



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 20, 2023 – 03:53 PM JST

PDB ID : 7COU
Title : Structure of cyanobacterial photosystem II in the dark S1 state
Authors : Li, H.; Shen, J.-R.; Suga, M.
Deposited on : 2020-08-05
Resolution : 2.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 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

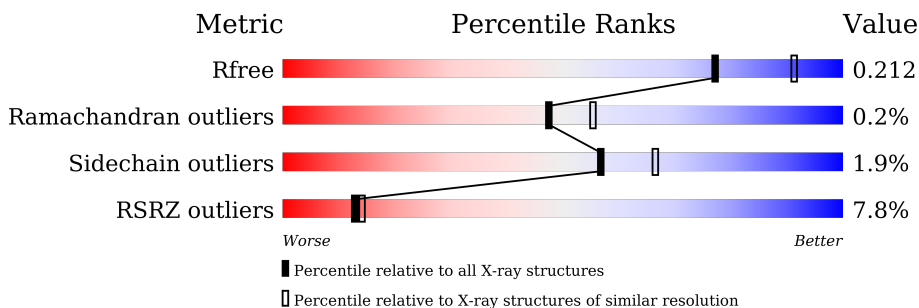
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	344	 4% (poor fit), 97% (0-3 outliers), 1% (4+ outliers), 1% (not modelled)
1	a	344	 6% (poor fit), 97% (0-3 outliers), 1% (4+ outliers), 1% (not modelled)
2	B	505	 5% (poor fit), 99% (0-3 outliers), 1% (4+ outliers), 1% (not modelled)
2	b	505	 10% (poor fit), 99% (0-3 outliers), 1% (4+ outliers), 1% (not modelled)
3	C	455	 5% (poor fit), 97% (0-3 outliers), 1% (4+ outliers), 1% (not modelled)
3	c	455	 8% (poor fit), 99% (0-3 outliers), 1% (4+ outliers), 1% (not modelled)
4	D	342	 3% (poor fit), 99% (0-3 outliers), 1% (4+ outliers), 1% (not modelled)

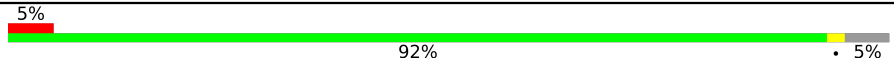
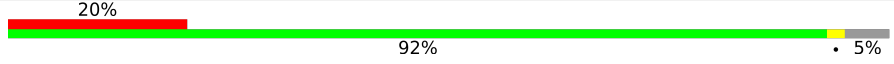
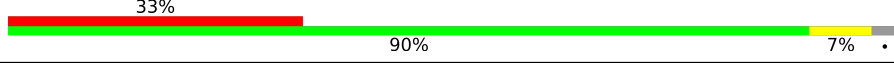
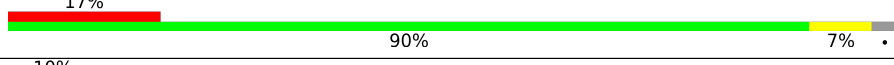
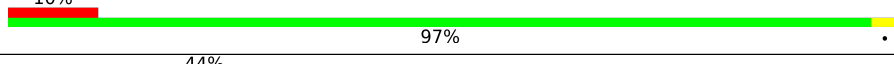
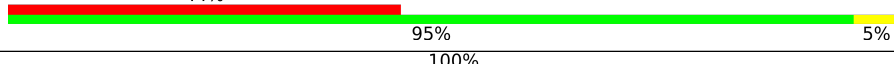

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Mol	Chain	Length	Quality of chain
4	d	342	5% 99%
5	E	84	10% 92% 5%
5	e	84	10% 90% 6%
6	F	44	5% 77% 23%
6	f	44	7% 70% 30%
7	H	65	94% 5%
7	h	65	6% 94% 5%
8	I	38	5% 92% 8%
8	i	38	3% 95% 5%
9	J	39	18% 90% 8%
9	j	39	13% 100%
10	K	37	92% 8%
10	k	37	8% 92% 8%
11	L	37	3% 97%
11	l	37	3% 97%
12	M	36	3% 89% 8%
12	m	36	6% 86% 8% 6%
13	O	244	10% 98%
13	o	244	17% 98%
14	T	32	88% 6% 6%
14	t	32	6% 91% 6%
15	U	104	3% 90% 8%
15	u	104	91% 7%
16	V	137	100%
16	v	137	4% 98%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	404	X	-	-	-
23	CLA	A	405	X	-	-	-
23	CLA	A	408	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	C	514	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	D	404	X	-	-	-
23	CLA	a	404	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	408	X	-	-	-
23	CLA	b	601	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	c	514	X	-	-	-
23	CLA	c	515	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-
26	GOL	B	629	-	-	-	X
30	UNL	A	414	-	-	-	X
30	UNL	b	626	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	LMG	C	522	-	-	-	X
32	LMG	c	522	-	-	-	X
33	HTG	b	623	-	-	-	X
34	LMT	C	526	-	-	-	X
34	LMT	E	102	-	-	-	X
34	LMT	a	418	-	-	-	X
34	LMT	e	101	-	-	-	X

2 Entry composition i

There are 40 unique types of molecules in this entry. The entry contains 53138 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	2634	1725	433	461	15	0	2	0
1	a	334	2642	1731	434	462	15	0	3	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	conflict	UNP P51765
a	279	PRO	ARG	conflict	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	4050	2650	677	710	13	0	10	0
2	b	504	3998	2622	665	698	13	0	4	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	3513	2295	588	617	13	0	4	0
3	c	455	3534	2311	591	619	13	0	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	342	2726	1805	445	464	12	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	d	341	2717	1800	444	461	12	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	81	668	435	108	125		0	1	0
5	e	79	648	424	105	119		0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	34	275	187	45	42	1	0	0	0
6	f	31	250	170	42	37	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	H	64	517	345	85	85	2	0	1	0
7	h	64	506	339	81	84	2	0	0	0

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
11	L	36	304	203	48	53	0	1	0
11	l	36	304	203	48	53	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	M	33	268	179	39	49	1	0	1	0
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	conflict	UNP P12312
m	8	LEU	PHE	conflict	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	1886	1177	318	386	5	0	3	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	o	243	Total	C	N	O	S	0	2	0
			1879	1173	317	384	5			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	96	Total	C	N	O	0	0	0
			765	486	128	151			
15	u	97	Total	C	N	O	0	0	0
			774	491	129	154			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	0	0	0
			273	186	47	40			

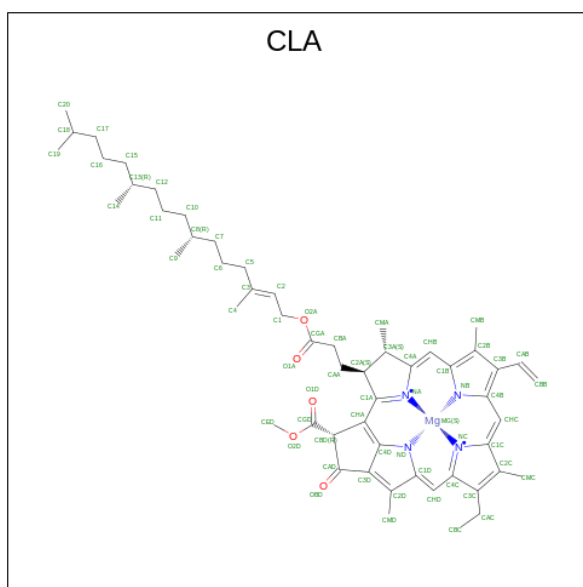
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

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

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

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



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

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

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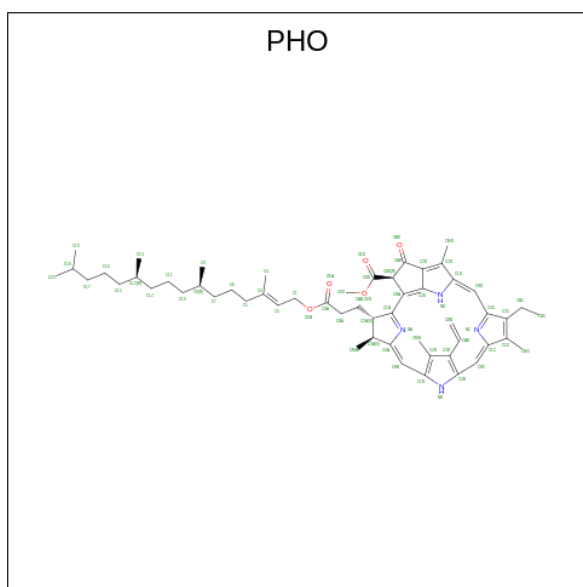
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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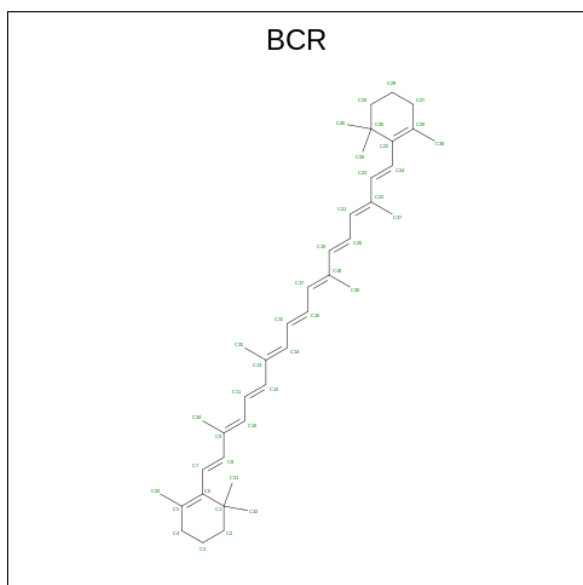
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



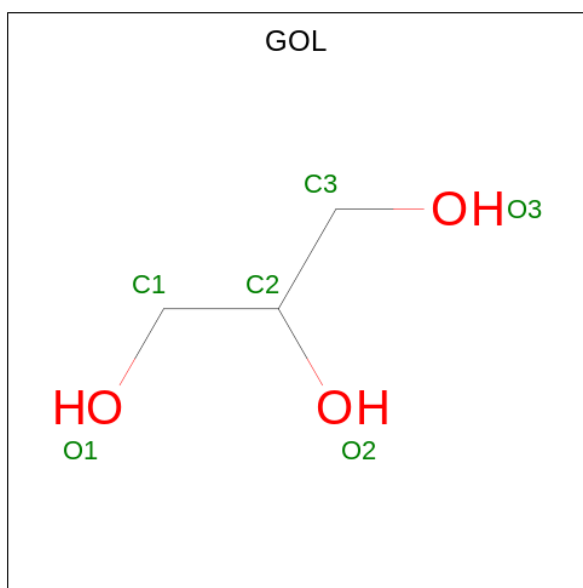
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
24	A	1	64	55	4	5	0	0
24	A	1	64	55	4	5	0	0
24	a	1	64	55	4	5	0	0
24	a	1	64	55	4	5	0	0

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



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

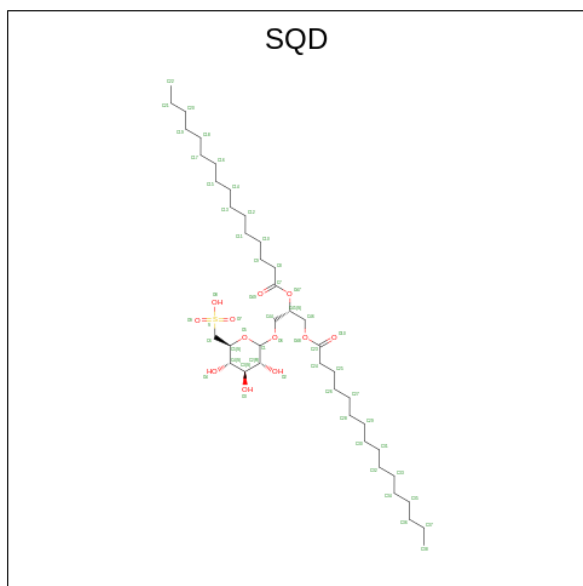
- Molecule 26 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O 6 3 3	0	0
26	B	1	Total C O 6 3 3	0	0
26	B	1	Total C O 6 3 3	0	0
26	B	1	Total C O 6 3 3	0	0
26	C	1	Total C O 6 3 3	0	0
26	O	1	Total C O 6 3 3	0	0
26	a	1	Total C O 6 3 3	0	0
26	b	1	Total C O 6 3 3	0	0
26	b	1	Total C O 6 3 3	0	0
26	c	1	Total C O 6 3 3	0	0
26	o	1	Total C O 6 3 3	0	0
26	v	1	Total C O 6 3 3	0	0

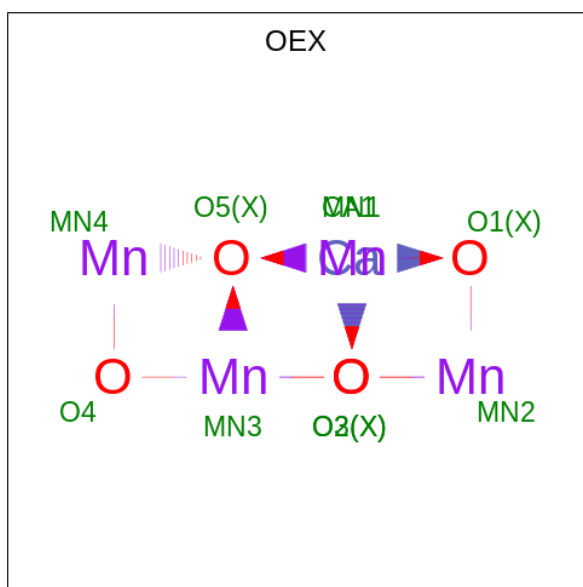
- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



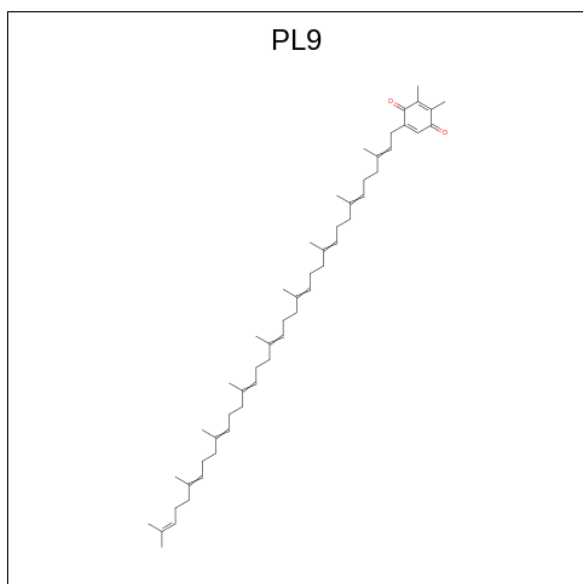
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	B	1	Total	C	O	S	0	0
			54	41	12	1		
27	C	1	Total	C	O	S	0	0
			54	41	12	1		
27	D	1	Total	C	O	S	0	0
			43	30	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	b	1	Total	C	O	S	0	0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

- Molecule 28 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn₄O₅).



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

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: C₅₃H₈₀O₂).



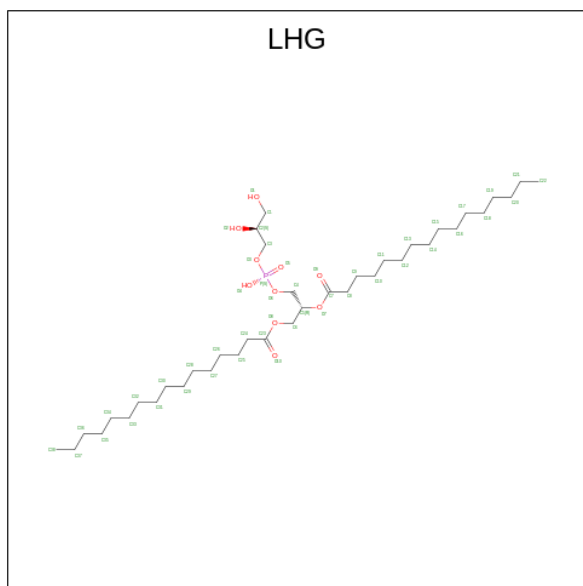
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			55	53	2		
29	D	1	Total	C	O	0	0
			55	53	2		
29	a	1	Total	C	O	0	0
			55	53	2		
29	d	1	Total	C	O	0	0
			55	53	2		

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

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

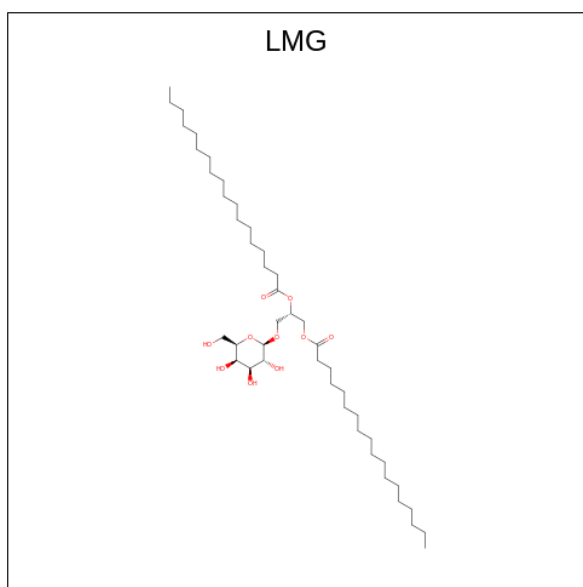
- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code:

LHG) (formula: C₃₈H₇₅O₁₀P).



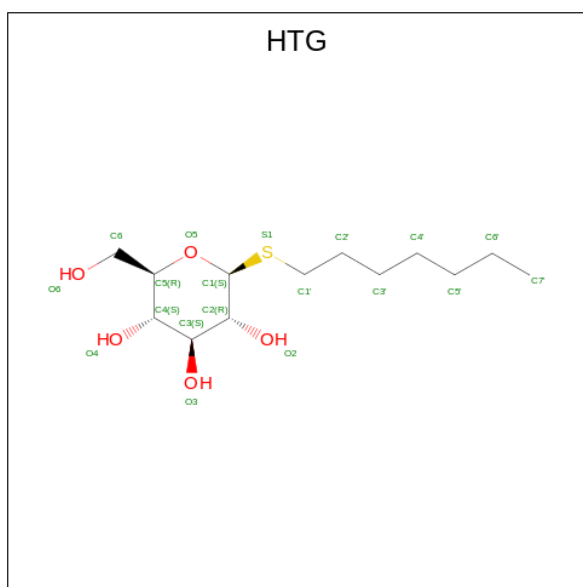
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	E	1	Total	C	O	P	0	0
			42	31	10	1		
31	L	1	Total	C	O	P	0	0
			49	38	10	1		
31	a	1	Total	C	O	P	0	0
			42	31	10	1		
31	b	1	Total	C	O	P	0	0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

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



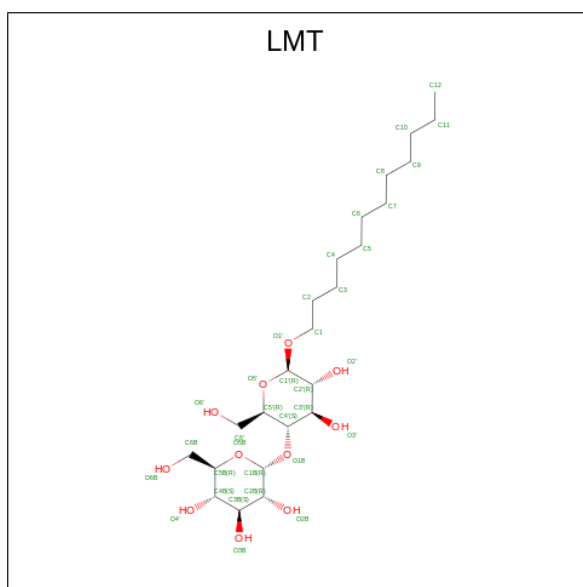
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	B	1	Total	C	O	0	0
			51	41	10		
32	C	1	Total	C	O	0	0
			51	41	10		
32	C	1	Total	C	O	0	0
			51	41	10		
32	C	1	Total	C	O	0	0
			51	41	10		
32	D	1	Total	C	O	0	0
			51	41	10		
32	Z	1	Total	C	O	0	0
			37	27	10		
32	c	1	Total	C	O	0	0
			51	41	10		
32	c	1	Total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

- Molecule 33 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



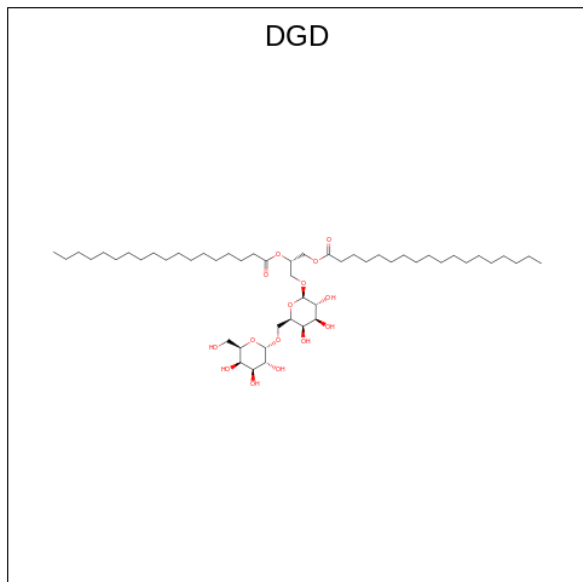
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	C	1	Total	C	O	S	0	0
			19	13	5	1		
33	D	1	Total	C	O	S	0	0
			16	10	5	1		
33	V	1	Total	C	O		0	0
			11	6	5			
33	b	1	Total	C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

- Molecule 34 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



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

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



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

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

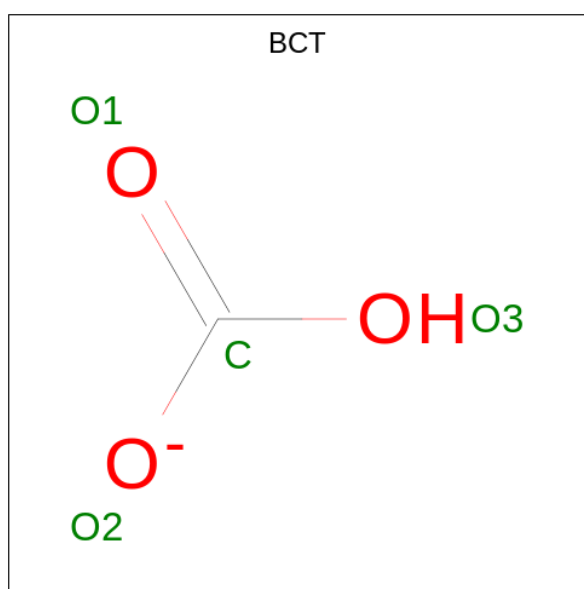
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	C	1	Total	Ca	0	0
			1	1		
36	F	1	Total	Ca	0	0
			1	1		

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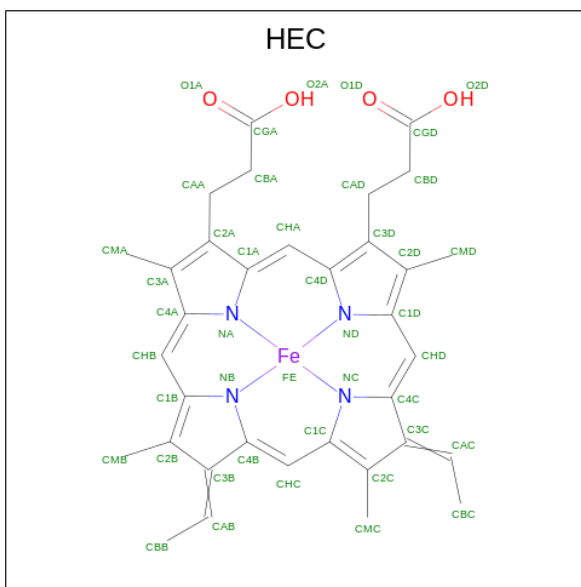
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	O	1	Total Ca 1 1	0	0
36	a	1	Total Ca 1 1	0	0
36	c	2	Total Ca 2 2	0	0
36	o	1	Total Ca 1 1	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	D	1	Total C O 4 1 3	0	0
37	d	1	Total C O 4 1 3	0	0

- Molecule 38 is HEME C (three-letter code: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



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

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

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

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	A	143	Total	O	0	0
			143	143		
40	B	223	Total	O	0	0
			223	223		
40	C	203	Total	O	0	0
			203	203		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	D	136	Total O 136 136	0	0
40	E	27	Total O 27 27	0	0
40	F	9	Total O 9 9	0	0
40	H	26	Total O 26 26	0	0
40	I	5	Total O 5 5	0	0
40	J	5	Total O 5 5	0	0
40	K	7	Total O 7 7	0	0
40	L	6	Total O 6 6	0	0
40	M	17	Total O 17 17	0	0
40	O	125	Total O 125 125	0	0
40	T	16	Total O 16 16	0	0
40	U	56	Total O 56 56	0	0
40	V	102	Total O 102 102	0	0
40	X	9	Total O 9 9	0	0
40	Y	1	Total O 1 1	0	0
40	R	1	Total O 1 1	0	0
40	a	143	Total O 143 143	0	0
40	b	234	Total O 234 234	0	0
40	c	174	Total O 174 174	0	0
40	d	125	Total O 125 125	0	0
40	e	16	Total O 16 16	0	0

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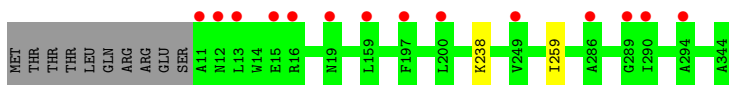
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	f	4	Total 4	O 4	0	0
40	h	23	Total 23	O 23	0	0
40	i	2	Total 2	O 2	0	0
40	j	3	Total 3	O 3	0	0
40	k	5	Total 5	O 5	0	0
40	l	7	Total 7	O 7	0	0
40	m	11	Total 11	O 11	0	0
40	o	99	Total 99	O 99	0	0
40	t	11	Total 11	O 11	0	0
40	u	71	Total 71	O 71	0	0
40	v	60	Total 60	O 60	0	0
40	x	9	Total 9	O 9	0	0
40	y	4	Total 4	O 4	0	0

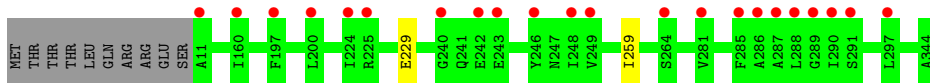
3 Residue-property plots [i](#)

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

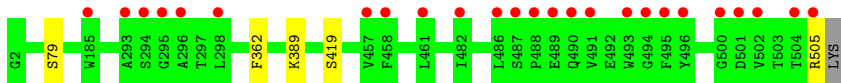
- Molecule 1: Photosystem II protein D1



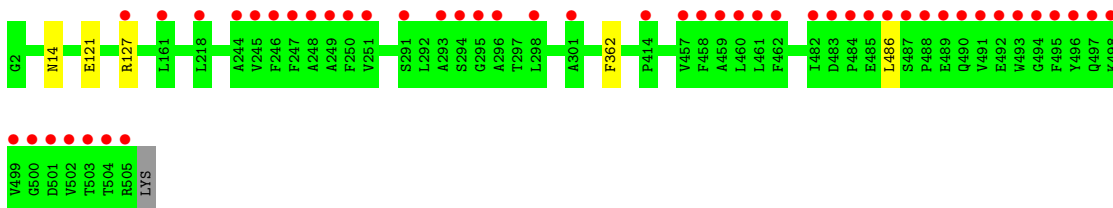
- Molecule 1: Photosystem II protein D1



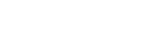
- Molecule 2: Photosystem II CP47 reaction center protein

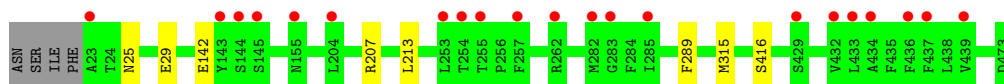


- Molecule 2: Photosystem II CP47 reaction center protein

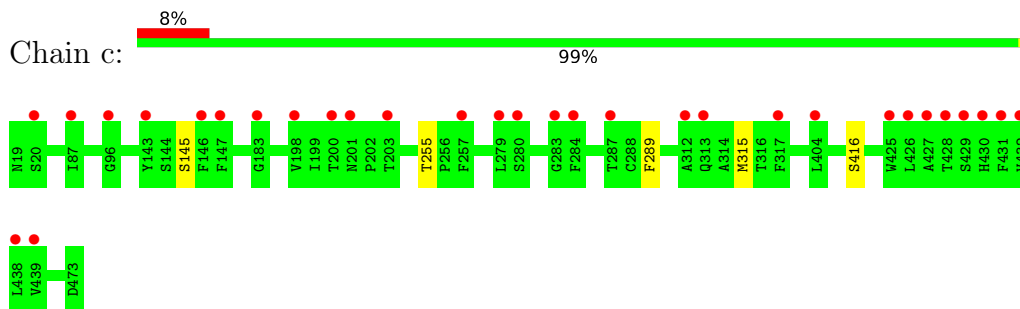


- Molecule 3: Photosystem II CP43 reaction center protein

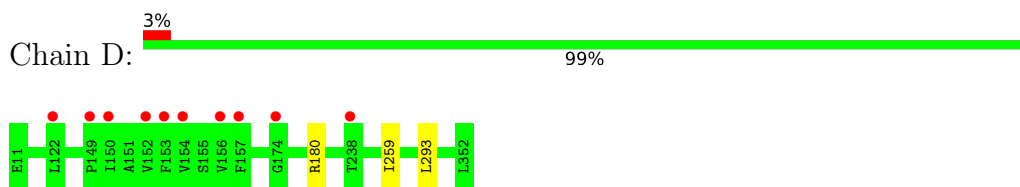




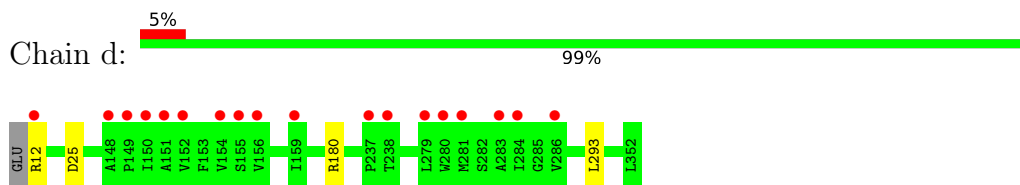
- Molecule 3: Photosystem II CP43 reaction center protein



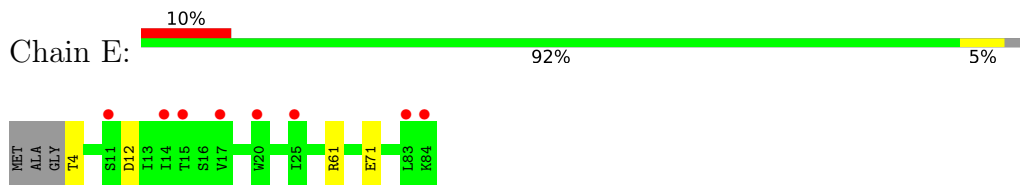
- Molecule 4: Photosystem II D2 protein



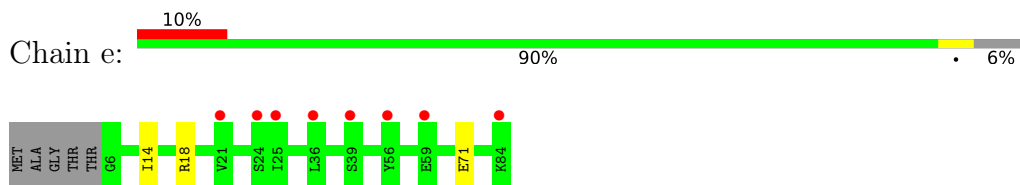
- Molecule 4: Photosystem II D2 protein



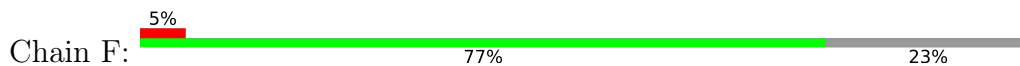
- Molecule 5: Cytochrome b559 subunit alpha

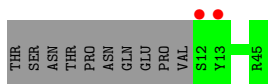


- Molecule 5: Cytochrome b559 subunit alpha

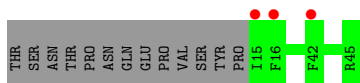


- Molecule 6: Cytochrome b559 subunit beta

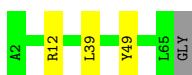




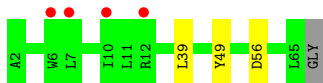
- Molecule 6: Cytochrome b559 subunit beta



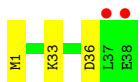
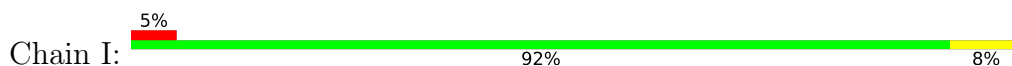
- Molecule 7: Photosystem II reaction center protein H



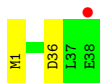
- Molecule 7: Photosystem II reaction center protein H



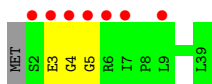
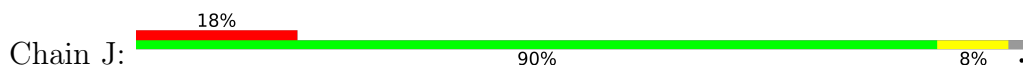
- Molecule 8: Photosystem II reaction center protein I



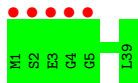
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



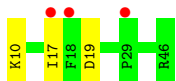
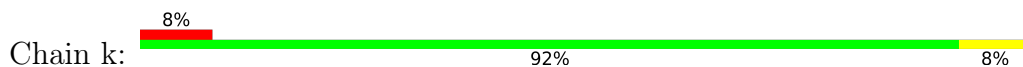
- Molecule 9: Photosystem II reaction center protein J



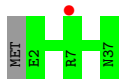
- Molecule 10: Photosystem II reaction center protein K



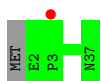
- Molecule 10: Photosystem II reaction center protein K



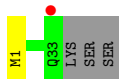
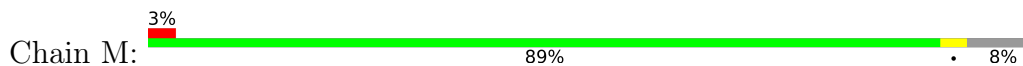
- Molecule 11: Photosystem II reaction center protein L



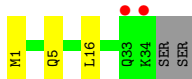
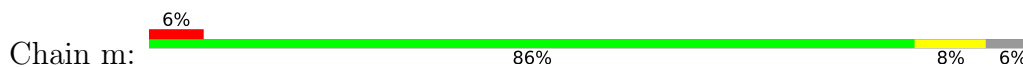
- Molecule 11: Photosystem II reaction center protein L



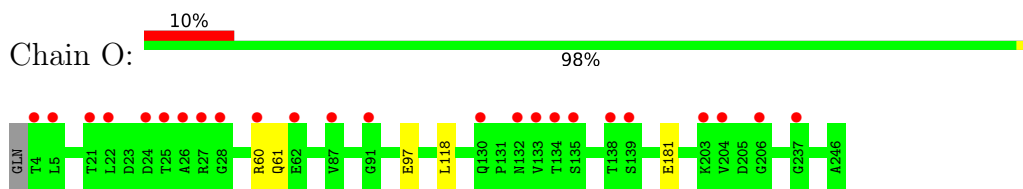
- Molecule 12: Photosystem II reaction center protein M



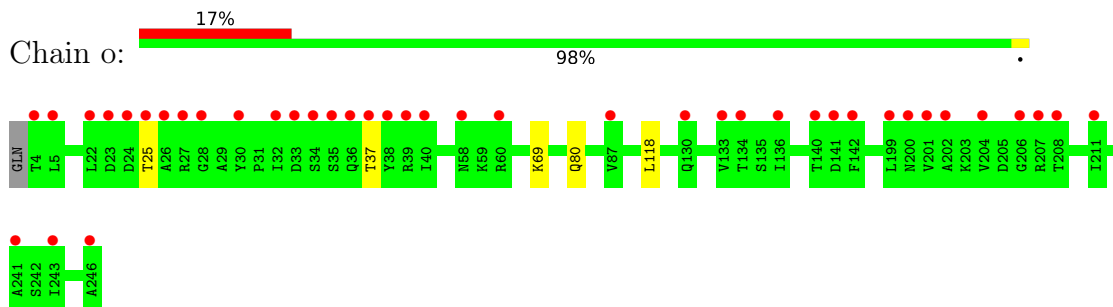
- Molecule 12: Photosystem II reaction center protein M



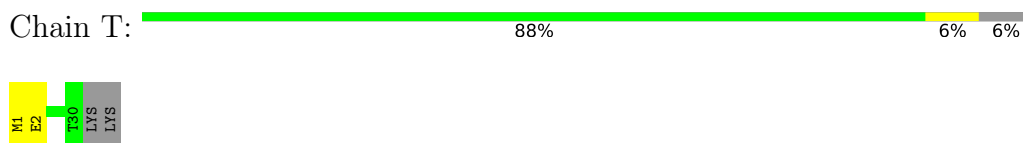
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



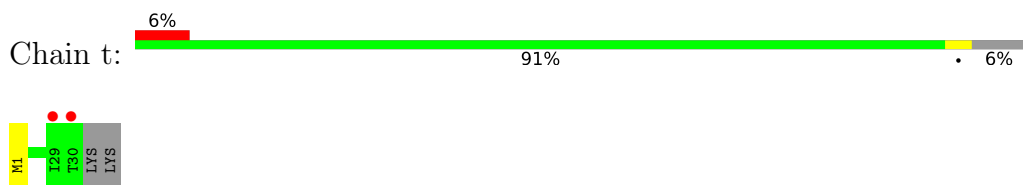
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



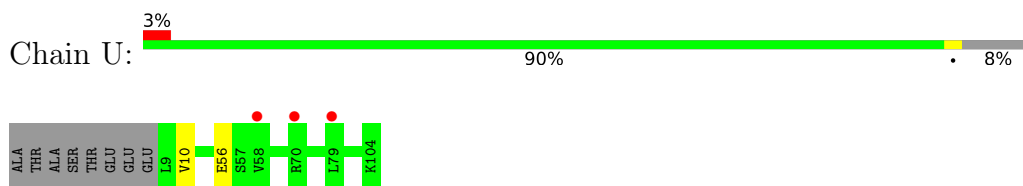
- Molecule 14: Photosystem II reaction center protein T



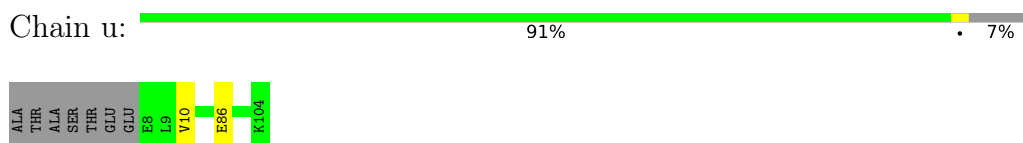
- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein

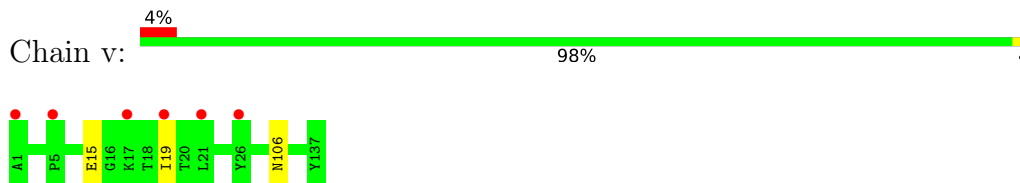


- Molecule 16: Cytochrome c-550

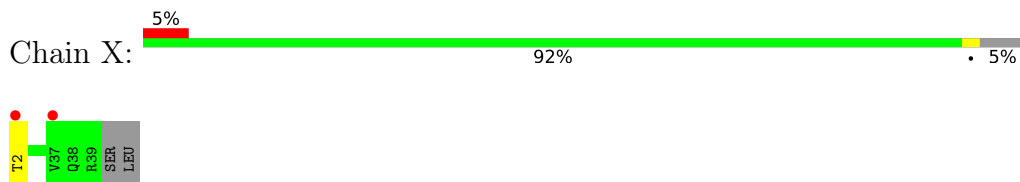


There are no outlier residues recorded for this chain.

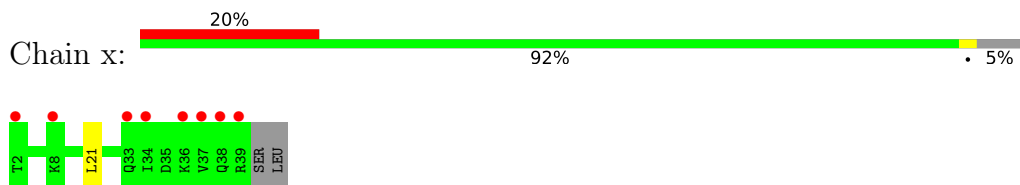
- Molecule 16: Cytochrome c-550



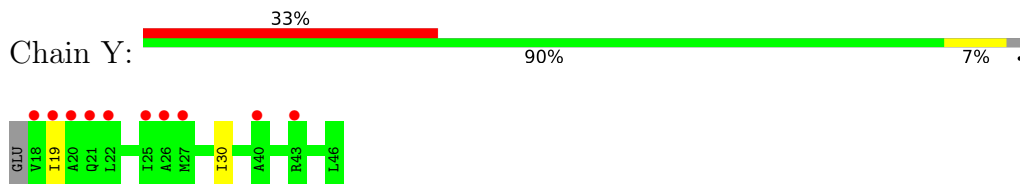
- Molecule 17: Photosystem II reaction center protein X



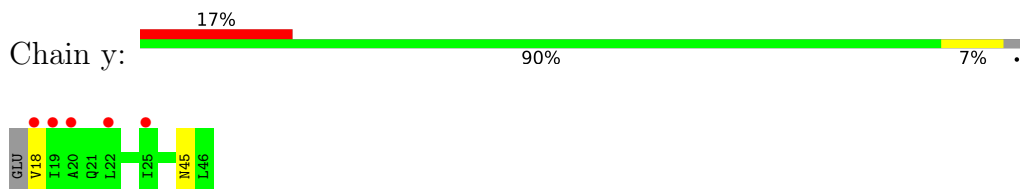
- Molecule 17: Photosystem II reaction center protein X



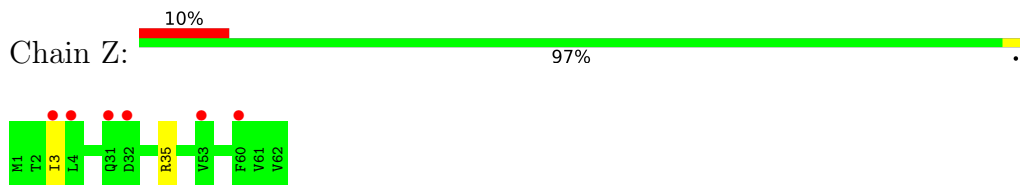
- Molecule 18: Photosystem II reaction center protein Ycf12



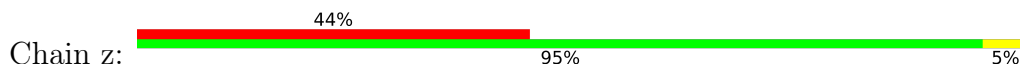
- Molecule 18: Photosystem II reaction center protein Ycf12

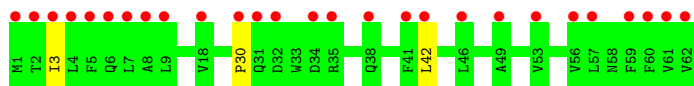


- Molecule 19: Photosystem II reaction center protein Z

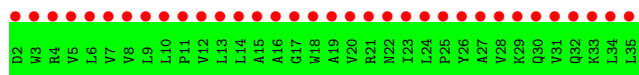


- Molecule 19: Photosystem II reaction center protein Z





- Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	126.15Å 232.70Å 288.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.97 – 2.25 52.83 – 2.25	Depositor EDS
% Data completeness (in resolution range)	96.0 (39.97-2.25) 85.6 (52.83-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.25Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.169 , 0.211 0.170 , 0.212	Depositor DCC
R_{free} test set	20023 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	43.9	Xtrriage
Anisotropy	0.424	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 70.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	53138	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.44	0/2719	0.56	0/3708
1	a	0.41	0/2727	0.54	0/3719
2	B	0.42	0/4190	0.55	0/5708
2	b	0.40	0/4138	0.53	0/5640
3	C	0.39	0/3626	0.51	0/4936
3	c	0.36	0/3648	0.49	0/4966
4	D	0.44	0/2821	0.55	0/3844
4	d	0.41	0/2812	0.53	0/3832
5	E	0.35	0/687	0.48	0/936
5	e	0.34	0/667	0.46	0/908
6	F	0.35	0/284	0.44	0/387
6	f	0.30	0/257	0.47	0/349
7	H	0.34	0/530	0.57	0/723
7	h	0.33	0/519	0.53	0/708
8	I	0.35	0/311	0.47	0/419
8	i	0.33	0/311	0.48	0/419
9	J	0.31	0/278	0.49	0/376
9	j	0.33	0/283	0.49	0/383
10	K	0.35	0/303	0.47	0/416
10	k	0.32	0/303	0.51	0/416
11	L	0.45	0/311	0.50	0/423
11	l	0.39	0/311	0.48	0/423
12	M	0.38	0/261	0.53	0/357
12	m	0.41	0/262	0.51	0/357
13	O	0.38	0/1917	0.58	0/2599
13	o	0.36	0/1910	0.57	0/2589
14	T	0.46	0/257	0.49	0/349
14	t	0.43	0/257	0.45	0/349
15	U	0.38	0/776	0.56	0/1052
15	u	0.36	0/785	0.59	0/1064
16	V	0.34	0/1085	0.52	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.33	0/1085	0.50	0/1473
17	X	0.29	0/284	0.47	0/384
17	x	0.28	0/284	0.43	0/384
18	Y	0.29	0/216	0.42	0/289
18	y	0.28	0/216	0.43	0/289
19	Z	0.30	0/490	0.39	0/669
19	z	0.29	0/490	0.41	0/669
20	R	0.26	0/279	0.40	0/383
All	All	0.39	0/42890	0.52	0/58368

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	334/344 (97%)	330 (99%)	3 (1%)	1 (0%)	41	46
1	a	335/344 (97%)	328 (98%)	6 (2%)	1 (0%)	41	46
2	B	512/505 (101%)	505 (99%)	7 (1%)	0	100	100
2	b	506/505 (100%)	497 (98%)	9 (2%)	0	100	100
3	C	453/455 (100%)	443 (98%)	8 (2%)	2 (0%)	34	37
3	c	455/455 (100%)	444 (98%)	10 (2%)	1 (0%)	47	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	340/342 (99%)	329 (97%)	11 (3%)	0	100	100
4	d	339/342 (99%)	331 (98%)	8 (2%)	0	100	100
5	E	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
5	e	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	29/44 (66%)	29 (100%)	0	0	100	100
7	H	63/65 (97%)	61 (97%)	2 (3%)	0	100	100
7	h	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
8	I	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
8	i	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
9	J	36/39 (92%)	33 (92%)	0	3 (8%)	1	0
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	32/36 (89%)	30 (94%)	2 (6%)	0	100	100
13	O	244/244 (100%)	237 (97%)	6 (2%)	1 (0%)	34	37
13	o	243/244 (100%)	236 (97%)	7 (3%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	94/104 (90%)	92 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
16	v	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
17	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
17	x	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
18	Y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
18	y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	9	4
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	5246/5384 (97%)	5129 (98%)	107 (2%)	10 (0%)	47	55

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416	SER
9	J	4	GLY
9	J	5	GLY

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	271/279 (97%)	270 (100%)	1 (0%)	91	94
1	a	272/279 (98%)	271 (100%)	1 (0%)	91	94
2	B	412/403 (102%)	407 (99%)	5 (1%)	71	80
2	b	406/403 (101%)	401 (99%)	5 (1%)	71	80
3	C	356/356 (100%)	349 (98%)	7 (2%)	55	64
3	c	358/356 (101%)	354 (99%)	4 (1%)	73	82
4	D	277/277 (100%)	274 (99%)	3 (1%)	73	82
4	d	276/277 (100%)	272 (99%)	4 (1%)	67	76
5	E	73/73 (100%)	69 (94%)	4 (6%)	21	21
5	e	70/73 (96%)	67 (96%)	3 (4%)	29	33
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	25/38 (66%)	25 (100%)	0	100	100
7	H	55/54 (102%)	51 (93%)	4 (7%)	14	12
7	h	54/54 (100%)	51 (94%)	3 (6%)	21	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	34/34 (100%)	32 (94%)	2 (6%)	19	19
8	i	34/34 (100%)	33 (97%)	1 (3%)	42	51
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	26/27 (96%)	26 (100%)	0	100	100
10	K	30/30 (100%)	27 (90%)	3 (10%)	7	5
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	5
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	30/32 (94%)	30 (100%)	0	100	100
12	m	30/32 (94%)	28 (93%)	2 (7%)	16	15
13	O	209/207 (101%)	205 (98%)	4 (2%)	57	66
13	o	208/207 (100%)	203 (98%)	5 (2%)	49	58
14	T	26/28 (93%)	25 (96%)	1 (4%)	33	39
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	83/89 (93%)	81 (98%)	2 (2%)	49	58
15	u	84/89 (94%)	82 (98%)	2 (2%)	49	58
16	V	117/117 (100%)	117 (100%)	0	100	100
16	v	117/117 (100%)	114 (97%)	3 (3%)	46	55
17	X	31/33 (94%)	30 (97%)	1 (3%)	39	47
17	x	31/33 (94%)	30 (97%)	1 (3%)	39	47
18	Y	22/23 (96%)	20 (91%)	2 (9%)	9	7
18	y	22/23 (96%)	20 (91%)	2 (9%)	9	7
19	Z	52/52 (100%)	50 (96%)	2 (4%)	33	39
19	z	52/52 (100%)	50 (96%)	2 (4%)	33	39
20	R	29/29 (100%)	29 (100%)	0	100	100
All	All	4352/4403 (99%)	4270 (98%)	82 (2%)	57	66

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	e	71	GLU
13	o	118	LEU
7	h	49	TYR

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Mol	Chain	Res	Type
12	m	5	GLN
16	v	19	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
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	$\# Z > 2$
14	FME	T	1	14	8,9,10	0.70	0	7,9,11	1.44	2 (28%)
8	FME	i	1	8	8,9,10	0.56	0	7,9,11	1.05	1 (14%)
14	FME	t	1	14	8,9,10	0.62	0	7,9,11	1.74	2 (28%)
12	FME	M	1	12	8,9,10	0.60	0	7,9,11	1.70	2 (28%)
12	FME	m	1	12	8,9,10	0.56	0	7,9,11	1.46	2 (28%)
8	FME	I	1	8	8,9,10	0.66	0	7,9,11	1.15	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	T	1	14	-	0/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	i	1	8	-	0/7/9/11	-
14	FME	t	1	14	-	2/7/9/11	-
12	FME	M	1	12	-	2/7/9/11	-
12	FME	m	1	12	-	2/7/9/11	-
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	CA-N-CN	-3.25	117.82	122.82
12	M	1	FME	CA-N-CN	-3.08	118.08	122.82
14	t	1	FME	O-C-CA	-2.60	117.96	124.78
14	T	1	FME	O-C-CA	-2.48	118.29	124.78
12	m	1	FME	C-CA-N	2.39	114.04	109.73

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

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

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 216 ligands modelled in this entry, 15 are monoatomic and 18 are unknown - leaving 183 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
27	SQD	f	101	-	42,43,54	1.17	3 (7%)	51,54,65	1.30	8 (15%)
23	CLA	b	601	40	65,73,73	2.14	16 (24%)	76,113,113	2.74	26 (34%)
23	CLA	c	510	-	65,73,73	2.14	16 (24%)	76,113,113	2.78	27 (35%)
26	GOL	o	302	-	5,5,5	0.82	0	5,5,5	1.04	0
23	CLA	b	614	-	65,73,73	2.01	16 (24%)	76,113,113	2.85	29 (38%)
23	CLA	b	607	40	65,73,73	2.00	17 (26%)	76,113,113	2.77	27 (35%)
33	HTG	h	101	-	16,16,19	1.14	2 (12%)	20,21,24	2.11	5 (25%)
26	GOL	B	624	-	5,5,5	0.89	0	5,5,5	1.02	0
23	CLA	C	510	-	65,73,73	2.07	17 (26%)	76,113,113	2.80	29 (38%)
23	CLA	C	514	-	65,73,73	2.08	16 (24%)	76,113,113	2.72	29 (38%)
35	DGD	c	519	-	63,63,67	0.85	2 (3%)	77,77,81	1.00	3 (3%)
23	CLA	B	603	-	65,73,73	2.04	16 (24%)	76,113,113	2.89	27 (35%)
25	BCR	B	619	-	41,41,41	1.03	1 (2%)	56,56,56	1.30	9 (16%)
27	SQD	D	412	-	42,43,54	1.15	3 (7%)	51,54,65	1.79	11 (21%)
23	CLA	a	404	-	65,73,73	2.02	16 (24%)	76,113,113	2.82	31 (40%)
34	LMT	e	101	-	36,36,36	0.53	1 (2%)	47,47,47	1.04	2 (4%)
29	PL9	D	406	-	55,55,55	0.67	2 (3%)	68,69,69	1.66	17 (25%)
27	SQD	b	620	-	53,54,54	1.03	3 (5%)	62,65,65	1.55	8 (12%)
23	CLA	b	609	-	65,73,73	2.04	18 (27%)	76,113,113	2.71	29 (38%)
23	CLA	b	613	-	65,73,73	2.05	15 (23%)	76,113,113	2.76	27 (35%)
35	DGD	c	518	-	63,63,67	0.89	2 (3%)	77,77,81	1.05	6 (7%)
26	GOL	b	628	-	5,5,5	0.97	0	5,5,5	1.07	0
23	CLA	B	601	40	65,73,73	2.10	17 (26%)	76,113,113	2.77	27 (35%)
32	LMG	c	501	-	51,51,55	0.92	2 (3%)	59,59,63	1.09	3 (5%)
34	LMT	a	413	-	36,36,36	0.59	1 (2%)	47,47,47	1.14	3 (6%)
26	GOL	B	627	-	5,5,5	0.99	0	5,5,5	1.15	0
31	LHG	D	408	-	48,48,48	0.90	2 (4%)	51,54,54	0.96	3 (5%)
23	CLA	D	403	-	65,73,73	2.00	16 (24%)	76,113,113	2.91	29 (38%)
23	CLA	d	402	-	65,73,73	2.01	16 (24%)	76,113,113	2.71	31 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	606	-	65,73,73	1.99	15 (23%)	76,113,113	2.92	29 (38%)
25	BCR	T	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.57	12 (21%)
24	PHO	a	417	-	51,69,69	1.85	8 (15%)	47,99,99	2.07	9 (19%)
25	BCR	H	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.36	7 (12%)
38	HEC	V	201	16	32,50,50	2.03	4 (12%)	24,82,82	1.95	6 (25%)
23	CLA	b	611	-	65,73,73	2.00	16 (24%)	76,113,113	2.82	27 (35%)
23	CLA	B	610	40	65,73,73	2.07	17 (26%)	76,113,113	2.79	26 (34%)
23	CLA	b	616	-	65,73,73	2.01	15 (23%)	76,113,113	2.86	30 (39%)
32	LMG	Z	101	-	37,37,55	1.01	3 (8%)	45,45,63	1.53	6 (13%)
23	CLA	B	616	-	65,73,73	1.98	16 (24%)	76,113,113	2.76	28 (36%)
25	BCR	b	618	-	41,41,41	1.03	1 (2%)	56,56,56	1.30	8 (14%)
23	CLA	b	612	-	65,73,73	2.05	17 (26%)	76,113,113	2.83	27 (35%)
25	BCR	a	409	-	41,41,41	1.08	1 (2%)	56,56,56	1.47	10 (17%)
23	CLA	c	503	-	65,73,73	2.01	17 (26%)	76,113,113	2.78	27 (35%)
23	CLA	B	614	-	65,73,73	1.95	17 (26%)	76,113,113	3.02	28 (36%)
35	DGD	c	520	-	63,63,67	0.88	2 (3%)	77,77,81	1.02	5 (6%)
23	CLA	C	507	-	65,73,73	1.98	16 (24%)	76,113,113	2.68	25 (32%)
26	GOL	O	302	-	5,5,5	0.86	0	5,5,5	1.01	0
34	LMT	M	101	-	36,36,36	0.45	0	47,47,47	0.97	3 (6%)
29	PL9	A	413	-	55,55,55	0.66	2 (3%)	68,69,69	1.87	21 (30%)
25	BCR	h	102	-	41,41,41	1.07	1 (2%)	56,56,56	1.31	7 (12%)
32	LMG	d	412	39	51,51,55	0.92	2 (3%)	59,59,63	0.87	2 (3%)
25	BCR	b	617	-	41,41,41	1.10	1 (2%)	56,56,56	1.50	7 (12%)
23	CLA	A	404	-	65,73,73	2.07	18 (27%)	76,113,113	2.80	31 (40%)
23	CLA	B	613	-	65,73,73	1.99	16 (24%)	76,113,113	2.76	27 (35%)
23	CLA	A	406	40	65,73,73	2.01	17 (26%)	76,113,113	2.73	25 (32%)
34	LMT	C	526	-	36,36,36	0.49	1 (2%)	47,47,47	1.04	3 (6%)
33	HTG	D	411	-	16,16,19	1.06	2 (12%)	20,21,24	1.33	1 (5%)
26	GOL	A	410	-	5,5,5	1.12	0	5,5,5	0.81	0
31	LHG	d	408	-	48,48,48	0.90	2 (4%)	51,54,54	1.07	3 (5%)
35	DGD	h	103	-	63,63,67	0.91	3 (4%)	77,77,81	1.01	3 (3%)
25	BCR	c	517	-	41,41,41	1.06	1 (2%)	56,56,56	1.44	11 (19%)
33	HTG	V	202	-	11,11,19	0.21	0	15,15,24	1.25	2 (13%)
23	CLA	C	511	-	65,73,73	2.14	18 (27%)	76,113,113	2.70	28 (36%)
33	HTG	B	623	-	19,19,19	0.81	1 (5%)	23,24,24	1.82	5 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LMG	D	413	39	51,51,55	0.83	2 (3%)	59,59,63	0.96	4 (6%)
25	BCR	B	617	-	41,41,41	1.06	1 (2%)	56,56,56	1.35	7 (12%)
24	PHO	a	407	-	51,69,69	1.85	9 (17%)	47,99,99	1.89	10 (21%)
32	LMG	c	522	-	51,51,55	0.96	2 (3%)	59,59,63	1.11	5 (8%)
31	LHG	A	416	-	48,48,48	0.89	2 (4%)	51,54,54	1.12	6 (11%)
31	LHG	d	407	-	48,48,48	0.89	2 (4%)	51,54,54	1.01	4 (7%)
27	SQD	B	620	-	53,54,54	1.04	3 (5%)	62,65,65	1.44	11 (17%)
23	CLA	C	506	40	65,73,73	1.99	17 (26%)	76,113,113	2.75	28 (36%)
23	CLA	c	514	-	65,73,73	2.04	16 (24%)	76,113,113	2.76	30 (39%)
23	CLA	B	611	-	65,73,73	2.04	16 (24%)	76,113,113	2.91	30 (39%)
23	CLA	b	610	40	65,73,73	2.04	17 (26%)	76,113,113	2.78	29 (38%)
38	HEC	e	102	5,6	32,50,50	1.57	4 (12%)	24,82,82	1.80	5 (20%)
31	LHG	D	407	-	48,48,48	0.88	2 (4%)	51,54,54	1.00	3 (5%)
25	BCR	k	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.45	11 (19%)
25	BCR	y	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.61	10 (17%)
31	LHG	L	101	-	48,48,48	0.92	3 (6%)	51,54,54	1.11	3 (5%)
23	CLA	D	404	-	65,73,73	2.02	16 (24%)	76,113,113	2.74	25 (32%)
23	CLA	a	405	40	65,73,73	2.08	15 (23%)	76,113,113	2.82	28 (36%)
23	CLA	B	605	-	65,73,73	2.01	15 (23%)	76,113,113	2.73	25 (32%)
23	CLA	B	615	-	65,73,73	1.95	15 (23%)	76,113,113	2.84	27 (35%)
23	CLA	a	406	40	65,73,73	1.93	14 (21%)	76,113,113	2.83	27 (35%)
34	LMT	b	621	-	25,25,36	0.51	0	30,30,47	0.58	0
26	GOL	b	624	-	5,5,5	0.95	0	5,5,5	1.06	0
27	SQD	a	410	-	53,54,54	0.98	3 (5%)	62,65,65	1.68	11 (17%)
23	CLA	B	609	-	65,73,73	1.97	16 (24%)	76,113,113	2.82	26 (34%)
34	LMT	m	103	-	36,36,36	0.46	0	47,47,47	0.99	4 (8%)
23	CLA	d	403	-	65,73,73	2.10	17 (26%)	76,113,113	2.81	30 (39%)
33	HTG	B	625	-	19,19,19	1.04	2 (10%)	23,24,24	1.11	1 (4%)
35	DGD	C	520	-	63,63,67	0.84	2 (3%)	77,77,81	1.04	5 (6%)
34	LMT	D	402	-	36,36,36	0.52	1 (2%)	47,47,47	0.85	1 (2%)
32	LMG	z	101	-	39,39,55	1.08	2 (5%)	47,47,63	1.10	3 (6%)
23	CLA	C	505	-	65,73,73	2.03	16 (24%)	76,113,113	2.84	24 (31%)
25	BCR	D	405	-	41,41,41	1.06	1 (2%)	56,56,56	1.64	12 (21%)
23	CLA	B	612	-	65,73,73	1.97	16 (24%)	76,113,113	2.97	28 (36%)
23	CLA	C	504	-	65,73,73	1.99	16 (24%)	76,113,113	2.69	27 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	LMT	t	101	-	26,26,36	0.55	1 (3%)	31,31,47	1.14	4 (12%)
23	CLA	C	513	3	65,73,73	2.07	19 (29%)	76,113,113	2.72	27 (35%)
33	HTG	b	625	-	19,19,19	0.99	2 (10%)	23,24,24	1.30	3 (13%)
26	GOL	a	411	-	5,5,5	0.87	0	5,5,5	1.04	0
35	DGD	H	102	-	63,63,67	0.83	3 (4%)	77,77,81	1.04	5 (6%)
33	HTG	b	623	-	19,19,19	1.00	1 (5%)	23,24,24	1.59	2 (8%)
23	CLA	b	615	-	65,73,73	1.99	15 (23%)	76,113,113	2.74	27 (35%)
23	CLA	c	511	-	65,73,73	2.11	17 (26%)	76,113,113	2.72	26 (34%)
31	LHG	E	101	-	41,41,48	1.04	2 (4%)	44,47,54	1.03	2 (4%)
32	LMG	m	101	-	51,51,55	0.89	2 (3%)	59,59,63	1.12	5 (8%)
37	BCT	d	401	21	2,3,3	0.58	0	2,3,3	1.69	1 (50%)
32	LMG	C	521	-	51,51,55	0.99	2 (3%)	59,59,63	1.03	3 (5%)
26	GOL	v	201	-	5,5,5	1.15	0	5,5,5	0.82	0
29	PL9	d	405	-	55,55,55	0.64	1 (1%)	68,69,69	1.66	16 (23%)
23	CLA	c	513	3	65,73,73	2.05	15 (23%)	76,113,113	2.85	28 (36%)
23	CLA	B	606	-	65,73,73	2.04	16 (24%)	76,113,113	2.85	28 (36%)
23	CLA	b	604	-	65,73,73	2.04	16 (24%)	76,113,113	2.70	29 (38%)
23	CLA	c	505	-	65,73,73	2.04	16 (24%)	76,113,113	2.74	25 (32%)
23	CLA	C	512	-	65,73,73	2.05	16 (24%)	76,113,113	2.76	28 (36%)
33	HTG	B	622	-	19,19,19	1.00	1 (5%)	23,24,24	1.59	5 (21%)
34	LMT	E	102	-	36,36,36	0.52	1 (2%)	47,47,47	0.85	1 (2%)
35	DGD	C	519	-	63,63,67	0.90	2 (3%)	77,77,81	1.10	4 (5%)
23	CLA	C	508	-	65,73,73	2.08	17 (26%)	76,113,113	2.73	30 (39%)
27	SQD	C	501	-	53,54,54	0.95	3 (5%)	62,65,65	1.90	10 (16%)
23	CLA	c	506	40	65,73,73	2.12	17 (26%)	76,113,113	2.83	30 (39%)
38	HEC	E	103	5,6	32,50,50	1.53	4 (12%)	24,82,82	1.93	6 (25%)
25	BCR	C	516	-	41,41,41	1.00	1 (2%)	56,56,56	1.62	10 (17%)
23	CLA	B	607	40	65,73,73	1.99	17 (26%)	76,113,113	2.73	28 (36%)
25	BCR	K	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.41	9 (16%)
32	LMG	C	522	-	51,51,55	1.01	3 (5%)	59,59,63	1.31	5 (8%)
23	CLA	c	515	-	65,73,73	2.07	16 (24%)	76,113,113	2.76	29 (38%)
23	CLA	c	512	-	65,73,73	2.00	16 (24%)	76,113,113	2.69	28 (36%)
34	LMT	B	628	-	36,36,36	0.42	0	47,47,47	1.10	3 (6%)
28	OEX	A	412	3,1,40	0,15,15	-	-	-	-	-
23	CLA	c	508	-	65,73,73	2.06	16 (24%)	76,113,113	2.76	29 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	PHO	A	415	-	51,69,69	1.87	7 (13%)	47,99,99	1.86	12 (25%)
23	CLA	A	405	40	65,73,73	2.00	17 (26%)	76,113,113	2.84	28 (36%)
25	BCR	c	516	-	41,41,41	1.03	1 (2%)	56,56,56	1.45	10 (17%)
25	BCR	A	409	-	41,41,41	1.03	1 (2%)	56,56,56	1.48	12 (21%)
33	HTG	c	523	-	19,19,19	0.96	2 (10%)	23,24,24	1.48	1 (4%)
23	CLA	b	602	-	65,73,73	2.10	16 (24%)	76,113,113	2.82	30 (39%)
23	CLA	B	608	-	65,73,73	2.02	16 (24%)	76,113,113	2.80	32 (42%)
31	LHG	d	406	-	48,48,48	0.88	2 (4%)	51,54,54	1.12	5 (9%)
34	LMT	a	418	-	36,36,36	0.45	0	47,47,47	0.92	1 (2%)
37	BCT	D	401	21	2,3,3	0.55	0	2,3,3	1.18	0
32	LMG	B	621	-	51,51,55	0.91	2 (3%)	59,59,63	1.16	4 (6%)
23	CLA	A	408	-	65,73,73	2.07	16 (24%)	76,113,113	2.71	30 (39%)
23	CLA	b	603	-	65,73,73	2.08	16 (24%)	76,113,113	2.86	28 (36%)
25	BCR	Y	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.84	17 (30%)
23	CLA	C	509	40	65,73,73	2.03	16 (24%)	76,113,113	2.74	25 (32%)
26	GOL	c	502	-	5,5,5	1.06	0	5,5,5	0.89	0
31	LHG	a	419	-	41,41,48	1.05	2 (4%)	44,47,54	0.97	2 (4%)
27	SQD	a	412	-	53,54,54	1.04	3 (5%)	62,65,65	1.28	6 (9%)
25	BCR	d	404	-	41,41,41	1.12	1 (2%)	56,56,56	1.73	11 (19%)
33	HTG	C	523	-	19,19,19	0.92	1 (5%)	23,24,24	1.41	1 (4%)
32	LMG	C	502	-	51,51,55	0.92	2 (3%)	59,59,63	1.02	2 (3%)
34	LMT	B	630	-	25,25,36	0.44	0	30,30,47	1.02	2 (6%)
23	CLA	c	504	-	65,73,73	2.05	15 (23%)	76,113,113	2.72	24 (31%)
25	BCR	C	517	-	41,41,41	1.01	1 (2%)	56,56,56	1.56	12 (21%)
35	DGD	C	518	-	63,63,67	0.88	2 (3%)	77,77,81	0.99	3 (3%)
23	CLA	B	602	-	65,73,73	2.05	16 (24%)	76,113,113	2.81	30 (39%)
23	CLA	C	503	-	65,73,73	1.99	16 (24%)	76,113,113	2.89	27 (35%)
34	LMT	M	103	-	36,36,36	0.46	0	47,47,47	1.03	2 (4%)
23	CLA	c	509	40	65,73,73	2.08	15 (23%)	76,113,113	2.83	28 (36%)
25	BCR	B	618	-	41,41,41	0.93	1 (2%)	56,56,56	1.41	7 (12%)
23	CLA	b	605	-	65,73,73	1.98	18 (27%)	76,113,113	2.94	24 (31%)
34	LMT	b	627	-	25,25,36	0.45	0	30,30,47	0.90	1 (3%)
23	CLA	B	604	-	65,73,73	2.04	18 (27%)	76,113,113	2.68	29 (38%)
26	GOL	C	524	-	5,5,5	1.08	0	5,5,5	0.94	0
28	OEX	a	414	3,1,40	0,15,15	-	-	-	-	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	608	-	65,73,73	2.07	16 (24%)	76,113,113	2.74	29 (38%)
24	PHO	A	407	-	51,69,69	1.80	8 (15%)	47,99,99	1.71	9 (19%)
23	CLA	c	507	-	65,73,73	2.01	16 (24%)	76,113,113	2.66	26 (34%)
32	LMG	c	521	-	51,51,55	0.92	2 (3%)	59,59,63	1.01	3 (5%)
25	BCR	b	619	-	41,41,41	1.16	2 (4%)	56,56,56	1.50	11 (19%)
23	CLA	a	408	-	65,73,73	1.99	16 (24%)	76,113,113	2.79	28 (36%)
26	GOL	B	629	-	5,5,5	1.01	0	5,5,5	0.87	0
25	BCR	t	102	-	41,41,41	1.06	1 (2%)	56,56,56	1.41	10 (17%)
31	LHG	b	629	-	48,48,48	0.90	2 (4%)	51,54,54	1.04	3 (5%)
23	CLA	C	515	-	65,73,73	2.05	16 (24%)	76,113,113	2.75	26 (34%)
27	SQD	A	411	-	53,54,54	1.04	3 (5%)	62,65,65	1.26	7 (11%)
38	HEC	v	202	16	32,50,50	2.09	4 (12%)	24,82,82	1.87	5 (20%)
29	PL9	a	415	-	55,55,55	0.65	2 (3%)	68,69,69	1.98	22 (32%)
33	HTG	b	622	-	19,19,19	1.10	1 (5%)	23,24,24	1.42	2 (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
27	SQD	f	101	-	-	19/38/58/69	0/1/1/1
23	CLA	b	601	40	1/1/15/20	15/37/115/115	-
23	CLA	c	510	-	1/1/15/20	10/37/115/115	-
26	GOL	o	302	-	-	2/4/4/4	-
23	CLA	b	614	-	1/1/15/20	13/37/115/115	-
23	CLA	b	607	40	1/1/15/20	1/37/115/115	-
33	HTG	h	101	-	-	2/7/27/30	0/1/1/1
26	GOL	B	624	-	-	2/4/4/4	-
23	CLA	C	510	-	1/1/15/20	5/37/115/115	-
23	CLA	C	514	-	1/1/15/20	14/37/115/115	-
35	DGD	c	519	-	-	17/51/91/95	0/2/2/2
23	CLA	B	603	-	1/1/15/20	6/37/115/115	-
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
27	SQD	D	412	-	-	15/38/58/69	0/1/1/1
23	CLA	a	404	-	1/1/15/20	6/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMT	e	101	-	-	9/21/61/61	0/2/2/2
29	PL9	D	406	-	-	8/53/73/73	0/1/1/1
27	SQD	b	620	-	-	24/49/69/69	0/1/1/1
23	CLA	b	609	-	1/1/15/20	6/37/115/115	-
23	CLA	b	613	-	1/1/15/20	7/37/115/115	-
35	DGD	c	518	-	-	18/51/91/95	0/2/2/2
26	GOL	b	628	-	-	0/4/4/4	-
23	CLA	B	601	40	1/1/15/20	10/37/115/115	-
32	LMG	c	501	-	-	18/46/66/70	0/1/1/1
34	LMT	a	413	-	-	7/21/61/61	0/2/2/2
26	GOL	B	627	-	-	0/4/4/4	-
31	LHG	D	408	-	-	13/53/53/53	-
23	CLA	D	403	-	1/1/15/20	4/37/115/115	-
23	CLA	d	402	-	1/1/15/20	3/37/115/115	-
23	CLA	b	606	-	1/1/15/20	11/37/115/115	-
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
24	PHO	a	417	-	-	3/37/103/103	0/5/6/6
25	BCR	H	101	-	-	1/29/63/63	0/2/2/2
38	HEC	V	201	16	-	2/10/54/54	-
23	CLA	b	611	-	1/1/15/20	5/37/115/115	-
23	CLA	B	610	40	1/1/15/20	8/37/115/115	-
23	CLA	b	616	-	1/1/15/20	7/37/115/115	-
32	LMG	Z	101	-	-	9/31/51/70	0/1/1/1
23	CLA	B	616	-	1/1/15/20	6/37/115/115	-
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
23	CLA	b	612	-	1/1/15/20	4/37/115/115	-
25	BCR	a	409	-	-	2/29/63/63	0/2/2/2
23	CLA	c	503	-	1/1/15/20	5/37/115/115	-
23	CLA	B	614	-	1/1/15/20	14/37/115/115	-
35	DGD	c	520	-	-	10/51/91/95	0/2/2/2
23	CLA	C	507	-	1/1/15/20	7/37/115/115	-
26	GOL	O	302	-	-	4/4/4/4	-
34	LMT	M	101	-	-	6/21/61/61	0/2/2/2
29	PL9	A	413	-	-	16/53/73/73	0/1/1/1
25	BCR	h	102	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LMG	d	412	39	-	9/46/66/70	0/1/1/1
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
23	CLA	A	404	-	1/1/15/20	2/37/115/115	-
23	CLA	B	613	-	1/1/15/20	8/37/115/115	-
23	CLA	A	406	40	-	4/37/115/115	-
34	LMT	C	526	-	-	8/21/61/61	0/2/2/2
33	HTG	D	411	-	-	2/7/27/30	0/1/1/1
26	GOL	A	410	-	-	2/4/4/4	-
31	LHG	d	408	-	-	10/53/53/53	-
35	DGD	h	103	-	-	14/51/91/95	0/2/2/2
25	BCR	c	517	-	-	0/29/63/63	0/2/2/2
33	HTG	V	202	-	-	1/2/19/30	0/1/1/1
23	CLA	C	511	-	1/1/15/20	5/37/115/115	-
33	HTG	B	623	-	-	4/10/30/30	0/1/1/1
32	LMG	D	413	39	-	8/46/66/70	0/1/1/1
25	BCR	B	617	-	-	0/29/63/63	0/2/2/2
24	PHO	a	407	-	-	5/37/103/103	0/5/6/6
32	LMG	c	522	-	-	11/46/66/70	0/1/1/1
31	LHG	A	416	-	-	16/53/53/53	-
31	LHG	d	407	-	-	20/53/53/53	-
27	SQD	B	620	-	-	17/49/69/69	0/1/1/1
23	CLA	C	506	40	1/1/15/20	6/37/115/115	-
23	CLA	c	514	-	1/1/15/20	13/37/115/115	-
23	CLA	B	611	-	1/1/15/20	3/37/115/115	-
23	CLA	b	610	40	1/1/15/20	9/37/115/115	-
38	HEC	e	102	5,6	-	3/10/54/54	-
31	LHG	D	407	-	-	12/53/53/53	-
25	BCR	k	101	-	-	2/29/63/63	0/2/2/2
25	BCR	y	101	-	-	6/29/63/63	0/2/2/2
31	LHG	L	101	-	-	14/53/53/53	-
23	CLA	D	404	-	1/1/15/20	10/37/115/115	-
23	CLA	a	405	40	1/1/15/20	11/37/115/115	-
23	CLA	B	605	-	1/1/15/20	4/37/115/115	-
23	CLA	B	615	-	1/1/15/20	7/37/115/115	-
23	CLA	a	406	40	-	6/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMT	b	621	-	-	7/17/37/61	0/1/1/2
26	GOL	b	624	-	-	3/4/4/4	-
27	SQD	a	410	-	-	14/49/69/69	0/1/1/1
23	CLA	B	609	-	1/1/15/20	5/37/115/115	-
34	LMT	m	103	-	-	7/21/61/61	0/2/2/2
23	CLA	d	403	-	1/1/15/20	8/37/115/115	-
33	HTG	B	625	-	-	3/10/30/30	0/1/1/1
35	DGD	C	520	-	-	10/51/91/95	0/2/2/2
34	LMT	D	402	-	-	8/21/61/61	0/2/2/2
32	LMG	z	101	-	-	8/34/54/70	0/1/1/1
23	CLA	C	505	-	1/1/15/20	4/37/115/115	-
25	BCR	D	405	-	-	8/29/63/63	0/2/2/2
23	CLA	B	612	-	1/1/15/20	3/37/115/115	-
23	CLA	C	504	-	-	8/37/115/115	-
34	LMT	t	101	-	-	6/17/38/61	0/1/1/2
23	CLA	C	513	3	1/1/15/20	2/37/115/115	-
33	HTG	b	625	-	-	4/10/30/30	0/1/1/1
26	GOL	a	411	-	-	4/4/4/4	-
35	DGD	H	102	-	-	11/51/91/95	0/2/2/2
33	HTG	b	623	-	-	2/10/30/30	0/1/1/1
23	CLA	b	615	-	1/1/15/20	8/37/115/115	-
23	CLA	c	511	-	1/1/15/20	14/37/115/115	-
31	LHG	E	101	-	-	15/46/46/53	-
32	LMG	m	101	-	-	10/46/66/70	0/1/1/1
32	LMG	C	521	-	-	10/46/66/70	0/1/1/1
26	GOL	v	201	-	-	2/4/4/4	-
29	PL9	d	405	-	-	7/53/73/73	0/1/1/1
23	CLA	c	513	3	1/1/15/20	8/37/115/115	-
23	CLA	B	606	-	1/1/15/20	11/37/115/115	-
23	CLA	b	604	-	1/1/15/20	11/37/115/115	-
23	CLA	c	505	-	1/1/15/20	1/37/115/115	-
23	CLA	C	512	-	1/1/15/20	10/37/115/115	-
33	HTG	B	622	-	-	5/10/30/30	0/1/1/1
34	LMT	E	102	-	-	7/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	DGD	C	519	-	-	16/51/91/95	0/2/2/2
23	CLA	C	508	-	1/1/15/20	11/37/115/115	-
27	SQD	C	501	-	-	12/49/69/69	0/1/1/1
23	CLA	c	506	40	1/1/15/20	6/37/115/115	-
38	HEC	E	103	5,6	-	4/10/54/54	-
25	BCR	C	516	-	-	3/29/63/63	0/2/2/2
23	CLA	B	607	40	1/1/15/20	2/37/115/115	-
25	BCR	K	101	-	-	1/29/63/63	0/2/2/2
32	LMG	C	522	-	-	12/46/66/70	0/1/1/1
23	CLA	c	515	-	1/1/15/20	7/37/115/115	-
23	CLA	c	512	-	1/1/15/20	7/37/115/115	-
34	LMT	B	628	-	-	10/21/61/61	0/2/2/2
23	CLA	c	508	-	1/1/15/20	10/37/115/115	-
24	PHO	A	415	-	-	3/37/103/103	0/5/6/6
23	CLA	A	405	40	1/1/15/20	5/37/115/115	-
25	BCR	c	516	-	-	0/29/63/63	0/2/2/2
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
33	HTG	c	523	-	-	3/10/30/30	0/1/1/1
23	CLA	b	602	-	1/1/15/20	3/37/115/115	-
23	CLA	B	608	-	-	2/37/115/115	-
31	LHG	d	406	-	-	15/53/53/53	-
34	LMT	a	418	-	-	4/21/61/61	0/2/2/2
32	LMG	B	621	-	-	11/46/66/70	0/1/1/1
23	CLA	A	408	-	1/1/15/20	9/37/115/115	-
23	CLA	b	603	-	1/1/15/20	3/37/115/115	-
25	BCR	Y	101	-	-	6/29/63/63	0/2/2/2
23	CLA	C	509	40	1/1/15/20	5/37/115/115	-
26	GOL	c	502	-	-	0/4/4/4	-
31	LHG	a	419	-	-	18/46/46/53	-
27	SQD	a	412	-	-	17/49/69/69	0/1/1/1
25	BCR	d	404	-	-	4/29/63/63	0/2/2/2
33	HTG	C	523	-	-	1/10/30/30	0/1/1/1
32	LMG	C	502	-	-	25/46/66/70	0/1/1/1
34	LMT	B	630	-	-	5/17/37/61	0/1/1/2
23	CLA	c	504	-	1/1/15/20	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	C	517	-	-	2/29/63/63	0/2/2/2
35	DGD	C	518	-	-	14/51/91/95	0/2/2/2
23	CLA	B	602	-	1/1/15/20	5/37/115/115	-
23	CLA	C	503	-	1/1/15/20	4/37/115/115	-
34	LMT	M	103	-	-	9/21/61/61	0/2/2/2
23	CLA	c	509	40	1/1/15/20	5/37/115/115	-
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
23	CLA	b	605	-	1/1/15/20	5/37/115/115	-
34	LMT	b	627	-	-	9/17/37/61	0/1/1/2
23	CLA	B	604	-	1/1/15/20	10/37/115/115	-
26	GOL	C	524	-	-	0/4/4/4	-
23	CLA	b	608	-	-	2/37/115/115	-
24	PHO	A	407	-	-	2/37/103/103	0/5/6/6
23	CLA	c	507	-	1/1/15/20	6/37/115/115	-
32	LMG	c	521	-	-	6/46/66/70	0/1/1/1
25	BCR	b	619	-	-	4/29/63/63	0/2/2/2
23	CLA	a	408	-	1/1/15/20	14/37/115/115	-
26	GOL	B	629	-	-	0/4/4/4	-
25	BCR	t	102	-	-	4/29/63/63	0/2/2/2
31	LHG	b	629	-	-	15/53/53/53	-
23	CLA	C	515	-	-	13/37/115/115	-
27	SQD	A	411	-	-	11/49/69/69	0/1/1/1
38	HEC	v	202	16	-	2/10/54/54	-
29	PL9	a	415	-	-	13/53/73/73	0/1/1/1
33	HTG	b	622	-	-	2/10/30/30	0/1/1/1

The worst 5 of 1325 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	506	CLA	C3B-C2B	6.93	1.50	1.40
23	b	612	CLA	C3B-C2B	6.85	1.49	1.40
24	A	415	PHO	C3B-C2B	6.75	1.49	1.40
23	C	510	CLA	C3B-C2B	6.73	1.49	1.40
23	c	510	CLA	C3B-C2B	6.61	1.49	1.40

The worst 5 of 2548 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	614	CLA	C2D-C1D-ND	10.44	117.80	110.10
23	c	513	CLA	C1D-ND-C4D	-10.37	98.97	106.33
23	b	605	CLA	C1D-ND-C4D	-10.34	98.99	106.33
23	B	614	CLA	C1D-ND-C4D	-10.29	99.02	106.33
23	B	612	CLA	C2D-C1D-ND	10.19	117.61	110.10

5 of 64 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404	CLA	ND
23	A	405	CLA	ND
23	A	408	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND

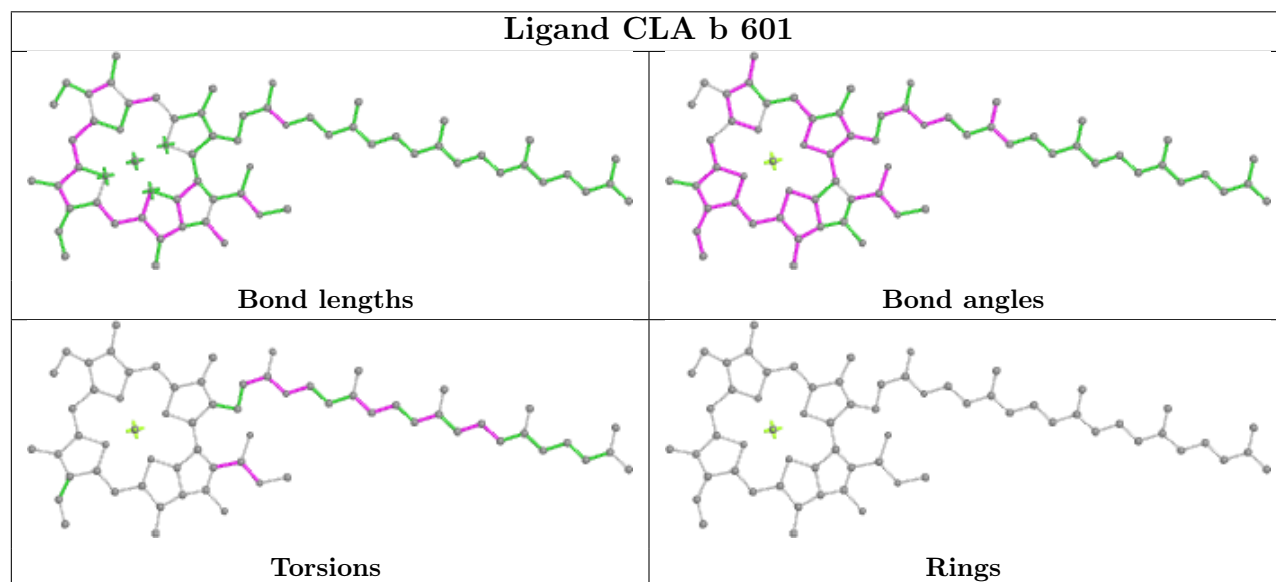
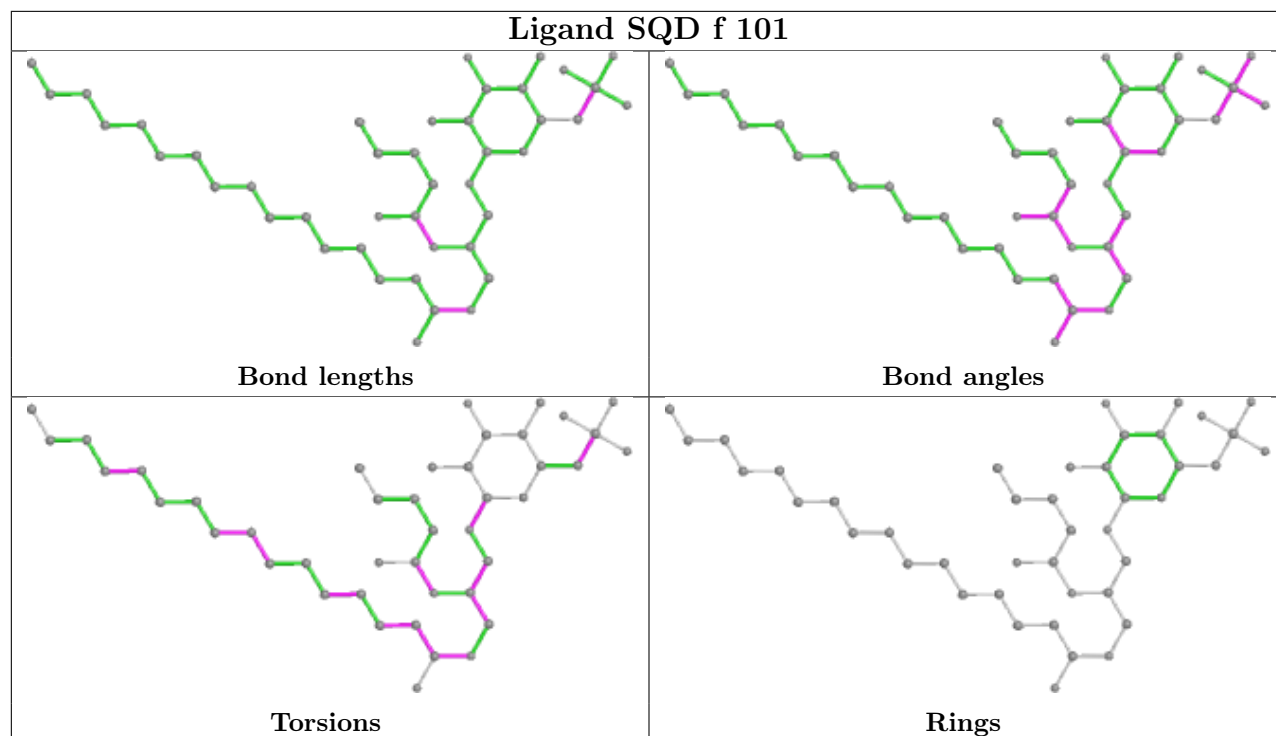
5 of 1275 torsion outliers are listed below:

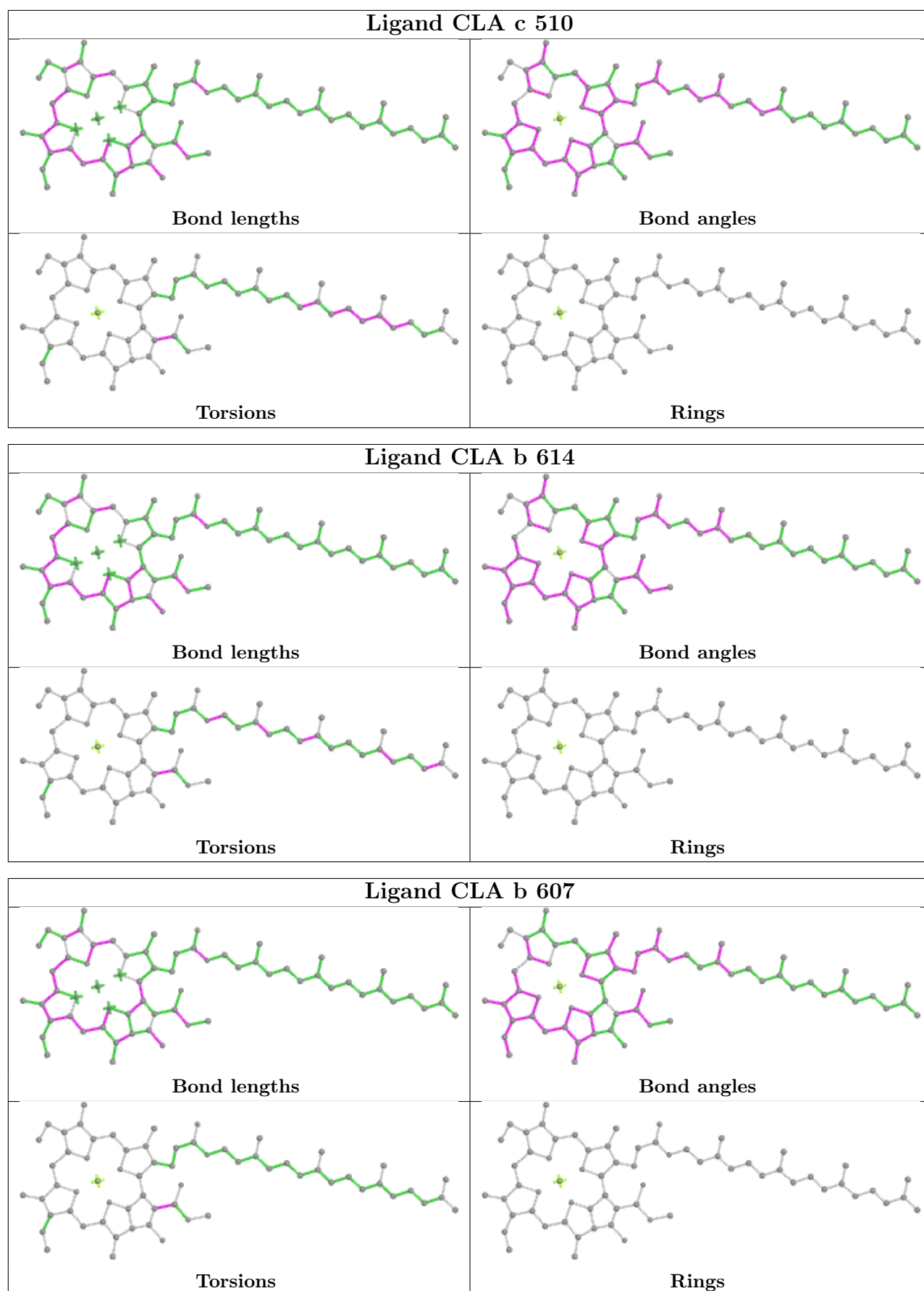
Mol	Chain	Res	Type	Atoms
23	B	605	CLA	C2-C3-C5-C6
23	B	605	CLA	C4-C3-C5-C6
23	B	606	CLA	CHA-CBD-CGD-O1D
23	B	606	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CHA-CBD-CGD-O1D

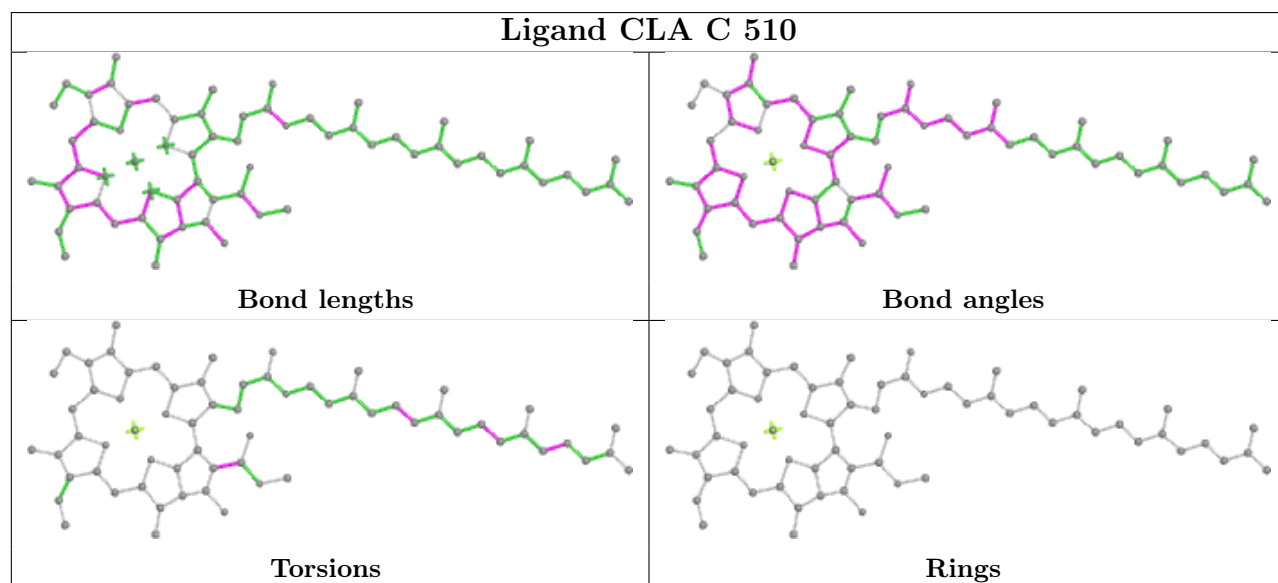
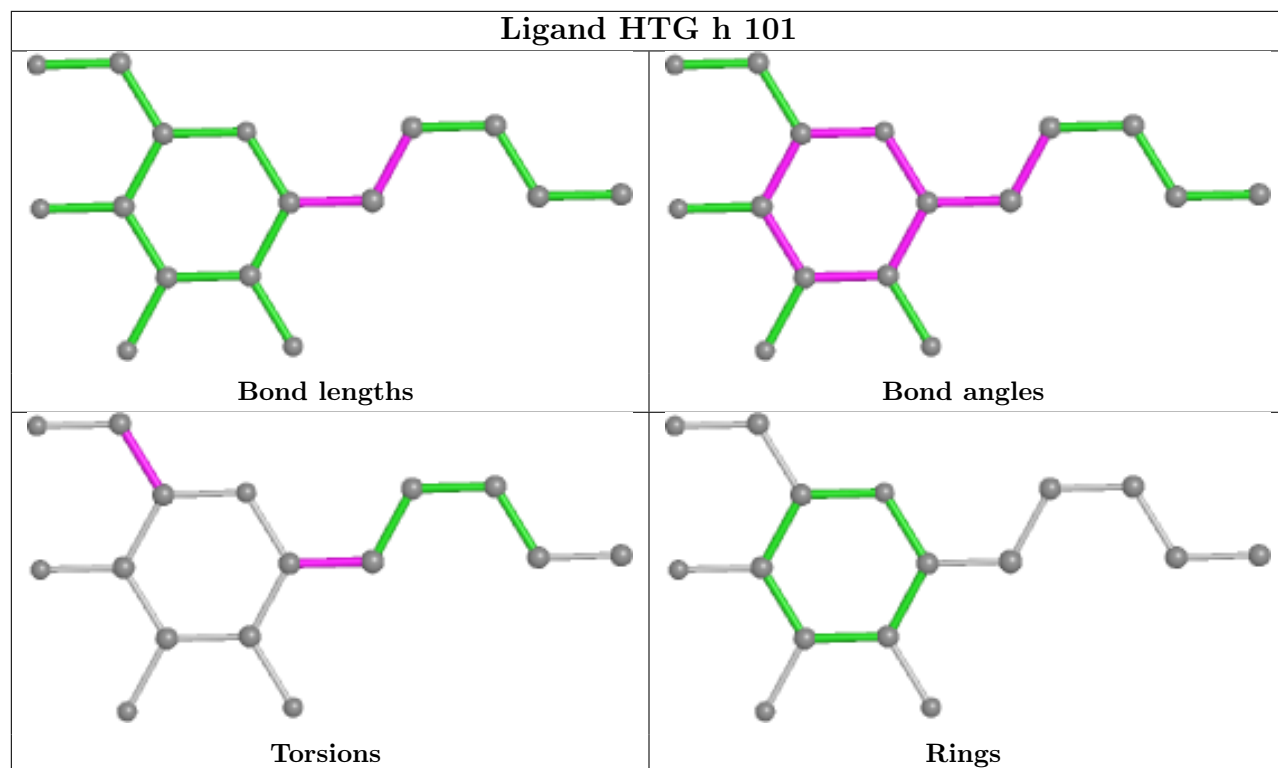
There are no ring outliers.

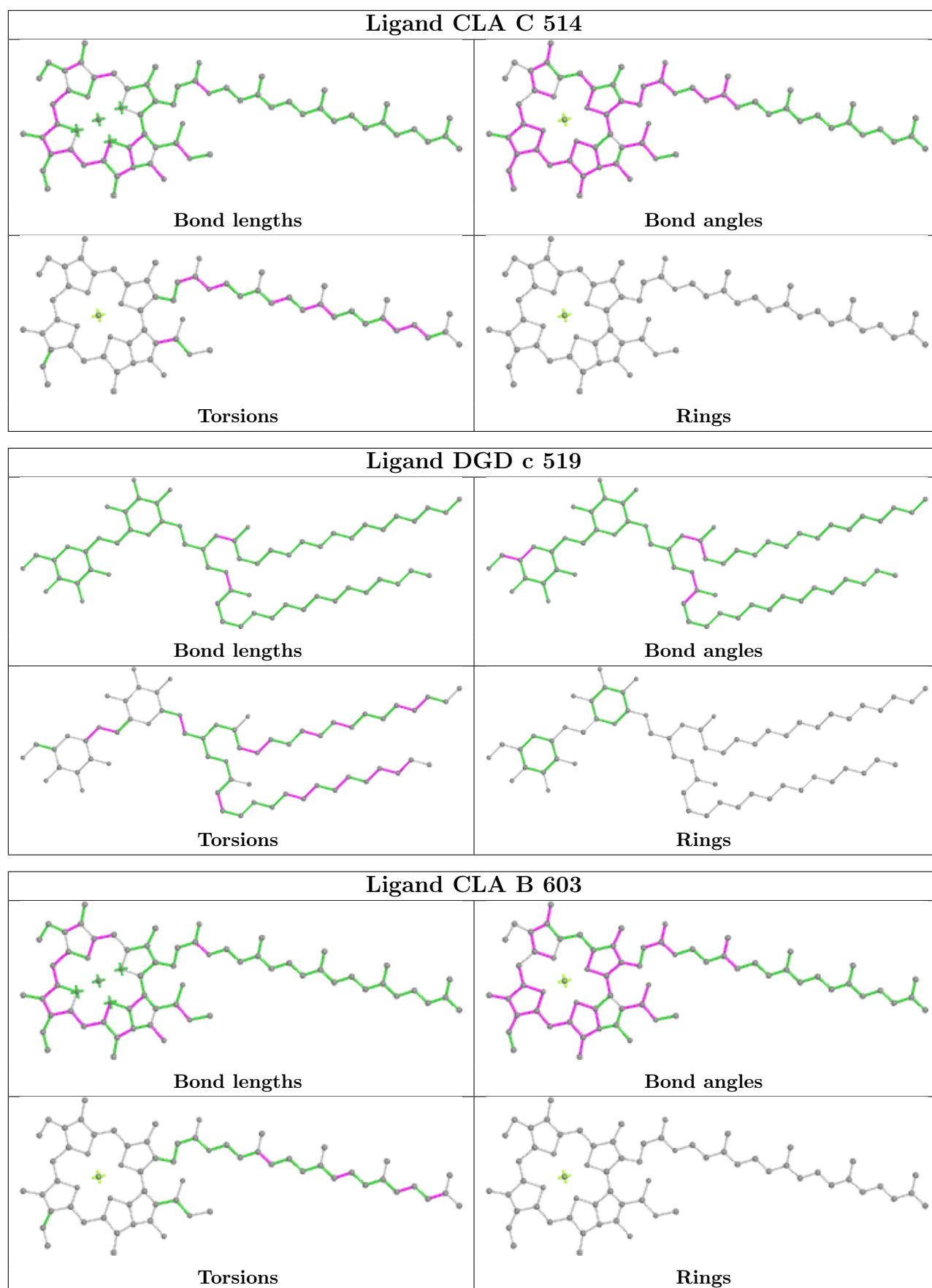
No monomer is involved in short contacts.

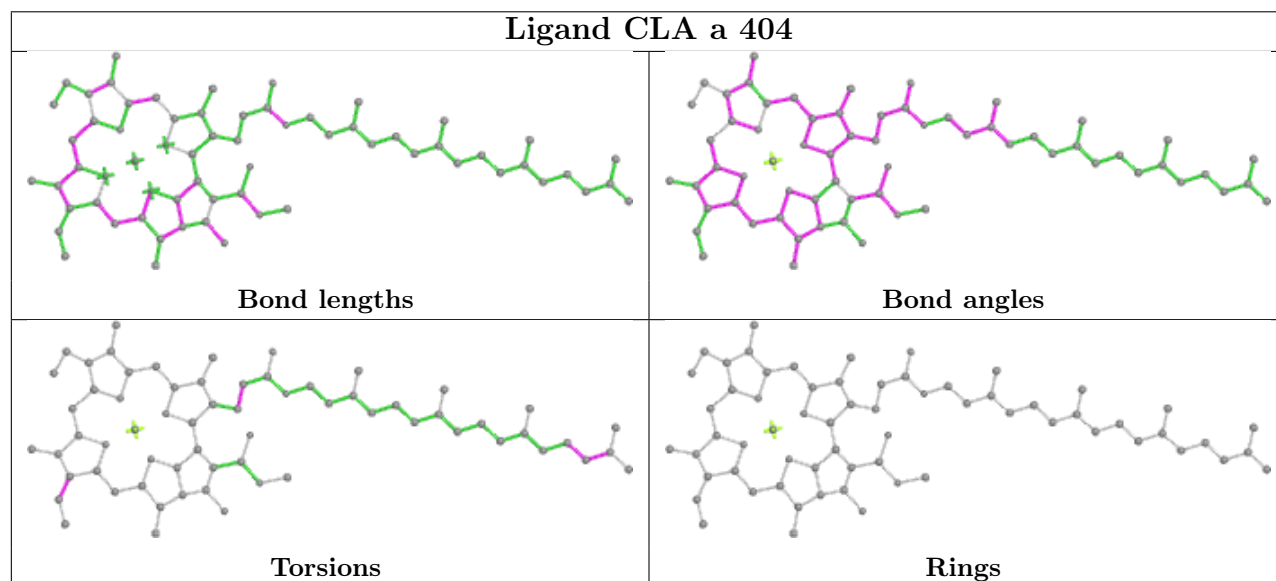
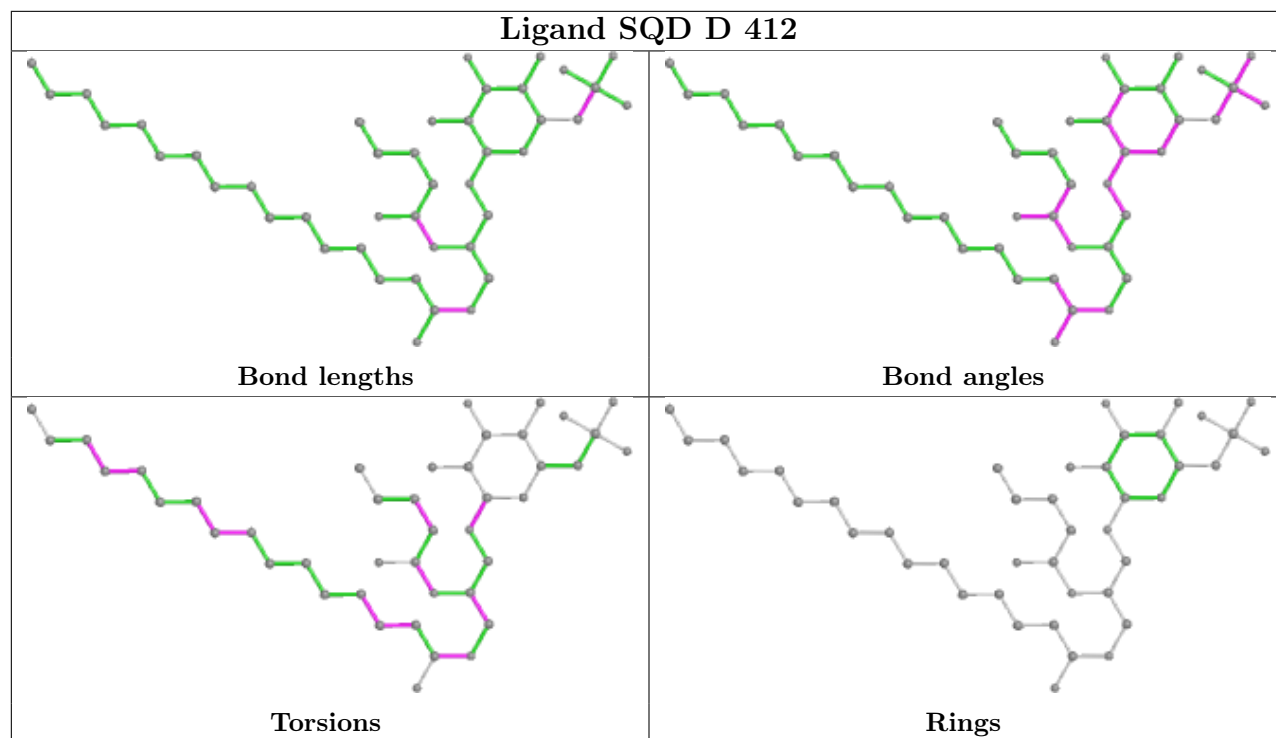
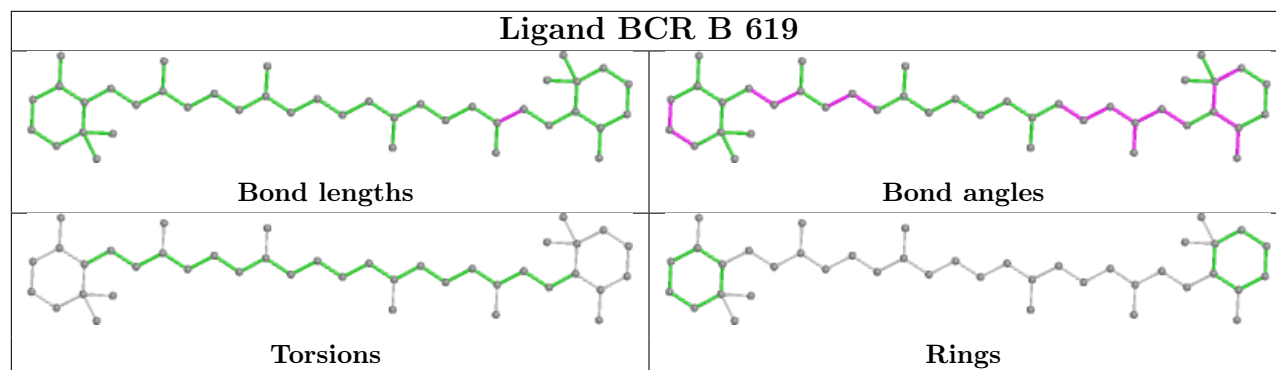
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

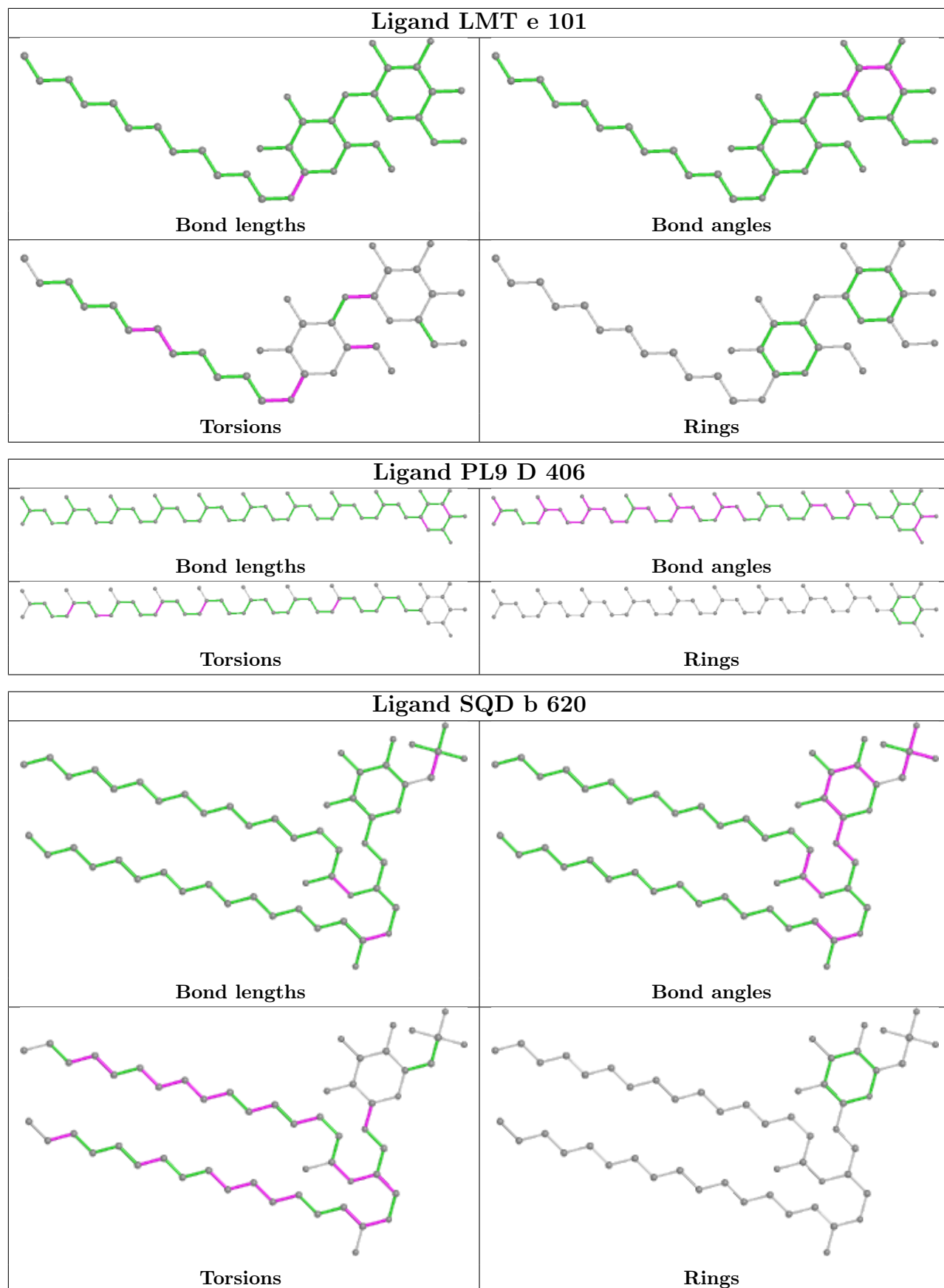


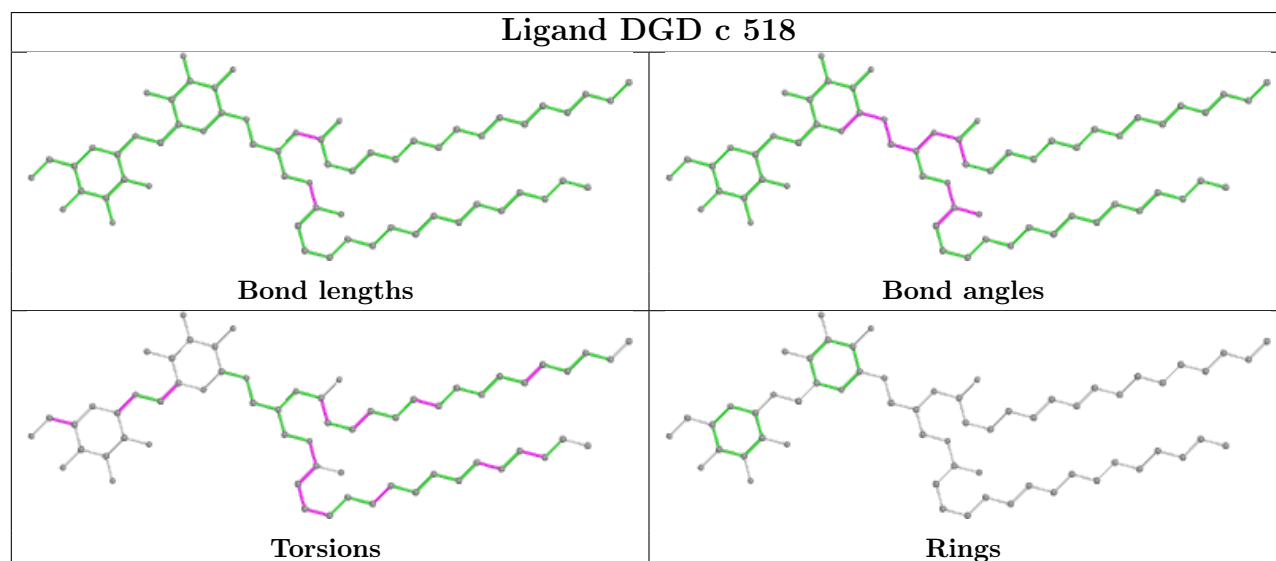
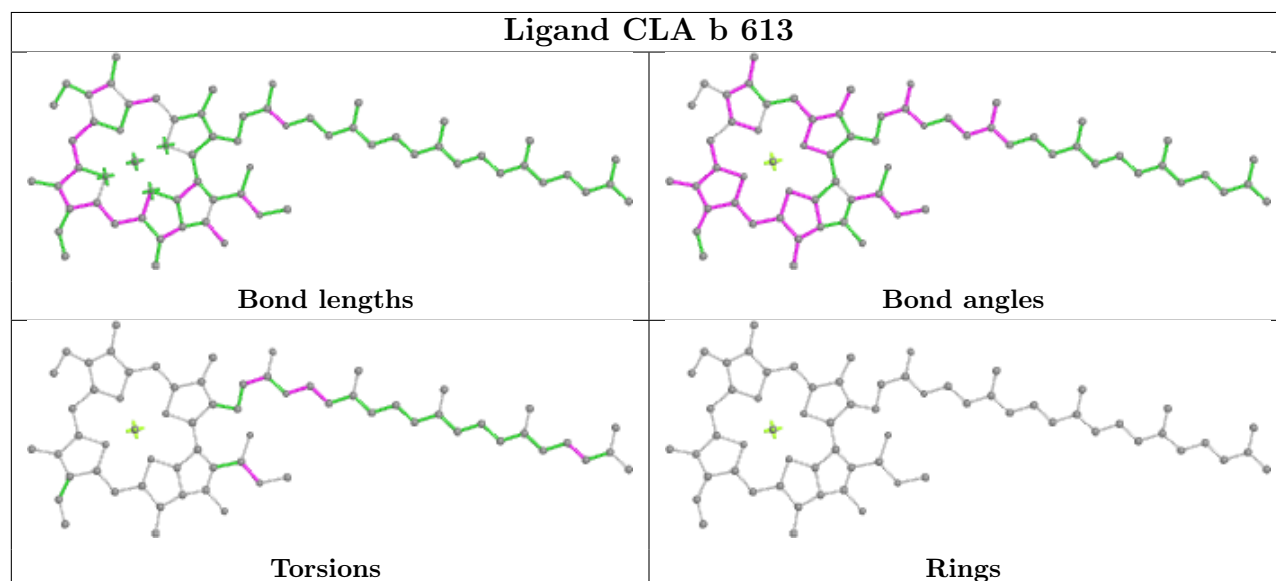
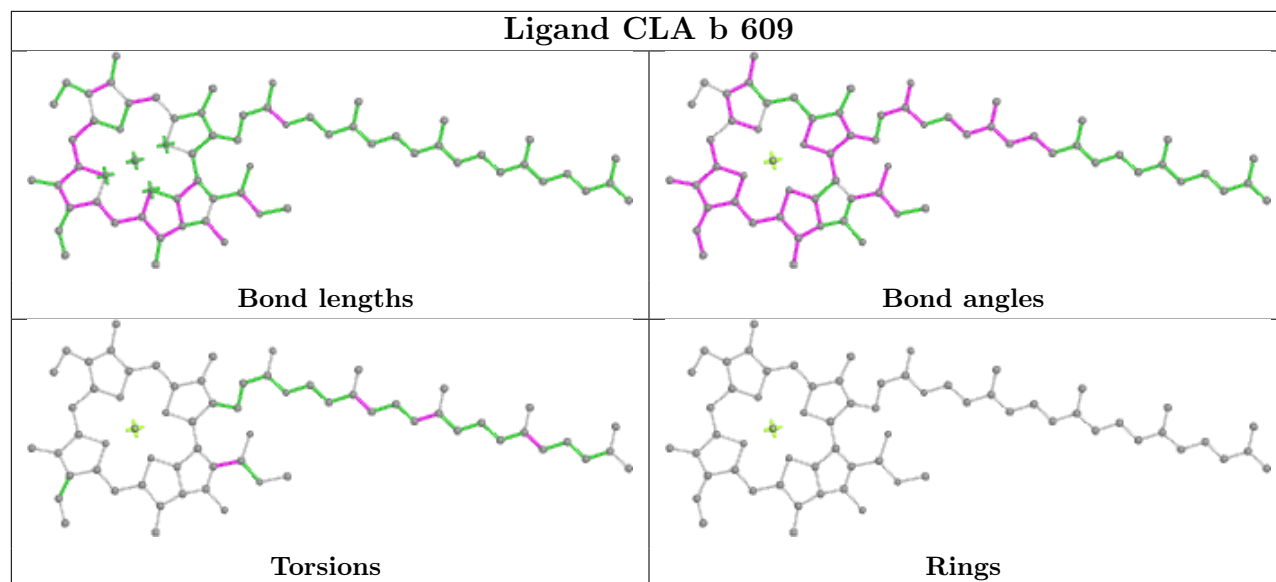


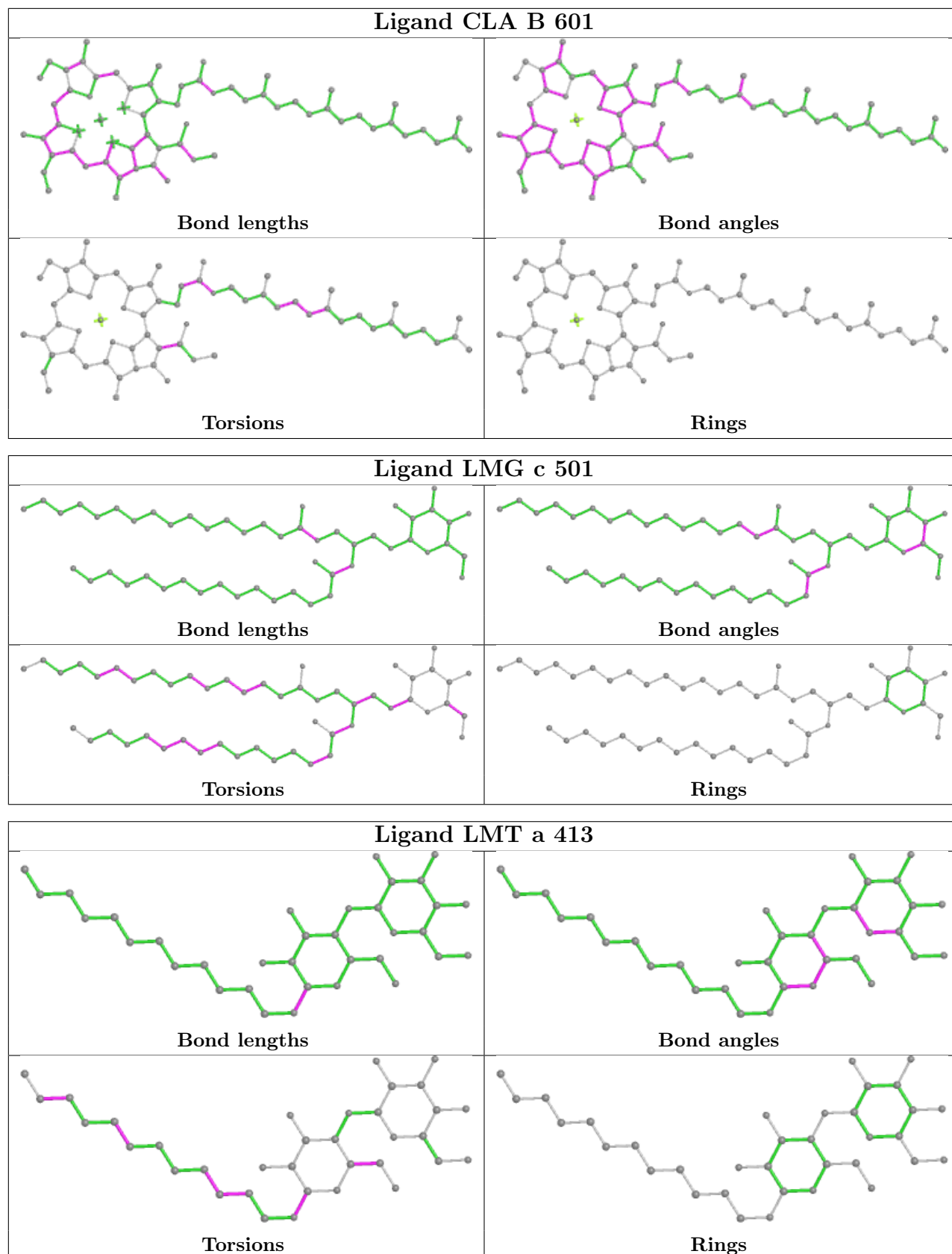


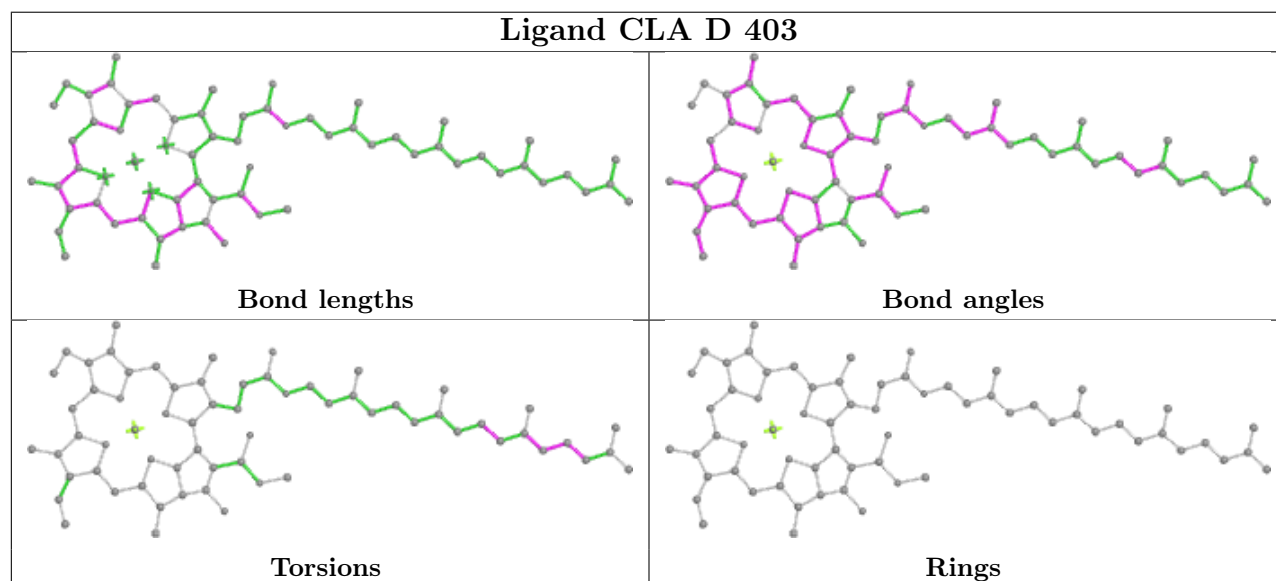
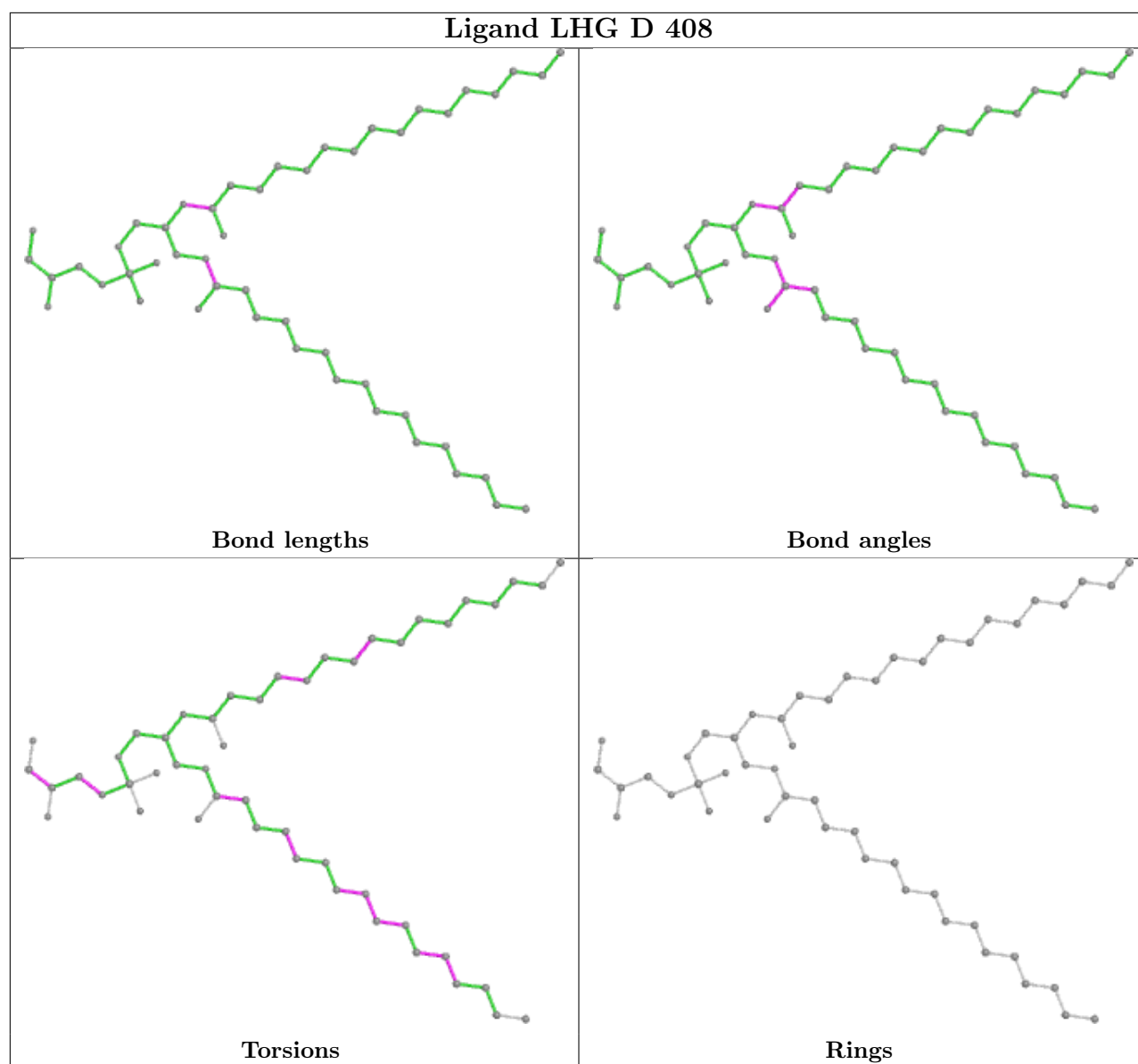


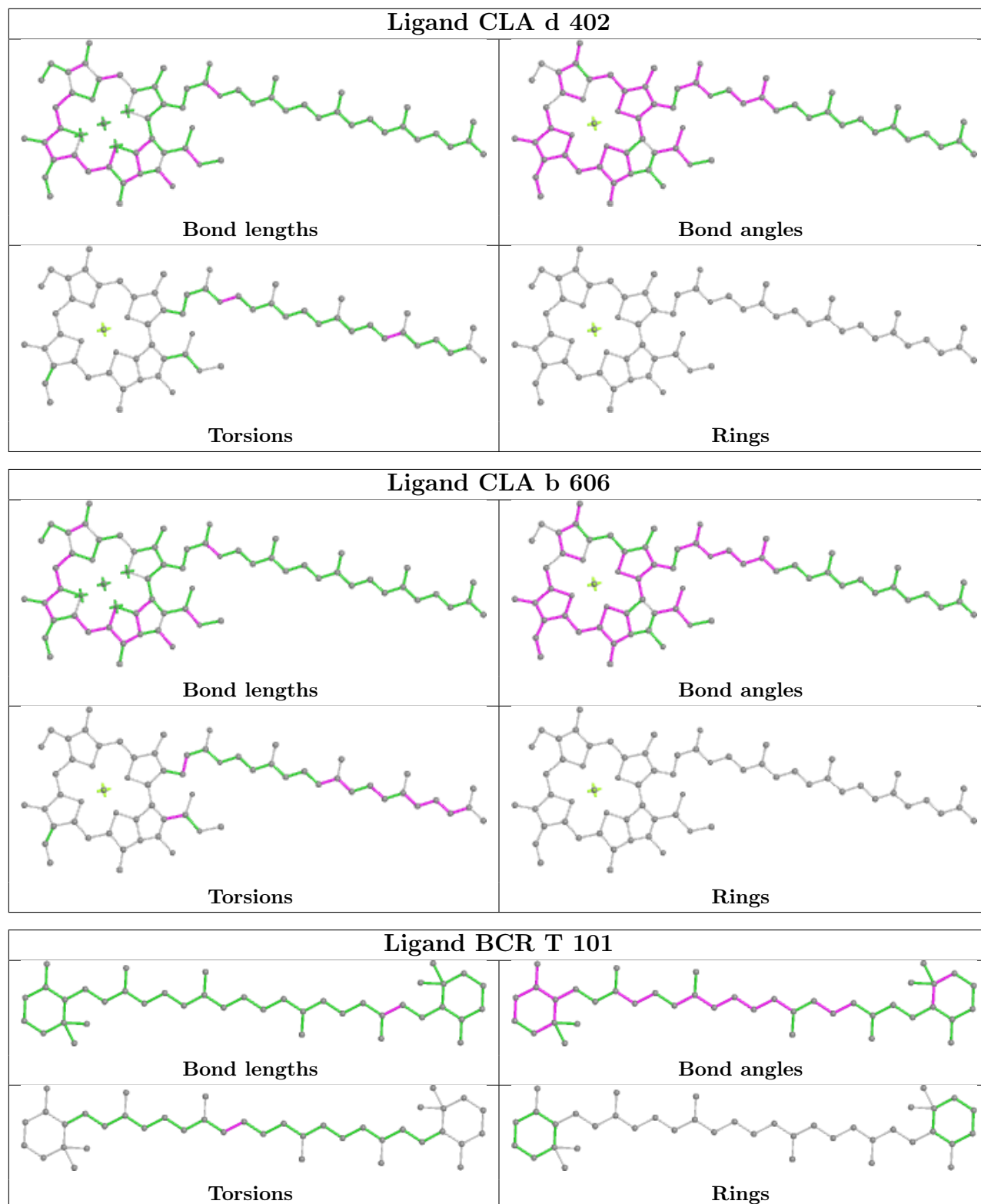


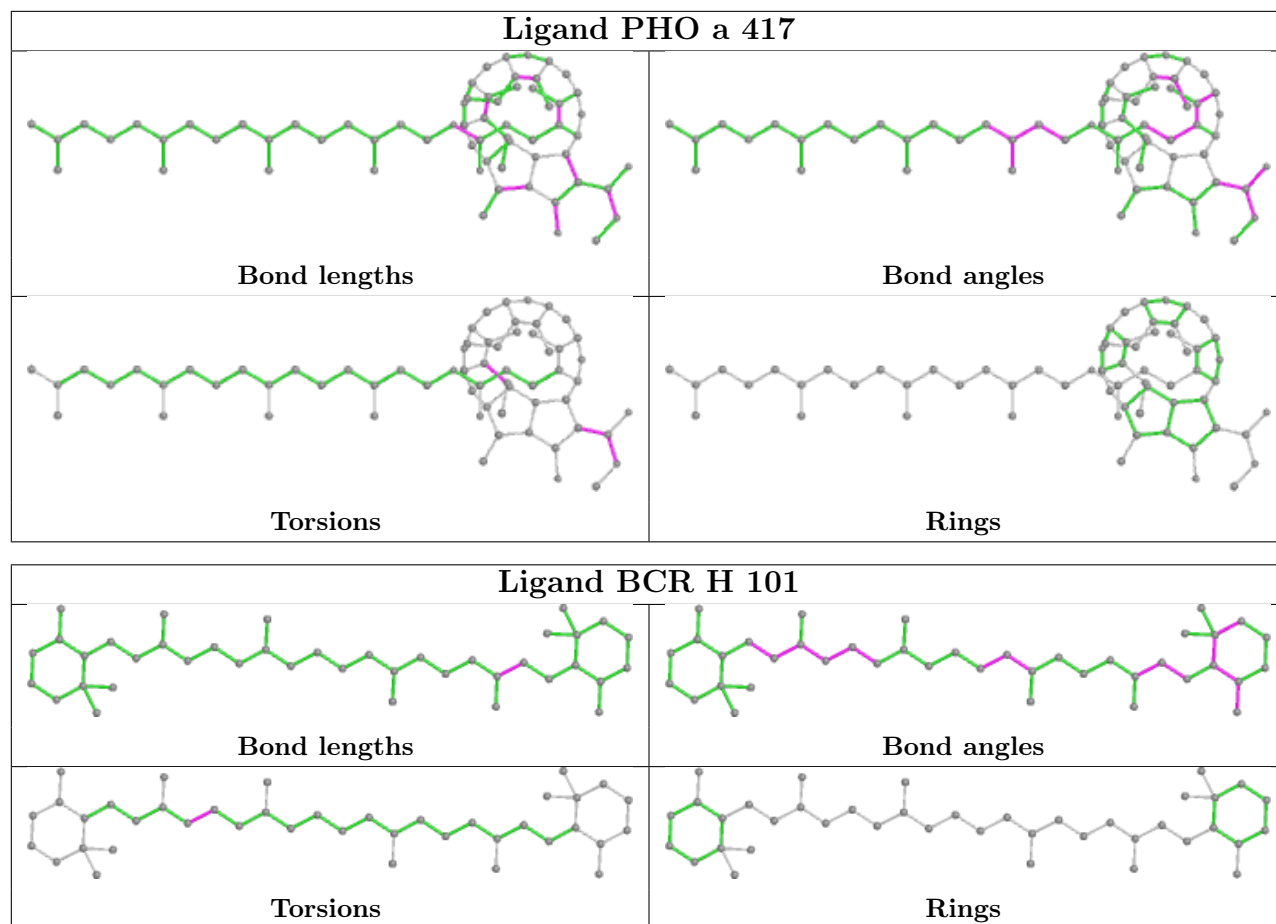


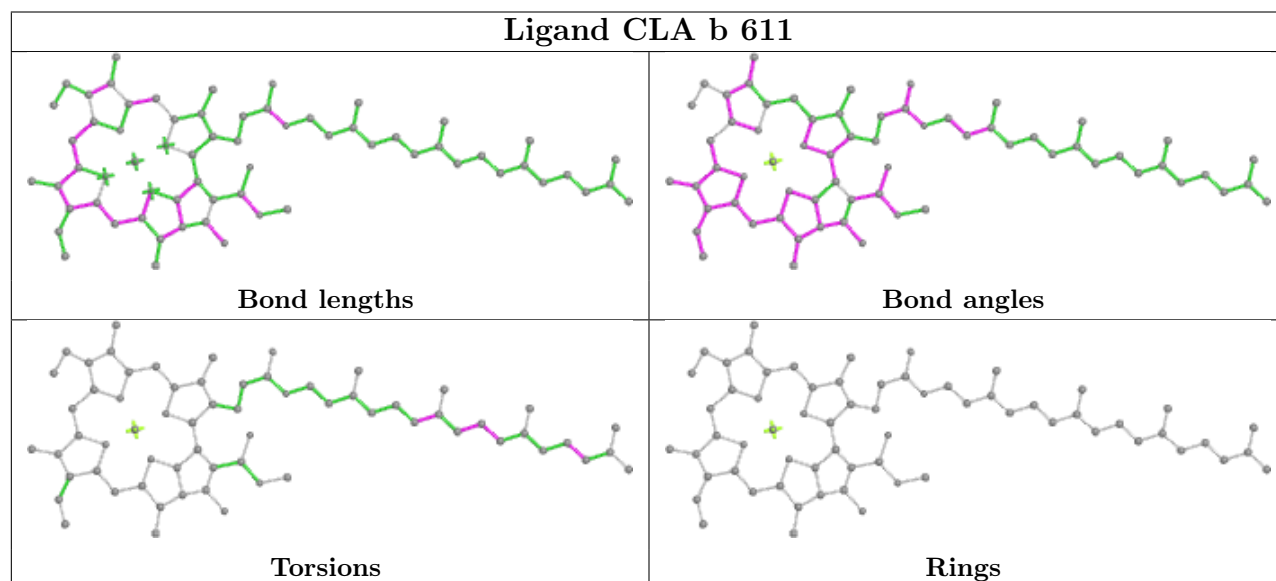
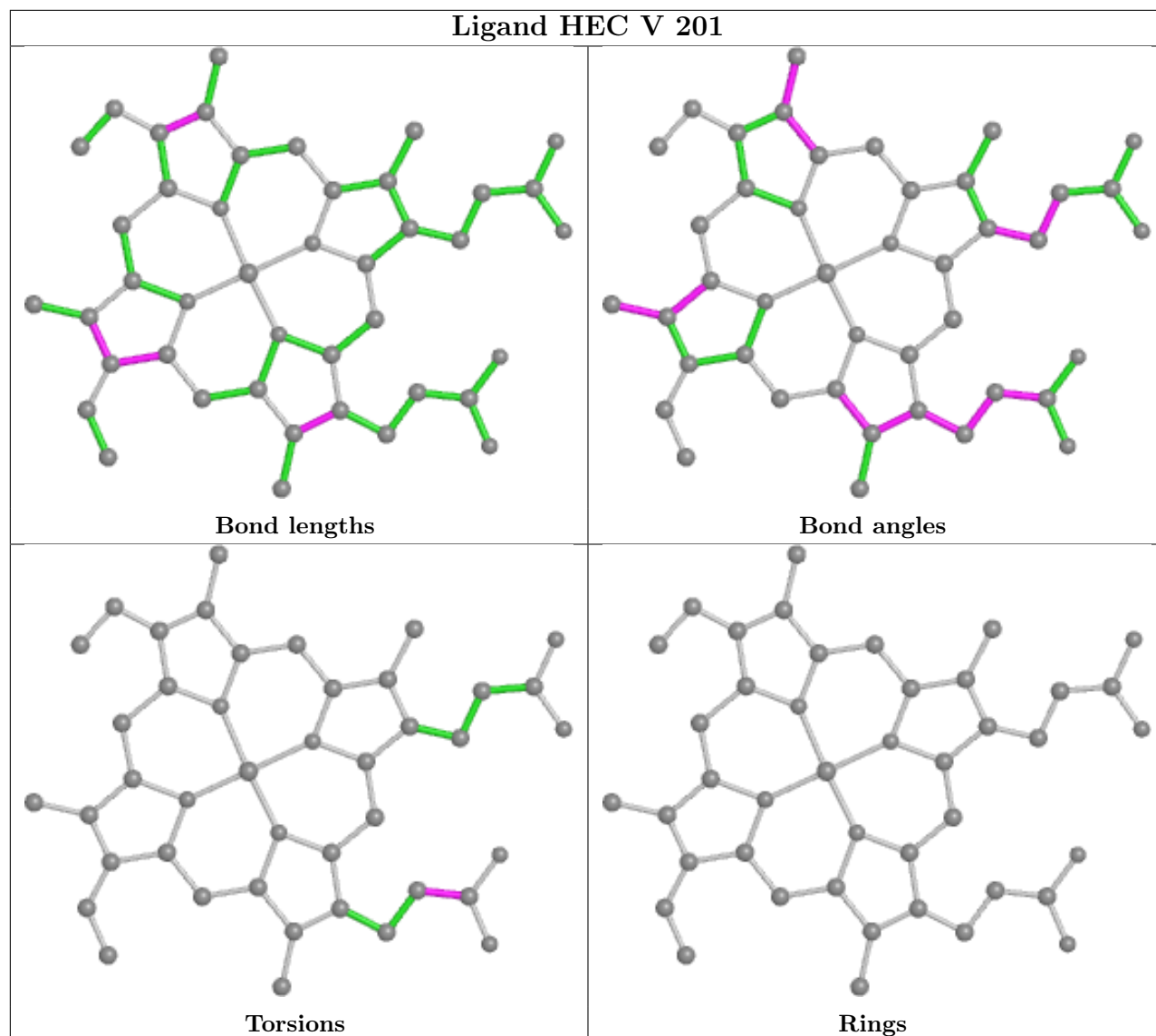


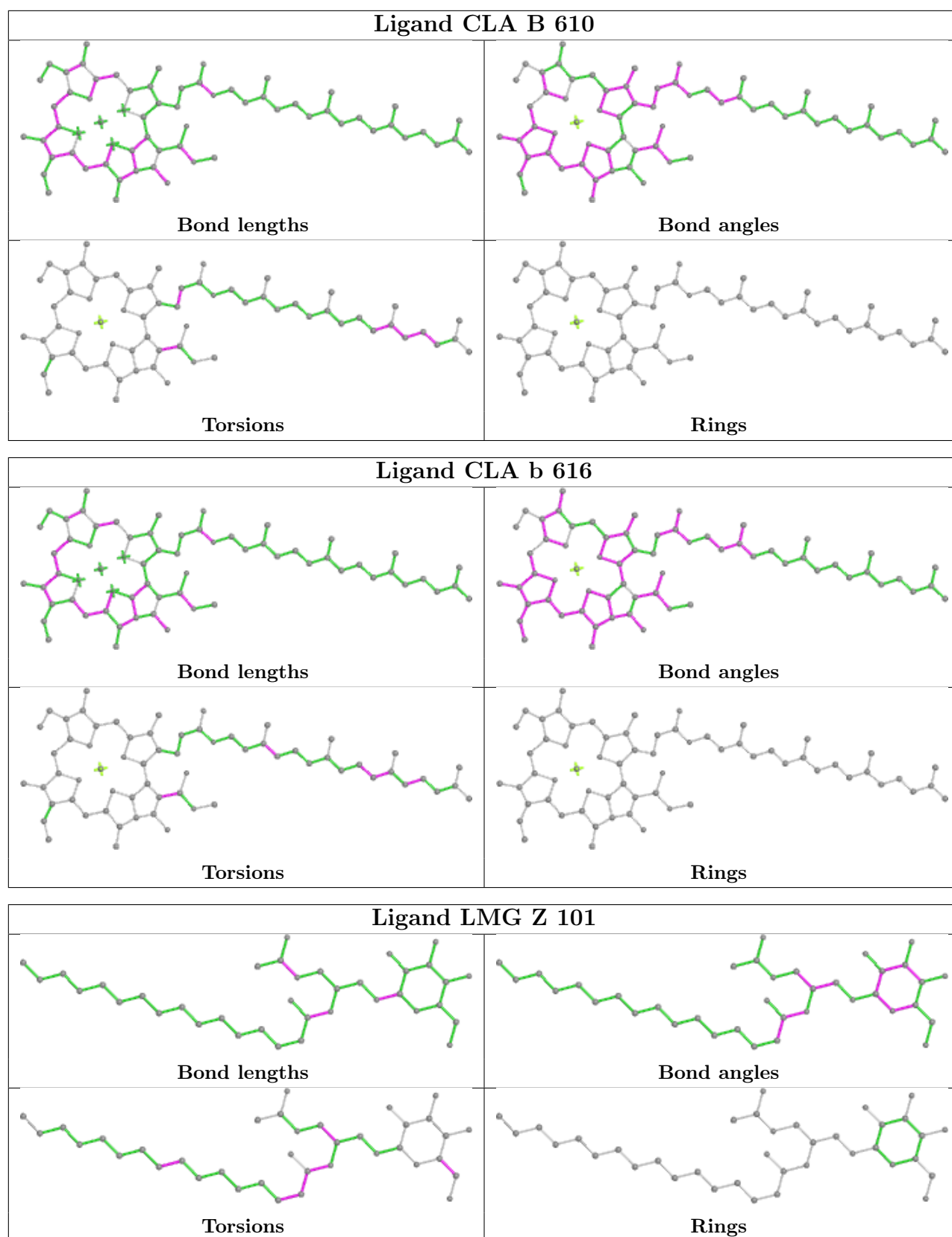


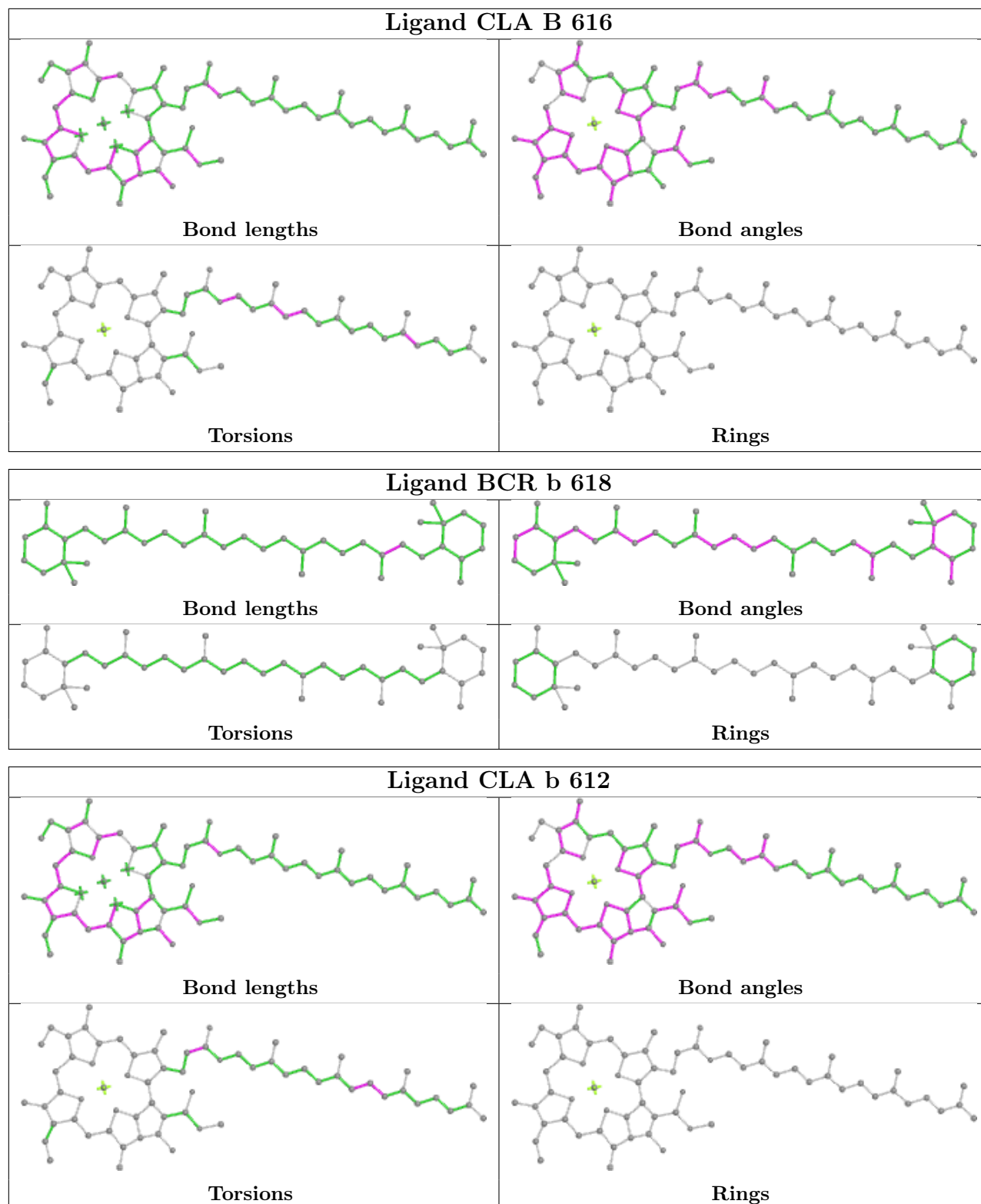


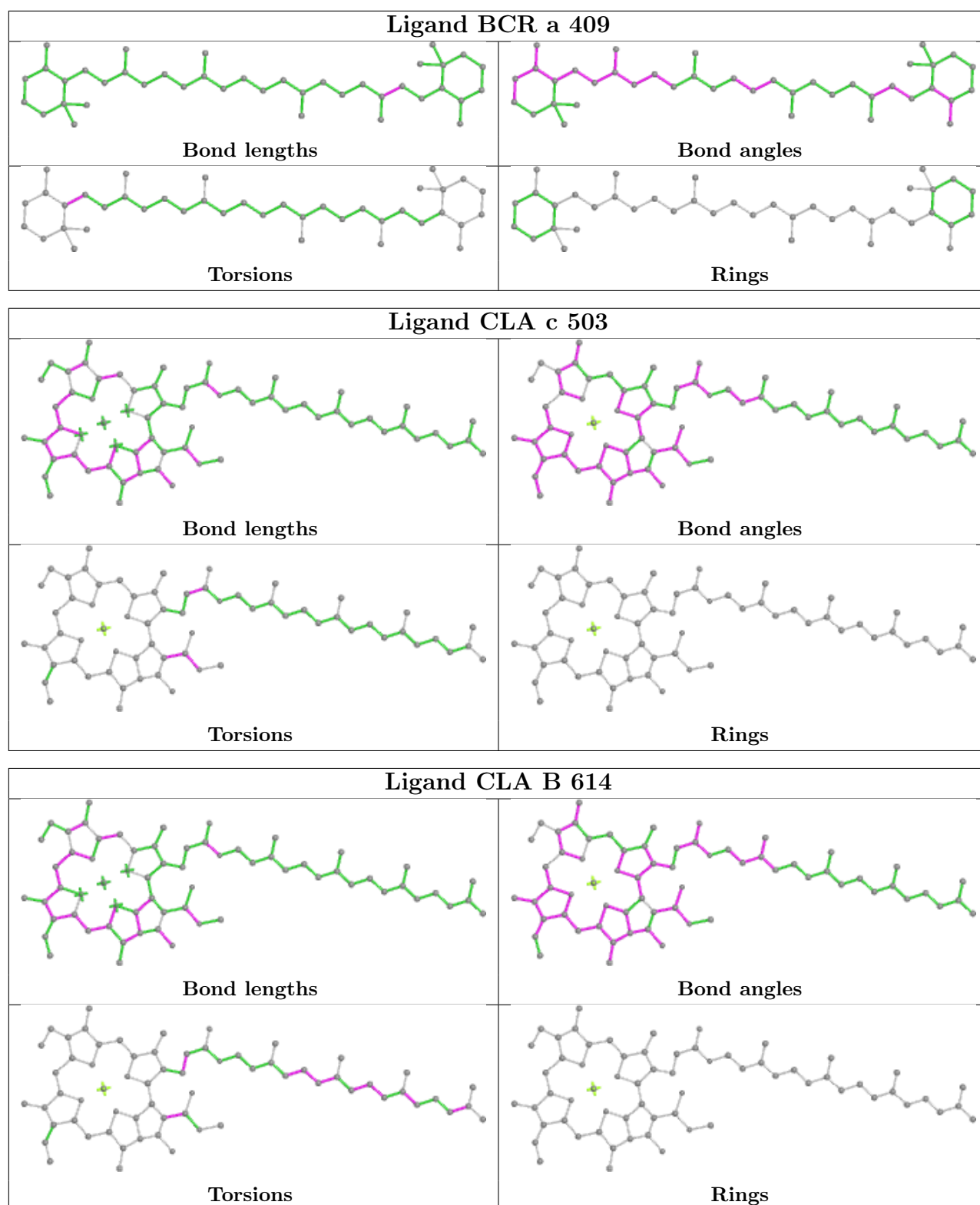


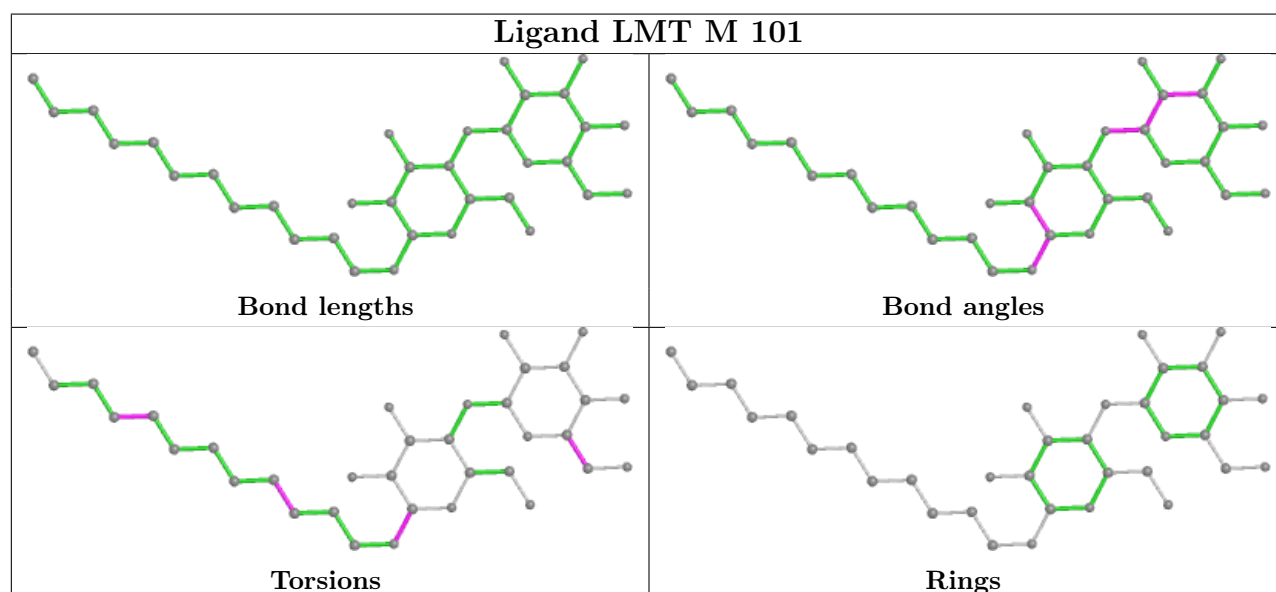
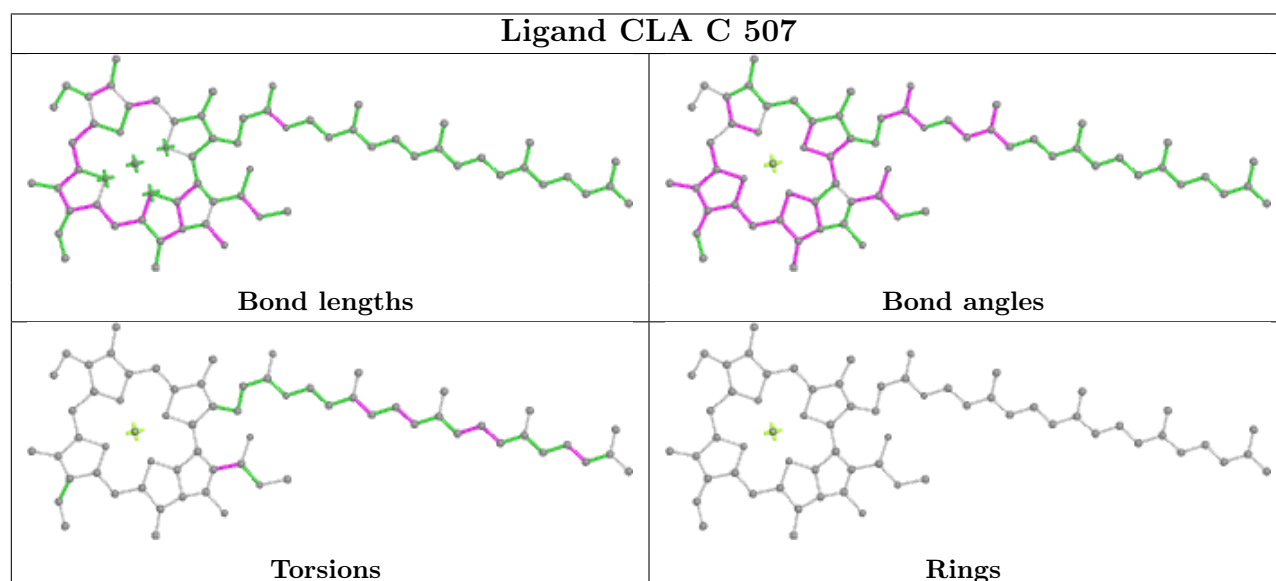
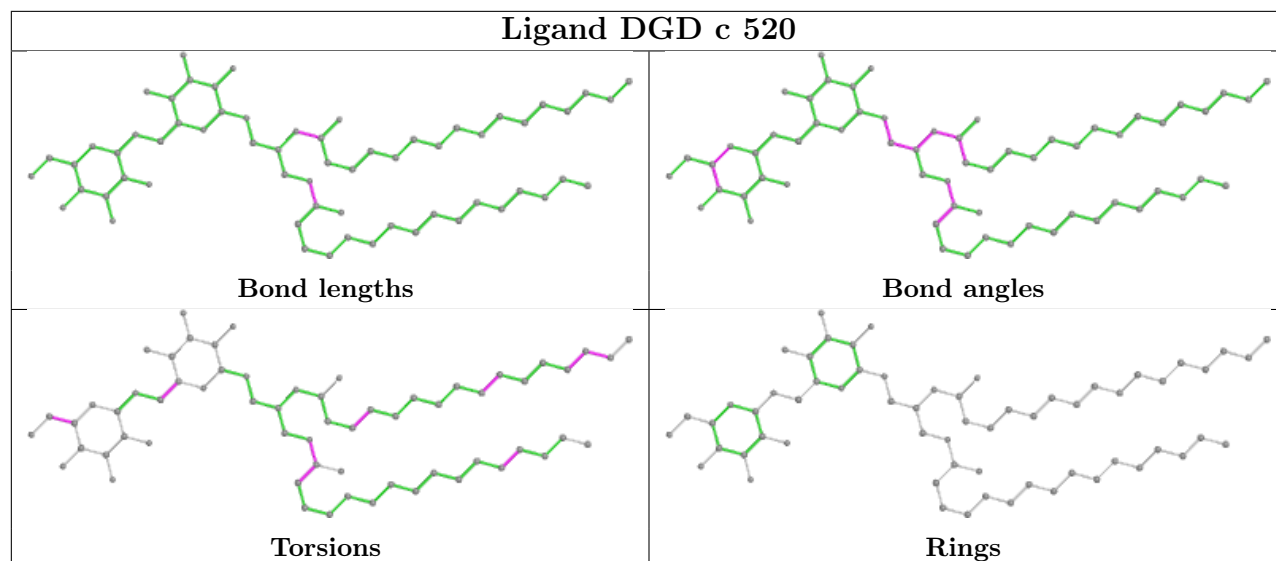


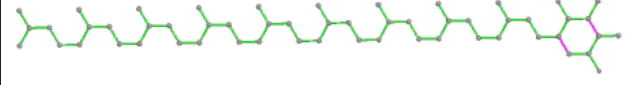
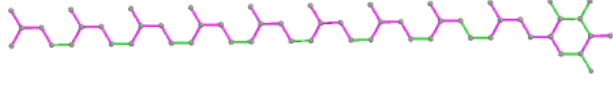
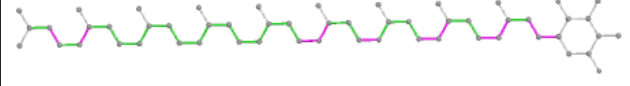
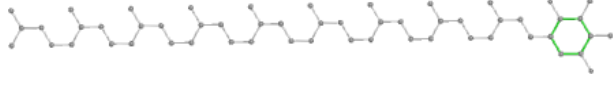
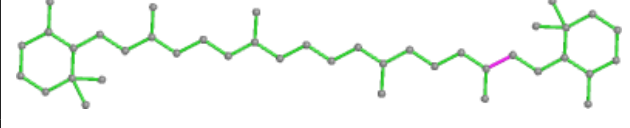
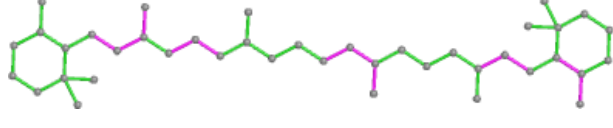
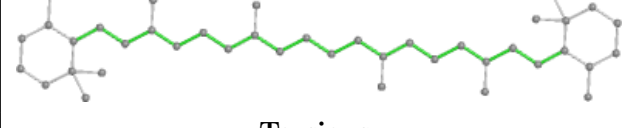
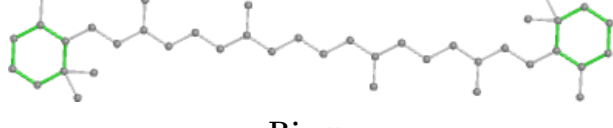
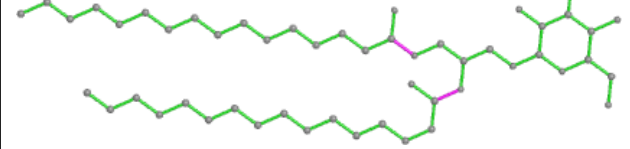
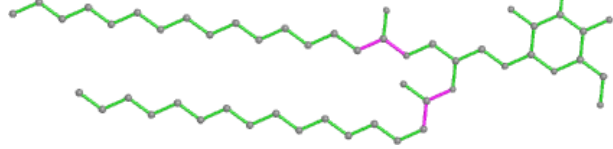
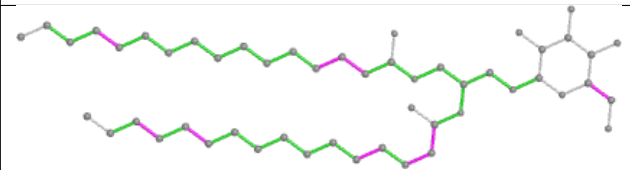
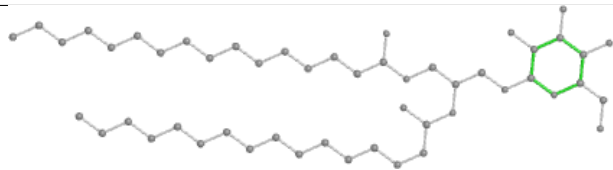
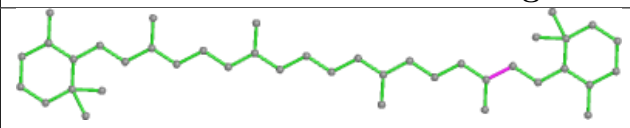
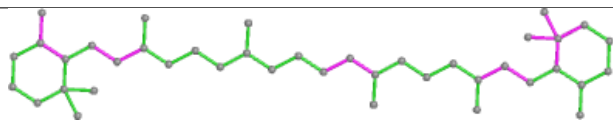
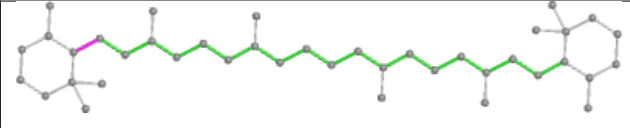
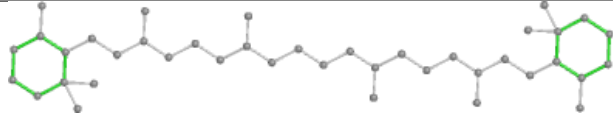


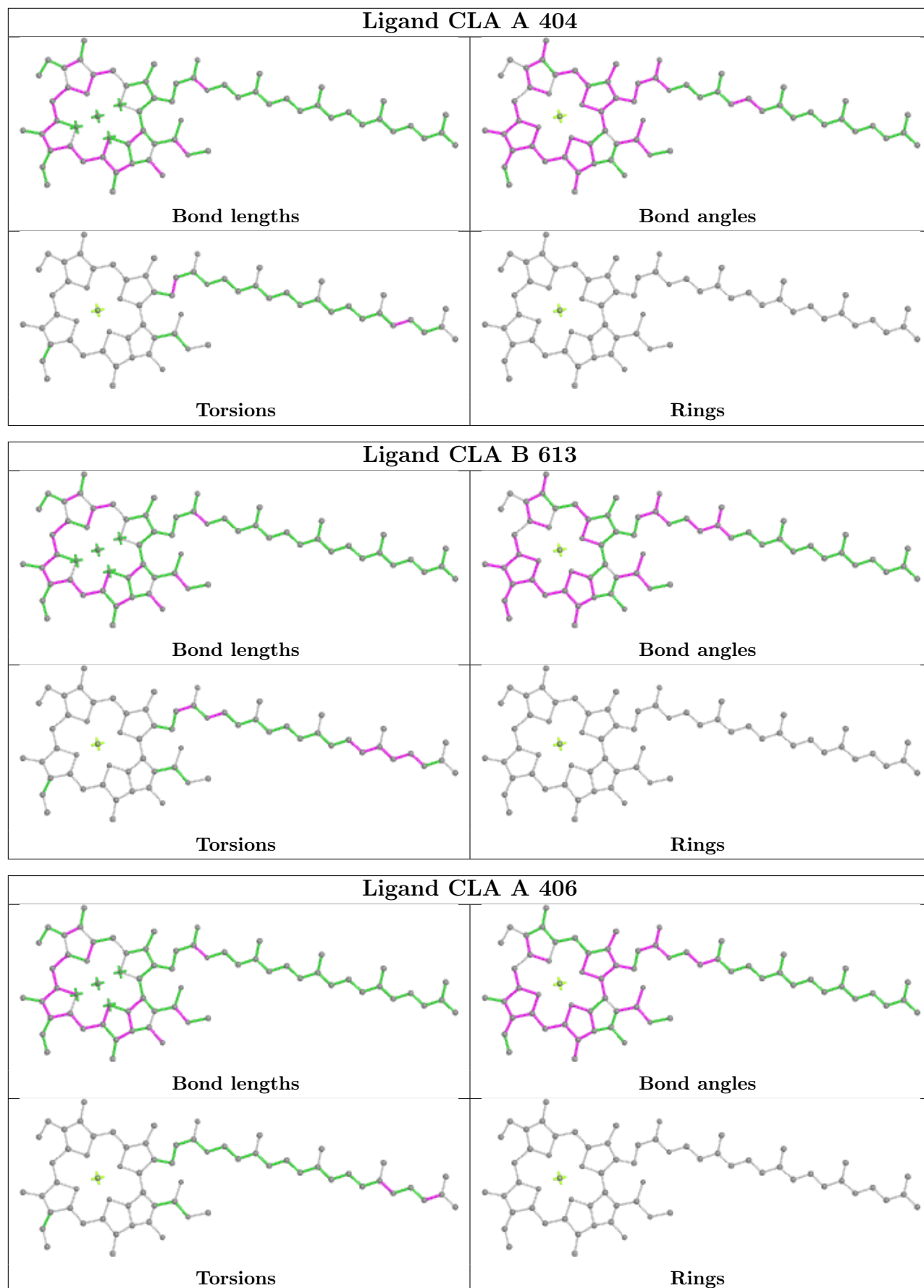


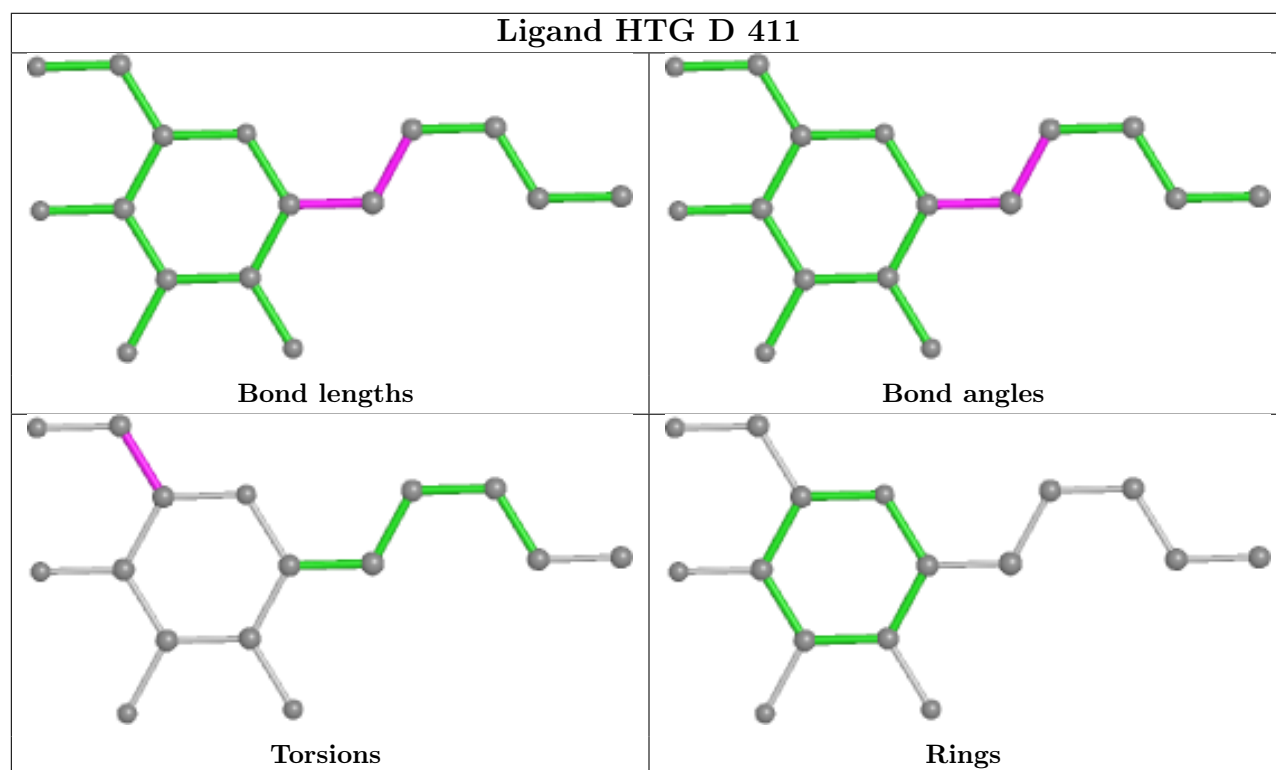
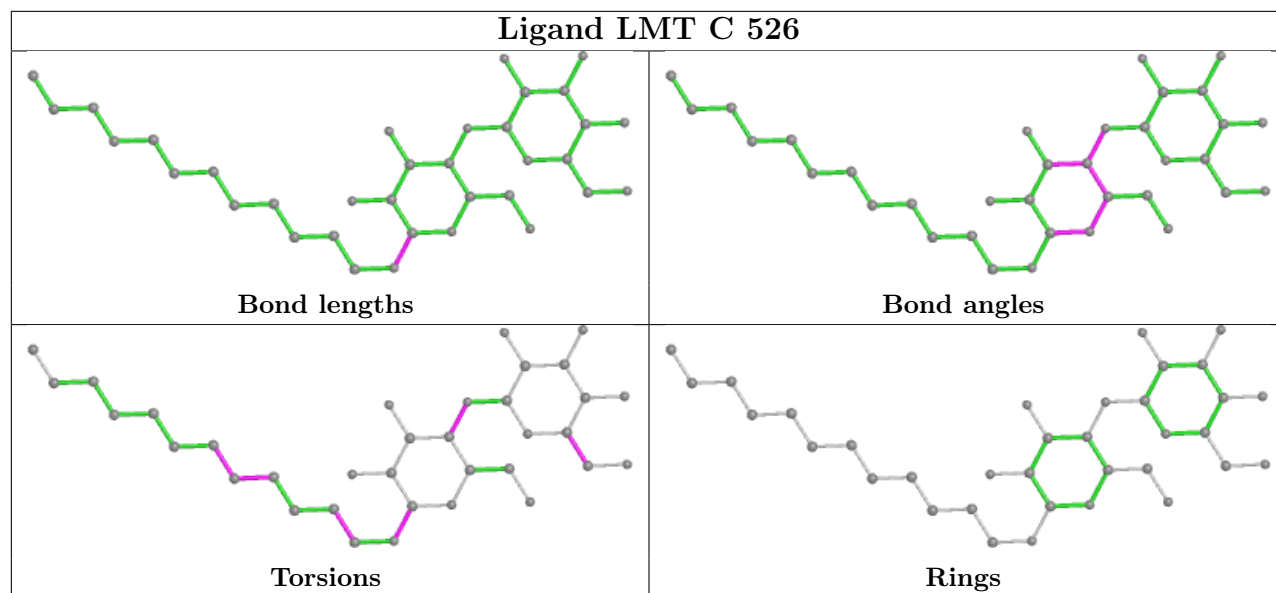


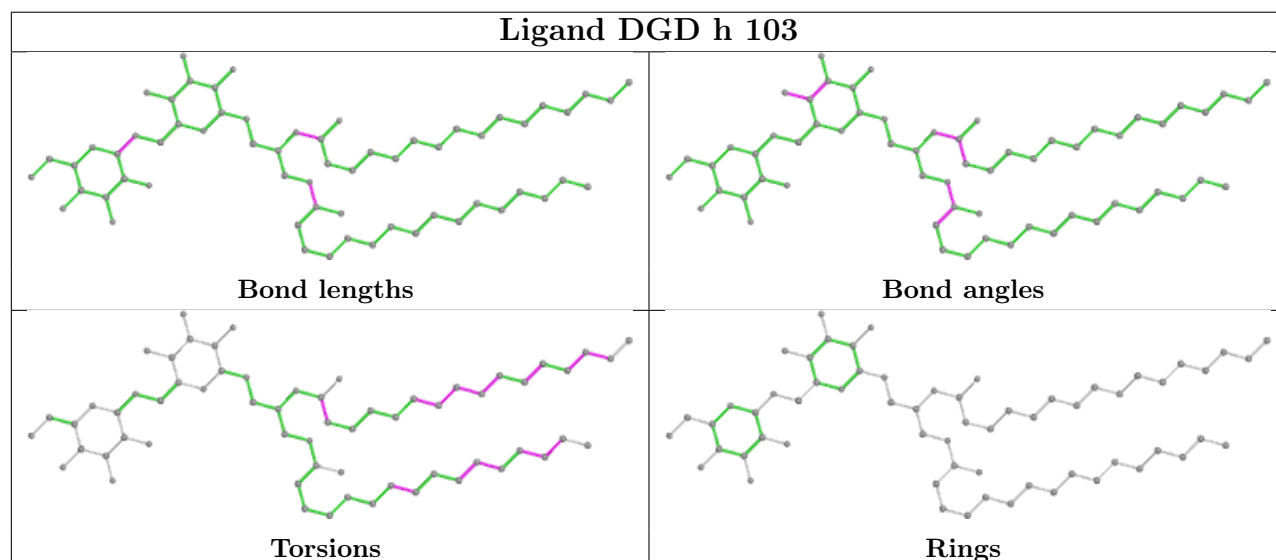
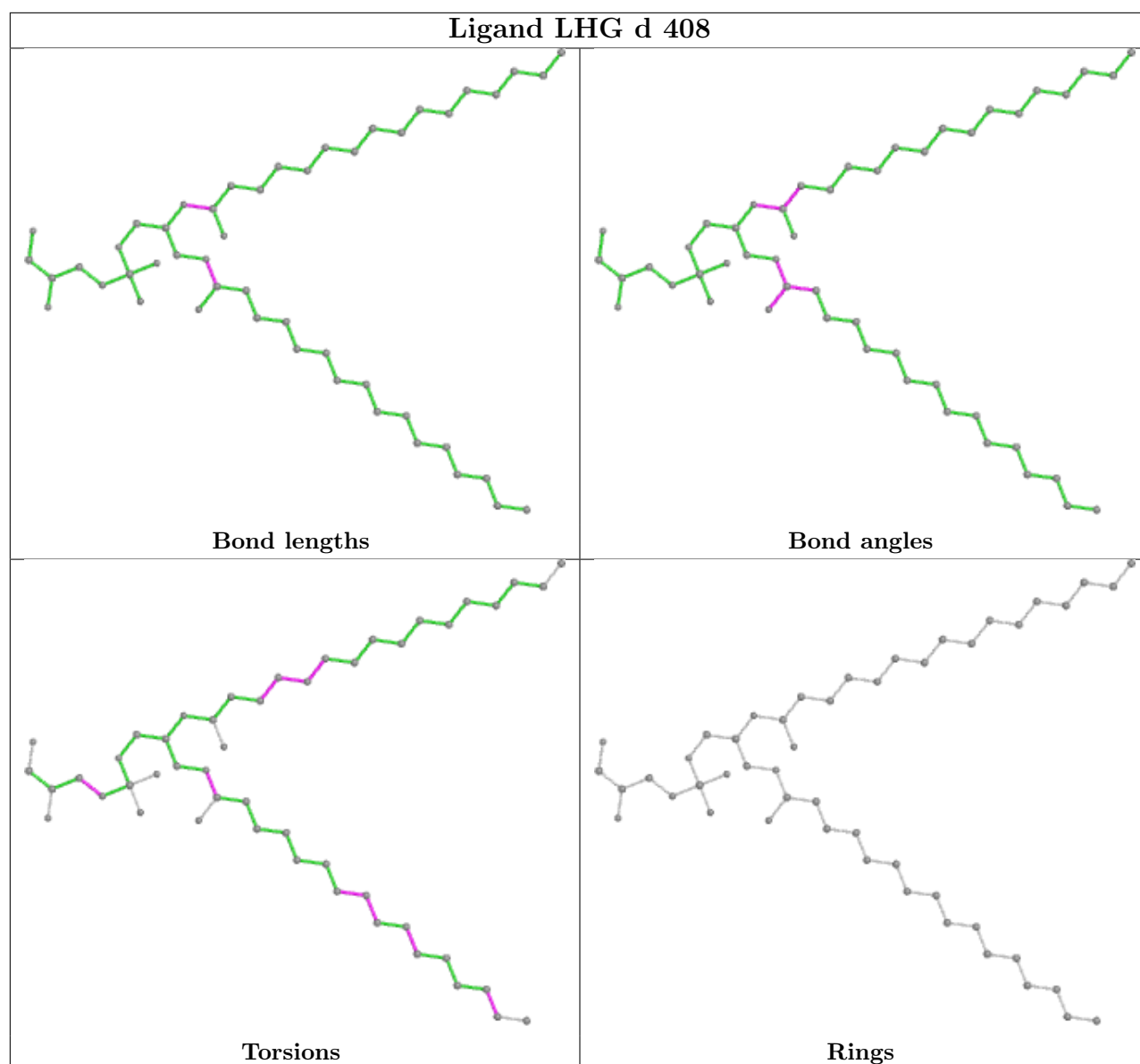


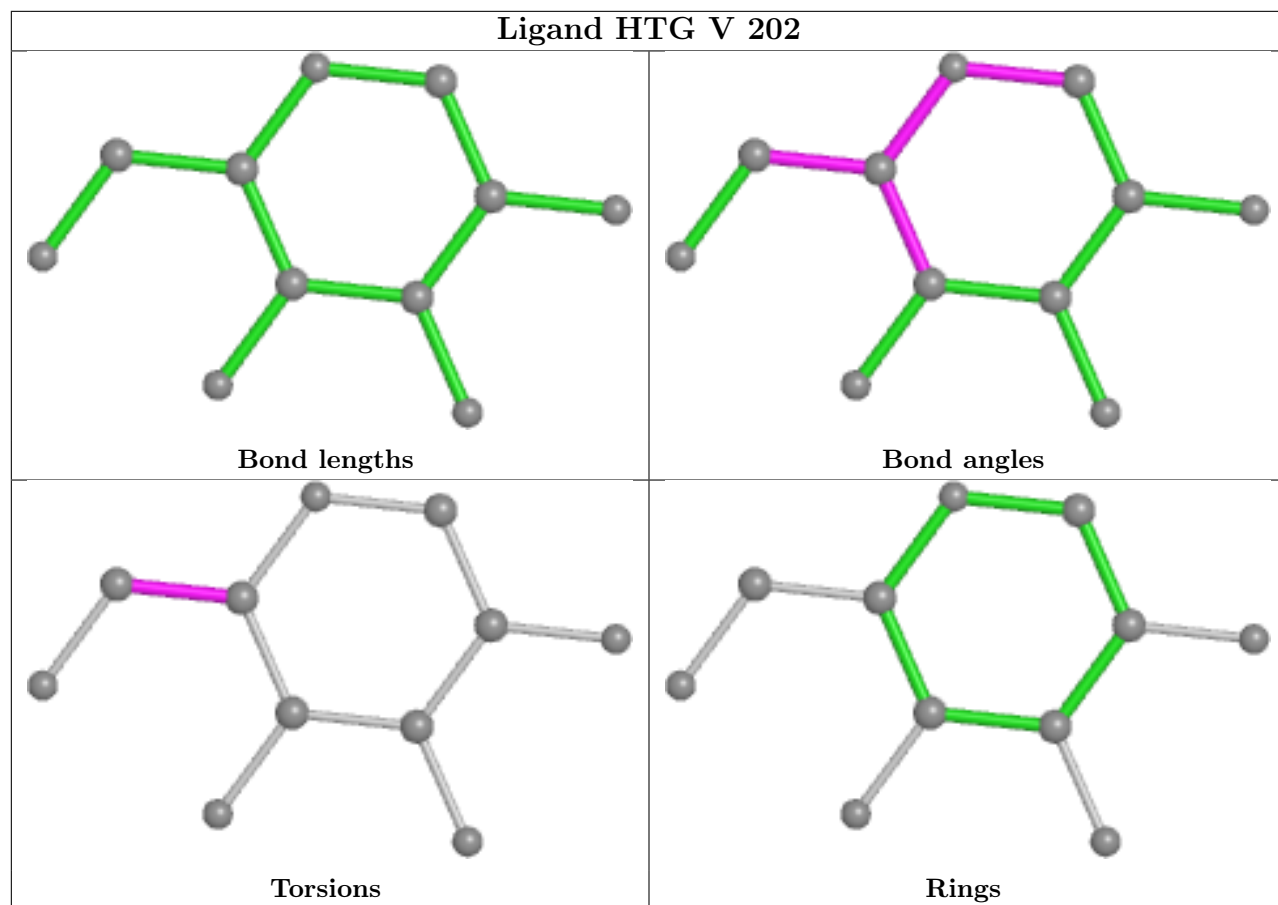
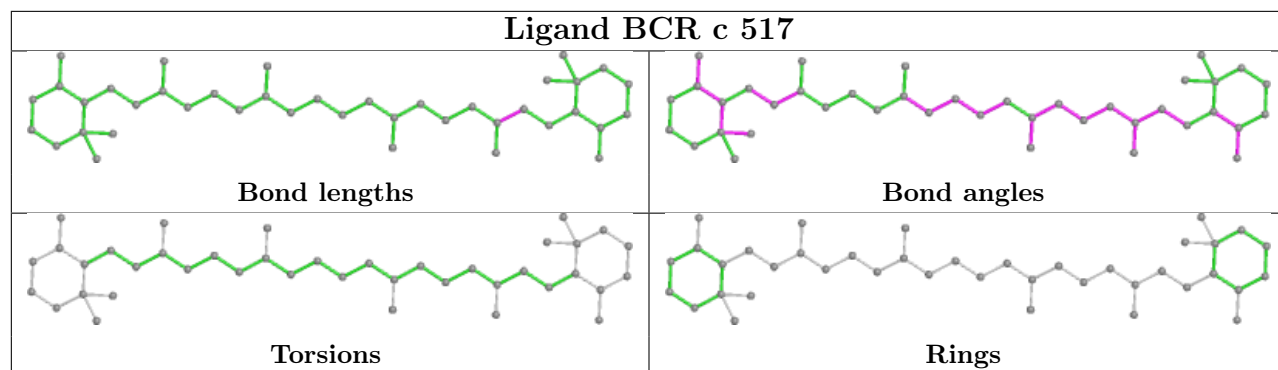


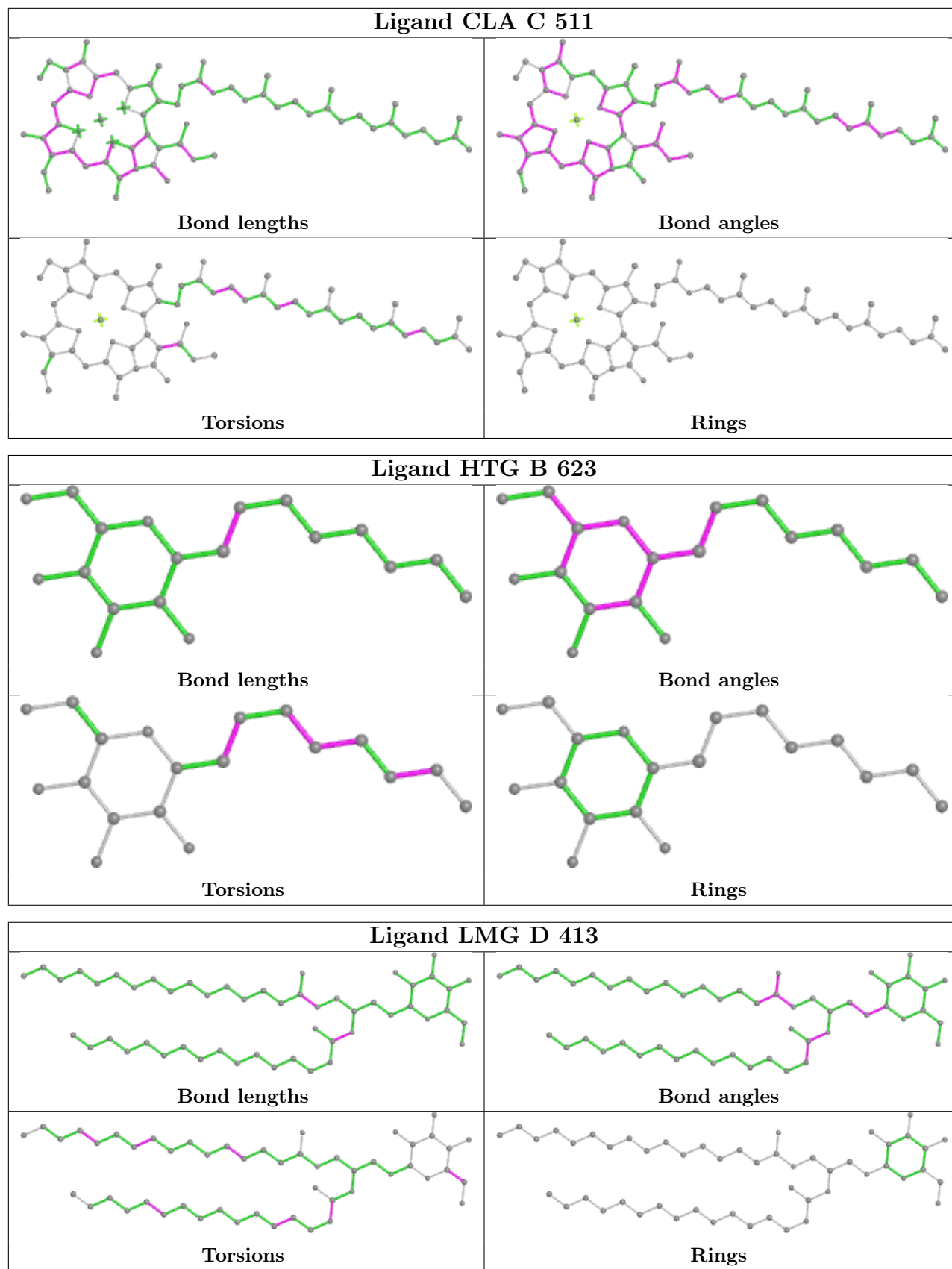
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 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR h 102	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LMG d 412	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
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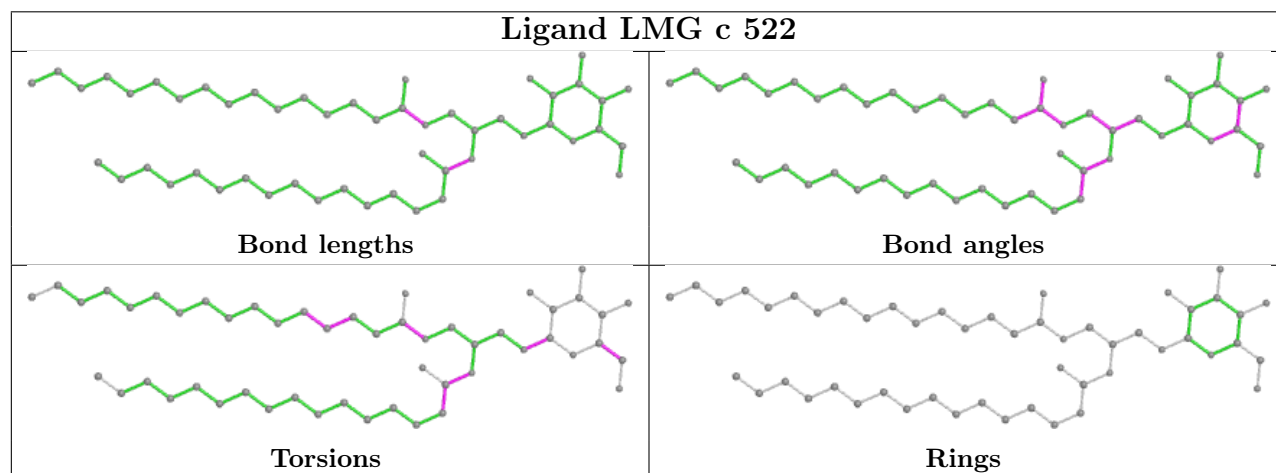
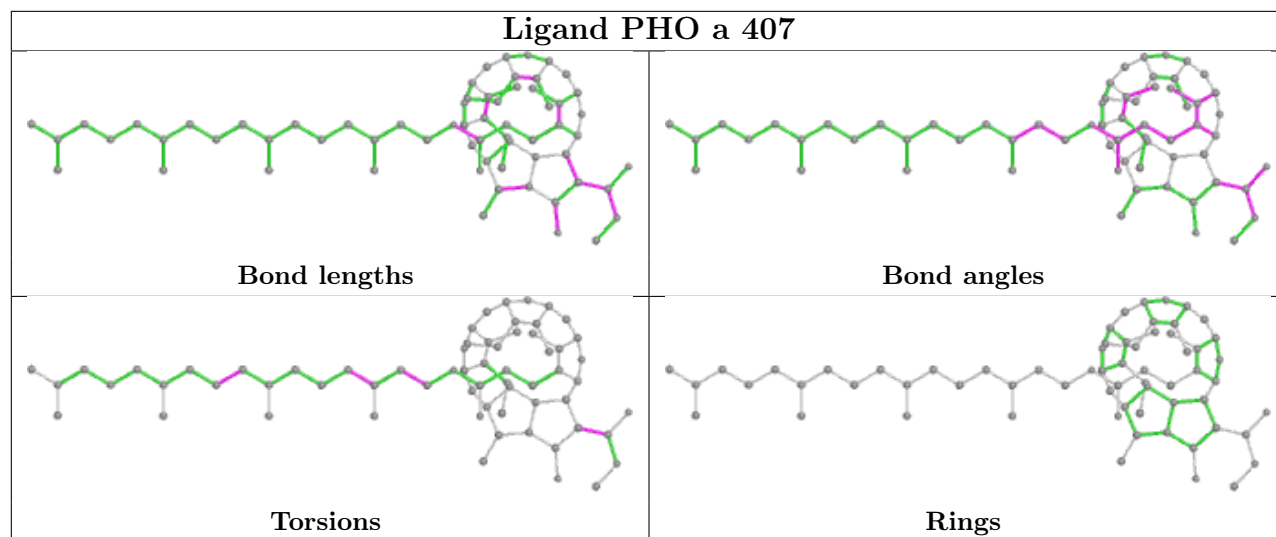
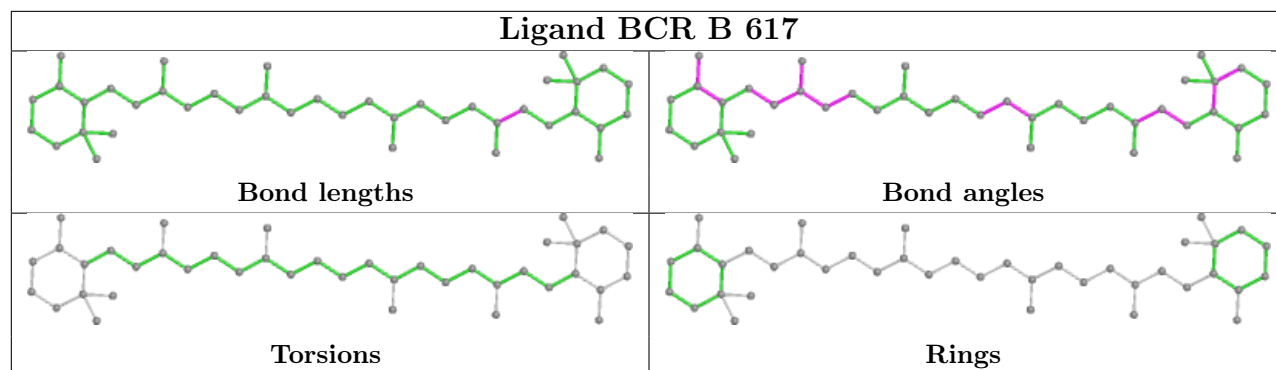


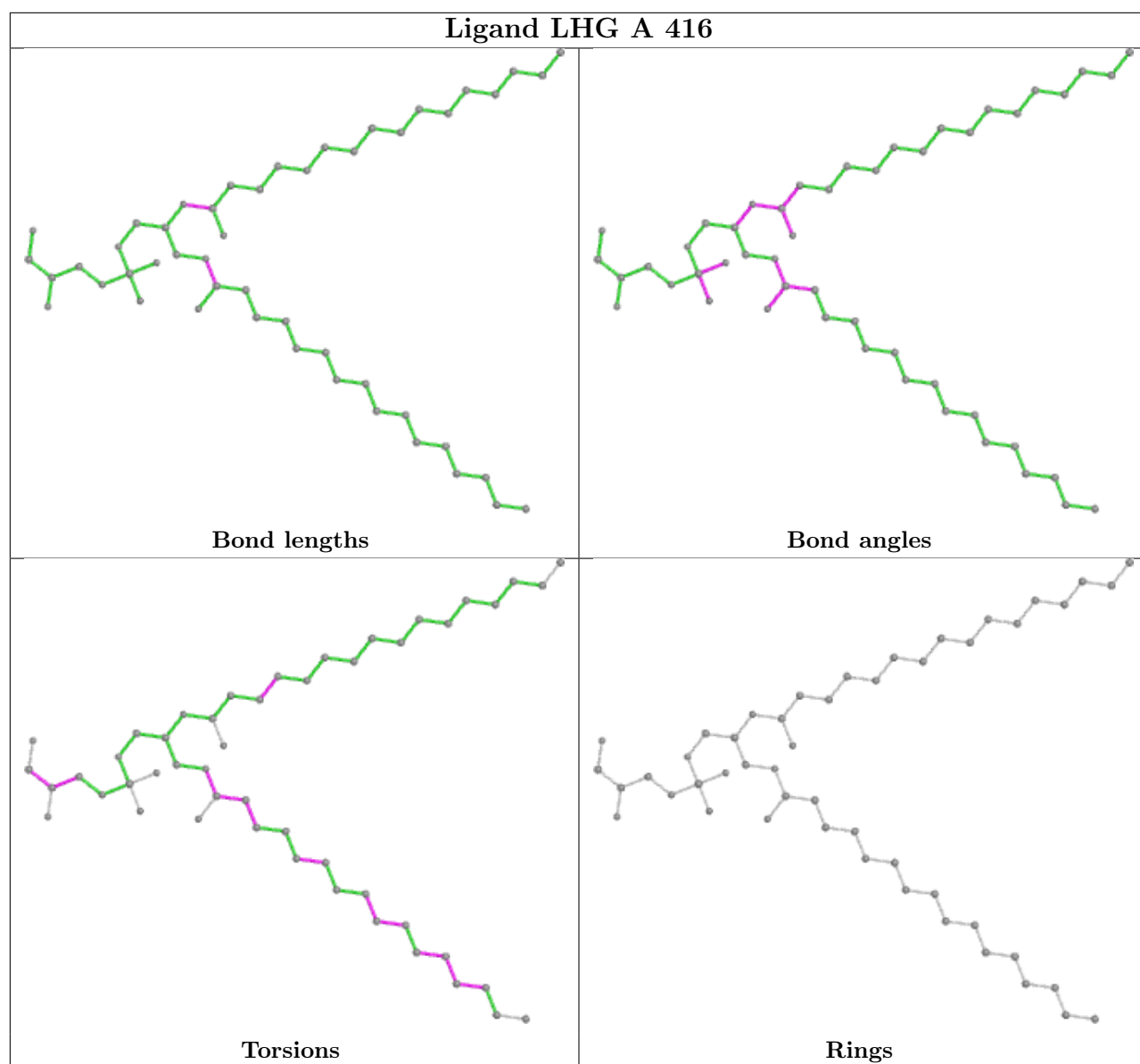


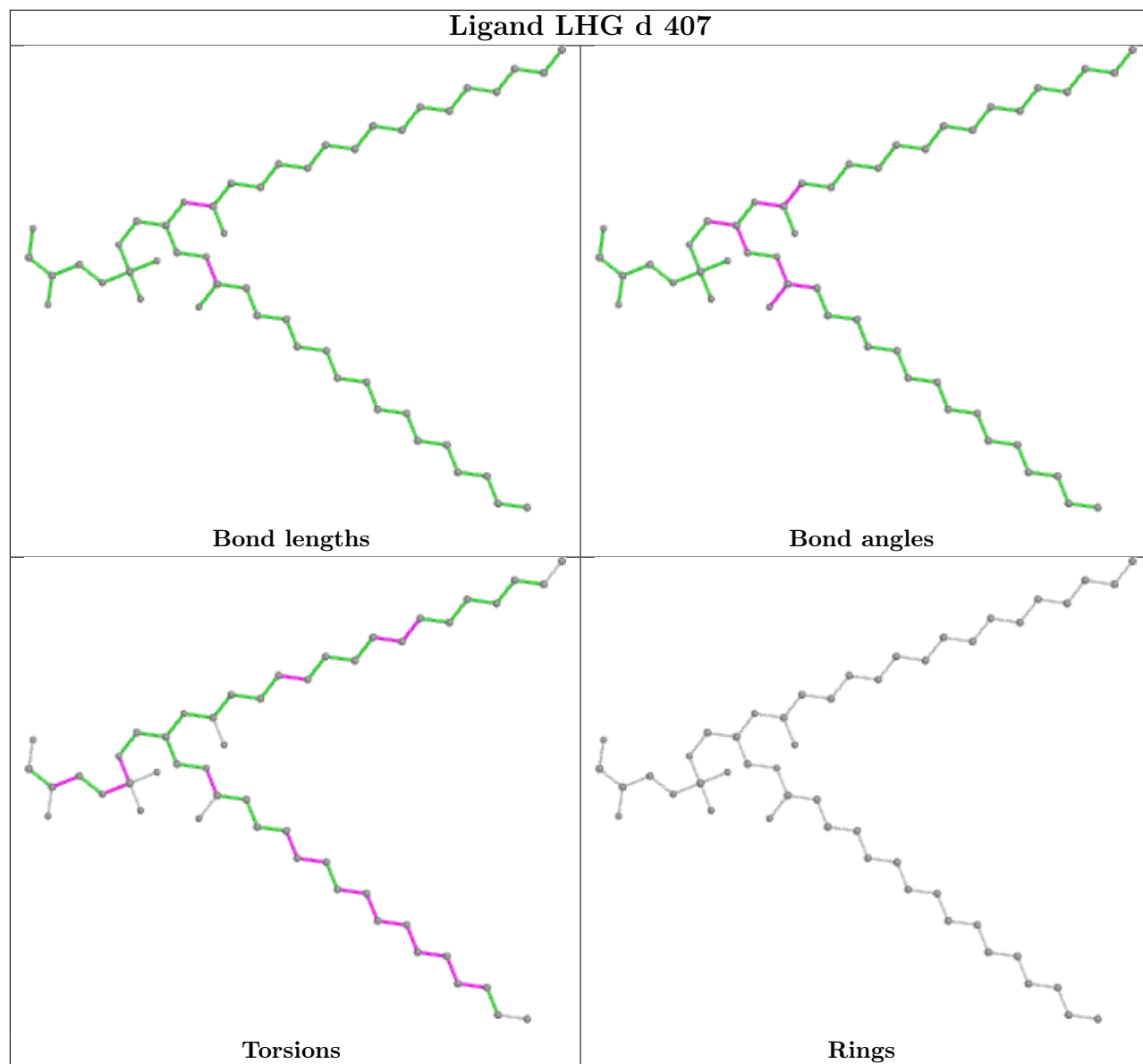


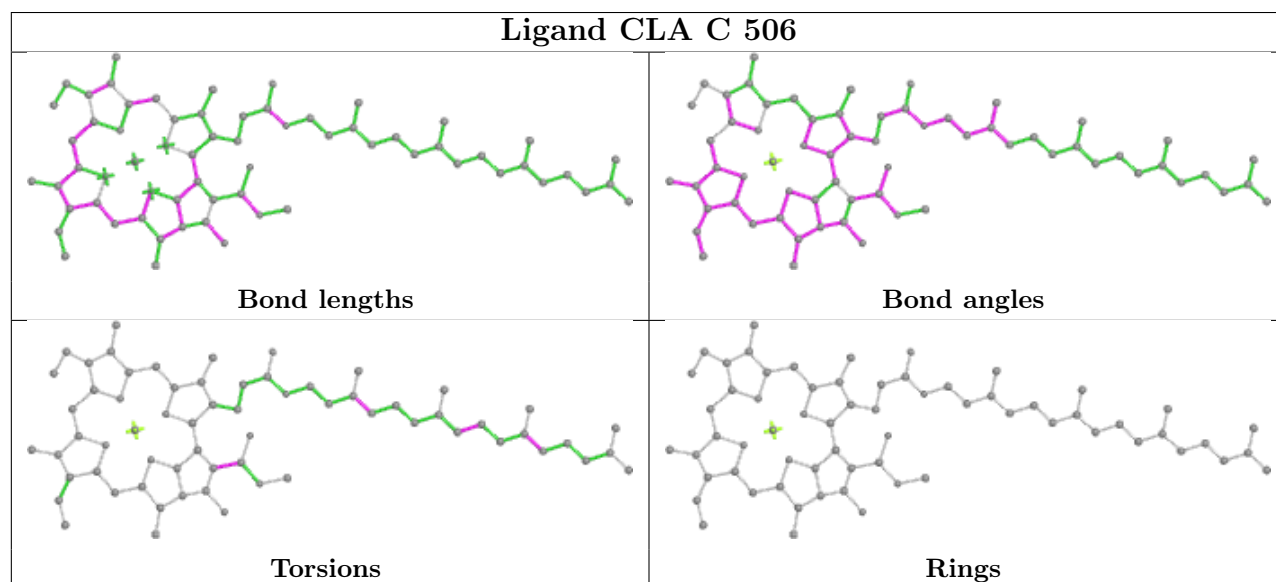
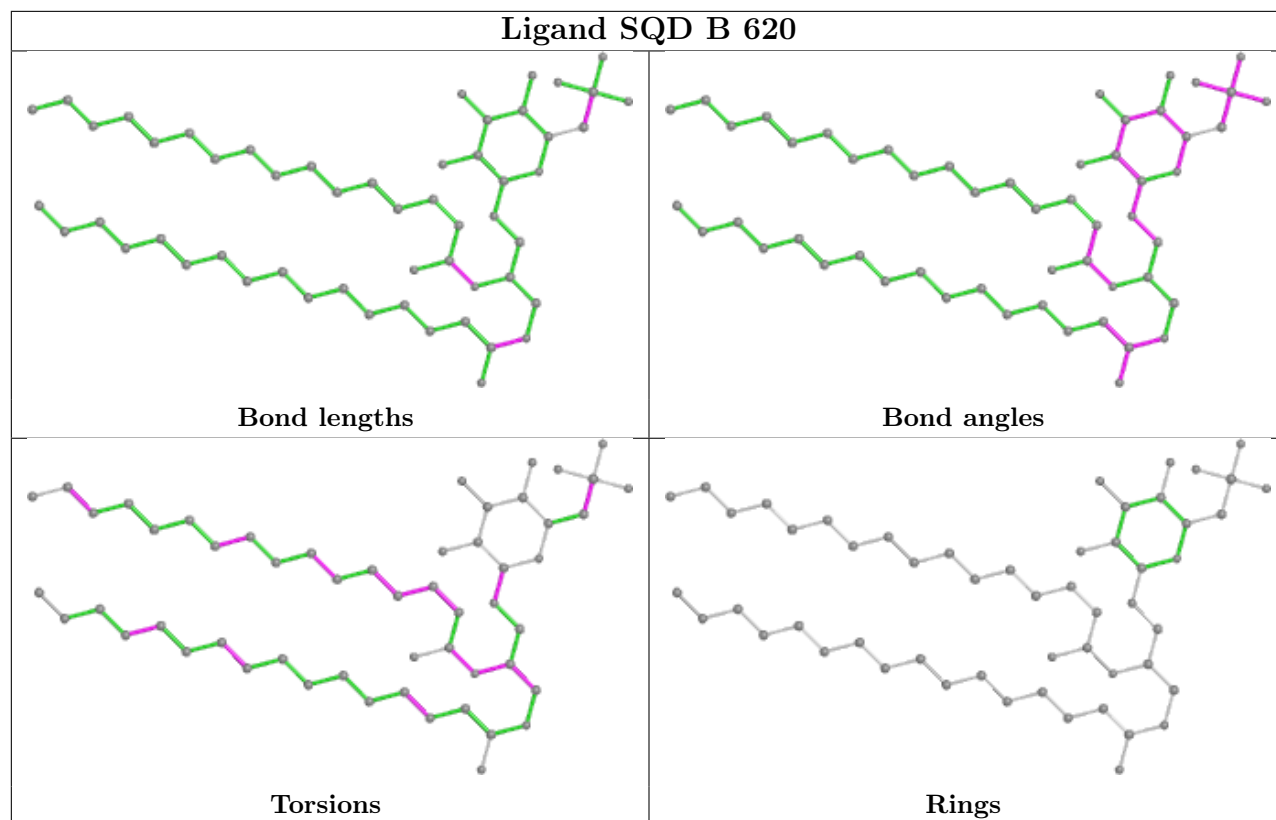


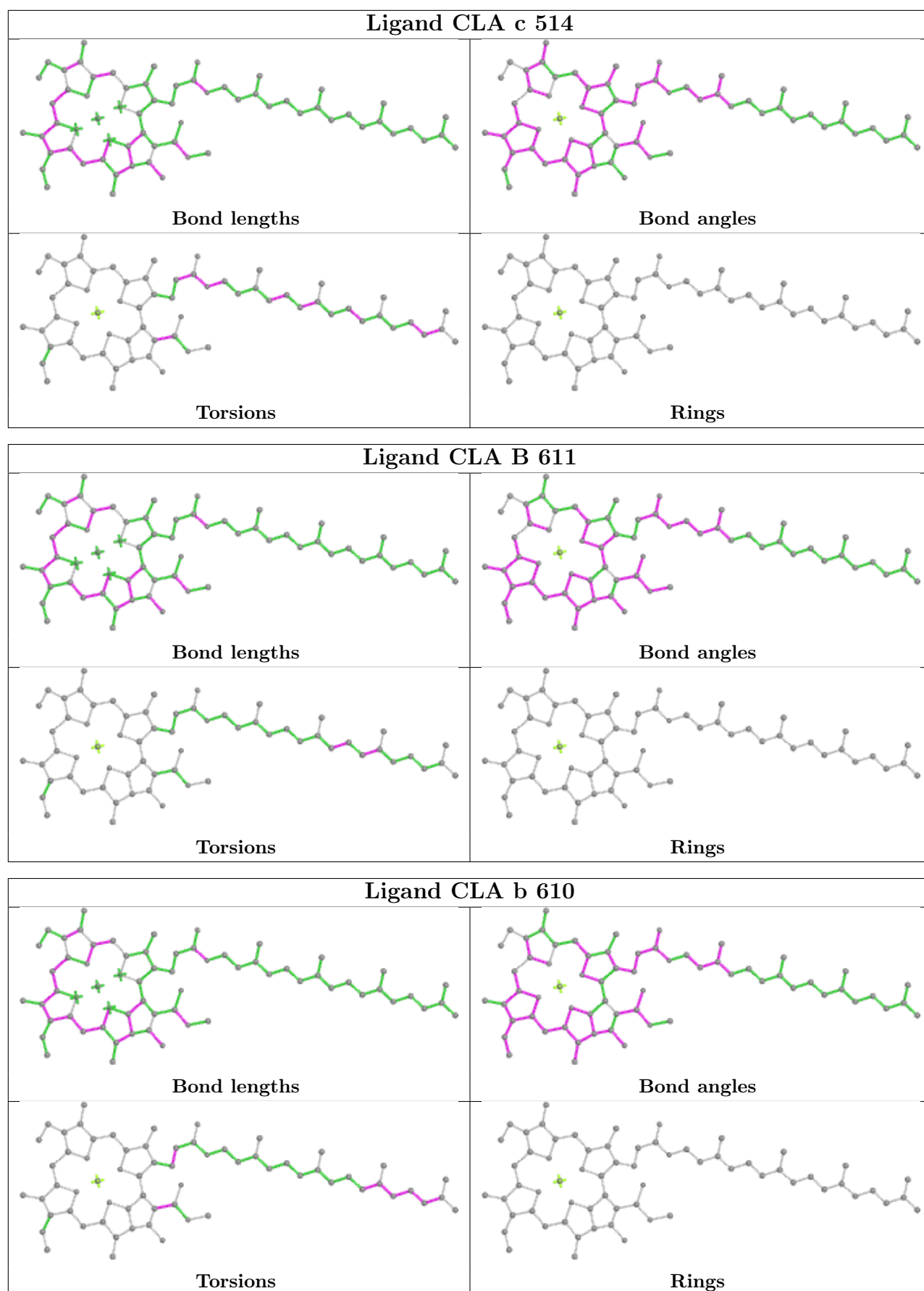


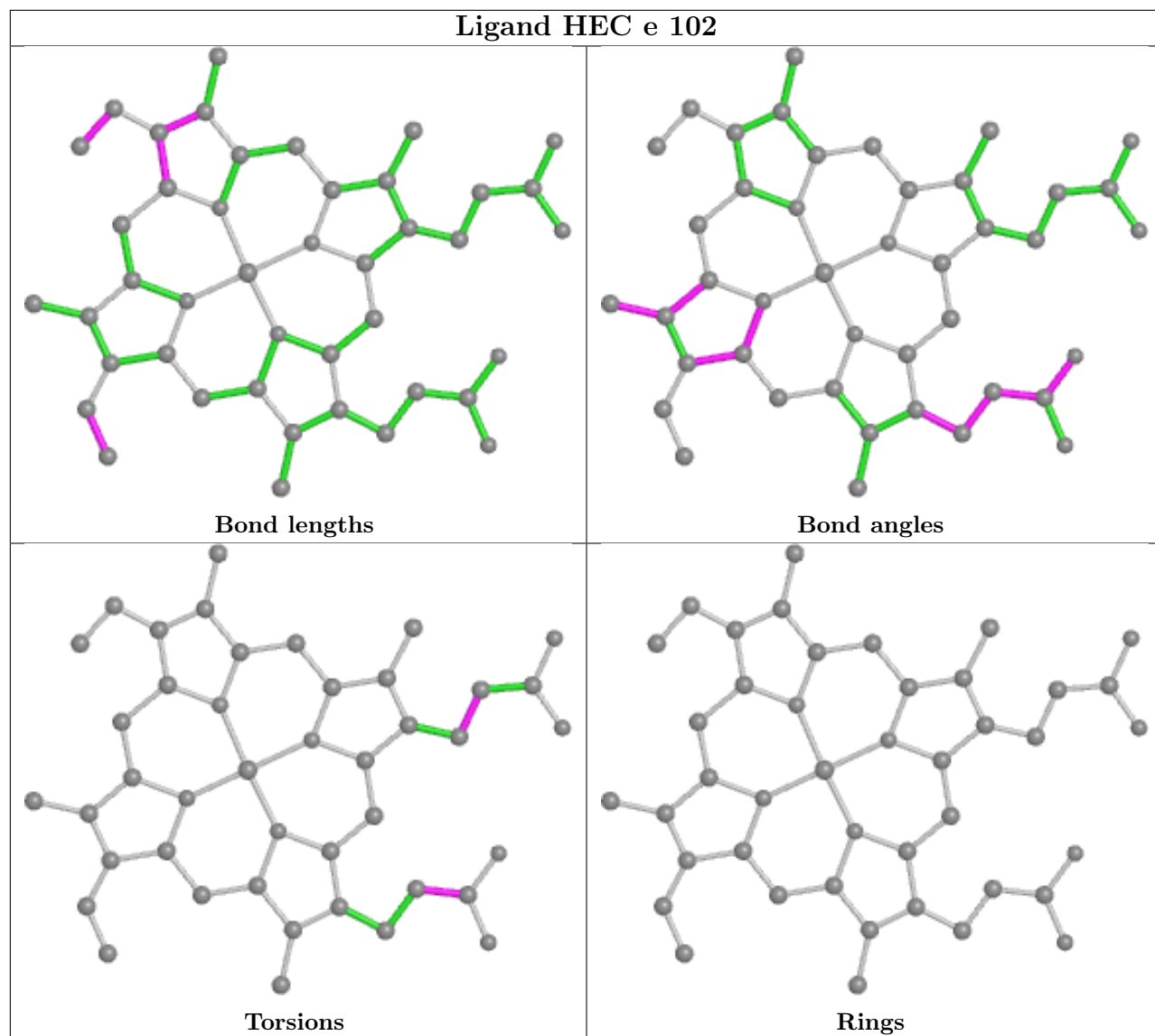


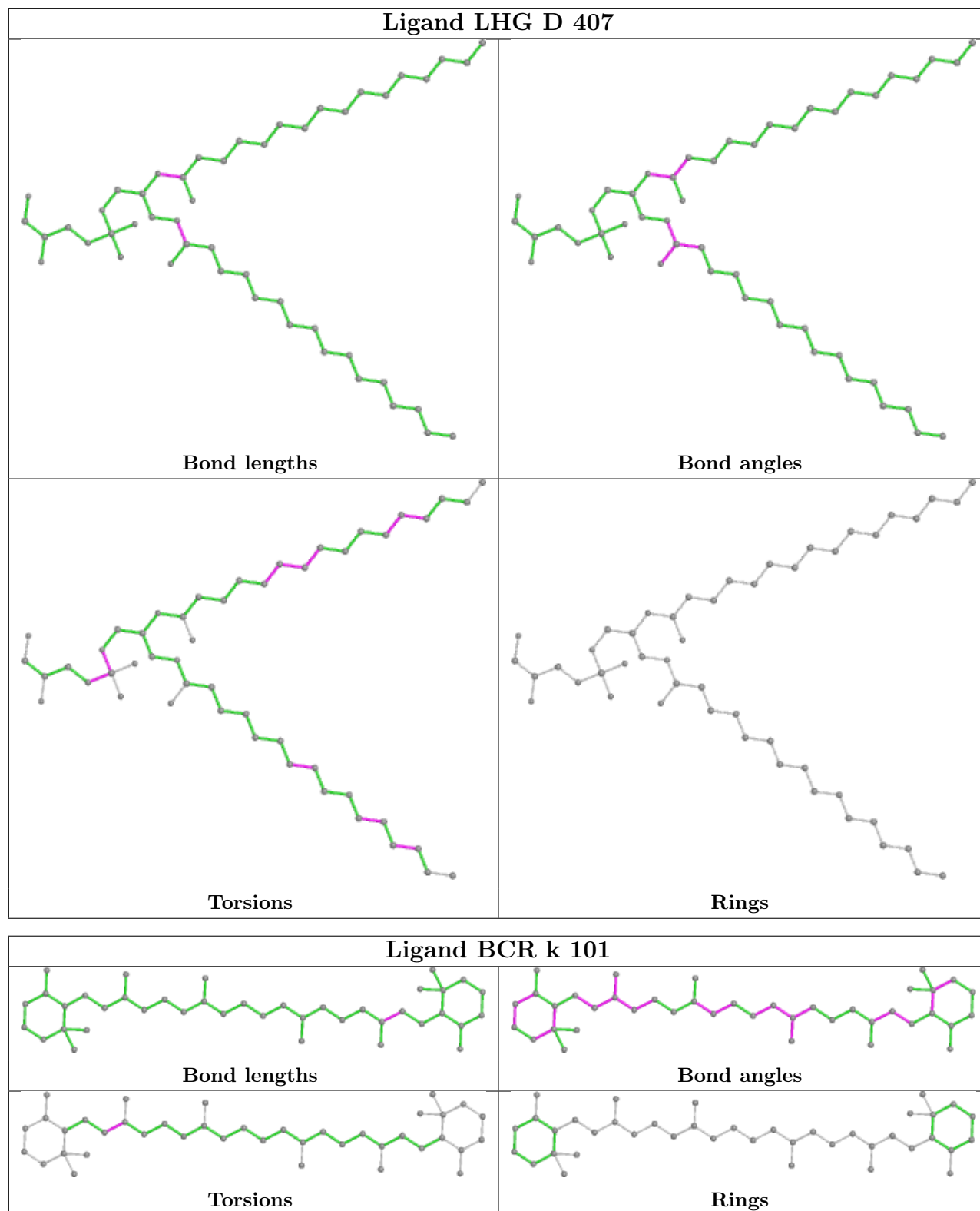


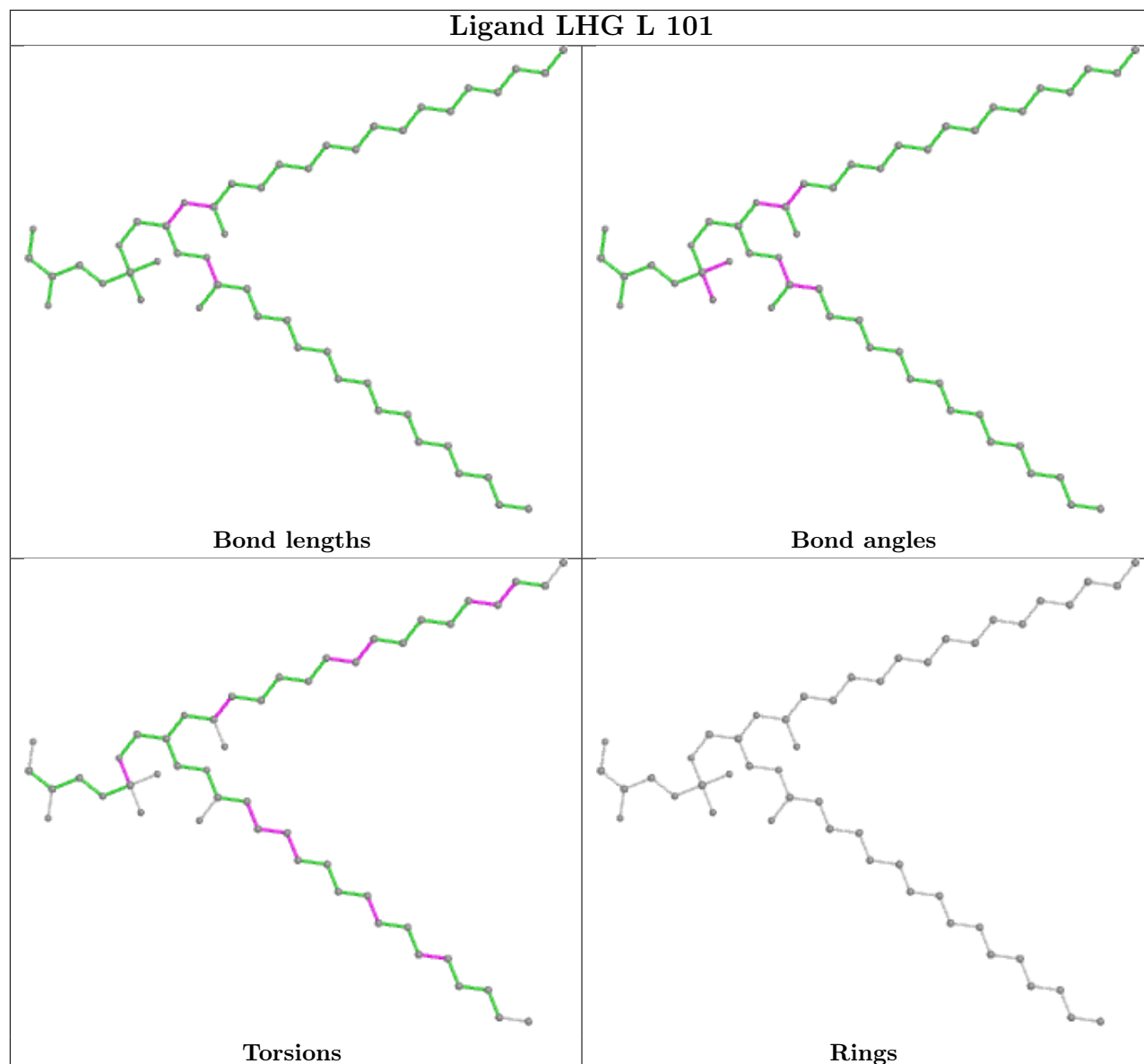
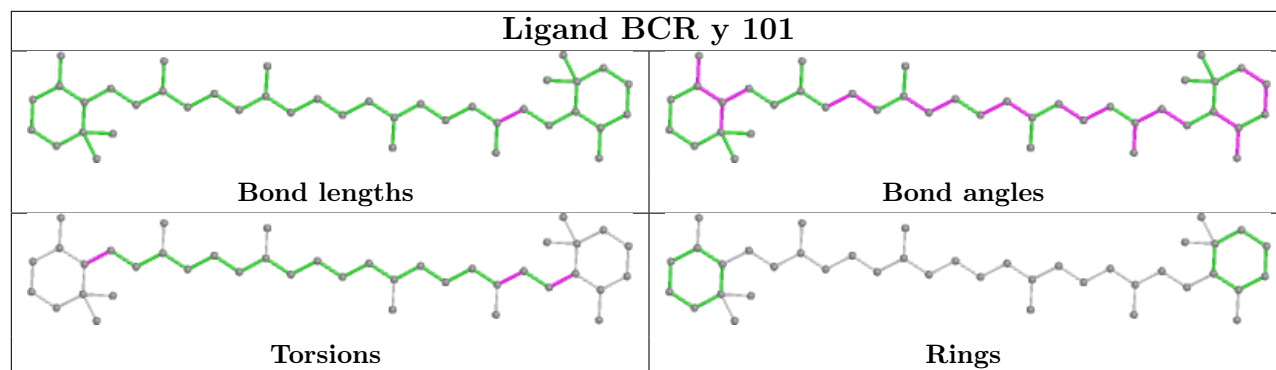


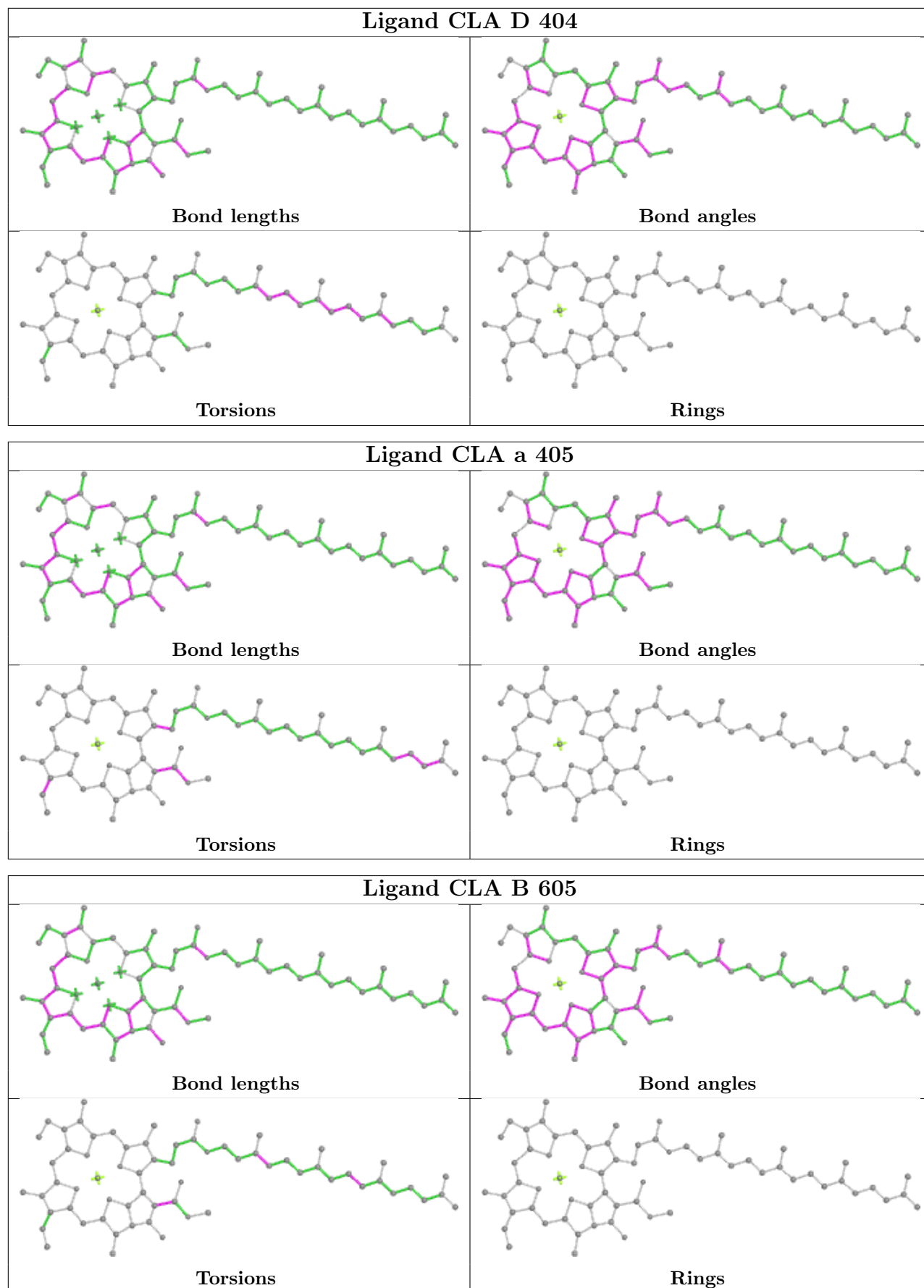


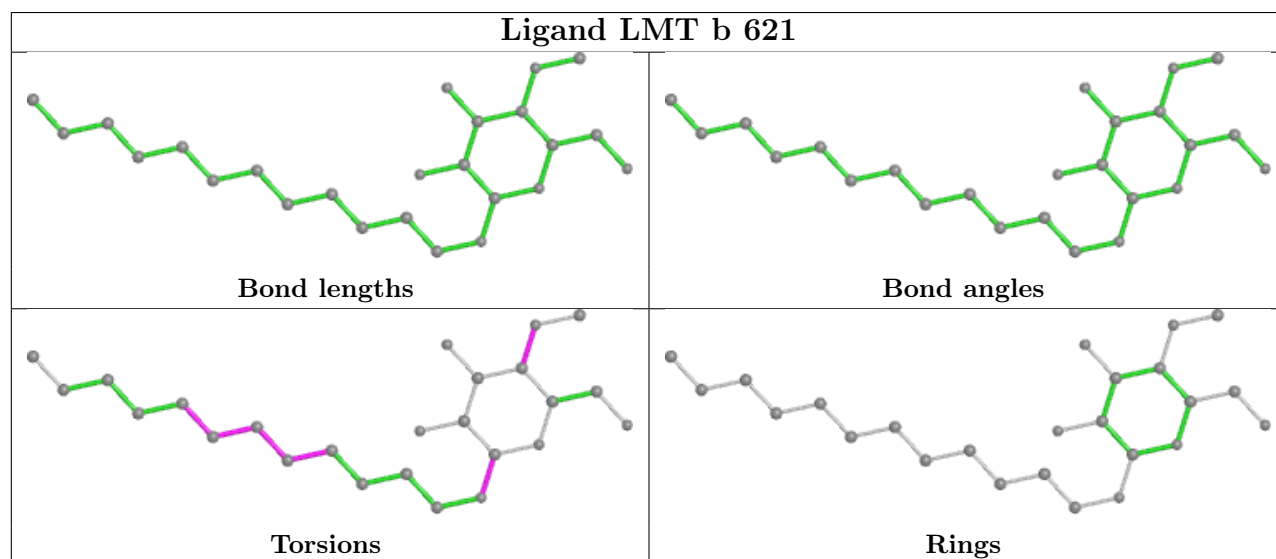
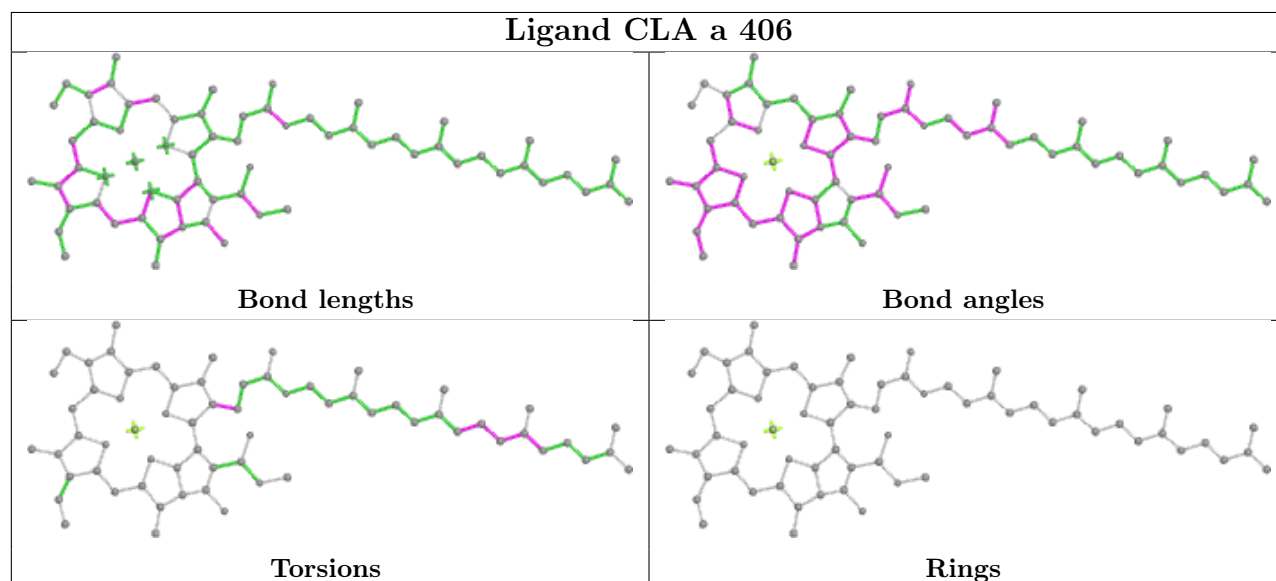
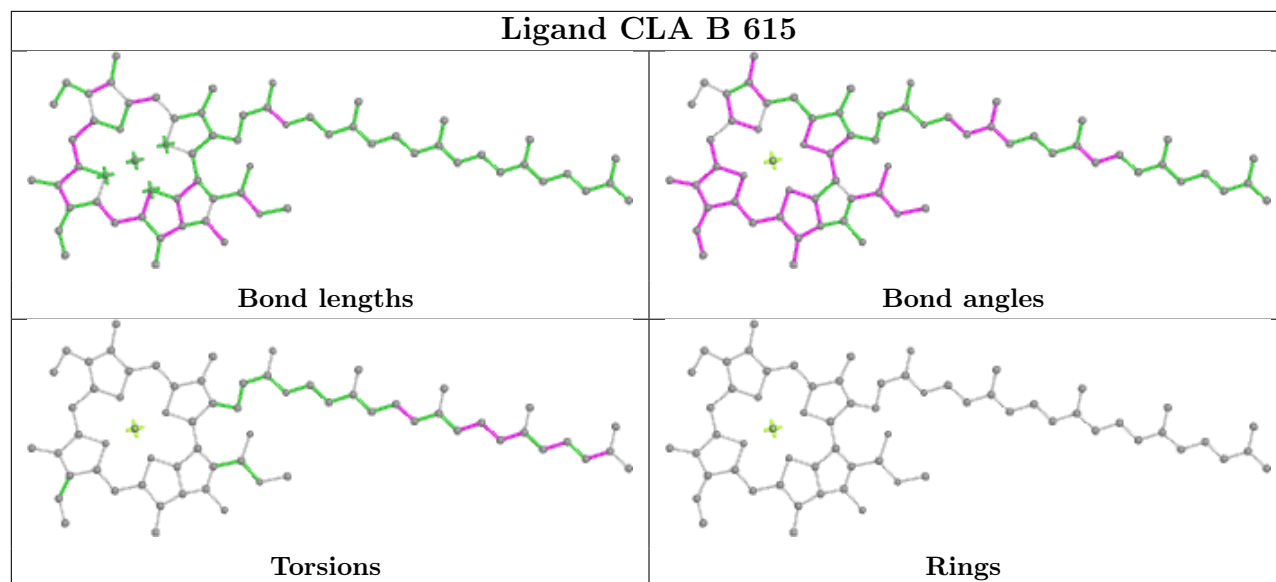


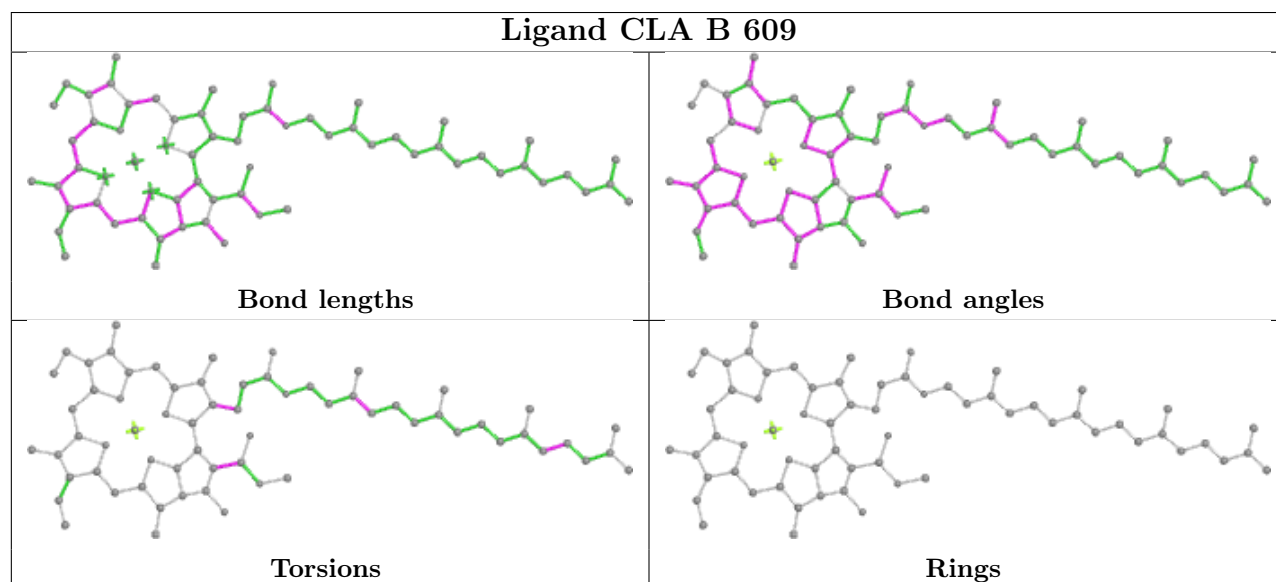
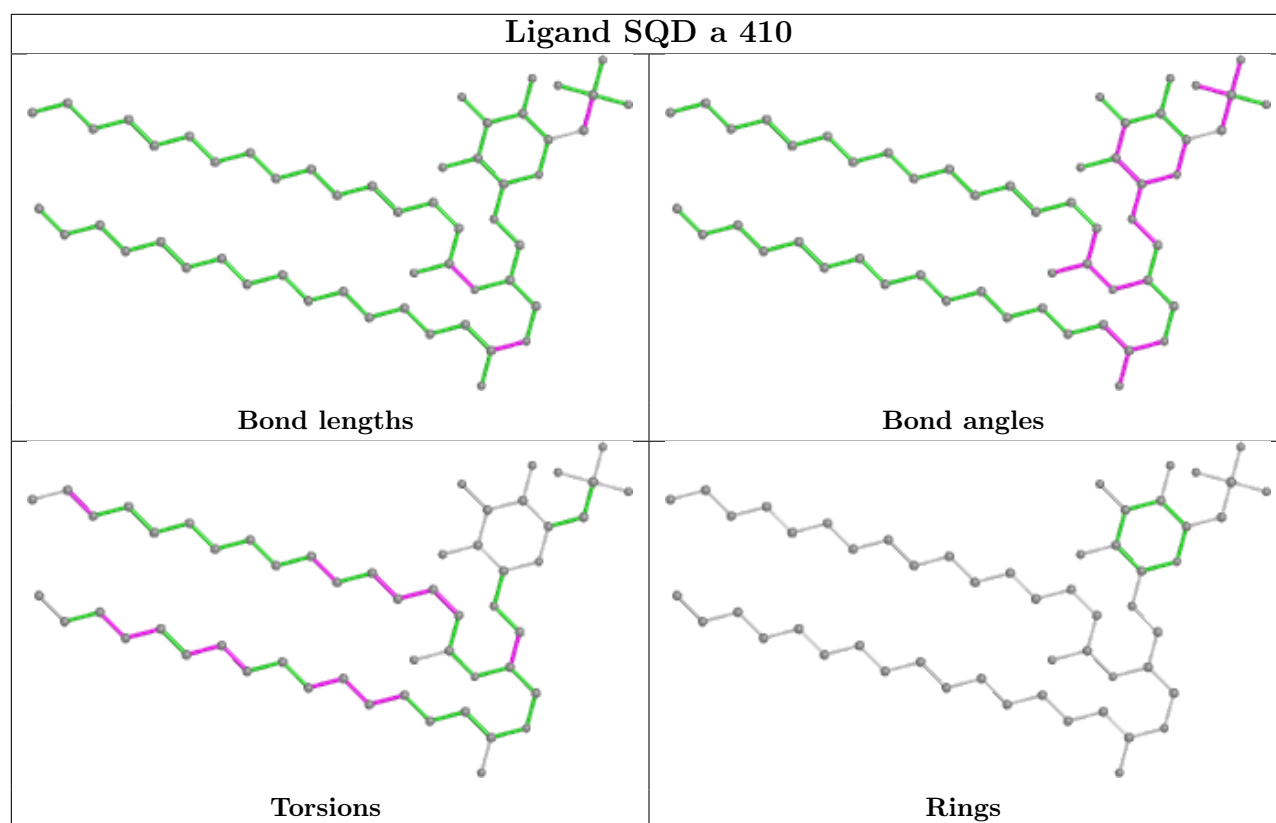


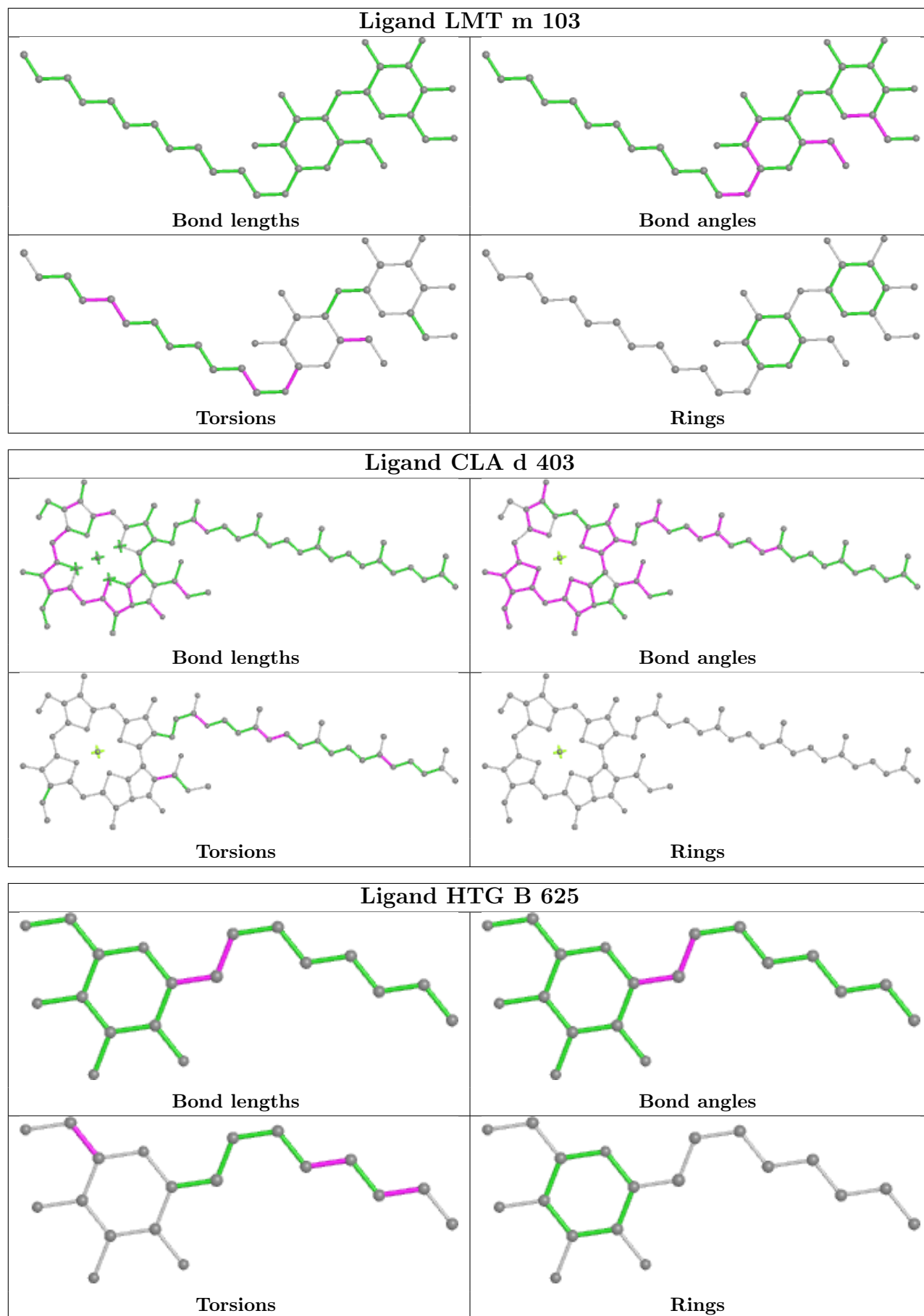


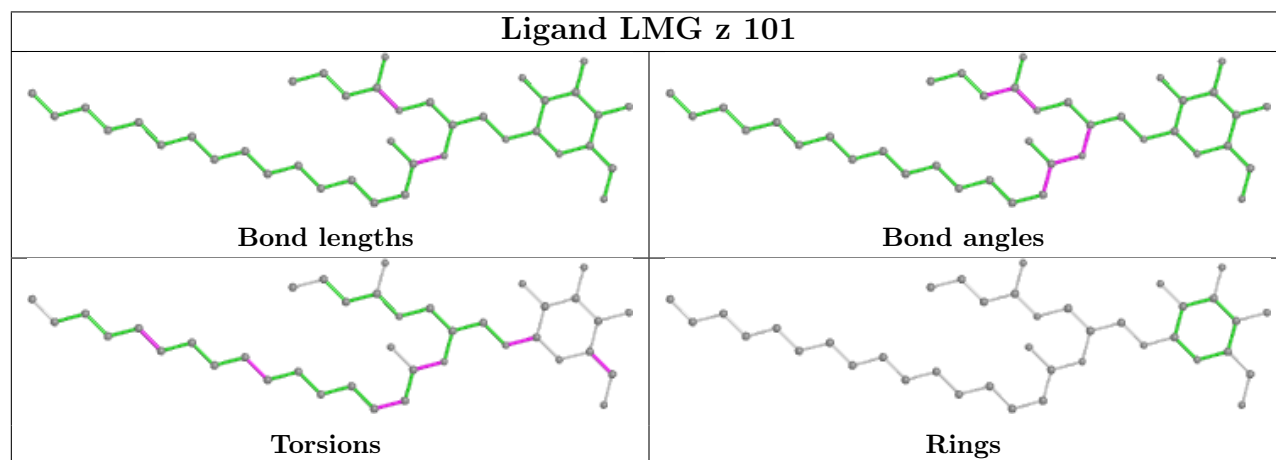
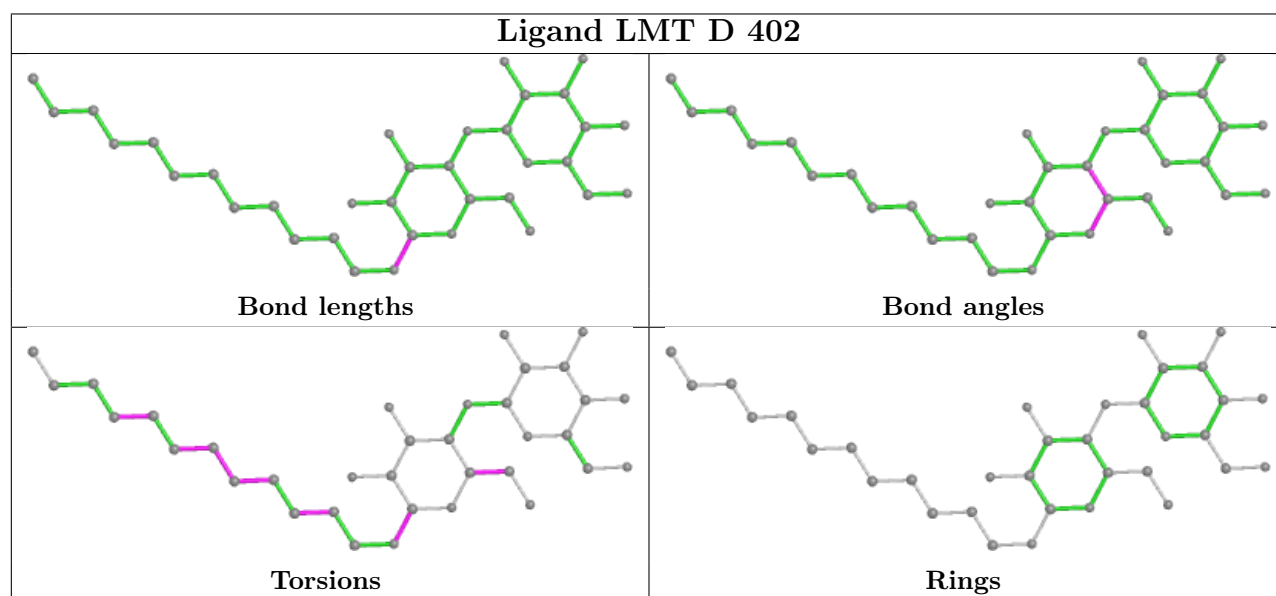
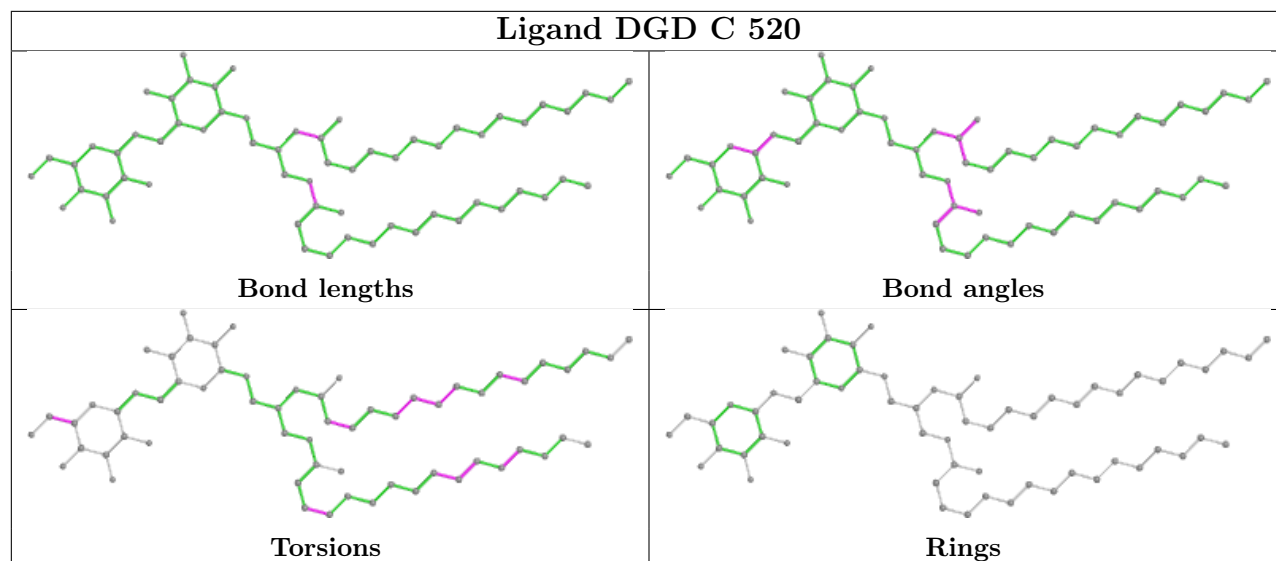


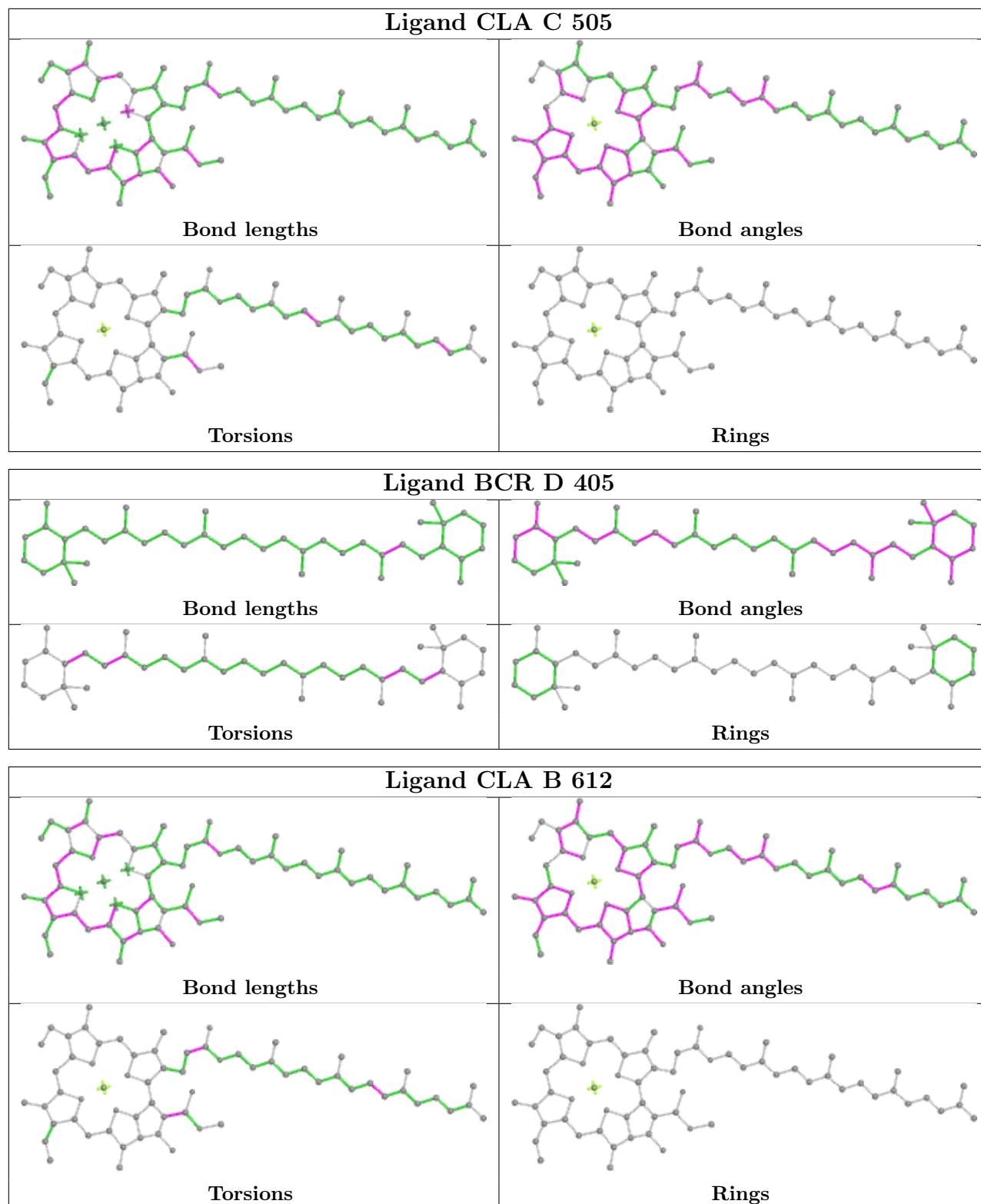


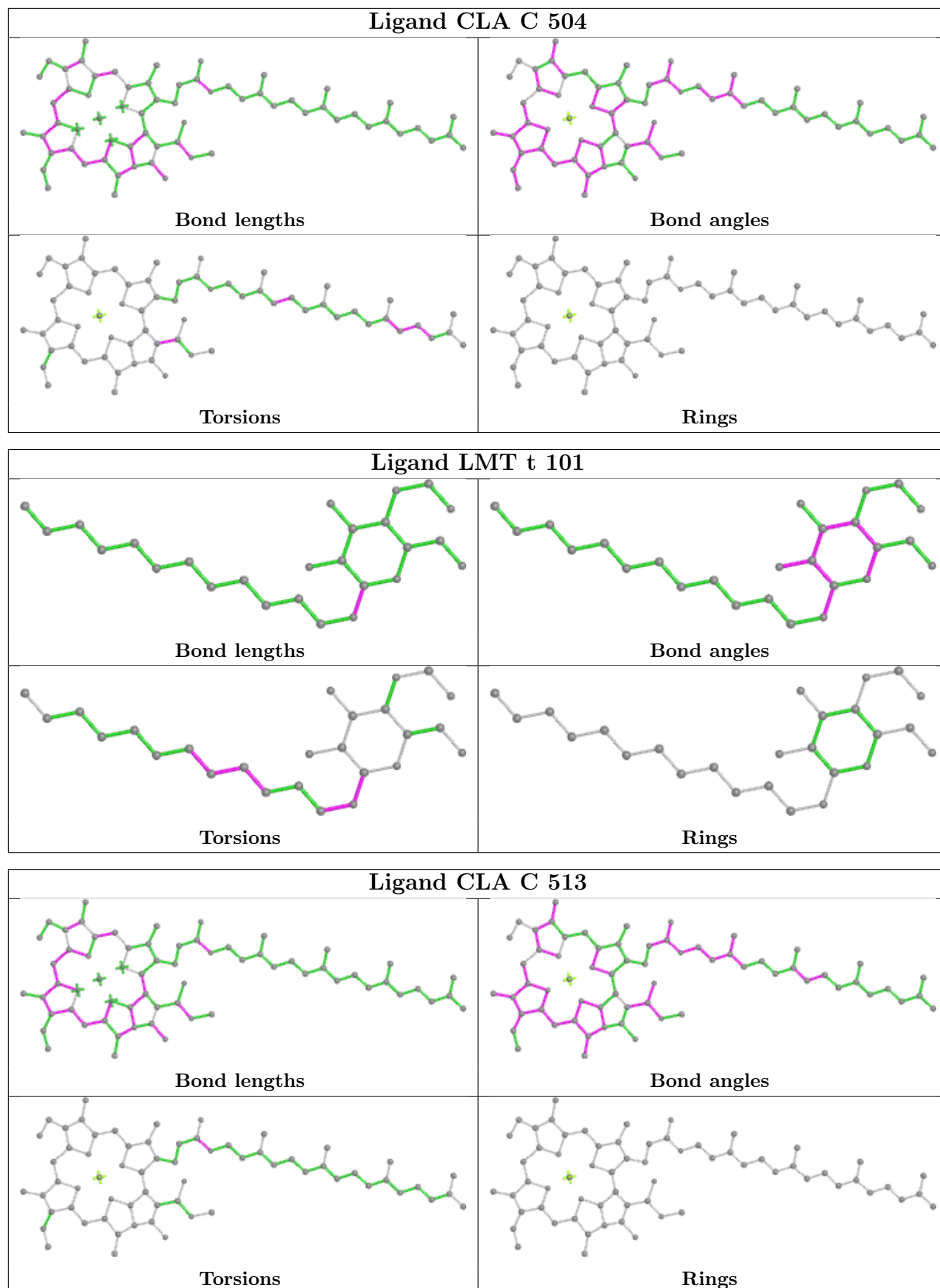


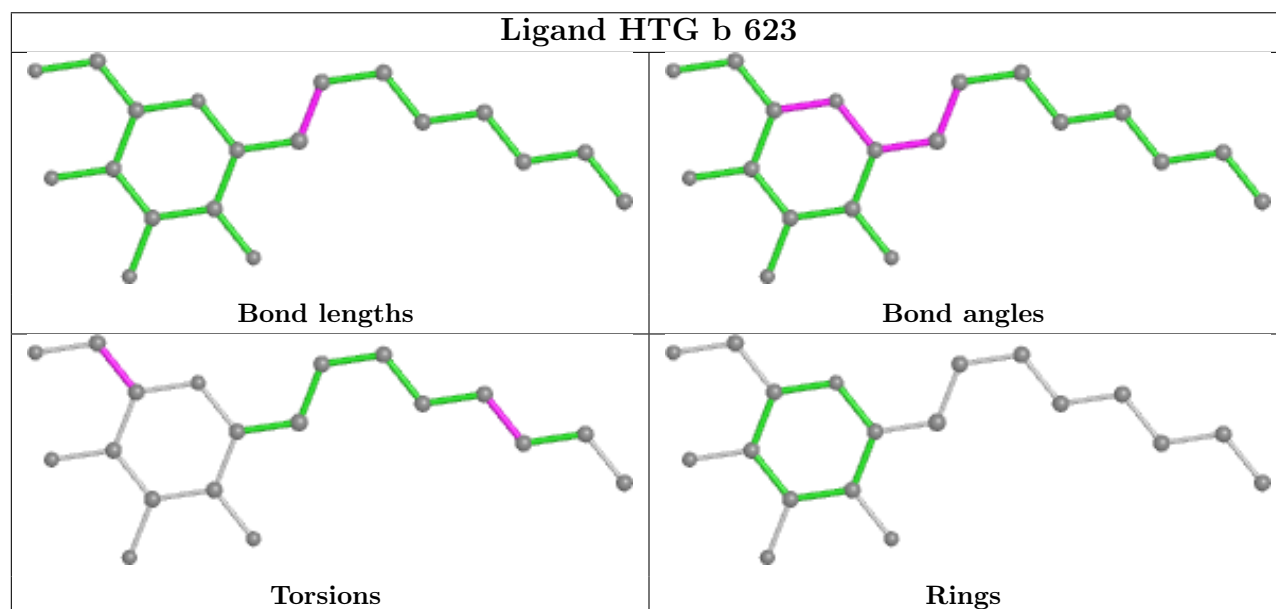
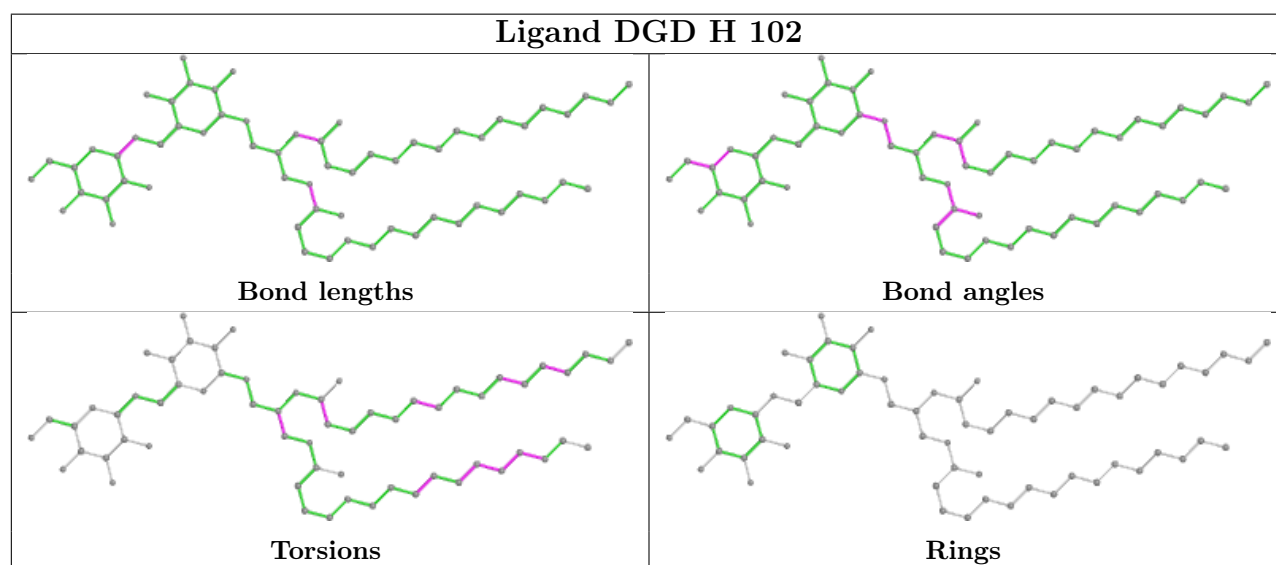
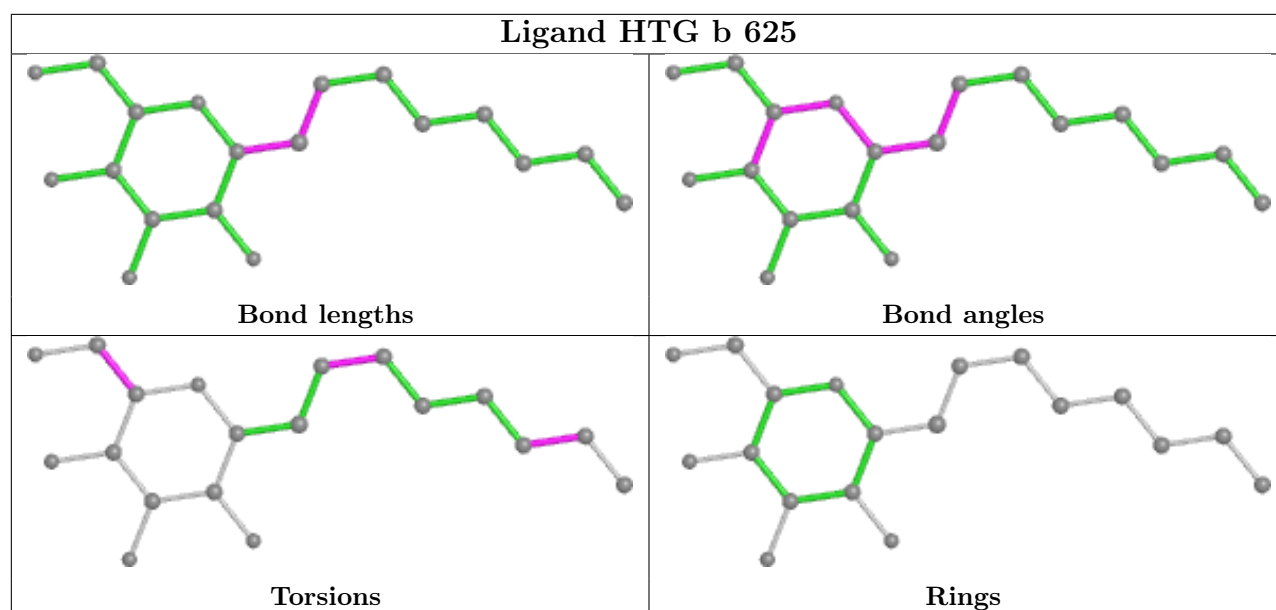


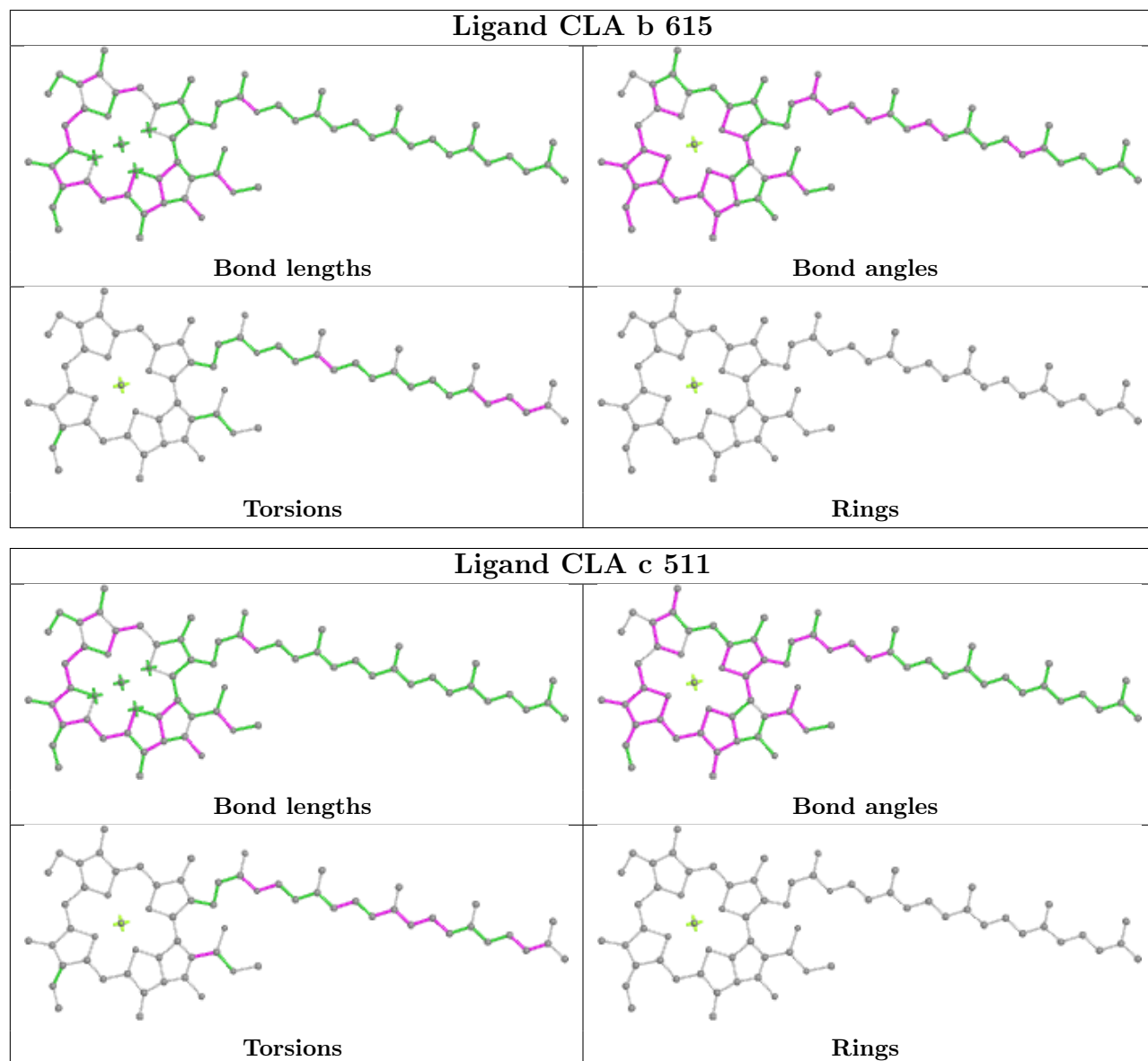


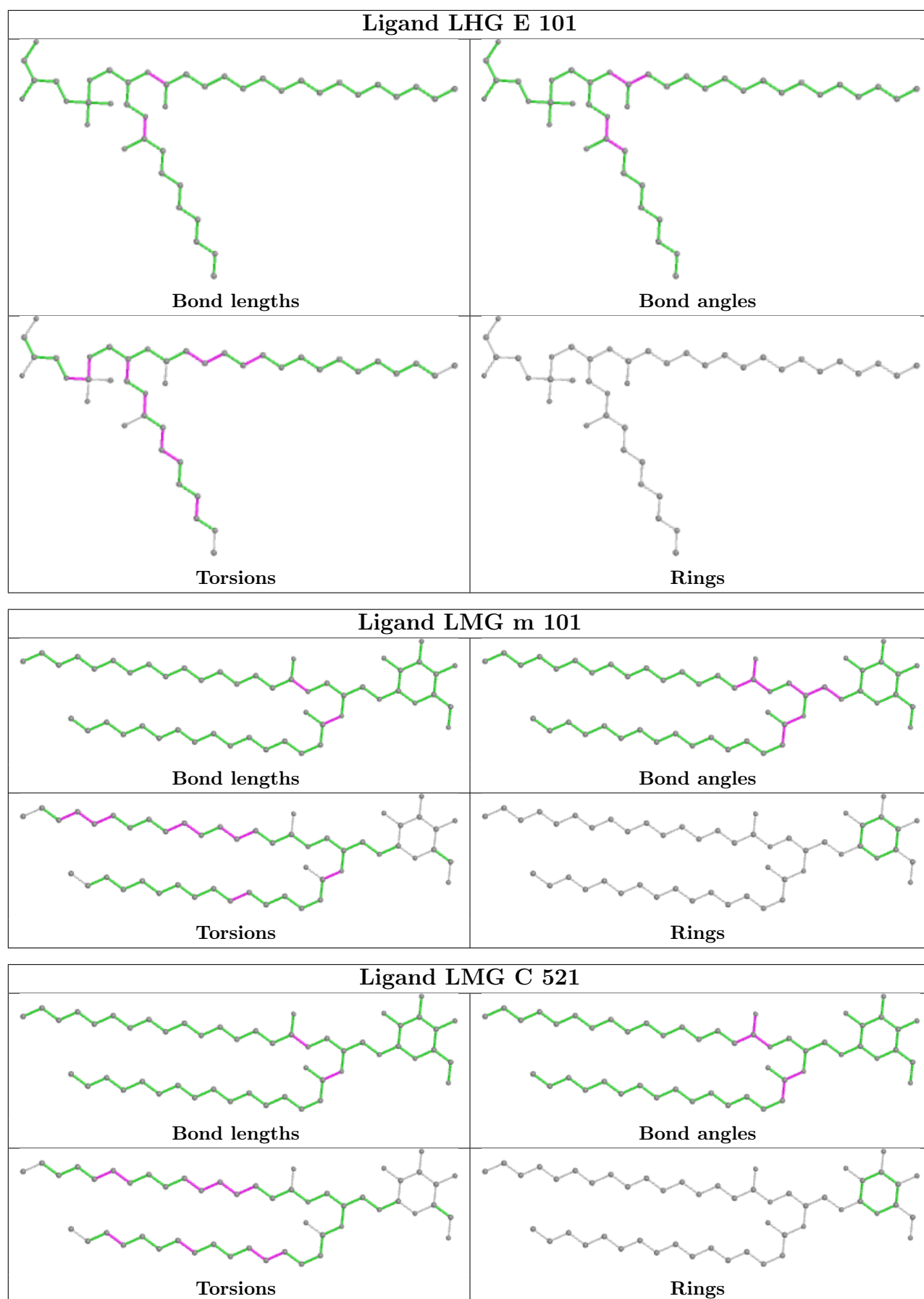


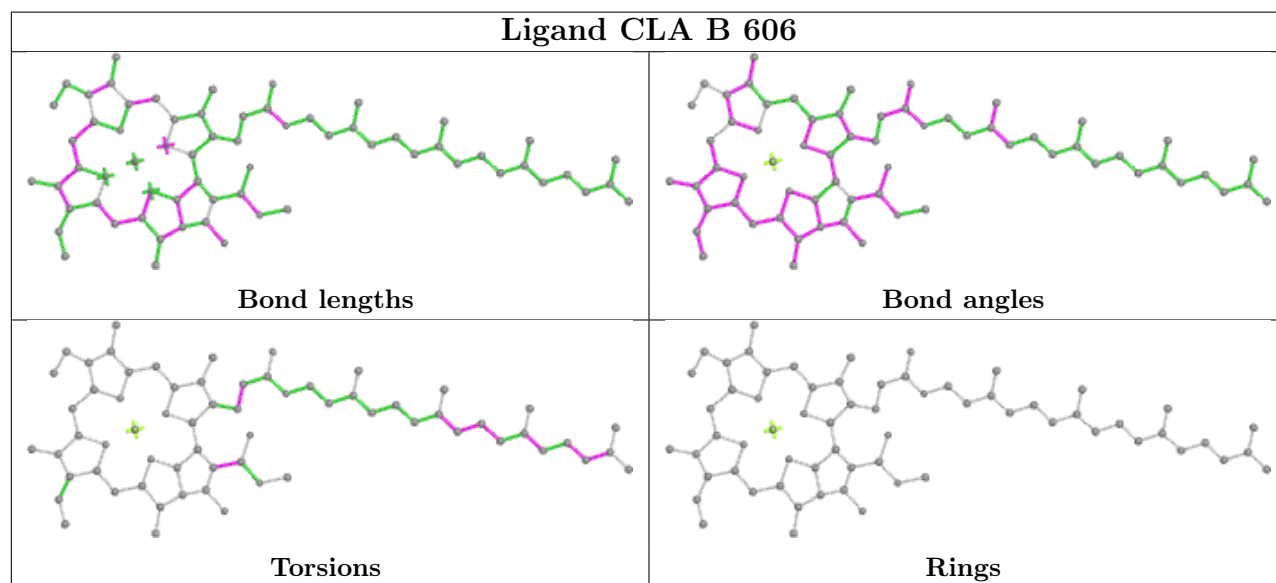
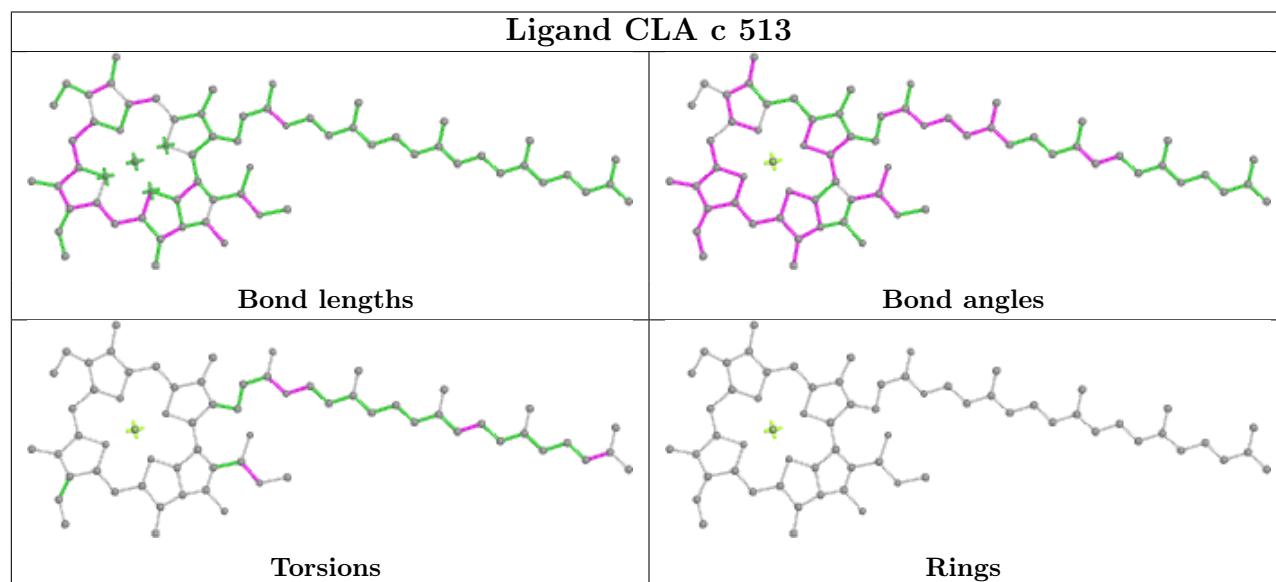
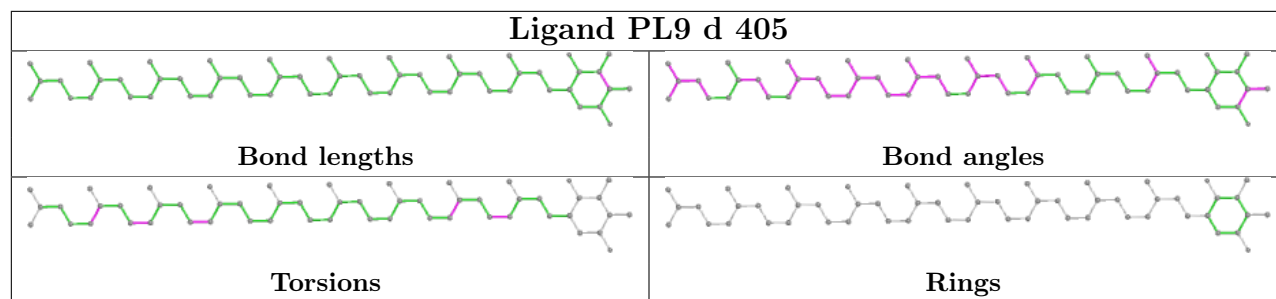


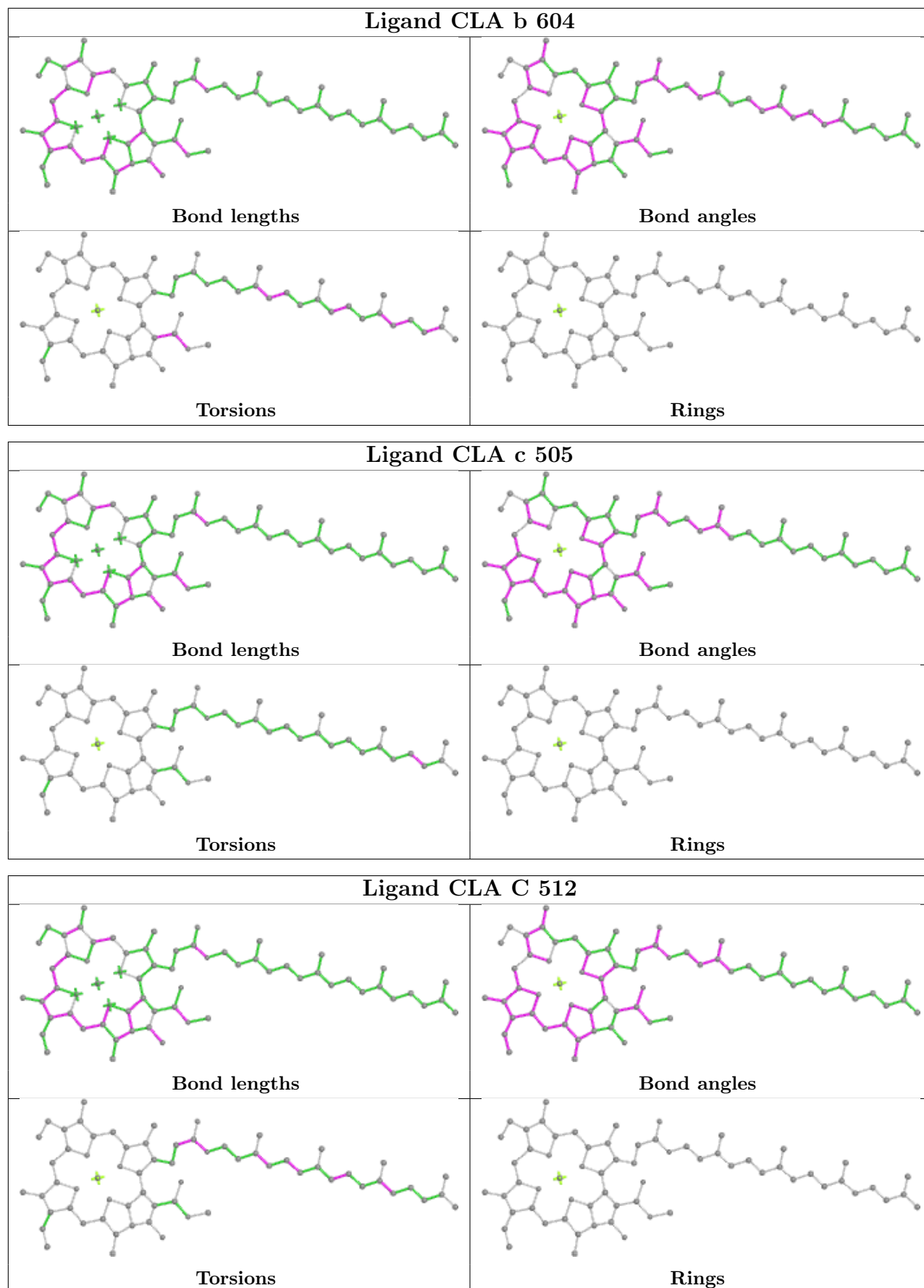


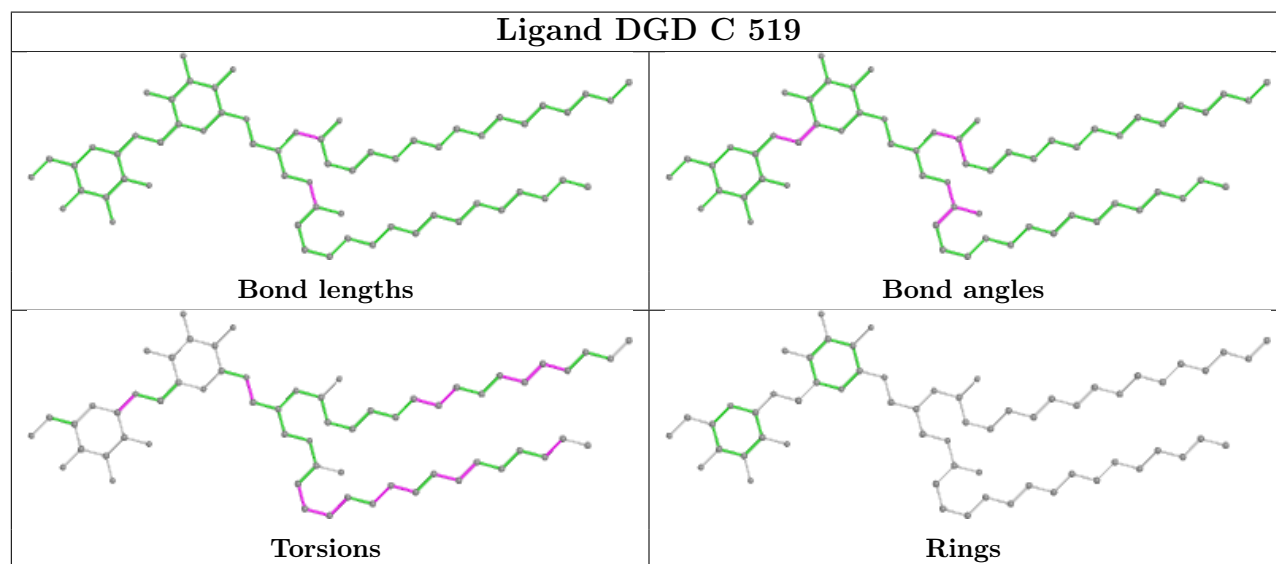
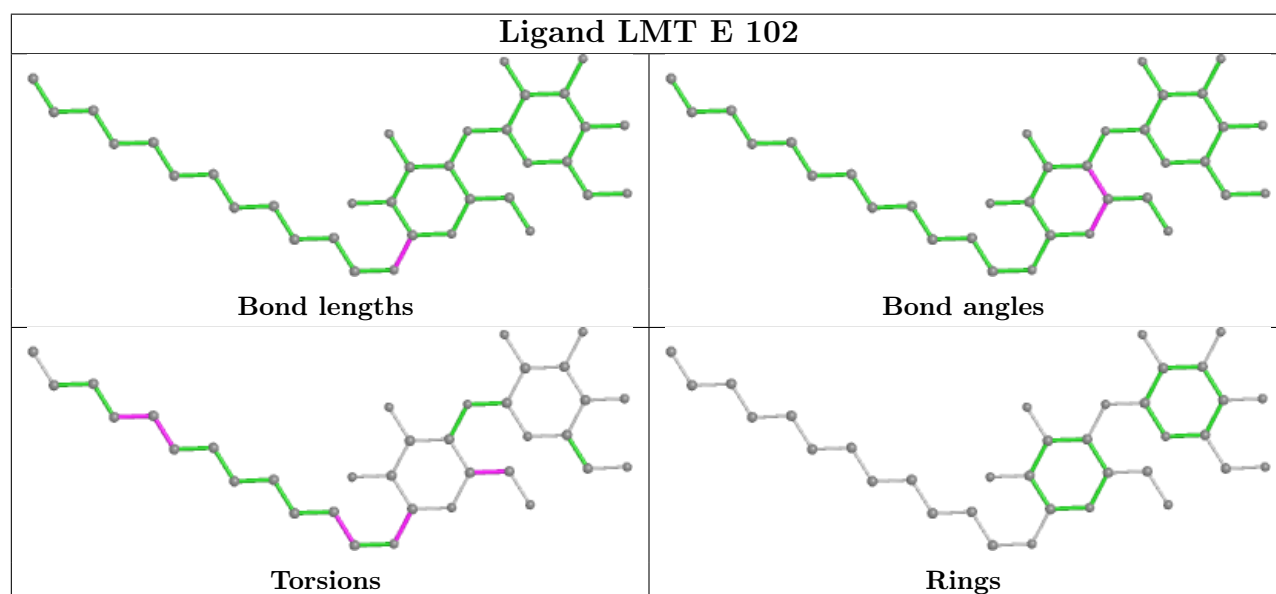
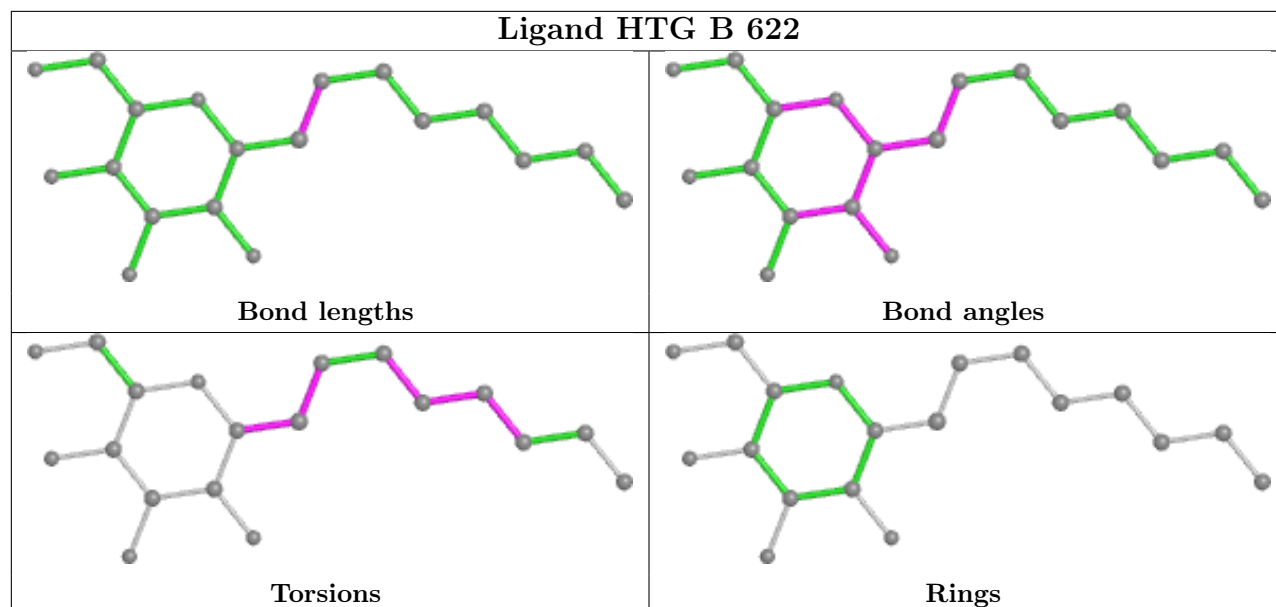


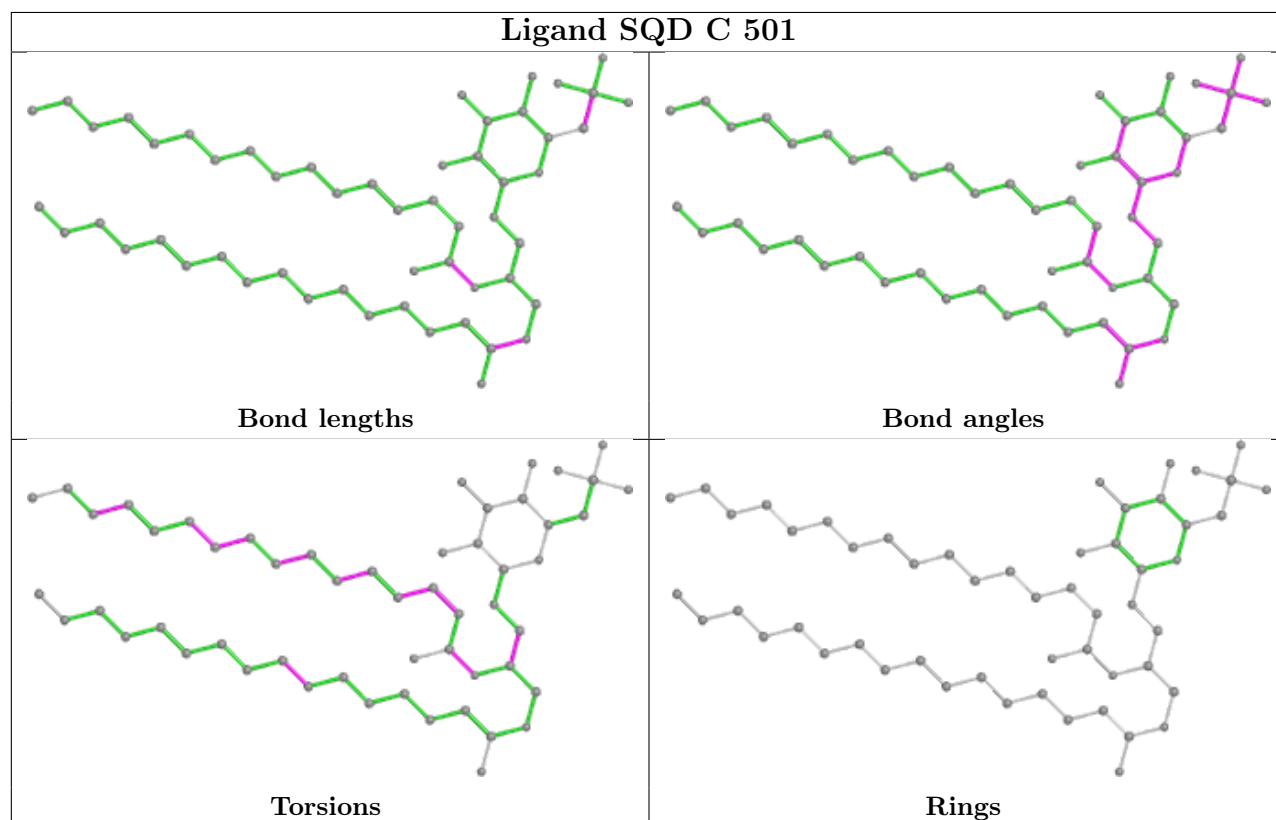
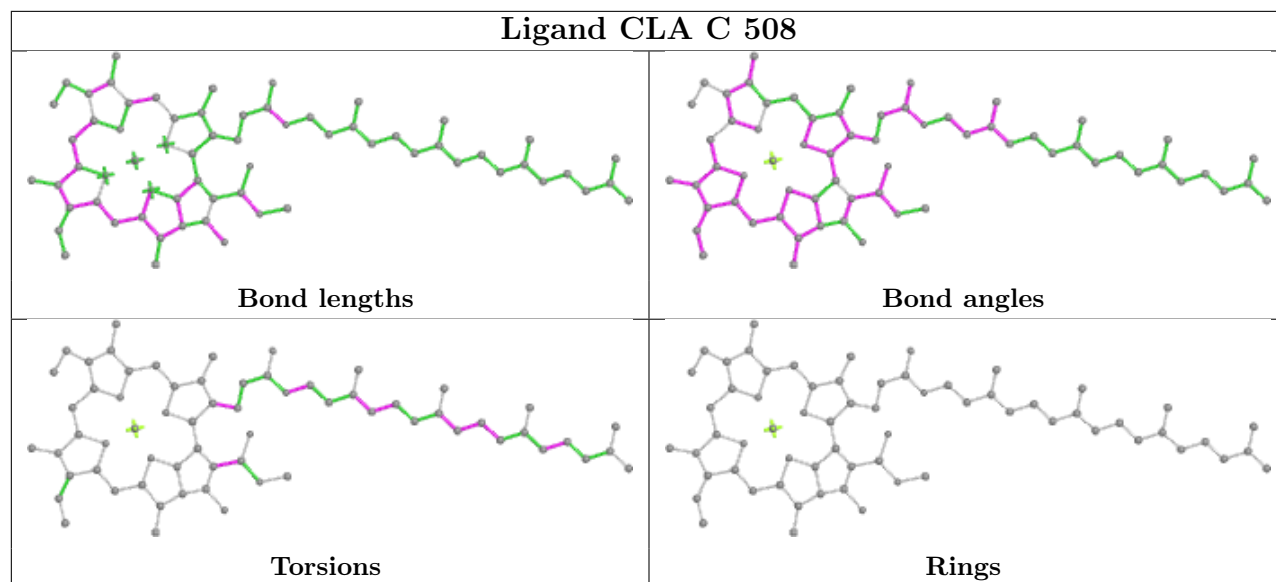


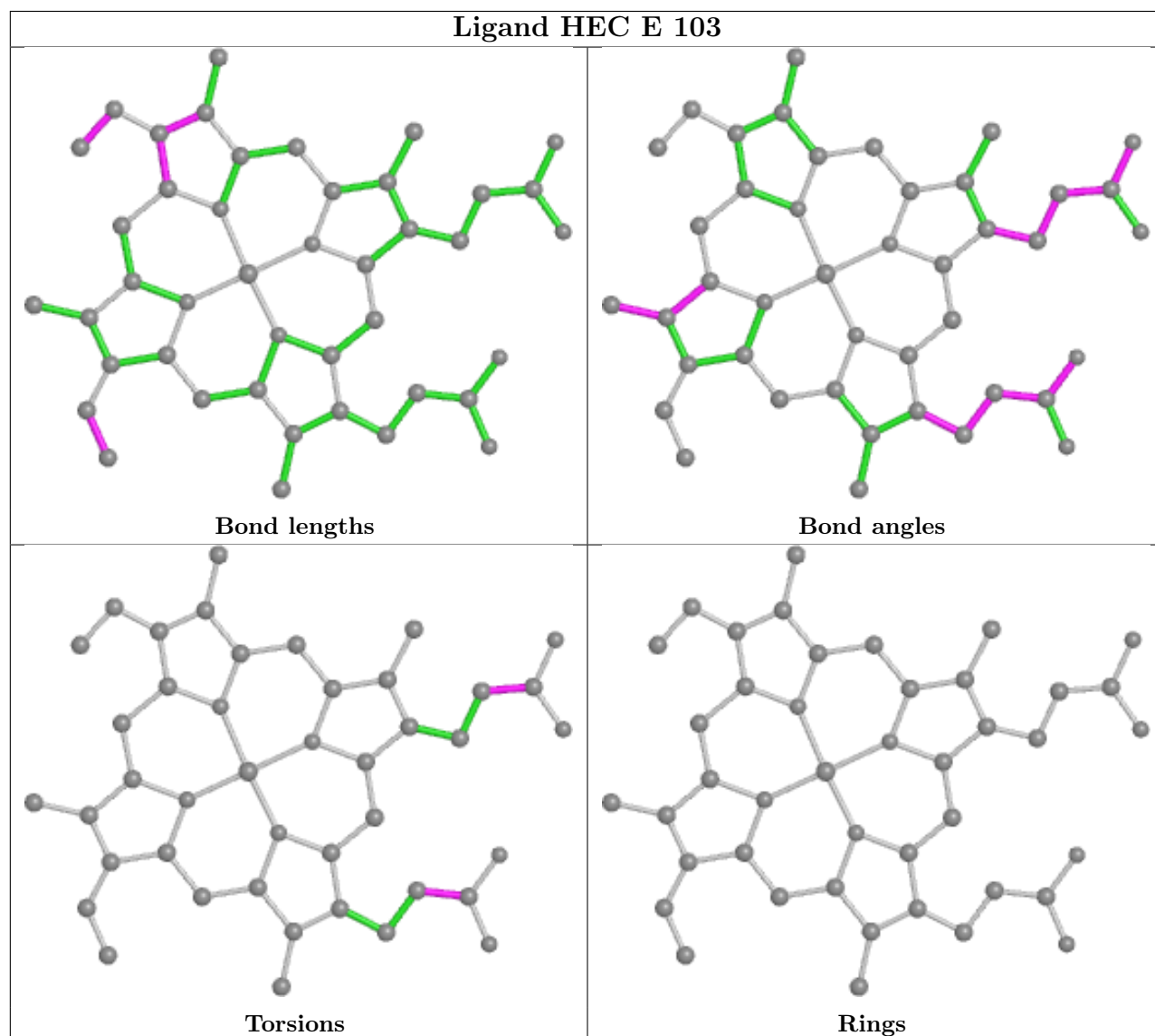
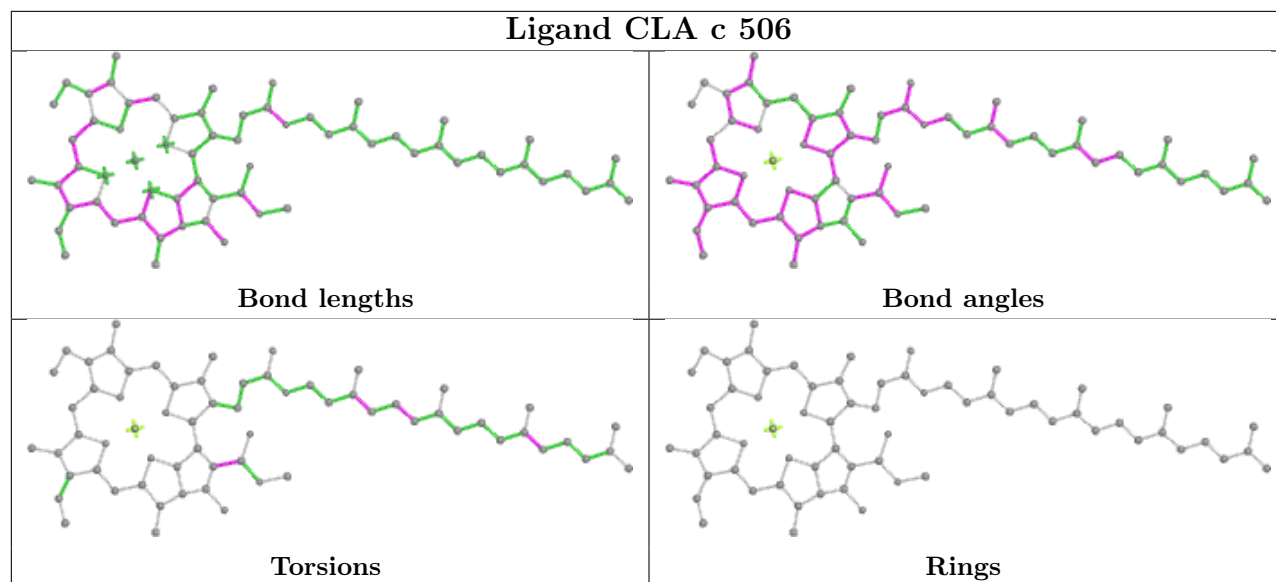


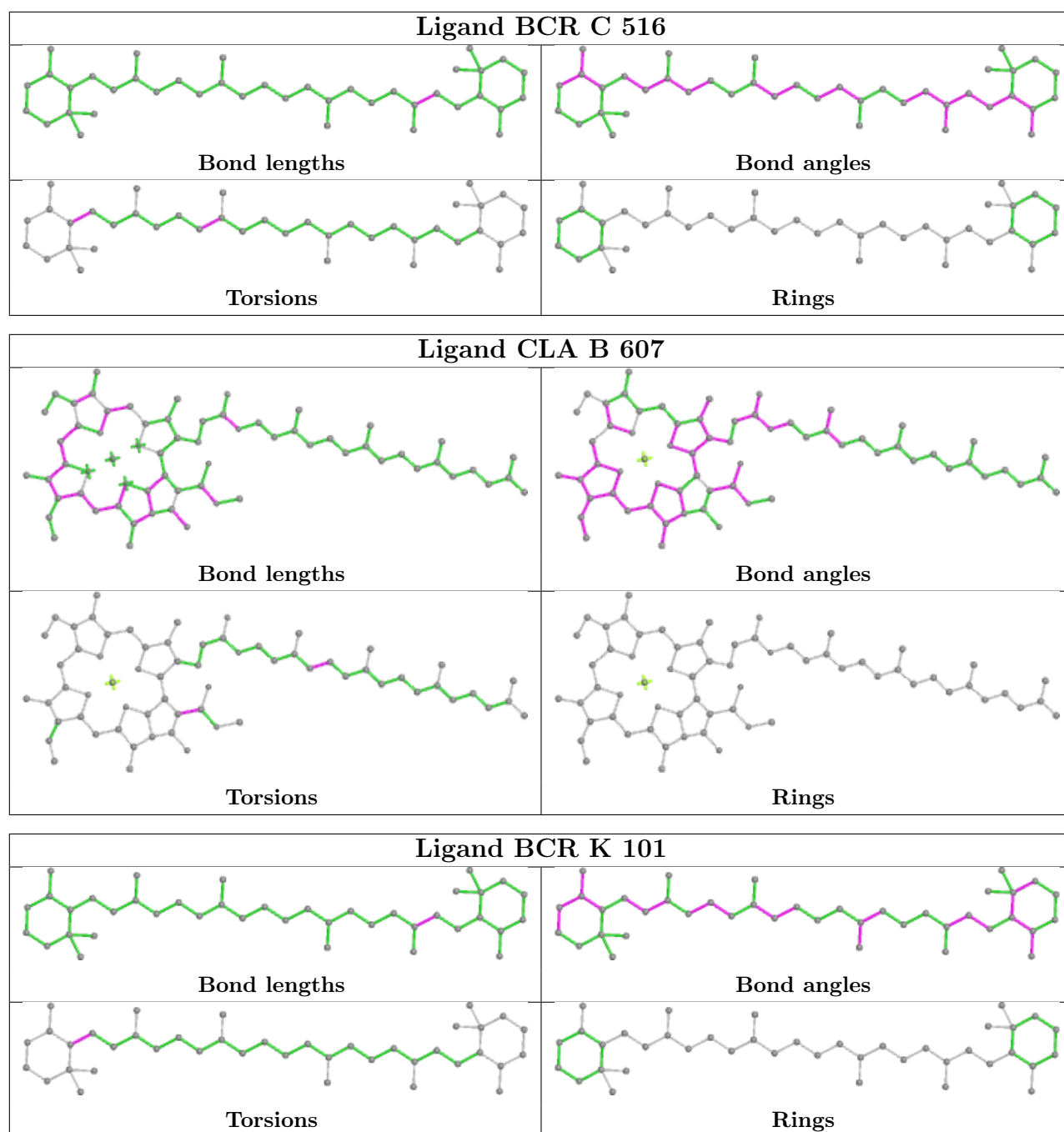


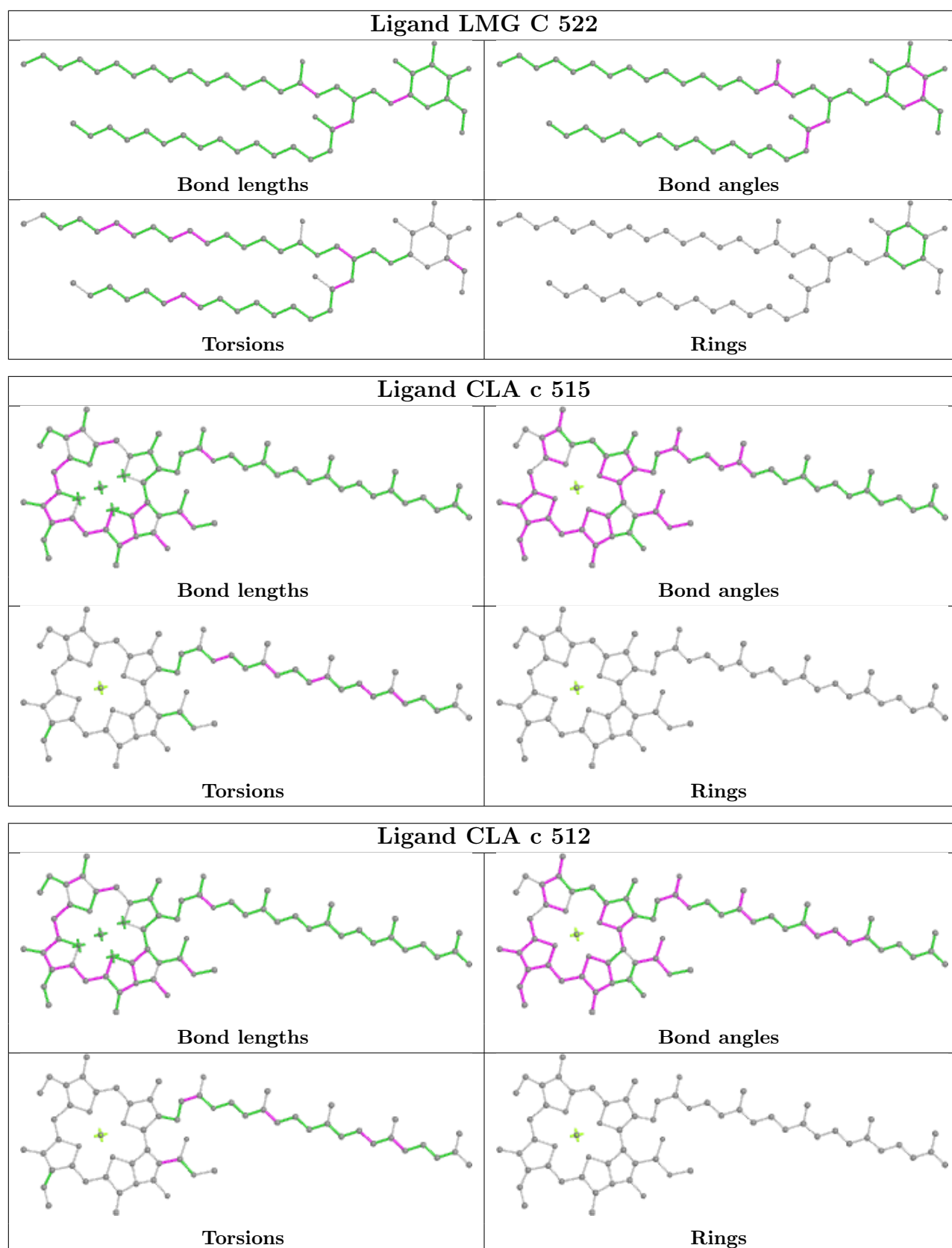


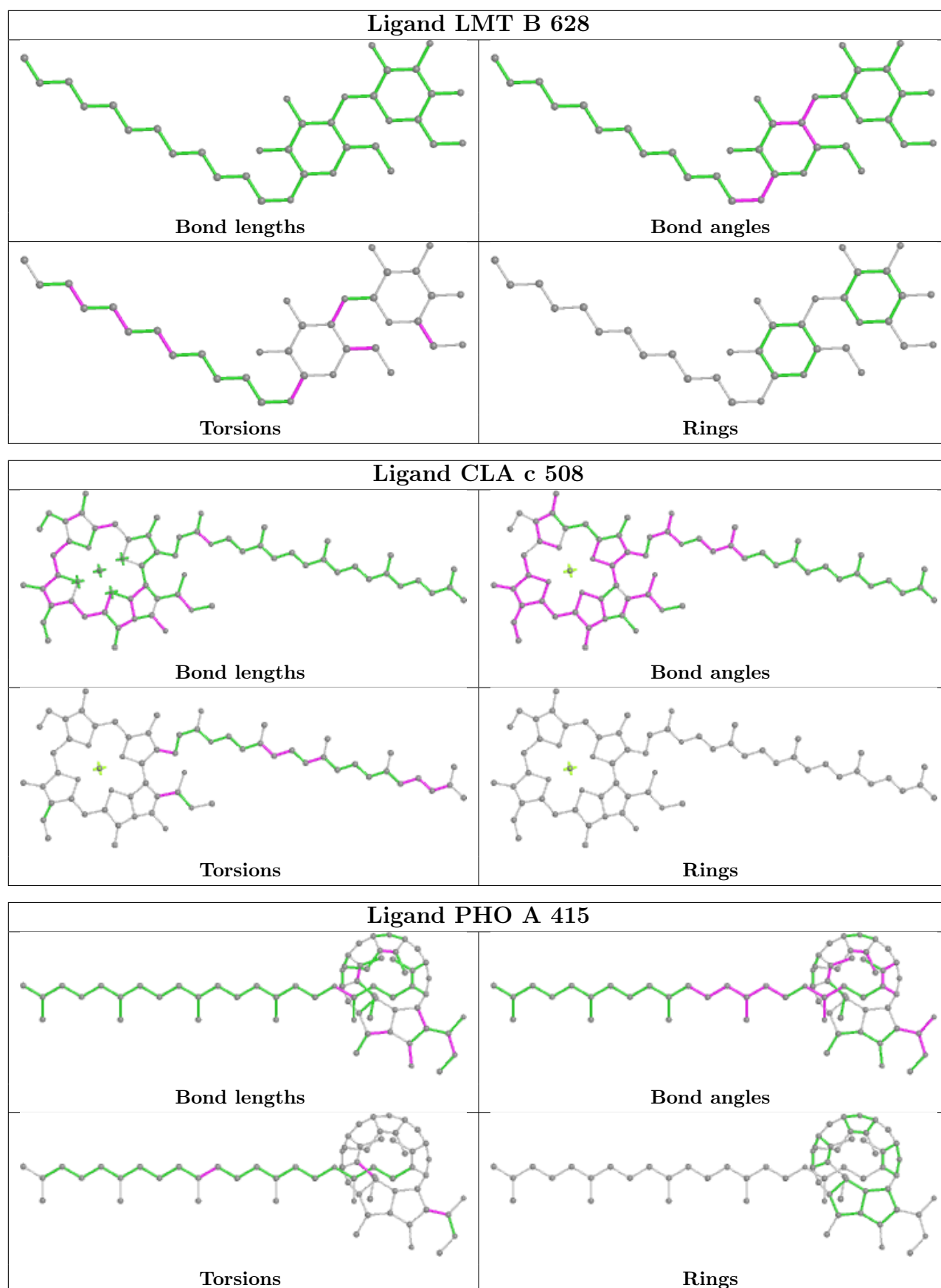


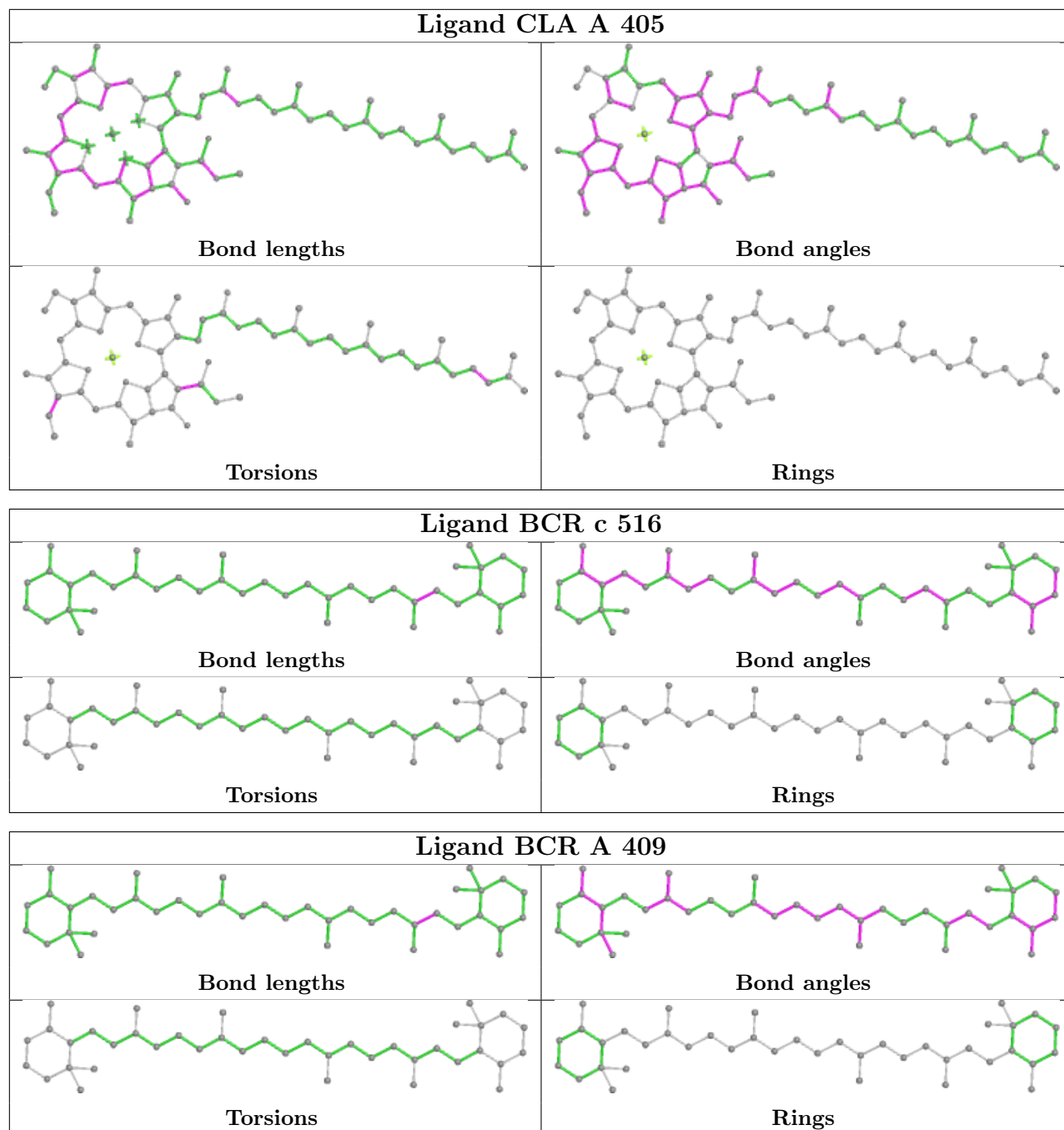


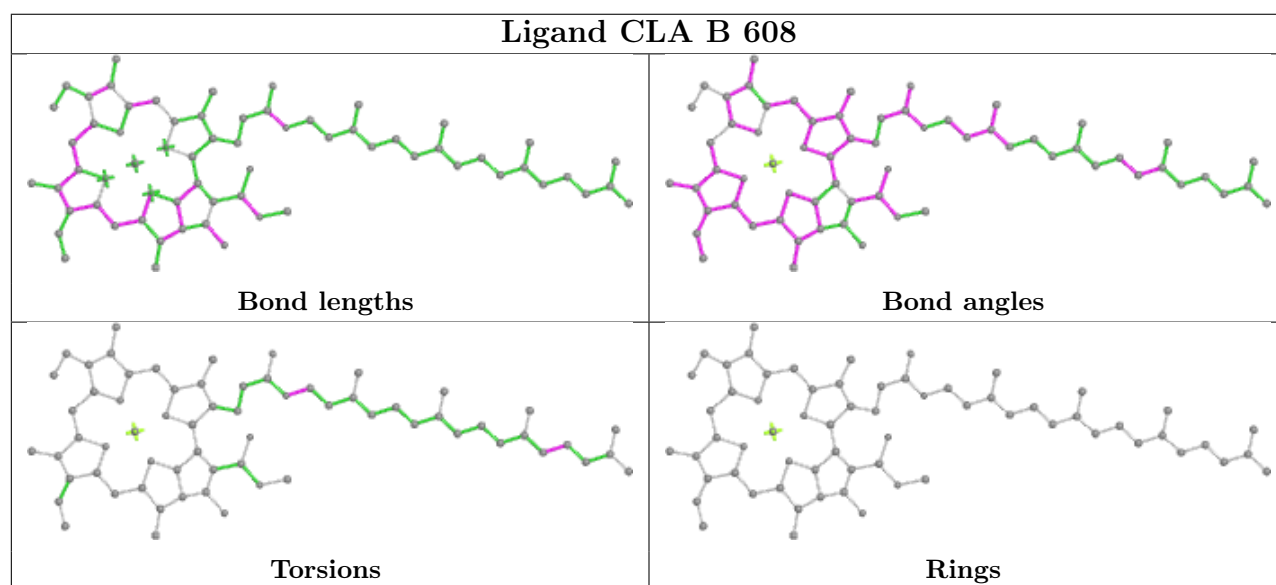
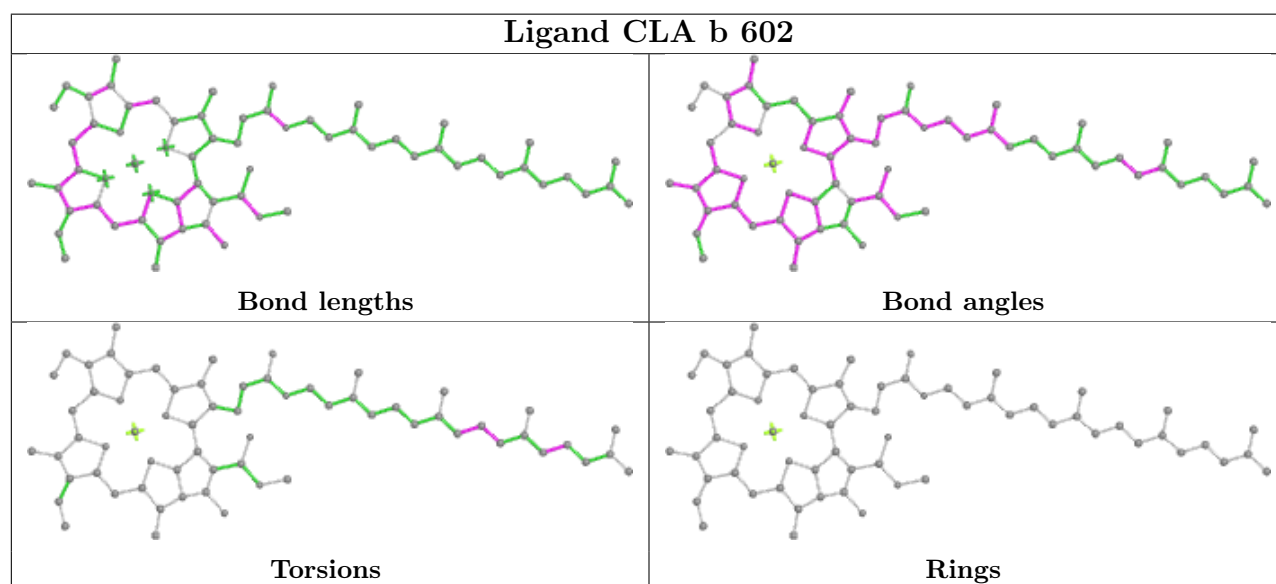
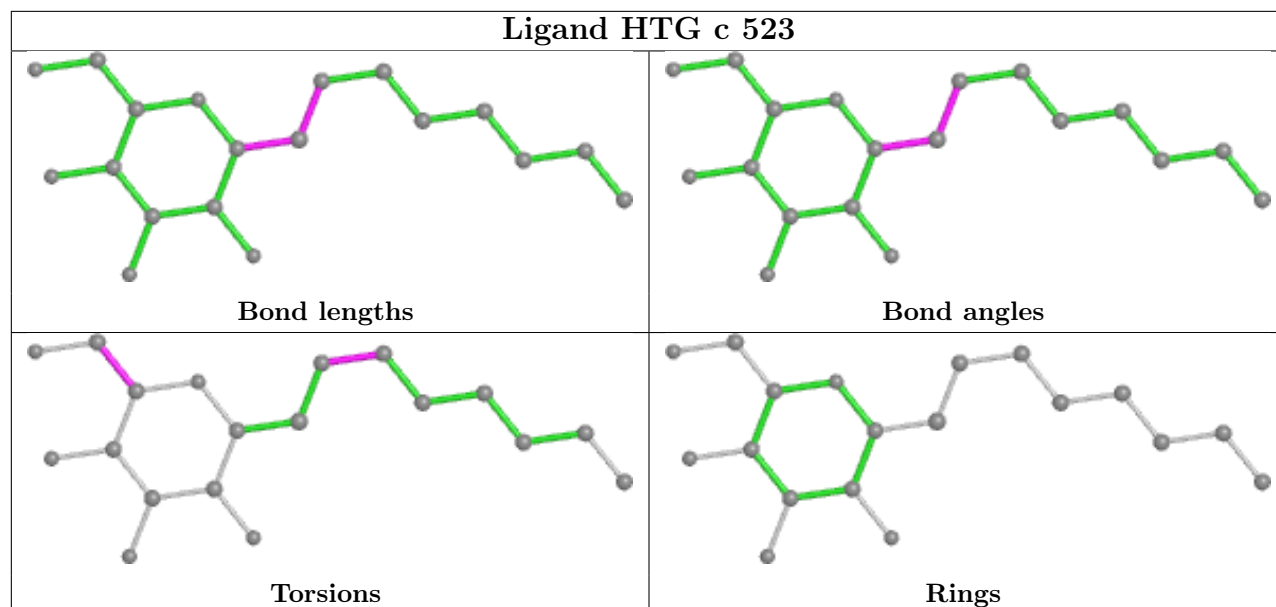


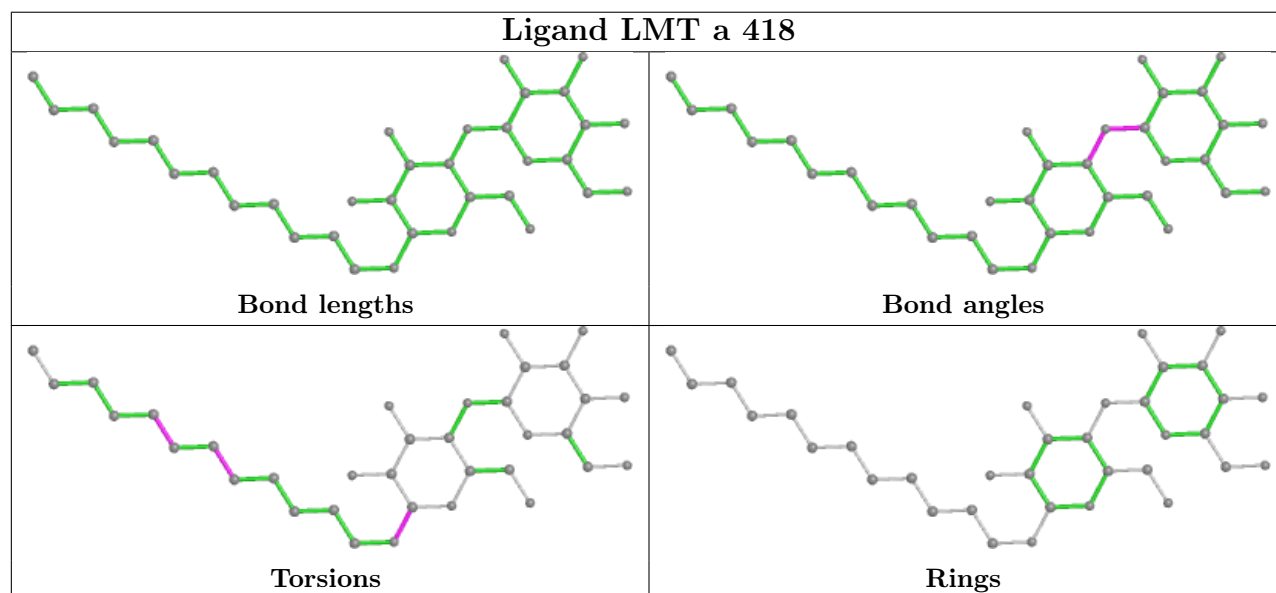
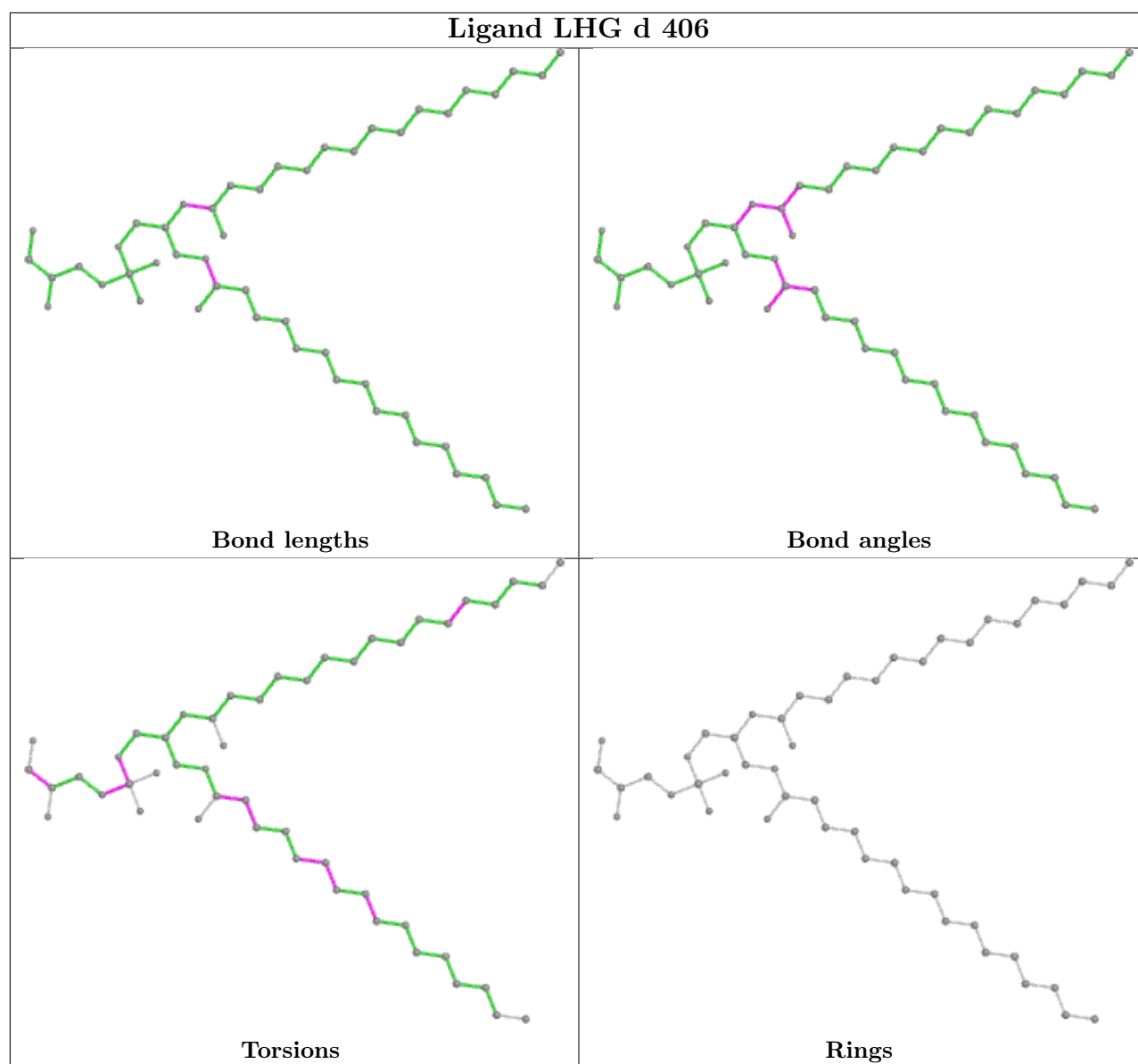


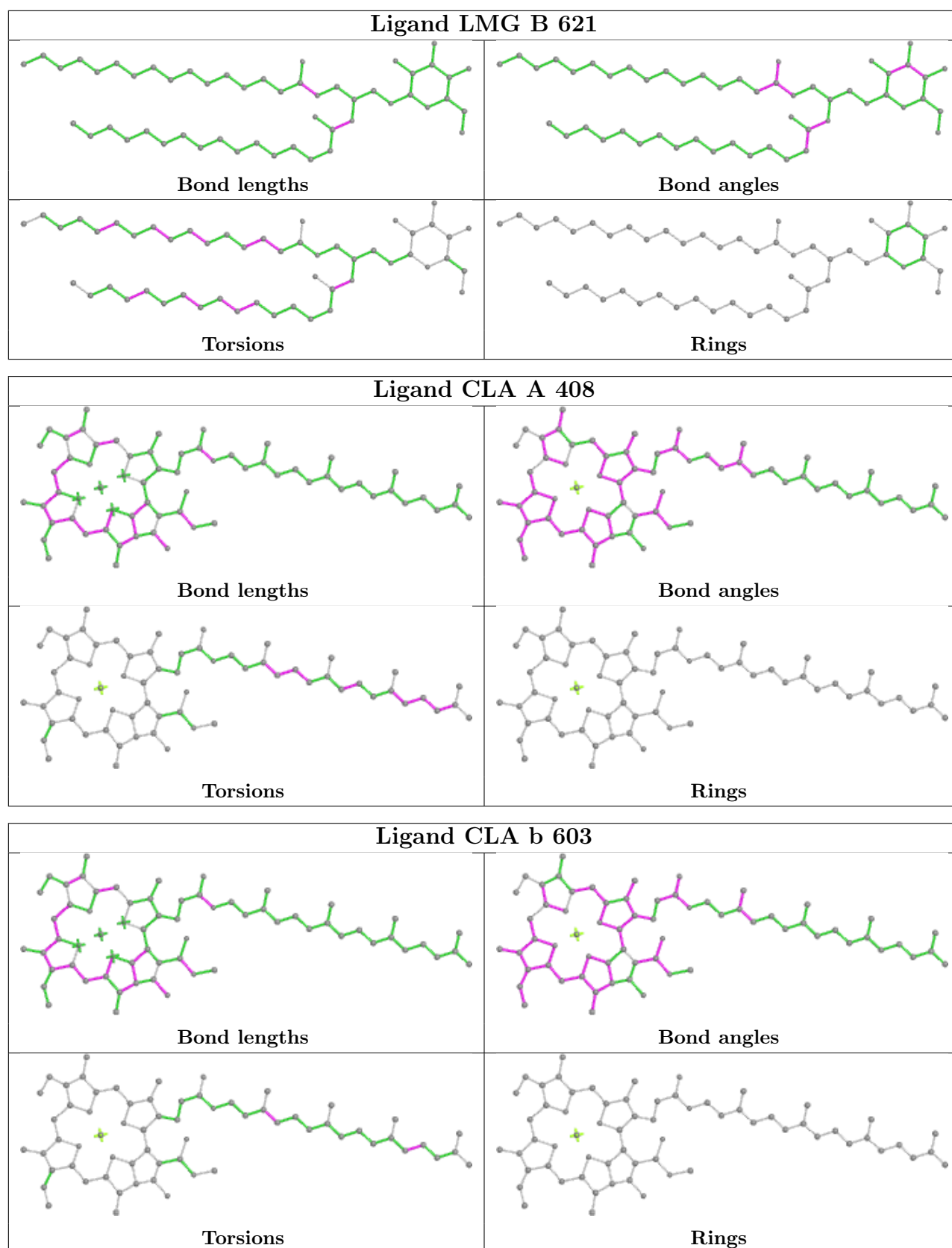


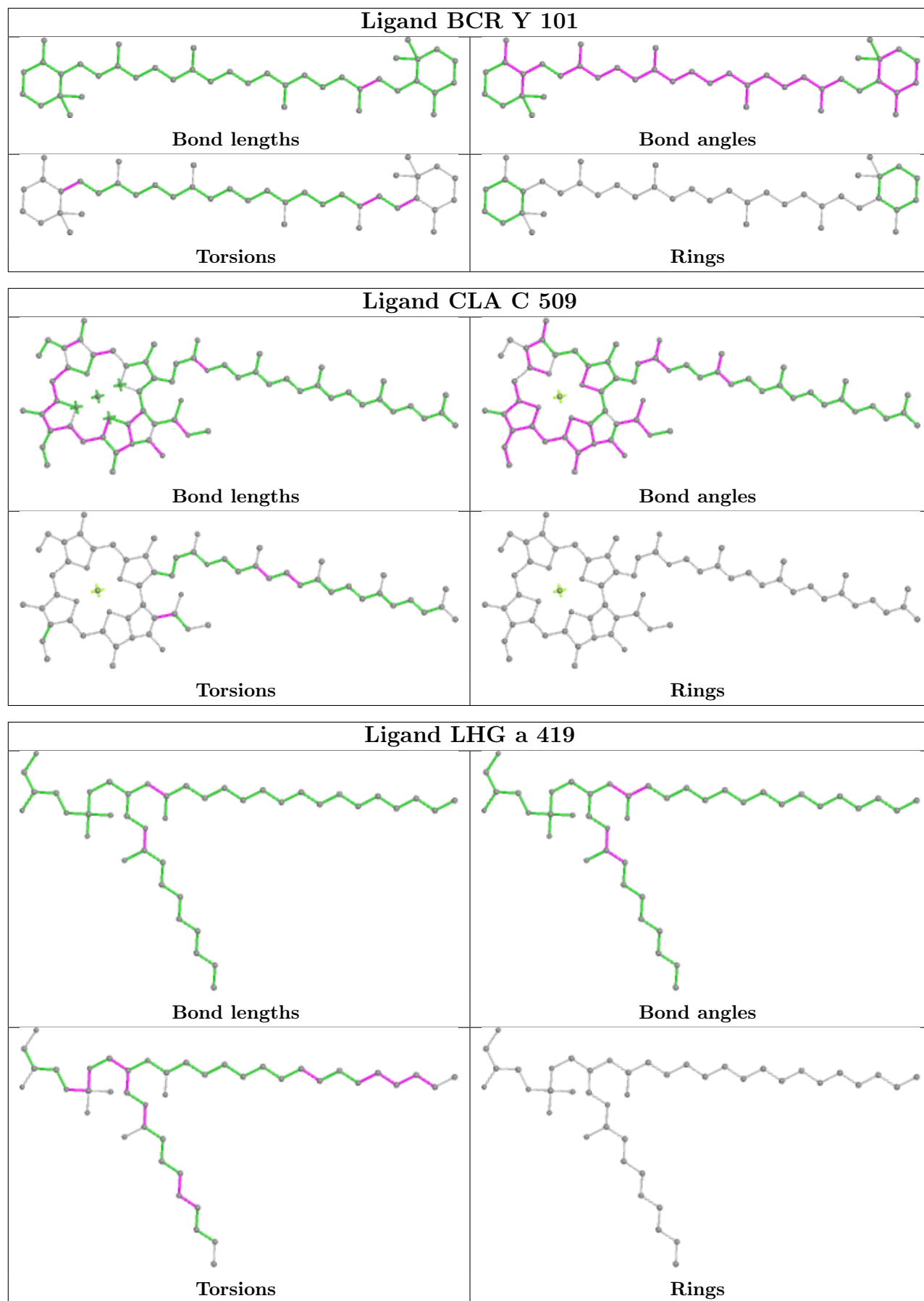


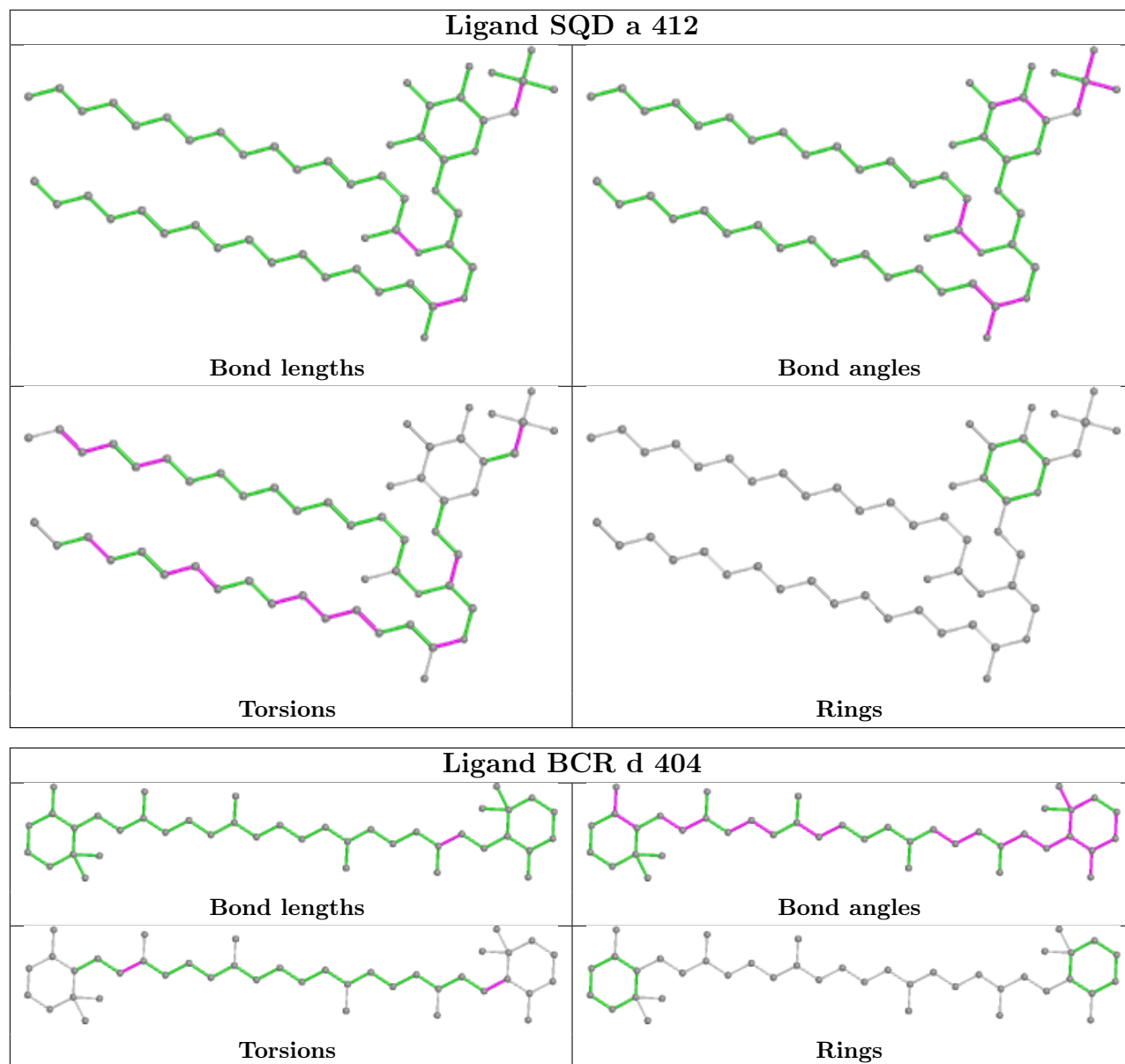


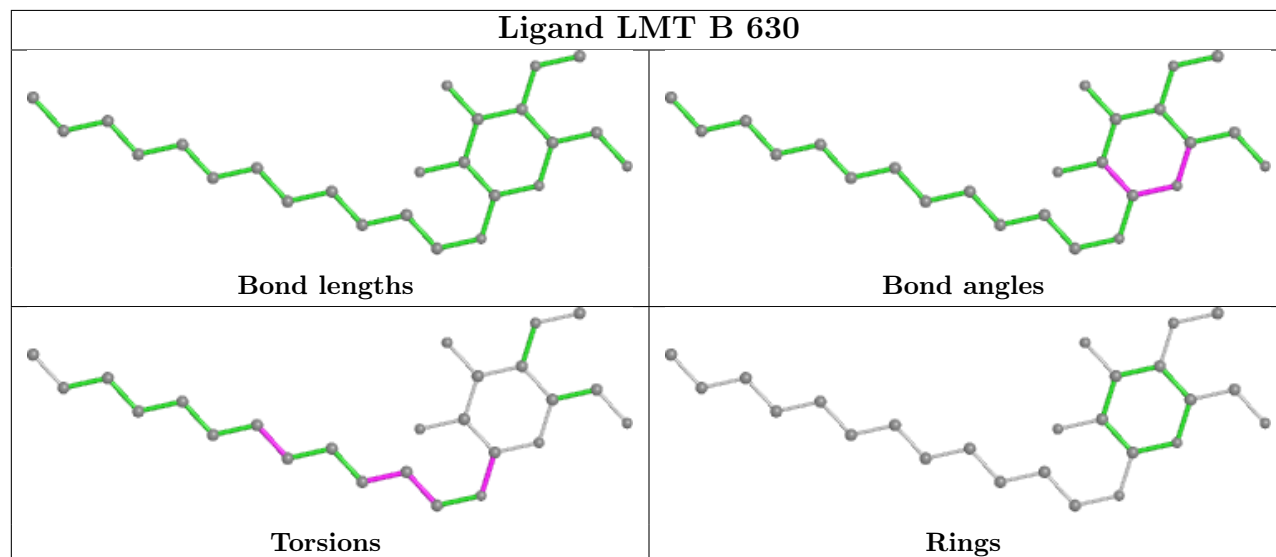
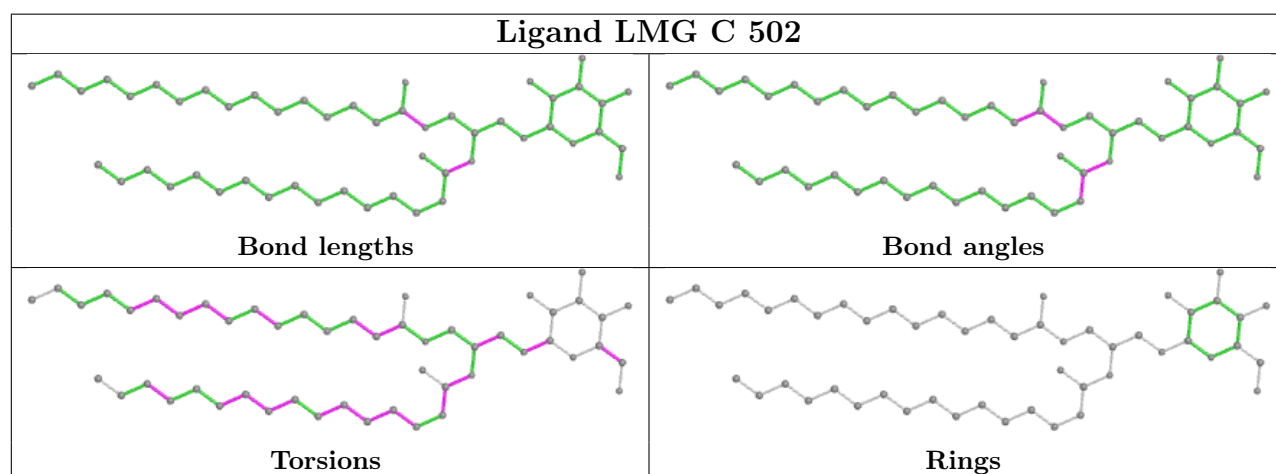
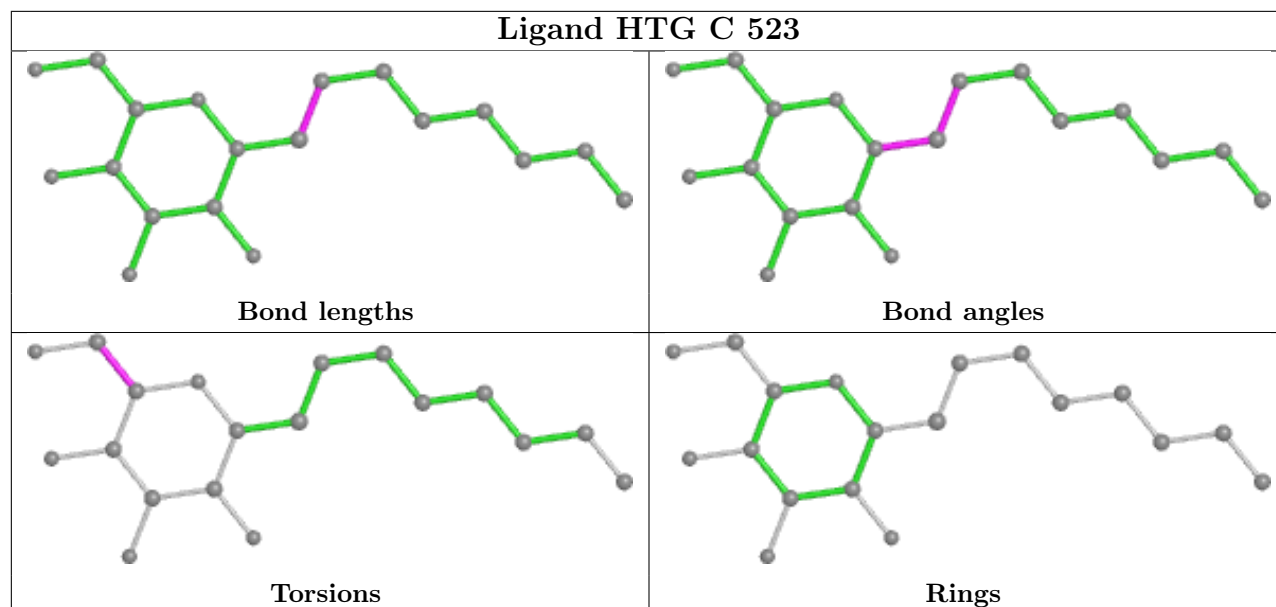


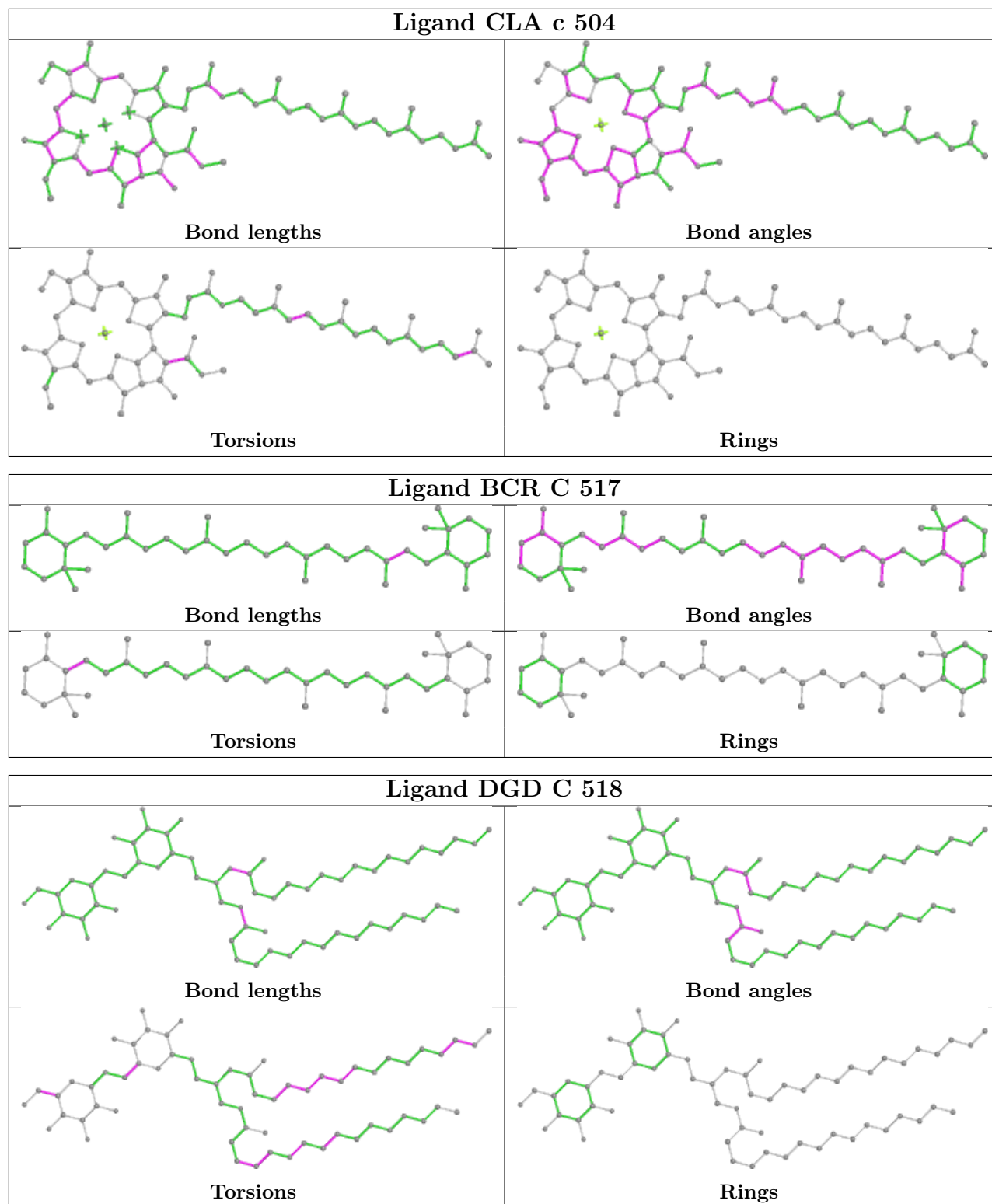


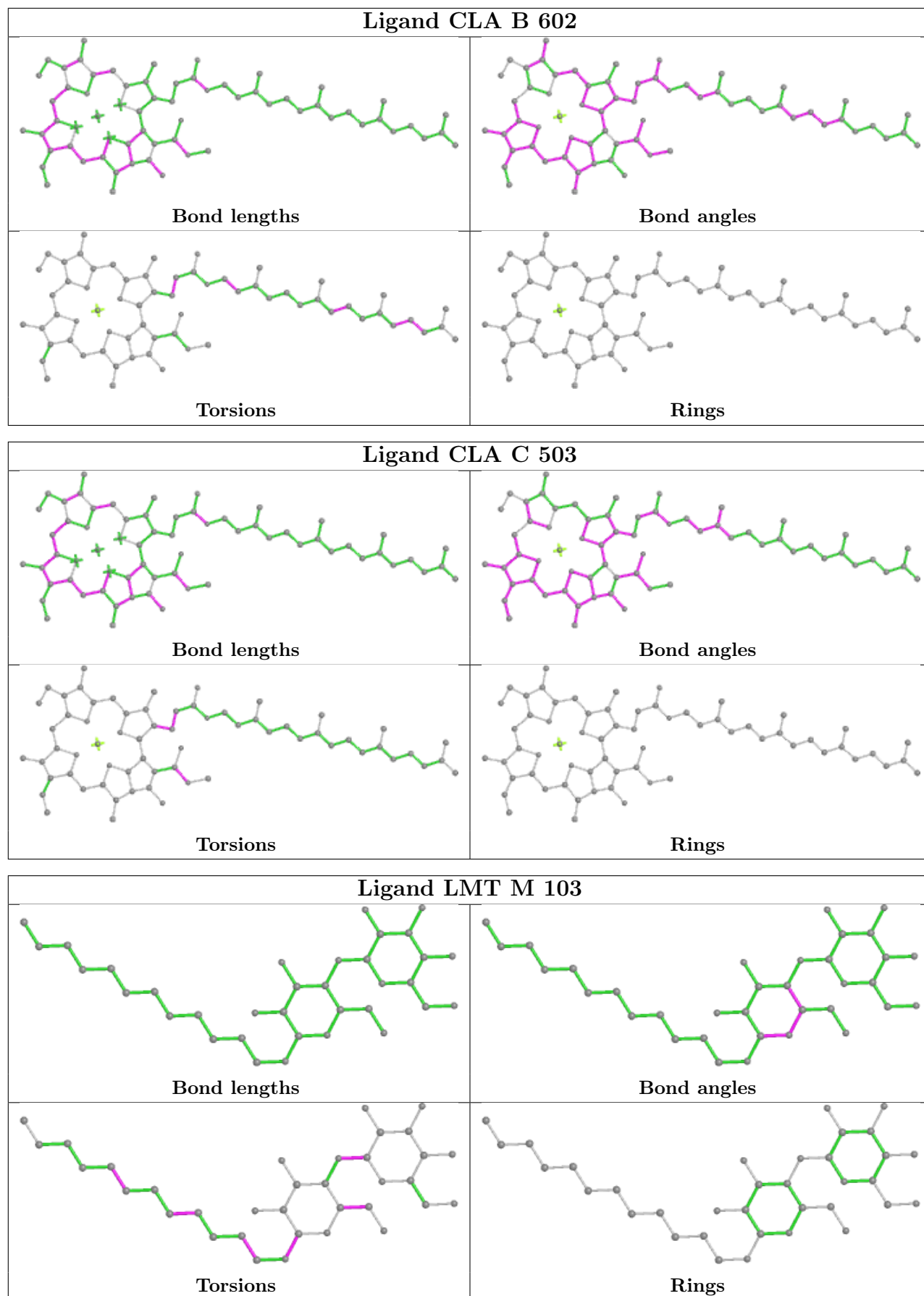


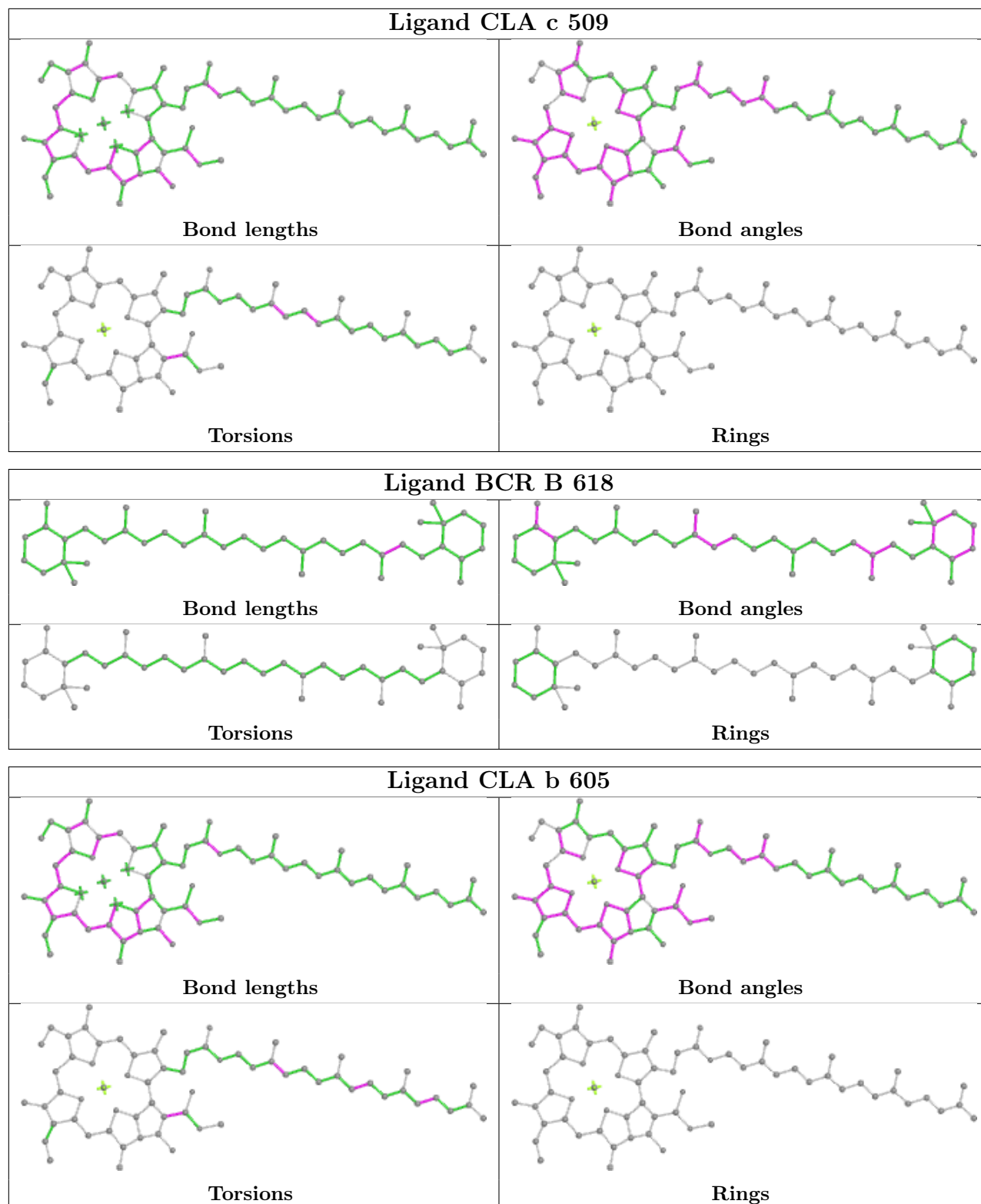


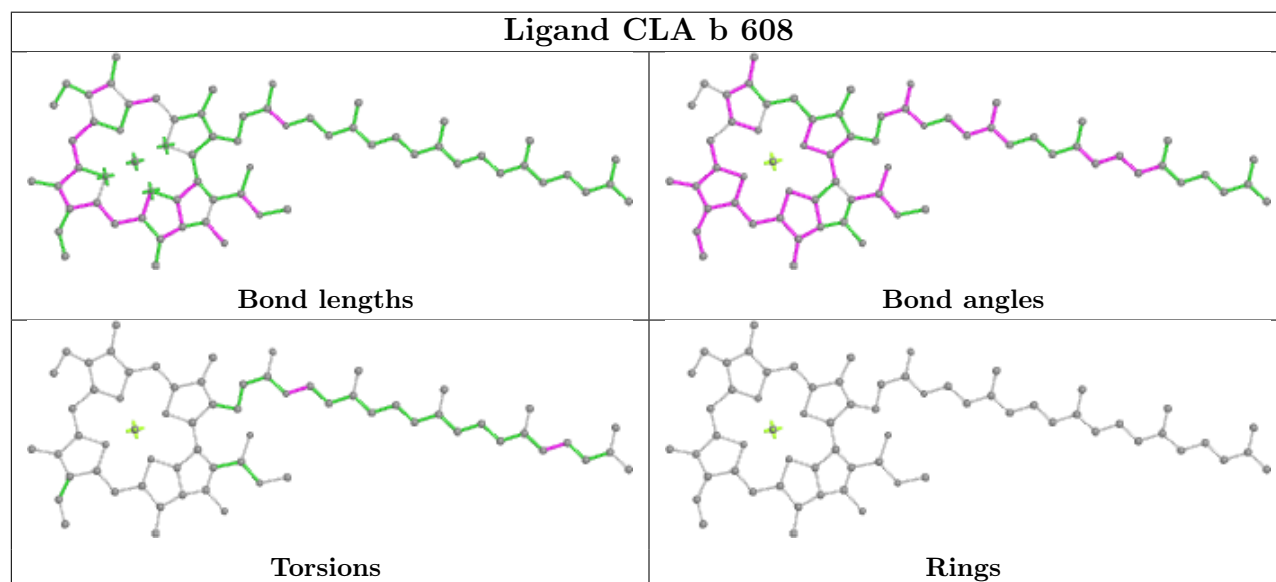
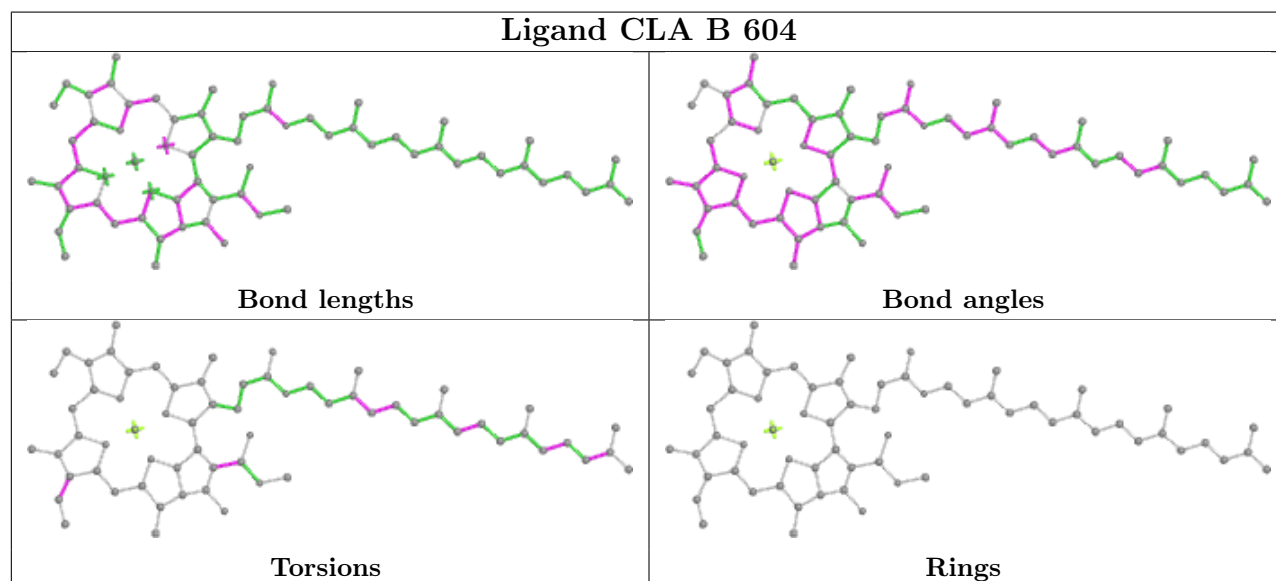
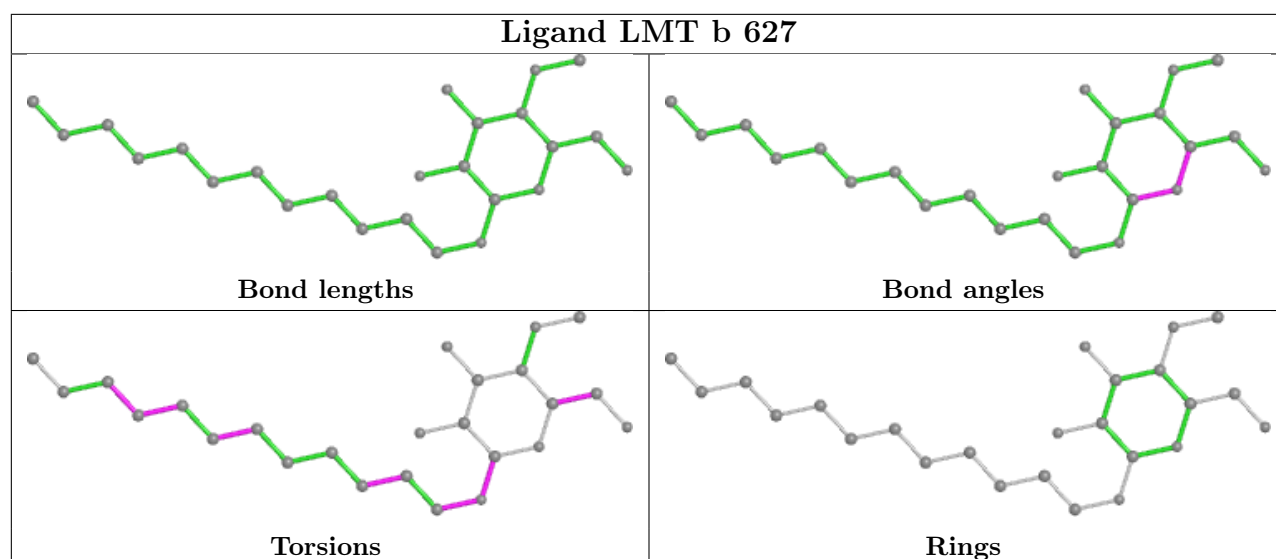


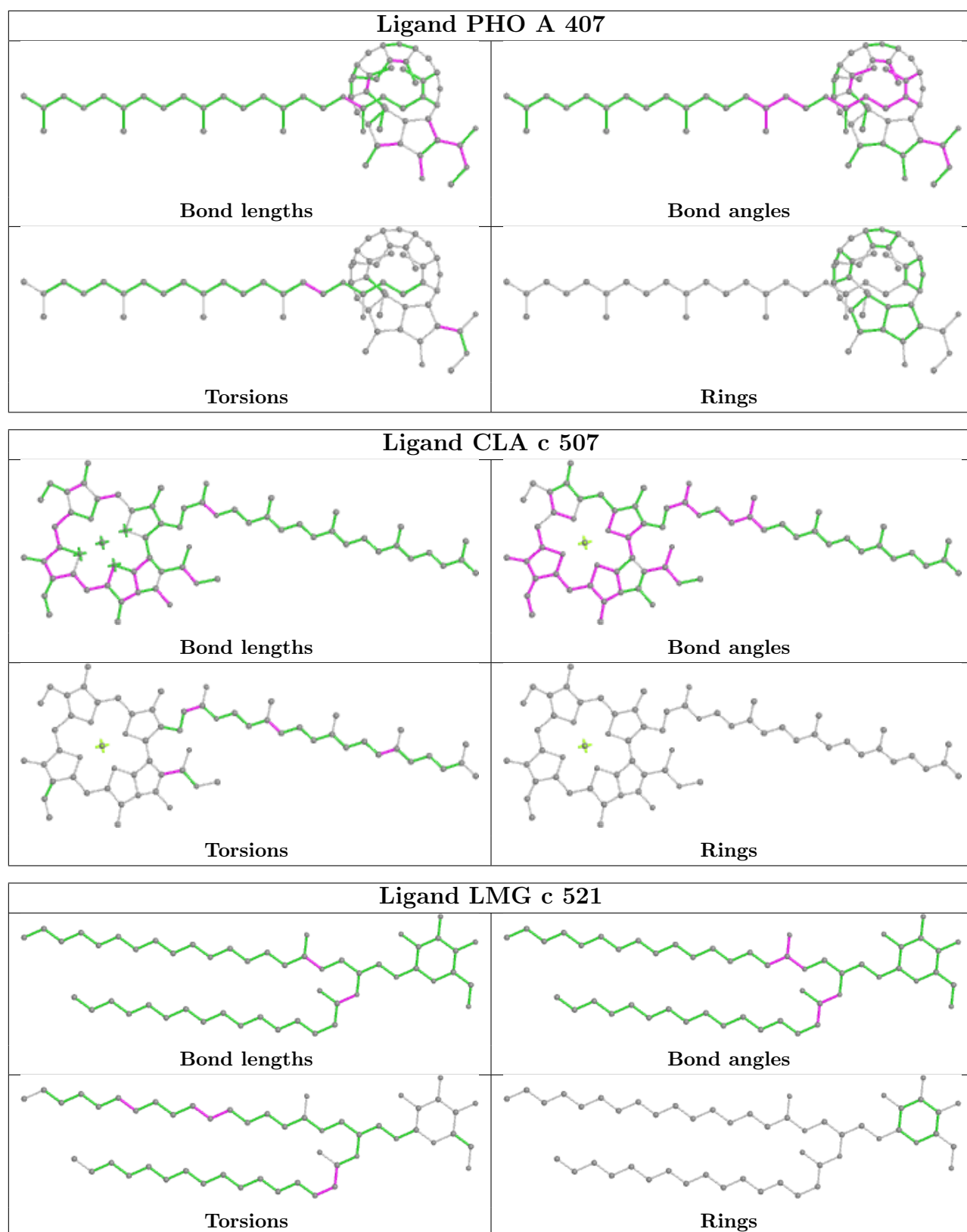


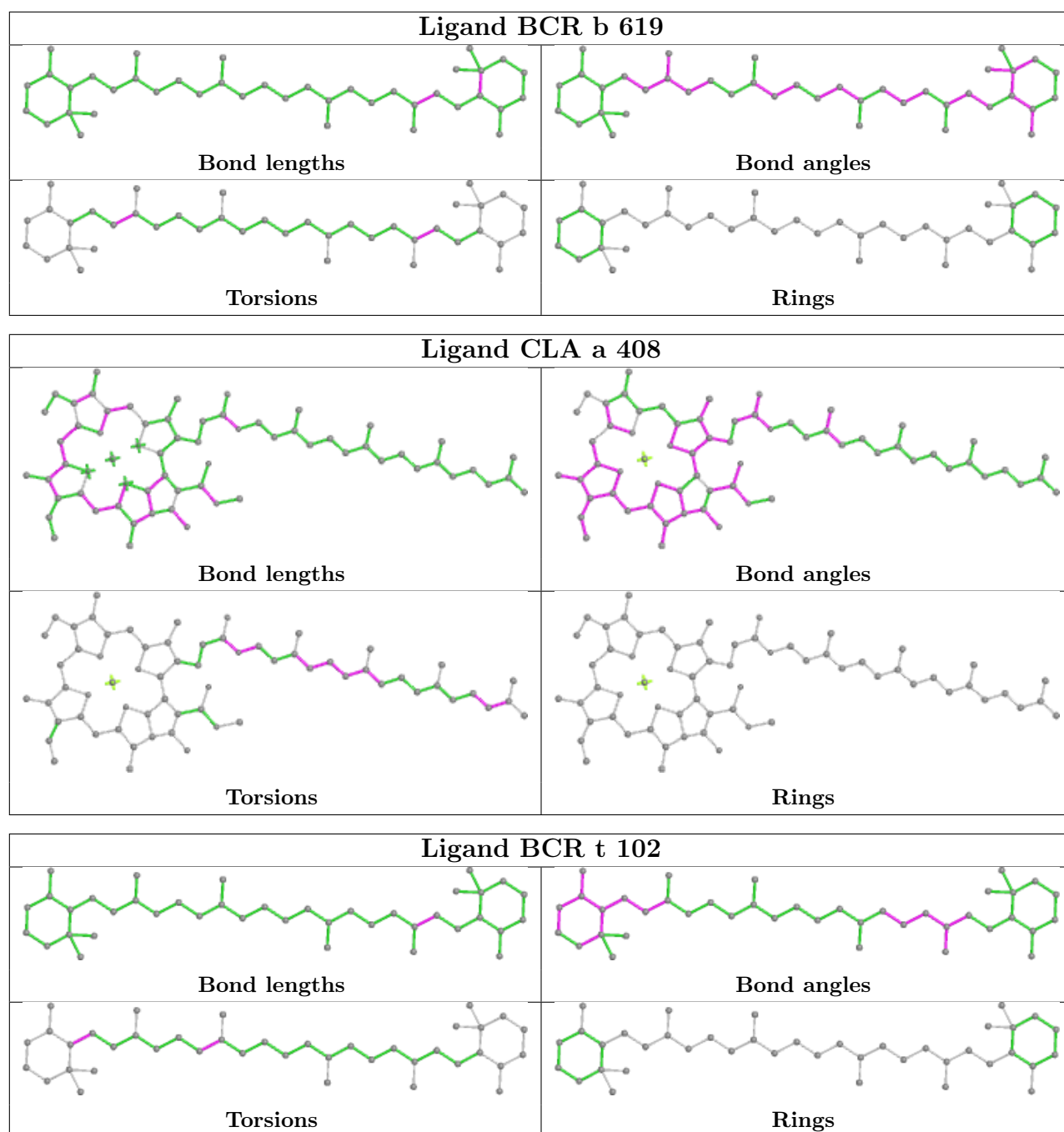


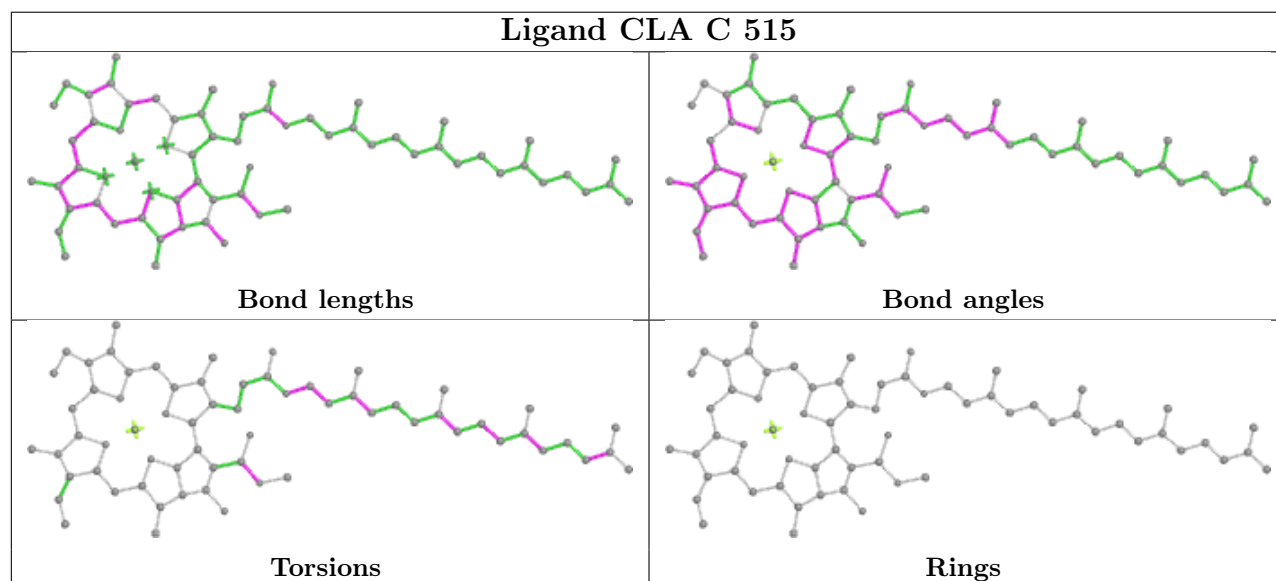
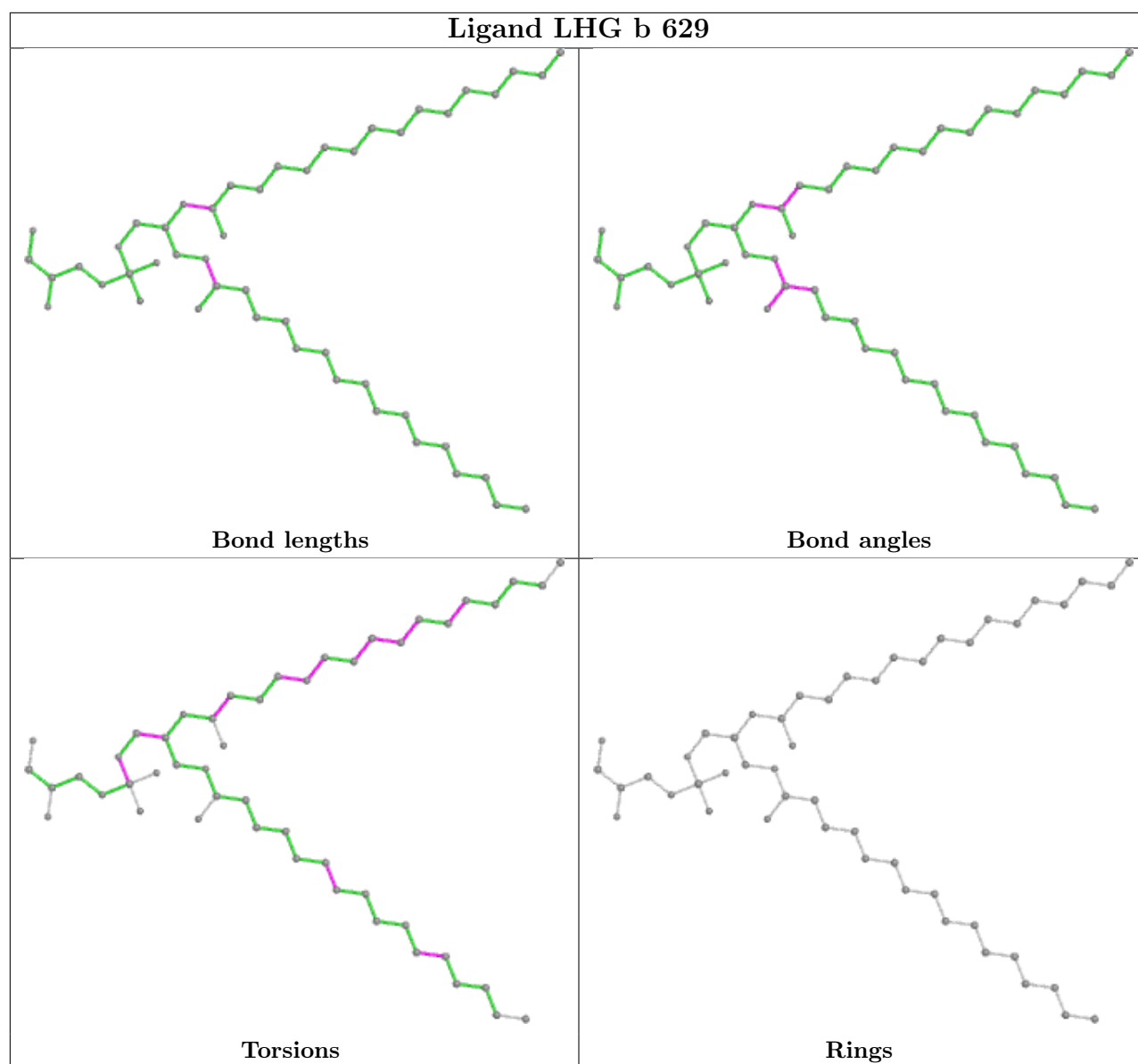


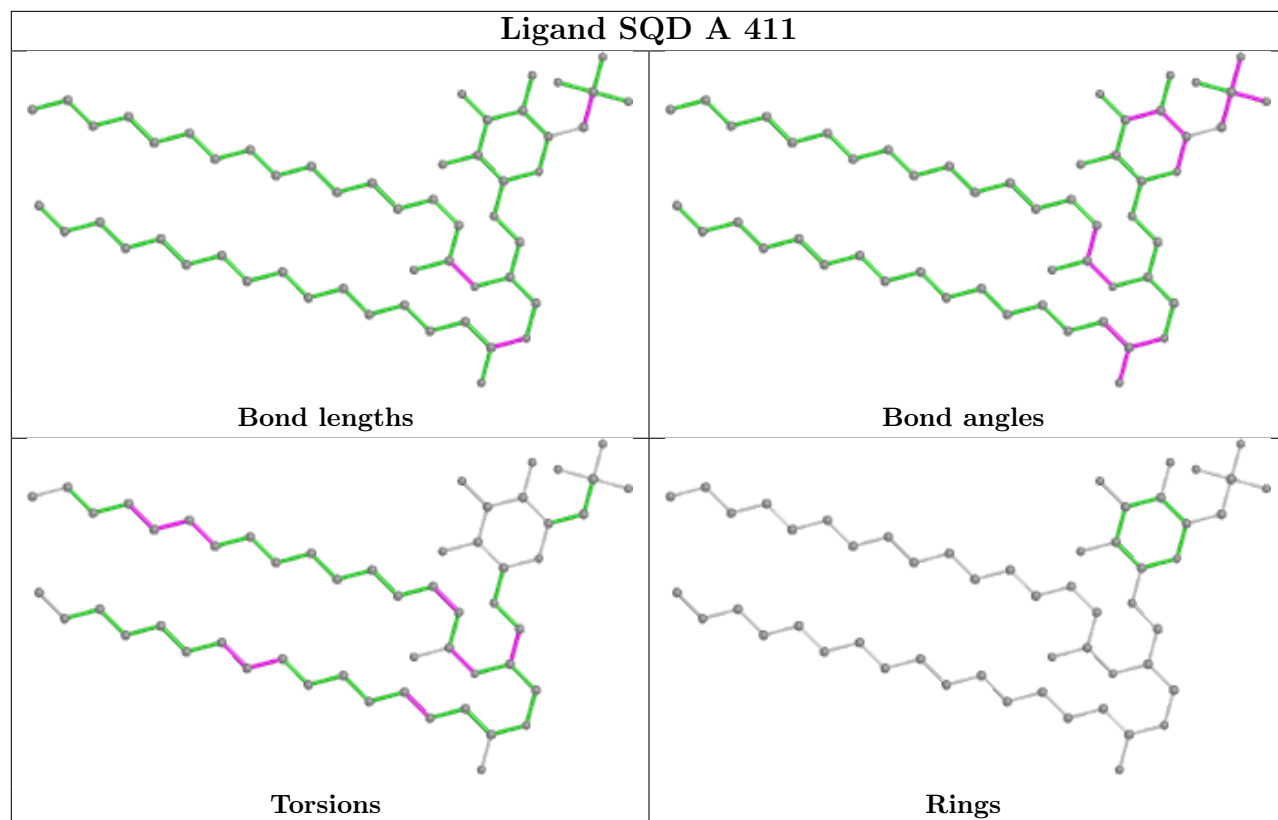


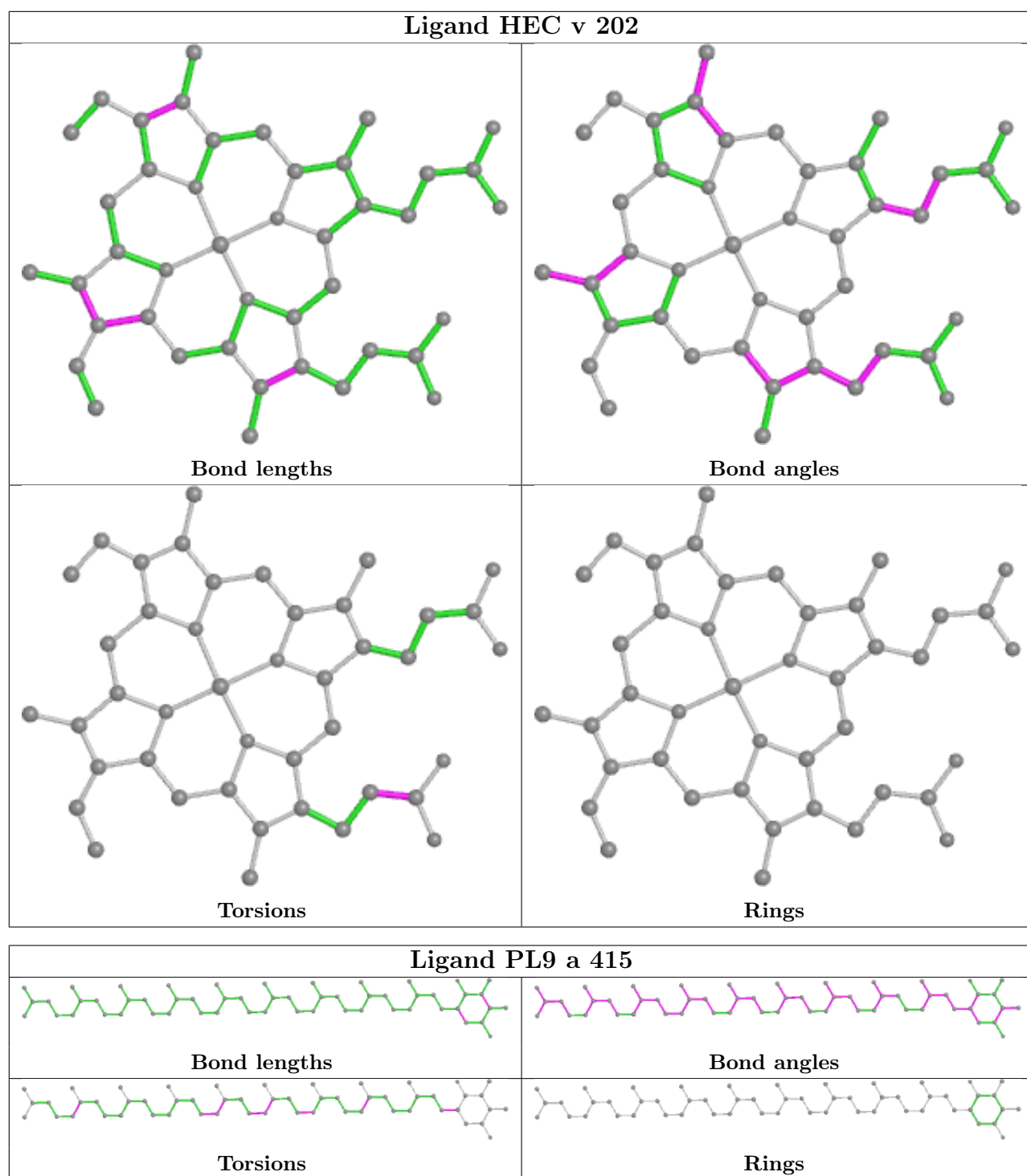


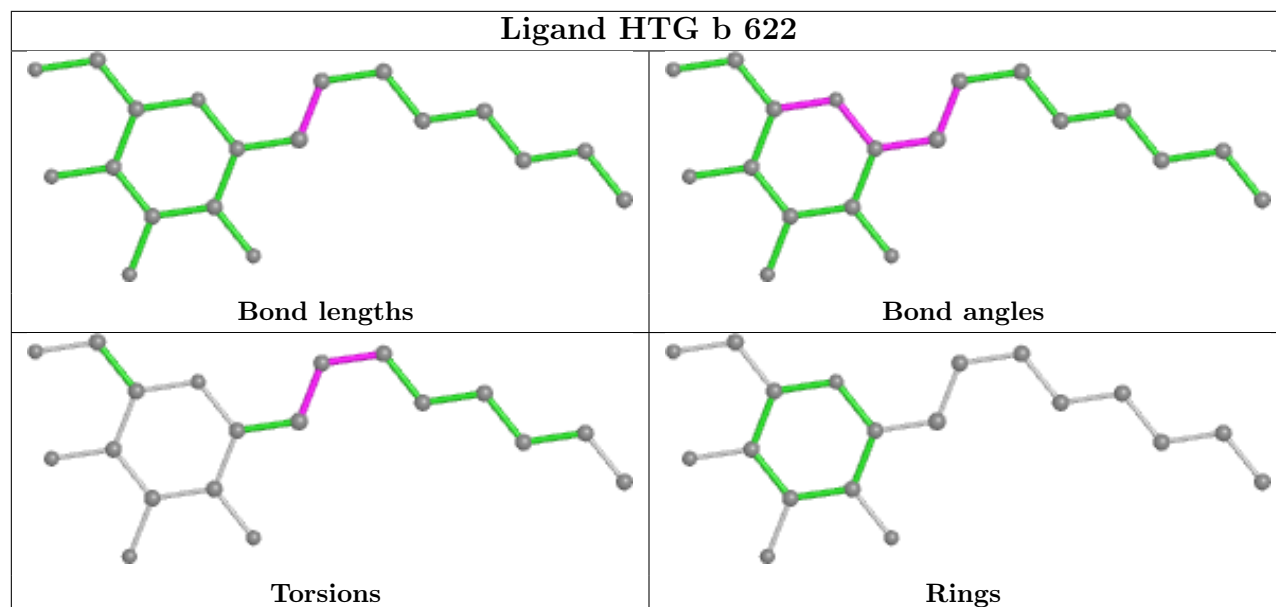












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	0.09	14 (4%) 36 38	33, 41, 67, 126	0
1	a	334/344 (97%)	0.17	22 (6%) 18 20	33, 46, 80, 122	0
2	B	504/505 (99%)	-0.18	25 (4%) 28 31	34, 47, 79, 129	0
2	b	504/505 (99%)	0.08	49 (9%) 7 8	35, 51, 92, 164	0
3	C	451/455 (99%)	-0.09	21 (4%) 31 34	38, 54, 77, 144	0
3	c	455/455 (100%)	0.16	36 (7%) 12 14	43, 62, 84, 127	0
4	D	342/342 (100%)	-0.00	10 (2%) 51 55	33, 43, 65, 134	0
4	d	341/342 (99%)	0.02	18 (5%) 26 29	35, 49, 74, 136	0
5	E	81/84 (96%)	0.31	8 (9%) 7 7	48, 66, 95, 140	0
5	e	79/84 (94%)	0.40	8 (10%) 7 7	57, 74, 117, 150	0
6	F	34/44 (77%)	-0.20	2 (5%) 22 24	48, 58, 92, 113	0
6	f	31/44 (70%)	-0.15	3 (9%) 7 8	57, 66, 93, 154	0
7	H	64/65 (98%)	-0.45	0 100 100	43, 58, 77, 105	0
7	h	64/65 (98%)	0.16	4 (6%) 20 22	51, 63, 85, 108	0
8	I	37/38 (97%)	-0.11	2 (5%) 25 28	47, 58, 120, 144	0
8	i	37/38 (97%)	-0.29	1 (2%) 54 57	49, 59, 117, 145	0
9	J	38/39 (97%)	0.27	7 (18%) 1 1	47, 66, 127, 181	0
9	j	39/39 (100%)	0.32	5 (12%) 3 3	55, 74, 135, 179	0
10	K	37/37 (100%)	-0.61	0 100 100	53, 65, 88, 102	0
10	k	37/37 (100%)	0.21	3 (8%) 12 13	66, 72, 94, 109	0
11	L	36/37 (97%)	-0.10	1 (2%) 53 55	34, 39, 95, 137	0
11	l	36/37 (97%)	0.12	1 (2%) 53 55	36, 40, 96, 132	0
12	M	32/36 (88%)	-0.12	1 (3%) 49 52	37, 42, 66, 135	0
12	m	33/36 (91%)	-0.09	2 (6%) 21 23	36, 43, 78, 125	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	0.12	24 (9%) 7 7	34, 57, 110, 186	0
13	o	243/244 (99%)	0.49	41 (16%) 1 1	38, 59, 124, 166	0
14	T	29/32 (90%)	-0.21	0 100 100	36, 40, 78, 109	0
14	t	29/32 (90%)	-0.03	2 (6%) 16 18	36, 43, 70, 137	0
15	U	96/104 (92%)	-0.30	3 (3%) 49 52	41, 53, 85, 90	0
15	u	97/104 (93%)	-0.53	0 100 100	46, 58, 80, 132	0
16	V	137/137 (100%)	-0.41	0 100 100	40, 53, 79, 115	0
16	v	137/137 (100%)	0.01	6 (4%) 34 37	47, 68, 96, 138	0
17	X	38/40 (95%)	-0.04	2 (5%) 26 29	56, 68, 93, 110	0
17	x	38/40 (95%)	0.64	8 (21%) 1 1	60, 74, 114, 163	0
18	Y	29/30 (96%)	1.62	10 (34%) 0 0	66, 82, 139, 159	0
18	y	29/30 (96%)	0.63	5 (17%) 1 1	77, 89, 119, 120	0
19	Z	62/62 (100%)	0.66	6 (9%) 7 8	66, 80, 132, 180	0
19	z	62/62 (100%)	1.92	27 (43%) 0 0	77, 94, 135, 178	0
20	R	34/34 (100%)	6.90	34 (100%) 0 0	102, 124, 154, 164	0
All	All	5283/5384 (98%)	0.11	411 (7%) 13 14	33, 54, 98, 186	0

The worst 5 of 411 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	R	6	LEU	11.3
20	R	14	LEU	10.7
20	R	18	TRP	10.5
20	R	5	VAL	9.6
20	R	35	LEU	9.5

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	T	1	10/11	0.96	0.08	40,46,63,64	0
8	FME	I	1	10/11	0.97	0.11	44,65,72,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	FME	M	1	10/11	0.98	0.10	37,50,80,87	0
8	FME	i	1	10/11	0.98	0.10	49,58,67,73	0
12	FME	m	1	10/11	0.98	0.07	41,53,62,76	0
14	FME	t	1	10/11	0.98	0.08	36,43,68,73	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
32	LMG	C	522	51/55	0.51	0.41	69,127,161,165	0
34	LMT	a	413	35/35	0.51	0.39	66,131,140,142	0
34	LMT	E	102	35/35	0.52	0.48	102,145,164,166	0
30	UNL	j	101	10/-	0.52	0.38	78,87,93,94	0
33	HTG	b	623	19/19	0.54	0.52	83,144,150,150	0
30	UNL	A	414	28/-	0.56	0.45	83,97,113,115	0
34	LMT	e	101	35/35	0.59	0.64	122,163,170,171	0
34	LMT	M	103	35/35	0.62	0.30	78,152,175,176	0
34	LMT	m	103	35/35	0.62	0.35	52,93,109,110	0
34	LMT	C	526	35/35	0.63	0.55	88,140,155,158	0
30	UNL	a	416	30/-	0.65	0.35	96,111,134,138	0
33	HTG	D	411	16/19	0.65	0.30	91,113,123,129	0
29	PL9	A	413	55/55	0.65	0.36	72,102,112,115	0
30	UNL	i	101	40/-	0.66	0.27	69,98,148,152	0
32	LMG	c	522	51/55	0.66	0.41	72,129,152,157	0
34	LMT	D	402	35/35	0.69	0.31	69,124,137,143	0
34	LMT	M	101	35/35	0.69	0.28	53,98,131,139	0
30	UNL	b	626	33/-	0.70	0.40	63,90,146,148	0
30	UNL	J	101	10/-	0.71	0.23	75,79,91,92	0
30	UNL	I	101	40/-	0.72	0.25	68,107,149,150	0
30	UNL	C	527	34/-	0.72	0.30	83,110,123,126	0
31	LHG	a	419	42/49	0.72	0.31	100,147,177,181	0
36	CA	F	101	1/1	0.72	0.06	115,115,115,115	0
32	LMG	Z	101	37/55	0.73	0.27	72,123,156,161	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	LMT	b	621	25/35	0.75	0.23	89,129,154,154	0
26	GOL	b	624	6/6	0.75	0.23	86,95,99,105	0
30	UNL	M	102	10/-	0.76	0.22	63,73,84,84	0
32	LMG	c	501	51/55	0.76	0.24	60,88,109,117	0
30	UNL	c	526	32/-	0.76	0.37	94,113,130,132	0
30	UNL	B	626	33/-	0.77	0.24	52,108,152,156	0
26	GOL	B	629	6/6	0.77	0.45	103,111,114,116	0
31	LHG	E	101	42/49	0.77	0.23	72,126,138,141	0
29	PL9	a	415	55/55	0.77	0.29	87,111,124,126	0
26	GOL	B	627	6/6	0.77	0.25	63,92,96,97	0
30	UNL	m	102	10/-	0.78	0.24	59,68,91,92	0
34	LMT	a	418	35/35	0.78	0.51	118,150,157,158	0
30	UNL	d	410	36/-	0.79	0.23	70,94,127,130	0
27	SQD	f	101	43/54	0.80	0.42	111,132,160,166	0
33	HTG	b	622	19/19	0.80	0.20	64,71,105,109	0
26	GOL	O	302	6/6	0.80	0.28	78,85,86,87	0
34	LMT	B	630	25/35	0.80	0.21	55,84,135,139	0
33	HTG	B	623	19/19	0.80	0.40	61,86,94,95	0
33	HTG	B	622	19/19	0.81	0.22	61,83,110,111	0
33	HTG	V	202	11/19	0.81	0.44	110,119,121,121	0
34	LMT	B	628	35/35	0.81	0.25	63,110,126,130	0
36	CA	a	420	1/1	0.81	0.29	105,105,105,105	0
27	SQD	B	620	54/54	0.82	0.19	54,88,124,129	0
33	HTG	h	101	16/19	0.82	0.29	103,133,139,143	0
27	SQD	b	620	54/54	0.83	0.19	59,88,112,115	0
30	UNL	d	411	18/-	0.83	0.25	74,78,109,112	0
32	LMG	z	101	39/55	0.83	0.32	80,128,136,139	0
30	UNL	D	410	40/-	0.83	0.23	56,85,125,129	0
30	UNL	X	101	18/-	0.84	0.18	60,68,98,99	0
34	LMT	t	101	26/35	0.84	0.20	77,117,136,140	0
34	LMT	b	627	25/35	0.85	0.22	50,75,135,136	0
26	GOL	o	302	6/6	0.85	0.49	110,113,118,120	0
25	BCR	h	102	40/40	0.85	0.17	50,61,74,75	0
27	SQD	A	411	54/54	0.86	0.16	60,82,123,130	0
26	GOL	A	410	6/6	0.86	0.19	68,68,74,81	0
33	HTG	c	523	19/19	0.86	0.27	119,138,143,144	0
32	LMG	B	621	51/55	0.86	0.18	49,65,92,114	0
25	BCR	H	101	40/40	0.87	0.17	44,61,71,74	0
32	LMG	C	521	51/55	0.87	0.20	52,87,119,120	0
32	LMG	c	521	51/55	0.87	0.26	68,92,125,127	0
26	GOL	v	201	6/6	0.87	0.24	51,70,78,80	0
32	LMG	m	101	51/55	0.87	0.20	51,68,96,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	DGD	h	103	62/66	0.88	0.22	50,59,68,71	0
26	GOL	a	411	6/6	0.88	0.20	57,68,80,81	0
33	HTG	C	523	19/19	0.88	0.31	106,118,127,127	0
32	LMG	C	502	51/55	0.89	0.18	57,84,104,106	0
31	LHG	A	416	49/49	0.89	0.22	41,57,80,87	0
35	DGD	H	102	62/66	0.89	0.20	40,55,67,69	0
27	SQD	a	412	54/54	0.89	0.16	59,85,125,127	0
29	PL9	d	405	55/55	0.89	0.19	35,46,56,61	0
25	BCR	k	101	40/40	0.89	0.17	58,70,81,81	0
23	CLA	C	515	65/65	0.90	0.16	59,70,111,114	0
25	BCR	y	101	40/40	0.90	0.12	57,70,83,86	0
26	GOL	b	628	6/6	0.90	0.25	94,100,102,103	0
23	CLA	c	504	65/65	0.91	0.28	48,56,73,83	0
26	GOL	c	502	6/6	0.91	0.23	61,75,77,81	0
35	DGD	C	519	62/66	0.91	0.17	42,62,116,121	0
30	UNL	d	409	17/-	0.91	0.21	67,82,97,97	0
23	CLA	c	505	65/65	0.91	0.22	53,63,73,77	0
30	UNL	D	409	17/-	0.91	0.29	56,77,114,114	0
23	CLA	B	602	65/65	0.91	0.14	39,48,72,77	0
23	CLA	C	514	65/65	0.92	0.15	55,65,114,119	0
23	CLA	C	508	65/65	0.92	0.13	51,63,123,130	0
35	DGD	c	519	62/66	0.92	0.19	50,70,107,118	0
23	CLA	c	509	65/65	0.92	0.14	53,63,73,83	0
23	CLA	c	514	65/65	0.92	0.18	64,77,112,122	0
23	CLA	b	609	65/65	0.92	0.13	49,57,78,100	0
23	CLA	b	602	65/65	0.93	0.19	43,54,70,80	0
31	LHG	b	629	49/49	0.93	0.17	40,55,71,78	0
33	HTG	B	625	19/19	0.93	0.11	65,75,82,87	0
31	LHG	d	407	49/49	0.93	0.14	41,51,68,78	0
23	CLA	c	515	65/65	0.93	0.27	64,83,117,119	0
23	CLA	d	403	65/65	0.93	0.15	48,58,115,123	0
23	CLA	C	509	65/65	0.93	0.12	50,57,76,80	0
27	SQD	C	501	54/54	0.93	0.17	59,79,105,107	0
32	LMG	D	413	51/55	0.93	0.17	44,64,111,123	0
27	SQD	D	412	43/54	0.93	0.21	74,111,131,138	0
35	DGD	C	520	62/66	0.93	0.16	40,53,95,108	0
27	SQD	a	410	54/54	0.93	0.19	64,83,117,118	0
25	BCR	b	618	40/40	0.93	0.20	37,50,67,72	0
23	CLA	C	506	65/65	0.93	0.16	42,51,85,95	0
23	CLA	B	609	65/65	0.93	0.12	43,51,74,81	0
23	CLA	D	404	65/65	0.93	0.16	44,54,126,133	0
25	BCR	b	617	40/40	0.94	0.15	35,43,56,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	CLA	C	513	65/65	0.94	0.12	49,62,77,78	0
25	BCR	c	516	40/40	0.94	0.17	68,83,90,94	0
25	BCR	d	404	40/40	0.94	0.11	52,63,87,92	0
23	CLA	b	601	65/65	0.94	0.20	58,80,120,129	0
23	CLA	c	506	65/65	0.94	0.24	49,58,103,110	0
23	CLA	B	611	65/65	0.94	0.16	34,39,61,68	0
23	CLA	c	510	65/65	0.94	0.24	47,57,127,132	0
26	GOL	B	624	6/6	0.94	0.14	76,87,95,97	0
32	LMG	d	412	51/55	0.94	0.13	53,67,111,119	0
23	CLA	c	513	65/65	0.94	0.14	55,65,81,85	0
29	PL9	D	406	55/55	0.94	0.16	32,42,54,60	0
23	CLA	b	604	65/65	0.94	0.23	34,43,111,119	0
23	CLA	B	601	65/65	0.94	0.21	52,72,115,121	0
23	CLA	b	610	65/65	0.94	0.15	43,50,62,73	0
25	BCR	C	516	40/40	0.94	0.11	59,74,81,83	0
23	CLA	b	612	65/65	0.94	0.17	38,46,61,70	0
25	BCR	K	101	40/40	0.94	0.13	54,63,69,71	0
35	DGD	c	518	62/66	0.94	0.20	45,58,90,95	0
31	LHG	d	406	49/49	0.94	0.25	50,61,76,81	0
35	DGD	c	520	62/66	0.94	0.15	48,60,98,111	0
25	BCR	Y	101	40/40	0.94	0.11	53,64,73,77	0
33	HTG	b	625	19/19	0.94	0.10	66,72,92,98	0
36	CA	O	301	1/1	0.94	0.18	103,103,103,103	0
31	LHG	d	408	49/49	0.94	0.20	53,65,117,122	0
36	CA	o	301	1/1	0.94	0.10	100,100,100,100	0
23	CLA	b	611	65/65	0.95	0.22	36,44,70,76	0
25	BCR	T	101	40/40	0.95	0.13	37,48,57,61	0
23	CLA	B	610	65/65	0.95	0.15	41,48,59,77	0
23	CLA	b	614	65/65	0.95	0.15	35,44,102,105	0
23	CLA	b	616	65/65	0.95	0.17	43,55,114,116	0
23	CLA	c	503	65/65	0.95	0.13	53,61,74,82	0
23	CLA	B	603	65/65	0.95	0.13	38,46,62,66	0
23	CLA	a	408	65/65	0.95	0.15	40,48,128,132	0
23	CLA	B	614	65/65	0.95	0.15	33,43,93,97	0
23	CLA	c	507	65/65	0.95	0.13	43,56,83,86	0
23	CLA	C	510	65/65	0.95	0.18	43,51,117,130	0
23	CLA	b	603	65/65	0.95	0.15	41,50,70,88	0
35	DGD	C	518	62/66	0.95	0.21	40,54,93,96	0
31	LHG	D	407	49/49	0.95	0.13	40,48,64,76	0
31	LHG	D	408	49/49	0.95	0.18	45,57,124,134	0
23	CLA	C	512	65/65	0.95	0.21	46,56,78,87	0
31	LHG	L	101	49/49	0.95	0.14	39,51,65,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	b	605	65/65	0.95	0.15	35,43,66,75	0
23	CLA	b	606	65/65	0.95	0.12	38,49,110,115	0
23	CLA	b	607	65/65	0.95	0.16	32,40,73,80	0
25	BCR	A	409	40/40	0.95	0.11	33,42,54,58	0
23	CLA	C	503	65/65	0.95	0.13	45,53,68,78	0
25	BCR	C	517	40/40	0.95	0.11	49,56,64,73	0
36	CA	c	525	1/1	0.95	0.02	80,80,80,80	0
23	CLA	C	505	65/65	0.95	0.14	47,55,67,72	0
23	CLA	c	508	65/65	0.96	0.12	56,69,121,126	0
23	CLA	B	607	65/65	0.96	0.15	31,40,64,69	0
25	BCR	a	409	40/40	0.96	0.09	36,45,56,59	0
23	CLA	A	408	65/65	0.96	0.12	38,45,111,119	0
23	CLA	c	511	65/65	0.96	0.20	54,62,86,88	0
25	BCR	b	619	40/40	0.96	0.10	46,53,74,84	0
23	CLA	c	512	65/65	0.96	0.31	52,59,73,76	0
25	BCR	c	517	40/40	0.96	0.10	53,65,71,71	0
23	CLA	b	613	65/65	0.96	0.26	33,42,84,88	0
23	CLA	C	507	65/65	0.96	0.15	43,52,86,93	0
23	CLA	b	615	65/65	0.96	0.11	42,50,74,79	0
25	BCR	t	102	40/40	0.96	0.13	37,51,66,70	0
23	CLA	B	616	65/65	0.96	0.17	41,52,136,137	0
24	PHO	A	407	64/64	0.96	0.14	32,37,47,52	0
24	PHO	A	415	64/64	0.96	0.22	35,43,52,54	0
23	CLA	B	606	65/65	0.96	0.11	38,46,101,108	0
25	BCR	B	619	40/40	0.96	0.10	43,53,72,75	0
26	GOL	C	524	6/6	0.96	0.13	53,56,60,61	0
23	CLA	a	406	65/65	0.96	0.21	39,49,114,118	0
23	CLA	b	608	65/65	0.96	0.19	45,52,69,76	0
25	BCR	D	405	40/40	0.96	0.17	45,58,95,103	0
36	CA	c	524	1/1	0.96	0.06	73,73,73,73	0
23	CLA	C	504	65/65	0.96	0.17	43,50,71,82	0
23	CLA	C	511	65/65	0.96	0.14	48,56,77,79	0
39	MG	j	102	1/1	0.96	0.11	60,60,60,60	0
24	PHO	a	407	64/64	0.97	0.14	35,42,47,50	0
24	PHO	a	417	64/64	0.97	0.19	39,47,55,60	0
23	CLA	a	404	65/65	0.97	0.19	37,41,64,73	0
25	BCR	B	617	40/40	0.97	0.14	34,45,55,58	0
25	BCR	B	618	40/40	0.97	0.15	35,50,63,72	0
23	CLA	a	405	65/65	0.97	0.14	34,40,57,62	0
23	CLA	B	613	65/65	0.97	0.20	34,41,89,94	0
23	CLA	A	405	65/65	0.97	0.17	31,37,52,56	0
23	CLA	B	615	65/65	0.97	0.12	40,46,77,83	0

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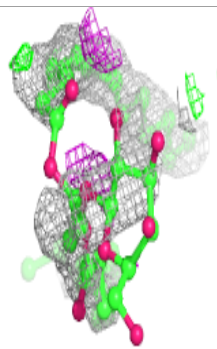
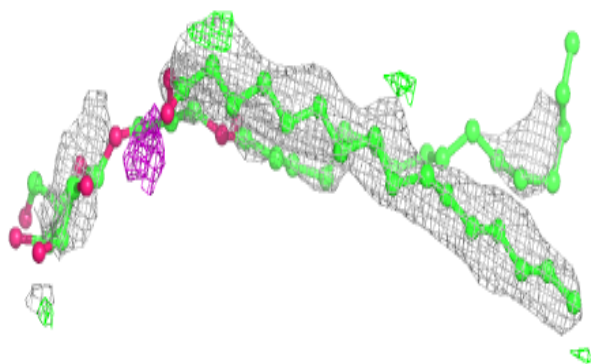
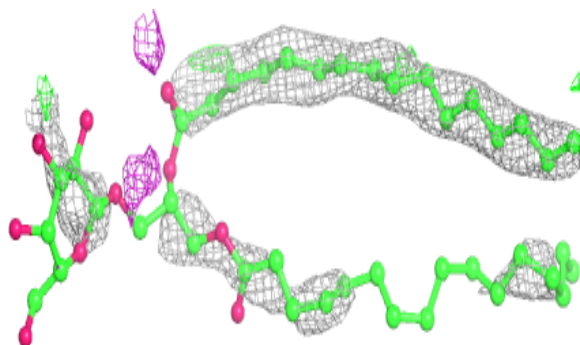
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	CA	C	525	1/1	0.97	0.20	66,66,66,66	0
23	CLA	A	406	65/65	0.97	0.20	34,42,114,117	0
23	CLA	B	608	65/65	0.97	0.17	39,47,62,65	0
23	CLA	A	404	65/65	0.97	0.22	33,36,61,75	0
23	CLA	B	604	65/65	0.97	0.19	32,39,110,116	0
23	CLA	B	605	65/65	0.97	0.12	35,41,61,73	0
23	CLA	D	403	65/65	0.97	0.24	32,37,53,62	0
38	HEC	E	103	43/43	0.97	0.11	57,65,80,93	0
38	HEC	e	102	43/43	0.97	0.17	64,78,119,130	0
38	HEC	v	202	43/43	0.97	0.11	52,58,63,64	0
23	CLA	B	612	65/65	0.97	0.15	35,44,54,59	0
38	HEC	V	201	43/43	0.98	0.09	43,46,51,54	0
28	OEX	A	412	10/10	0.98	0.11	35,38,45,46	0
37	BCT	D	401	4/4	0.98	0.06	51,57,61,62	0
39	MG	J	102	1/1	0.98	0.07	50,50,50,50	0
23	CLA	d	402	65/65	0.98	0.23	36,40,68,77	0
22	CL	A	403	1/1	0.99	0.11	40,40,40,40	0
37	BCT	d	401	4/4	0.99	0.07	52,54,62,64	0
22	CL	a	402	1/1	0.99	0.06	42,42,42,42	0
22	CL	a	403	1/1	0.99	0.09	44,44,44,44	0
21	FE2	A	401	1/1	0.99	0.03	53,53,53,53	0
21	FE2	a	401	1/1	0.99	0.03	57,57,57,57	0
22	CL	A	402	1/1	0.99	0.05	35,35,35,35	0
28	OEX	a	414	10/10	0.99	0.11	39,45,49,49	0

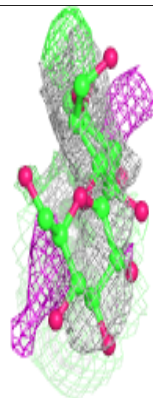
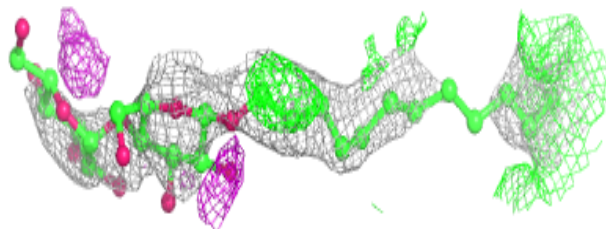
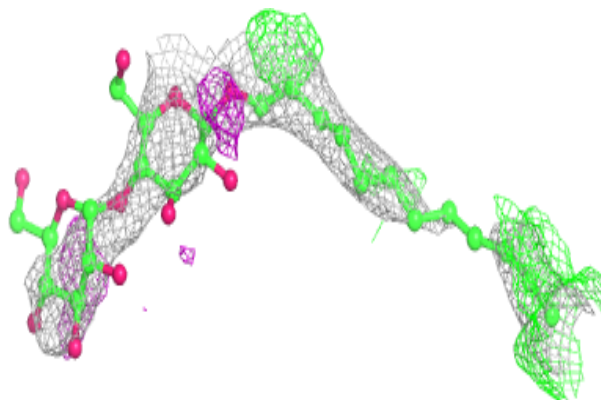
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

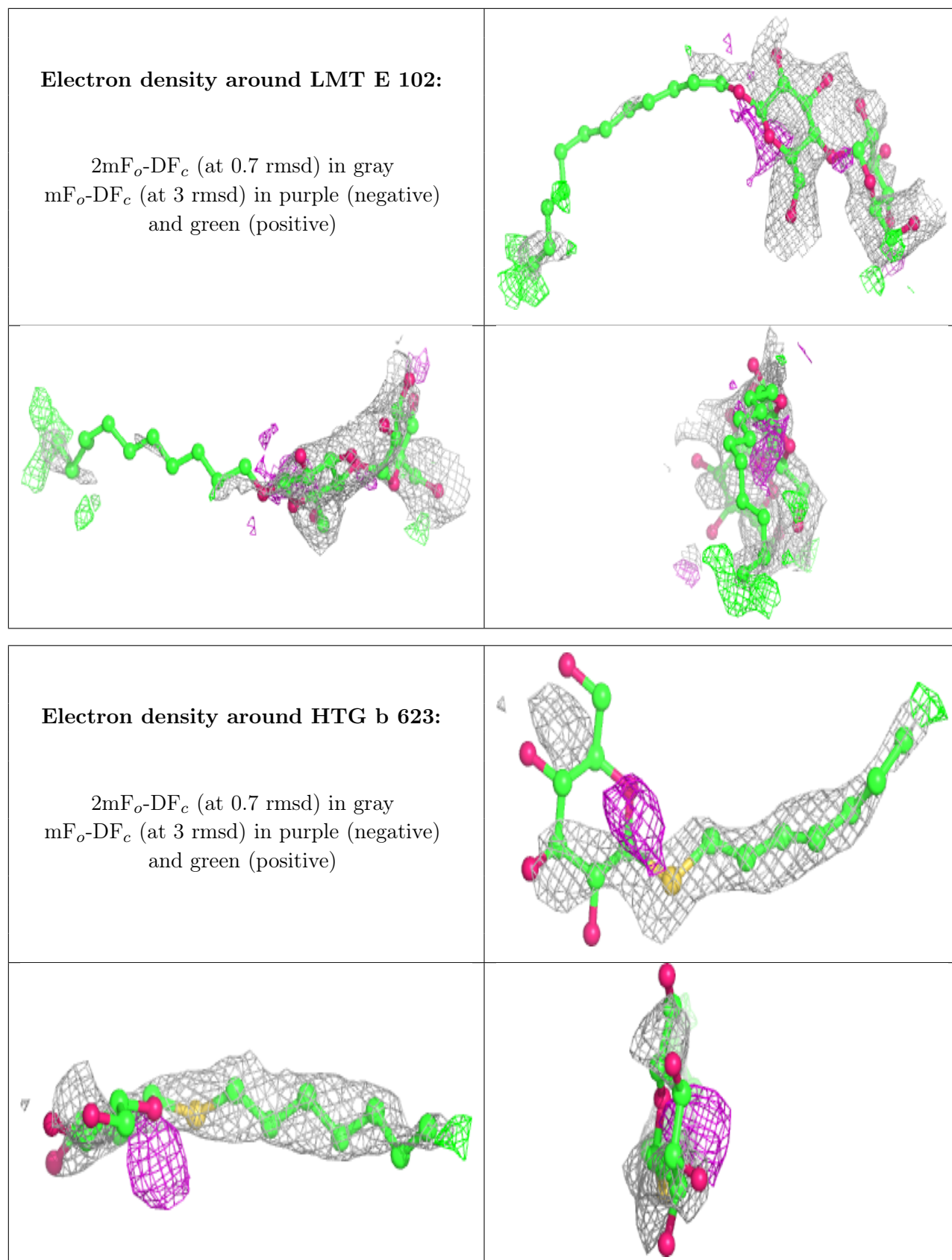
Electron density around LMG C 522:

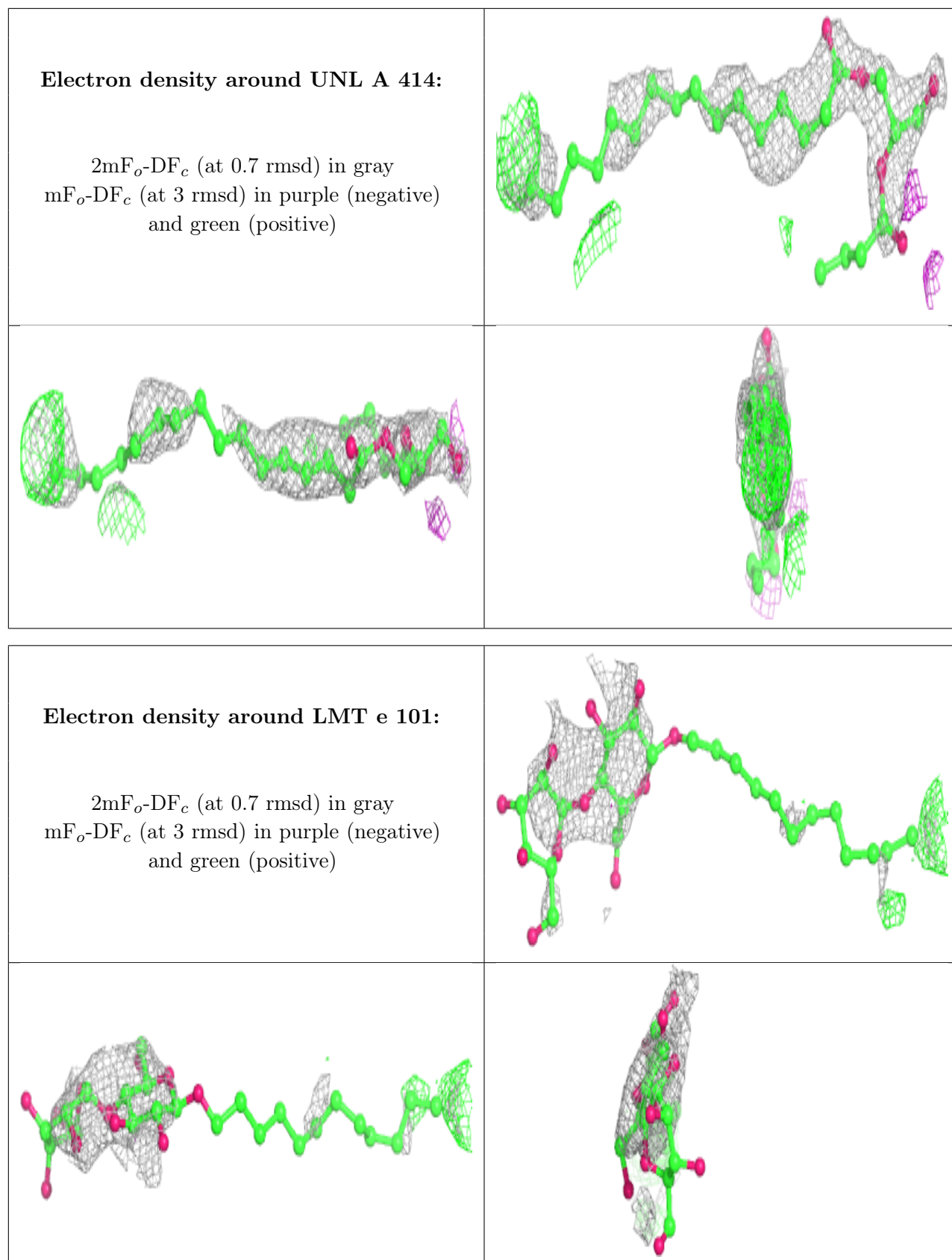
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

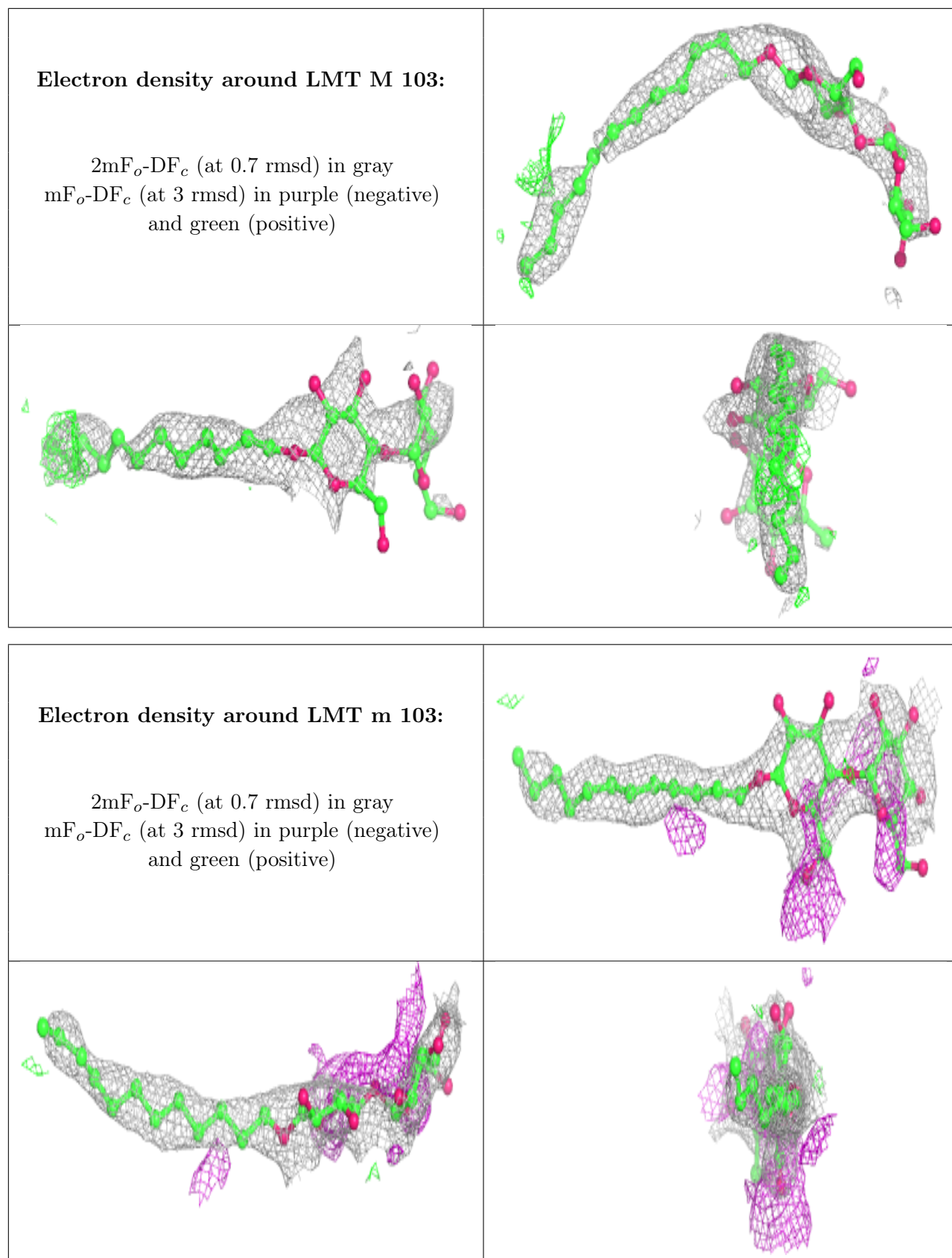
**Electron density around LMT a 413:**

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



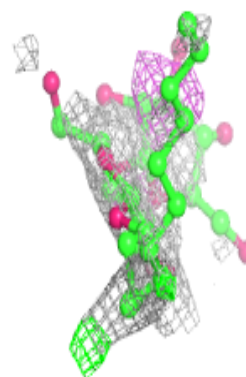
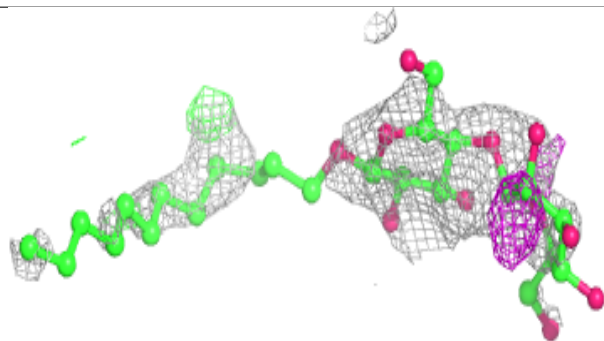
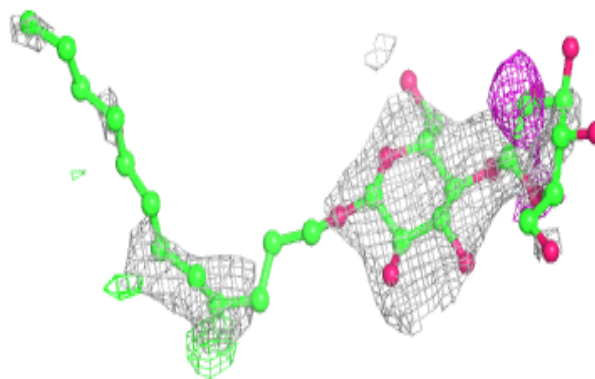




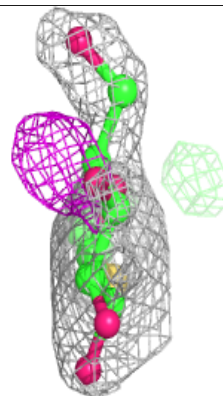
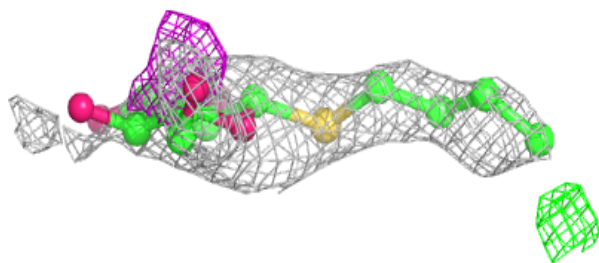
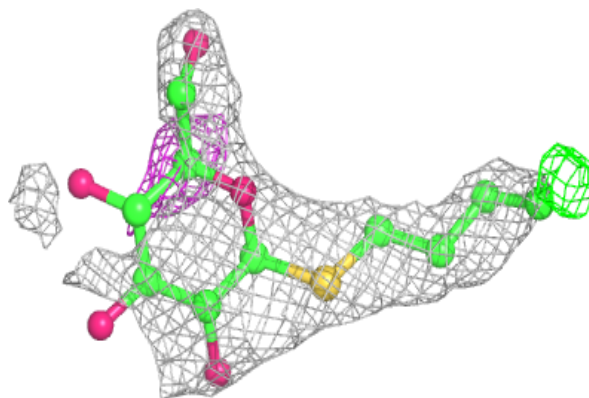


Electron density around LMT C 526:

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

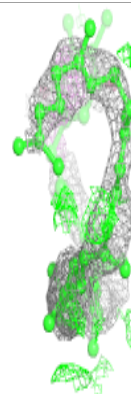
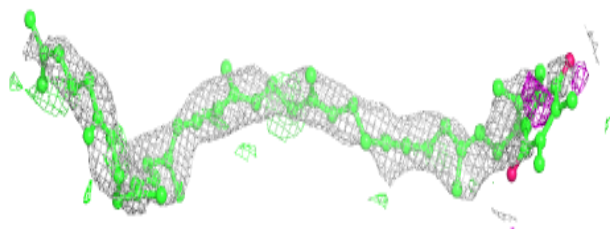
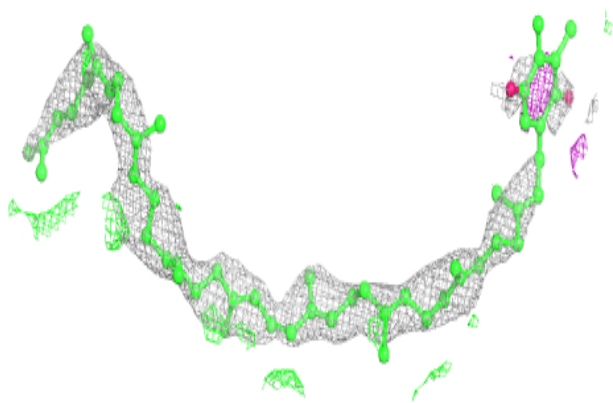
**Electron density around HTG D 411:**

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

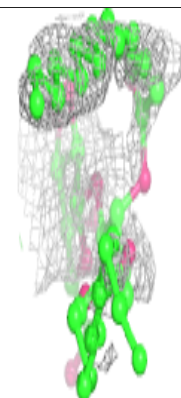
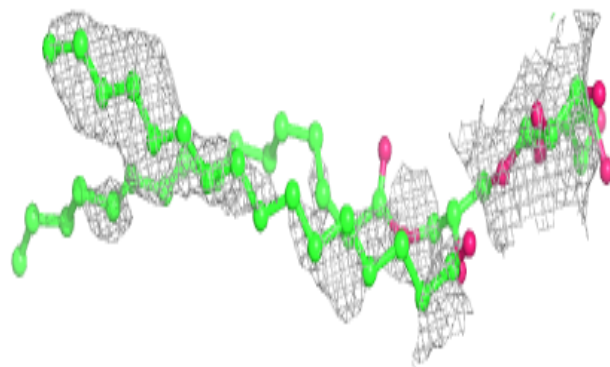
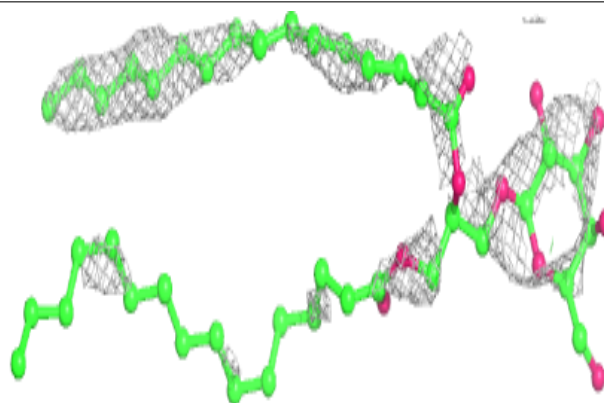


Electron density around PL9 A 413:

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

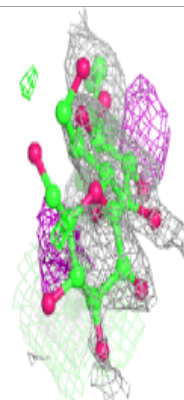
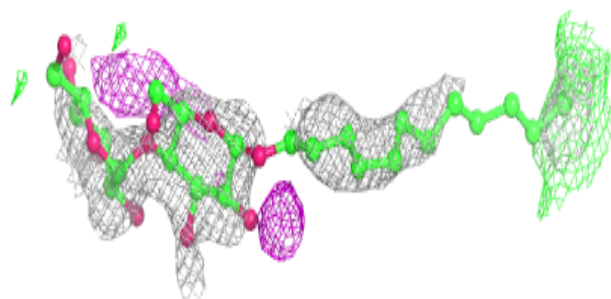
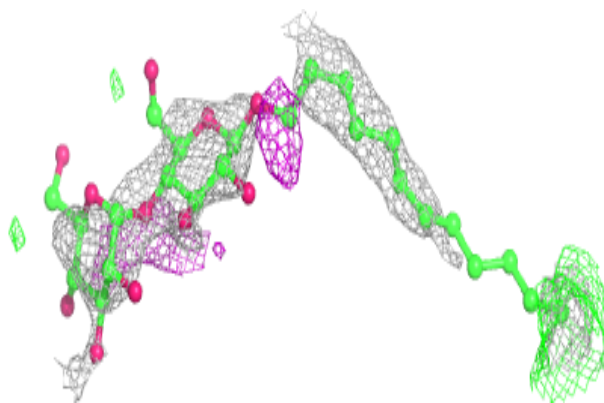
**Electron density around LMG c 522:**

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

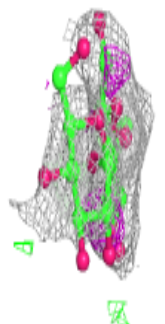
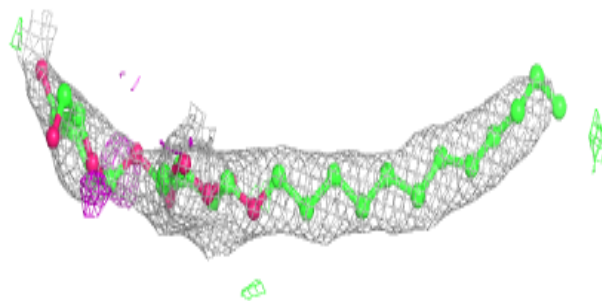
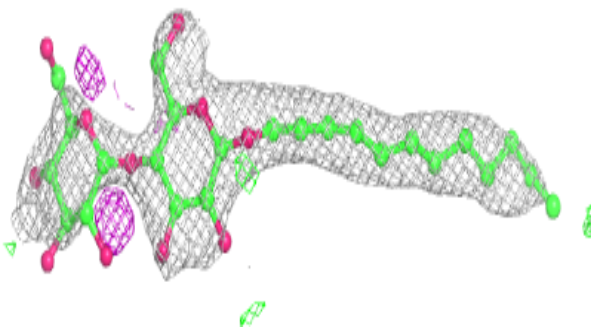


Electron density around LMT D 402:

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

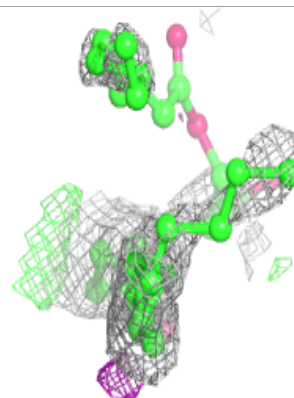
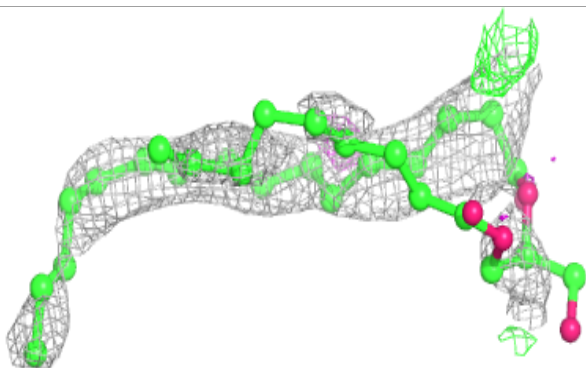
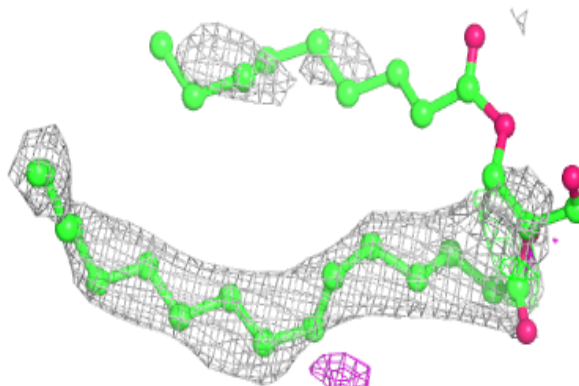
**Electron density around LMT M 101:**

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

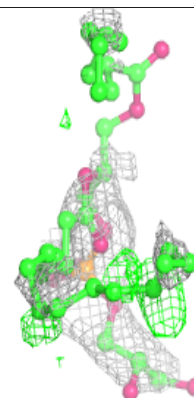
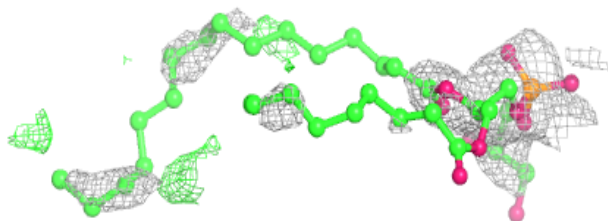
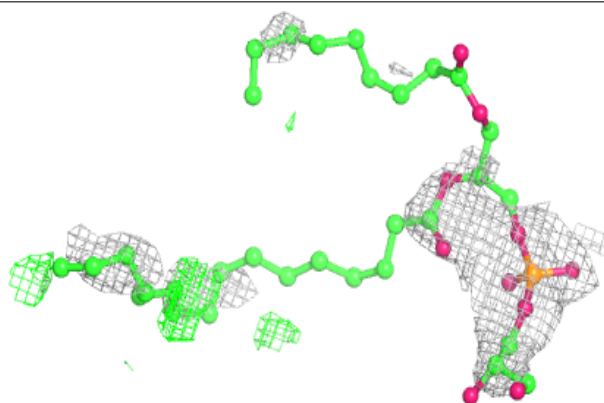


Electron density around UNL b 626:

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

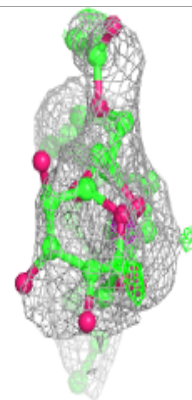
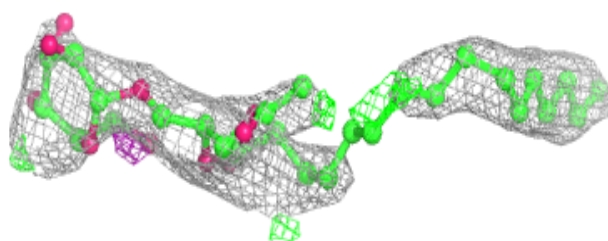
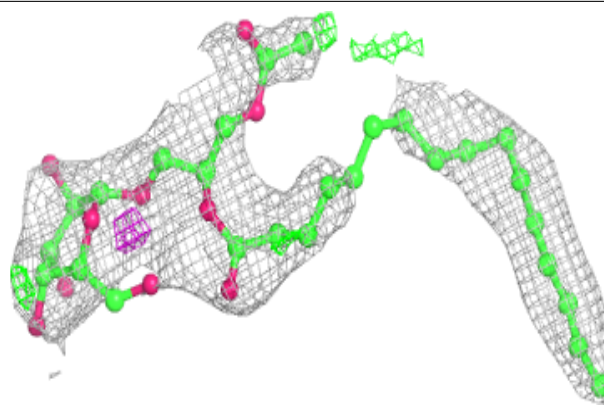
**Electron density around LHG a 419:**

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

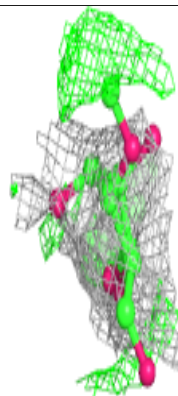
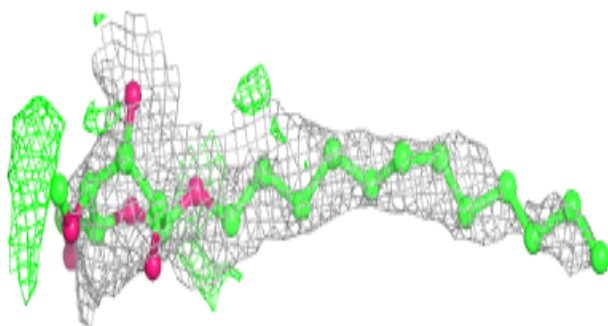
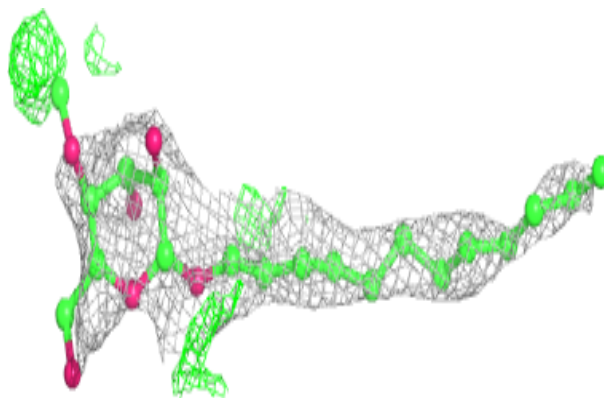


Electron density around LMG Z 101:

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

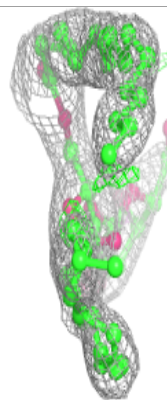
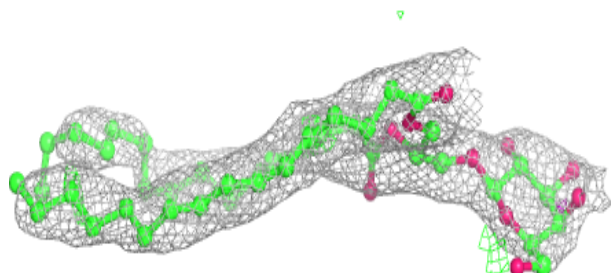
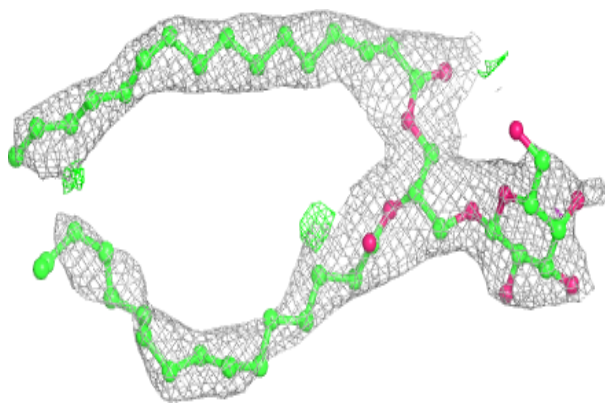
**Electron density around LMT b 621:**

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

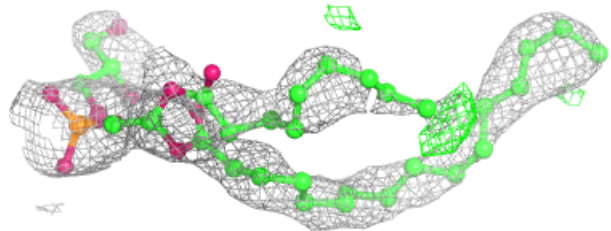
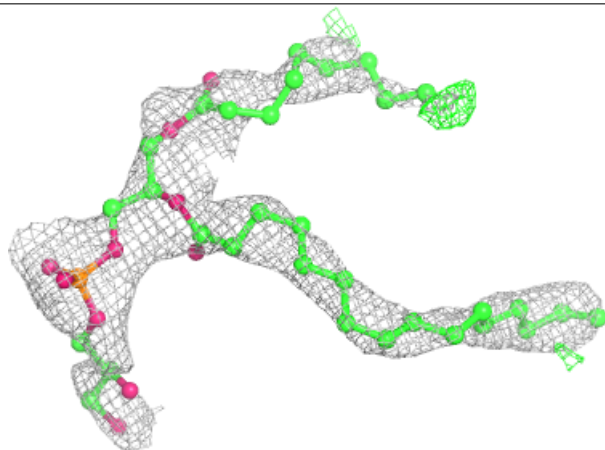


Electron density around LMG c 501:

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

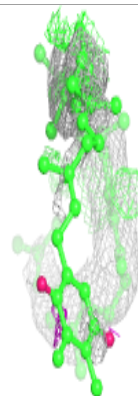
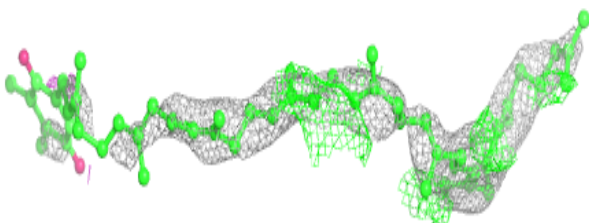
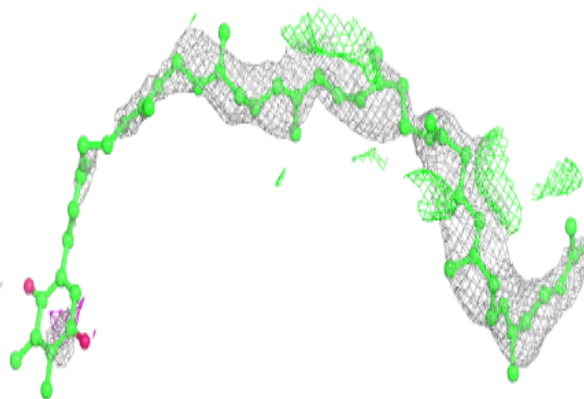
**Electron density around LHG E 101:**

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

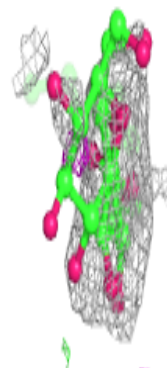
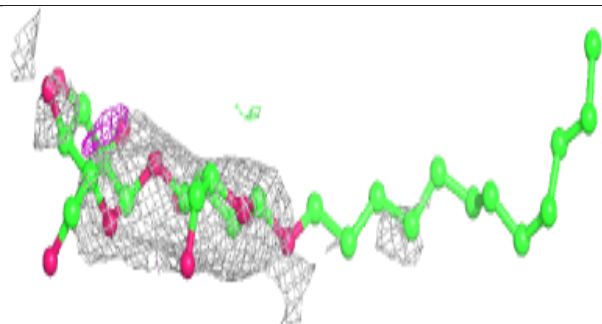
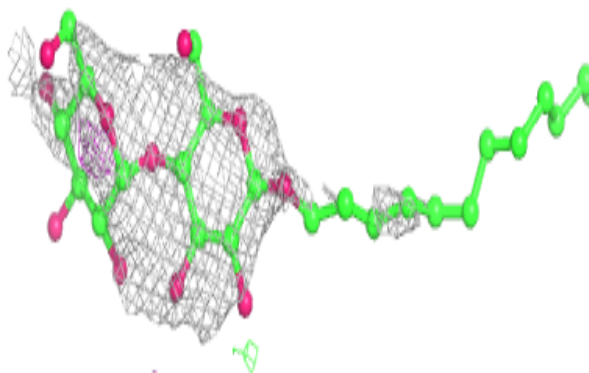


Electron density around PL9 a 415:

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

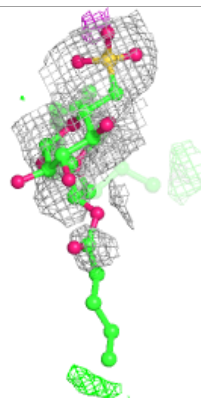
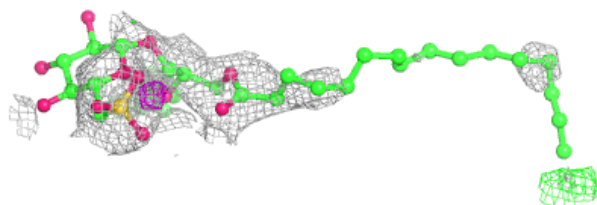
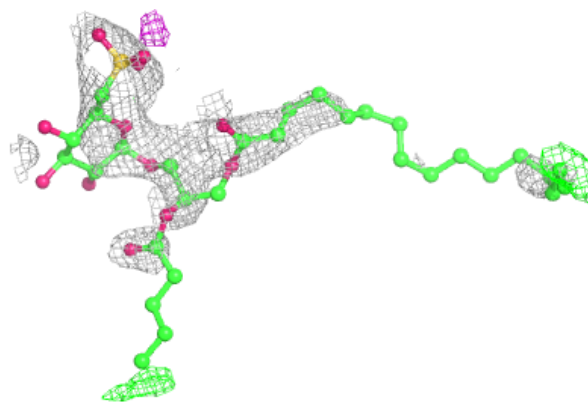
**Electron density around LMT a 418:**

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

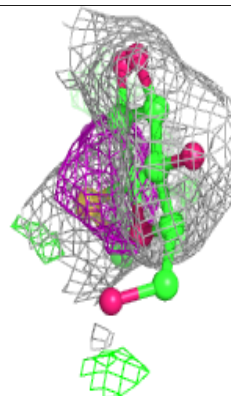
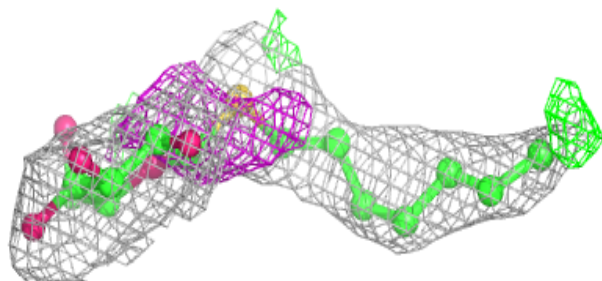
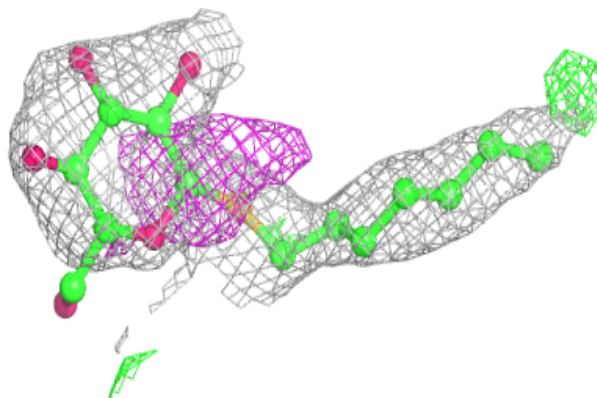


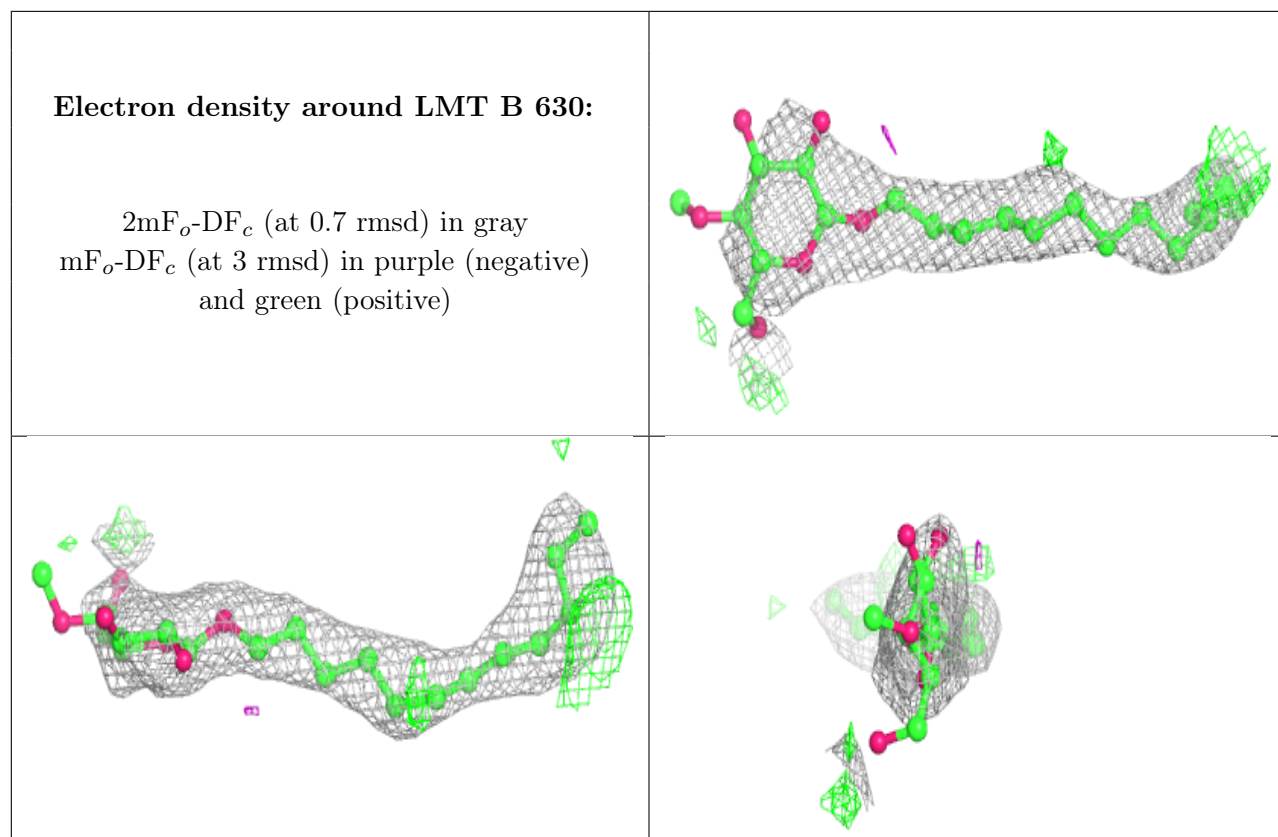
Electron density around SQD f 101:

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

**Electron density around HTG b 622:**

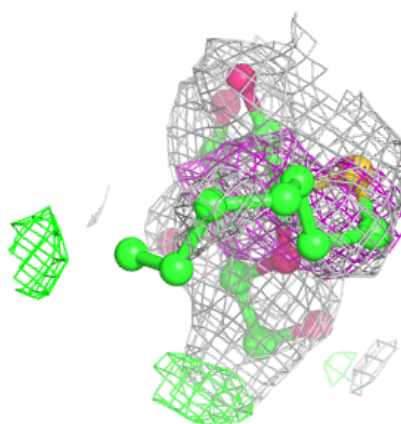
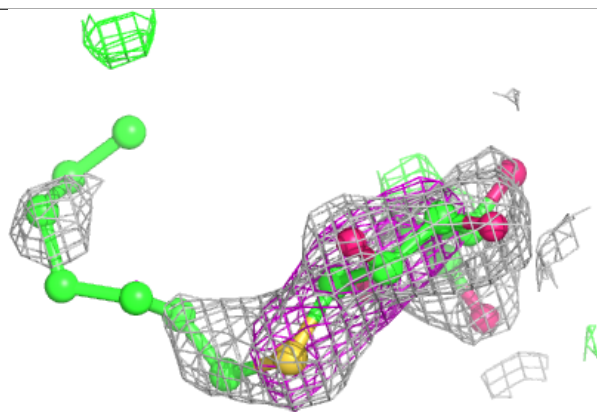
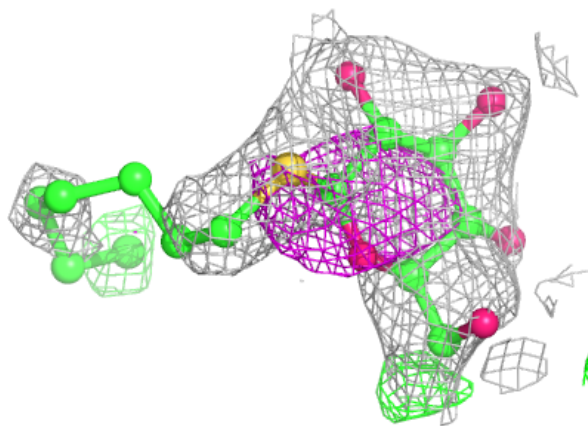
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





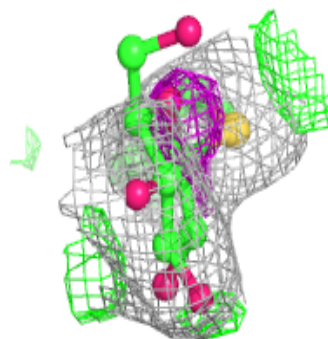
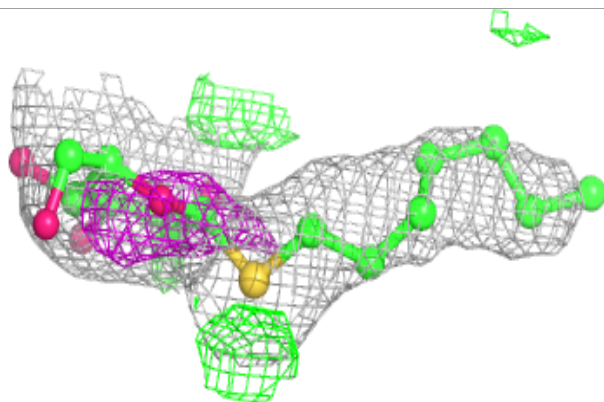
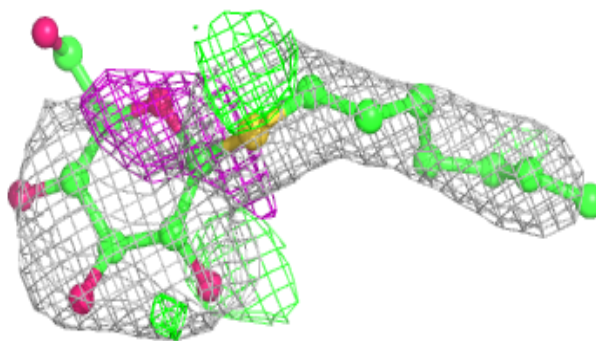
Electron density around HTG B 623:

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



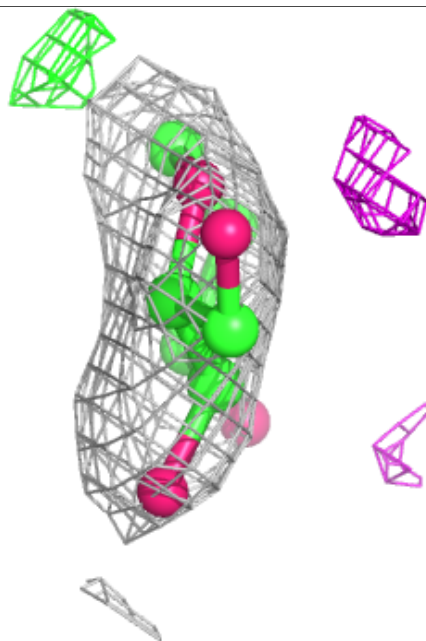
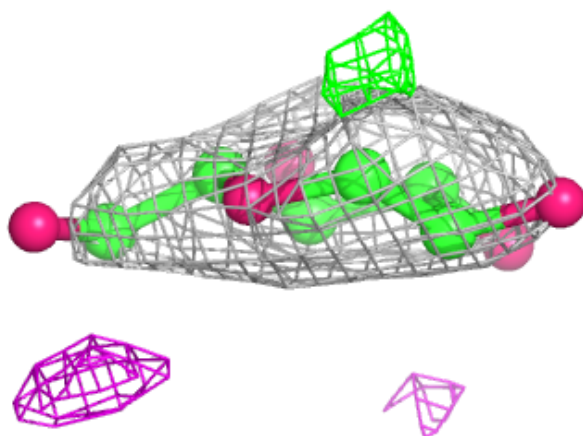
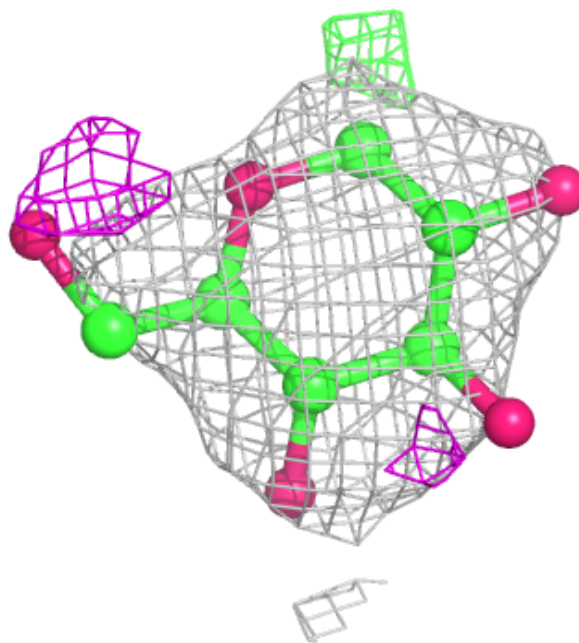
Electron density around HTG B 622:

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



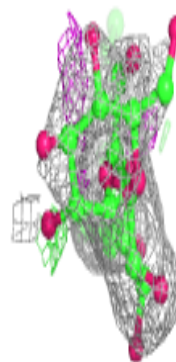
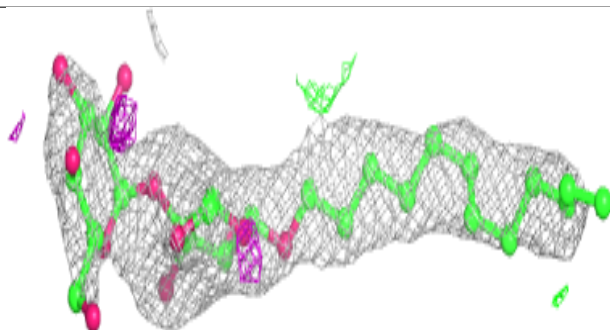
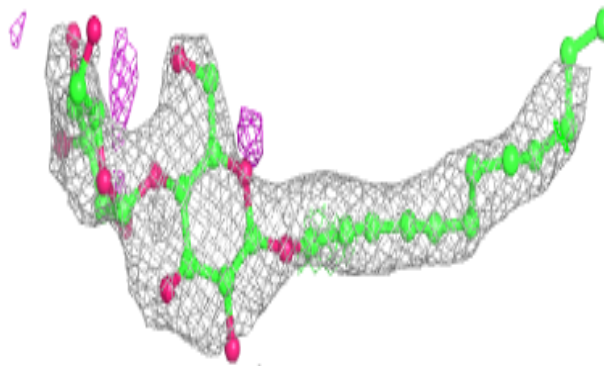
Electron density around HTG V 202:

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

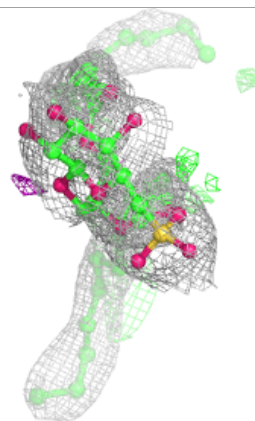
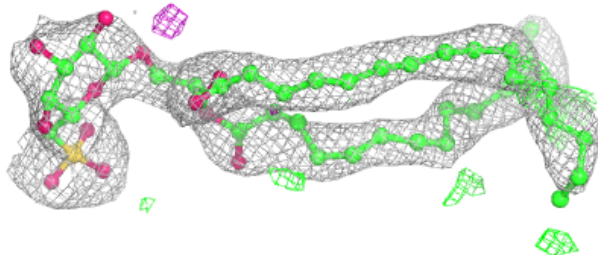
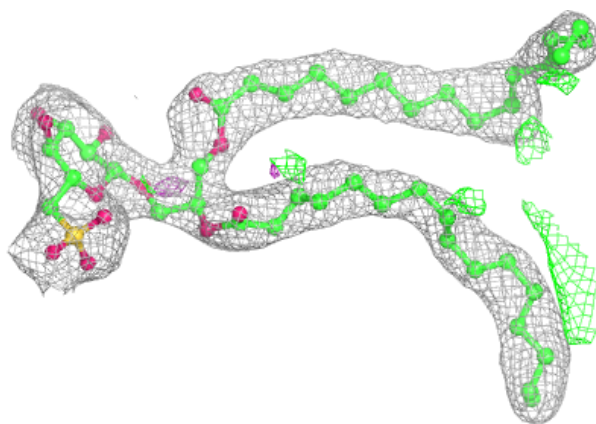


Electron density around LMT B 628:

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

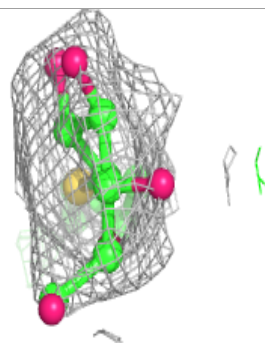
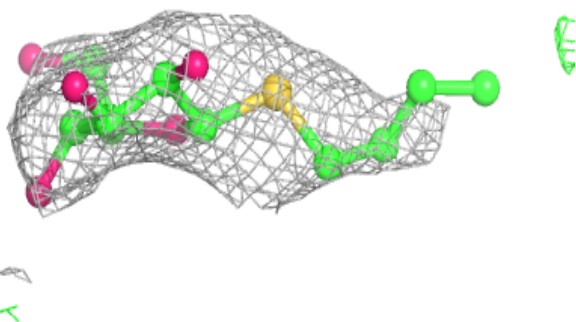
**Electron density around SQD B 620:**

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

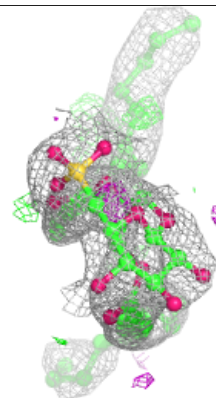
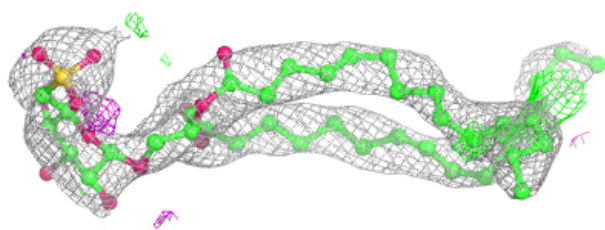
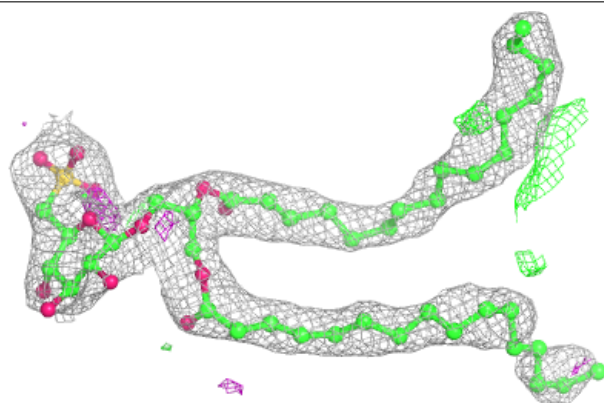


Electron density around HTG h 101:

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

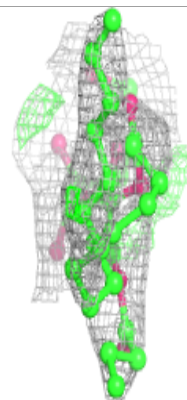
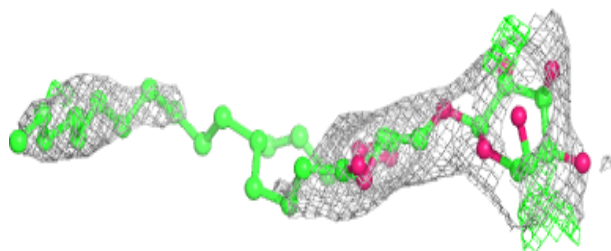
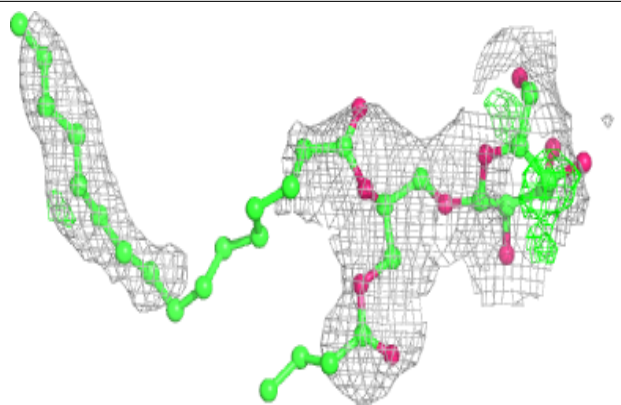
**Electron density around SQD b 620:**

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

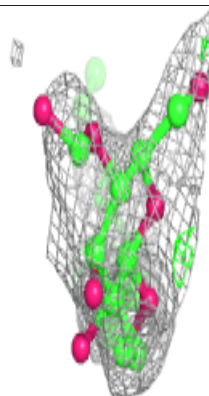
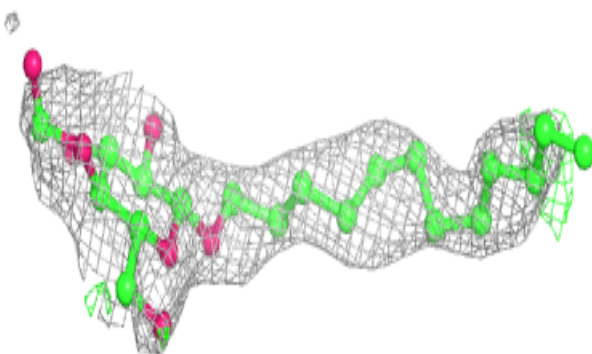
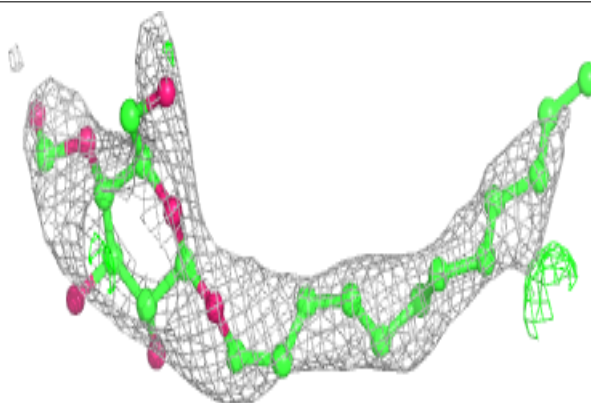


Electron density around LMG z 101:

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

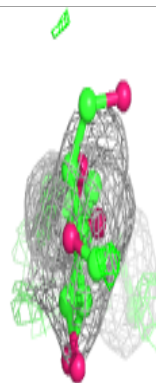
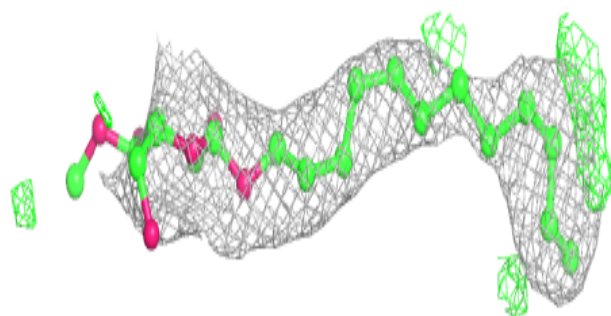
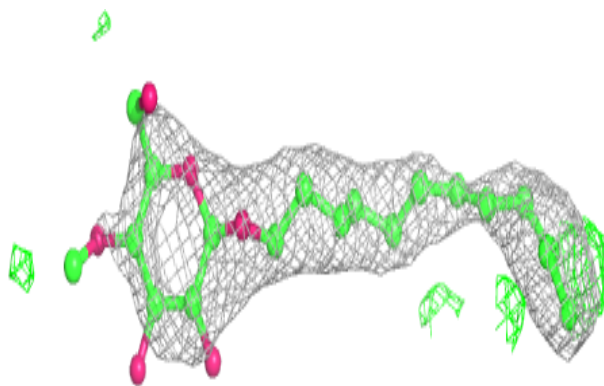
**Electron density around LMT t 101:**

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

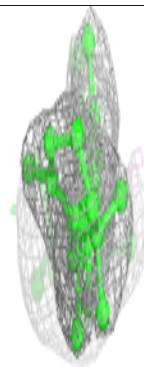
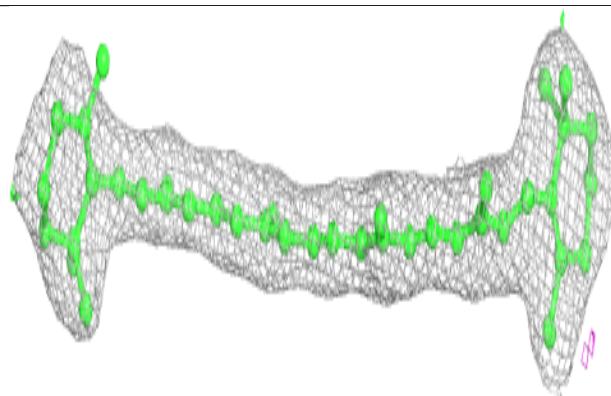
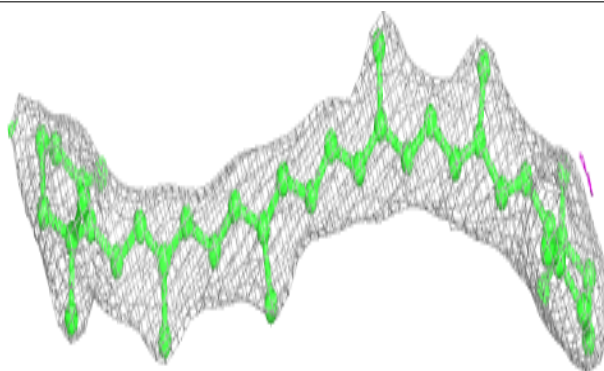


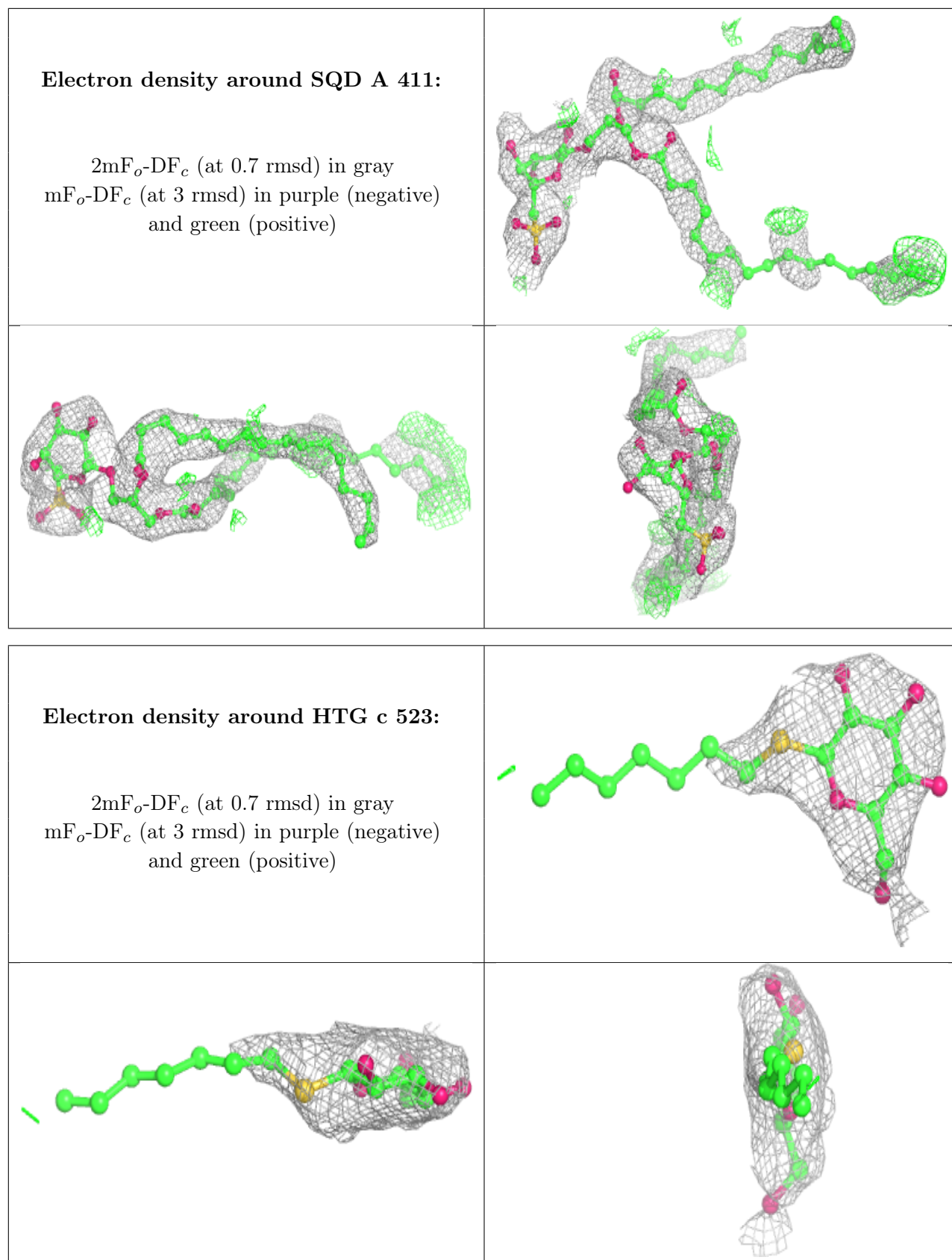
Electron density around LMT b 627:

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

**Electron density around BCR h 102:**

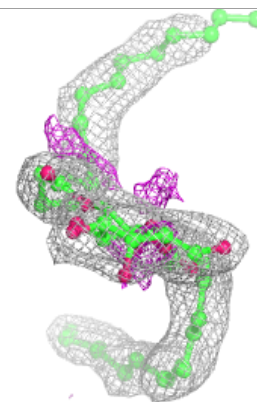
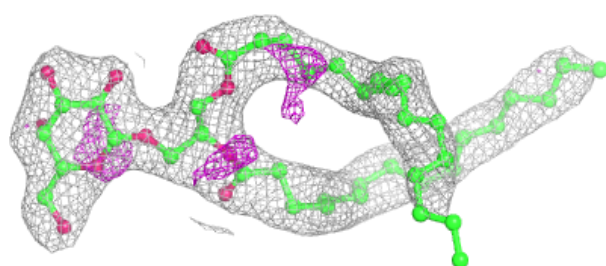
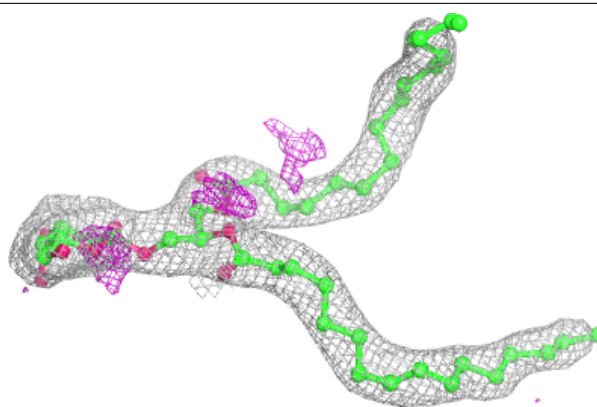
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



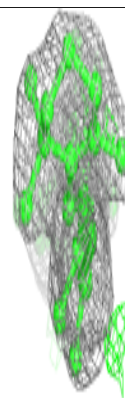
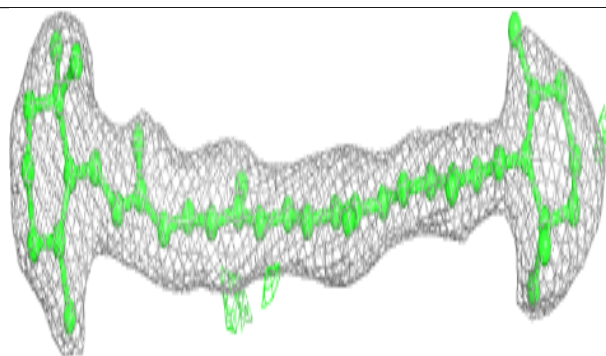
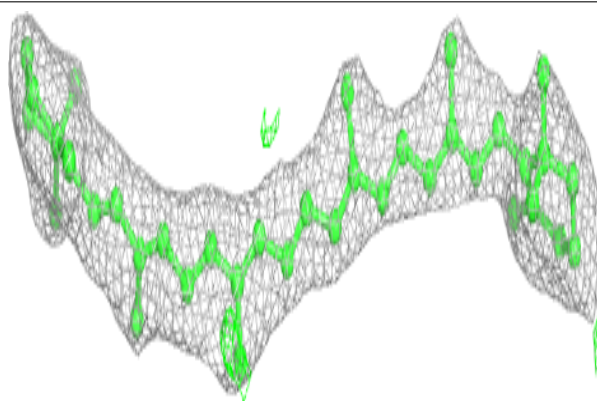


Electron density around LMG B 621:

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

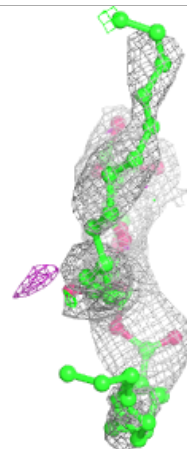
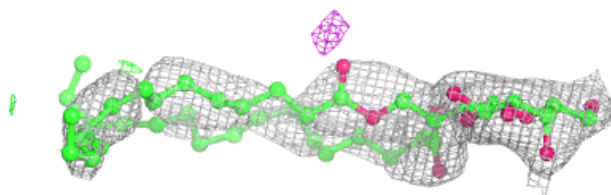
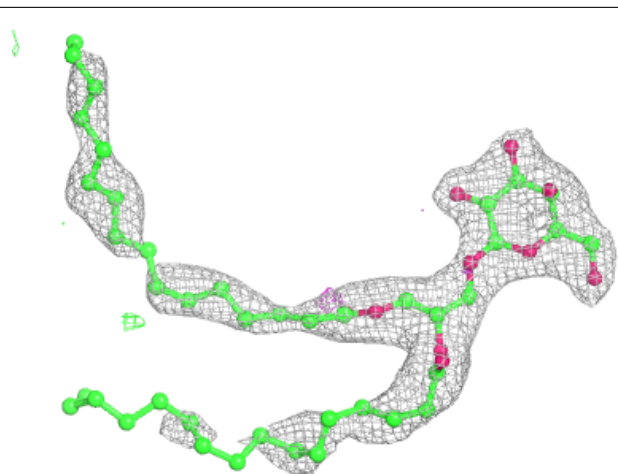
**Electron density around BCR H 101:**

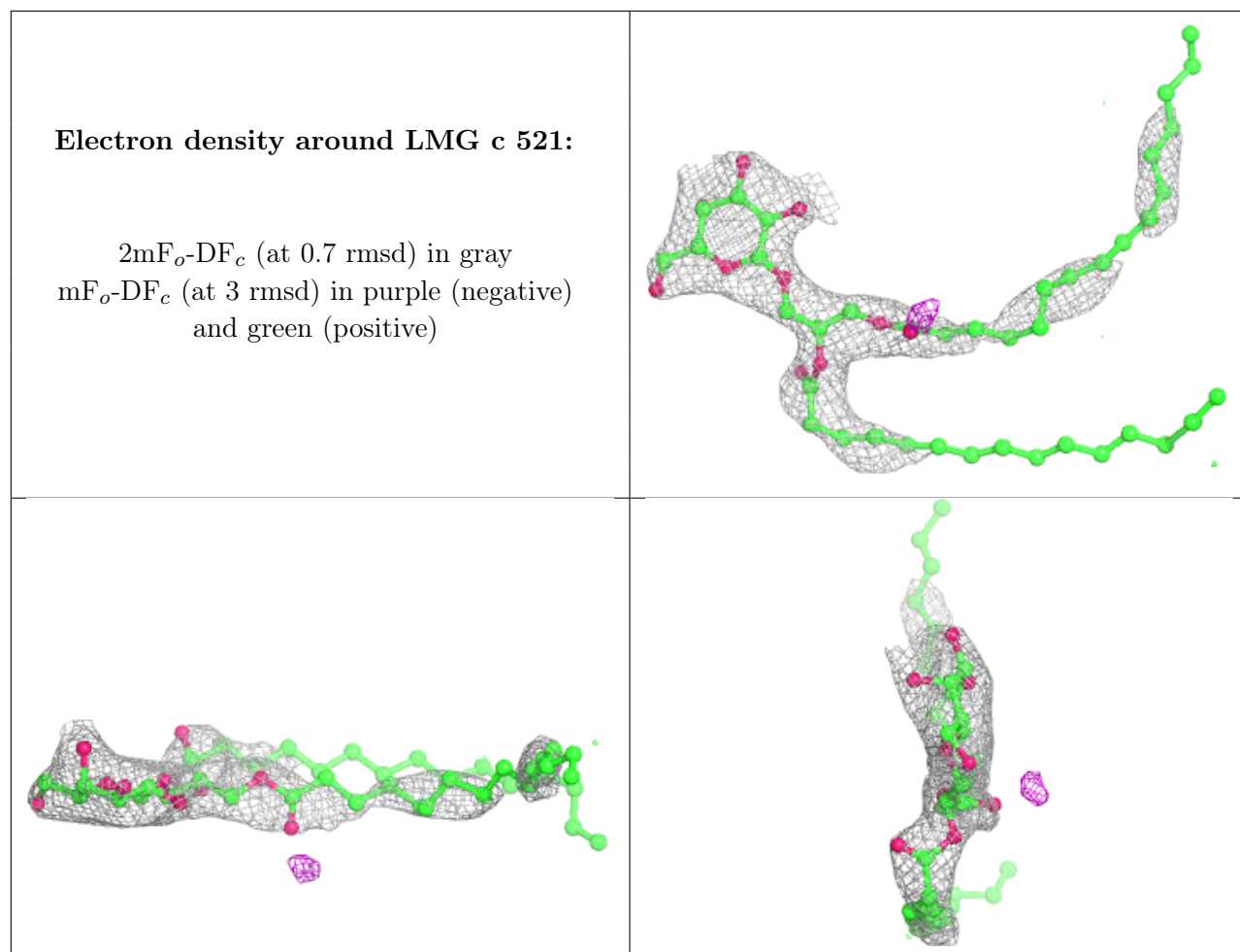
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LMG C 521:

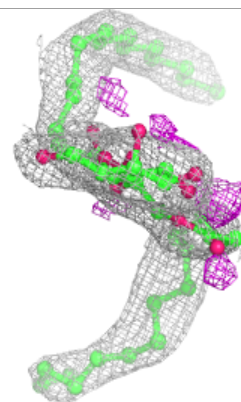
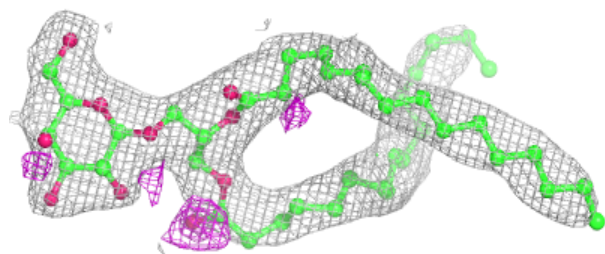
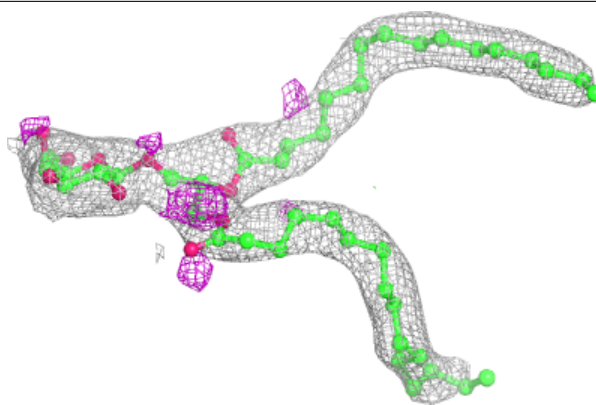
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



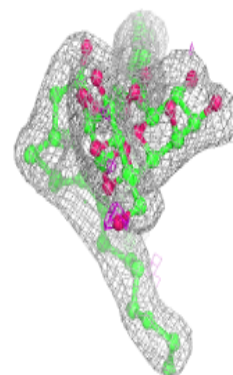
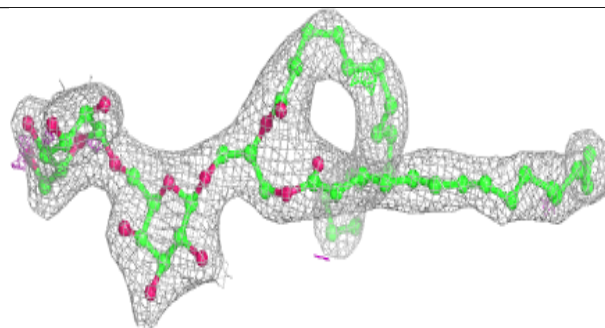
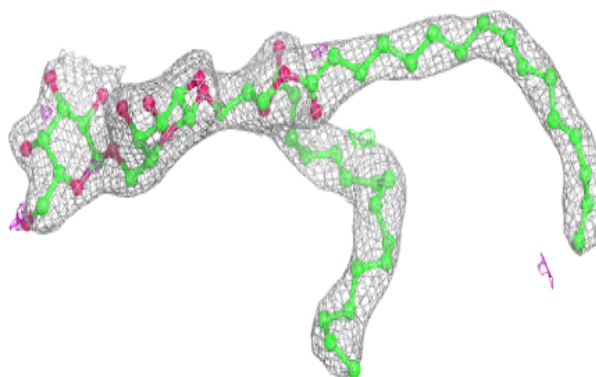


Electron density around LMG m 101:

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

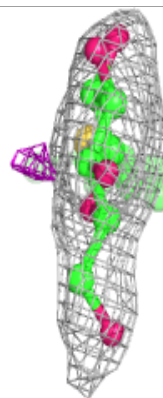
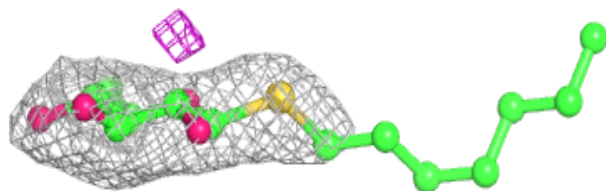
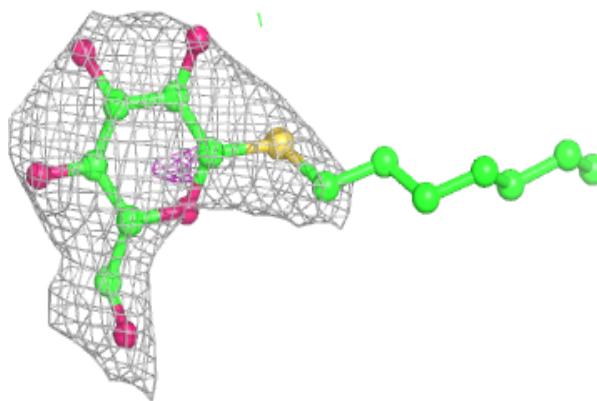
**Electron density around DGD h 103:**

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

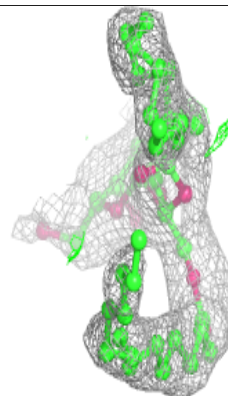
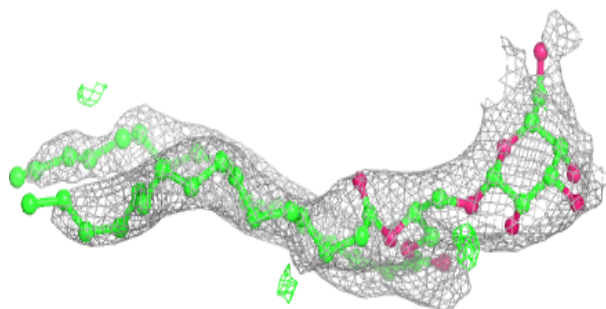
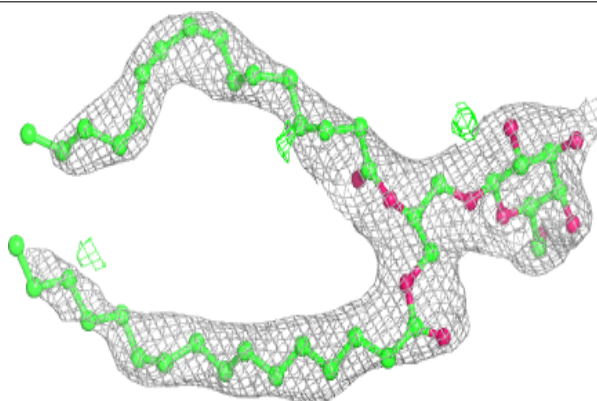


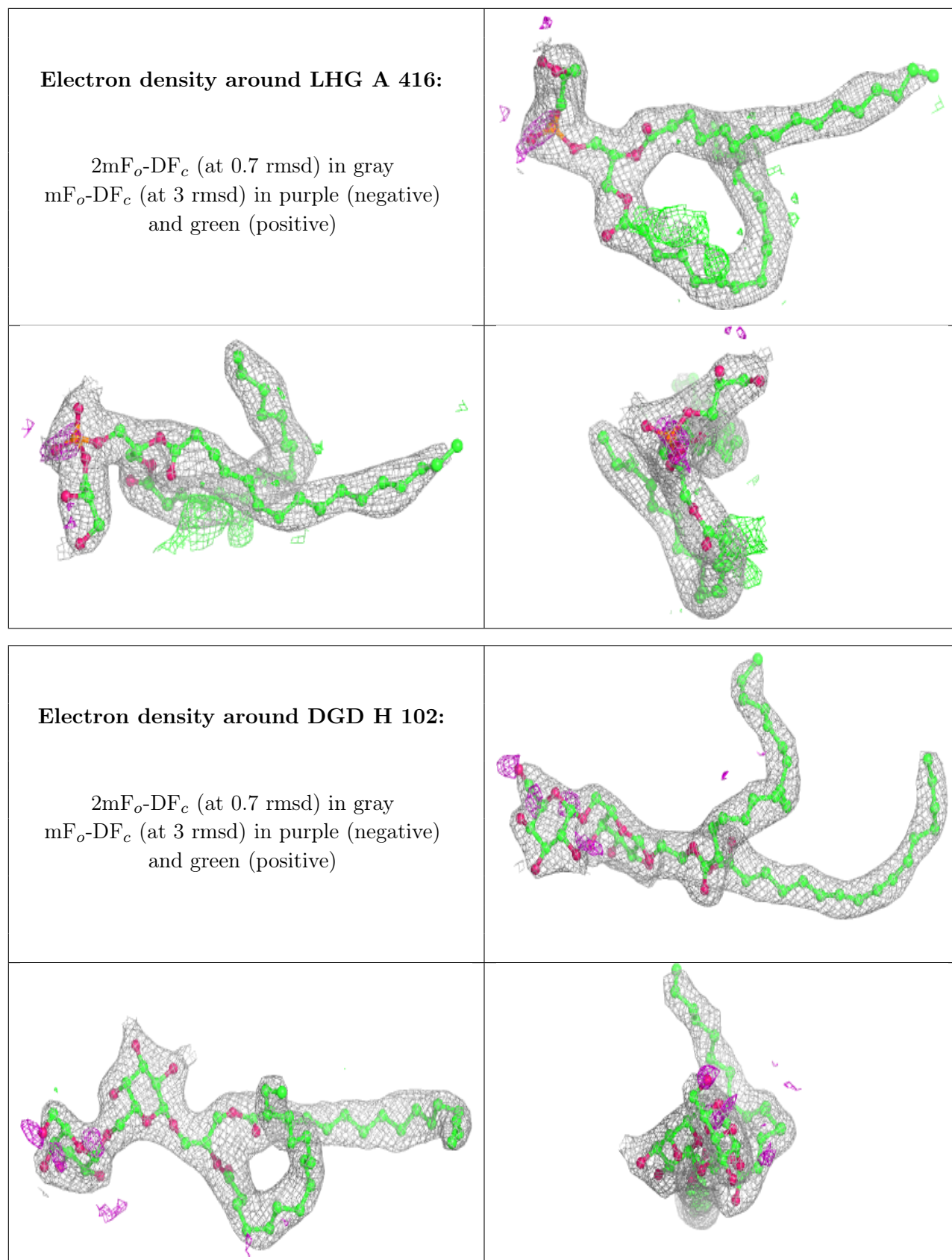
Electron density around HTG C 523:

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

**Electron density around LMG C 502:**

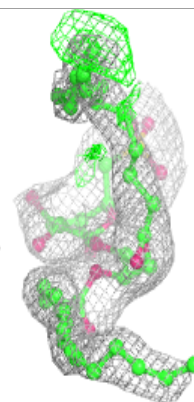
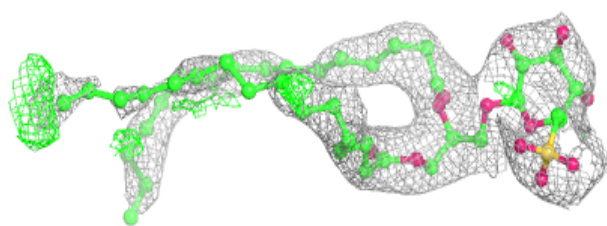
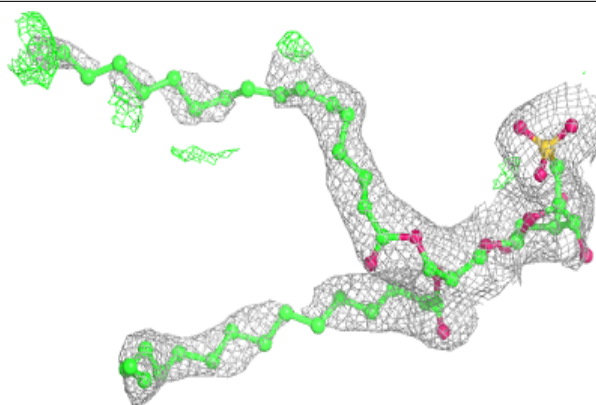
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



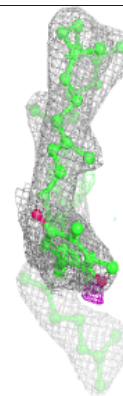
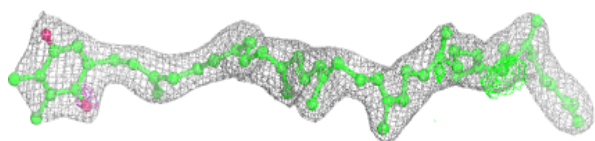
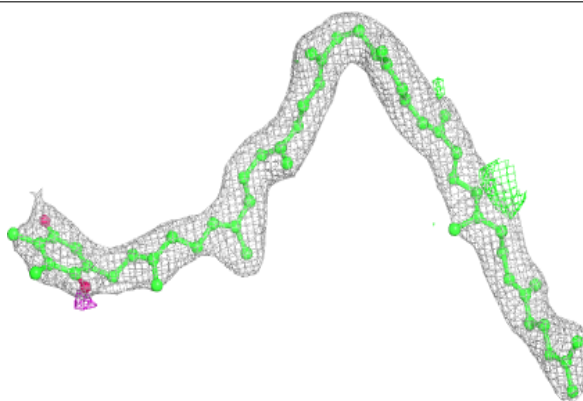


Electron density around SQD a 412:

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

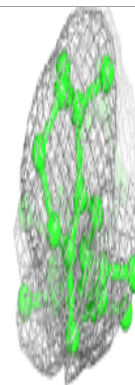
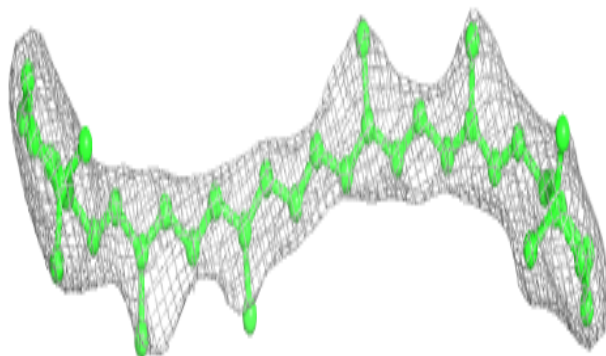
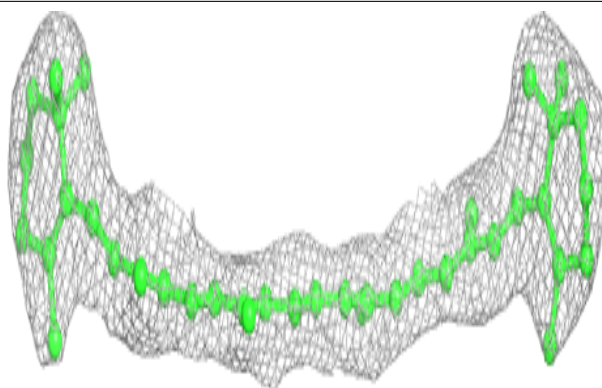
**Electron density around PL9 d 405:**

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

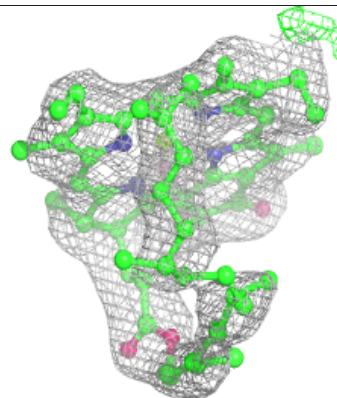
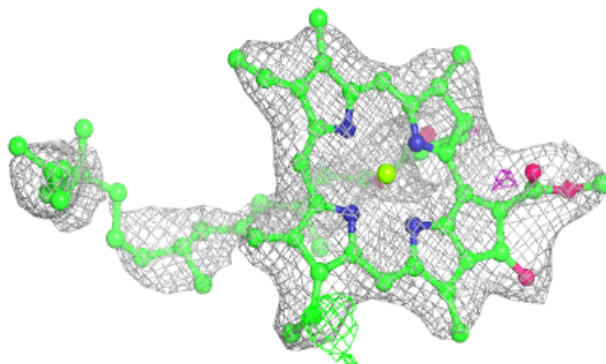
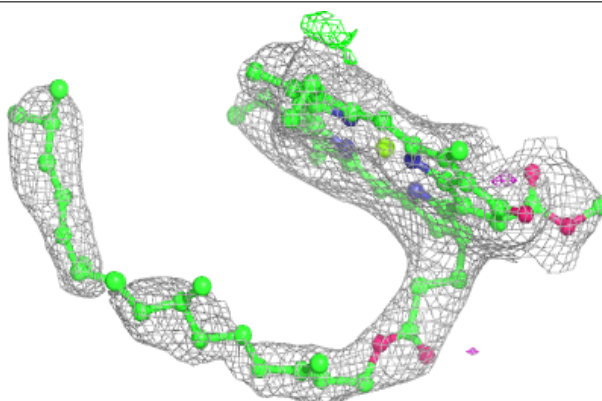


Electron density around BCR k 101:

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

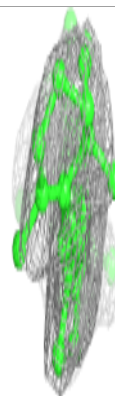
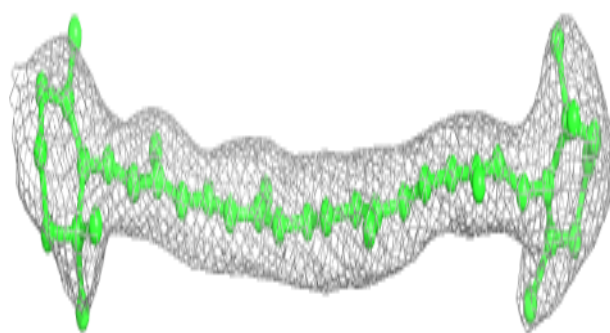
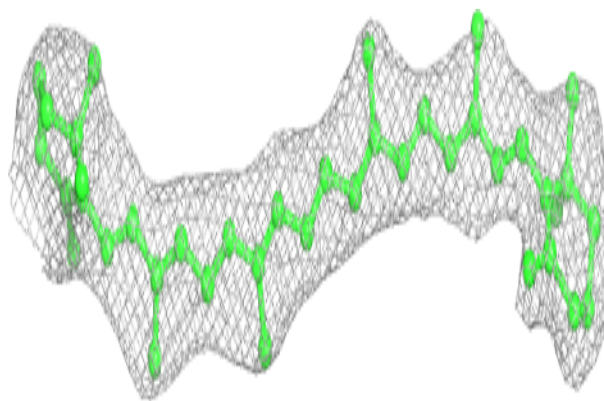
**Electron density around CLA C 515:**

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

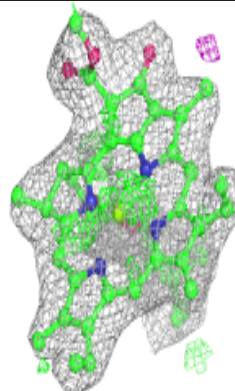
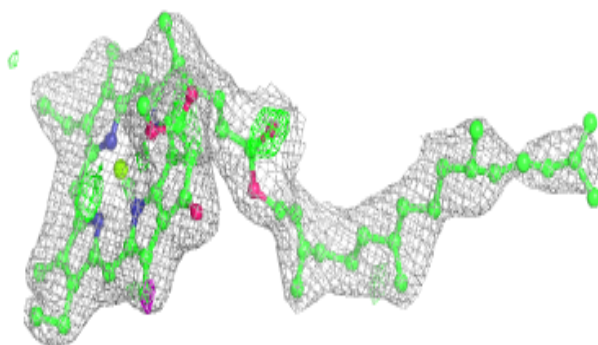
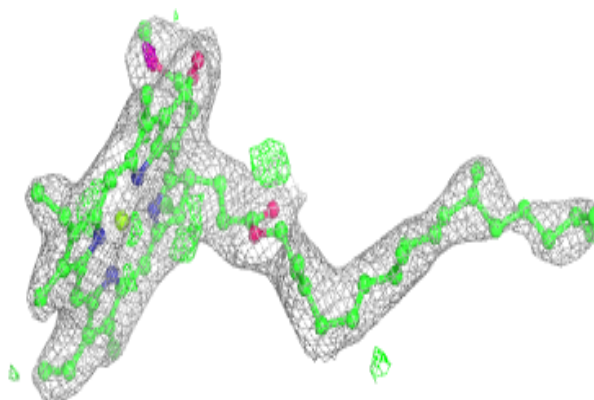


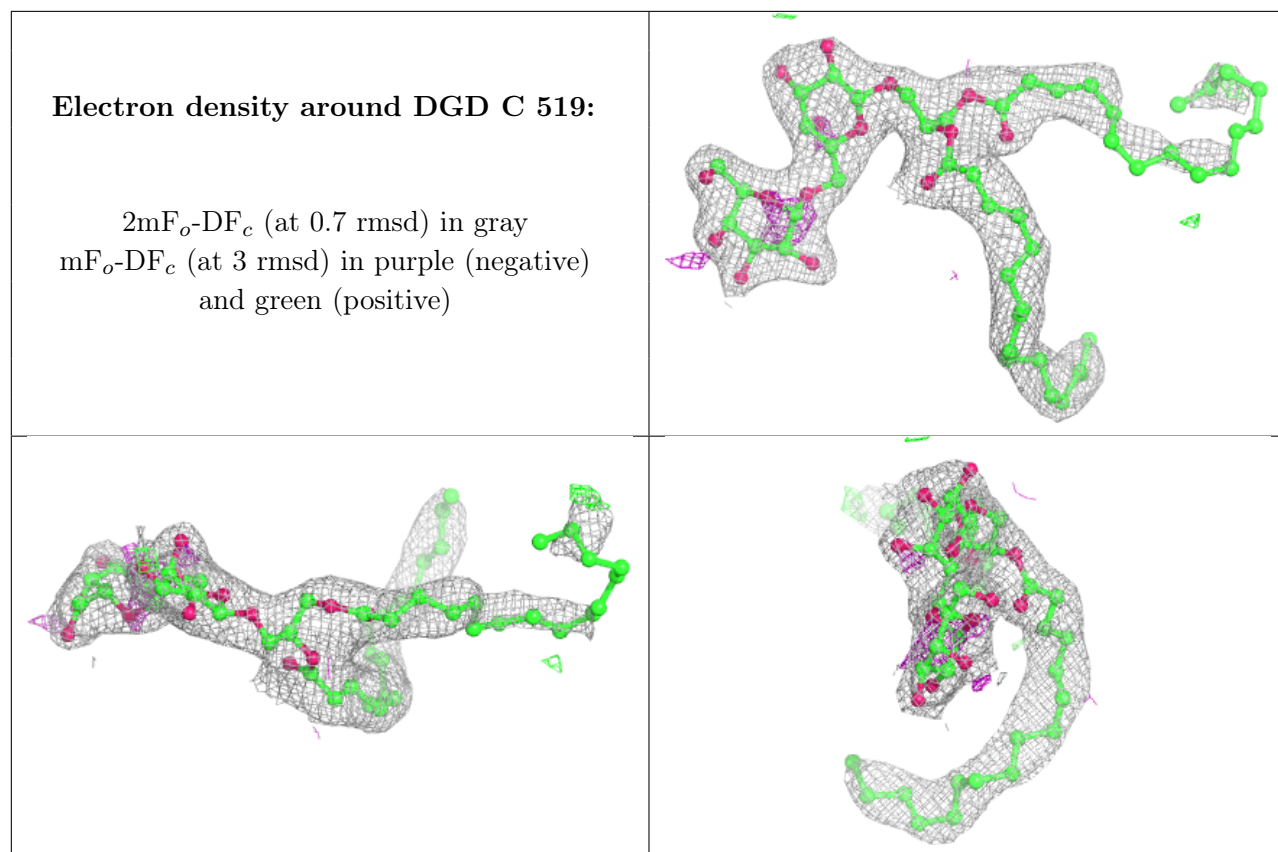
Electron density around BCR y 101:

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

**Electron density around CLA c 504:**

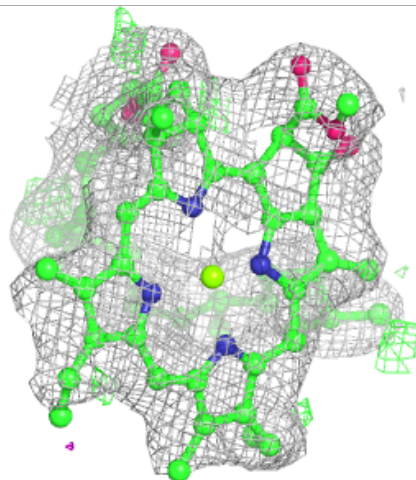
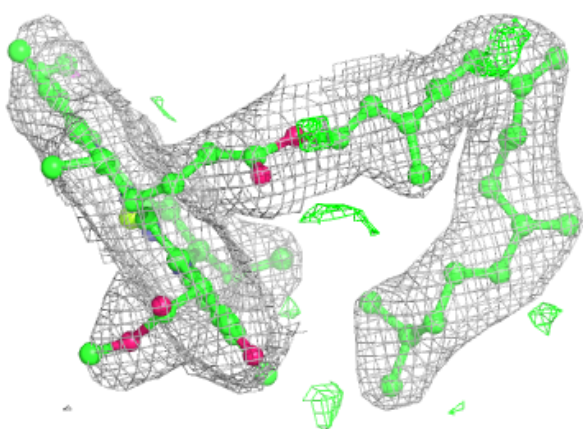
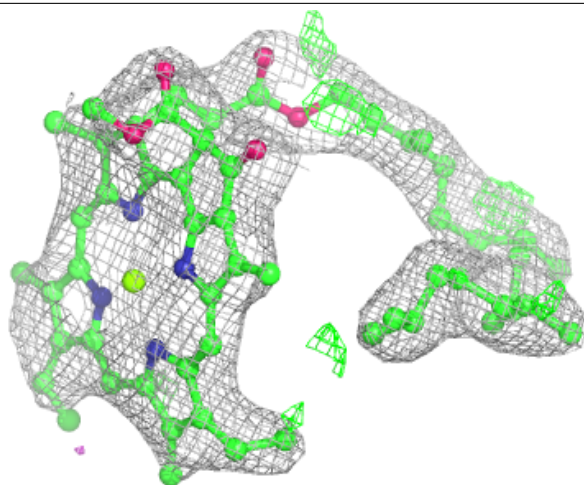
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

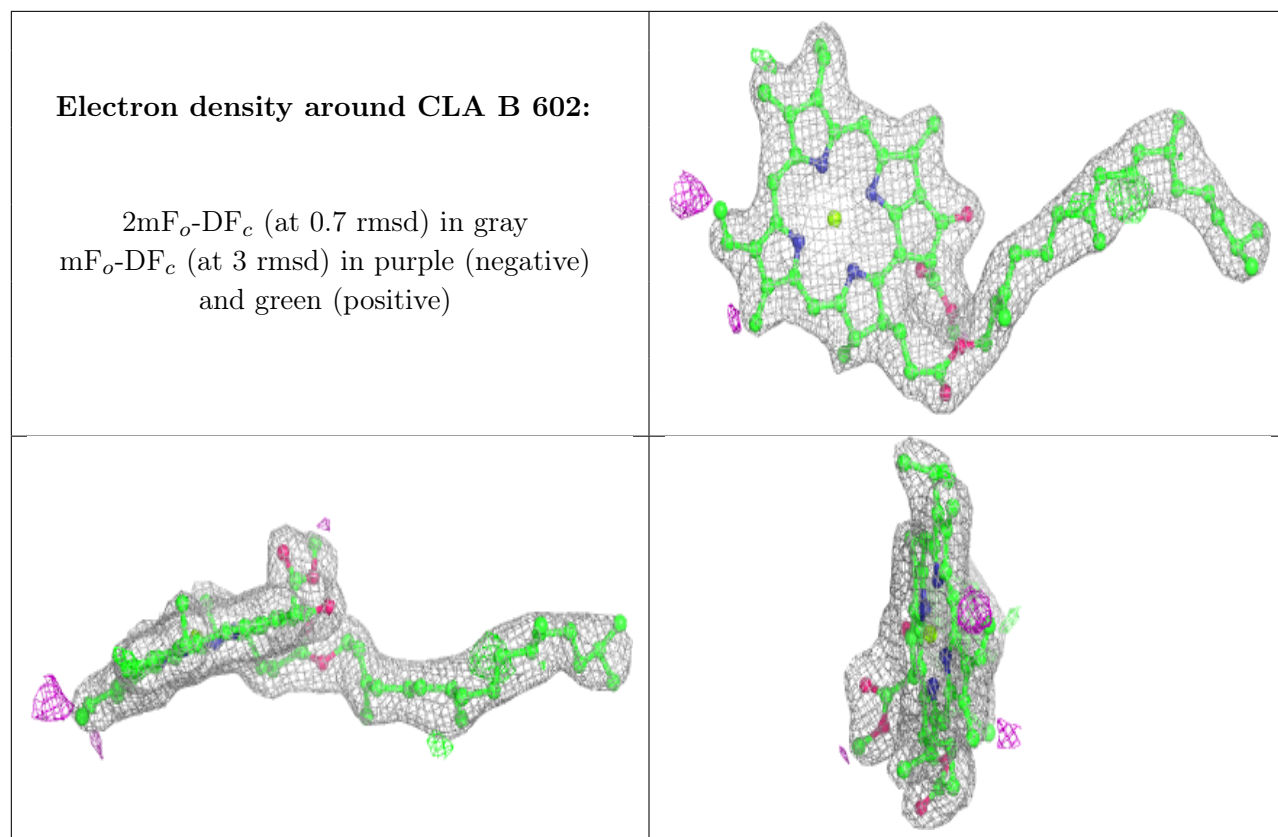




Electron density around CLA c 505:

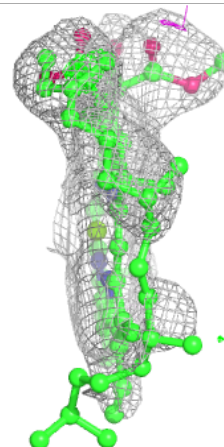
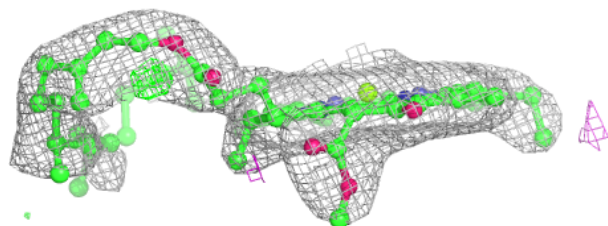
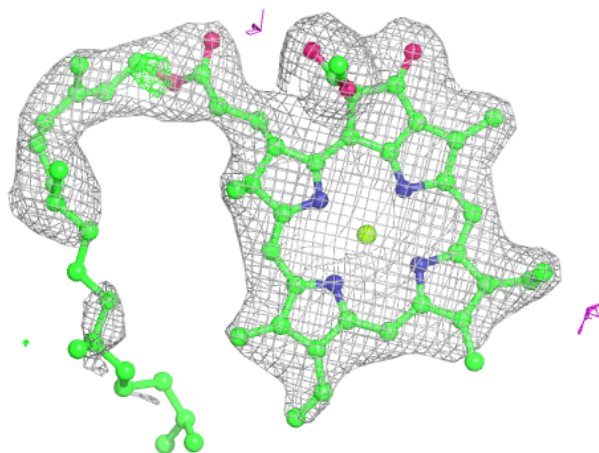
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





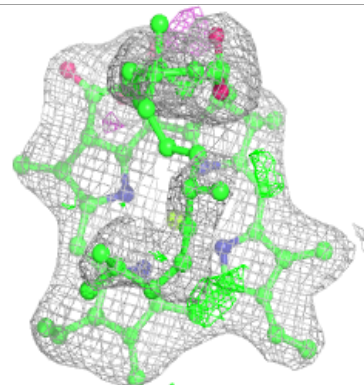
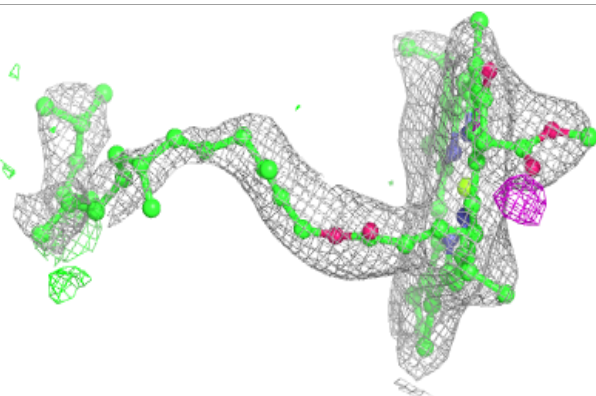
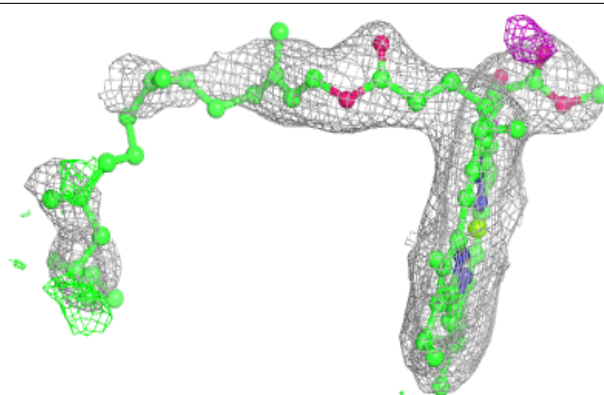
Electron density around CLA C 514:

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

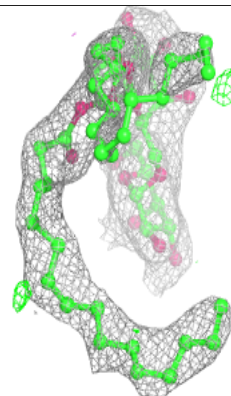
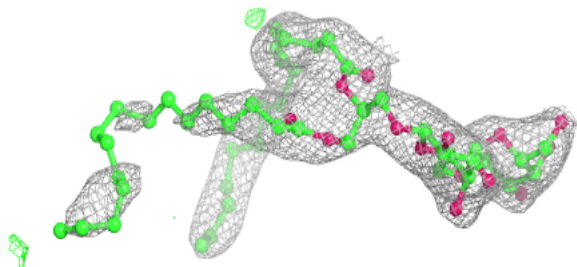
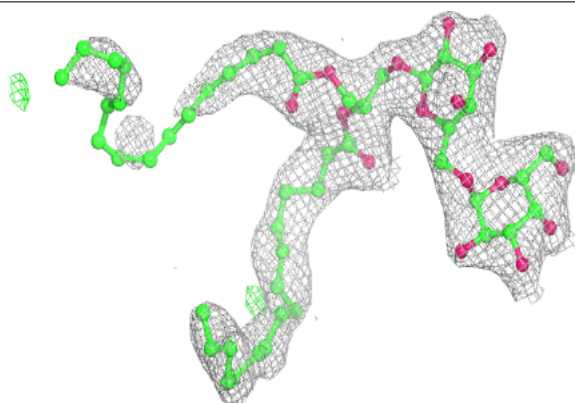


Electron density around CLA C 508:

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

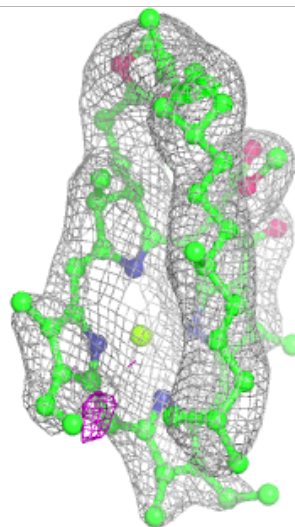
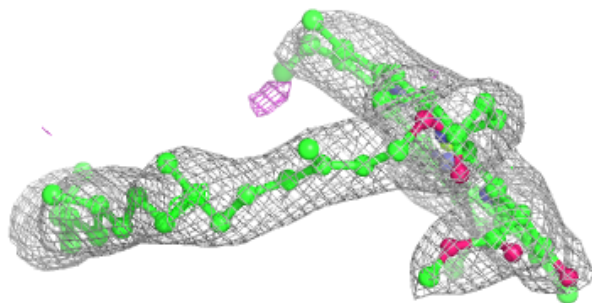
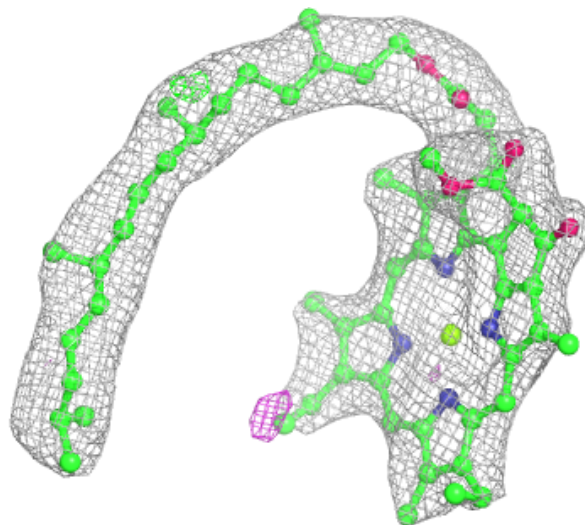
**Electron density around DGD c 519:**

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



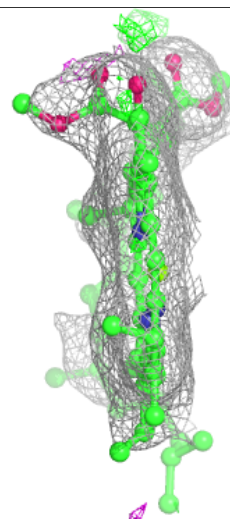
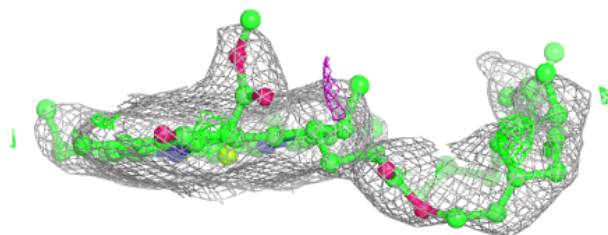
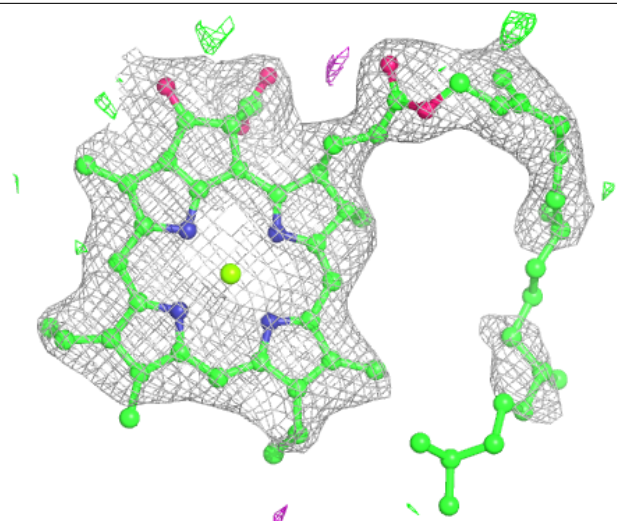
Electron density around CLA c 509:

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



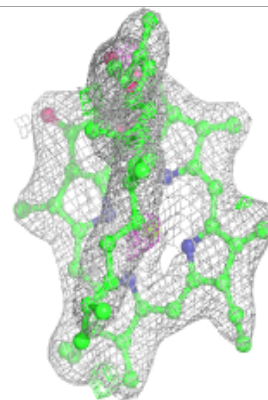
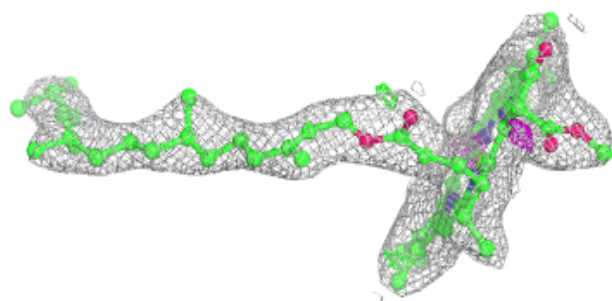
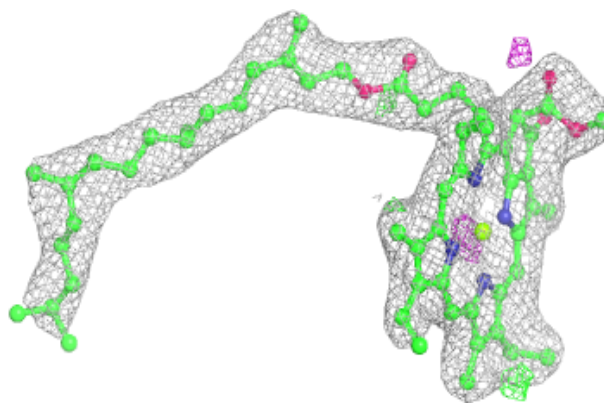
Electron density around CLA c 514:

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

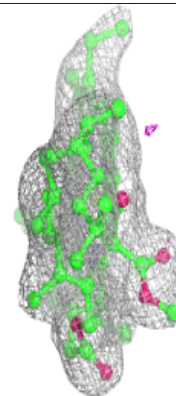
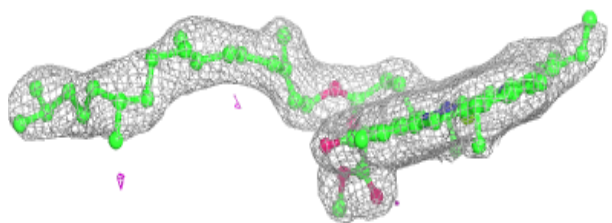
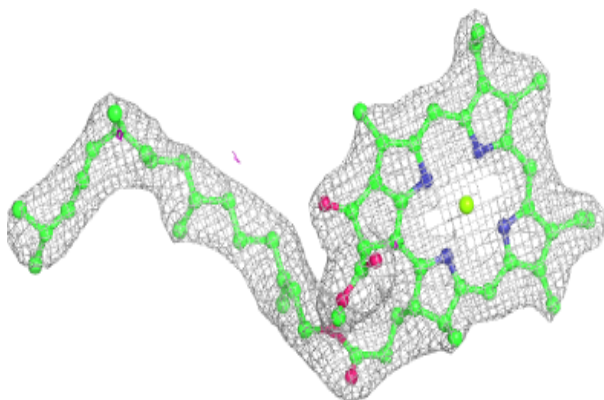


Electron density around CLA b 609:

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

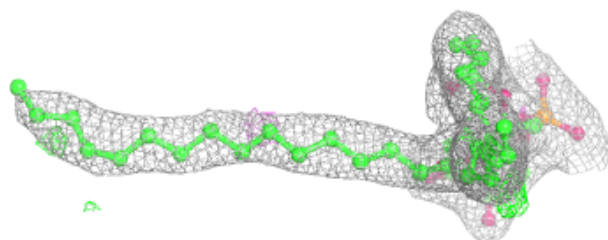
**Electron density around CLA b 602:**

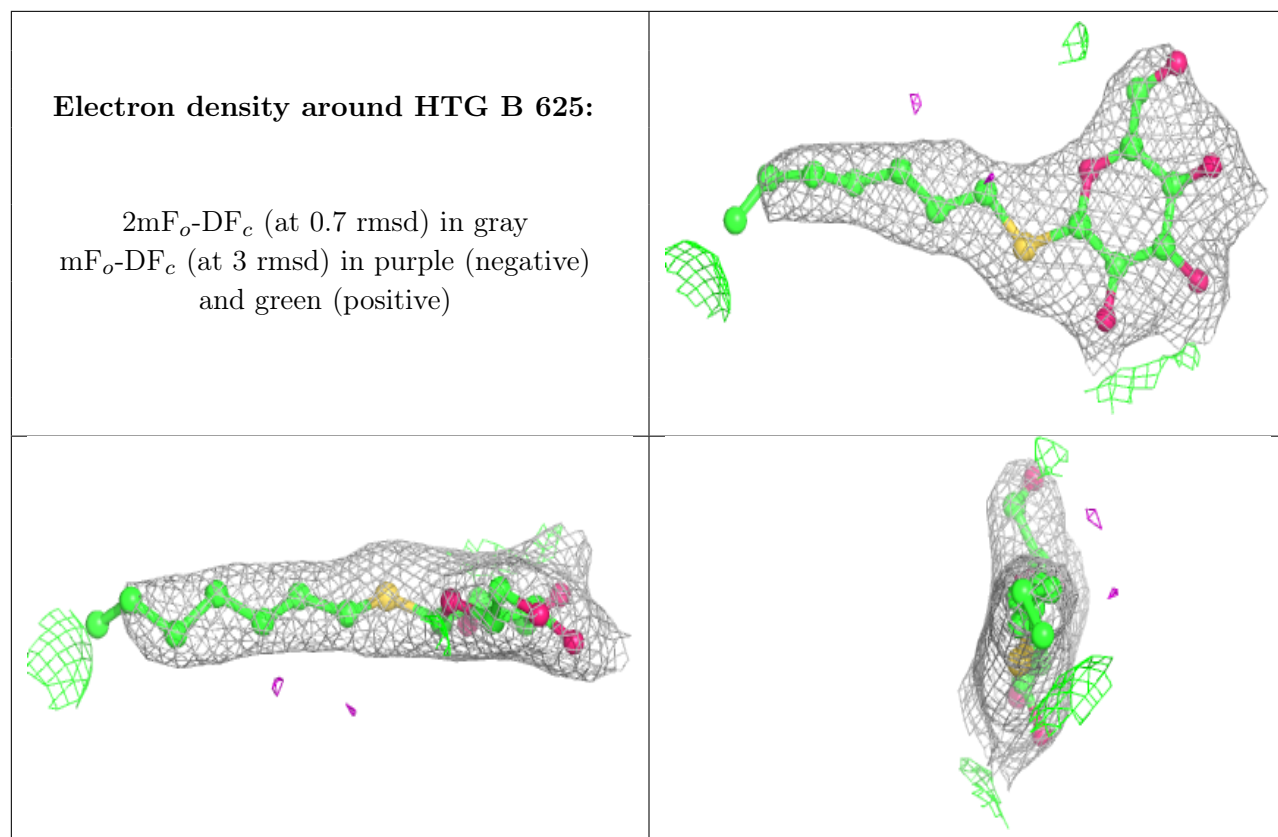
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LHG b 629:

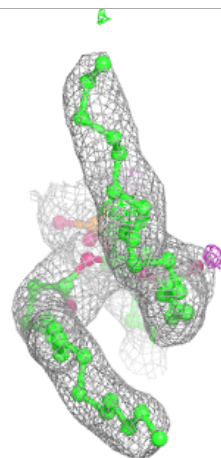
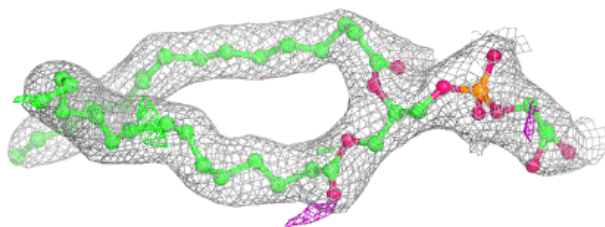
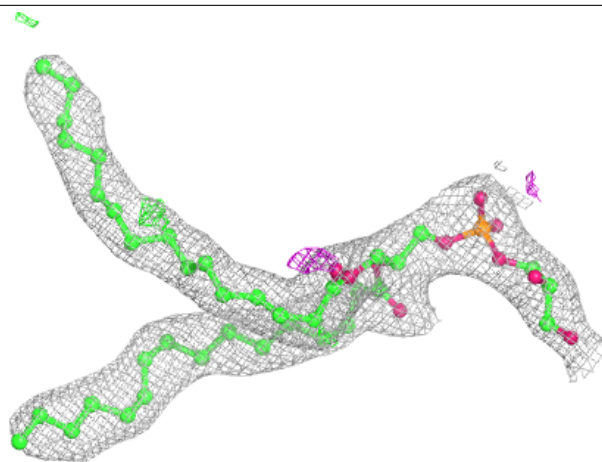
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





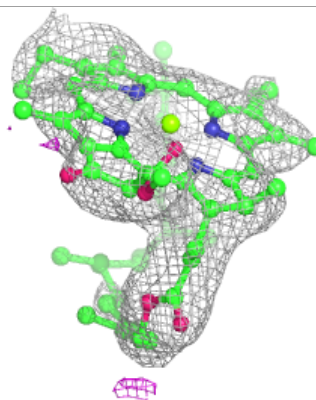
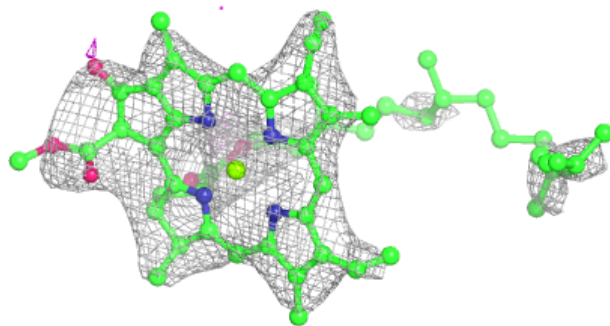
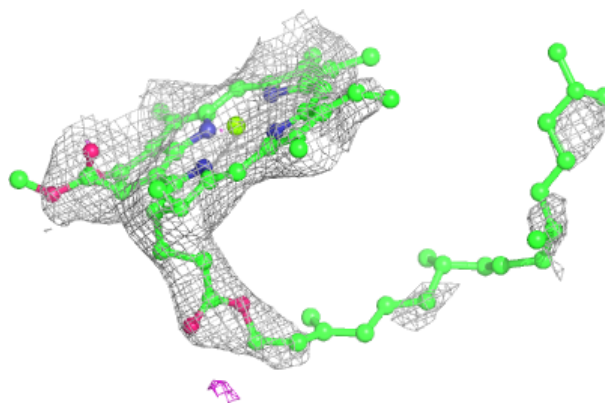
Electron density around LHG d 407:

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

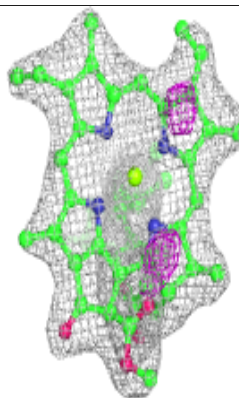
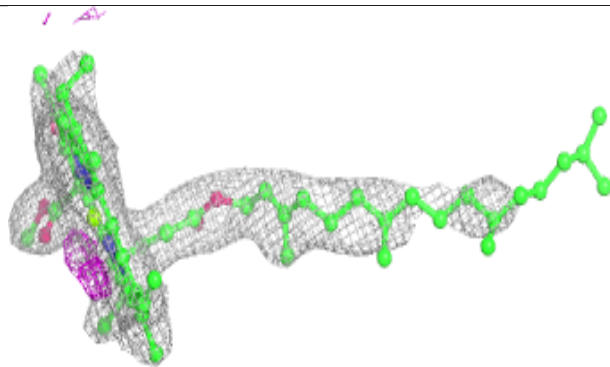
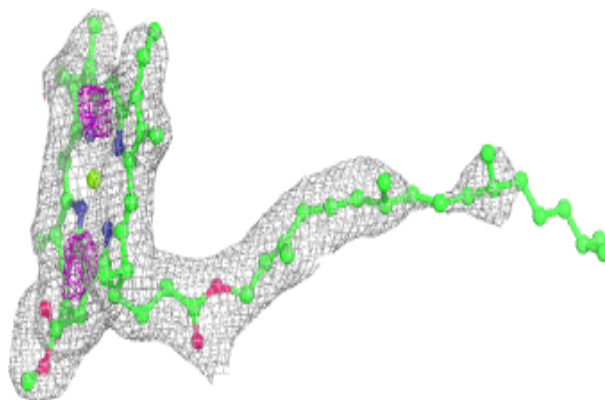


Electron density around CLA c 515:

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

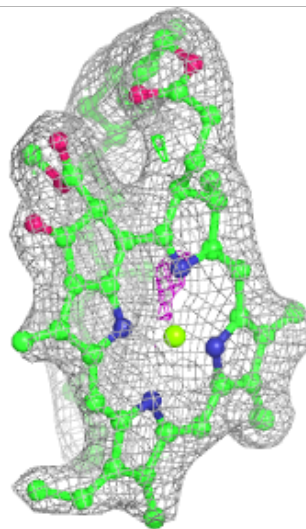
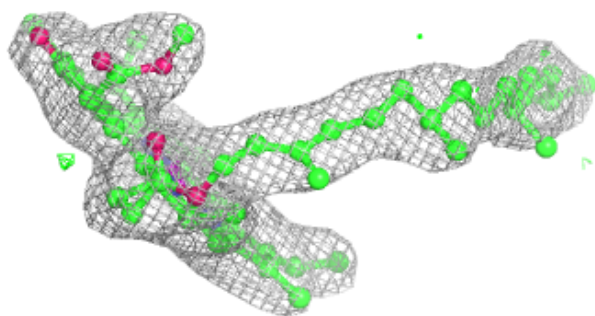
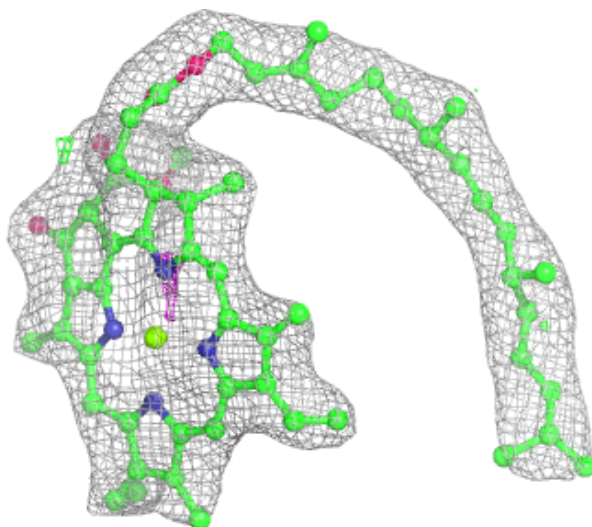
**Electron density around CLA d 403:**

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



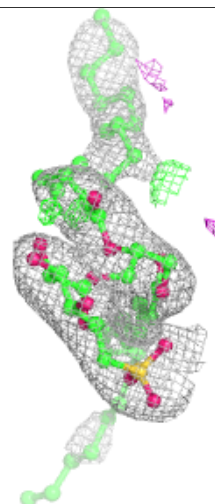
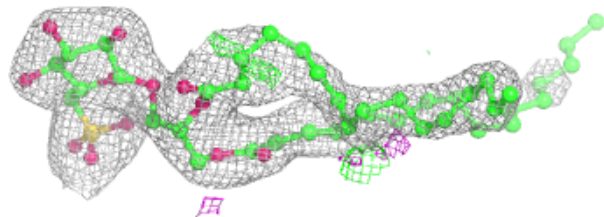
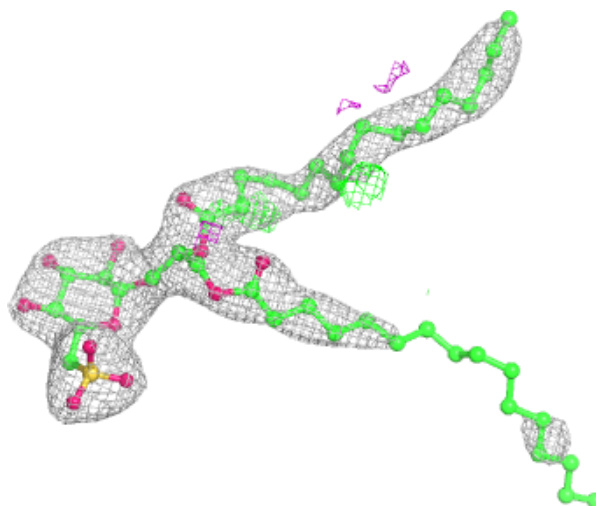
Electron density around CLA C 509:

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



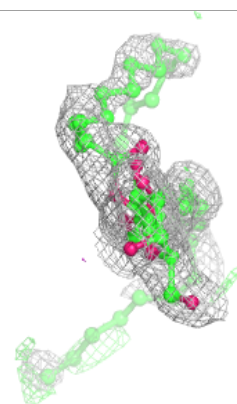
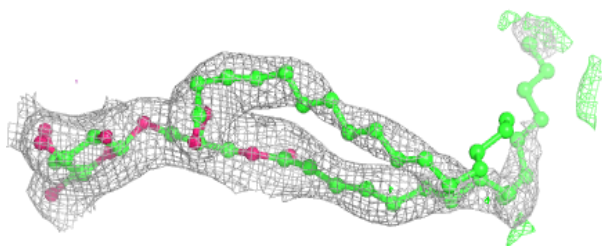
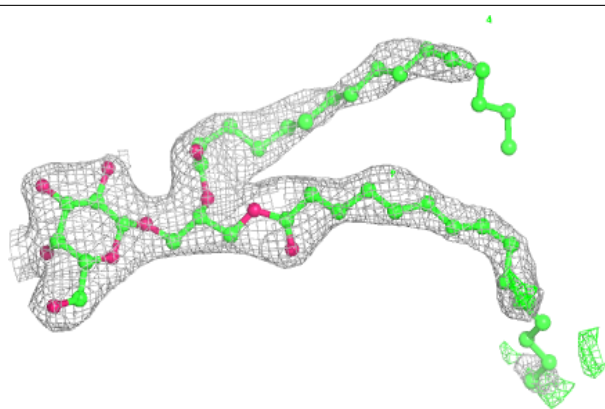
Electron density around SQD C 501:

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

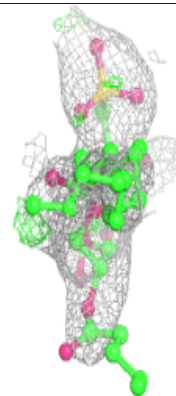
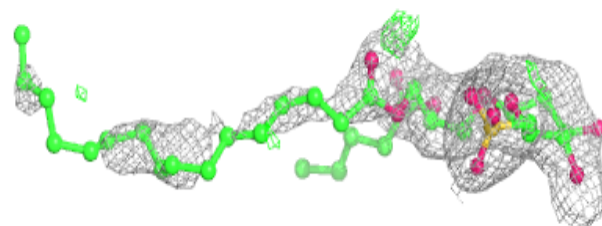
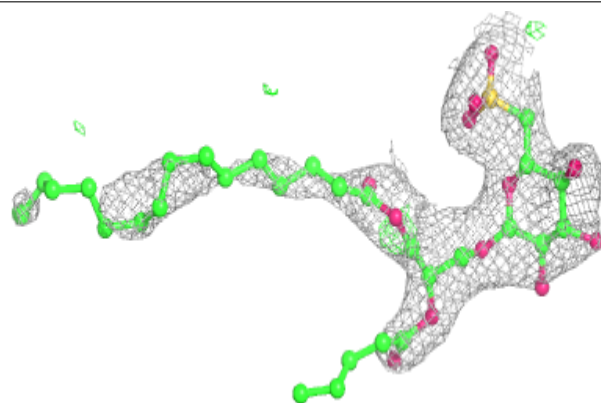


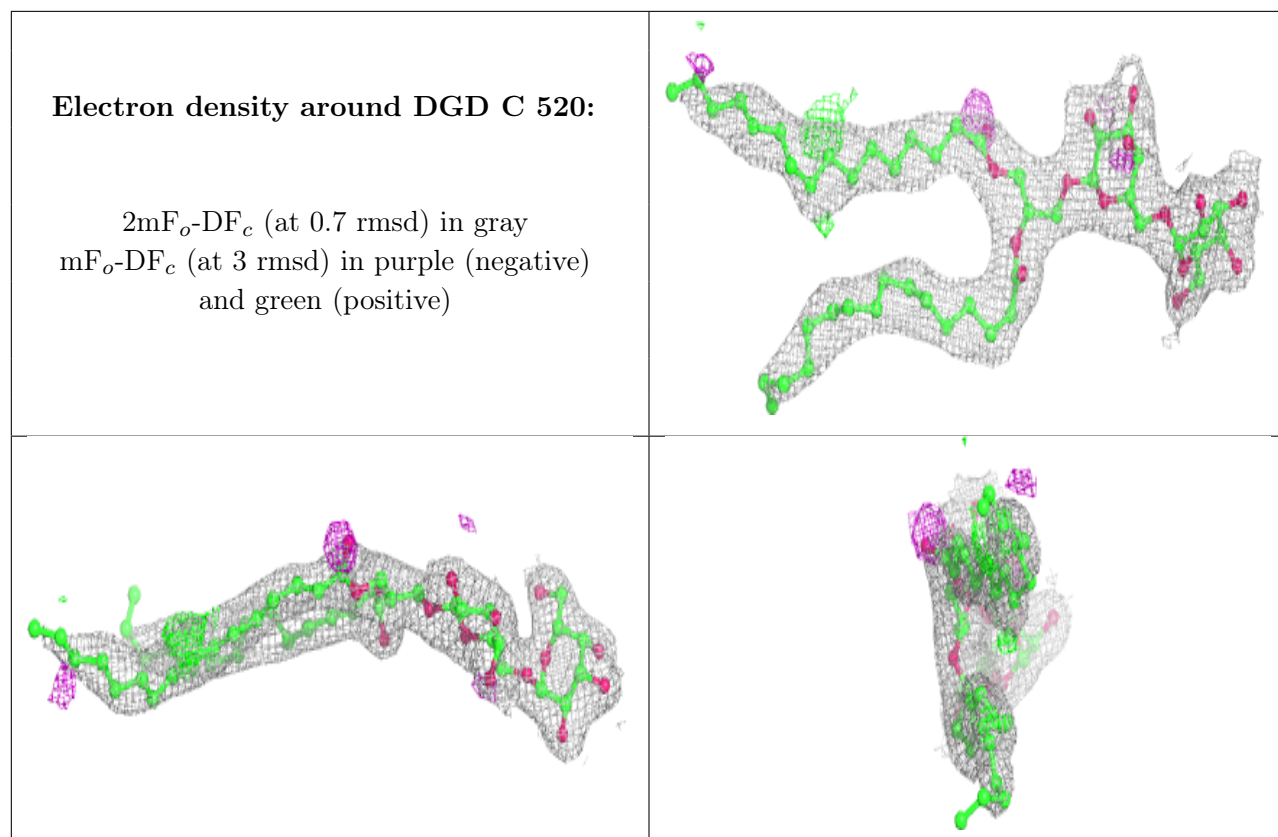
Electron density around LMG D 413:

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

**Electron density around SQD D 412:**

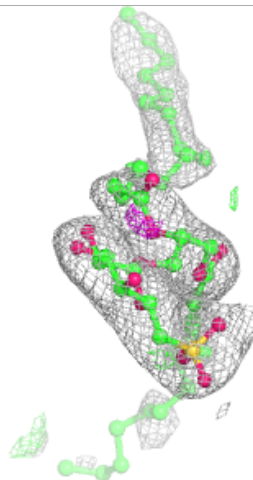
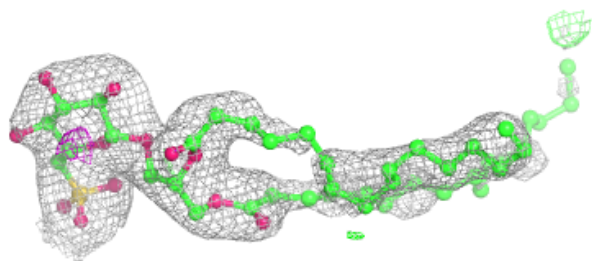
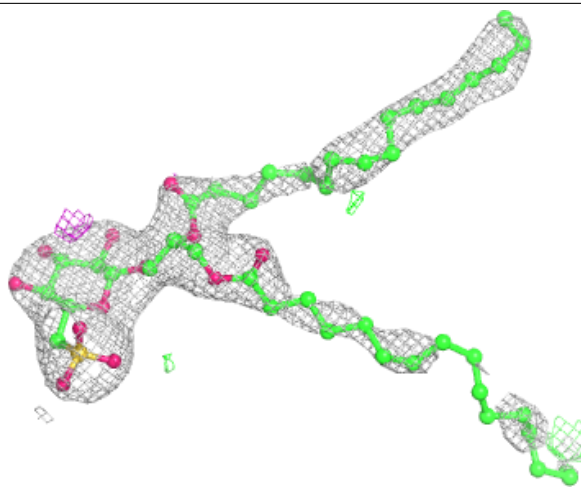
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





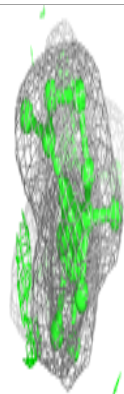
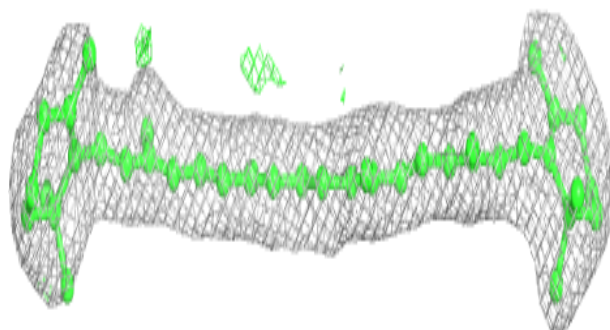
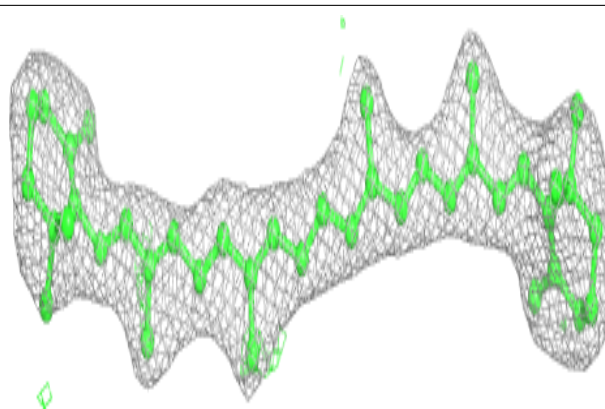
Electron density around SQD a 410:

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

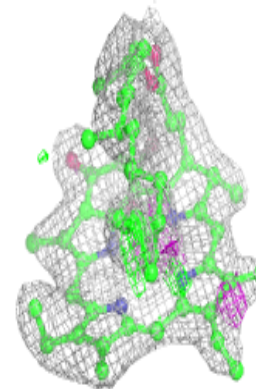
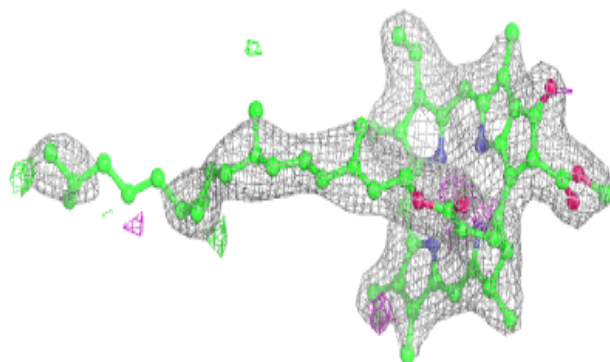
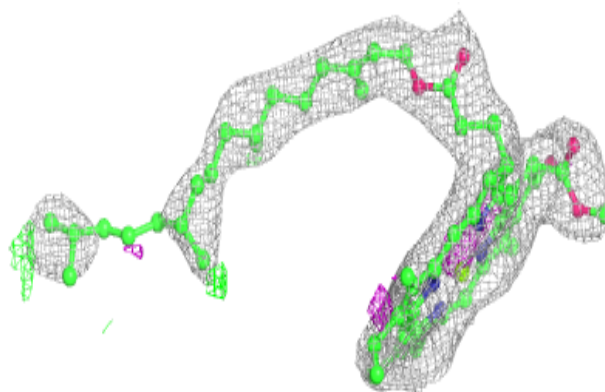


Electron density around BCR b 618:

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

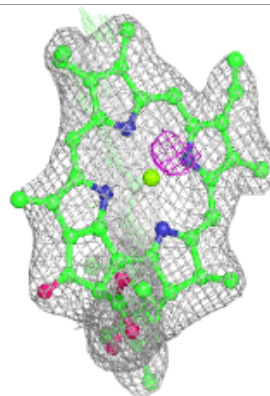
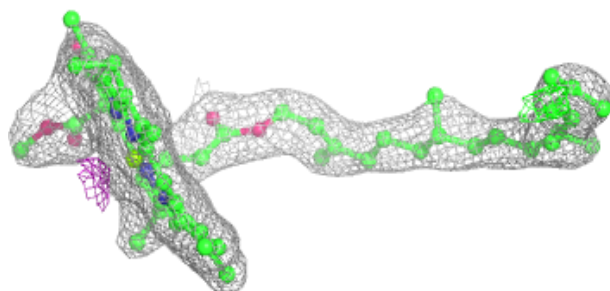
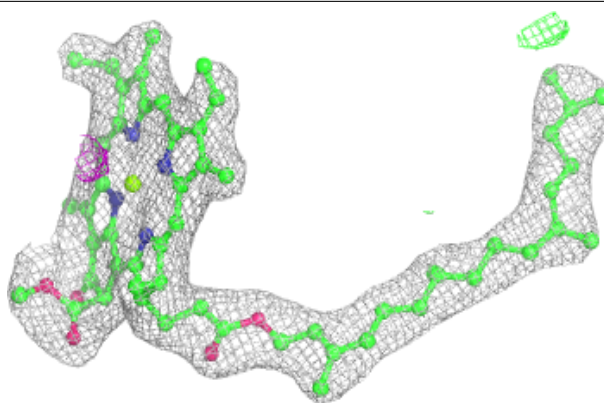
**Electron density around CLA C 506:**

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

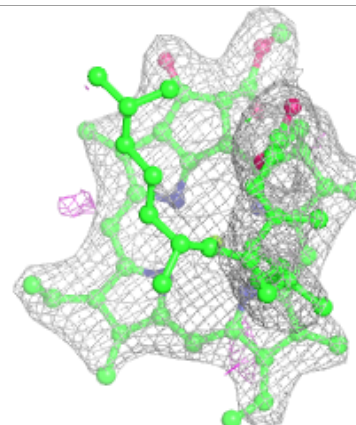
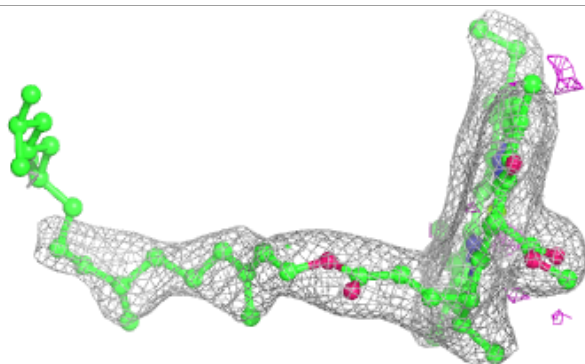
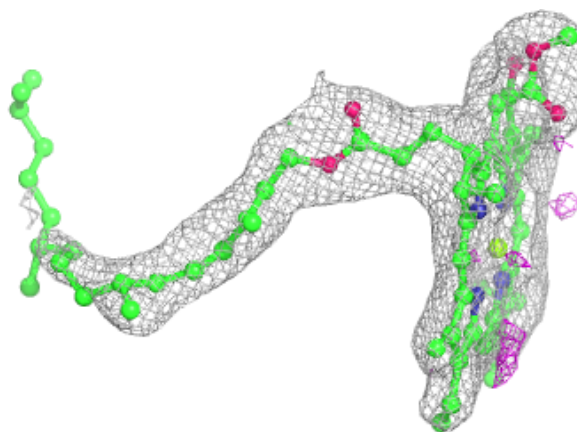


Electron density around CLA B 609:

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

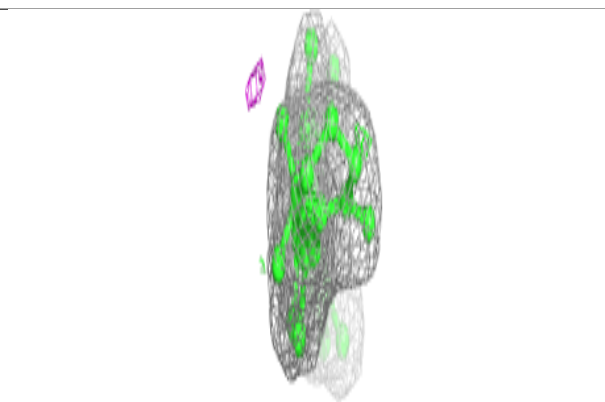
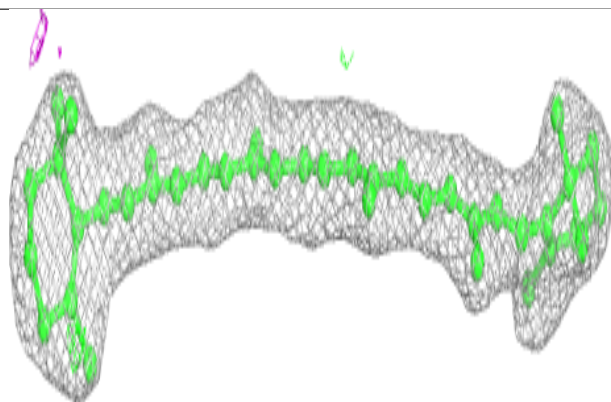
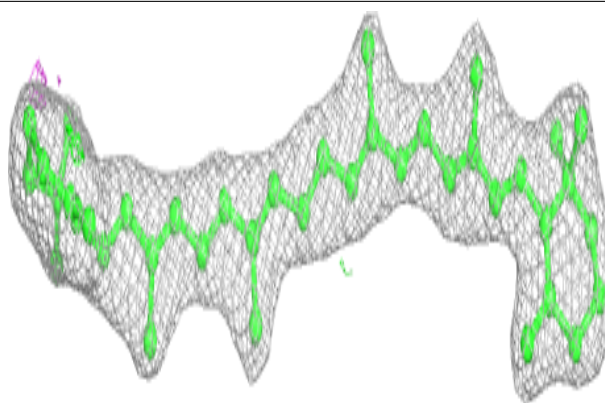
**Electron density around CLA D 404:**

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

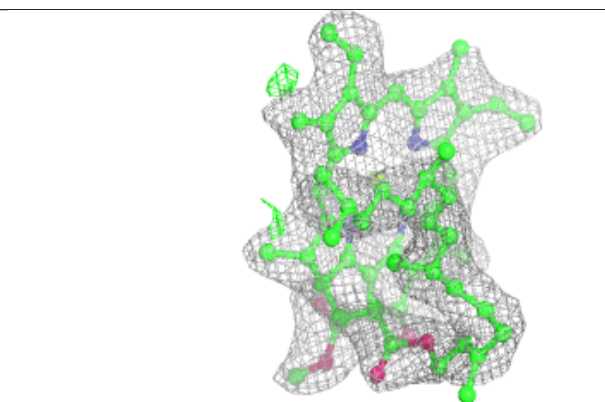
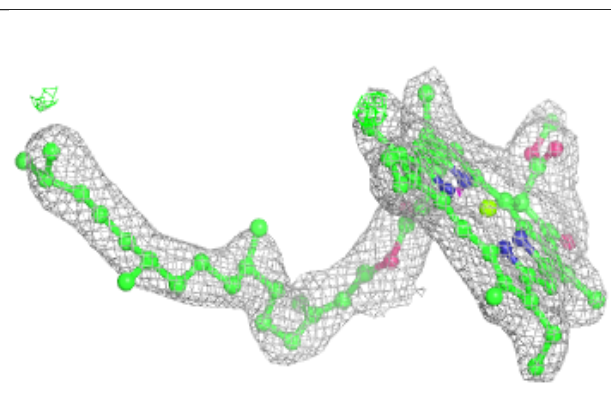
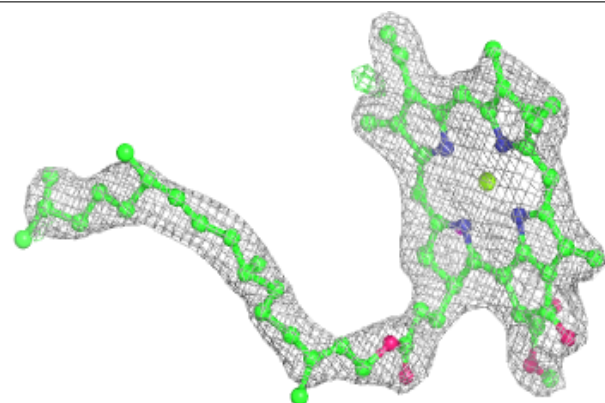


Electron density around BCR b 617:

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

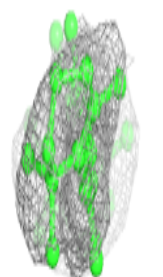
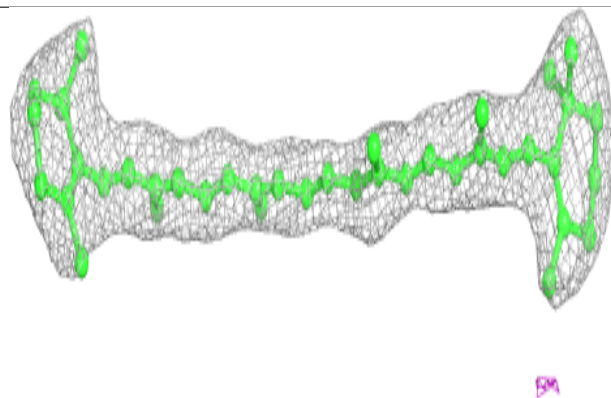
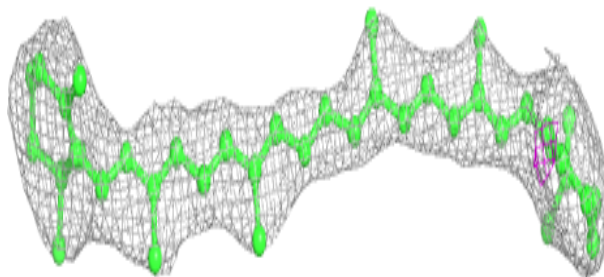
**Electron density around CLA C 513:**

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

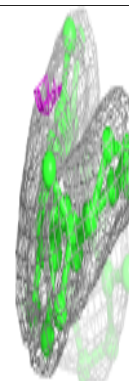
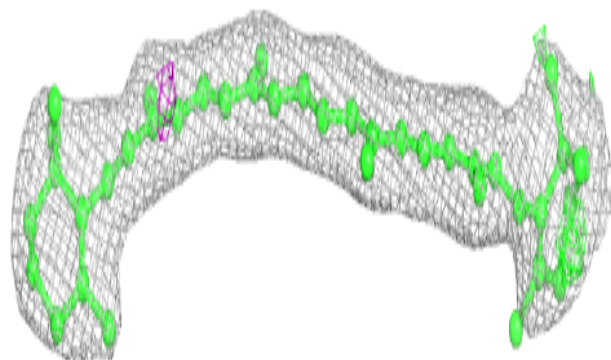
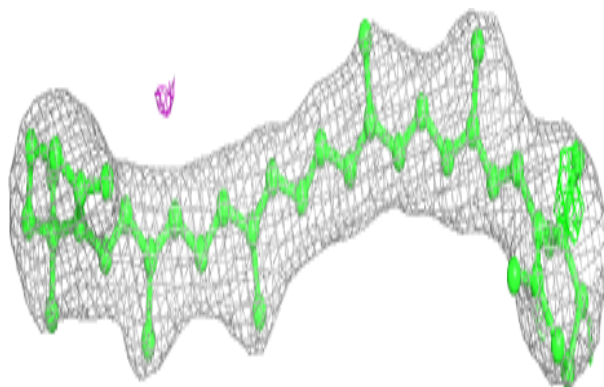


Electron density around BCR c 516:

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

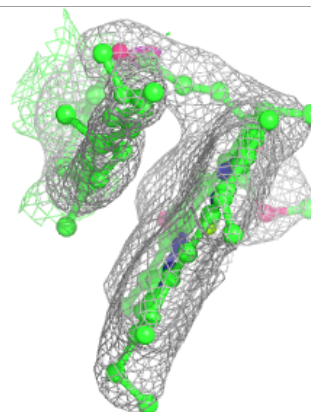
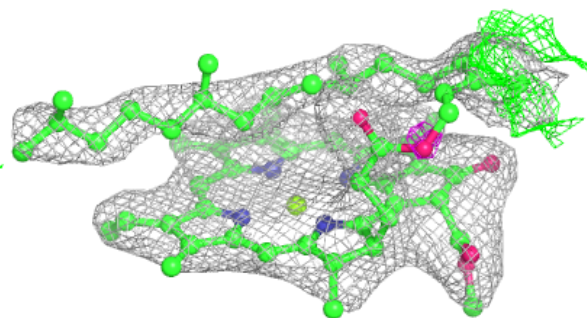
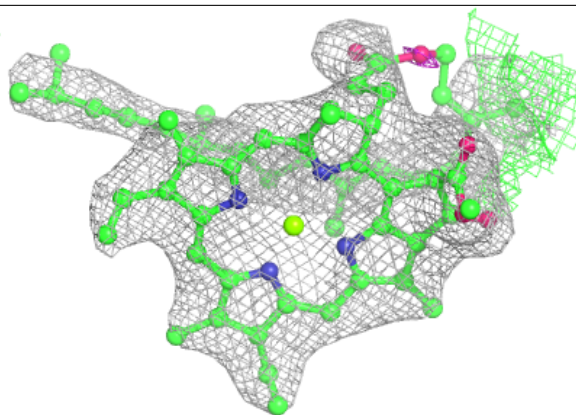
**Electron density around BCR d 404:**

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

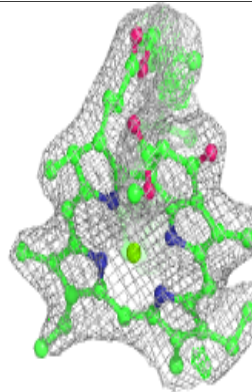
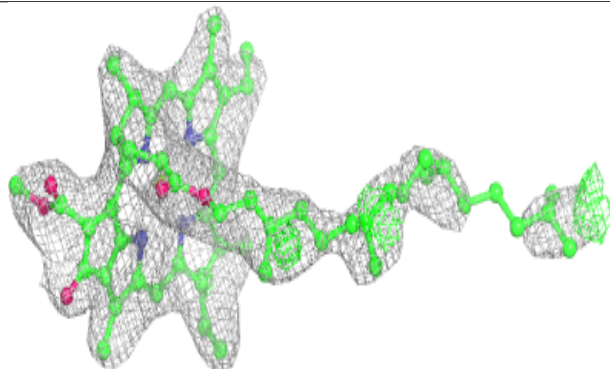
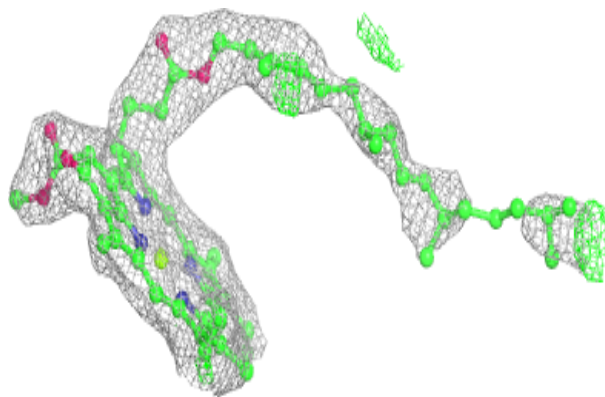


Electron density around CLA b 601:

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

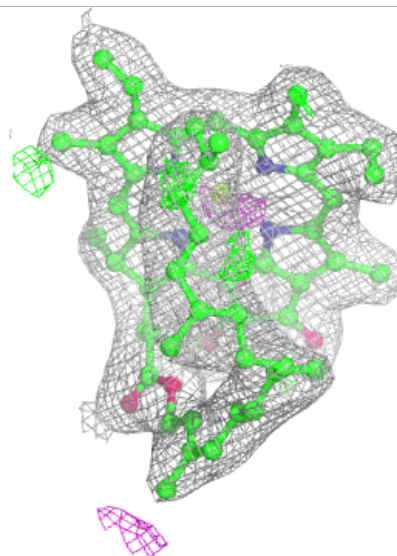
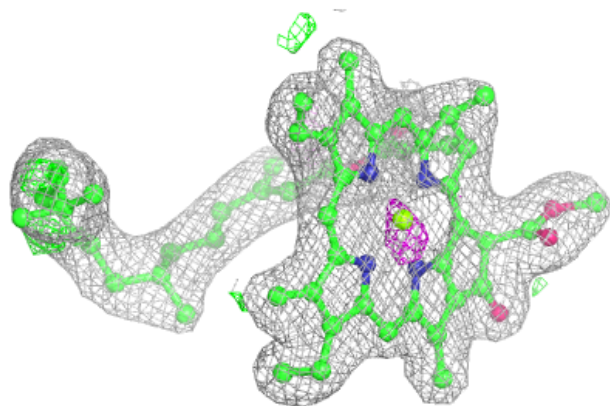
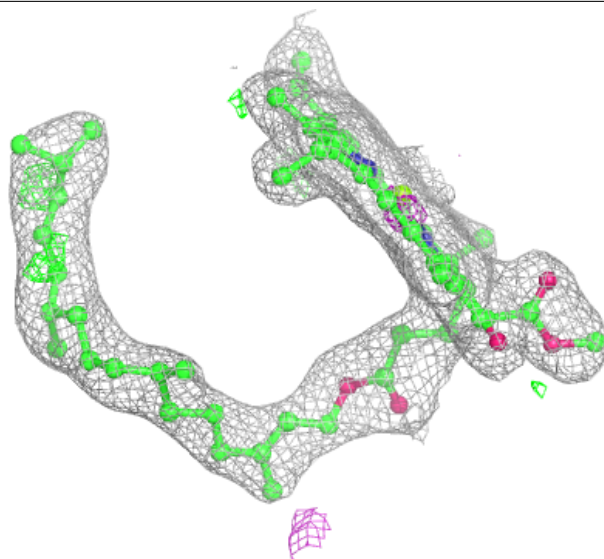
**Electron density around CLA c 506:**

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



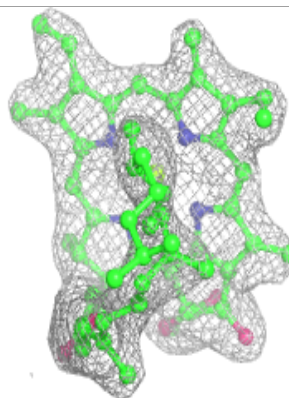
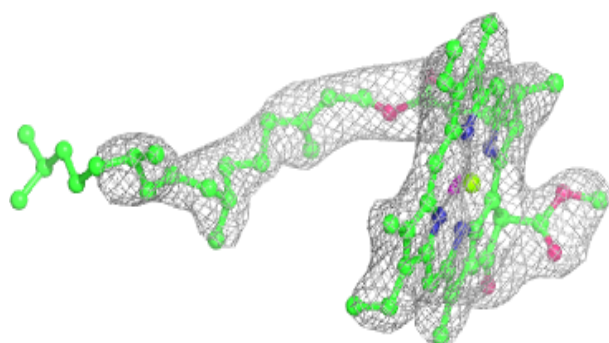
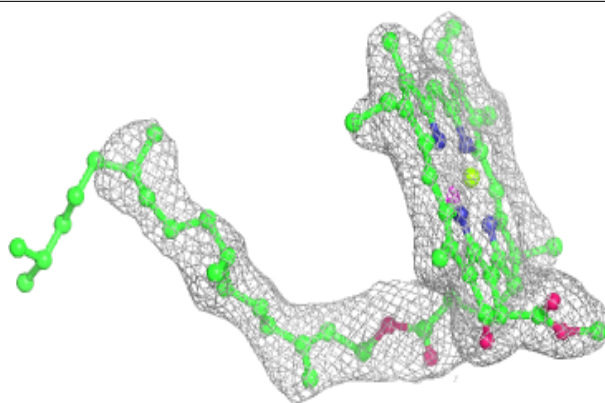
Electron density around CLA B 611:

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

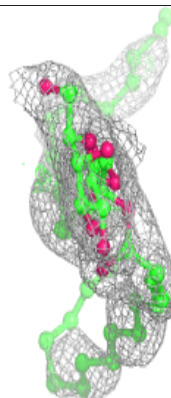
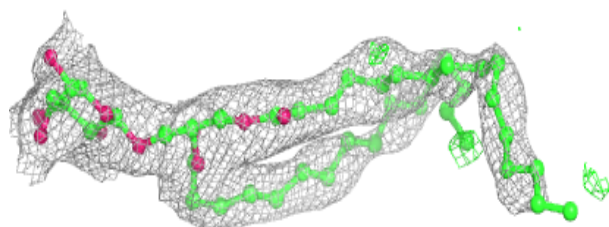
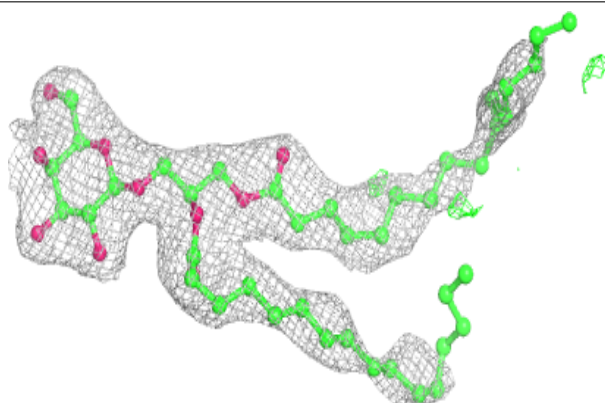


Electron density around CLA c 510:

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

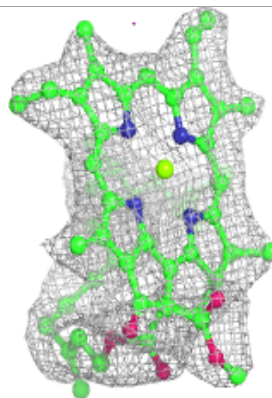
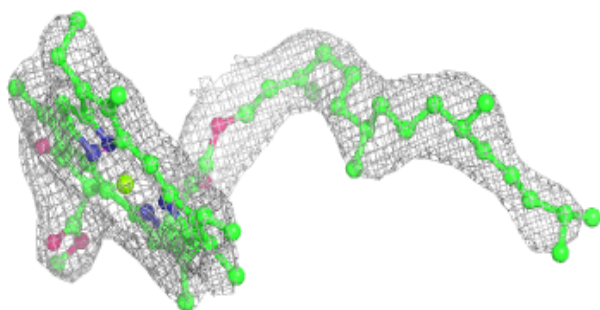
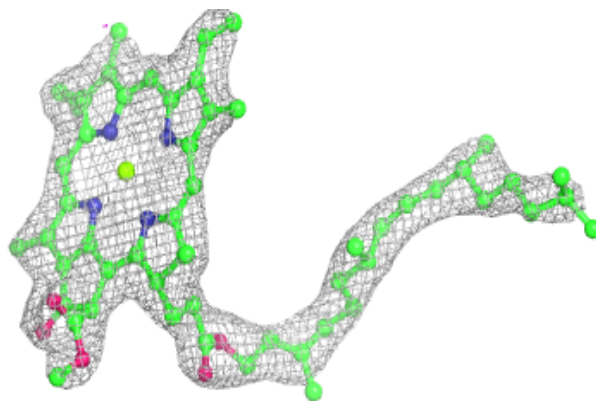
**Electron density around LMG d 412:**

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

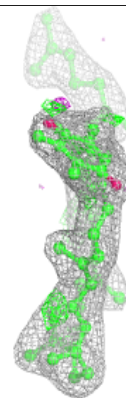
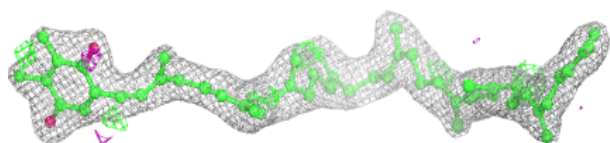
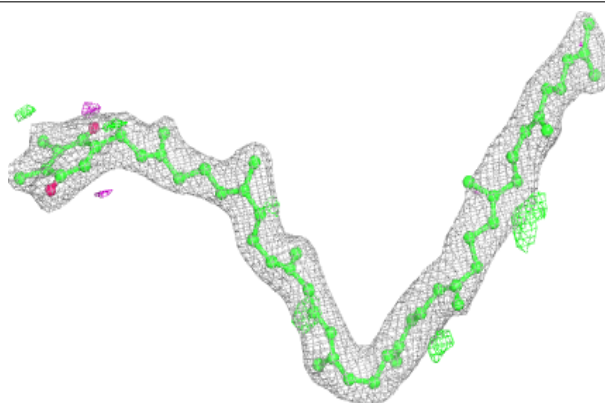


Electron density around CLA c 513:

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

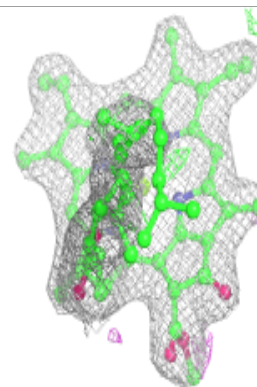
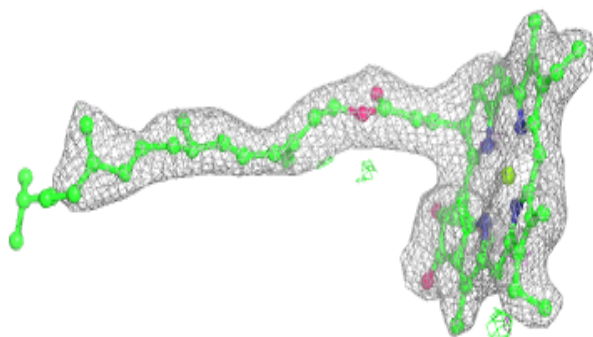
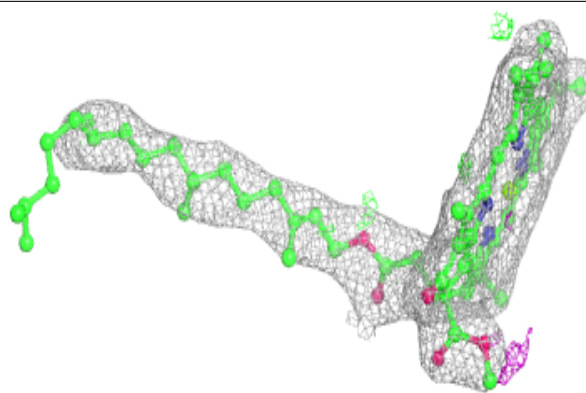
**Electron density around PL9 D 406:**

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

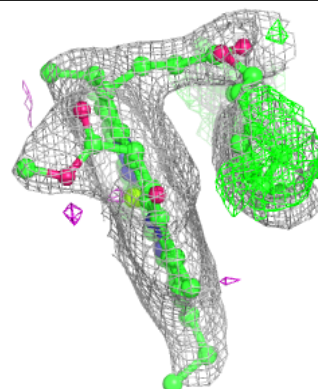
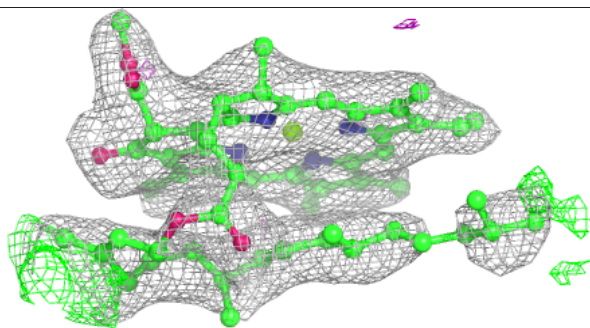
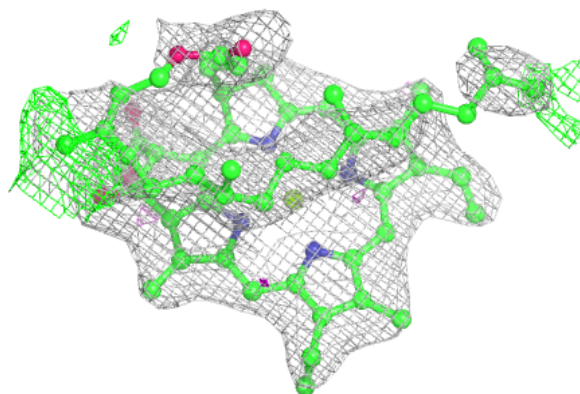


Electron density around CLA b 604:

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

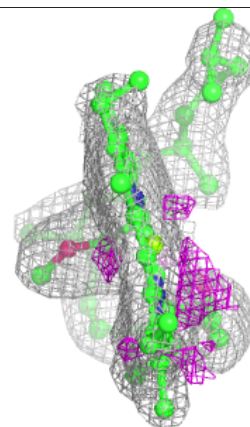
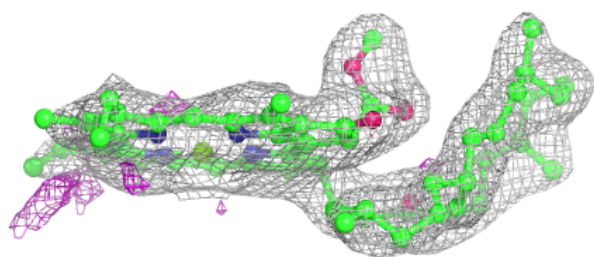
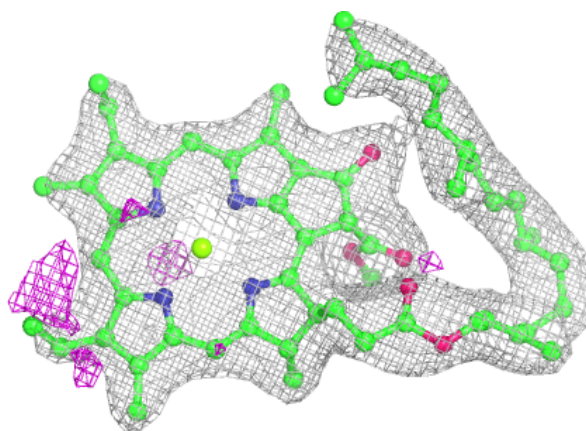
**Electron density around CLA B 601:**

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

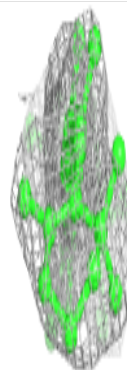
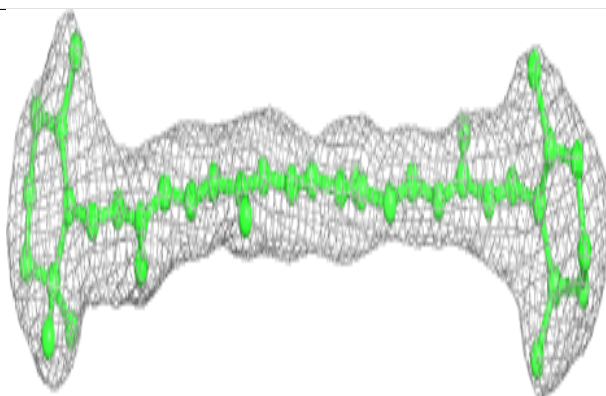
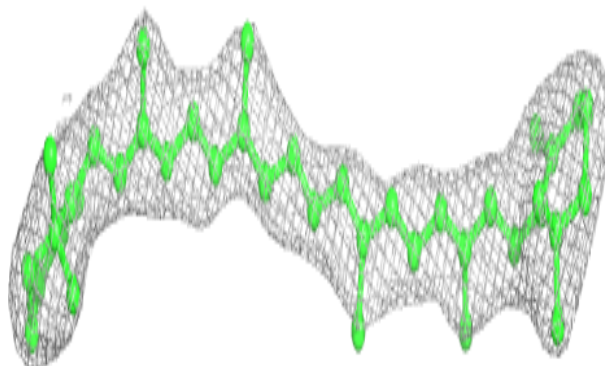


Electron density around CLA b 610:

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

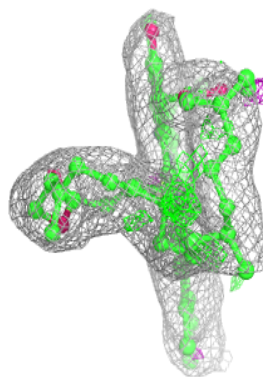
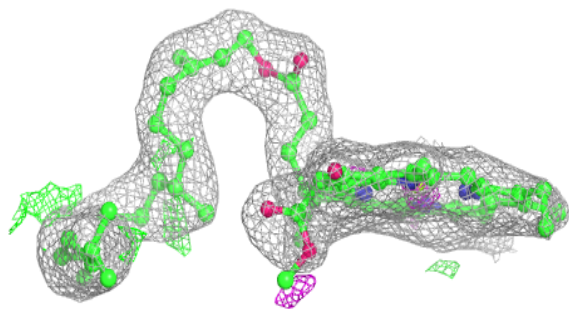
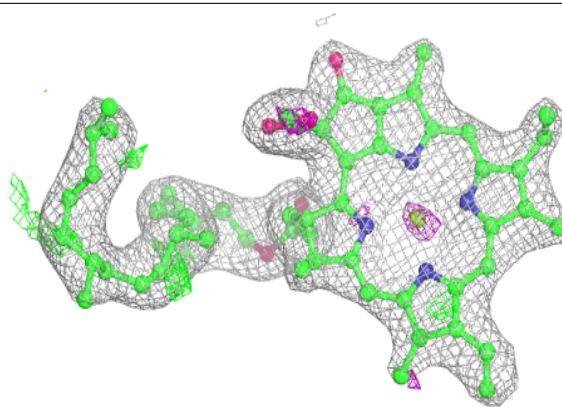
**Electron density around BCR C 516:**

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

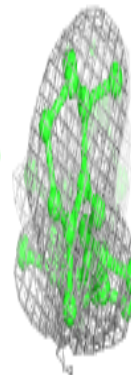
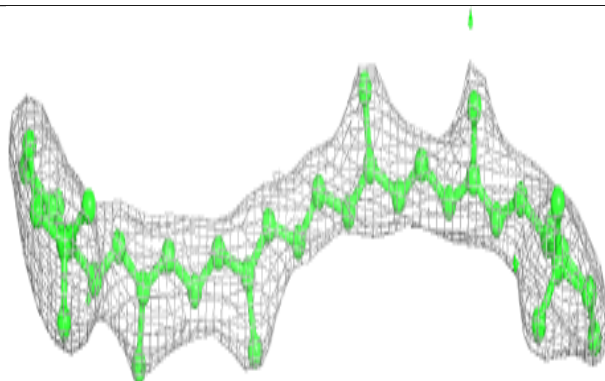
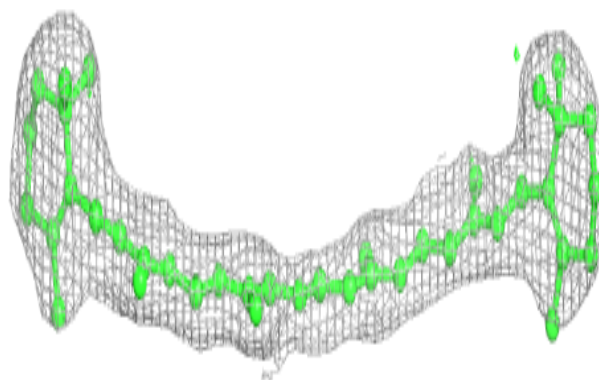


Electron density around CLA b 612:

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

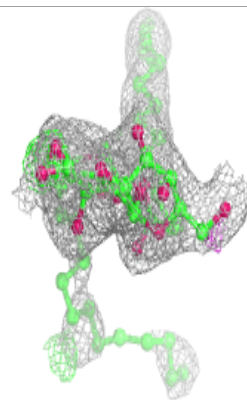
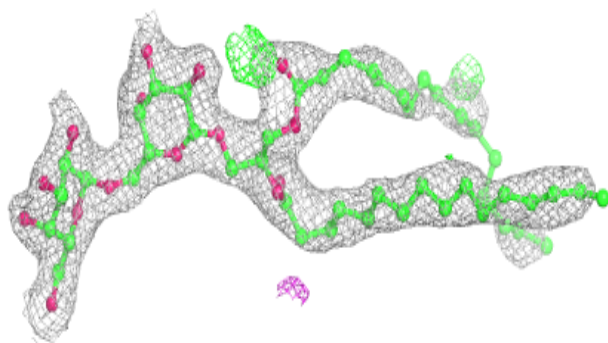
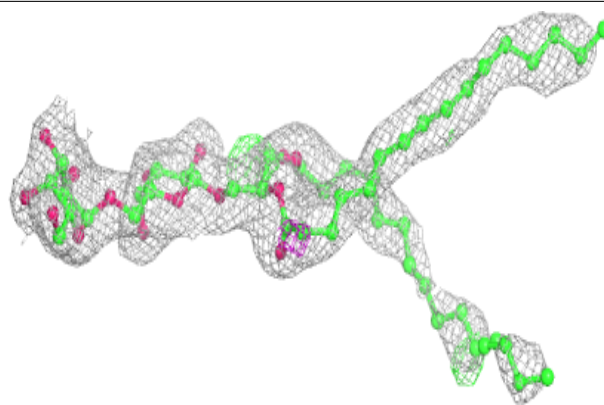
**Electron density around BCR K 101:**

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

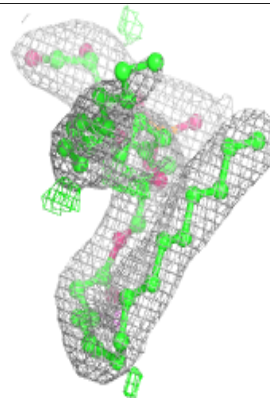
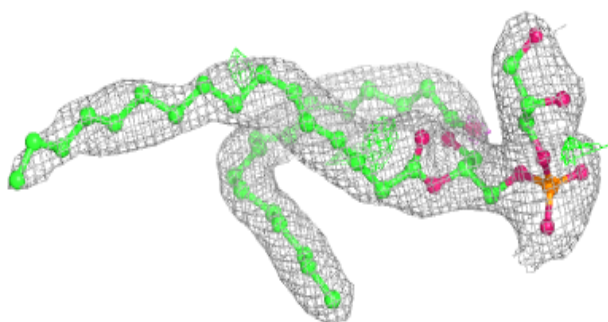
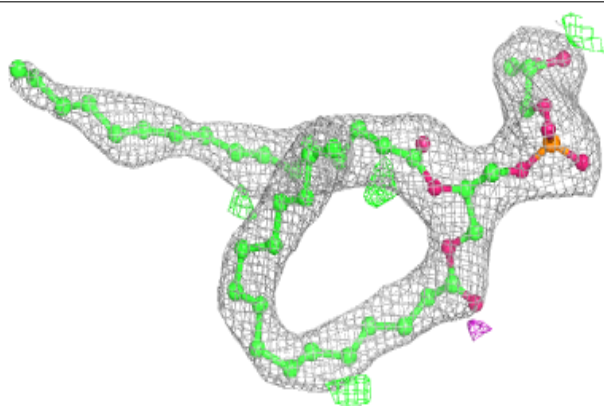


Electron density around DGD c 518:

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

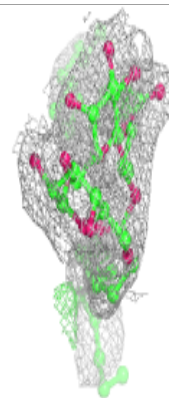
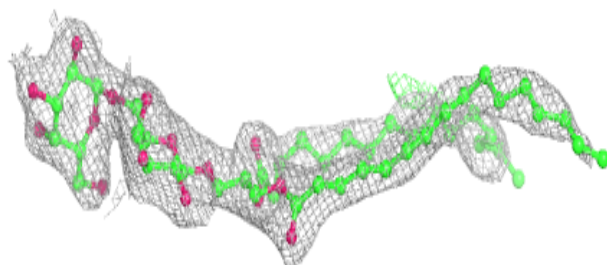
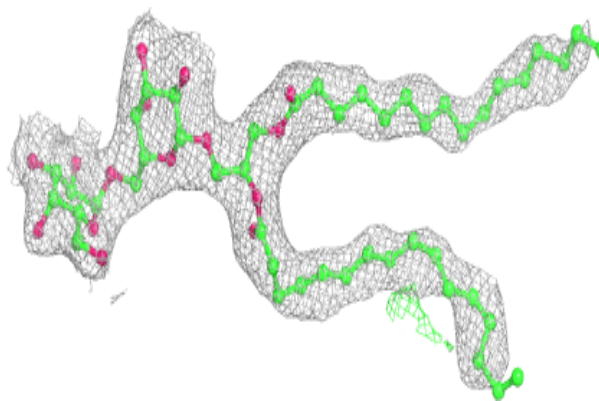
**Electron density around LHG d 406:**

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

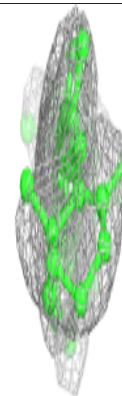
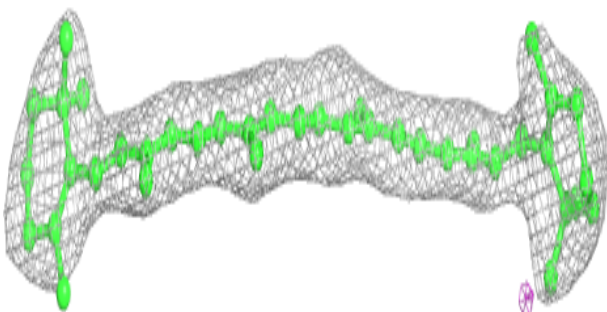
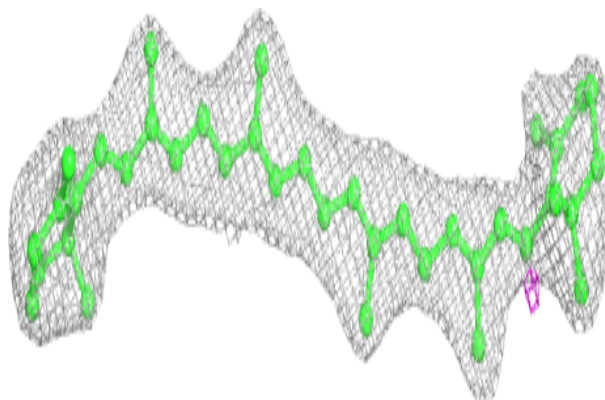


Electron density around DGD c 520:

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

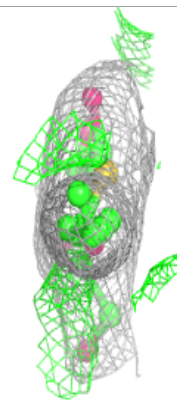
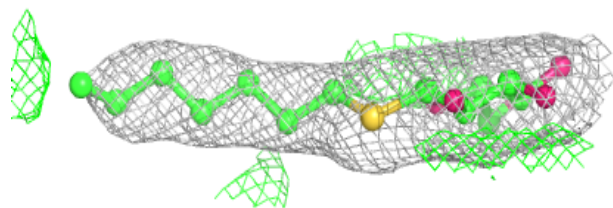
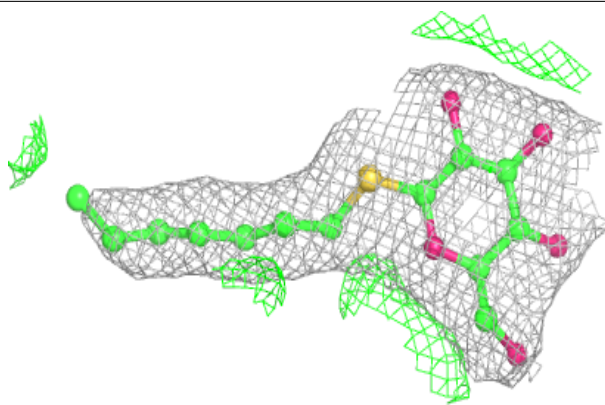
**Electron density around BCR Y 101:**

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

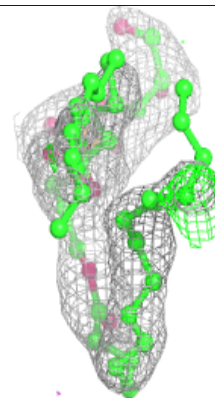
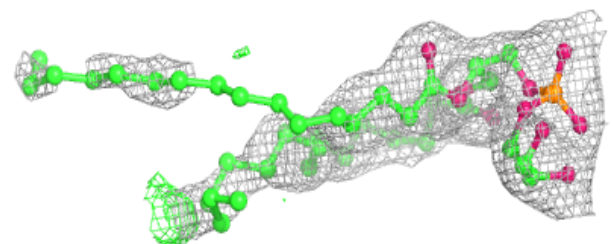
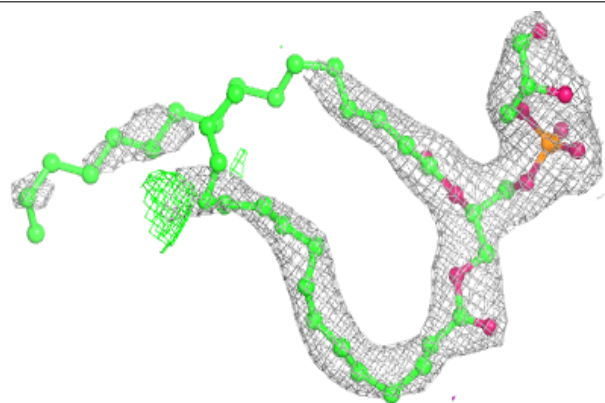


Electron density around HTG b 625:

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

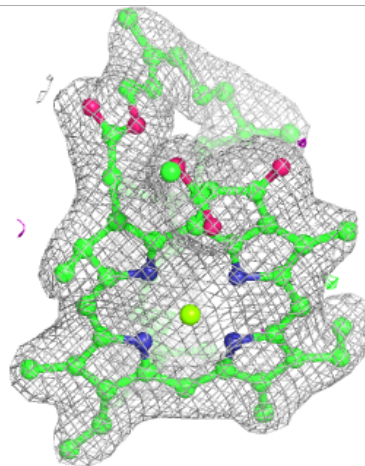
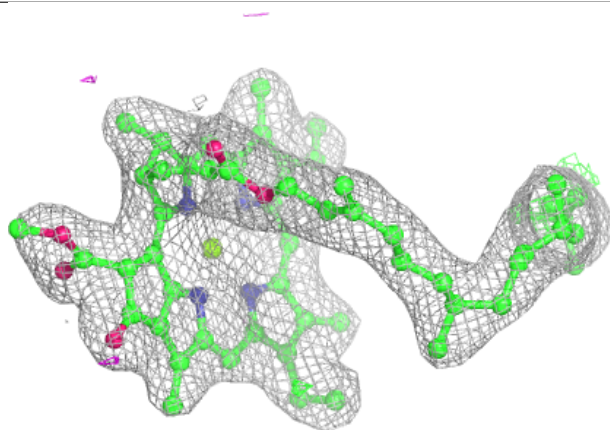
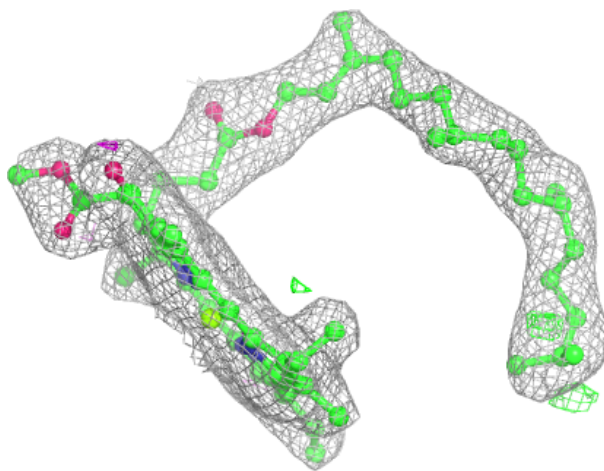
**Electron density around LHG d 408:**

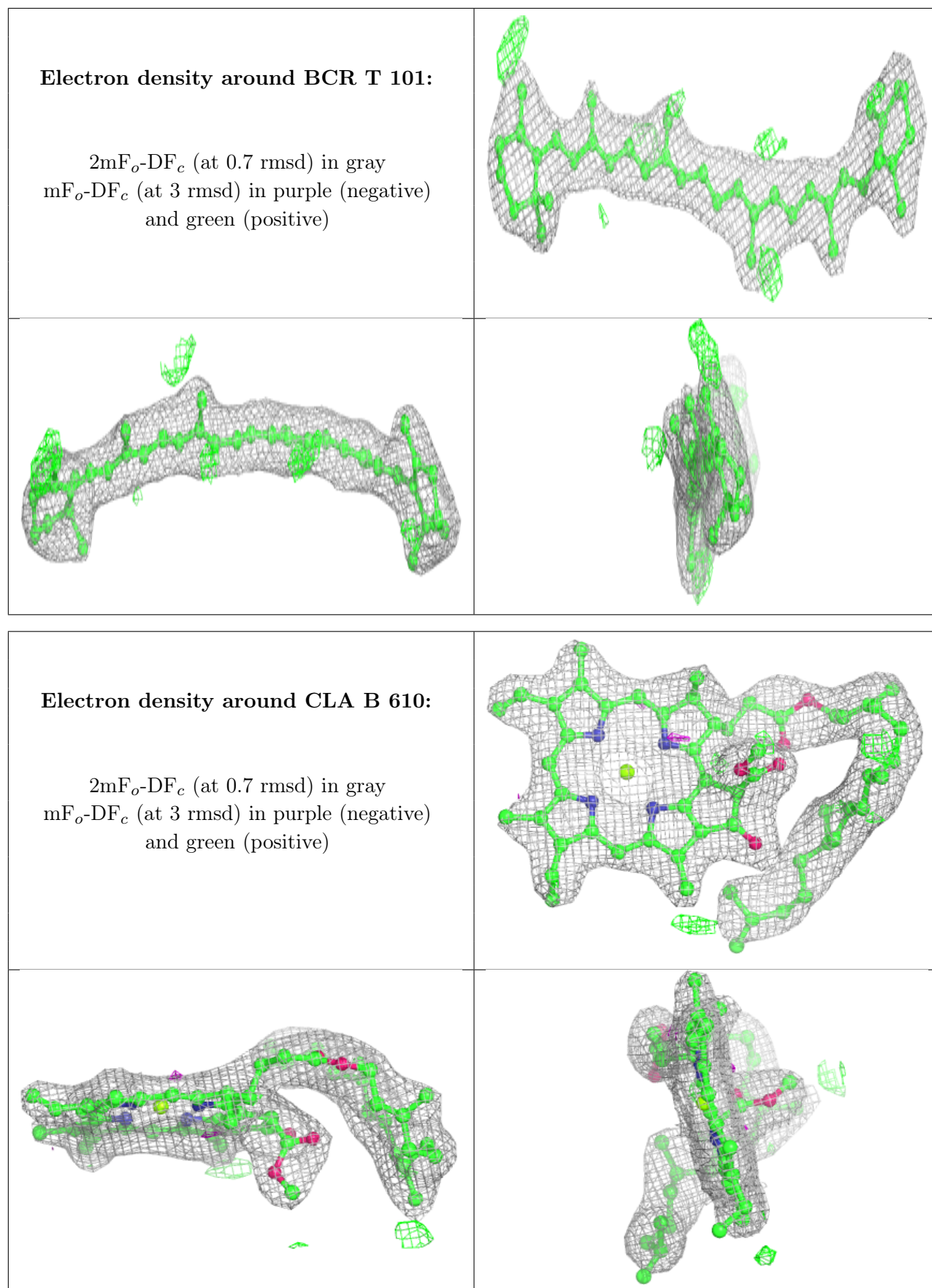
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA b 611:

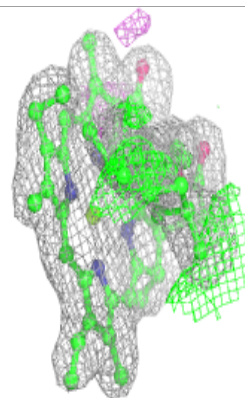
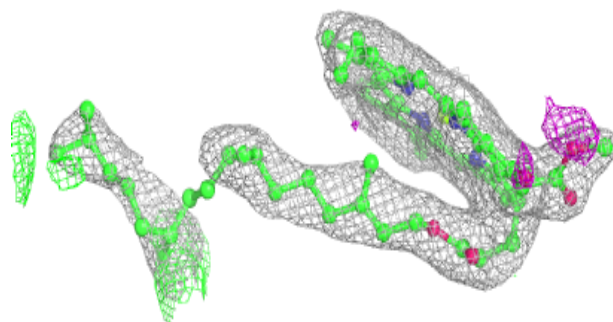
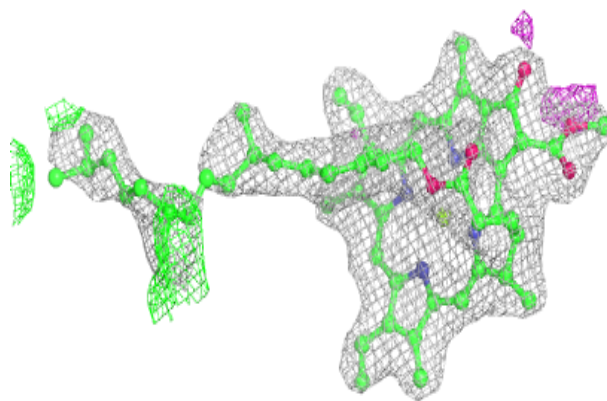
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





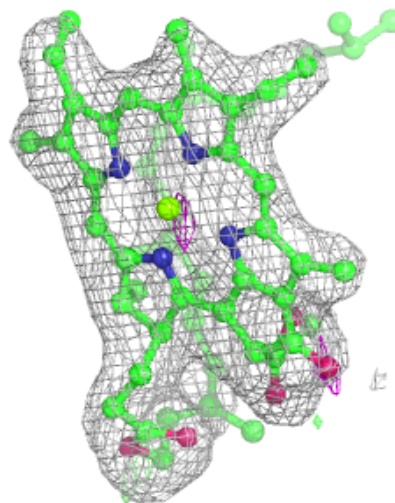
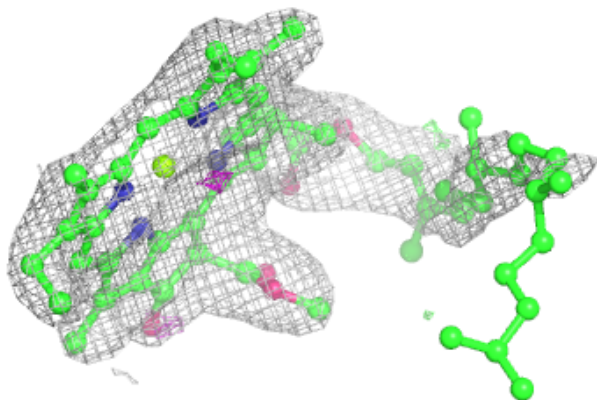
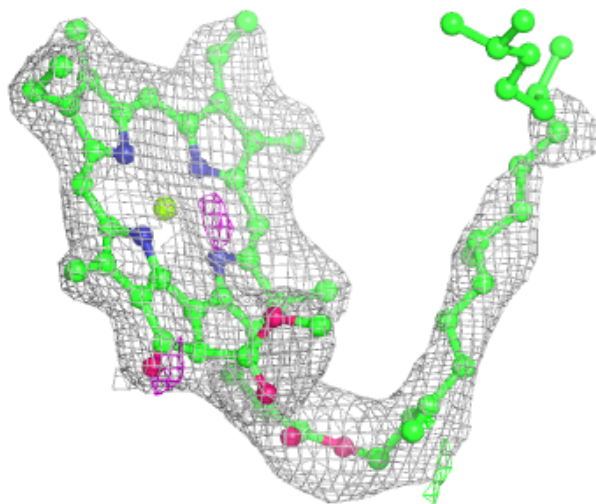
Electron density around CLA b 614:

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



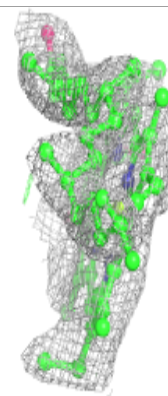
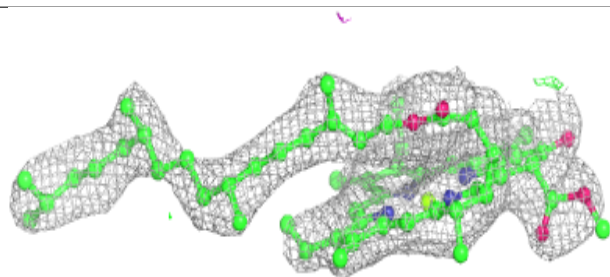
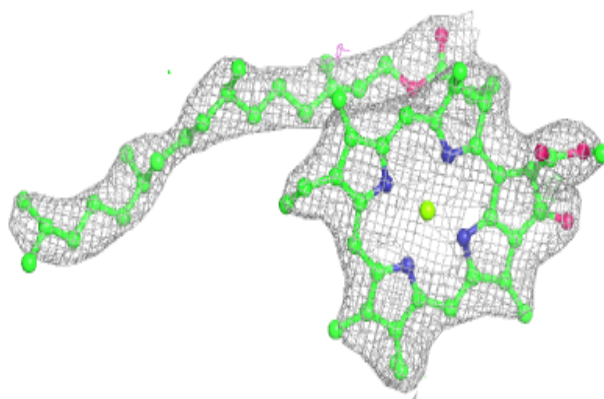
Electron density around CLA b 616:

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

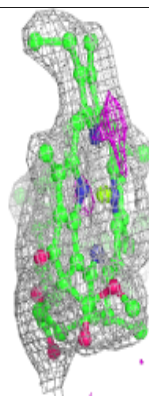
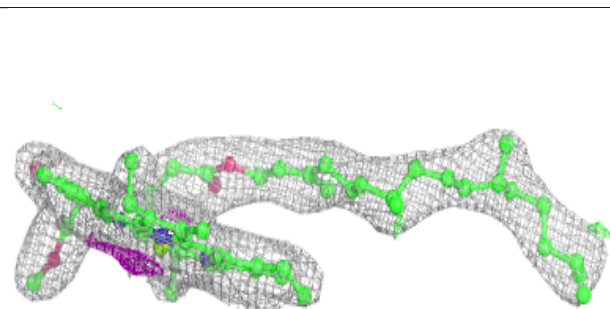
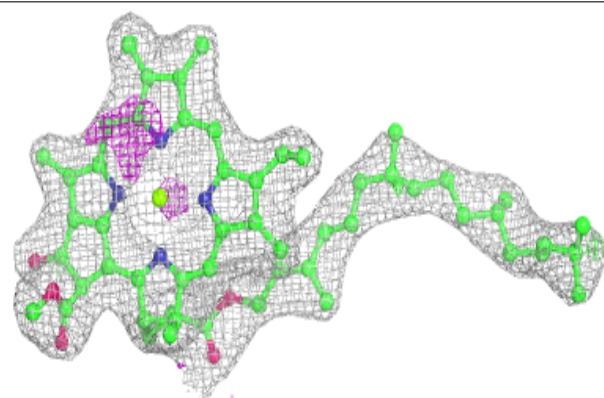


Electron density around CLA c 503:

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

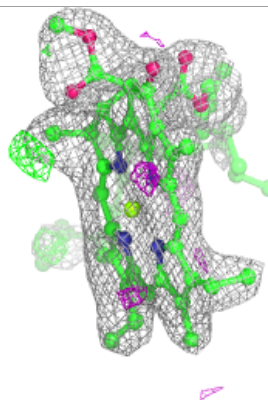
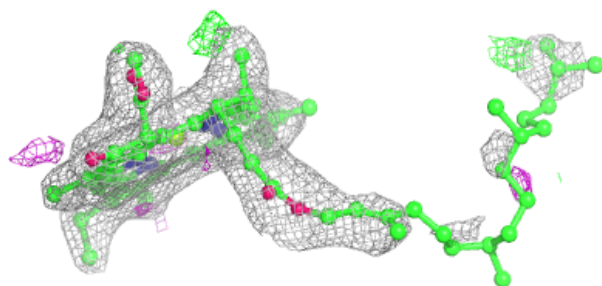
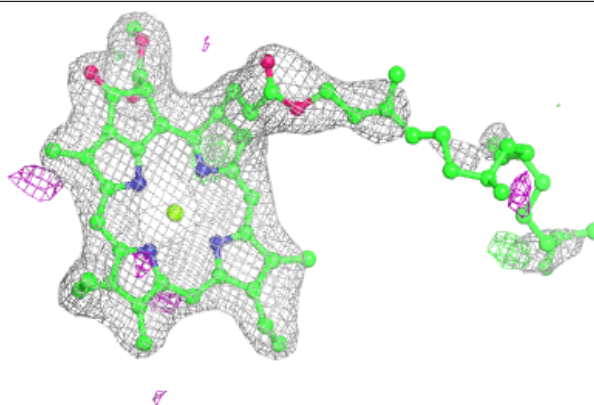
**Electron density around CLA B 603:**

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

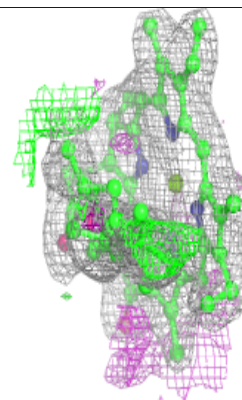
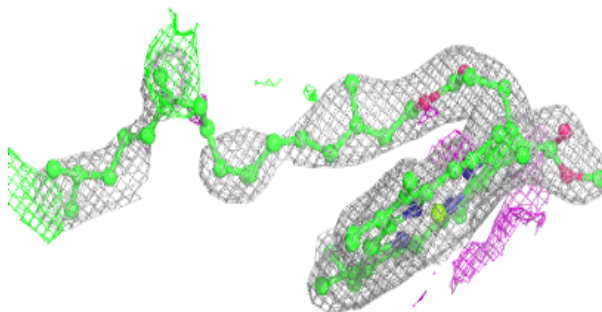
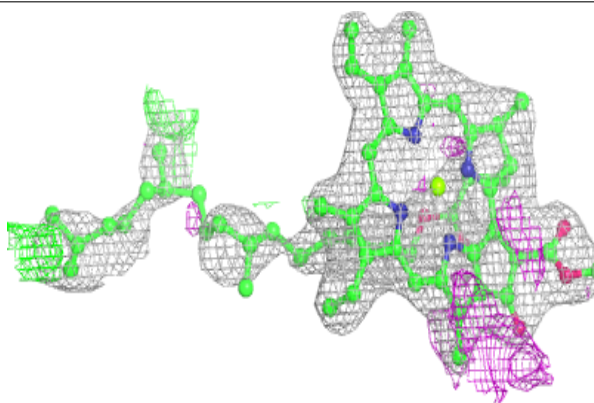


Electron density around CLA a 408:

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

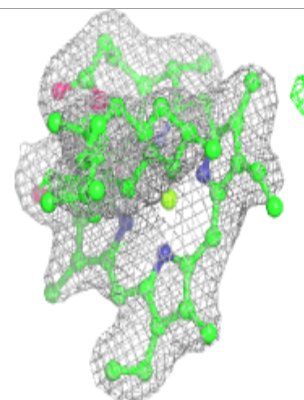
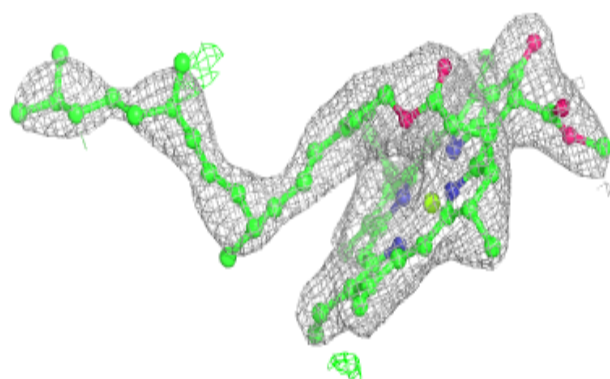
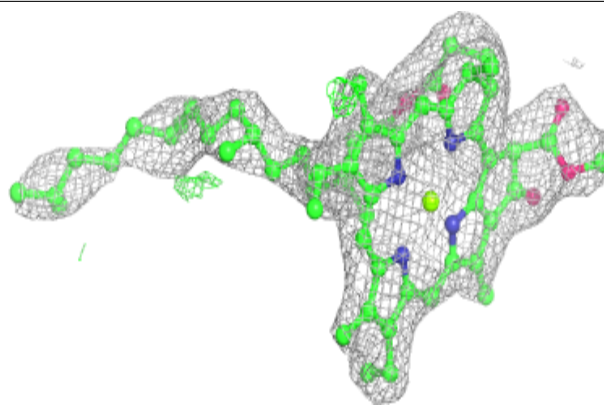
**Electron density around CLA B 614:**

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

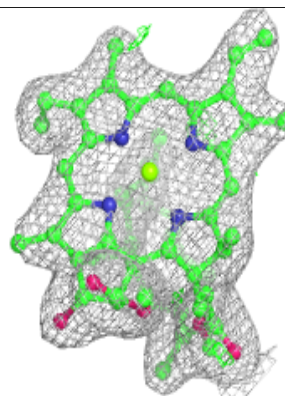
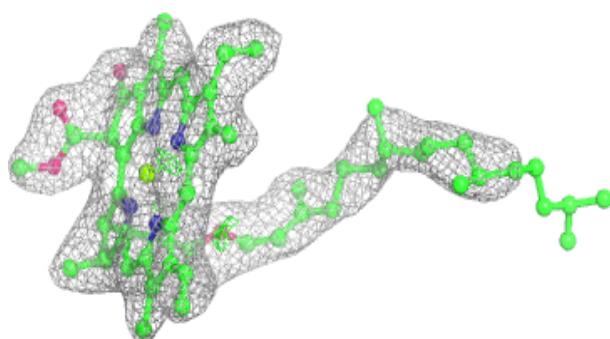
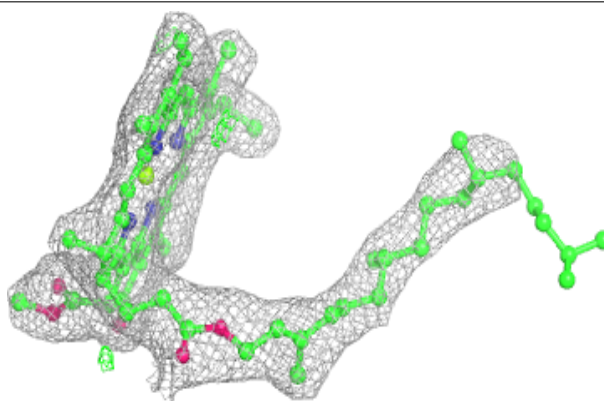


Electron density around CLA c 507:

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

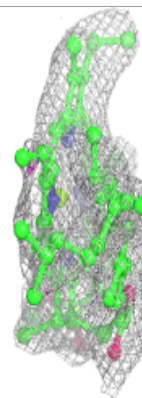
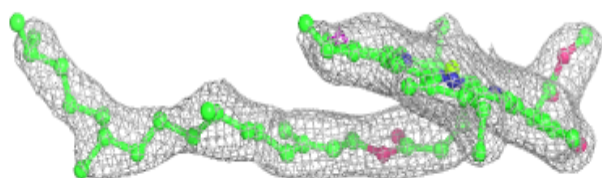
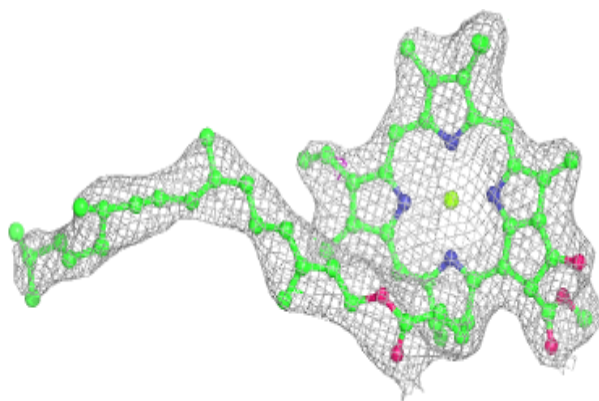
**Electron density around CLA C 510:**

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

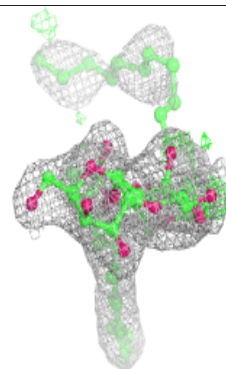
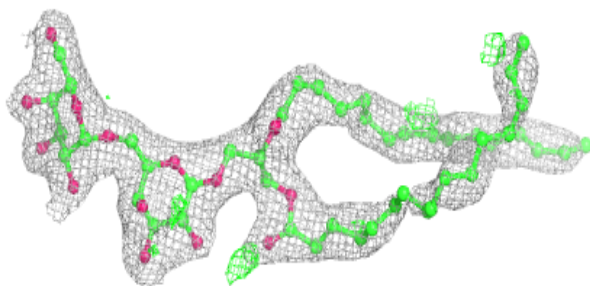
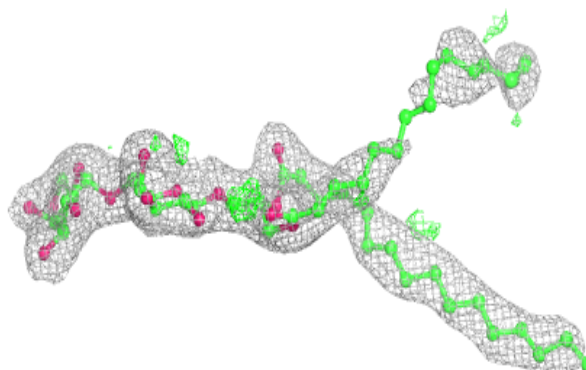


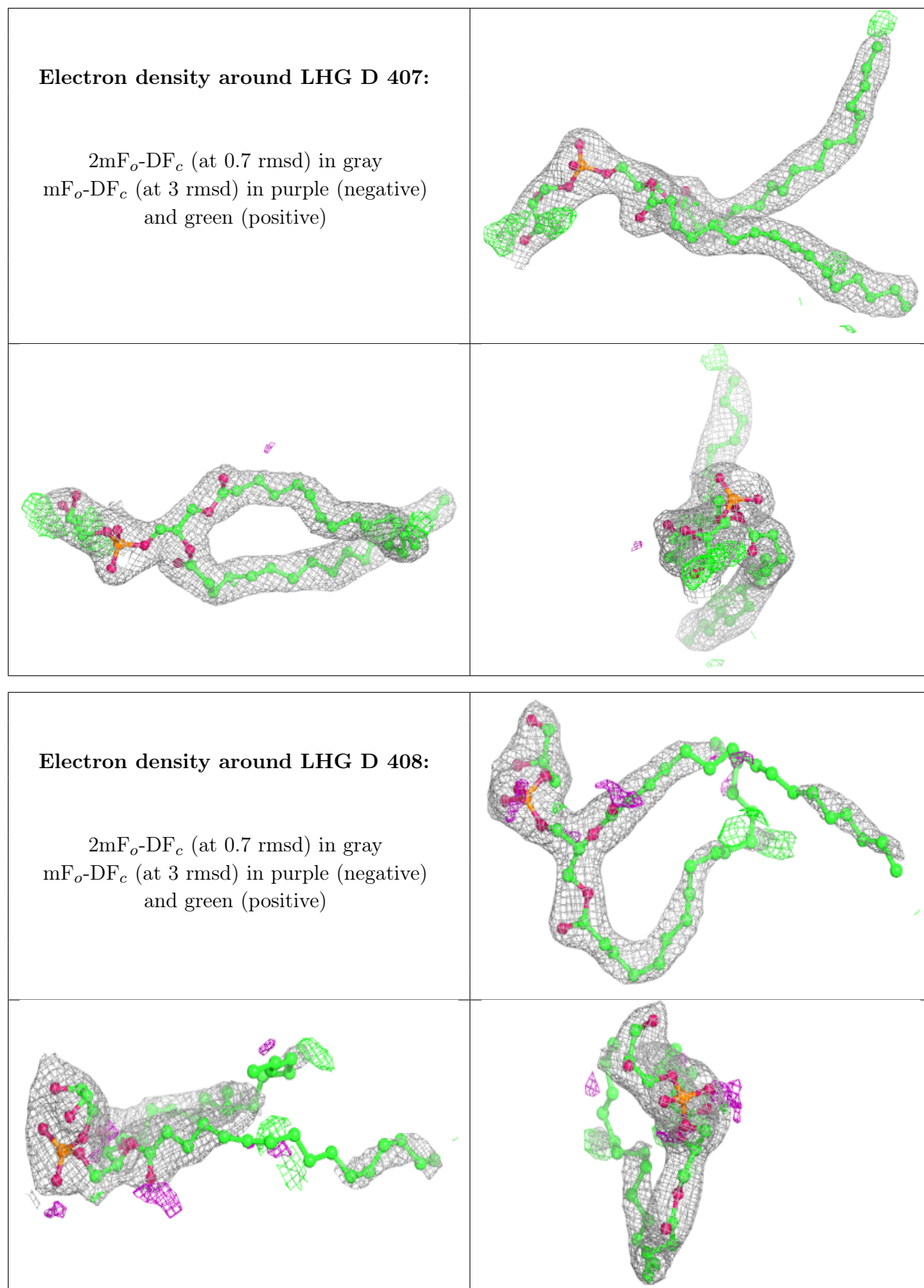
Electron density around CLA b 603:

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

**Electron density around DGD C 518:**

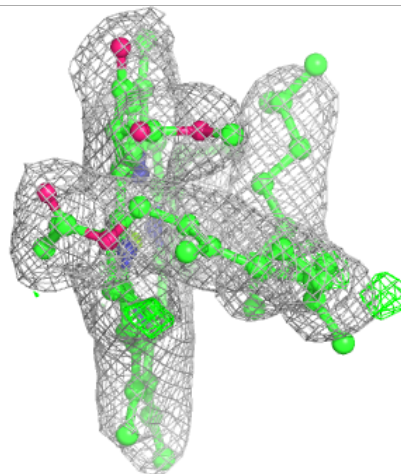
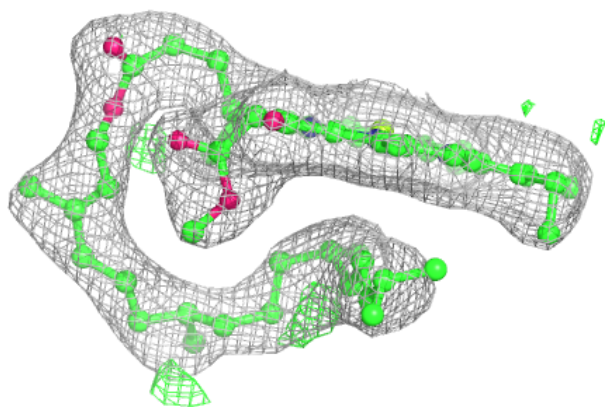
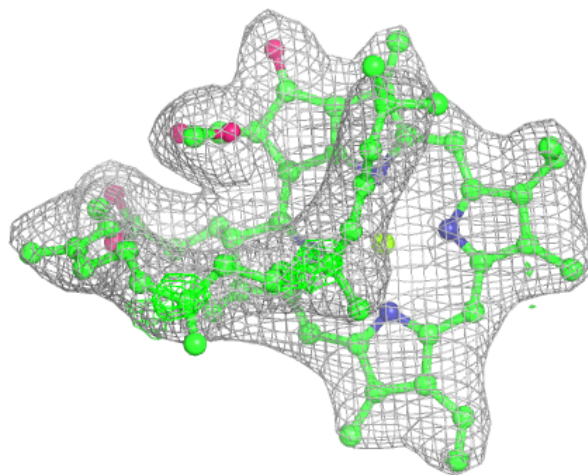
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





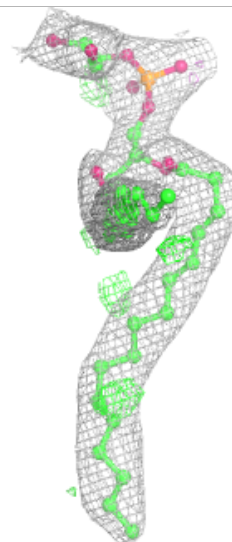
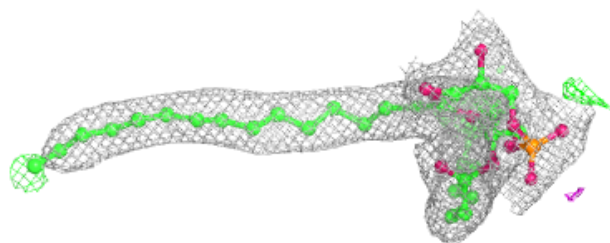
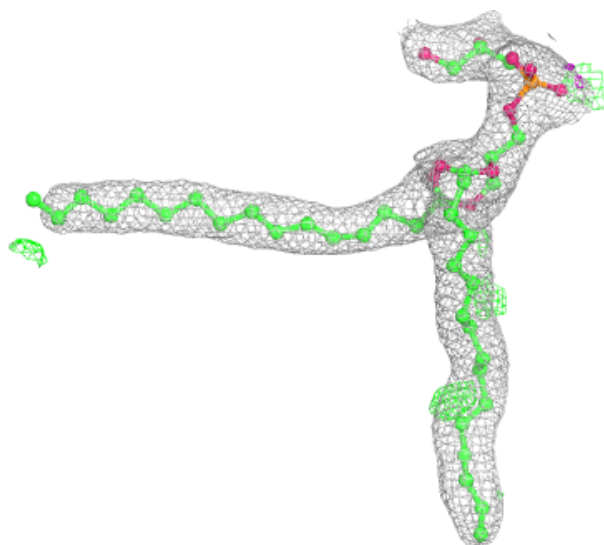
Electron density around CLA C 512:

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



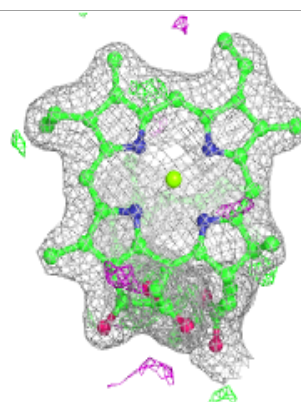
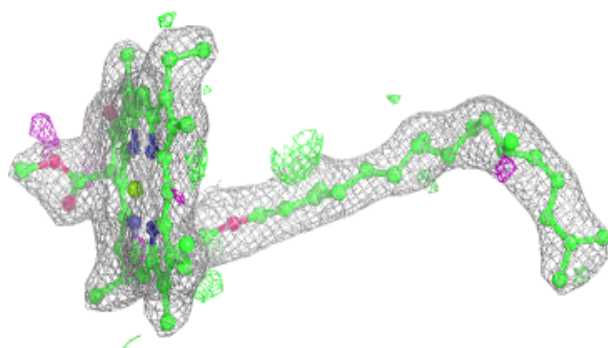
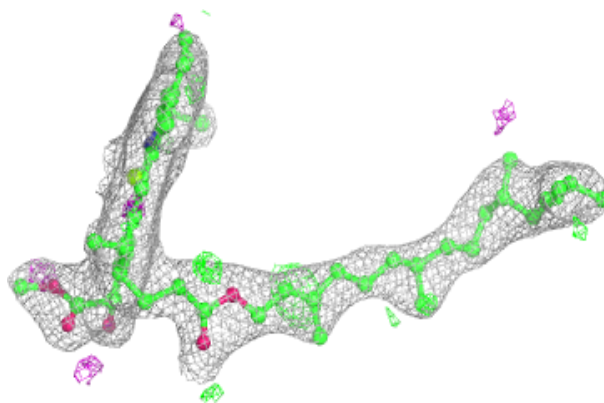
Electron density around LHG L 101:

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

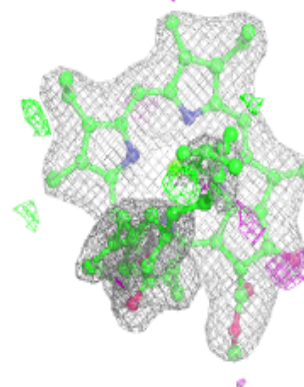
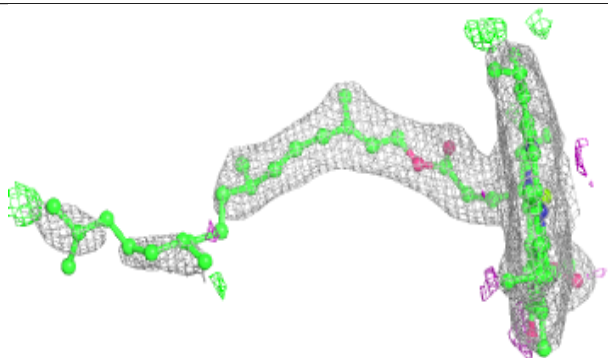
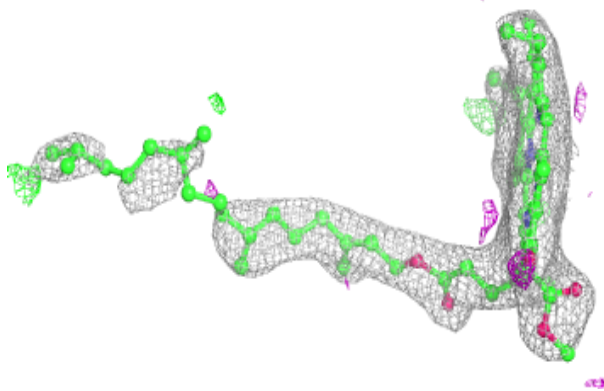


Electron density around CLA b 605:

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

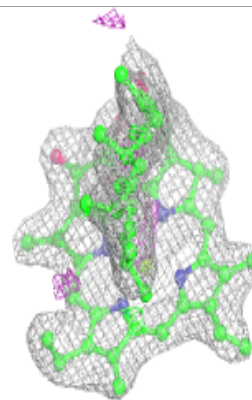
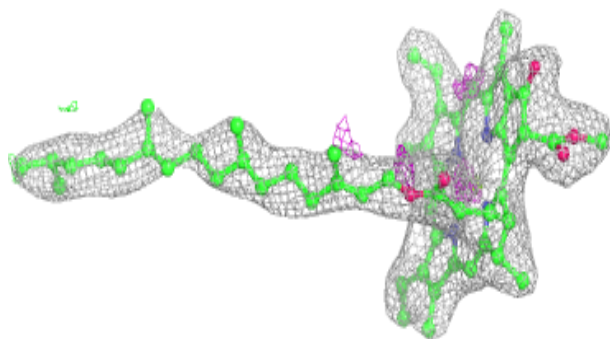
**Electron density around CLA b 606:**

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

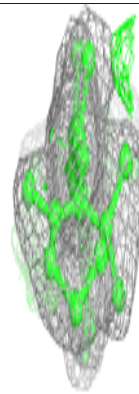
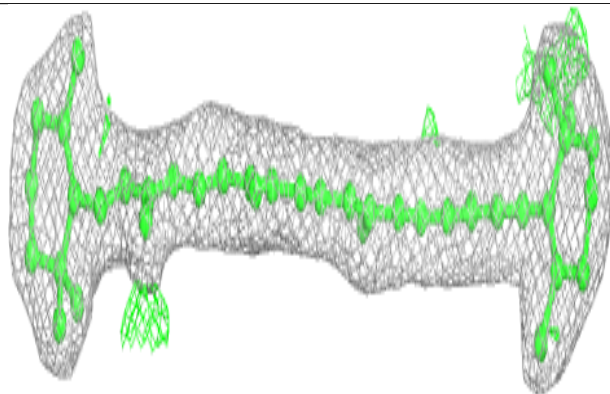
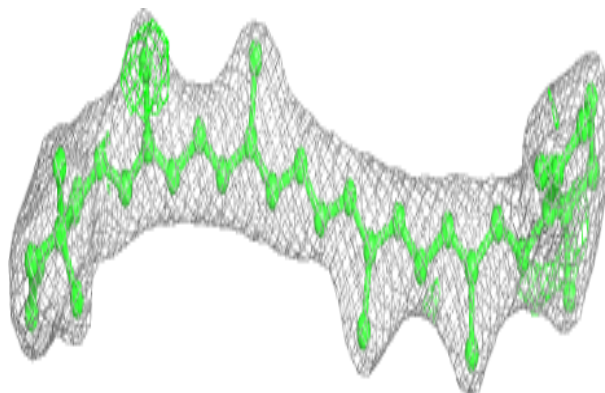


Electron density around CLA b 607:

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

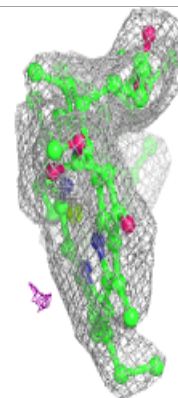
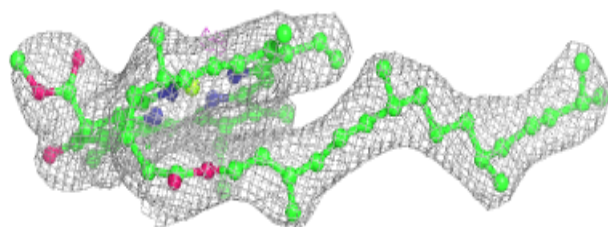
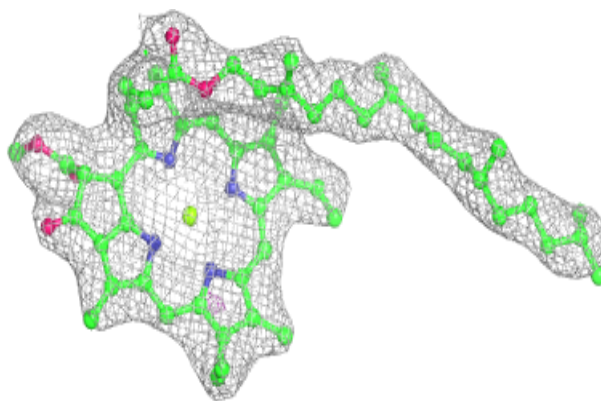
**Electron density around BCR A 409:**

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

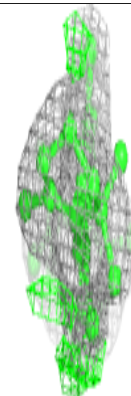
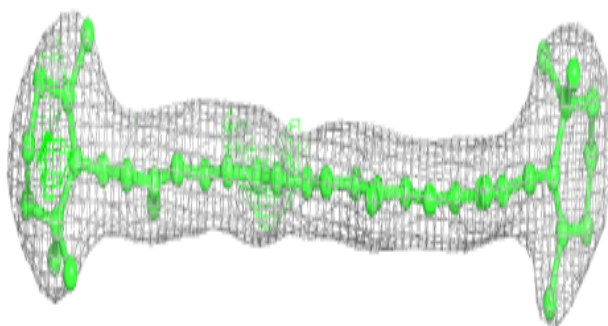
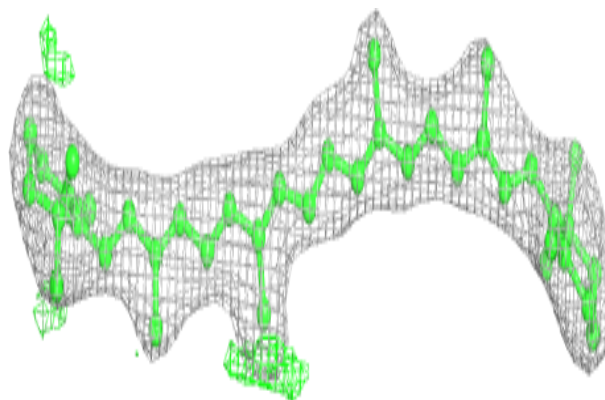


Electron density around CLA C 503:

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

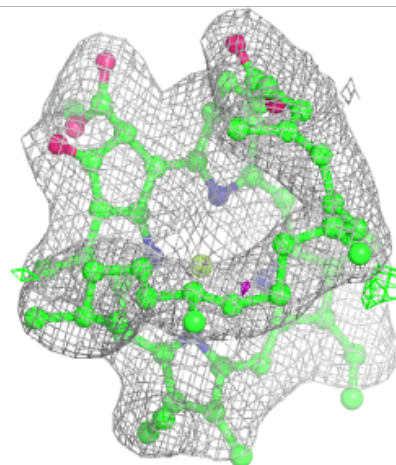
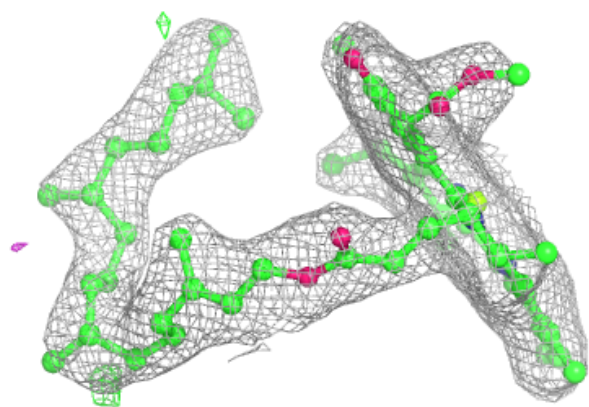
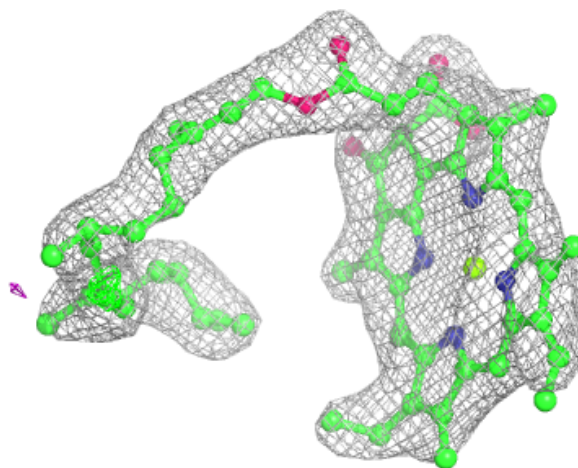
**Electron density around BCR C 517:**

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



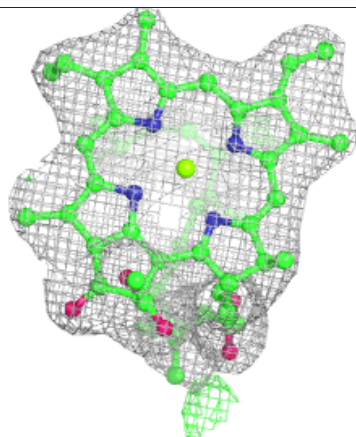
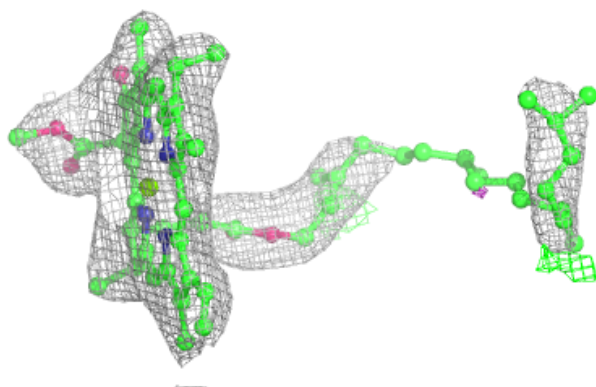
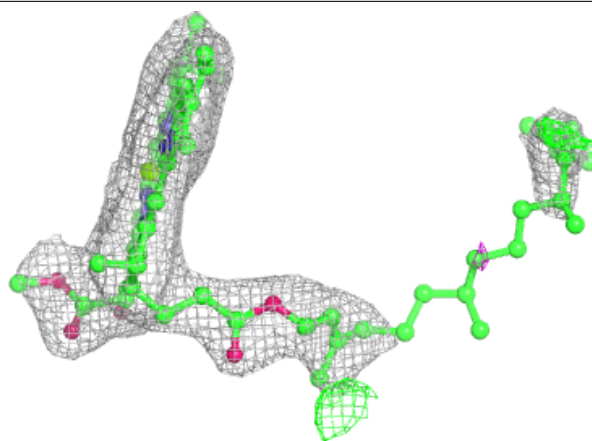
Electron density around CLA C 505:

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

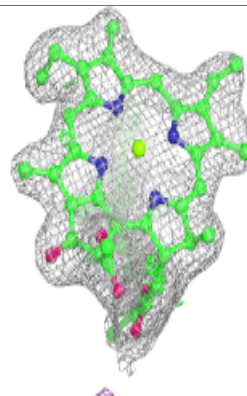
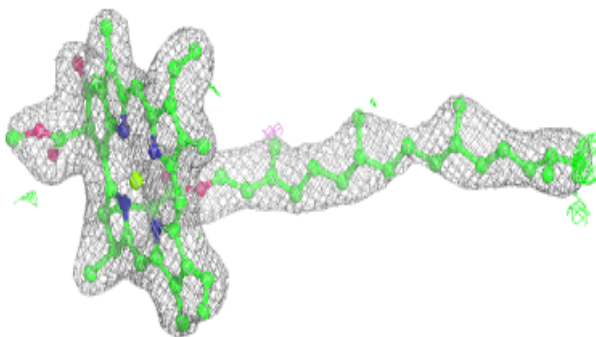
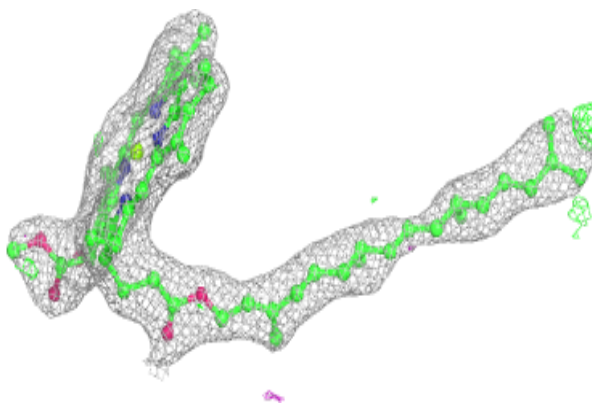


Electron density around CLA c 508:

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

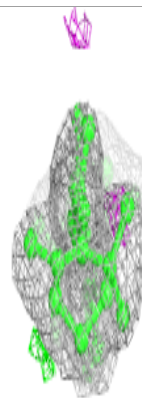
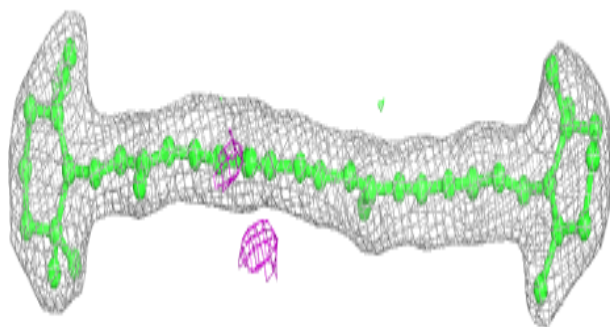
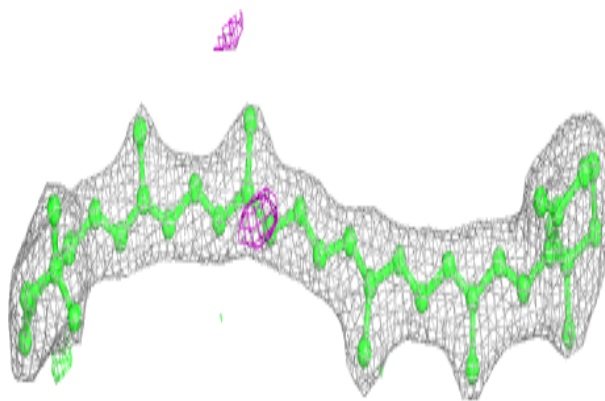
**Electron density around CLA B 607:**

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

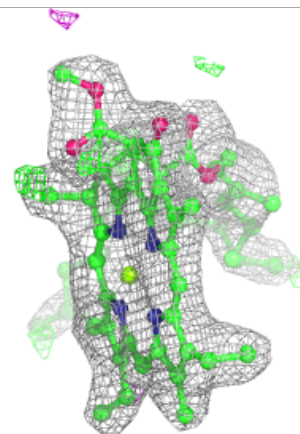
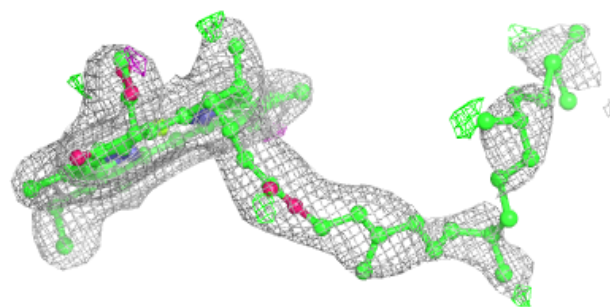
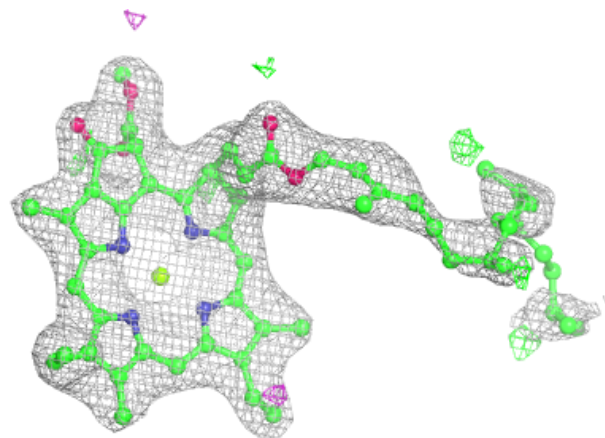


Electron density around BCR a 409:

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

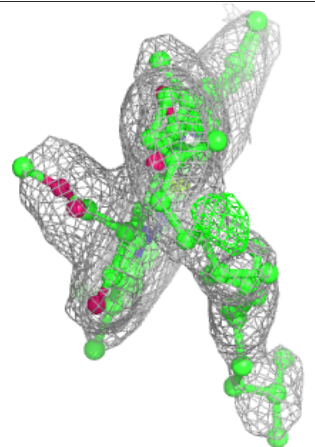
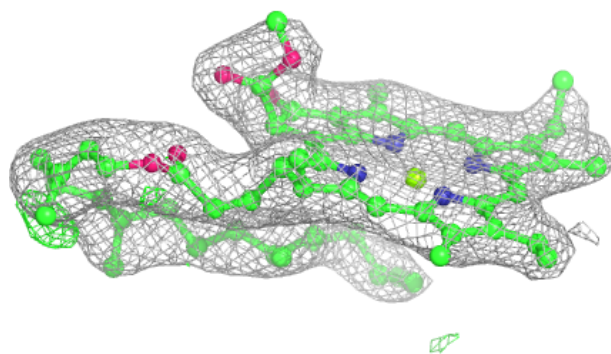
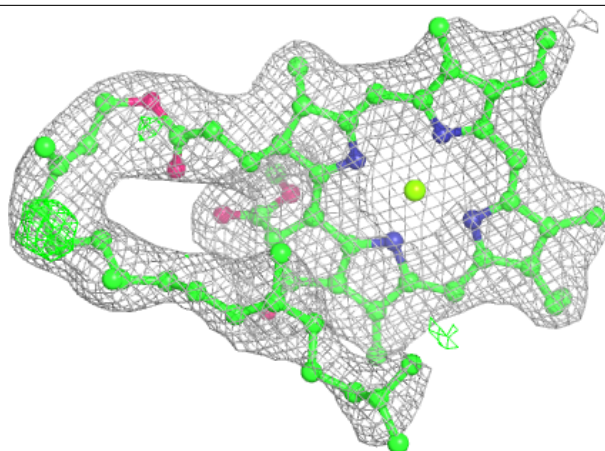
**Electron density around CLA A 408:**

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

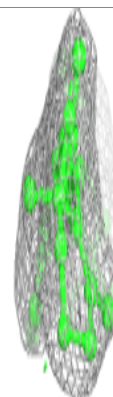
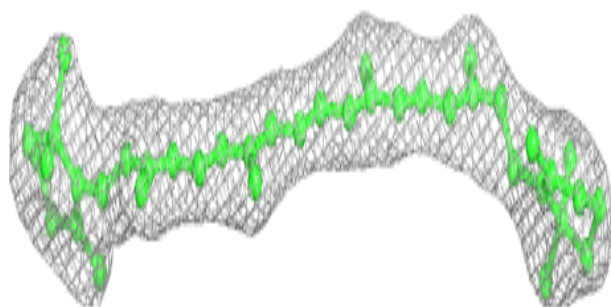
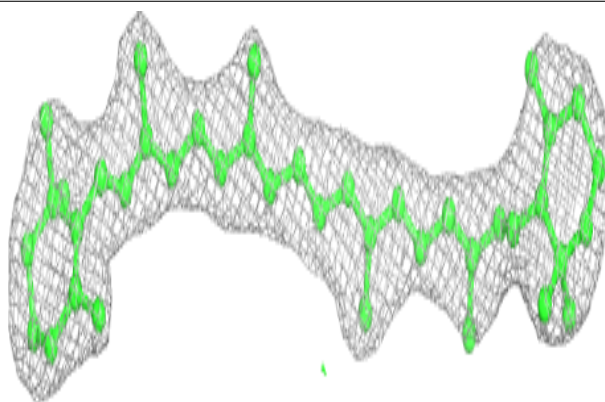


Electron density around CLA c 511:

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

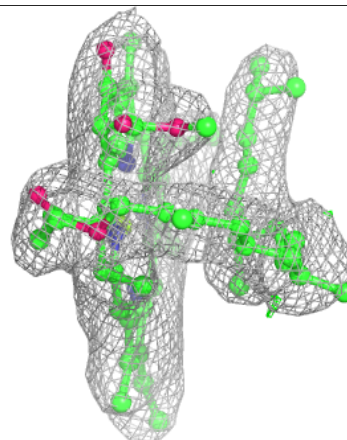
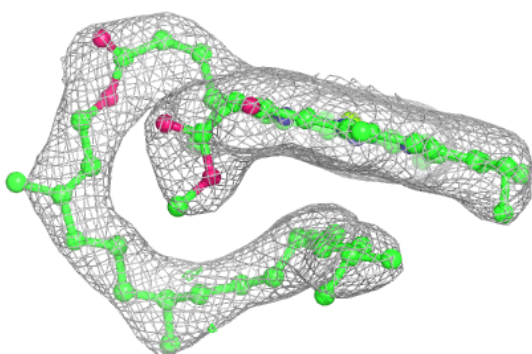
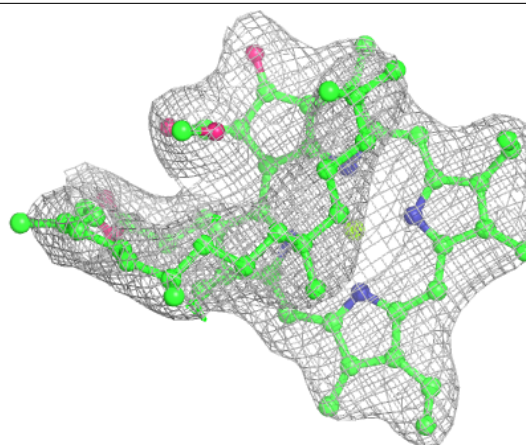
**Electron density around BCR b 619:**

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

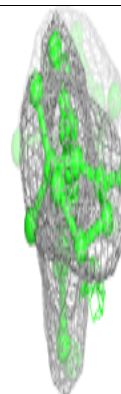
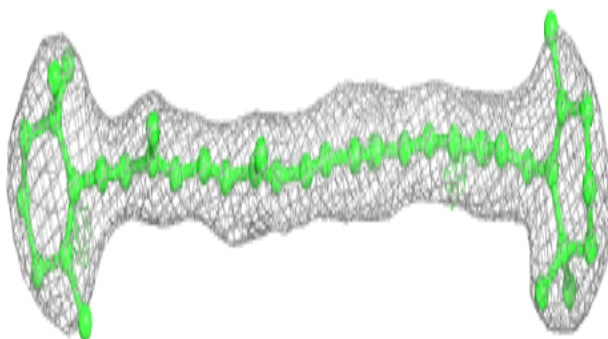
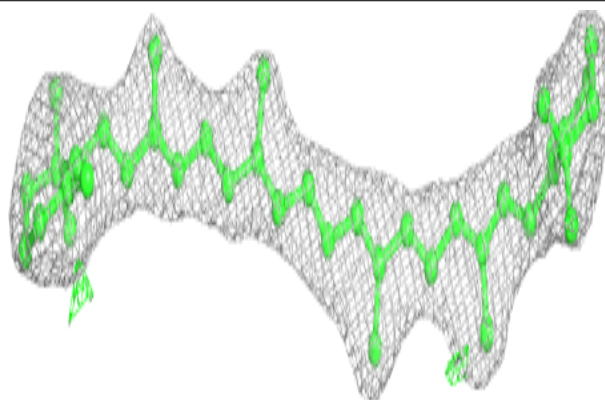


Electron density around CLA c 512:

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

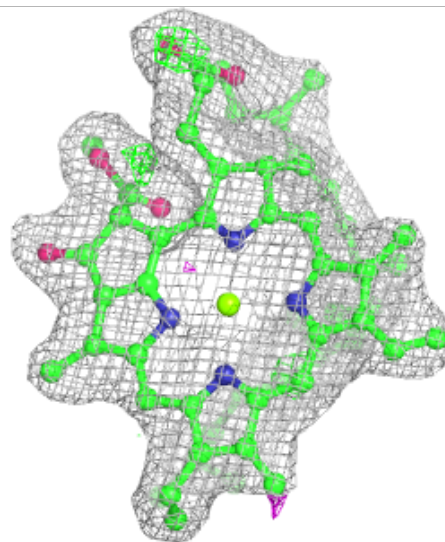
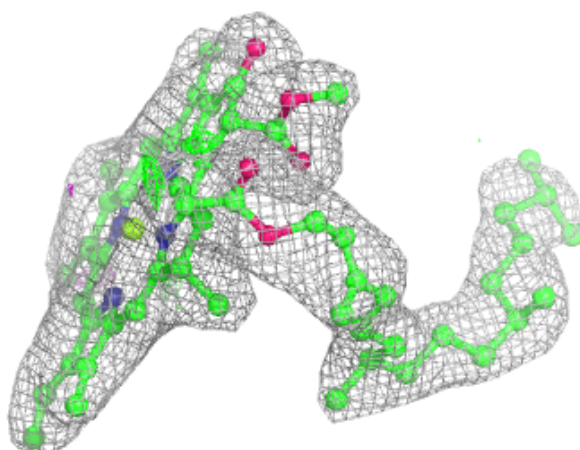
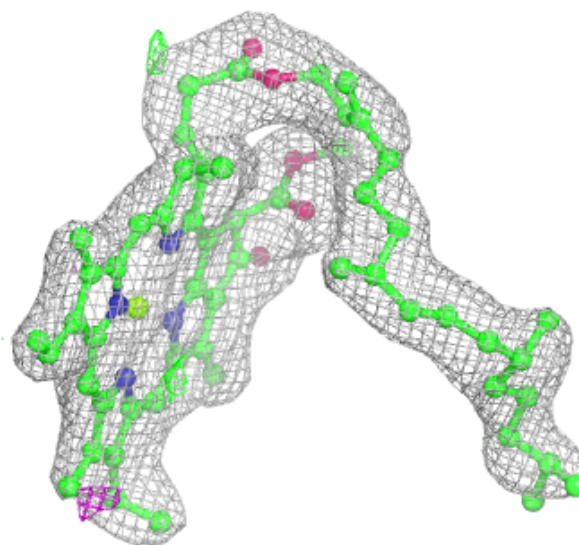
**Electron density around BCR c 517:**

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



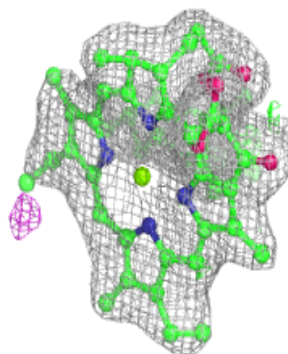
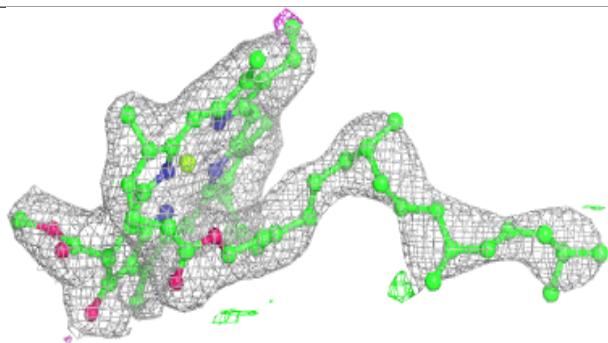
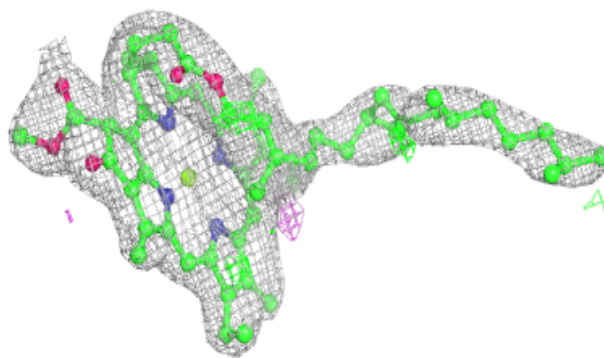
Electron density around CLA b 613:

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

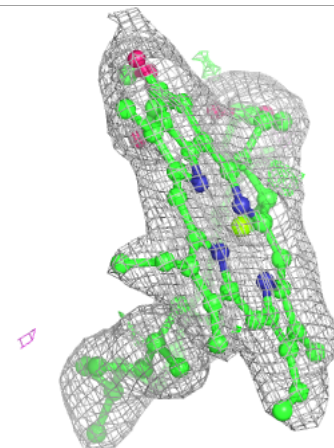
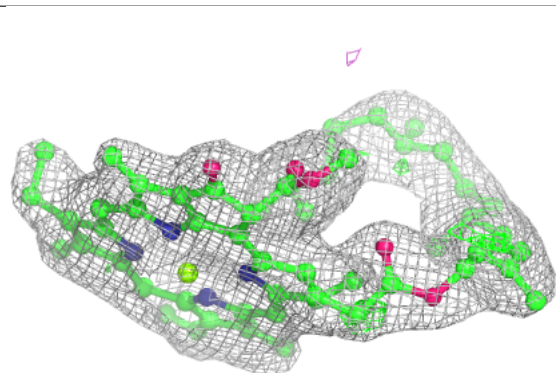
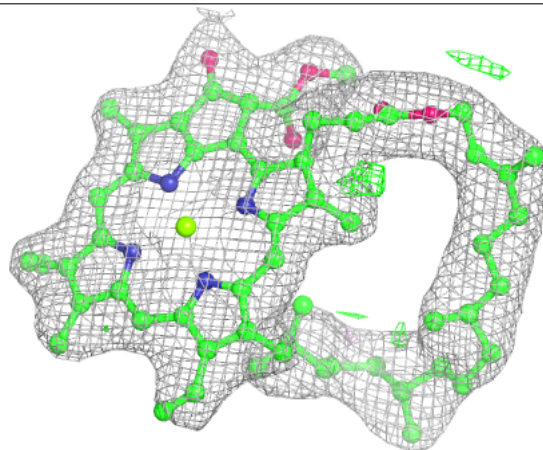


Electron density around CLA C 507:

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

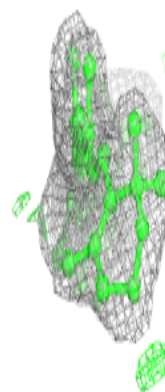
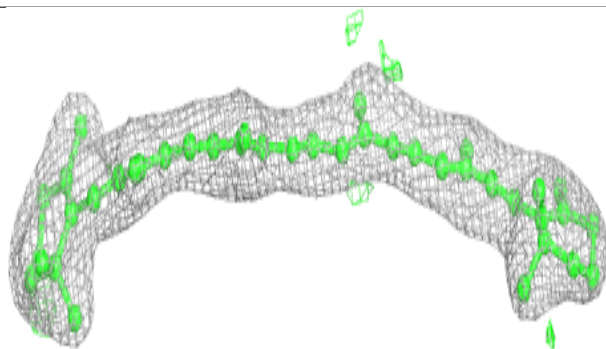
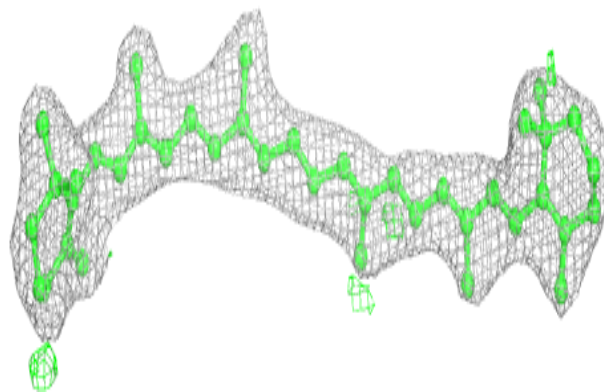
**Electron density around CLA b 615:**

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



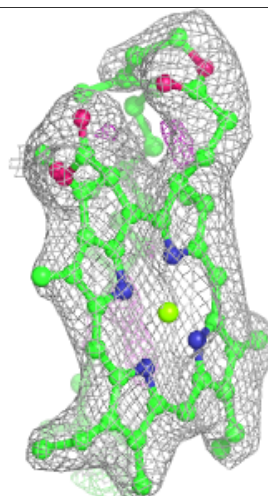
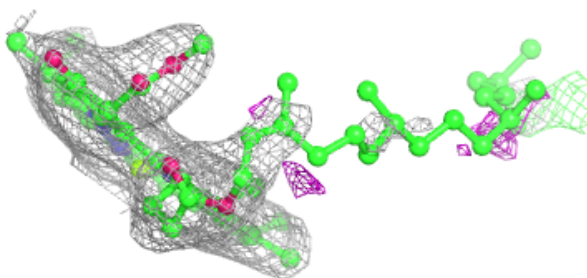
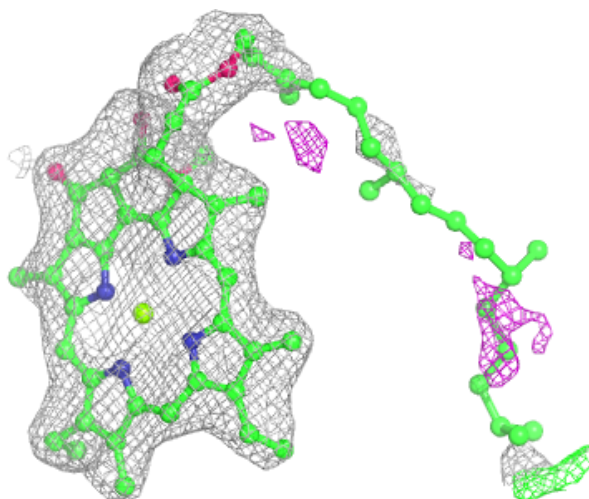
Electron density around BCR t 102:

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



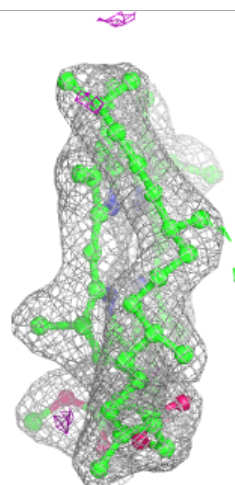
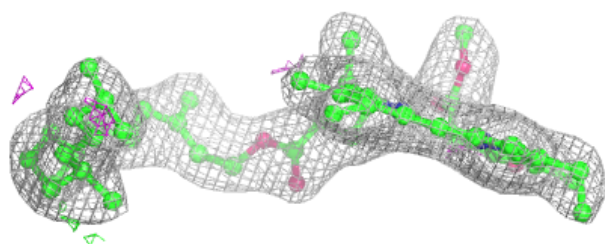
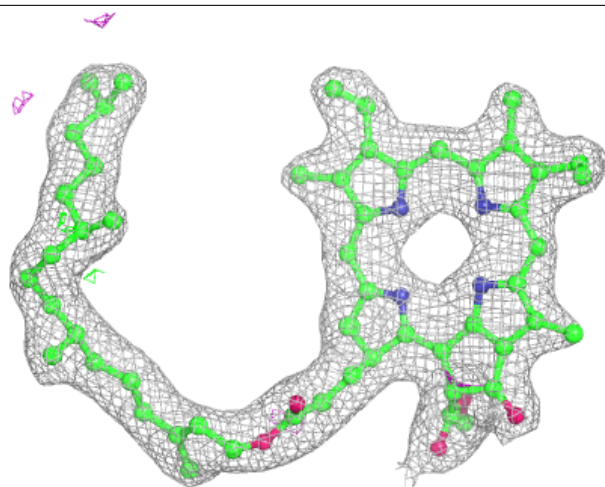
Electron density around CLA B 616:

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



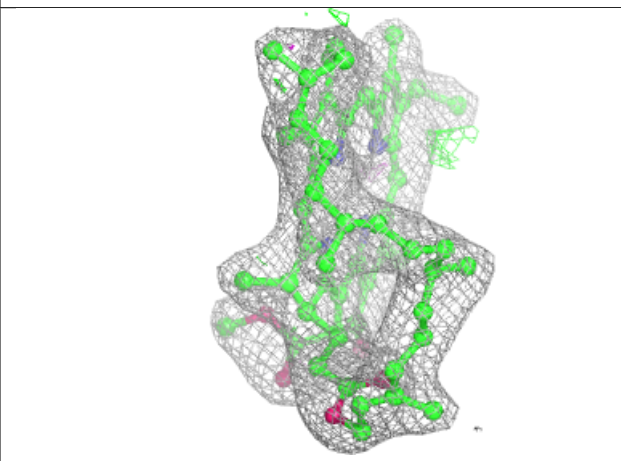
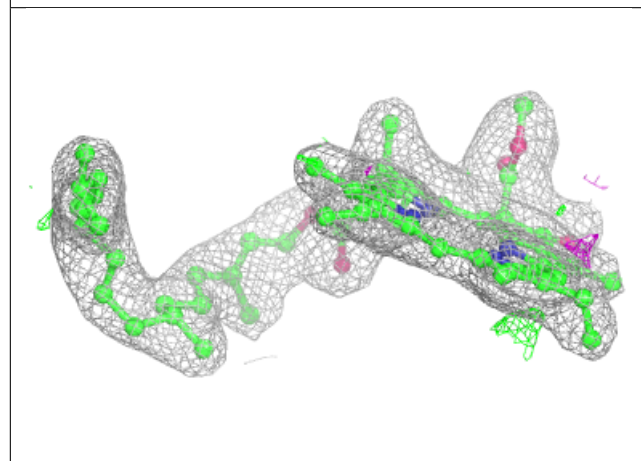
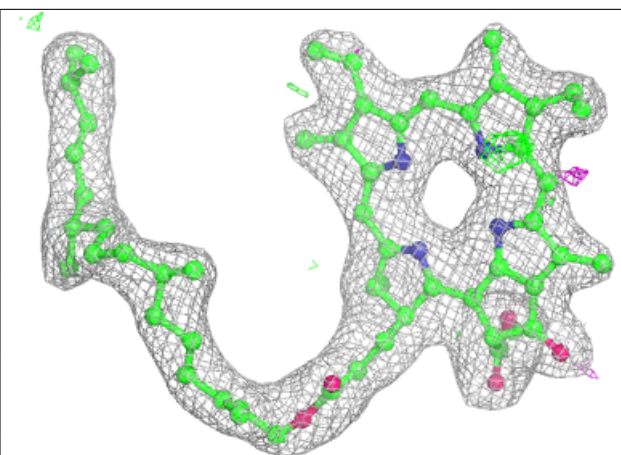
Electron density around PHO A 407:

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

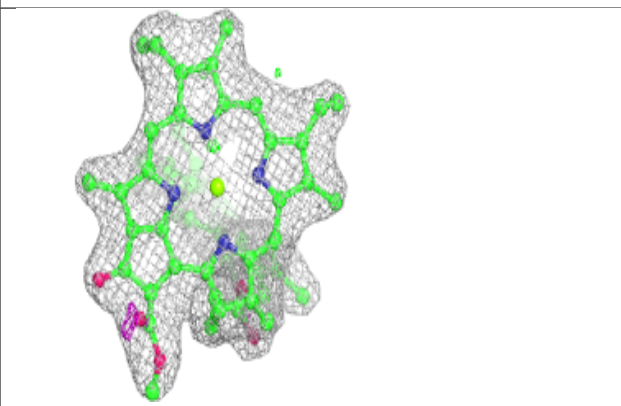
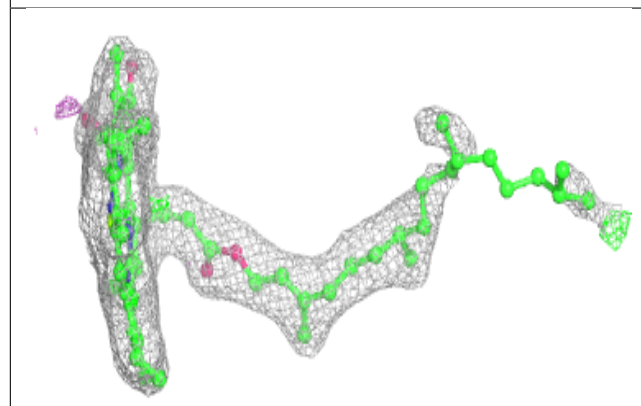
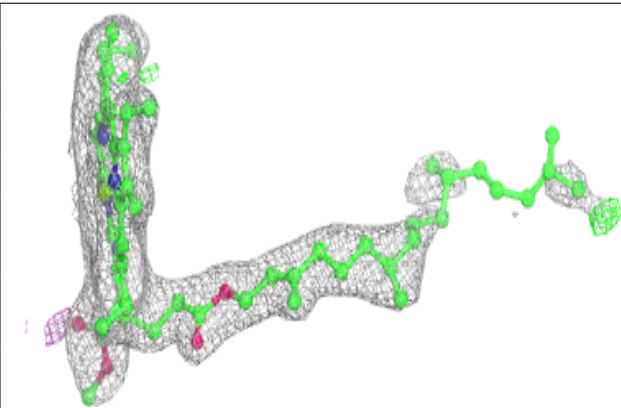


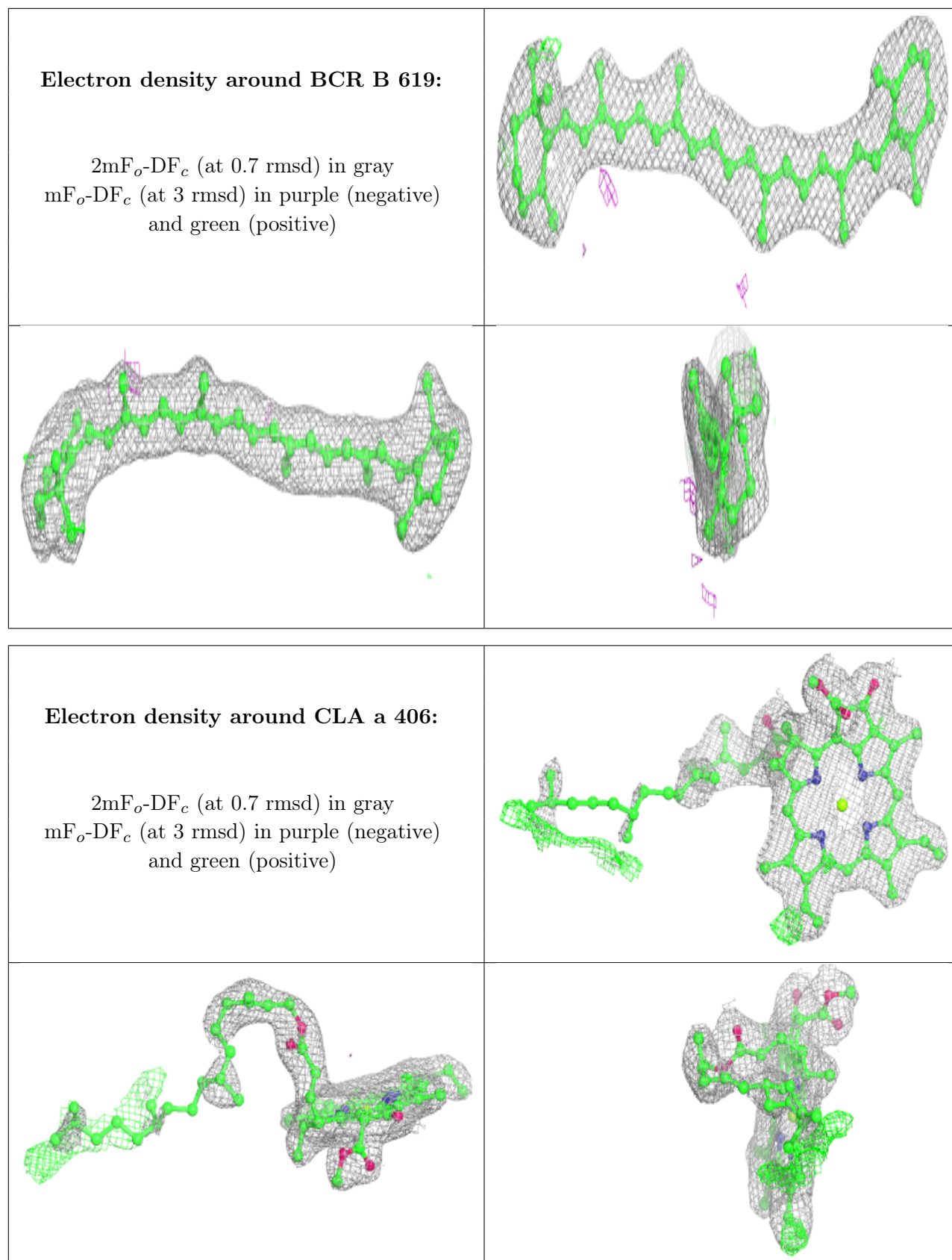
Electron density around PHO A 415:

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

**Electron density around CLA B 606:**

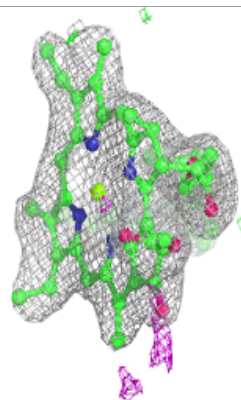
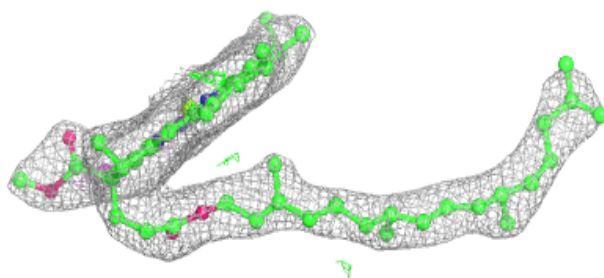
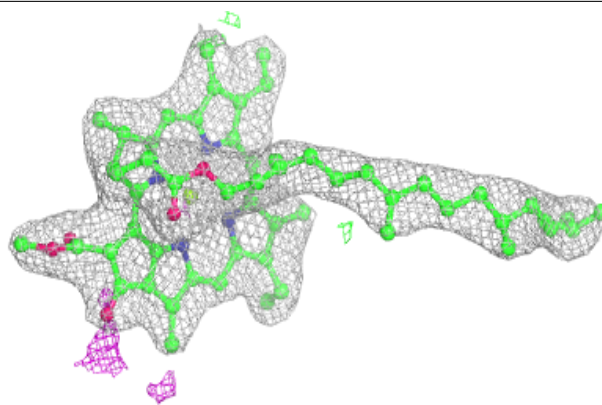
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



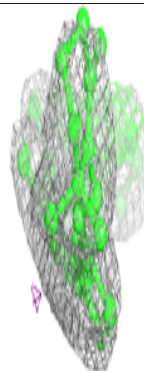
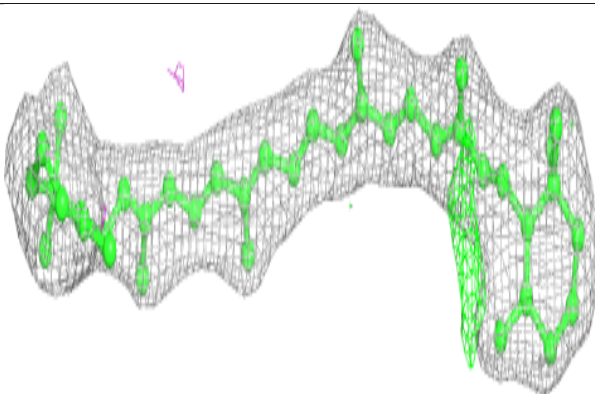
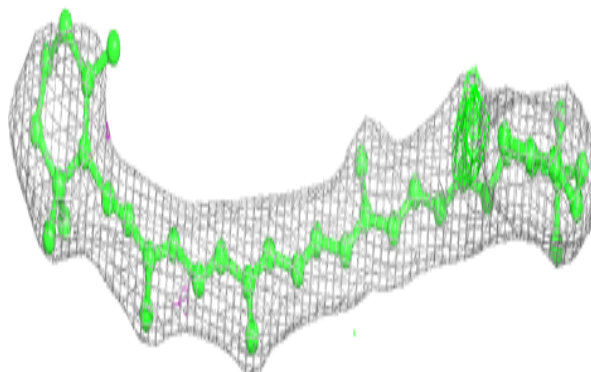


Electron density around CLA b 608:

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

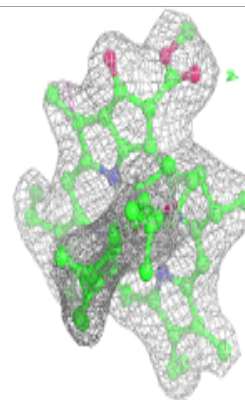
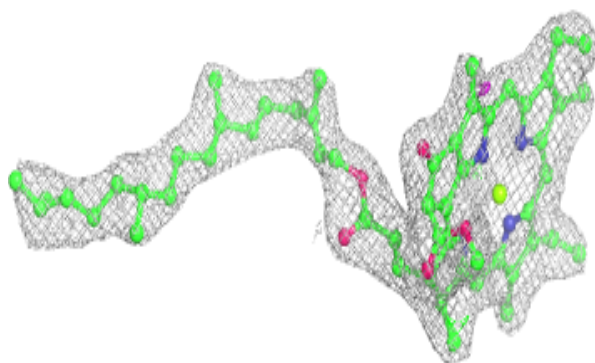
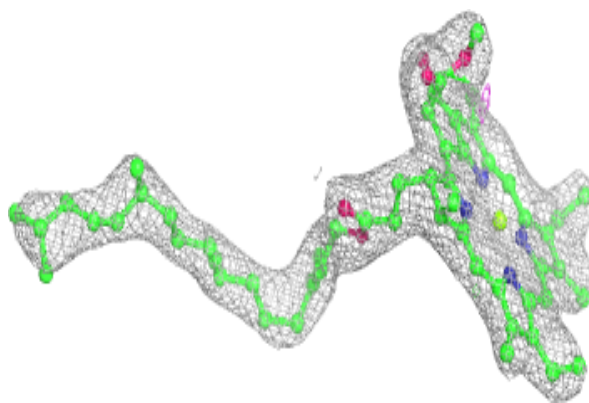
**Electron density around BCR D 405:**

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

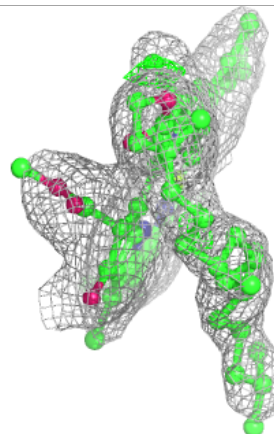
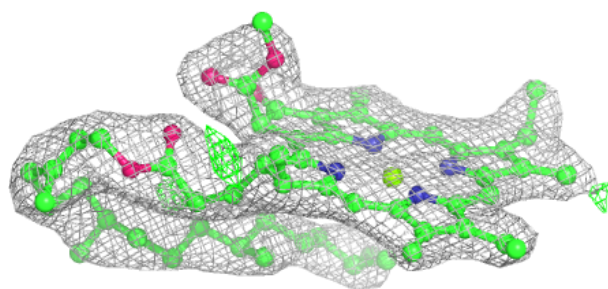
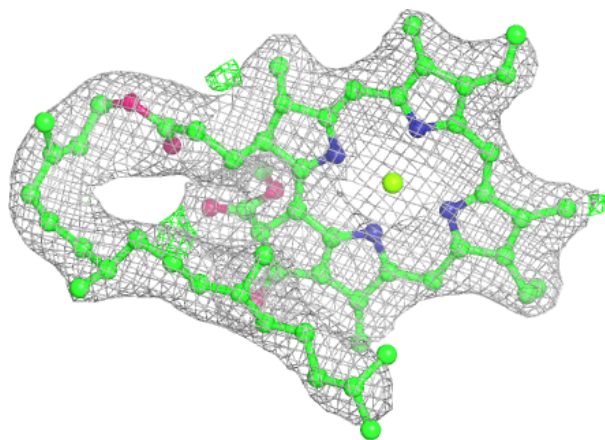


Electron density around CLA C 504:

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

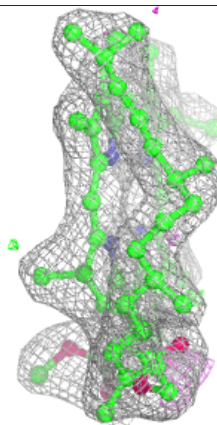
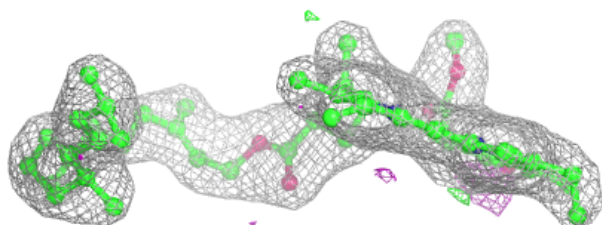
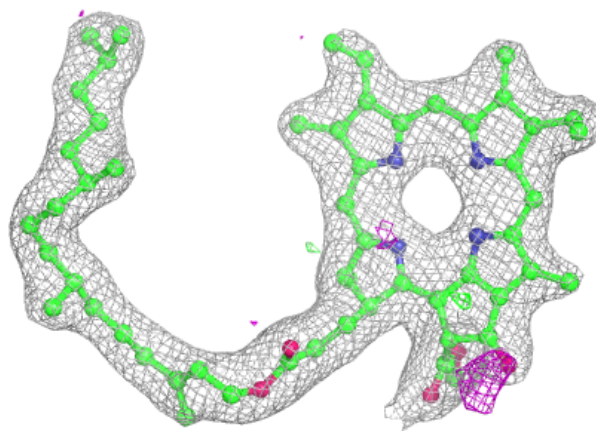
**Electron density around CLA C 511:**

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



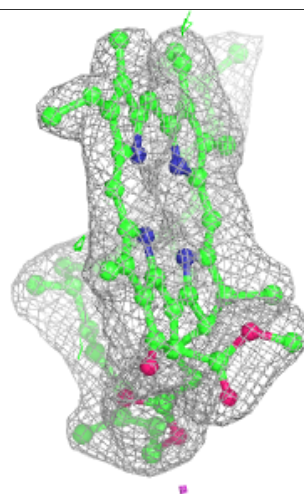
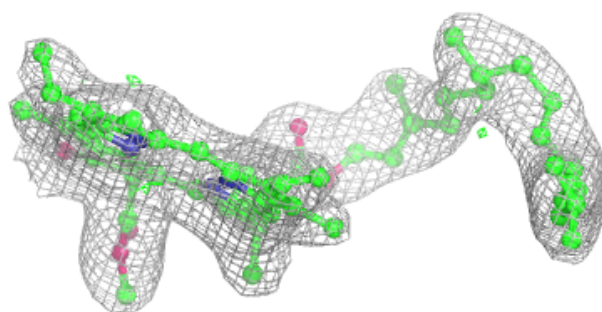
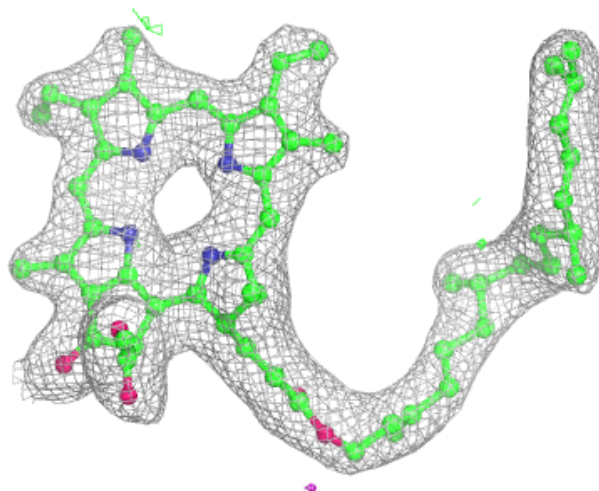
Electron density around PHO a 407:

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



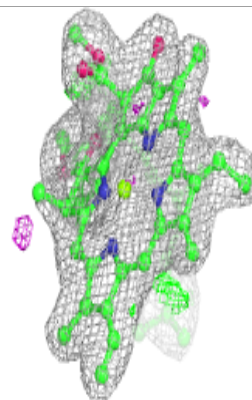
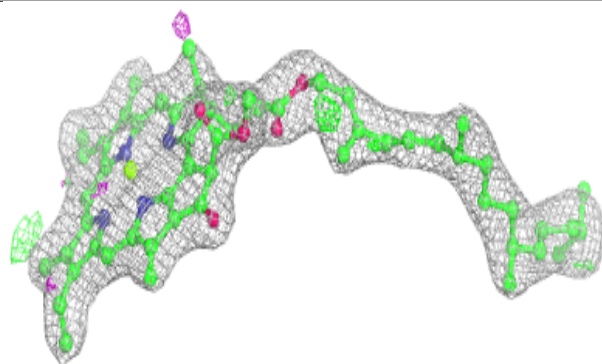
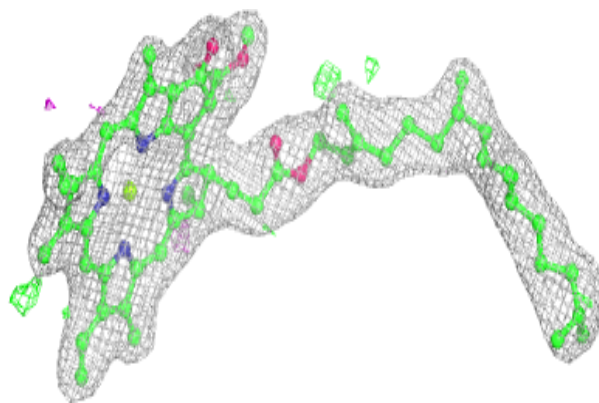
Electron density around PHO a 417:

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

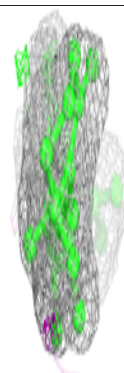
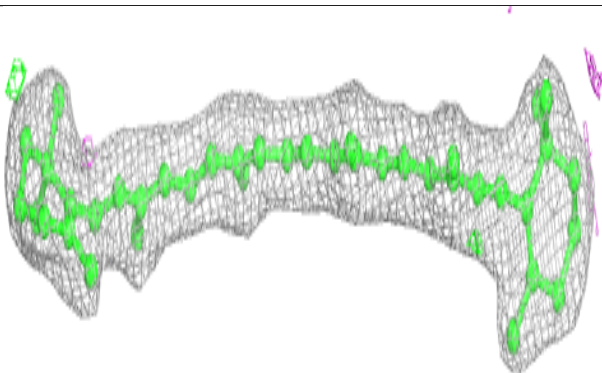
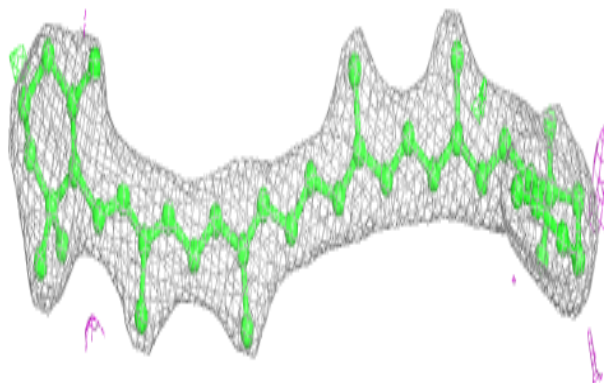


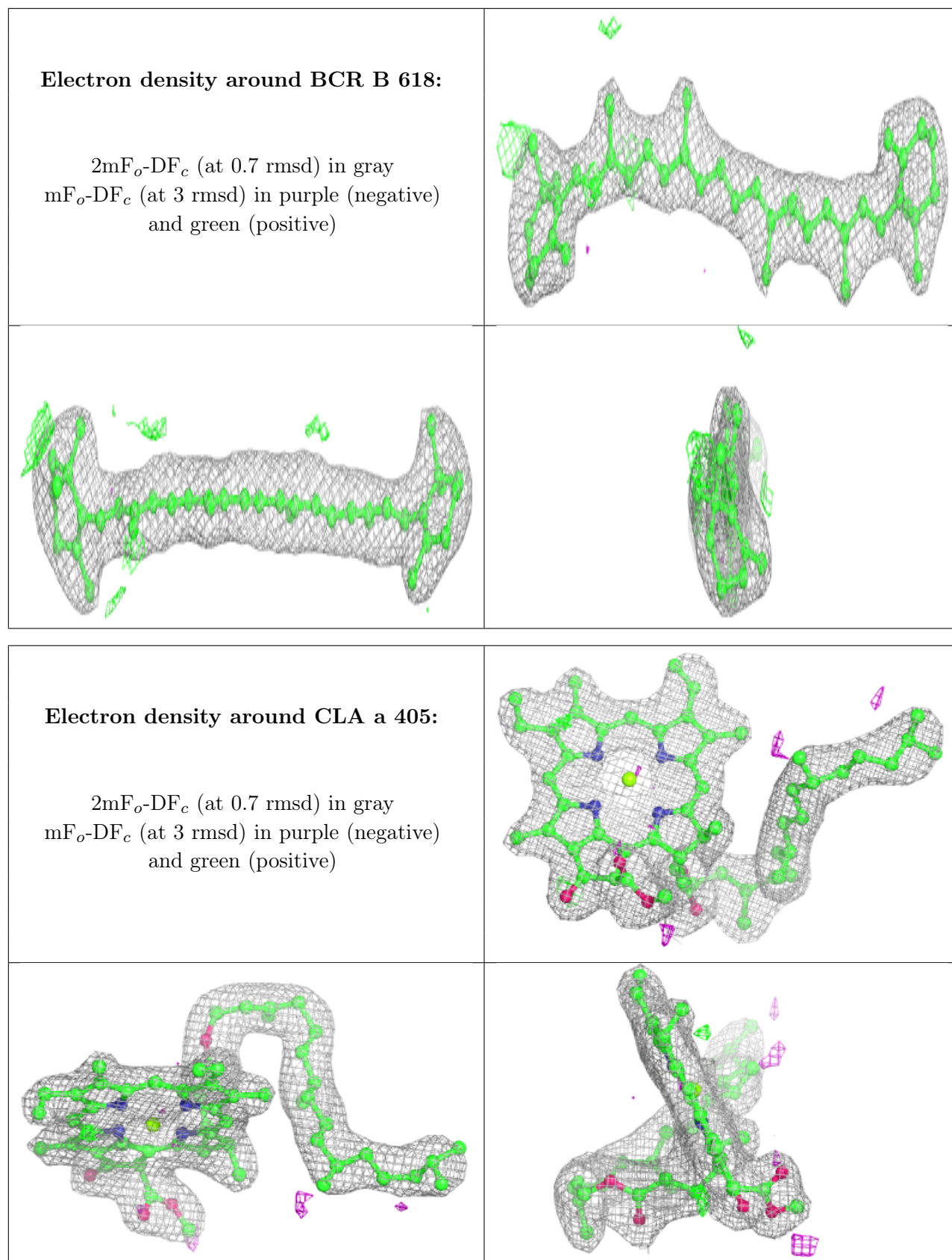
Electron density around CLA a 404:

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

**Electron density around BCR B 617:**

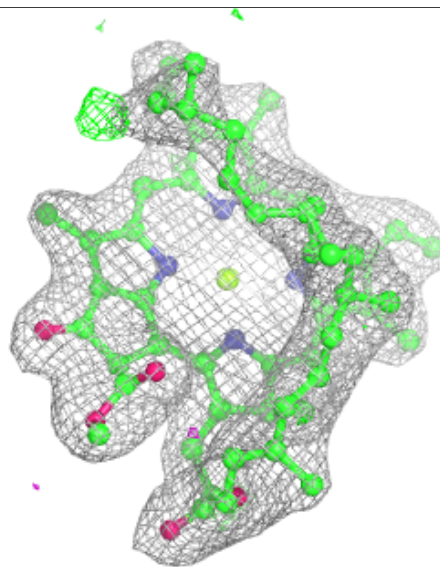
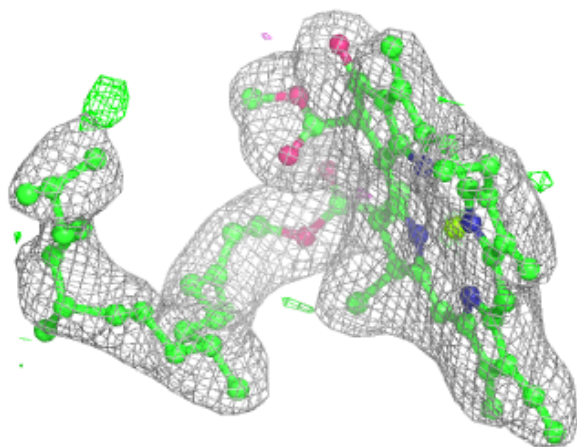
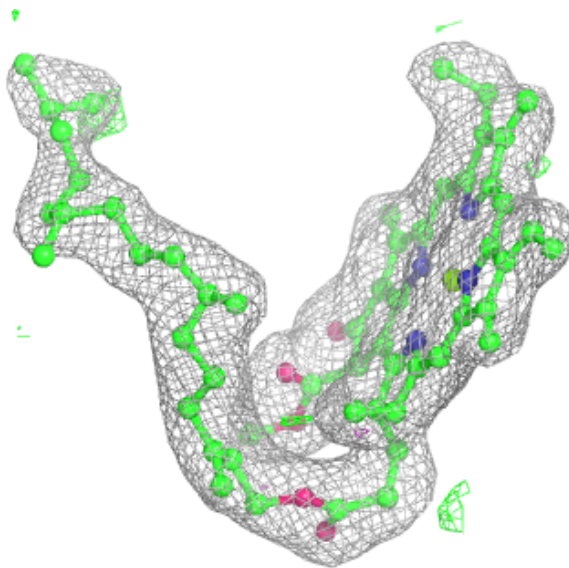
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

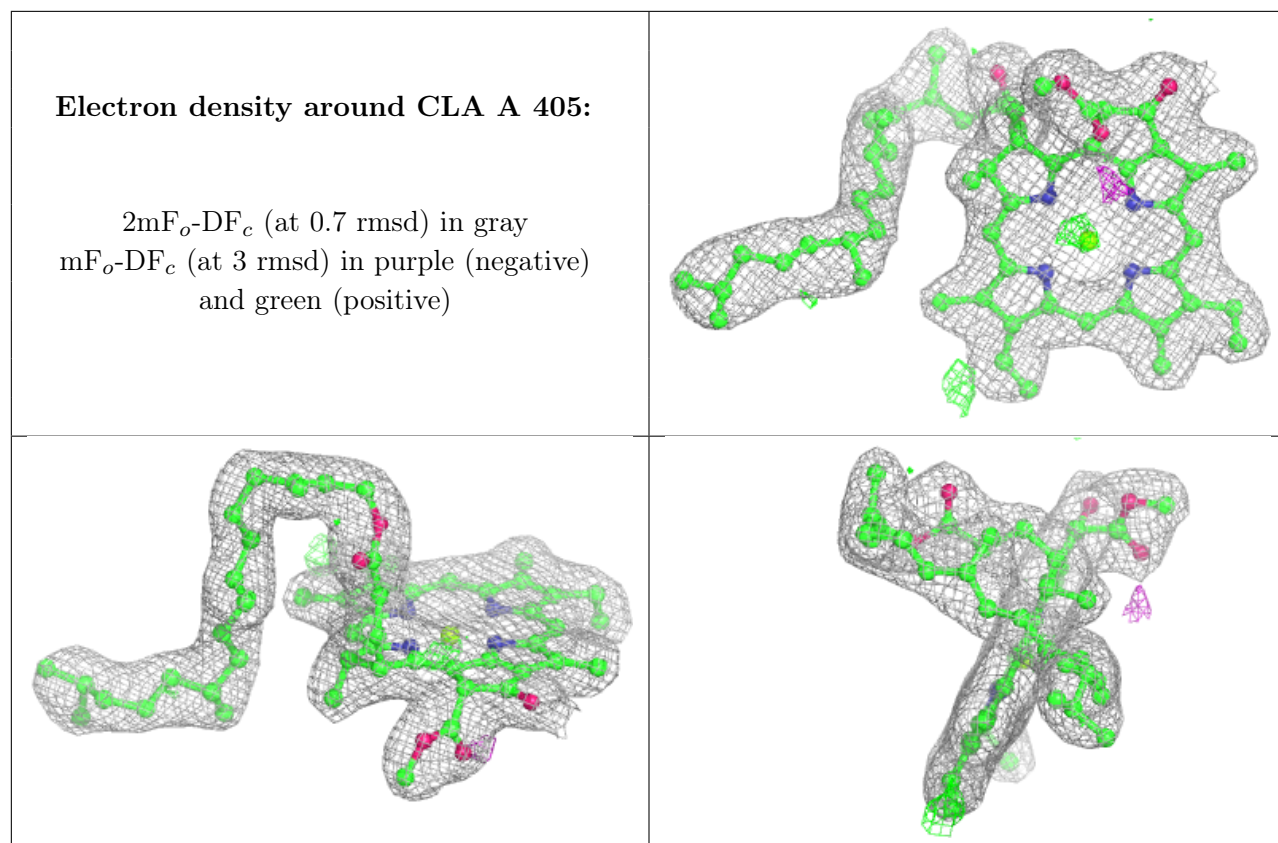




Electron density around CLA B 613:

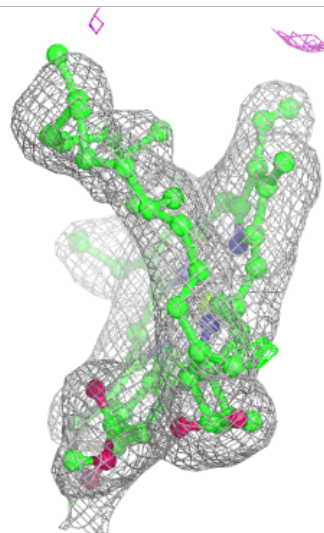
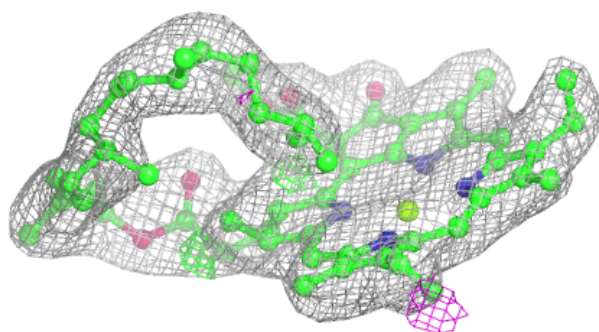
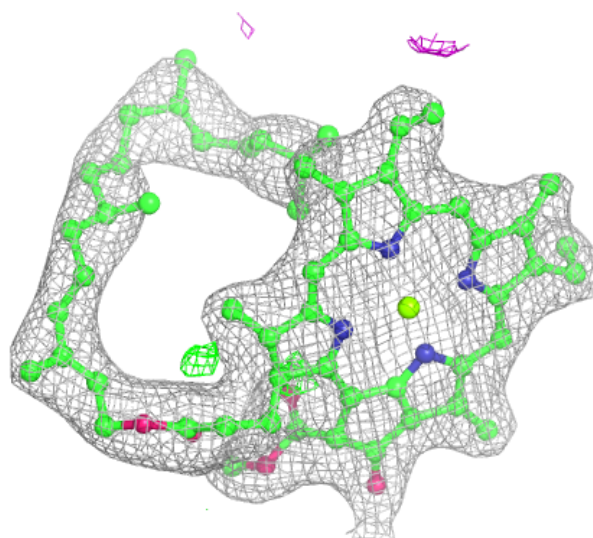
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





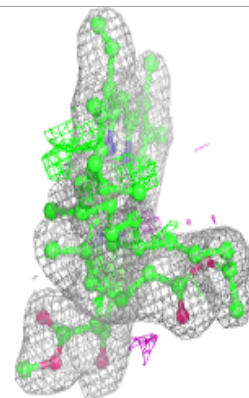
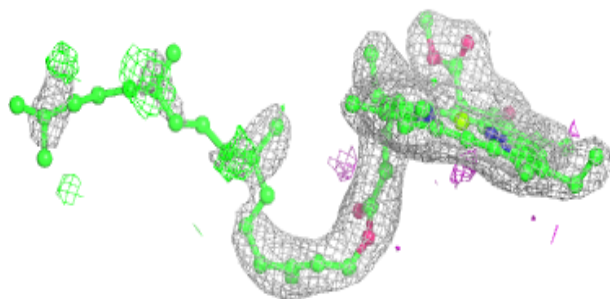
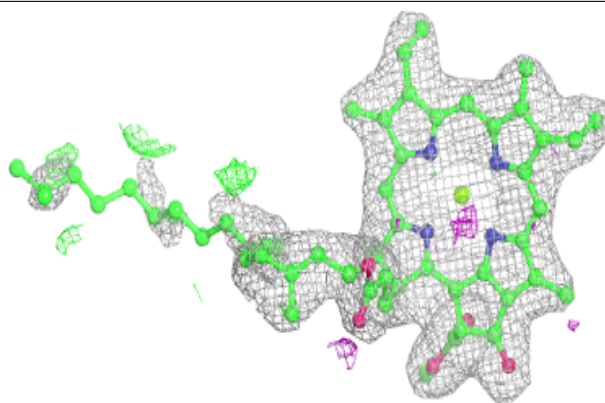
Electron density around CLA B 615:

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

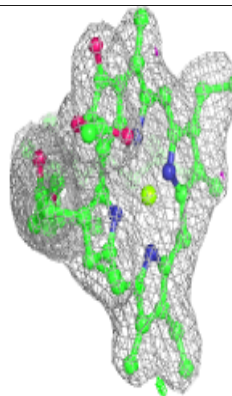
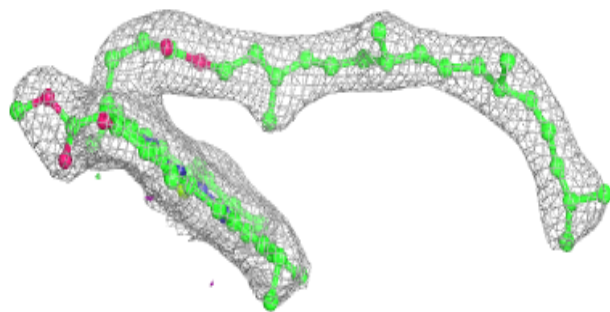
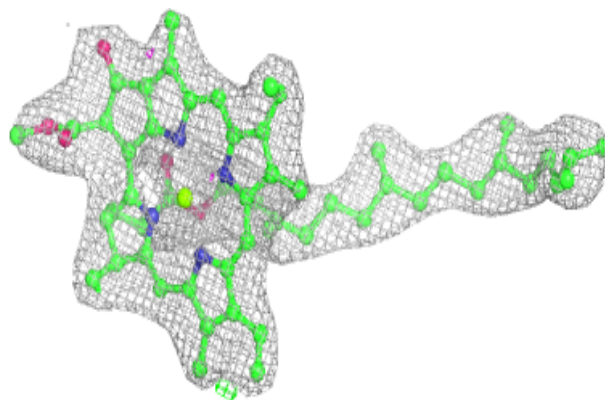


Electron density around CLA A 406:

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

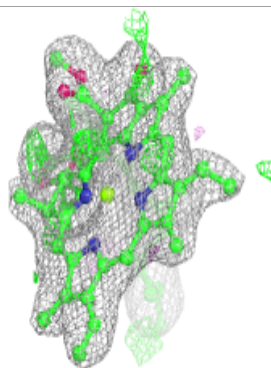
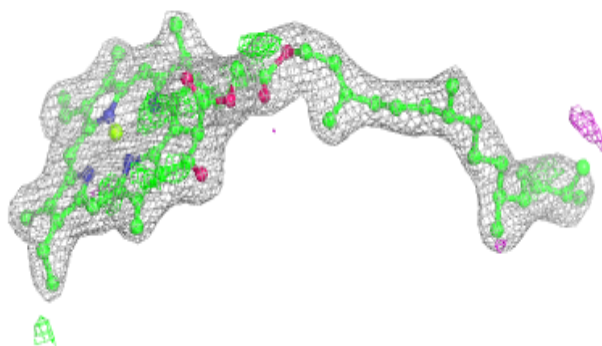
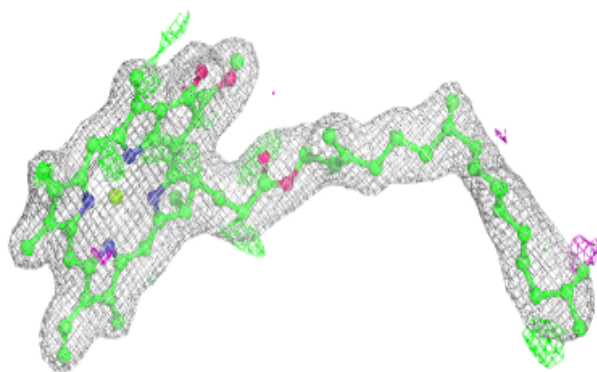
**Electron density around CLA B 608:**

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

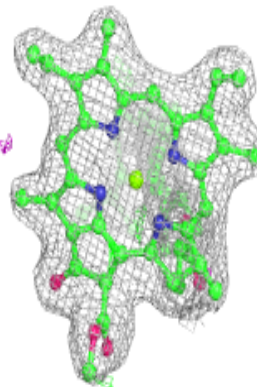
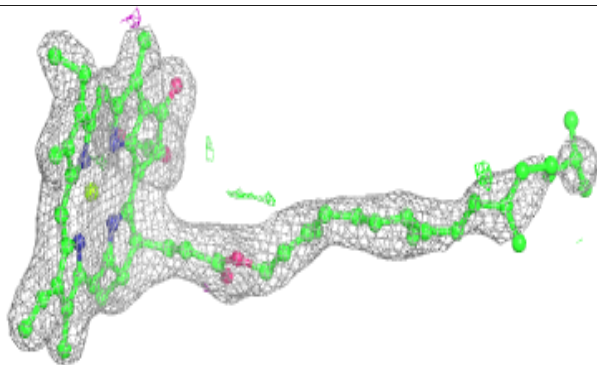
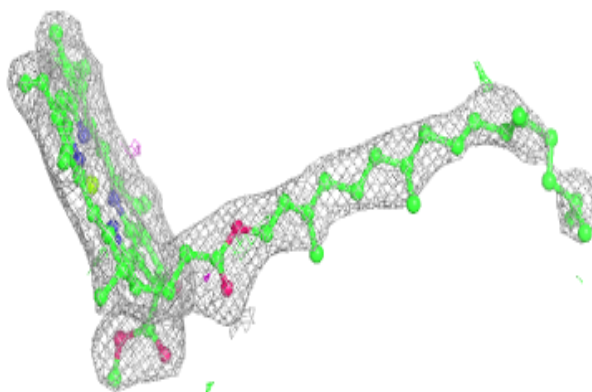


Electron density around CLA A 404:

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

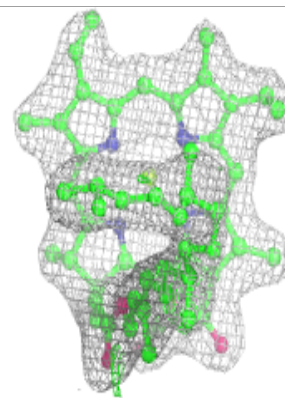
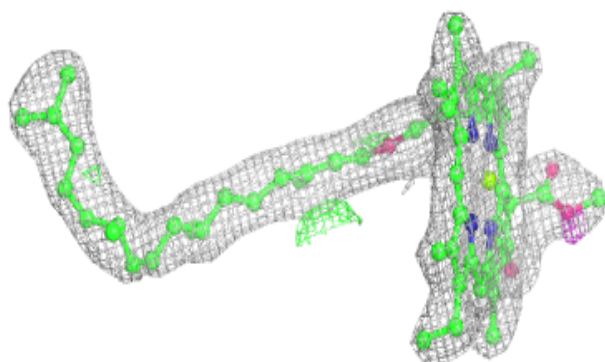
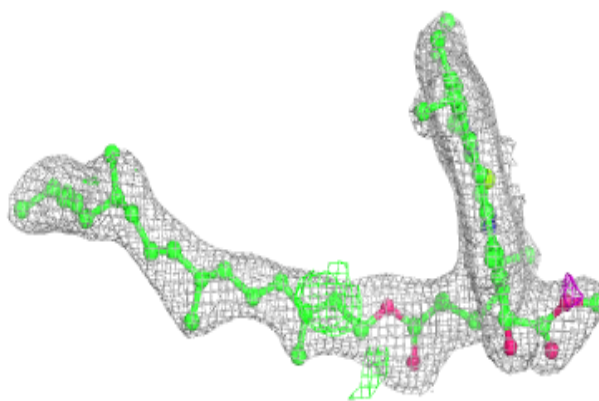
**Electron density around CLA B 604:**

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

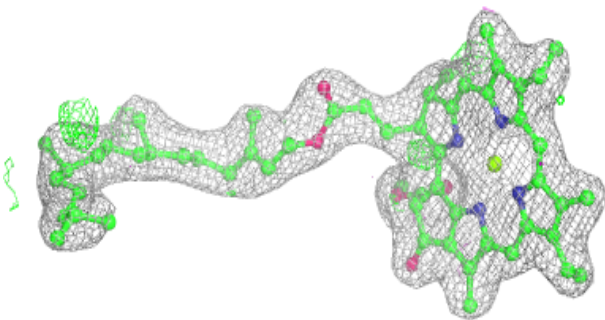
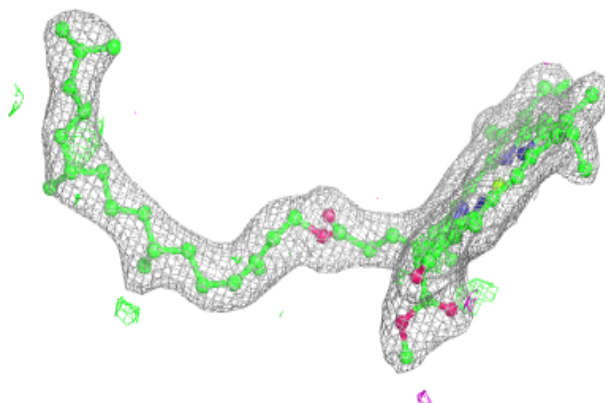


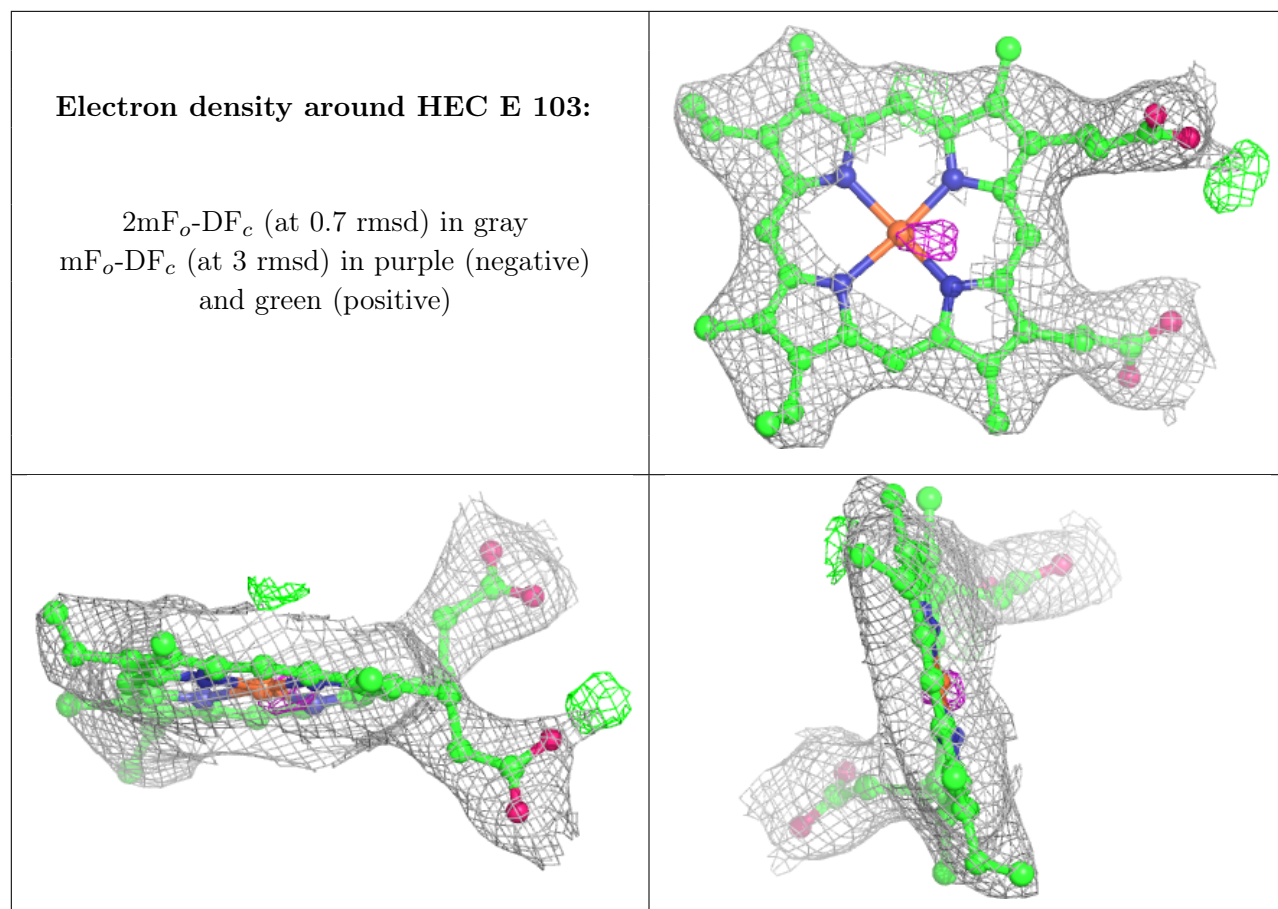
Electron density around CLA B 605:

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

**Electron density around CLA D 403:**

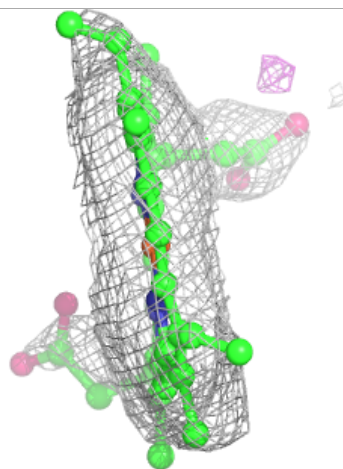
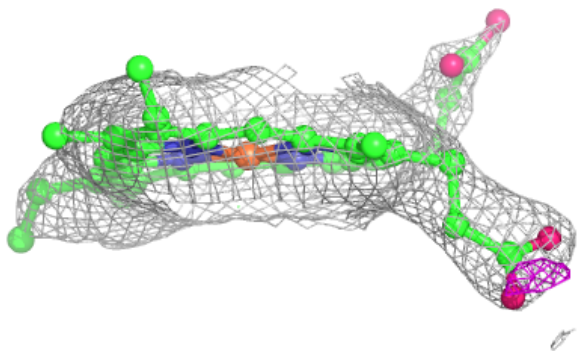
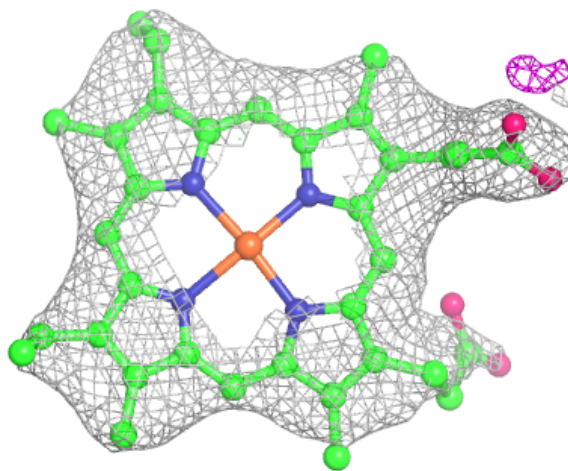
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





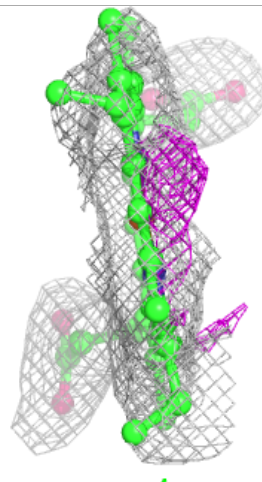
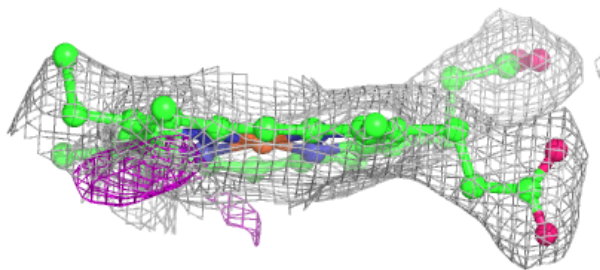
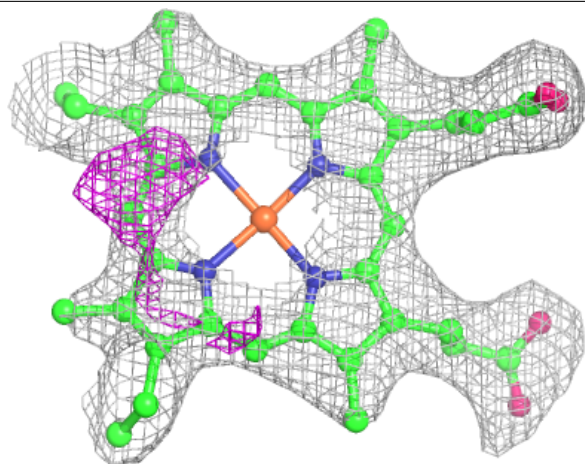
Electron density around HEC e 102:

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



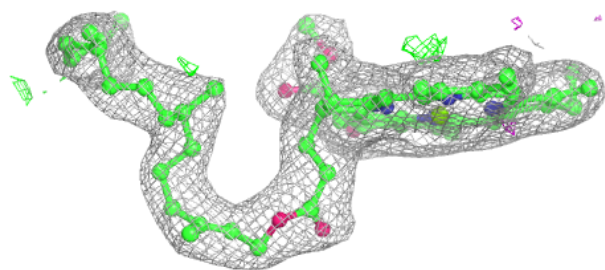
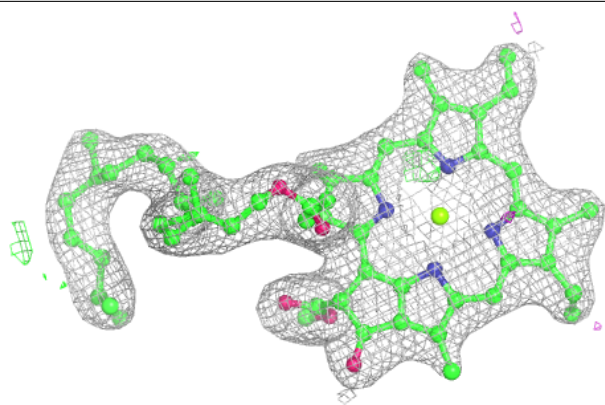
Electron density around HEC v 202:

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



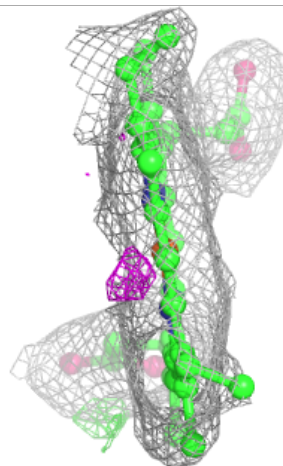
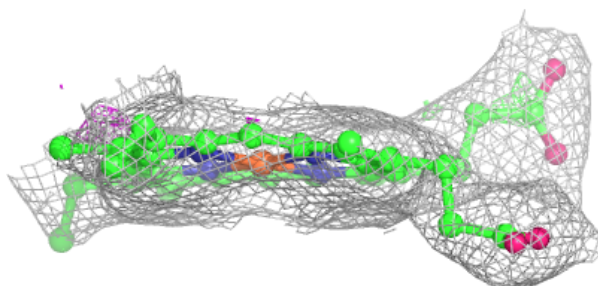
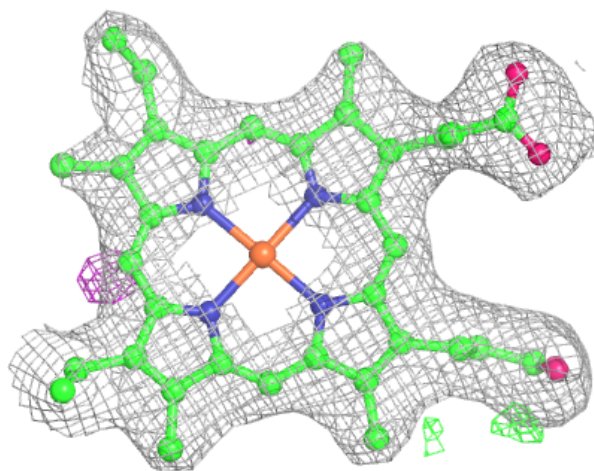
Electron density around CLA B 612:

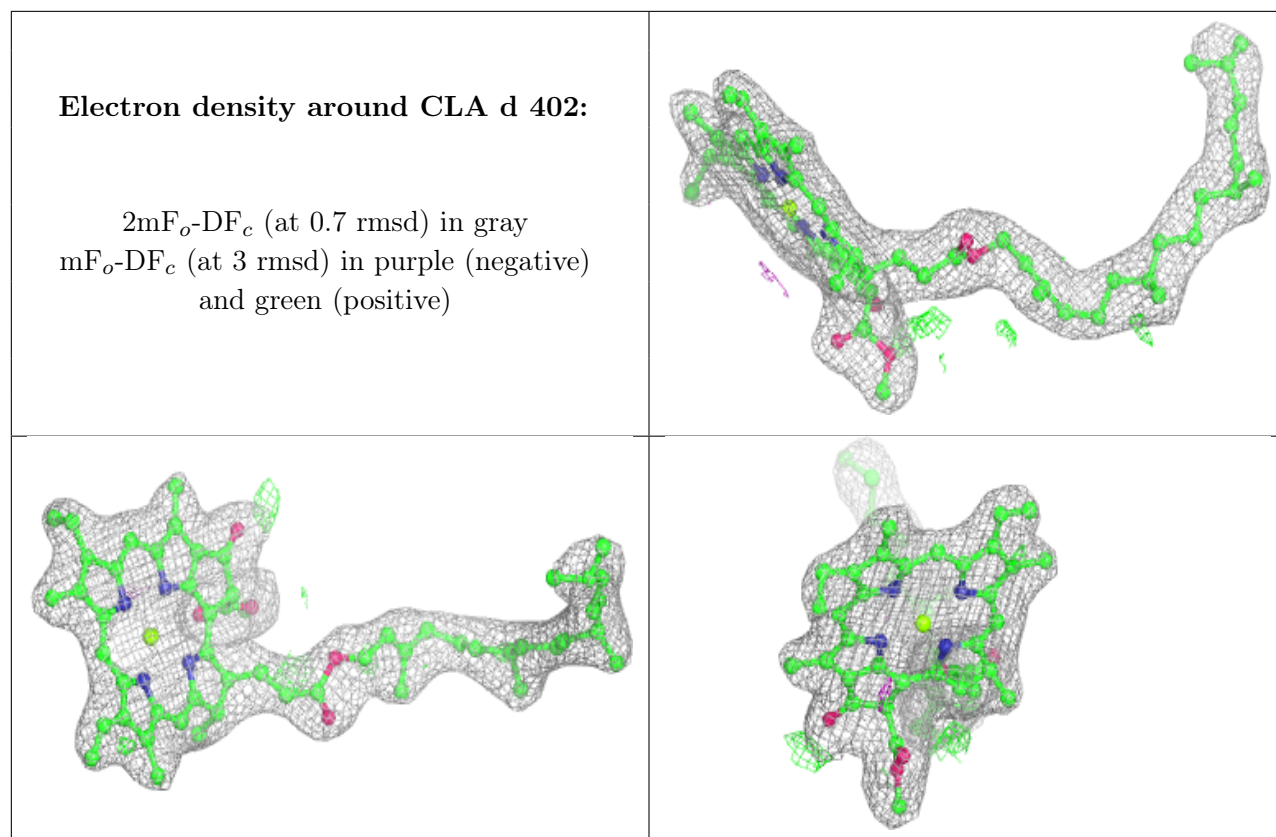
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC V 201:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.