



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 15, 2023 – 06:12 PM JST

PDB ID : 6JLN  
Title : XFEL structure of cyanobacterial photosystem II (1F state, dataset2)  
Authors : Suga, M.; Shen, J.R.  
Deposited on : 2019-03-06  
Resolution : 2.40 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

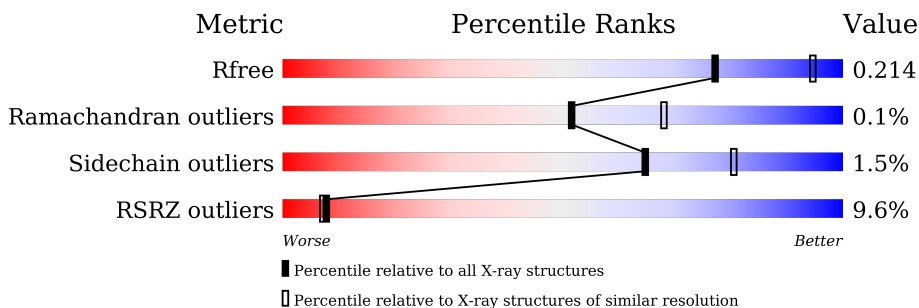
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3907 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	3% 97% ..
1	a	344	3% 97% ..
2	B	505	5% 99% .
2	b	505	8% 98% .
3	C	455	7% 98% ..
3	c	455	8% 98% .
4	D	342	4% 99% .

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Mol	Chain	Length	Quality of chain
4	d	342	3% 99%
5	E	84	44% 96%
5	e	84	12% 95%
6	F	44	18% 77% 23%
6	f	44	2% 70% 27%
7	H	65	8% 97%
7	h	65	12% 98%
8	I	38	11% 92% 8%
8	i	38	13% 92% 8%
9	J	39	21% 97%
9	j	39	8% 97%
10	K	37	11% 97%
10	k	37	5% 97%
11	L	37	32% 97%
11	l	37	38% 100%
12	M	36	44% 89% 6% 6%
12	m	36	44% 92% 6%
13	O	244	4% 98%
13	o	244	11% 97%
14	T	32	22% 88% 6% 6%
14	t	32	25% 88% 6% 6%
15	U	104	91% 7%
15	u	104	92% 7%
16	V	137	100%
16	v	137	2% 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	
20	R	34	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	A	405	X	-	-	-
24	CLA	A	406	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	B	617	X	-	-	-
24	CLA	C	501	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	D	404	X	-	-	-
24	CLA	D	405	X	-	-	-
24	CLA	a	409	X	-	-	-
24	CLA	a	412	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	618	X	-	-	-
24	CLA	b	619	X	-	-	-
24	CLA	b	620	X	-	-	-
24	CLA	b	621	X	-	-	-
24	CLA	b	622	X	-	-	-
24	CLA	b	623	X	-	-	-
24	CLA	b	624	X	-	-	-
24	CLA	b	625	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	c	514	X	-	-	-
24	CLA	c	515	X	-	-	-
24	CLA	c	516	X	-	-	-
24	CLA	d	403	X	-	-	-
24	CLA	d	404	X	-	-	-
24	CLA	d	405	X	-	-	-
27	SQD	B	621	-	-	-	X
28	GOL	V	201	-	-	-	X
29	LMT	E	102	-	-	-	X
29	LMT	M	104	-	-	-	X

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
29	LMT	T	104	-	-	-	X
29	LMT	a	419	-	-	-	X
29	LMT	m	103	-	-	-	X
29	LMT	t	101	-	-	-	X
33	UNL	M	103	-	-	-	X
33	UNL	c	525	-	-	-	X
33	UNL	j	101	-	-	-	X
33	UNL	m	101	-	-	-	X
34	LMG	z	101	-	-	-	X
36	HTG	C	523	-	-	-	X
36	HTG	b	632	-	-	-	X
36	HTG	c	524	-	-	-	X
37	DGD	D	408	-	-	-	X
37	DGD	e	101	-	-	-	X

## 2 Entry composition i

There are 41 unique types of molecules in this entry. The entry contains 55631 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
			Total	C	N	O	S			
1	A	334	Total 3019	C 1966	N 498	O 537	S 18	0	53	0
1	a	334	Total 3027	C 1973	N 498	O 538	S 18	0	55	0

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
			Total	C	N	O	S			
2	B	504	Total 4021	C 2639	N 667	O 702	S 13	0	10	0
2	b	503	Total 4022	C 2644	N 664	O 701	S 13	0	12	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	451	Total 3518	C 2300	N 587	O 618	S 13	0	7	0
3	c	455	Total 3598	C 2356	N 599	O 629	S 14	0	13	0

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	341	Total	C	N	O	S	0	16	0
			2849	1884	469	483	13			
4	d	341	Total	C	N	O	S	0	16	0
			2849	1884	469	483	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	S	0	2	0
			668	436	107	125				
5	e	81	Total	C	N	O	S	0	2	0
			670	439	107	124				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	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	65	Total	C	N	O	S	0	1	0
			519	346	85	86	2			
7	h	65	Total	C	N	O	S	0	0	0
			511	341	82	86	2			

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



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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	39	Total	C	N	O	S	0	0	0
			280	187	43	48	2			

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			
11	l	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	1	0
			274	184	40	49	1			

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

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
			Total	C	N	O	S			
13	O	243	1903	1191	315	392	5	0	8	0
13	o	243	1891	1183	315	388	5	0	5	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	T	30	264	185	36	41	2	0	1	0
14	t	30	264	185	36	41	2	0	1	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	V	137	1085	689	181	211	4	0	2	0
16	v	137	1077	684	178	211	4	0	1	0

- 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
			215	142	37	33	3			
17	y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	39	Total	C	N	O	S	0	0	0
			287	191	46	50				
18	x	38	Total	C	N	O	S	0	0	0
			281	188	45	48				

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	30	Total	C	N	O	S	98	0	0
			239	163	41	35				

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total	Fe	0	1
			2	2		
21	a	1	Total	Fe	0	1
			2	2		

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

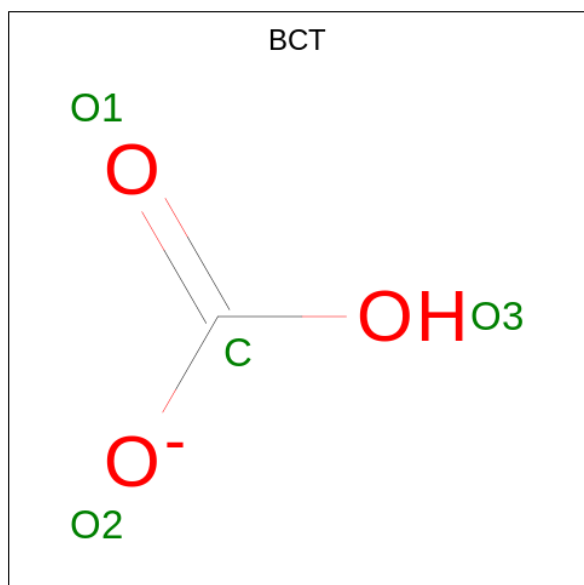
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	2
			4	4		
22	U	1	Total	Cl	0	0
			1	1		

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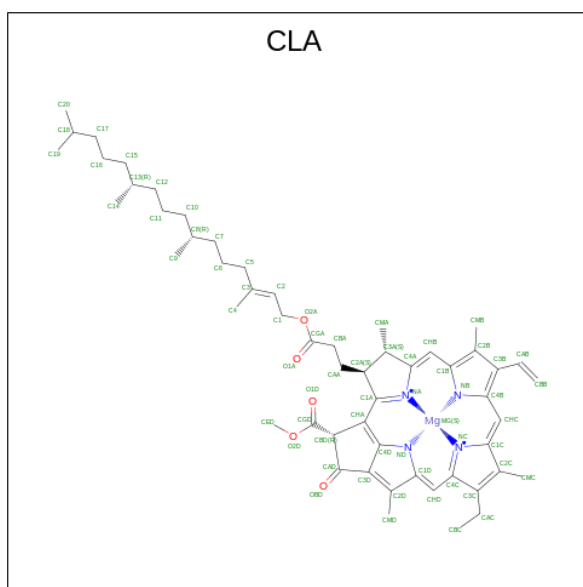
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	a	2	Total Cl 4 4	0	2
22	v	1	Total Cl 1 1	0	0

- Molecule 23 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O 8 2 6	0	1
23	d	1	Total C O 8 2 6	0	1

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$ ).



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

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

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

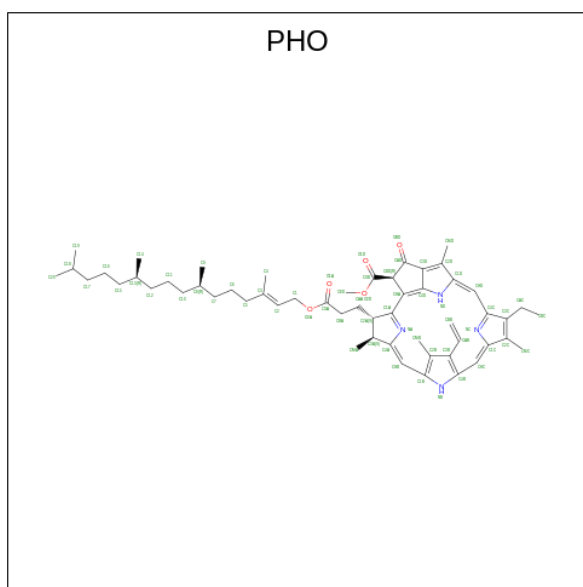
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65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

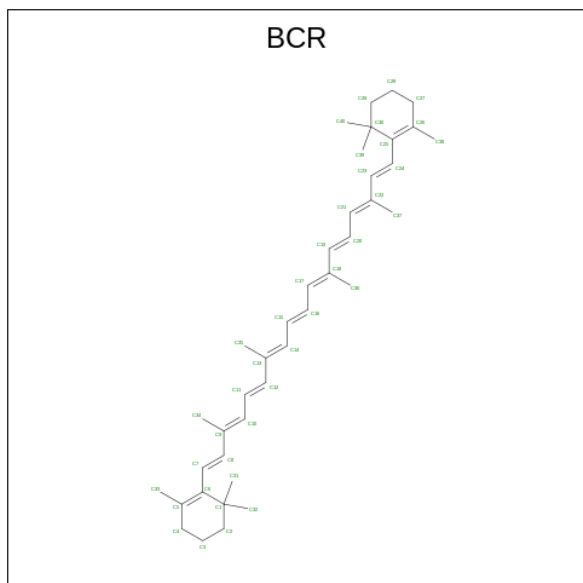
- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).





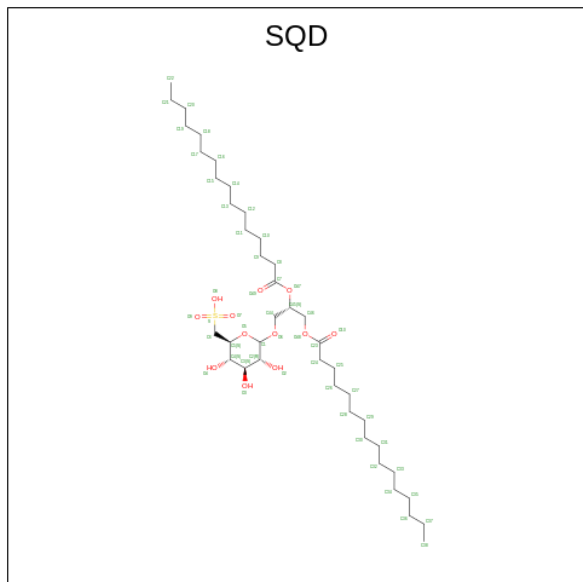
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
25	A	1	Total 64	C 55	N 4	O 5	0	0
25	D	1	Total 128	C 110	N 8	O 10	0	1
25	a	1	Total 64	C 55	N 4	O 5	0	0
25	d	1	Total 128	C 110	N 8	O 10	0	1

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).



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

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
27	A	1	54	41	12	1	0	0
27	A	1	54	41	12	1	0	0
27	B	1	54	41	12	1	0	0
27	F	1	43	30	12	1	0	0
27	L	1	54	41	12	1	0	0
27	a	1	54	41	12	1	0	0
27	a	1	54	41	12	1	0	0
27	f	1	43	30	12	1	0	0

- Molecule 28 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



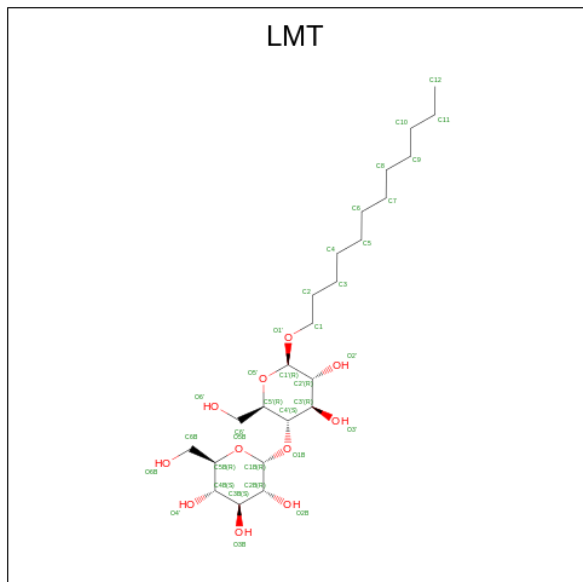
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	C	1	Total C O 6 3 3	0	0
28	C	1	Total C O 6 3 3	0	0
28	D	1	Total C O 6 3 3	0	0
28	F	1	Total C O 6 3 3	0	0
28	O	1	Total C O 6 3 3	0	0
28	T	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	T	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	a	1	Total 6	C 3	O 3	0	0
28	a	1	Total 6	C 3	O 3	0	0
28	a	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	c	1	Total 6	C 3	O 3	0	0
28	c	1	Total 6	C 3	O 3	0	0
28	o	1	Total 6	C 3	O 3	0	0
28	t	1	Total 6	C 3	O 3	0	0
28	v	1	Total 6	C 3	O 3	0	0
28	v	1	Total 6	C 3	O 3	0	0
28	v	1	Total 6	C 3	O 3	0	0
28	v	1	Total 6	C 3	O 3	0	0

- Molecule 29 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



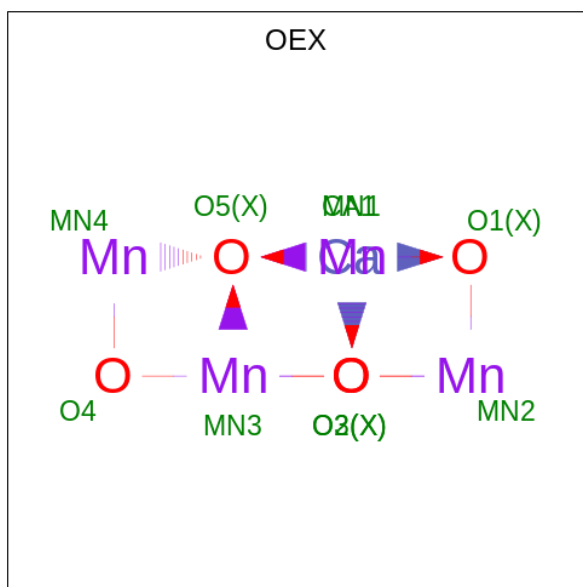
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C O 35 24 11	0	0
29	C	1	Total C O 35 24 11	0	0
29	D	1	Total C O 35 24 11	0	0
29	E	1	Total C O 35 24 11	0	0
29	M	1	Total C O 35 24 11	0	0
29	M	1	Total C O 35 24 11	0	0
29	T	1	Total C O 25 19 6	0	0
29	a	1	Total C O 35 24 11	0	0
29	a	1	Total C O 35 24 11	0	0
29	b	1	Total C O 25 19 6	0	0
29	e	1	Total C O 35 24 11	0	0
29	m	1	Total C O 35 24 11	0	0

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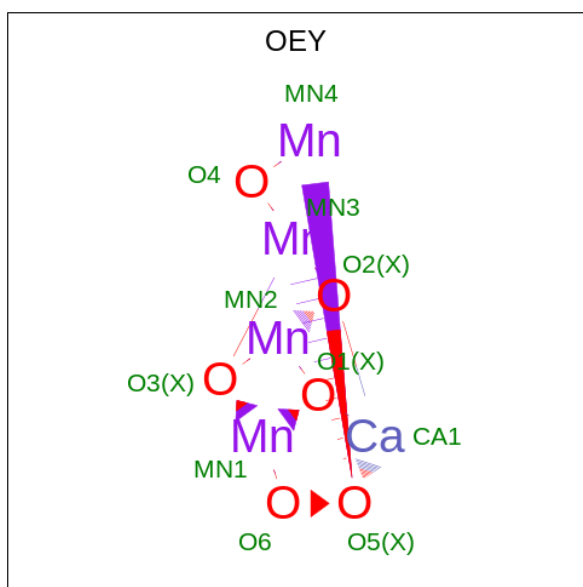
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	m	1	Total	C	O	0	0
			35	24	11		
29	t	1	Total	C	O	0	0
			25	19	6		

- Molecule 30 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



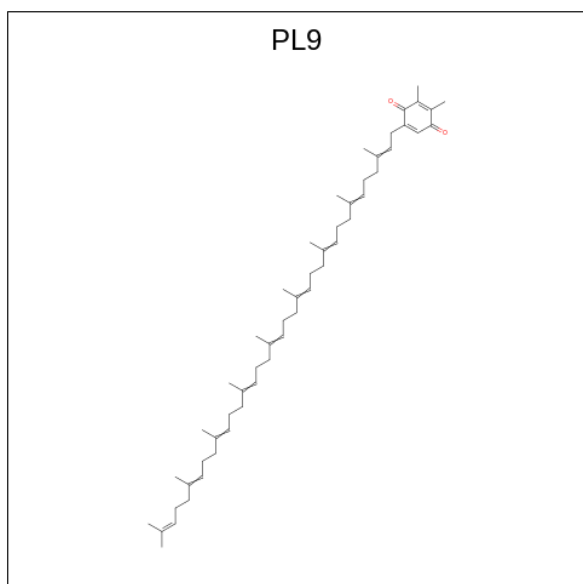
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
30	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 31 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula:  $\text{CaMn}_4\text{O}_6$ ).



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

- Molecule 32 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:  $C_{53}H_{80}O_2$ ).





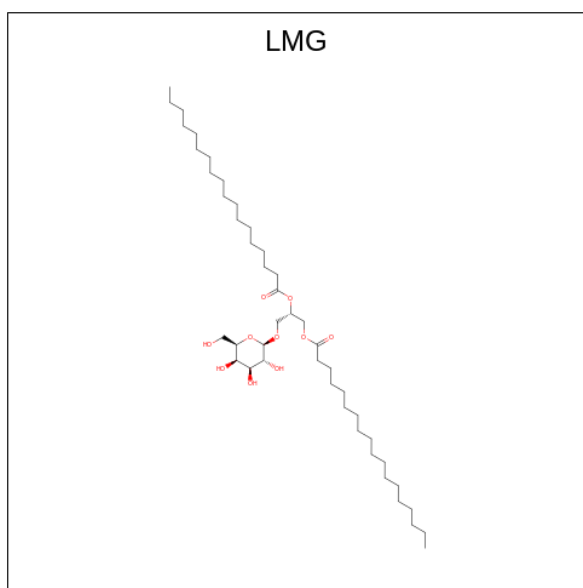
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	1
			110	106	4		
32	D	1	Total	C	O	0	1
			110	106	4		
32	a	1	Total	C	O	0	1
			110	106	4		
32	d	1	Total	C	O	0	1
			110	106	4		

- Molecule 33 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

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

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter

code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).

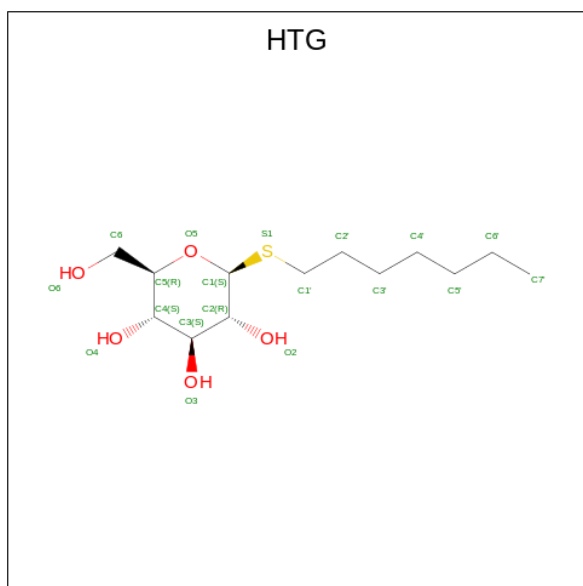


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	A	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	D	1	Total	C	O	0	0
			51	41	10		
34	M	1	Total	C	O	0	0
			51	41	10		
34	Z	1	Total	C	O	0	0
			37	27	10		
34	a	1	Total	C	O	0	0
			51	41	10		
34	b	1	Total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

- Molecule 35 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	B	1	Total Ca 1 1	0	0
35	C	1	Total Ca 1 1	0	0
35	F	1	Total Ca 1 1	0	0
35	O	1	Total Ca 1 1	0	0
35	b	1	Total Ca 1 1	0	0
35	c	2	Total Ca 2 2	0	0
35	f	1	Total Ca 1 1	0	0
35	o	1	Total Ca 1 1	0	0

- Molecule 36 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: C<sub>13</sub>H<sub>26</sub>O<sub>5</sub>S).



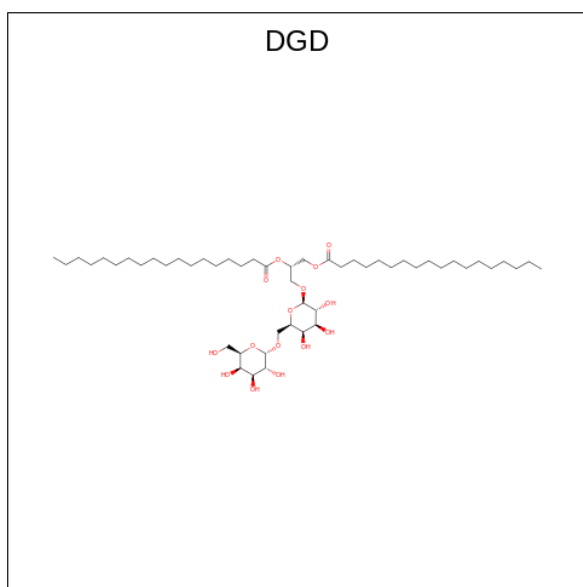
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	B	1	Total C O S 19 13 5 1	0	0
36	B	1	Total C O S 19 13 5 1	0	0
36	B	1	Total C O S 19 13 5 1	0	0

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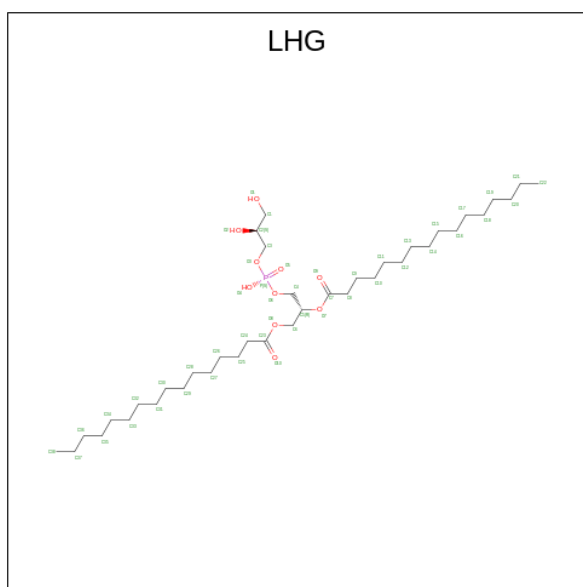
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	D	1	Total	C	O	S	0	0
			16	10	5	1		
36	V	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19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

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



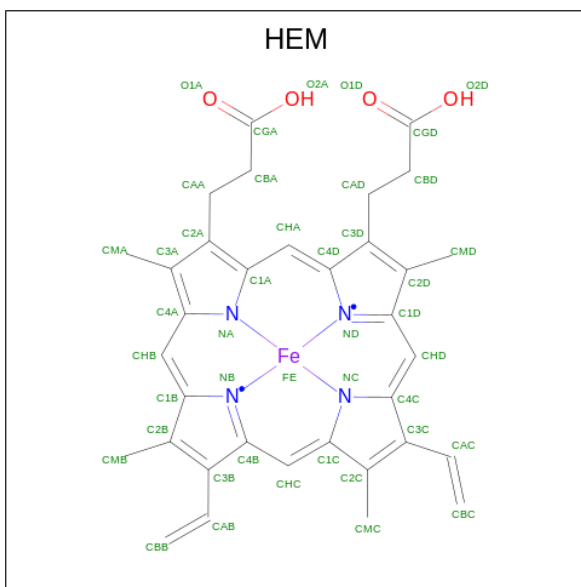
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	C	1	Total	C	O	0	0
			62	47	15		
37	C	1	Total	C	O	0	0
			62	47	15		
37	C	1	Total	C	O	0	0
			62	47	15		
37	D	1	Total	C	O	0	0
			52	42	10		
37	H	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	e	1	Total	C	O	0	0
			62	47	15		
37	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 38 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



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

- Molecule 39 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 40 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	162	Total	O	0	15
			175	175		
41	B	284	Total	O	0	4
			288	288		
41	C	232	Total	O	0	6
			236	236		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	D	144	Total O 149 149	0	5
41	E	36	Total O 37 37	0	1
41	F	7	Total O 7 7	0	0
41	H	41	Total O 41 41	0	0
41	I	4	Total O 4 4	0	0
41	J	10	Total O 10 10	0	0
41	K	8	Total O 8 8	0	0
41	L	16	Total O 17 17	0	1
41	M	23	Total O 23 23	0	0
41	O	177	Total O 179 179	0	2
41	T	15	Total O 16 16	0	1
41	U	83	Total O 83 83	0	0
41	V	114	Total O 116 116	0	2
41	Y	4	Total O 4 4	0	0
41	X	8	Total O 8 8	0	0
41	Z	1	Total O 1 1	0	0
41	a	157	Total O 168 168	0	13
41	b	261	Total O 264 264	0	3
41	c	200	Total O 206 206	0	8
41	d	134	Total O 137 137	0	3
41	e	20	Total O 20 20	0	0

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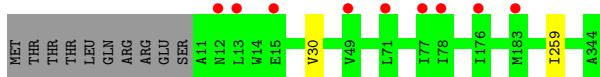
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	f	6	Total O 6 6	0	0
41	h	42	Total O 42 42	0	0
41	i	5	Total O 5 5	0	0
41	j	7	Total O 7 7	0	0
41	k	8	Total O 8 8	0	0
41	l	7	Total O 7 7	0	0
41	m	15	Total O 15 15	0	0
41	o	152	Total O 152 152	0	0
41	t	14	Total O 14 14	0	0
41	u	95	Total O 95 95	0	0
41	v	85	Total O 86 86	0	1
41	y	2	Total O 2 2	0	0
41	x	6	Total O 6 6	0	0

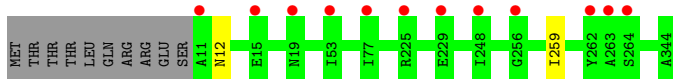
### 3 Residue-property plots [i](#)

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

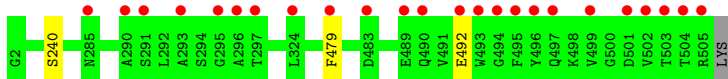
- Molecule 1: Photosystem II protein D1



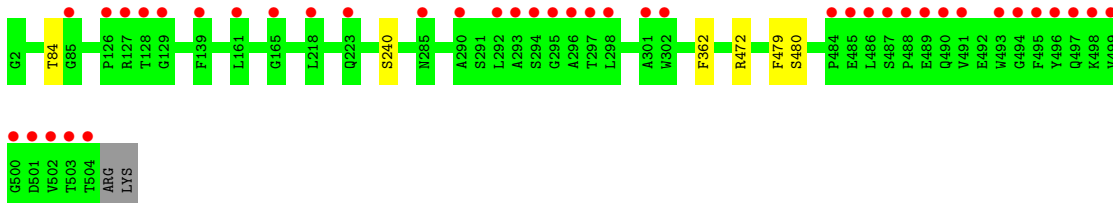
- Molecule 1: Photosystem II protein D1



- Molecule 2: Photosystem II CP47 reaction center protein

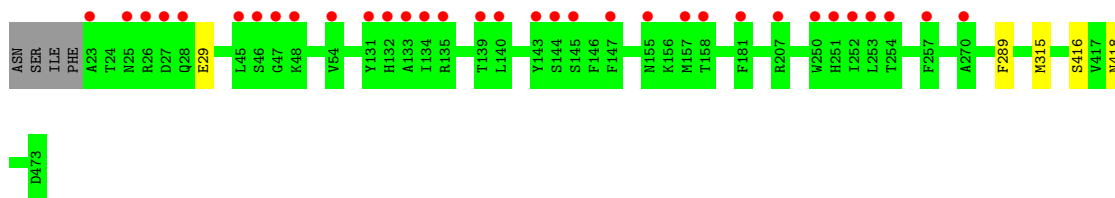


- Molecule 2: Photosystem II CP47 reaction center protein

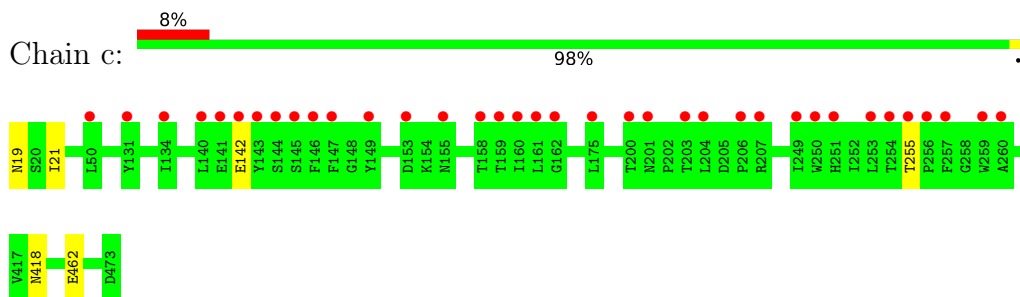


- Molecule 3: Photosystem II CP43 reaction center protein

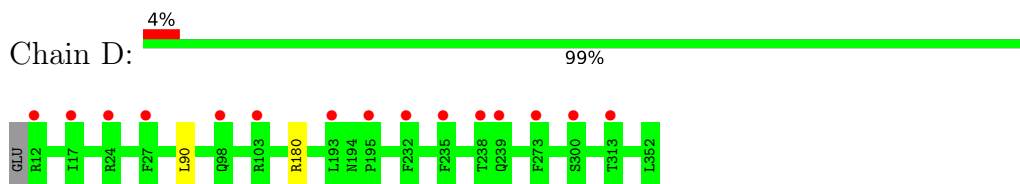




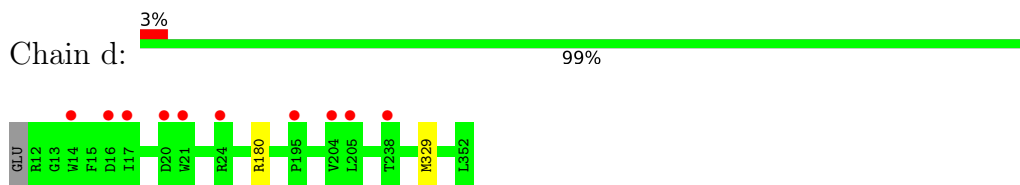
- Molecule 3: Photosystem II CP43 reaction center protein



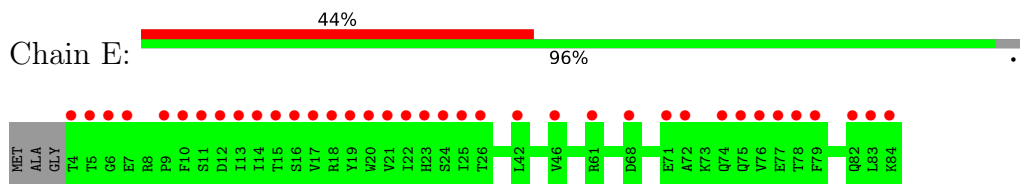
- Molecule 4: Photosystem II D2 protein



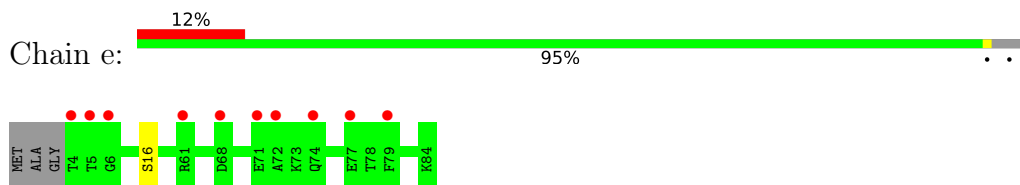
- Molecule 4: Photosystem II D2 protein



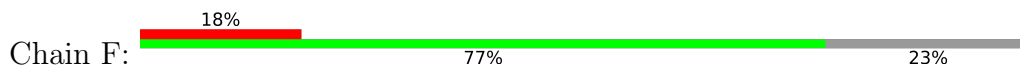
- Molecule 5: Cytochrome b559 subunit alpha

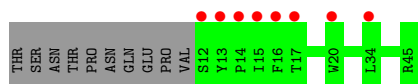


- Molecule 5: Cytochrome b559 subunit alpha

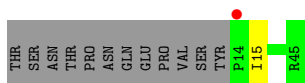


- Molecule 6: Cytochrome b559 subunit beta

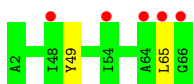




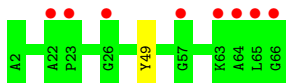
- Molecule 6: Cytochrome b559 subunit beta



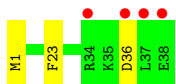
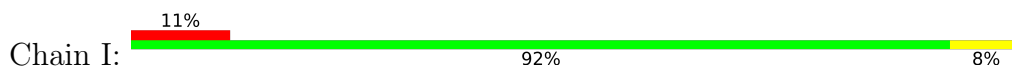
- Molecule 7: Photosystem II reaction center protein H



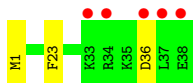
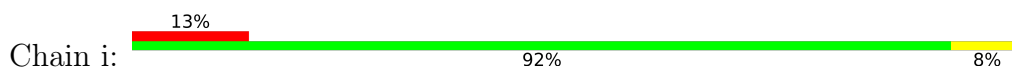
- Molecule 7: Photosystem II reaction center protein H



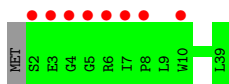
- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



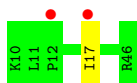
- Molecule 9: Photosystem II reaction center protein J



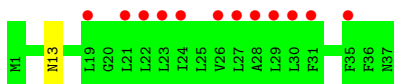
- Molecule 10: Photosystem II reaction center protein K



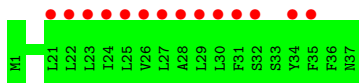
- Molecule 10: Photosystem II reaction center protein K



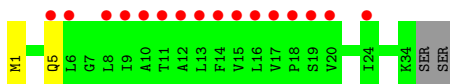
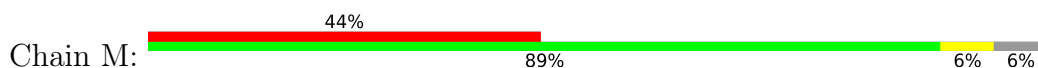
- Molecule 11: Photosystem II reaction center protein L



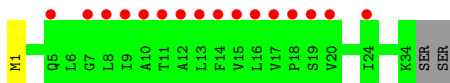
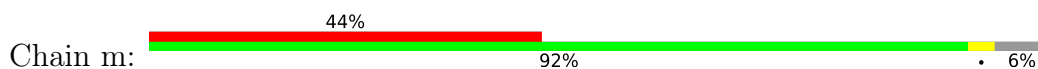
- Molecule 11: Photosystem II reaction center protein L



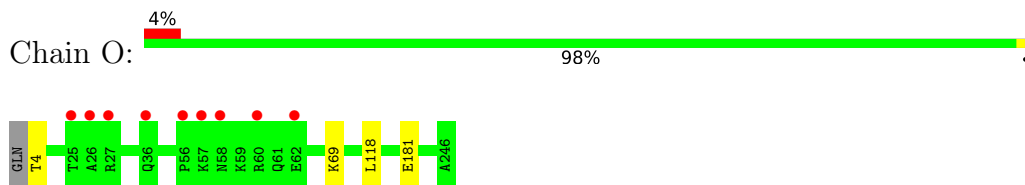
- Molecule 12: Photosystem II reaction center protein M



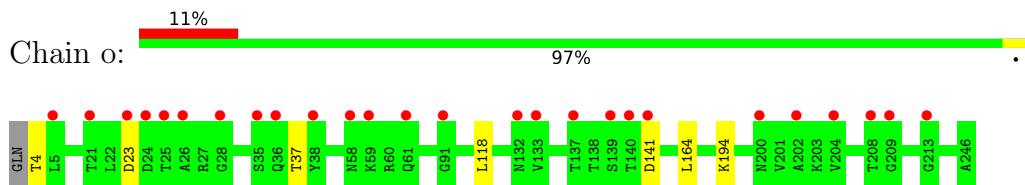
- Molecule 12: Photosystem II reaction center protein M



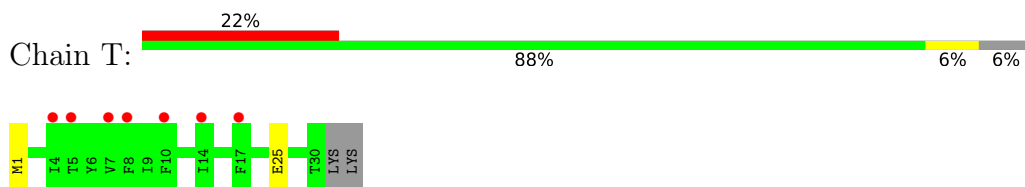
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



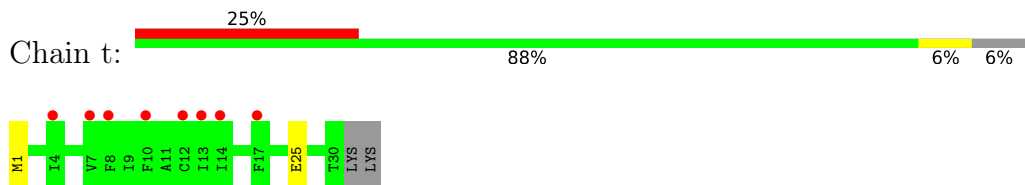
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



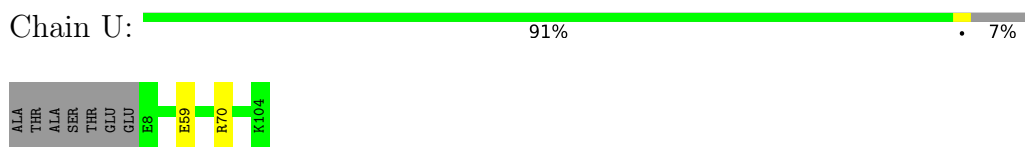
- Molecule 14: Photosystem II reaction center protein T



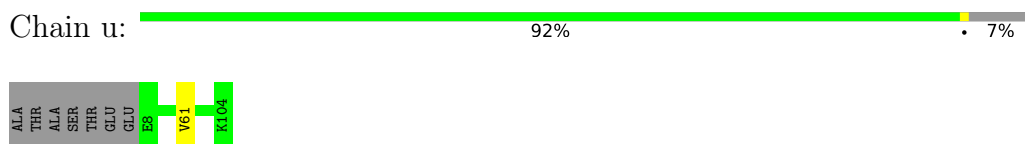
- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein

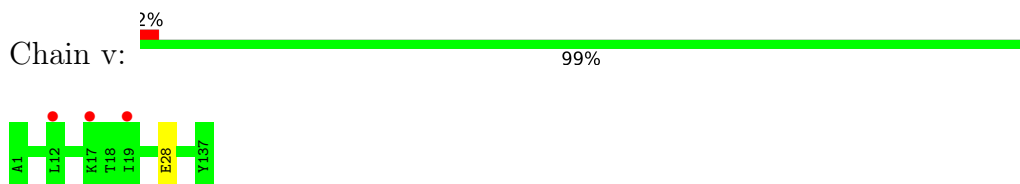


- Molecule 16: Cytochrome c-550

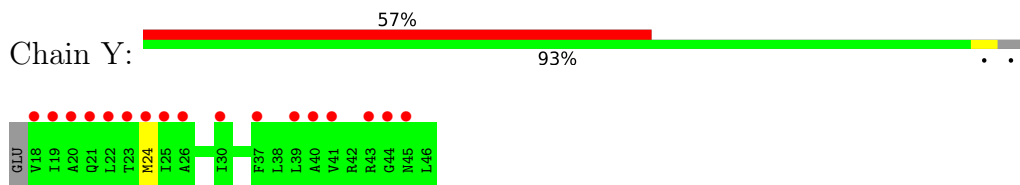


There are no outlier residues recorded for this chain.

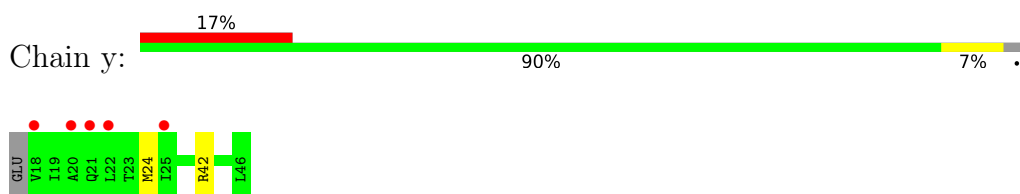
- Molecule 16: Cytochrome c-550



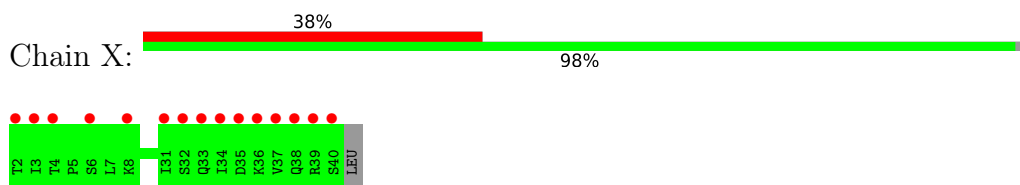
- Molecule 17: Photosystem II reaction center protein Ycf12



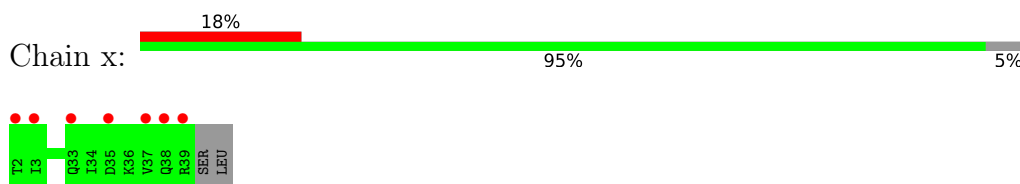
- Molecule 17: Photosystem II reaction center protein Ycf12



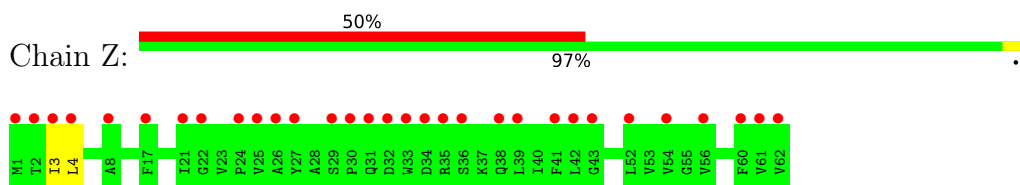
- Molecule 18: Photosystem II reaction center protein X



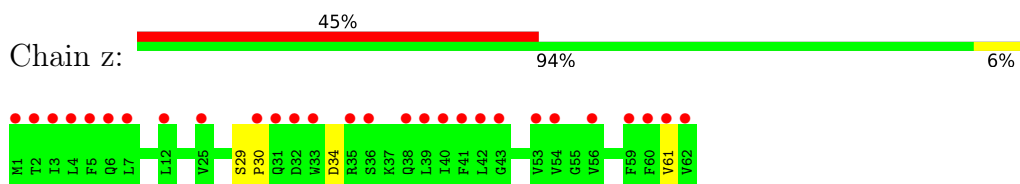
- Molecule 18: Photosystem II reaction center protein X




- Molecule 19: Photosystem II reaction center protein Z

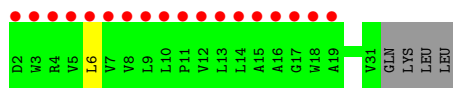


- Molecule 19: Photosystem II reaction center protein Z



## ● Molecule 20: Photosystem II protein Y

Chain R:  53% 85% 12%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.04Å 228.84Å 286.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.40 92.96 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.99-2.40) 99.2 (92.96-2.29)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.22 (at 2.29Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.154 , 0.212 0.158 , 0.214	Depositor DCC
$R_{free}$ test set	17838 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.9	Xtrriage
Anisotropy	0.604	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 79.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	55631	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.44	0/3121	0.56	0/4250
1	a	0.44	0/3135	0.56	0/4269
2	B	0.42	0/4191	0.54	0/5709
2	b	0.43	0/4198	0.54	0/5720
3	C	0.38	0/3643	0.49	0/4958
3	c	0.38	0/3731	0.51	0/5076
4	D	0.46	0/2952	0.54	0/4021
4	d	0.46	0/2952	0.55	0/4021
5	E	0.34	0/693	0.49	0/944
5	e	0.33	0/695	0.50	0/948
6	F	0.38	0/284	0.52	0/387
6	f	0.39	0/265	0.51	0/360
7	H	0.36	0/535	0.53	0/728
7	h	0.35	0/524	0.51	0/713
8	I	0.37	0/311	0.49	0/419
8	i	0.35	0/311	0.48	0/419
9	J	0.38	0/278	0.42	0/376
9	j	0.33	0/286	0.45	0/386
10	K	0.33	0/303	0.51	0/416
10	k	0.36	0/303	0.49	0/416
11	L	0.44	0/319	0.51	0/433
11	l	0.42	0/319	0.46	0/433
12	M	0.47	0/270	0.57	0/368
12	m	0.44	0/262	0.59	0/357
13	O	0.38	0/1958	0.56	0/2654
13	o	0.38	0/1937	0.55	0/2625
14	T	0.45	0/266	0.53	0/362
14	t	0.51	0/266	0.54	0/362
15	U	0.38	0/785	0.54	0/1064
15	u	0.38	0/785	0.55	0/1064
16	V	0.37	0/1109	0.51	0/1502

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	v	0.37	0/1098	0.52	0/1488
17	Y	0.35	0/216	0.49	0/289
17	y	0.32	0/216	0.47	0/289
18	X	0.34	0/290	0.45	0/392
18	x	0.33	0/284	0.49	0/384
19	Z	0.30	0/490	0.43	0/669
19	z	0.29	0/490	0.45	0/669
20	R	0.26	0/245	0.38	0/338
All	All	0.41	0/44316	0.53	0/60278

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	384/344 (112%)	377 (98%)	5 (1%)	2 (0%)	29	41
1	a	386/344 (112%)	378 (98%)	7 (2%)	1 (0%)	41	55
2	B	512/505 (101%)	505 (99%)	7 (1%)	0	100	100
2	b	513/505 (102%)	503 (98%)	10 (2%)	0	100	100
3	C	456/455 (100%)	446 (98%)	8 (2%)	2 (0%)	34	48
3	c	466/455 (102%)	450 (97%)	14 (3%)	2 (0%)	34	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	355/342 (104%)	343 (97%)	12 (3%)	0	100	100
4	d	355/342 (104%)	346 (98%)	9 (2%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
6	F	32/44 (73%)	30 (94%)	2 (6%)	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	64/65 (98%)	58 (91%)	6 (9%)	0	100	100
7	h	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
9	J	36/39 (92%)	36 (100%)	0	0	100	100
9	j	37/39 (95%)	34 (92%)	3 (8%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/36 (92%)	33 (100%)	0	0	100	100
12	m	32/36 (89%)	32 (100%)	0	0	100	100
13	O	249/244 (102%)	241 (97%)	8 (3%)	0	100	100
13	o	246/244 (101%)	235 (96%)	11 (4%)	0	100	100
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	29/32 (91%)	29 (100%)	0	0	100	100
15	U	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
16	V	136/137 (99%)	130 (96%)	6 (4%)	0	100	100
16	v	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
17	Y	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
17	y	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
18	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
18	x	36/40 (90%)	34 (94%)	2 (6%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	z	60/62 (97%)	57 (95%)	1 (2%)	2 (3%)	4	3
20	R	28/34 (82%)	28 (100%)	0	0	100	100
All	All	5419/5384 (101%)	5272 (97%)	138 (2%)	9 (0%)	51	62

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
1	a	259	ILE

### 5.3.2 Protein sidechains [i](#)

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	312/279 (112%)	312 (100%)	0	100	100
1	a	314/279 (112%)	313 (100%)	1 (0%)	92	97
2	B	412/403 (102%)	409 (99%)	3 (1%)	84	92
2	b	413/403 (102%)	407 (98%)	6 (2%)	65	80
3	C	357/356 (100%)	353 (99%)	4 (1%)	73	87
3	c	367/356 (103%)	356 (97%)	11 (3%)	41	61
4	D	290/277 (105%)	288 (99%)	2 (1%)	84	92
4	d	290/277 (105%)	288 (99%)	2 (1%)	84	92
5	E	74/73 (101%)	74 (100%)	0	100	100
5	e	74/73 (101%)	73 (99%)	1 (1%)	67	82
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	26/38 (68%)	25 (96%)	1 (4%)	33	51
7	H	55/54 (102%)	53 (96%)	2 (4%)	35	54
7	h	54/54 (100%)	53 (98%)	1 (2%)	57	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	34/34 (100%)	32 (94%)	2 (6%)	19	32
8	i	34/34 (100%)	32 (94%)	2 (6%)	19	32
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	27/27 (100%)	26 (96%)	1 (4%)	34	53
10	K	30/30 (100%)	29 (97%)	1 (3%)	38	57
10	k	30/30 (100%)	29 (97%)	1 (3%)	38	57
11	L	36/35 (103%)	35 (97%)	1 (3%)	43	63
11	l	36/35 (103%)	36 (100%)	0	100	100
12	M	31/32 (97%)	30 (97%)	1 (3%)	39	59
12	m	30/32 (94%)	30 (100%)	0	100	100
13	O	214/207 (103%)	209 (98%)	5 (2%)	50	70
13	o	211/207 (102%)	204 (97%)	7 (3%)	38	57
14	T	27/28 (96%)	25 (93%)	2 (7%)	13	22
14	t	27/28 (96%)	25 (93%)	2 (7%)	13	22
15	U	84/89 (94%)	82 (98%)	2 (2%)	49	68
15	u	84/89 (94%)	83 (99%)	1 (1%)	71	85
16	V	119/117 (102%)	119 (100%)	0	100	100
16	v	118/117 (101%)	117 (99%)	1 (1%)	81	91
17	Y	22/23 (96%)	21 (96%)	1 (4%)	27	44
17	y	22/23 (96%)	20 (91%)	2 (9%)	9	14
18	X	32/33 (97%)	32 (100%)	0	100	100
18	x	31/33 (94%)	31 (100%)	0	100	100
19	Z	52/52 (100%)	50 (96%)	2 (4%)	33	51
19	z	52/52 (100%)	50 (96%)	2 (4%)	33	51
20	R	25/29 (86%)	24 (96%)	1 (4%)	31	49
All	All	4500/4403 (102%)	4429 (98%)	71 (2%)	65	79

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	o	23	ASP
13	o	118	LEU
15	u	61	VAL

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Mol	Chain	Res	Type
15	U	70	ARG
15	U	59	GLU

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

Mol	Chain	Res	Type
1	a	12	ASN
2	b	331	ASN
13	o	147	ASN
2	b	53	ASN
2	b	490	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
12	FME	M	1	12	8,9,10	0.70	0	7,9,11	1.36	2 (28%)
14	FME	T	1	14	8,9,10	0.70	0	7,9,11	1.32	1 (14%)
14	FME	t	1	14	8,9,10	0.79	0	7,9,11	2.10	3 (42%)
12	FME	m	1	12	8,9,10	0.61	0	7,9,11	1.37	1 (14%)
8	FME	i	1	8	8,9,10	0.66	0	7,9,11	1.22	1 (14%)
8	FME	I	1	8	8,9,10	0.75	0	7,9,11	1.44	2 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	M	1	12	-	2/7/9/11	-
14	FME	T	1	14	-	0/7/9/11	-
14	FME	t	1	14	-	2/7/9/11	-
12	FME	m	1	12	-	2/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	C-CA-N	3.25	115.61	109.73
14	t	1	FME	CA-N-CN	-2.77	118.57	122.82
8	I	1	FME	CA-N-CN	-2.50	118.97	122.82
14	T	1	FME	O-C-CA	-2.41	118.45	124.78
14	t	1	FME	O-C-CA	-2.37	118.57	124.78

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 267 ligands modelled in this entry, 25 are monoatomic and 18 are unknown - leaving 224 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$
26	BCR	C	514	-	41,41,41	1.06	1 (2%)	56,56,56	1.42	8 (14%)
28	GOL	B	634	-	5,5,5	0.45	0	5,5,5	0.45	0
36	HTG	B	624	-	19,19,19	1.05	2 (10%)	23,24,24	2.06	4 (17%)
24	CLA	B	607	-	65,73,73	2.04	16 (24%)	76,113,113	2.85	28 (36%)
25	PHO	A	408	-	51,69,69	1.83	8 (15%)	47,99,99	1.80	12 (25%)
28	GOL	b	604	-	5,5,5	0.33	0	5,5,5	0.26	0
28	GOL	B	630	-	5,5,5	0.37	0	5,5,5	0.28	0
29	LMT	b	630	-	25,25,36	0.50	0	30,30,47	0.66	0
31	OEY	a	418[B]	3,1,41	0,14,16	-	-	-	-	-
36	HTG	B	632	-	19,19,19	1.05	2 (10%)	23,24,24	1.43	2 (8%)
37	DGD	C	517	-	63,63,67	0.88	2 (3%)	77,77,81	1.05	9 (11%)
28	GOL	b	601	-	5,5,5	0.38	0	5,5,5	0.44	0
24	CLA	B	612	-	65,73,73	2.02	16 (24%)	76,113,113	2.76	29 (38%)
24	CLA	B	603	-	65,73,73	2.10	17 (26%)	76,113,113	2.82	29 (38%)
24	CLA	b	612	-	65,73,73	2.02	16 (24%)	76,113,113	2.81	28 (36%)
26	BCR	Y	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.76	11 (19%)
28	GOL	B	628	-	5,5,5	0.34	0	5,5,5	0.39	0
29	LMT	T	104	-	25,25,36	0.55	1 (4%)	30,30,47	1.06	2 (6%)
34	LMG	d	415	40	51,51,55	0.94	2 (3%)	59,59,63	1.12	7 (11%)
26	BCR	A	410	-	41,41,41	1.07	1 (2%)	56,56,56	1.15	3 (5%)
24	CLA	c	512	-	65,73,73	2.05	16 (24%)	76,113,113	2.72	27 (35%)
38	LHG	L	101	-	48,48,48	0.92	2 (4%)	51,54,54	1.10	5 (9%)
24	CLA	C	512	-	65,73,73	2.07	16 (24%)	76,113,113	2.73	27 (35%)
38	LHG	a	420	-	41,41,48	1.03	2 (4%)	44,47,54	0.93	2 (4%)
24	CLA	c	508	41	65,73,73	2.04	17 (26%)	76,113,113	2.77	29 (38%)
29	LMT	t	101	-	25,25,36	0.52	0	30,30,47	0.76	1 (3%)
24	CLA	C	507	41	65,73,73	2.04	15 (23%)	76,113,113	2.64	25 (32%)
34	LMG	z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.13	4 (8%)
24	CLA	b	617	-	65,73,73	2.06	16 (24%)	76,113,113	2.72	29 (38%)
27	SQD	A	413	-	53,54,54	1.02	3 (5%)	62,65,65	1.15	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	HTG	B	622	-	19,19,19	1.10	1 (5%)	23,24,24	1.35	1 (4%)
24	CLA	B	604	-	65,73,73	2.06	17 (26%)	76,113,113	2.75	27 (35%)
24	CLA	C	511	3	65,73,73	2.13	16 (24%)	76,113,113	2.72	27 (35%)
30	OEX	A	415[A]	3,1,41	0,15,15	-	-	-	-	-
34	LMG	Z	101	-	37,37,55	0.98	3 (8%)	45,45,63	1.36	7 (15%)
28	GOL	B	629	-	5,5,5	0.44	0	5,5,5	0.30	0
39	HEM	E	103	6,5	41,50,50	1.28	4 (9%)	45,82,82	1.99	9 (20%)
24	CLA	B	611	41	65,73,73	2.13	16 (24%)	76,113,113	2.83	32 (42%)
24	CLA	c	513	-	65,73,73	2.14	16 (24%)	76,113,113	2.70	28 (36%)
36	HTG	C	523	-	19,19,19	0.97	1 (5%)	23,24,24	1.74	4 (17%)
38	LHG	D	411	-	48,48,48	0.99	2 (4%)	51,54,54	1.12	3 (5%)
24	CLA	D	404	-	65,73,73	2.00	16 (24%)	76,113,113	2.86	27 (35%)
26	BCR	H	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.56	7 (12%)
28	GOL	v	202	-	5,5,5	0.36	0	5,5,5	0.32	0
28	GOL	o	301	-	5,5,5	0.41	0	5,5,5	0.34	0
34	LMG	k	101	-	51,51,55	0.89	2 (3%)	59,59,63	1.08	5 (8%)
39	HEM	f	101	6,5	41,50,50	1.29	4 (9%)	45,82,82	1.77	10 (22%)
24	CLA	c	507	-	65,73,73	2.06	16 (24%)	76,113,113	2.72	26 (34%)
24	CLA	c	509	-	65,73,73	2.03	16 (24%)	76,113,113	2.70	25 (32%)
24	CLA	B	602	41	65,73,73	2.11	18 (27%)	76,113,113	2.74	25 (32%)
36	HTG	B	631	-	19,19,19	1.03	2 (10%)	23,24,24	1.36	2 (8%)
29	LMT	M	104	-	36,36,36	0.54	1 (2%)	47,47,47	1.14	5 (10%)
24	CLA	c	506	-	65,73,73	2.07	17 (26%)	76,113,113	2.60	23 (30%)
24	CLA	b	625	-	65,73,73	2.06	15 (23%)	76,113,113	2.71	28 (36%)
28	GOL	D	402	-	5,5,5	0.42	0	5,5,5	0.29	0
26	BCR	B	618	-	41,41,41	1.05	1 (2%)	56,56,56	1.37	8 (14%)
26	BCR	k	102	-	41,41,41	1.05	1 (2%)	56,56,56	1.52	11 (19%)
36	HTG	d	413	-	16,16,19	1.23	2 (12%)	20,21,24	1.81	2 (10%)
26	BCR	a	413	-	41,41,41	1.03	1 (2%)	56,56,56	1.48	9 (16%)
28	GOL	T	101	-	5,5,5	0.39	0	5,5,5	0.28	0
36	HTG	B	623	-	19,19,19	0.85	1 (5%)	23,24,24	1.48	1 (4%)
28	GOL	b	606	-	5,5,5	0.38	0	5,5,5	0.22	0
28	GOL	V	201	-	5,5,5	0.37	0	5,5,5	0.31	0
28	GOL	A	412	-	5,5,5	0.40	0	5,5,5	0.15	0
26	BCR	y	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.57	10 (17%)
24	CLA	a	410	41	65,73,73	2.04	16 (24%)	76,113,113	2.81	28 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	HTG	b	602	-	19,19,19	0.95	1 (5%)	23,24,24	1.07	2 (8%)
24	CLA	A	405	-	65,73,73	2.14	16 (24%)	76,113,113	2.70	28 (36%)
24	CLA	b	616	41	65,73,73	2.03	16 (24%)	76,113,113	2.71	26 (34%)
25	PHO	d	402[A]	-	51,69,69	1.81	8 (15%)	47,99,99	1.98	8 (17%)
26	BCR	h	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.33	8 (14%)
27	SQD	L	102	-	53,54,54	1.05	3 (5%)	62,65,65	1.59	12 (19%)
26	BCR	b	627	-	41,41,41	1.00	1 (2%)	56,56,56	1.40	7 (12%)
29	LMT	a	419	-	36,36,36	0.43	0	47,47,47	0.78	1 (2%)
24	CLA	b	615	-	65,73,73	2.06	16 (24%)	76,113,113	2.75	28 (36%)
26	BCR	D	406	-	41,41,41	1.05	1 (2%)	56,56,56	1.76	13 (23%)
29	LMT	C	521	-	36,36,36	0.49	0	47,47,47	1.11	3 (6%)
28	GOL	V	202	-	5,5,5	0.33	0	5,5,5	0.36	0
34	LMG	C	519	-	51,51,55	0.95	2 (3%)	59,59,63	1.02	5 (8%)
37	DGD	c	521	-	63,63,67	0.86	2 (3%)	77,77,81	1.02	3 (3%)
29	LMT	m	103	-	36,36,36	0.51	0	47,47,47	1.06	4 (8%)
23	BCT	A	404[B]	21	2,3,3	0.66	0	2,3,3	1.00	0
28	GOL	b	605	-	5,5,5	0.38	0	5,5,5	0.32	0
26	BCR	c	526	-	41,41,41	1.05	1 (2%)	56,56,56	1.57	9 (16%)
26	BCR	K	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.56	13 (23%)
38	LHG	E	101	-	41,41,48	1.04	2 (4%)	44,47,54	1.15	4 (9%)
24	CLA	d	405	-	65,73,73	2.04	15 (23%)	76,113,113	2.72	26 (34%)
26	BCR	B	620	-	41,41,41	1.01	1 (2%)	56,56,56	1.59	12 (21%)
28	GOL	a	402	-	5,5,5	0.38	0	5,5,5	0.33	0
25	PHO	a	411	-	51,69,69	1.94	9 (17%)	47,99,99	1.74	10 (21%)
34	LMG	a	415	-	51,51,55	0.91	2 (3%)	59,59,63	1.18	5 (8%)
23	BCT	d	401[A]	21	2,3,3	0.65	0	2,3,3	0.80	0
34	LMG	D	415	40	51,51,55	0.89	2 (3%)	59,59,63	0.96	3 (5%)
27	SQD	a	414	-	53,54,54	0.95	3 (5%)	62,65,65	1.57	11 (17%)
28	GOL	T	102	-	5,5,5	0.40	0	5,5,5	0.29	0
28	GOL	v	201	-	5,5,5	0.33	0	5,5,5	0.32	0
25	PHO	D	401[B]	-	51,69,69	1.88	8 (15%)	47,99,99	1.67	8 (17%)
37	DGD	C	518	-	63,63,67	0.90	2 (3%)	77,77,81	0.98	4 (5%)
24	CLA	c	510	-	65,73,73	2.07	16 (24%)	76,113,113	2.71	27 (35%)
24	CLA	C	510	-	65,73,73	2.12	16 (24%)	76,113,113	2.68	30 (39%)
23	BCT	A	404[A]	21	2,3,3	0.59	0	2,3,3	1.28	0
24	CLA	B	616	-	65,73,73	2.02	15 (23%)	76,113,113	2.71	25 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
28	GOL	b	603	-	5,5,5	0.40	0	5,5,5	0.37	0
39	HEM	V	205	16	41,50,50	1.38	6 (14%)	45,82,82	1.80	9 (20%)
38	LHG	d	408	-	48,48,48	0.90	3 (6%)	51,54,54	1.06	5 (9%)
28	GOL	B	626	-	5,5,5	0.33	0	5,5,5	0.37	0
24	CLA	b	613	-	65,73,73	2.05	16 (24%)	76,113,113	2.75	25 (32%)
25	PHO	D	401[A]	-	51,69,69	1.88	8 (15%)	47,99,99	1.80	9 (19%)
28	GOL	V	204	-	5,5,5	0.35	0	5,5,5	0.28	0
24	CLA	C	504	41	65,73,73	2.10	16 (24%)	76,113,113	2.79	26 (34%)
36	HTG	c	523	-	19,19,19	0.99	2 (10%)	23,24,24	1.46	2 (8%)
24	CLA	c	514	-	65,73,73	2.09	16 (24%)	76,113,113	2.74	28 (36%)
34	LMG	M	101	-	51,51,55	0.93	2 (3%)	59,59,63	0.97	3 (5%)
24	CLA	b	621	-	65,73,73	2.06	16 (24%)	76,113,113	2.86	27 (35%)
24	CLA	B	617	-	65,73,73	2.06	15 (23%)	76,113,113	2.69	25 (32%)
25	PHO	d	402[B]	-	51,69,69	1.86	8 (15%)	47,99,99	1.89	11 (23%)
37	DGD	C	516	-	63,63,67	0.86	2 (3%)	77,77,81	1.09	6 (7%)
36	HTG	b	607	-	19,19,19	1.00	1 (5%)	23,24,24	1.39	4 (17%)
24	CLA	c	515	3	65,73,73	2.01	16 (24%)	76,113,113	2.74	27 (35%)
26	BCR	T	103	-	41,41,41	1.01	1 (2%)	56,56,56	1.77	14 (25%)
29	LMT	E	102	-	36,36,36	0.49	0	47,47,47	0.94	1 (2%)
24	CLA	B	610	-	65,73,73	1.99	16 (24%)	76,113,113	2.72	27 (35%)
24	CLA	b	610	41	65,73,73	2.13	15 (23%)	76,113,113	2.71	27 (35%)
29	LMT	A	414	-	36,36,36	0.57	1 (2%)	47,47,47	1.27	4 (8%)
38	LHG	D	409	-	48,48,48	0.86	2 (4%)	51,54,54	1.00	3 (5%)
24	CLA	B	608	41	65,73,73	2.09	17 (26%)	76,113,113	2.70	27 (35%)
24	CLA	b	624	-	65,73,73	2.08	16 (24%)	76,113,113	2.70	23 (30%)
32	PL9	a	416[B]	-	55,55,55	0.64	2 (3%)	68,69,69	1.84	19 (27%)
37	DGD	c	519	-	63,63,67	0.83	2 (3%)	77,77,81	1.04	6 (7%)
28	GOL	C	525	-	5,5,5	0.42	0	5,5,5	0.41	0
23	BCT	d	401[B]	21	2,3,3	0.66	0	2,3,3	0.78	0
24	CLA	b	618	-	65,73,73	2.05	16 (24%)	76,113,113	2.80	28 (36%)
32	PL9	D	407[B]	-	55,55,55	0.63	1 (1%)	68,69,69	1.81	22 (32%)
28	GOL	F	103	35	5,5,5	0.36	0	5,5,5	0.24	0
28	GOL	v	203	-	5,5,5	0.33	0	5,5,5	0.47	0
32	PL9	d	407[B]	-	55,55,55	0.66	1 (1%)	68,69,69	1.64	17 (25%)
29	LMT	e	102	-	36,36,36	0.49	0	47,47,47	0.84	1 (2%)
32	PL9	A	417[B]	-	55,55,55	0.64	2 (3%)	68,69,69	1.80	22 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	PL9	a	416[A]	-	55,55,55	0.63	2 (3%)	68,69,69	1.91	20 (29%)
26	BCR	c	518	-	41,41,41	1.04	1 (2%)	56,56,56	1.60	11 (19%)
27	SQD	a	405	-	53,54,54	1.08	3 (5%)	62,65,65	1.19	4 (6%)
24	CLA	C	502	-	65,73,73	2.07	16 (24%)	76,113,113	2.70	27 (35%)
24	CLA	C	506	-	65,73,73	2.03	17 (26%)	76,113,113	2.66	28 (36%)
32	PL9	D	407[A]	-	55,55,55	0.66	1 (1%)	68,69,69	1.74	20 (29%)
24	CLA	C	501	-	65,73,73	2.06	16 (24%)	76,113,113	2.77	26 (34%)
28	GOL	B	627	-	5,5,5	0.36	0	5,5,5	0.51	0
32	PL9	d	407[A]	-	55,55,55	0.69	2 (3%)	68,69,69	1.54	15 (22%)
27	SQD	B	621	-	53,54,54	1.01	3 (5%)	62,65,65	1.41	5 (8%)
28	GOL	c	502	-	5,5,5	0.39	0	5,5,5	0.37	0
24	CLA	C	508	-	65,73,73	2.11	16 (24%)	76,113,113	2.72	30 (39%)
28	GOL	O	301	-	5,5,5	0.36	0	5,5,5	0.36	0
38	LHG	d	409	-	48,48,48	0.88	2 (4%)	51,54,54	1.01	5 (9%)
32	PL9	A	417[A]	-	55,55,55	0.64	2 (3%)	68,69,69	1.77	22 (32%)
24	CLA	B	606	-	65,73,73	2.06	17 (26%)	76,113,113	2.78	24 (31%)
24	CLA	C	513	-	65,73,73	2.07	17 (26%)	76,113,113	2.68	27 (35%)
24	CLA	B	605	-	65,73,73	1.99	16 (24%)	76,113,113	2.71	26 (34%)
24	CLA	B	615	-	65,73,73	2.06	15 (23%)	76,113,113	2.86	30 (39%)
24	CLA	d	404	-	65,73,73	2.00	17 (26%)	76,113,113	2.77	28 (36%)
36	HTG	V	206	-	19,19,19	1.02	2 (10%)	23,24,24	1.44	4 (17%)
37	DGD	e	101	-	63,63,67	0.95	3 (4%)	77,77,81	1.28	7 (9%)
24	CLA	c	511	41	65,73,73	2.05	16 (24%)	76,113,113	2.77	26 (34%)
24	CLA	b	614	-	65,73,73	2.03	17 (26%)	76,113,113	2.87	27 (35%)
24	CLA	a	412	-	65,73,73	2.01	17 (26%)	76,113,113	2.78	27 (35%)
38	LHG	b	634	-	48,48,48	0.93	2 (4%)	51,54,54	0.96	2 (3%)
24	CLA	b	619	41	65,73,73	2.09	18 (27%)	76,113,113	2.77	30 (39%)
26	BCR	b	626	-	41,41,41	1.01	1 (2%)	56,56,56	1.59	11 (19%)
27	SQD	F	101	-	42,43,54	1.17	3 (7%)	51,54,65	1.69	11 (21%)
29	LMT	D	403	-	36,36,36	0.43	0	47,47,47	1.00	1 (2%)
29	LMT	M	102	-	36,36,36	0.42	0	47,47,47	0.87	1 (2%)
36	HTG	D	414	-	16,16,19	1.07	2 (12%)	20,21,24	1.32	1 (5%)
24	CLA	b	611	-	65,73,73	2.09	17 (26%)	76,113,113	2.87	30 (39%)
36	HTG	c	524	-	19,19,19	1.02	2 (10%)	23,24,24	1.50	2 (8%)
26	BCR	B	619	-	41,41,41	1.01	1 (2%)	56,56,56	1.37	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	B	609	-	65,73,73	2.06	16 (24%)	76,113,113	2.67	27 (35%)
38	LHG	d	410	-	48,48,48	0.91	2 (4%)	51,54,54	1.07	3 (5%)
24	CLA	D	405	-	65,73,73	2.02	17 (26%)	76,113,113	2.74	27 (35%)
37	DGD	H	102	-	63,63,67	0.90	2 (3%)	77,77,81	1.03	5 (6%)
24	CLA	C	509	-	65,73,73	2.12	16 (24%)	76,113,113	2.75	28 (36%)
24	CLA	A	406	41	65,73,73	2.08	18 (27%)	76,113,113	2.89	28 (36%)
26	BCR	C	515	-	41,41,41	1.04	1 (2%)	56,56,56	1.53	10 (17%)
28	GOL	v	204	-	5,5,5	0.37	0	5,5,5	0.24	0
24	CLA	b	623	-	65,73,73	2.06	17 (26%)	76,113,113	2.80	28 (36%)
24	CLA	d	403	41	65,73,73	2.04	15 (23%)	76,113,113	2.83	27 (35%)
28	GOL	C	524	-	5,5,5	0.36	0	5,5,5	0.75	0
28	GOL	t	103	-	5,5,5	0.41	0	5,5,5	0.23	0
24	CLA	B	613	-	65,73,73	1.98	14 (21%)	76,113,113	2.82	26 (34%)
34	LMG	A	419	-	51,51,55	0.92	2 (3%)	59,59,63	1.08	3 (5%)
37	DGD	D	408	-	52,52,67	1.03	3 (5%)	60,60,81	1.19	5 (8%)
37	DGD	h	102	-	63,63,67	0.90	3 (4%)	77,77,81	0.96	3 (3%)
27	SQD	f	102	-	42,43,54	1.19	3 (7%)	51,54,65	1.45	7 (13%)
36	HTG	b	632	-	19,19,19	1.19	2 (10%)	23,24,24	1.68	3 (13%)
24	CLA	A	407	41	65,73,73	2.01	16 (24%)	76,113,113	2.80	29 (38%)
38	LHG	D	410	-	48,48,48	0.93	2 (4%)	51,54,54	0.73	2 (3%)
36	HTG	C	522	-	19,19,19	1.03	2 (10%)	23,24,24	1.67	1 (4%)
26	BCR	d	406	-	41,41,41	1.08	1 (2%)	56,56,56	1.66	15 (26%)
24	CLA	C	503	-	65,73,73	2.09	16 (24%)	76,113,113	2.81	25 (32%)
24	CLA	c	517	-	65,73,73	2.06	16 (24%)	76,113,113	2.76	27 (35%)
36	HTG	b	631	-	19,19,19	0.80	1 (5%)	23,24,24	1.35	1 (4%)
28	GOL	V	203	-	5,5,5	0.42	0	5,5,5	0.24	0
29	LMT	m	102	-	36,36,36	0.46	0	47,47,47	0.87	0
24	CLA	B	614	-	65,73,73	2.12	15 (23%)	76,113,113	2.73	28 (36%)
28	GOL	a	401	-	5,5,5	0.39	0	5,5,5	0.24	0
28	GOL	B	625	-	5,5,5	0.40	0	5,5,5	0.15	0
30	OEX	a	417[A]	3,1,41	0,15,15	-	-	-	-	-
28	GOL	c	501	-	5,5,5	0.40	0	5,5,5	0.23	0
31	OEY	A	416[B]	3,1,41	0,14,16	-	-	-	-	-
34	LMG	c	522	-	51,51,55	0.95	2 (3%)	59,59,63	1.17	7 (11%)
37	DGD	c	520	-	63,63,67	0.88	3 (4%)	77,77,81	1.03	6 (7%)
26	BCR	t	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.70	15 (26%)
39	HEM	v	206	16	41,50,50	1.32	5 (12%)	45,82,82	1.83	11 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	b	622	-	65,73,73	2.09	15 (23%)	76,113,113	2.68	26 (34%)
24	CLA	A	409	-	65,73,73	2.06	17 (26%)	76,113,113	2.65	28 (36%)
28	GOL	a	421	35	5,5,5	0.33	0	5,5,5	0.43	0
24	CLA	a	409	-	65,73,73	2.09	16 (24%)	76,113,113	2.76	30 (39%)
24	CLA	b	620	-	65,73,73	1.98	15 (23%)	76,113,113	2.65	27 (35%)
24	CLA	c	516	-	65,73,73	2.08	16 (24%)	76,113,113	2.79	28 (36%)
34	LMG	C	520	-	51,51,55	0.95	2 (3%)	59,59,63	1.12	3 (5%)
26	BCR	b	628	-	41,41,41	1.06	1 (2%)	56,56,56	1.42	10 (17%)
24	CLA	c	505	-	65,73,73	2.05	17 (26%)	76,113,113	2.71	27 (35%)
24	CLA	C	505	-	65,73,73	2.01	17 (26%)	76,113,113	2.63	24 (31%)
27	SQD	A	411	-	53,54,54	0.98	3 (5%)	62,65,65	1.53	11 (17%)
29	LMT	a	404	-	36,36,36	0.47	1 (2%)	47,47,47	1.16	3 (6%)
36	HTG	b	608	-	19,19,19	1.05	2 (10%)	23,24,24	1.11	3 (13%)
34	LMG	b	629	-	51,51,55	0.91	3 (5%)	59,59,63	1.07	5 (8%)

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
26	BCR	C	514	-	-	1/29/63/63	0/2/2/2
28	GOL	B	634	-	-	0/4/4/4	-
36	HTG	B	624	-	-	4/10/30/30	0/1/1/1
24	CLA	B	607	-	1/1/15/20	5/37/115/115	-
25	PHO	A	408	-	-	3/37/103/103	0/5/6/6
28	GOL	b	604	-	-	2/4/4/4	-
28	GOL	B	630	-	-	0/4/4/4	-
29	LMT	b	630	-	-	4/17/37/61	0/1/1/2
36	HTG	B	632	-	-	0/10/30/30	0/1/1/1
37	DGD	C	517	-	-	20/51/91/95	0/2/2/2
28	GOL	b	601	-	-	0/4/4/4	-
24	CLA	B	612	-	1/1/15/20	1/37/115/115	-
24	CLA	B	603	-	1/1/15/20	3/37/115/115	-
24	CLA	b	612	-	1/1/15/20	10/37/115/115	-
26	BCR	Y	101	-	-	6/29/63/63	0/2/2/2
28	GOL	B	628	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMT	T	104	-	-	9/17/37/61	0/1/1/2
34	LMG	d	415	40	-	10/46/66/70	0/1/1/1
26	BCR	A	410	-	-	0/29/63/63	0/2/2/2
24	CLA	c	512	-	1/1/15/20	4/37/115/115	-
38	LHG	L	101	-	-	13/53/53/53	-
24	CLA	C	512	-	1/1/15/20	6/37/115/115	-
38	LHG	a	420	-	-	18/46/46/53	-
24	CLA	c	508	41	1/1/15/20	9/37/115/115	-
29	LMT	t	101	-	-	7/17/37/61	0/1/1/2
24	CLA	C	507	41	1/1/15/20	4/37/115/115	-
34	LMG	z	101	-	-	12/34/54/70	0/1/1/1
24	CLA	b	617	-	-	2/37/115/115	-
27	SQD	A	413	-	-	17/49/69/69	0/1/1/1
36	HTG	B	622	-	-	2/10/30/30	0/1/1/1
24	CLA	B	604	-	1/1/15/20	5/37/115/115	-
24	CLA	C	511	3	-	2/37/115/115	-
34	LMG	Z	101	-	-	14/31/51/70	0/1/1/1
28	GOL	B	629	-	-	4/4/4/4	-
39	HEM	E	103	6,5	-	4/12/54/54	-
24	CLA	B	611	41	1/1/15/20	4/37/115/115	-
24	CLA	c	513	-	1/1/15/20	15/37/115/115	-
36	HTG	C	523	-	-	3/10/30/30	0/1/1/1
38	LHG	D	411	-	-	12/53/53/53	-
24	CLA	D	404	-	1/1/15/20	2/37/115/115	-
26	BCR	H	101	-	-	6/29/63/63	0/2/2/2
28	GOL	v	202	-	-	2/4/4/4	-
28	GOL	o	301	-	-	2/4/4/4	-
34	LMG	k	101	-	-	14/46/66/70	0/1/1/1
39	HEM	f	101	6,5	-	7/12/54/54	-
24	CLA	c	507	-	1/1/15/20	6/37/115/115	-
24	CLA	c	509	-	1/1/15/20	3/37/115/115	-
24	CLA	B	602	41	1/1/15/20	15/37/115/115	-
36	HTG	B	631	-	-	1/10/30/30	0/1/1/1
29	LMT	M	104	-	-	10/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	506	-	1/1/15/20	4/37/115/115	-
24	CLA	b	625	-	1/1/15/20	11/37/115/115	-
28	GOL	D	402	-	-	4/4/4/4	-
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
26	BCR	k	102	-	-	1/29/63/63	0/2/2/2
36	HTG	d	413	-	-	1/7/27/30	0/1/1/1
26	BCR	a	413	-	-	0/29/63/63	0/2/2/2
28	GOL	T	101	-	-	0/4/4/4	-
36	HTG	B	623	-	-	6/10/30/30	0/1/1/1
28	GOL	b	606	-	-	2/4/4/4	-
28	GOL	V	201	-	-	2/4/4/4	-
28	GOL	A	412	-	-	1/4/4/4	-
26	BCR	y	101	-	-	2/29/63/63	0/2/2/2
24	CLA	a	410	41	-	10/37/115/115	-
36	HTG	b	602	-	-	3/10/30/30	0/1/1/1
24	CLA	A	405	-	1/1/15/20	4/37/115/115	-
24	CLA	b	616	41	1/1/15/20	1/37/115/115	-
25	PHO	d	402[A]	-	-	1/37/103/103	0/5/6/6
26	BCR	h	101	-	-	1/29/63/63	0/2/2/2
27	SQD	L	102	-	-	20/49/69/69	0/1/1/1
26	BCR	b	627	-	-	1/29/63/63	0/2/2/2
29	LMT	a	419	-	-	4/21/61/61	0/2/2/2
24	CLA	b	615	-	1/1/15/20	11/37/115/115	-
26	BCR	D	406	-	-	6/29/63/63	0/2/2/2
29	LMT	C	521	-	-	9/21/61/61	0/2/2/2
28	GOL	V	202	-	-	2/4/4/4	-
34	LMG	C	519	-	-	8/46/66/70	0/1/1/1
37	DGD	c	521	-	-	14/51/91/95	0/2/2/2
29	LMT	m	103	-	-	8/21/61/61	0/2/2/2
28	GOL	b	605	-	-	2/4/4/4	-
26	BCR	c	526	-	-	1/29/63/63	0/2/2/2
26	BCR	K	101	-	-	2/29/63/63	0/2/2/2
38	LHG	E	101	-	-	23/46/46/53	-
24	CLA	d	405	-	1/1/15/20	6/37/115/115	-
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
28	GOL	a	402	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PHO	a	411	-	-	5/37/103/103	0/5/6/6
34	LMG	a	415	-	-	17/46/66/70	0/1/1/1
34	LMG	D	415	40	-	8/46/66/70	0/1/1/1
27	SQD	a	414	-	-	15/49/69/69	0/1/1/1
28	GOL	T	102	-	-	2/4/4/4	-
28	GOL	v	201	-	-	1/4/4/4	-
25	PHO	D	401[B]	-	-	0/37/103/103	0/5/6/6
37	DGD	C	518	-	-	12/51/91/95	0/2/2/2
24	CLA	c	510	-	1/1/15/20	13/37/115/115	-
24	CLA	C	510	-	1/1/15/20	11/37/115/115	-
24	CLA	B	616	-	1/1/15/20	9/37/115/115	-
28	GOL	b	603	-	-	0/4/4/4	-
39	HEM	V	205	16	-	4/12/54/54	-
38	LHG	d	408	-	-	13/53/53/53	-
28	GOL	B	626	-	-	2/4/4/4	-
24	CLA	b	613	-	1/1/15/20	5/37/115/115	-
25	PHO	D	401[A]	-	-	0/37/103/103	0/5/6/6
28	GOL	V	204	-	-	4/4/4/4	-
24	CLA	C	504	41	1/1/15/20	6/37/115/115	-
36	HTG	c	523	-	-	3/10/30/30	0/1/1/1
24	CLA	c	514	-	1/1/15/20	8/37/115/115	-
34	LMG	M	101	-	-	12/46/66/70	0/1/1/1
24	CLA	b	621	-	1/1/15/20	1/37/115/115	-
24	CLA	B	617	-	1/1/15/20	6/37/115/115	-
25	PHO	d	402[B]	-	-	2/37/103/103	0/5/6/6
37	DGD	C	516	-	-	14/51/91/95	0/2/2/2
36	HTG	b	607	-	-	3/10/30/30	0/1/1/1
24	CLA	c	515	3	1/1/15/20	6/37/115/115	-
26	BCR	T	103	-	-	2/29/63/63	0/2/2/2
29	LMT	E	102	-	-	4/21/61/61	0/2/2/2
24	CLA	B	610	-	1/1/15/20	6/37/115/115	-
24	CLA	b	610	41	1/1/15/20	15/37/115/115	-
29	LMT	A	414	-	-	6/21/61/61	0/2/2/2
38	LHG	D	409	-	-	14/53/53/53	-
24	CLA	B	608	41	1/1/15/20	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	624	-	1/1/15/20	5/37/115/115	-
32	PL9	a	416[B]	-	-	15/53/73/73	0/1/1/1
37	DGD	c	519	-	-	15/51/91/95	0/2/2/2
28	GOL	C	525	-	-	2/4/4/4	-
24	CLA	b	618	-	1/1/15/20	3/37/115/115	-
32	PL9	D	407[B]	-	-	9/53/73/73	0/1/1/1
28	GOL	F	103	35	-	1/4/4/4	-
28	GOL	v	203	-	-	2/4/4/4	-
32	PL9	d	407[B]	-	-	8/53/73/73	0/1/1/1
29	LMT	e	102	-	-	10/21/61/61	0/2/2/2
32	PL9	A	417[B]	-	-	10/53/73/73	0/1/1/1
32	PL9	a	416[A]	-	-	18/53/73/73	0/1/1/1
26	BCR	c	518	-	-	4/29/63/63	0/2/2/2
27	SQD	a	405	-	-	12/49/69/69	0/1/1/1
24	CLA	C	502	-	1/1/15/20	5/37/115/115	-
24	CLA	C	506	-	1/1/15/20	10/37/115/115	-
32	PL9	D	407[A]	-	-	7/53/73/73	0/1/1/1
24	CLA	C	501	-	1/1/15/20	12/37/115/115	-
28	GOL	B	627	-	-	2/4/4/4	-
32	PL9	d	407[A]	-	-	5/53/73/73	0/1/1/1
27	SQD	B	621	-	-	20/49/69/69	0/1/1/1
28	GOL	c	502	-	-	2/4/4/4	-
24	CLA	C	508	-	1/1/15/20	7/37/115/115	-
28	GOL	O	301	-	-	3/4/4/4	-
38	LHG	d	409	-	-	10/53/53/53	-
32	PL9	A	417[A]	-	-	14/53/73/73	0/1/1/1
24	CLA	B	606	-	1/1/15/20	7/37/115/115	-
24	CLA	C	513	-	1/1/15/20	7/37/115/115	-
24	CLA	B	605	-	1/1/15/20	5/37/115/115	-
24	CLA	B	615	-	1/1/15/20	17/37/115/115	-
24	CLA	d	404	-	1/1/15/20	3/37/115/115	-
36	HTG	V	206	-	-	4/10/30/30	0/1/1/1
37	DGD	e	101	-	-	26/51/91/95	0/2/2/2
24	CLA	c	511	41	1/1/15/20	3/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	614	-	1/1/15/20	7/37/115/115	-
24	CLA	a	412	-	1/1/15/20	10/37/115/115	-
38	LHG	b	634	-	-	15/53/53/53	-
24	CLA	b	619	41	1/1/15/20	7/37/115/115	-
26	BCR	b	626	-	-	3/29/63/63	0/2/2/2
27	SQD	F	101	-	-	14/38/58/69	0/1/1/1
29	LMT	D	403	-	-	10/21/61/61	0/2/2/2
29	LMT	M	102	-	-	10/21/61/61	0/2/2/2
36	HTG	D	414	-	-	0/7/27/30	0/1/1/1
24	CLA	b	611	-	1/1/15/20	4/37/115/115	-
36	HTG	c	524	-	-	2/10/30/30	0/1/1/1
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
24	CLA	B	609	-	-	0/37/115/115	-
38	LHG	d	410	-	-	16/53/53/53	-
24	CLA	D	405	-	1/1/15/20	4/37/115/115	-
37	DGD	H	102	-	-	10/51/91/95	0/2/2/2
24	CLA	C	509	-	1/1/15/20	14/37/115/115	-
24	CLA	A	406	41	1/1/15/20	5/37/115/115	-
26	BCR	C	515	-	-	6/29/63/63	0/2/2/2
28	GOL	v	204	-	-	2/4/4/4	-
24	CLA	b	623	-	1/1/15/20	21/37/115/115	-
24	CLA	d	403	41	1/1/15/20	8/37/115/115	-
28	GOL	C	524	-	-	1/4/4/4	-
28	GOL	t	103	-	-	0/4/4/4	-
24	CLA	B	613	-	1/1/15/20	3/37/115/115	-
34	LMG	A	419	-	-	19/46/66/70	0/1/1/1
37	DGD	D	408	-	-	21/47/67/95	0/1/1/2
37	DGD	h	102	-	-	10/51/91/95	0/2/2/2
27	SQD	f	102	-	-	15/38/58/69	0/1/1/1
36	HTG	b	632	-	-	4/10/30/30	0/1/1/1
24	CLA	A	407	41	-	5/37/115/115	-
38	LHG	D	410	-	-	6/53/53/53	-
36	HTG	C	522	-	-	1/10/30/30	0/1/1/1
26	BCR	d	406	-	-	4/29/63/63	0/2/2/2
24	CLA	C	503	-	1/1/15/20	3/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	517	-	-	5/37/115/115	-
36	HTG	b	631	-	-	2/10/30/30	0/1/1/1
28	GOL	V	203	-	-	0/4/4/4	-
29	LMT	m	102	-	-	10/21/61/61	0/2/2/2
24	CLA	B	614	-	1/1/15/20	8/37/115/115	-
28	GOL	a	401	-	-	2/4/4/4	-
28	GOL	B	625	-	-	0/4/4/4	-
28	GOL	c	501	-	-	0/4/4/4	-
34	LMG	c	522	-	-	7/46/66/70	0/1/1/1
37	DGD	c	520	-	-	18/51/91/95	0/2/2/2
26	BCR	t	102	-	-	7/29/63/63	0/2/2/2
39	HEM	v	206	16	-	4/12/54/54	-
24	CLA	b	622	-	1/1/15/20	11/37/115/115	-
24	CLA	A	409	-	-	10/37/115/115	-
28	GOL	a	421	35	-	2/4/4/4	-
24	CLA	a	409	-	1/1/15/20	6/37/115/115	-
24	CLA	b	620	-	1/1/15/20	7/37/115/115	-
24	CLA	c	516	-	1/1/15/20	8/37/115/115	-
34	LMG	C	520	-	-	13/46/66/70	0/1/1/1
26	BCR	b	628	-	-	2/29/63/63	0/2/2/2
24	CLA	c	505	-	1/1/15/20	3/37/115/115	-
24	CLA	C	505	-	1/1/15/20	6/37/115/115	-
27	SQD	A	411	-	-	12/49/69/69	0/1/1/1
29	LMT	a	404	-	-	7/21/61/61	0/2/2/2
36	HTG	b	608	-	-	0/10/30/30	0/1/1/1
34	LMG	b	629	-	-	11/46/66/70	0/1/1/1

The worst 5 of 1360 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	614	CLA	C3B-C2B	6.56	1.49	1.40
24	B	613	CLA	C3B-C2B	6.55	1.49	1.40
24	c	513	CLA	C3B-C2B	6.49	1.49	1.40
24	C	511	CLA	C3B-C2B	6.48	1.49	1.40
24	D	404	CLA	C3B-C2B	6.47	1.49	1.40

The worst 5 of 2659 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	613	CLA	C1D-ND-C4D	-10.18	99.11	106.33
24	b	621	CLA	C1D-ND-C4D	-10.11	99.16	106.33
24	B	606	CLA	C1D-ND-C4D	-9.99	99.24	106.33
24	A	407	CLA	C1D-ND-C4D	-9.93	99.28	106.33
24	a	412	CLA	C1D-ND-C4D	-9.86	99.33	106.33

5 of 63 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	405	CLA	ND
24	A	406	CLA	ND
24	B	602	CLA	ND
24	B	603	CLA	ND
24	B	604	CLA	ND

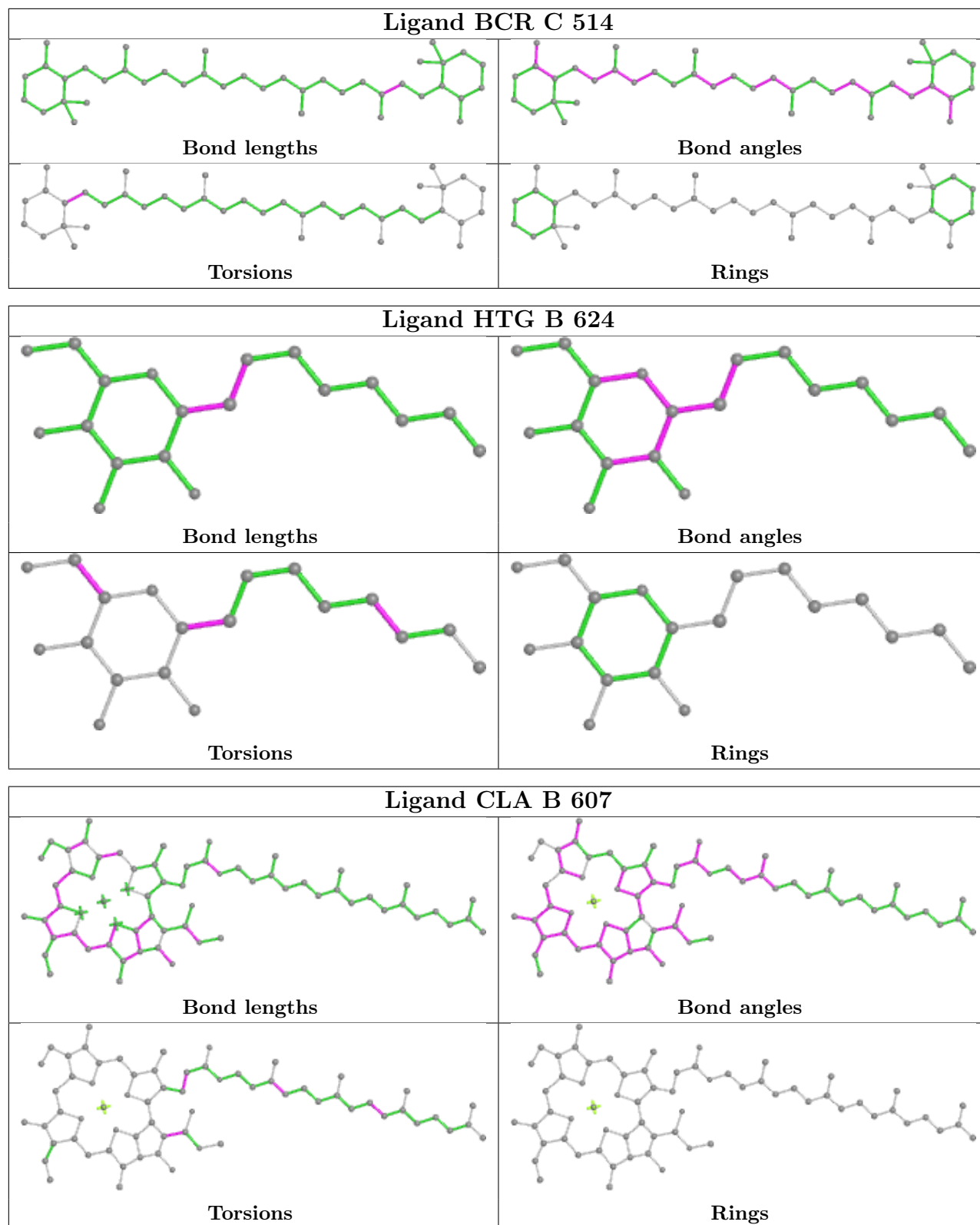
5 of 1418 torsion outliers are listed below:

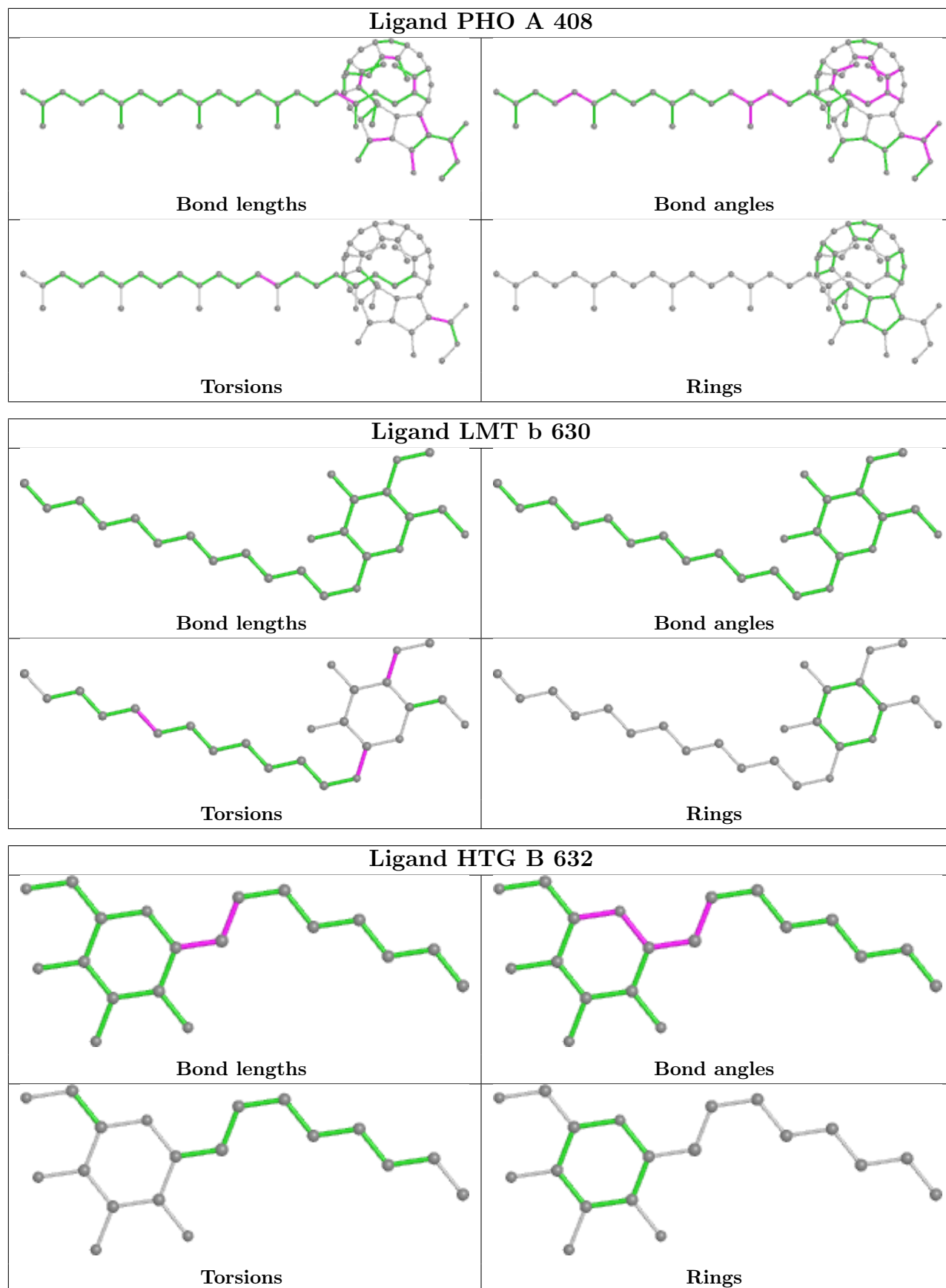
Mol	Chain	Res	Type	Atoms
24	B	607	CLA	CHA-CBD-CGD-O1D
24	B	607	CLA	CHA-CBD-CGD-O2D
24	B	615	CLA	CAD-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O2D
24	B	615	CLA	C2-C3-C5-C6

There are no ring outliers.

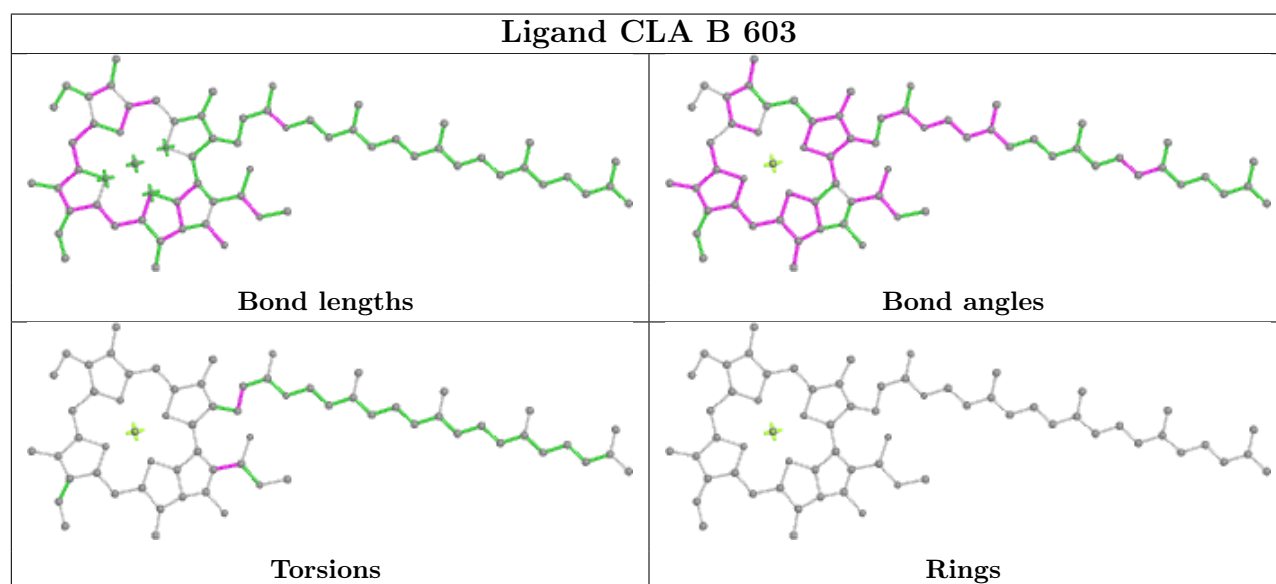
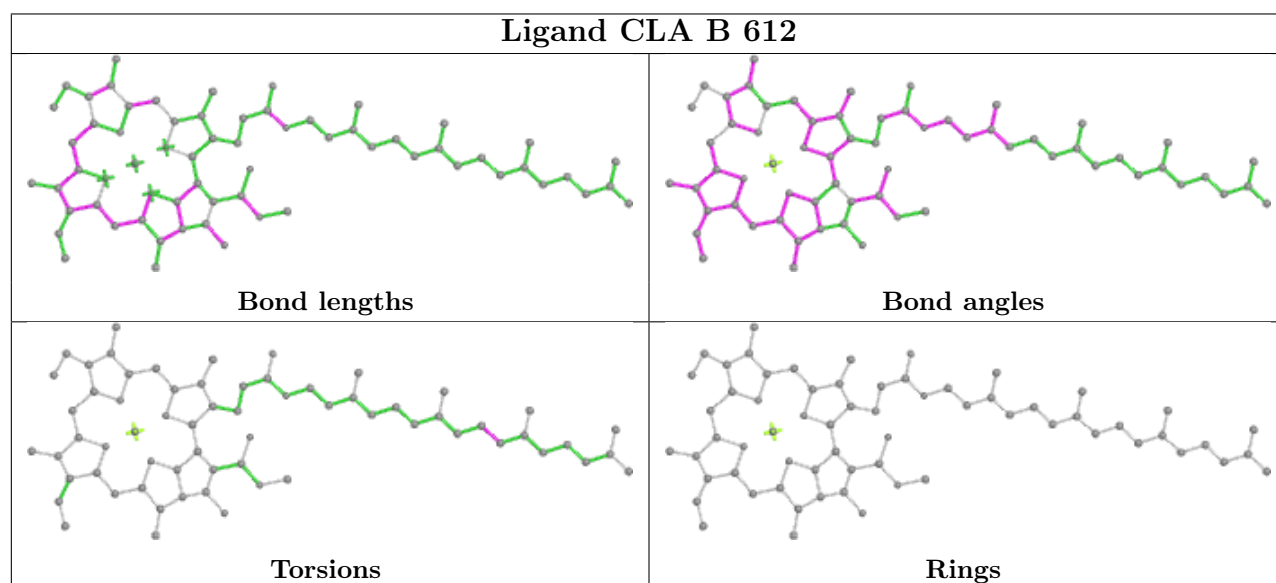
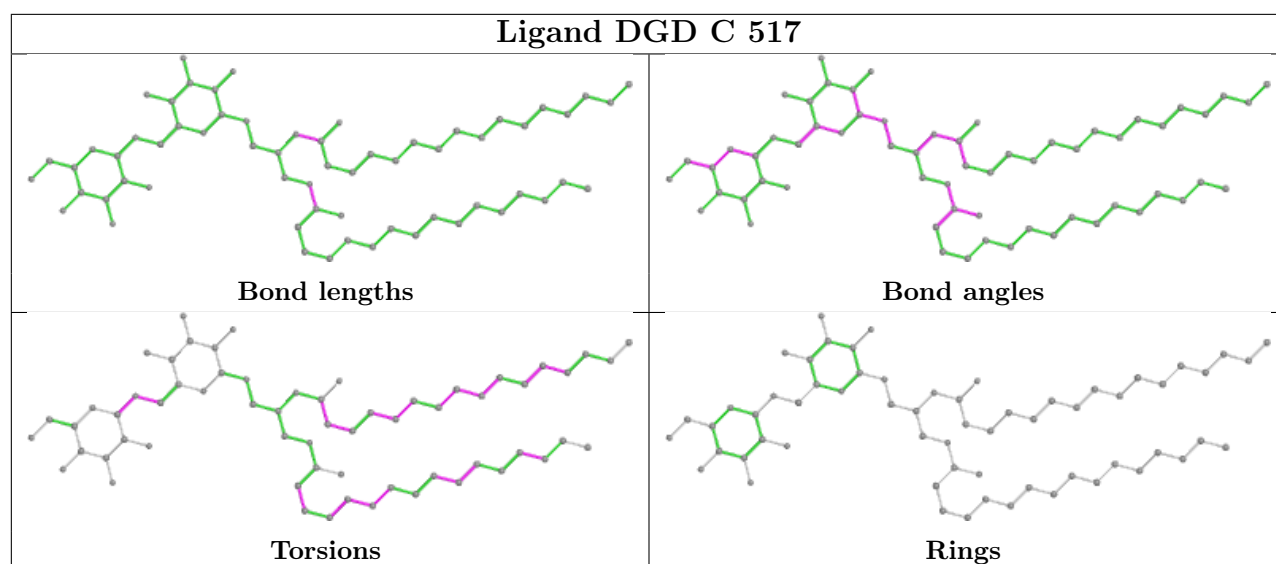
No monomer is involved in short contacts.

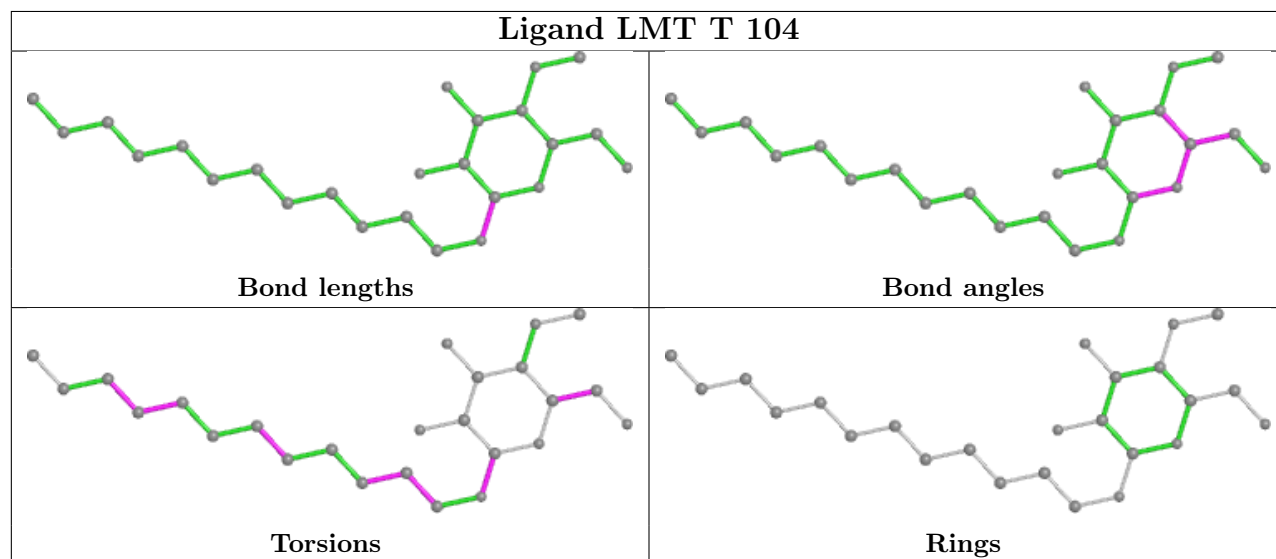
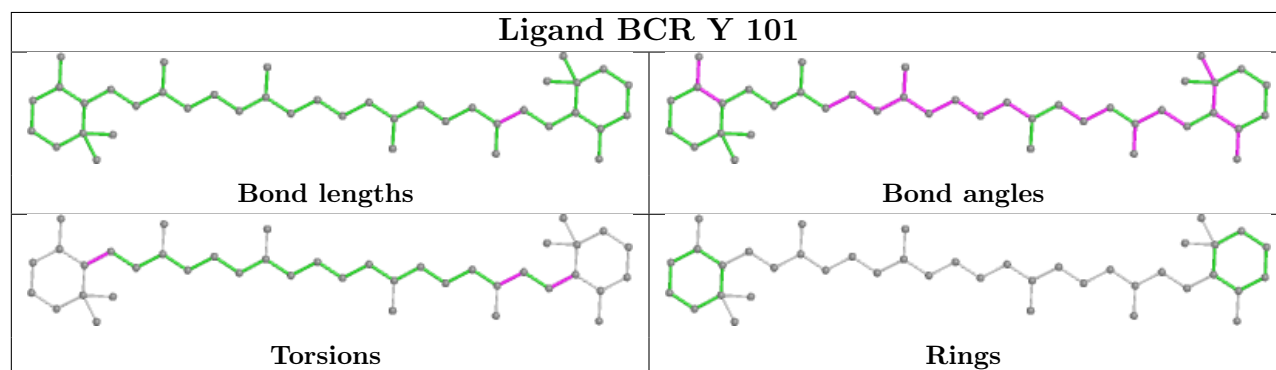
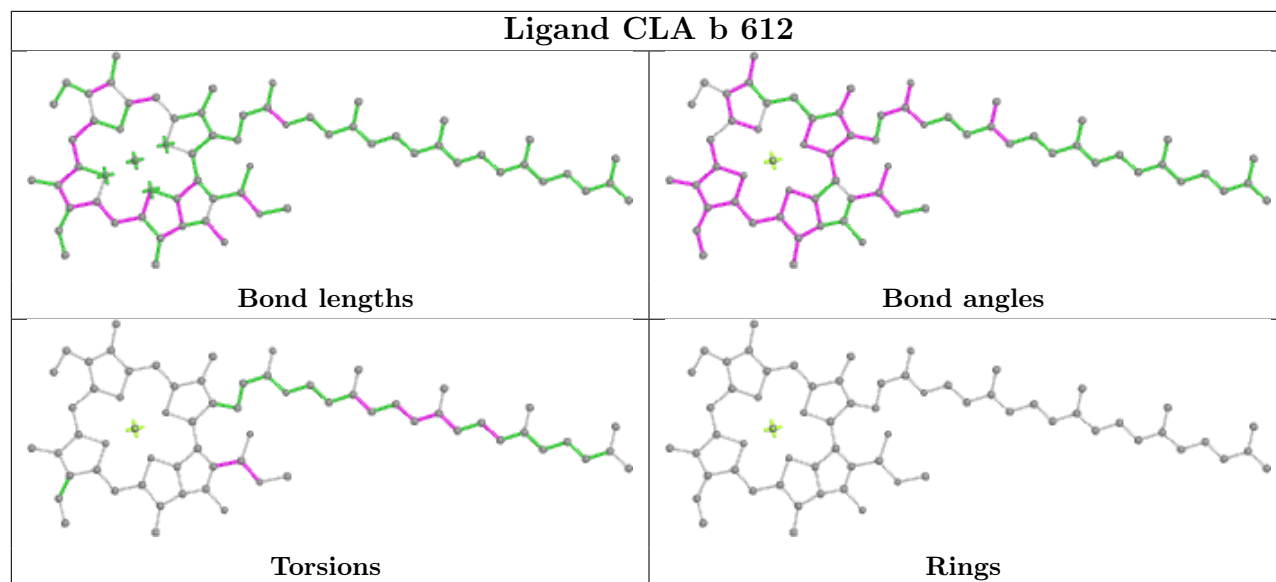
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

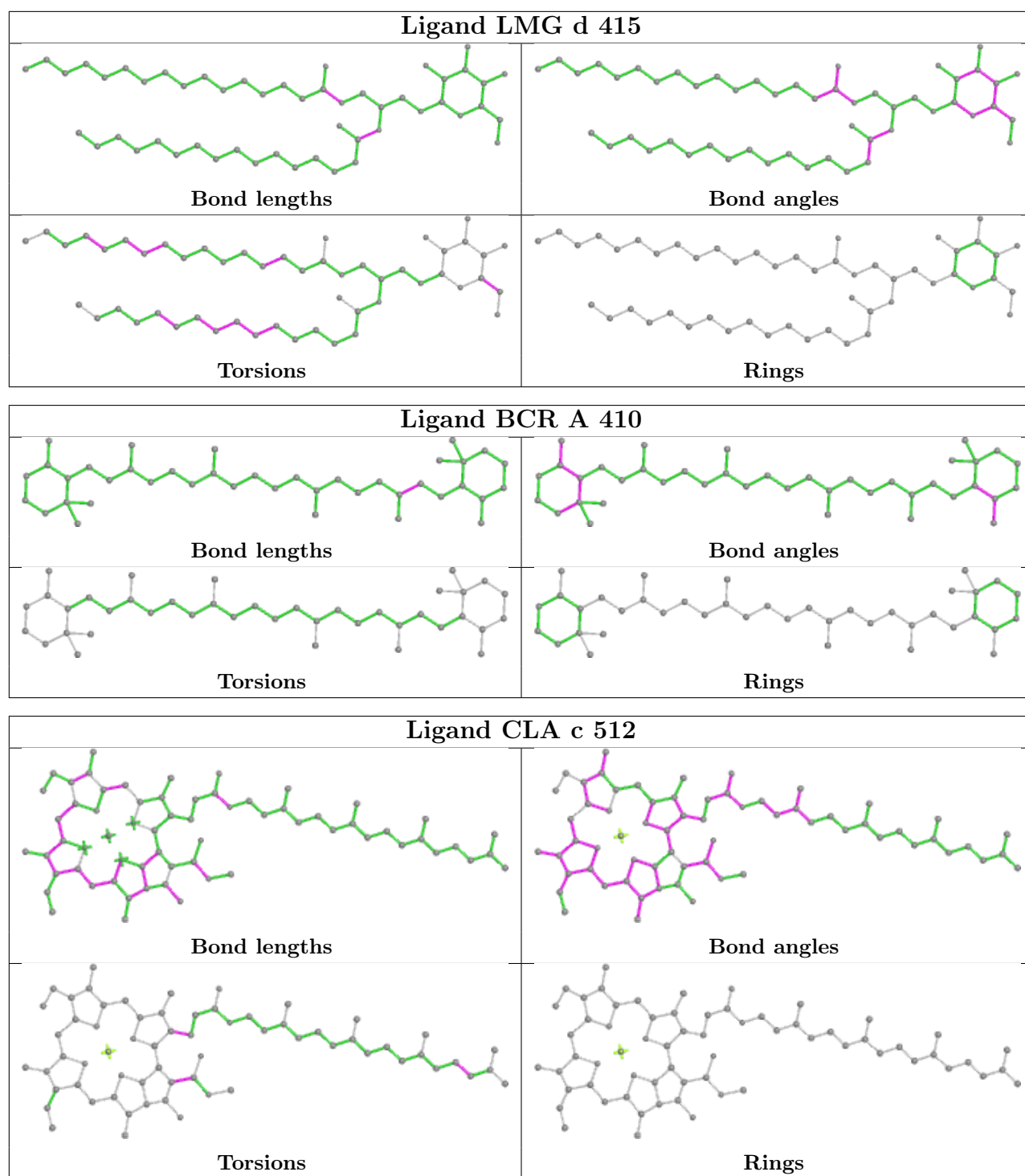


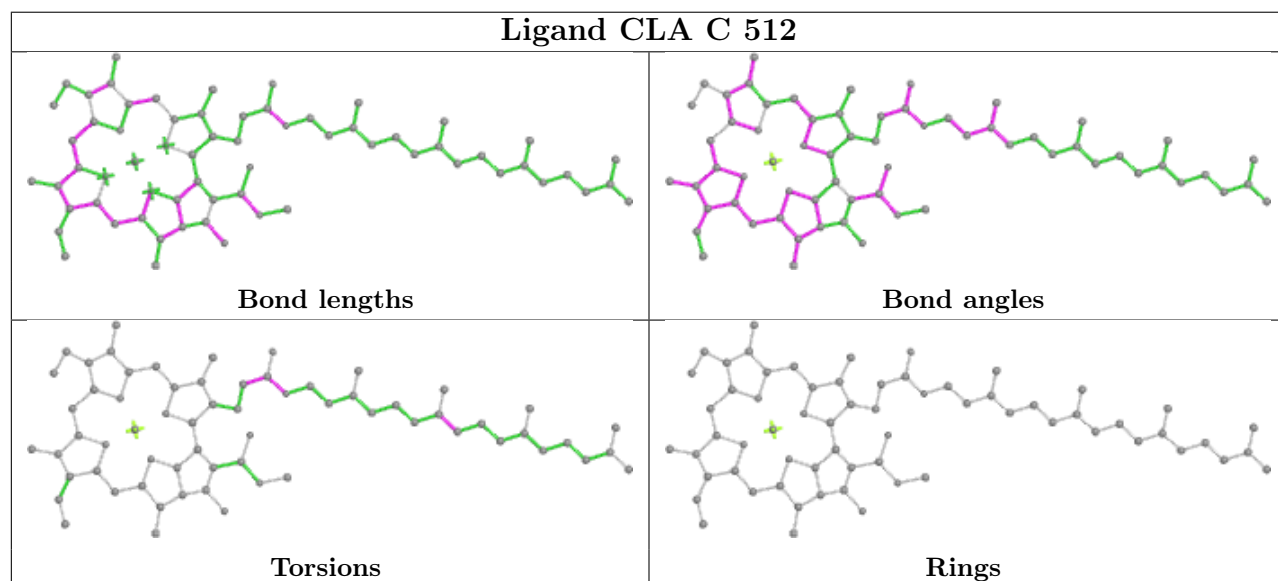
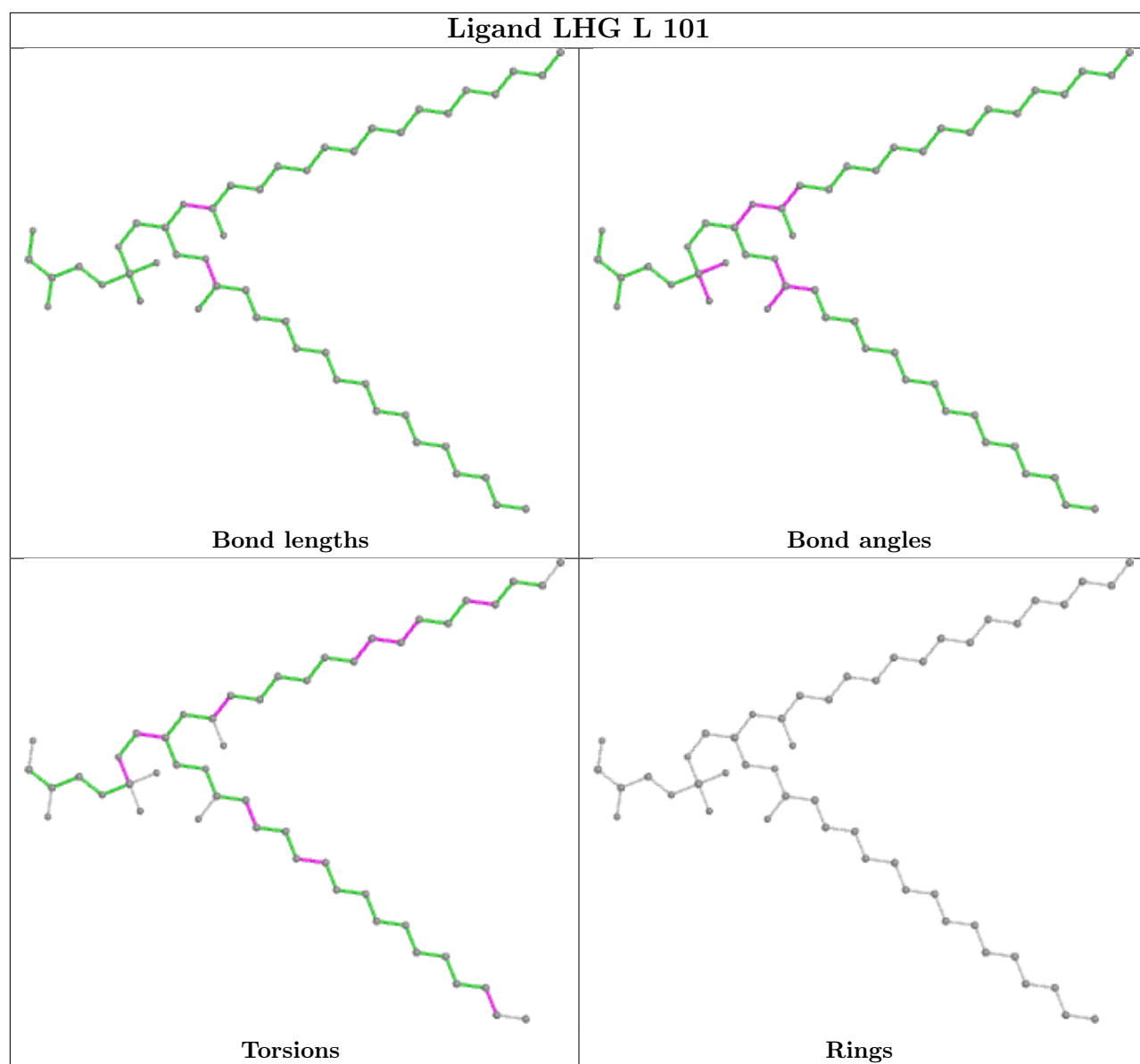


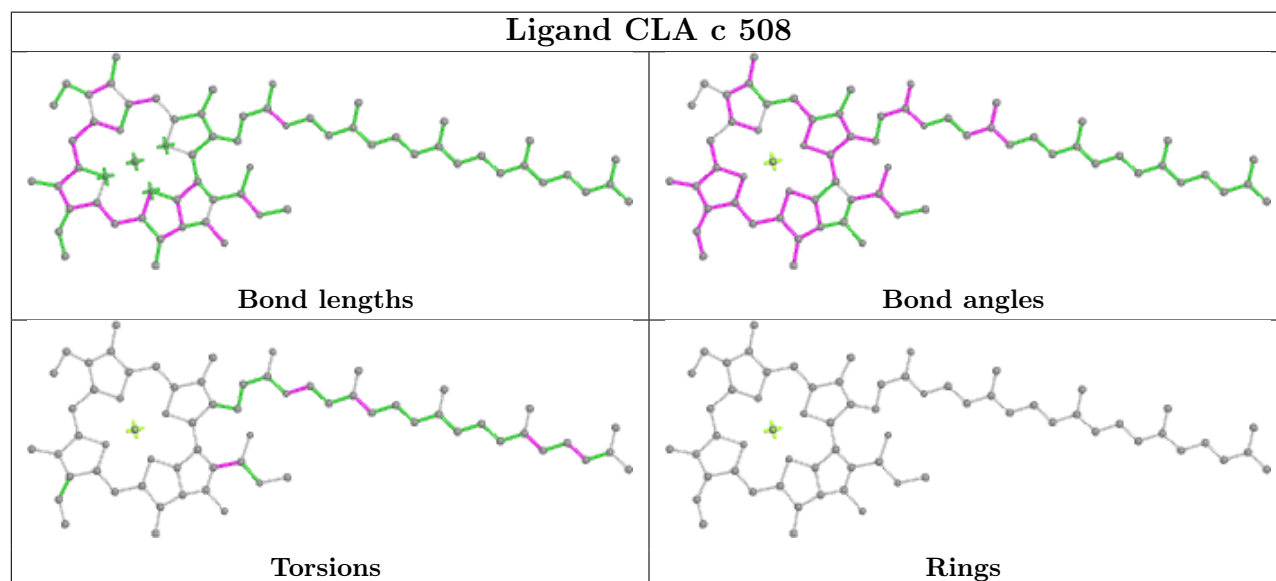
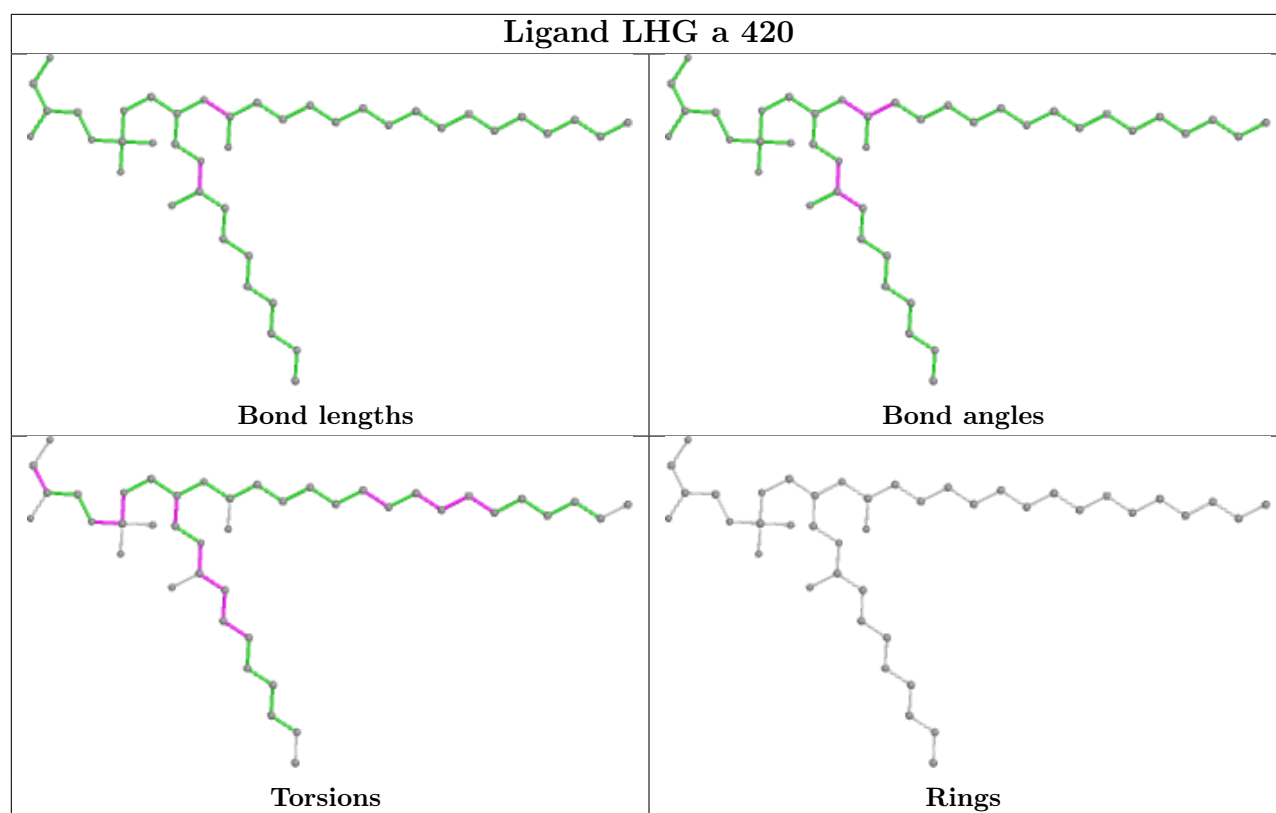


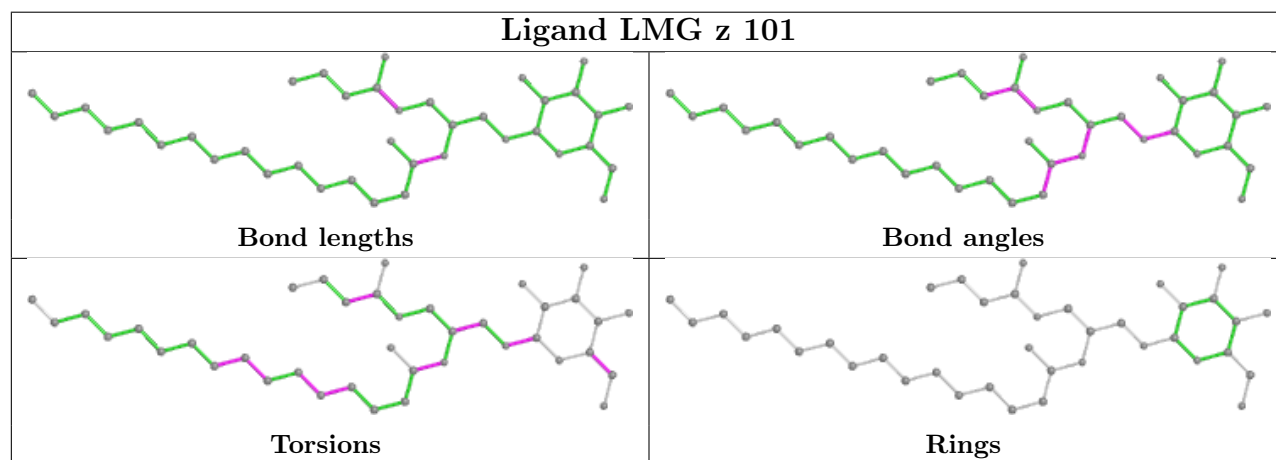
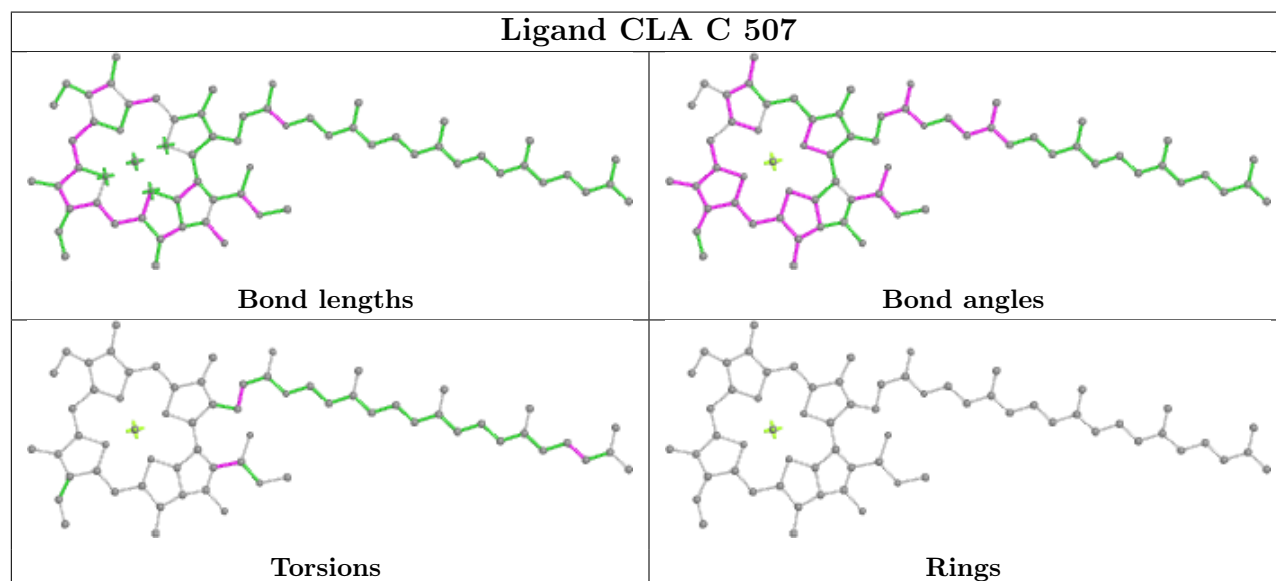
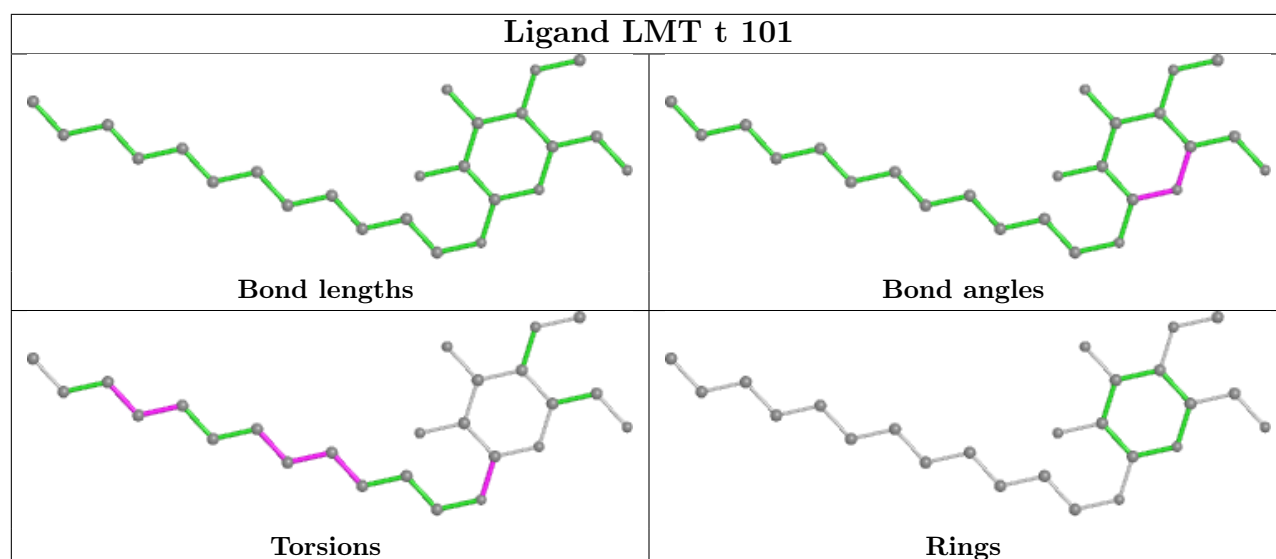


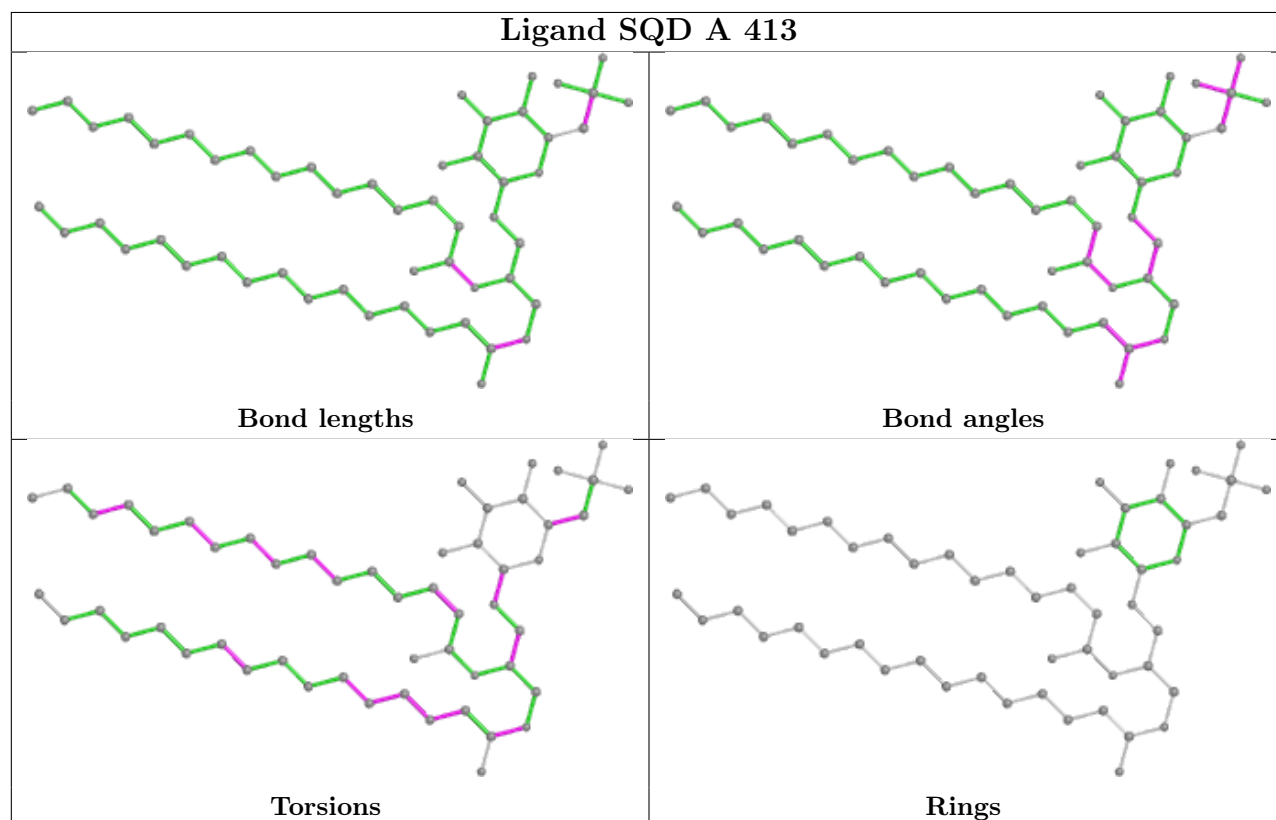
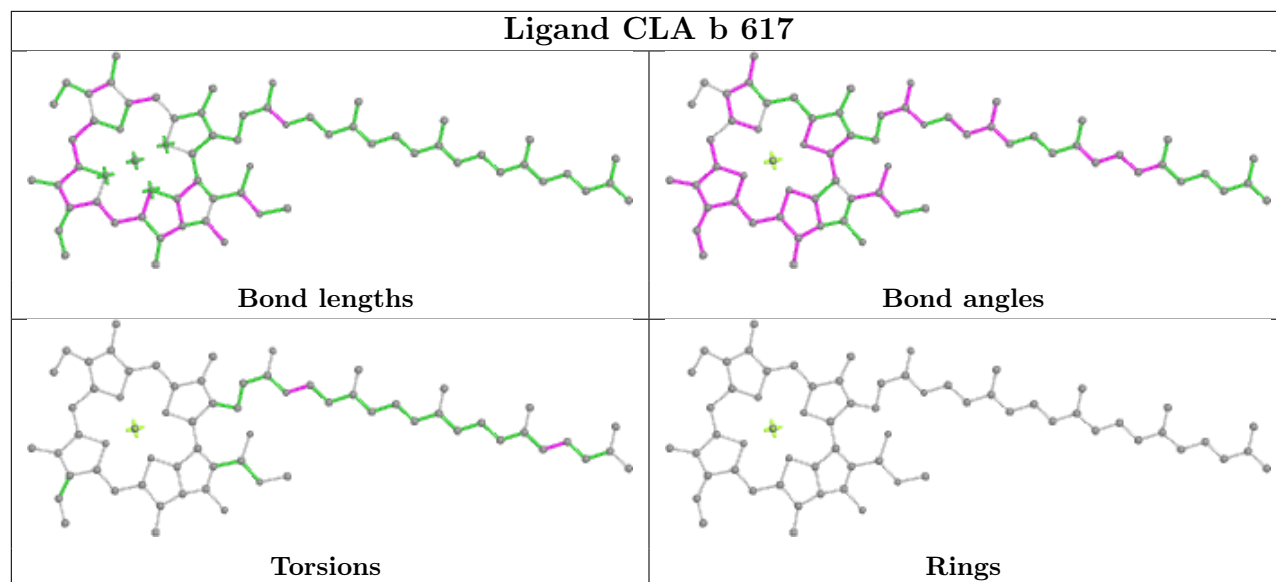


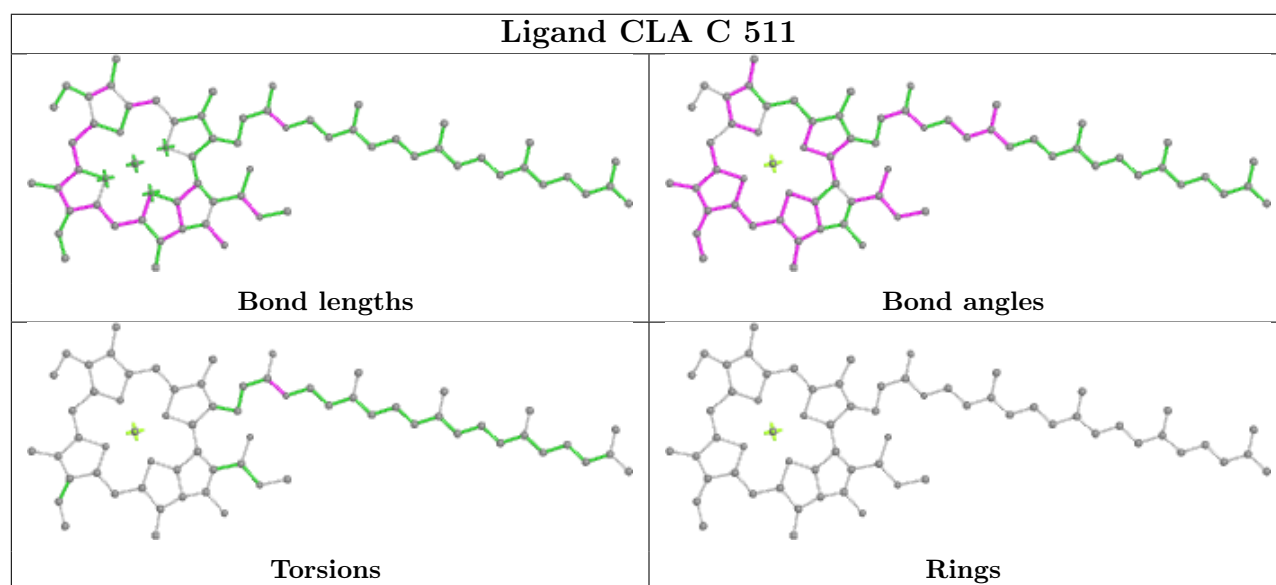
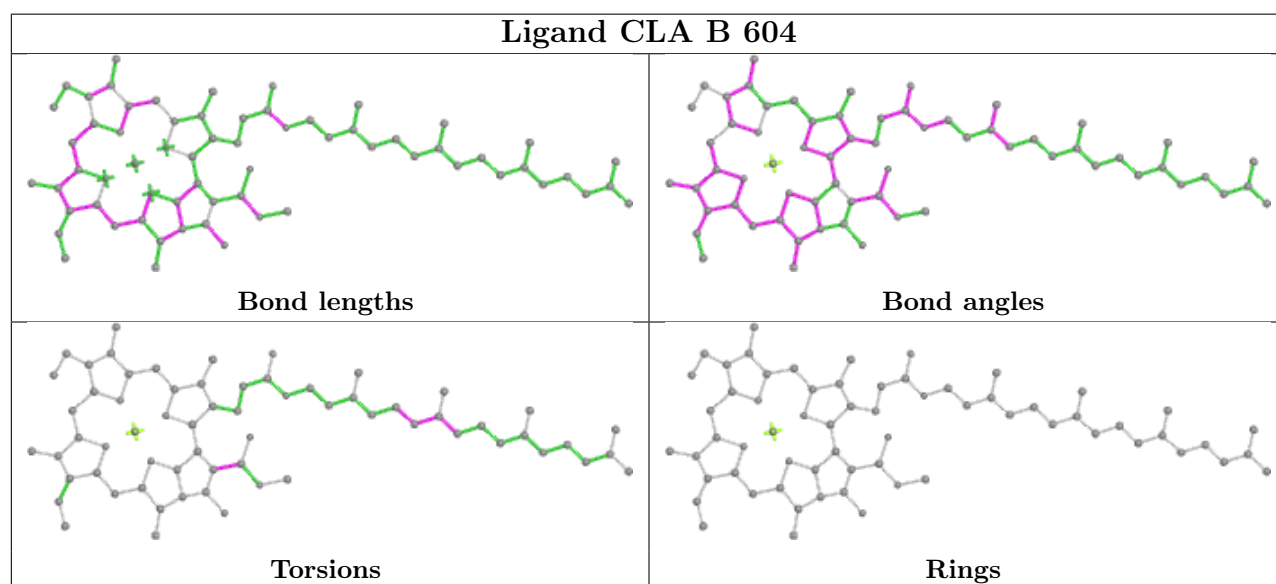
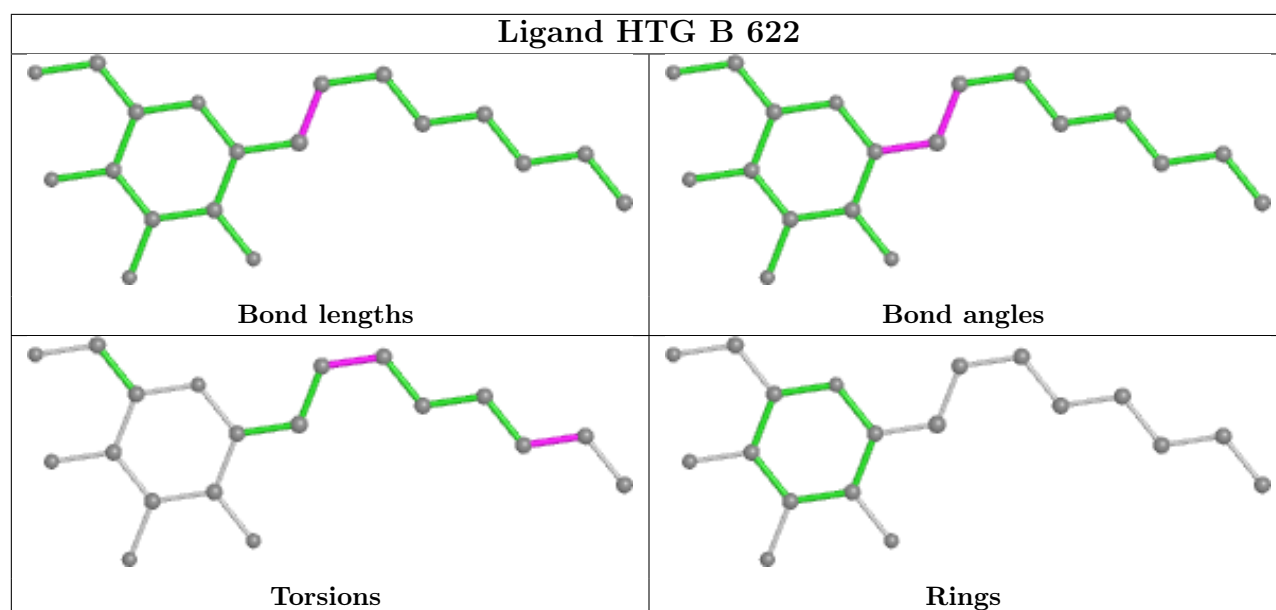




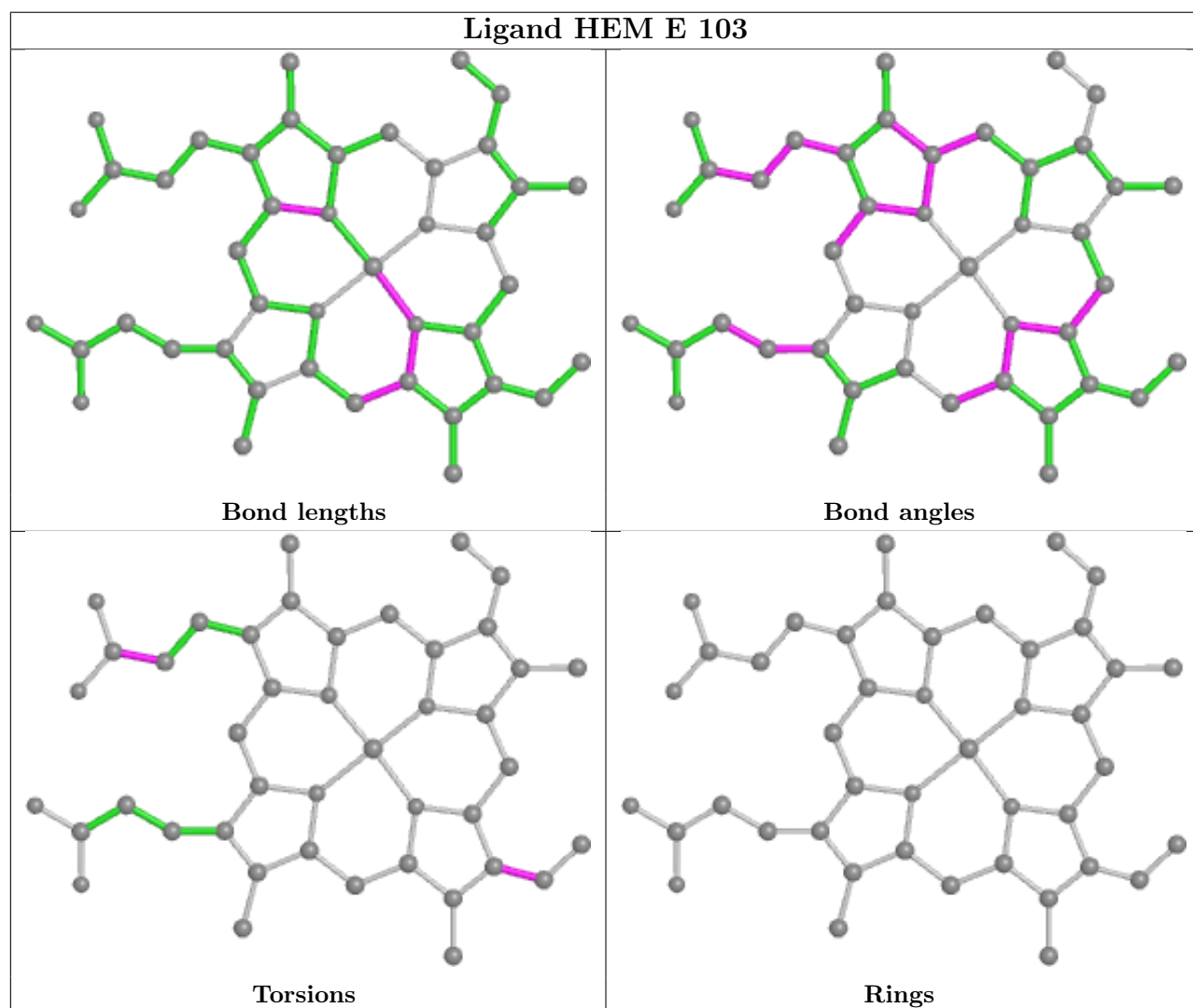
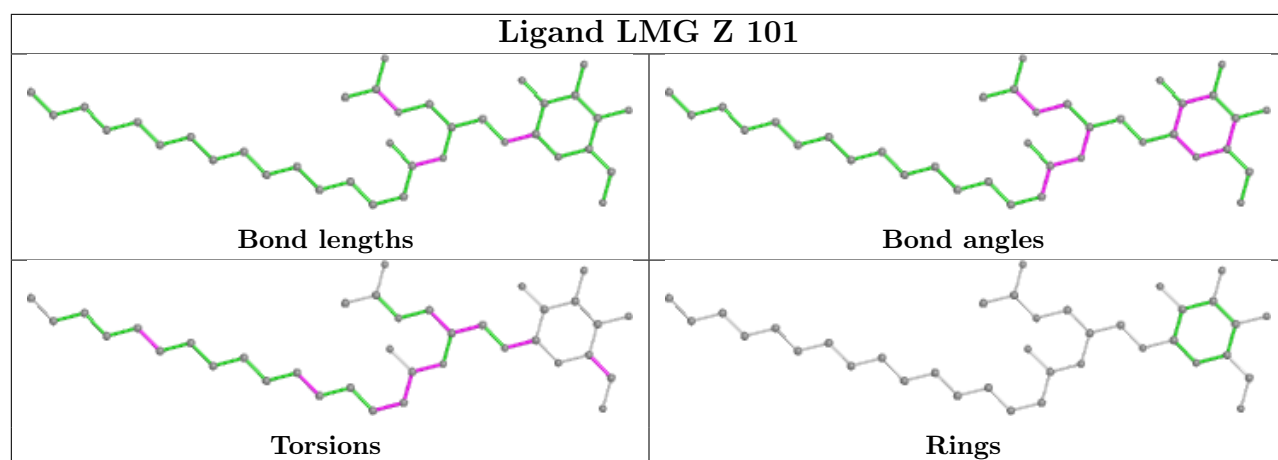


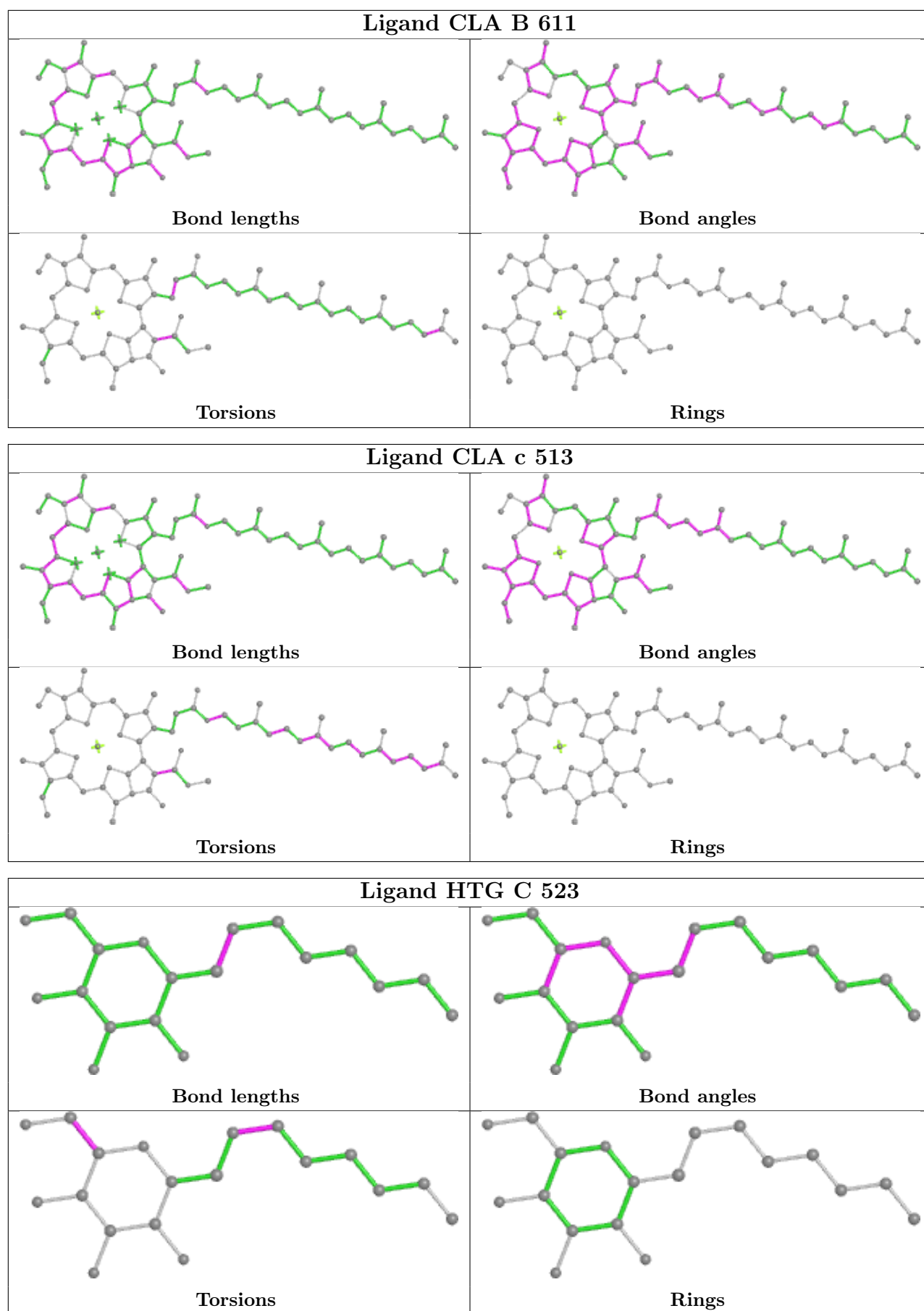


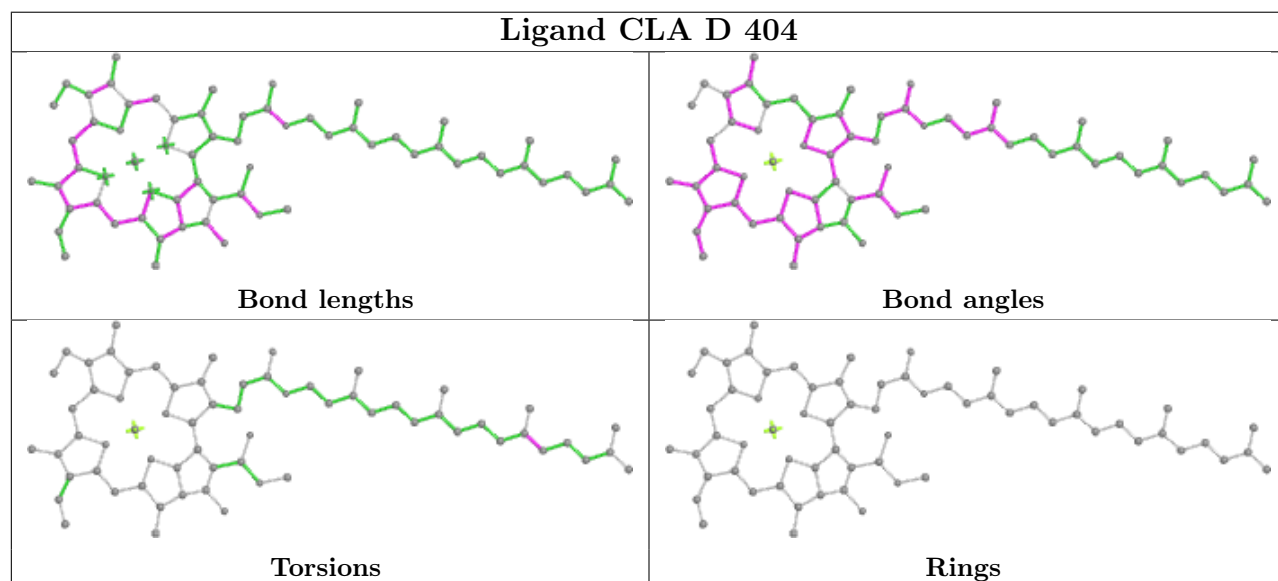
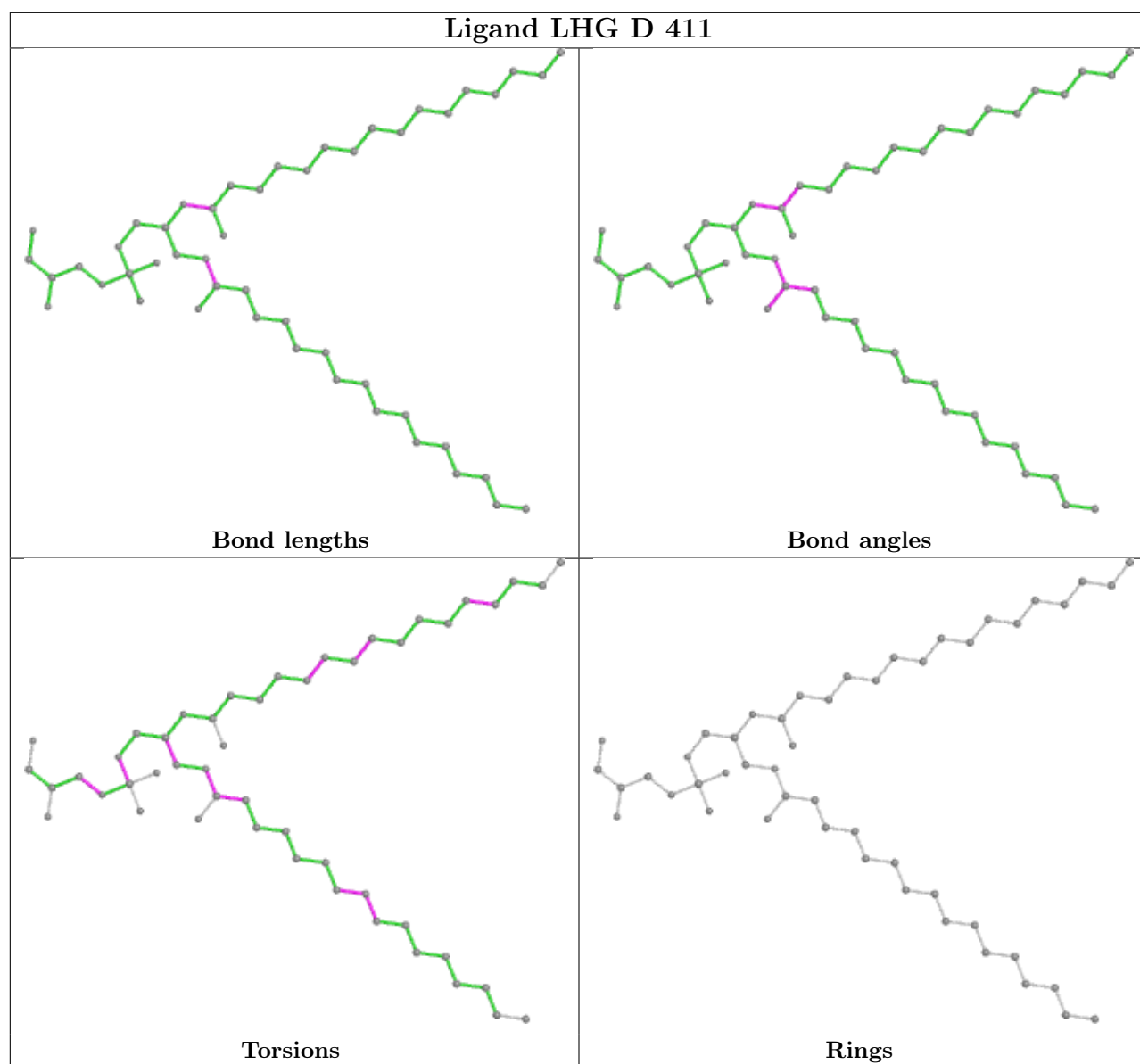


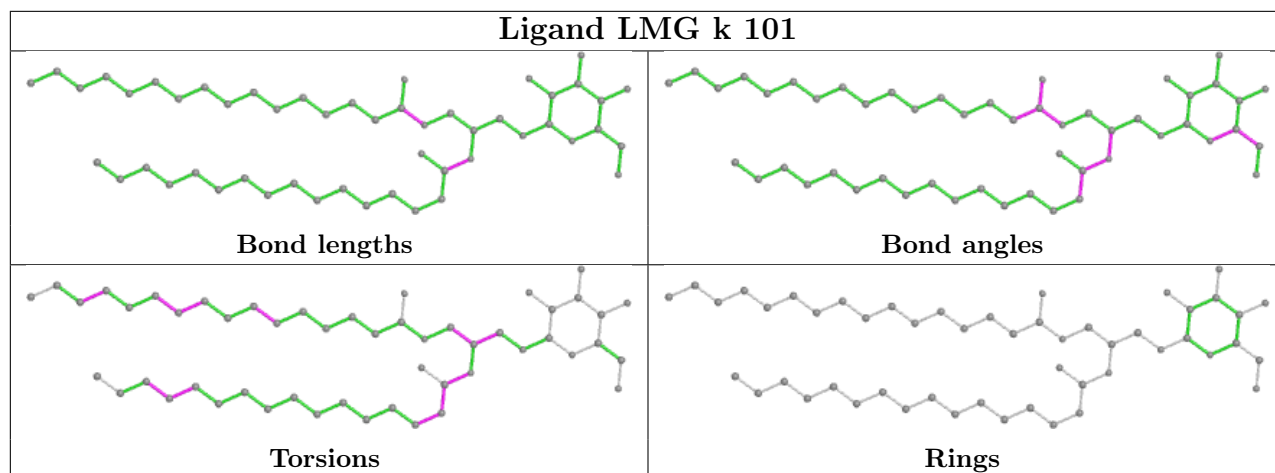
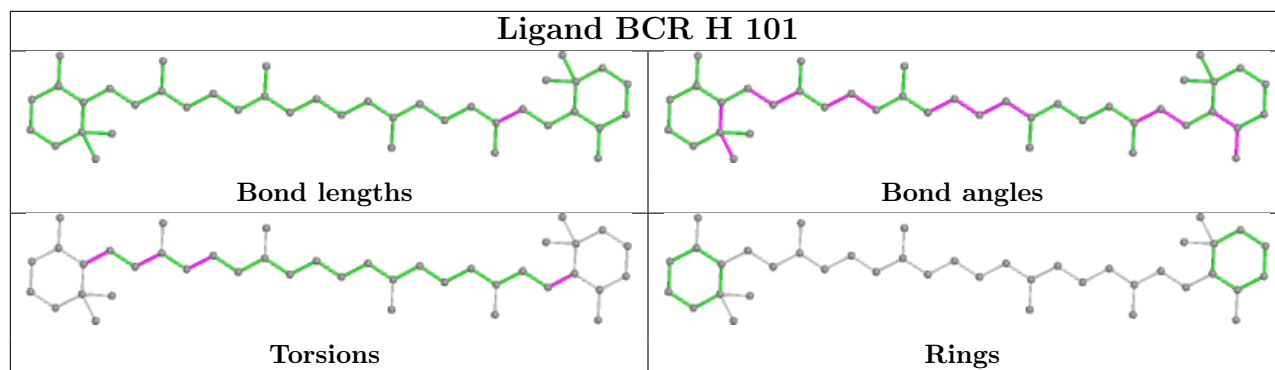


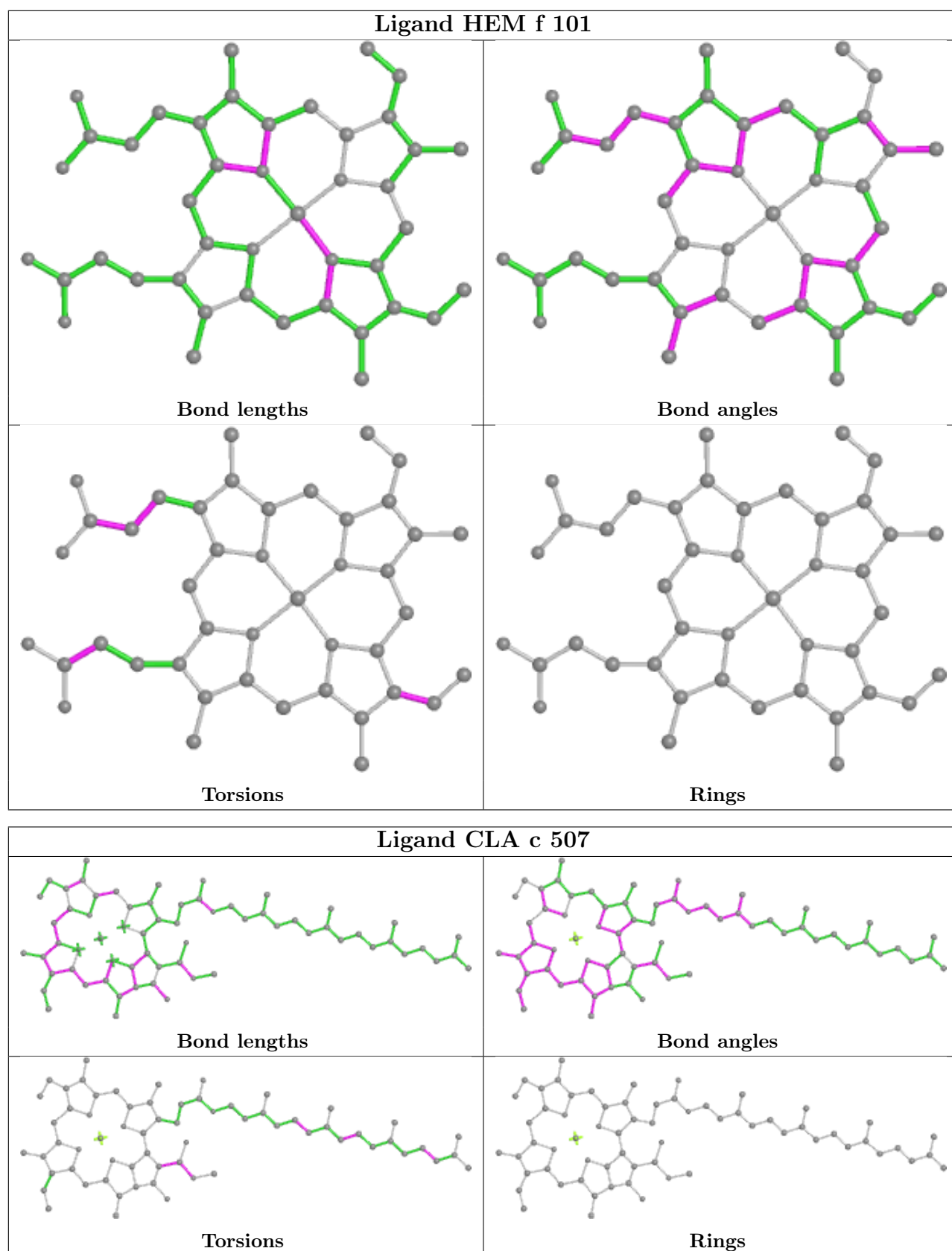


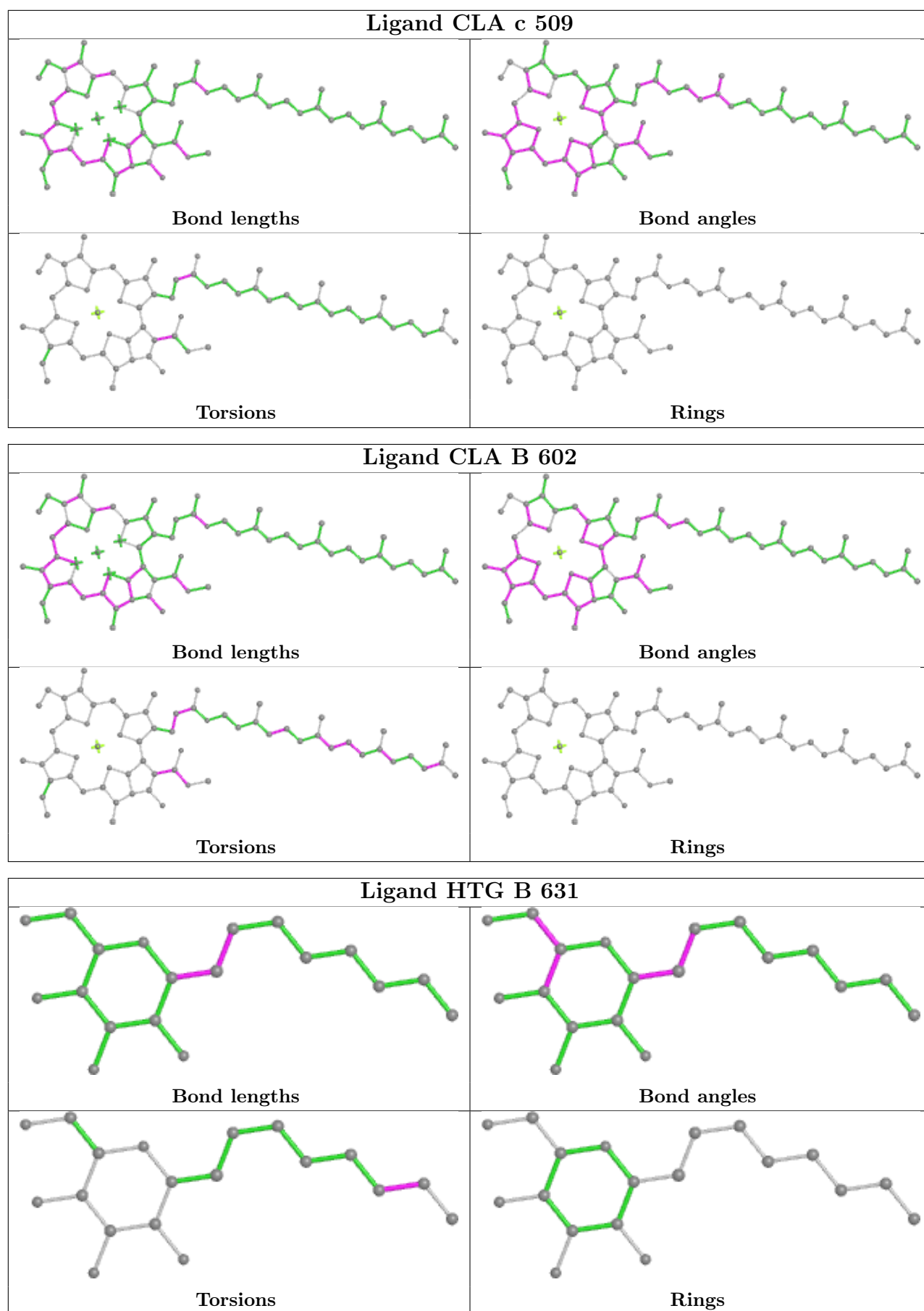


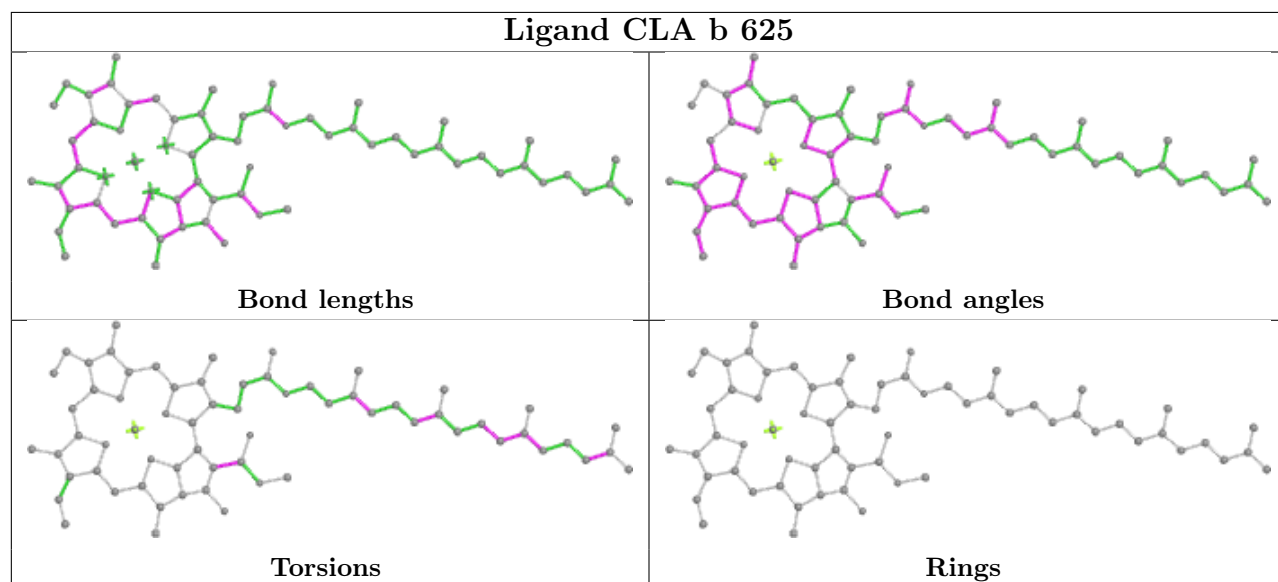
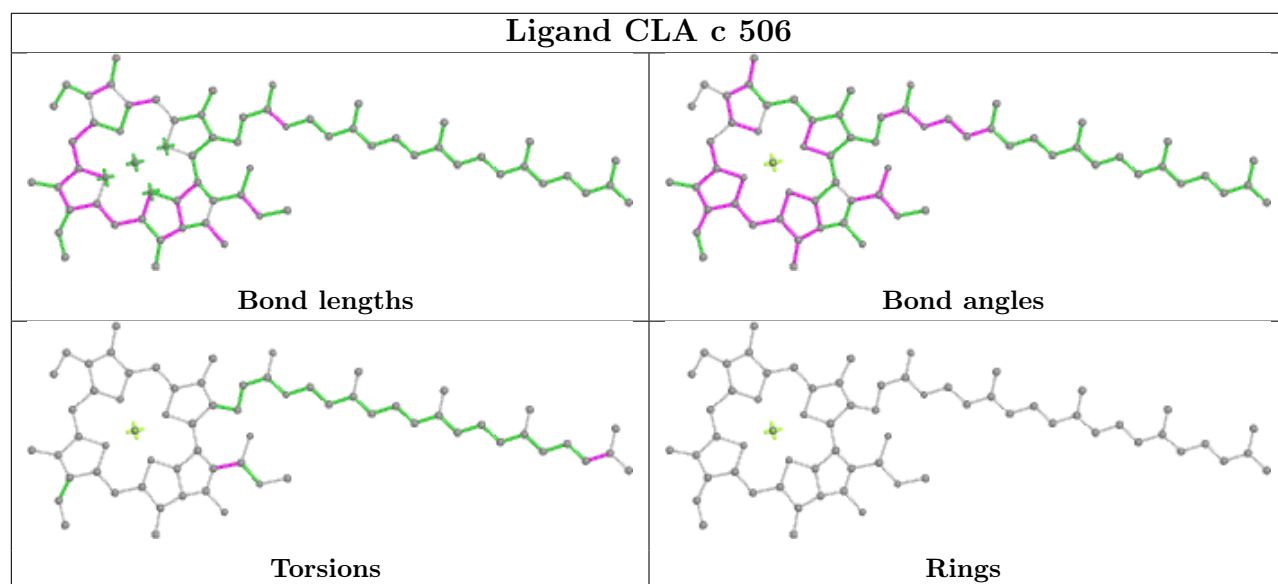
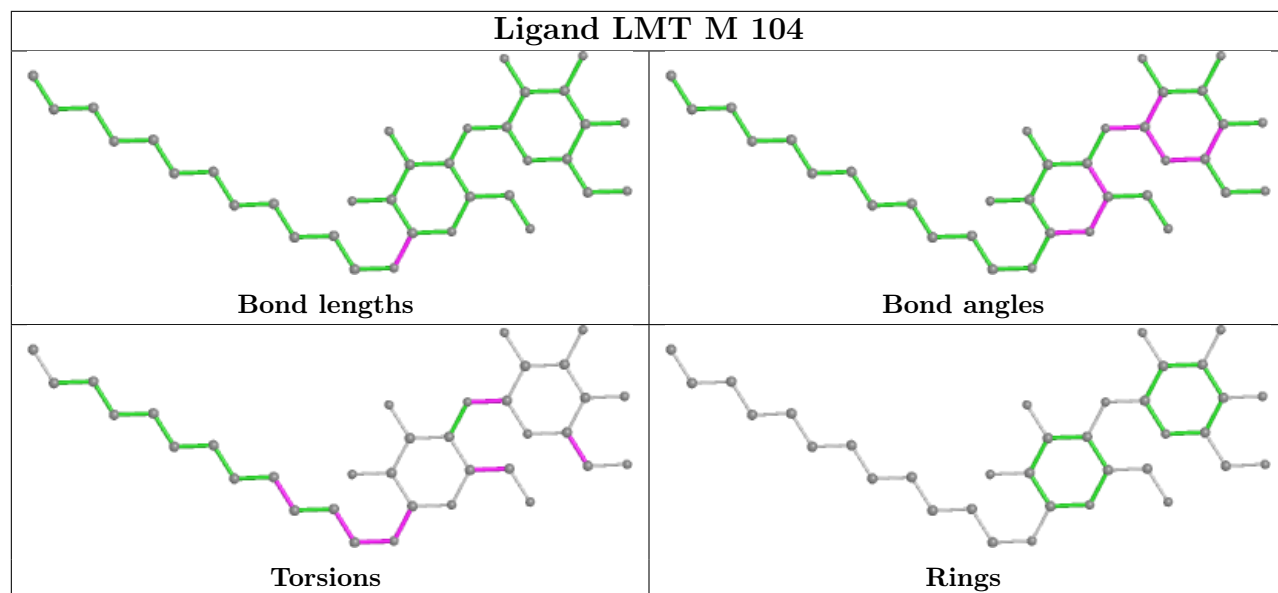


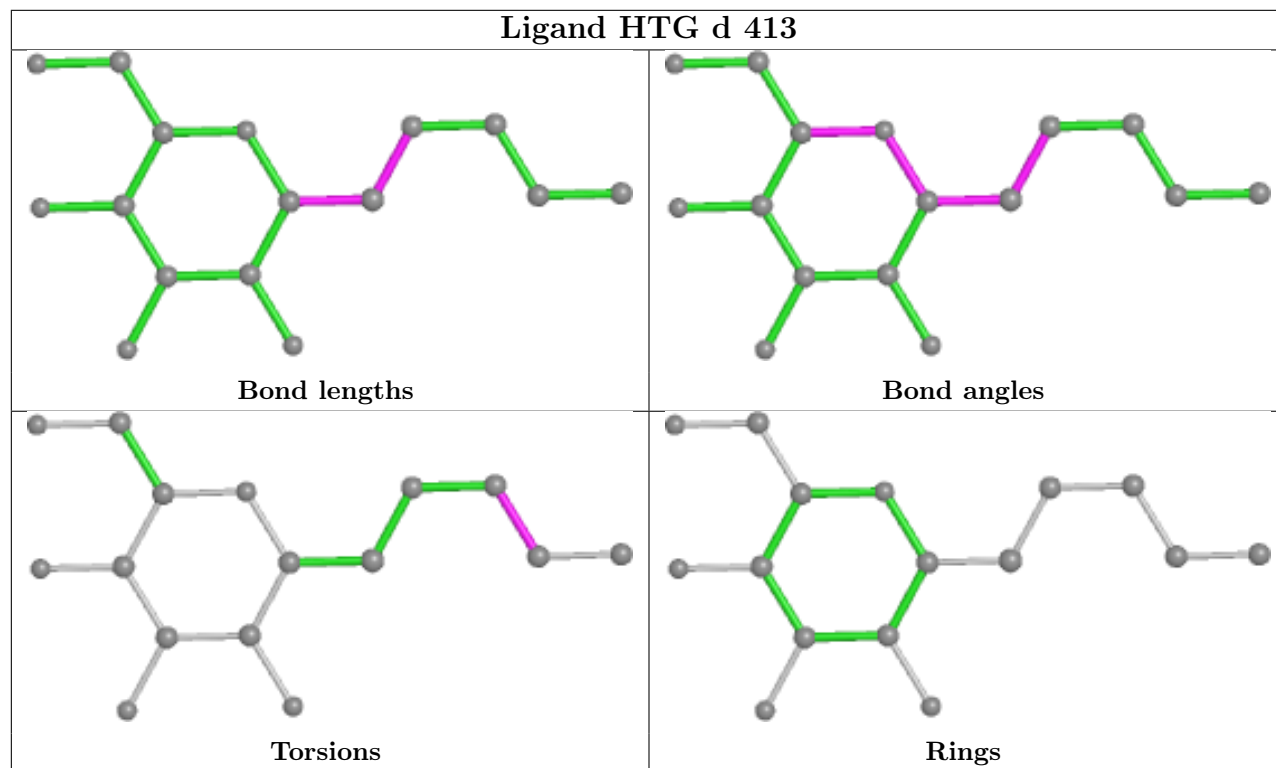
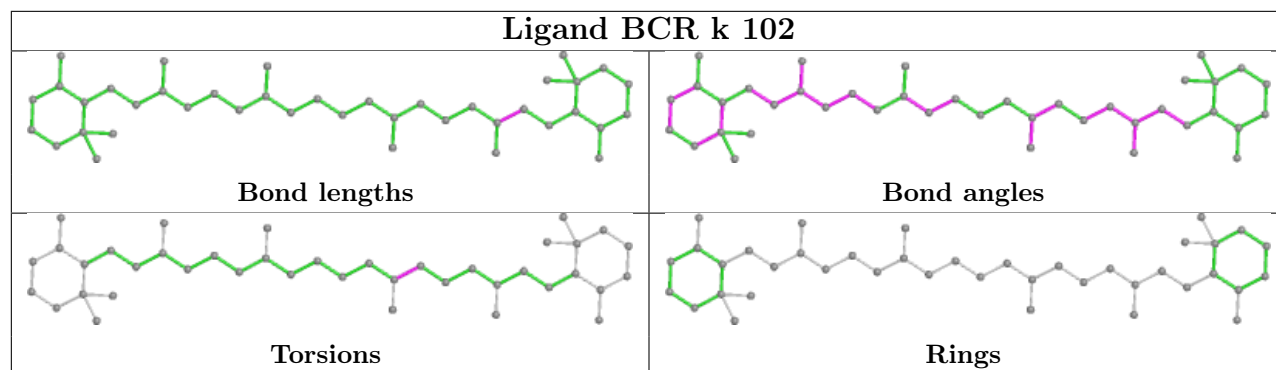
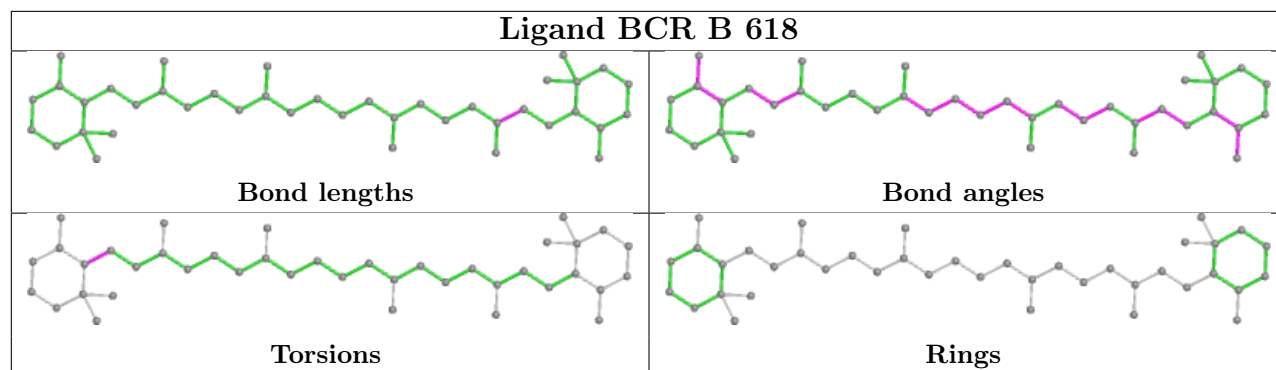




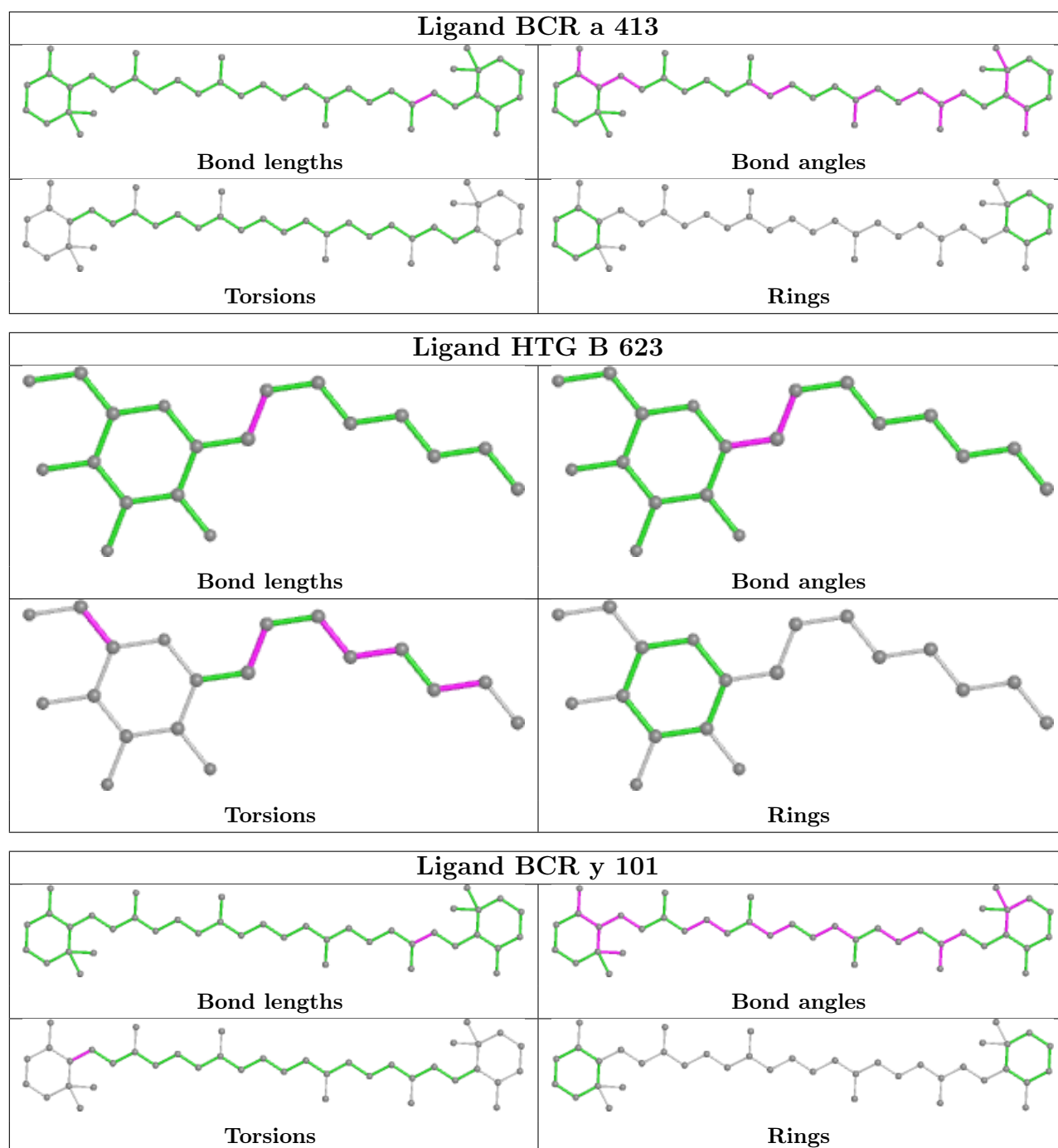


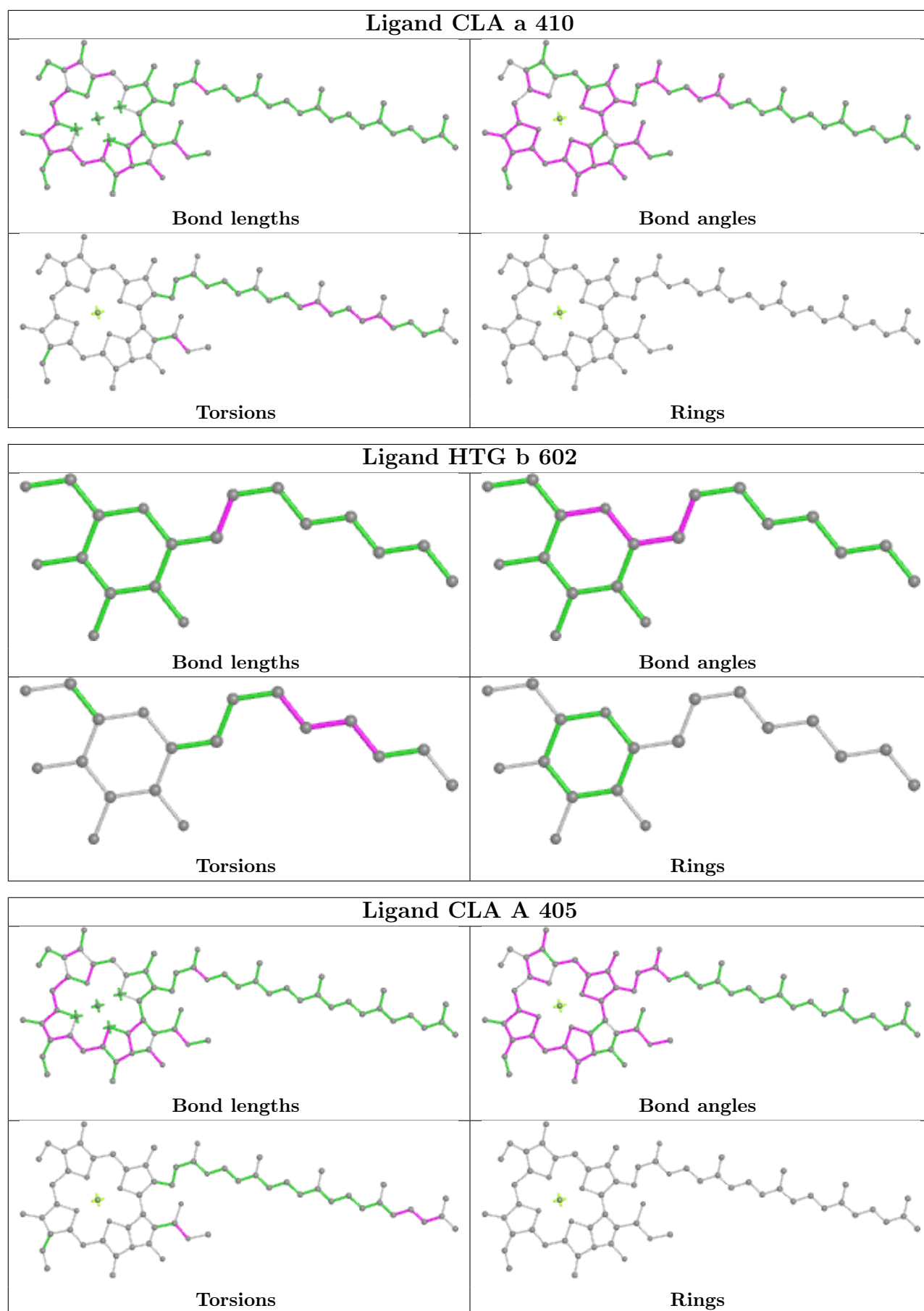


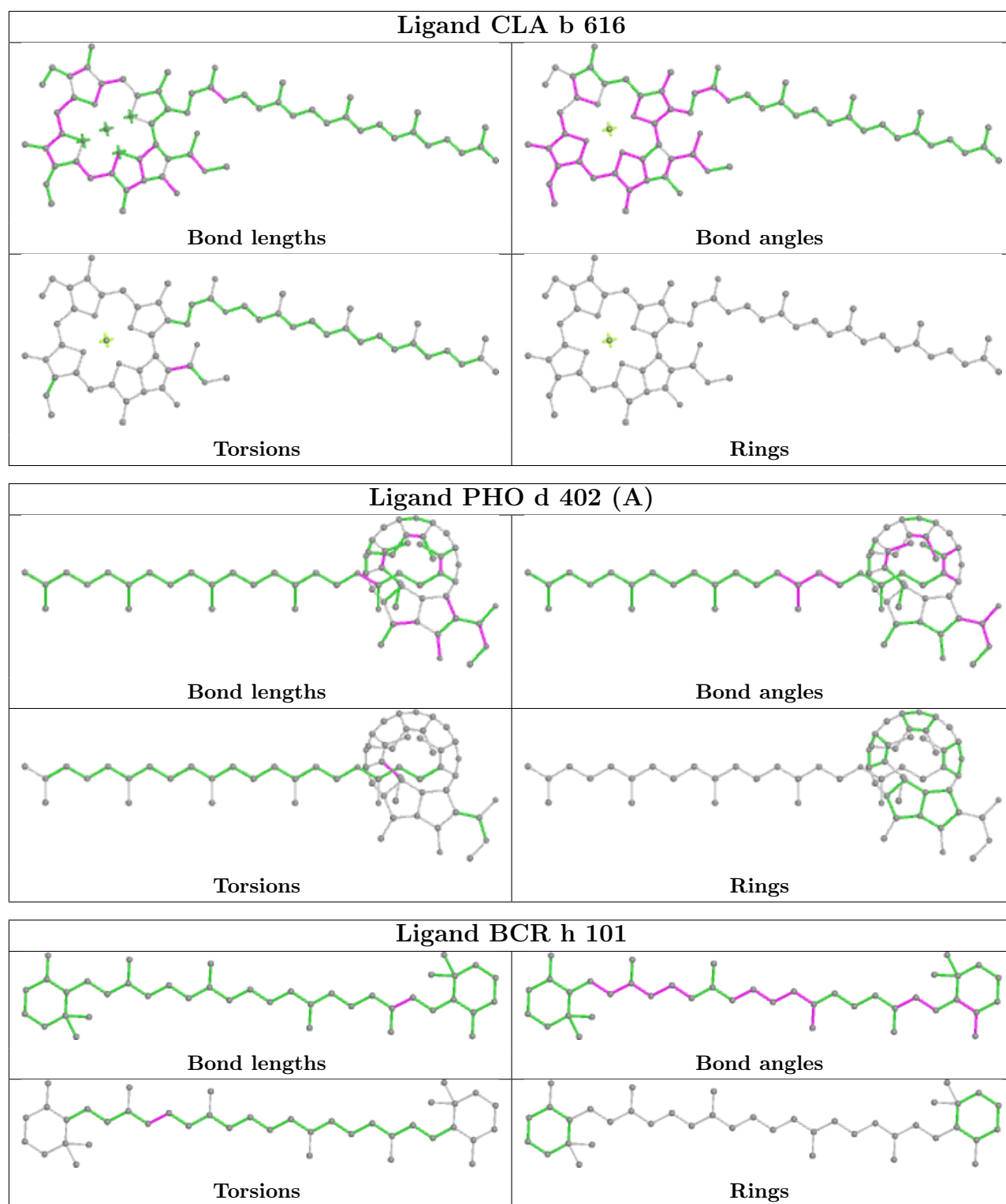


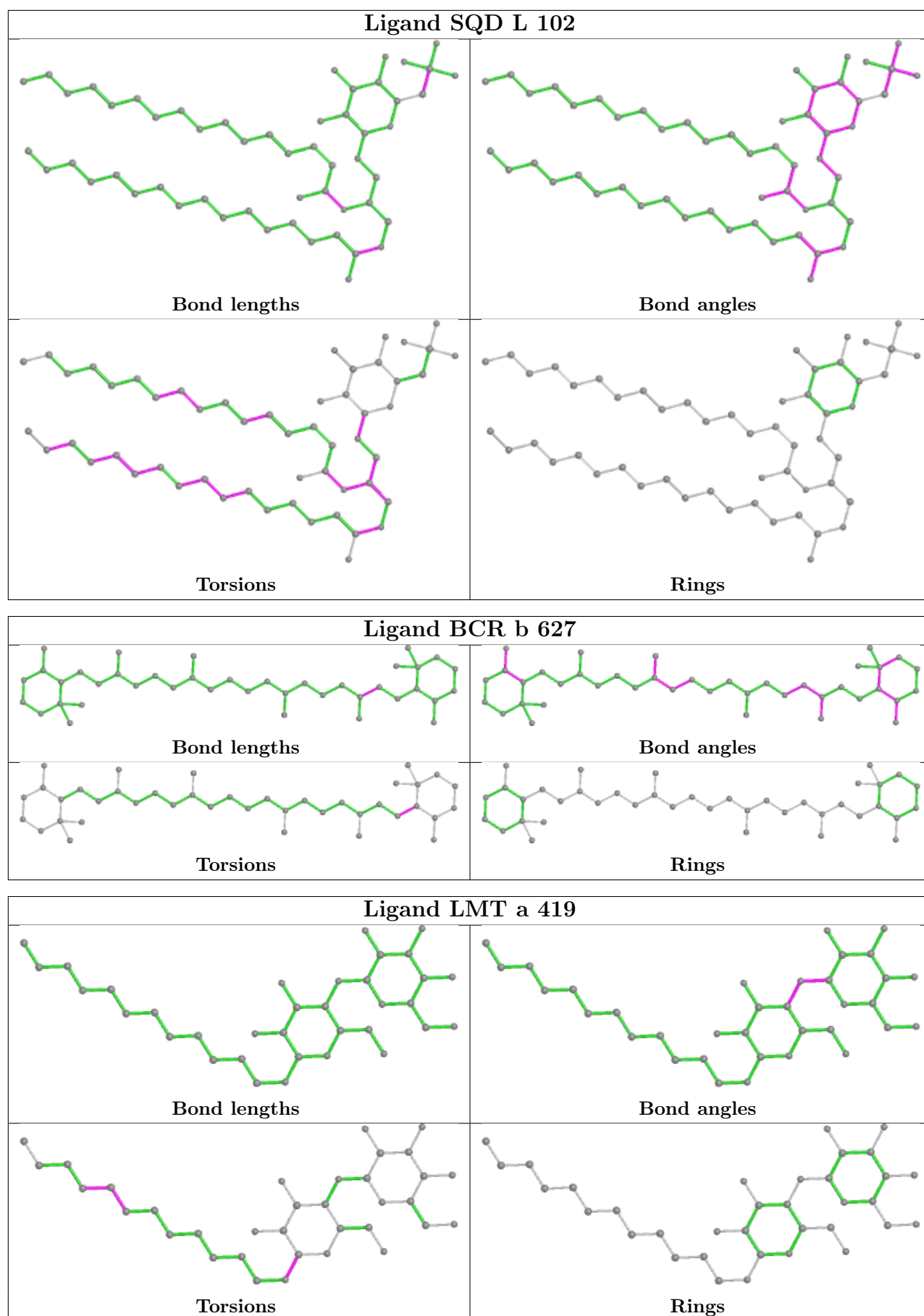


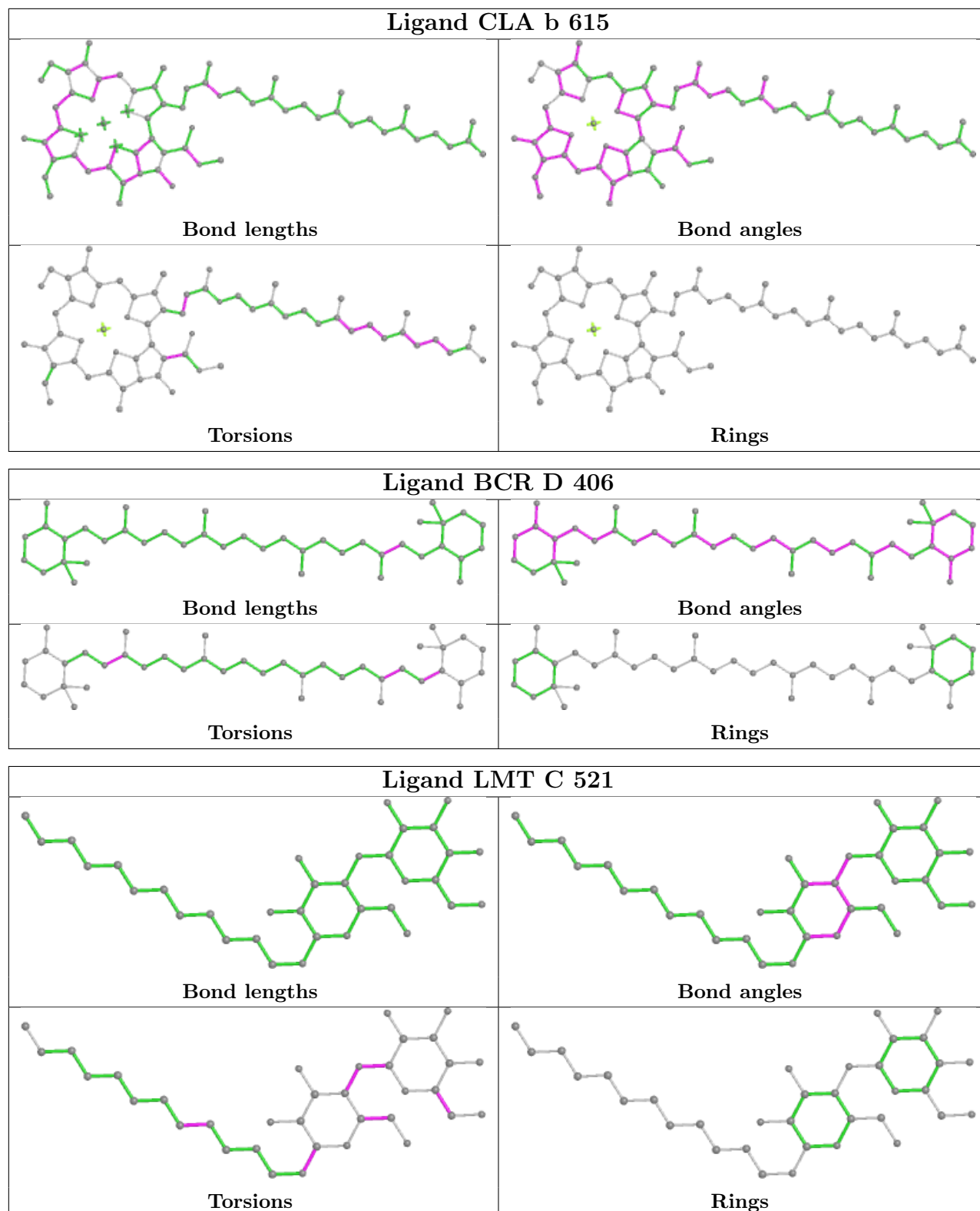


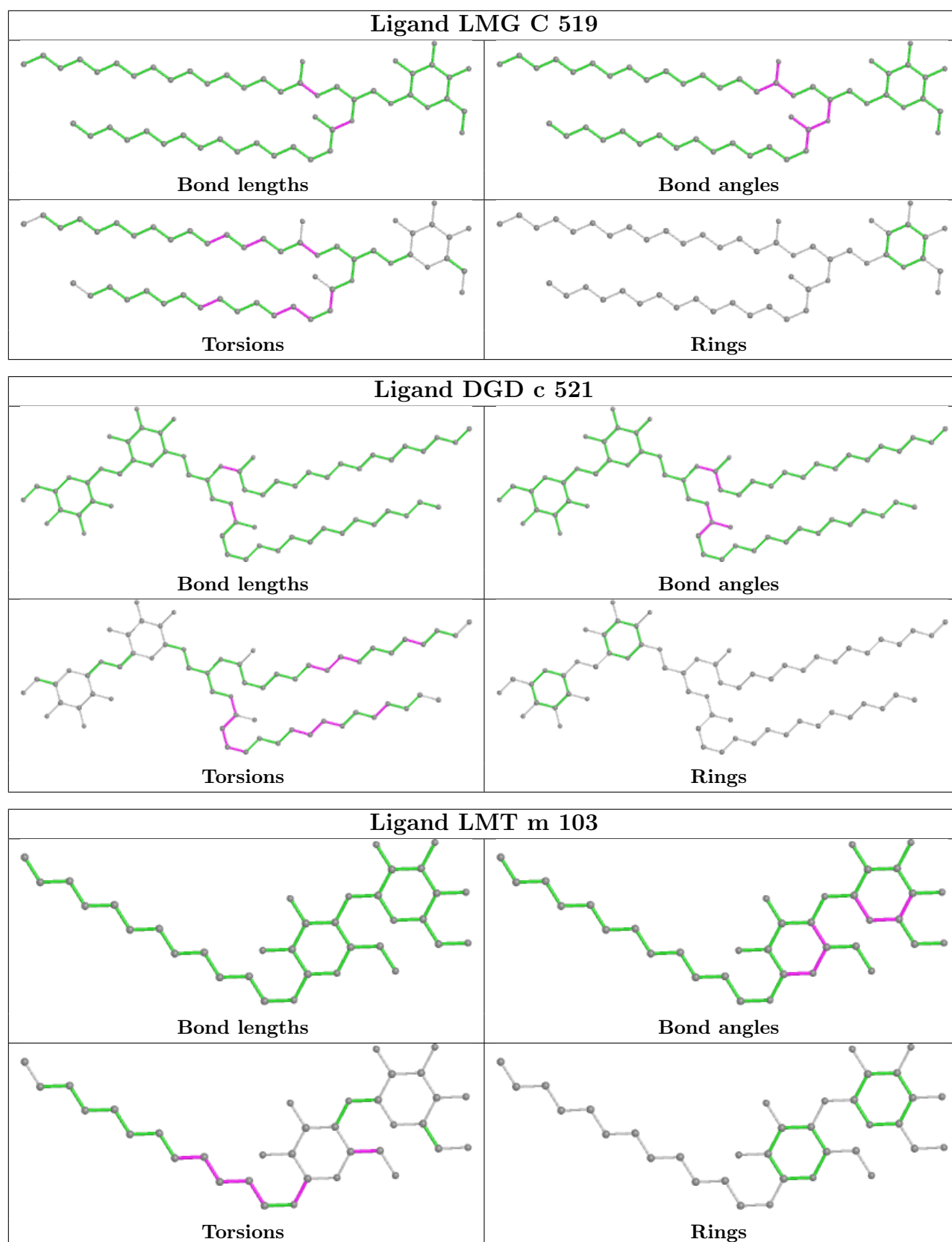


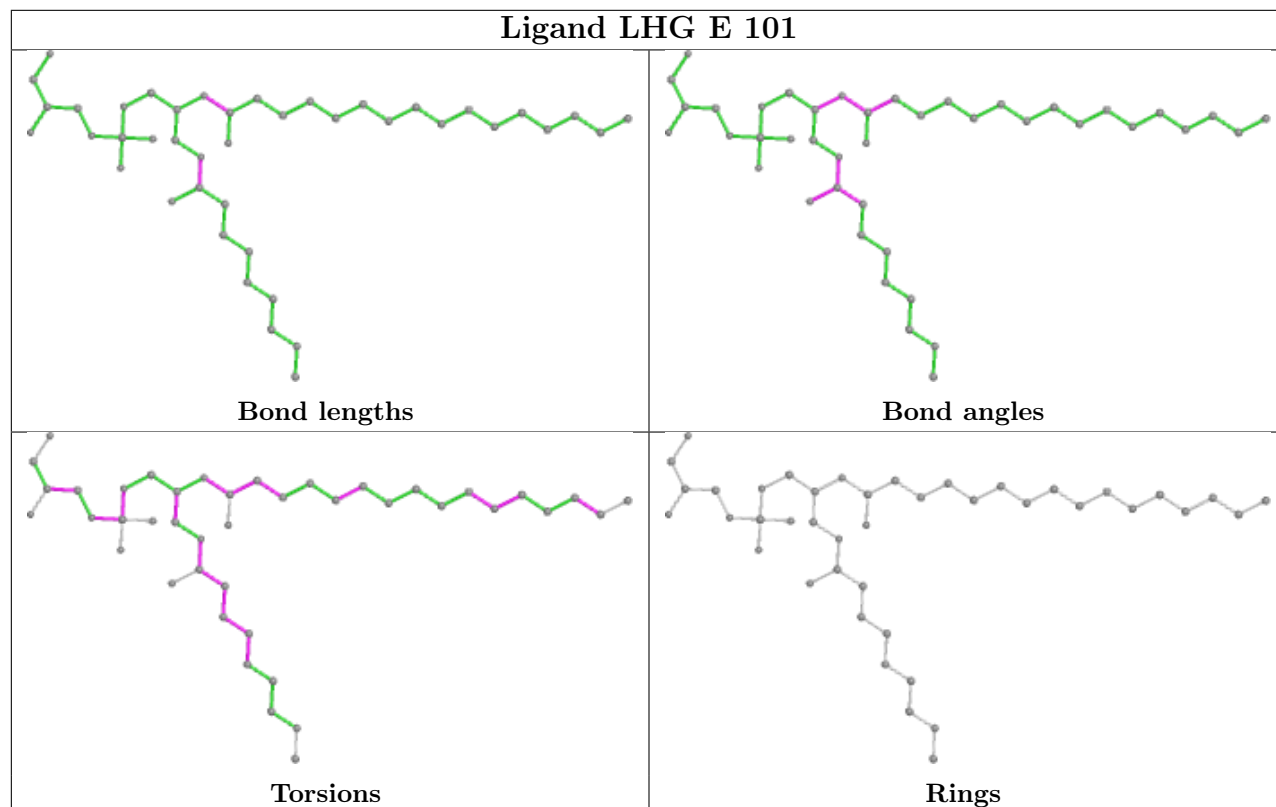
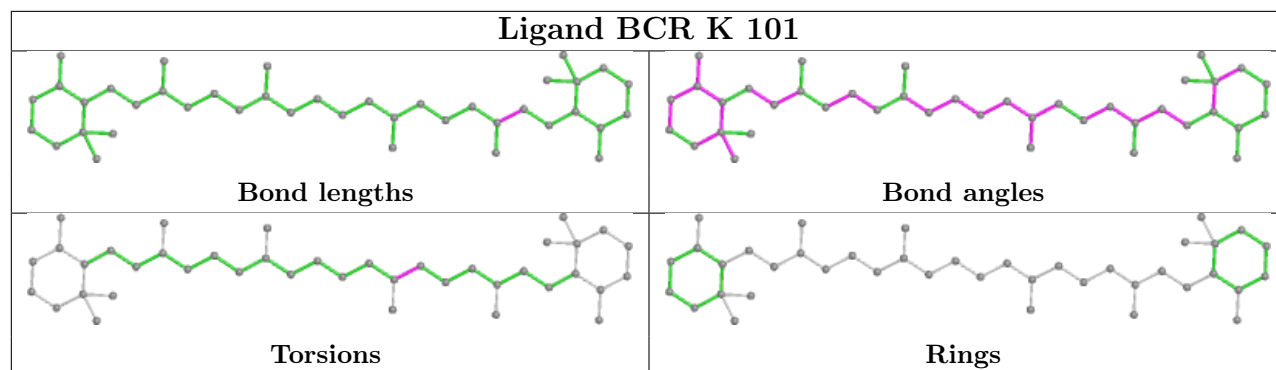
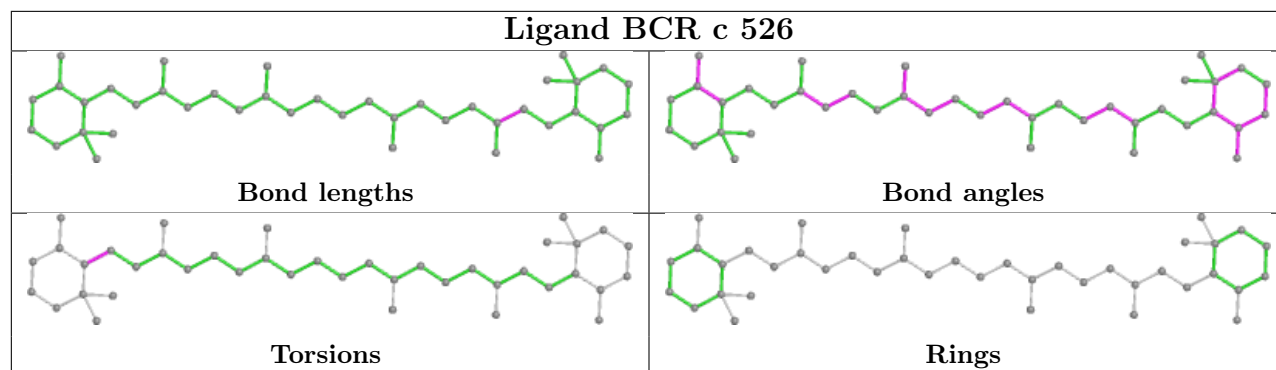


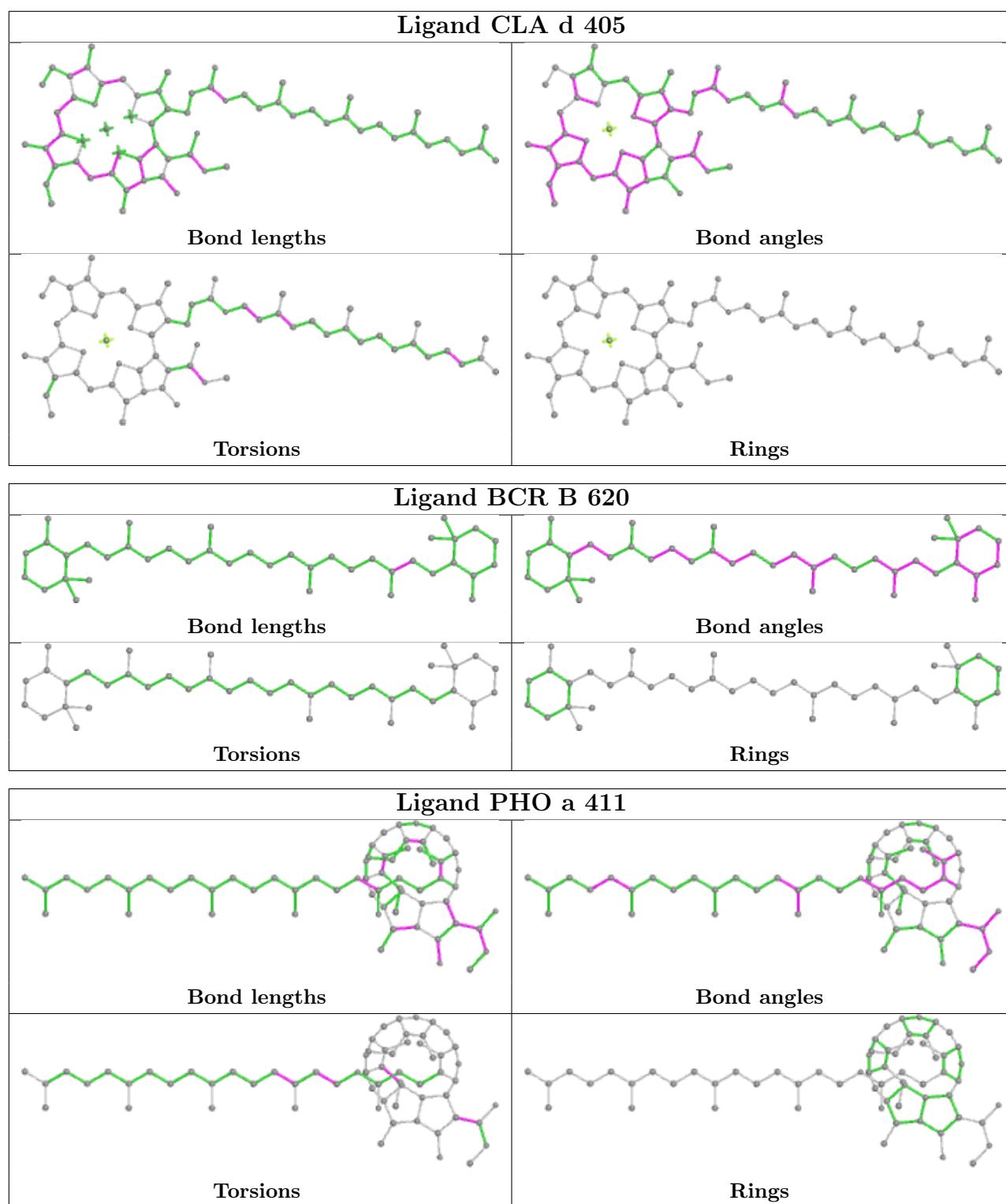




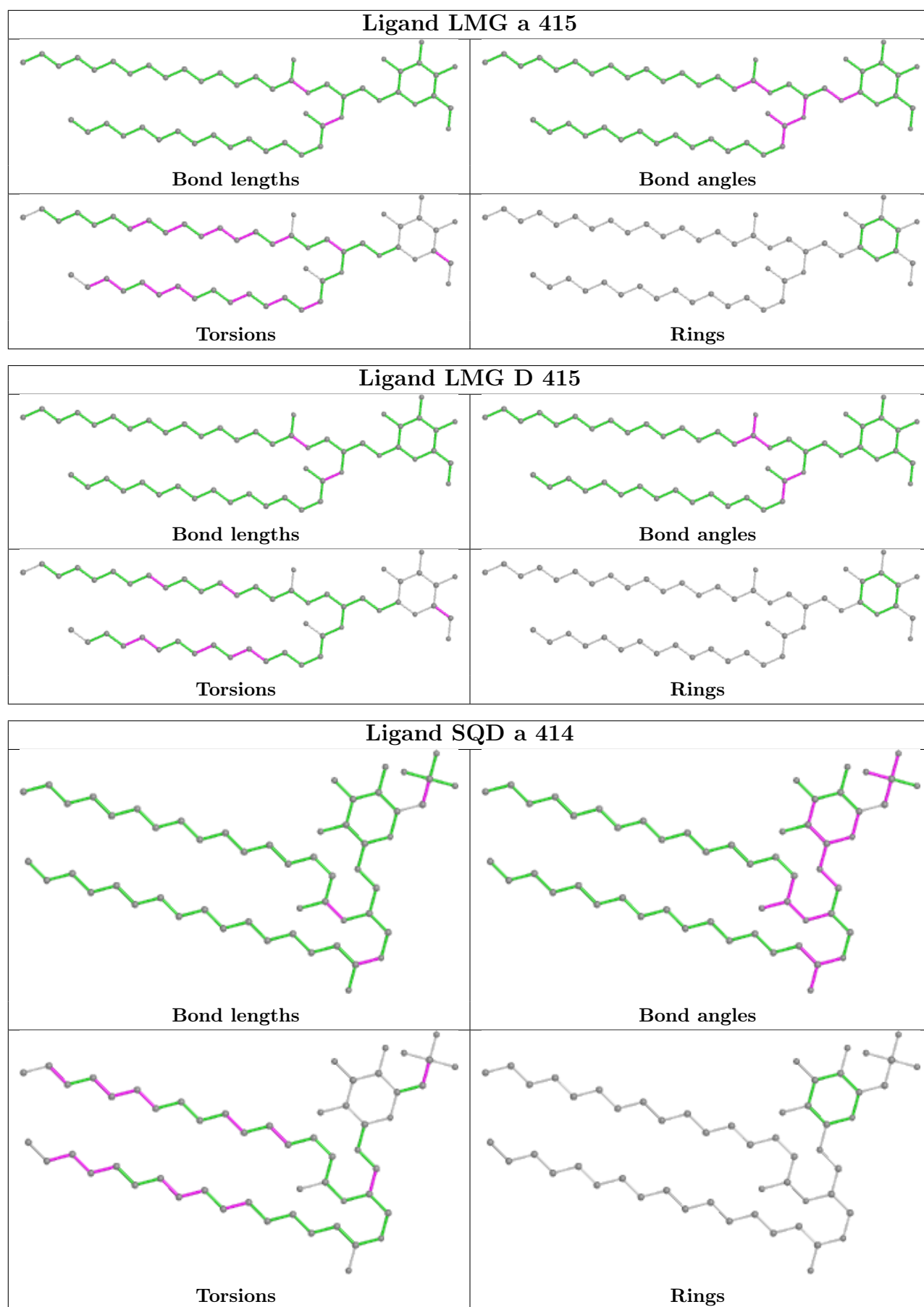


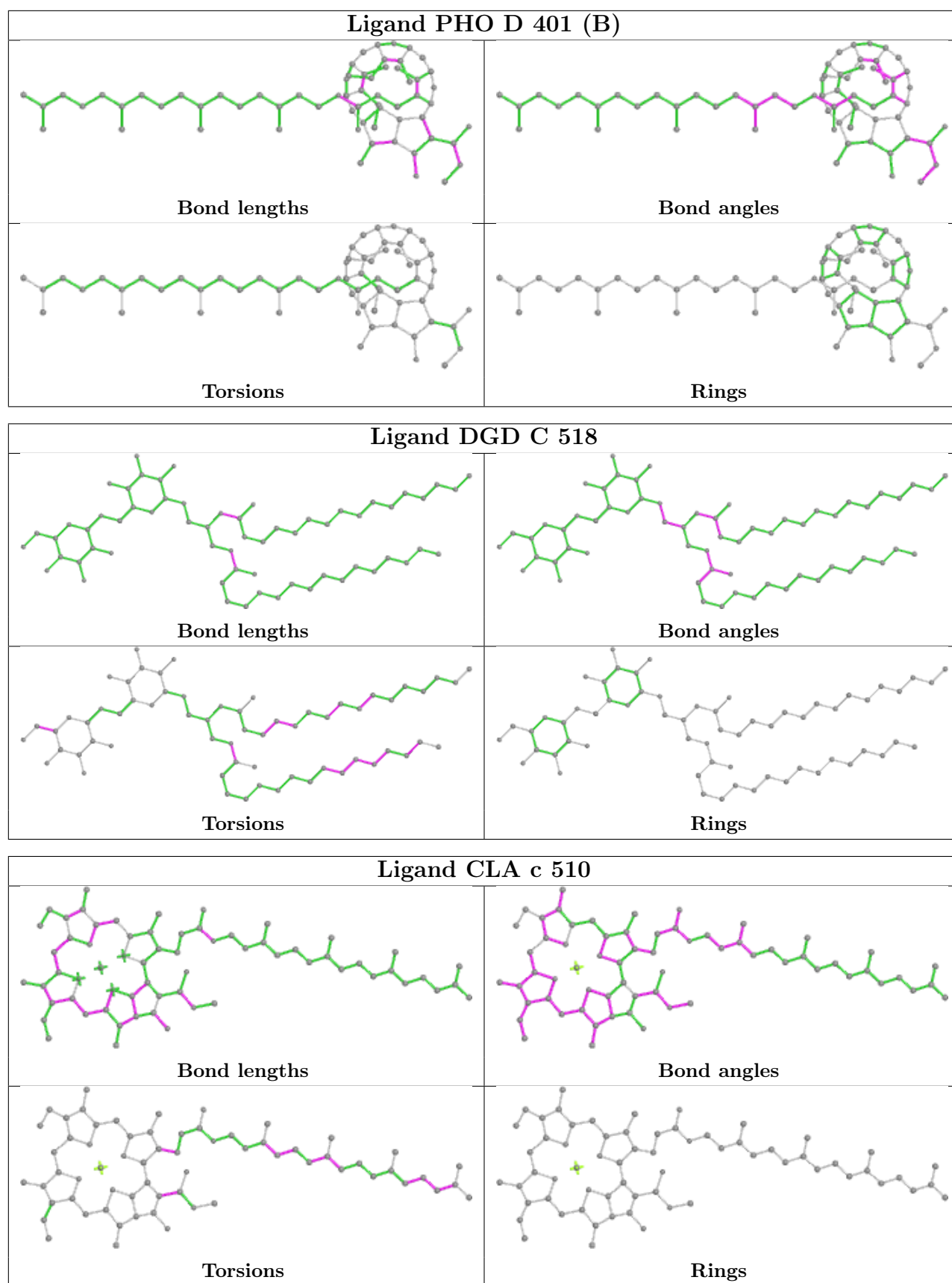


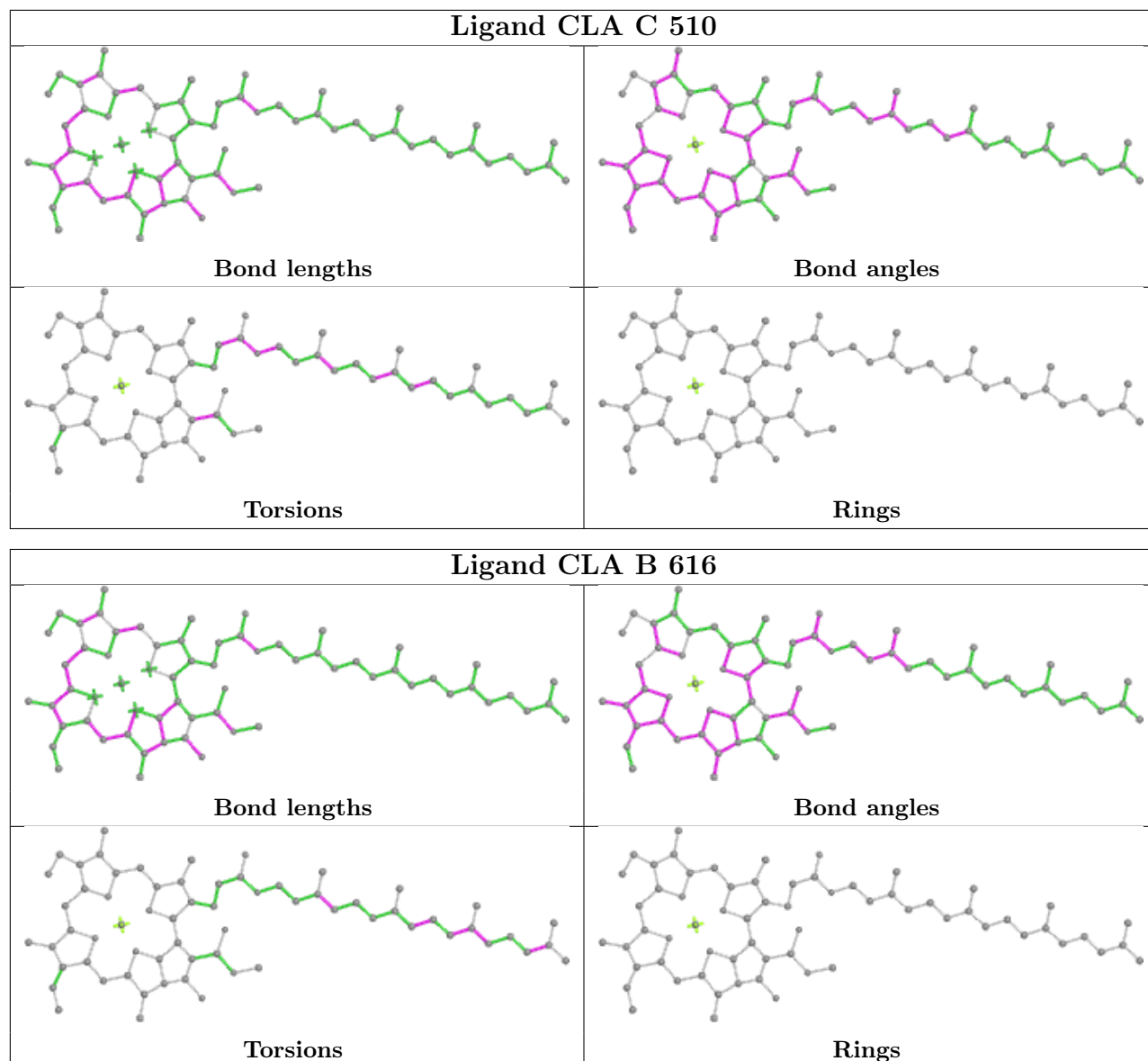


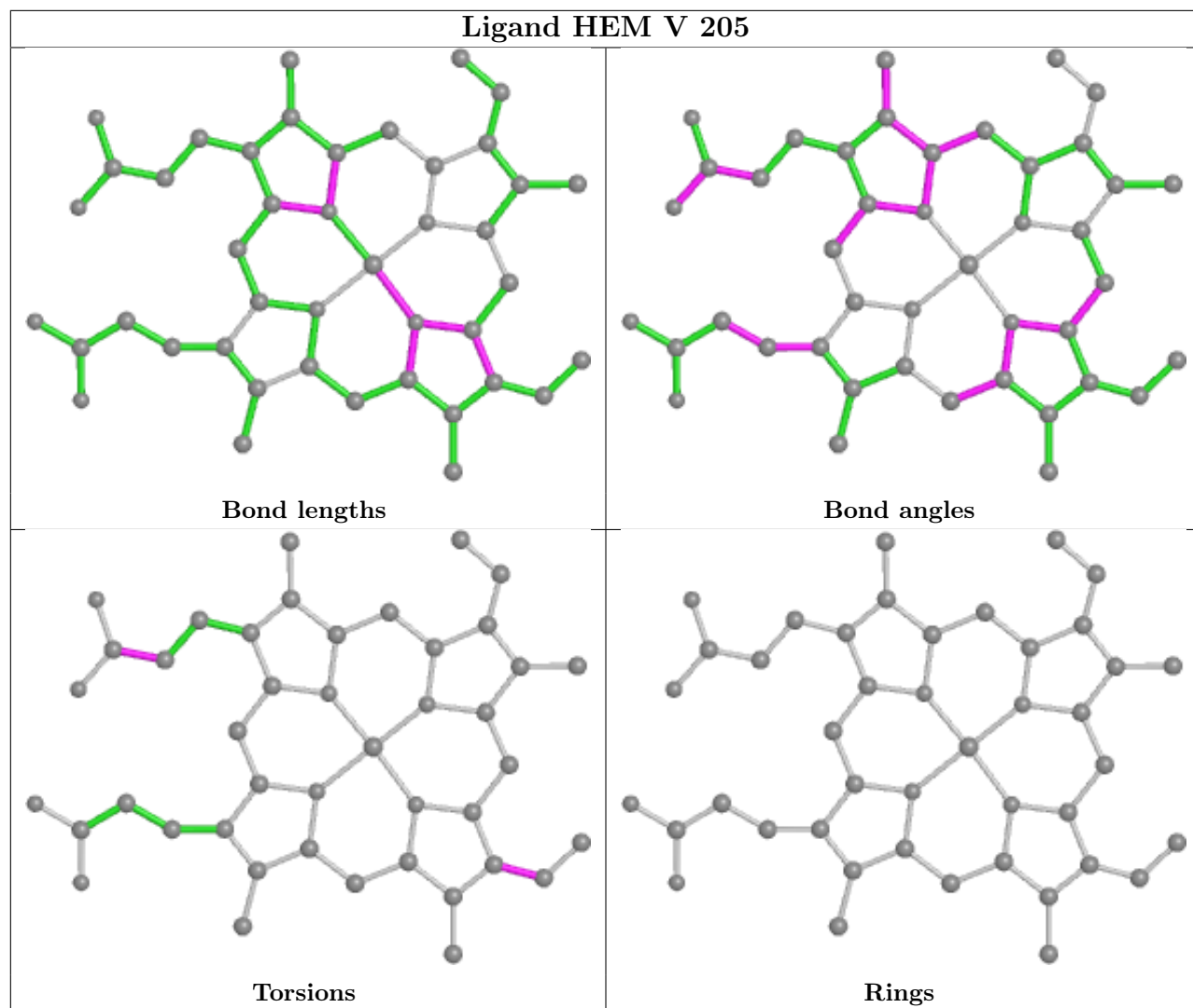


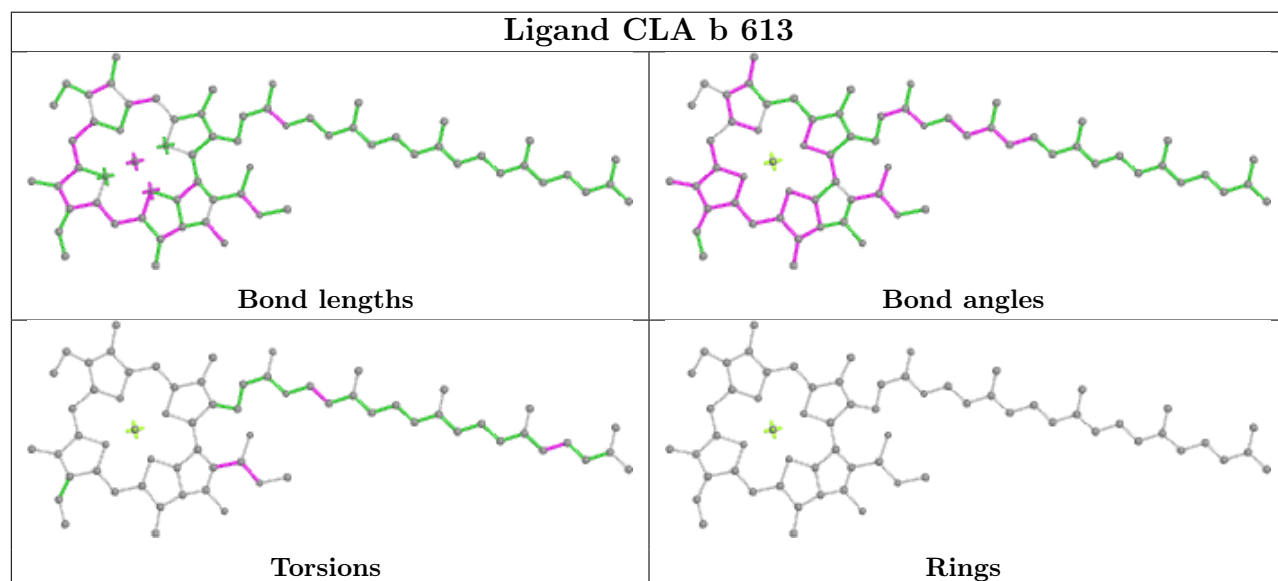
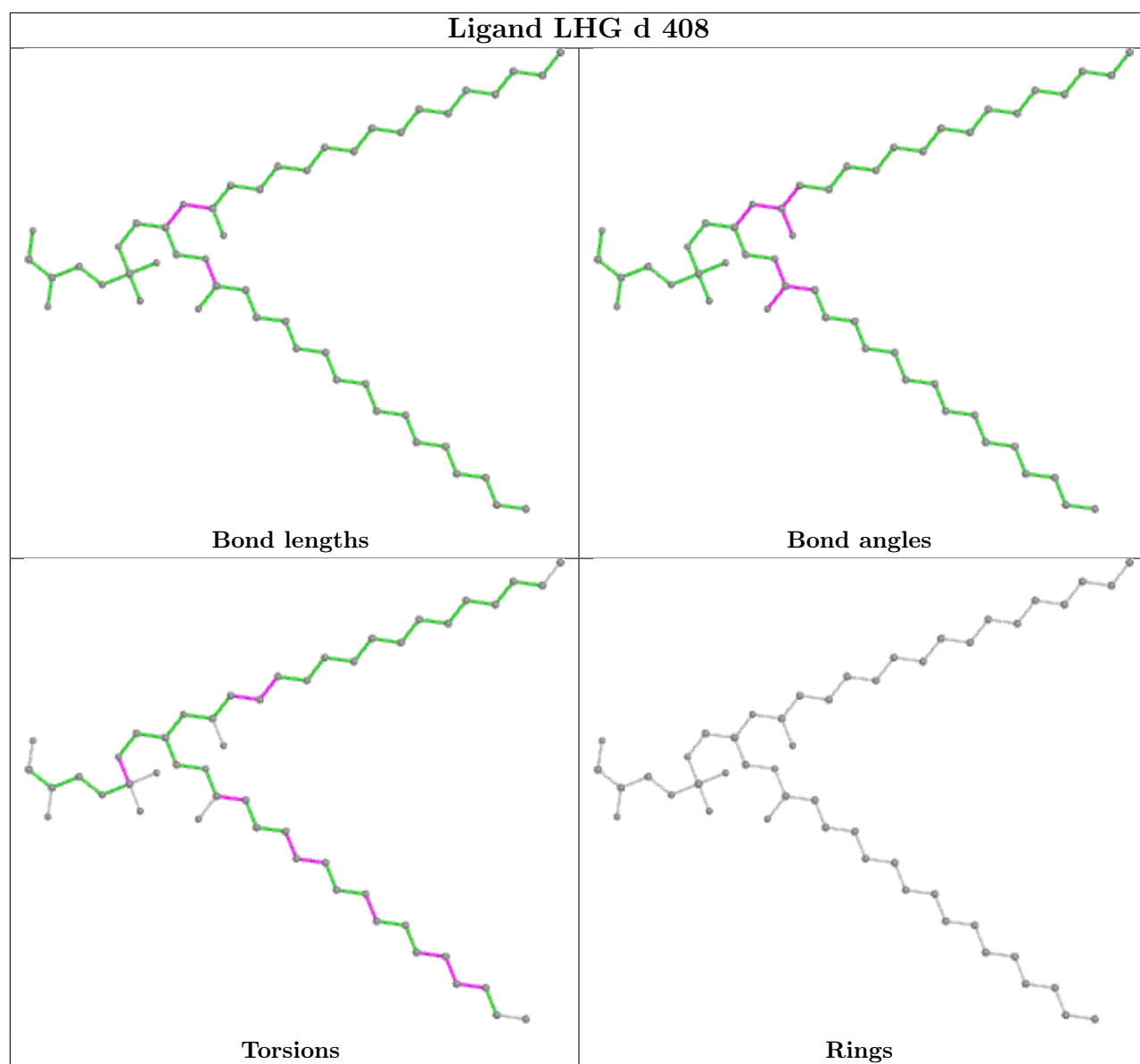


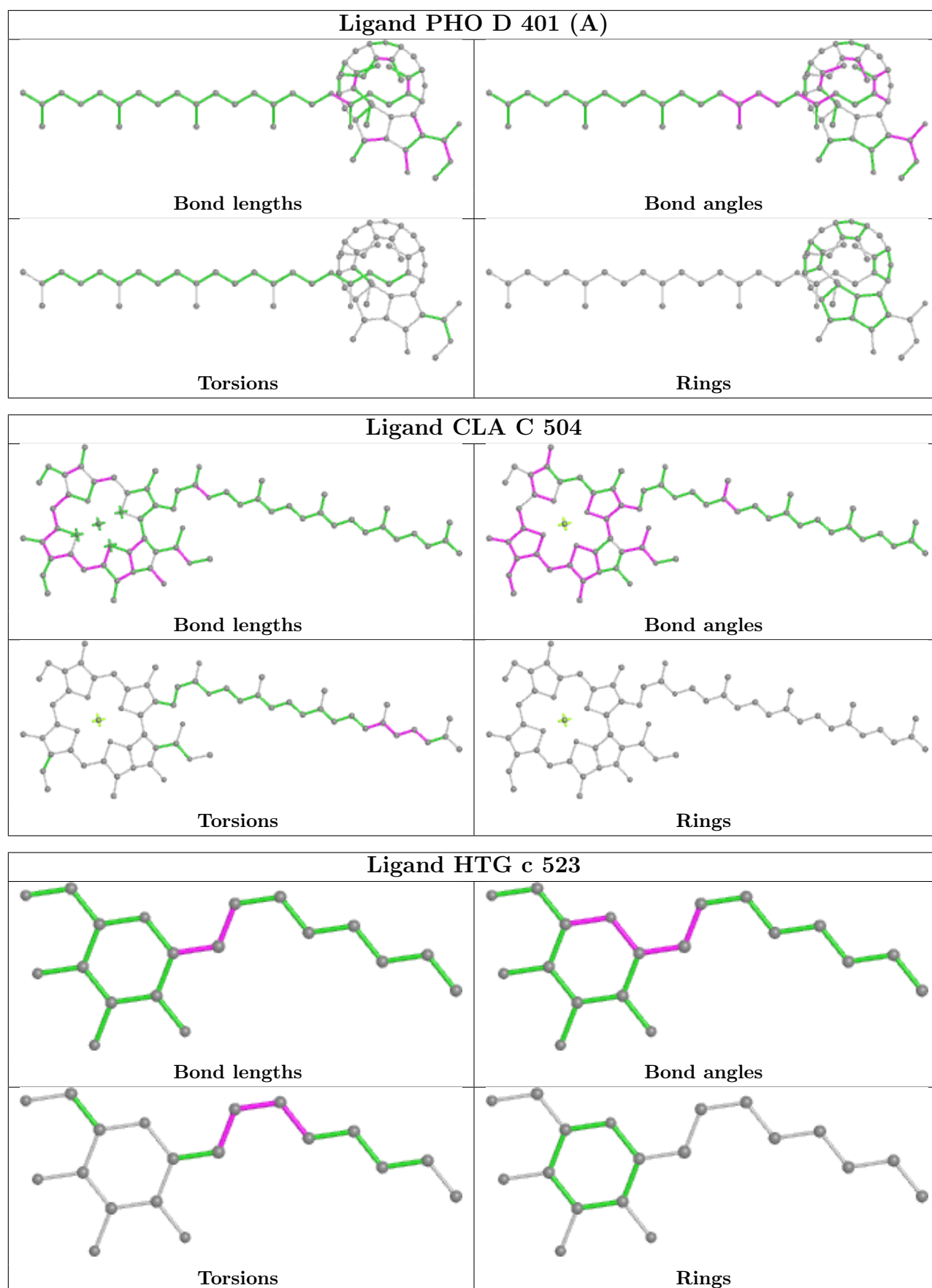


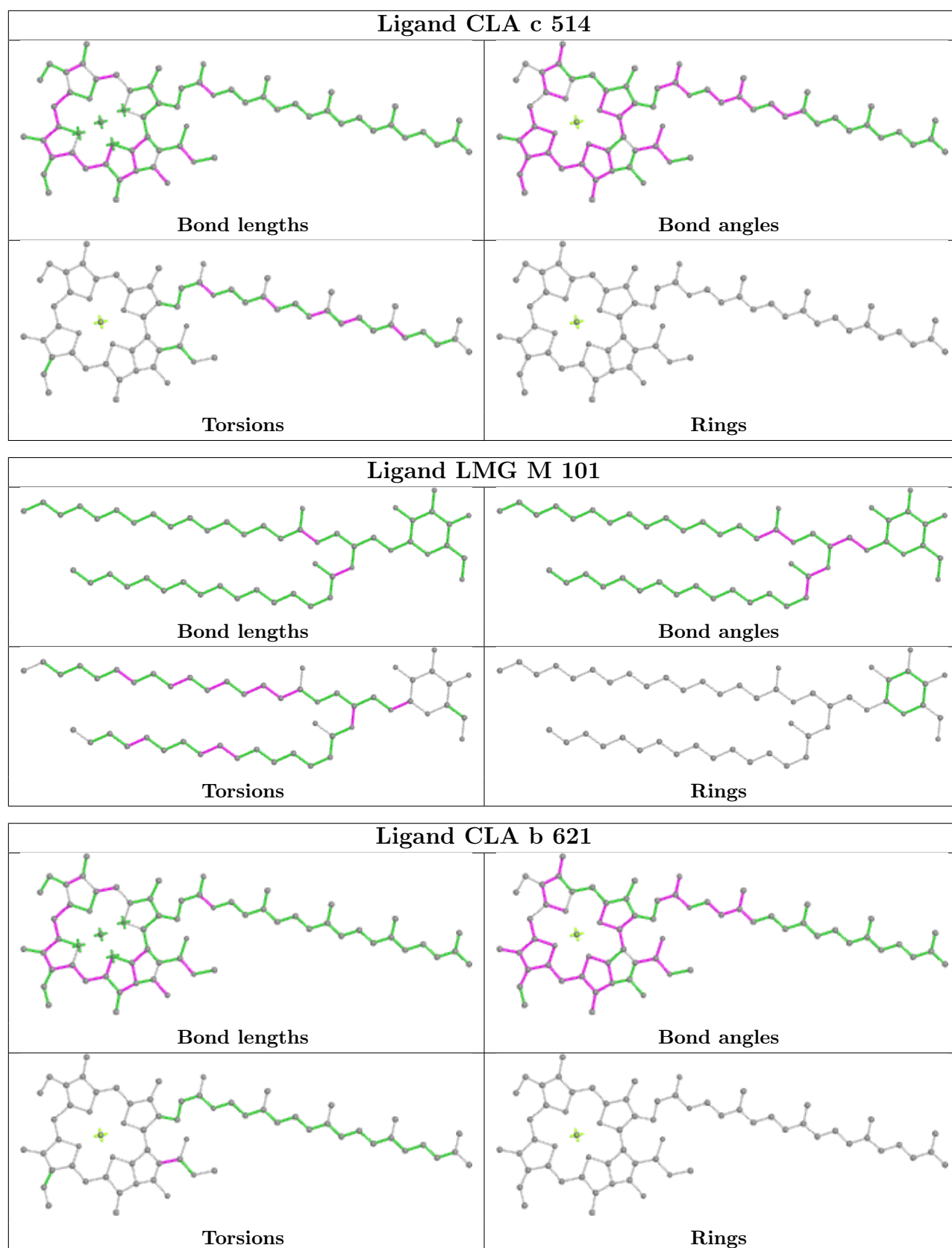


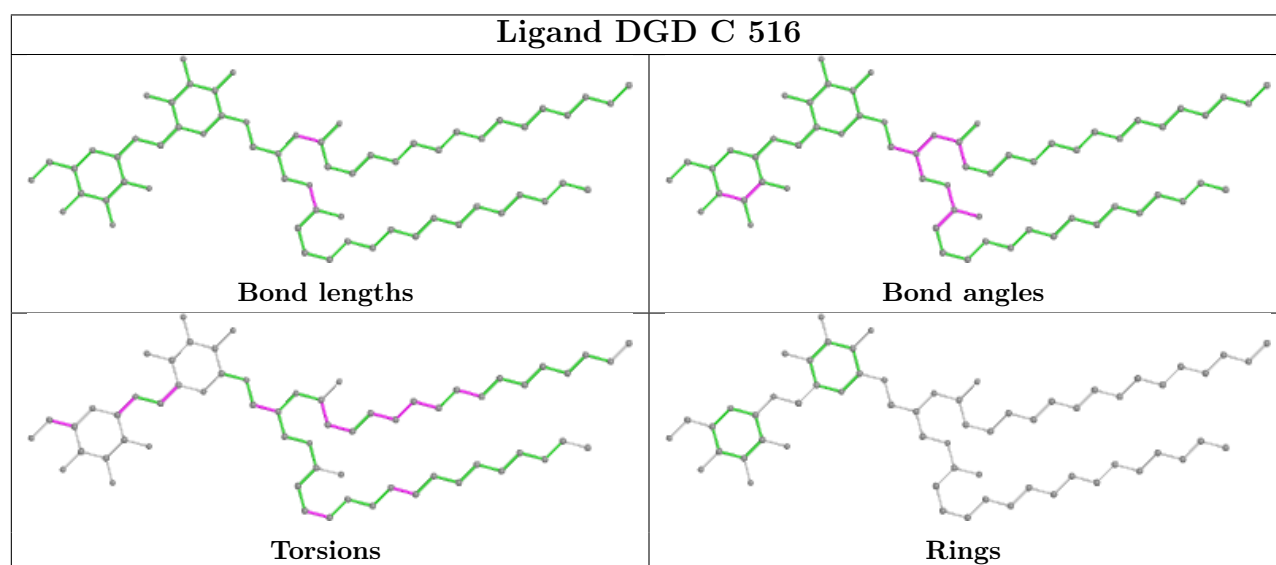
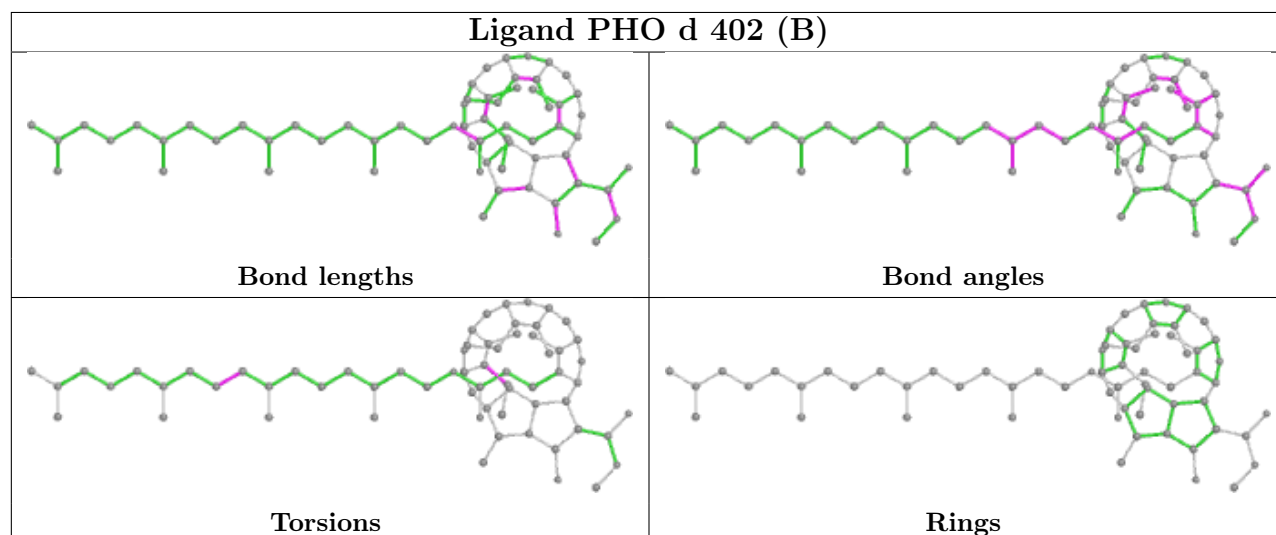
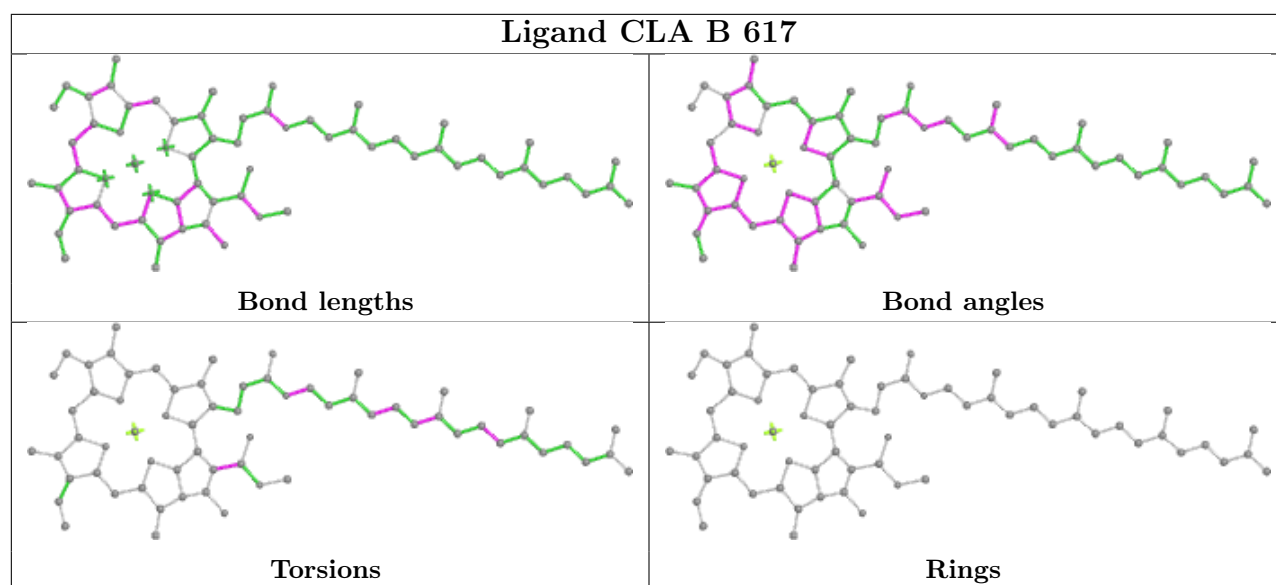




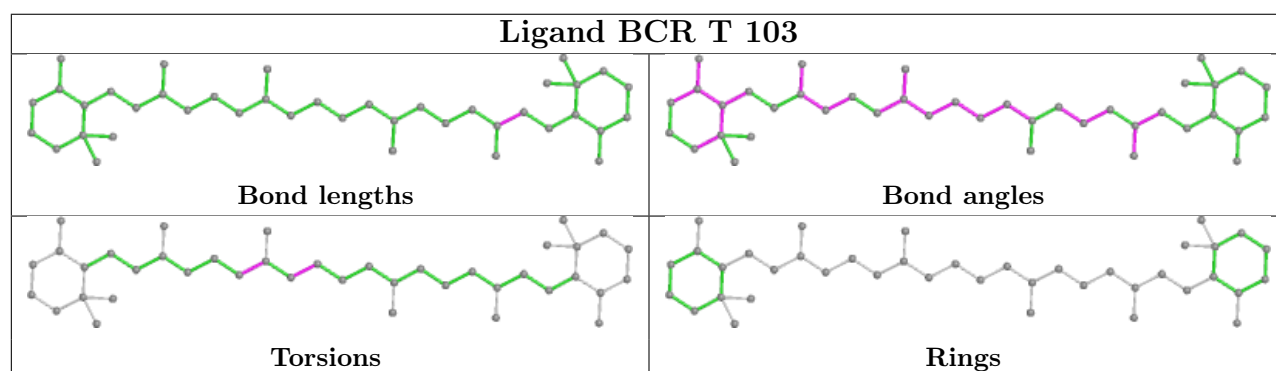
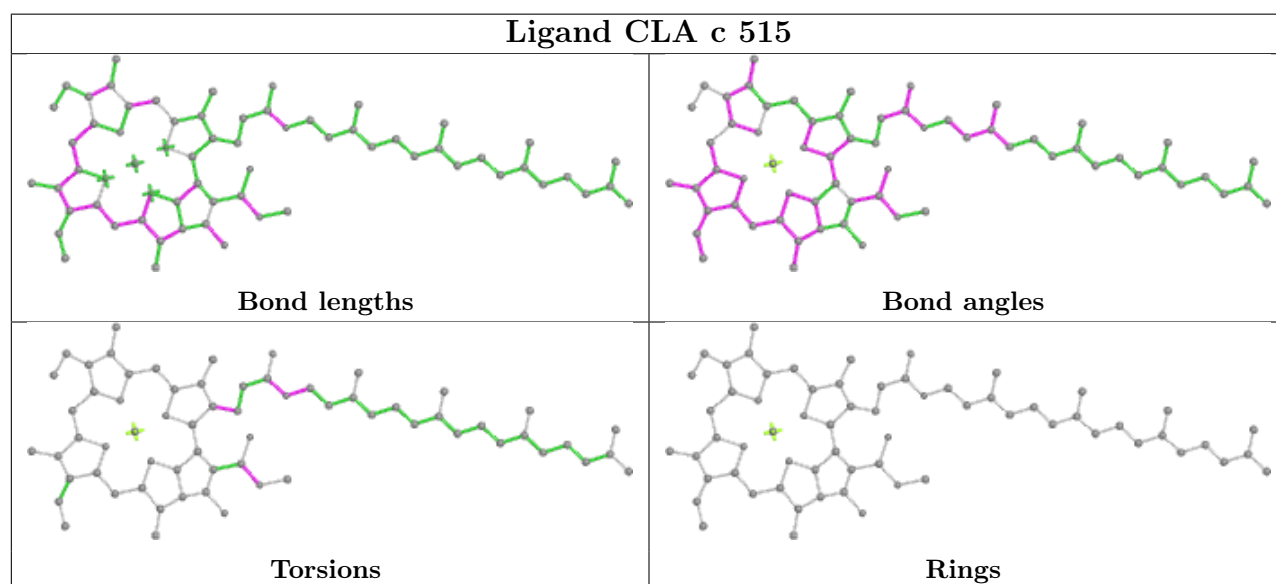
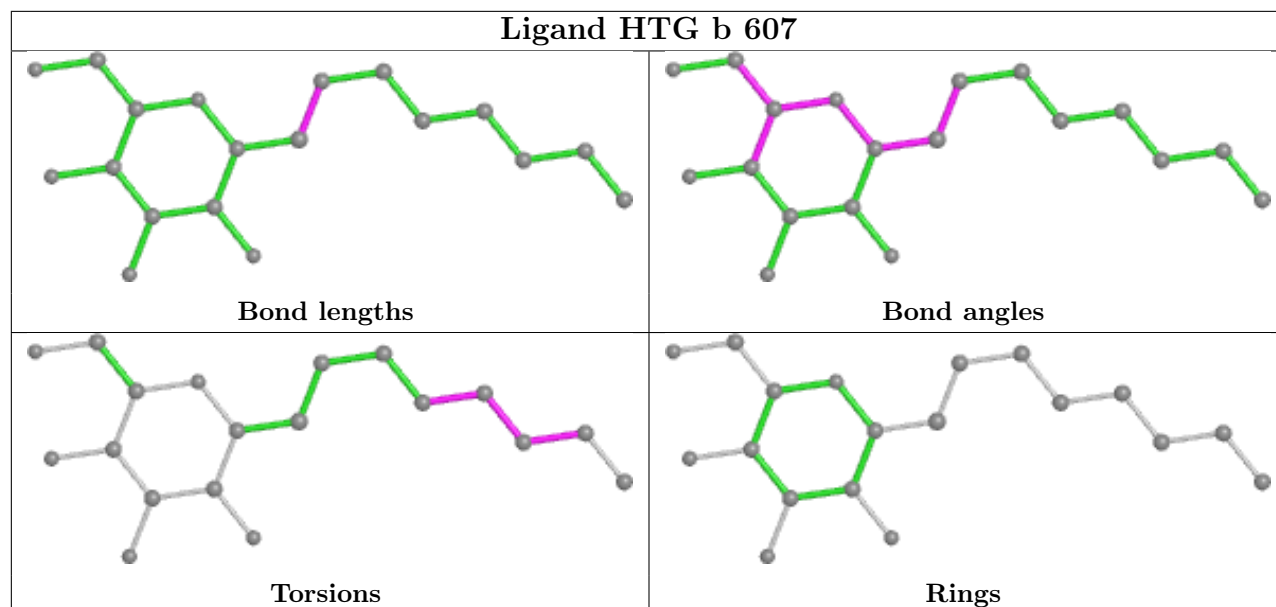


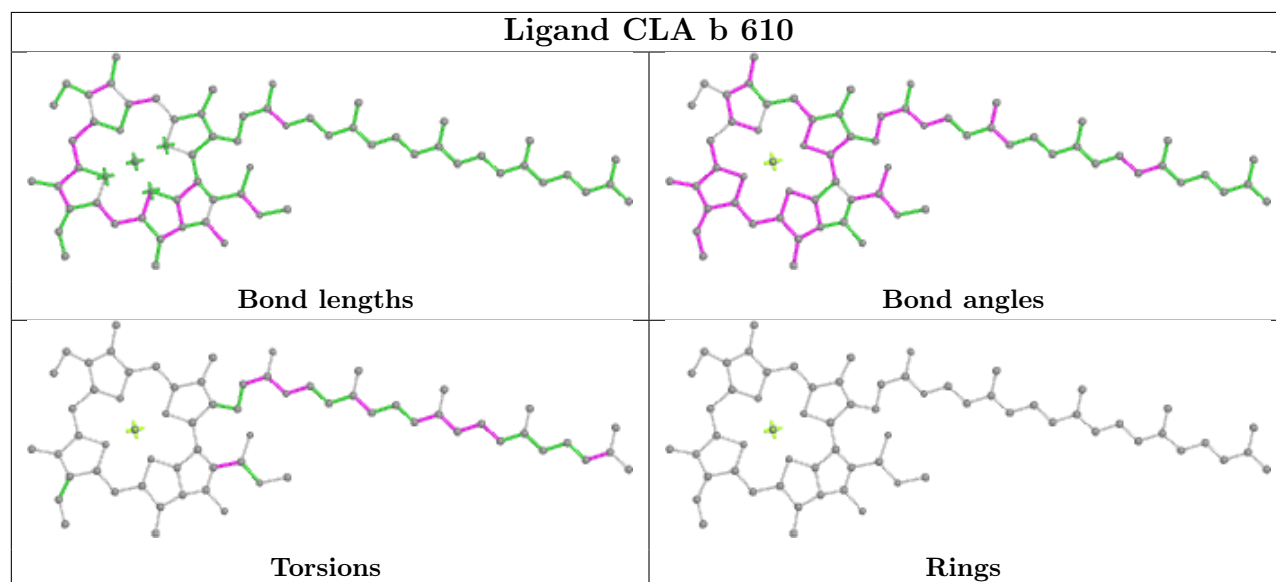
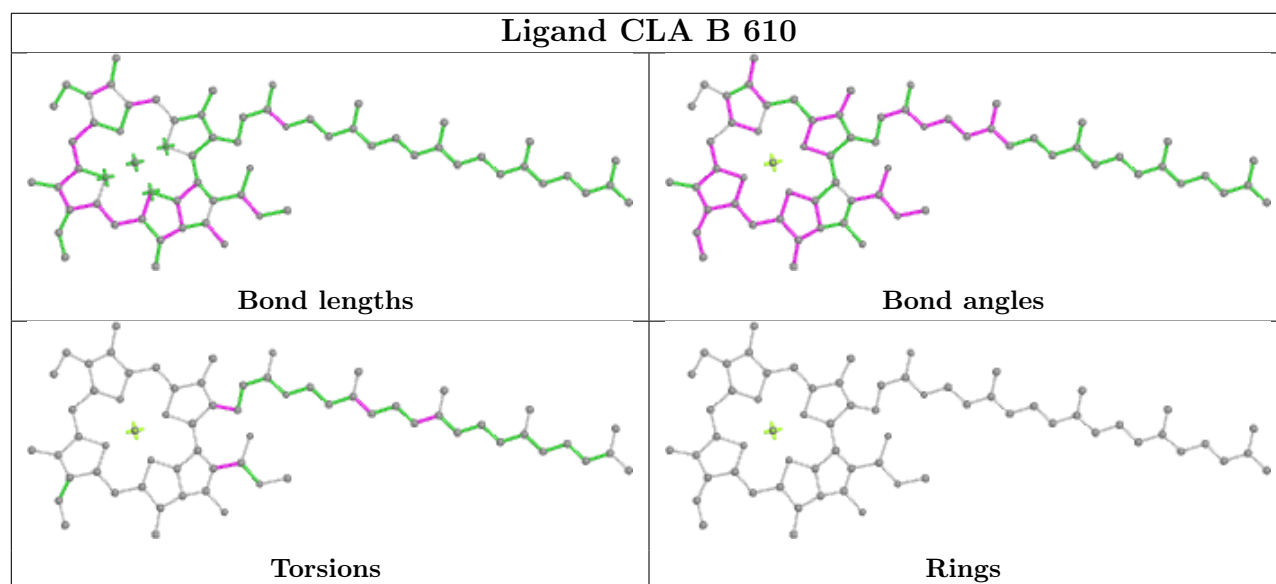
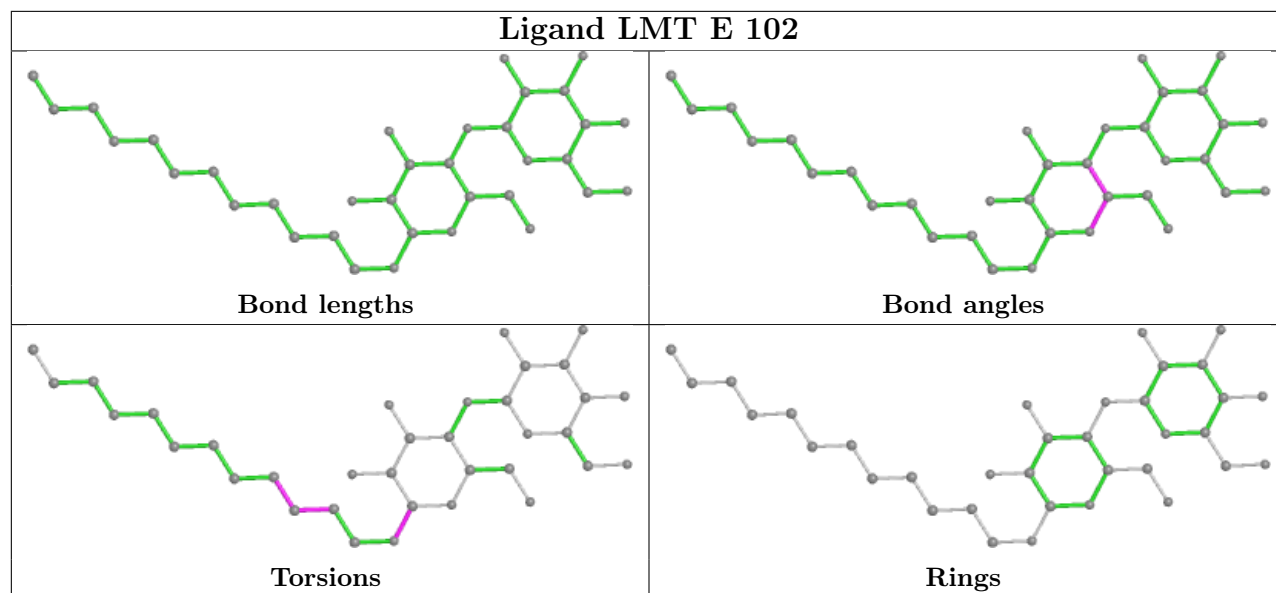


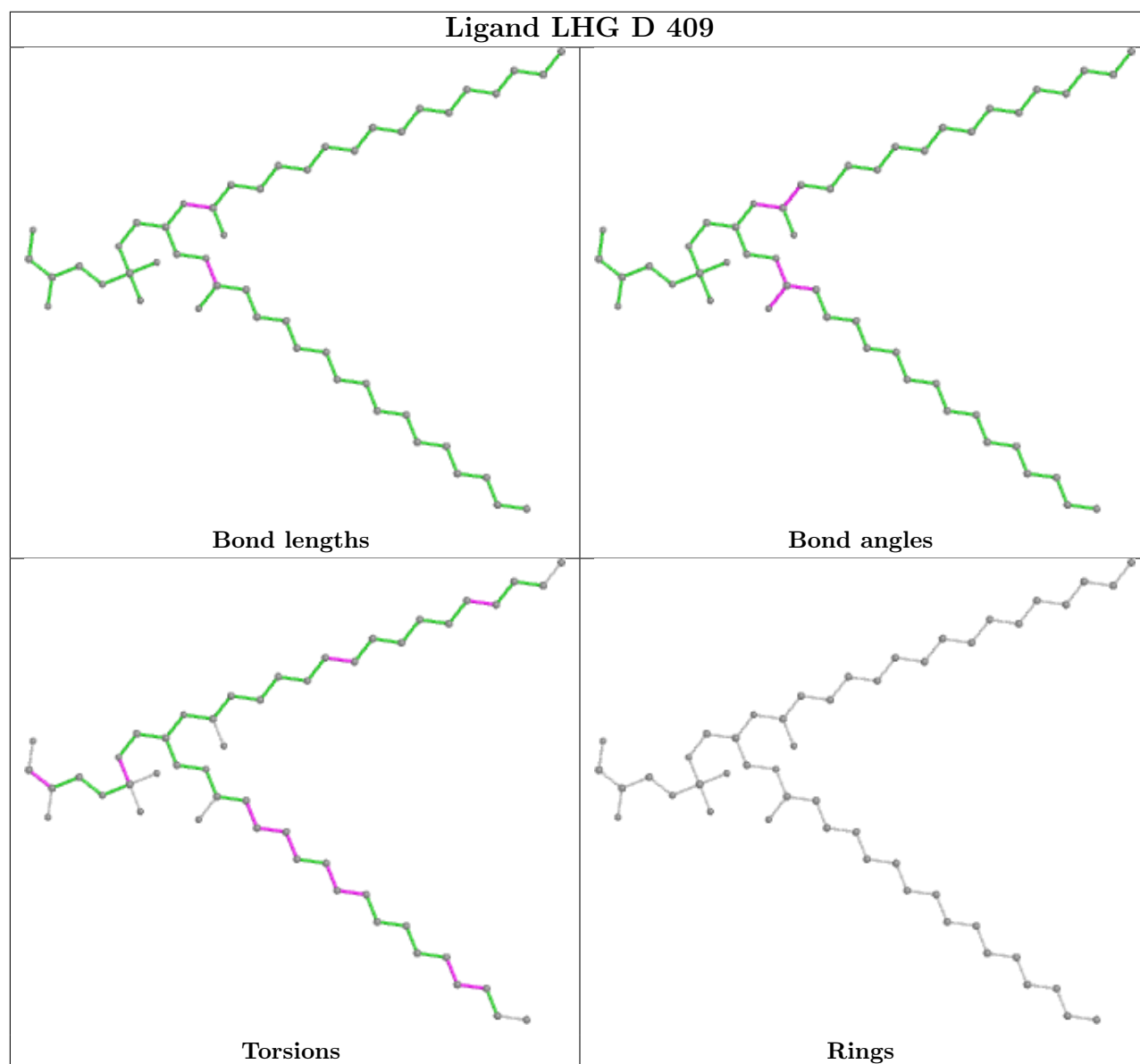
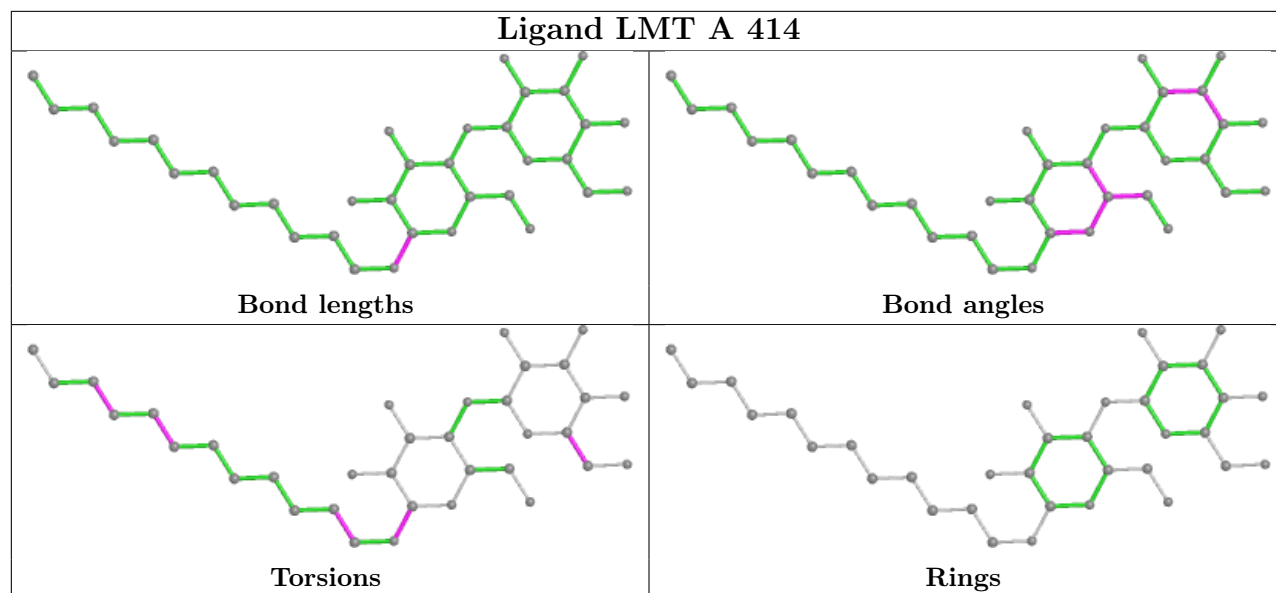


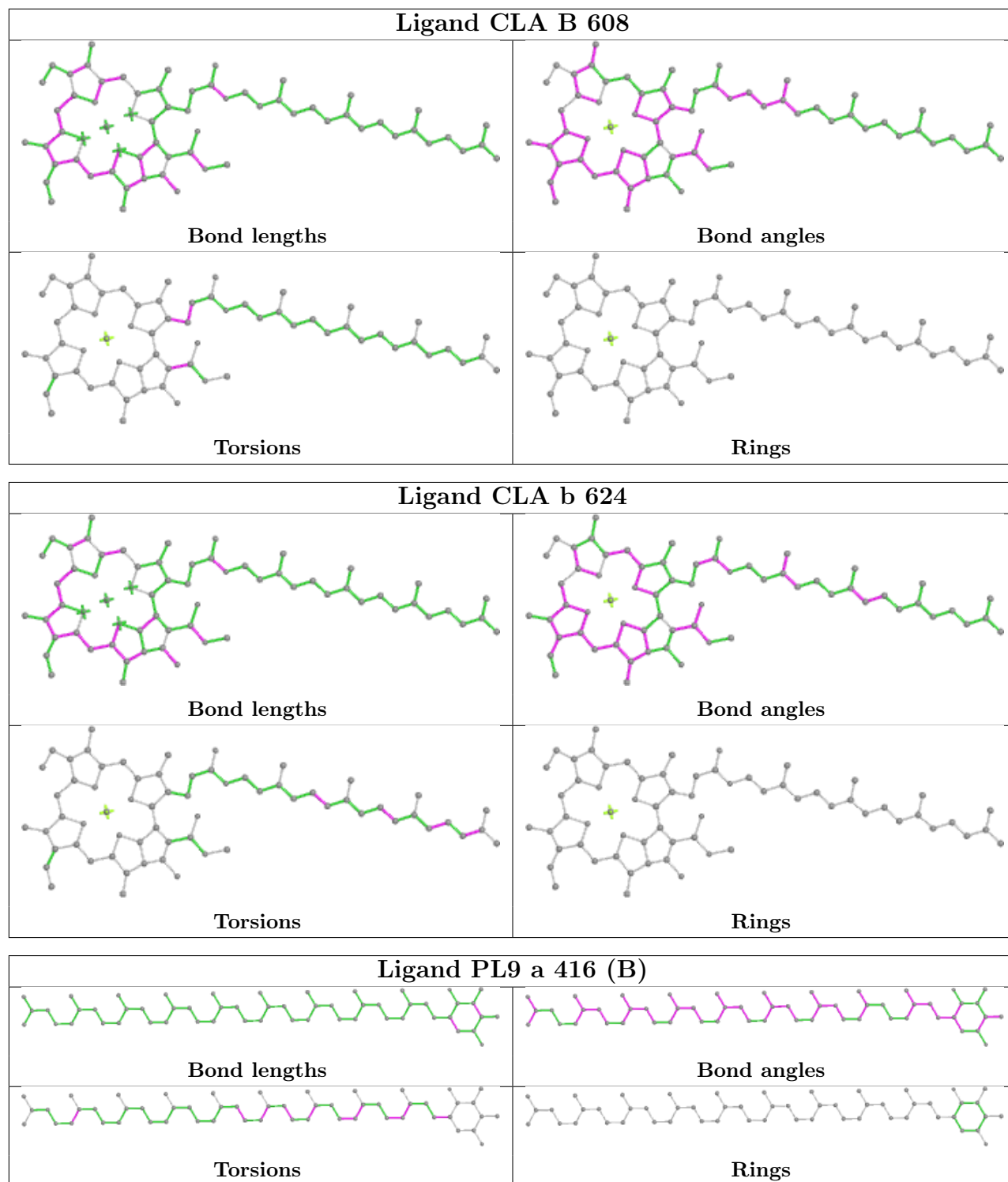


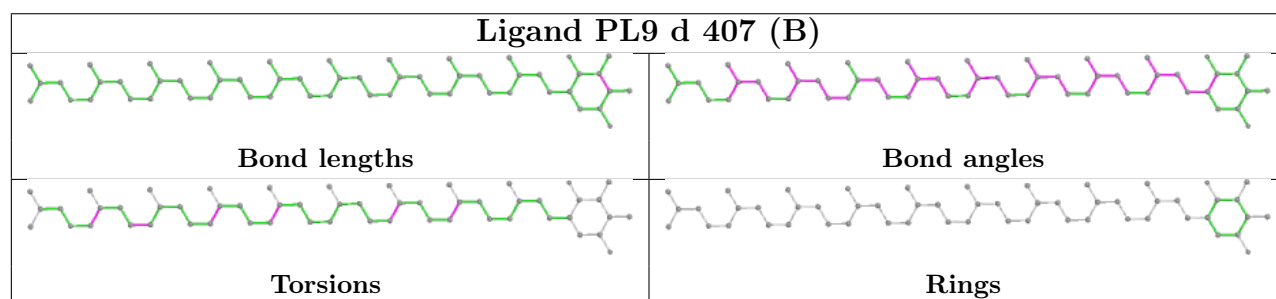
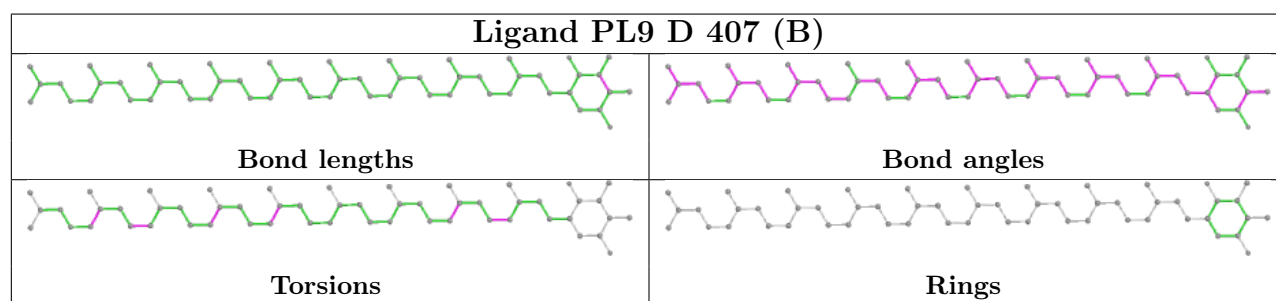
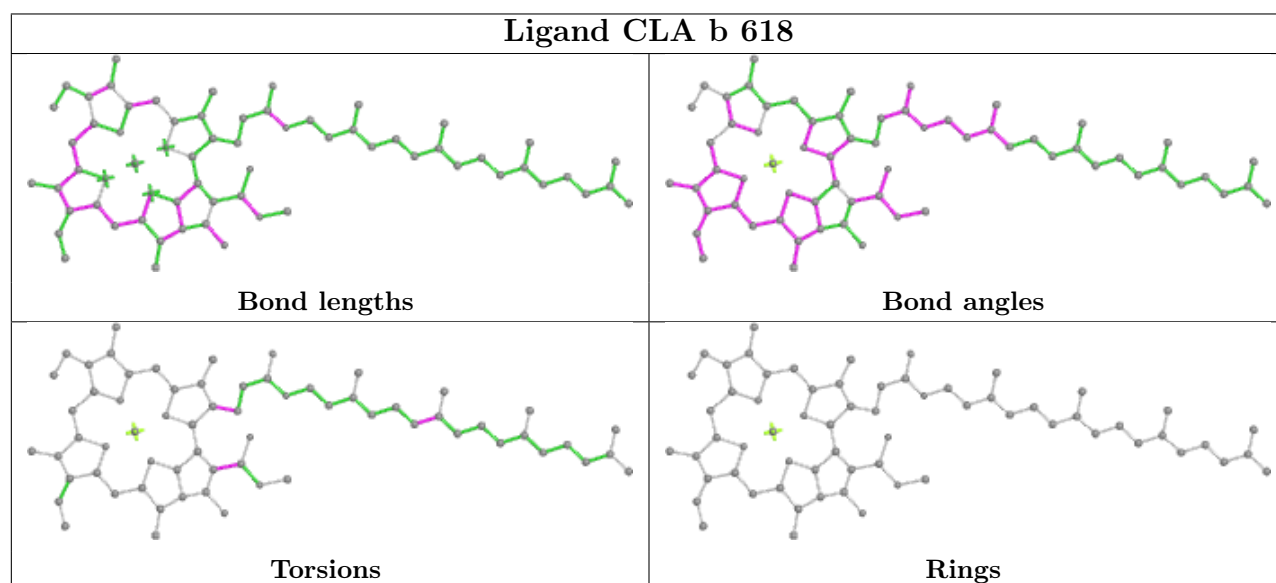
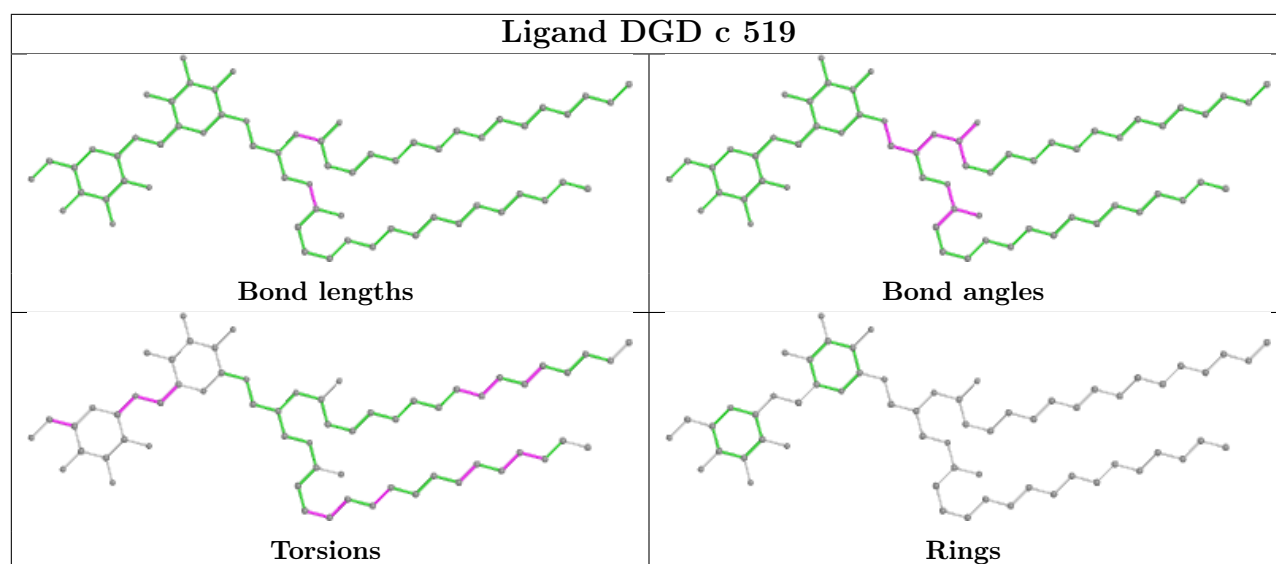


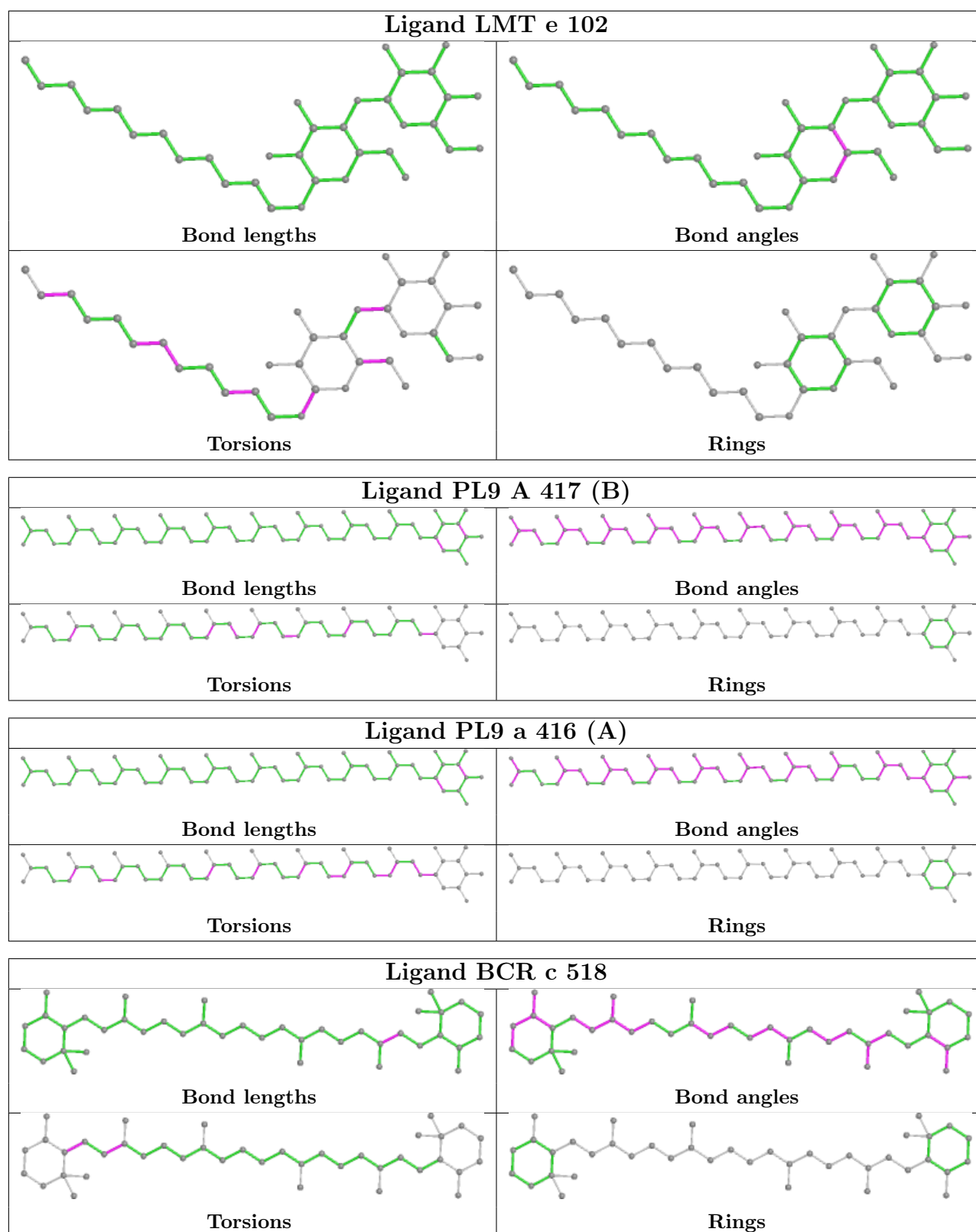


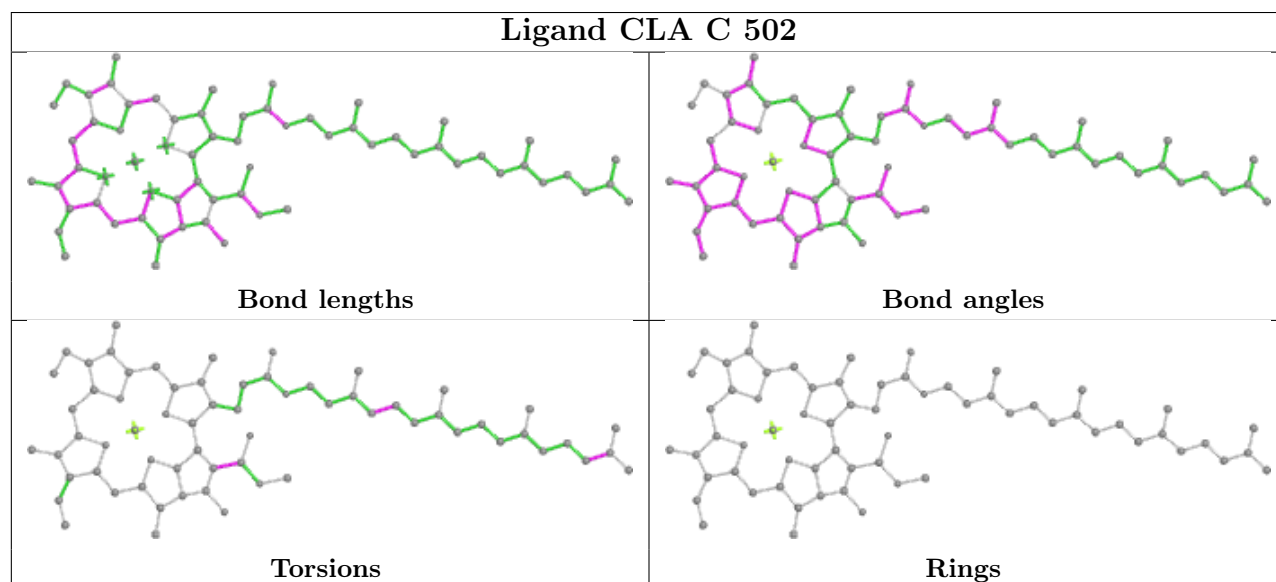
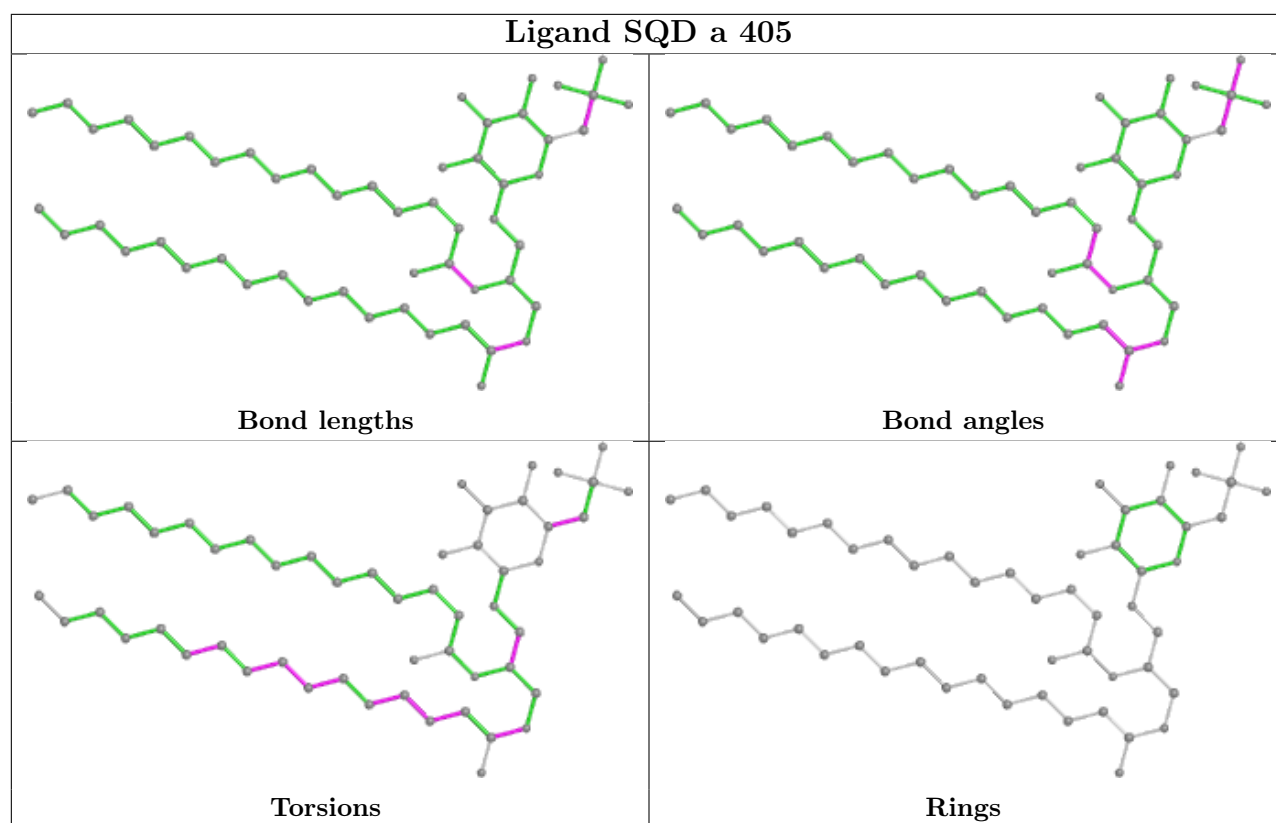


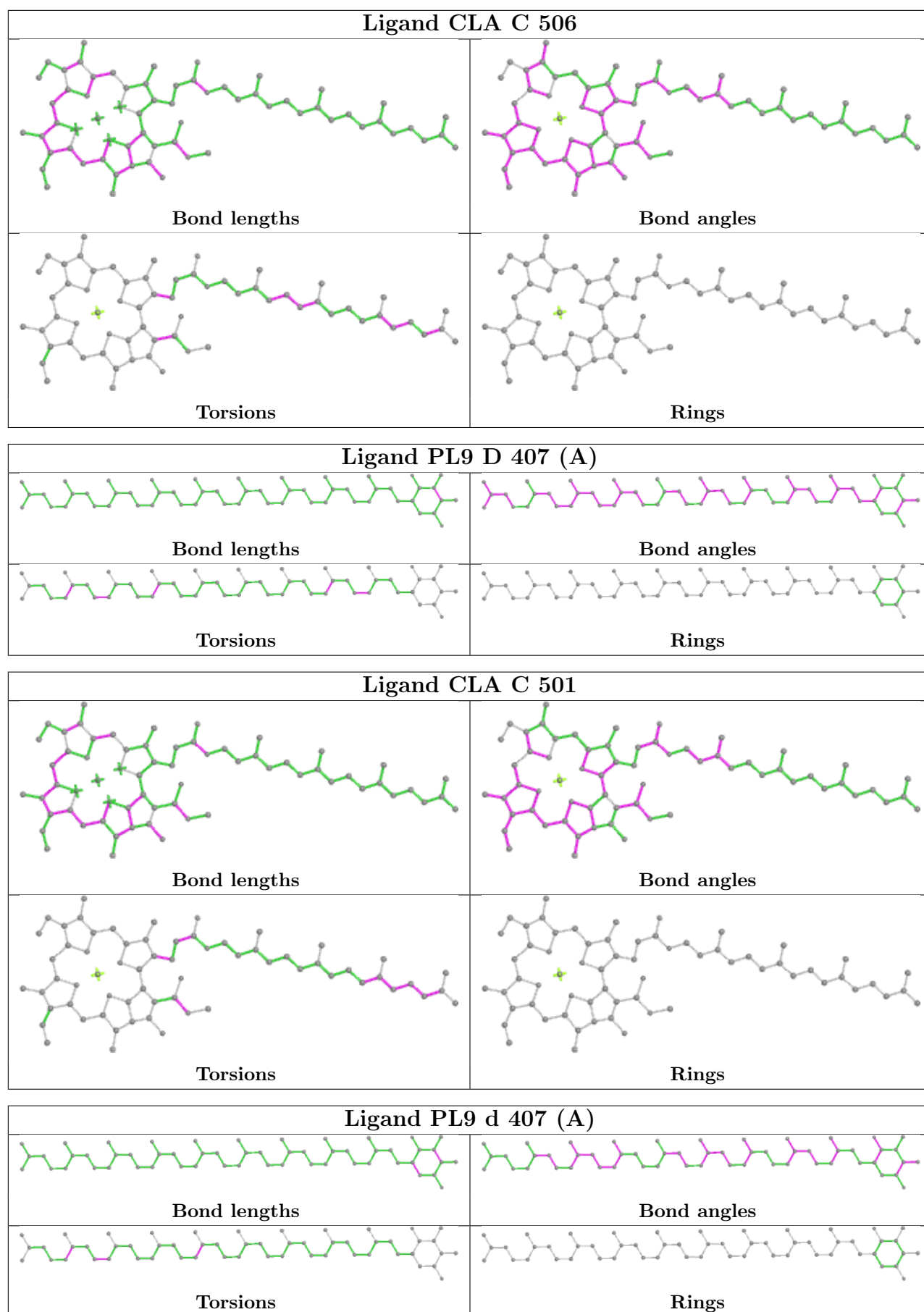




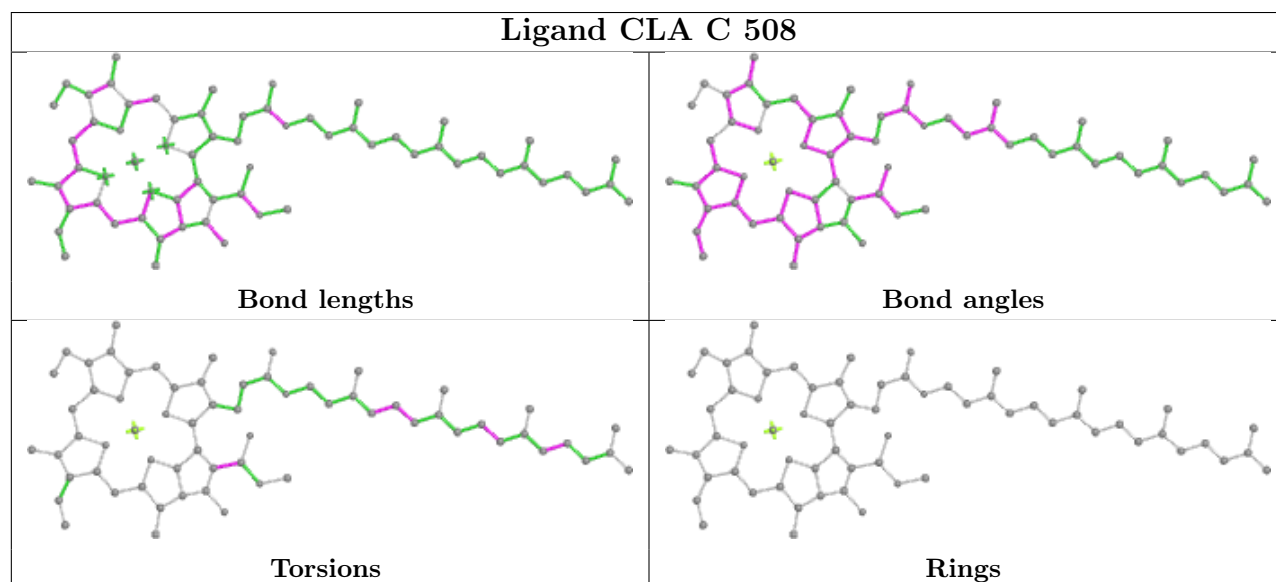
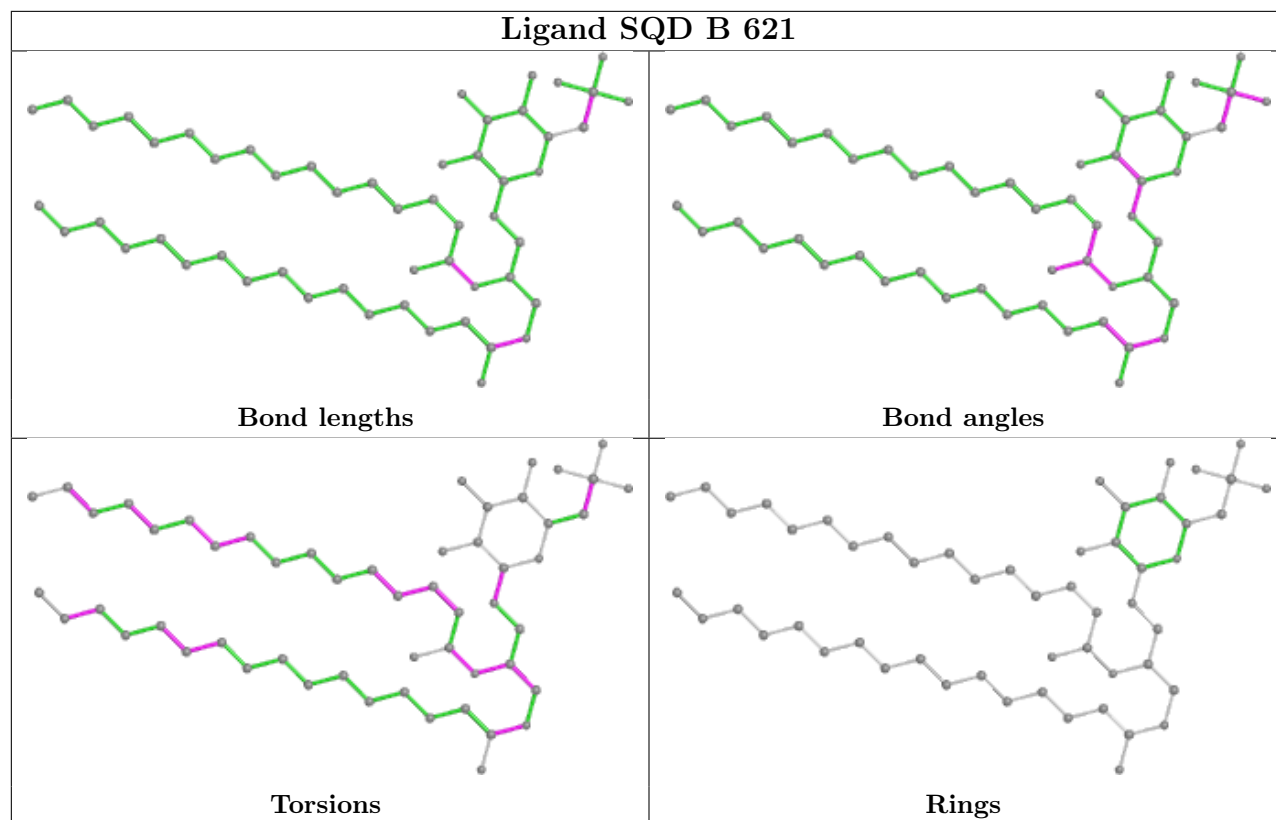


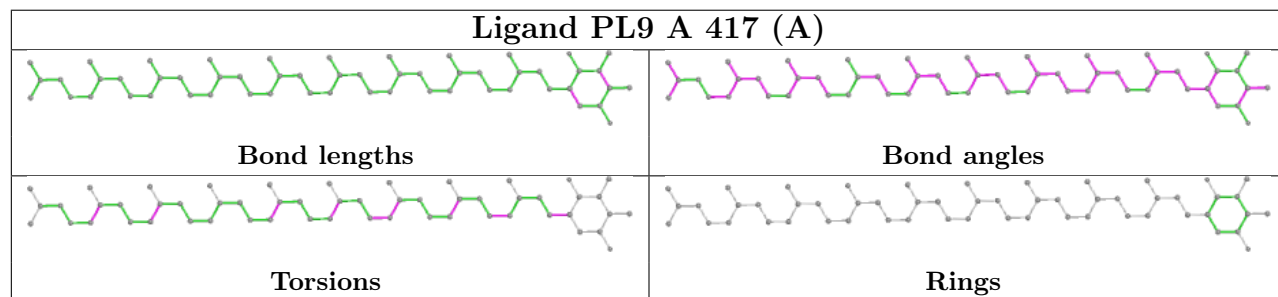
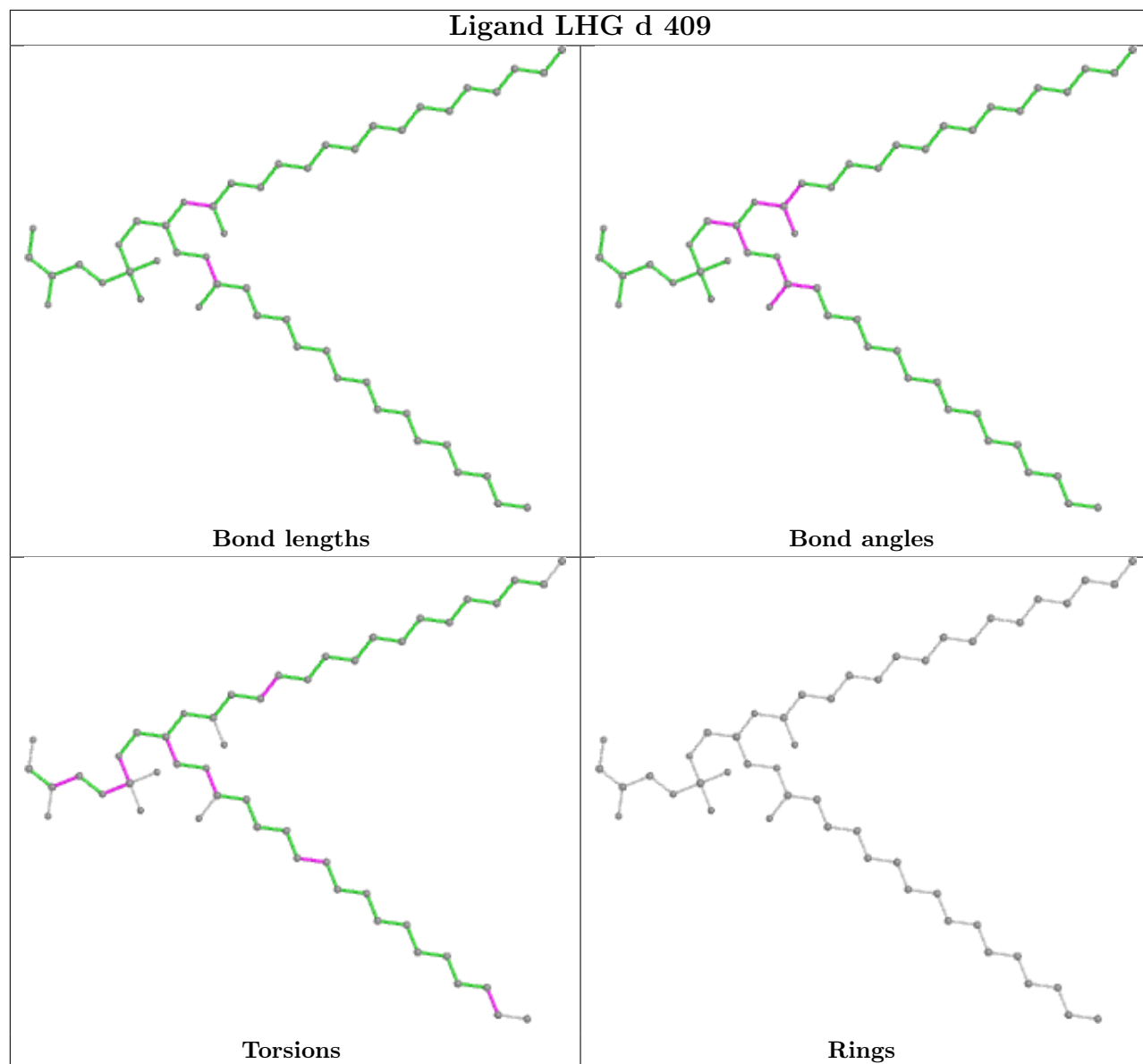


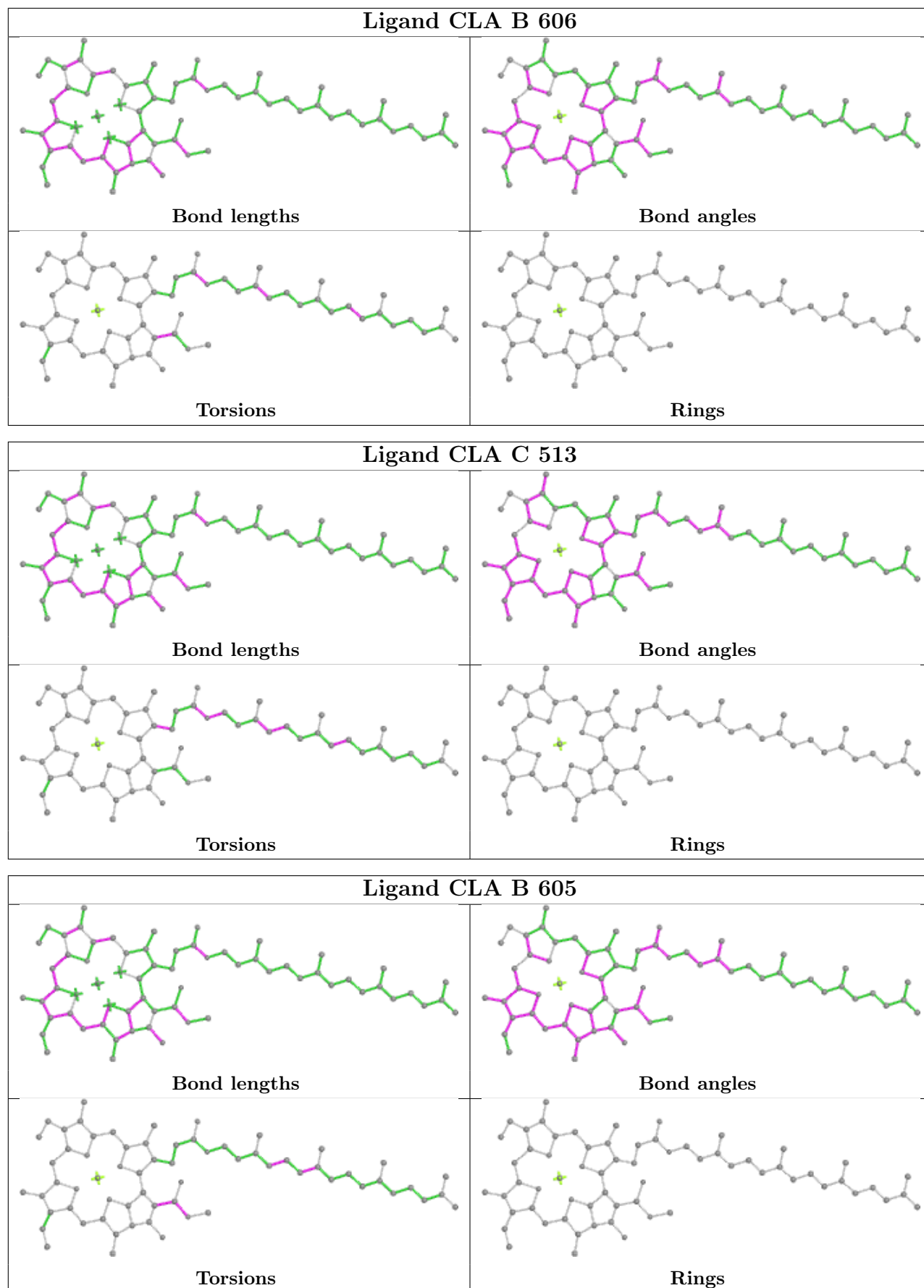


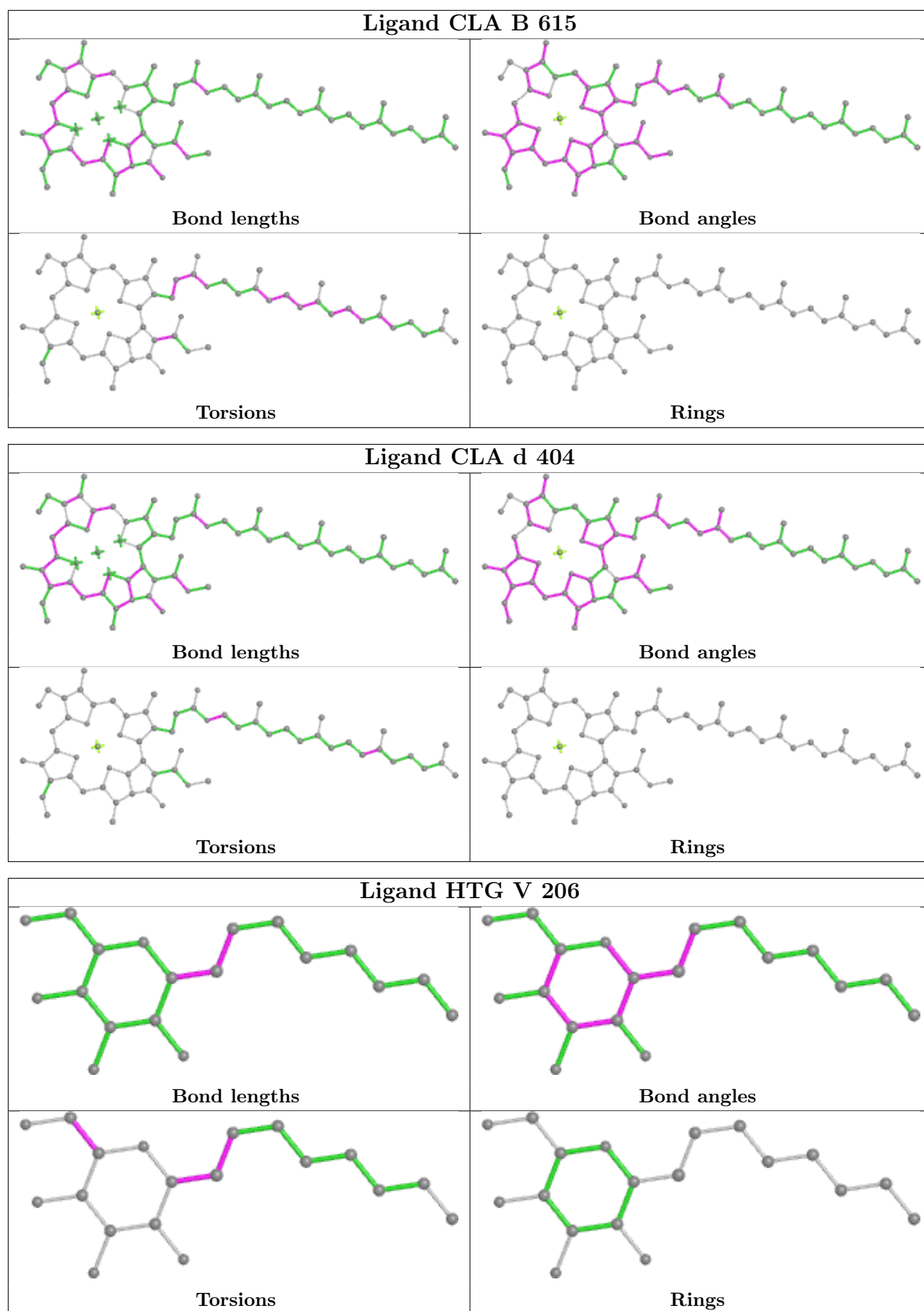


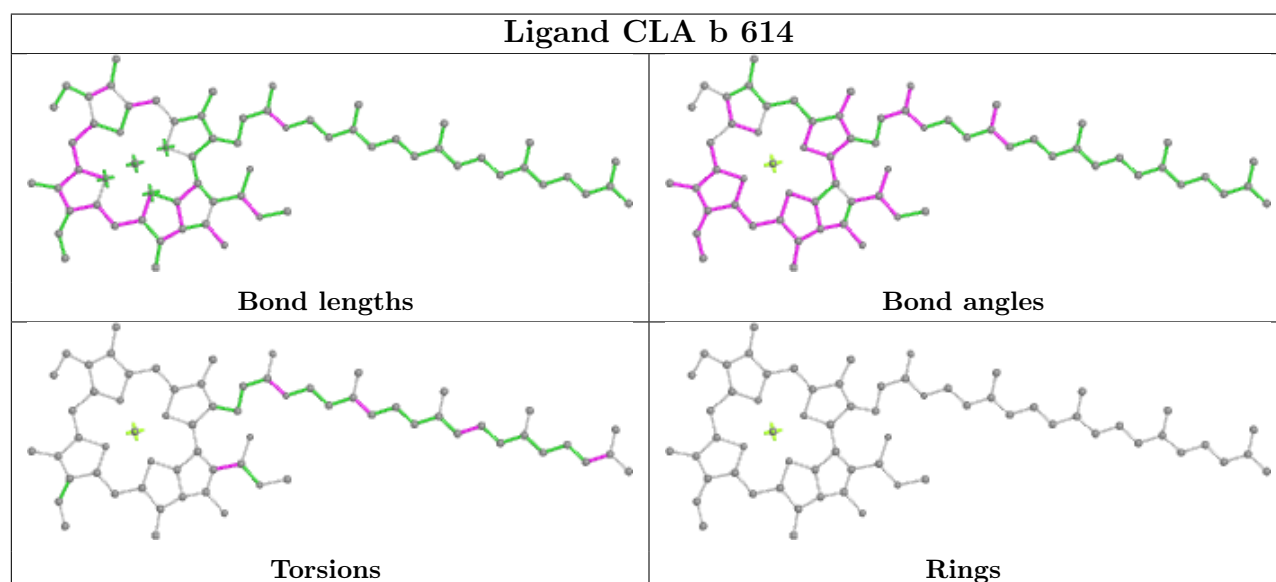
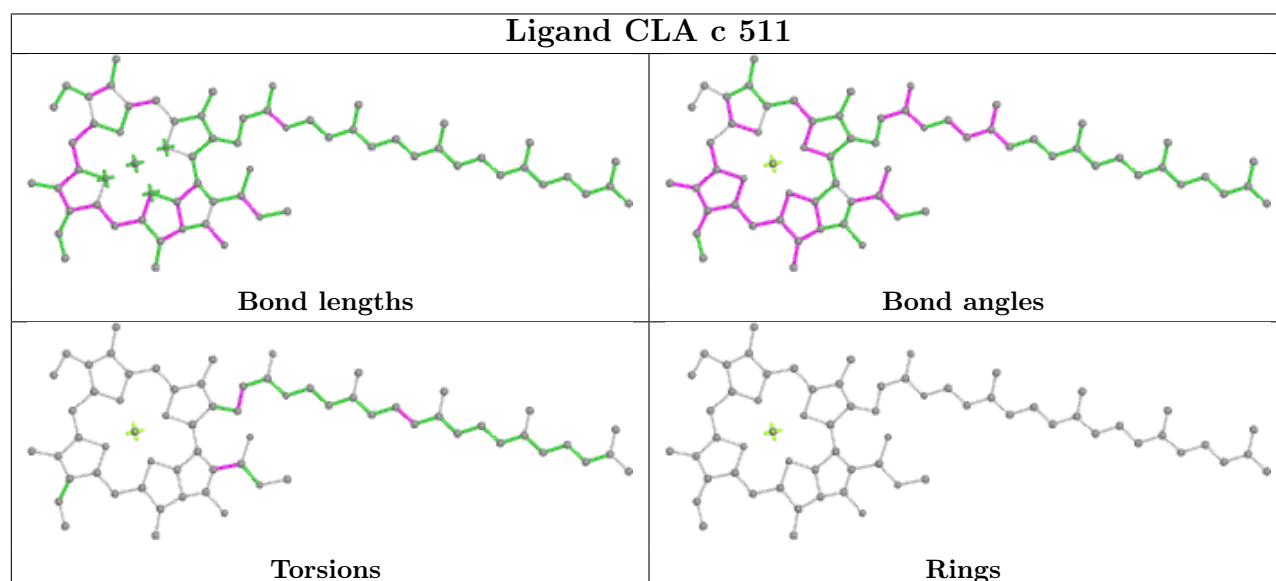
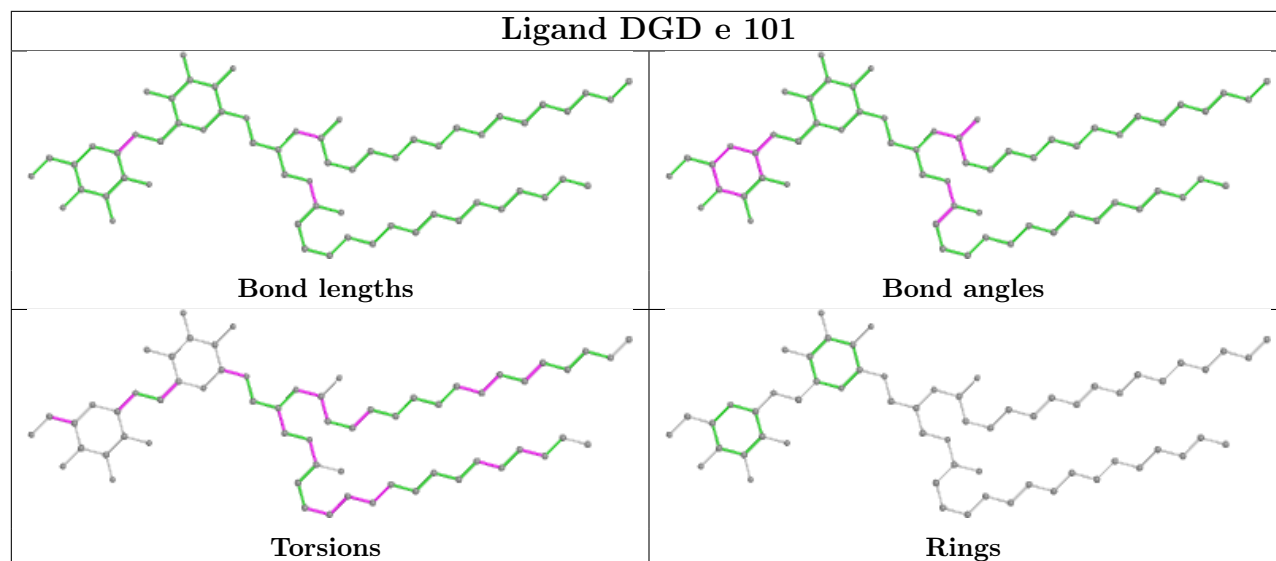


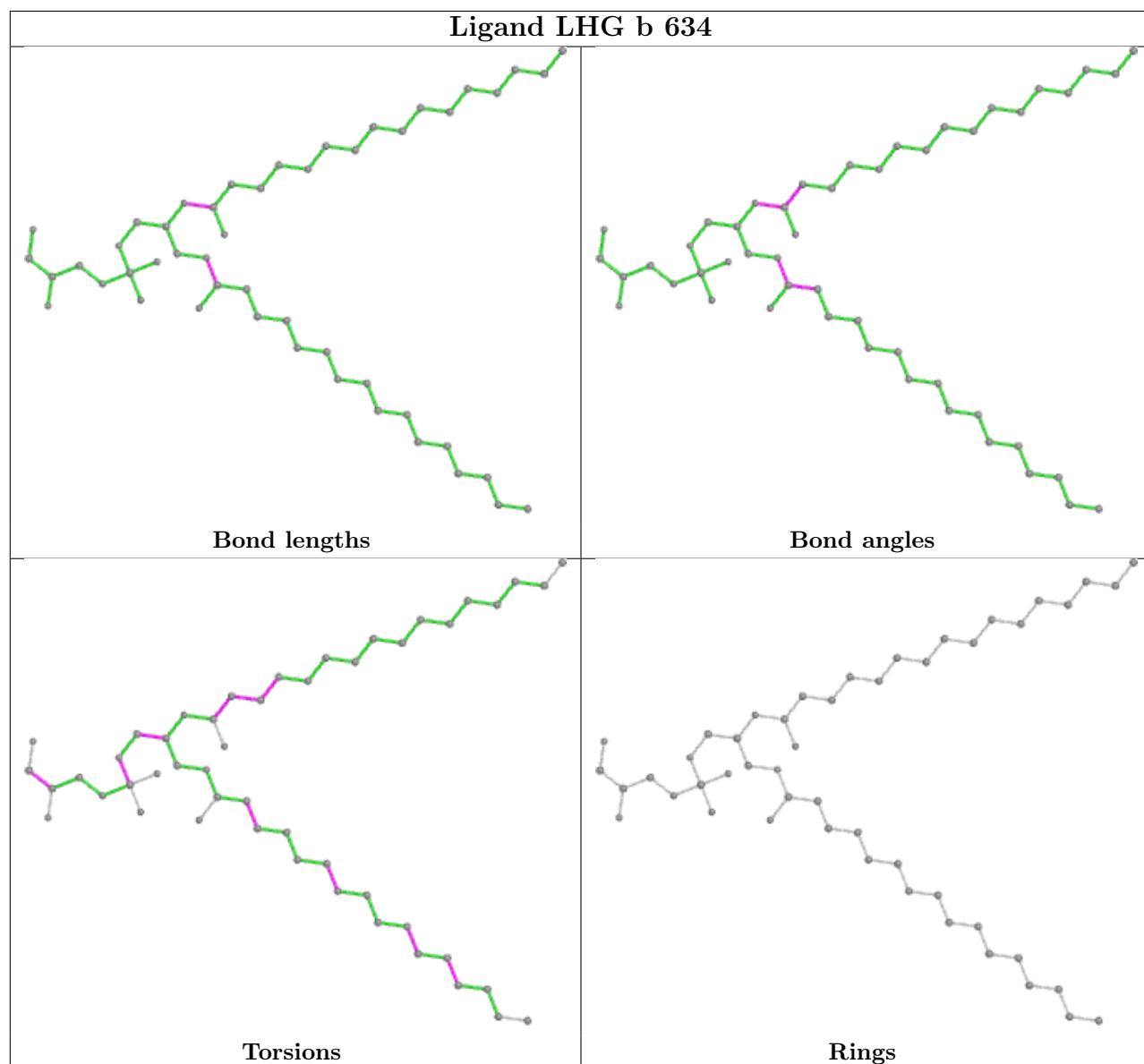
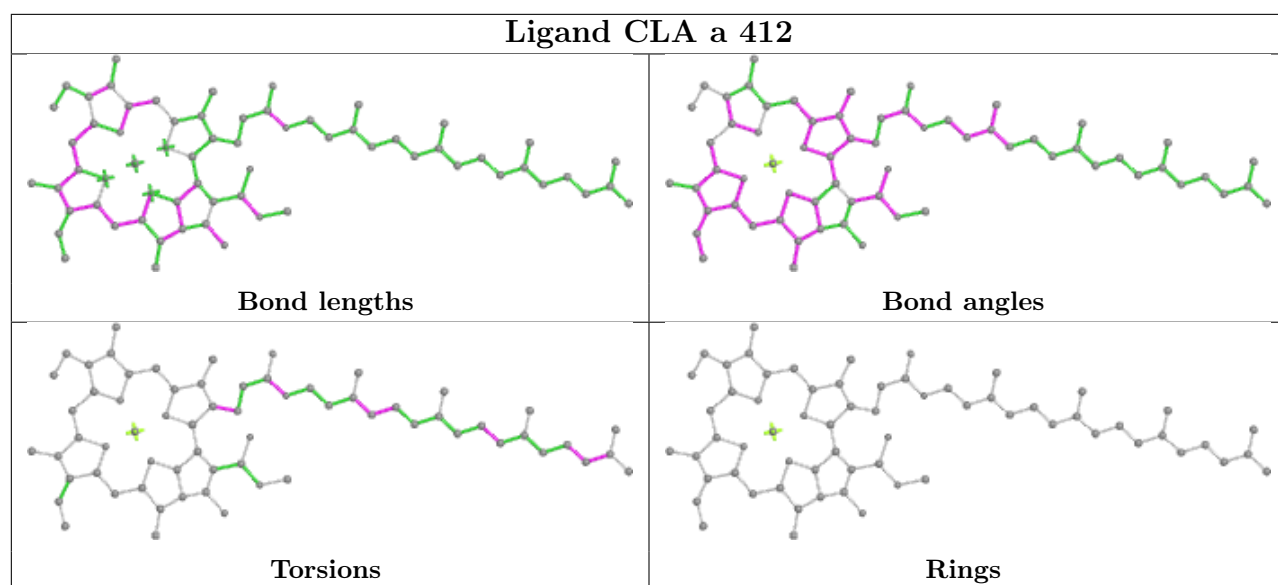


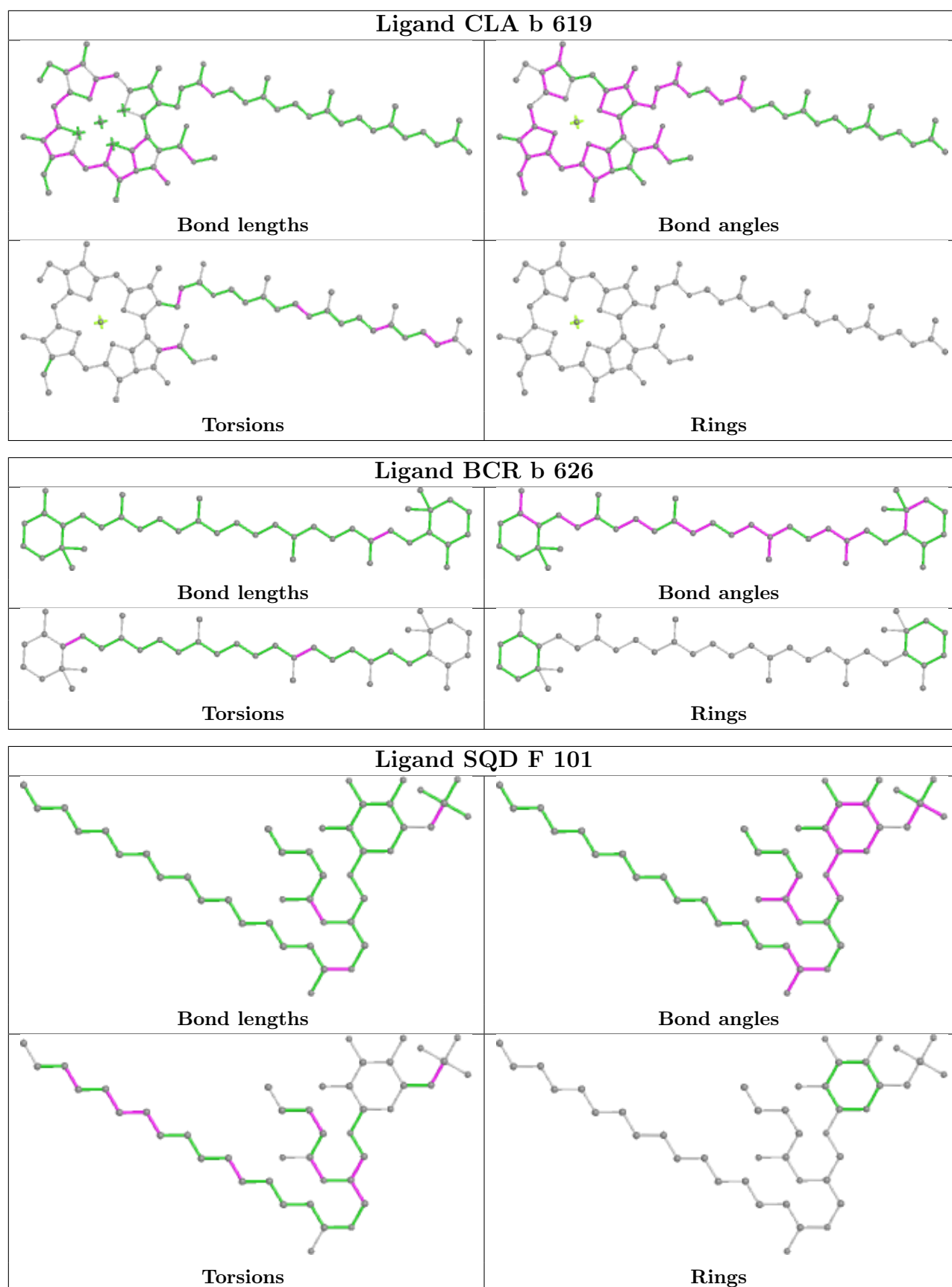


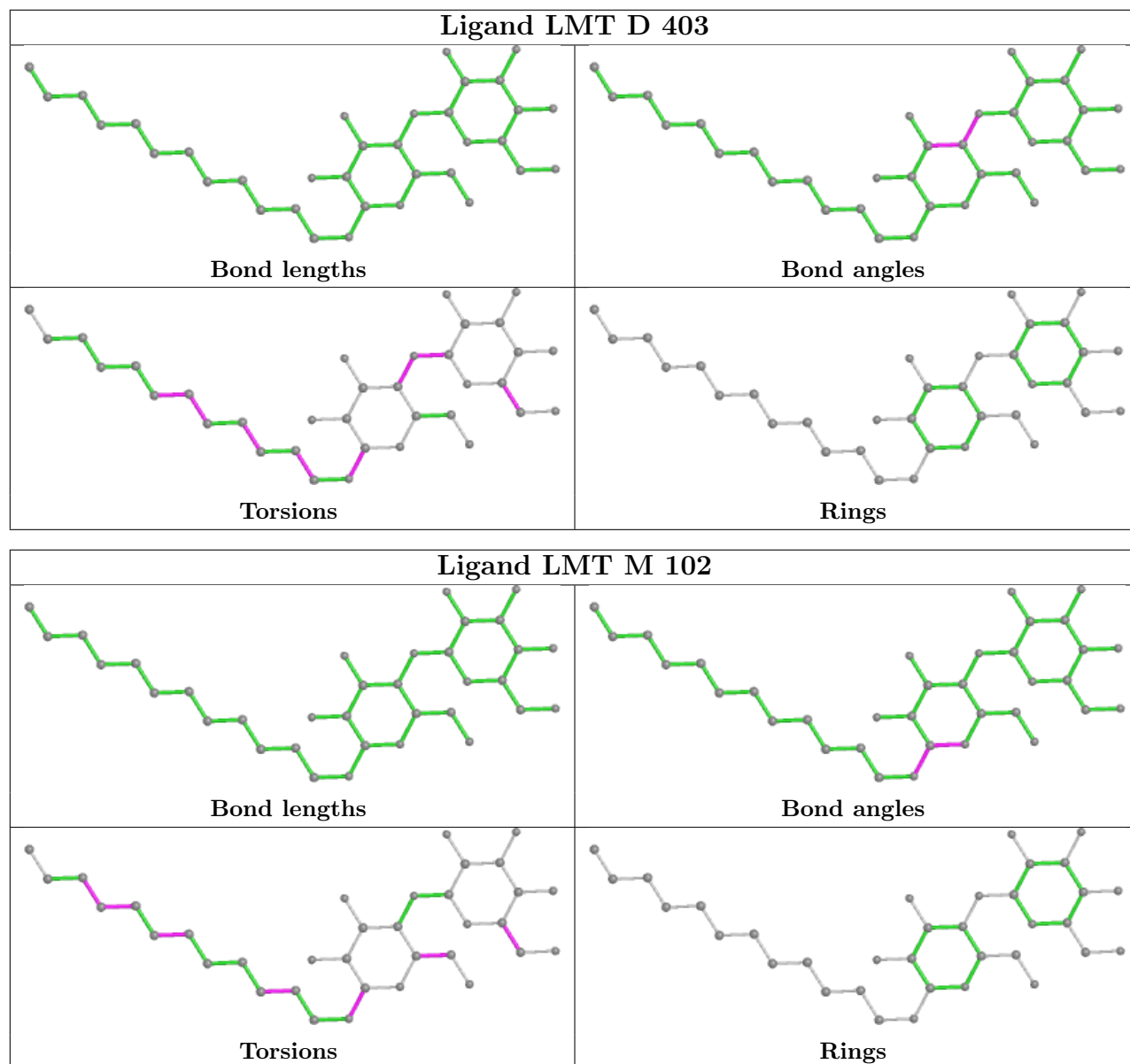




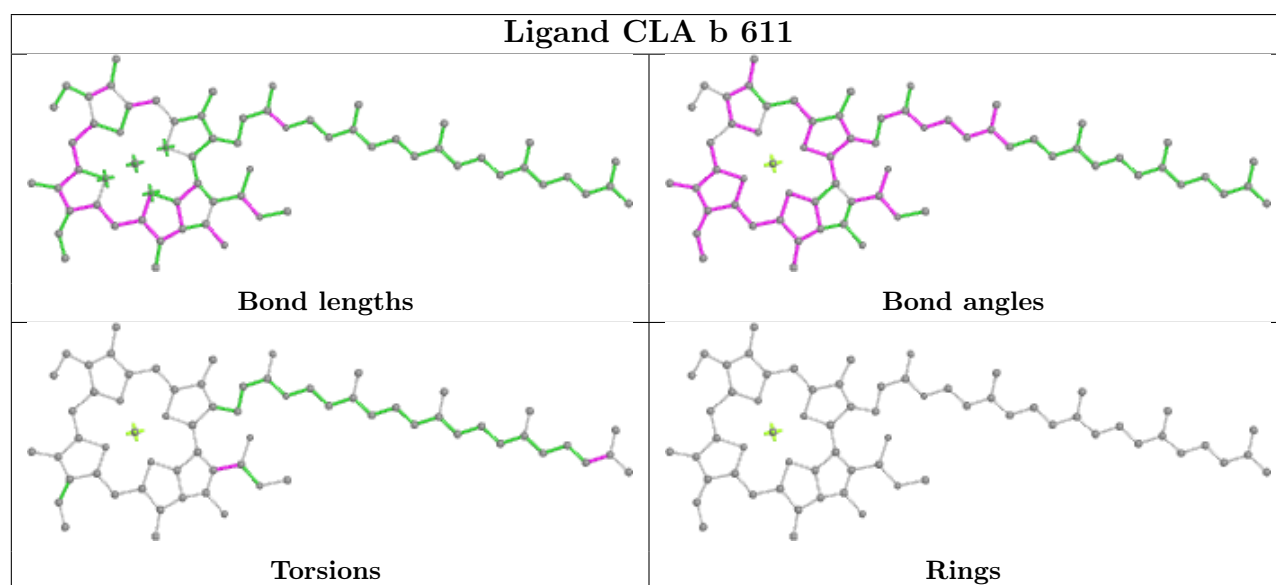
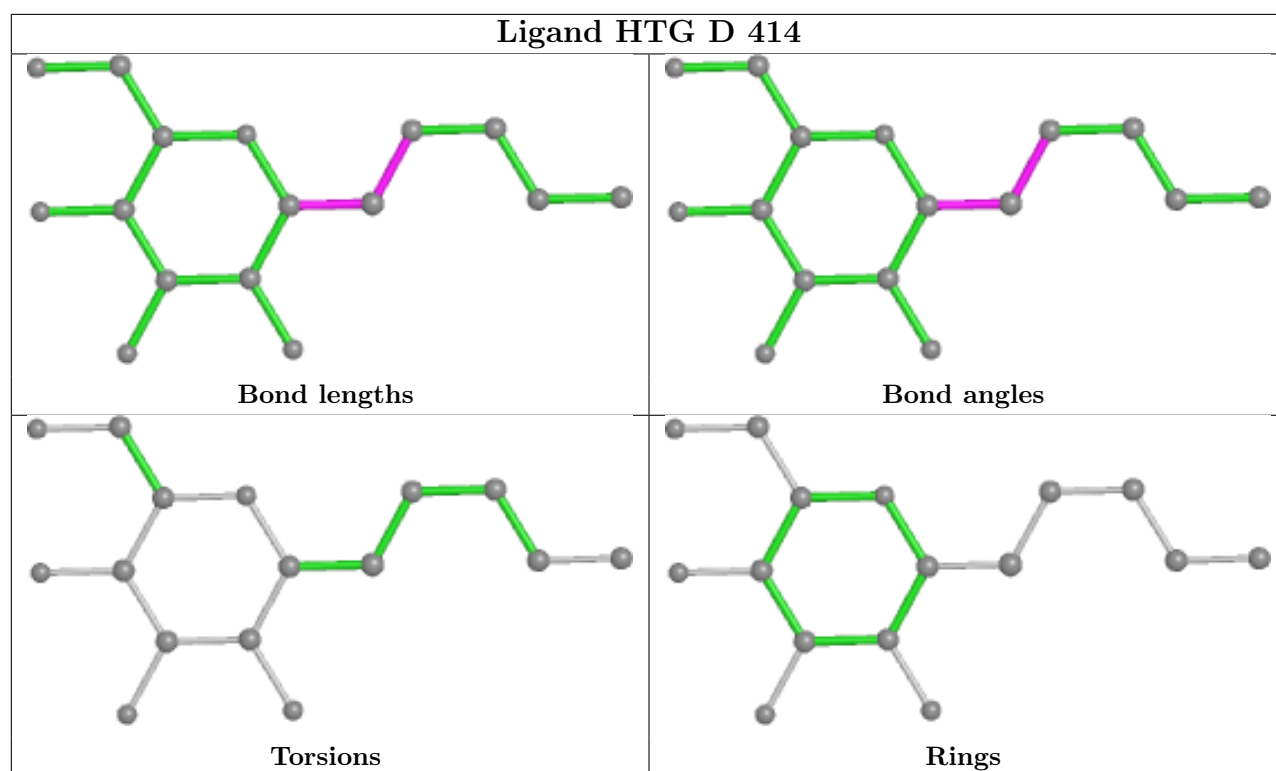


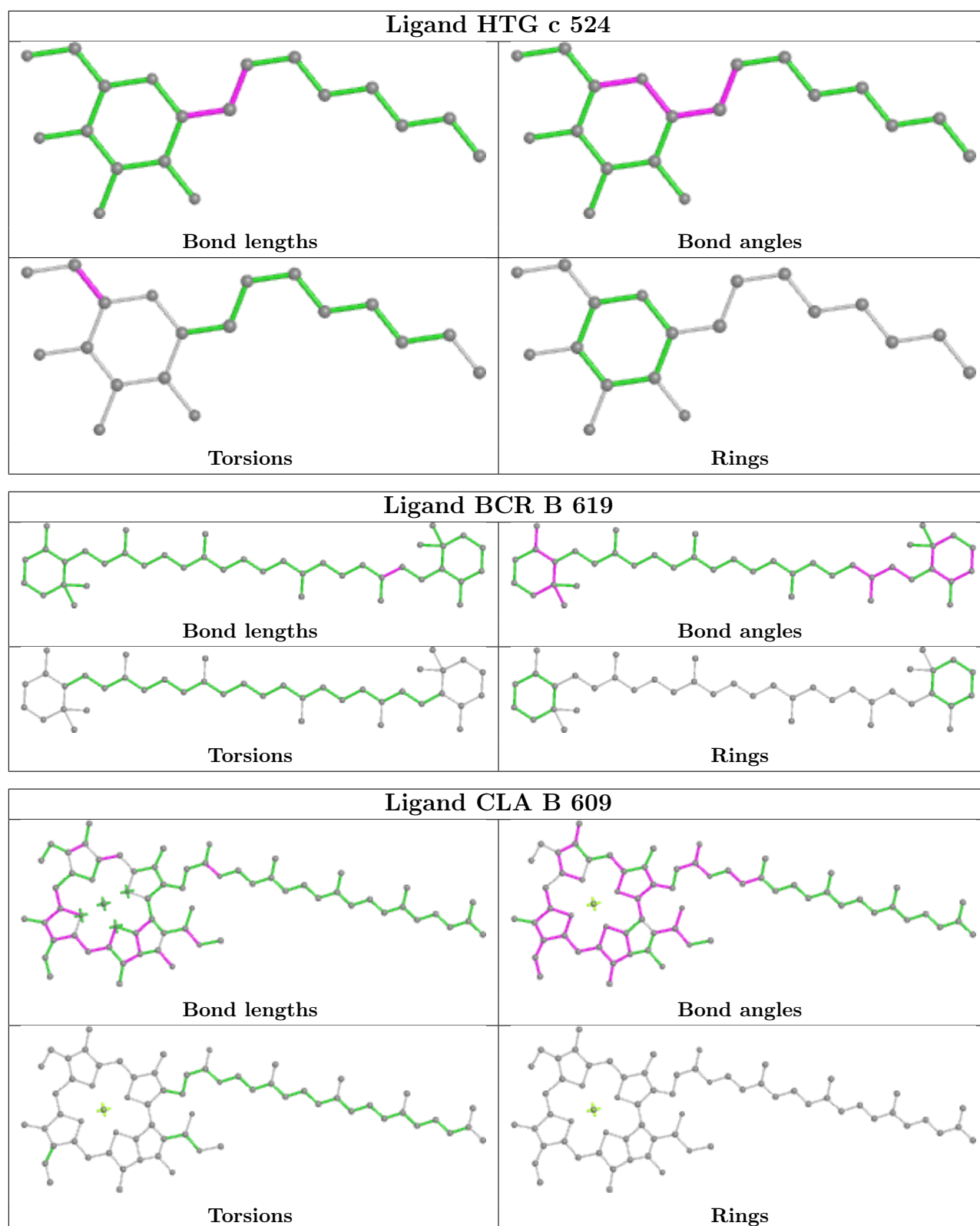


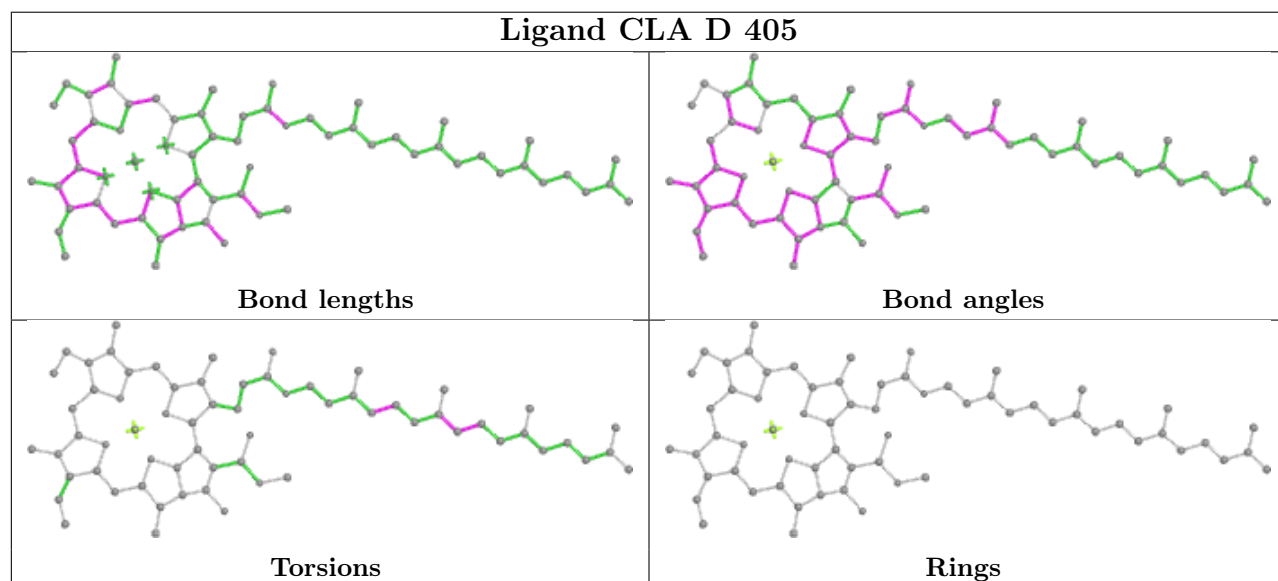
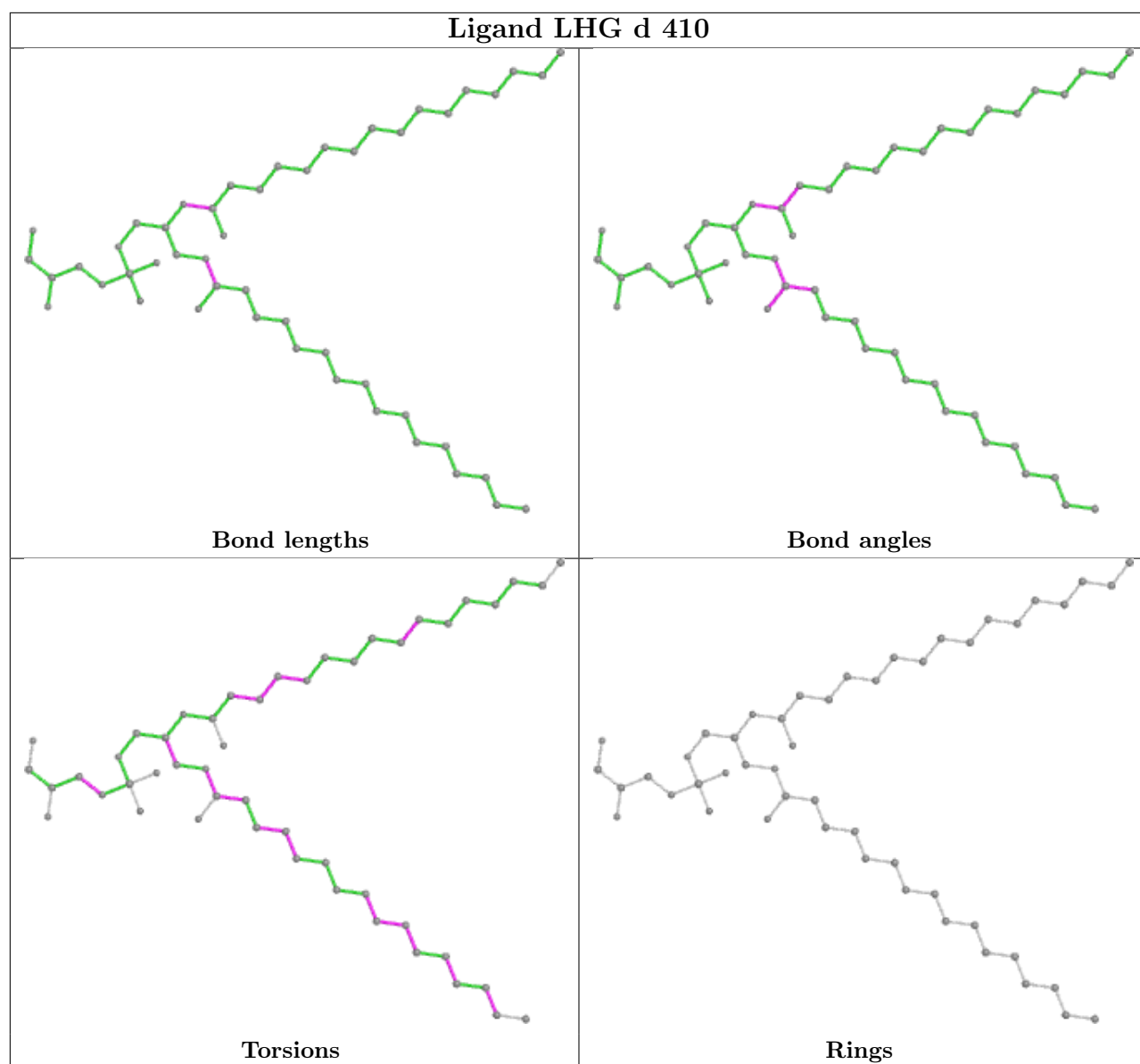


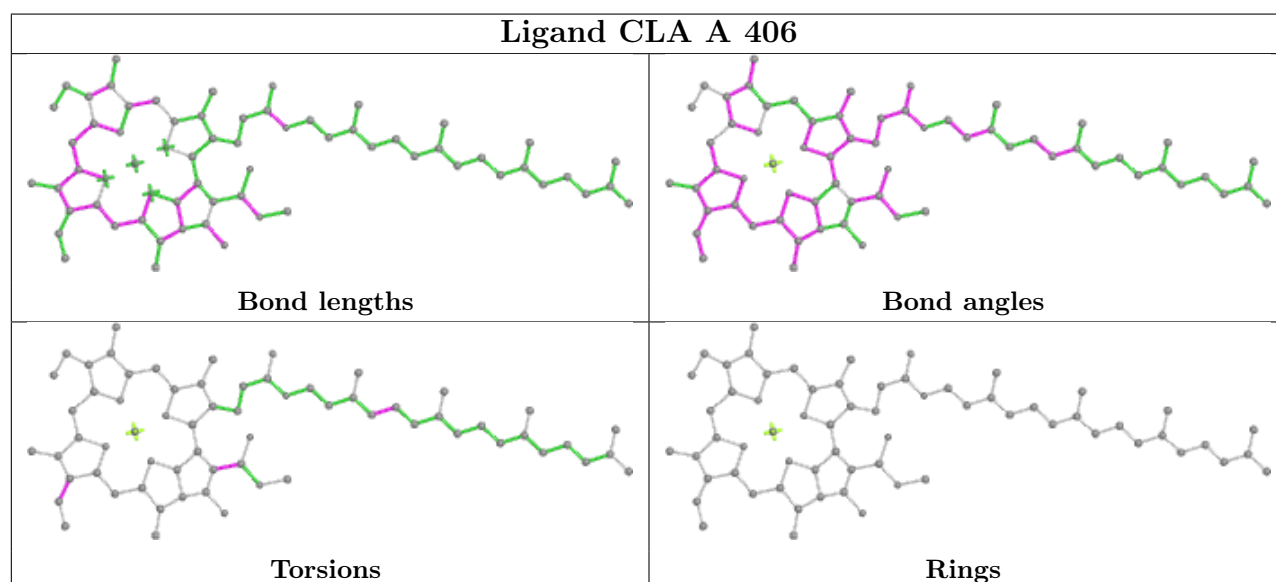
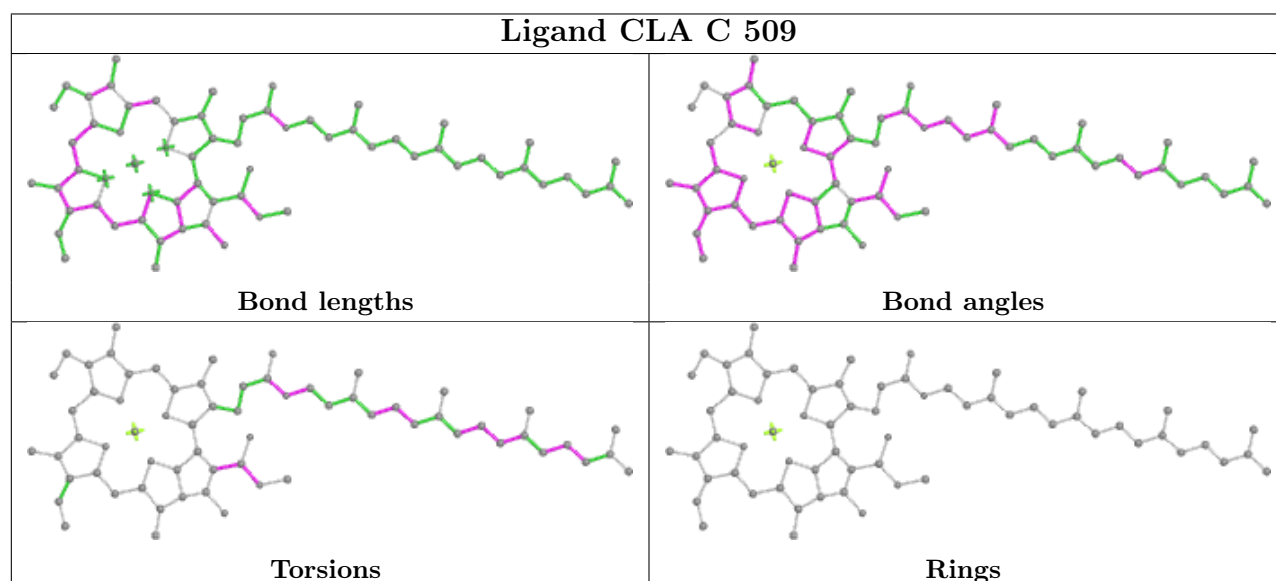
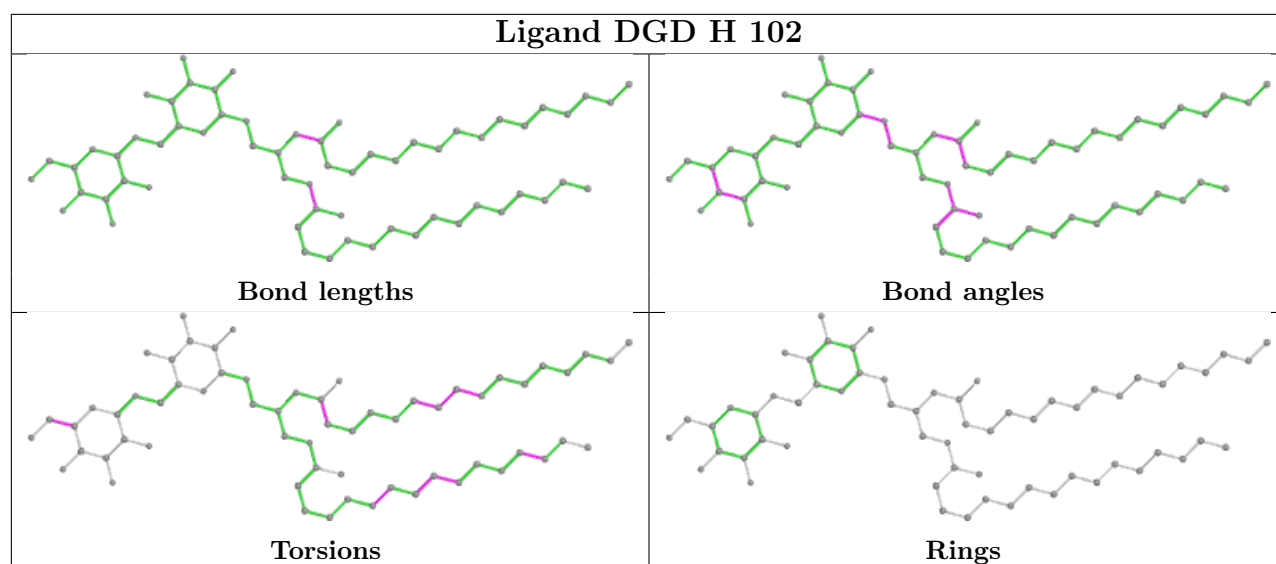


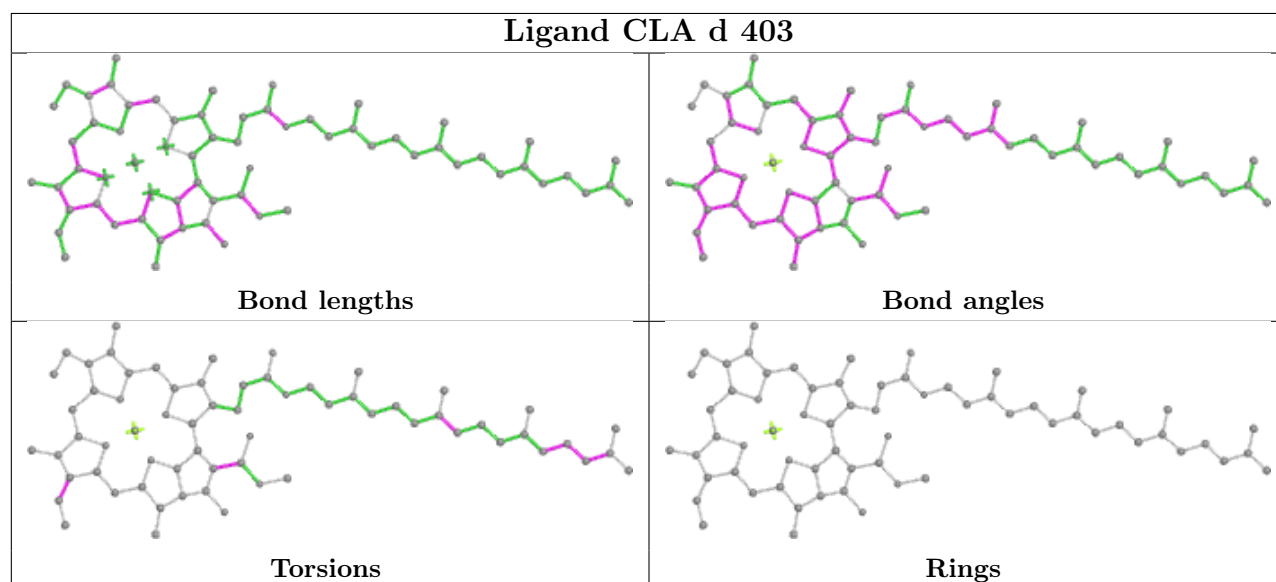
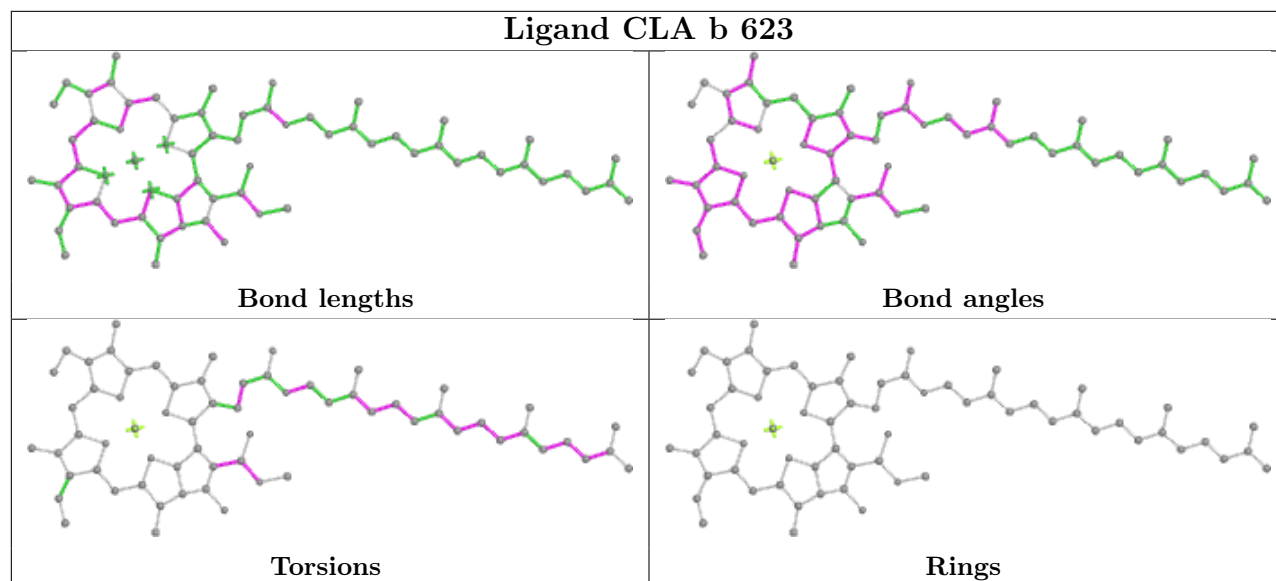
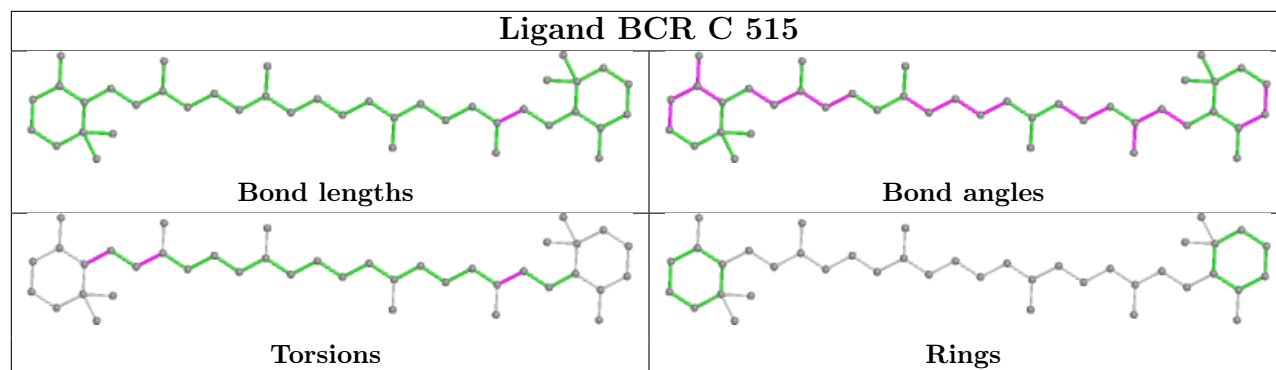


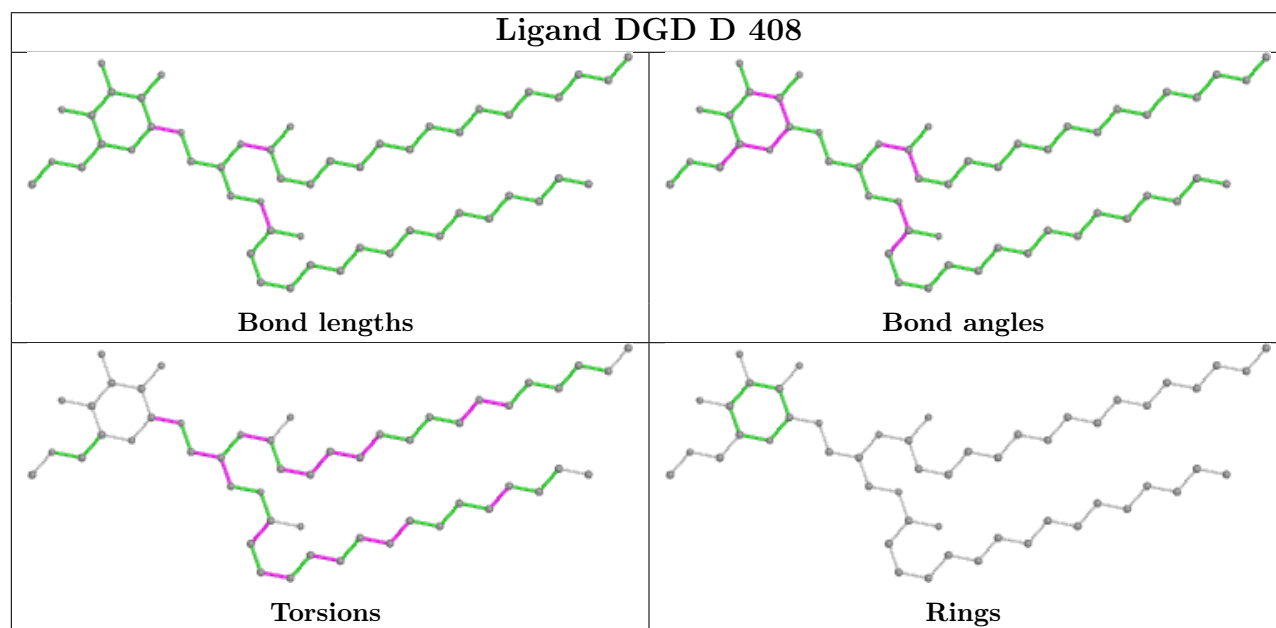
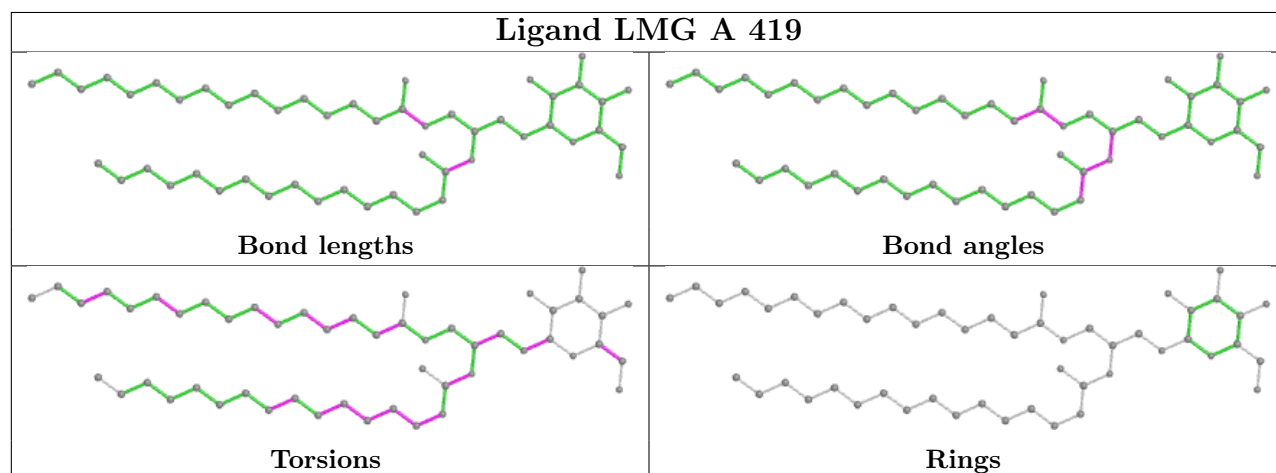
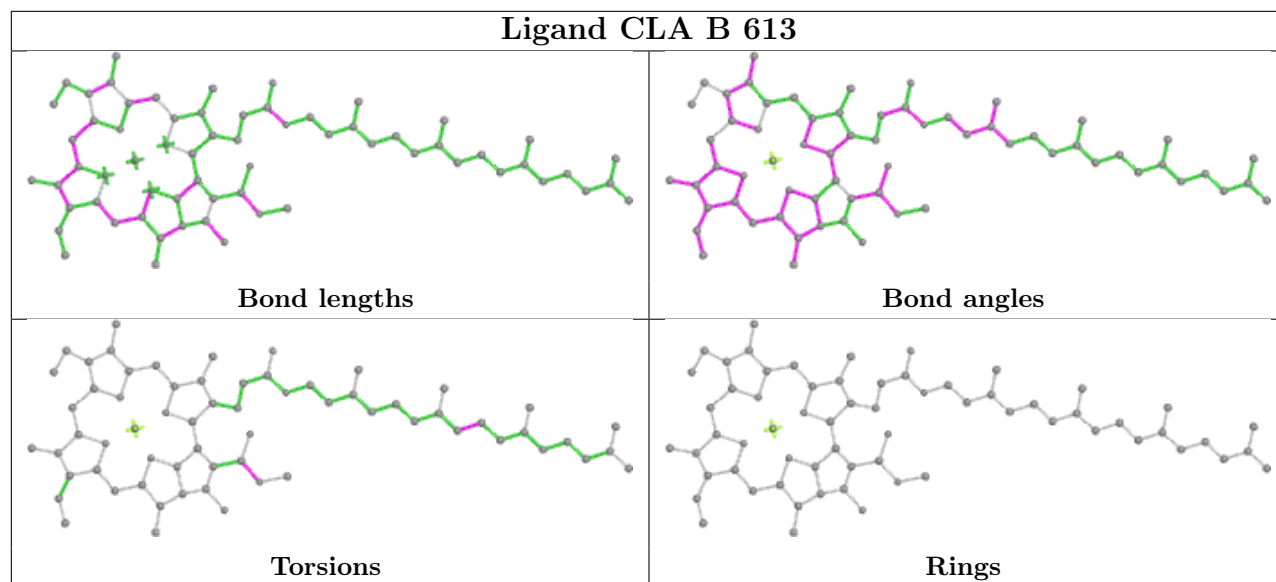


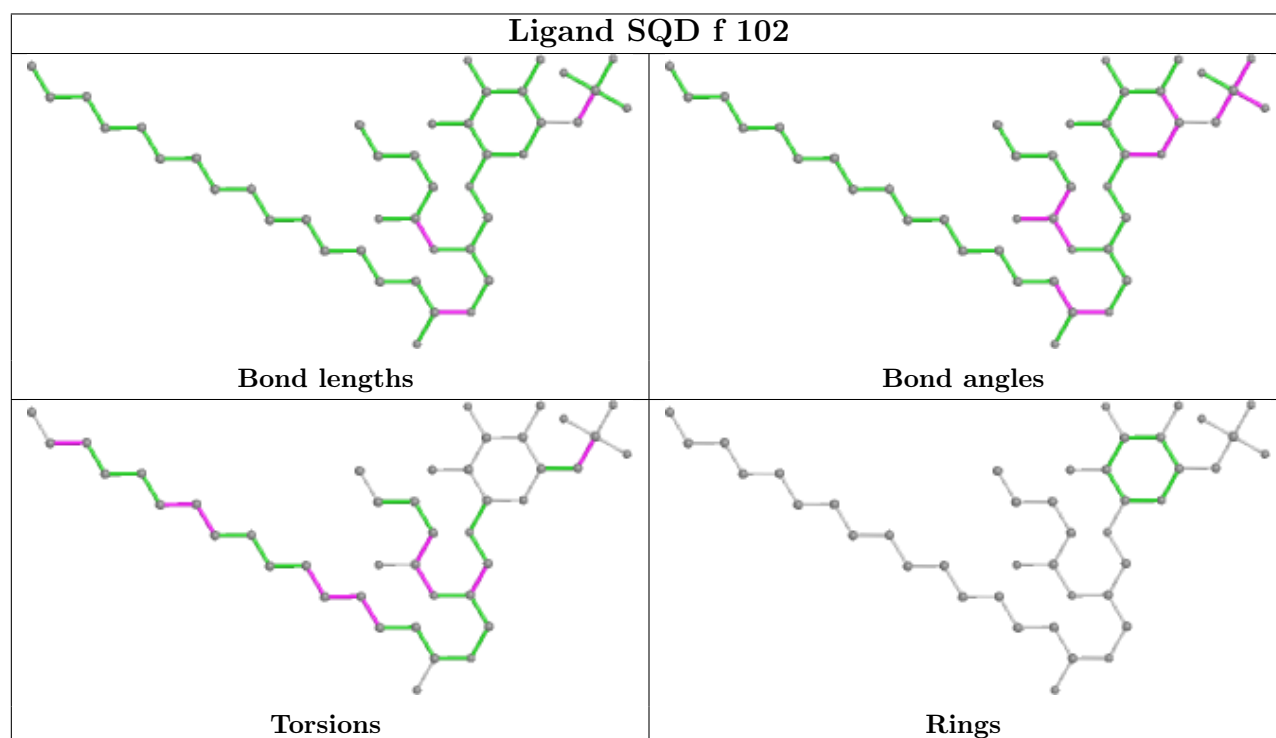
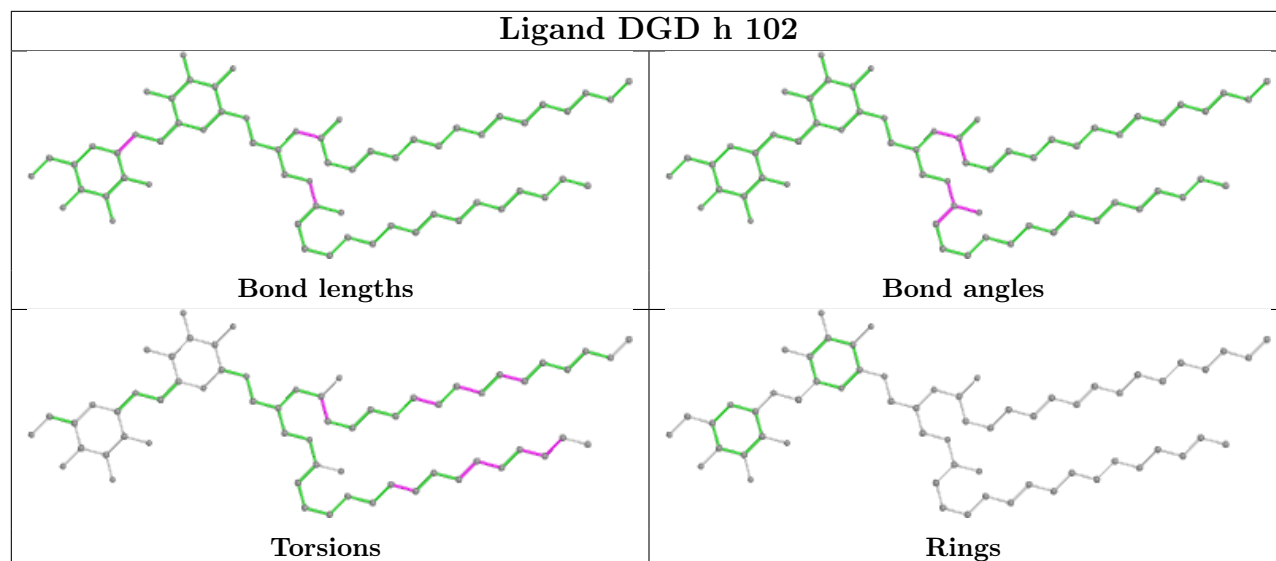


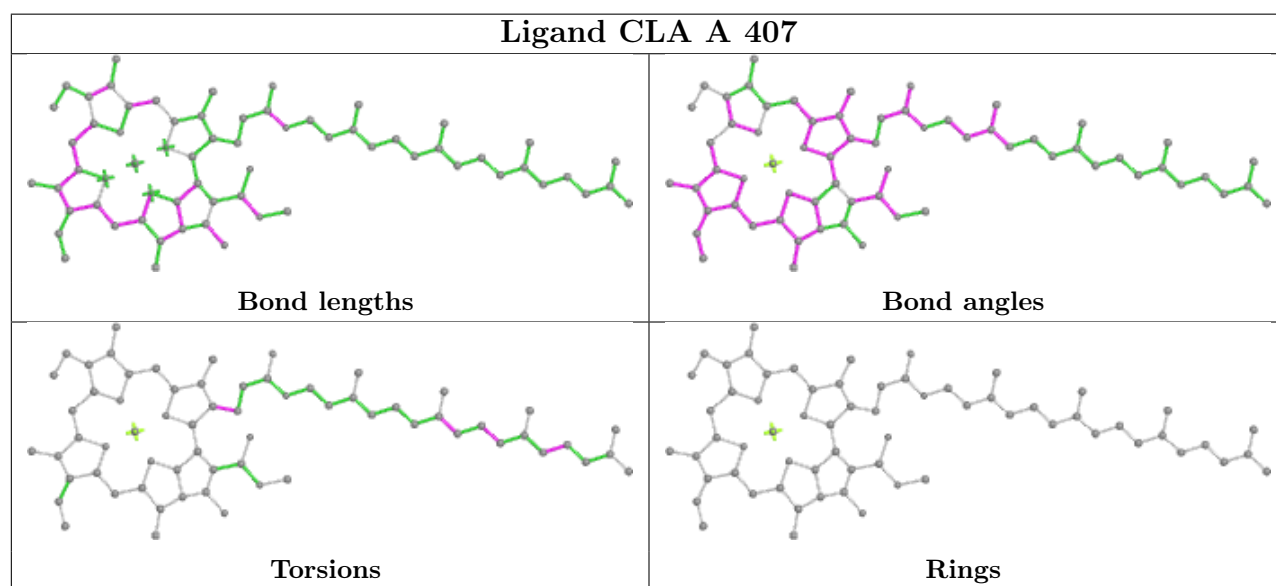
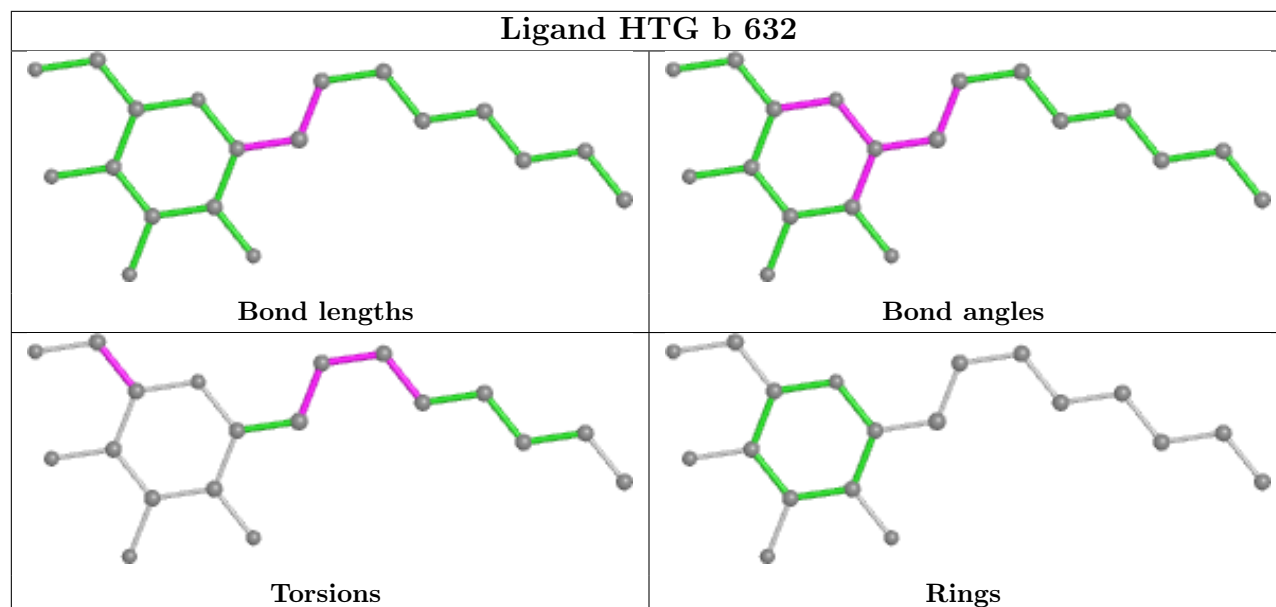




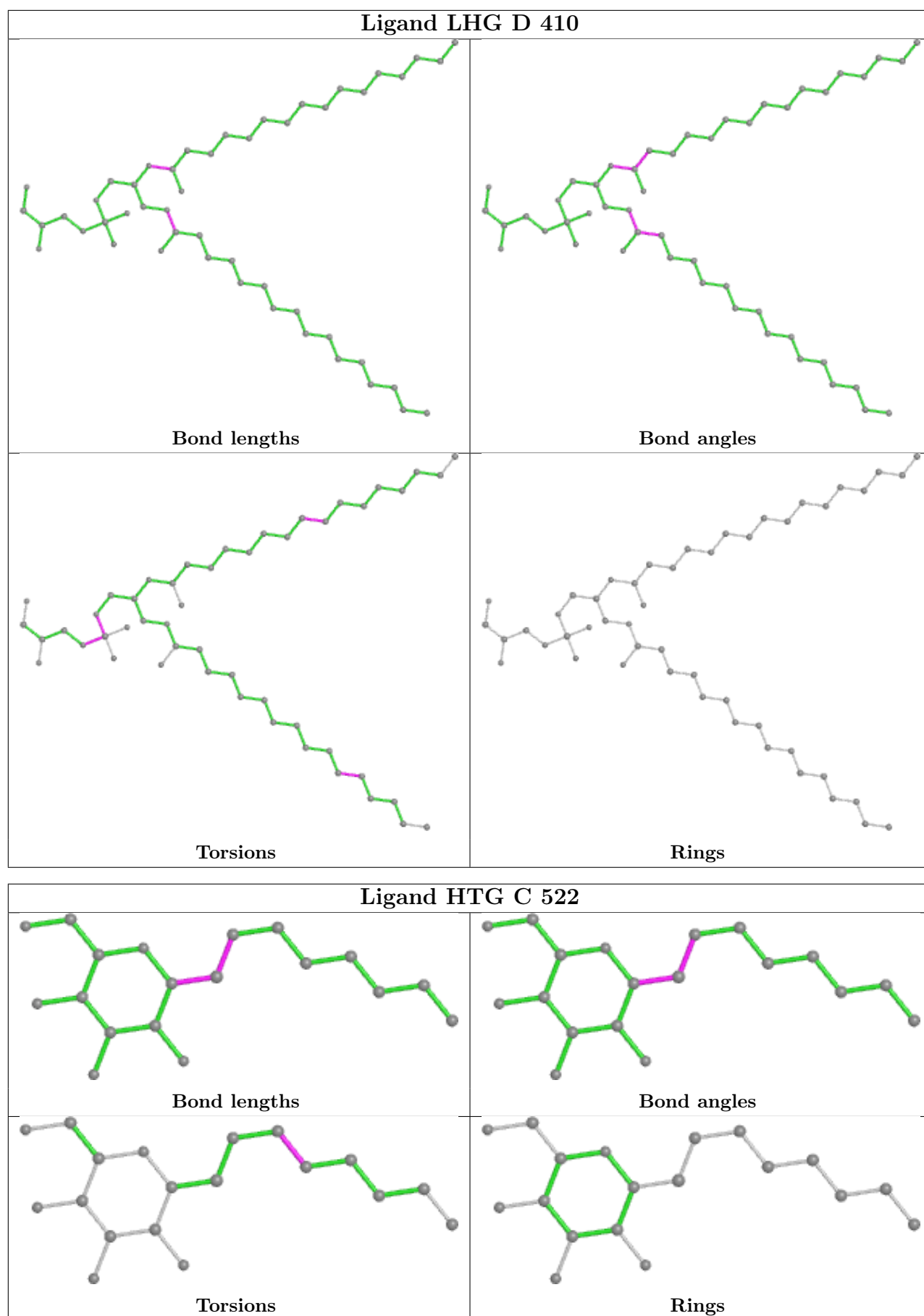


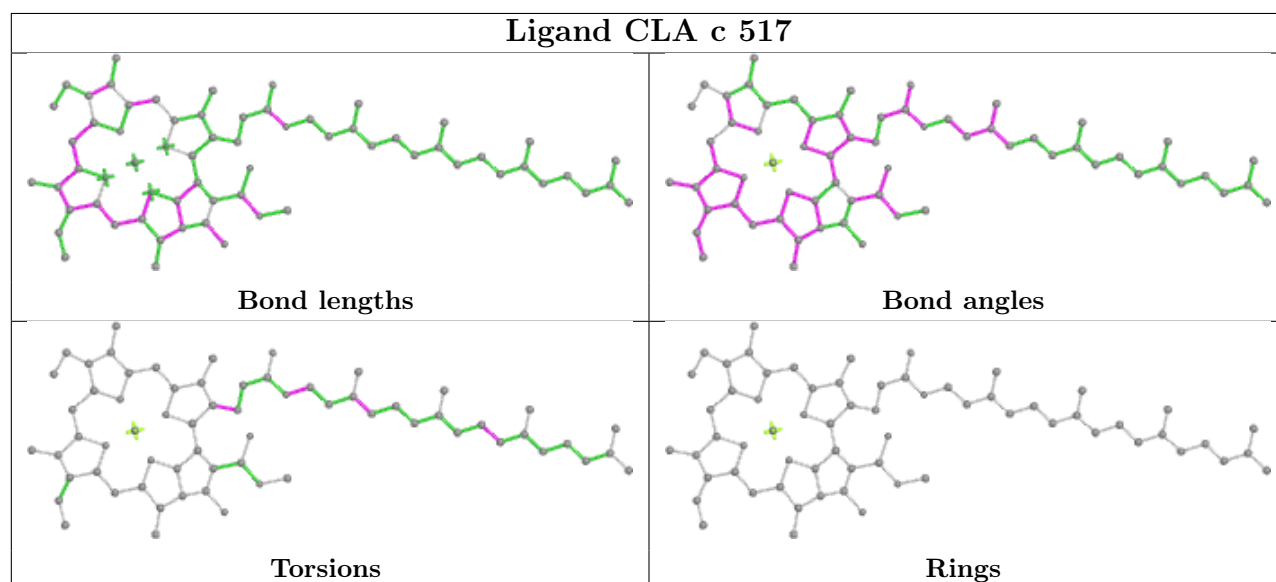
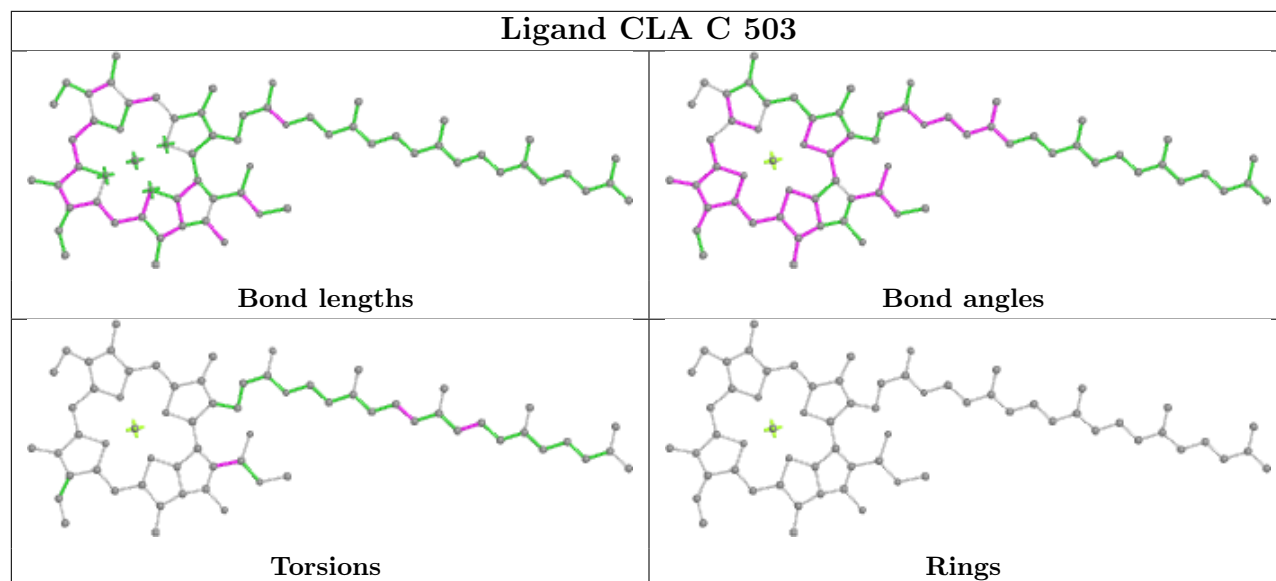
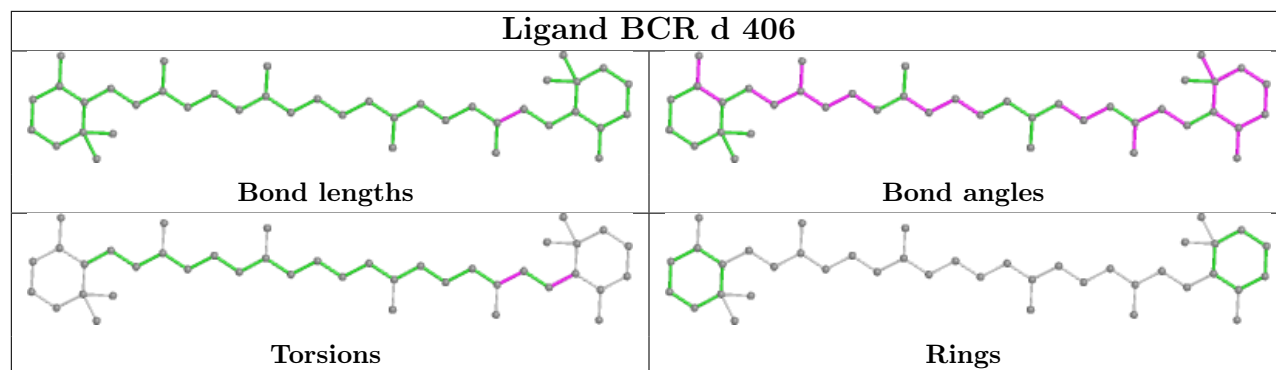


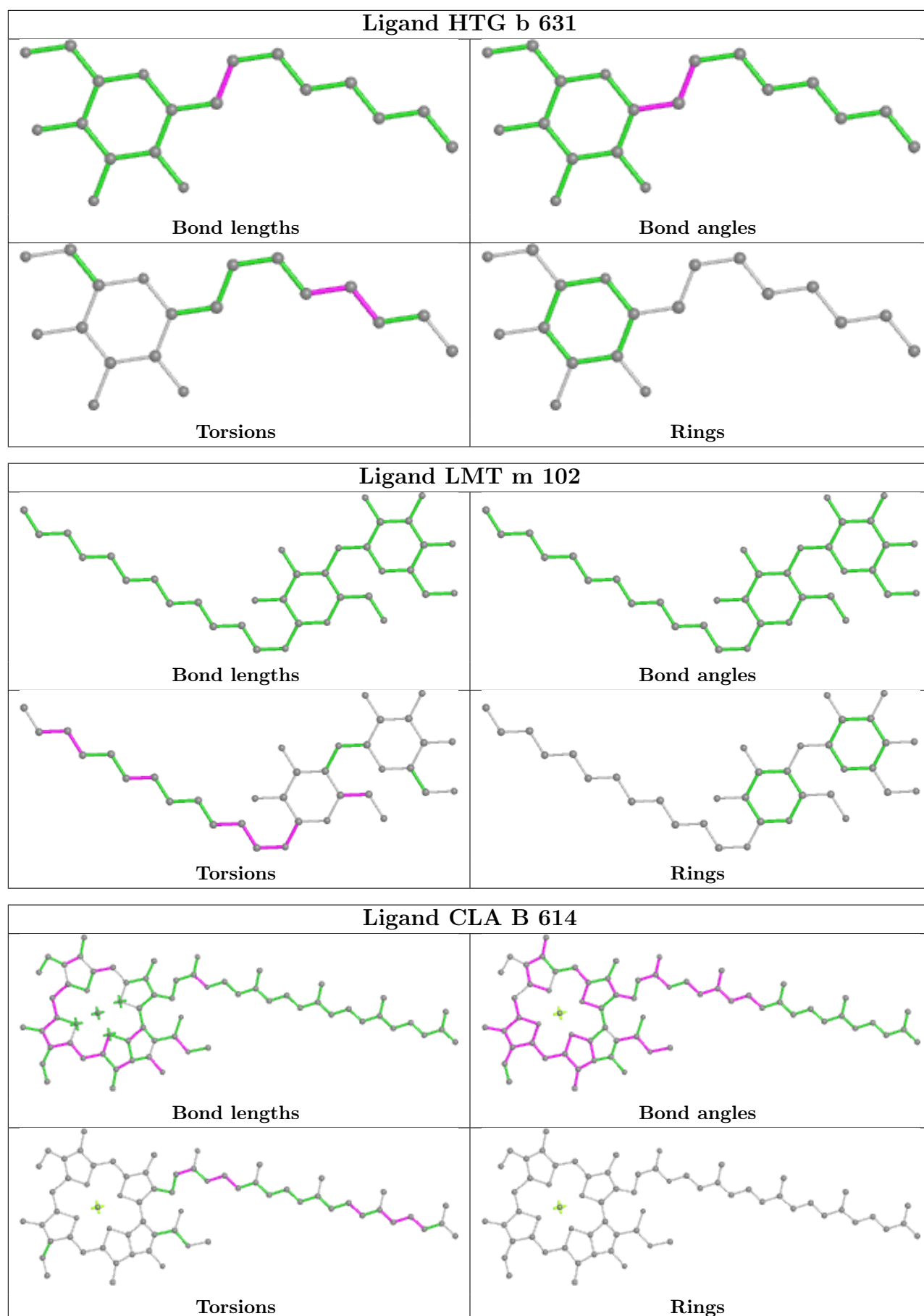


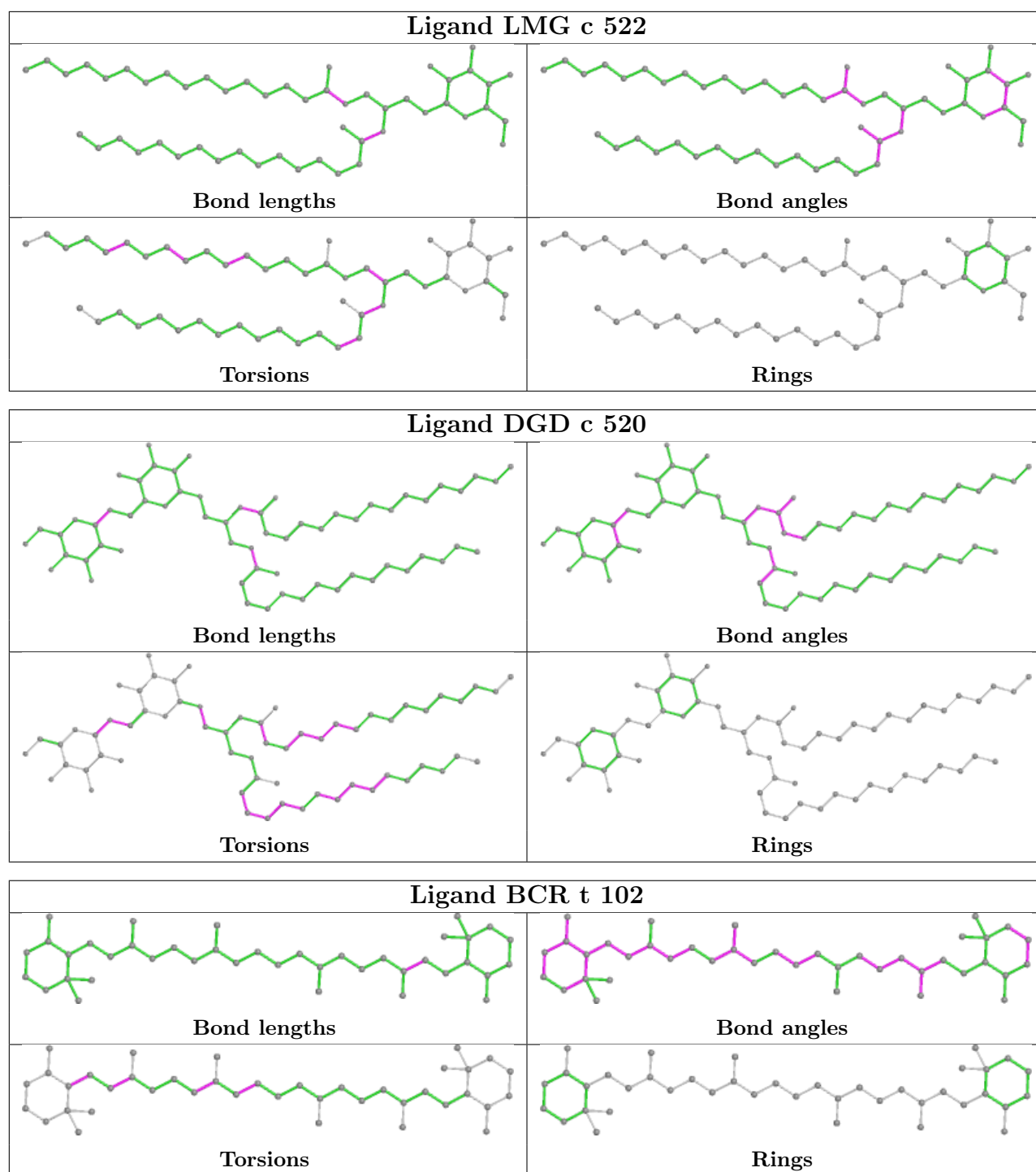


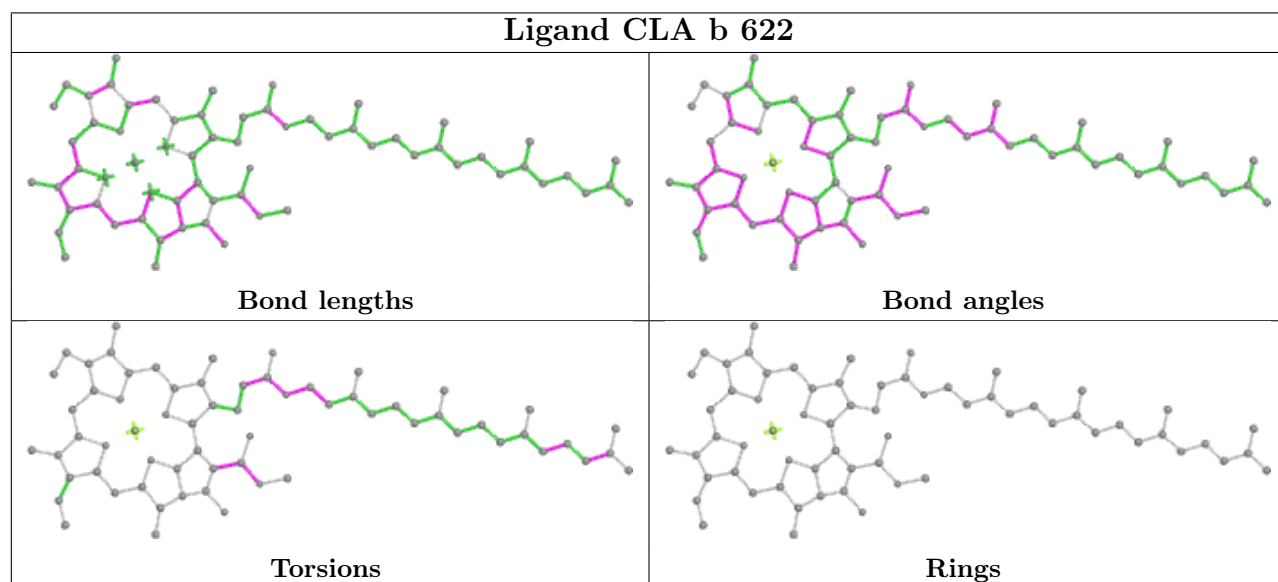
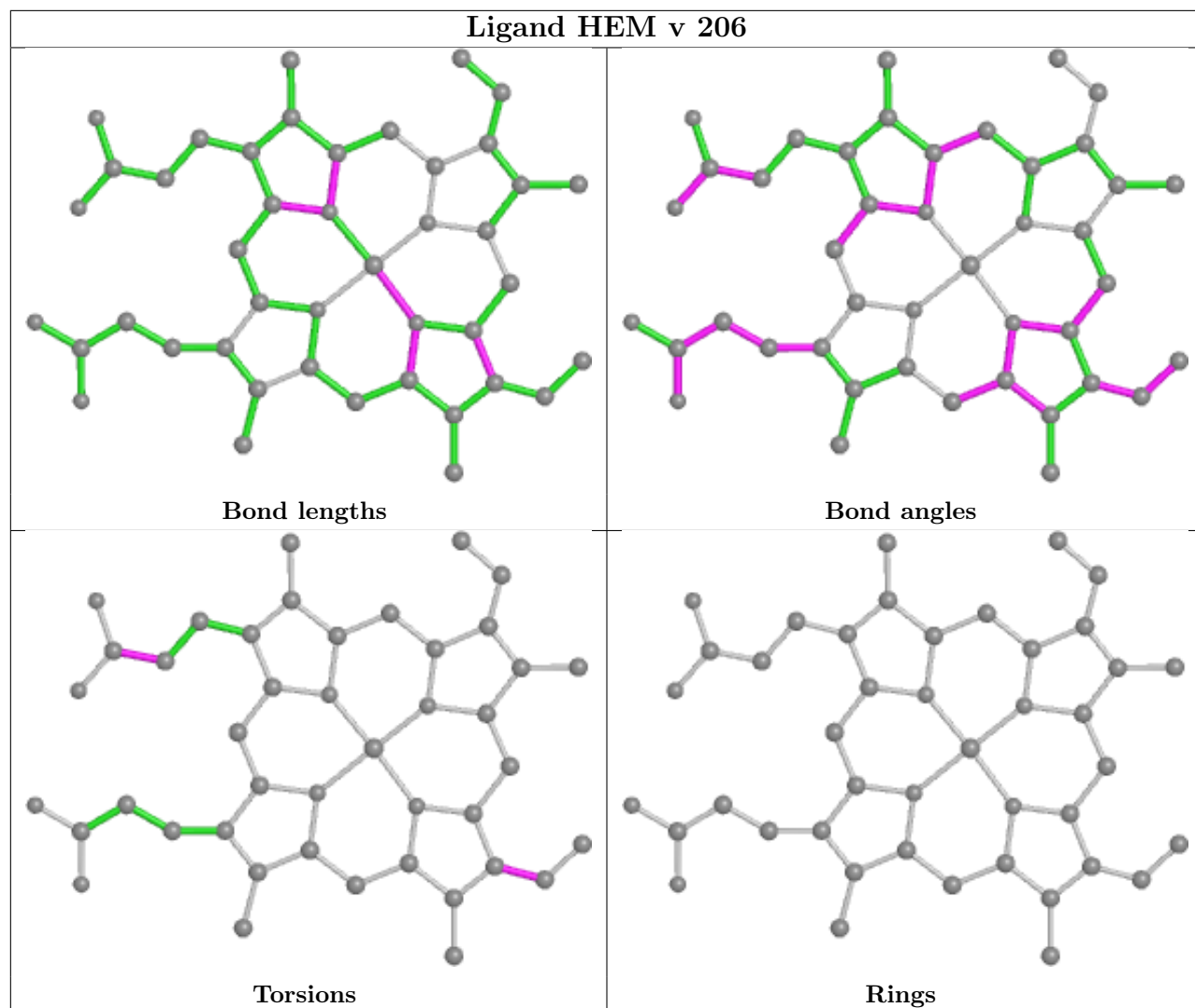


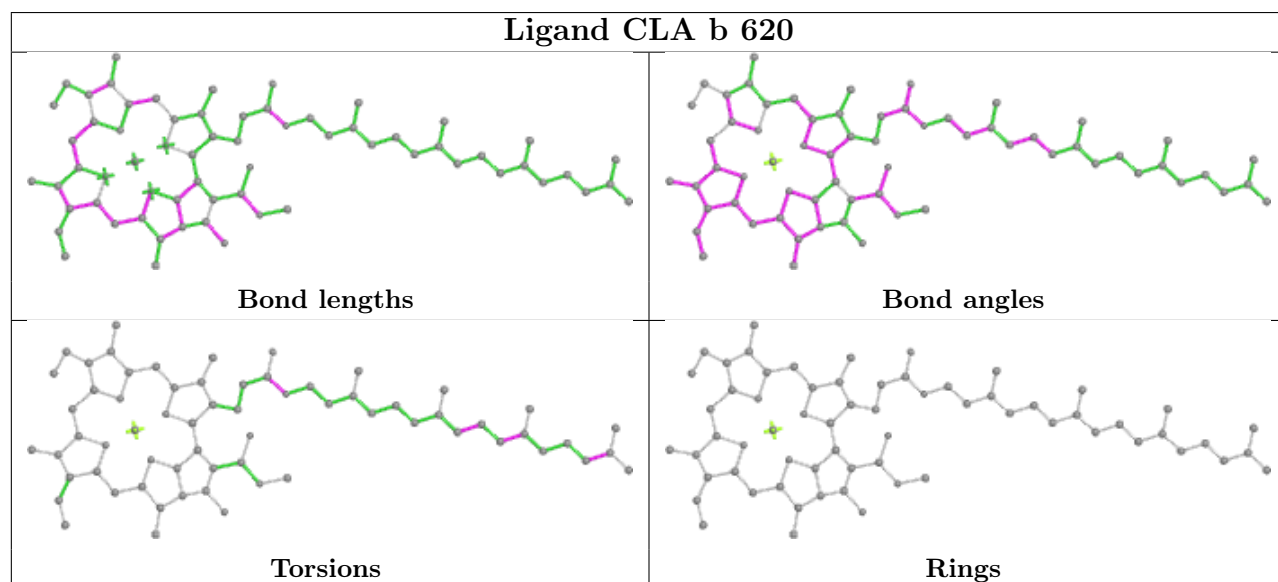
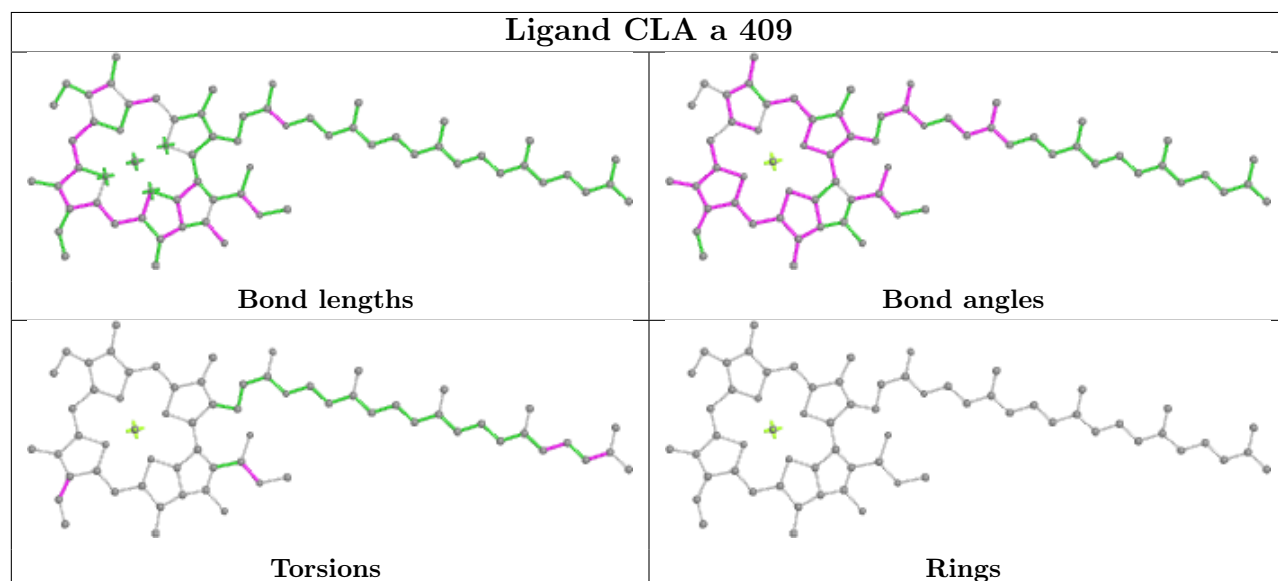
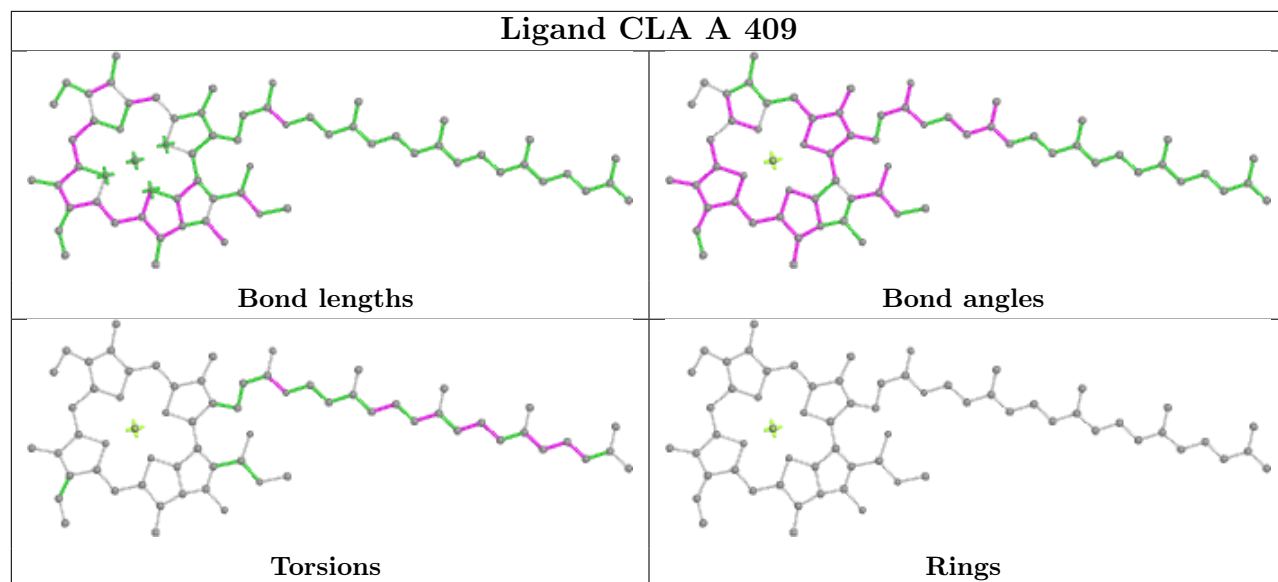


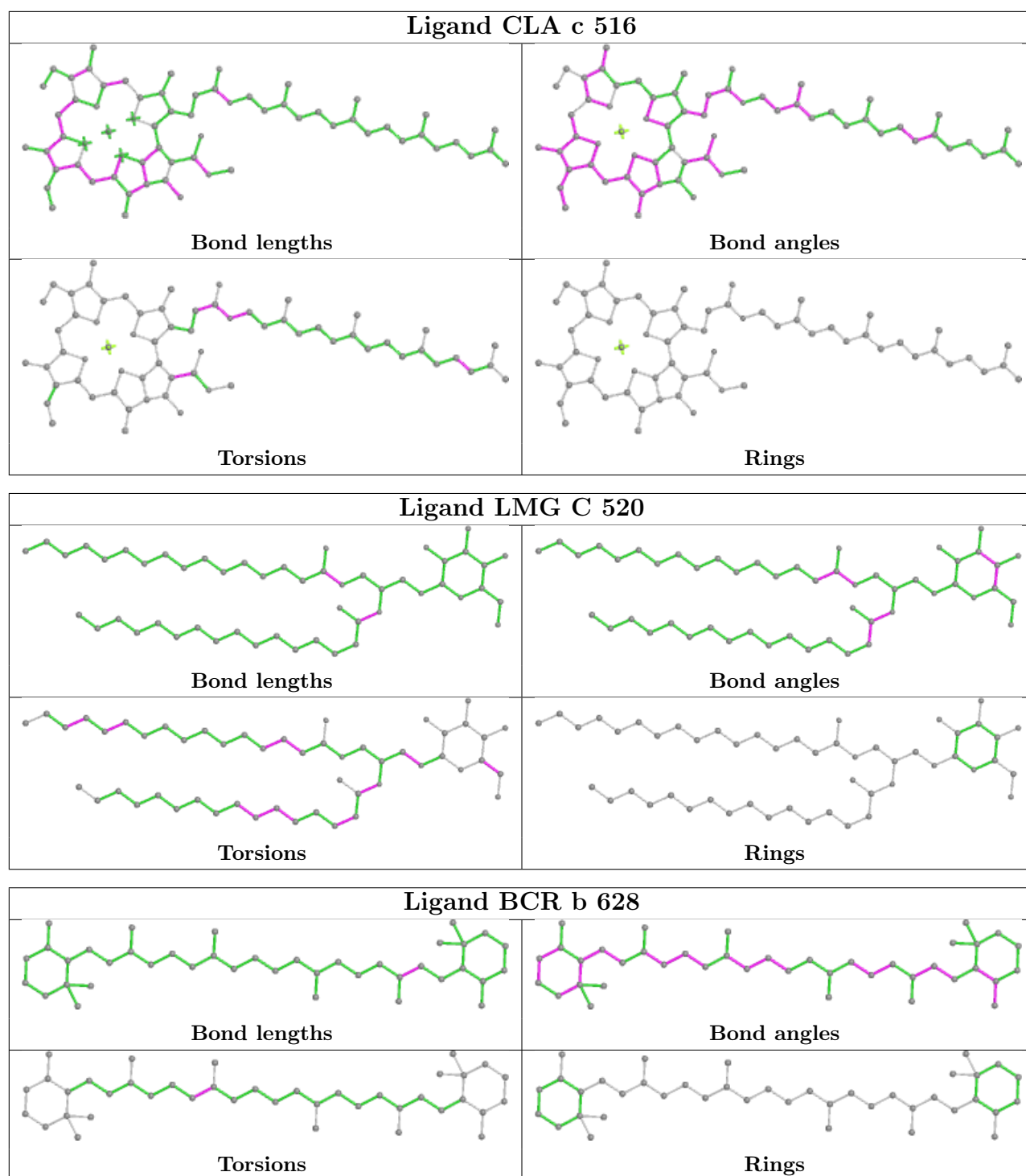


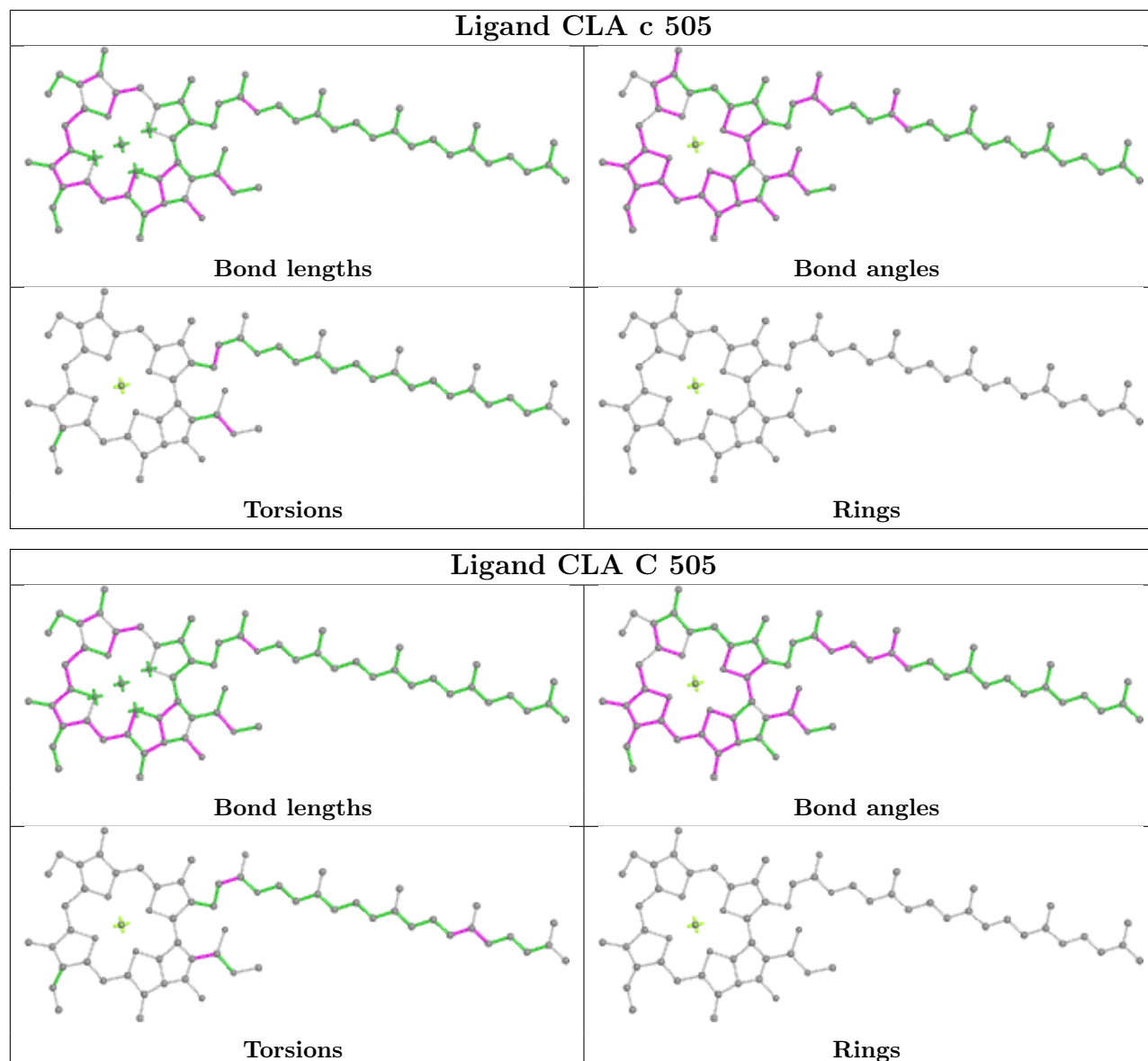




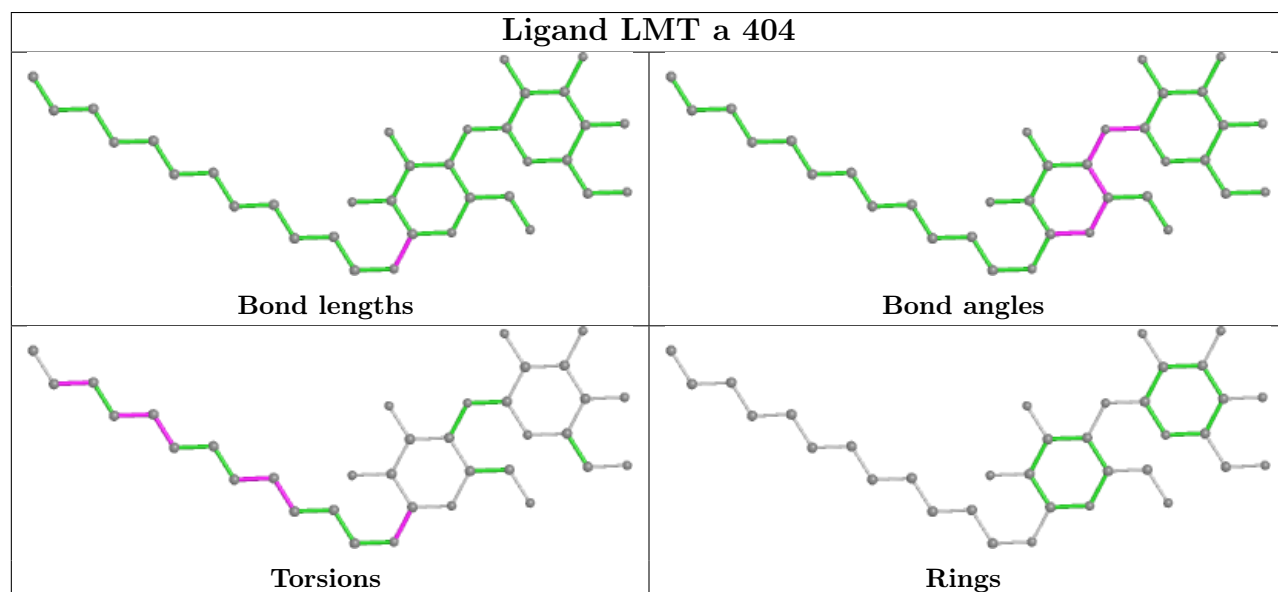
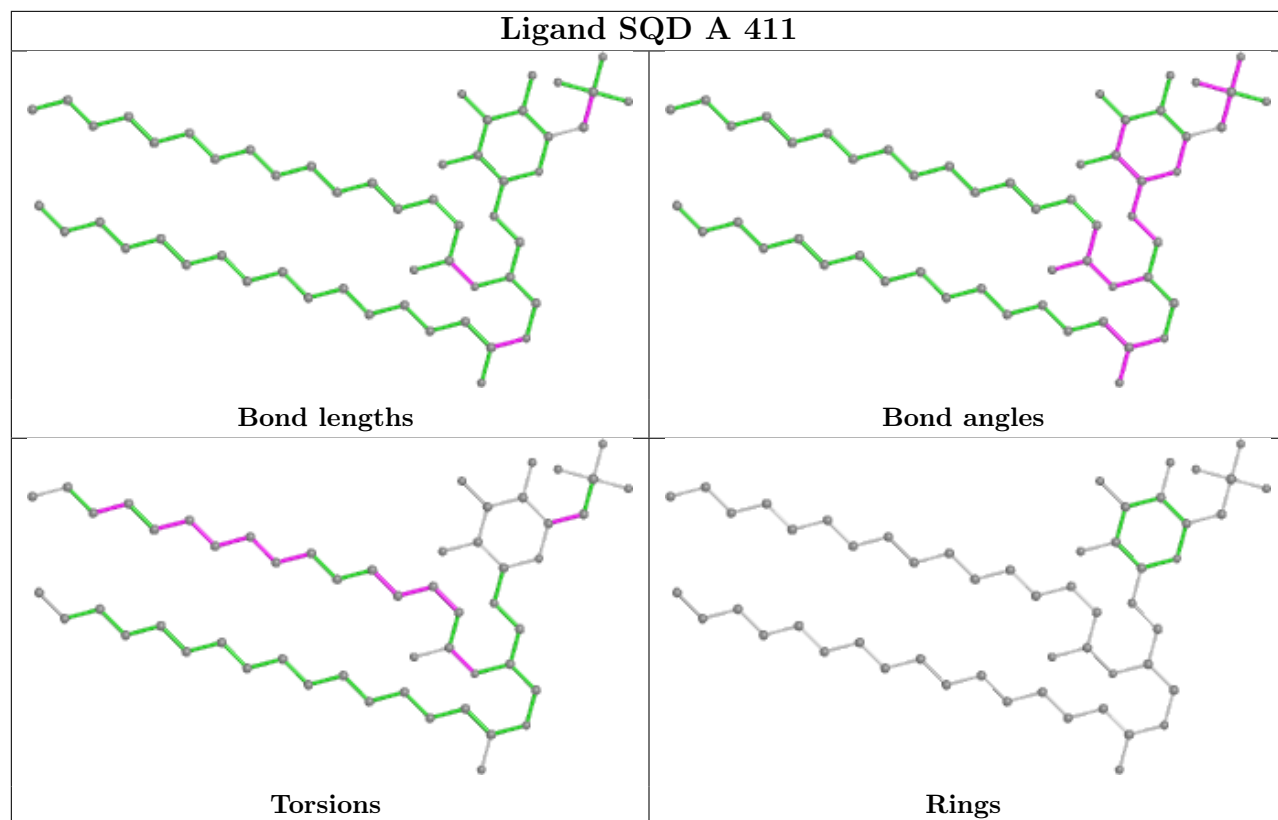


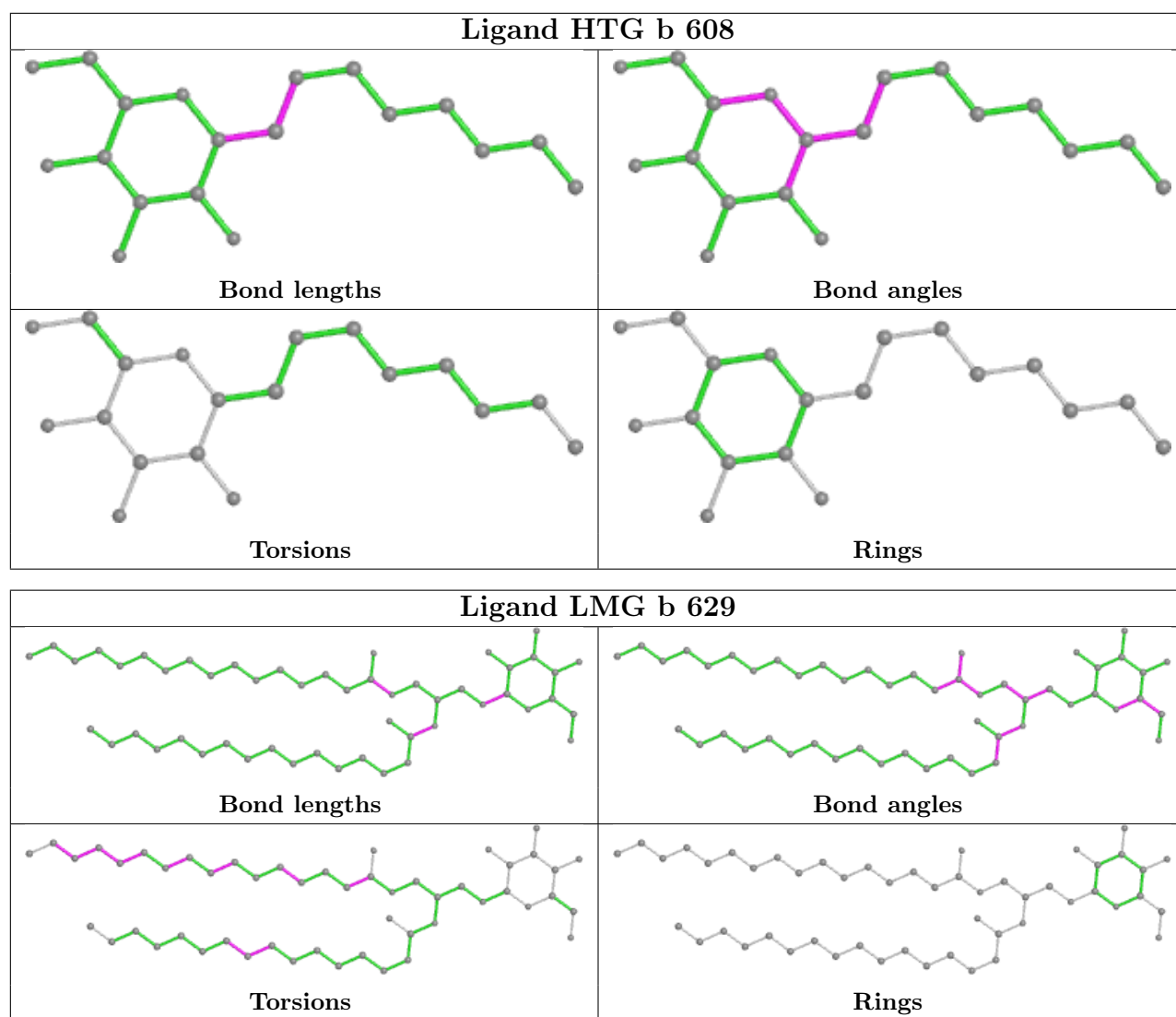












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.25	9 (2%) 54 52	37, 49, 79, 117	0
1	a	334/344 (97%)	0.27	12 (3%) 42 42	37, 50, 87, 160	0
2	B	504/505 (99%)	0.20	24 (4%) 30 29	39, 54, 93, 141	0
2	b	503/505 (99%)	0.37	41 (8%) 11 10	41, 54, 99, 194	0
3	C	451/455 (99%)	0.22	33 (7%) 15 13	42, 63, 87, 140	0
3	c	455/455 (100%)	0.23	36 (7%) 12 11	46, 66, 87, 139	0
4	D	341/342 (99%)	0.24	15 (4%) 34 33	38, 51, 79, 139	0
4	d	341/342 (99%)	0.11	10 (2%) 51 50	39, 52, 79, 122	0
5	E	81/84 (96%)	2.26	37 (45%) 0 0	58, 79, 113, 169	0
5	e	81/84 (96%)	0.38	10 (12%) 4 3	58, 80, 131, 187	0
6	F	34/44 (77%)	1.07	8 (23%) 0 0	59, 70, 111, 118	0
6	f	32/44 (72%)	-0.01	1 (3%) 49 47	57, 69, 132, 154	0
7	H	65/65 (100%)	-0.06	5 (7%) 13 12	52, 65, 86, 160	0
7	h	65/65 (100%)	0.53	8 (12%) 4 3	54, 67, 85, 172	0
8	I	37/38 (97%)	0.13	4 (10%) 5 5	53, 67, 127, 178	0
8	i	37/38 (97%)	0.16	5 (13%) 3 2	49, 64, 131, 156	0
9	J	38/39 (97%)	1.17	8 (21%) 1 0	58, 76, 160, 184	0
9	j	39/39 (100%)	0.28	3 (7%) 13 12	59, 71, 147, 178	0
10	K	37/37 (100%)	0.41	4 (10%) 5 5	65, 77, 94, 113	0
10	k	37/37 (100%)	0.17	2 (5%) 25 24	65, 76, 98, 113	0
11	L	37/37 (100%)	1.17	12 (32%) 0 0	39, 44, 98, 137	0
11	l	37/37 (100%)	1.28	14 (37%) 0 0	40, 46, 98, 140	0
12	M	33/36 (91%)	1.85	16 (48%) 0 0	39, 46, 80, 122	0
12	m	33/36 (91%)	1.74	16 (48%) 0 0	39, 48, 87, 122	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/244 (99%)	0.13	9 (3%) 41 41	41, 59, 100, 159	0
13	o	243/244 (99%)	0.33	26 (10%) 6 5	43, 63, 115, 176	0
14	T	29/32 (90%)	1.09	7 (24%) 0 0	39, 45, 78, 136	0
14	t	29/32 (90%)	1.18	8 (27%) 0 0	39, 45, 71, 137	0
15	U	97/104 (93%)	-0.28	0 100 100	46, 59, 89, 121	0
15	u	97/104 (93%)	-0.37	0 100 100	47, 61, 81, 129	0
16	V	137/137 (100%)	-0.23	0 100 100	46, 59, 83, 119	0
16	v	137/137 (100%)	-0.05	3 (2%) 62 60	48, 69, 98, 139	0
17	Y	29/30 (96%)	4.06	17 (58%) 0 0	81, 91, 187, 209	0
17	y	29/30 (96%)	0.64	5 (17%) 1 1	82, 96, 146, 162	0
18	X	39/40 (97%)	1.34	15 (38%) 0 0	62, 73, 120, 151	0
18	x	38/40 (95%)	0.81	7 (18%) 1 1	63, 72, 133, 157	0
19	Z	62/62 (100%)	2.37	31 (50%) 0 0	78, 93, 132, 152	0
19	z	62/62 (100%)	2.22	28 (45%) 0 0	83, 97, 151, 188	0
20	R	18/34 (52%)	7.41	18 (100%) 0 0	96, 143, 171, 174	0
All	All	5275/5384 (97%)	0.39	507 (9%) 8 7	37, 59, 107, 209	0

The worst 5 of 507 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	Y	18	VAL	23.2
17	Y	19	ILE	12.6
20	R	8	VAL	12.3
20	R	18	TRP	11.5
17	Y	20	ALA	10.8

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	0.91	0.30	40,51,58,129	0
8	FME	i	1	10/11	0.93	0.17	45,62,71,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
14	FME	t	1	10/11	0.93	0.29	33,45,52,103	0
12	FME	m	1	10/11	0.95	0.27	37,59,100,111	0
8	FME	I	1	10/11	0.95	0.13	36,59,66,70	0
12	FME	M	1	10/11	0.97	0.24	38,56,95,98	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(Å <sup>2</sup> )	Q<0.9
37	DGD	e	101	62/66	0.28	0.48	89,127,190,192	0
33	UNL	C	527	34/-	0.38	0.33	92,125,135,139	0
29	LMT	E	102	35/35	0.44	0.46	116,153,169,172	0
33	UNL	a	403	30/-	0.46	0.35	77,96,125,131	0
33	UNL	A	418	28/-	0.53	0.28	65,94,113,117	0
37	DGD	D	408	52/66	0.53	0.46	75,107,156,165	0
29	LMT	b	630	25/35	0.53	0.39	80,112,160,160	0
29	LMT	m	102	35/35	0.54	0.38	56,93,121,125	0
33	UNL	j	101	10/-	0.56	0.42	76,91,98,99	0
38	LHG	E	101	42/49	0.56	0.34	73,119,141,142	0
33	UNL	B	633	33/-	0.57	0.30	62,87,128,133	0
29	LMT	C	521	35/35	0.58	0.39	96,134,162,166	0
33	UNL	c	525	32/-	0.58	0.40	85,102,136,143	0
38	LHG	a	420	42/49	0.58	0.33	75,138,182,183	0
36	HTG	D	414	16/19	0.59	0.28	81,137,154,157	0
36	HTG	d	413	16/19	0.59	0.32	72,110,117,122	0
27	SQD	f	102	43/54	0.60	0.31	109,123,162,167	0
29	LMT	a	419	35/35	0.61	0.49	104,129,159,162	0
29	LMT	e	102	35/35	0.62	0.31	86,143,166,167	0
29	LMT	M	102	35/35	0.62	0.31	46,102,124,132	0
29	LMT	m	103	35/35	0.62	0.45	46,103,128,129	0
33	UNL	J	101	10/-	0.64	0.27	61,84,93,93	0
22	CL	v	205	1/1	0.66	0.22	128,128,128,128	0
34	LMG	Z	101	37/55	0.66	0.39	72,131,146,147	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
29	LMT	D	403	35/35	0.67	0.31	75,127,151,153	0
29	LMT	A	414	35/35	0.67	0.34	59,96,114,123	0
36	HTG	B	632	19/19	0.67	0.25	55,118,140,210	0
29	LMT	M	104	35/35	0.68	0.58	56,102,155,159	0
32	PL9	A	417[A]	55/55	0.68	0.31	85,104,120,121	55
32	PL9	A	417[B]	55/55	0.68	0.31	84,104,120,121	55
36	HTG	B	624	19/19	0.69	0.35	78,133,147,176	0
29	LMT	a	404	35/35	0.69	0.38	42,99,122,150	0
34	LMG	C	519	51/55	0.70	0.23	62,99,117,120	0
27	SQD	L	102	54/54	0.70	0.34	54,82,126,138	0
36	HTG	c	524	19/19	0.71	0.44	90,122,133,164	0
36	HTG	C	523	19/19	0.71	0.42	78,117,141,143	0
34	LMG	z	101	39/55	0.71	0.41	77,125,148,160	0
32	PL9	a	416[B]	55/55	0.72	0.31	87,114,123,124	55
33	UNL	i	101	40/-	0.72	0.24	54,88,139,142	0
32	PL9	a	416[A]	55/55	0.72	0.31	87,114,123,124	55
33	UNL	b	633	33/-	0.72	0.24	58,97,147,148	0
27	SQD	B	621	54/54	0.73	0.46	56,82,141,145	0
36	HTG	b	608	19/19	0.73	0.21	55,112,147,160	0
27	SQD	A	413	54/54	0.74	0.27	56,81,130,137	0
33	UNL	m	101	10/-	0.74	0.75	64,66,90,92	0
33	UNL	d	412	36/-	0.75	0.21	69,89,135,139	0
37	DGD	h	102	62/66	0.76	0.20	44,60,79,85	0
36	HTG	b	607	19/19	0.76	0.22	52,88,101,103	0
27	SQD	a	405	54/54	0.76	0.30	40,83,122,127	0
33	UNL	I	101	40/-	0.77	0.25	60,95,150,153	0
29	LMT	t	101	25/35	0.77	0.55	52,86,147,149	0
22	CL	U	201	1/1	0.77	0.31	117,117,117,117	0
28	GOL	A	412	6/6	0.77	0.23	76,86,88,92	0
29	LMT	T	104	25/35	0.77	0.44	43,83,140,150	0
37	DGD	C	517	62/66	0.78	0.21	55,71,102,113	0
28	GOL	v	202	6/6	0.78	0.29	83,96,98,100	0
33	UNL	D	413	40/-	0.78	0.18	63,88,132,140	0
34	LMG	k	101	51/55	0.79	0.24	62,94,123,126	0
36	HTG	b	632	19/19	0.79	0.41	77,138,158,165	0
33	UNL	M	103	10/-	0.79	0.52	48,53,74,76	0
34	LMG	a	415	51/55	0.79	0.21	61,90,100,101	0
36	HTG	B	631	19/19	0.79	0.20	52,105,123,128	0
34	LMG	A	419	51/55	0.80	0.23	57,90,109,115	0
28	GOL	T	101	6/6	0.80	0.34	70,88,93,93	0
34	LMG	C	520	51/55	0.80	0.30	67,122,137,143	0
28	GOL	V	201	6/6	0.80	0.47	81,91,96,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	UNL	d	414	18/-	0.80	0.25	76,84,116,118	0
34	LMG	c	522	51/55	0.80	0.34	59,111,124,132	0
35	CA	F	102	1/1	0.81	0.05	119,119,119,119	0
35	CA	f	103	1/1	0.81	0.07	124,124,124,124	0
36	HTG	B	623	19/19	0.81	0.20	60,79,91,92	0
37	DGD	H	102	62/66	0.81	0.20	41,58,95,103	0
27	SQD	F	101	43/54	0.81	0.37	80,119,134,139	0
36	HTG	b	631	19/19	0.81	0.25	67,83,98,102	0
28	GOL	O	301	6/6	0.81	0.15	74,89,90,93	0
28	GOL	b	606	6/6	0.81	0.22	70,91,98,100	0
27	SQD	A	411	54/54	0.82	0.23	52,94,103,105	0
37	DGD	c	520	62/66	0.82	0.23	47,65,115,133	0
28	GOL	t	103	6/6	0.82	0.29	60,88,99,102	0
28	GOL	V	204	6/6	0.83	0.15	90,103,105,112	0
34	LMG	M	101	51/55	0.83	0.41	41,61,83,89	0
24	CLA	C	513	65/65	0.83	0.39	61,87,117,123	0
24	CLA	C	504	65/65	0.83	0.19	45,67,93,102	0
34	LMG	b	629	51/55	0.83	0.35	40,57,76,83	0
27	SQD	a	414	54/54	0.84	0.25	54,87,114,116	0
33	UNL	X	101	18/-	0.84	0.22	70,77,101,105	0
36	HTG	c	523	19/19	0.84	0.27	91,114,126,129	0
28	GOL	B	629	6/6	0.84	0.23	55,69,74,78	0
24	CLA	b	611	65/65	0.84	0.18	41,57,65,73	0
28	GOL	v	203	6/6	0.84	0.28	96,105,112,124	0
37	DGD	C	518	62/66	0.84	0.19	45,63,82,96	0
28	GOL	T	102	6/6	0.85	0.29	104,114,118,118	0
38	LHG	D	409	49/49	0.85	0.39	39,56,65,72	0
36	HTG	b	602	19/19	0.85	0.19	46,64,75,77	0
26	BCR	H	101	40/40	0.85	0.19	45,64,78,85	0
37	DGD	c	521	62/66	0.86	0.23	51,62,87,100	0
24	CLA	c	517	65/65	0.86	0.33	76,94,106,111	0
34	LMG	d	415	51/55	0.86	0.27	53,70,112,122	0
28	GOL	a	402	6/6	0.86	0.20	93,97,103,103	0
28	GOL	b	601	6/6	0.86	0.20	55,59,64,68	0
24	CLA	C	506	65/65	0.86	0.18	52,75,116,119	0
24	CLA	b	616	65/65	0.87	0.26	31,42,54,62	0
35	CA	b	609	1/1	0.87	0.40	134,134,134,134	0
24	CLA	b	618	65/65	0.87	0.18	45,57,67,77	0
24	CLA	c	507	65/65	0.87	0.20	50,62,75,87	0
36	HTG	V	206	19/19	0.87	0.22	62,103,129,237	0
24	CLA	c	510	65/65	0.87	0.18	52,74,96,102	0
38	LHG	d	408	49/49	0.87	0.31	44,60,70,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
28	GOL	D	402	6/6	0.88	0.29	55,64,73,77	0
26	BCR	C	514	40/40	0.88	0.21	58,81,93,94	0
24	CLA	b	615	65/65	0.88	0.18	41,54,100,112	0
34	LMG	D	415	51/55	0.88	0.19	51,73,119,129	0
38	LHG	D	411	49/49	0.88	0.23	51,71,118,127	0
24	CLA	c	512	65/65	0.88	0.16	44,59,125,141	0
28	GOL	o	301	6/6	0.88	0.23	84,90,97,98	0
38	LHG	b	634	49/49	0.88	0.32	39,54,68,82	0
24	CLA	B	607	65/65	0.88	0.17	40,54,94,98	0
24	CLA	c	509	65/65	0.89	0.14	43,56,75,78	0
24	CLA	B	603	65/65	0.89	0.15	40,53,62,66	0
24	CLA	B	602	65/65	0.89	0.23	57,74,114,132	0
24	CLA	C	511	65/65	0.89	0.20	56,74,89,101	0
24	CLA	B	614	65/65	0.89	0.30	31,45,67,82	0
24	CLA	b	624	65/65	0.89	0.14	42,56,74,78	0
24	CLA	b	610	65/65	0.89	0.34	57,79,127,133	0
24	CLA	c	508	65/65	0.89	0.18	49,62,85,99	0
28	GOL	C	524	6/6	0.89	0.23	86,89,104,108	0
37	DGD	c	519	62/66	0.89	0.16	41,62,97,101	0
38	LHG	d	410	49/49	0.89	0.24	42,65,113,119	0
28	GOL	F	103	6/6	0.90	0.23	88,95,100,104	0
24	CLA	c	515	65/65	0.90	0.17	51,73,89,101	0
24	CLA	C	503	65/65	0.90	0.19	50,62,77,82	0
24	CLA	B	615	65/65	0.90	0.30	34,46,97,100	0
36	HTG	C	522	19/19	0.90	0.22	91,102,119,121	0
24	CLA	C	501	65/65	0.90	0.15	50,62,87,97	0
26	BCR	c	526	40/40	0.90	0.21	72,87,94,96	0
26	BCR	d	406	40/40	0.90	0.23	48,61,83,91	0
32	PL9	D	407[A]	55/55	0.90	0.38	34,45,52,64	55
32	PL9	D	407[B]	55/55	0.90	0.38	34,45,53,67	55
28	GOL	a	421	6/6	0.90	0.26	88,100,106,106	0
24	CLA	b	620	65/65	0.90	0.18	35,49,59,65	0
24	CLA	c	511	65/65	0.90	0.16	53,68,79,83	0
28	GOL	c	502	6/6	0.90	0.27	85,111,119,127	0
24	CLA	C	510	65/65	0.90	0.14	55,71,84,92	0
38	LHG	d	409	49/49	0.90	0.34	35,51,69,90	0
36	HTG	B	622	19/19	0.90	0.23	53,65,88,92	0
26	BCR	b	627	40/40	0.91	0.29	37,52,68,78	0
24	CLA	C	508	65/65	0.91	0.14	46,66,133,146	0
28	GOL	V	203	6/6	0.91	0.18	68,76,82,85	0
32	PL9	d	407[A]	55/55	0.91	0.34	31,46,53,59	55
32	PL9	d	407[B]	55/55	0.91	0.34	31,45,55,63	55

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
38	LHG	L	101	49/49	0.91	0.38	39,52,64,67	0
24	CLA	b	625	65/65	0.91	0.15	40,61,106,112	0
28	GOL	v	201	6/6	0.91	0.16	74,84,87,96	0
24	CLA	B	612	65/65	0.91	0.25	35,46,54,63	0
26	BCR	D	406	40/40	0.91	0.15	52,65,99,107	0
24	CLA	b	623	65/65	0.91	0.22	31,47,93,106	0
24	CLA	C	507	65/65	0.92	0.17	51,71,84,91	0
24	CLA	b	622	65/65	0.92	0.22	36,49,62,68	0
24	CLA	C	512	65/65	0.92	0.20	62,81,95,102	0
33	UNL	D	412	17/-	0.92	0.15	46,71,89,96	0
35	CA	B	601	1/1	0.92	0.36	135,135,135,135	0
28	GOL	b	603	6/6	0.92	0.30	60,73,78,87	0
24	CLA	B	610	65/65	0.92	0.15	38,58,67,75	0
38	LHG	D	410	49/49	0.92	0.33	34,49,75,92	0
26	BCR	b	626	40/40	0.92	0.29	36,49,59,64	0
24	CLA	b	617	65/65	0.92	0.12	43,57,64,73	0
24	CLA	c	514	65/65	0.92	0.14	47,64,74,80	0
24	CLA	B	608	65/65	0.92	0.32	32,45,58,70	0
37	DGD	C	516	62/66	0.92	0.20	40,58,89,91	0
26	BCR	y	101	40/40	0.92	0.15	58,70,81,83	0
28	GOL	B	626	6/6	0.92	0.24	56,67,87,100	0
33	UNL	d	411	17/-	0.92	0.17	57,77,101,101	0
24	CLA	d	403	65/65	0.93	0.26	35,44,53,57	0
24	CLA	d	405	65/65	0.93	0.14	49,64,115,122	0
24	CLA	b	619	65/65	0.93	0.14	41,58,66,77	0
28	GOL	b	605	6/6	0.93	0.20	66,82,107,110	0
24	CLA	B	613	65/65	0.93	0.16	32,47,57,60	0
24	CLA	c	513	65/65	0.93	0.17	53,68,85,94	0
26	BCR	K	101	40/40	0.93	0.14	58,71,80,87	0
26	BCR	Y	101	40/40	0.93	0.15	62,72,92,98	0
24	CLA	D	405	65/65	0.93	0.17	47,62,111,116	0
28	GOL	V	202	6/6	0.93	0.19	54,65,76,78	0
24	CLA	B	616	65/65	0.93	0.16	40,56,68,77	0
24	CLA	c	516	65/65	0.93	0.24	63,79,91,99	0
24	CLA	C	509	65/65	0.93	0.16	49,72,86,92	0
24	CLA	b	612	65/65	0.94	0.13	45,55,63,71	0
24	CLA	c	505	65/65	0.94	0.14	50,67,75,77	0
28	GOL	b	604	6/6	0.94	0.33	62,73,80,84	0
24	CLA	c	506	65/65	0.94	0.15	47,61,79,88	0
25	PHO	A	408	64/64	0.94	0.25	28,44,52,61	0
25	PHO	D	401[A]	64/64	0.94	0.18	41,51,60,63	64
25	PHO	D	401[B]	64/64	0.94	0.18	40,50,59,64	64

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	PHO	d	402[A]	64/64	0.94	0.20	39,50,56,59	64
25	PHO	d	402[B]	64/64	0.94	0.20	40,50,56,60	64
26	BCR	B	619	40/40	0.94	0.36	37,51,64,71	0
24	CLA	B	604	65/65	0.94	0.16	43,55,63,68	0
28	GOL	v	204	6/6	0.94	0.15	59,64,71,78	0
24	CLA	C	502	65/65	0.94	0.14	45,66,73,81	0
24	CLA	B	605	65/65	0.94	0.18	31,45,75,79	0
24	CLA	A	405	65/65	0.94	0.25	32,41,52,62	0
35	CA	c	504	1/1	0.94	0.06	84,84,84,84	0
26	BCR	T	103	40/40	0.94	0.27	32,51,66,72	0
24	CLA	C	505	65/65	0.94	0.13	48,60,75,91	0
23	BCT	A	404[A]	4/4	0.94	0.17	72,74,78,88	4
24	CLA	b	621	65/65	0.94	0.13	35,50,59,63	0
26	BCR	c	518	40/40	0.94	0.14	49,63,73,78	0
24	CLA	a	409	65/65	0.94	0.26	34,44,56,71	0
23	BCT	A	404[B]	4/4	0.94	0.17	71,72,78,90	4
26	BCR	h	101	40/40	0.94	0.17	46,66,76,77	0
28	GOL	a	401	6/6	0.94	0.26	55,63,75,82	0
26	BCR	k	102	40/40	0.94	0.17	54,75,85,87	0
24	CLA	B	617	65/65	0.94	0.21	45,62,136,139	0
40	MG	j	102	1/1	0.94	0.13	70,70,70,70	0
26	BCR	A	410	40/40	0.95	0.20	37,48,57,65	0
26	BCR	B	618	40/40	0.95	0.41	36,49,59,62	0
28	GOL	B	627	6/6	0.95	0.22	71,86,88,88	0
28	GOL	B	628	6/6	0.95	0.17	56,69,75,78	0
24	CLA	A	409	65/65	0.95	0.16	40,58,123,132	0
28	GOL	B	634	6/6	0.95	0.19	56,58,65,66	0
26	BCR	B	620	40/40	0.95	0.20	39,53,64,79	0
24	CLA	B	609	65/65	0.95	0.15	42,53,62,66	0
26	BCR	t	102	40/40	0.95	0.38	36,53,75,77	0
26	BCR	C	515	40/40	0.95	0.16	47,63,75,80	0
24	CLA	B	606	65/65	0.95	0.16	36,47,58,61	0
24	CLA	b	613	65/65	0.95	0.14	32,48,75,84	0
24	CLA	b	614	65/65	0.95	0.14	36,46,60,70	0
24	CLA	B	611	65/65	0.95	0.18	42,56,67,71	0
24	CLA	A	406	65/65	0.95	0.29	31,42,51,53	0
24	CLA	a	410	65/65	0.95	0.24	38,51,113,120	0
24	CLA	a	412	65/65	0.95	0.18	40,59,116,123	0
26	BCR	b	628	40/40	0.95	0.15	41,59,69,72	0
24	CLA	A	407	65/65	0.96	0.16	33,47,101,110	0
23	BCT	d	401[A]	4/4	0.96	0.20	86,88,90,94	4
28	GOL	B	630	6/6	0.96	0.25	59,95,102,108	0

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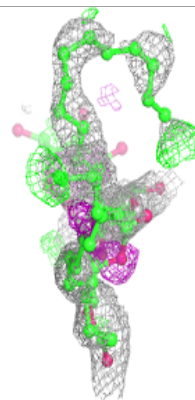
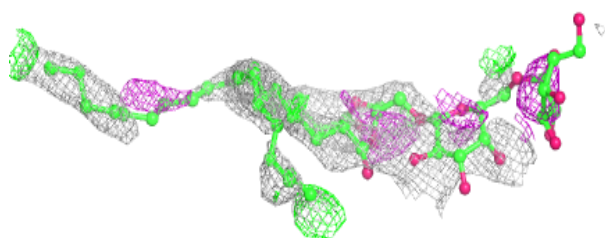
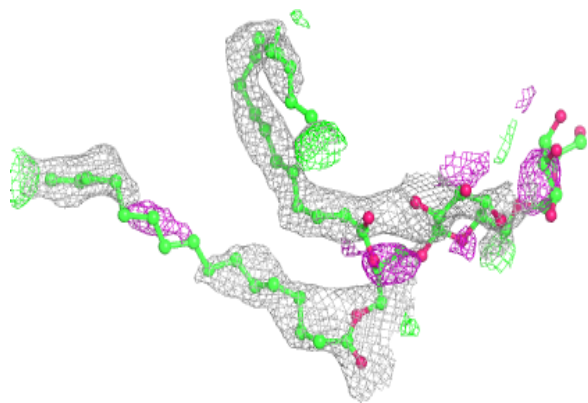
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
26	BCR	a	413	40/40	0.96	0.20	34,47,58,61	0
24	CLA	d	404	65/65	0.96	0.22	32,45,58,73	0
25	PHO	a	411	64/64	0.96	0.28	38,45,54,63	0
35	CA	O	302	1/1	0.96	0.13	100,100,100,100	0
39	HEM	E	103	43/43	0.96	0.28	63,82,103,115	0
23	BCT	d	401[B]	4/4	0.96	0.20	85,85,88,93	4
28	GOL	B	625	6/6	0.97	0.12	55,65,74,83	0
22	CL	A	403[A]	1/1	0.97	0.12	47,47,47,47	1
35	CA	o	302	1/1	0.97	0.07	97,97,97,97	0
28	GOL	c	501	6/6	0.97	0.17	47,52,56,58	0
24	CLA	D	404	65/65	0.97	0.21	30,42,61,69	0
22	CL	A	403[B]	1/1	0.97	0.12	45,45,45,45	1
39	HEM	V	205	43/43	0.97	0.14	44,53,65,67	0
39	HEM	f	101	43/43	0.97	0.13	66,90,130,144	0
40	MG	J	102	1/1	0.97	0.09	71,71,71,71	0
28	GOL	C	525	6/6	0.97	0.22	52,54,59,60	0
30	OEX	a	417[A]	10/10	0.98	0.13	47,51,57,61	10
35	CA	C	526	1/1	0.98	0.24	87,87,87,87	0
31	OEY	a	418[B]	10/11	0.98	0.13	47,51,57,60	10
39	HEM	v	206	43/43	0.98	0.11	51,65,74,75	0
22	CL	a	408[A]	1/1	0.98	0.14	49,49,49,49	1
22	CL	a	408[B]	1/1	0.98	0.14	49,49,49,49	1
22	CL	A	402[A]	1/1	0.99	0.25	41,41,41,41	1
30	OEX	A	415[A]	10/10	0.99	0.12	47,57,59,70	10
22	CL	A	402[B]	1/1	0.99	0.25	41,41,41,41	1
31	OEY	A	416[B]	10/11	0.99	0.12	43,52,60,68	10
21	FE2	A	401[A]	1/1	0.99	0.10	66,66,66,66	1
21	FE2	A	401[B]	1/1	0.99	0.10	65,65,65,65	1
21	FE2	a	406[A]	1/1	0.99	0.11	62,62,62,62	1
22	CL	a	407[A]	1/1	0.99	0.16	43,43,43,43	1
35	CA	c	503	1/1	0.99	0.21	77,77,77,77	0
22	CL	a	407[B]	1/1	0.99	0.16	45,45,45,45	1
21	FE2	a	406[B]	1/1	0.99	0.11	62,62,62,62	1

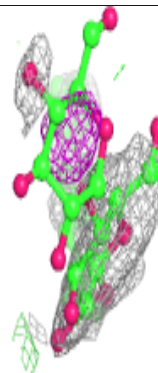
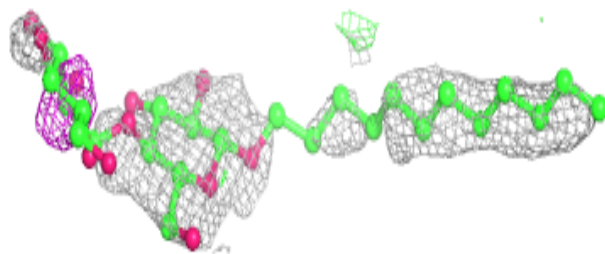
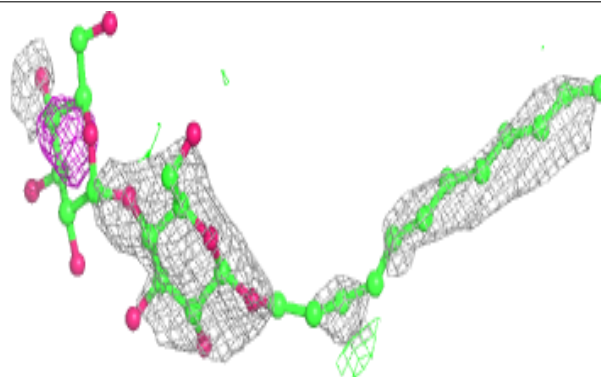
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around DGD e 101:**

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

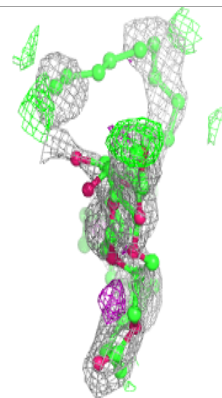
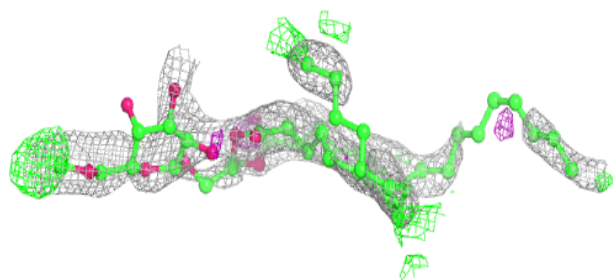
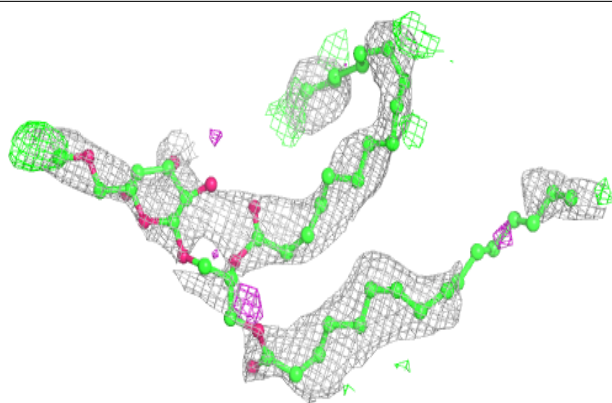
**Electron density around LMT E 102:**

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

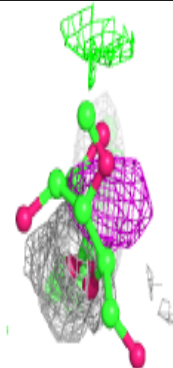
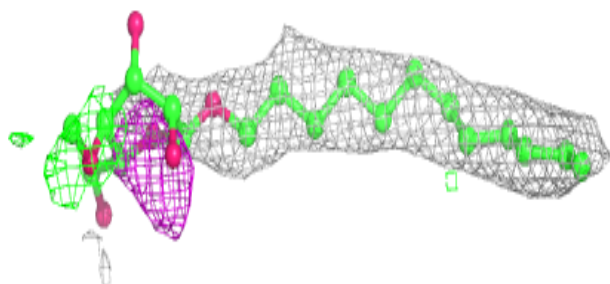
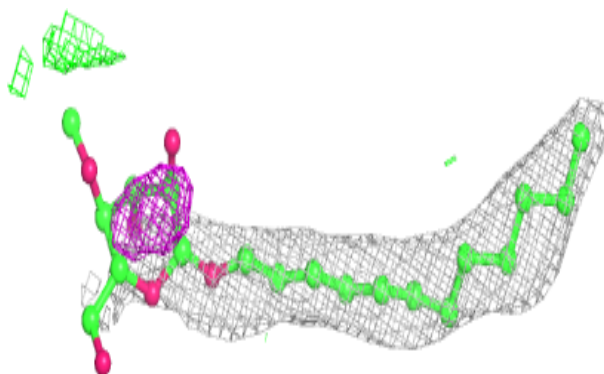


**Electron density around DGD D 408:**

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

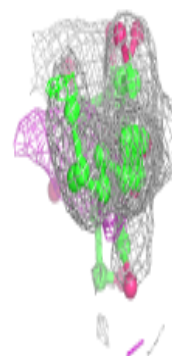
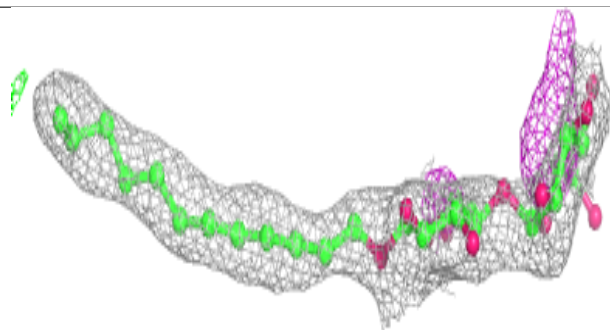
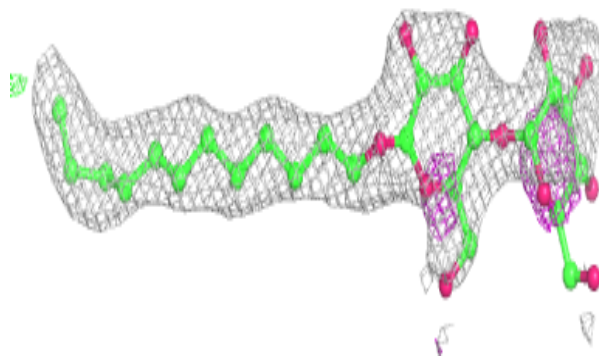
**Electron density around LMT b 630:**

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

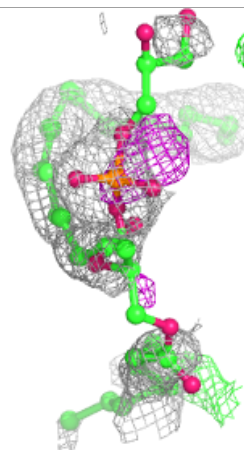
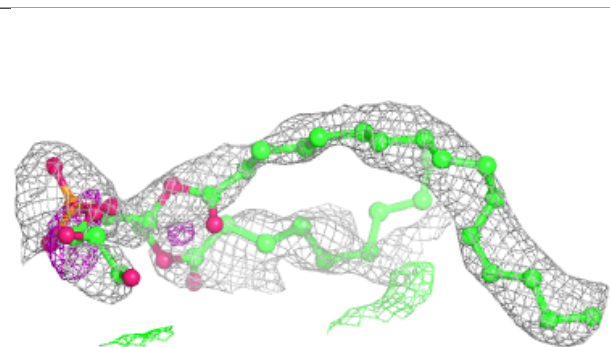
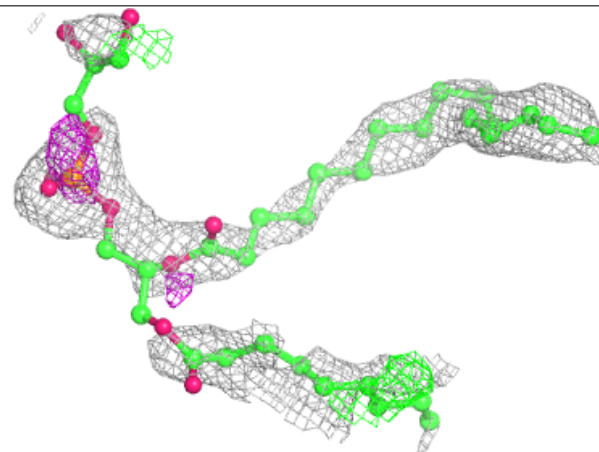


**Electron density around LMT m 102:**

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

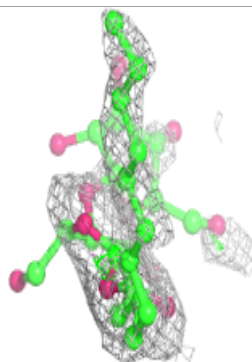
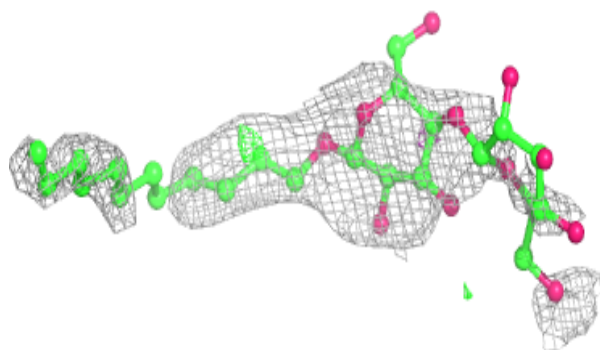
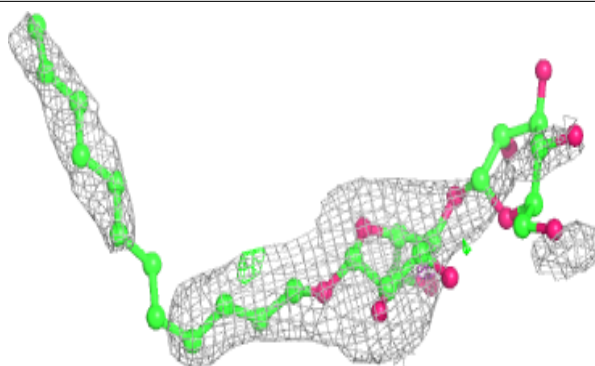
**Electron density around LHG E 101:**

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

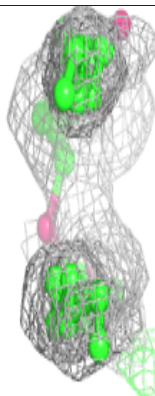
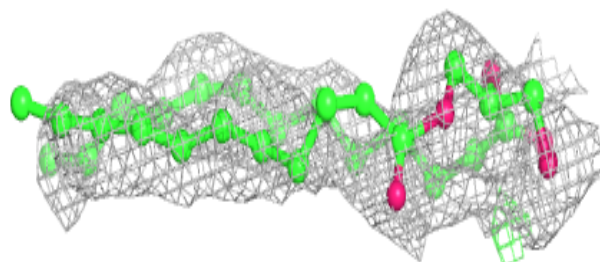
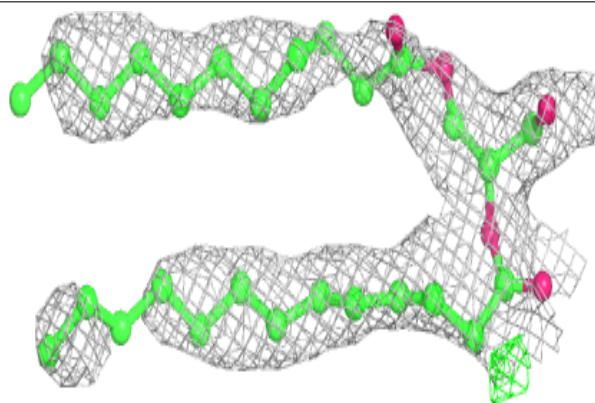


**Electron density around LMT C 521:**

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

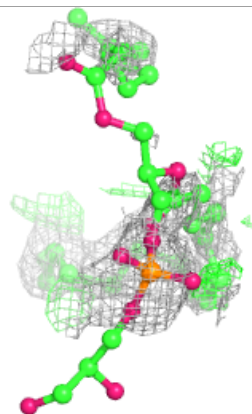
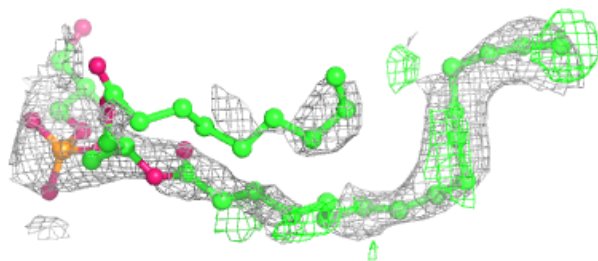
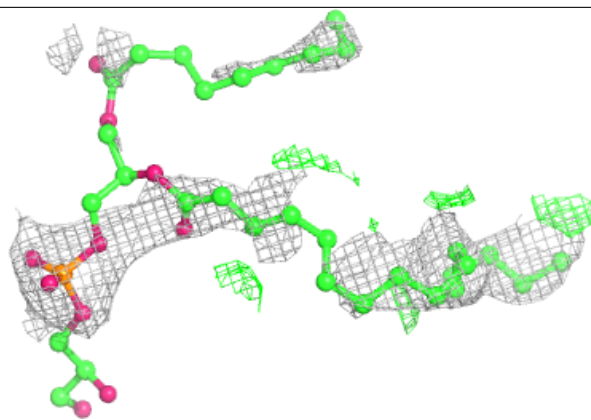
**Electron density around UNL c 525:**

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

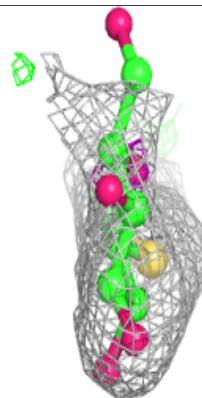
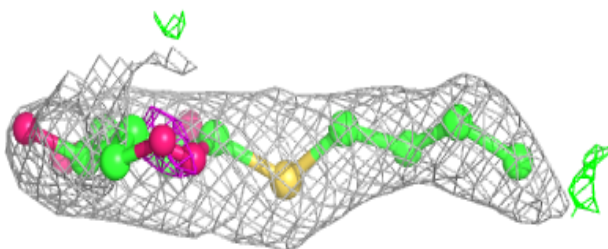
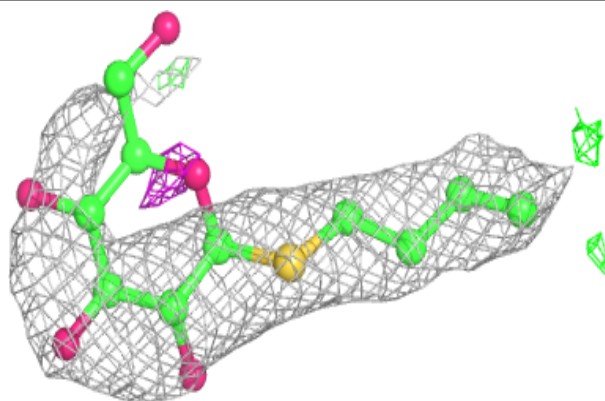


**Electron density around LHG a 420:**

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

**Electron density around HTG D 414:**

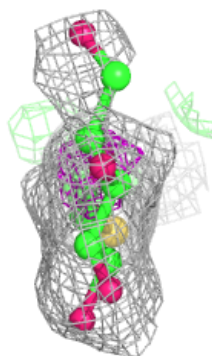
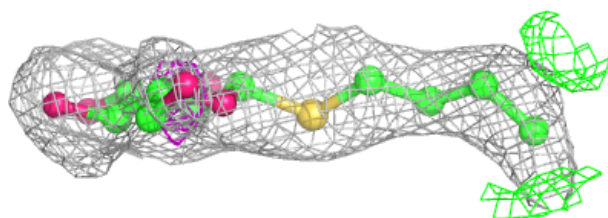
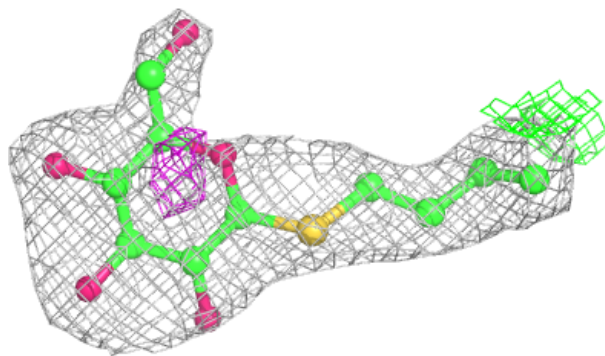
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



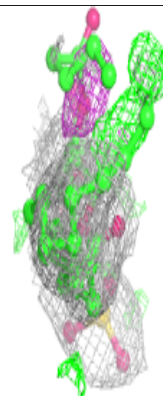
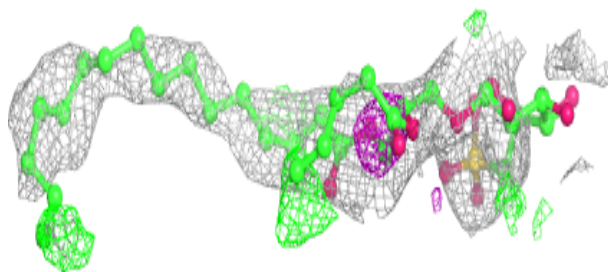
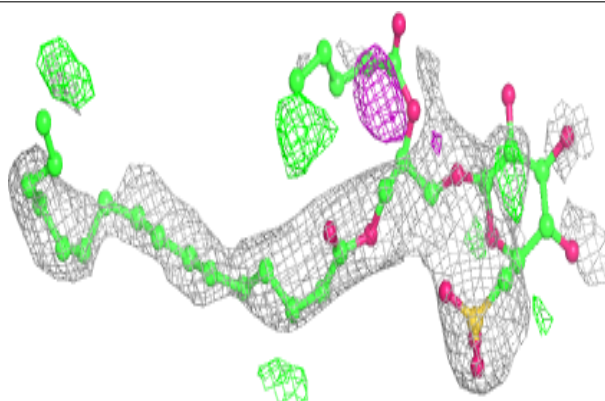


**Electron density around HTG d 413:**

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

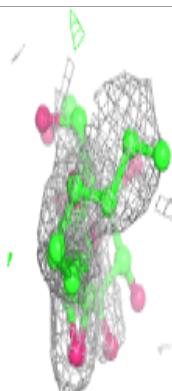
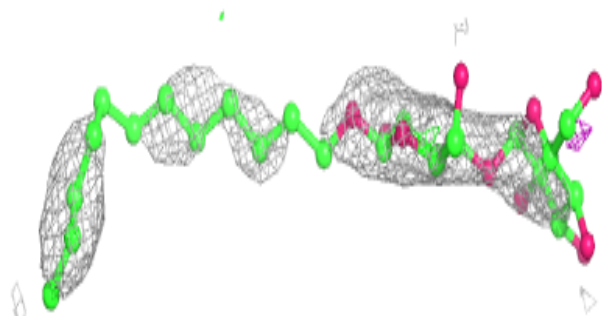
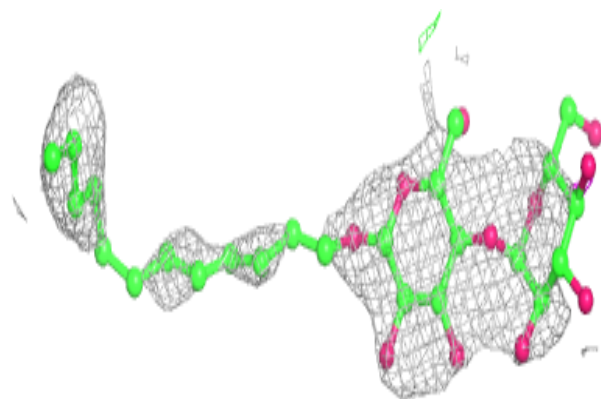
**Electron density around SQD f 102:**

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

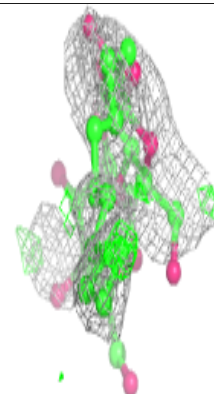
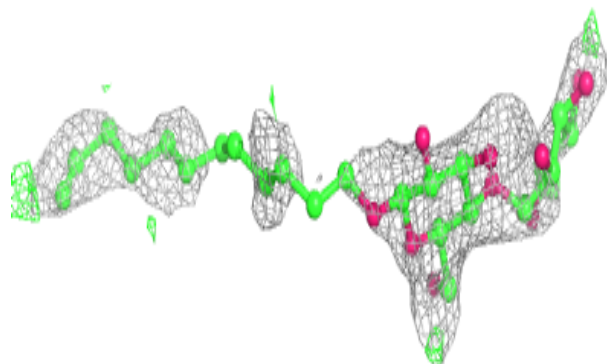
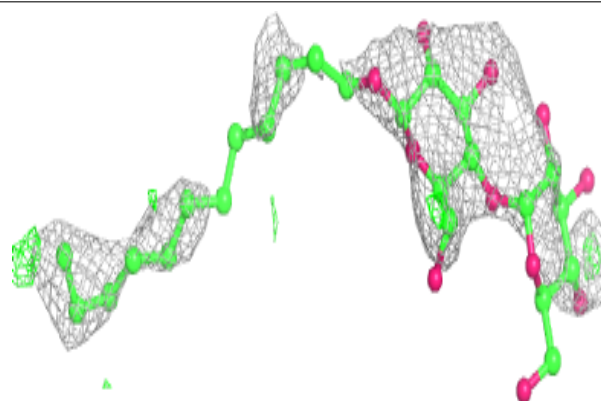


**Electron density around LMT a 419:**

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

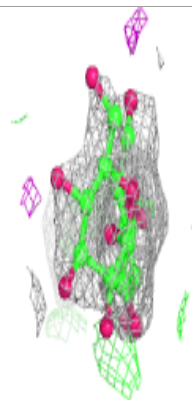
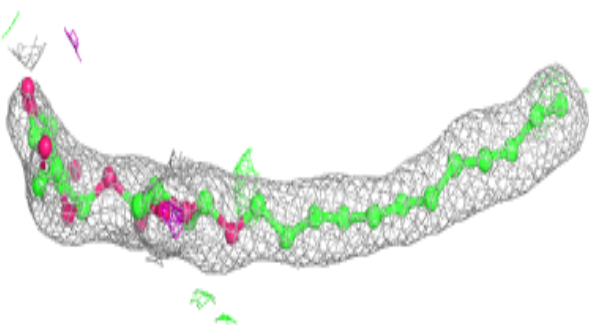
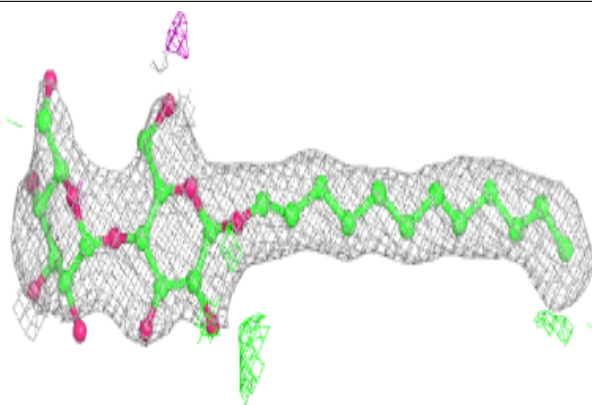
**Electron density around LMT e 102:**

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

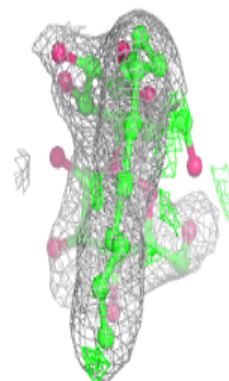
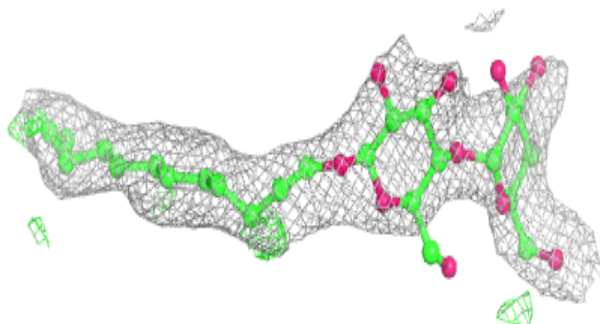
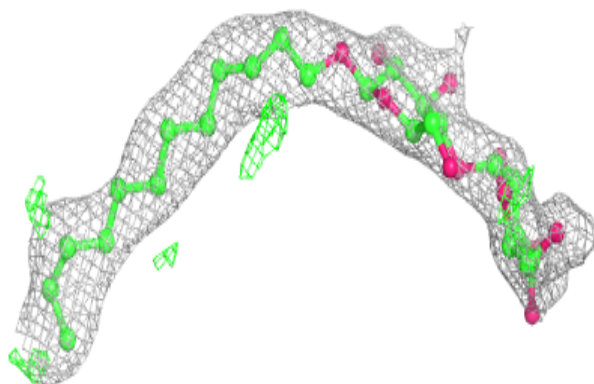


**Electron density around LMT M 102:**

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

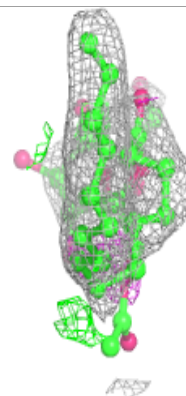
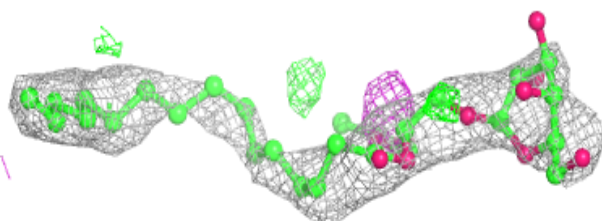
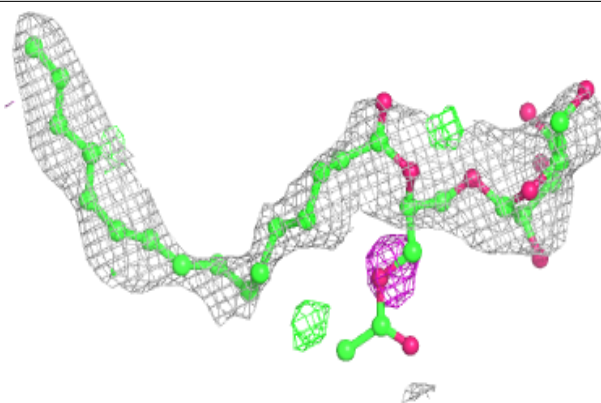
**Electron density around LMT m 103:**

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

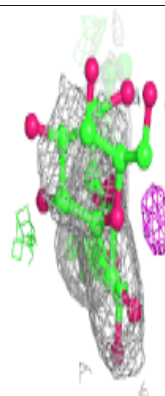
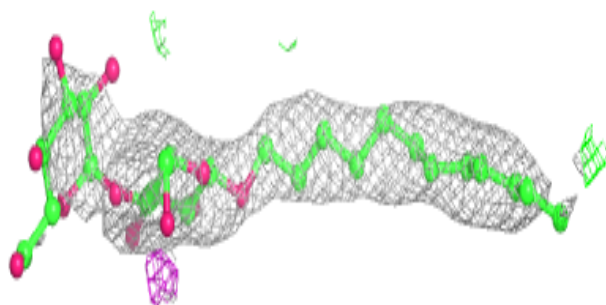
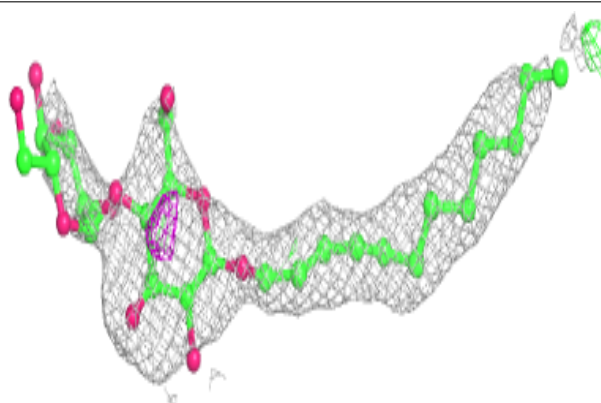


**Electron density around LMG Z 101:**

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

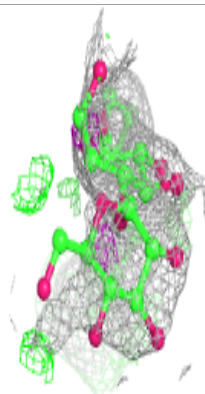
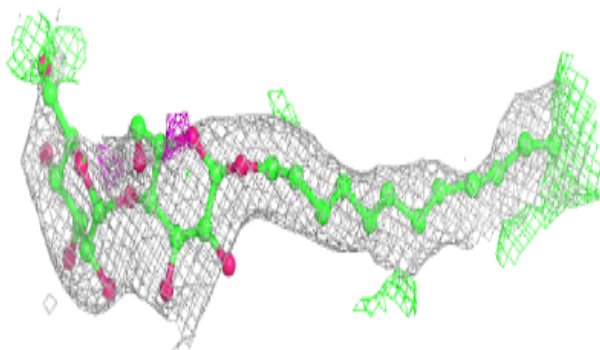
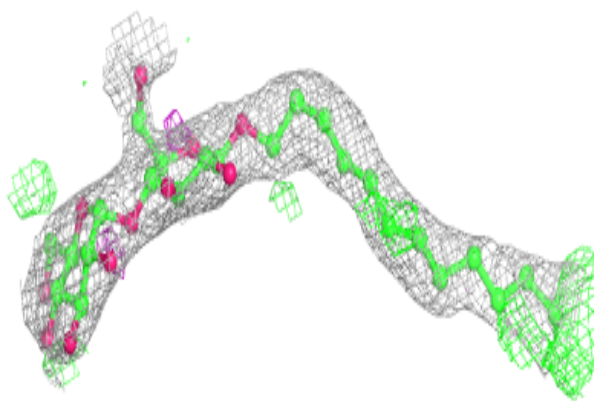
**Electron density around LMT D 403:**

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

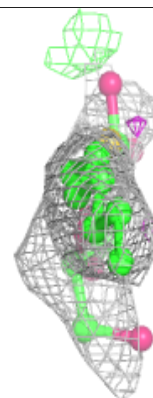
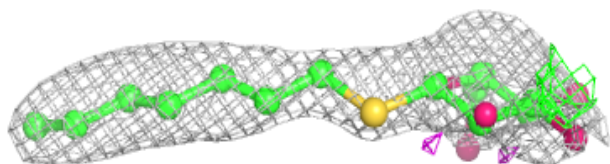
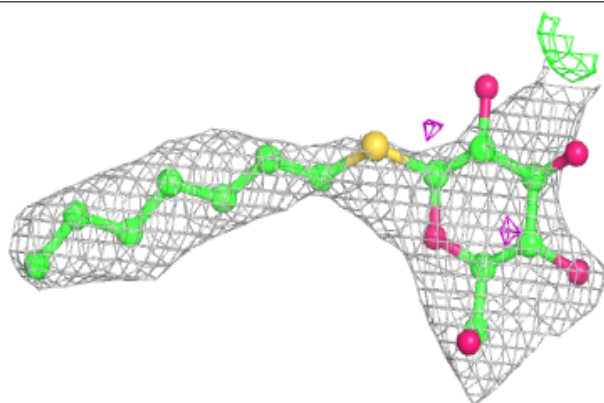


**Electron density around LMT A 414:**

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

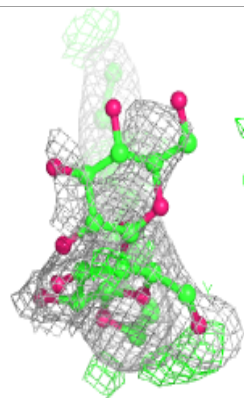
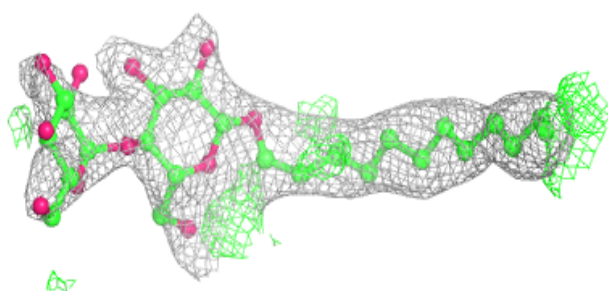
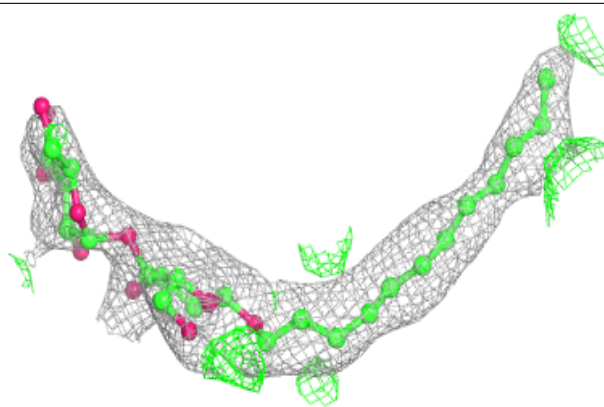
**Electron density around HTG B 632:**

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

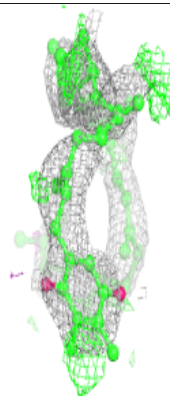
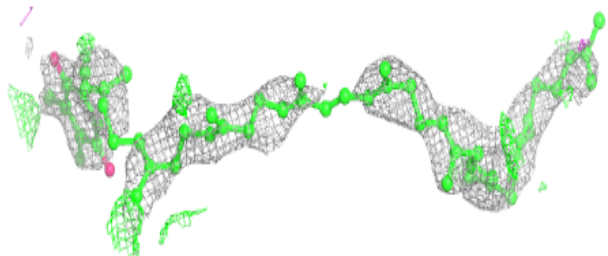
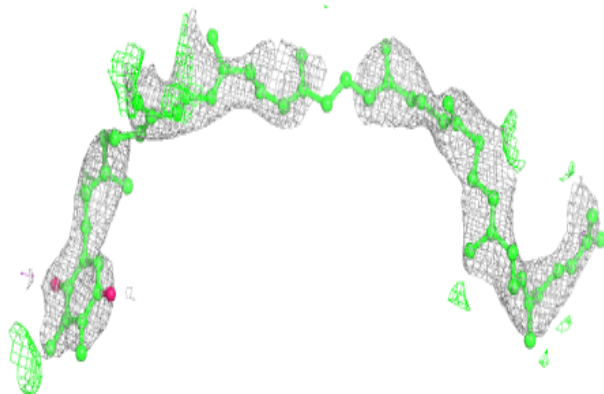


**Electron density around LMT M 104:**

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

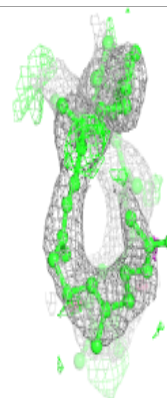
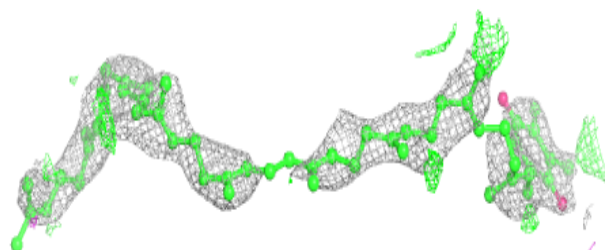
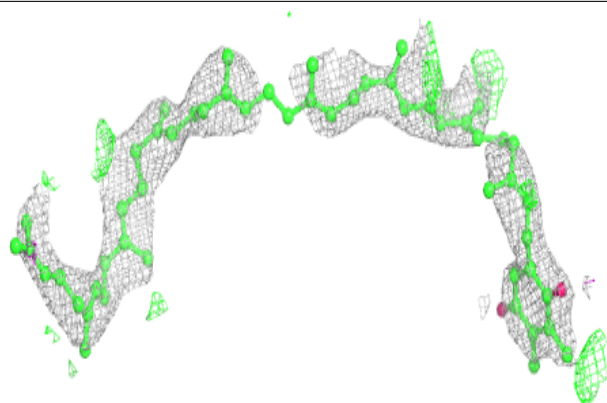
**Electron density around PL9 A 417 (A):**

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

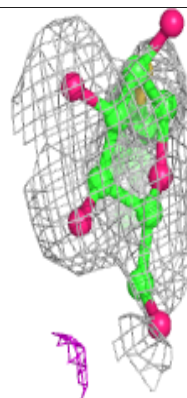
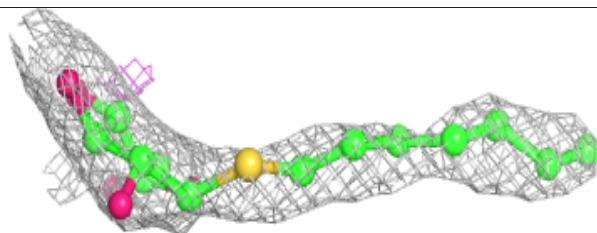
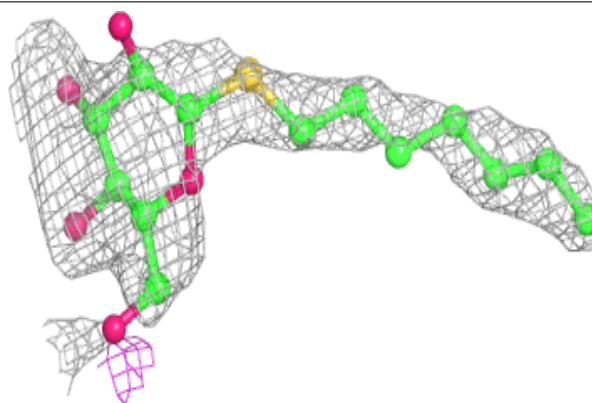


**Electron density around PL9 A 417 (B):**

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

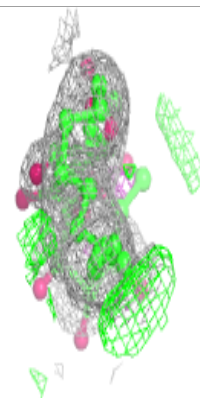
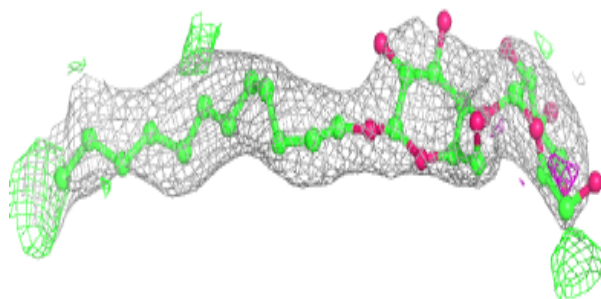
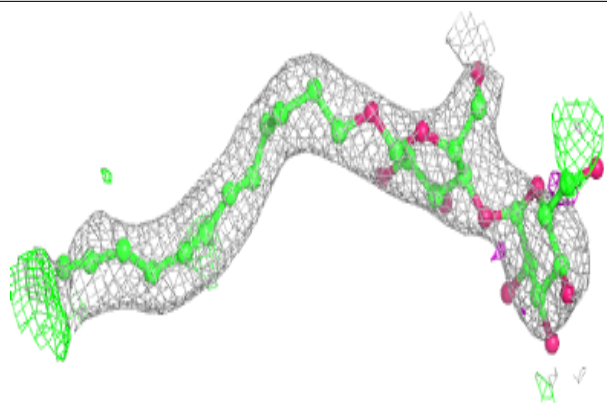
**Electron density around HTG B 624:**

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



**Electron density around LMT a 404:**

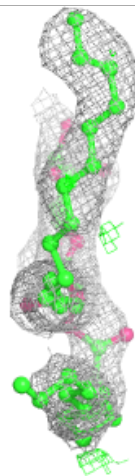
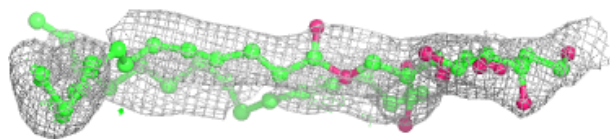
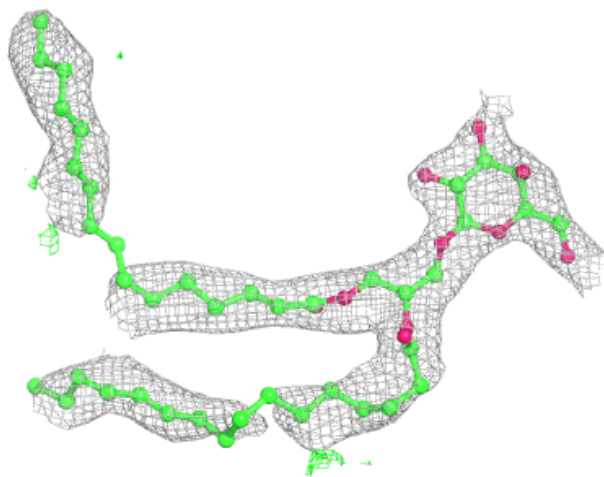
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





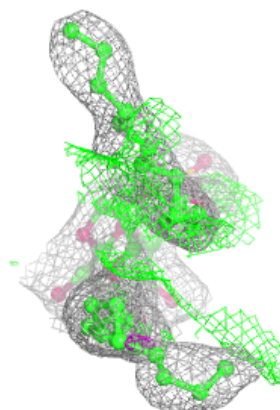
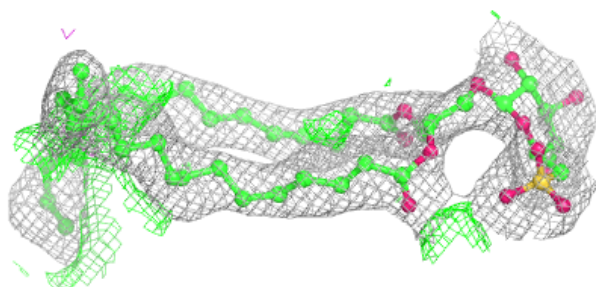
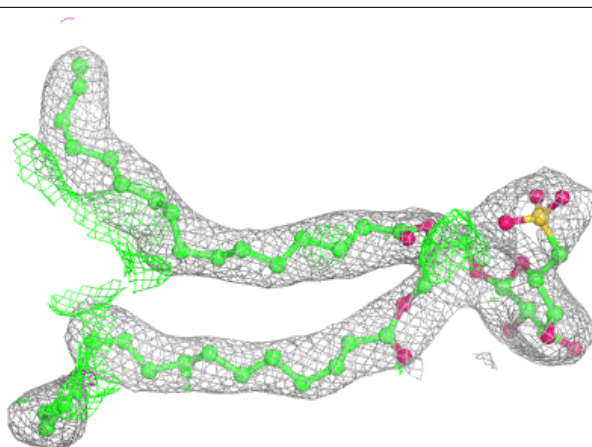
**Electron density around LMG C 519:**

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

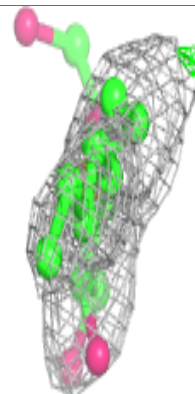
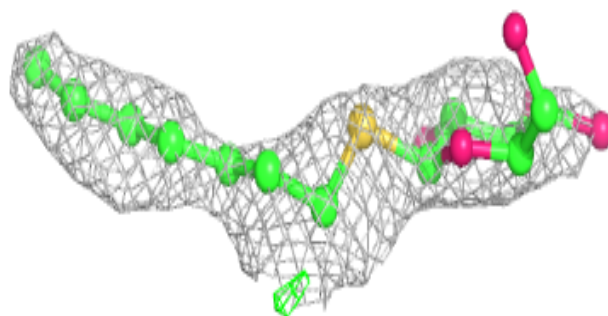
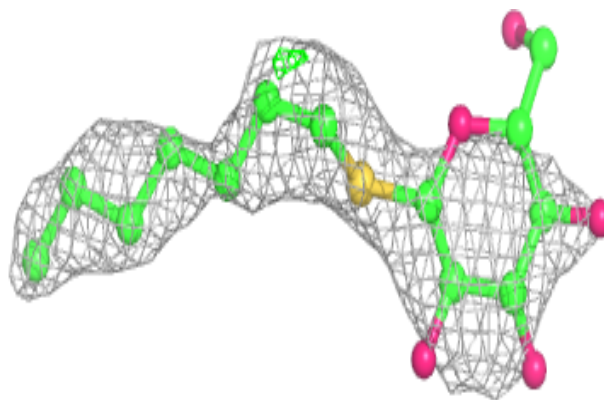


**Electron density around SQD L 102:**

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

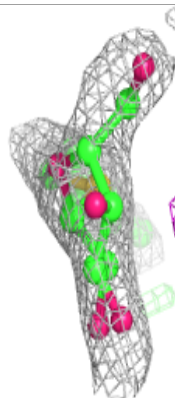
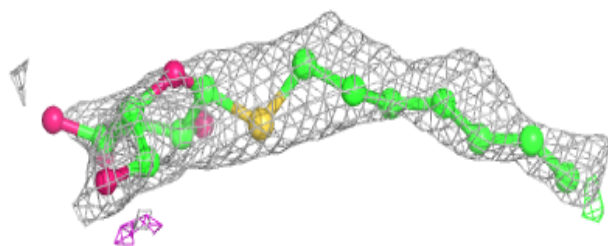
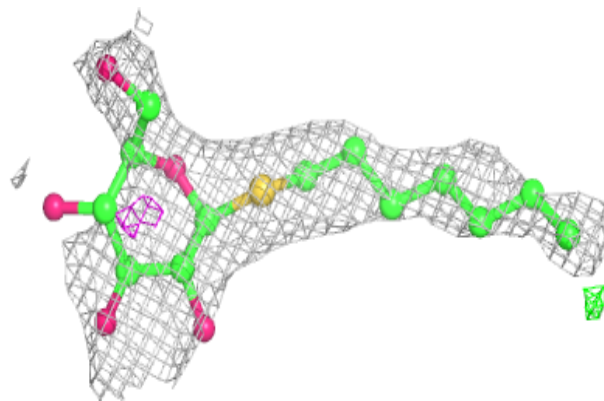
**Electron density around HTG c 524:**

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

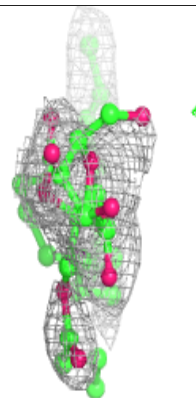
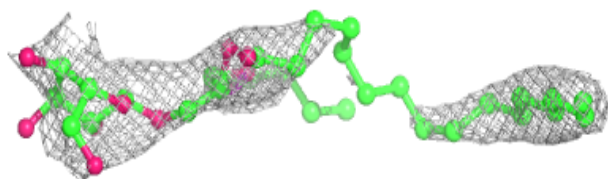
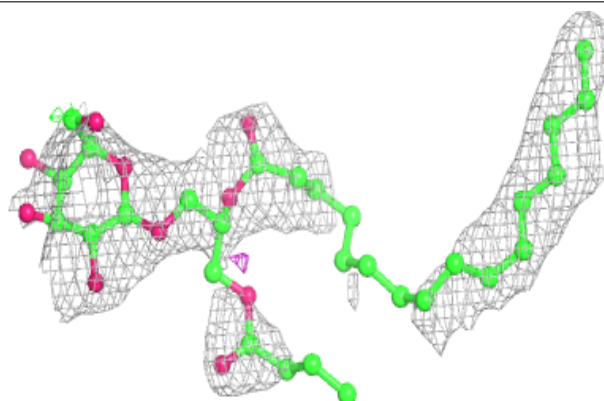


**Electron density around HTG C 523:**

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

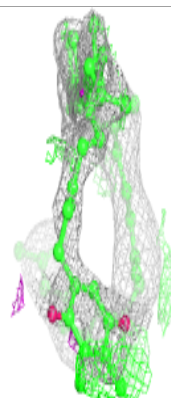
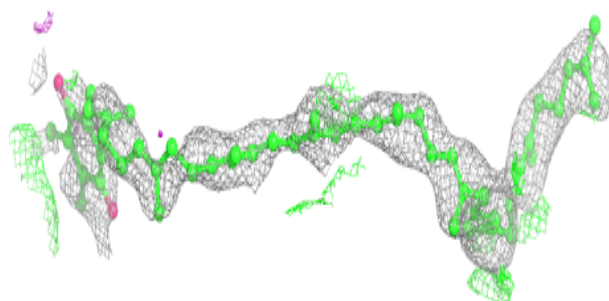
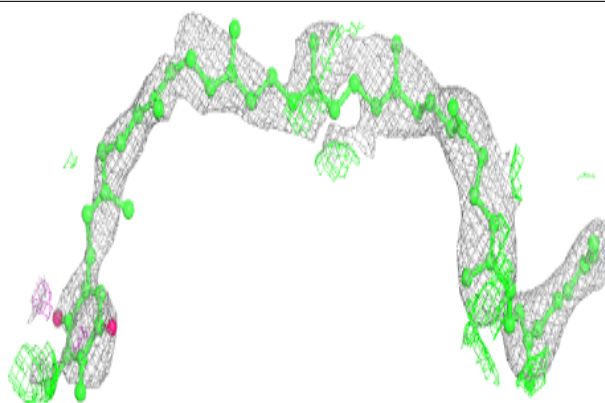
**Electron density around LMG z 101:**

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

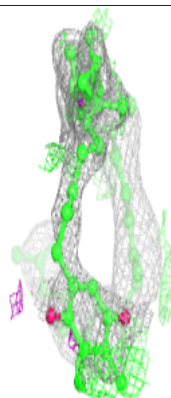
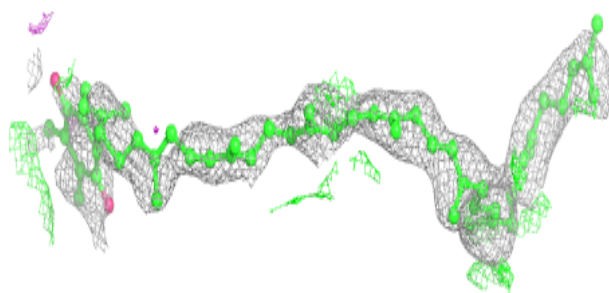
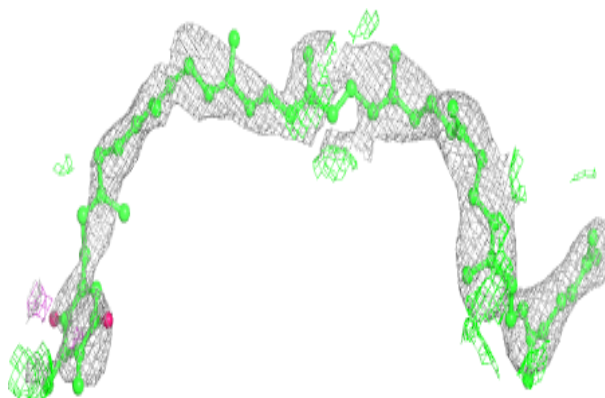


**Electron density around PL9 a 416 (B):**

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

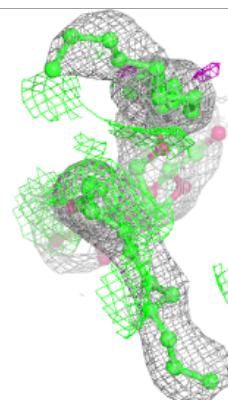
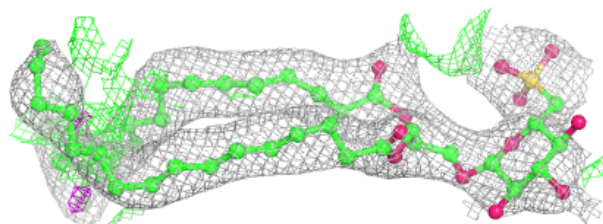
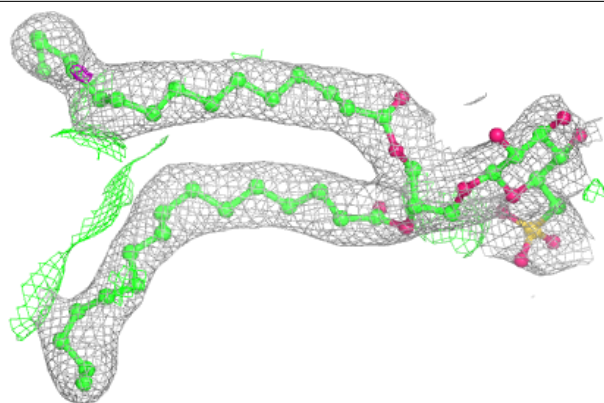
**Electron density around PL9 a 416 (A):**

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

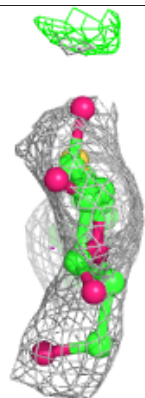
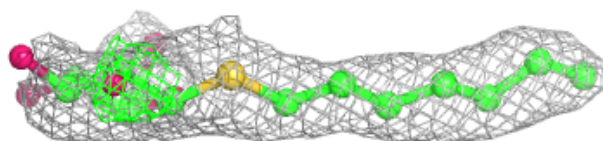
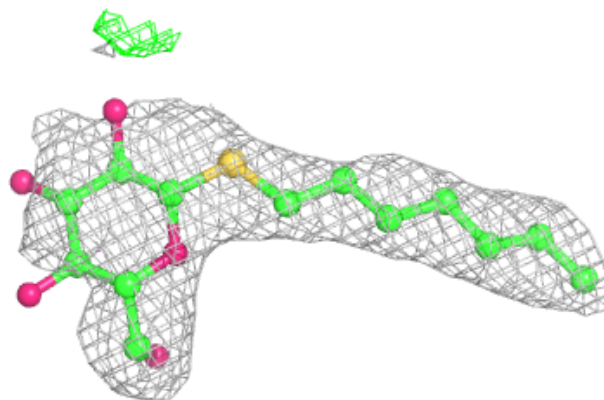


**Electron density around SQD B 621:**

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

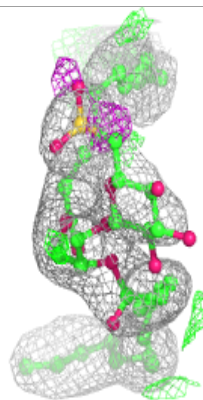
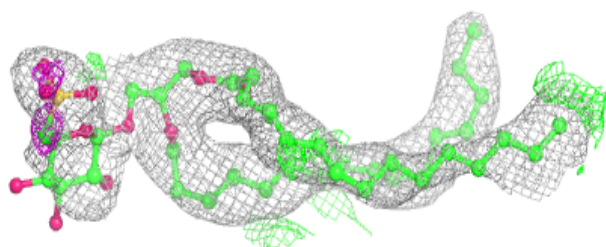
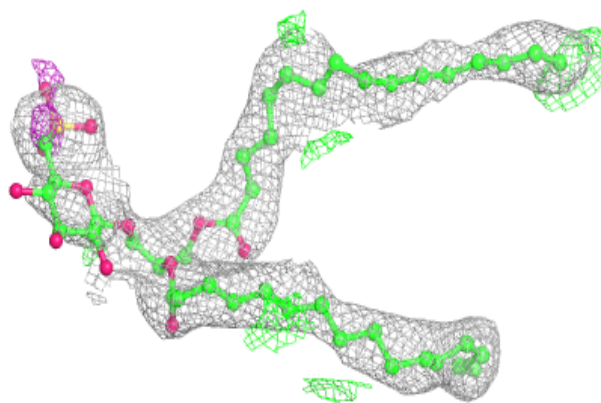
**Electron density around HTG b 608:**

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

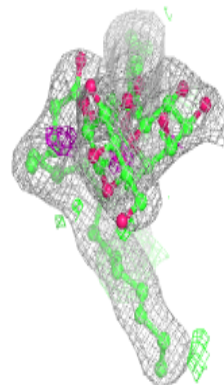
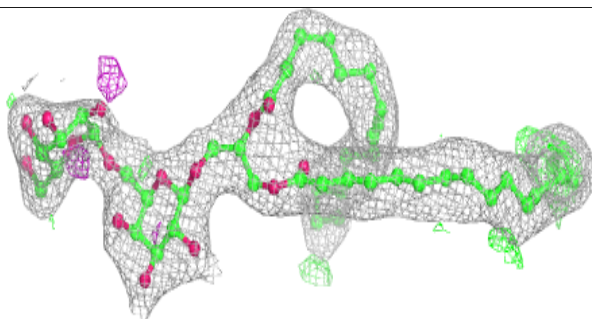
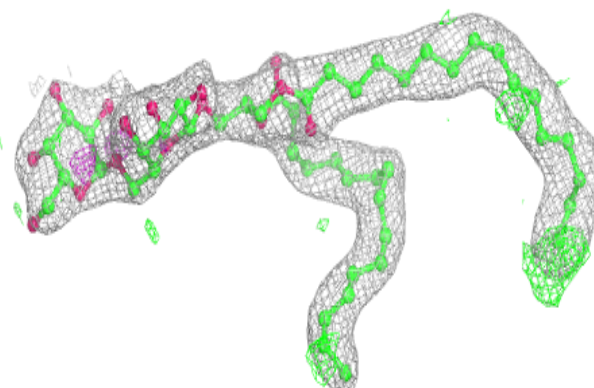


**Electron density around SQD A 413:**

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

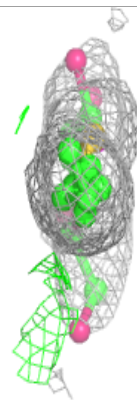
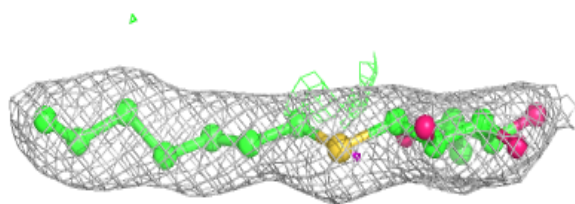
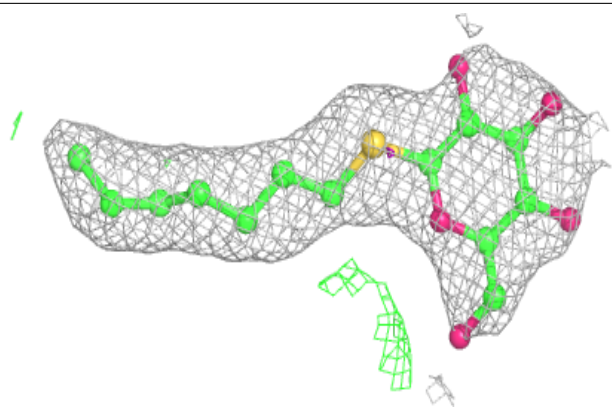
**Electron density around DGD h 102:**

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

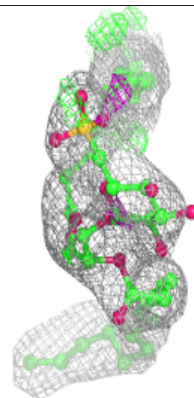
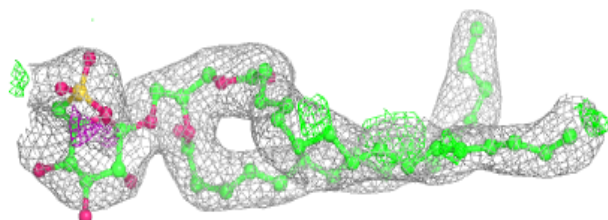
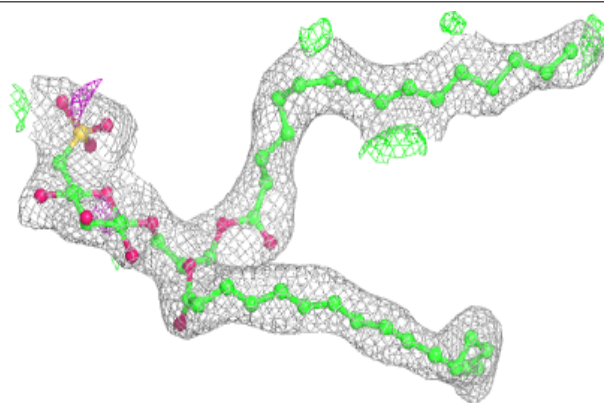


**Electron density around HTG b 607:**

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

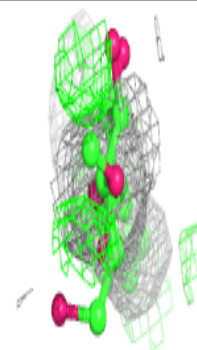
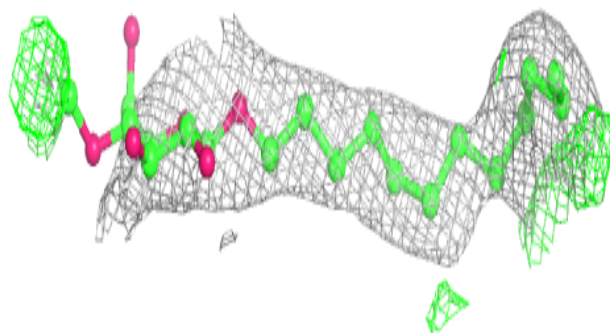
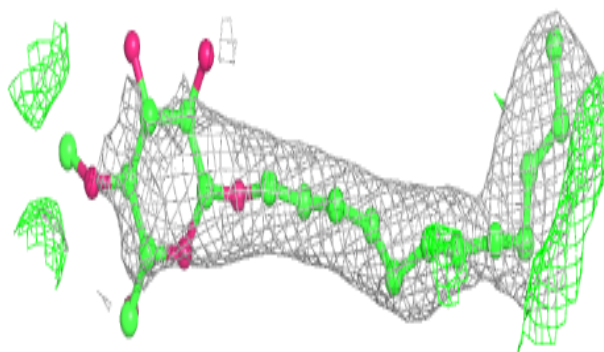
**Electron density around SQD a 405:**

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

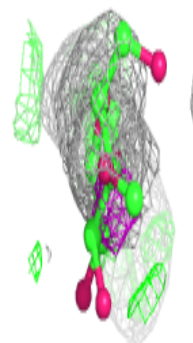
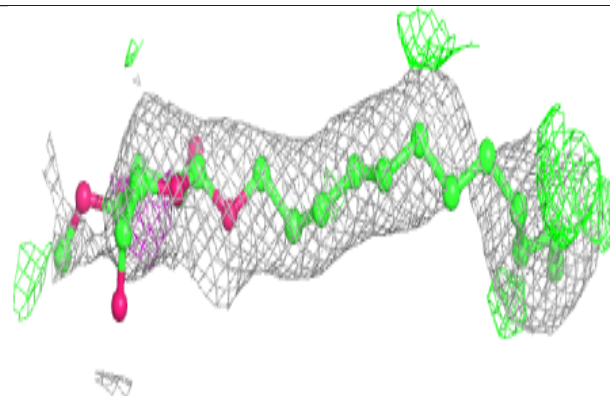
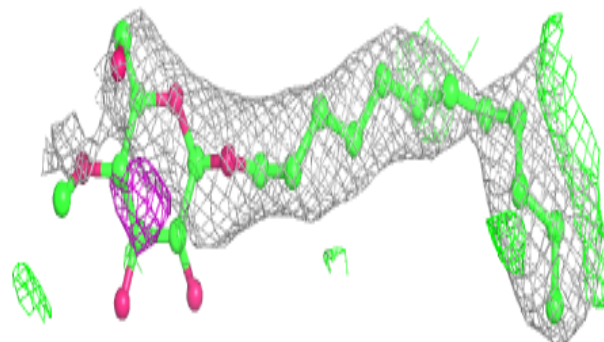


**Electron density around LMT t 101:**

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

**Electron density around LMT T 104:**

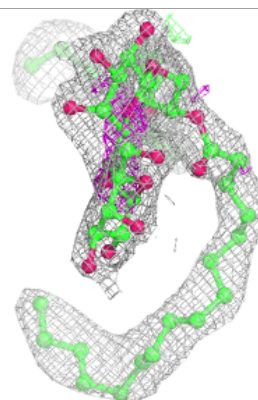
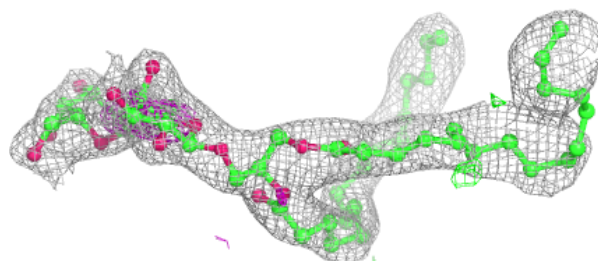
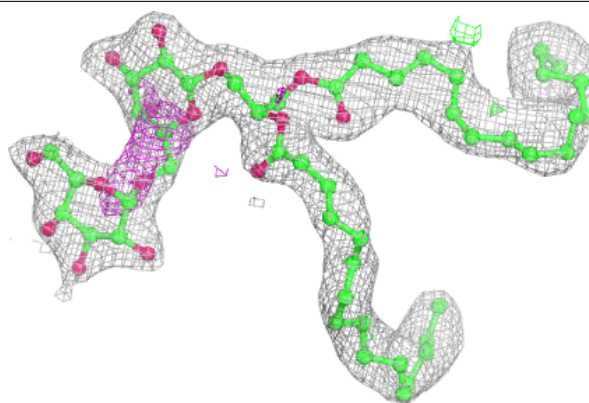
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



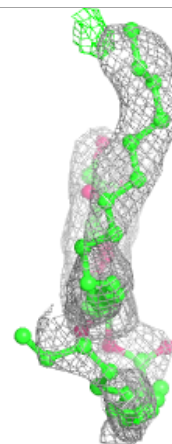
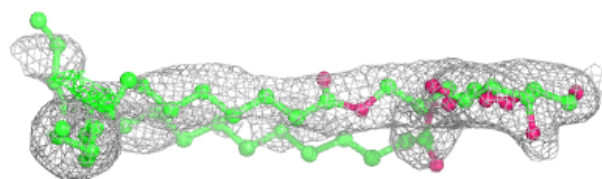
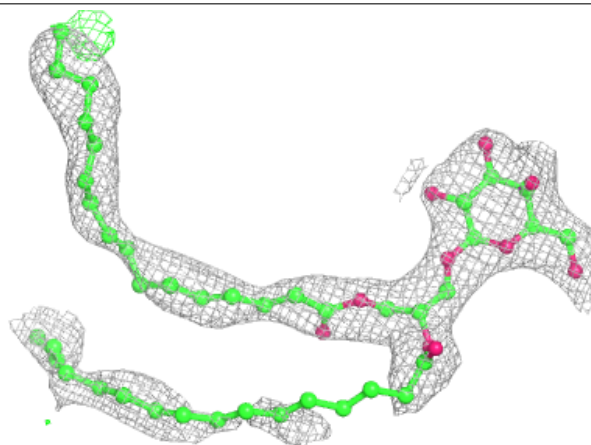


**Electron density around DGD C 517:**

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

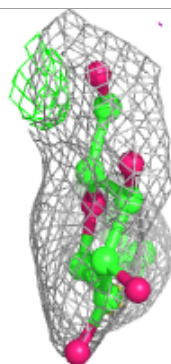
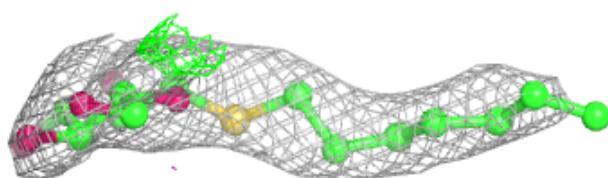
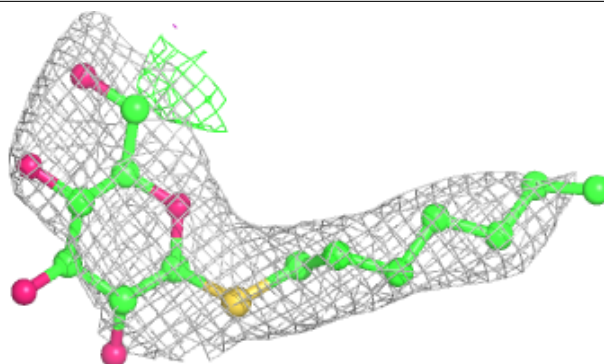
**Electron density around LMG k 101:**

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

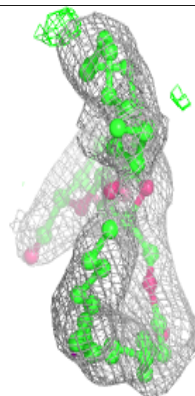
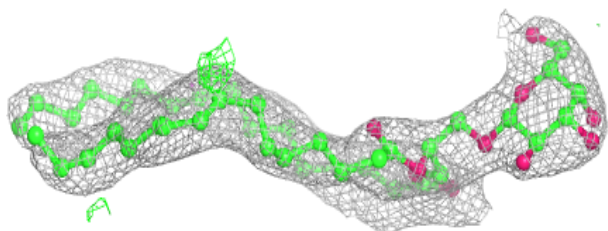
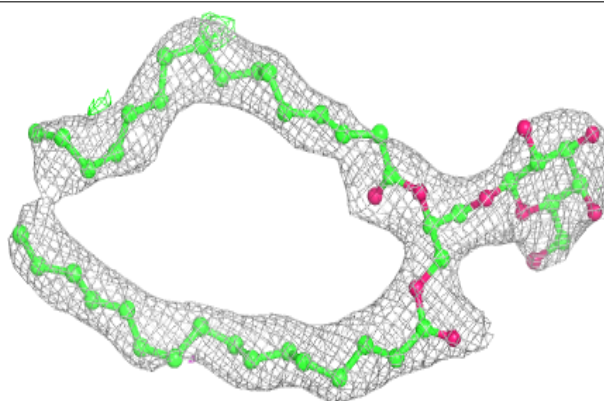


**Electron density around HTG b 632:**

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

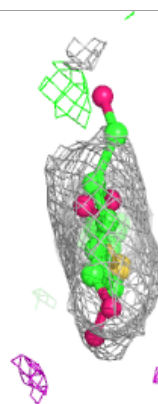
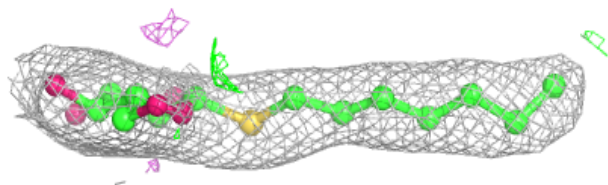
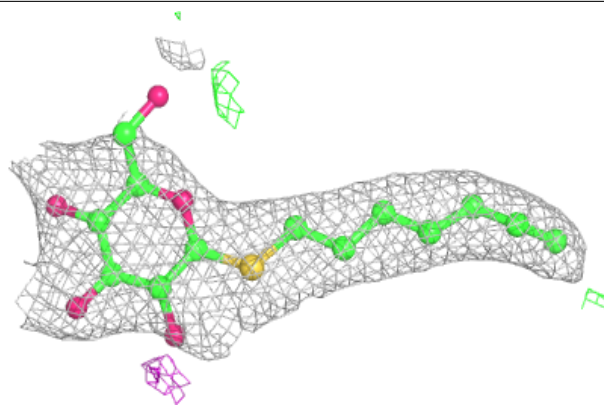
**Electron density around LMG a 415:**

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

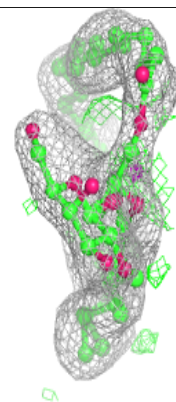
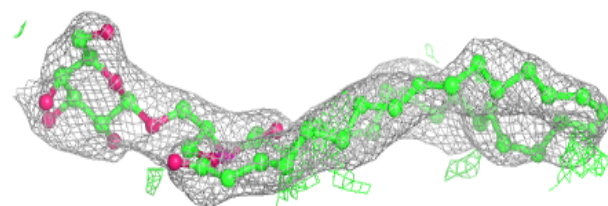
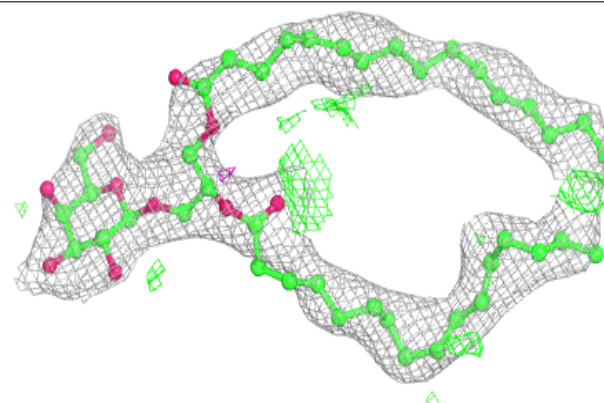


**Electron density around HTG B 631:**

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

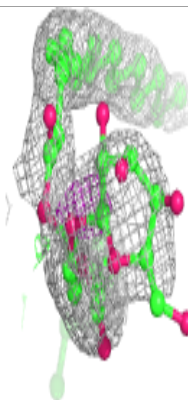
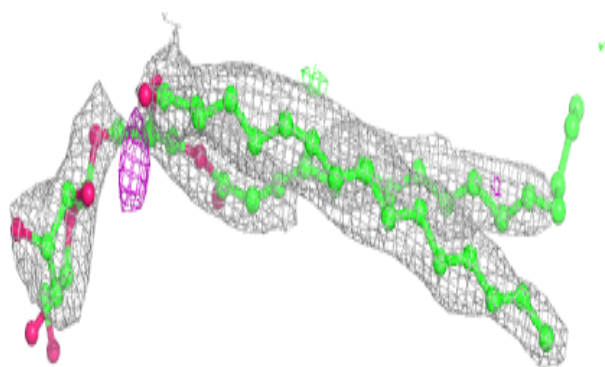
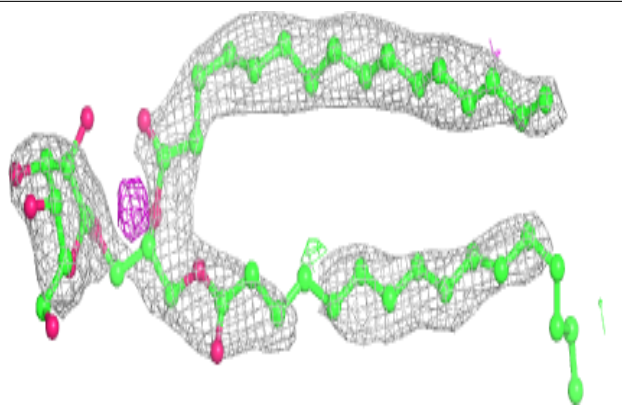
**Electron density around LMG A 419:**

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

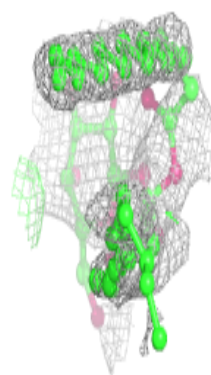
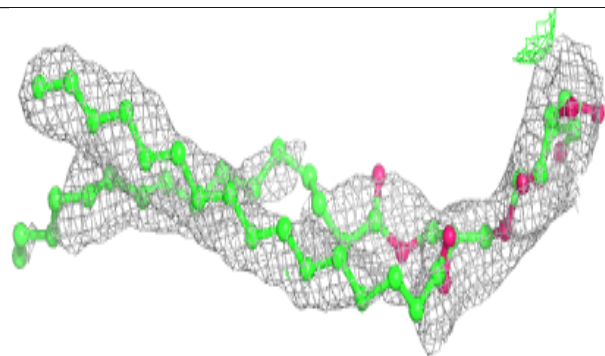
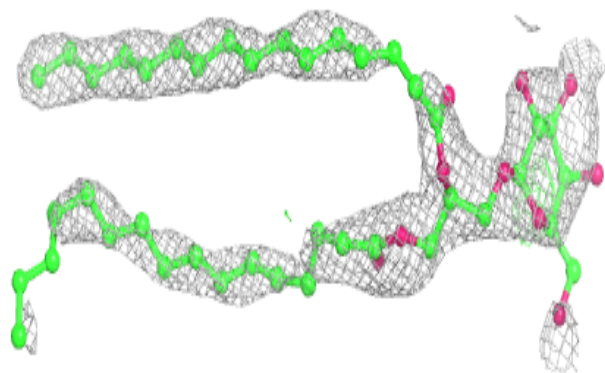


**Electron density around LMG C 520:**

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

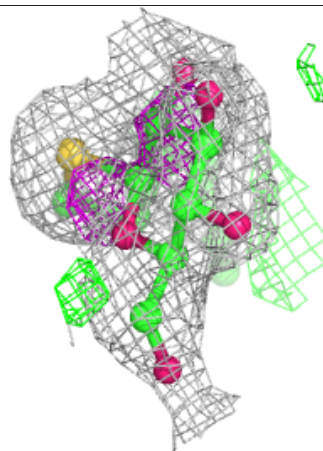
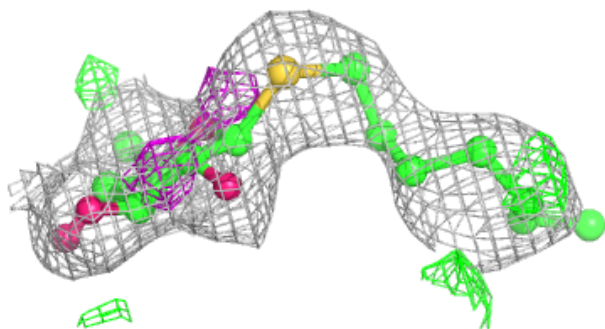
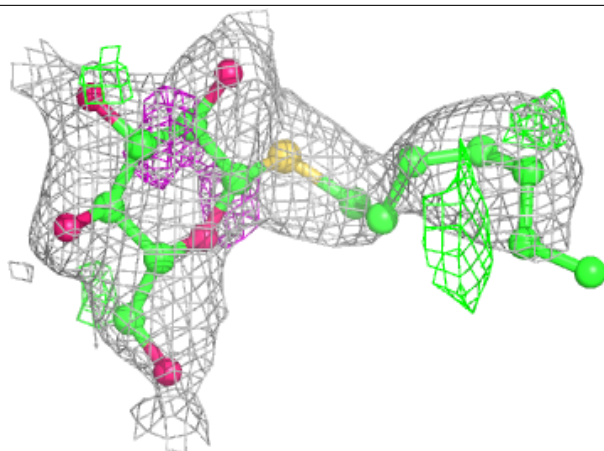
**Electron density around LMG c 522:**

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

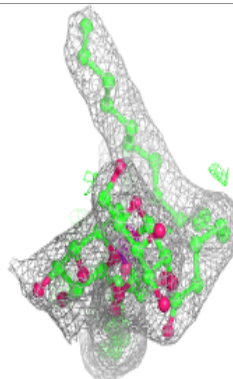
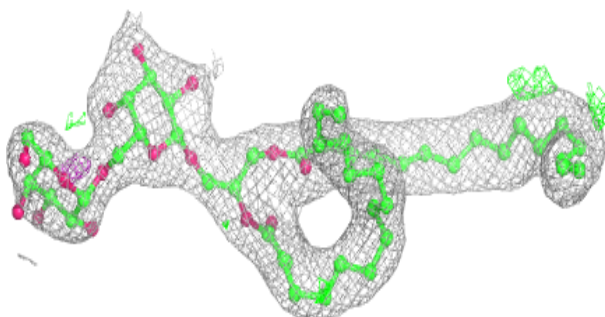
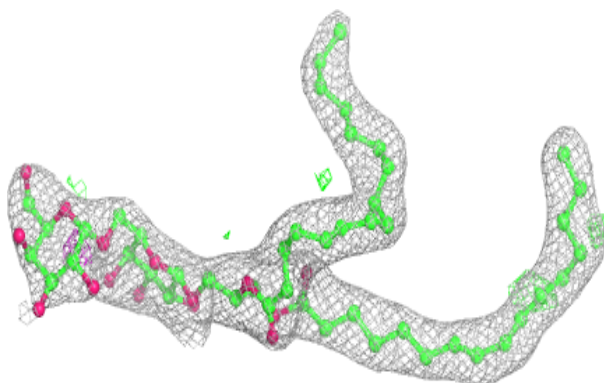


**Electron density around HTG B 623:**

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

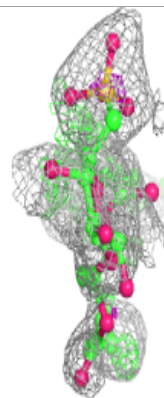
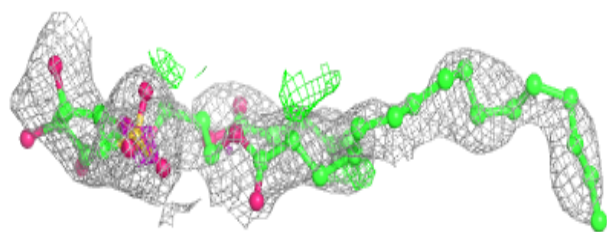
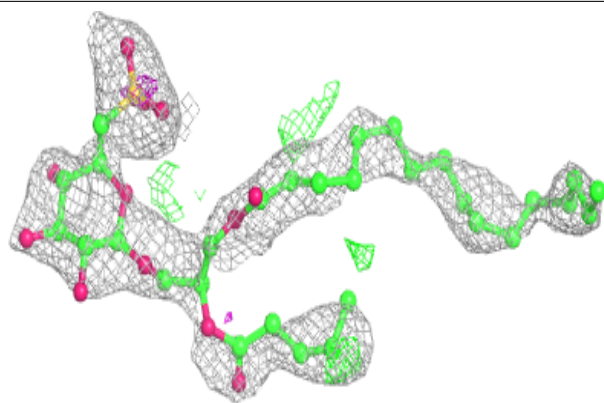
**Electron density around DGD H 102:**

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

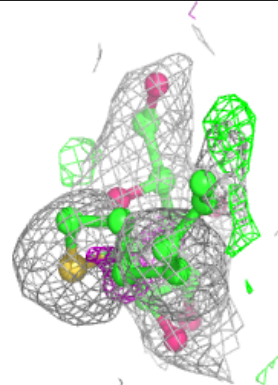
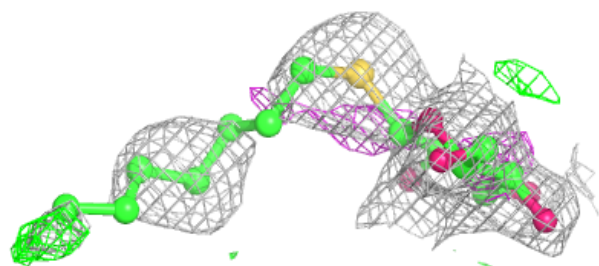
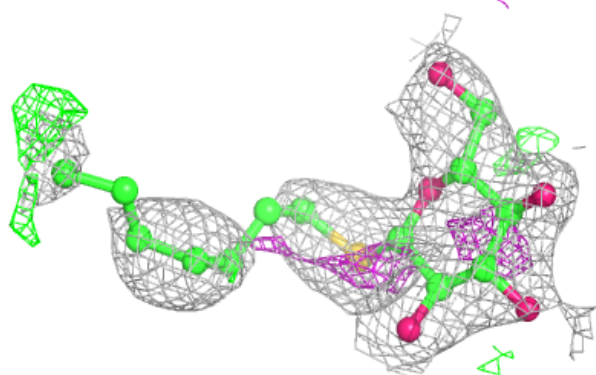


**Electron density around SQD F 101:**

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

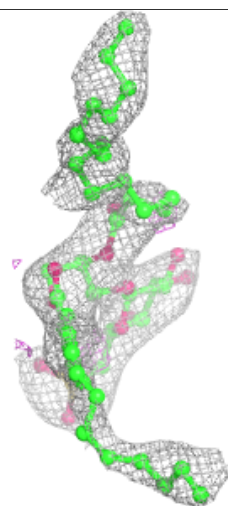
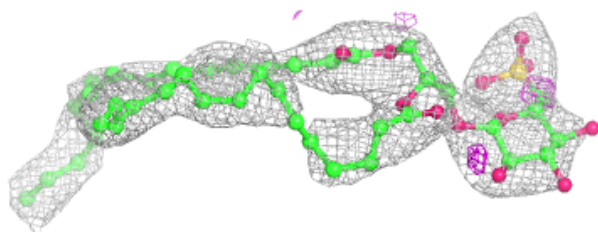
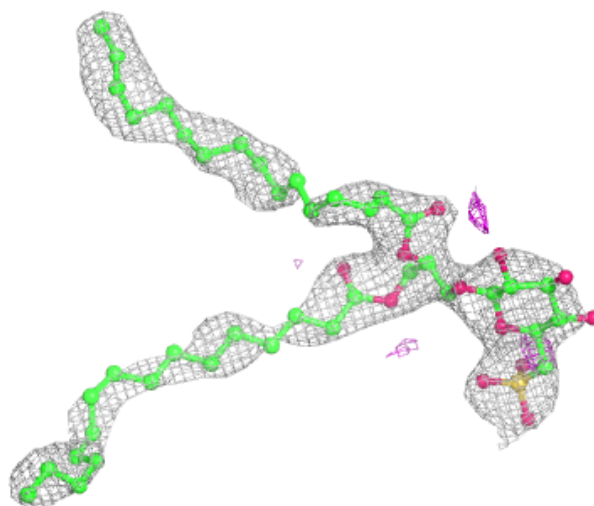
**Electron density around HTG b 631:**

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



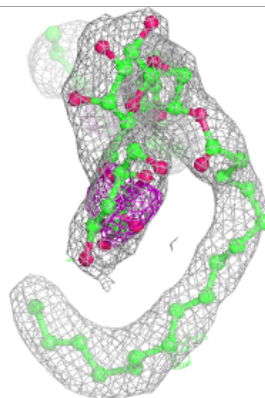
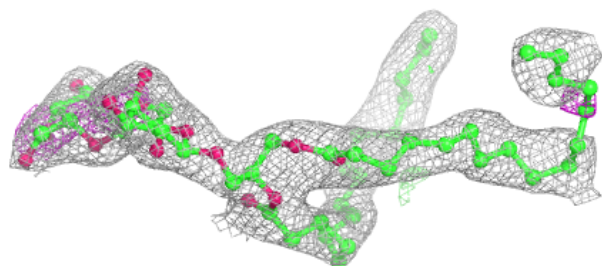
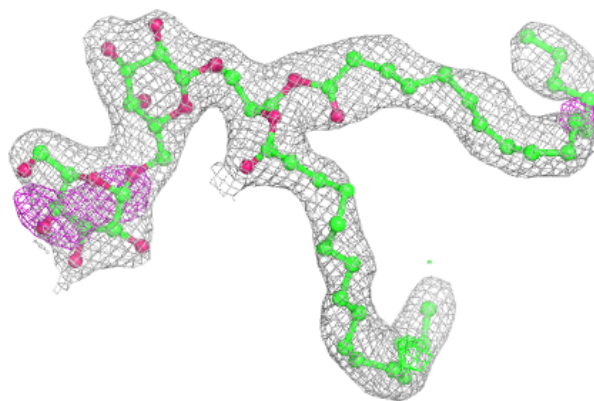
**Electron density around SQD A 411:**

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

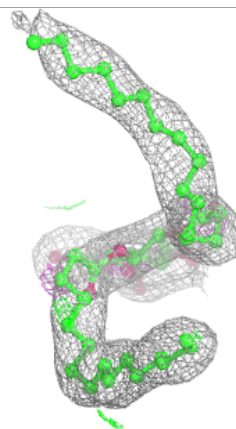
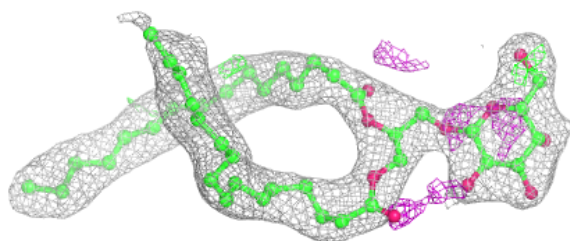
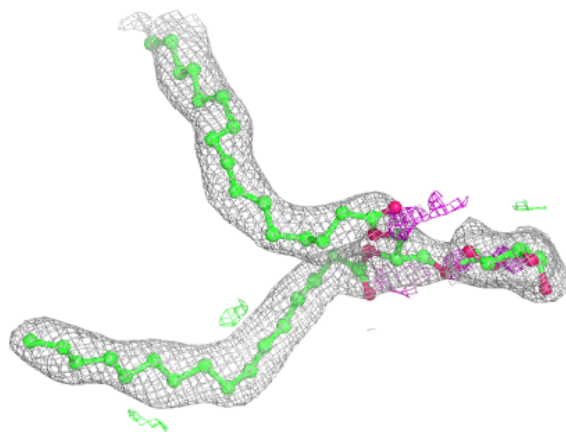


**Electron density around DGD c 520:**

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

**Electron density around LMG M 101:**

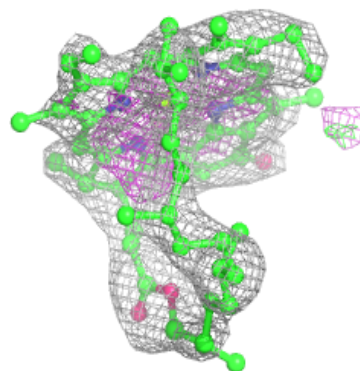
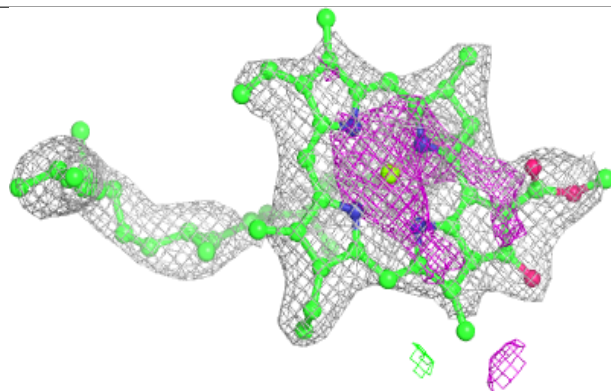
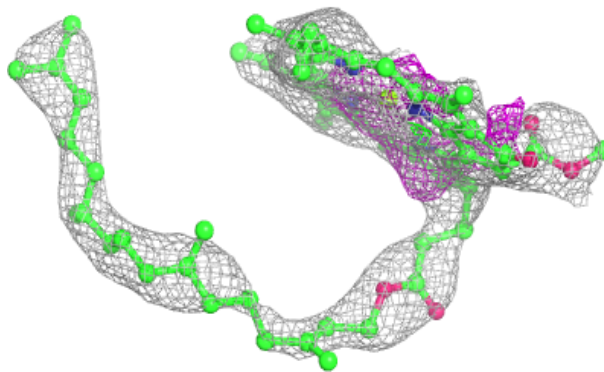
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



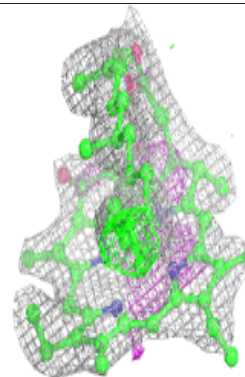
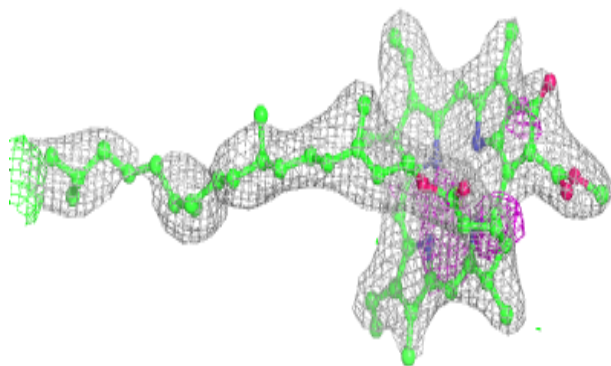
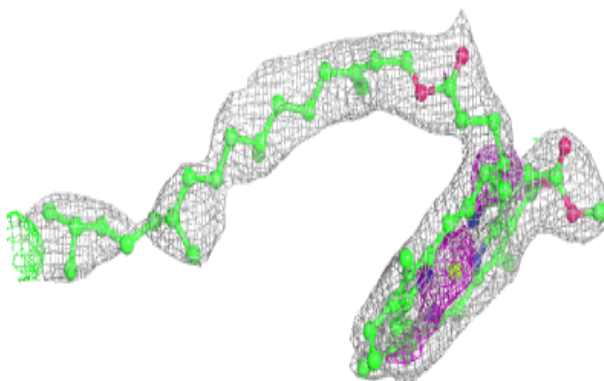


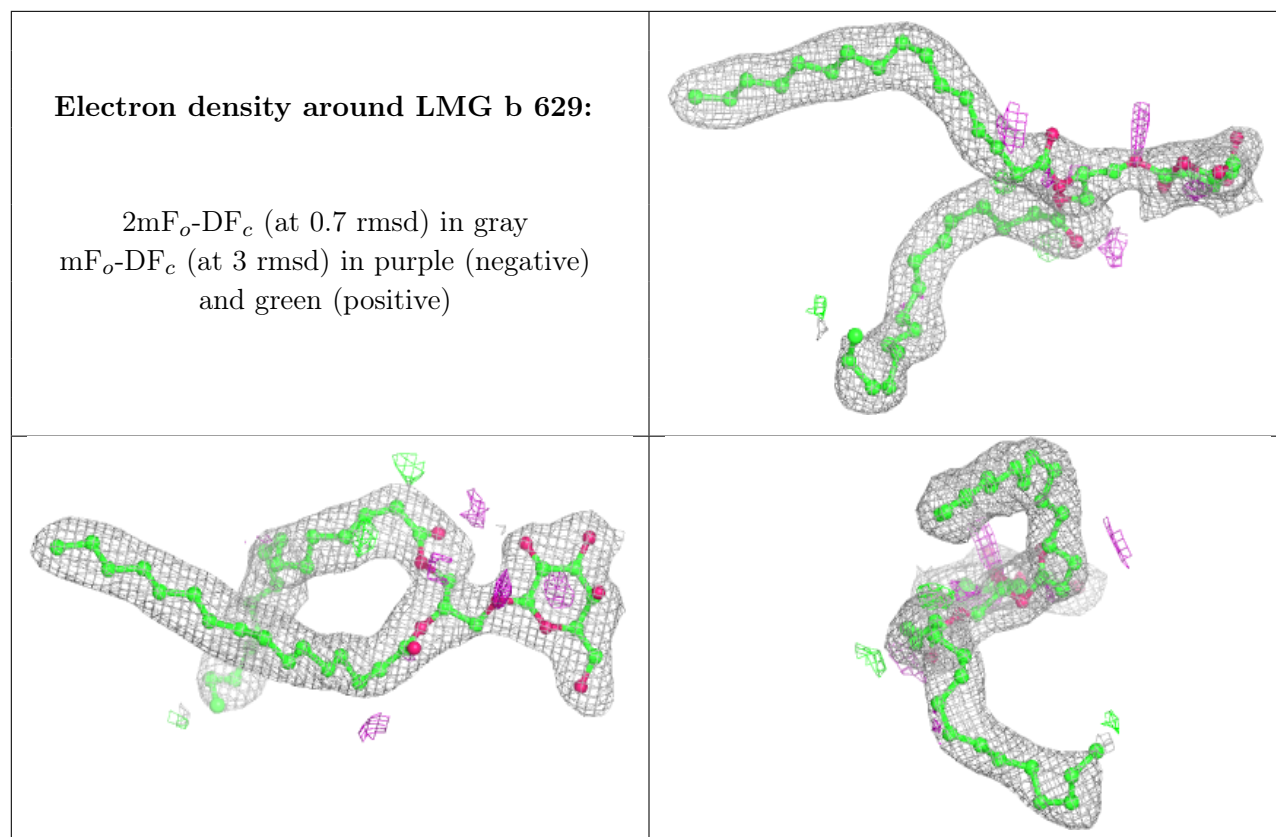
**Electron density around CLA C 513:**

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

**Electron density around CLA C 504:**

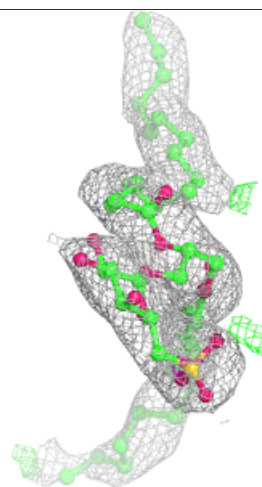
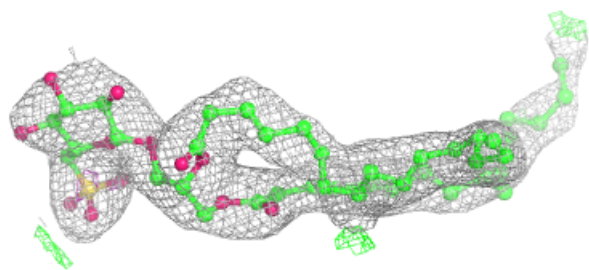
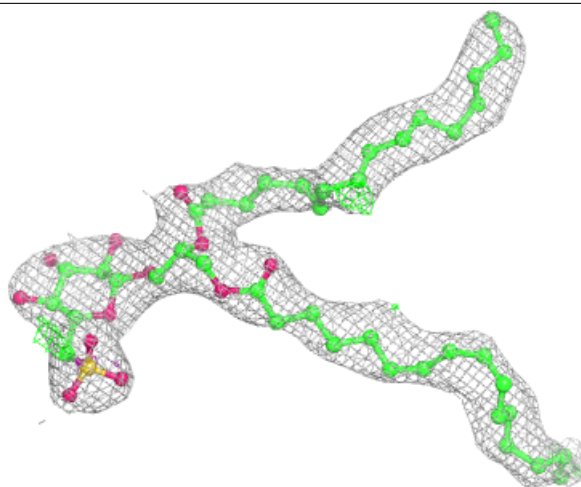
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





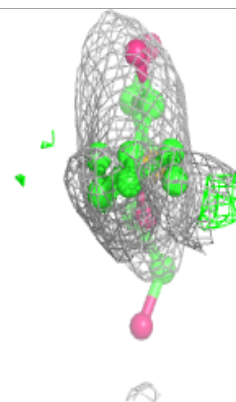
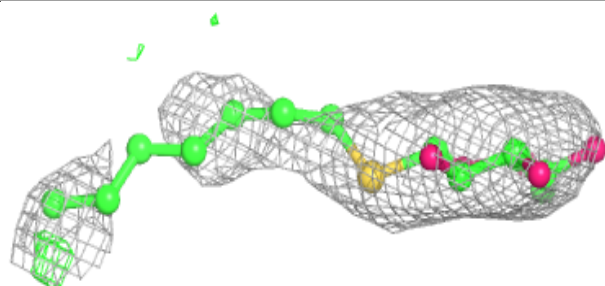
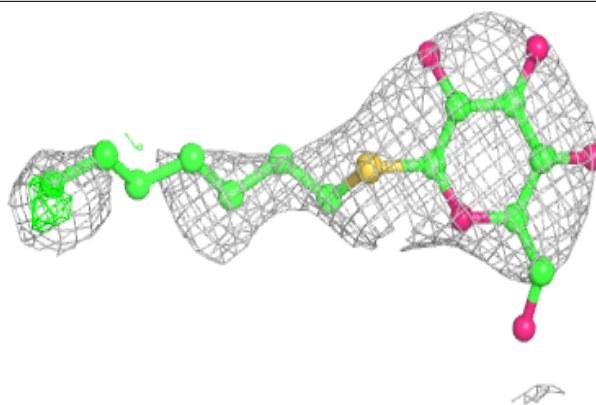
**Electron density around SQD a 414:**

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

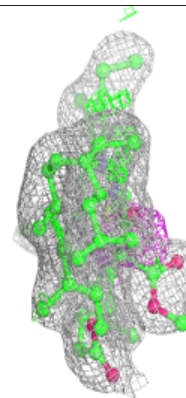
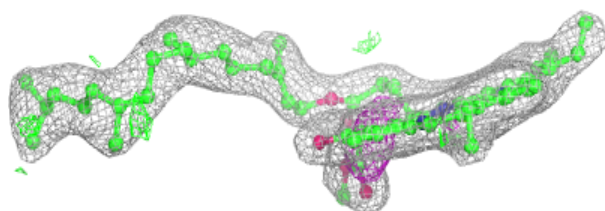
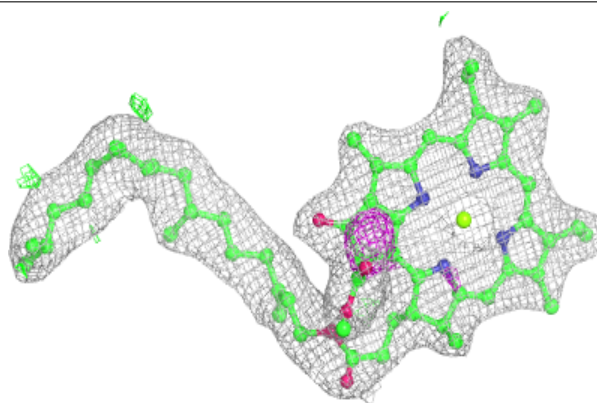


**Electron density around HTG c 523:**

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

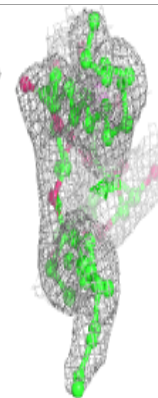
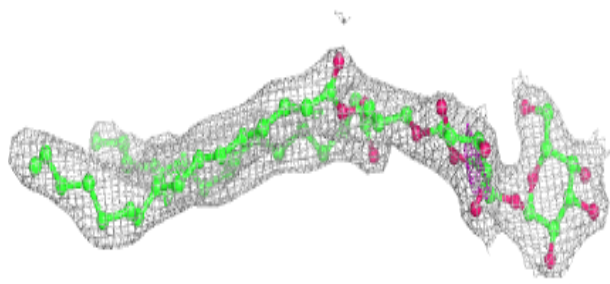
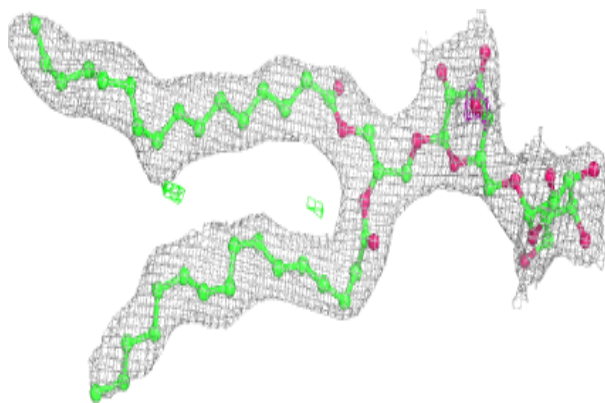
**Electron density around CLA b 611:**

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

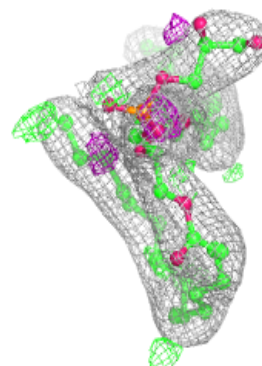
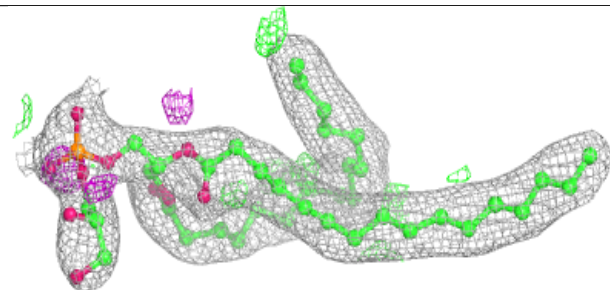
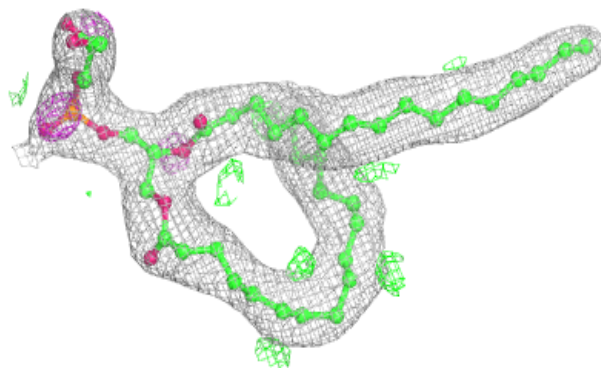


**Electron density around DGD C 518:**

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

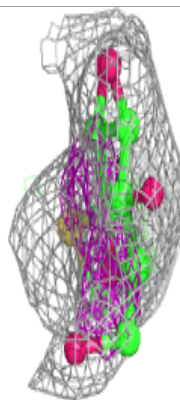
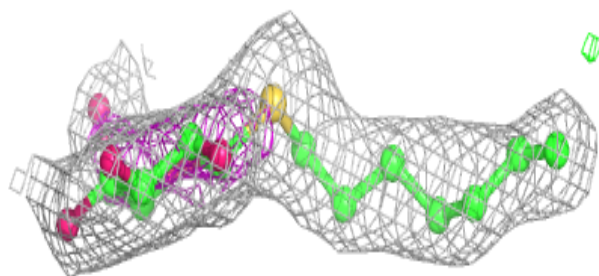
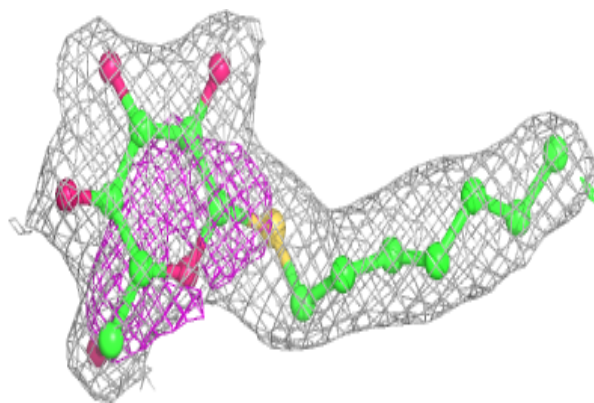
**Electron density around LHG D 409:**

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

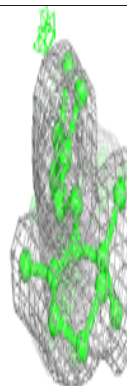
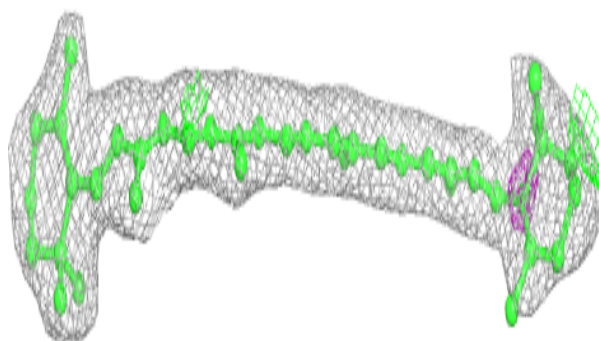
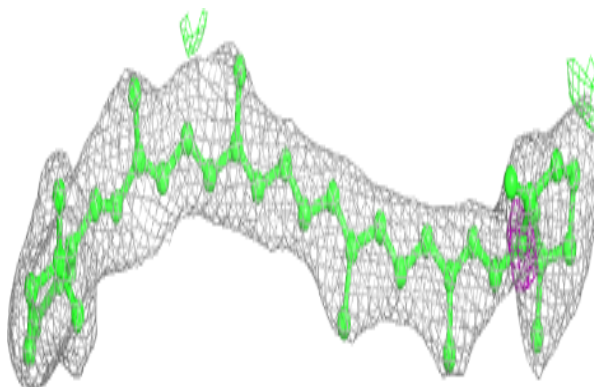


**Electron density around HTG b 602:**

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

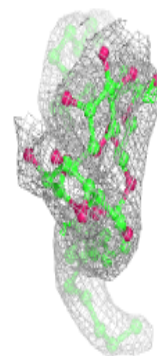
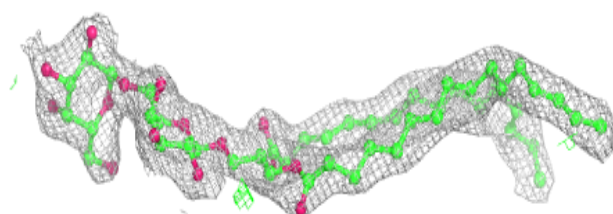
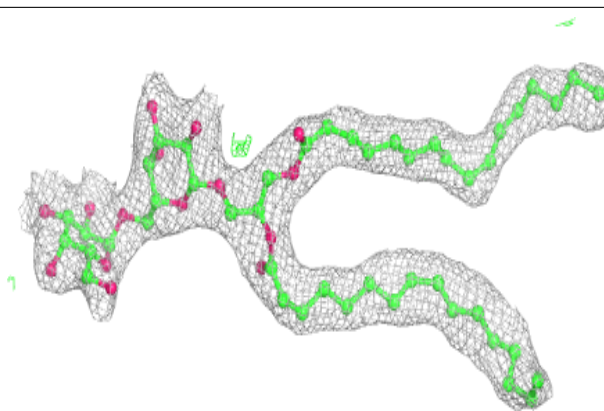
**Electron density around BCR H 101:**

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

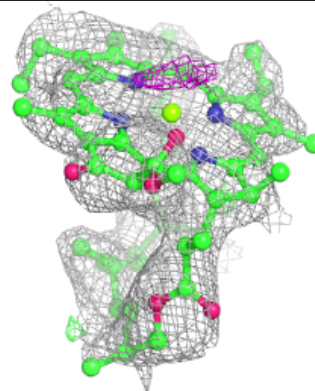
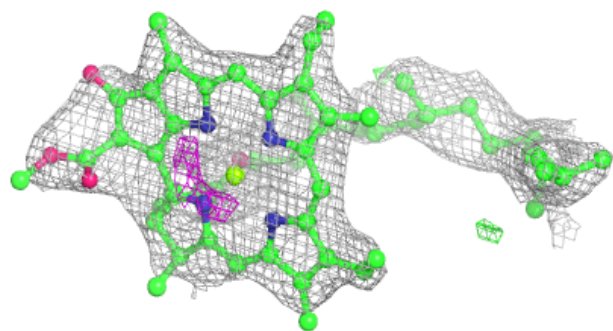
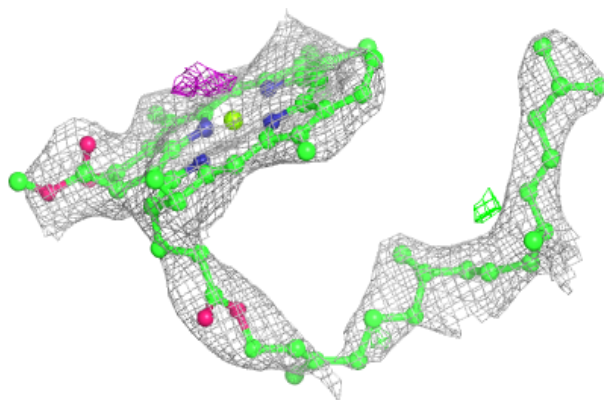


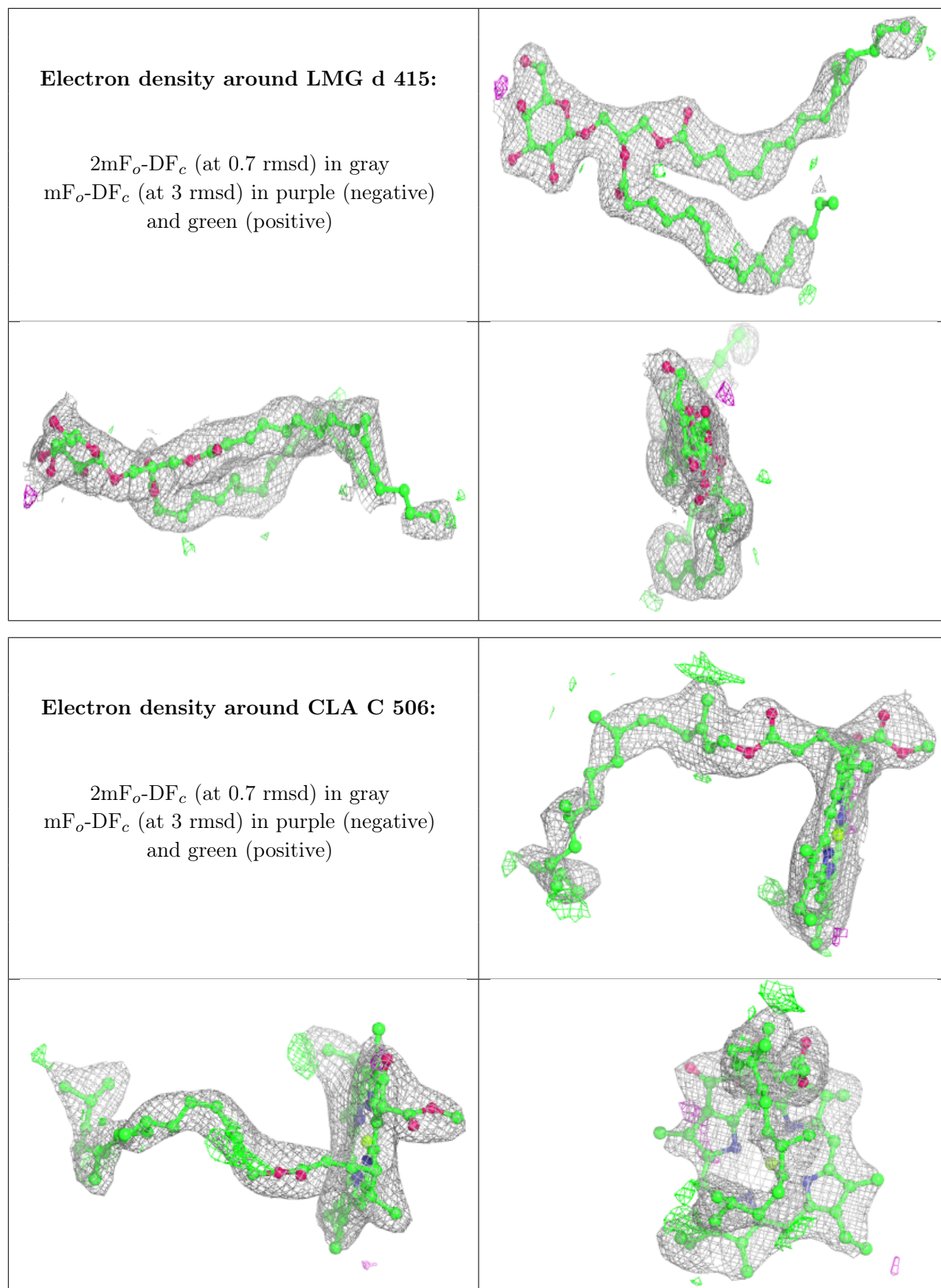
**Electron density around DGD c 521:**

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

**Electron density around CLA c 517:**

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

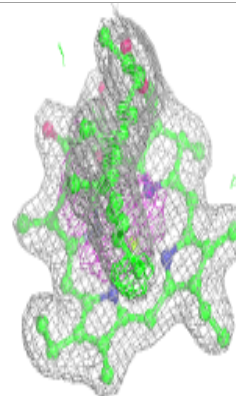
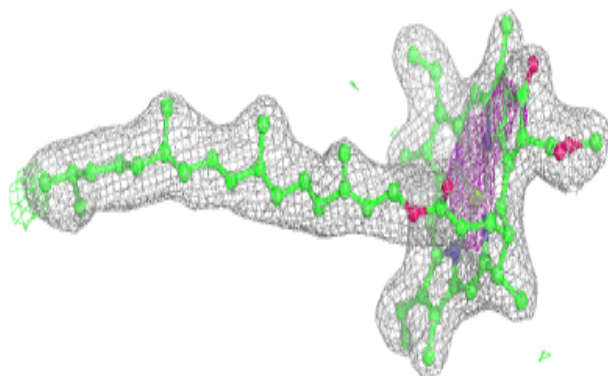
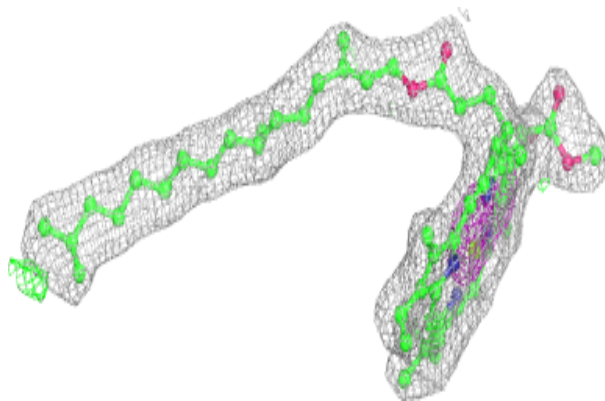




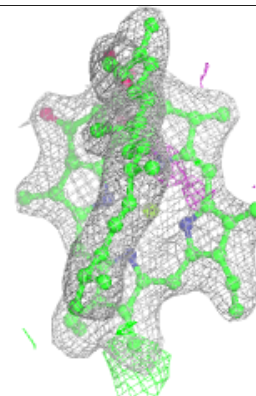
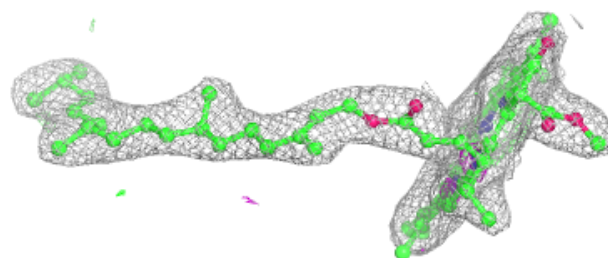
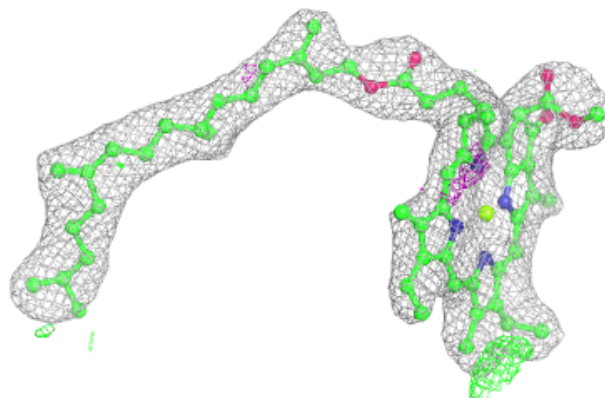


**Electron density around CLA b 616:**

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

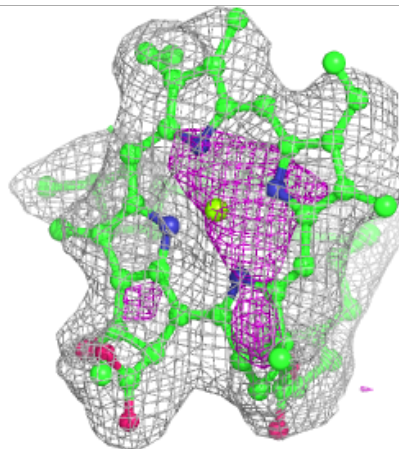
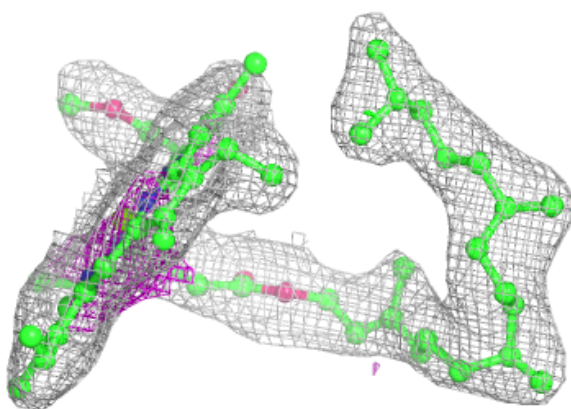
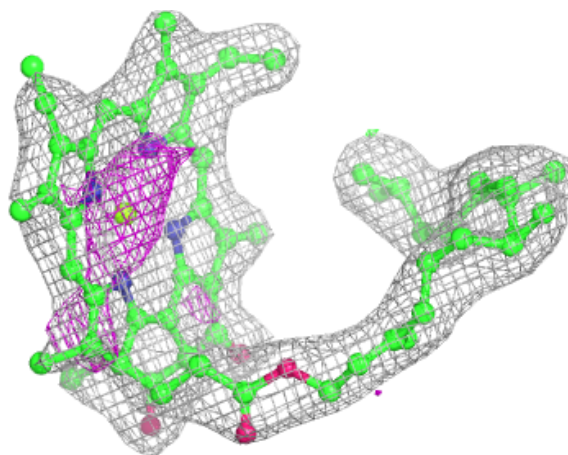
**Electron density around CLA b 618:**

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



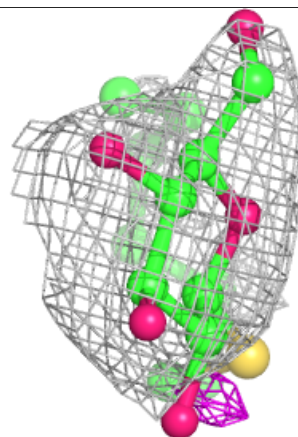
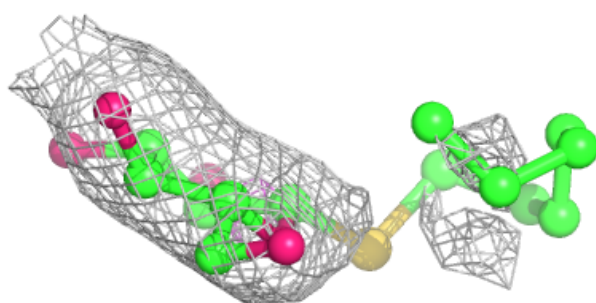
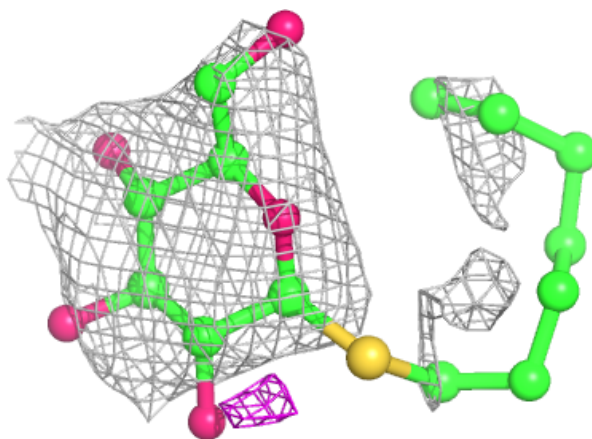
**Electron density around CLA c 507:**

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

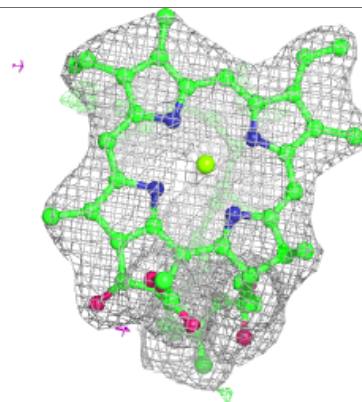
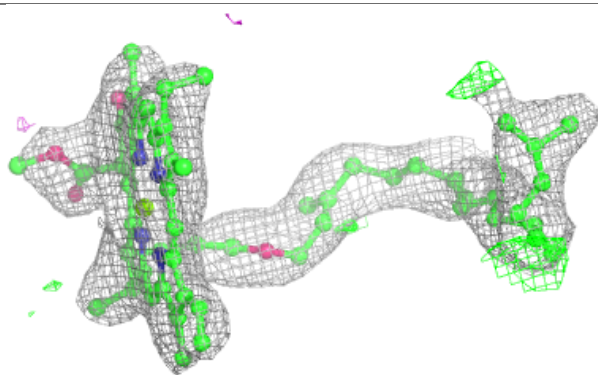
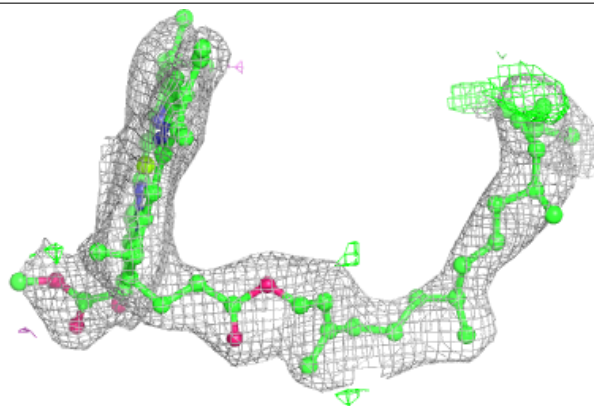


**Electron density around HTG V 206:**

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

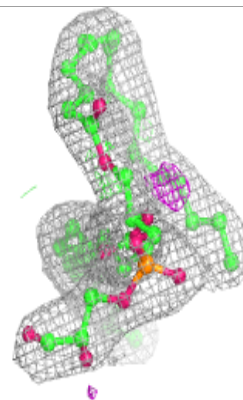
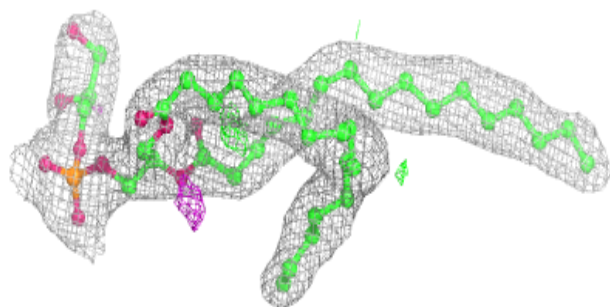
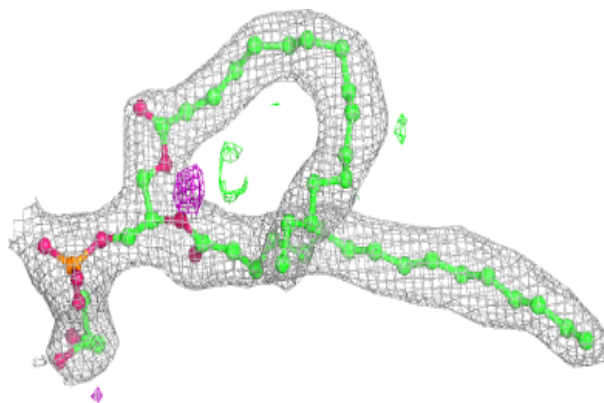
**Electron density around CLA c 510:**

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

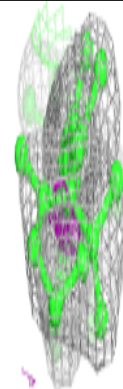
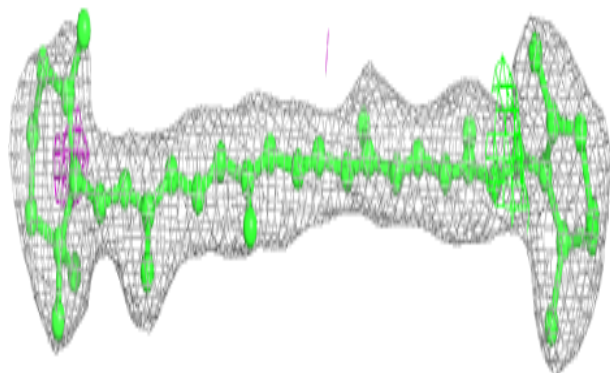
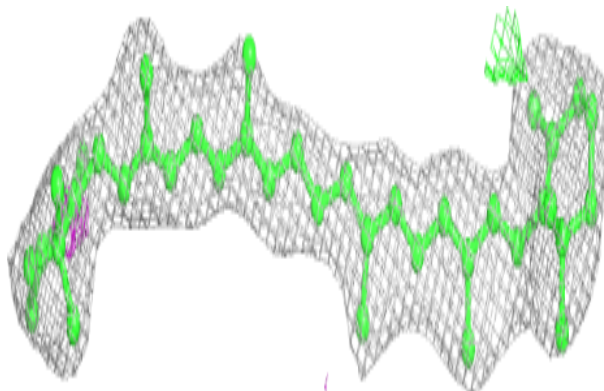


**Electron density around LHG d 408:**

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

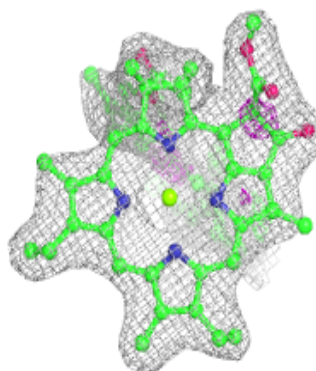
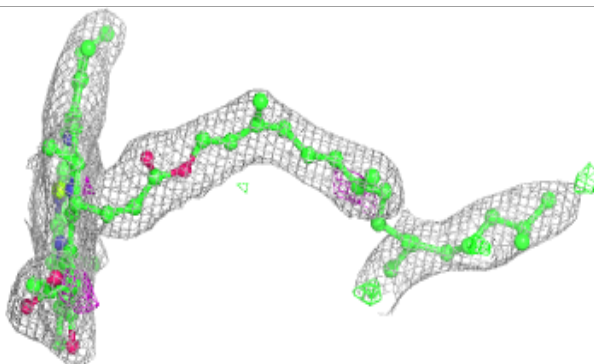
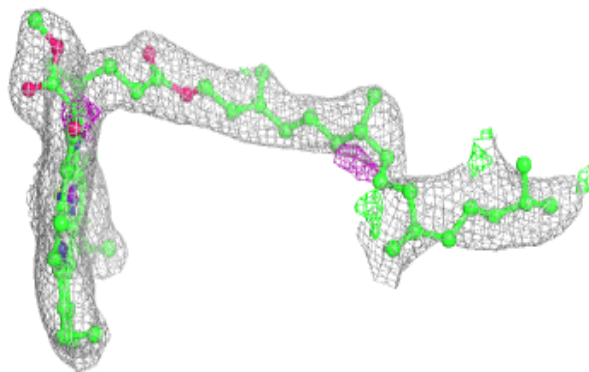
**Electron density around BCR C 514:**

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

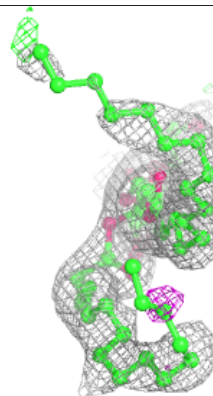
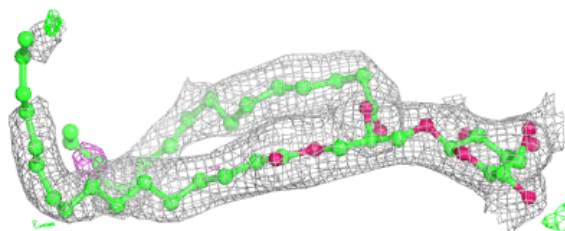
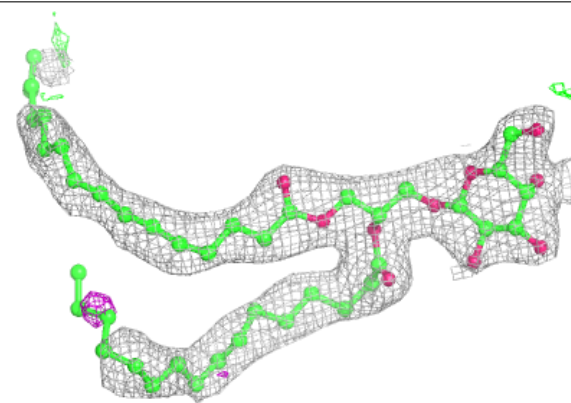


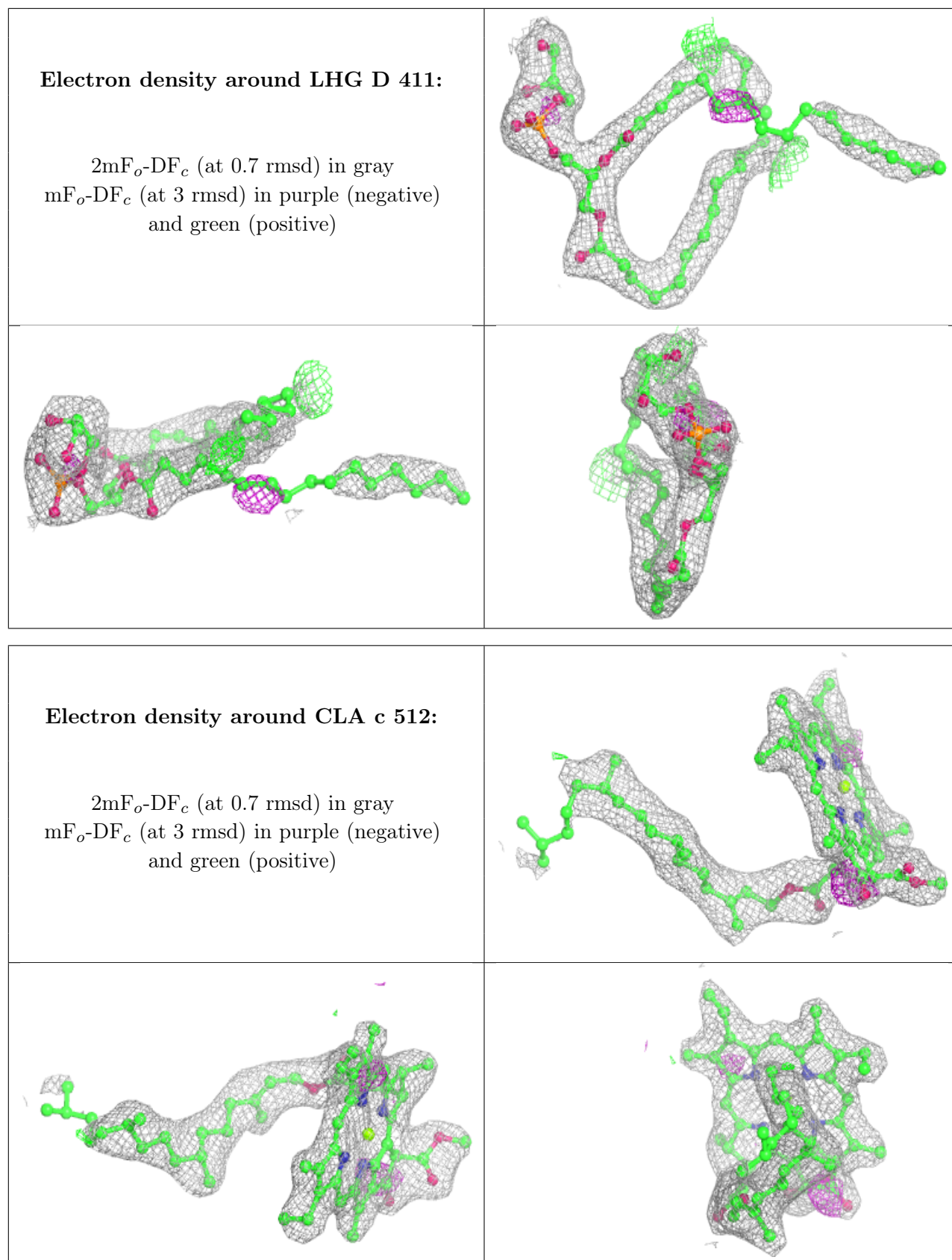
**Electron density around CLA b 615:**

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

**Electron density around LMG D 415:**

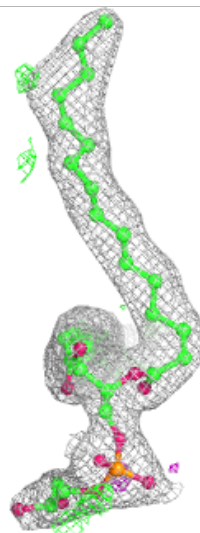
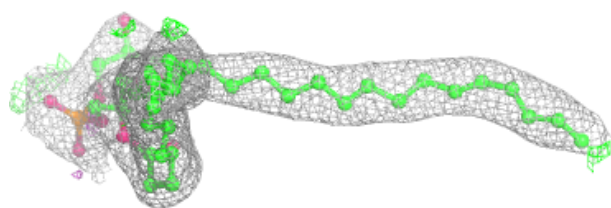
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





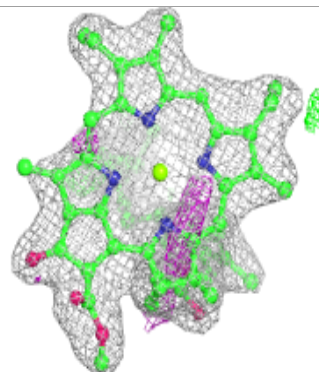
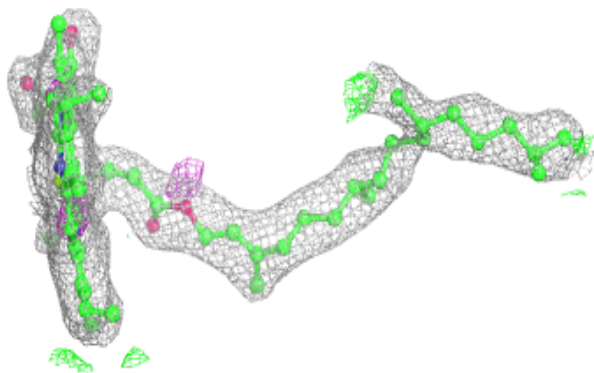
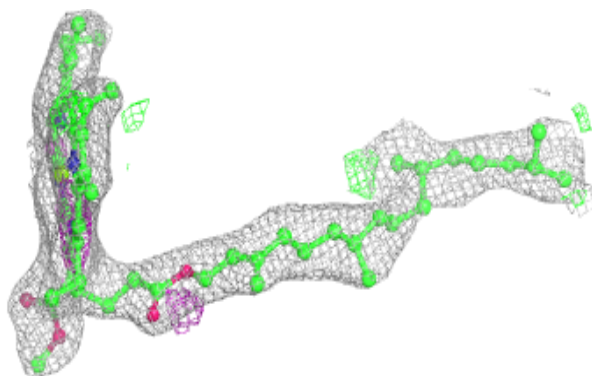
**Electron density around LHG b 634:**

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

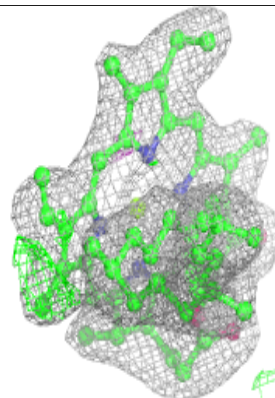
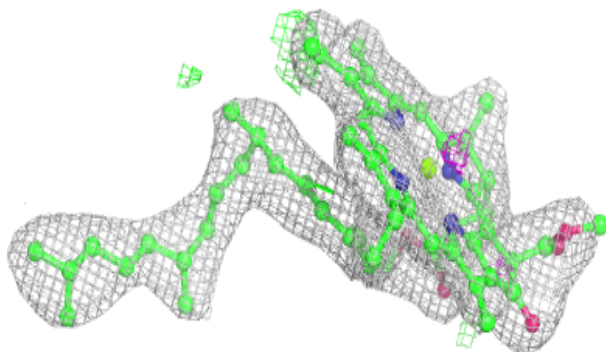
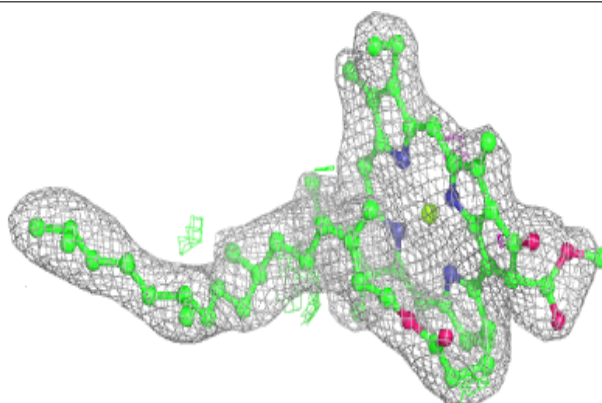


**Electron density around CLA B 607:**

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

**Electron density around CLA c 509:**

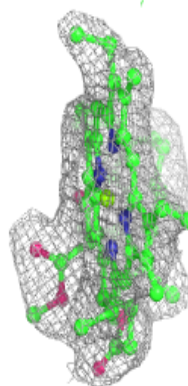
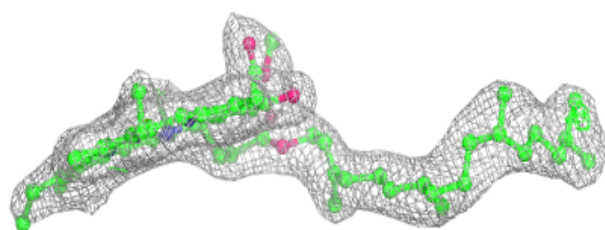
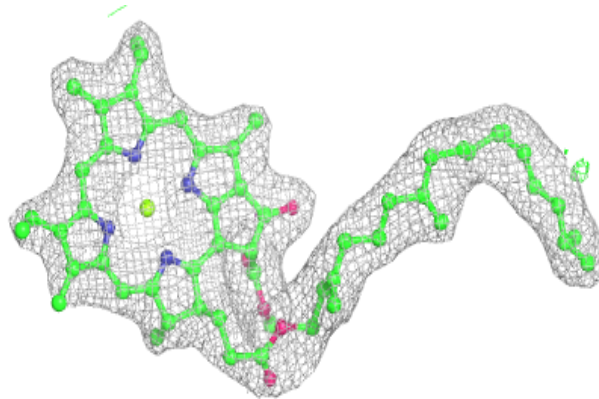
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



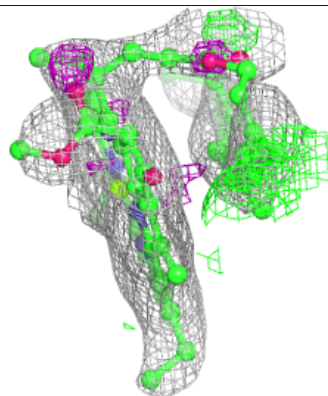
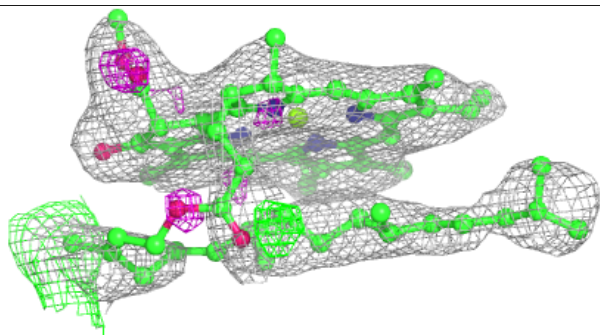
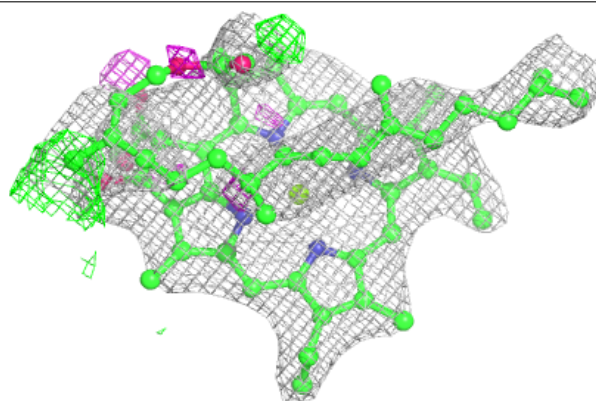


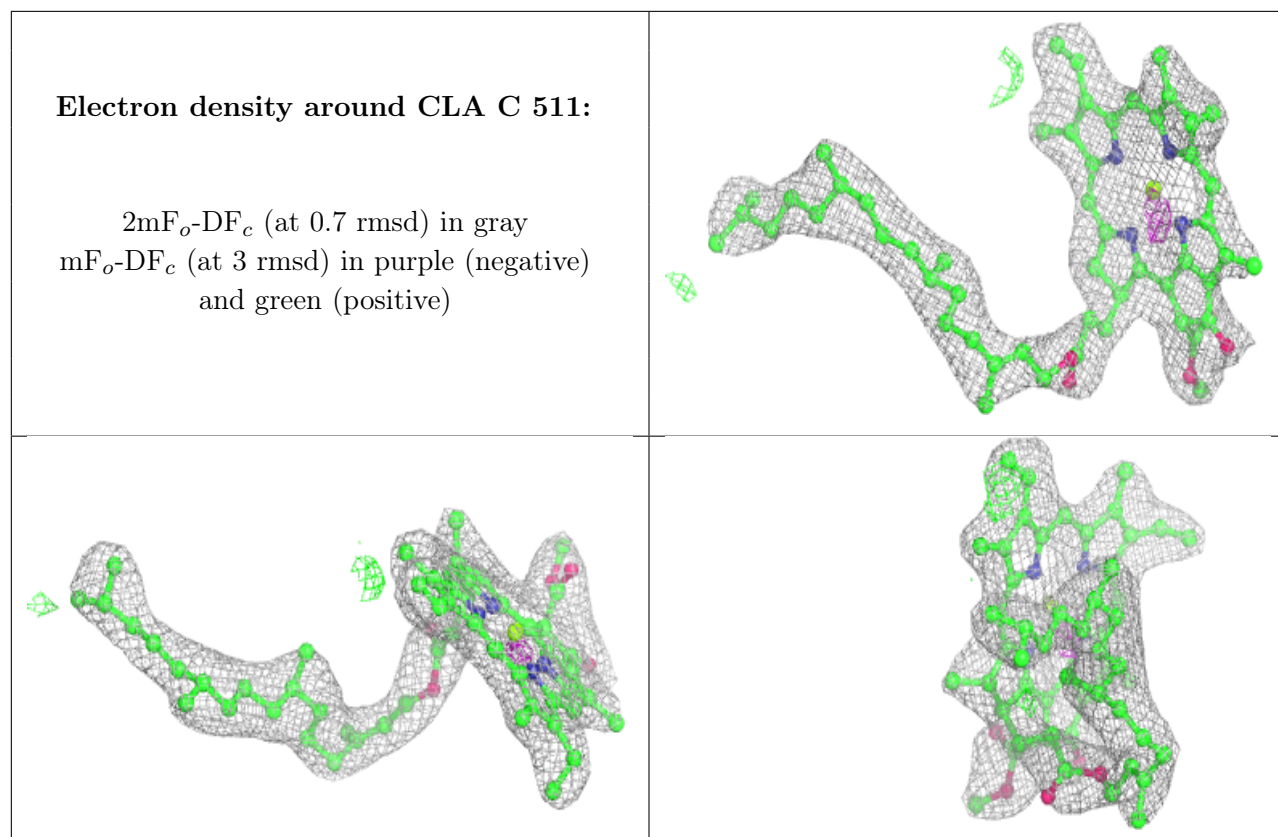
**Electron density around CLA B 603:**

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

**Electron density around CLA B 602:**

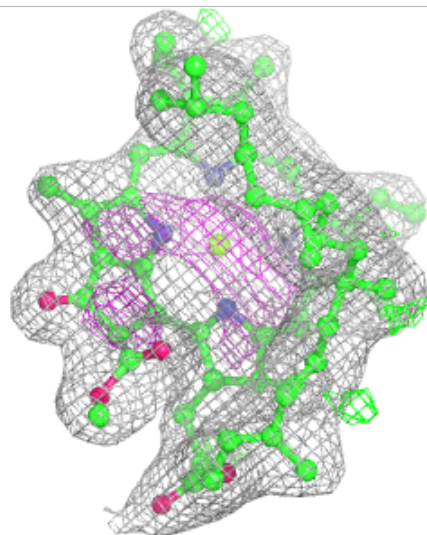
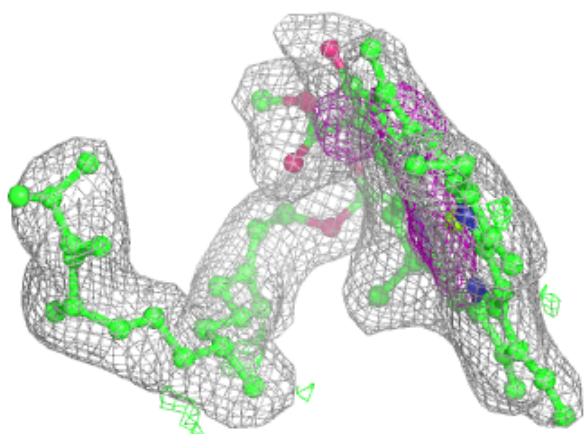
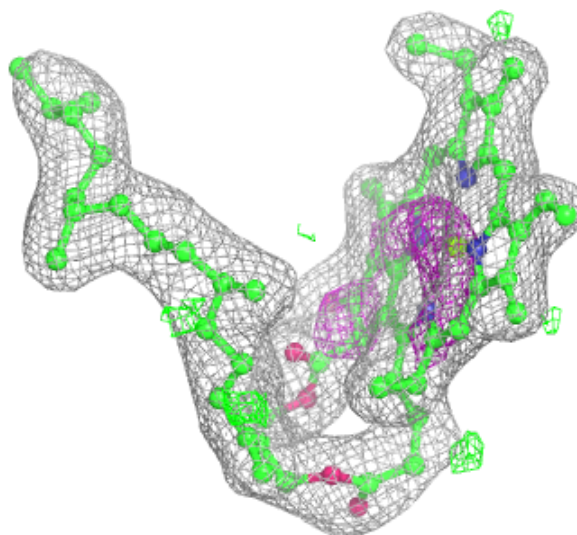
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





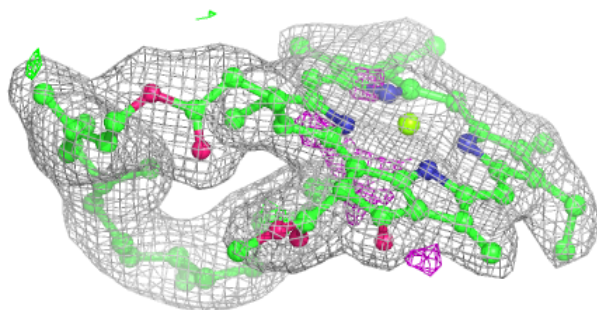
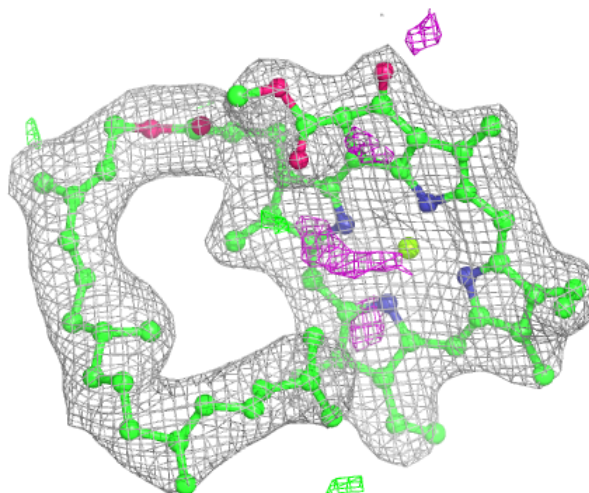
**Electron density around CLA B 614:**

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



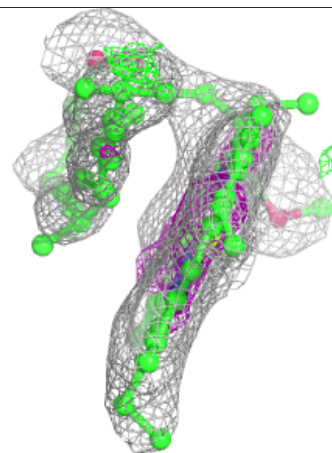
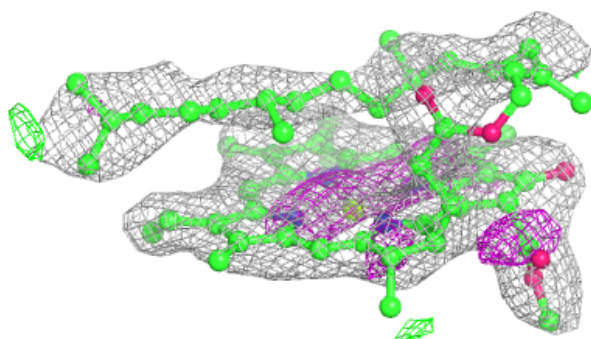
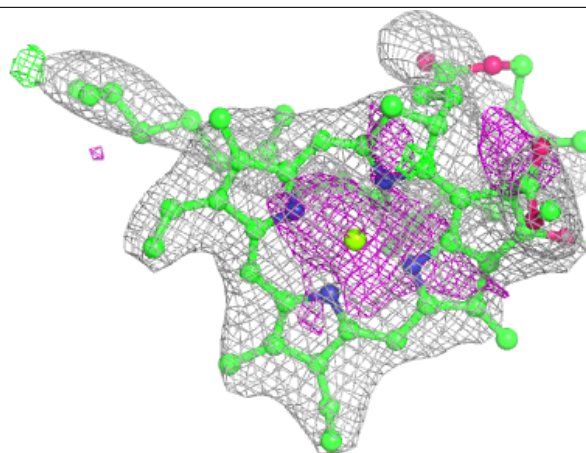
**Electron density around CLA b 624:**

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

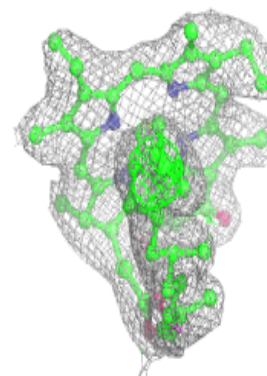
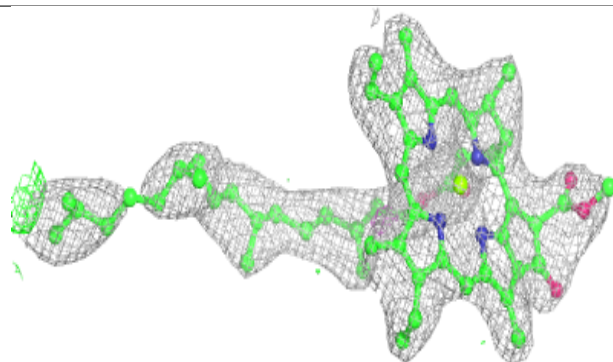
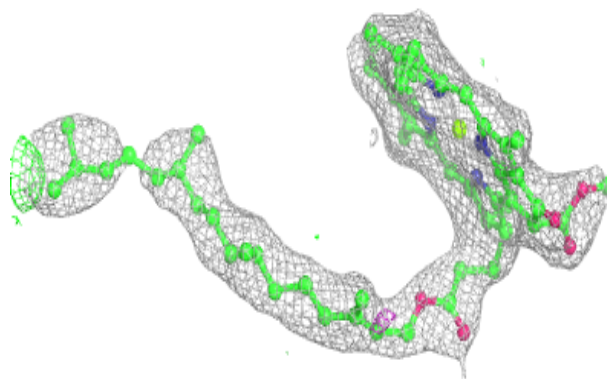


**Electron density around CLA b 610:**

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

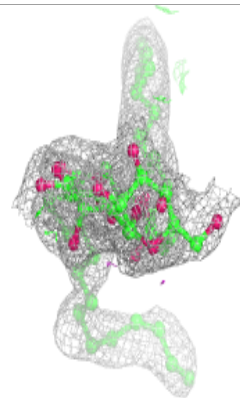
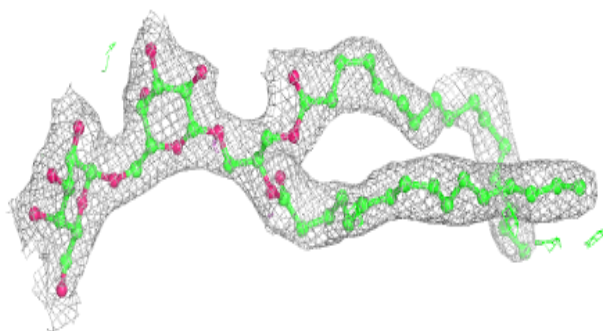
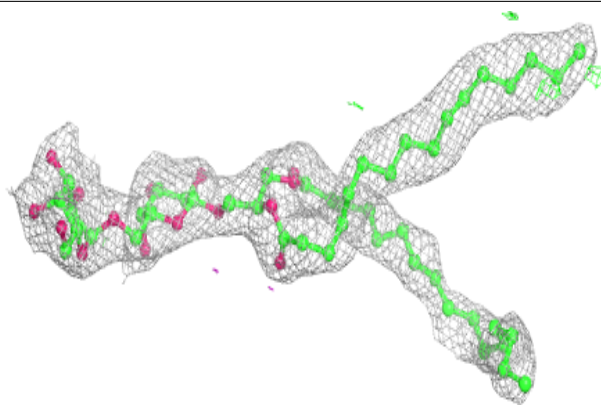
**Electron density around CLA c 508:**

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

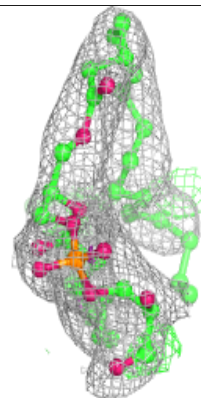
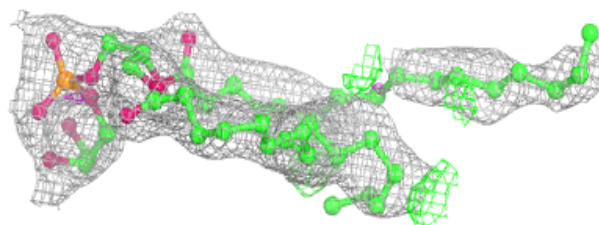
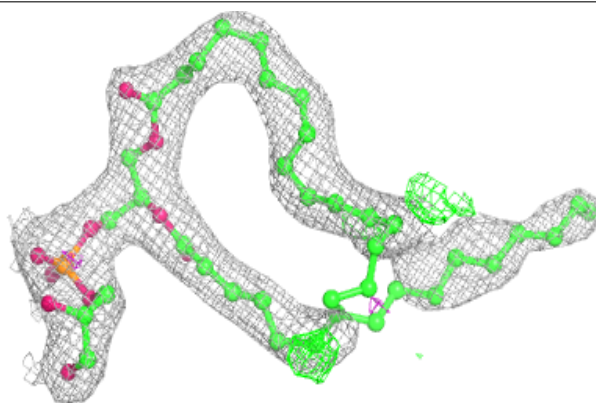


**Electron density around DGD c 519:**

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

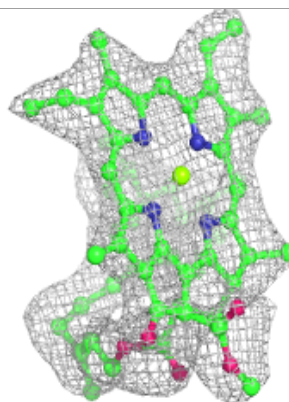
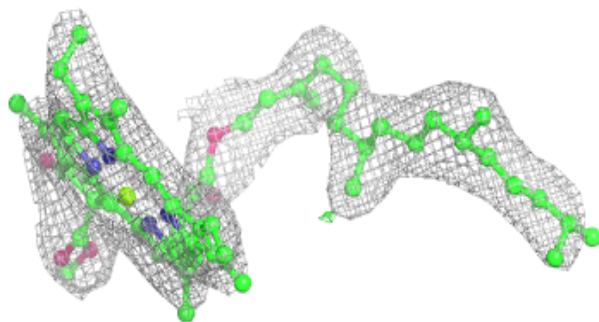
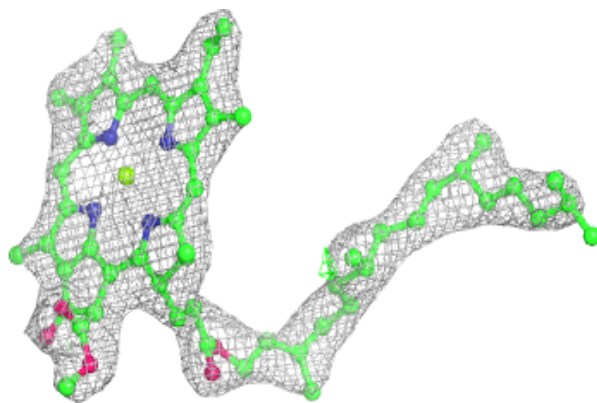
**Electron density around LHG d 410:**

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



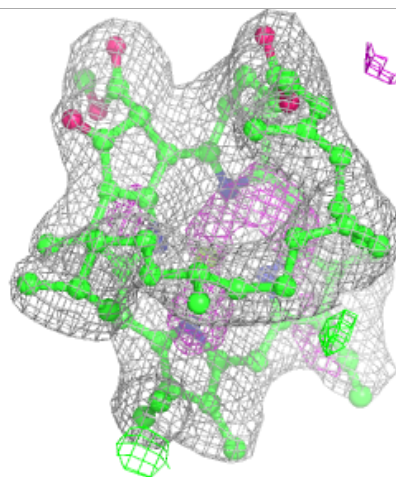
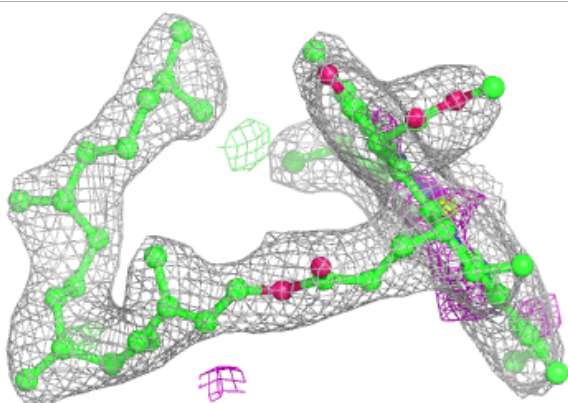
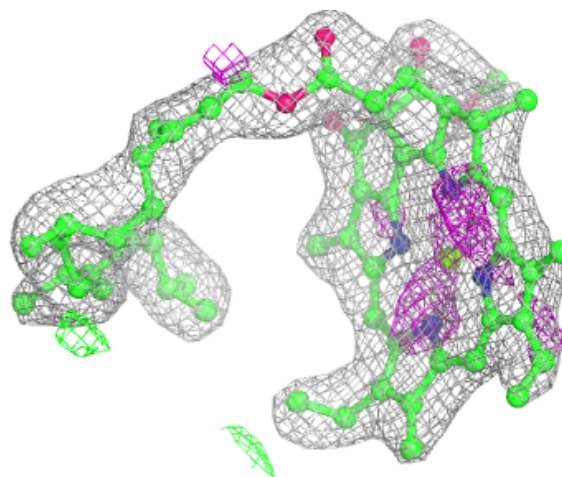
**Electron density around CLA c 515:**

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



**Electron density around CLA C 503:**

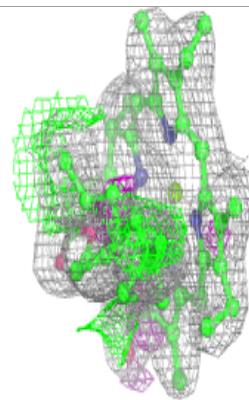
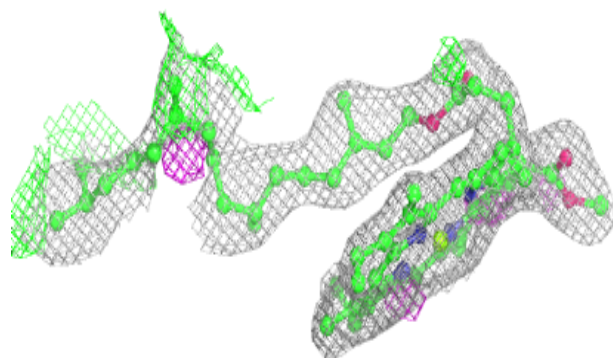
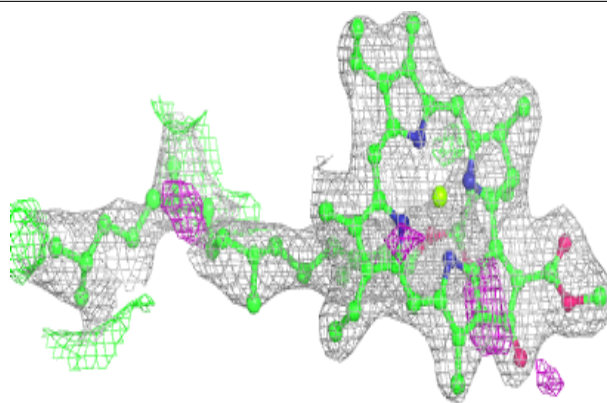
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



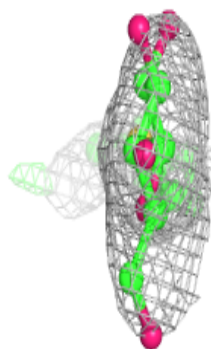
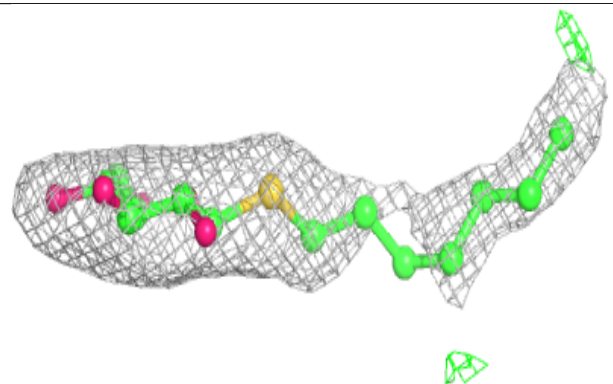
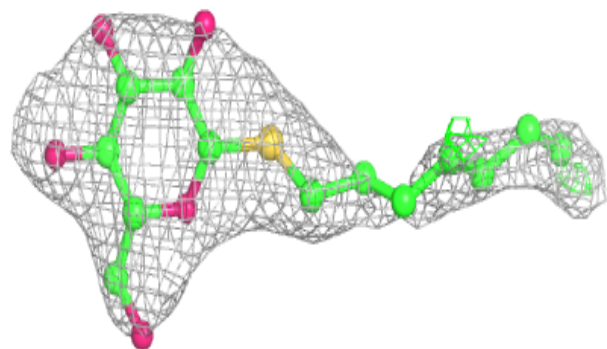


**Electron density around CLA B 615:**

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

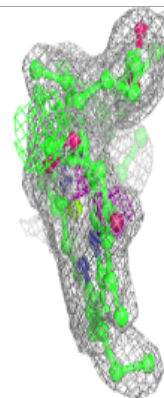
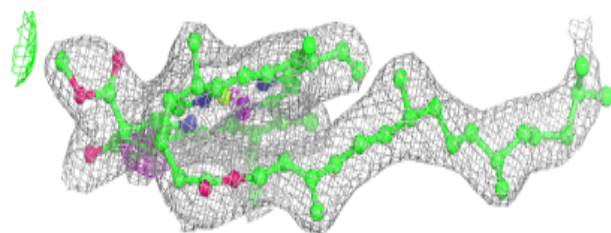
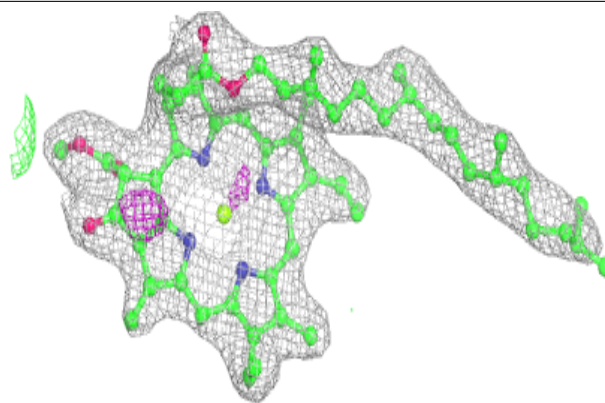
**Electron density around HTG C 522:**

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

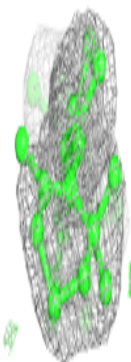
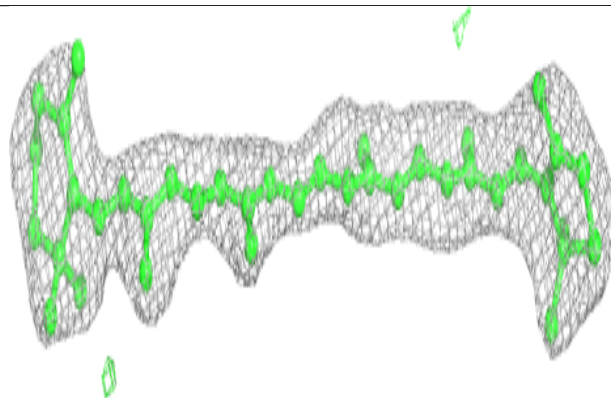
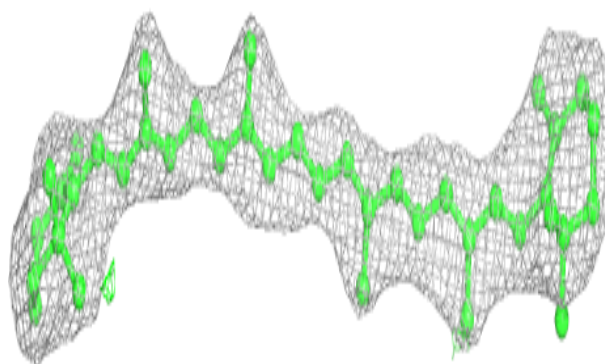


**Electron density around CLA C 501:**

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

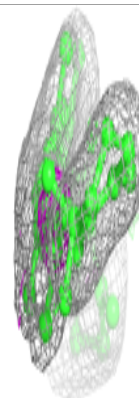
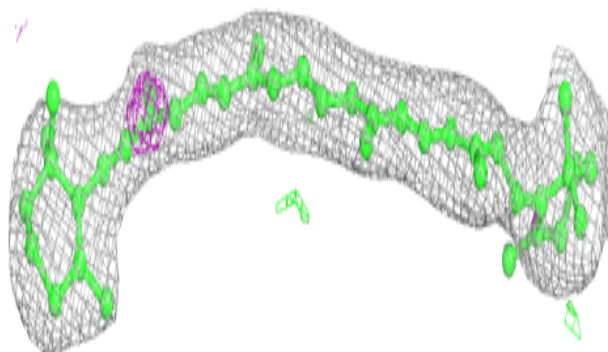
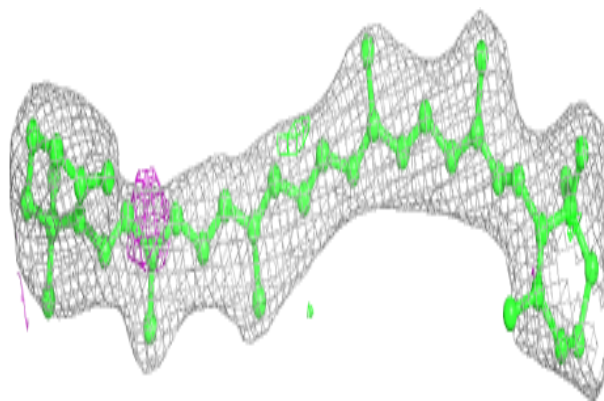
**Electron density around BCR c 526:**

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

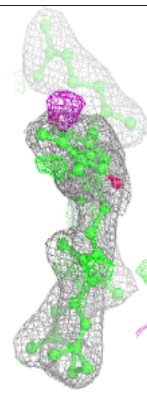
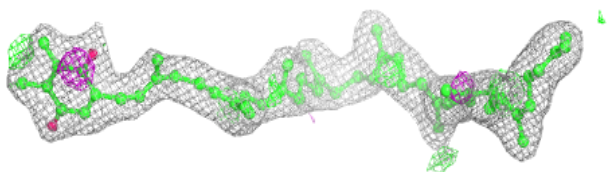
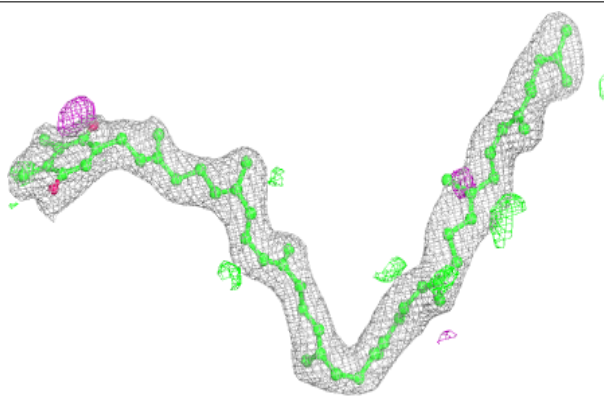


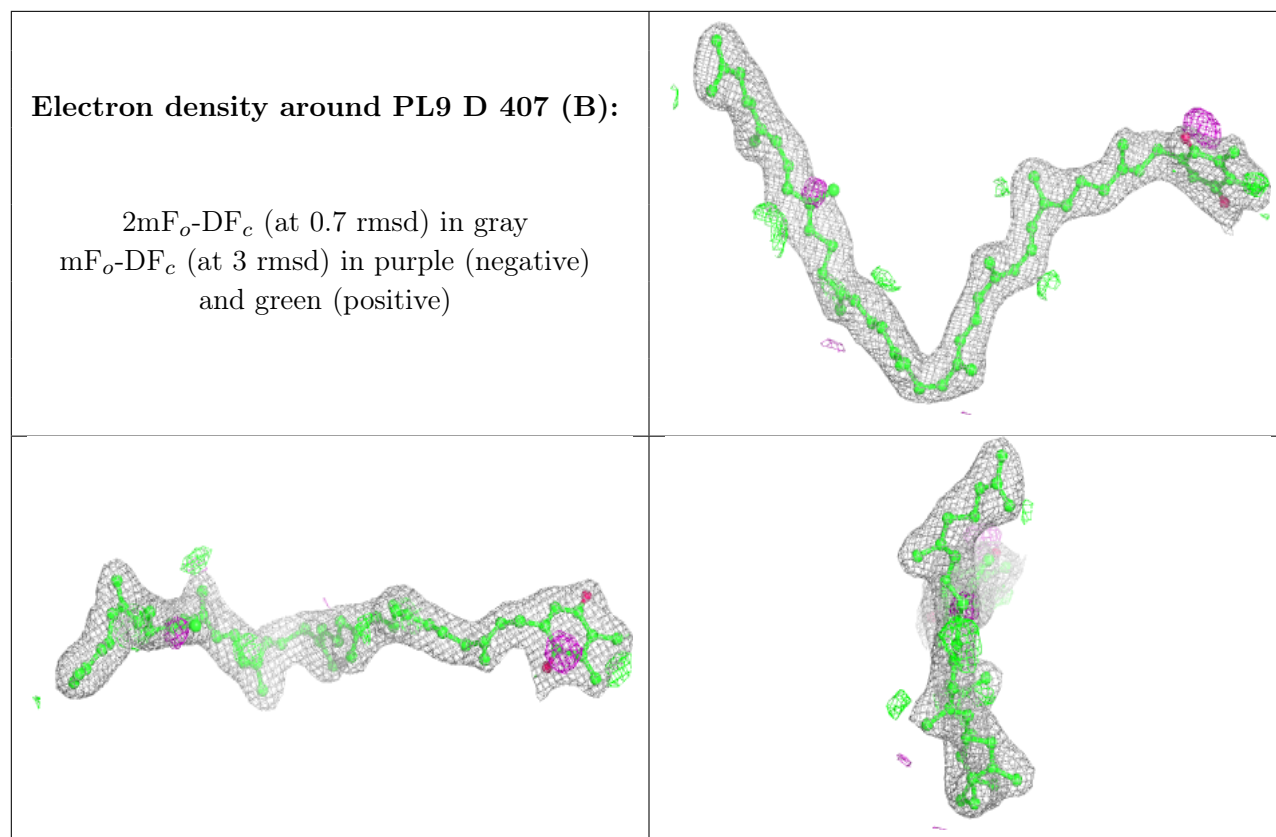
**Electron density around BCR d 406:**

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

**Electron density around PL9 D 407 (A):**

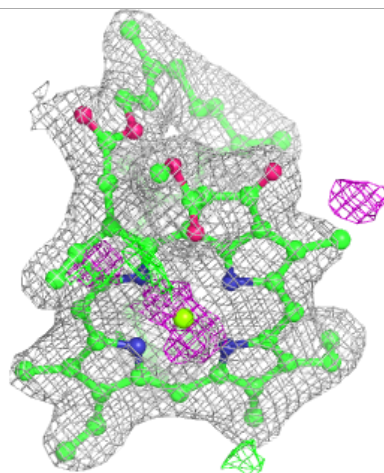
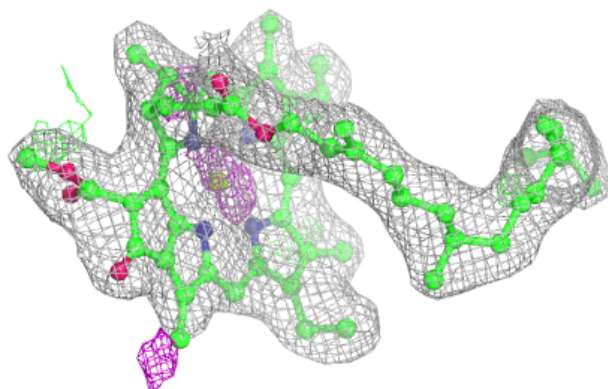
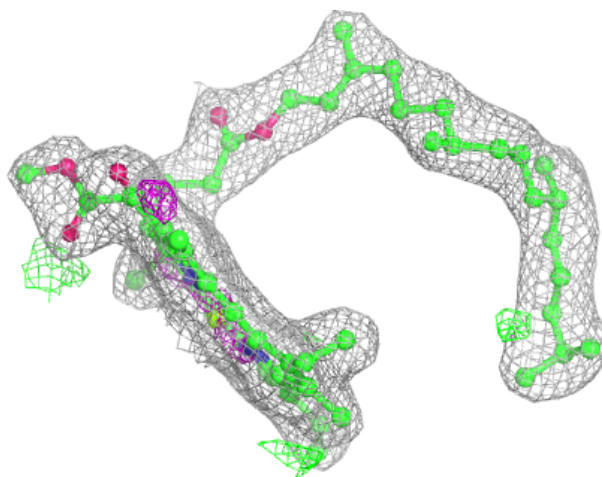
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





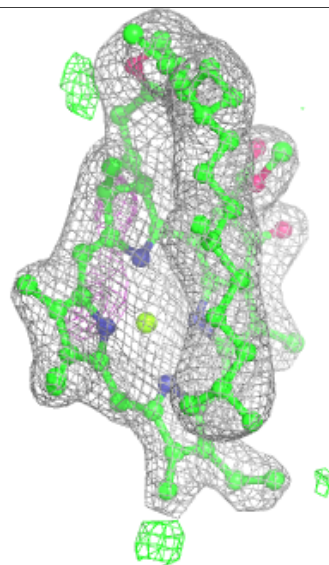
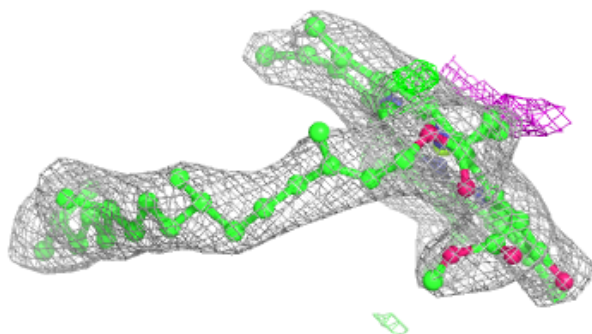
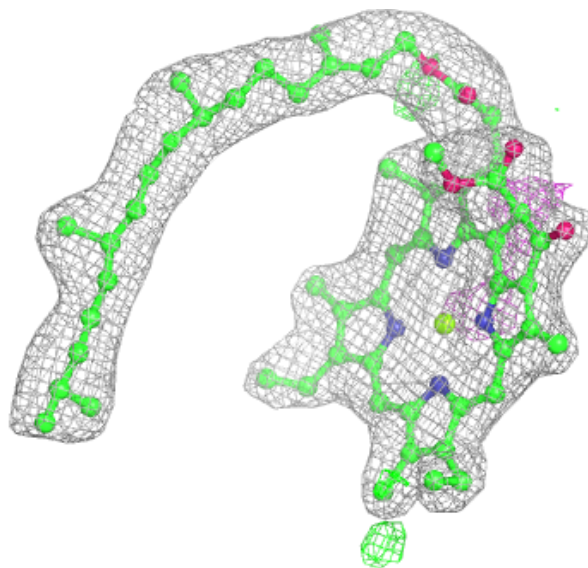
**Electron density around CLA b 620:**

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



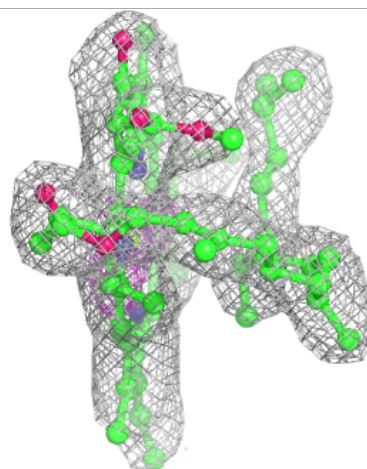
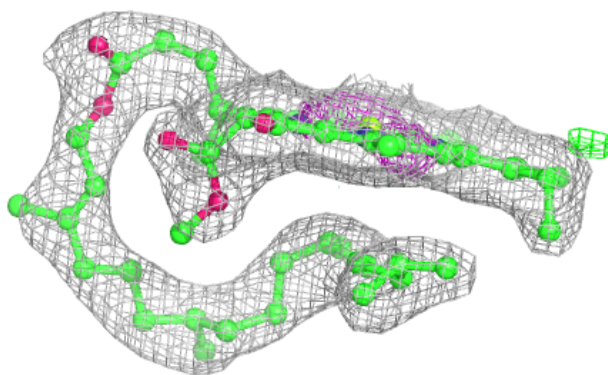
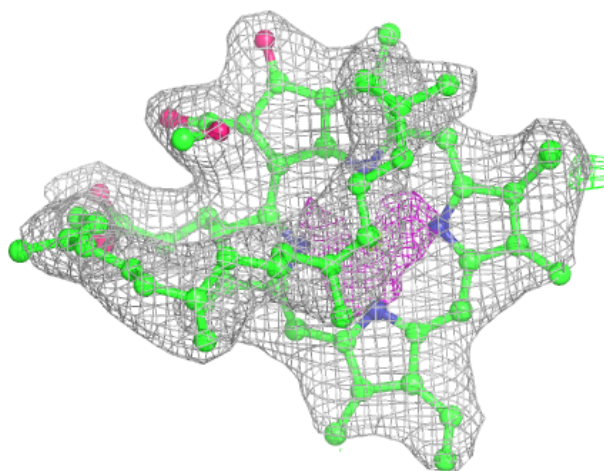
**Electron density around CLA c 511:**

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



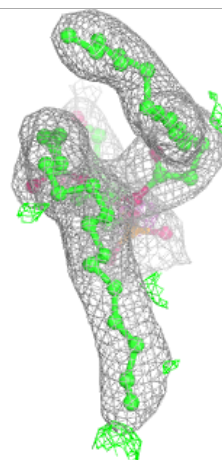
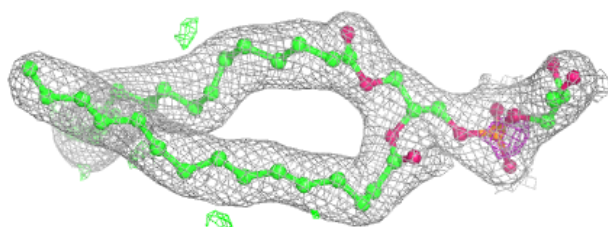
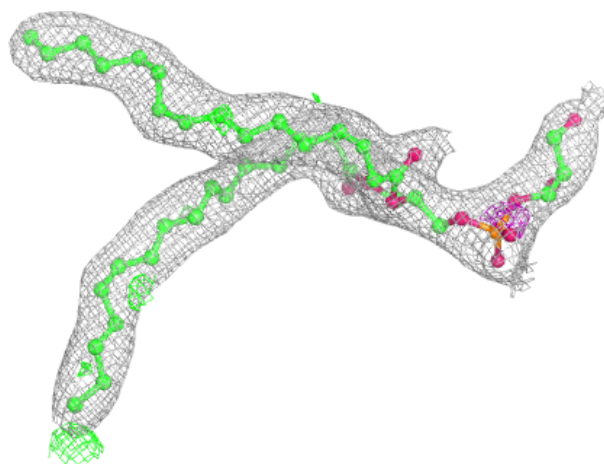
**Electron density around CLA C 510:**

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



**Electron density around LHG d 409:**

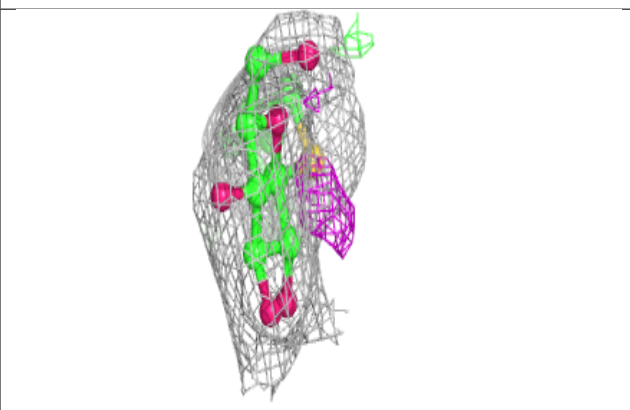
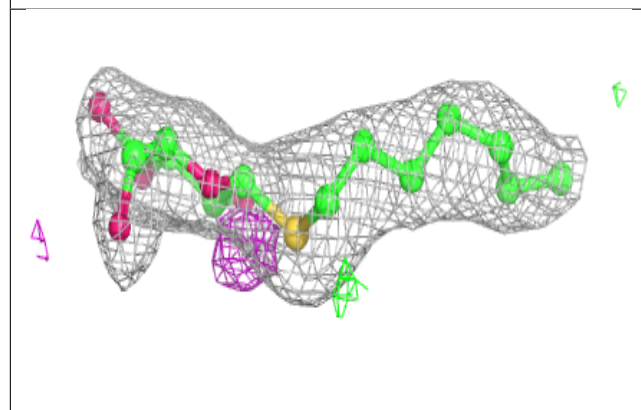
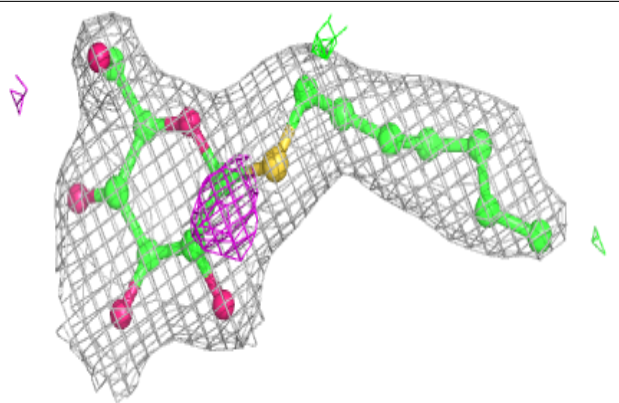
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



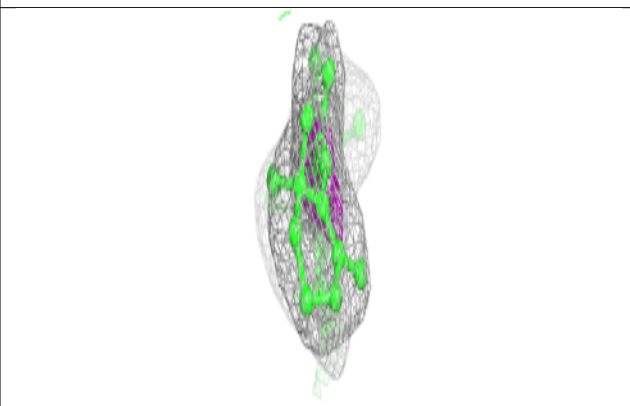
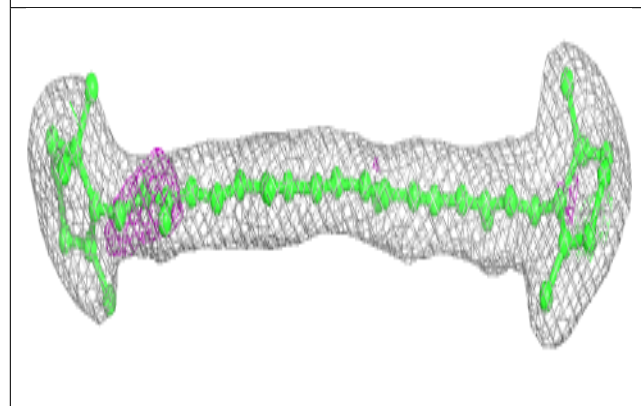
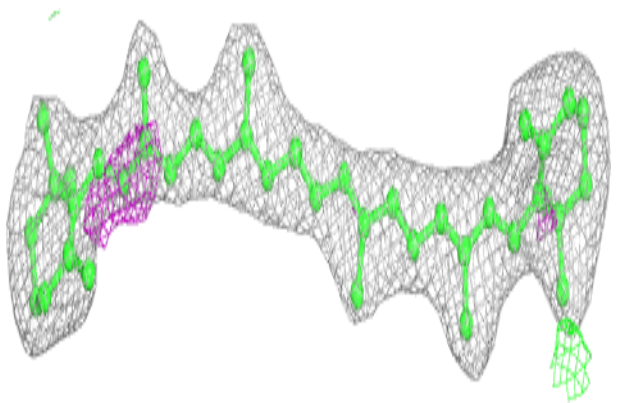


**Electron density around HTG B 622:**

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

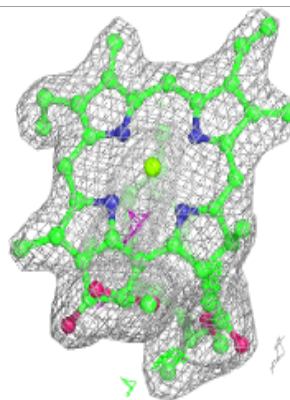
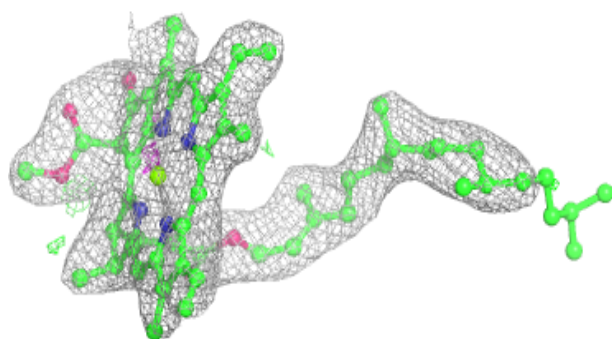
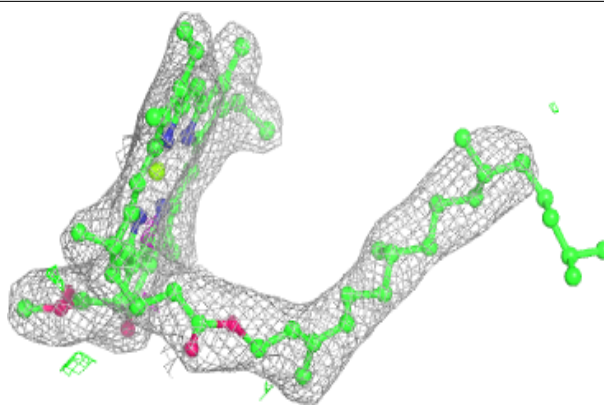
**Electron density around BCR b 627:**

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

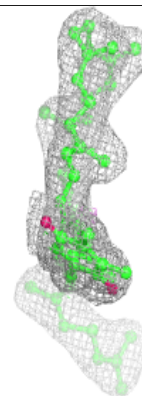
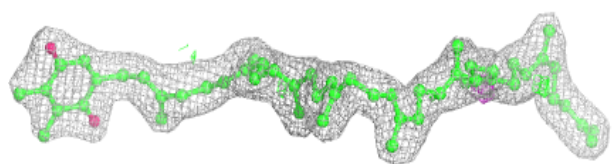
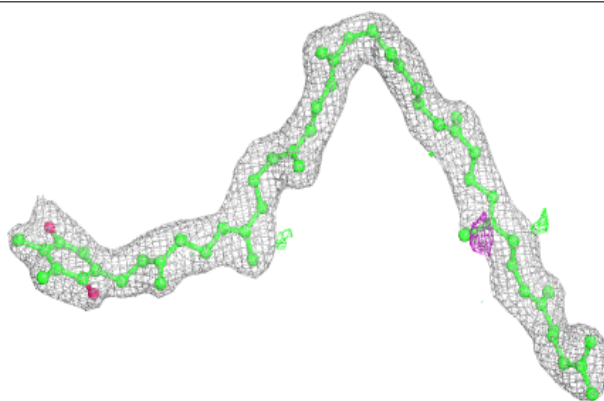


**Electron density around CLA C 508:**

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

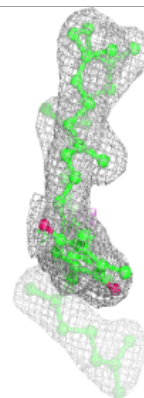
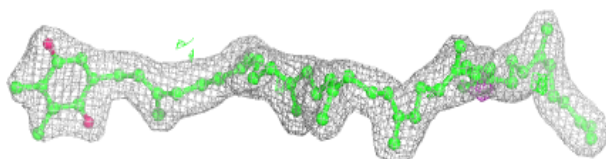
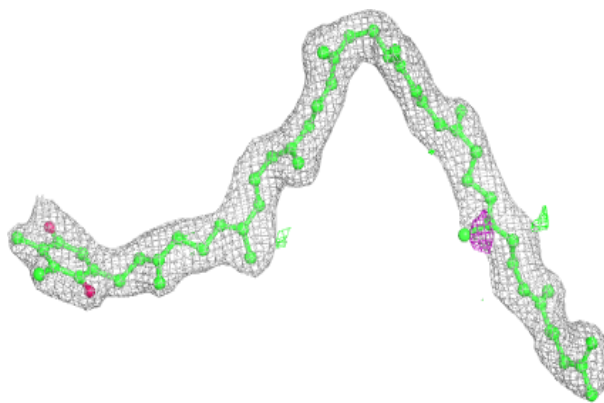
**Electron density around PL9 d 407 (A):**

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



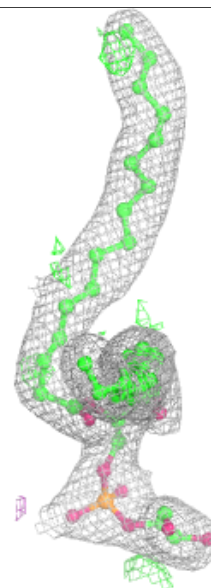
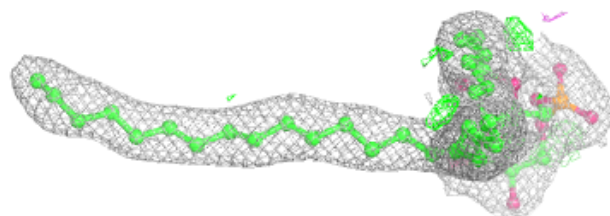
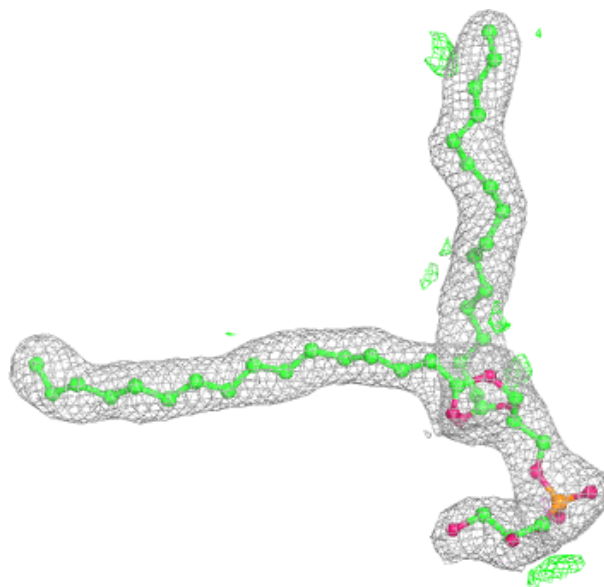
**Electron density around PL9 d 407 (B):**

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



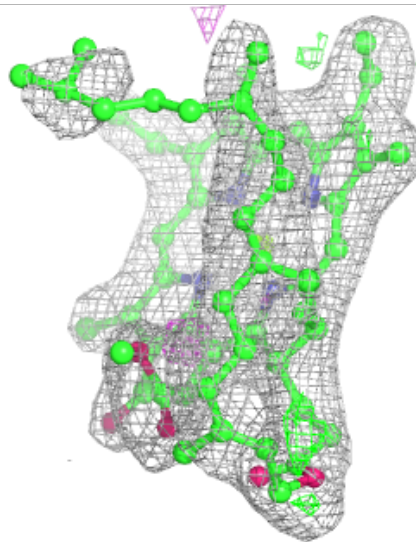
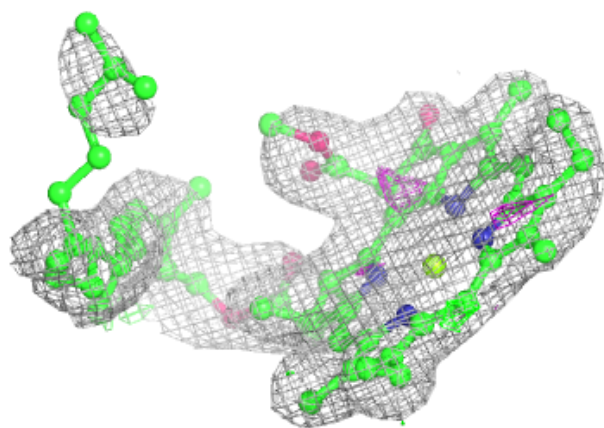
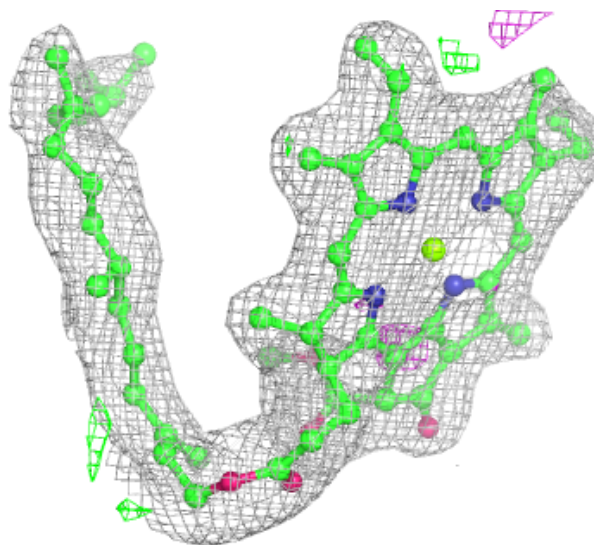
**Electron density around LHG L 101:**

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



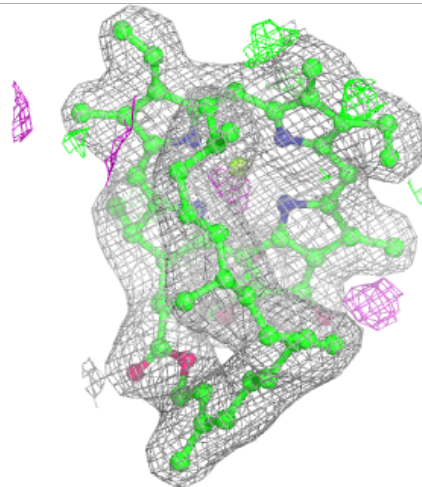
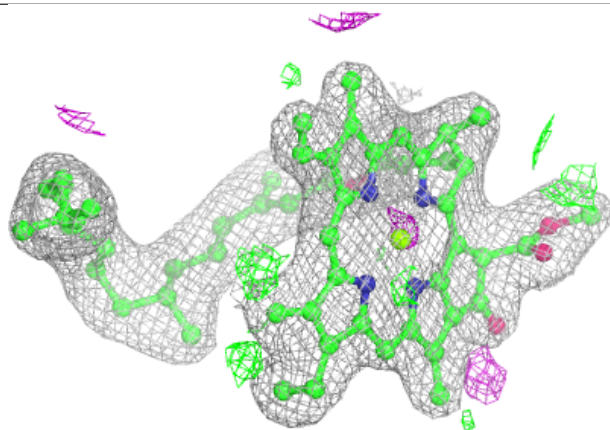
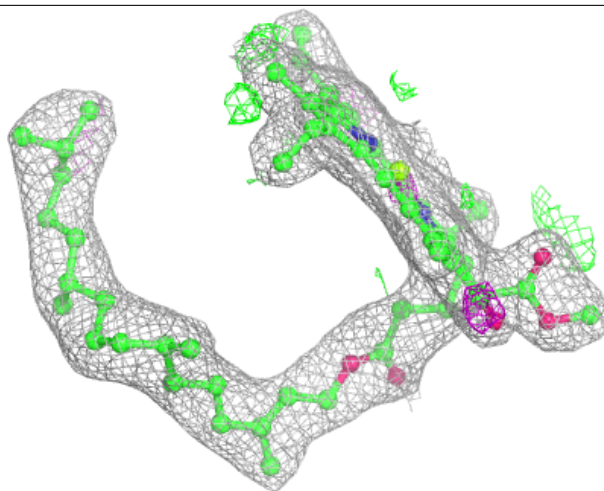
**Electron density around CLA b 625:**

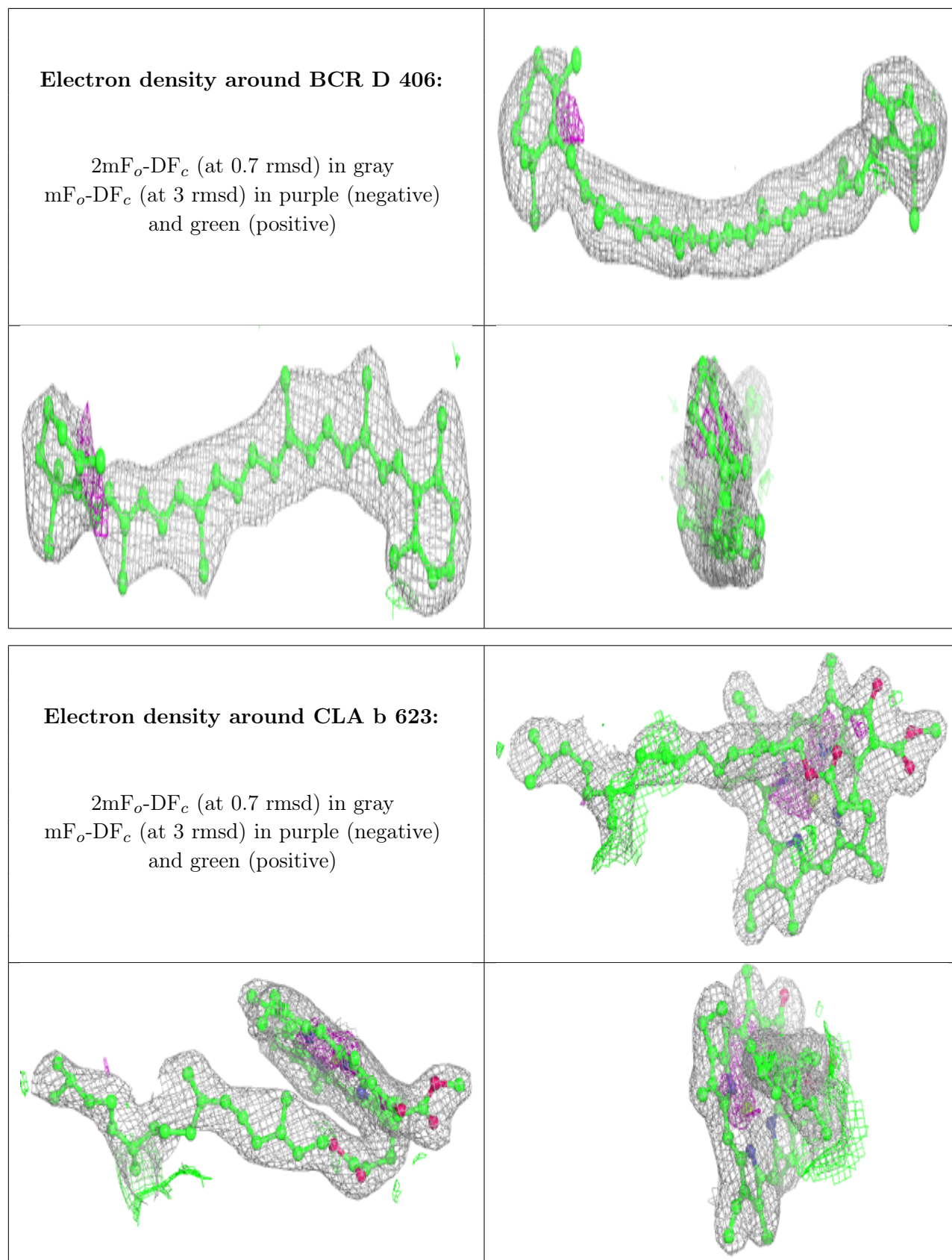
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 612:**

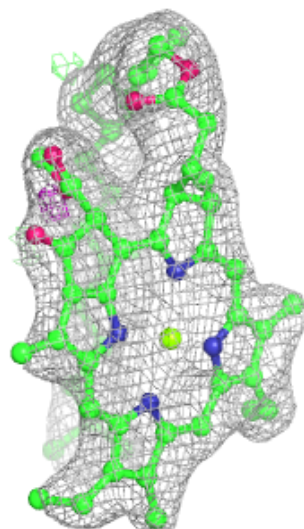
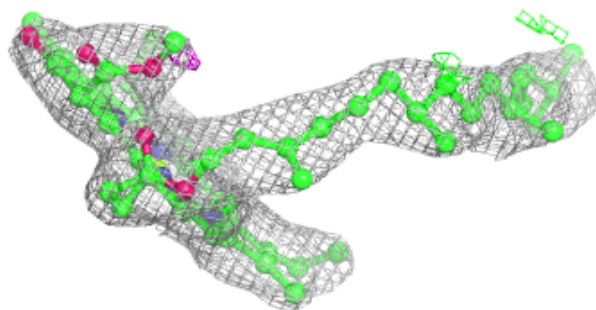
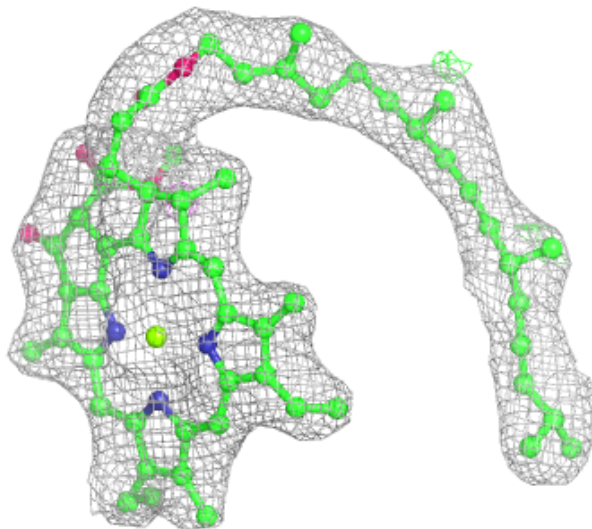
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA C 507:**

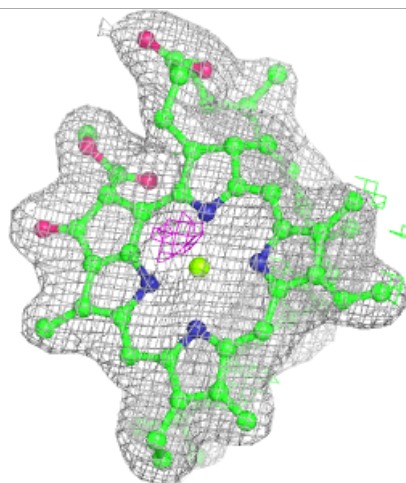
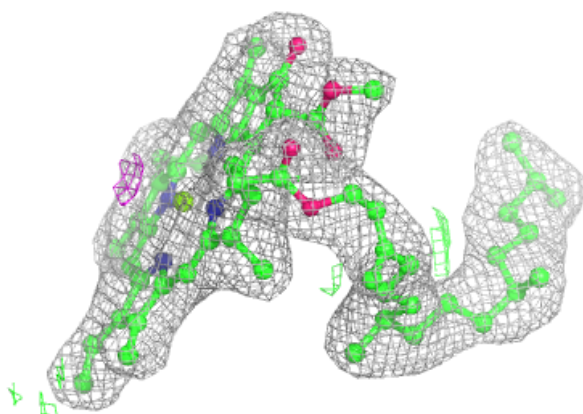
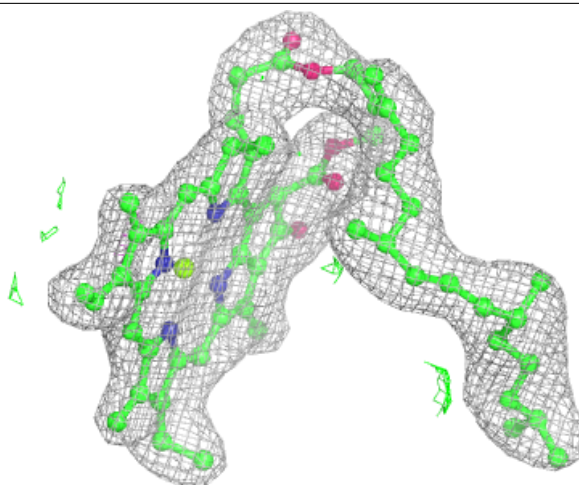
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





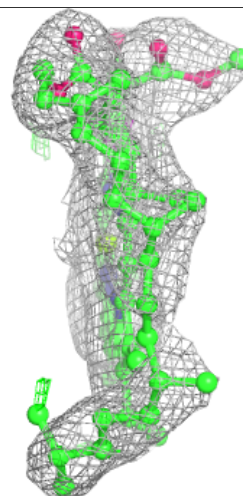
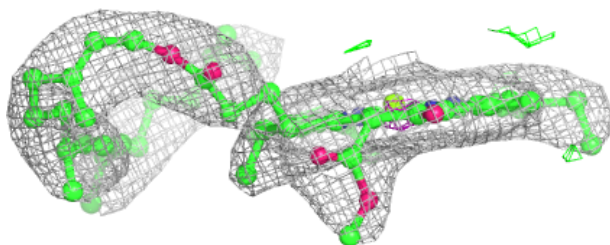
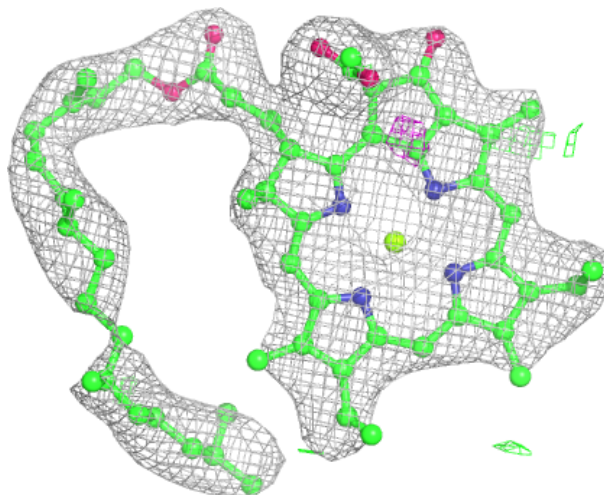
**Electron density around CLA b 622:**

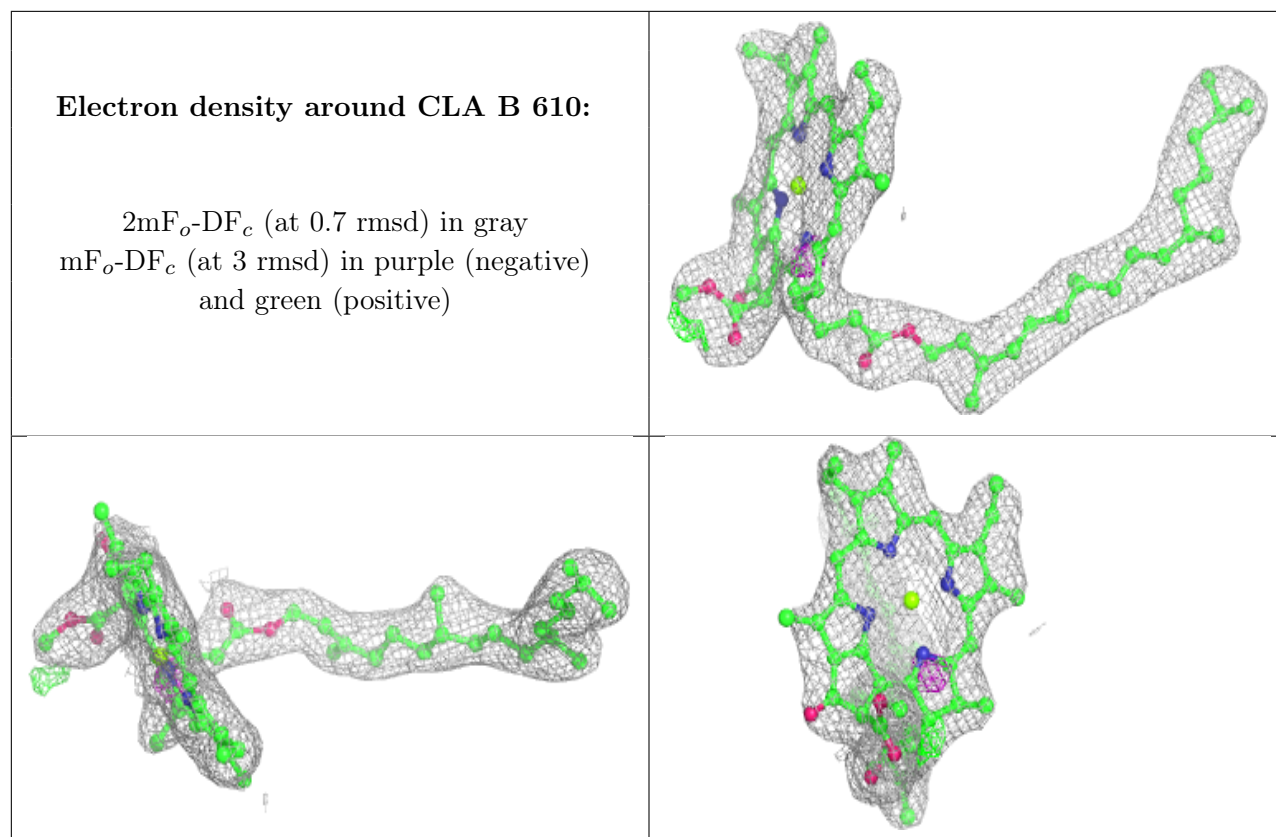
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA C 512:**

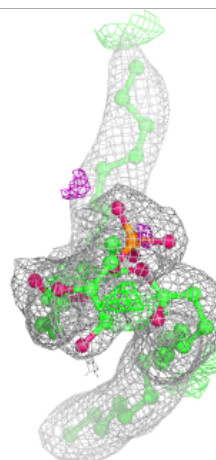
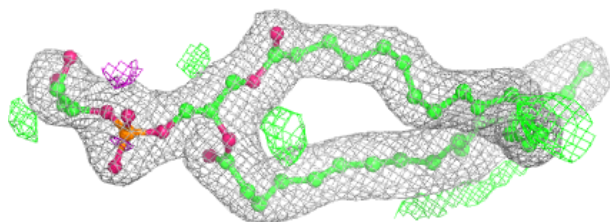
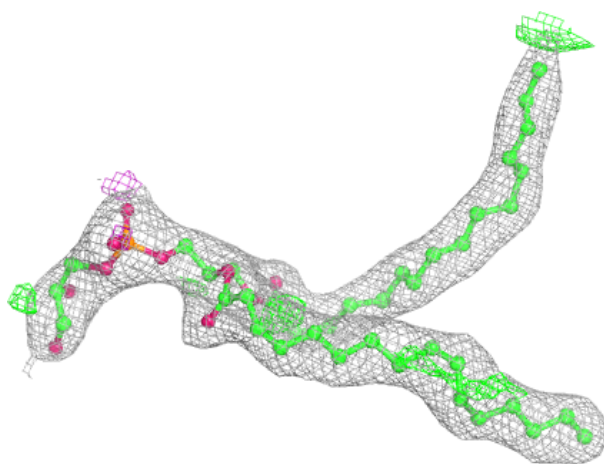
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





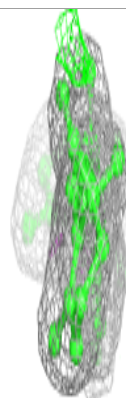
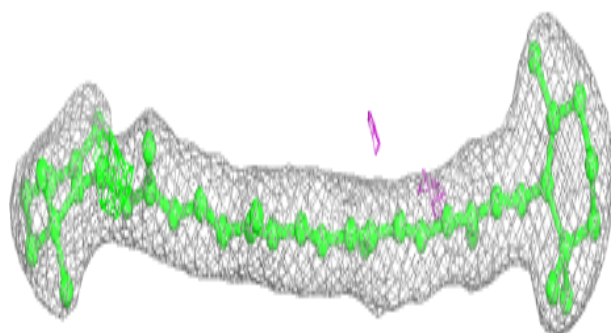
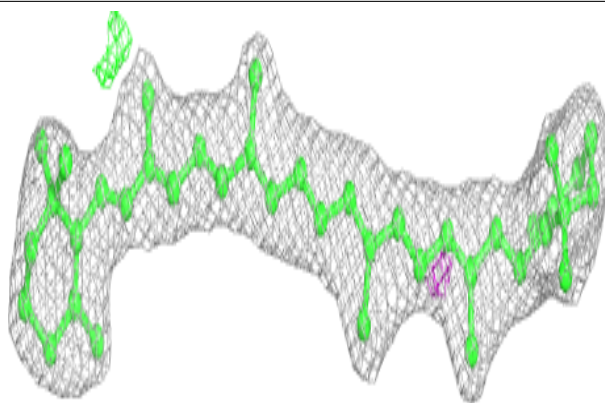
**Electron density around LHG D 410:**

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

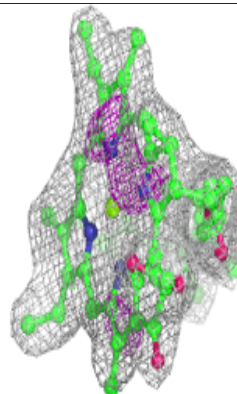
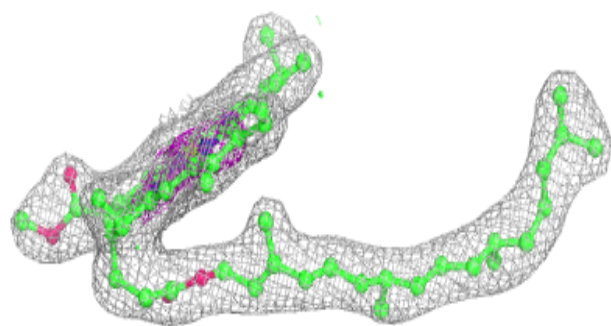
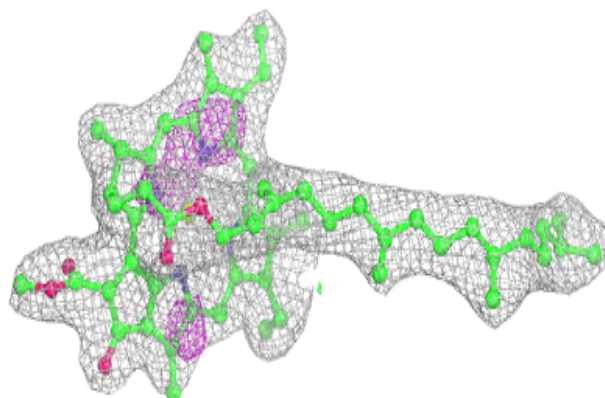


**Electron density around BCR b 626:**

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

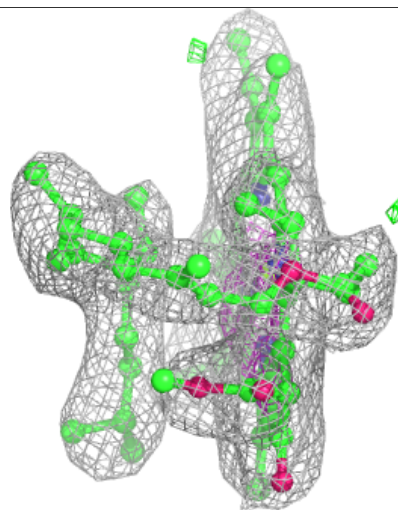
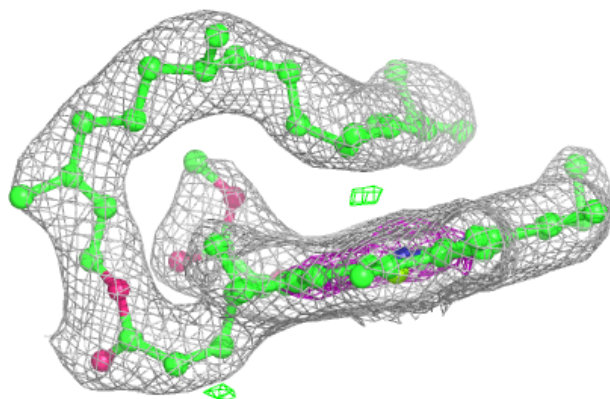
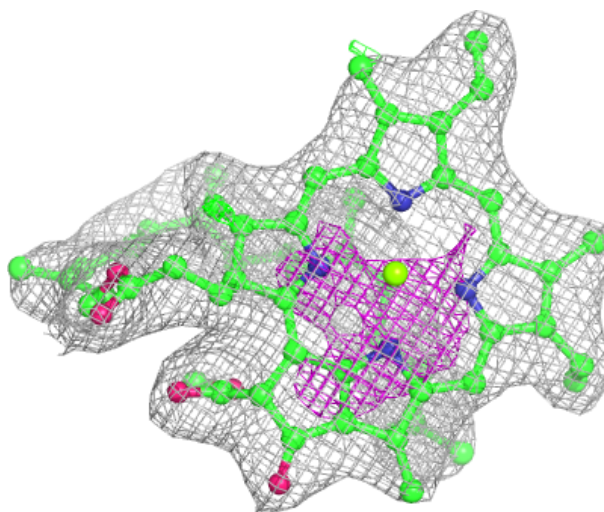
**Electron density around CLA b 617:**

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



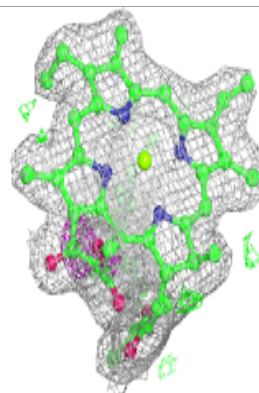
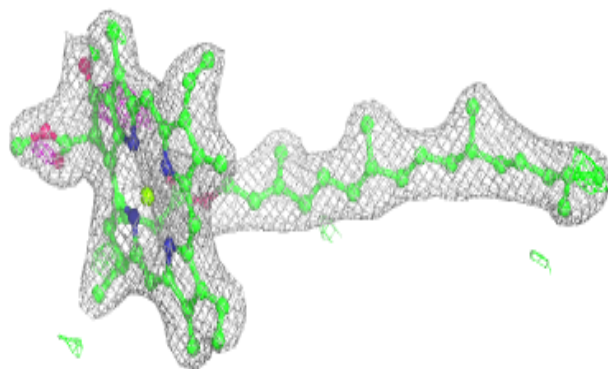
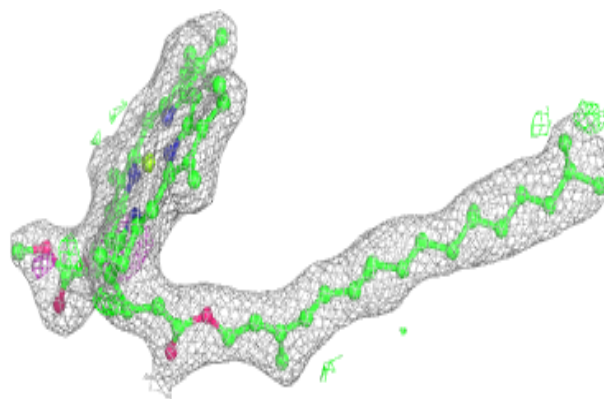
**Electron density around CLA c 514:**

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

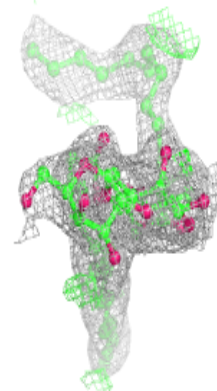
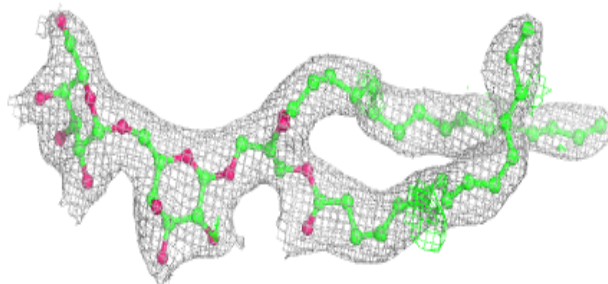
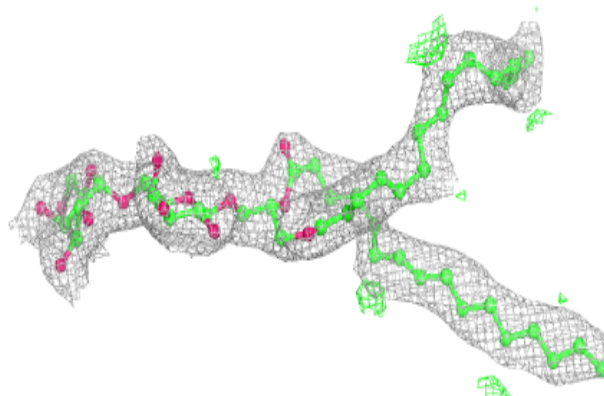


**Electron density around CLA B 608:**

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

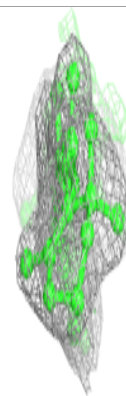
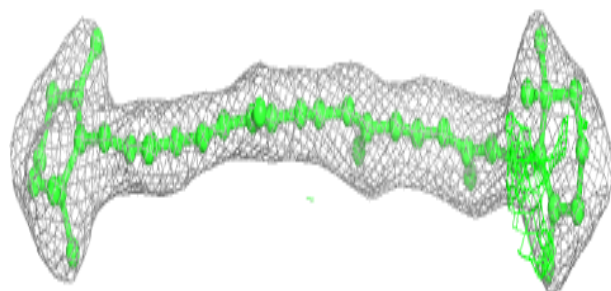
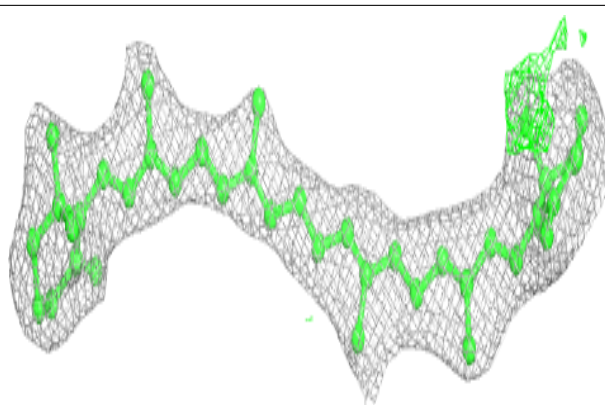
**Electron density around DGD C 516:**

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

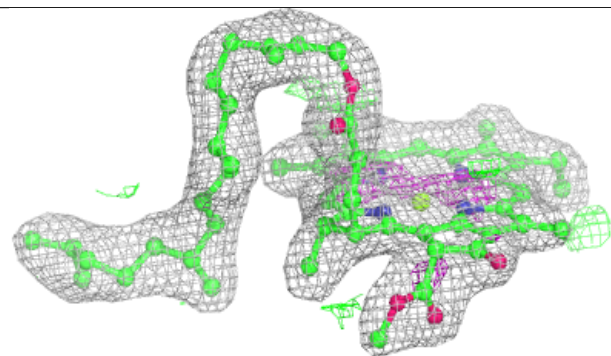
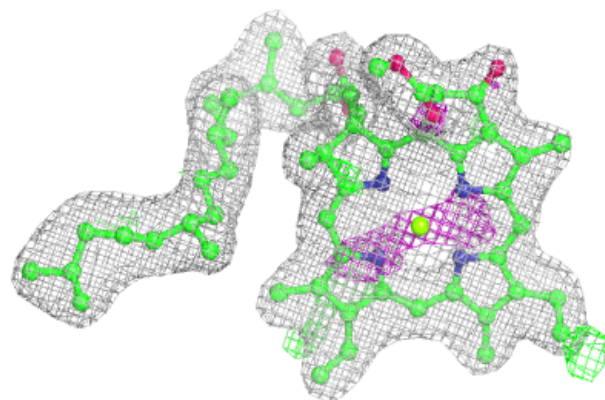


**Electron density around BCR y 101:**

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

**Electron density around CLA d 403:**

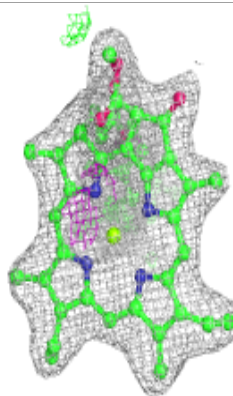
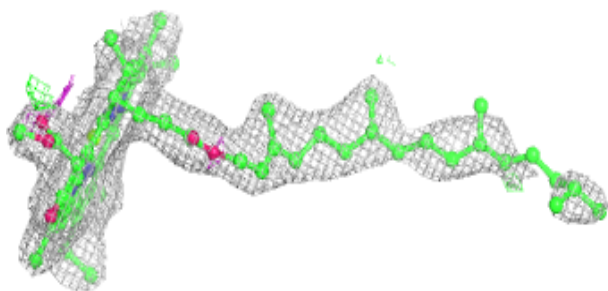
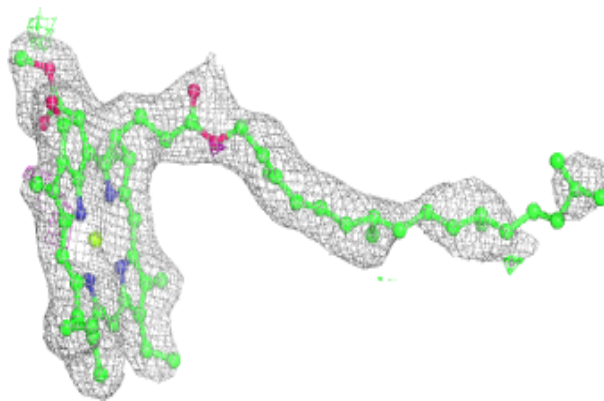
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



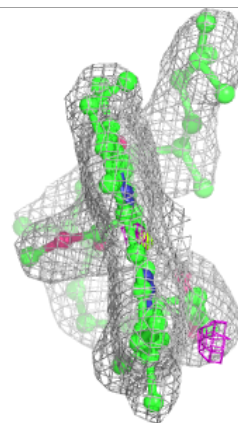
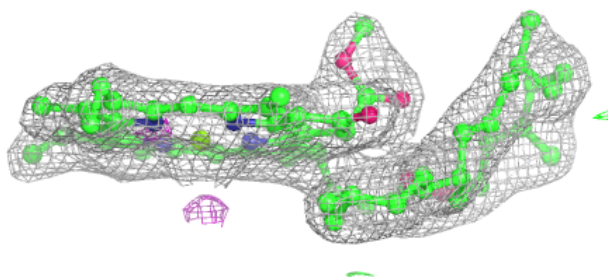
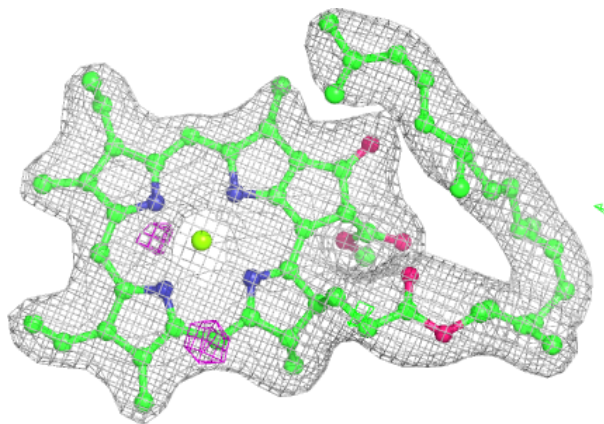


**Electron density around CLA d 405:**

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

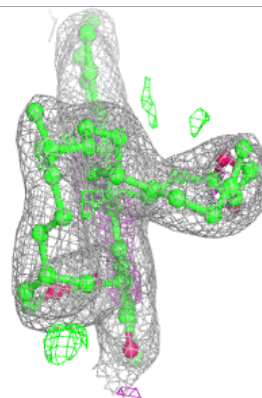
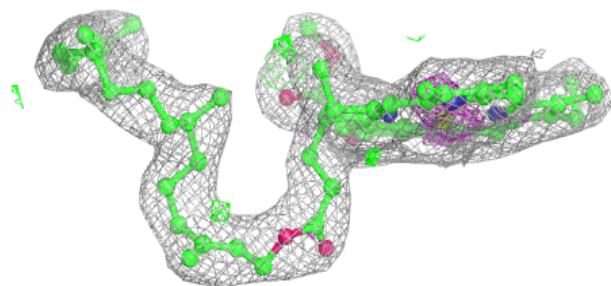
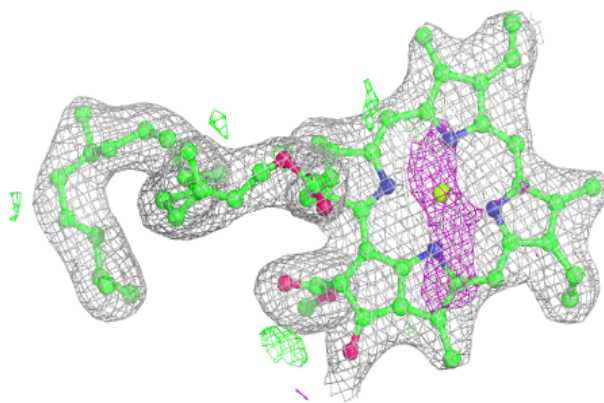
**Electron density around CLA b 619:**

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

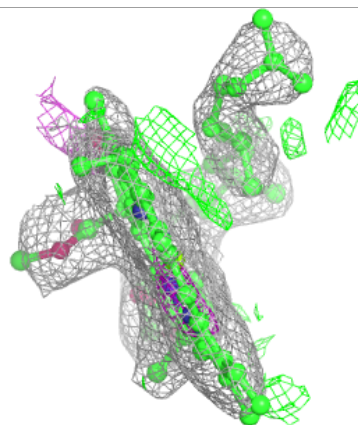
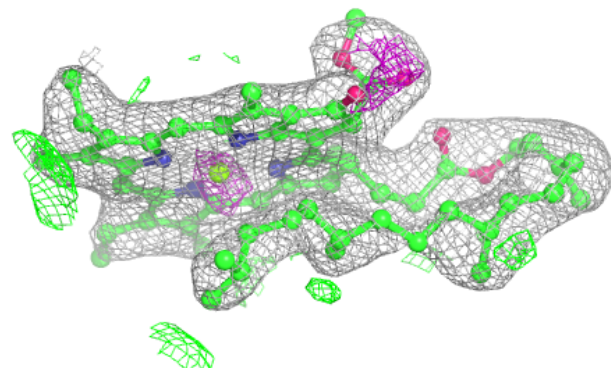
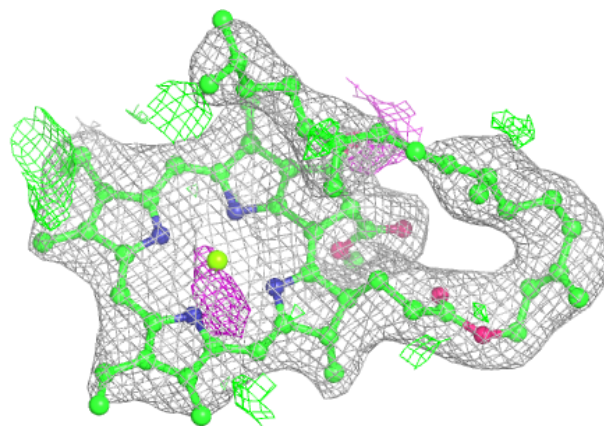


**Electron density around CLA B 613:**

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

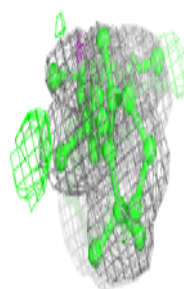
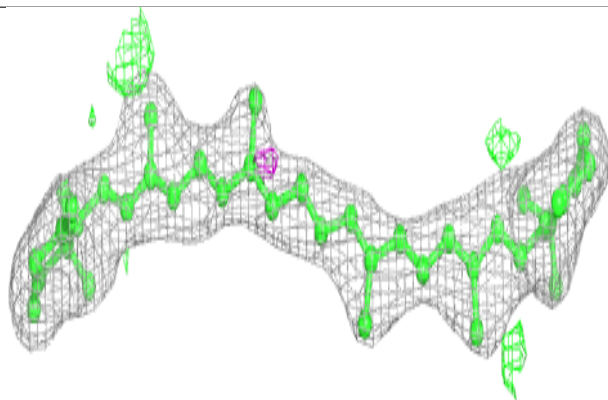
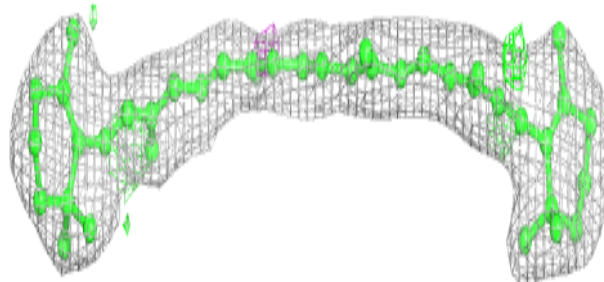
**Electron density around CLA c 513:**

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

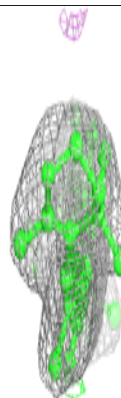
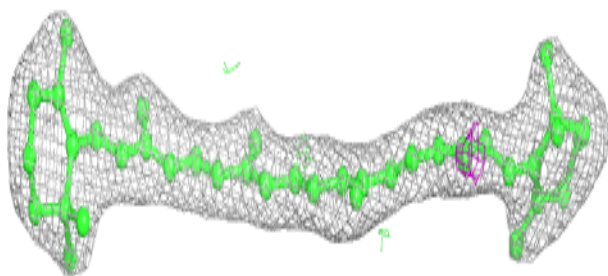
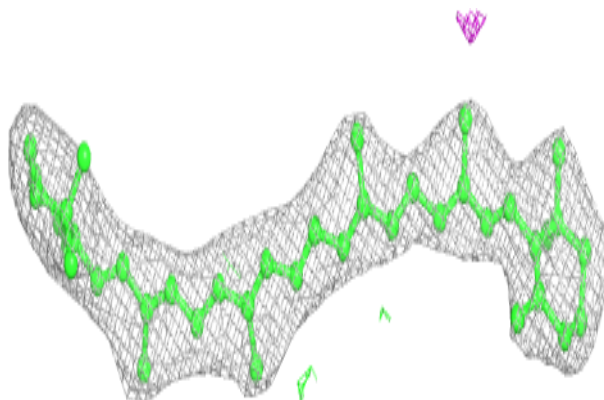


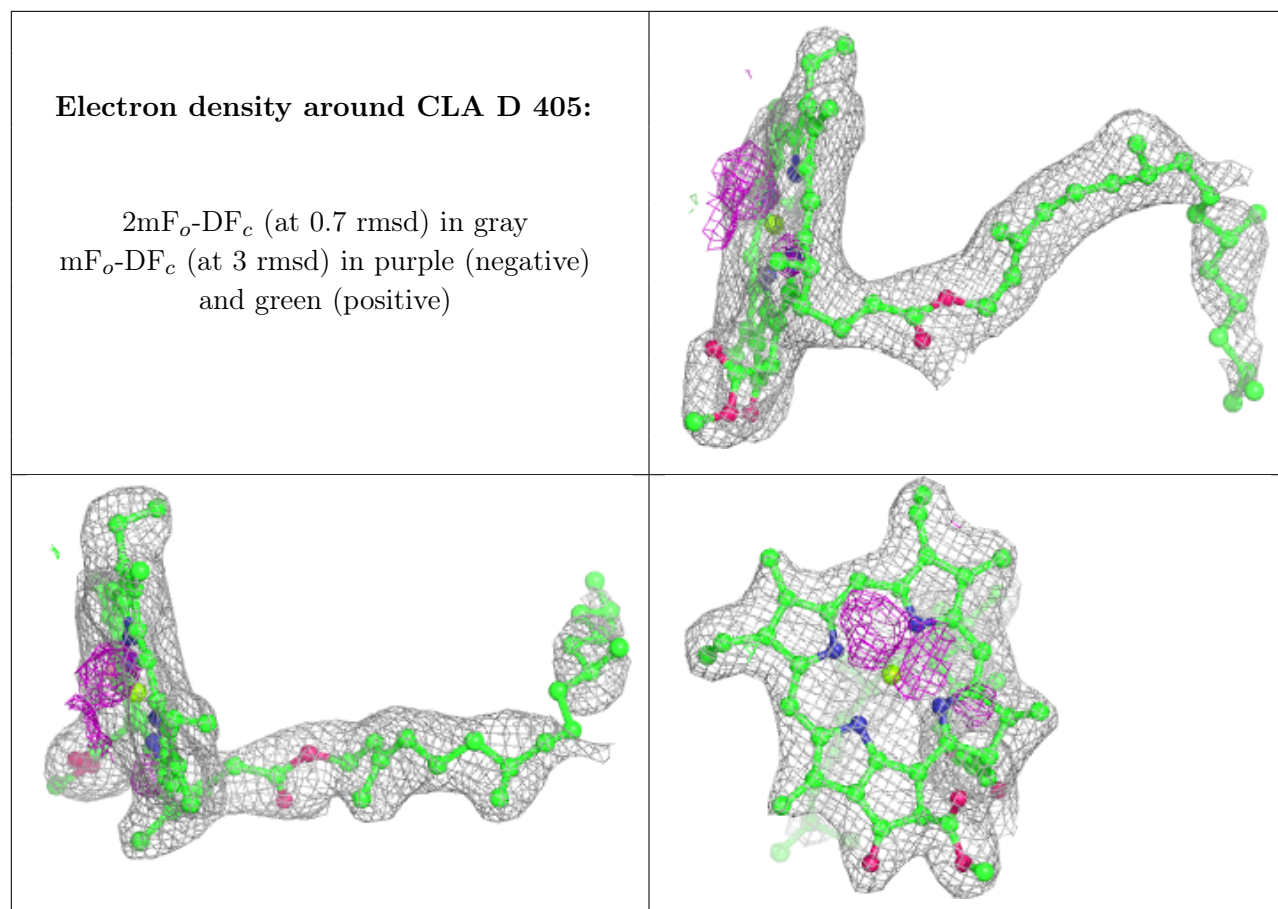
**Electron density around BCR K 101:**

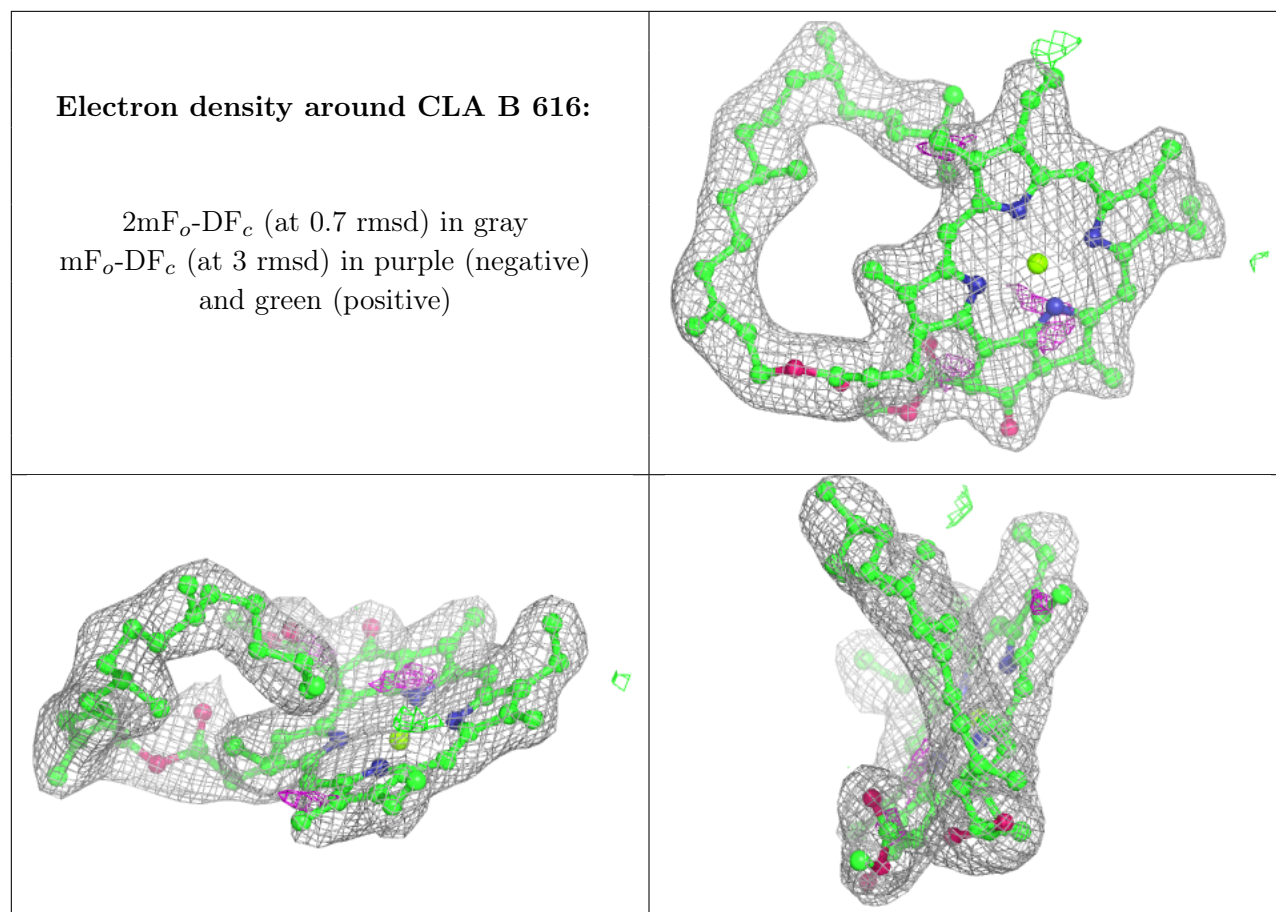
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around BCR Y 101:**

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

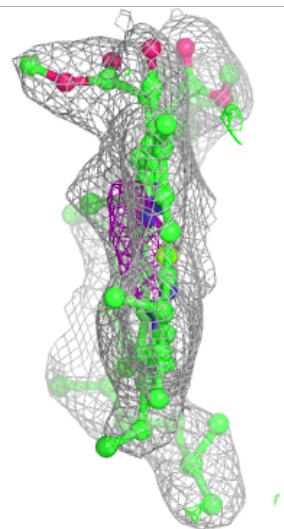
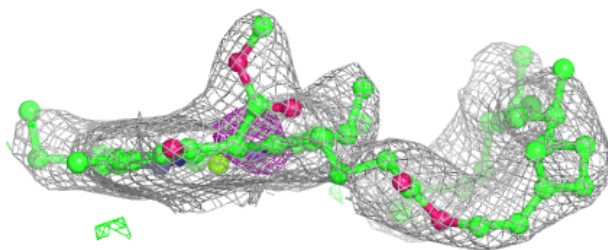
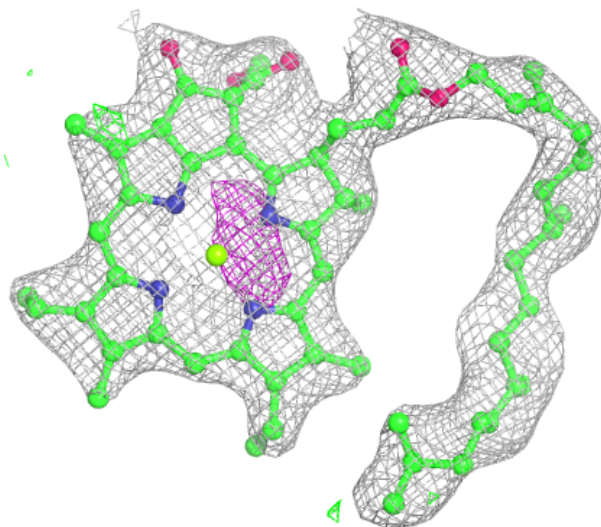






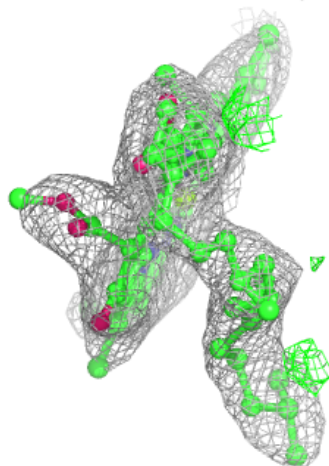
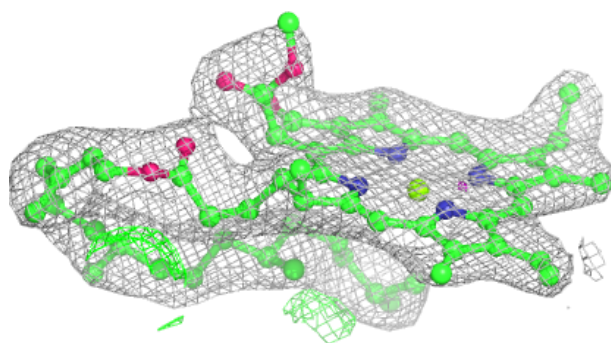
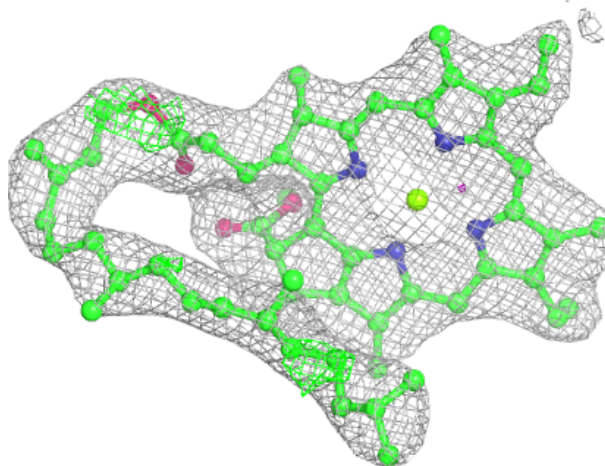
**Electron density around CLA c 516:**

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



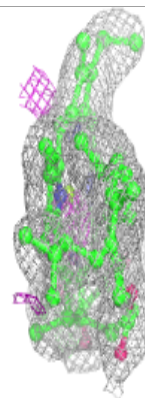
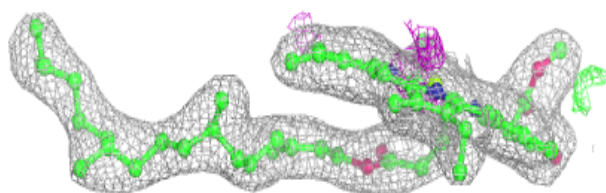
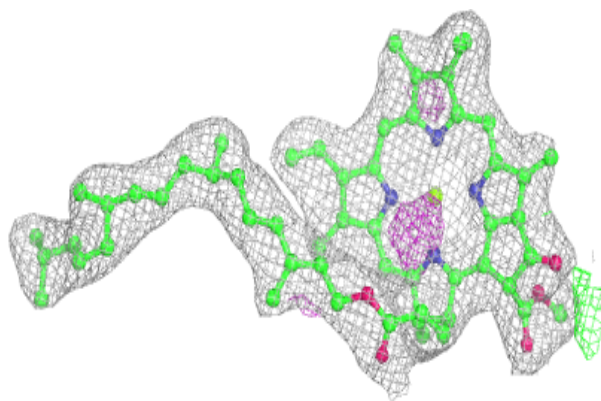
**Electron density around CLA C 509:**

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

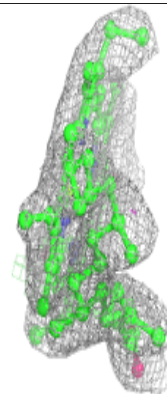
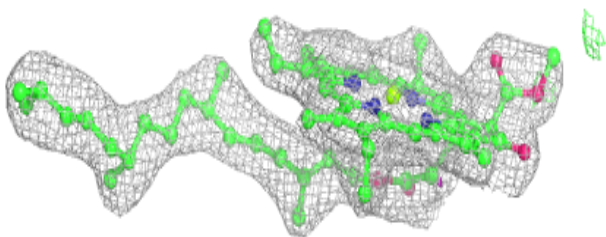
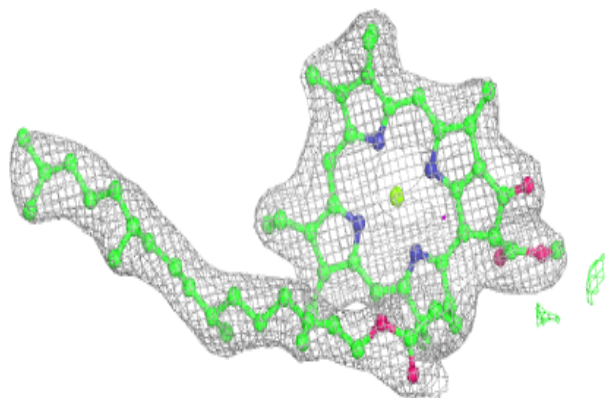


**Electron density around CLA b 612:**

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

**Electron density around CLA c 505:**

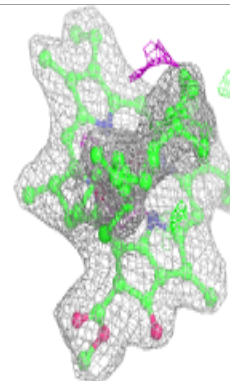
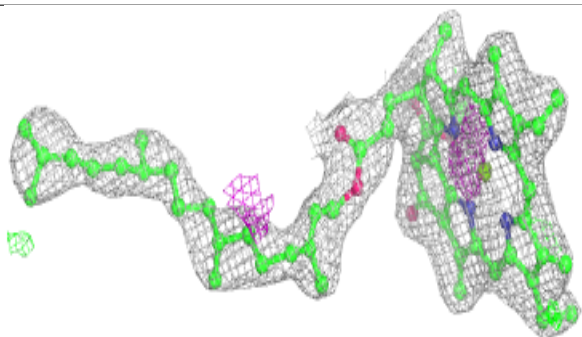
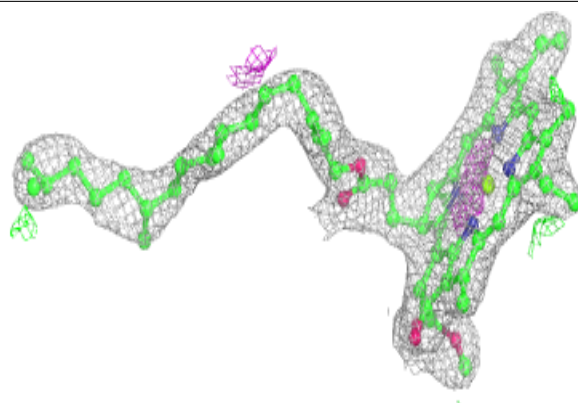
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



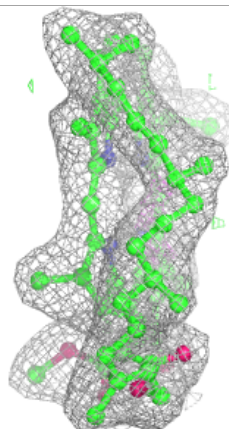
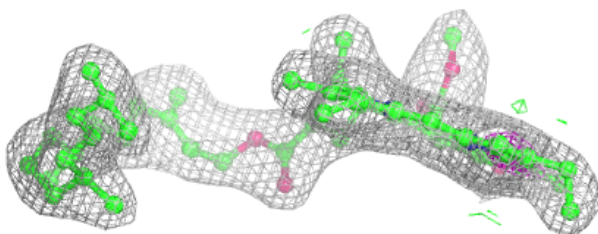
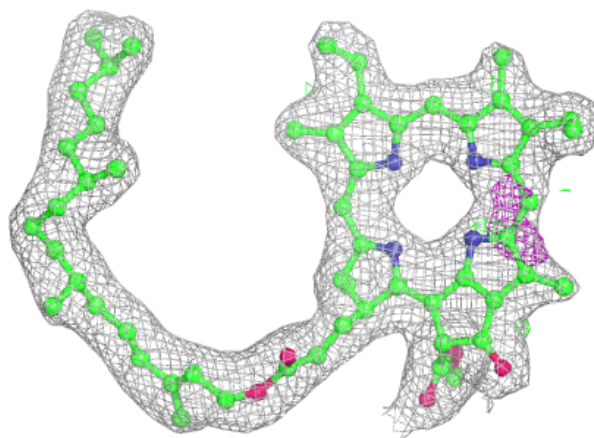


**Electron density around CLA c 506:**

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

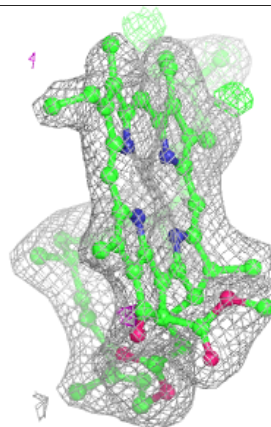
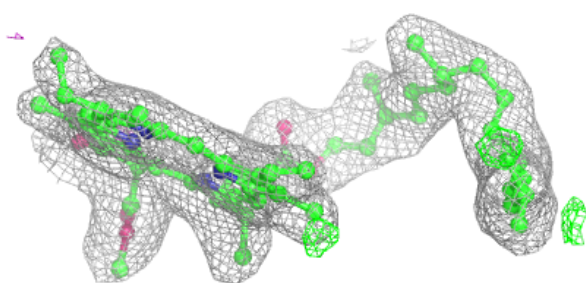
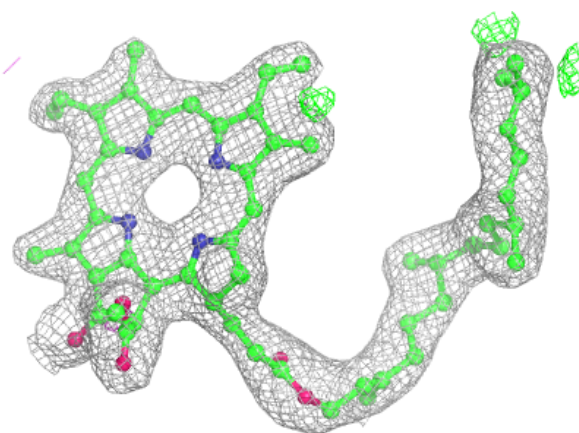
**Electron density around PHO A 408:**

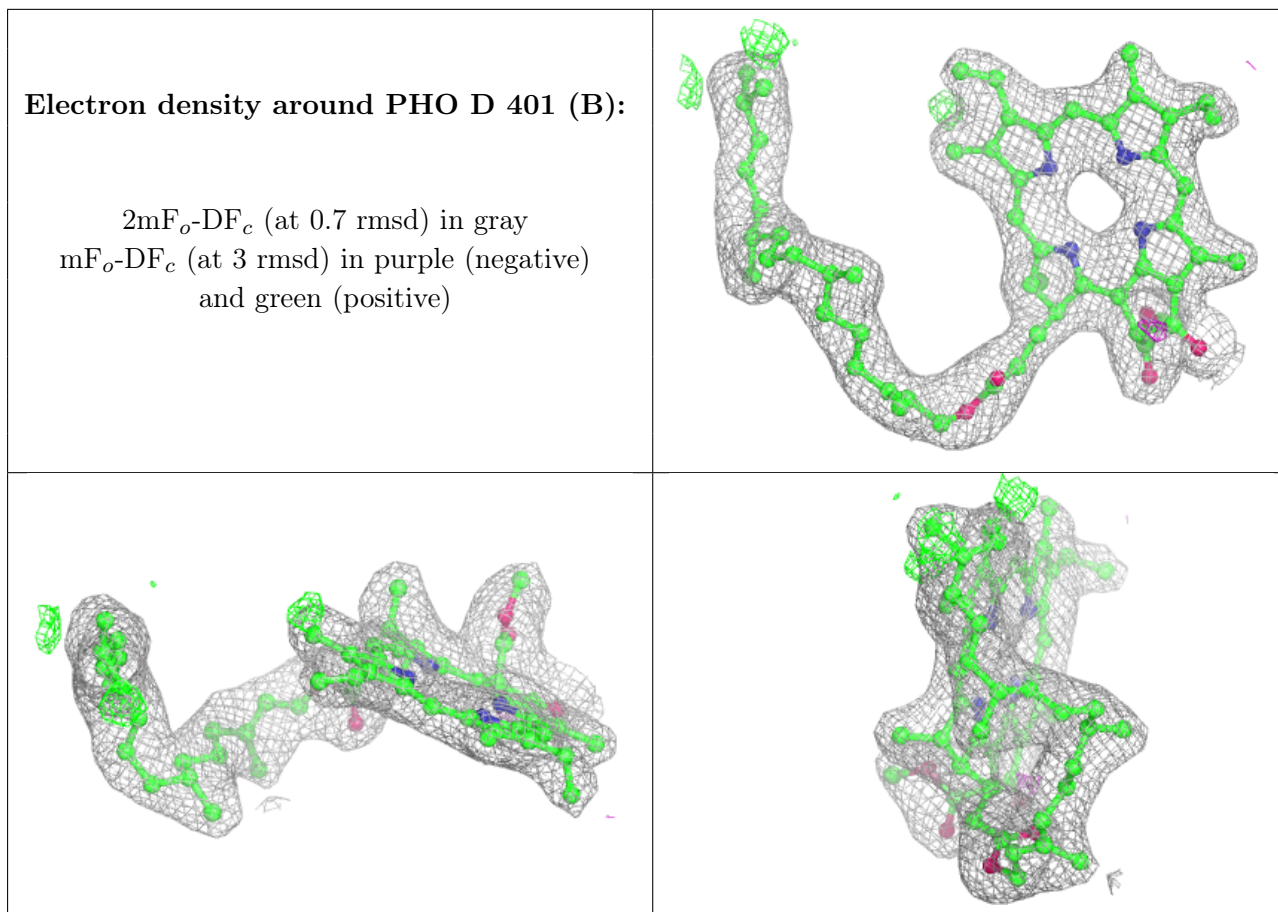
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PHO D 401 (A):**

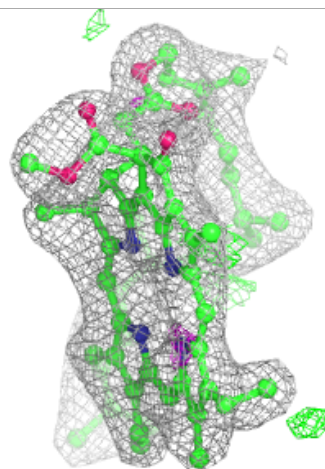
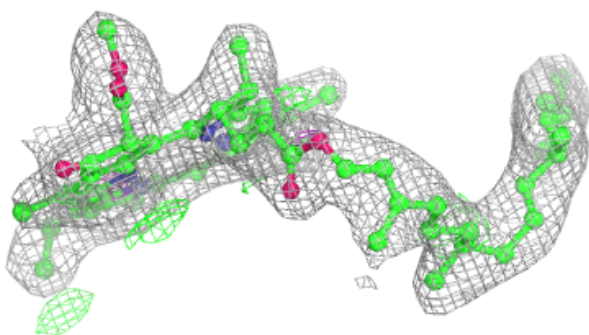
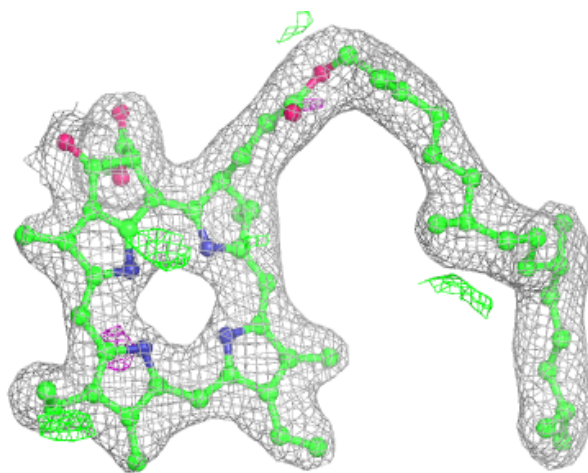
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





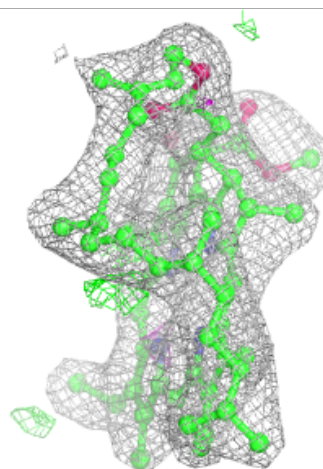
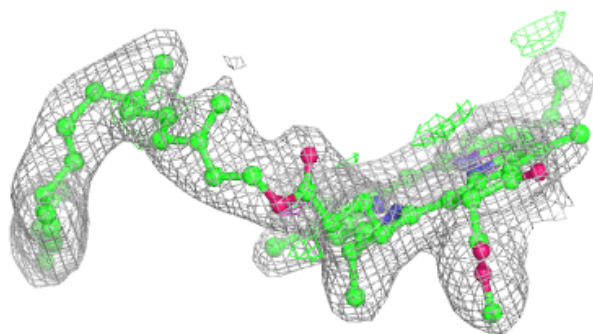
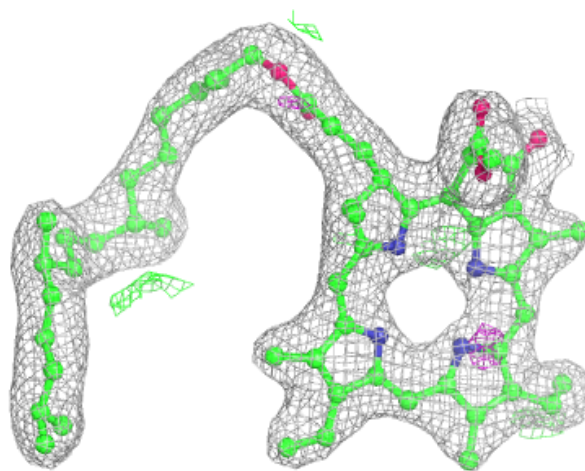
**Electron density around PHO d 402 (A):**

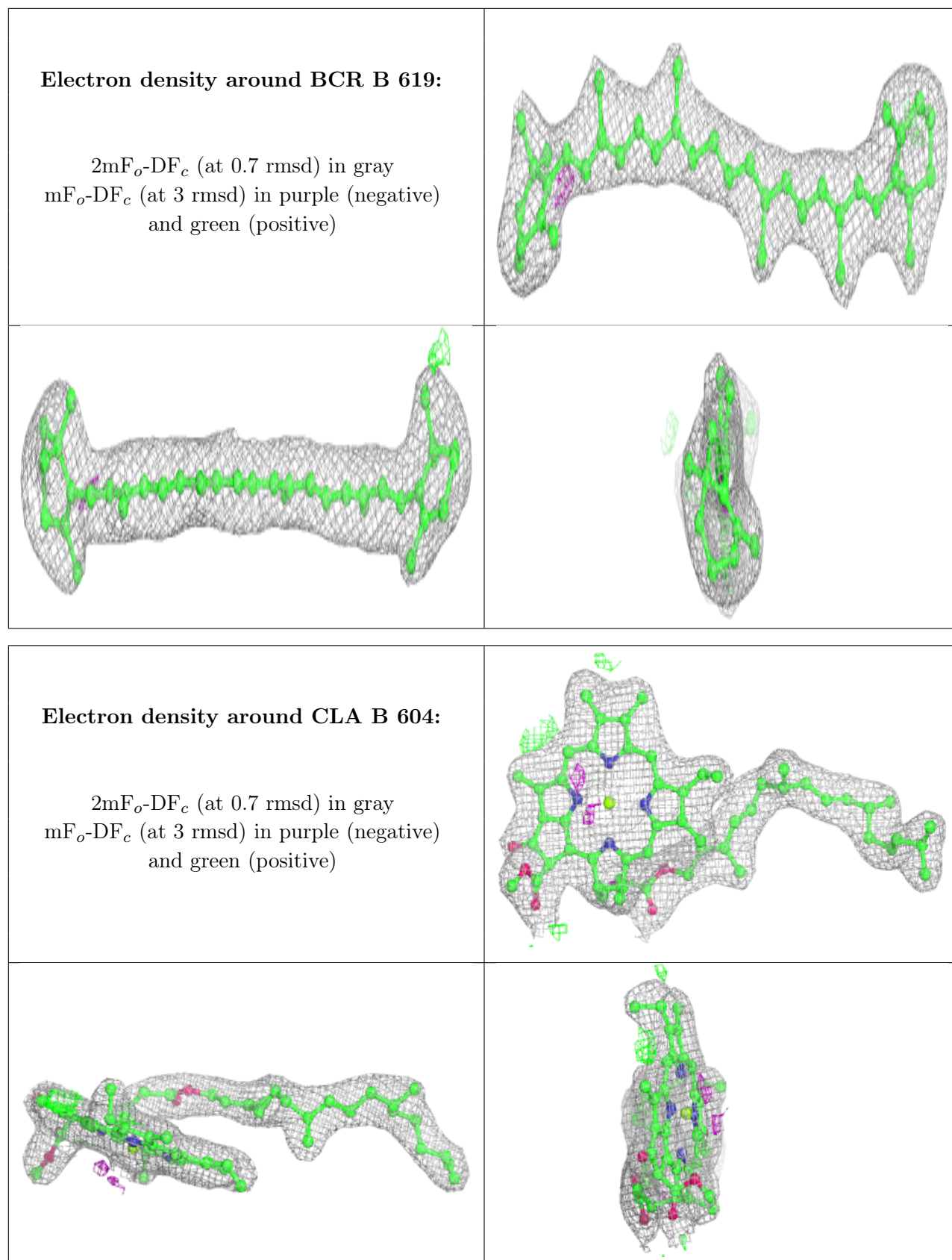
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PHO d 402 (B):**

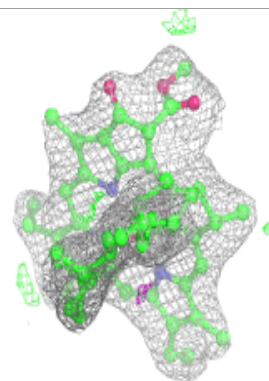
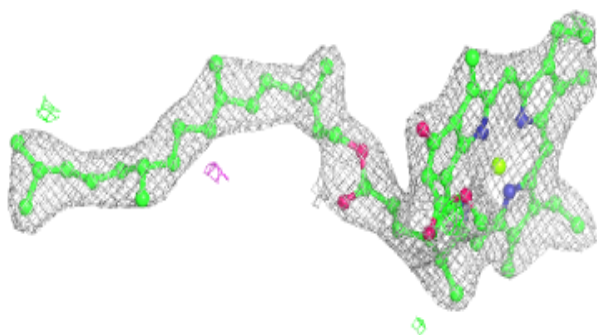
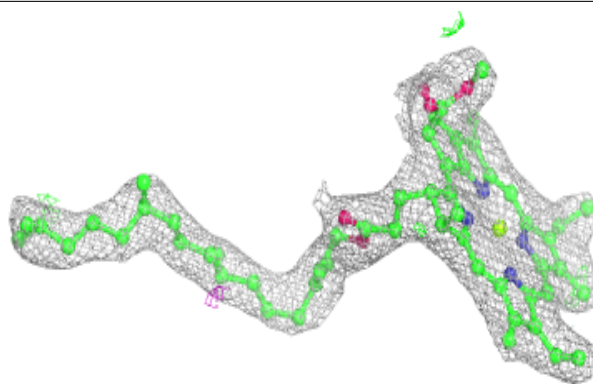
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



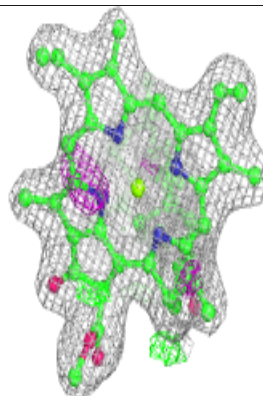
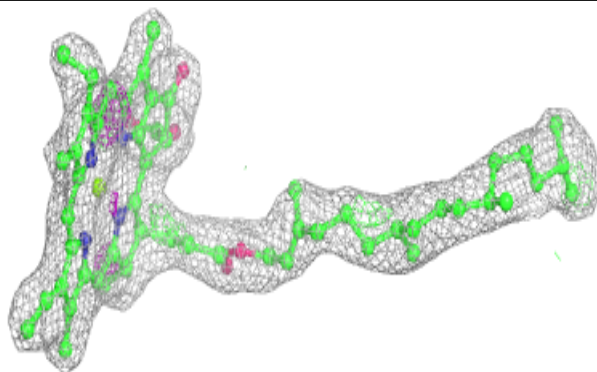
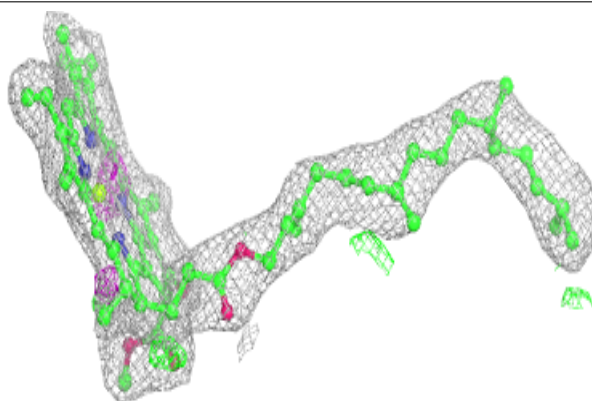


**Electron density around CLA C 502:**

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

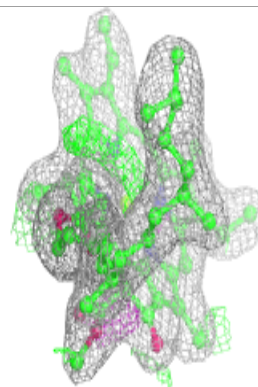
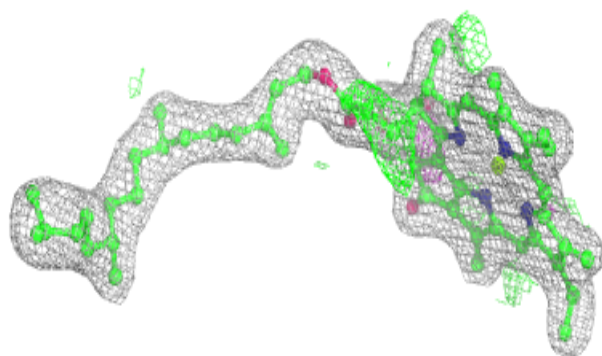
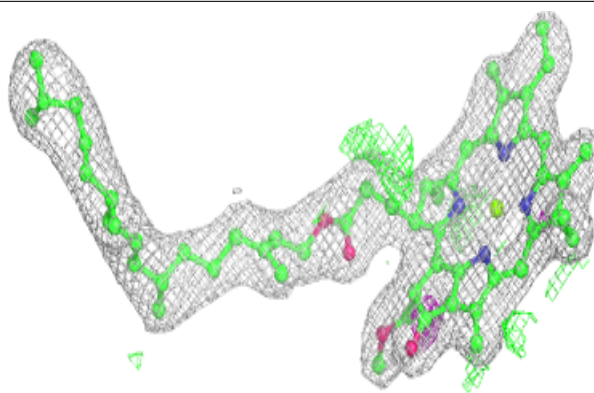
**Electron density around CLA B 605:**

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

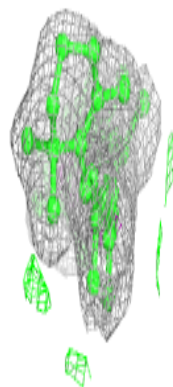
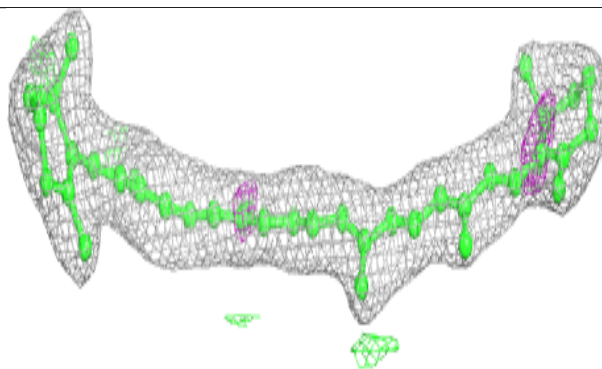
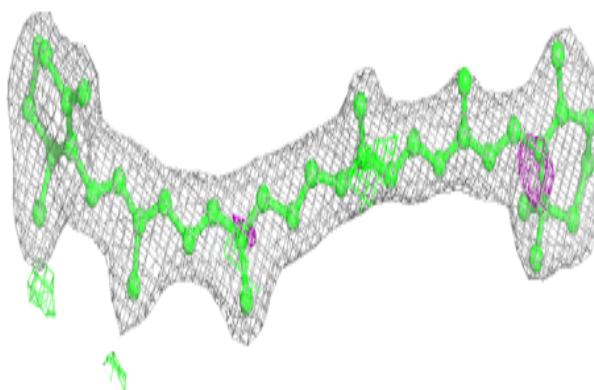


**Electron density around CLA A 405:**

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

**Electron density around BCR T 103:**

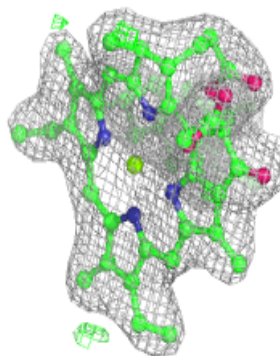
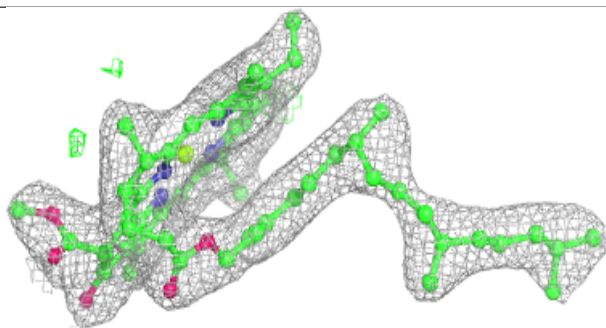
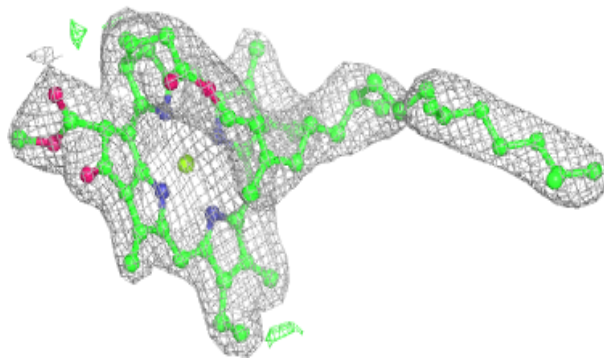
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



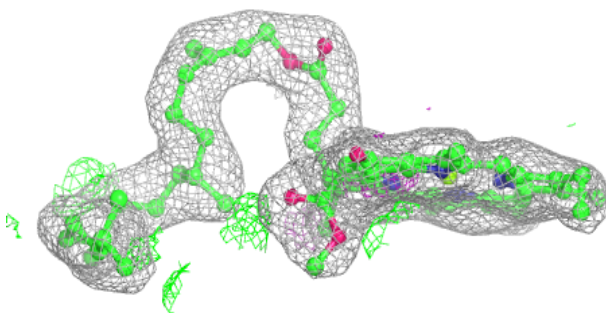
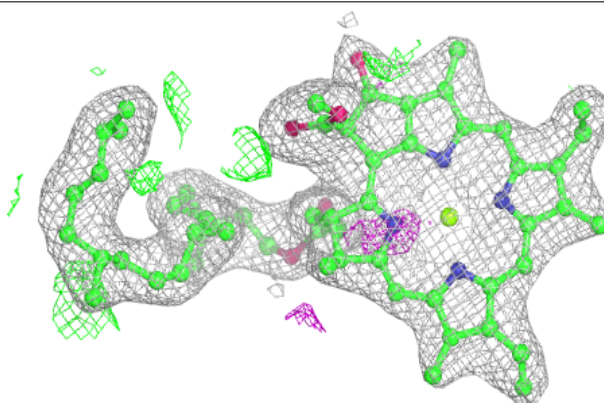


**Electron density around CLA C 505:**

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

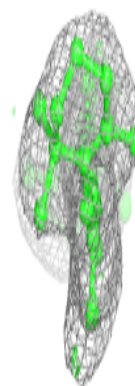
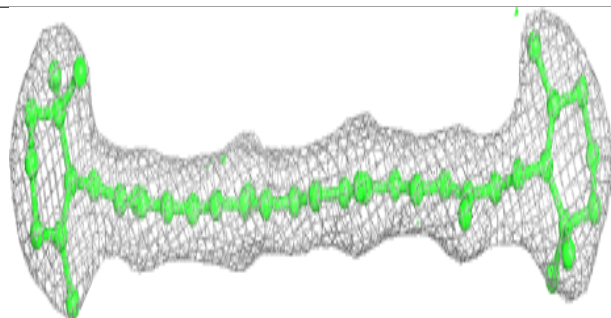
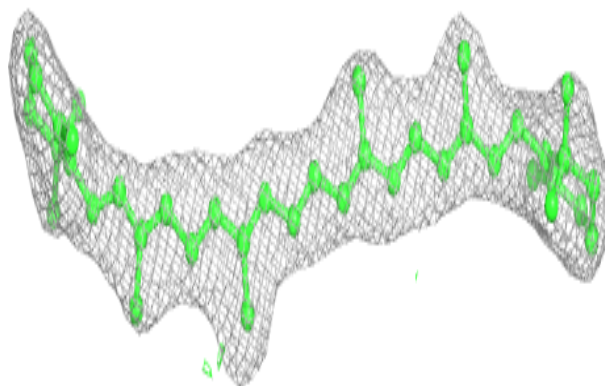
**Electron density around CLA b 621:**

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

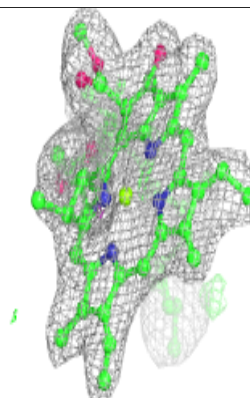
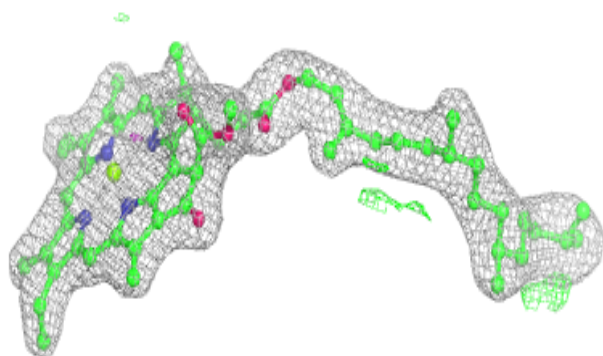
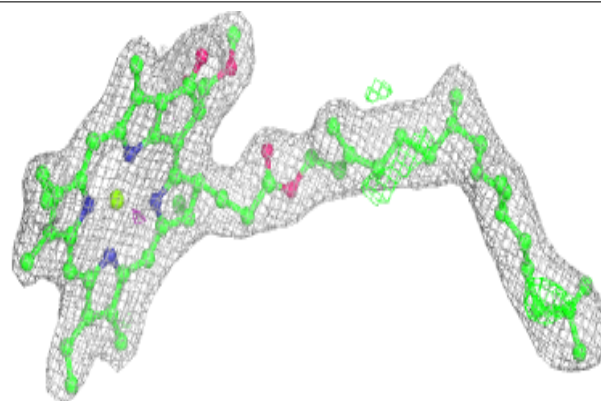


**Electron density around BCR c 518:**

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

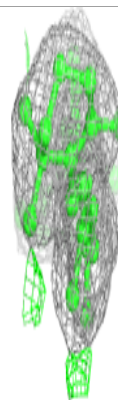
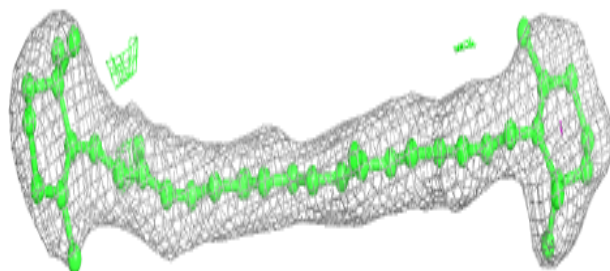
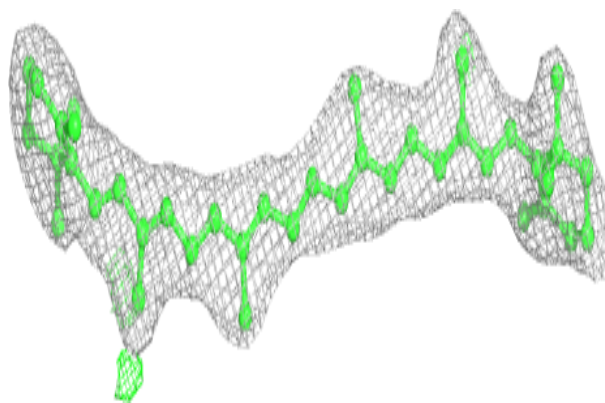
**Electron density around CLA a 409:**

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

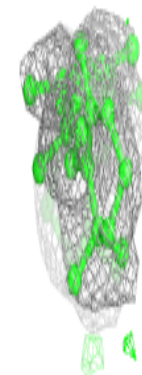
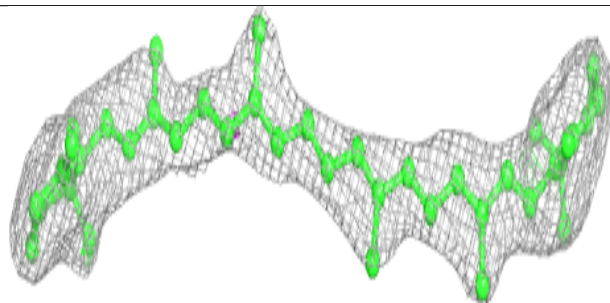
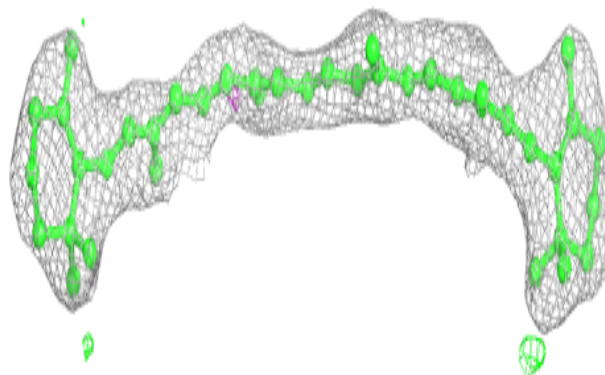


**Electron density around BCR h 101:**

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

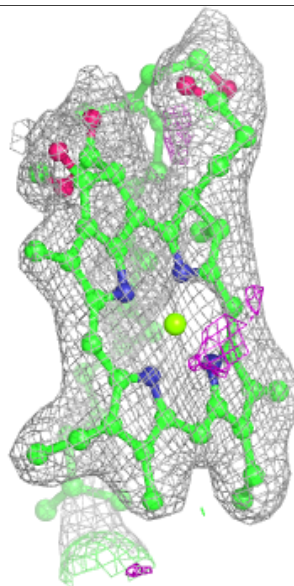
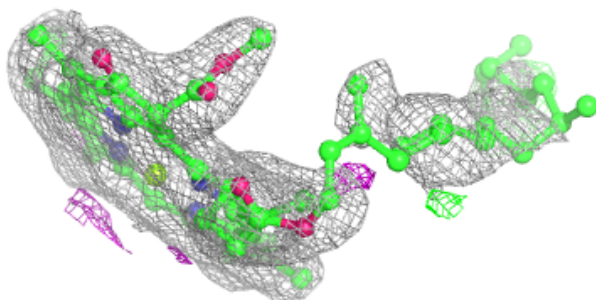
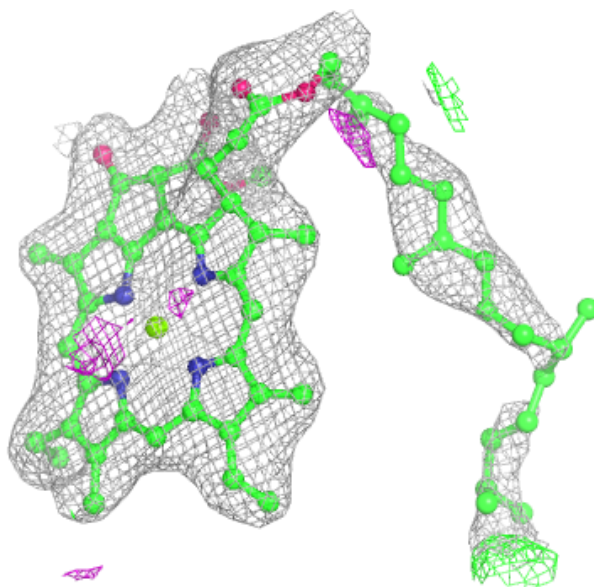
**Electron density around BCR k 102:**

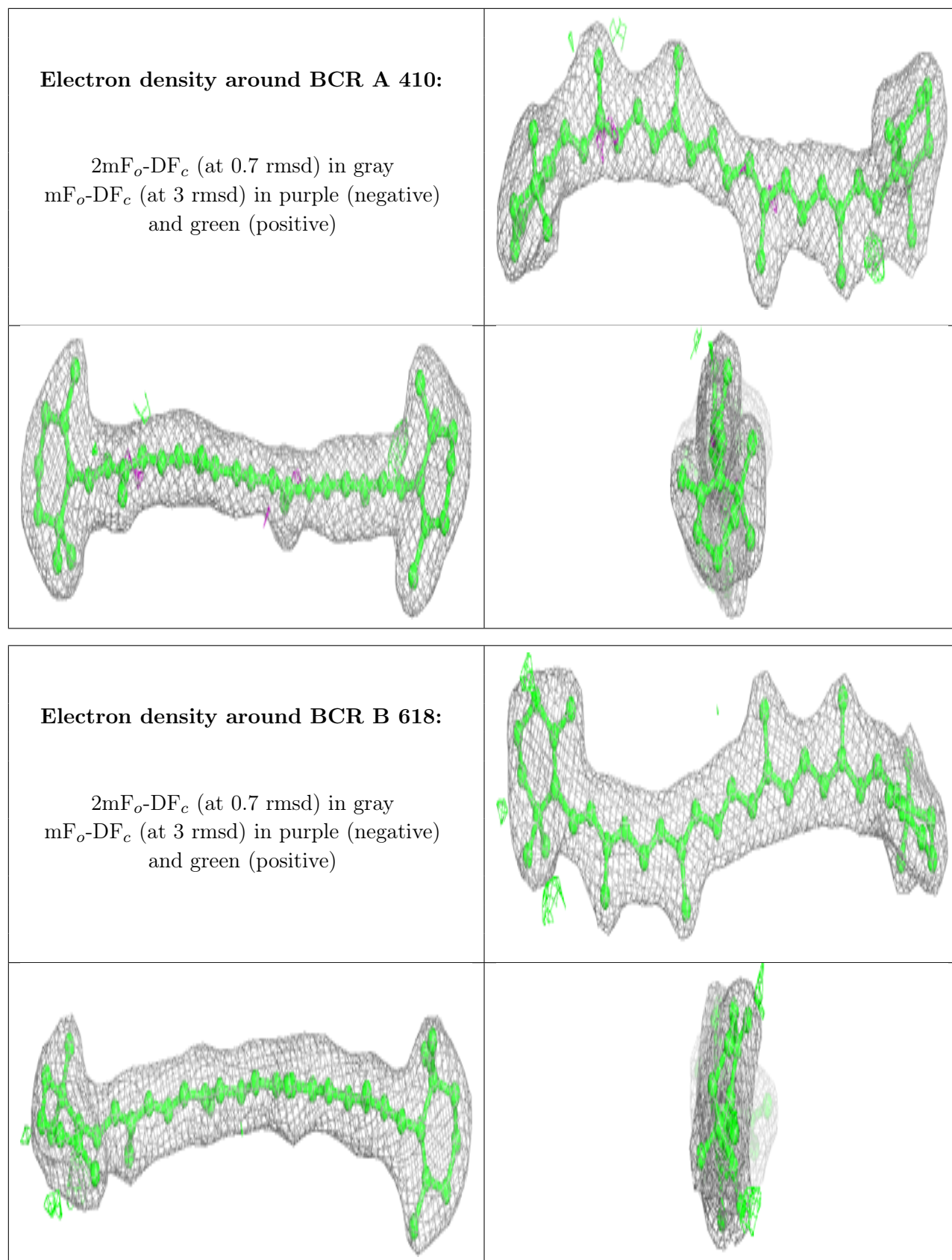
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 617:**

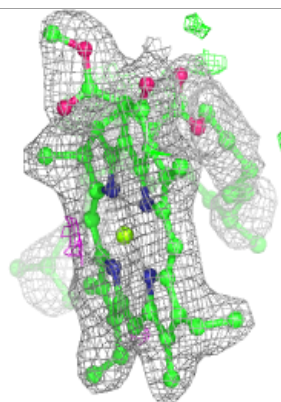
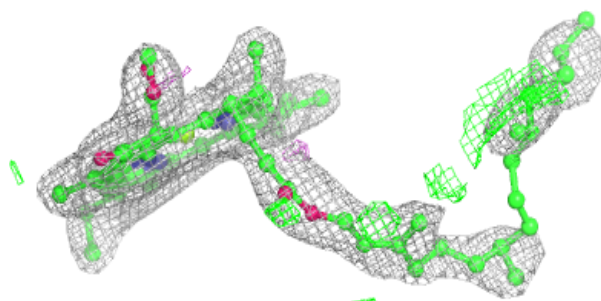
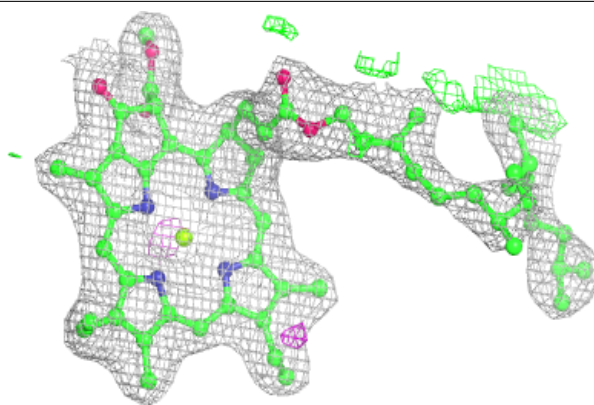
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



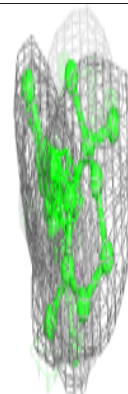
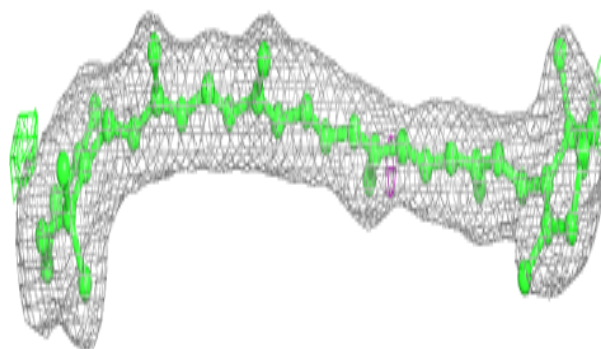
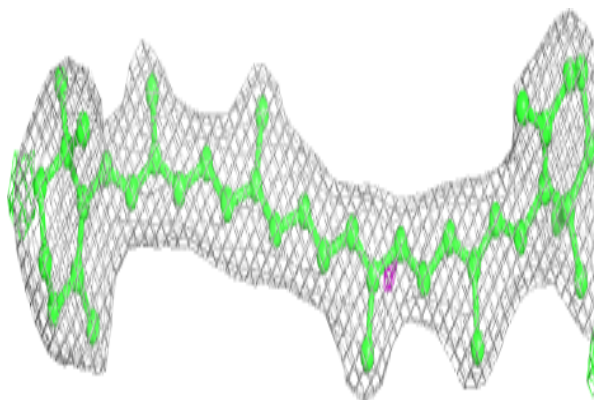


**Electron density around CLA A 409:**

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

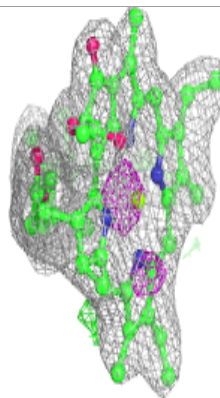
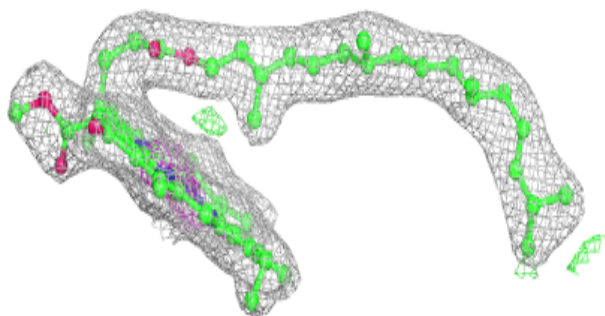
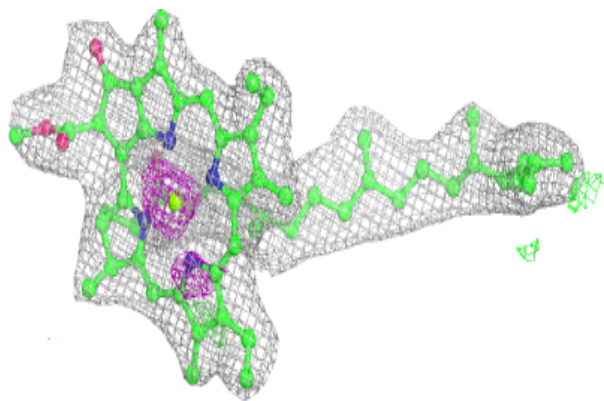
**Electron density around BCR B 620:**

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

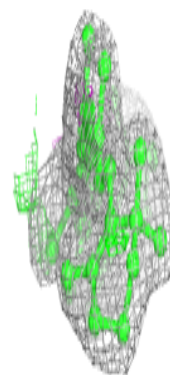
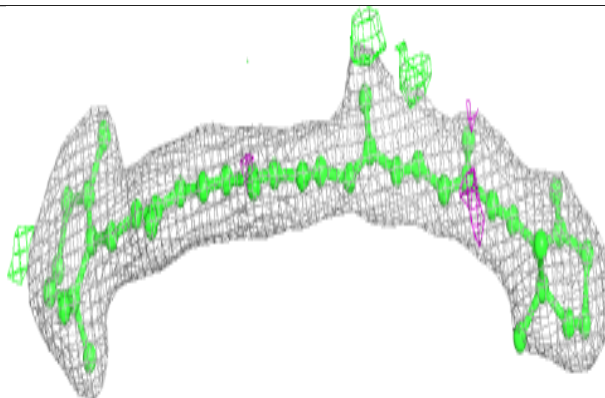
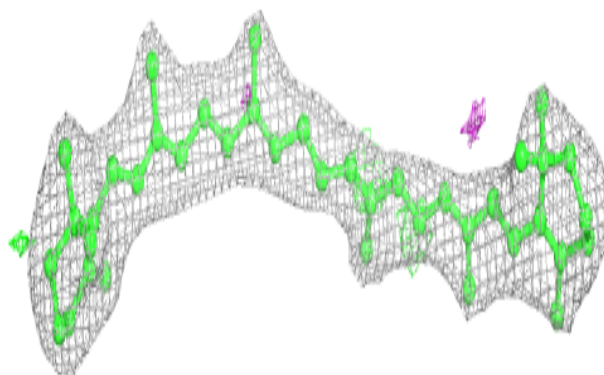


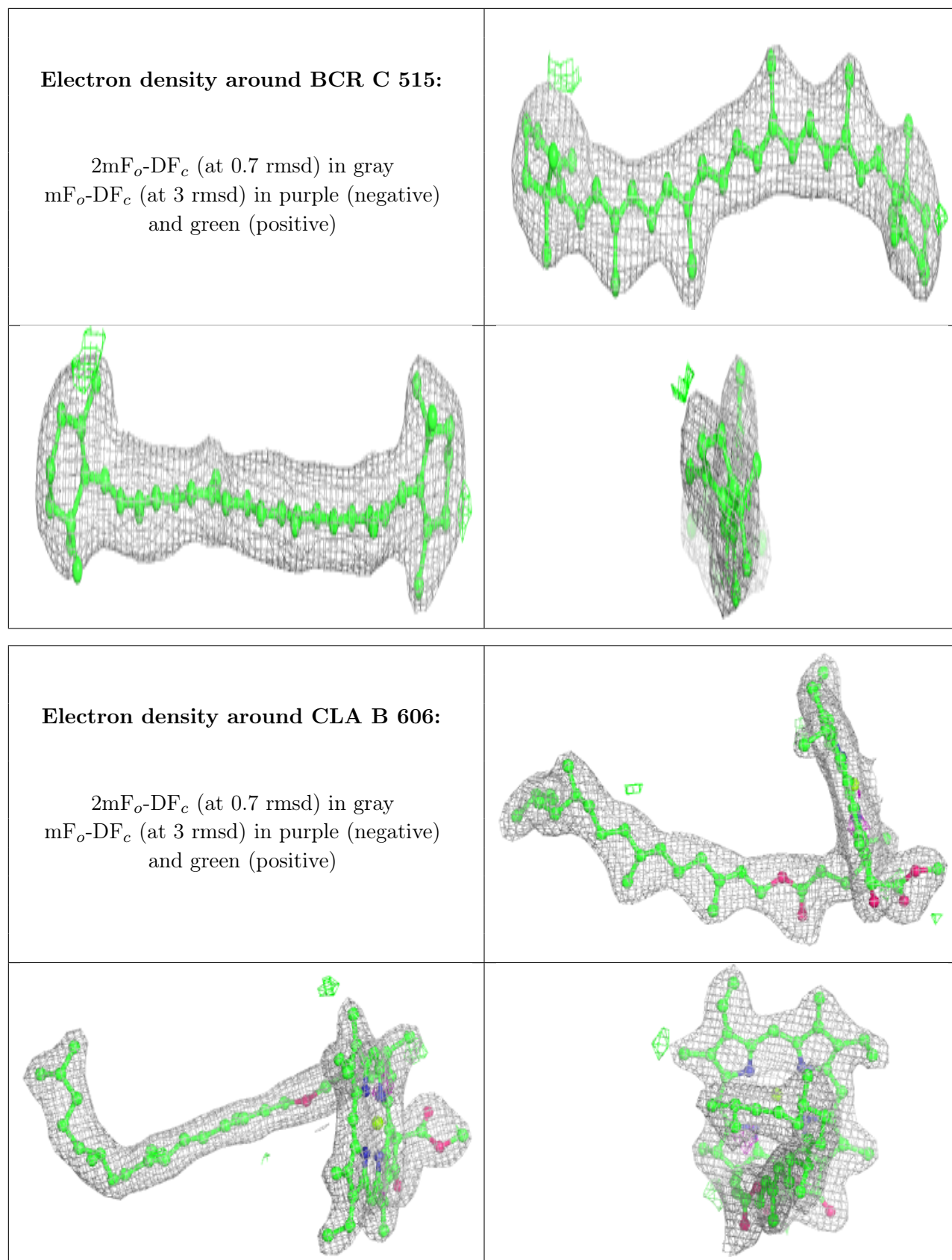
**Electron density around CLA B 609:**

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

**Electron density around BCR 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)

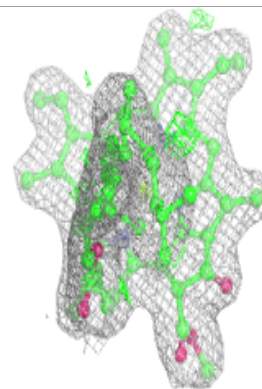
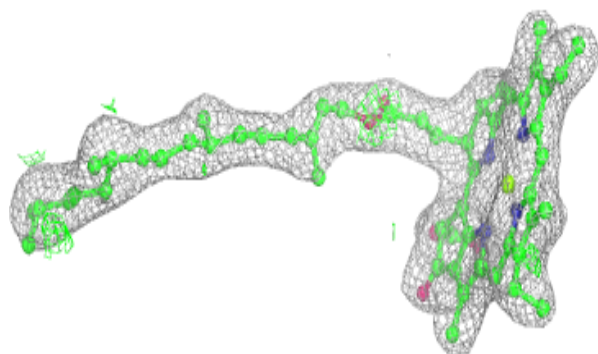
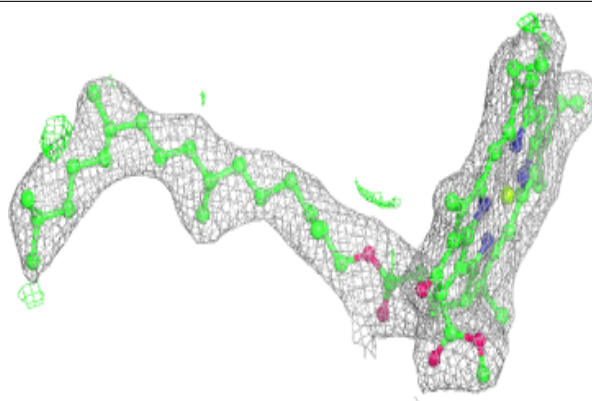




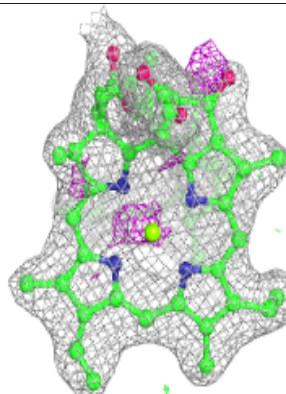
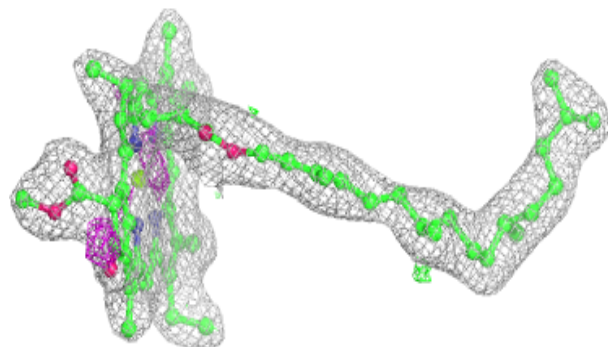
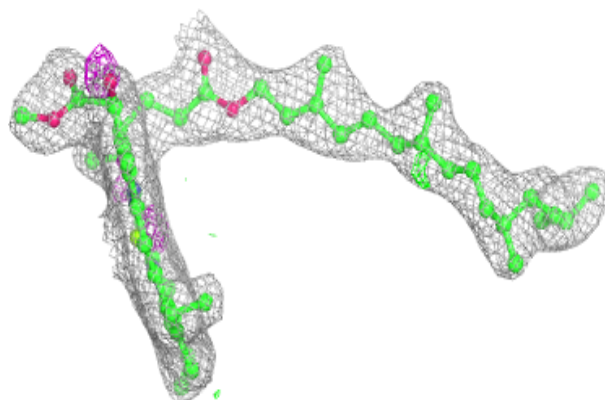


**Electron density around CLA b 613:**

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

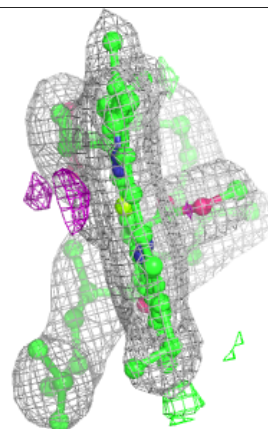
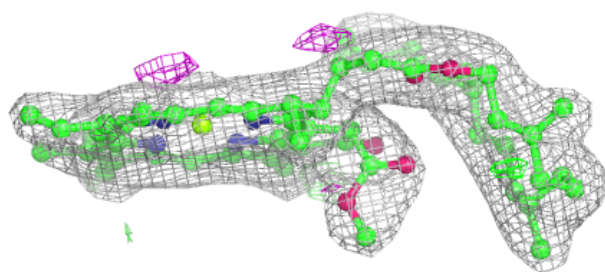
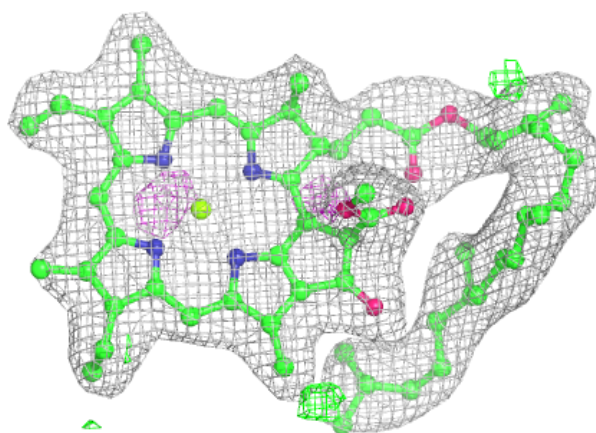
**Electron density around CLA b 614:**

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

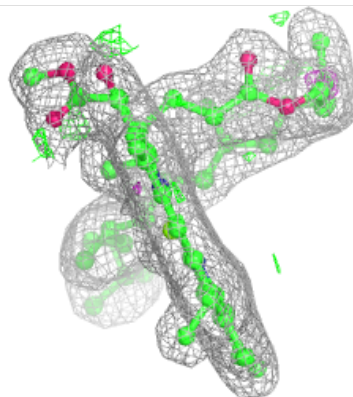
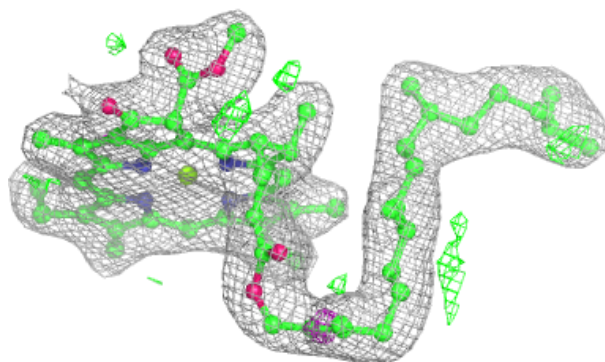
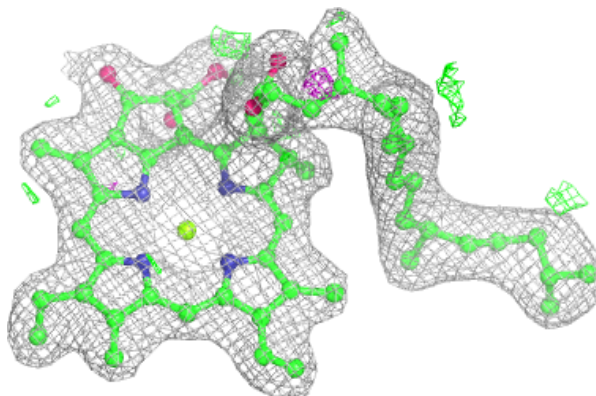


**Electron density around CLA B 611:**

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

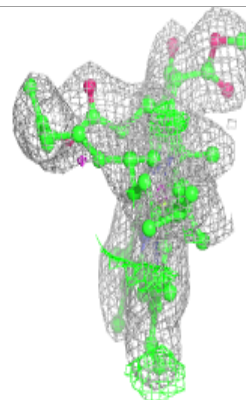
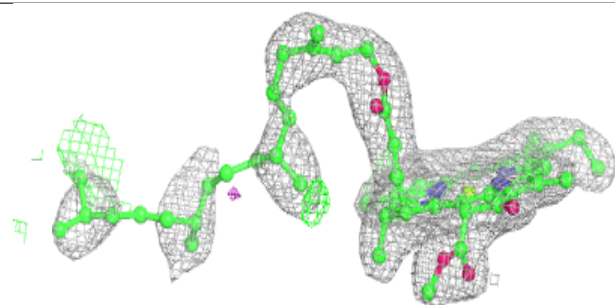
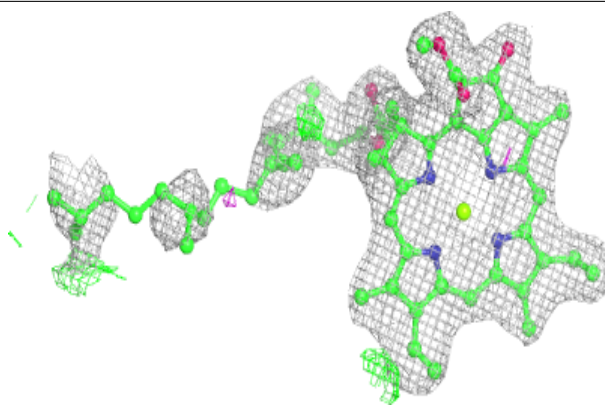
**Electron density around CLA A 406:**

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

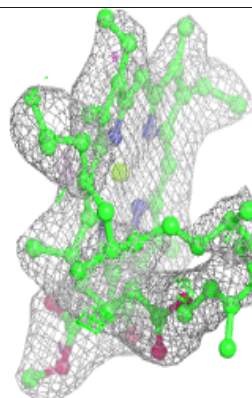
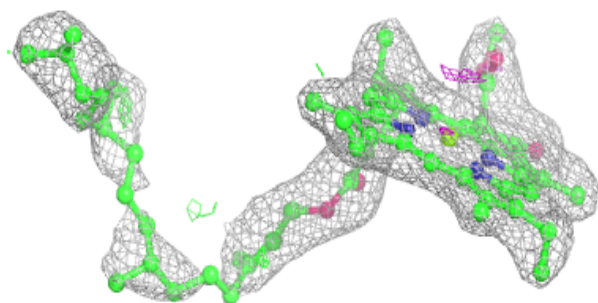
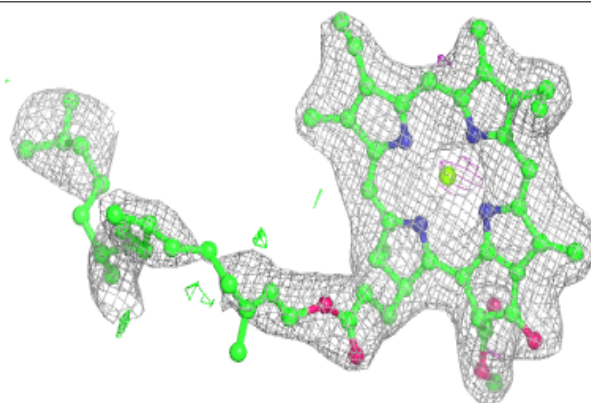


**Electron density around CLA a 410:**

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

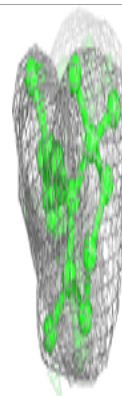
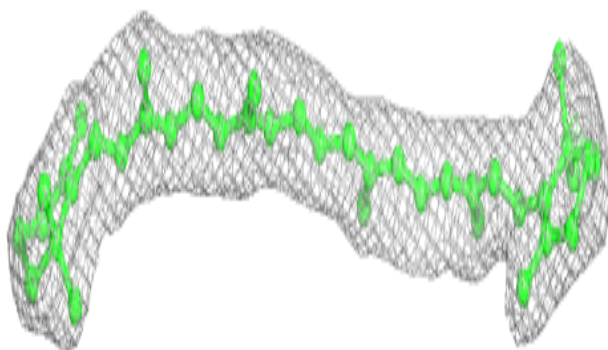
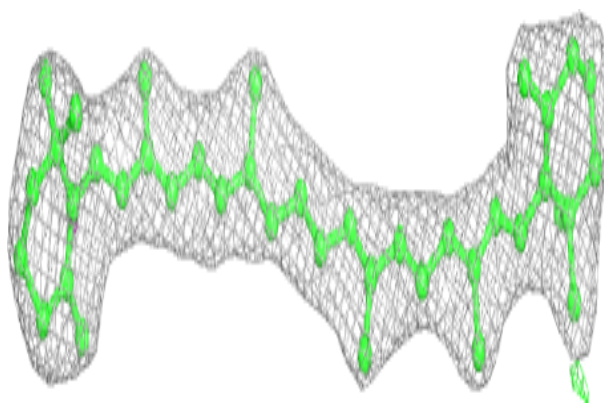
**Electron density around CLA a 412:**

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

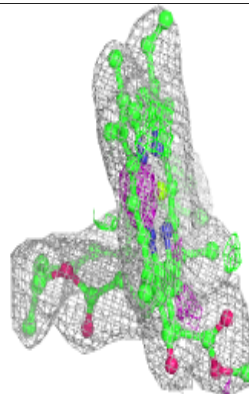
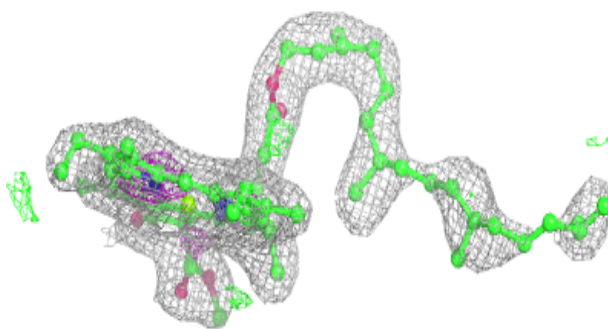
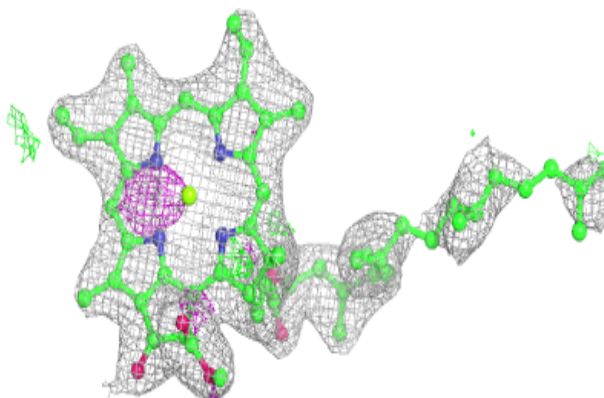


**Electron density around BCR b 628:**

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

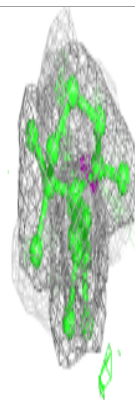
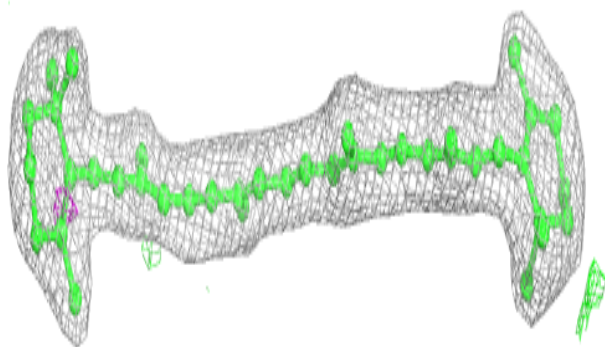
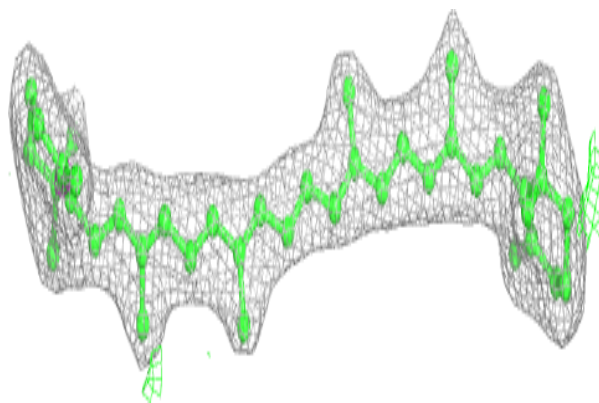
**Electron density around CLA A 407:**

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

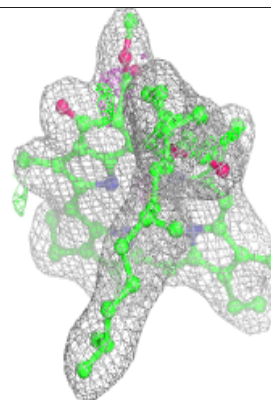
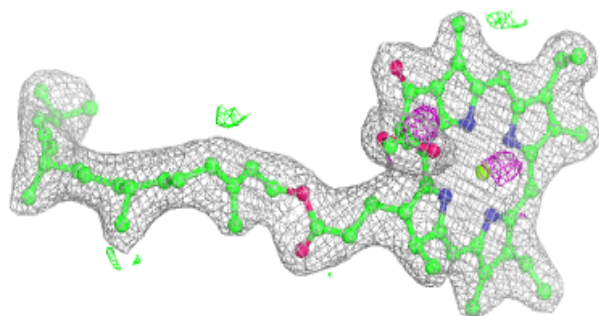
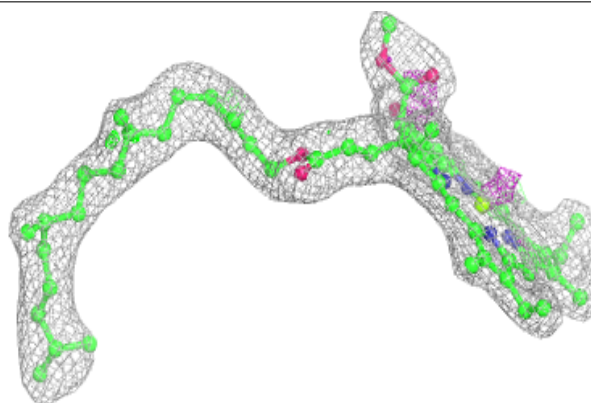


**Electron density around BCR a 413:**

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

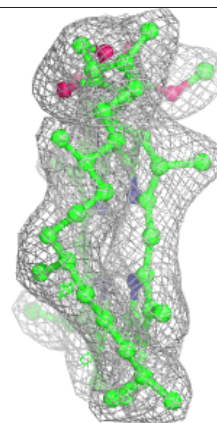
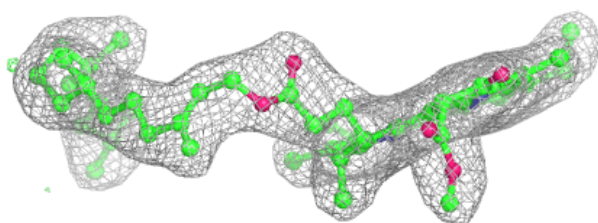
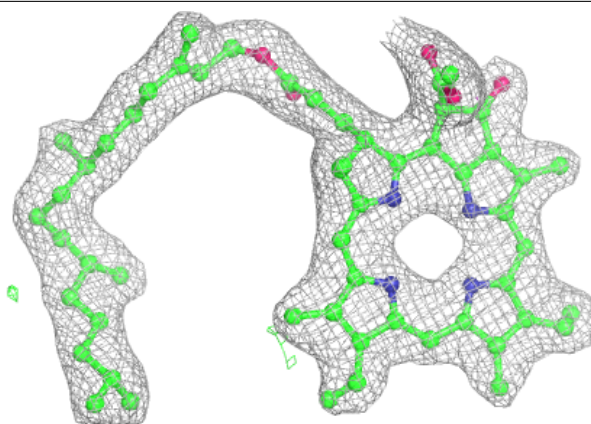
**Electron density around CLA d 404:**

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

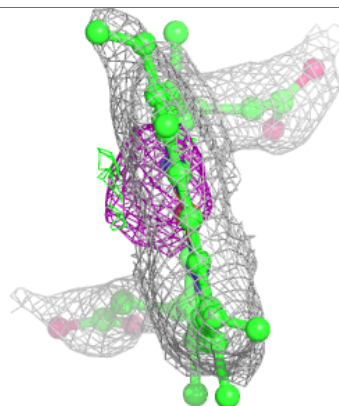
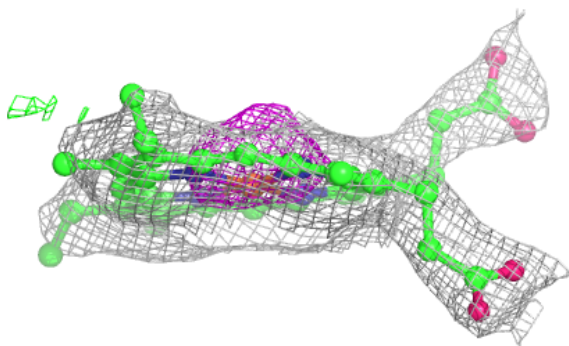
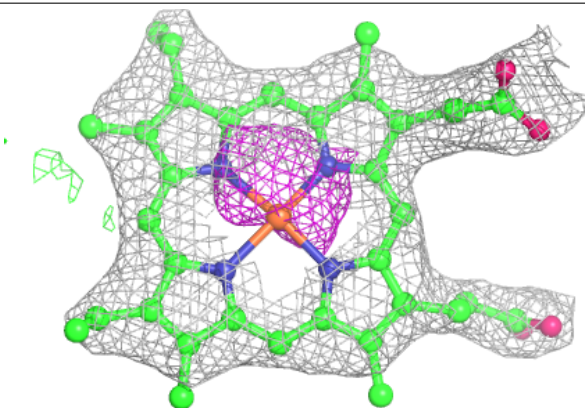


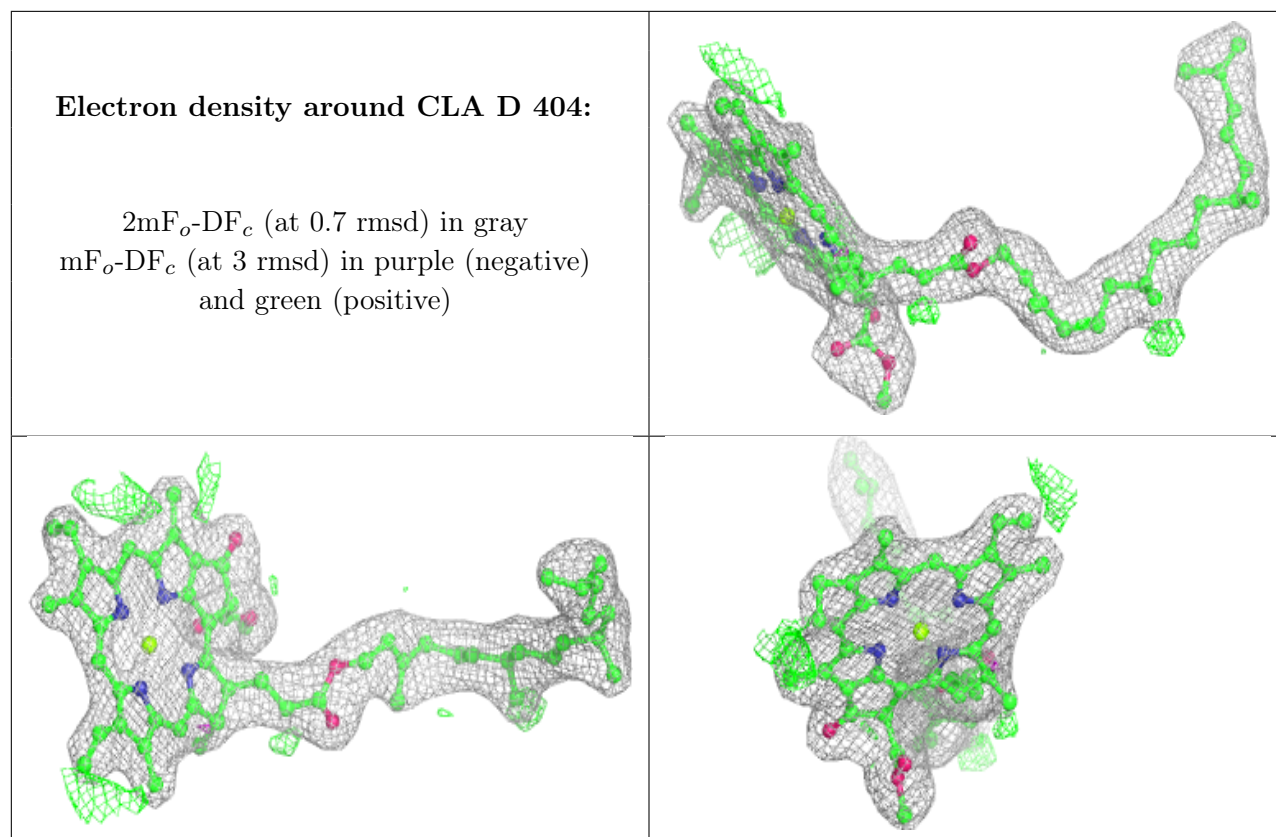
**Electron density around PHO a 411:**

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

**Electron density around HEM E 103:**

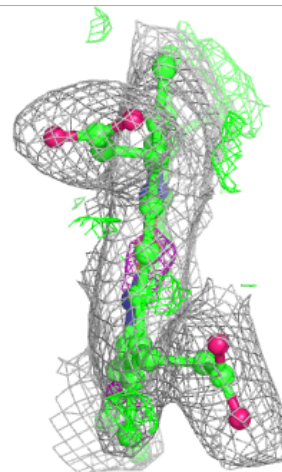
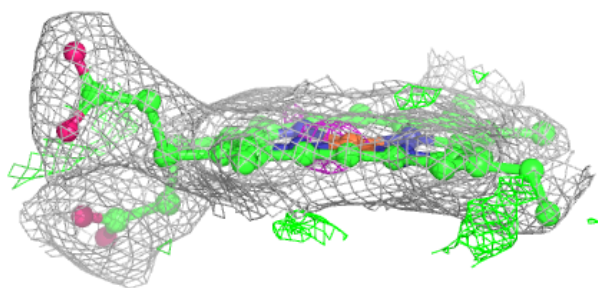
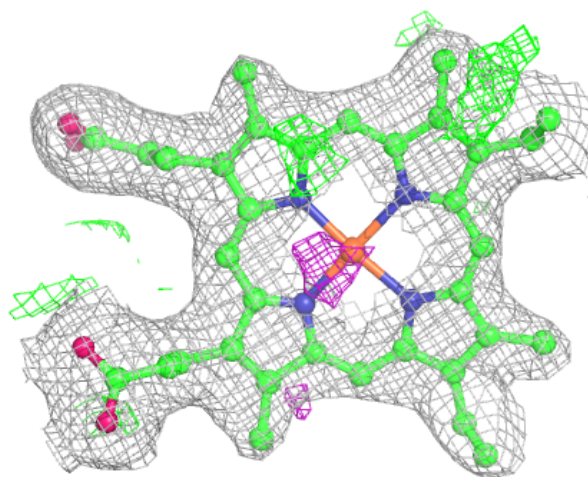
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEM V 205:**

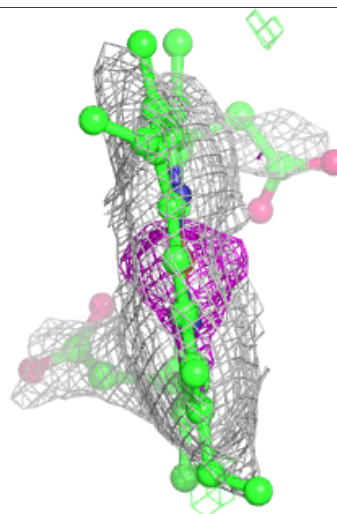
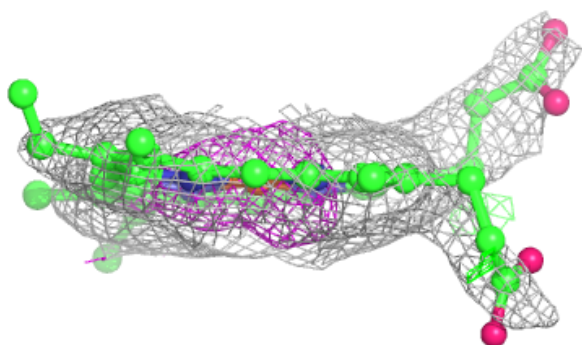
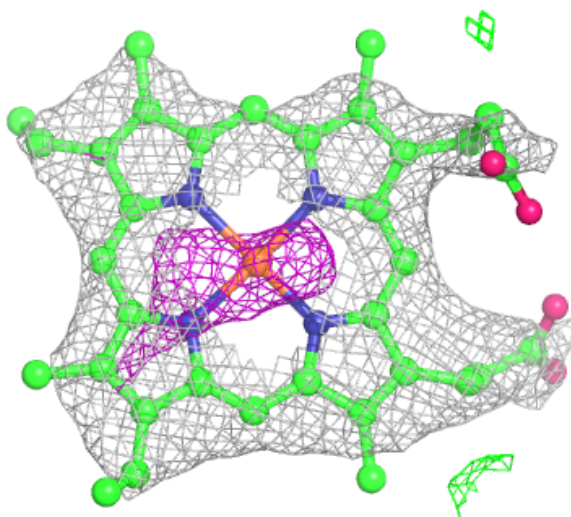
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

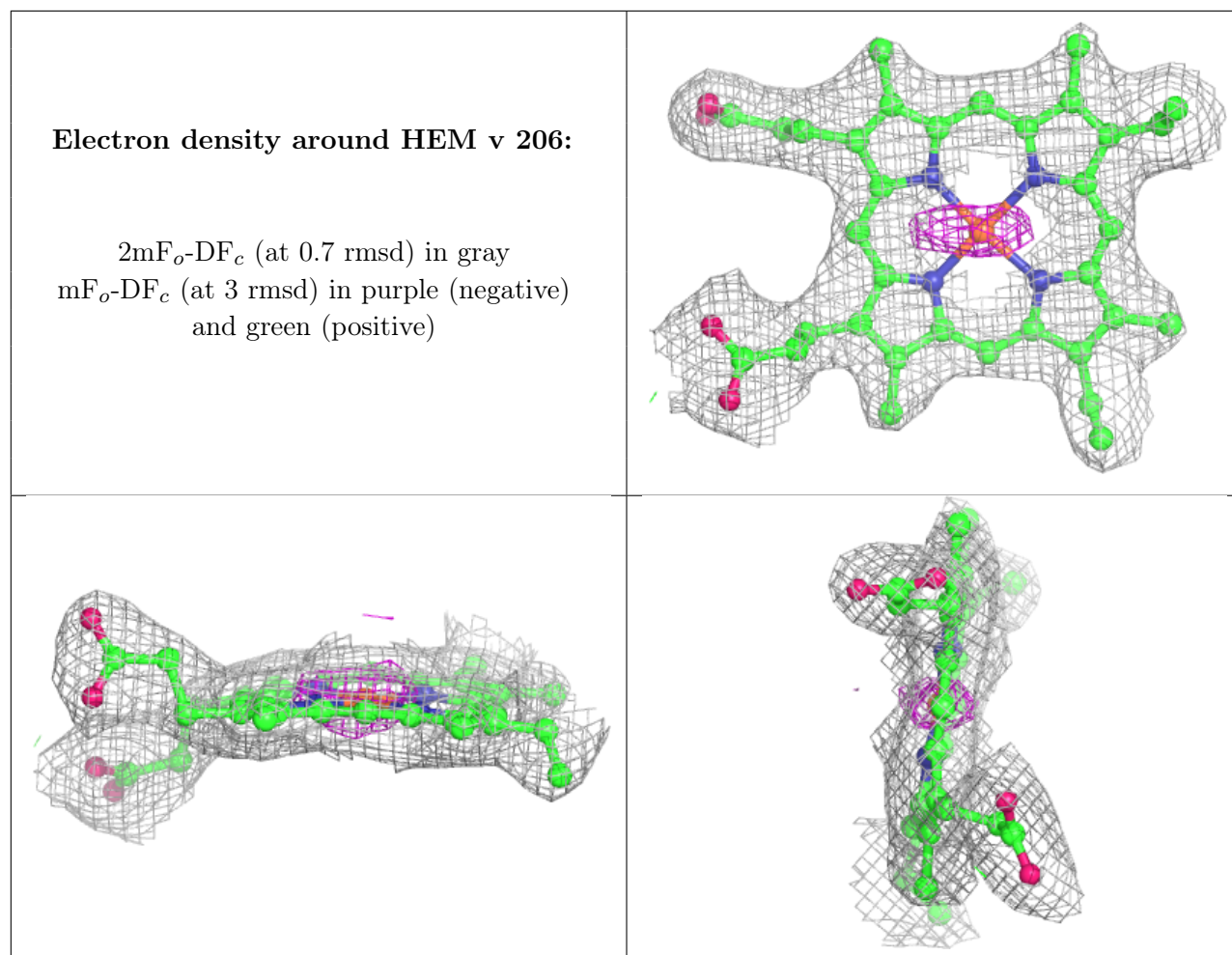




**Electron density around HEM f 101:**

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





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

There are no such residues in this entry.