



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 19, 2024 – 01:35 PM EDT

PDB ID : 3WU2
Title : Crystal structure analysis of Photosystem II complex
Authors : Umena, Y.; Kawakami, K.; Shen, J.R.; Kamiya, N.
Deposited on : 2014-04-21
Resolution : 1.90 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

<http://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 : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 2.37.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

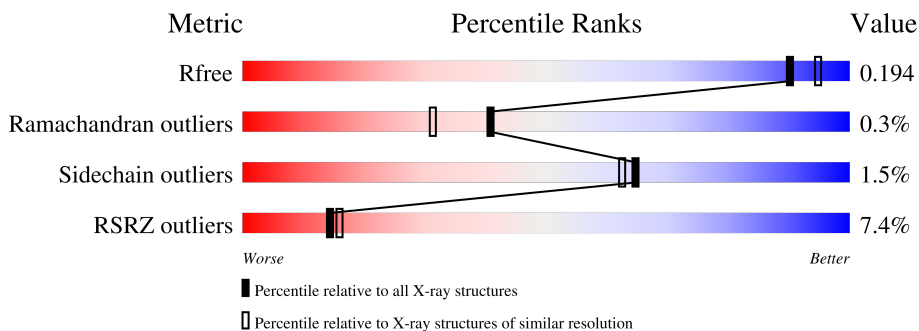
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	
1	a	344	
2	B	504	
2	b	504	
3	C	455	
3	c	455	

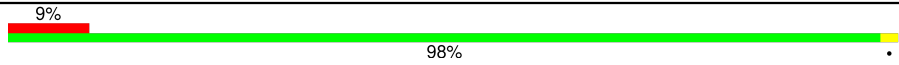

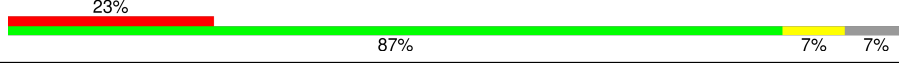
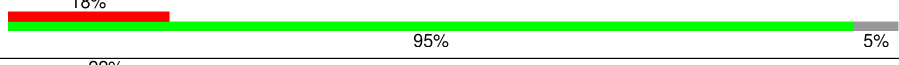
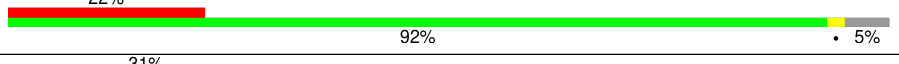
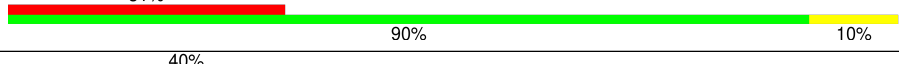
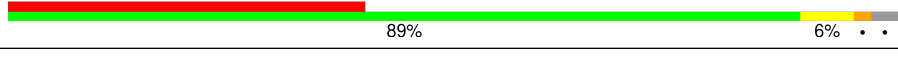
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Mol	Chain	Length	Quality of chain
4	D	342	2% 96% .
4	d	342	2% 95% .
5	E	83	20% 96% ..
5	e	83	27% 92% . 5%
6	F	44	11% 73% 5% 23%
6	f	44	7% 68% 5% 27%
7	H	63	2% 97% .
7	h	63	8% 94% 6%
8	I	38	95% 5%
8	i	38	5% 89% 11%
9	J	40	10% 90% 10%
9	j	40	20% 95% ..
10	K	37	97% .
10	k	37	8% 95% 5%
11	L	37	8% 100%
11	l	37	5% 97% .
12	M	36	3% 89% . 8%
12	m	36	6% 92% . 6%
13	O	244	14% 98% .
13	o	244	16% 96% ..
14	T	32	3% 88% 6% 6%
14	t	32	3% 88% 6% 6%
15	U	104	90% . 7%
15	u	104	% 93% 7%
16	V	137	99% .

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Mol	Chain	Length	Quality of chain
16	v	137	
17	Y	30	
17	y	30	
18	X	40	
18	x	40	
19	Z	62	
19	z	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	405	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	B	617	X	-	-	-
23	CLA	C	501	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	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	D	402	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	a	409	X	-	-	-
23	CLA	a	410	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	b	618	X	-	-	-
23	CLA	b	619	X	-	-	-
23	CLA	c	902	X	-	-	-
23	CLA	c	903	X	-	-	-
23	CLA	c	905	X	-	-	-
23	CLA	c	906	X	-	-	-
23	CLA	c	907	X	-	-	-
23	CLA	c	908	X	-	-	-
23	CLA	c	910	X	-	-	-
23	CLA	c	911	X	-	-	-
23	CLA	c	913	X	-	-	-
23	CLA	d	402	X	-	-	-
29	UNL	T	102	-	-	-	X
29	UNL	t	103	-	-	-	X
33	HTG	B	626	-	-	-	X
33	HTG	c	924	-	-	-	X

2 Entry composition [i](#)

There are 41 unique types of molecules in this entry. The entry contains 54036 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 Q(B) protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	334	2633	1729	429	460	15	0	4	0
1	a	334	2625	1722	431	457	15	0	4	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	SEE REMARK 999	UNP P51765
a	279	PRO	ARG	SEE REMARK 999	UNP P51765

- Molecule 2 is a protein called Photosystem II CP47 chlorophyll apoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	504	4009	2633	668	695	13	0	10	0
2	b	501	3964	2605	658	688	13	0	11	0

- Molecule 3 is a protein called Photosystem II 44 kDa reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	451	3502	2291	588	610	13	0	3	0
3	c	455	3536	2315	593	615	13	0	4	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	SEE REMARK 999	UNP D0VWR7
C	20	SER	-	SEE REMARK 999	UNP D0VWR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	SEE REMARK 999	UNP D0VWR7
C	22	PHE	-	SEE REMARK 999	UNP D0VWR7
c	19	ASN	-	SEE REMARK 999	UNP D0VWR7
c	20	SER	-	SEE REMARK 999	UNP D0VWR7
c	21	ILE	-	SEE REMARK 999	UNP D0VWR7
c	22	PHE	-	SEE REMARK 999	UNP D0VWR7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	2	0
			2726	1809	443	462	12			
4	d	341	Total	C	N	O	S	0	4	0
			2741	1817	449	463	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	S	0	0	0
			657	429	106	122				
5	e	79	Total	C	N	O	S	0	0	0
			639	419	103	117				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			274	187	45	41	1			
6	f	32	Total	C	N	O	S	0	0	0
			257	175	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			
7	h	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total	C	N	O	S	0	0	0
			294	199	45	49	1			
8	i	38	Total	C	N	O	S	0	0	0
			311	210	48	52	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			251	171	37	42	1			
9	j	39	Total	C	N	O	S	0	0	0
			271	182	40	48	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	1	0
			290	202	42	46			
10	k	37	Total	C	N	O	0	0	0
			286	198	42	46			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	SEE REMARK 999	UNP P19054
K	39	TRP	VAL	SEE REMARK 999	UNP P19054
k	33	LEU	PHE	SEE REMARK 999	UNP P19054
k	39	TRP	VAL	SEE REMARK 999	UNP P19054

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	0	1	0
			302	203	48	51			
11	l	37	Total	C	N	O	0	2	0
			300	204	45	51			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			261	176	37	47	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	2	0
			271	184	38	48	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	SEE REMARK 999	UNP P12312
m	8	LEU	PHE	SEE REMARK 999	UNP P12312

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	N	O	S	0	5	0
			1878	1177	314	382	5			
13	o	241	Total	C	N	O	S	0	5	0
			1855	1163	305	381	6			

- 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
			256	180	36	38	2			
14	t	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	0	0	0
			770	489	129	152			
15	u	97	Total	C	N	O	0	1	0
			772	490	129	153			

- 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	2	0
			1066	677	180	205	4			
16	v	137	Total	C	N	O	S	0	1	0
			1060	671	177	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	27	Total	C	N	O	S	0	0	0
			196	130	32	31	3			
17	y	28	Total	C	N	O	S	0	0	0
			196	128	33	32	3			

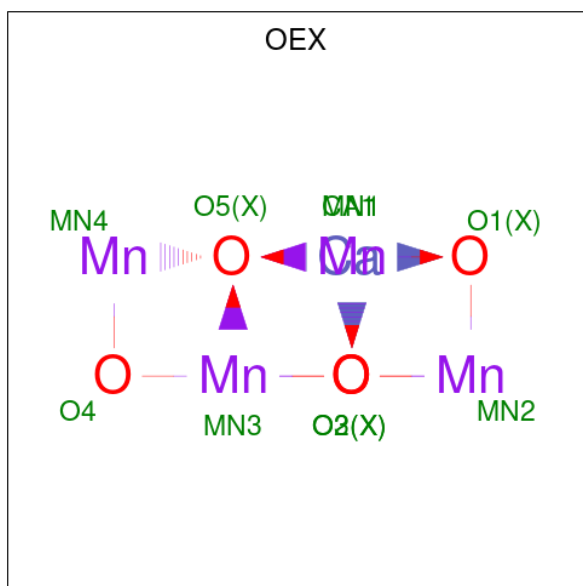
- Molecule 18 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O	S	0	1	0
			280	190	44	46				
18	x	38	Total	C	N	O	S	0	1	0
			280	190	44	46				

- 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
			459	318	67	73	1			
19	z	60	Total	C	N	O	S	0	0	0
			431	301	64	65	1			

- Molecule 20 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



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

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

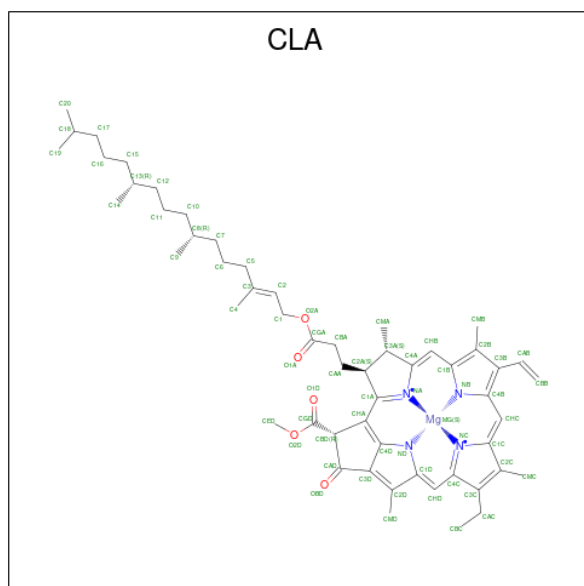
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

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

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

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



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

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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	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		
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		

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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	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		
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		

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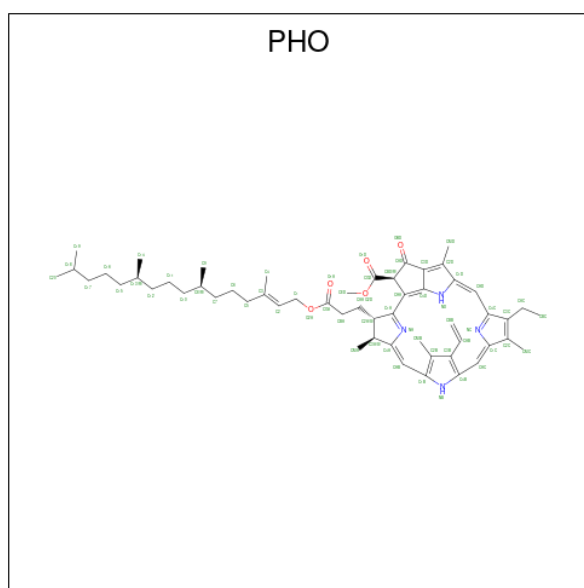
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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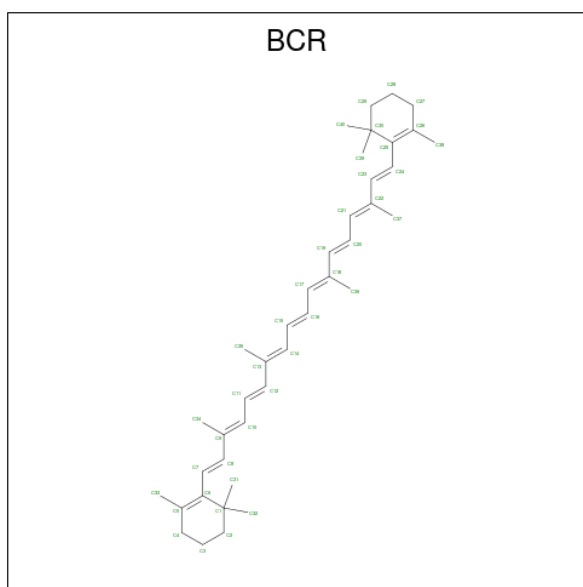
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



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

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



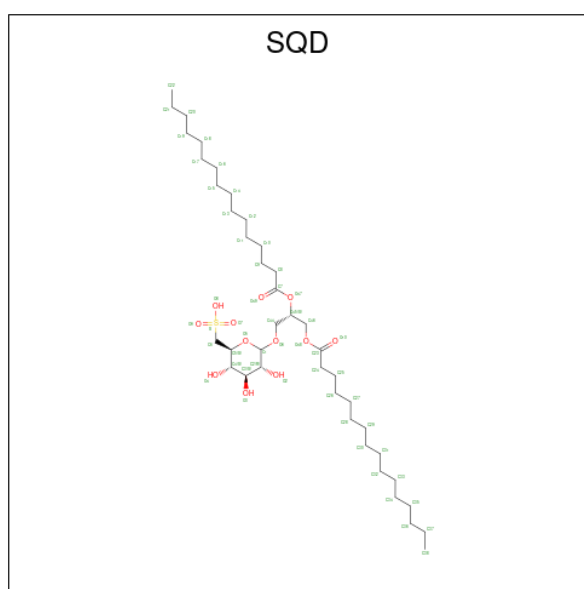
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	a	1	Total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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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	k	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

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



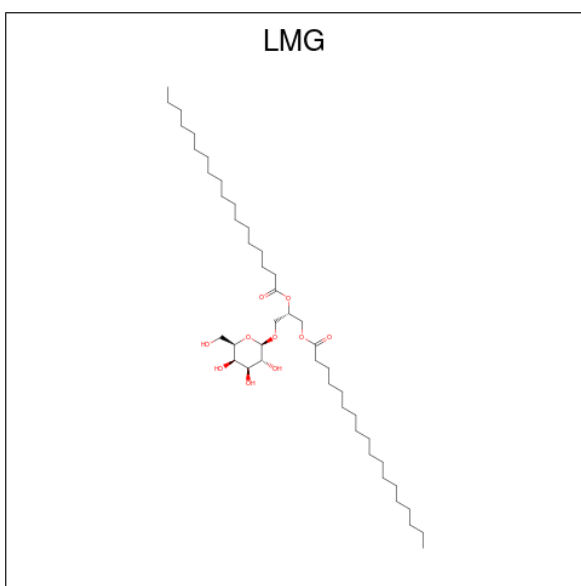
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O S 54 41 12 1	0	0
26	A	1	Total C O S 54 41 12 1	0	0
26	B	1	Total C O S 54 41 12 1	0	0
26	D	1	Total C O S 45 32 12 1	0	0
26	L	1	Total C O S 54 41 12 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
26	a	1	Total 54	C 41	O 12	S 1	0	0
26	a	1	Total 54	C 41	O 12	S 1	0	0
26	f	1	Total 33	C 23	O 9	S 1	0	0

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



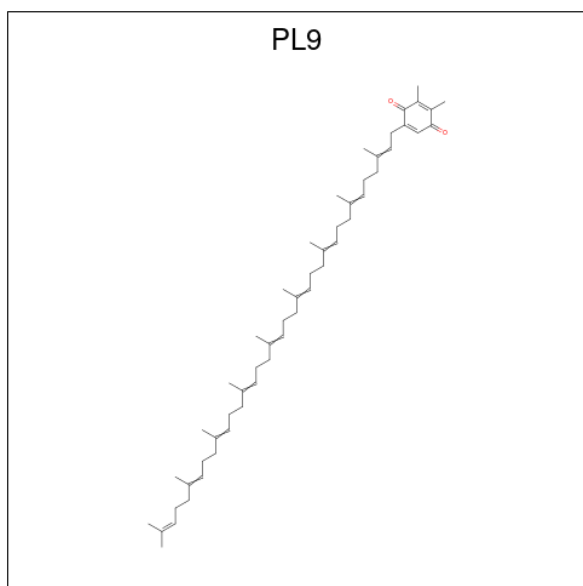
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
27	A	1	Total 51	C 41	O 10	0	0
27	B	1	Total 51	C 41	O 10	0	0
27	C	1	Total 51	C 41	O 10	0	0
27	D	1	Total 51	C 41	O 10	0	0
27	Z	1	Total 51	C 41	O 10	0	0
27	a	1	Total 51	C 41	O 10	0	0
27	b	1	Total 51	C 41	O 10	0	0
27	c	1	Total 51	C 41	O 10	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	c	1	Total	C	O	0	0
			51	41	10		
27	d	1	Total	C	O	0	0
			51	41	10		

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



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

- Molecule 29 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

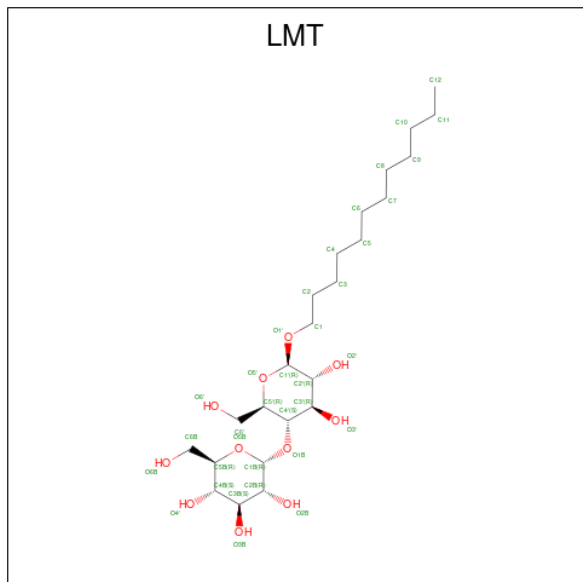
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	4	Total	C	O	0	0
			69	64	5		
29	B	4	Total	C		0	0
			56	56			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	C	1	Total	C	O	0	0
			34	29	5		
29	D	2	Total	C	O	0	0
			56	51	5		
29	E	2	Total	C		0	0
			27	27			
29	H	1	Total	C		0	0
			10	10			
29	I	2	Total	C		0	0
			24	24			
29	J	2	Total	C		0	0
			26	26			
29	L	1	Total	C		0	0
			14	14			
29	M	1	Total	C		0	0
			16	16			
29	T	1	Total	C		0	0
			13	13			
29	X	1	Total	C		0	0
			16	16			
29	Z	1	Total	C		0	0
			16	16			
29	a	3	Total	C	O	0	0
			56	51	5		
29	b	4	Total	C	O	0	0
			84	79	5		
29	c	2	Total	C	O	0	0
			40	35	5		
29	d	1	Total	C		0	0
			16	16			
29	e	1	Total	C		0	0
			11	11			
29	i	4	Total	C		0	0
			55	55			
29	j	2	Total	C		0	0
			28	28			
29	t	1	Total	C		0	0
			16	16			
29	x	1	Total	C		0	0
			16	16			
29	z	1	Total	C		0	0
			16	16			

- Molecule 30 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



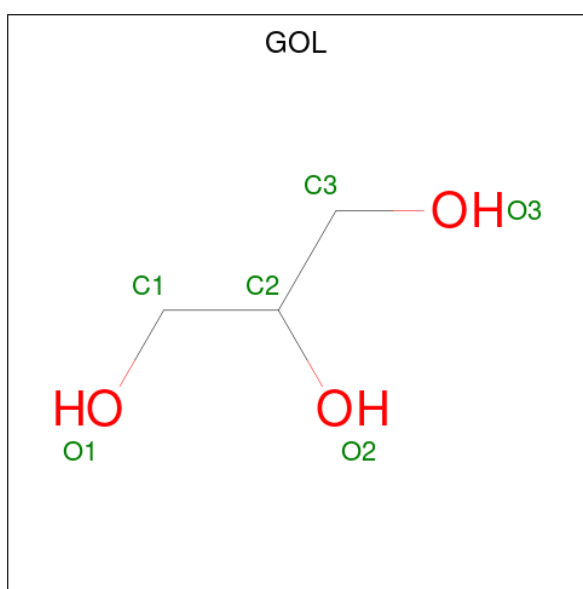
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	1	Total C O 35 24 11	0	0
30	B	1	Total C O 35 24 11	0	0
30	C	1	Total C O 35 24 11	0	0
30	F	1	Total C O 35 24 11	0	0
30	J	1	Total C O 24 18 6	0	0
30	M	1	Total C O 35 24 11	0	0
30	M	1	Total C O 35 24 11	0	0
30	Z	1	Total C O 35 24 11	0	0
30	a	1	Total C O 35 24 11	0	0
30	b	1	Total C O 25 19 6	0	0
30	b	1	Total C O 24 18 6	0	0
30	c	1	Total C O 35 24 11	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	m	1	Total	C	O	0	0
			35	24	11		
30	m	1	Total	C	O	0	0
			35	24	11		
30	t	1	Total	C	O	0	0
			24	18	6		
30	z	1	Total	C	O	0	0
			32	21	11		

- Molecule 31 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			6	3	3		
31	A	1	Total	C	O	0	0
			6	3	3		
31	A	1	Total	C	O	0	0
			6	3	3		
31	B	1	Total	C	O	0	0
			6	3	3		
31	B	1	Total	C	O	0	0
			6	3	3		
31	B	1	Total	C	O	0	0
			6	3	3		
31	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total 6	C 3	O 3	0	0
31	B	1	Total 6	C 3	O 3	0	0
31	C	1	Total 6	C 3	O 3	0	0
31	C	1	Total 6	C 3	O 3	0	0
31	C	1	Total 6	C 3	O 3	0	0
31	D	1	Total 6	C 3	O 3	0	0
31	L	1	Total 6	C 3	O 3	0	0
31	O	1	Total 6	C 3	O 3	0	0
31	V	1	Total 6	C 3	O 3	0	0
31	V	1	Total 6	C 3	O 3	0	0
31	V	1	Total 6	C 3	O 3	0	0
31	a	1	Total 6	C 3	O 3	0	0
31	a	1	Total 6	C 3	O 3	0	0
31	a	1	Total 6	C 3	O 3	0	0
31	b	1	Total 6	C 3	O 3	0	0
31	b	1	Total 6	C 3	O 3	0	0
31	b	1	Total 6	C 3	O 3	0	0
31	b	1	Total 6	C 3	O 3	0	0
31	b	1	Total 6	C 3	O 3	0	0
31	c	1	Total 6	C 3	O 3	0	0
31	c	1	Total 6	C 3	O 3	0	0

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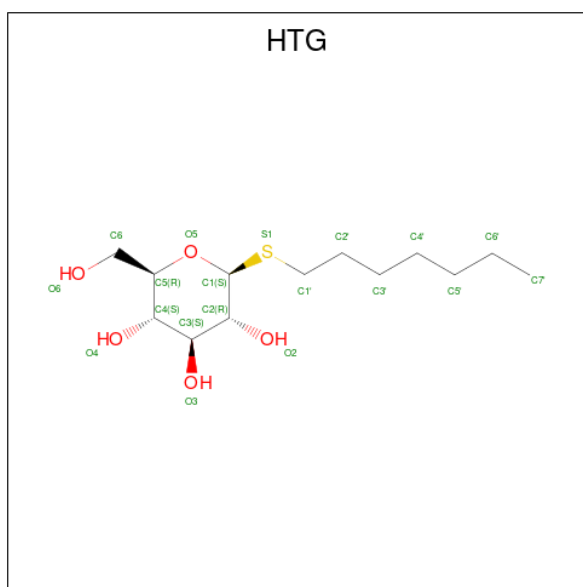
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	c	1	Total C O 6 3 3	0	0
31	c	1	Total C O 6 3 3	0	0
31	f	1	Total C O 6 3 3	0	0
31	h	1	Total C O 6 3 3	0	0
31	l	1	Total C O 6 3 3	0	0
31	v	1	Total C O 6 3 3	0	0
31	v	1	Total C O 6 3 3	0	0
31	v	1	Total C O 6 3 3	0	0

- Molecule 32 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 33 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: C₁₃H₂₆O₅S).



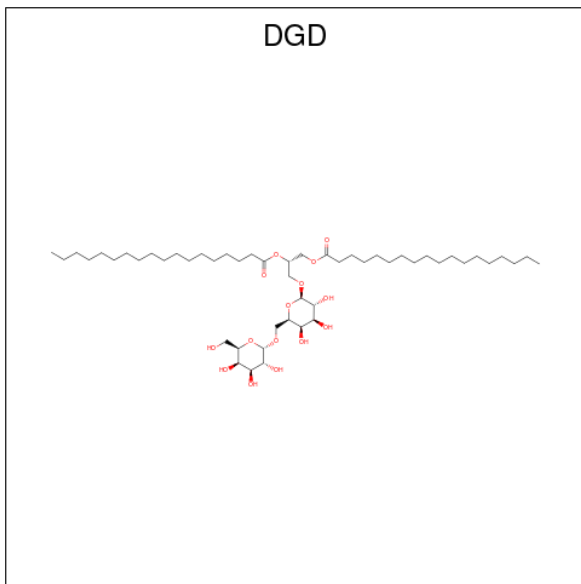
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	C	1	Total	C	O	S	0	0
			19	13	5	1		
33	C	1	Total	C	O	S	0	0
			19	13	5	1		
33	D	1	Total	C	O	S	0	0
			19	13	5	1		
33	O	1	Total	C	O	S	0	0
			19	13	5	1		
33	U	1	Total	C	S		0	0
			9	8	1			
33	V	1	Total	C	O	S	0	0
			13	7	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	b	1	Total	C	O	S	0	0
			19	13	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
33	b	1	Total 19	C 13	O 5	S 1	0	0
33	c	1	Total 19	C 13	O 5	S 1	0	0
33	c	1	Total 19	C 13	O 5	S 1	0	0
33	d	1	Total 19	C 13	O 5	S 1	0	0
33	u	1	Total 14	C 10	O 3	S 1	0	0

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



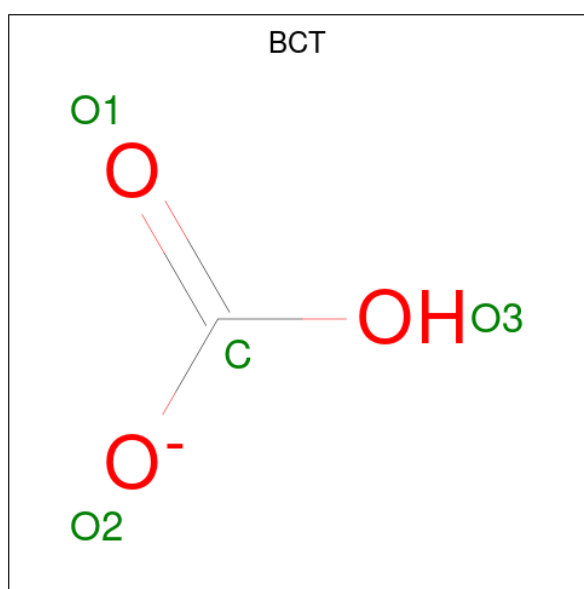
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
34	C	1	Total 62	C 47	O 15	0	0
34	C	1	Total 62	C 47	O 15	0	0
34	C	1	Total 62	C 47	O 15	0	0
34	D	1	Total 53	C 42	O 11	0	0
34	H	1	Total 62	C 47	O 15	0	0
34	c	1	Total 62	C 47	O 15	0	0

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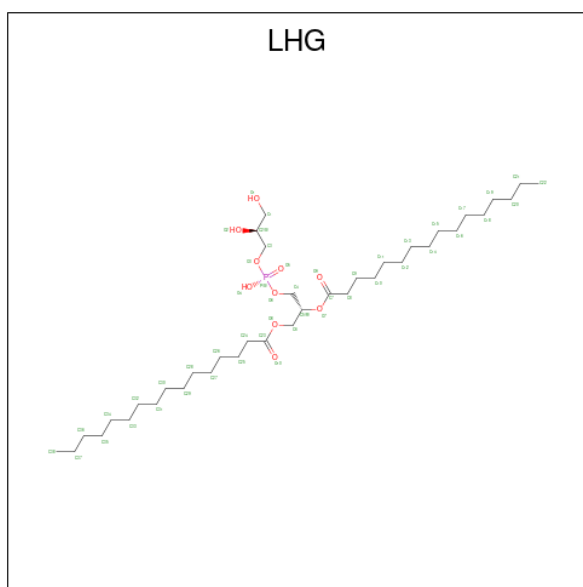
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	c	1	Total	C	O	0	0
			62	47	15		
34	c	1	Total	C	O	0	0
			62	47	15		
34	d	1	Total	C	O	0	0
			50	41	9		
34	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 35 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	D	1	Total	C	O	0	0
			4	1	3		
35	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 36 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $\text{C}_{38}\text{H}_{75}\text{O}_{10}\text{P}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
36	D	1	49	38	10	1	0	0
36	D	1	49	38	10	1	0	0
36	D	1	46	35	10	1	0	0
36	E	1	49	38	10	1	0	0
36	L	1	49	38	10	1	0	0
36	a	1	40	29	10	1	0	0
36	d	1	49	38	10	1	0	0
36	d	1	49	38	10	1	0	0
36	d	1	49	38	10	1	0	0
36	l	1	49	38	10	1	0	0

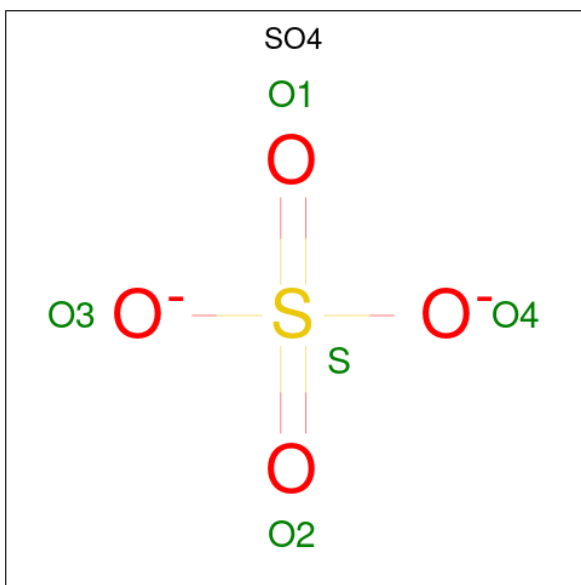
- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

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

- 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 SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
40	O	1	Total	O	S	0	0
			5	4	1		

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	168	Total	O	0	2
			170	170		
41	B	311	Total	O	0	8
			319	319		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	C	253	Total O 263 263	0	10
41	D	156	Total O 161 161	0	5
41	E	32	Total O 35 35	0	3
41	F	12	Total O 12 12	0	0
41	H	50	Total O 52 52	0	2
41	I	8	Total O 8 8	0	0
41	J	9	Total O 9 9	0	0
41	K	8	Total O 8 8	0	0
41	L	23	Total O 24 24	0	1
41	M	15	Total O 16 16	0	1
41	O	193	Total O 202 202	0	9
41	T	10	Total O 10 10	0	0
41	U	98	Total O 100 100	0	2
41	V	140	Total O 144 144	0	4
41	Y	6	Total O 6 6	0	0
41	X	13	Total O 14 14	0	1
41	Z	1	Total O 1 1	0	0
41	a	153	Total O 155 155	0	2
41	b	295	Total O 306 306	0	11
41	c	238	Total O 245 245	0	7
41	d	156	Total O 160 160	0	4

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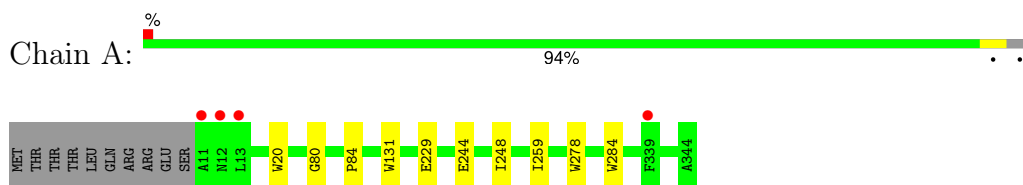
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	e	22	Total O 22 22	0	0
41	f	13	Total O 14 14	0	1
41	h	48	Total O 53 53	0	5
41	i	13	Total O 14 14	0	1
41	j	9	Total O 9 9	0	0
41	k	5	Total O 5 5	0	0
41	l	17	Total O 18 18	0	1
41	m	15	Total O 16 16	0	1
41	o	167	Total O 175 175	0	8
41	t	12	Total O 12 12	0	0
41	u	102	Total O 106 106	0	4
41	v	98	Total O 104 104	0	6
41	y	7	Total O 7 7	0	0
41	x	6	Total O 6 6	0	0
41	z	2	Total O 2 2	0	0

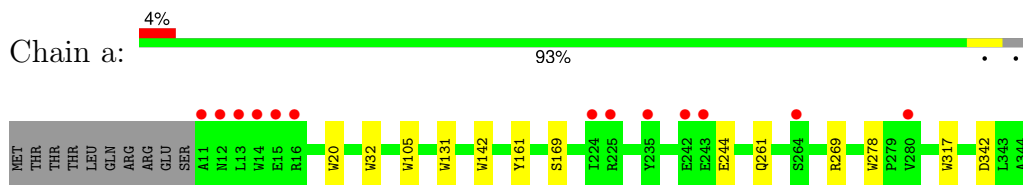
3 Residue-property plots [i](#)

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

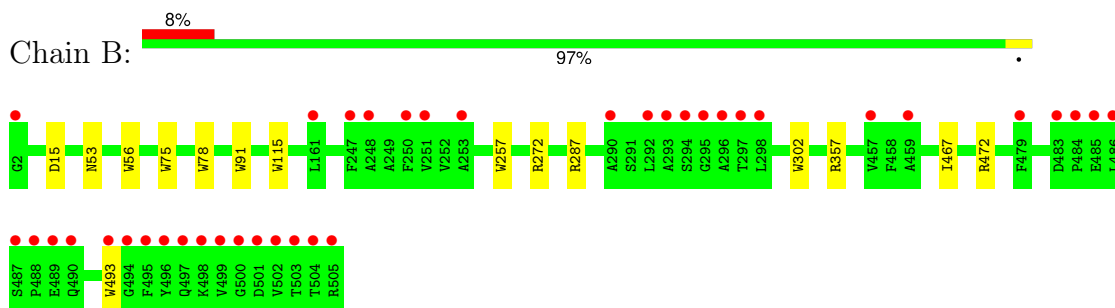
- Molecule 1: Photosystem Q(B) protein



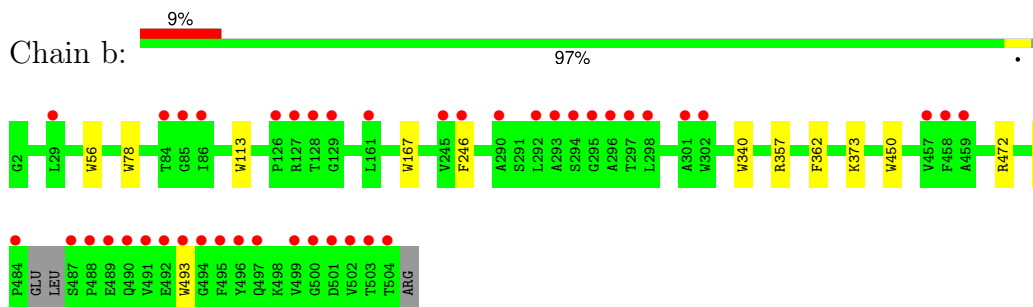
- Molecule 1: Photosystem Q(B) protein



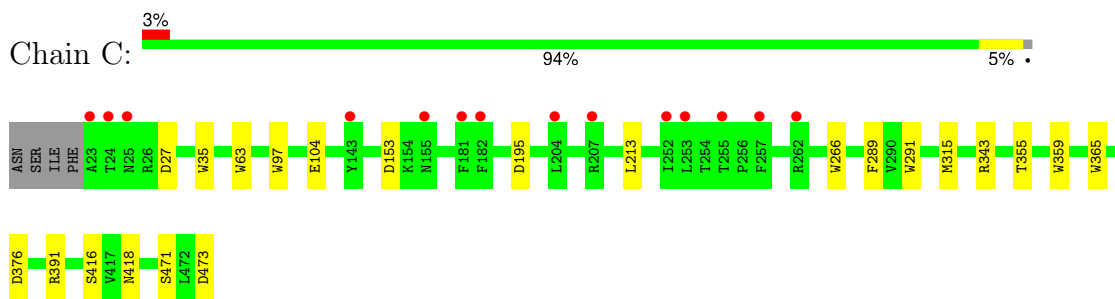
- Molecule 2: Photosystem II CP47 chlorophyll apoprotein



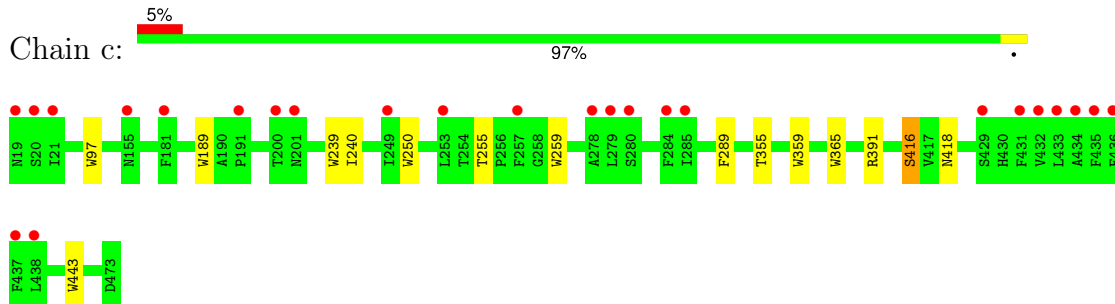
- Molecule 2: Photosystem II CP47 chlorophyll apoprotein



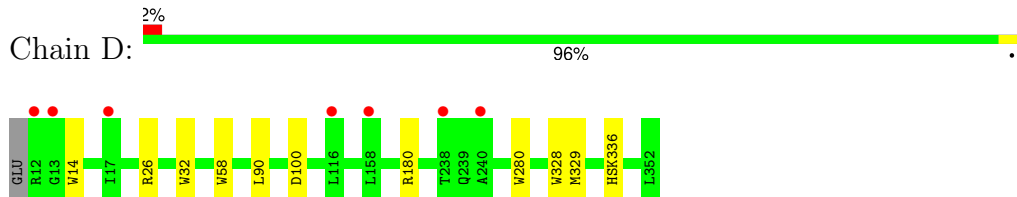
- Molecule 3: Photosystem II 44 kDa reaction center protein



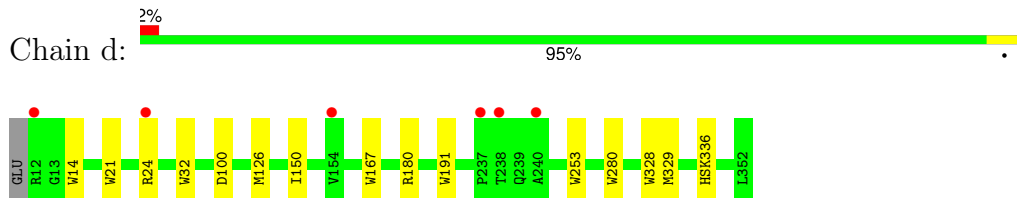
● Molecule 3: Photosystem II 44 kDa reaction center protein



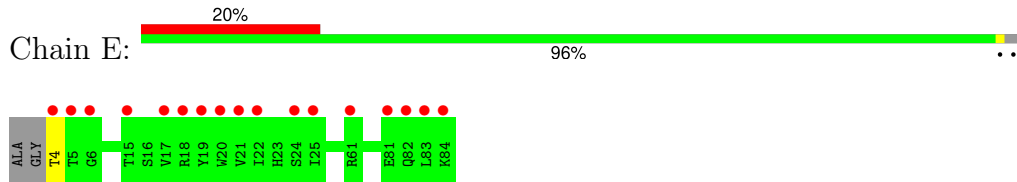
● Molecule 4: Photosystem II D2 protein



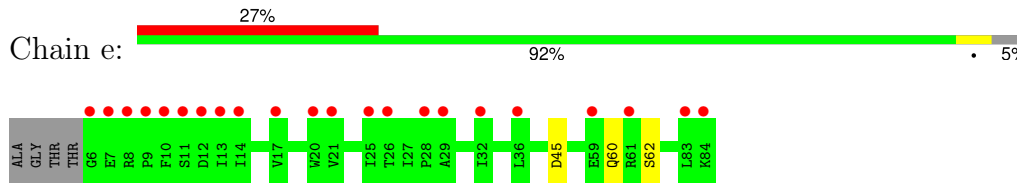
● Molecule 4: Photosystem II D2 protein



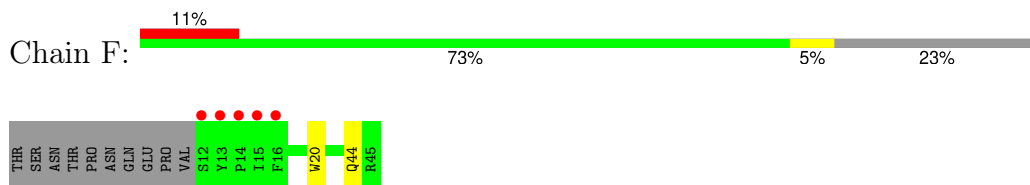
● Molecule 5: Cytochrome b559 subunit alpha



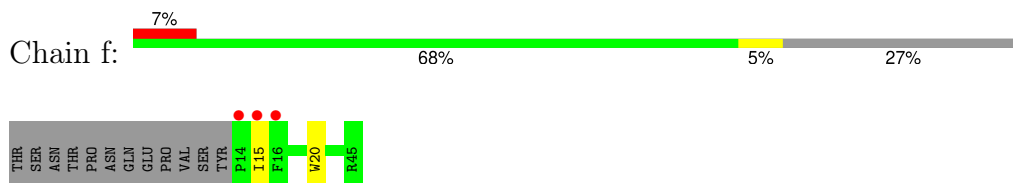
● Molecule 5: Cytochrome b559 subunit alpha



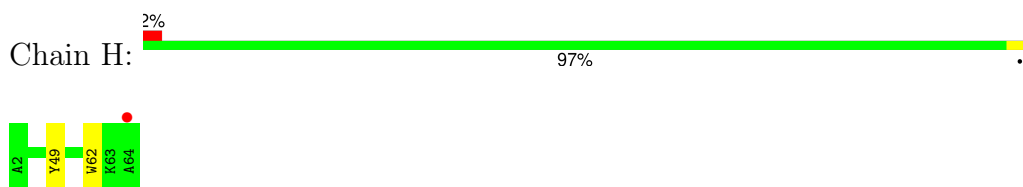
- Molecule 6: Cytochrome b559 subunit beta



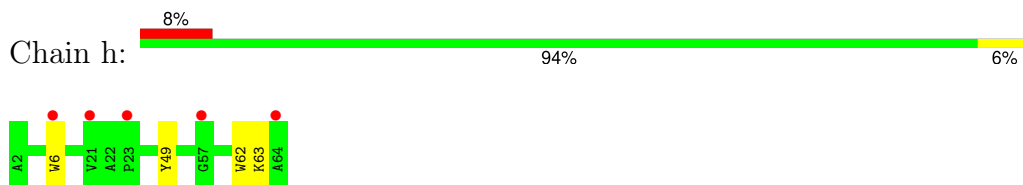
- Molecule 6: Cytochrome b559 subunit beta



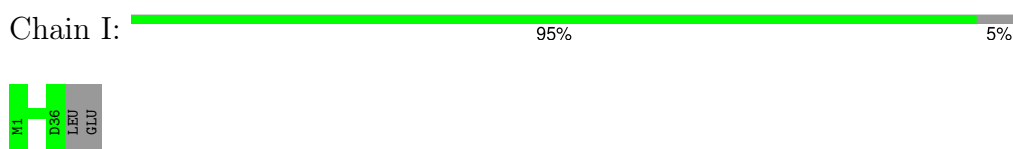
- Molecule 7: Photosystem II reaction center protein H



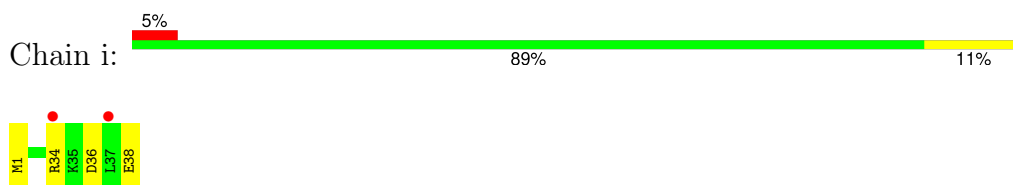
- Molecule 7: Photosystem II reaction center protein H



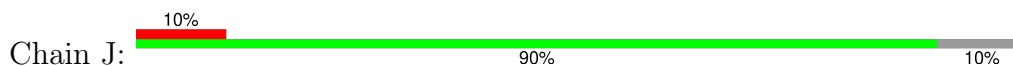
- Molecule 8: Photosystem II reaction center protein I

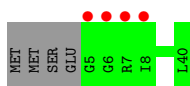


- Molecule 8: Photosystem II reaction center protein I

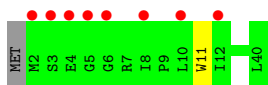


- Molecule 9: Photosystem II reaction center protein J





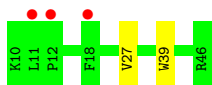
- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K



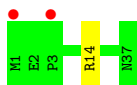
- Molecule 10: Photosystem II reaction center protein K



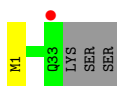
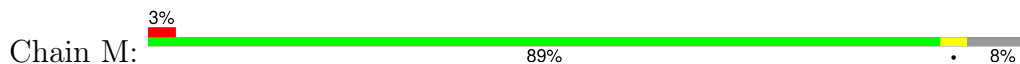
- Molecule 11: Photosystem II reaction center protein L



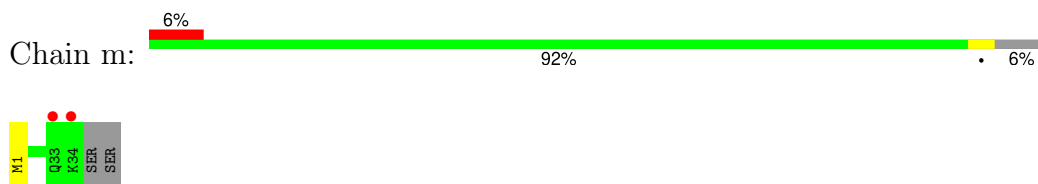
- Molecule 11: Photosystem II reaction center protein L



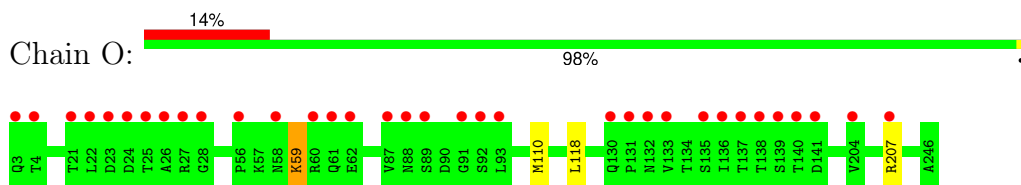
- Molecule 12: Photosystem II reaction center protein M



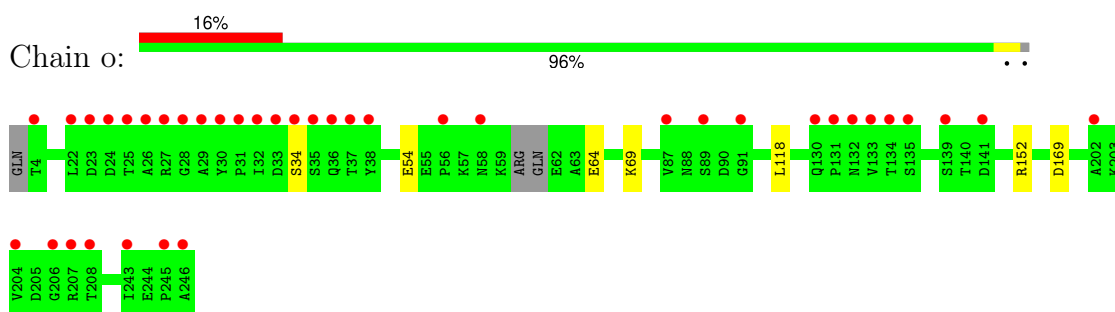
- Molecule 12: Photosystem II reaction center protein M



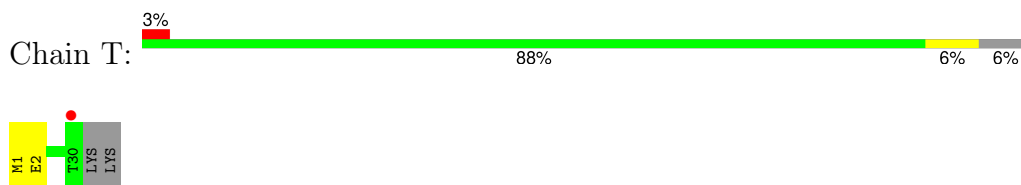
• Molecule 13: Photosystem II manganese-stabilizing polypeptide



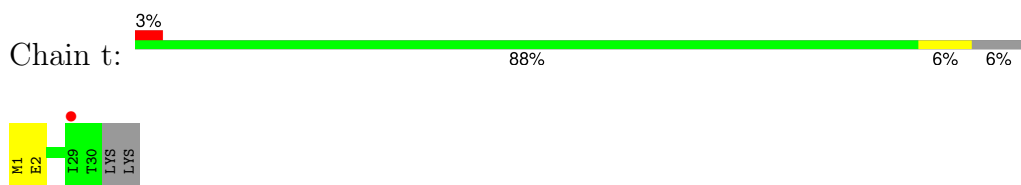
• Molecule 13: Photosystem II manganese-stabilizing polypeptide



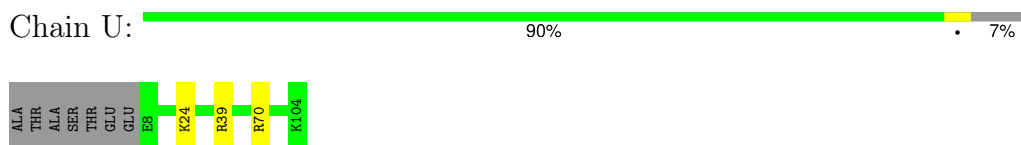
• Molecule 14: Photosystem II reaction center protein T



• Molecule 14: Photosystem II reaction center protein T

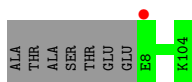


• Molecule 15: Photosystem II 12 kDa extrinsic protein



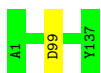
• Molecule 15: Photosystem II 12 kDa extrinsic protein





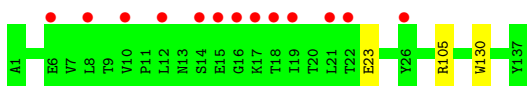
- Molecule 16: Cytochrome c-550

Chain V: 99%



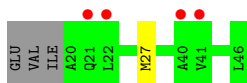
- Molecule 16: Cytochrome c-550

Chain v: 9% 98%



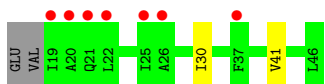
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y: 13% 87% 10%



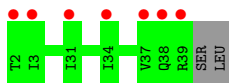
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y: 23% 87% 7% 7%



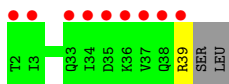
- Molecule 18: Photosystem II reaction center protein X

Chain X: 18% 95% 5%

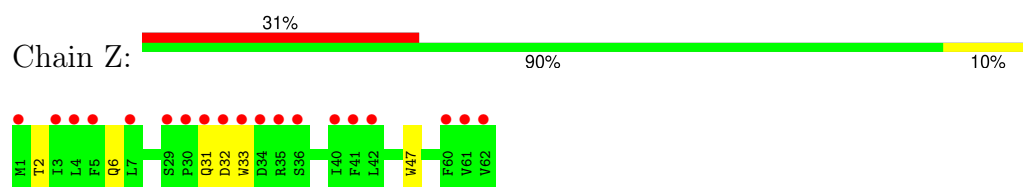


- Molecule 18: Photosystem II reaction center protein X

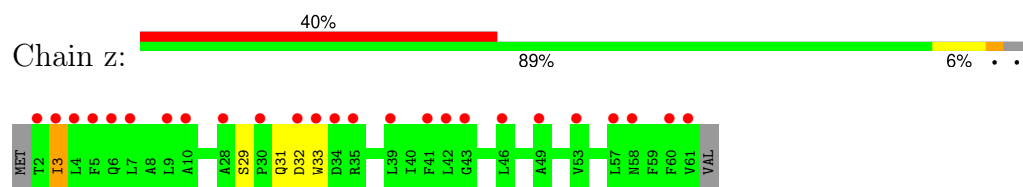
Chain x: 22% 92% 5%



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	122.19Å 228.51Å 286.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 49.02 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-1.90) 99.8 (49.02-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 1.90Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.156 , 0.194 0.157 , 0.194	Depositor DCC
R_{free} test set	31215 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtrriage
Anisotropy	0.575	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 66.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	54036	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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: PHO, CA, SQD, FME, BCT, HSK, OEX, PL9, MG, HEM, LHG, DGD, RRX, GOL, CL, FE2, CLA, UNL, BCR, LMT, SO4, HTG, LMG

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	1.08	4/2730 (0.1%)	0.90	1/3723 (0.0%)
1	a	1.06	9/2721 (0.3%)	0.86	4/3711 (0.1%)
2	B	1.03	9/4179 (0.2%)	0.89	5/5693 (0.1%)
2	b	1.01	7/4134 (0.2%)	0.85	2/5633 (0.0%)
3	C	1.00	7/3624 (0.2%)	0.84	9/4933 (0.2%)
3	c	0.96	8/3662 (0.2%)	0.81	0/4986
4	D	1.13	5/2804 (0.2%)	0.93	3/3820 (0.1%)
4	d	1.05	8/2825 (0.3%)	0.87	2/3847 (0.1%)
5	E	0.81	0/676	0.82	0/924
5	e	0.81	0/658	0.78	1/899 (0.1%)
6	F	0.90	1/283 (0.4%)	0.71	0/386
6	f	0.92	1/265 (0.4%)	0.69	0/360
7	H	0.98	1/511 (0.2%)	0.79	0/697
7	h	0.94	2/511 (0.4%)	0.81	0/697
8	I	0.77	0/291	0.78	0/394
8	i	0.75	0/308	0.77	0/415
9	J	0.94	0/257	0.68	0/349
9	j	0.81	1/277 (0.4%)	0.69	0/376
10	K	0.76	1/303 (0.3%)	0.75	0/418
10	k	0.79	1/296 (0.3%)	0.77	0/408
11	L	1.05	0/312	0.88	0/425
11	l	1.00	0/313	0.84	1/428 (0.2%)
12	M	0.85	0/257	0.91	0/352
12	m	0.86	0/270	0.80	0/370
13	O	0.84	0/1924	0.89	0/2610
13	o	0.79	0/1900	0.86	3/2577 (0.1%)
14	T	0.93	0/255	0.86	0/346
14	t	0.99	0/255	0.92	0/346
15	U	0.93	0/781	0.90	1/1059 (0.1%)
15	u	0.95	0/786	0.91	0/1067
16	V	0.97	0/1093	0.89	1/1485 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.88	1/1084 (0.1%)	0.85	1/1475 (0.1%)
17	Y	0.55	0/197	0.66	0/263
17	y	0.50	0/197	0.75	0/264
18	X	0.72	0/286	0.75	0/387
18	x	0.67	0/286	0.75	0/387
19	Z	0.76	2/470 (0.4%)	0.74	0/645
19	z	0.68	1/442 (0.2%)	0.71	0/608
All	All	0.97	69/42423 (0.2%)	0.85	34/57763 (0.1%)

The worst 5 of 69 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	78	TRP	CD2-CE2	7.33	1.50	1.41
7	H	62	TRP	CD2-CE2	6.81	1.49	1.41
3	c	443	TRP	CD2-CE2	6.79	1.49	1.41
1	A	284	TRP	CD2-CE2	6.79	1.49	1.41
3	C	359	TRP	CD2-CE2	6.46	1.49	1.41

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	272	ARG	NE-CZ-NH1	-7.88	116.36	120.30
13	o	152	ARG	NE-CZ-NH1	-7.53	116.54	120.30
2	B	357	ARG	NE-CZ-NH2	-7.36	116.62	120.30
3	C	153	ASP	CB-CG-OD1	7.03	124.63	118.30
4	D	100	ASP	CB-CG-OD2	7.02	124.62	118.30

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	336/344 (98%)	330 (98%)	5 (2%)	1 (0%)	41	31
1	a	336/344 (98%)	329 (98%)	7 (2%)	0	100	100
2	B	512/504 (102%)	503 (98%)	9 (2%)	0	100	100
2	b	508/504 (101%)	497 (98%)	11 (2%)	0	100	100
3	C	452/455 (99%)	442 (98%)	9 (2%)	1 (0%)	47	38
3	c	457/455 (100%)	442 (97%)	13 (3%)	2 (0%)	34	24
4	D	339/342 (99%)	332 (98%)	7 (2%)	0	100	100
4	d	341/342 (100%)	334 (98%)	7 (2%)	0	100	100
5	E	79/83 (95%)	78 (99%)	1 (1%)	0	100	100
5	e	77/83 (93%)	75 (97%)	2 (3%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
7	h	61/63 (97%)	55 (90%)	5 (8%)	1 (2%)	9	2
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	36/38 (95%)	32 (89%)	2 (6%)	2 (6%)	2	0
9	J	34/40 (85%)	34 (100%)	0	0	100	100
9	j	37/40 (92%)	35 (95%)	2 (5%)	0	100	100
10	K	36/37 (97%)	36 (100%)	0	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	37/37 (100%)	37 (100%)	0	0	100	100
12	M	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
12	m	34/36 (94%)	34 (100%)	0	0	100	100
13	O	247/244 (101%)	238 (96%)	8 (3%)	1 (0%)	34	24
13	o	242/244 (99%)	232 (96%)	9 (4%)	1 (0%)	34	24
14	T	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
14	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
15	U	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
15	u	96/104 (92%)	93 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	V	137/137 (100%)	132 (96%)	5 (4%)	0	100	100
16	v	136/137 (99%)	129 (95%)	7 (5%)	0	100	100
17	Y	25/30 (83%)	25 (100%)	0	0	100	100
17	y	26/30 (87%)	25 (96%)	1 (4%)	0	100	100
18	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
18	x	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	55 (92%)	2 (3%)	3 (5%)	2	0
19	z	58/62 (94%)	50 (86%)	5 (9%)	3 (5%)	2	0
All	All	5224/5344 (98%)	5075 (97%)	134 (3%)	15 (0%)	41	31

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	59	LYS
19	Z	31	GLN
19	Z	32	ASP
8	i	36	ASP
19	z	31	GLN

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	272/279 (98%)	267 (98%)	5 (2%)	59	55
1	a	271/279 (97%)	269 (99%)	2 (1%)	84	84
2	B	407/402 (101%)	404 (99%)	3 (1%)	84	84
2	b	399/402 (99%)	393 (98%)	6 (2%)	65	62
3	C	355/356 (100%)	347 (98%)	8 (2%)	50	45
3	c	358/356 (101%)	349 (98%)	9 (2%)	47	41
4	D	275/276 (100%)	273 (99%)	2 (1%)	84	84
4	d	278/276 (101%)	274 (99%)	4 (1%)	67	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	71/72 (99%)	70 (99%)	1 (1%)	67	65
5	e	68/72 (94%)	66 (97%)	2 (3%)	42	35
6	F	27/38 (71%)	26 (96%)	1 (4%)	34	25
6	f	26/38 (68%)	25 (96%)	1 (4%)	33	24
7	H	53/53 (100%)	52 (98%)	1 (2%)	57	53
7	h	53/53 (100%)	52 (98%)	1 (2%)	57	53
8	I	31/34 (91%)	31 (100%)	0	100	100
8	i	33/34 (97%)	32 (97%)	1 (3%)	41	33
9	J	23/28 (82%)	23 (100%)	0	100	100
9	j	25/28 (89%)	25 (100%)	0	100	100
10	K	29/30 (97%)	29 (100%)	0	100	100
10	k	28/30 (93%)	27 (96%)	1 (4%)	35	26
11	L	34/35 (97%)	34 (100%)	0	100	100
11	l	34/35 (97%)	34 (100%)	0	100	100
12	M	29/32 (91%)	29 (100%)	0	100	100
12	m	30/32 (94%)	30 (100%)	0	100	100
13	O	207/207 (100%)	203 (98%)	4 (2%)	57	53
13	o	206/207 (100%)	203 (98%)	3 (2%)	65	62
14	T	25/28 (89%)	24 (96%)	1 (4%)	31	22
14	t	25/28 (89%)	24 (96%)	1 (4%)	31	22
15	U	83/89 (93%)	81 (98%)	2 (2%)	49	43
15	u	83/89 (93%)	83 (100%)	0	100	100
16	V	116/117 (99%)	116 (100%)	0	100	100
16	v	115/117 (98%)	114 (99%)	1 (1%)	78	79
17	Y	19/23 (83%)	18 (95%)	1 (5%)	22	13
17	y	18/23 (78%)	16 (89%)	2 (11%)	6	2
18	X	30/33 (91%)	30 (100%)	0	100	100
18	x	30/33 (91%)	29 (97%)	1 (3%)	38	29
19	Z	47/52 (90%)	46 (98%)	1 (2%)	53	48
19	z	40/52 (77%)	38 (95%)	2 (5%)	24	15
All	All	4253/4368 (97%)	4186 (98%)	67 (2%)	65	60

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	o	54	GLU
13	o	118	LEU
19	z	3	ILE
13	O	207	ARG
13	O	118	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	331	ASN
4	d	332	GLN
13	o	104	GLN
13	o	36	GLN
3	c	311	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](#)

10 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	$\# Z > 2$
4	HSK	D	336[A]	-	8,10,12	3.80	2 (25%)	4,12,16	1.77	1 (25%)
12	FME	m	1	12	8,9,10	0.89	0	8,9,11	1.53	1 (12%)
4	HSK	D	336[B]	-	8,11,12	2.21	2 (25%)	4,14,16	1.44	1 (25%)
4	HSK	d	336[A]	-	8,10,12	3.31	2 (25%)	4,12,16	2.11	1 (25%)
14	FME	T	1	14	8,9,10	0.48	0	8,9,11	1.26	1 (12%)
8	FME	i	1	8	8,9,10	0.42	0	8,9,11	1.38	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HSK	d	336[B]	-	8,11,12	1.91	2 (25%)	4,14,16	1.77	2 (50%)
14	FME	t	1	14	8,9,10	0.83	0	8,9,11	1.38	2 (25%)
12	FME	M	1	12	8,9,10	0.83	0	8,9,11	1.55	2 (25%)
8	FME	I	1	8	8,9,10	0.62	0	8,9,11	1.05	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HSK	D	336[A]	-	-	0/5/6/8	0/1/1/1
12	FME	m	1	12	-	2/7/9/11	-
4	HSK	D	336[B]	-	-	0/5/6/8	0/1/1/1
4	HSK	d	336[A]	-	-	0/5/6/8	0/1/1/1
14	FME	T	1	14	-	2/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
4	HSK	d	336[B]	-	-	0/5/6/8	0/1/1/1
14	FME	t	1	14	-	5/7/9/11	-
12	FME	M	1	12	-	2/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	336[A]	HSK	OM-ND1	-10.36	1.16	1.37
4	d	336[A]	HSK	OM-ND1	-8.93	1.19	1.37
4	D	336[B]	HSK	OM-ND1	5.08	1.47	1.37
4	d	336[B]	HSK	OM-ND1	4.22	1.45	1.37
4	D	336[B]	HSK	CE1-ND1	-3.25	1.32	1.36

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	336[A]	HSK	CG-CB-CA	-3.38	105.54	114.00
12	M	1	FME	CG-CB-CA	2.59	120.80	112.87
12	m	1	FME	CG-CB-CA	2.56	120.69	112.87
4	D	336[B]	HSK	CD2-NE2-CE1	2.47	109.62	105.72
4	d	336[B]	HSK	CD2-NE2-CE1	2.44	109.58	105.72

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	O1-CN-N-CA
12	M	1	FME	O-C-CA-CB
14	T	1	FME	O1-CN-N-CA
12	m	1	FME	O1-CN-N-CA
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 276 ligands modelled in this entry, 15 are monoatomic and 43 are unknown - leaving 218 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	LMG	Z	101	-	51,51,55	1.11	3 (5%)	59,59,63	1.37	7 (11%)
23	CLA	B	613	-	63,73,73	2.11	17 (26%)	74,113,113	2.07	23 (31%)
23	CLA	b	618	-	63,73,73	2.31	15 (23%)	74,113,113	2.33	24 (32%)
38	RRX	h	101	-	42,42,42	0.96	1 (2%)	56,58,58	1.34	8 (14%)
31	GOL	C	524	-	5,5,5	0.36	0	5,5,5	1.69	1 (20%)
23	CLA	C	511	3	63,73,73	2.43	20 (31%)	74,113,113	2.52	23 (31%)
34	DGD	h	102	-	63,63,67	1.00	3 (4%)	77,77,81	1.27	11 (14%)
25	BCR	k	101	-	41,41,41	0.86	0	56,56,56	1.49	12 (21%)
27	LMG	a	418	-	51,51,55	0.94	2 (3%)	59,59,63	1.34	5 (8%)
31	GOL	C	526	-	5,5,5	0.68	0	5,5,5	0.50	0
23	CLA	b	610	41	63,73,73	2.37	16 (25%)	74,113,113	2.03	24 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	PHO	a	413	-	50,69,69	1.59	8 (16%)	48,99,99	2.10	11 (22%)
23	CLA	b	604	41	63,73,73	2.43	18 (28%)	74,113,113	2.27	21 (28%)
28	PL9	a	419	-	55,55,55	0.86	3 (5%)	68,69,69	1.76	18 (26%)
36	LHG	a	417	-	39,39,48	1.17	2 (5%)	42,45,54	1.00	2 (4%)
23	CLA	A	410	-	63,73,73	1.97	17 (26%)	74,113,113	2.43	24 (32%)
23	CLA	A	406	41	63,73,73	2.07	17 (26%)	74,113,113	2.47	30 (40%)
23	CLA	B	614	-	63,73,73	2.09	17 (26%)	74,113,113	2.05	23 (31%)
31	GOL	V	203	-	5,5,5	1.03	0	5,5,5	0.84	0
26	SQD	A	418	-	52,54,54	1.09	2 (3%)	62,65,65	1.62	12 (19%)
31	GOL	v	203	-	5,5,5	0.75	0	5,5,5	0.51	0
34	DGD	C	517	-	63,63,67	0.91	2 (3%)	77,77,81	1.06	3 (3%)
37	HEM	V	201	16	42,50,50	2.03	13 (30%)	46,82,82	1.65	9 (19%)
30	LMT	a	402	-	36,36,36	0.77	1 (2%)	47,47,47	1.60	10 (21%)
34	DGD	c	919	-	63,63,67	1.06	5 (7%)	77,77,81	1.37	10 (12%)
23	CLA	B	610	-	63,73,73	2.02	17 (26%)	74,113,113	2.16	23 (31%)
27	LMG	d	410	39	51,51,55	1.02	3 (5%)	59,59,63	1.15	7 (11%)
24	PHO	a	412	-	50,69,69	1.68	8 (16%)	48,99,99	1.95	9 (18%)
23	CLA	b	606	-	63,73,73	2.12	16 (25%)	74,113,113	2.38	25 (33%)
25	BCR	a	415	-	41,41,41	1.22	5 (12%)	56,56,56	1.46	8 (14%)
31	GOL	A	423	32	5,5,5	0.33	0	5,5,5	0.83	0
33	HTG	C	522	-	19,19,19	0.95	2 (10%)	23,24,24	2.00	3 (13%)
20	OEX	a	404	1,3,41	0,15,15	-	-	-	-	-
23	CLA	D	402	-	63,73,73	2.31	16 (25%)	74,113,113	2.40	28 (37%)
28	PL9	A	414	-	55,55,55	0.93	3 (5%)	68,69,69	1.51	11 (16%)
23	CLA	C	502	-	63,73,73	1.99	16 (25%)	74,113,113	2.24	24 (32%)
30	LMT	M	101	-	36,36,36	0.87	1 (2%)	47,47,47	1.23	6 (12%)
23	CLA	B	608	41	63,73,73	2.27	19 (30%)	74,113,113	2.06	24 (32%)
23	CLA	c	902	-	63,73,73	2.16	16 (25%)	74,113,113	2.60	24 (32%)
24	PHO	A	408	-	50,69,69	1.50	6 (12%)	48,99,99	1.63	10 (20%)
30	LMT	b	625	-	24,24,36	0.54	0	29,29,47	1.25	4 (13%)
31	GOL	B	638	-	5,5,5	0.53	0	5,5,5	0.92	0
25	BCR	B	618	-	41,41,41	1.13	5 (12%)	56,56,56	1.60	9 (16%)
31	GOL	a	424	-	5,5,5	0.68	0	5,5,5	0.79	0
23	CLA	a	410	41	63,73,73	2.07	18 (28%)	74,113,113	2.09	20 (27%)
33	HTG	b	627	-	19,19,19	1.05	2 (10%)	23,24,24	1.42	1 (4%)
24	PHO	A	409	-	50,69,69	1.73	7 (14%)	48,99,99	1.68	12 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	612	-	63,73,73	2.31	19 (30%)	74,113,113	1.92	20 (27%)
31	GOL	C	525	-	5,5,5	0.82	0	5,5,5	0.93	0
36	LHG	d	408	-	48,48,48	0.79	2 (4%)	51,54,54	1.34	9 (17%)
23	CLA	C	510	-	63,73,73	2.23	18 (28%)	74,113,113	2.24	22 (29%)
23	CLA	b	615	-	63,73,73	2.25	16 (25%)	74,113,113	2.51	21 (28%)
23	CLA	C	509	-	63,73,73	2.22	17 (26%)	74,113,113	2.19	24 (32%)
25	BCR	B	619	-	41,41,41	1.20	4 (9%)	56,56,56	1.25	8 (14%)
31	GOL	b	632	-	5,5,5	0.54	0	5,5,5	1.38	0
23	CLA	A	405	-	63,73,73	2.07	17 (26%)	74,113,113	2.09	25 (33%)
26	SQD	A	412	-	52,54,54	0.86	2 (3%)	62,65,65	2.15	17 (27%)
23	CLA	c	909	-	63,73,73	2.41	17 (26%)	74,113,113	2.27	24 (32%)
38	RRX	H	101	-	42,42,42	1.10	3 (7%)	56,58,58	1.62	10 (17%)
30	LMT	c	922	-	36,36,36	0.75	1 (2%)	47,47,47	0.96	3 (6%)
34	DGD	D	406	-	53,53,67	1.20	3 (5%)	61,61,81	1.38	8 (13%)
26	SQD	f	102	-	31,32,54	2.00	3 (9%)	33,36,65	1.61	5 (15%)
36	LHG	l	101	-	48,48,48	0.84	2 (4%)	51,54,54	1.12	5 (9%)
31	GOL	h	103	-	5,5,5	0.37	0	5,5,5	0.29	0
27	LMG	D	411	39	51,51,55	0.87	2 (3%)	59,59,63	1.04	2 (3%)
23	CLA	C	512	-	63,73,73	2.49	17 (26%)	74,113,113	2.24	25 (33%)
23	CLA	b	616	-	63,73,73	2.14	17 (26%)	74,113,113	2.32	24 (32%)
31	GOL	b	633	-	5,5,5	0.40	0	5,5,5	0.94	0
27	LMG	B	622	-	51,51,55	0.95	2 (3%)	59,59,63	1.63	9 (15%)
23	CLA	b	611	-	63,73,73	2.05	15 (23%)	74,113,113	2.07	22 (29%)
31	GOL	D	415	-	5,5,5	0.73	0	5,5,5	1.33	1 (20%)
25	BCR	B	620	-	41,41,41	1.03	1 (2%)	56,56,56	1.67	12 (21%)
30	LMT	A	419	-	36,36,36	0.84	1 (2%)	47,47,47	1.35	5 (10%)
33	HTG	C	521	-	19,19,19	0.85	1 (5%)	23,24,24	1.21	1 (4%)
23	CLA	a	414	-	63,73,73	2.01	17 (26%)	74,113,113	2.41	29 (39%)
23	CLA	c	913	-	63,73,73	2.52	18 (28%)	74,113,113	2.17	23 (31%)
25	BCR	K	102	-	41,41,41	0.97	1 (2%)	56,56,56	1.69	9 (16%)
23	CLA	B	602	41	63,73,73	2.37	19 (30%)	74,113,113	2.58	26 (35%)
34	DGD	c	918	-	63,63,67	1.01	4 (6%)	77,77,81	1.23	10 (12%)
25	BCR	C	515	-	41,41,41	0.95	1 (2%)	56,56,56	1.47	7 (12%)
23	CLA	B	611	41	63,73,73	2.13	19 (30%)	74,113,113	2.45	26 (35%)
25	BCR	b	622	-	41,41,41	0.96	2 (4%)	56,56,56	1.28	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	506	-	63,73,73	2.34	16 (25%)	74,113,113	2.30	25 (33%)
23	CLA	a	411	41	63,73,73	1.92	17 (26%)	74,113,113	2.34	29 (39%)
25	BCR	K	101	-	41,41,41	0.91	0	56,56,56	1.70	12 (21%)
23	CLA	c	910	-	63,73,73	2.43	18 (28%)	74,113,113	2.34	28 (37%)
31	GOL	B	637	-	5,5,5	0.48	0	5,5,5	1.18	1 (20%)
33	HTG	B	624	-	19,19,19	1.07	1 (5%)	23,24,24	1.40	6 (26%)
23	CLA	C	503	-	63,73,73	2.31	18 (28%)	74,113,113	2.08	21 (28%)
37	HEM	v	201	16	42,50,50	2.02	7 (16%)	46,82,82	1.84	10 (21%)
30	LMT	Z	102	-	36,36,36	0.68	1 (2%)	47,47,47	0.90	0
23	CLA	c	905	41	63,73,73	2.47	18 (28%)	74,113,113	2.44	24 (32%)
27	LMG	C	519	-	51,51,55	1.03	3 (5%)	59,59,63	1.48	9 (15%)
36	LHG	d	407	-	48,48,48	0.81	2 (4%)	51,54,54	1.41	6 (11%)
30	LMT	t	102	-	24,24,36	0.69	0	29,29,47	1.32	3 (10%)
30	LMT	M	102	-	36,36,36	0.62	0	47,47,47	1.35	7 (14%)
31	GOL	B	635	-	5,5,5	0.54	0	5,5,5	1.11	0
26	SQD	a	401	-	52,54,54	1.13	2 (3%)	62,65,65	1.59	9 (14%)
33	HTG	c	924	-	19,19,19	0.94	1 (5%)	23,24,24	2.17	4 (17%)
26	SQD	B	621	-	52,54,54	1.10	4 (7%)	62,65,65	1.84	12 (19%)
23	CLA	b	617	-	63,73,73	1.98	17 (26%)	74,113,113	2.76	30 (40%)
31	GOL	A	422	-	5,5,5	0.44	0	5,5,5	0.52	0
30	LMT	b	624	-	25,25,36	0.75	1 (4%)	30,30,47	1.39	5 (16%)
23	CLA	C	504	41	63,73,73	2.22	16 (25%)	74,113,113	2.18	22 (29%)
31	GOL	B	636	-	5,5,5	0.48	0	5,5,5	0.79	0
33	HTG	b	602	-	19,19,19	0.74	0	23,24,24	1.09	2 (8%)
23	CLA	b	614	-	63,73,73	2.21	15 (23%)	74,113,113	2.25	25 (33%)
27	LMG	A	413	-	51,51,55	1.00	2 (3%)	59,59,63	1.22	4 (6%)
35	BCT	a	408	21	3,3,3	1.14	0	2,3,3	2.98	1 (50%)
23	CLA	b	619	-	63,73,73	2.24	19 (30%)	74,113,113	2.29	25 (33%)
23	CLA	c	906	-	63,73,73	2.10	17 (26%)	74,113,113	2.17	26 (35%)
33	HTG	V	202	-	12,13,19	0.73	0	17,18,24	3.30	7 (41%)
23	CLA	B	617	-	63,73,73	1.93	18 (28%)	74,113,113	2.22	20 (27%)
23	CLA	a	409	-	63,73,73	1.87	12 (19%)	74,113,113	2.21	25 (33%)
30	LMT	m	102	-	36,36,36	0.73	1 (2%)	47,47,47	1.09	3 (6%)
25	BCR	A	411	-	41,41,41	1.05	0	56,56,56	1.50	11 (19%)
26	SQD	D	407	-	43,45,54	1.26	3 (6%)	53,56,65	2.12	15 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	914	-	63,73,73	2.78	17 (26%)	74,113,113	1.95	23 (31%)
31	GOL	v	204	-	5,5,5	0.30	0	5,5,5	0.73	0
36	LHG	d	409	-	48,48,48	0.93	3 (6%)	51,54,54	1.09	4 (7%)
27	LMG	c	921	-	51,51,55	1.10	3 (5%)	59,59,63	1.23	6 (10%)
36	LHG	D	409	-	48,48,48	0.84	2 (4%)	51,54,54	1.14	5 (9%)
31	GOL	b	636	-	5,5,5	0.59	0	5,5,5	1.05	0
23	CLA	A	407	41	63,73,73	2.03	13 (20%)	74,113,113	2.26	25 (33%)
25	BCR	b	621	-	41,41,41	1.14	2 (4%)	56,56,56	1.31	7 (12%)
33	HTG	B	626	-	19,19,19	0.87	1 (5%)	23,24,24	1.59	2 (8%)
36	LHG	E	101	-	48,48,48	1.02	2 (4%)	51,54,54	0.94	2 (3%)
23	CLA	d	403	-	63,73,73	2.17	18 (28%)	74,113,113	2.25	26 (35%)
36	LHG	D	410	-	45,45,48	1.04	2 (4%)	48,51,54	1.06	3 (6%)
23	CLA	C	505	-	63,73,73	2.11	17 (26%)	74,113,113	1.99	23 (31%)
27	LMG	b	623	-	51,51,55	0.87	2 (3%)	59,59,63	1.47	7 (11%)
33	HTG	U	201	-	8,8,19	0.30	0	7,7,24	0.97	0
31	GOL	B	634	-	5,5,5	0.85	0	5,5,5	0.71	0
25	BCR	t	101	-	41,41,41	1.04	3 (7%)	56,56,56	1.86	15 (26%)
33	HTG	B	625	-	19,19,19	0.93	1 (5%)	23,24,24	1.38	4 (17%)
30	LMT	J	102	-	24,24,36	0.84	1 (4%)	29,29,47	1.13	2 (6%)
23	CLA	D	403	-	63,73,73	2.26	17 (26%)	74,113,113	2.22	25 (33%)
25	BCR	c	915	-	41,41,41	0.87	1 (2%)	56,56,56	1.26	6 (10%)
30	LMT	B	623	-	36,36,36	1.00	2 (5%)	47,47,47	1.39	8 (17%)
23	CLA	C	513	-	63,73,73	2.67	17 (26%)	74,113,113	2.16	22 (29%)
23	CLA	C	508	-	63,73,73	2.51	17 (26%)	74,113,113	2.02	20 (27%)
23	CLA	c	904	-	63,73,73	2.59	19 (30%)	74,113,113	2.24	23 (31%)
23	CLA	B	616	-	63,73,73	2.33	14 (22%)	74,113,113	2.23	22 (29%)
33	HTG	O	303	-	19,19,19	1.13	2 (10%)	23,24,24	1.22	1 (4%)
31	GOL	a	422	-	5,5,5	0.69	0	5,5,5	0.82	0
26	SQD	a	416	-	52,54,54	0.89	2 (3%)	62,65,65	2.19	14 (22%)
31	GOL	A	421	-	5,5,5	0.91	0	5,5,5	0.53	0
25	BCR	d	404	-	41,41,41	1.03	3 (7%)	56,56,56	1.83	15 (26%)
28	PL9	D	405	-	55,55,55	1.38	9 (16%)	68,69,69	1.53	12 (17%)
31	GOL	l	102	-	5,5,5	0.49	0	5,5,5	1.08	0
34	DGD	C	516	-	63,63,67	0.92	3 (4%)	77,77,81	1.36	12 (15%)
37	HEM	F	101	6,5	42,50,50	1.80	8 (19%)	46,82,82	2.07	14 (30%)
34	DGD	C	518	-	63,63,67	0.79	3 (4%)	77,77,81	1.31	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	507	41	63,73,73	2.47	18 (28%)	74,113,113	2.23	21 (28%)
23	CLA	c	907	-	63,73,73	2.22	17 (26%)	74,113,113	2.46	25 (33%)
23	CLA	c	903	-	63,73,73	2.31	17 (26%)	74,113,113	2.50	25 (33%)
34	DGD	c	917	-	63,63,67	0.91	4 (6%)	77,77,81	1.27	9 (11%)
31	GOL	B	633	-	5,5,5	0.34	0	5,5,5	1.46	1 (20%)
31	GOL	c	930	-	5,5,5	0.47	0	5,5,5	0.71	0
25	BCR	k	102	-	41,41,41	1.00	2 (4%)	56,56,56	1.33	7 (12%)
23	CLA	b	613	41	63,73,73	2.25	17 (26%)	74,113,113	2.37	21 (28%)
23	CLA	B	607	-	63,73,73	2.29	13 (20%)	74,113,113	2.57	28 (37%)
31	GOL	c	928	-	5,5,5	0.23	0	5,5,5	0.86	0
33	HTG	D	414	-	19,19,19	0.99	1 (5%)	23,24,24	1.04	1 (4%)
36	LHG	L	101	-	48,48,48	0.83	2 (4%)	51,54,54	1.56	7 (13%)
33	HTG	B	630	-	19,19,19	0.99	2 (10%)	23,24,24	1.42	3 (13%)
23	CLA	B	609	-	63,73,73	1.74	14 (22%)	74,113,113	2.43	24 (32%)
31	GOL	a	423	-	5,5,5	0.60	0	5,5,5	0.63	0
25	BCR	b	620	-	41,41,41	1.08	1 (2%)	56,56,56	1.76	15 (26%)
31	GOL	c	927	-	5,5,5	0.64	0	5,5,5	0.43	0
23	CLA	B	603	-	63,73,73	2.32	16 (25%)	74,113,113	1.96	25 (33%)
23	CLA	B	612	-	63,73,73	2.06	15 (23%)	74,113,113	2.38	24 (32%)
34	DGD	d	406	-	50,50,67	1.20	3 (6%)	58,58,81	1.38	9 (15%)
33	HTG	b	626	-	19,19,19	0.97	1 (5%)	23,24,24	1.37	3 (13%)
34	DGD	H	102	-	63,63,67	1.13	3 (4%)	77,77,81	1.36	12 (15%)
30	LMT	C	520	-	36,36,36	0.62	1 (2%)	47,47,47	1.49	7 (14%)
25	BCR	D	404	-	41,41,41	1.17	4 (9%)	56,56,56	2.10	18 (32%)
31	GOL	O	304	-	5,5,5	0.56	0	5,5,5	0.64	0
23	CLA	b	607	-	63,73,73	2.16	15 (23%)	74,113,113	2.46	23 (31%)
30	LMT	m	101	-	36,36,36	0.74	0	47,47,47	1.39	8 (17%)
31	GOL	V	204	-	5,5,5	0.31	0	5,5,5	0.47	0
31	GOL	b	635	-	5,5,5	0.81	0	5,5,5	0.96	0
31	GOL	c	929	-	5,5,5	0.56	0	5,5,5	0.90	0
27	LMG	c	920	-	51,51,55	1.12	4 (7%)	59,59,63	1.28	9 (15%)
20	OEX	A	401	1,3,41	0,15,15	-	-	-	-	-
23	CLA	B	605	-	63,73,73	2.03	14 (22%)	74,113,113	2.22	26 (35%)
26	SQD	L	103	-	52,54,54	1.09	2 (3%)	62,65,65	1.66	12 (19%)
23	CLA	c	911	-	63,73,73	2.19	18 (28%)	74,113,113	2.03	22 (29%)
28	PL9	d	405	-	55,55,55	1.27	9 (16%)	68,69,69	1.53	13 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	HTG	c	923	-	19,19,19	0.93	2 (10%)	23,24,24	1.37	2 (8%)
31	GOL	f	104	32	5,5,5	0.55	0	5,5,5	0.45	0
23	CLA	B	615	-	63,73,73	2.11	15 (23%)	74,113,113	2.27	24 (32%)
40	SO4	O	302	-	4,4,4	0.60	0	6,6,6	0.40	0
33	HTG	B	631	-	19,19,19	0.80	1 (5%)	23,24,24	1.68	3 (13%)
23	CLA	b	608	-	63,73,73	1.93	13 (20%)	74,113,113	2.42	23 (31%)
23	CLA	d	402	-	63,73,73	1.97	15 (23%)	74,113,113	2.17	24 (32%)
31	GOL	b	634	-	5,5,5	0.51	0	5,5,5	0.25	0
30	LMT	F	102	-	36,36,36	0.75	1 (2%)	47,47,47	1.19	3 (6%)
23	CLA	c	908	41	63,73,73	2.36	20 (31%)	74,113,113	2.38	26 (35%)
23	CLA	b	609	-	63,73,73	2.43	19 (30%)	74,113,113	2.42	25 (33%)
33	HTG	b	601	-	19,19,19	0.92	2 (10%)	23,24,24	1.24	3 (13%)
30	LMT	z	101	-	32,32,36	0.70	1 (3%)	42,42,47	1.01	4 (9%)
31	GOL	L	104	-	5,5,5	0.52	0	5,5,5	0.64	0
31	GOL	v	202	-	5,5,5	0.59	0	5,5,5	0.55	0
23	CLA	b	605	-	63,73,73	2.17	15 (23%)	74,113,113	2.21	27 (36%)
33	HTG	d	401	-	19,19,19	1.01	1 (5%)	23,24,24	1.25	1 (4%)
25	BCR	T	101	-	41,41,41	0.92	0	56,56,56	1.69	15 (26%)
25	BCR	c	916	-	41,41,41	0.99	1 (2%)	56,56,56	1.40	7 (12%)
33	HTG	u	201	-	10,13,19	0.76	0	13,14,24	1.69	2 (15%)
35	BCT	D	401	21	3,3,3	1.13	0	2,3,3	1.11	0
37	HEM	f	101	6,5	42,50,50	1.89	11 (26%)	46,82,82	1.91	10 (21%)
23	CLA	B	604	-	63,73,73	2.10	16 (25%)	74,113,113	2.53	26 (35%)
25	BCR	C	514	-	41,41,41	0.91	0	56,56,56	1.33	9 (16%)
23	CLA	B	606	-	63,73,73	2.09	16 (25%)	74,113,113	2.07	21 (28%)
23	CLA	C	501	-	63,73,73	2.00	17 (26%)	74,113,113	2.63	25 (33%)
23	CLA	c	912	3	63,73,73	2.40	18 (28%)	74,113,113	2.37	24 (32%)
31	GOL	V	205	-	5,5,5	0.67	0	5,5,5	0.34	0
36	LHG	D	408	-	48,48,48	0.80	1 (2%)	51,54,54	1.50	6 (11%)

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	LMG	Z	101	-	-	25/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	613	-	1/1/15/20	2/37/115/115	-
23	CLA	b	618	-	1/1/15/20	9/37/115/115	-
38	RRX	h	101	-	-	1/29/65/65	0/2/2/2
31	GOL	C	524	-	-	2/4/4/4	-
23	CLA	C	511	3	1/1/15/20	0/37/115/115	-
34	DGD	h	102	-	-	10/51/91/95	0/2/2/2
25	BCR	k	101	-	-	1/29/63/63	0/2/2/2
27	LMG	a	418	-	-	19/46/66/70	0/1/1/1
31	GOL	C	526	-	-	0/4/4/4	-
23	CLA	b	610	41	1/1/15/20	2/37/115/115	-
24	PHO	a	413	-	-	3/37/103/103	0/5/6/6
23	CLA	b	604	41	1/1/15/20	14/37/115/115	-
28	PL9	a	419	-	-	11/53/73/73	0/1/1/1
36	LHG	a	417	-	-	29/44/44/53	-
23	CLA	A	410	-	-	13/37/115/115	-
23	CLA	A	406	41	-	4/37/115/115	-
23	CLA	B	614	-	1/1/15/20	6/37/115/115	-
31	GOL	V	203	-	-	2/4/4/4	-
26	SQD	A	418	-	-	16/49/69/69	0/1/1/1
31	GOL	v	203	-	-	2/4/4/4	-
34	DGD	C	517	-	-	22/51/91/95	0/2/2/2
37	HEM	V	201	16	-	4/12/54/54	-
30	LMT	a	402	-	-	10/21/61/61	0/2/2/2
34	DGD	c	919	-	-	16/51/91/95	0/2/2/2
23	CLA	B	610	-	1/1/15/20	3/37/115/115	-
27	LMG	d	410	39	-	10/46/66/70	0/1/1/1
24	PHO	a	412	-	-	1/37/103/103	0/5/6/6
23	CLA	b	606	-	1/1/15/20	4/37/115/115	-
25	BCR	a	415	-	-	1/29/63/63	0/2/2/2
31	GOL	A	423	32	-	0/4/4/4	-
33	HTG	C	522	-	-	2/10/30/30	0/1/1/1
23	CLA	D	402	-	1/1/15/20	6/37/115/115	-
28	PL9	A	414	-	-	11/53/73/73	0/1/1/1
30	LMT	M	101	-	-	7/21/61/61	0/2/2/2
23	CLA	C	502	-	-	6/37/115/115	-
23	CLA	B	608	41	1/1/15/20	1/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	902	-	1/1/15/20	4/37/115/115	-
24	PHO	A	408	-	-	0/37/103/103	0/5/6/6
30	LMT	b	625	-	-	11/15/35/61	0/1/1/2
31	GOL	B	638	-	-	2/4/4/4	-
25	BCR	B	618	-	-	2/29/63/63	0/2/2/2
31	GOL	a	424	-	-	3/4/4/4	-
23	CLA	a	410	41	1/1/15/20	3/37/115/115	-
33	HTG	b	627	-	-	5/10/30/30	0/1/1/1
24	PHO	A	409	-	-	4/37/103/103	0/5/6/6
23	CLA	b	612	-	-	0/37/115/115	-
31	GOL	C	525	-	-	0/4/4/4	-
36	LHG	d	408	-	-	9/53/53/53	-
23	CLA	C	510	-	1/1/15/20	3/37/115/115	-
23	CLA	b	615	-	1/1/15/20	6/37/115/115	-
23	CLA	C	509	-	1/1/15/20	6/37/115/115	-
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
31	GOL	b	632	-	-	4/4/4/4	-
23	CLA	A	405	-	1/1/15/20	3/37/115/115	-
26	SQD	A	412	-	-	18/49/69/69	0/1/1/1
23	CLA	c	909	-	-	1/37/115/115	-
38	RRX	H	101	-	-	1/29/65/65	0/2/2/2
30	LMT	c	922	-	-	5/21/61/61	0/2/2/2
34	DGD	D	406	-	-	26/47/68/95	0/1/1/2
26	SQD	f	102	-	-	13/33/33/69	-
36	LHG	l	101	-	-	17/53/53/53	-
31	GOL	h	103	-	-	1/4/4/4	-
27	LMG	D	411	39	-	9/46/66/70	0/1/1/1
23	CLA	C	512	-	1/1/15/20	7/37/115/115	-
23	CLA	b	616	-	1/1/15/20	4/37/115/115	-
31	GOL	b	633	-	-	3/4/4/4	-
27	LMG	B	622	-	-	15/46/66/70	0/1/1/1
23	CLA	b	611	-	-	1/37/115/115	-
31	GOL	D	415	-	-	2/4/4/4	-
25	BCR	B	620	-	-	0/29/63/63	0/2/2/2
30	LMT	A	419	-	-	5/21/61/61	0/2/2/2
33	HTG	C	521	-	-	3/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	a	414	-	-	12/37/115/115	-
23	CLA	c	913	-	1/1/15/20	8/37/115/115	-
25	BCR	K	102	-	-	2/29/63/63	0/2/2/2
23	CLA	B	602	41	1/1/15/20	18/37/115/115	-
34	DGD	c	918	-	-	21/51/91/95	0/2/2/2
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
23	CLA	B	611	41	1/1/15/20	8/37/115/115	-
25	BCR	b	622	-	-	0/29/63/63	0/2/2/2
23	CLA	C	506	-	1/1/15/20	11/37/115/115	-
23	CLA	a	411	41	-	6/37/115/115	-
25	BCR	K	101	-	-	3/29/63/63	0/2/2/2
23	CLA	c	910	-	1/1/15/20	11/37/115/115	-
31	GOL	B	637	-	-	0/4/4/4	-
33	HTG	B	624	-	-	2/10/30/30	0/1/1/1
23	CLA	C	503	-	1/1/15/20	1/37/115/115	-
37	HEM	v	201	16	-	4/12/54/54	-
30	LMT	Z	102	-	-	13/21/61/61	0/2/2/2
23	CLA	c	905	41	1/1/15/20	10/37/115/115	-
27	LMG	C	519	-	-	22/46/66/70	0/1/1/1
36	LHG	d	407	-	-	6/53/53/53	-
30	LMT	t	102	-	-	8/15/35/61	0/1/1/2
30	LMT	M	102	-	-	2/21/61/61	0/2/2/2
31	GOL	B	635	-	-	4/4/4/4	-
26	SQD	a	401	-	-	23/49/69/69	0/1/1/1
33	HTG	c	924	-	-	1/10/30/30	0/1/1/1
26	SQD	B	621	-	-	29/49/69/69	0/1/1/1
23	CLA	b	617	-	1/1/15/20	16/37/115/115	-
31	GOL	A	422	-	-	0/4/4/4	-
30	LMT	b	624	-	-	9/17/37/61	0/1/1/2
23	CLA	C	504	41	1/1/15/20	10/37/115/115	-
31	GOL	B	636	-	-	0/4/4/4	-
33	HTG	b	602	-	-	1/10/30/30	0/1/1/1
23	CLA	b	614	-	-	5/37/115/115	-
27	LMG	A	413	-	-	25/46/66/70	0/1/1/1
23	CLA	b	619	-	1/1/15/20	6/37/115/115	-
23	CLA	c	906	-	1/1/15/20	3/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	HTG	V	202	-	-	2/4/24/30	0/1/1/1
23	CLA	B	617	-	1/1/15/20	15/37/115/115	-
23	CLA	a	409	-	1/1/15/20	4/37/115/115	-
30	LMT	m	102	-	-	6/21/61/61	0/2/2/2
25	BCR	A	411	-	-	0/29/63/63	0/2/2/2
26	SQD	D	407	-	-	13/40/60/69	0/1/1/1
23	CLA	c	914	-	-	11/37/115/115	-
31	GOL	v	204	-	-	0/4/4/4	-
36	LHG	d	409	-	-	16/53/53/53	-
27	LMG	c	921	-	-	13/46/66/70	0/1/1/1
36	LHG	D	409	-	-	13/53/53/53	-
31	GOL	b	636	-	-	2/4/4/4	-
23	CLA	A	407	41	-	6/37/115/115	-
25	BCR	b	621	-	-	0/29/63/63	0/2/2/2
33	HTG	B	626	-	-	5/10/30/30	0/1/1/1
36	LHG	E	101	-	-	27/53/53/53	-
23	CLA	d	403	-	-	8/37/115/115	-
36	LHG	D	410	-	-	13/50/50/53	-
23	CLA	C	505	-	1/1/15/20	2/37/115/115	-
27	LMG	b	623	-	-	19/46/66/70	0/1/1/1
33	HTG	U	201	-	-	4/6/6/30	-
31	GOL	B	634	-	-	0/4/4/4	-
25	BCR	t	101	-	-	1/29/63/63	0/2/2/2
33	HTG	B	625	-	-	4/10/30/30	0/1/1/1
30	LMT	J	102	-	-	7/15/35/61	0/1/1/2
23	CLA	D	403	-	1/1/15/20	12/37/115/115	-
25	BCR	c	915	-	-	5/29/63/63	0/2/2/2
30	LMT	B	623	-	-	12/21/61/61	0/2/2/2
23	CLA	C	513	-	-	13/37/115/115	-
23	CLA	C	508	-	-	3/37/115/115	-
23	CLA	c	904	-	-	1/37/115/115	-
23	CLA	B	616	-	1/1/15/20	5/37/115/115	-
33	HTG	O	303	-	-	3/10/30/30	0/1/1/1
31	GOL	a	422	-	-	0/4/4/4	-
26	SQD	a	416	-	-	20/49/69/69	0/1/1/1
31	GOL	A	421	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	d	404	-	-	4/29/63/63	0/2/2/2
28	PL9	D	405	-	-	1/53/73/73	0/1/1/1
31	GOL	l	102	-	-	0/4/4/4	-
34	DGD	C	516	-	-	17/51/91/95	0/2/2/2
37	HEM	F	101	6,5	-	2/12/54/54	-
34	DGD	C	518	-	-	13/51/91/95	0/2/2/2
23	CLA	C	507	41	1/1/15/20	11/37/115/115	-
23	CLA	c	907	-	1/1/15/20	12/37/115/115	-
23	CLA	c	903	-	1/1/15/20	4/37/115/115	-
34	DGD	c	917	-	-	14/51/91/95	0/2/2/2
31	GOL	B	633	-	-	2/4/4/4	-
31	GOL	c	930	-	-	4/4/4/4	-
25	BCR	k	102	-	-	3/29/63/63	0/2/2/2
23	CLA	b	613	41	1/1/15/20	3/37/115/115	-
23	CLA	B	607	-	1/1/15/20	6/37/115/115	-
31	GOL	c	928	-	-	1/4/4/4	-
33	HTG	D	414	-	-	2/10/30/30	0/1/1/1
36	LHG	L	101	-	-	10/53/53/53	-
33	HTG	B	630	-	-	4/10/30/30	0/1/1/1
23	CLA	B	609	-	-	1/37/115/115	-
31	GOL	a	423	-	-	2/4/4/4	-
25	BCR	b	620	-	-	2/29/63/63	0/2/2/2
31	GOL	c	927	-	-	2/4/4/4	-
23	CLA	B	603	-	1/1/15/20	3/37/115/115	-
23	CLA	B	612	-	-	1/37/115/115	-
34	DGD	d	406	-	-	26/44/64/95	0/1/1/2
33	HTG	b	626	-	-	4/10/30/30	0/1/1/1
34	DGD	H	102	-	-	16/51/91/95	0/2/2/2
30	LMT	C	520	-	-	10/21/61/61	0/2/2/2
25	BCR	D	404	-	-	2/29/63/63	0/2/2/2
31	GOL	O	304	-	-	2/4/4/4	-
23	CLA	b	607	-	1/1/15/20	5/37/115/115	-
30	LMT	m	101	-	-	3/21/61/61	0/2/2/2
31	GOL	V	204	-	-	0/4/4/4	-
31	GOL	b	635	-	-	1/4/4/4	-
31	GOL	c	929	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	c	920	-	-	18/46/66/70	0/1/1/1
23	CLA	B	605	-	1/1/15/20	5/37/115/115	-
26	SQD	L	103	-	-	28/49/69/69	0/1/1/1
23	CLA	c	911	-	1/1/15/20	6/37/115/115	-
28	PL9	d	405	-	-	2/53/73/73	0/1/1/1
33	HTG	c	923	-	-	4/10/30/30	0/1/1/1
31	GOL	f	104	32	-	2/4/4/4	-
23	CLA	B	615	-	1/1/15/20	11/37/115/115	-
33	HTG	B	631	-	-	5/10/30/30	0/1/1/1
23	CLA	b	608	-	1/1/15/20	3/37/115/115	-
23	CLA	d	402	-	1/1/15/20	1/37/115/115	-
31	GOL	b	634	-	-	0/4/4/4	-
30	LMT	F	102	-	-	11/21/61/61	0/2/2/2
23	CLA	c	908	41	1/1/15/20	8/37/115/115	-
23	CLA	b	609	-	1/1/15/20	10/37/115/115	-
33	HTG	b	601	-	-	3/10/30/30	0/1/1/1
30	LMT	z	101	-	-	8/15/55/61	0/2/2/2
31	GOL	L	104	-	-	1/4/4/4	-
31	GOL	v	202	-	-	0/4/4/4	-
23	CLA	b	605	-	1/1/15/20	2/37/115/115	-
33	HTG	d	401	-	-	5/10/30/30	0/1/1/1
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
25	BCR	c	916	-	-	0/29/63/63	0/2/2/2
33	HTG	u	201	-	-	6/12/14/30	-
37	HEM	f	101	6,5	-	1/12/54/54	-
23	CLA	B	604	-	1/1/15/20	4/37/115/115	-
25	BCR	C	514	-	-	2/29/63/63	0/2/2/2
23	CLA	B	606	-	1/1/15/20	6/37/115/115	-
23	CLA	C	501	-	1/1/15/20	3/37/115/115	-
23	CLA	c	912	3	-	6/37/115/115	-
31	GOL	V	205	-	-	0/4/4/4	-
36	LHG	D	408	-	-	9/53/53/53	-

The worst 5 of 1434 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	513	CLA	MG-NA	12.57	2.36	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	914	CLA	MG-NC	11.74	2.34	2.06
23	C	512	CLA	MG-NA	11.26	2.33	2.06
23	C	511	CLA	MG-NA	11.02	2.32	2.06
23	B	616	CLA	MG-NA	10.89	2.32	2.06

The worst 5 of 2489 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	511	CLA	C4A-NA-C1A	13.12	112.67	106.68
23	b	609	CLA	C4A-NA-C1A	11.80	112.06	106.68
23	C	501	CLA	O2D-CGD-O1D	-10.54	103.33	123.85
23	c	904	CLA	C4A-NA-C1A	10.52	111.48	106.68
23	c	902	CLA	C4A-NA-C1A	10.03	111.25	106.68

5 of 52 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	405	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND
23	B	604	CLA	ND
23	B	605	CLA	ND

5 of 1400 torsion outliers are listed below:

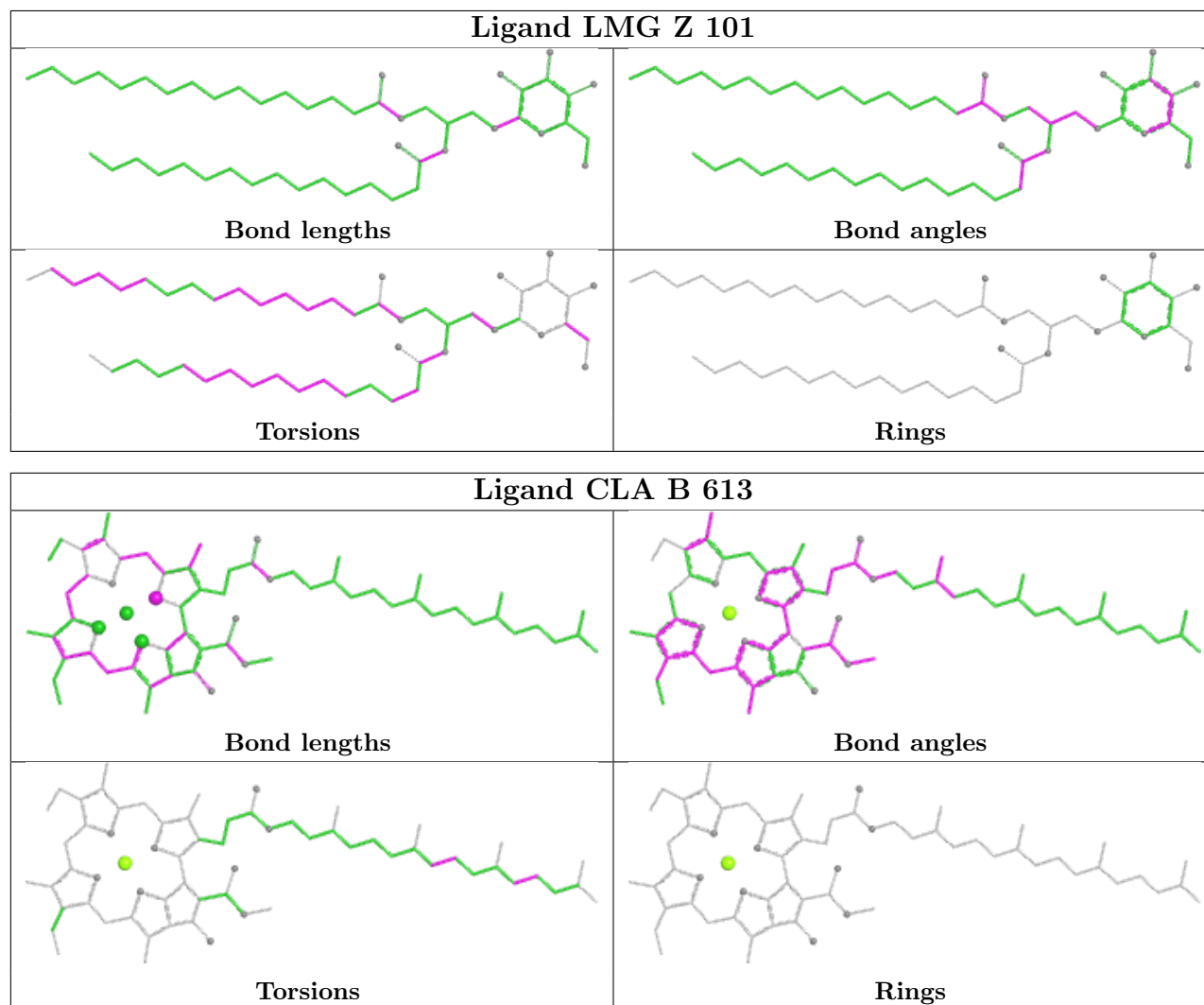
Mol	Chain	Res	Type	Atoms
23	B	602	CLA	CAD-CBD-CGD-O1D
23	B	602	CLA	C11-C10-C8-C9
23	B	615	CLA	CAD-CBD-CGD-O1D
23	B	615	CLA	CAD-CBD-CGD-O2D
23	B	617	CLA	CHA-CBD-CGD-O1D

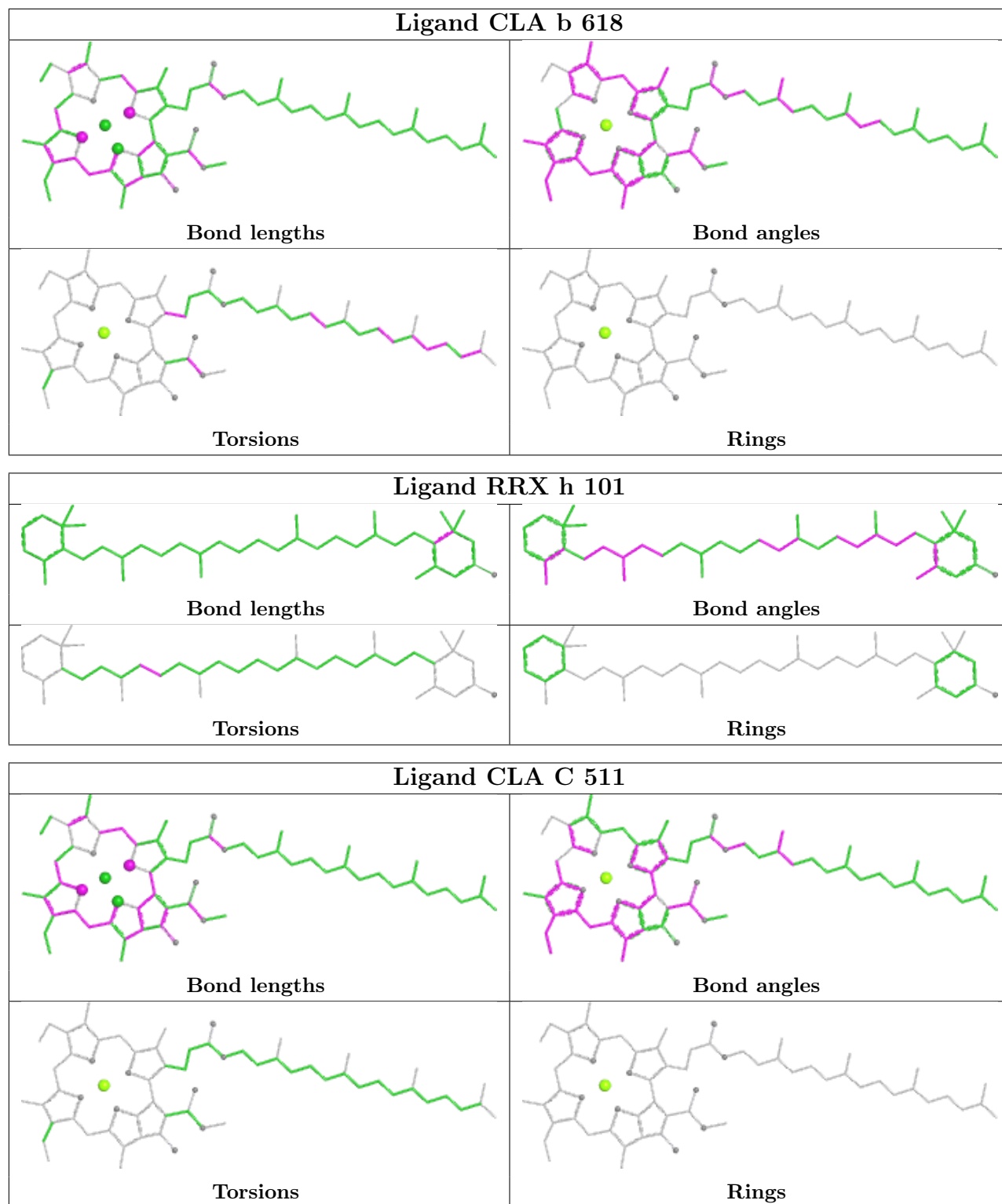
There are no ring outliers.

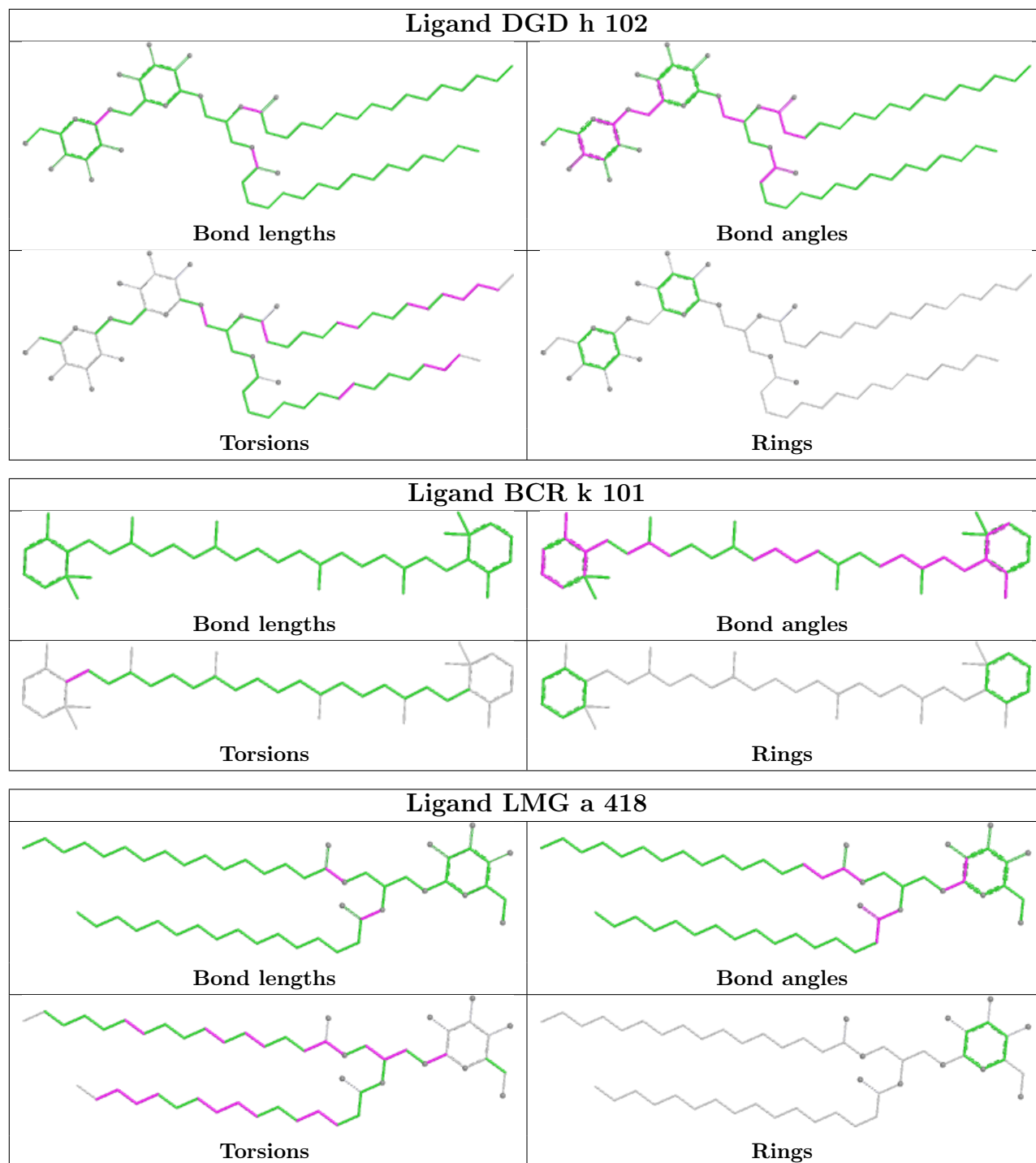
No monomer is involved in short contacts.

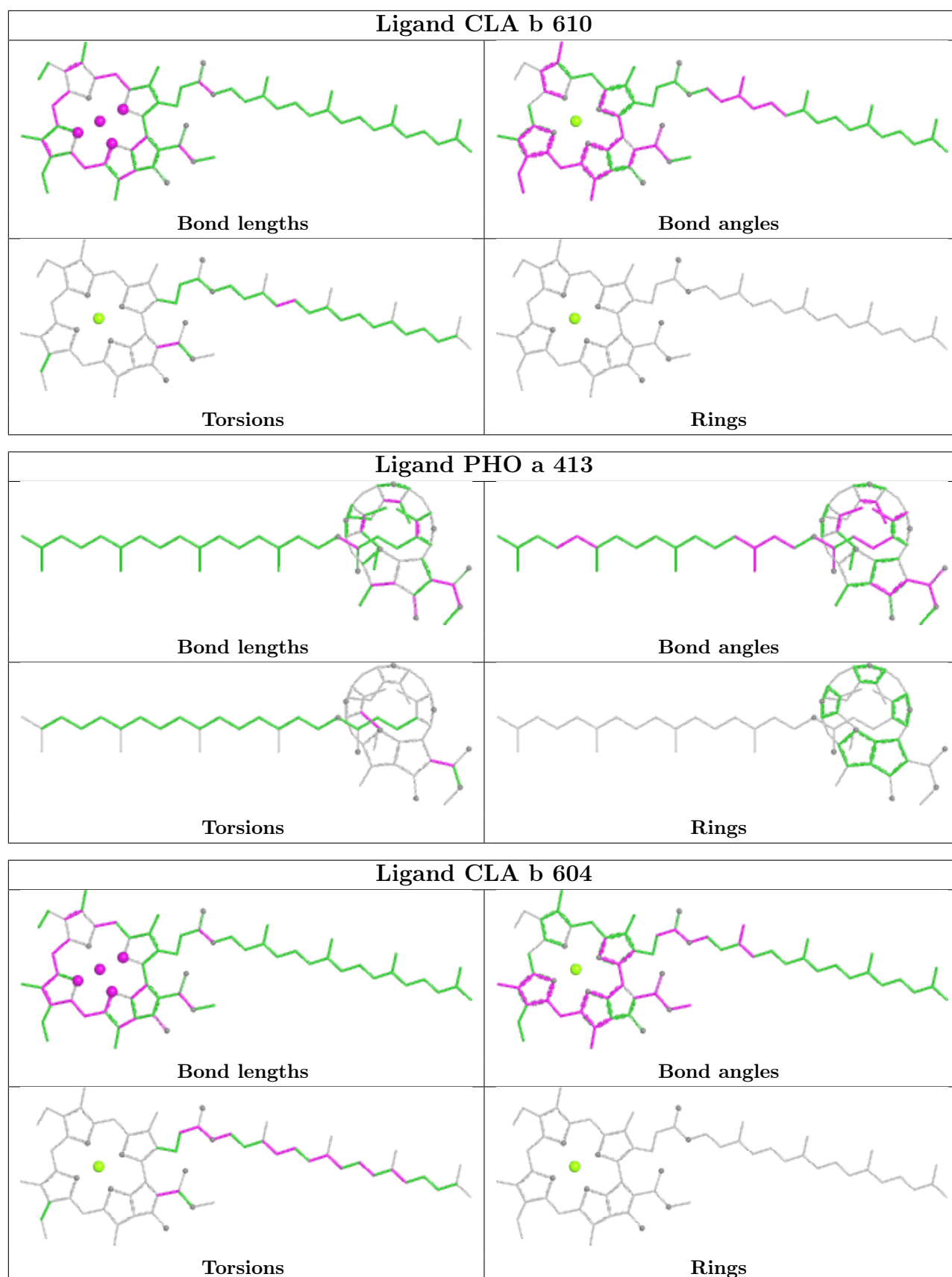
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

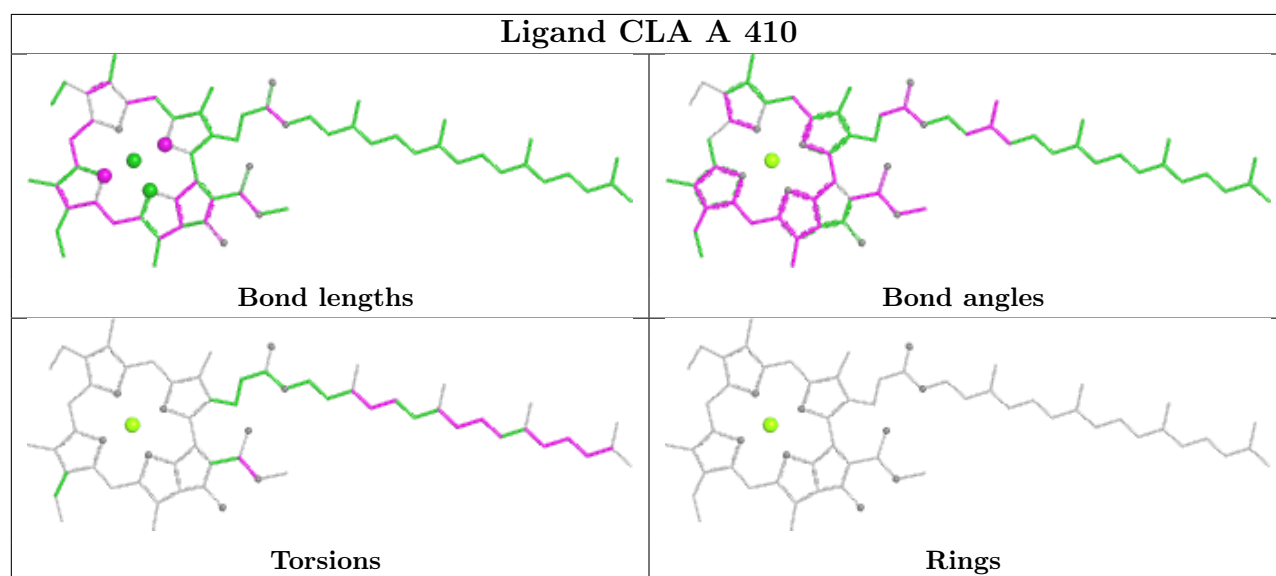
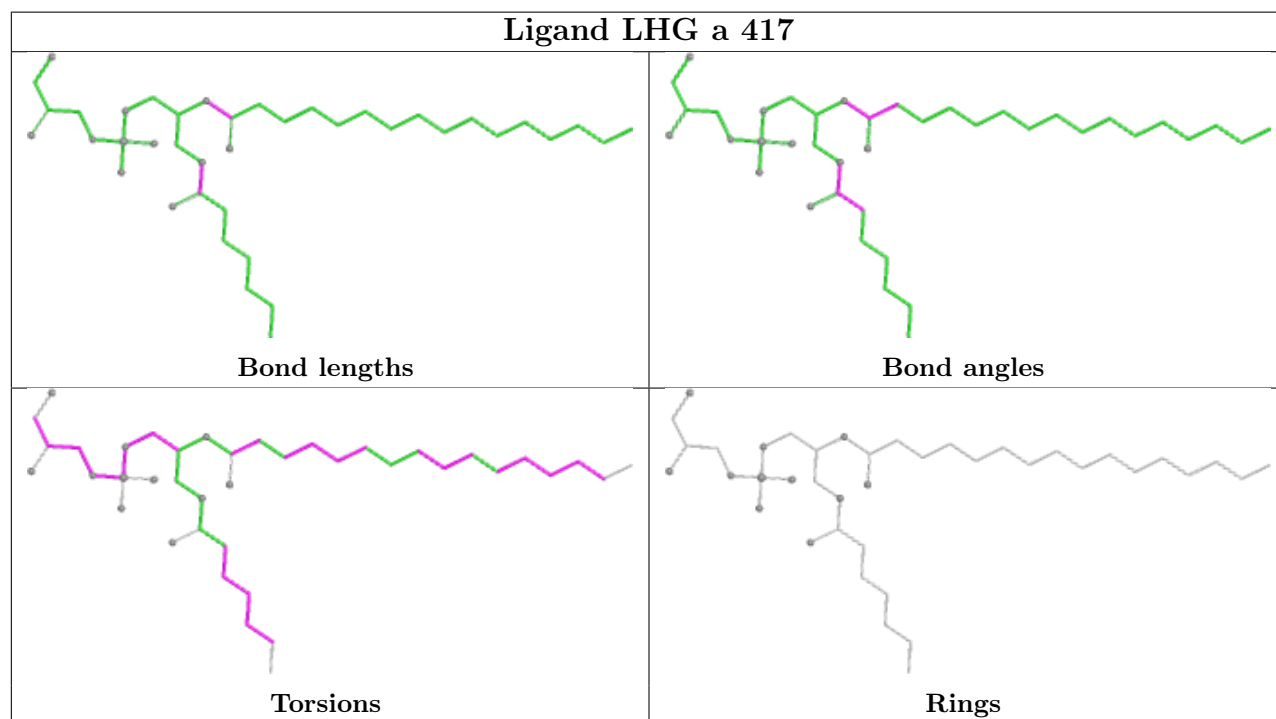
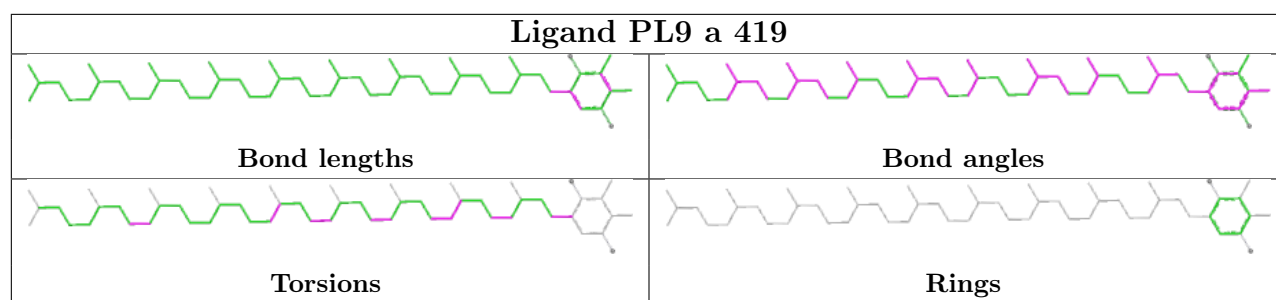
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

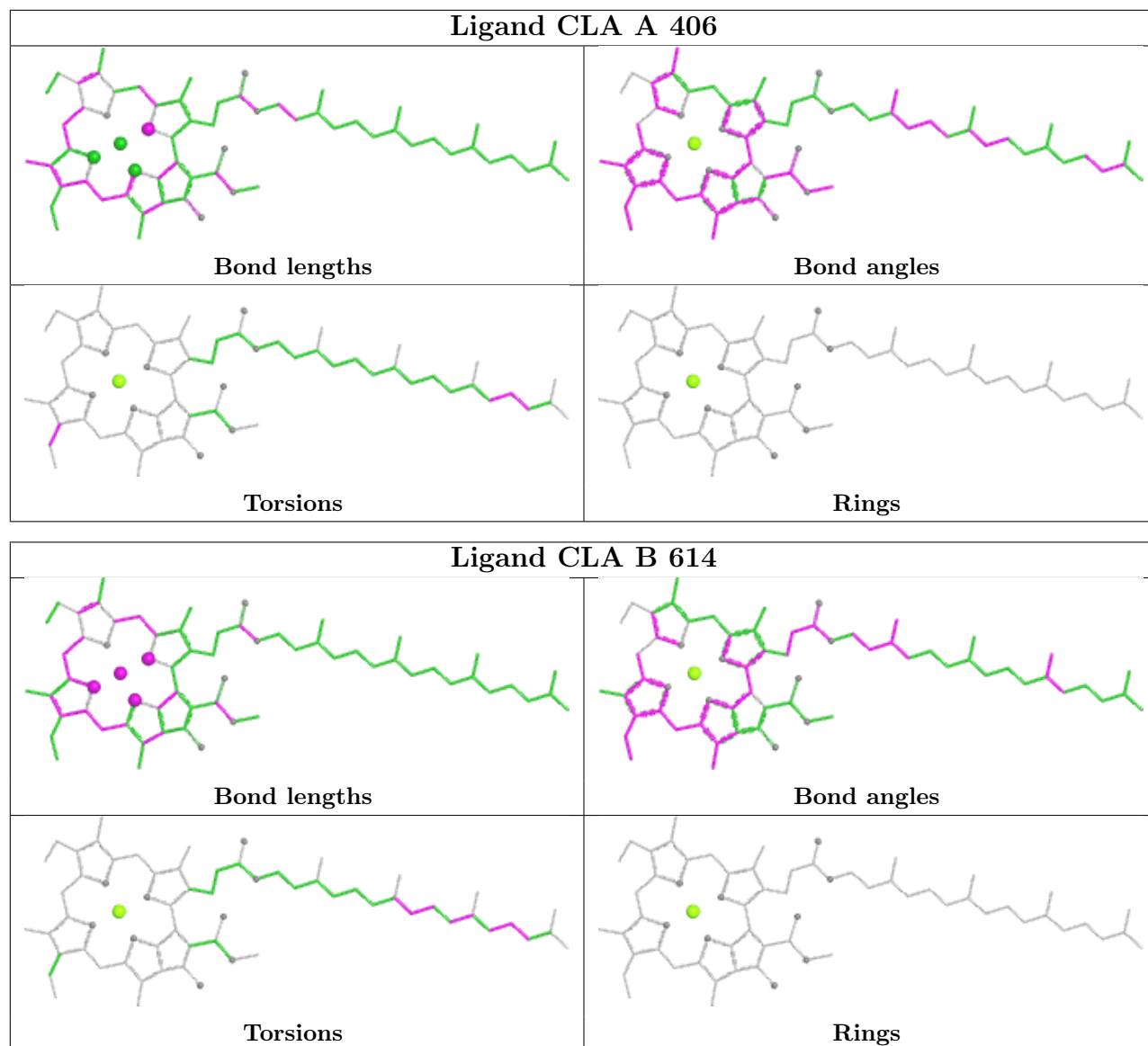


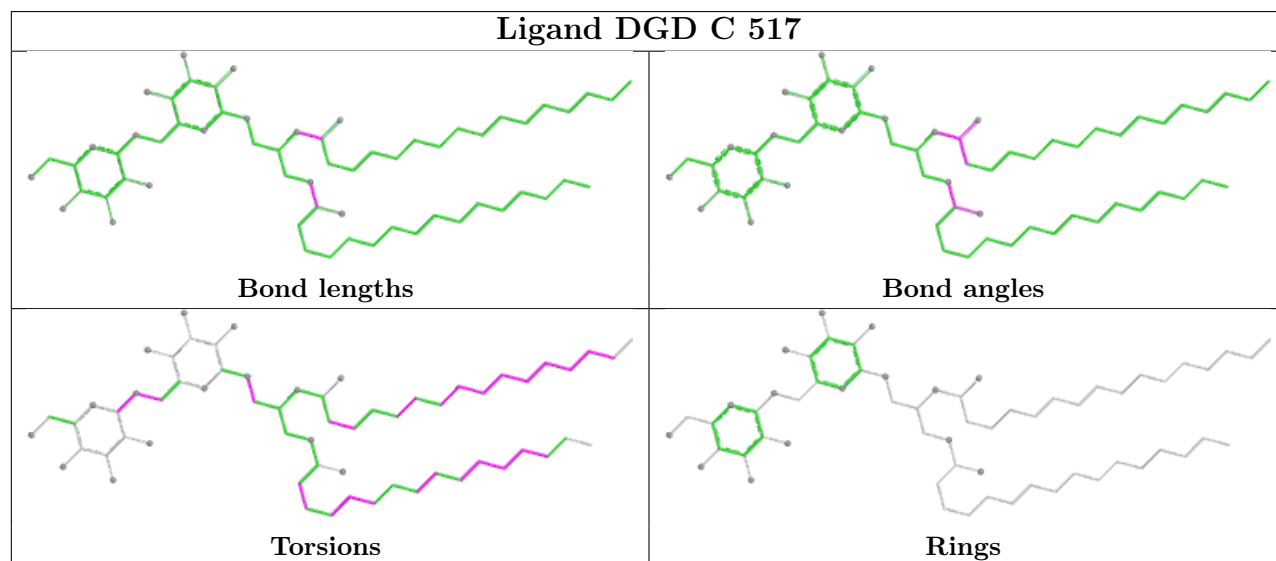
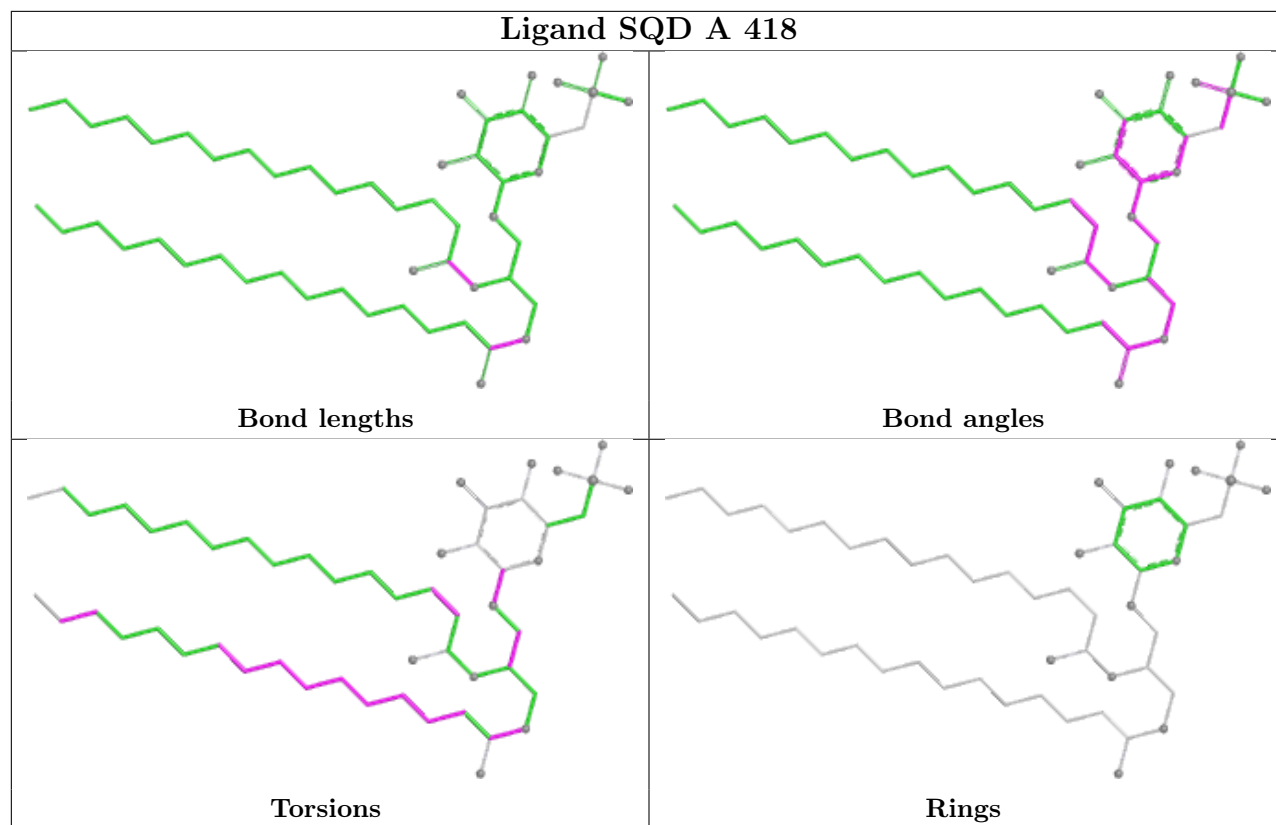


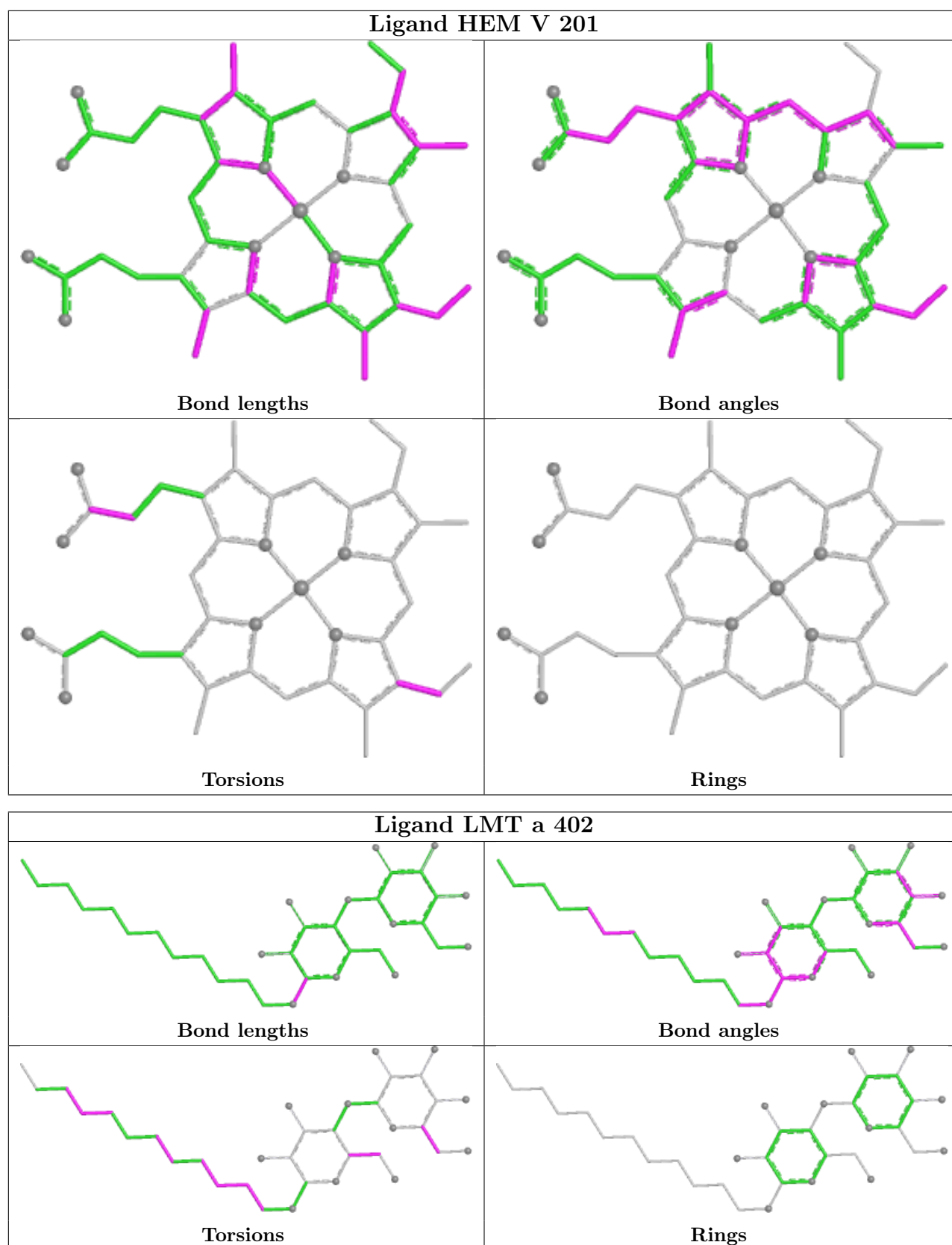


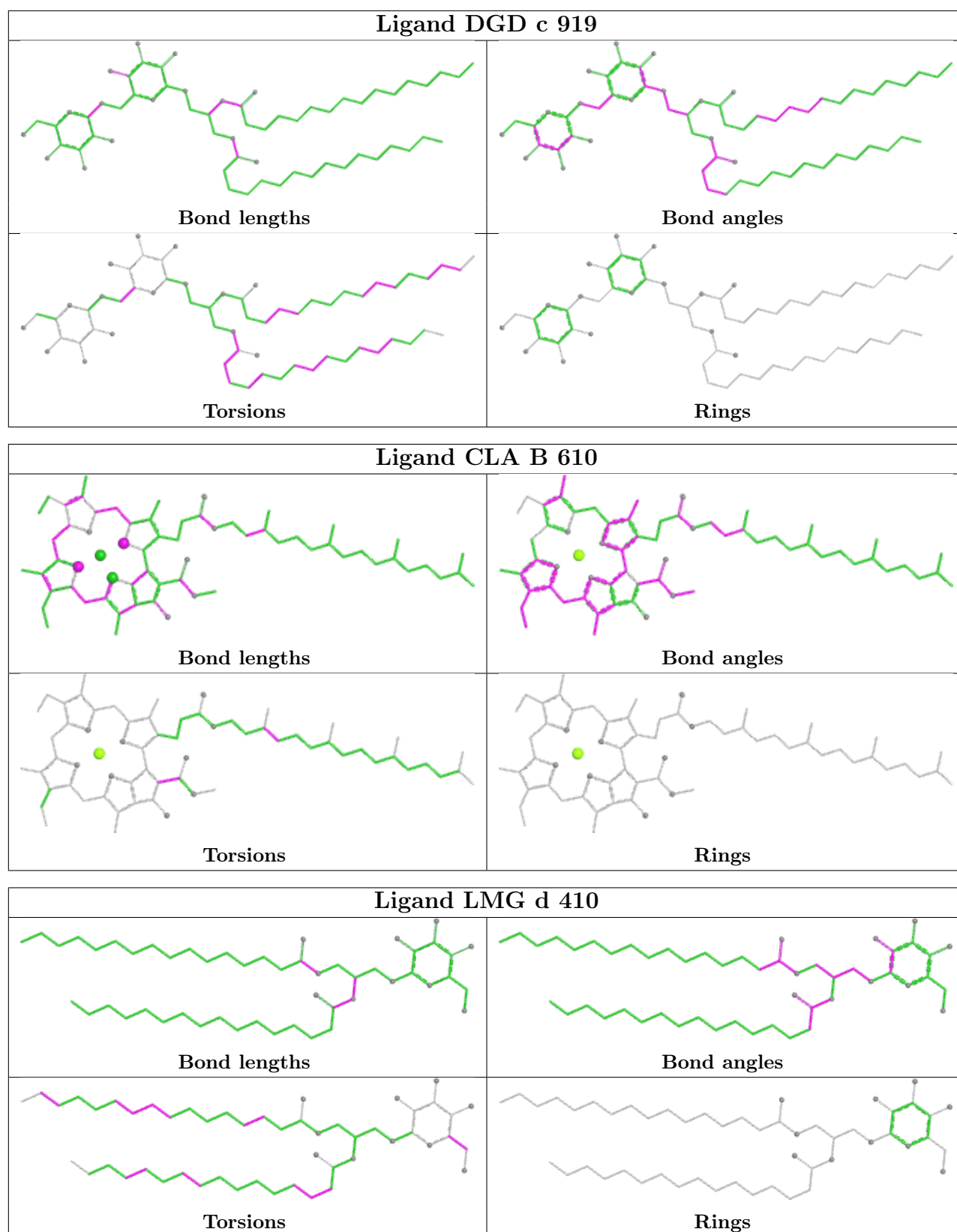


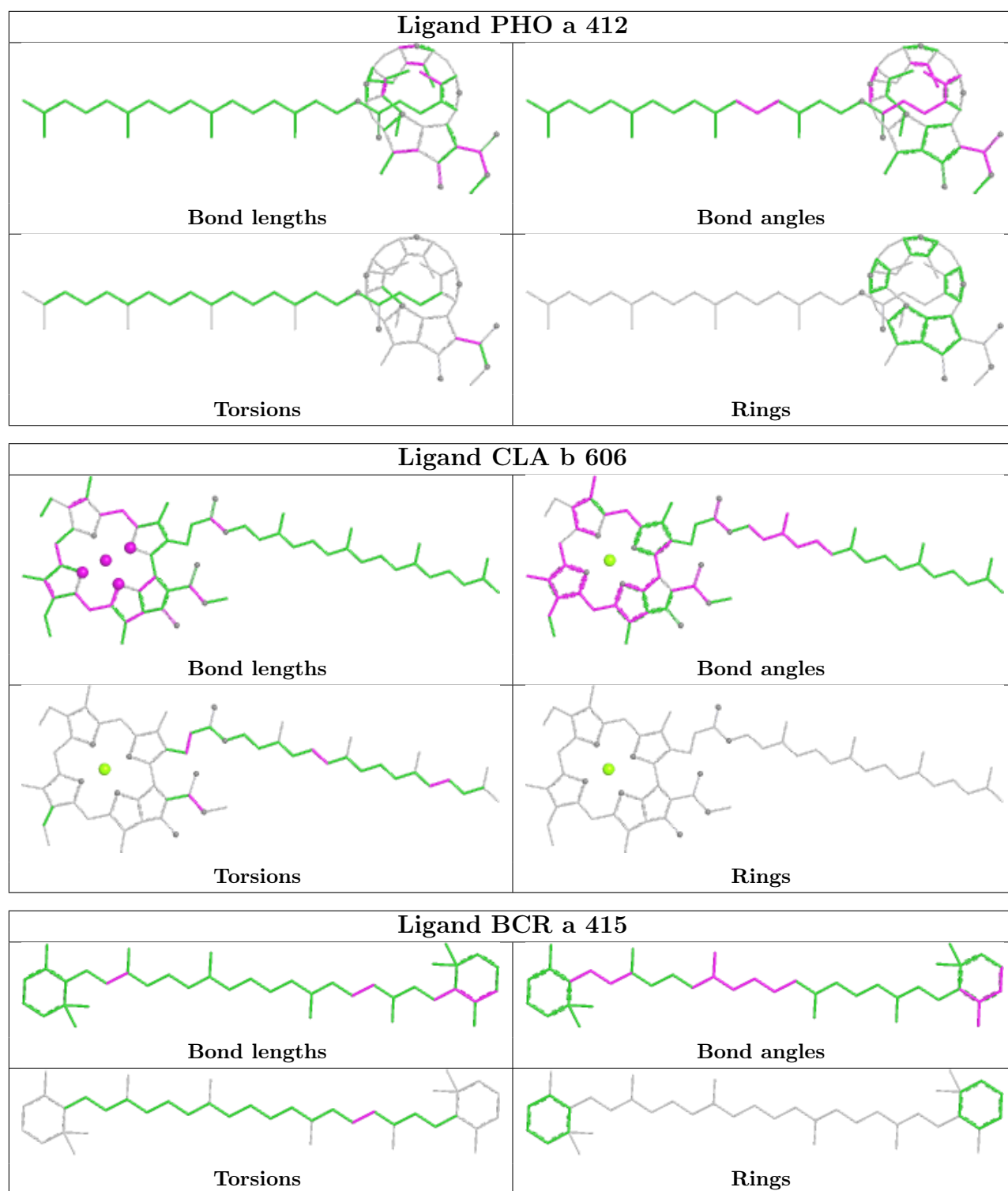


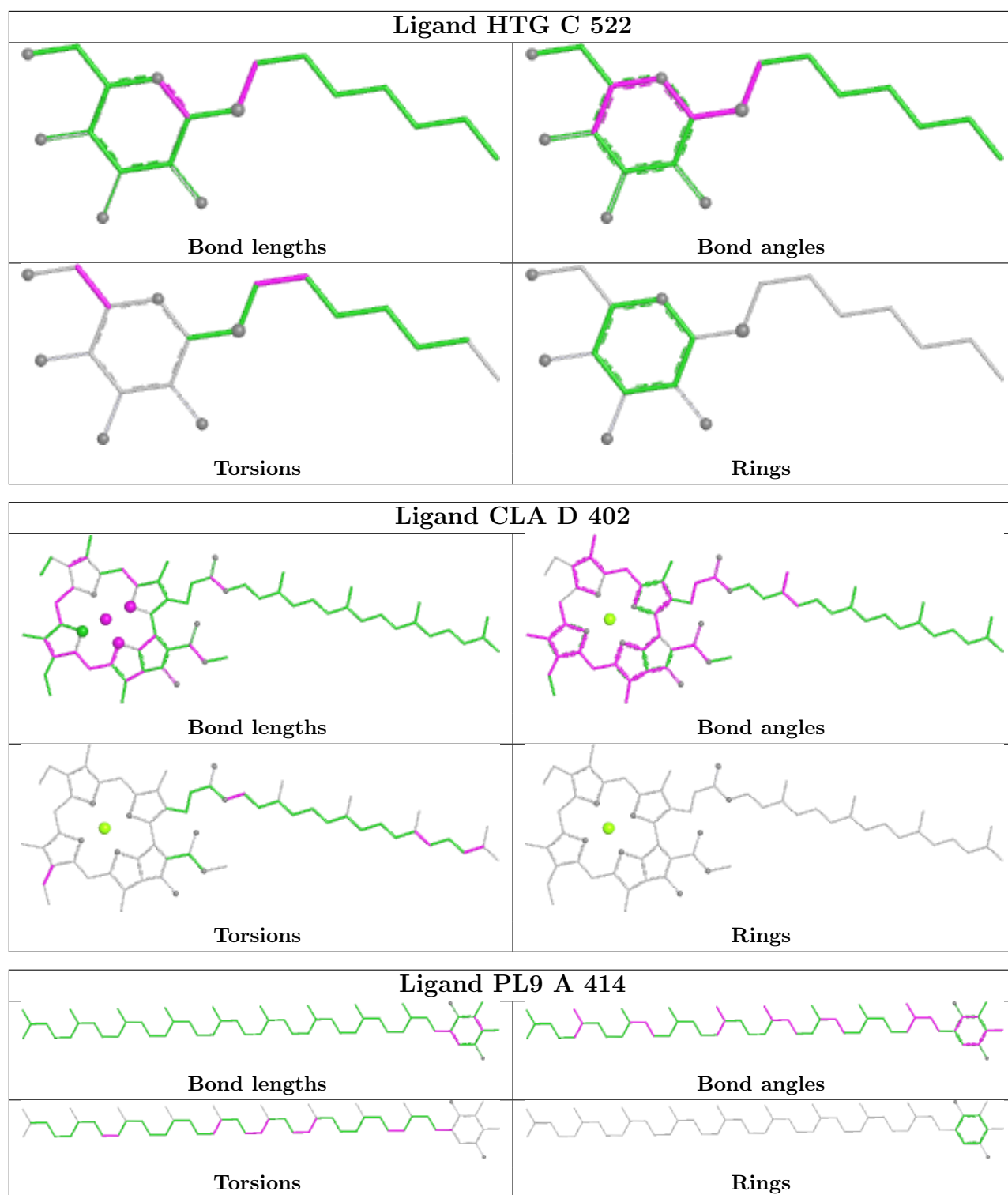


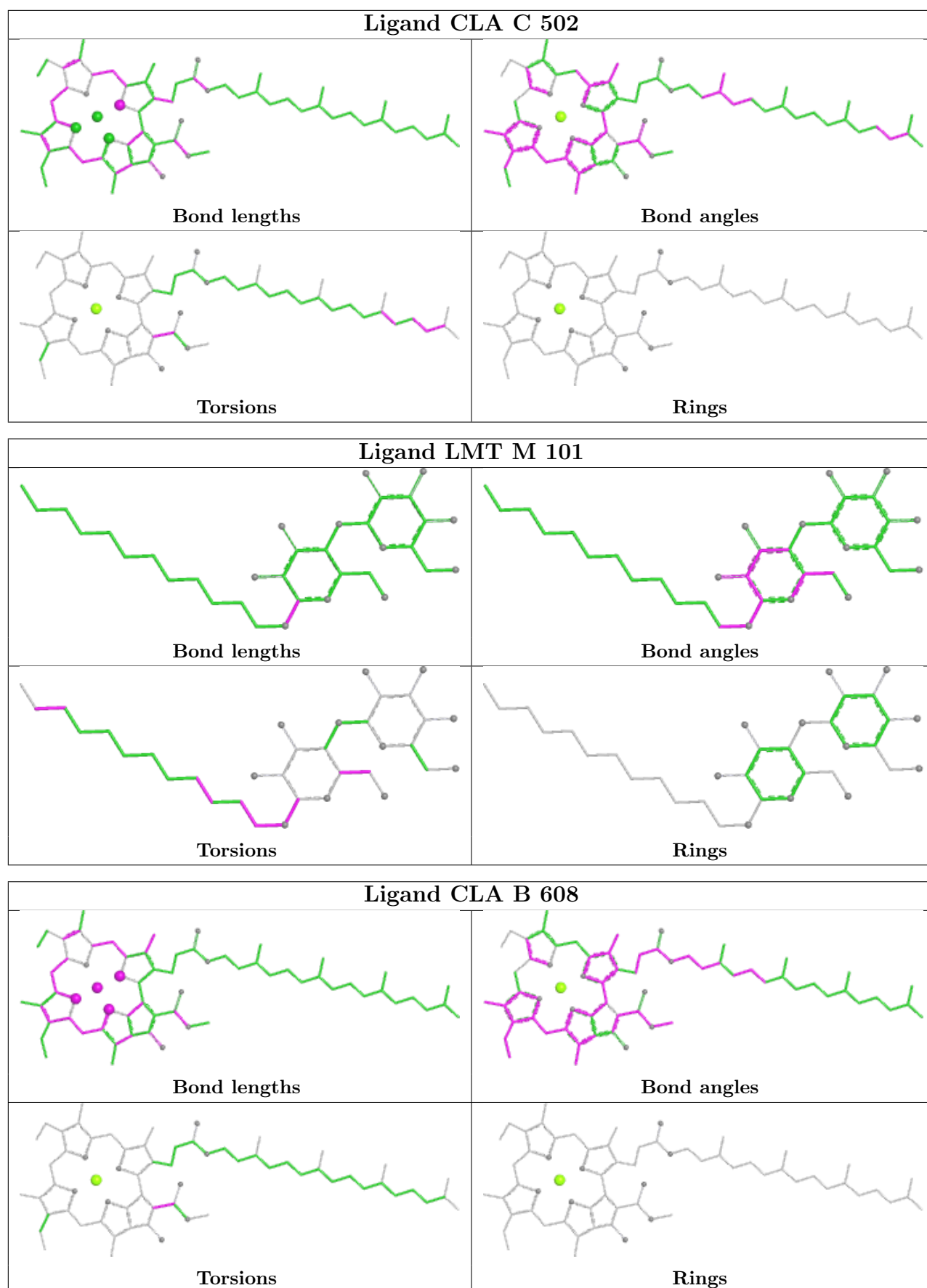


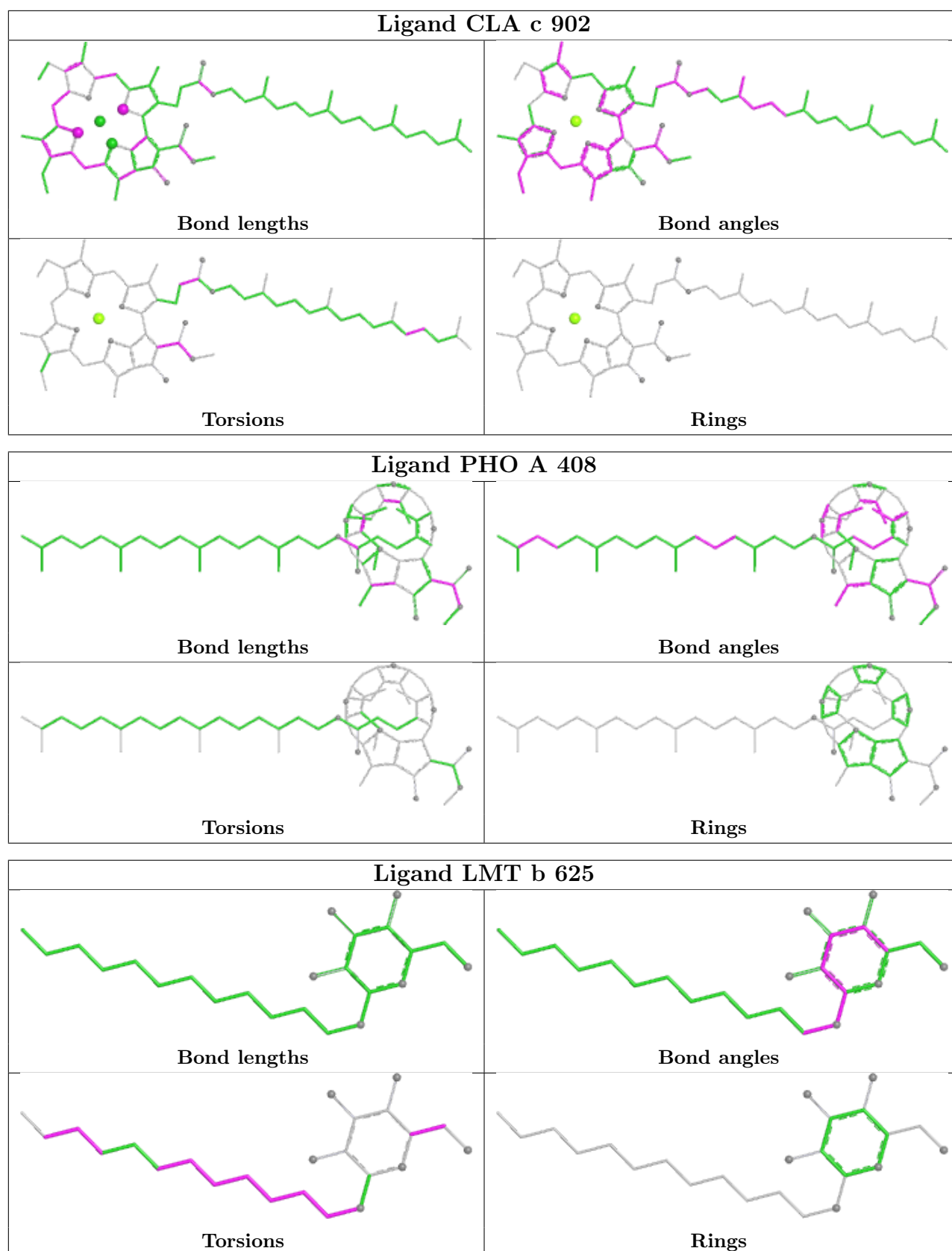


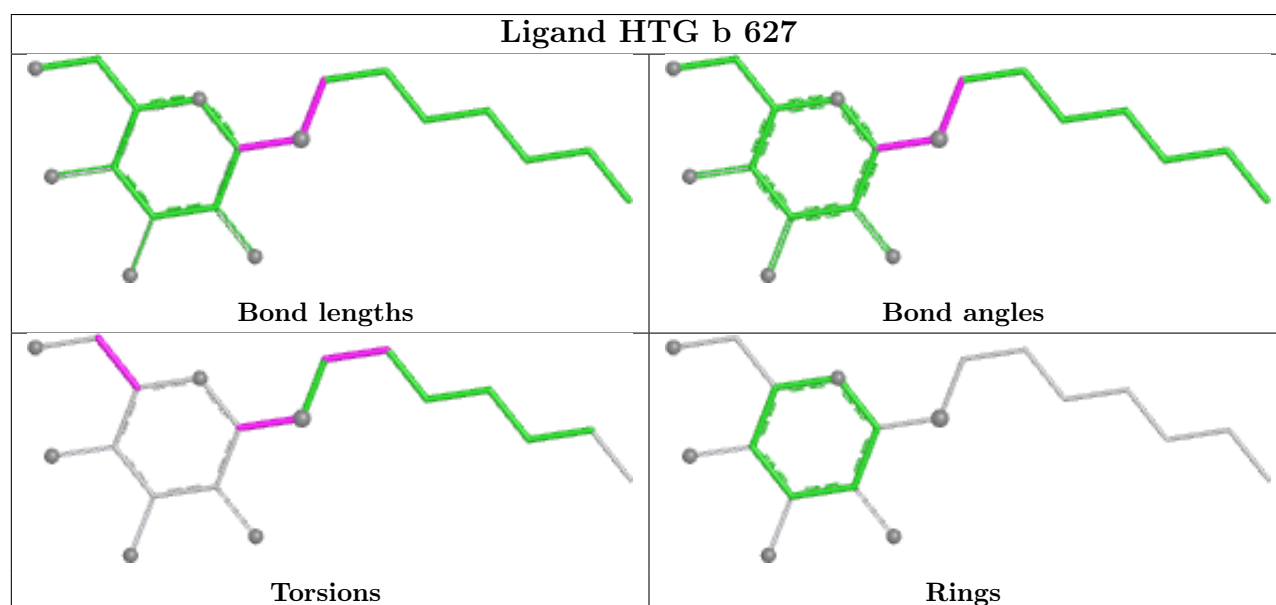
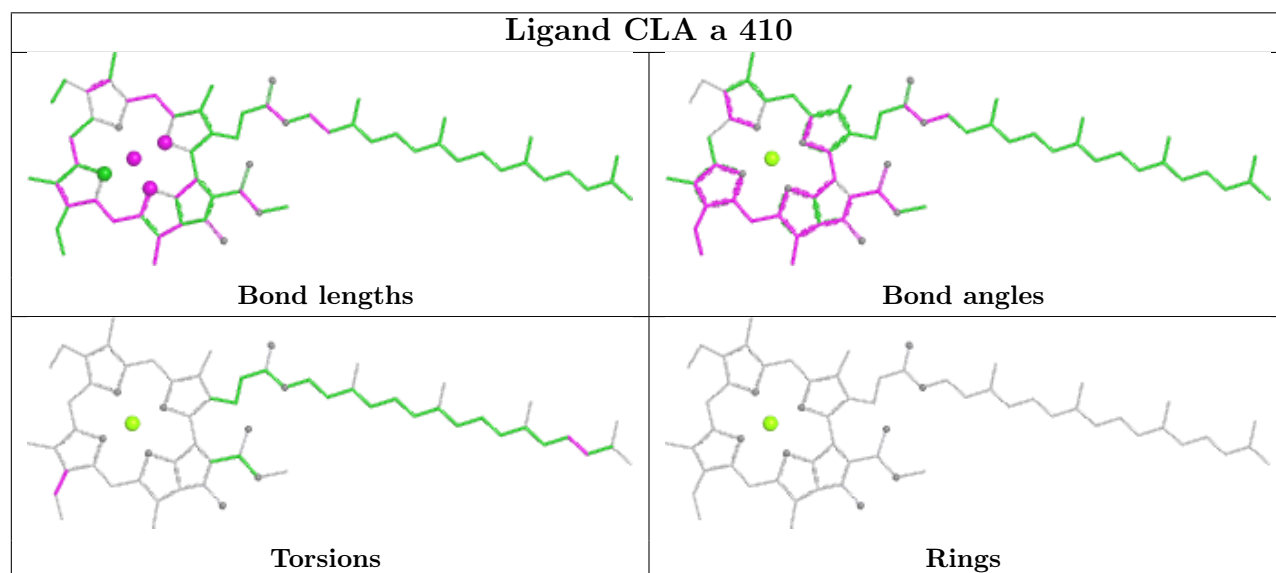
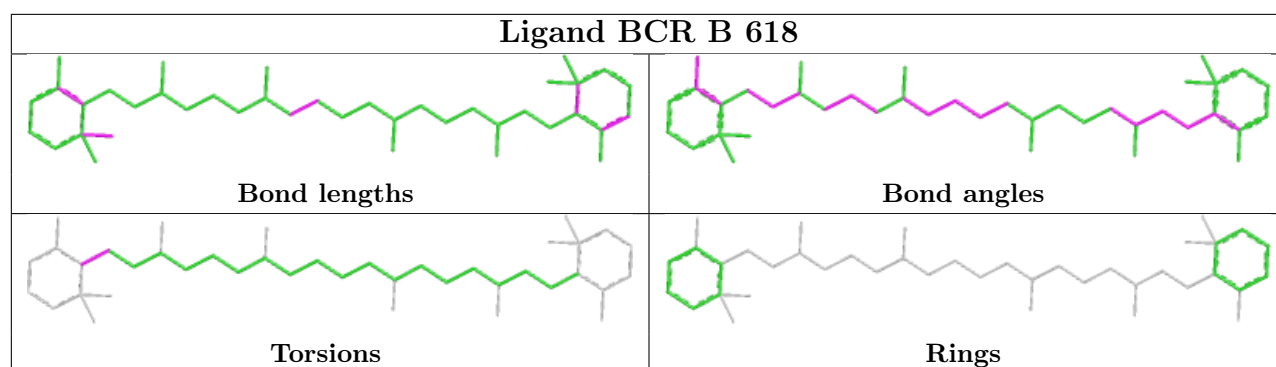


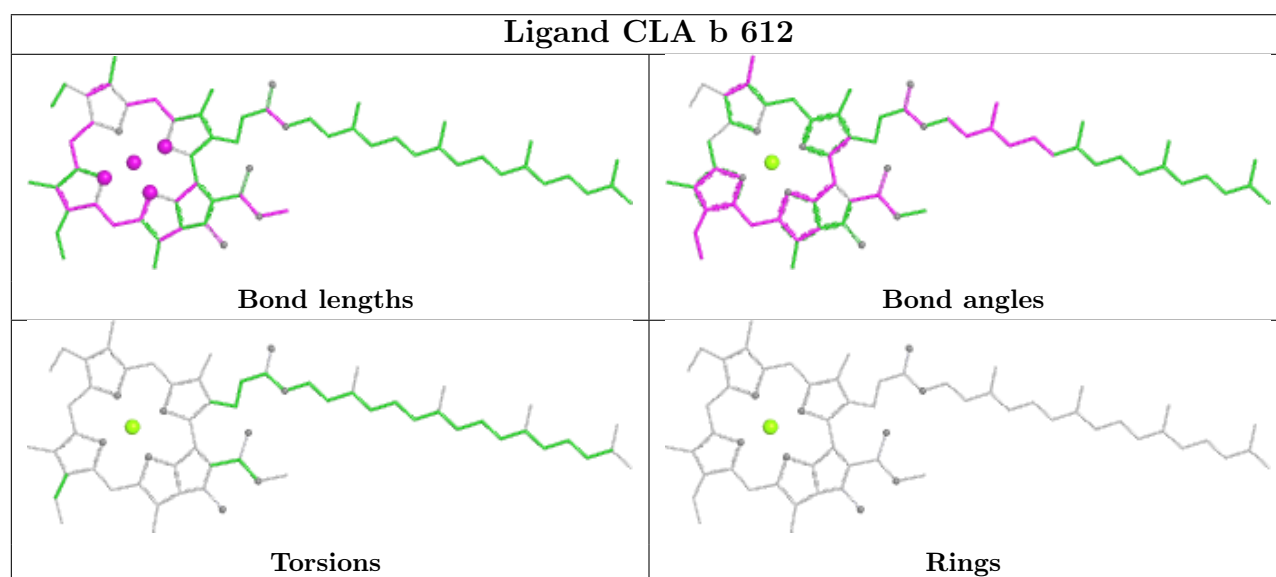
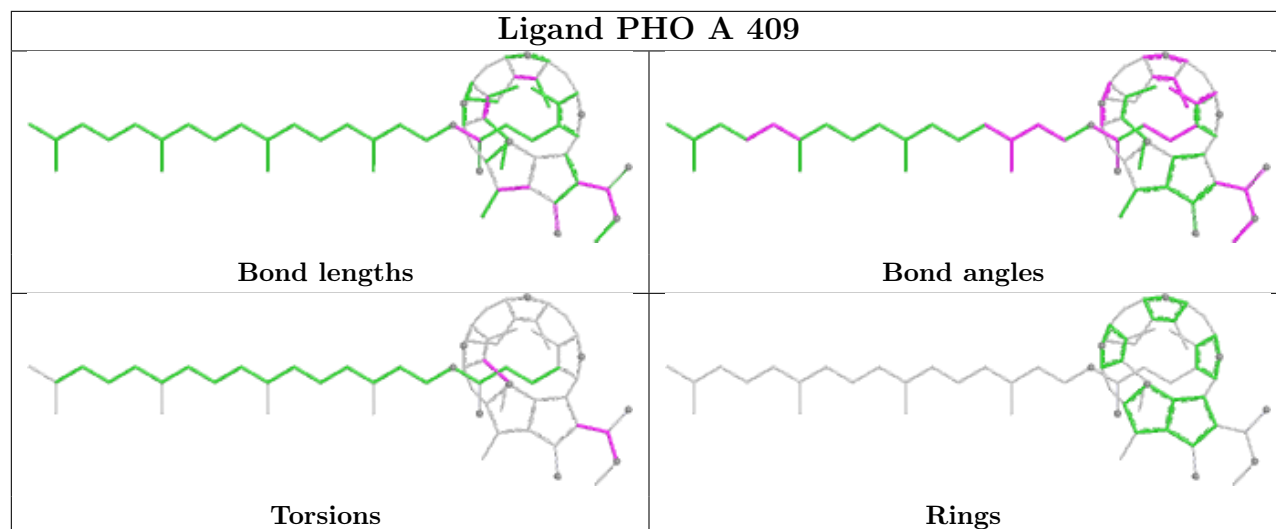


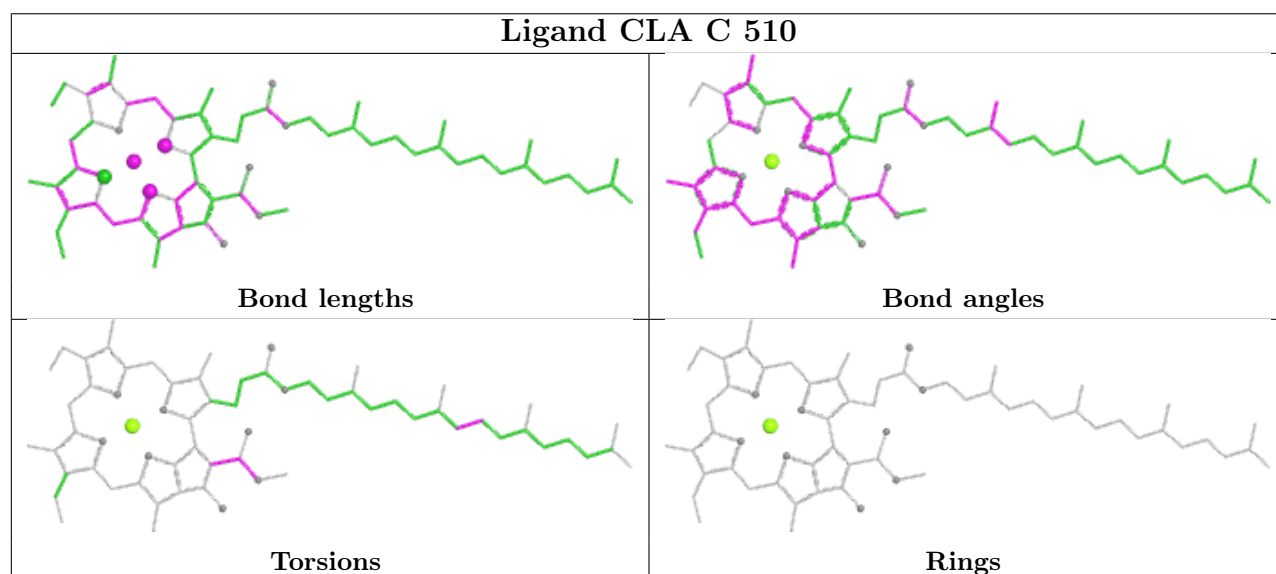
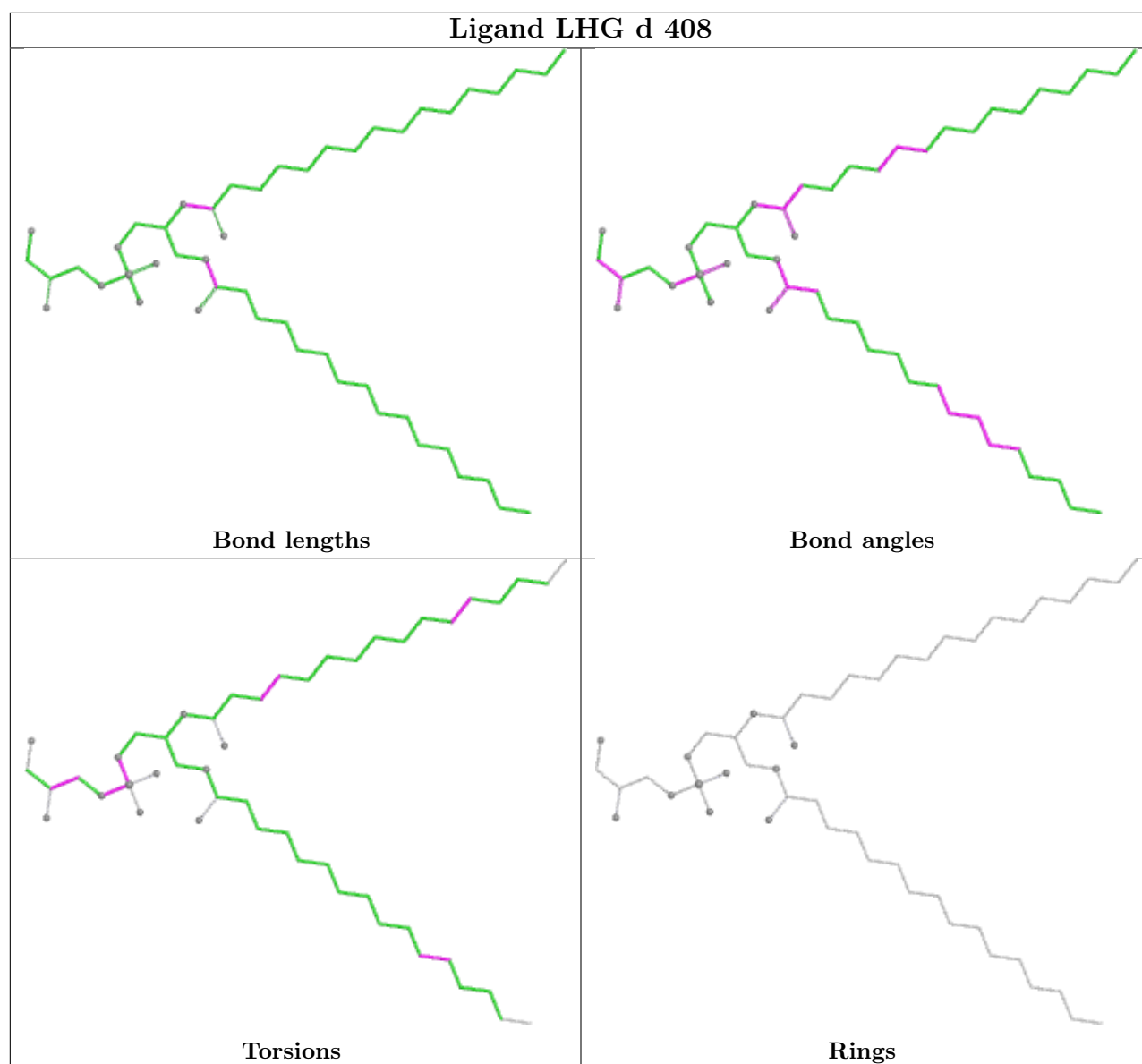


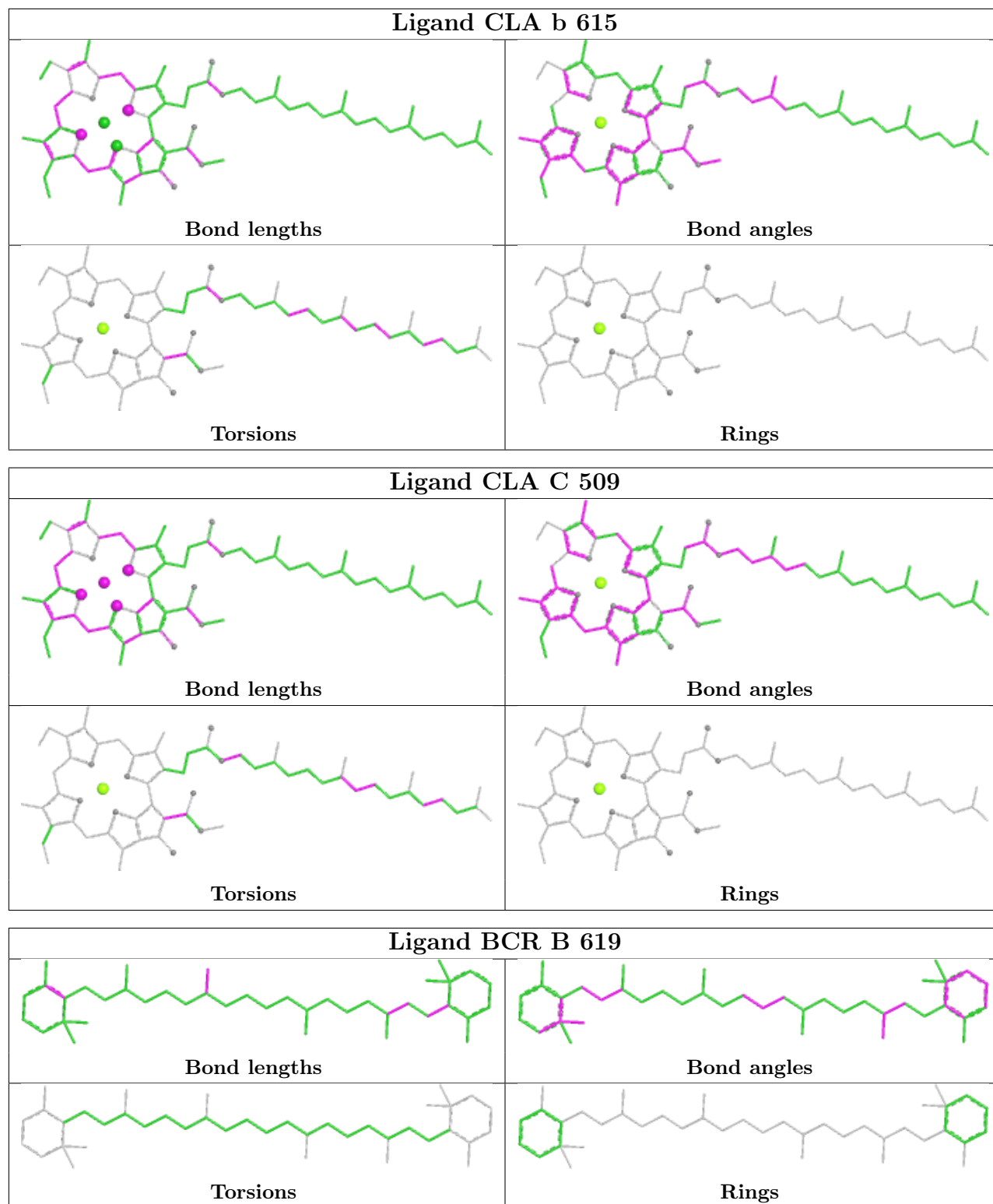


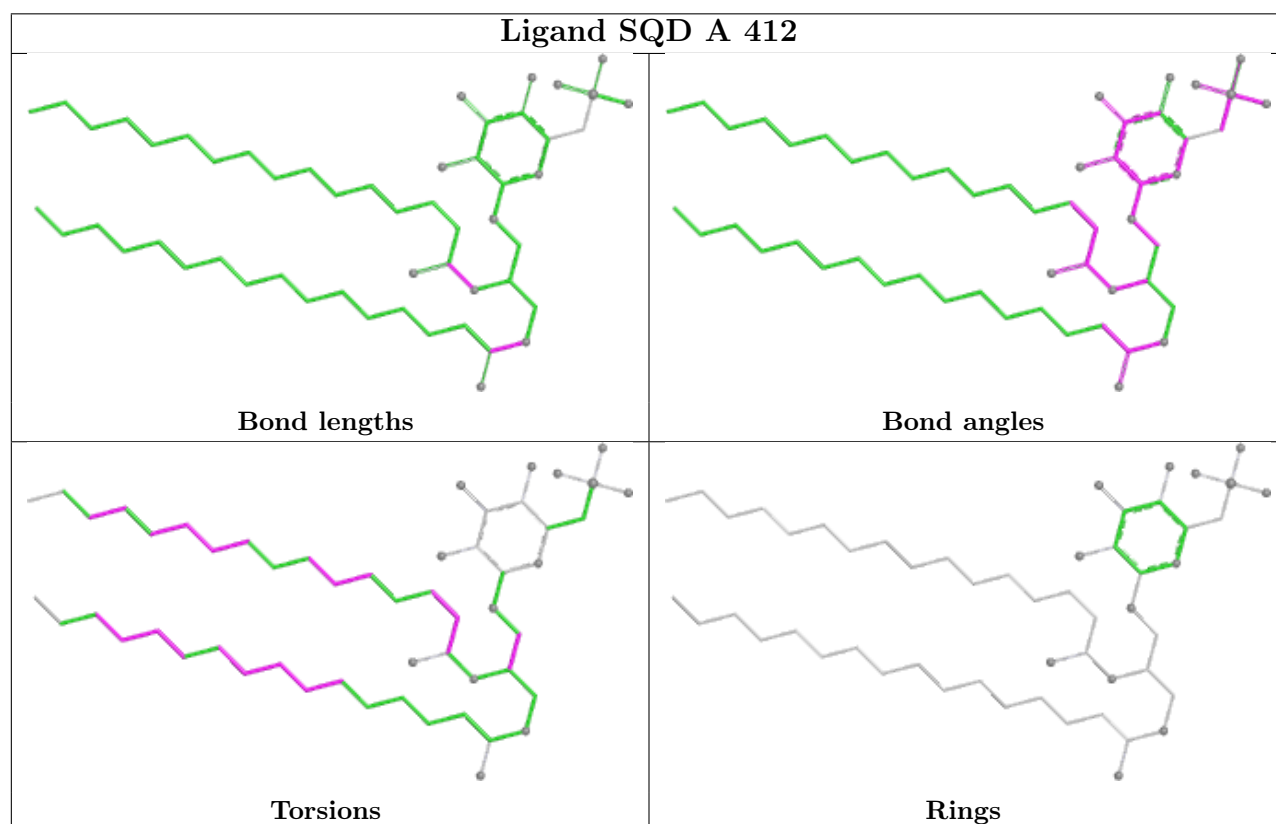
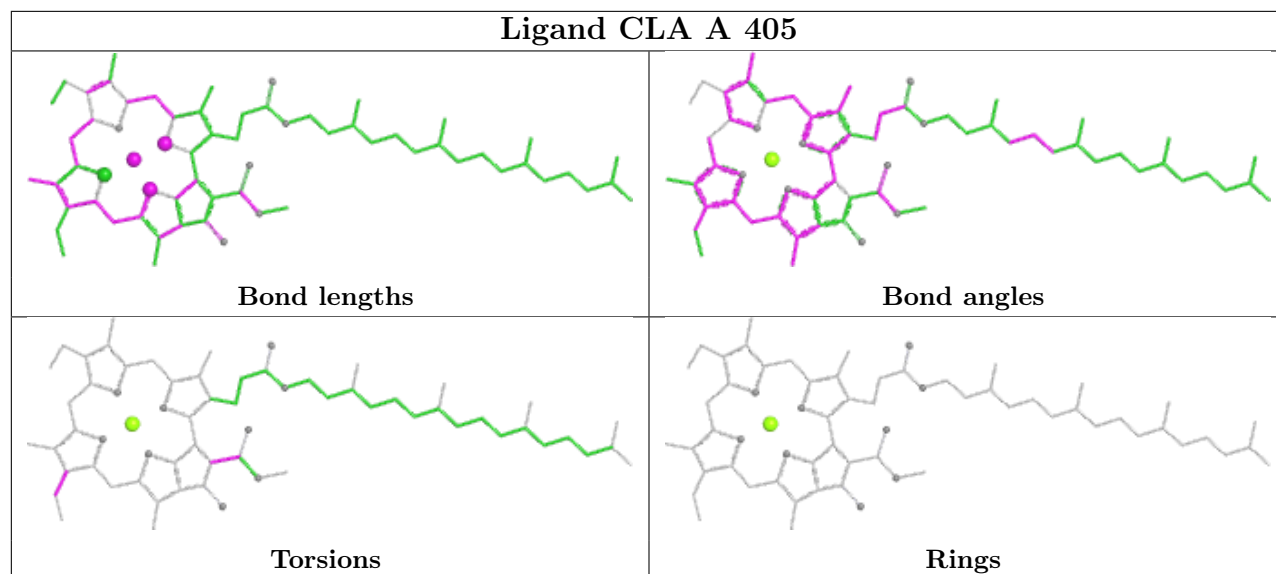


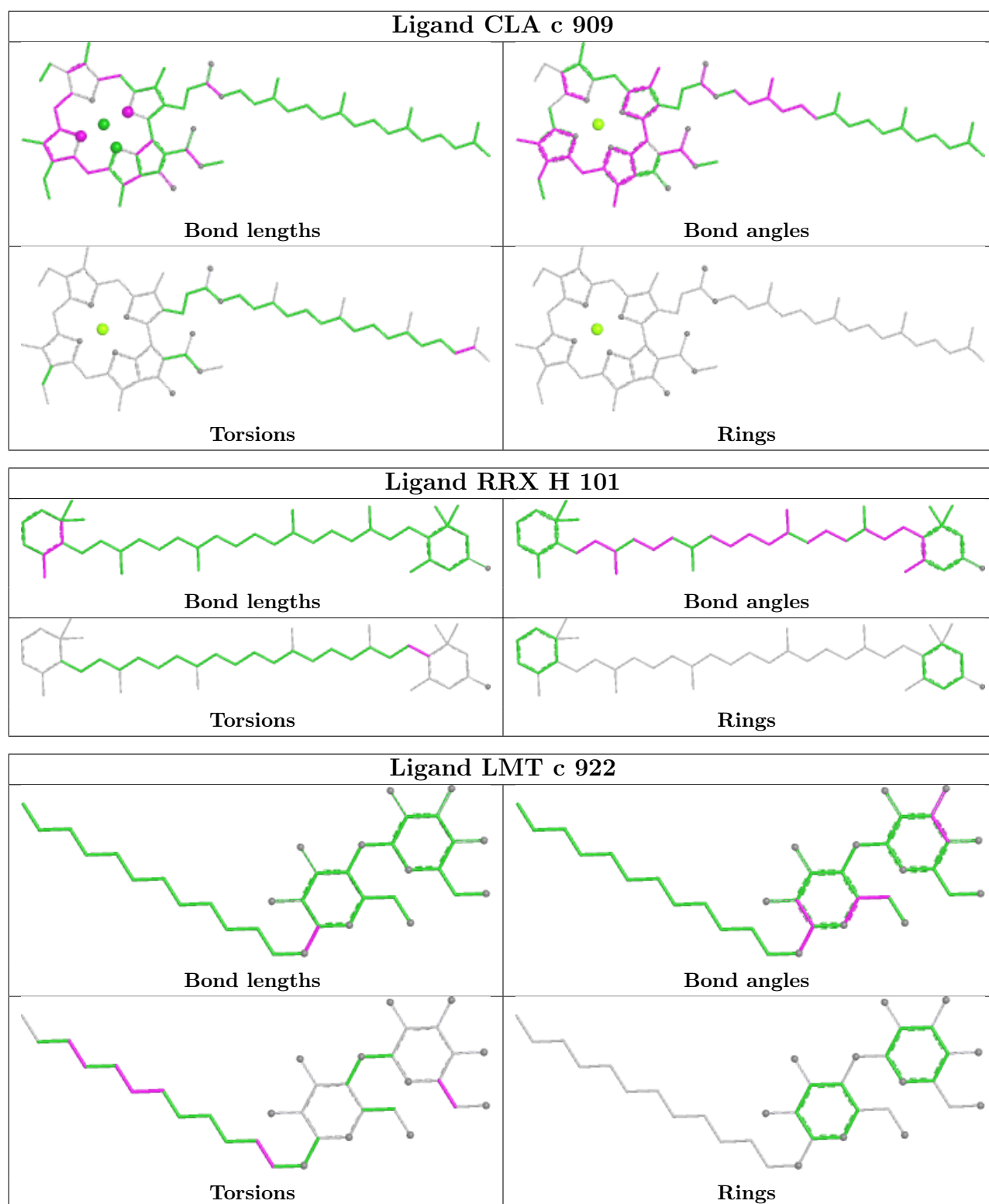


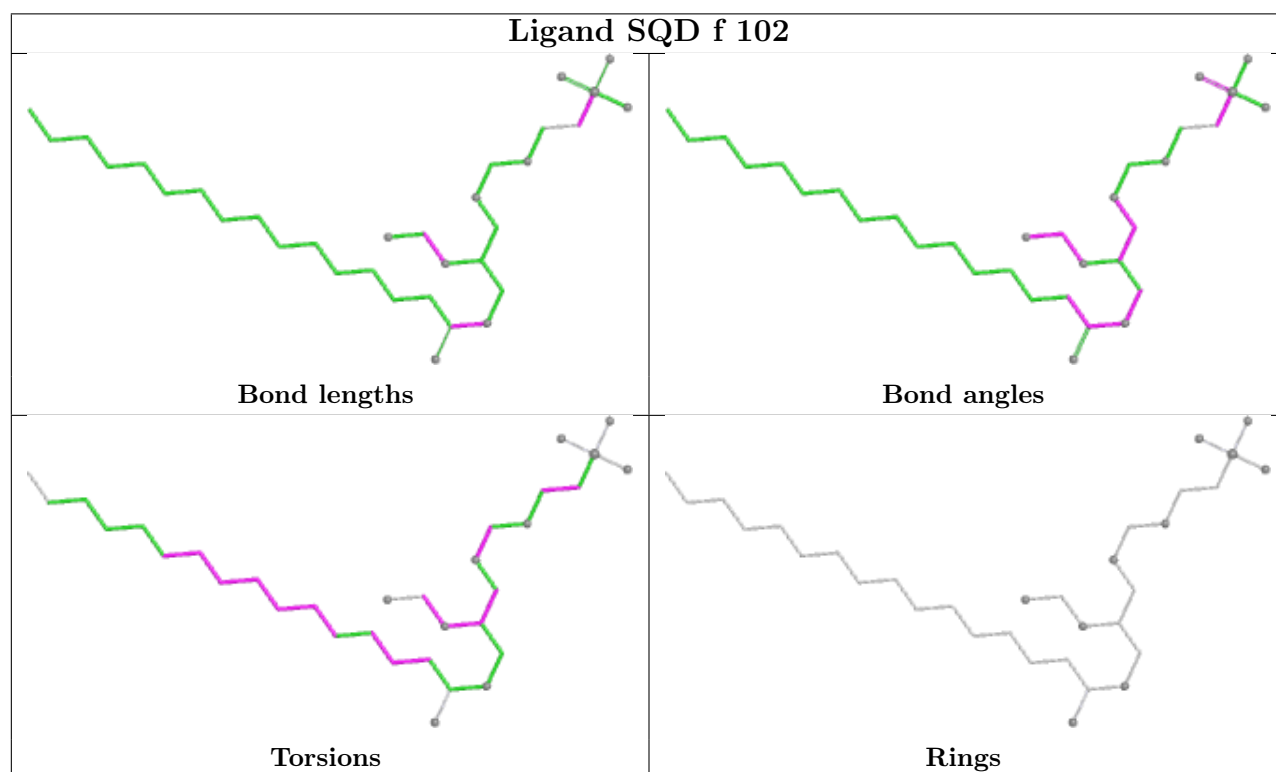
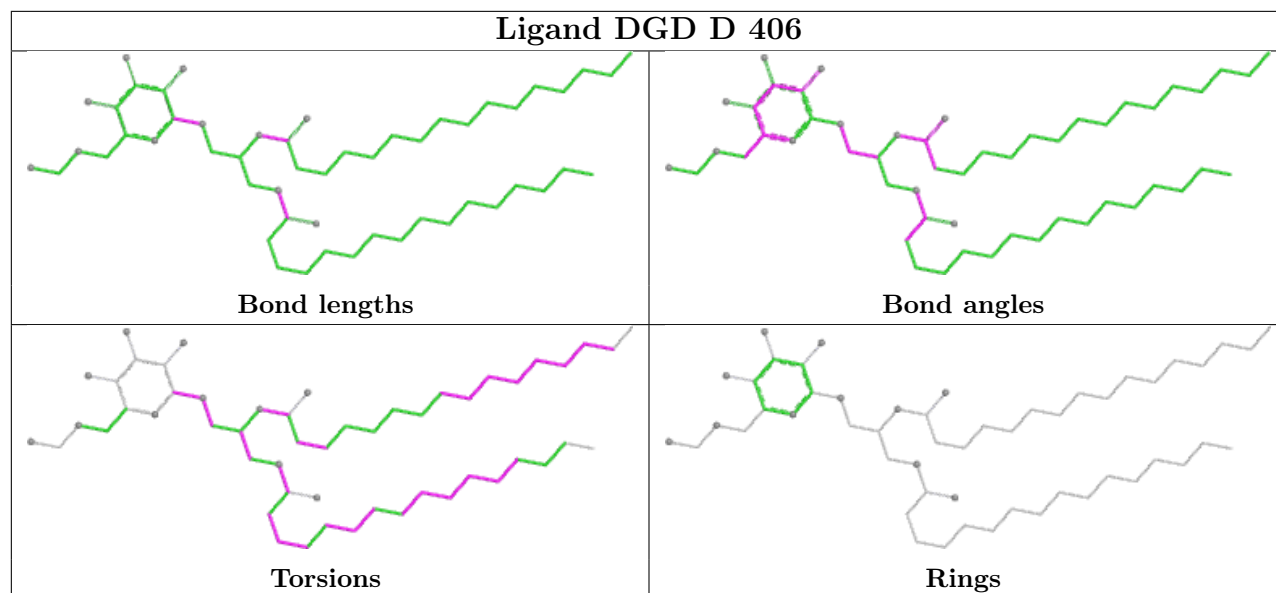


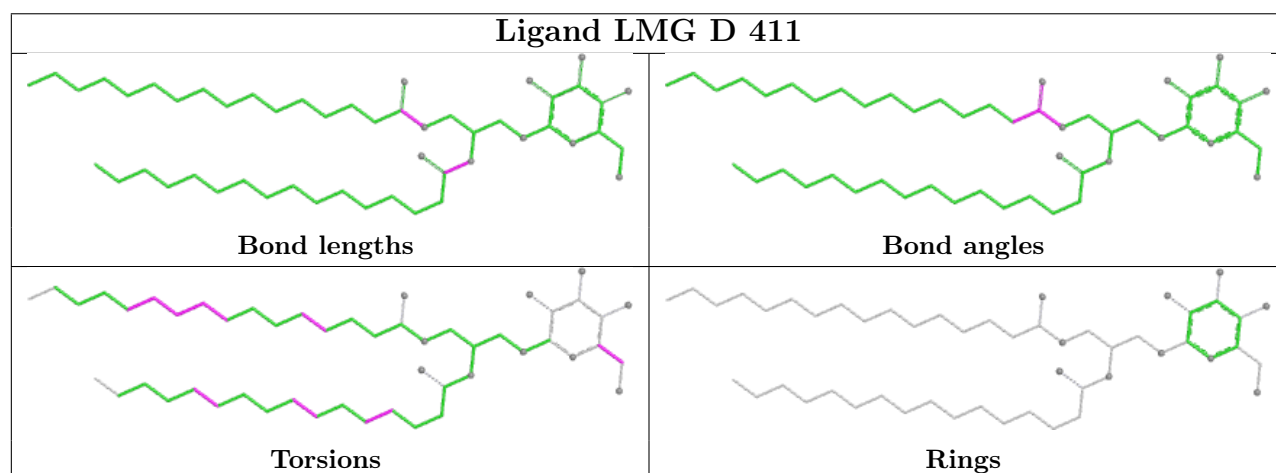
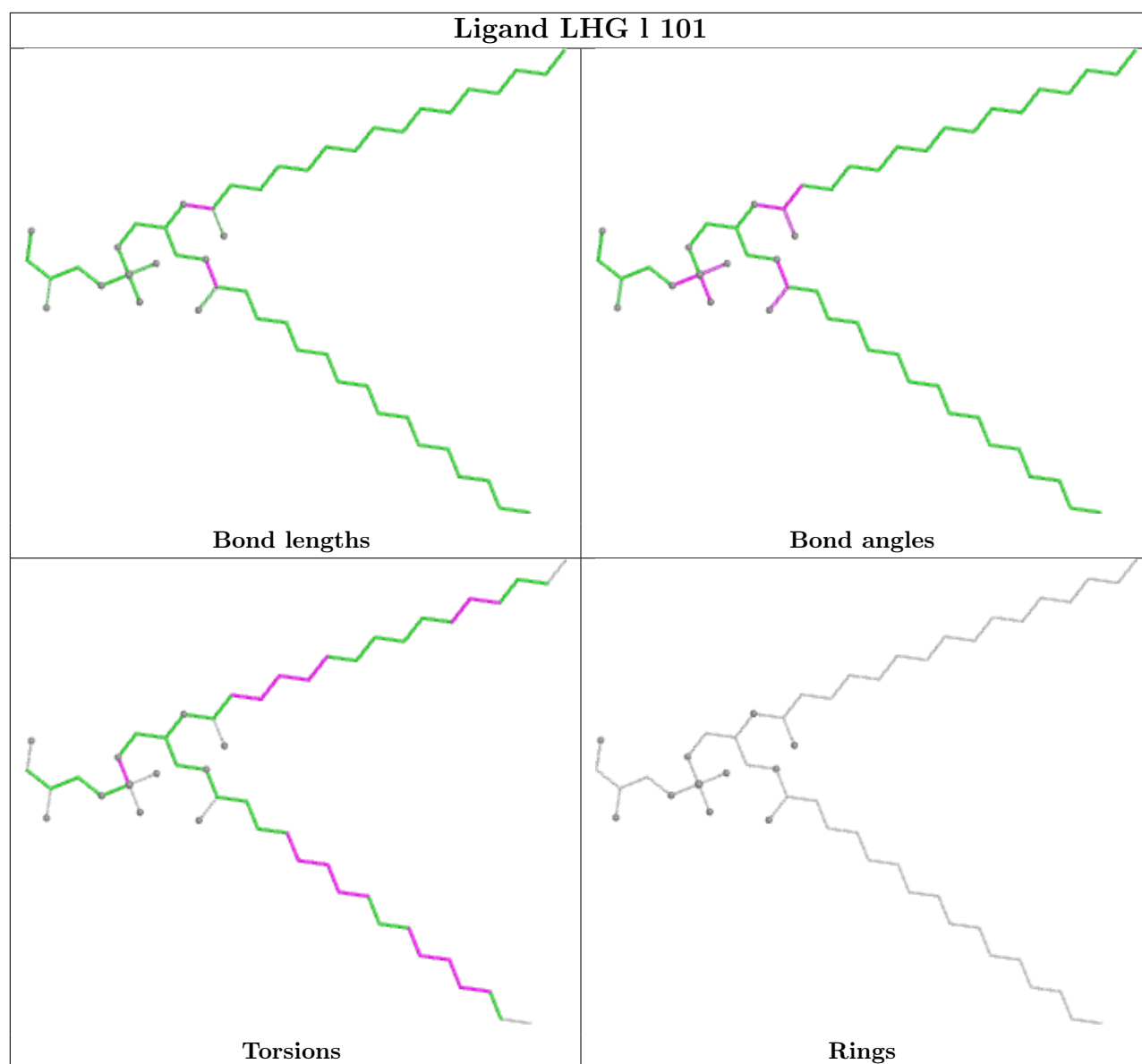


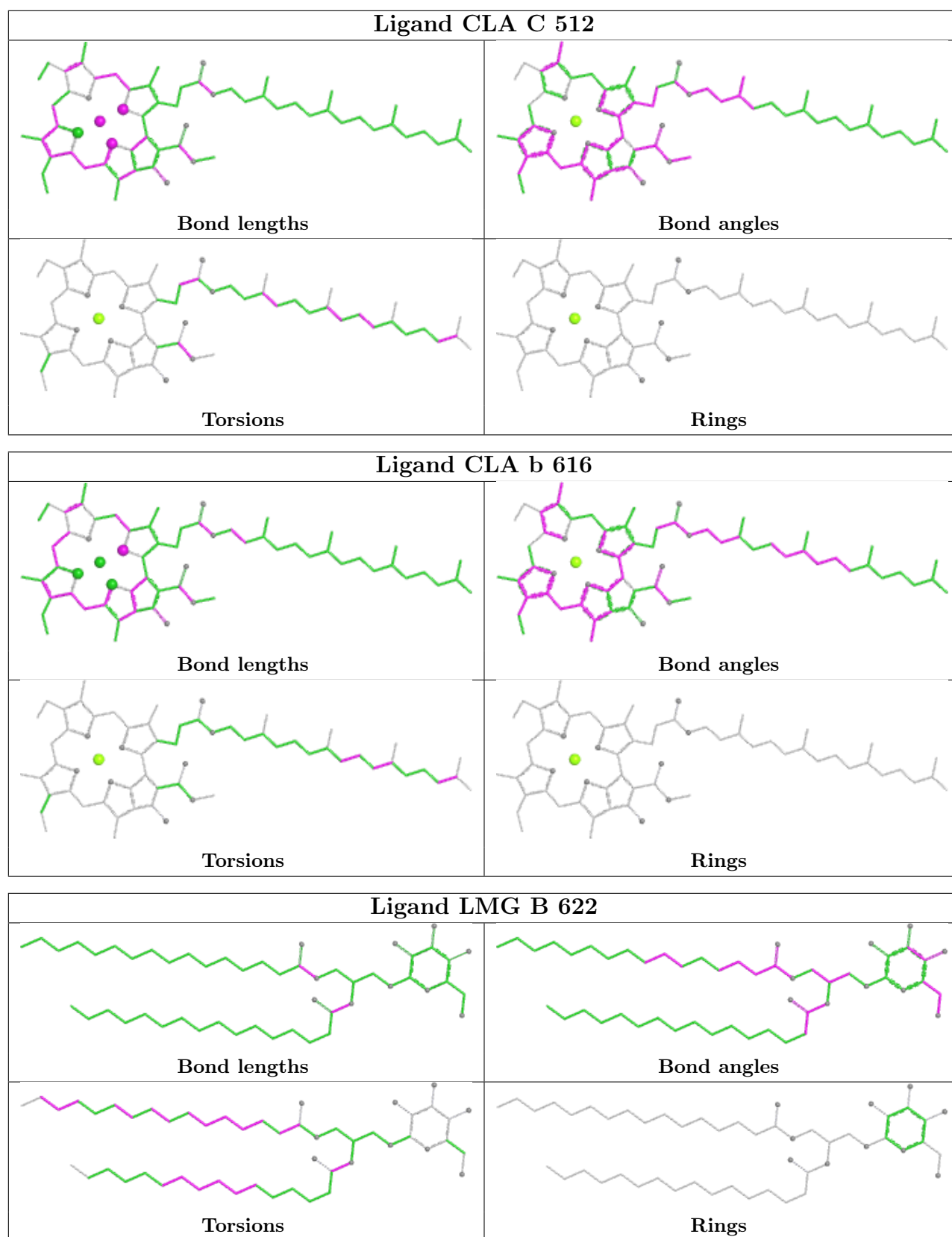


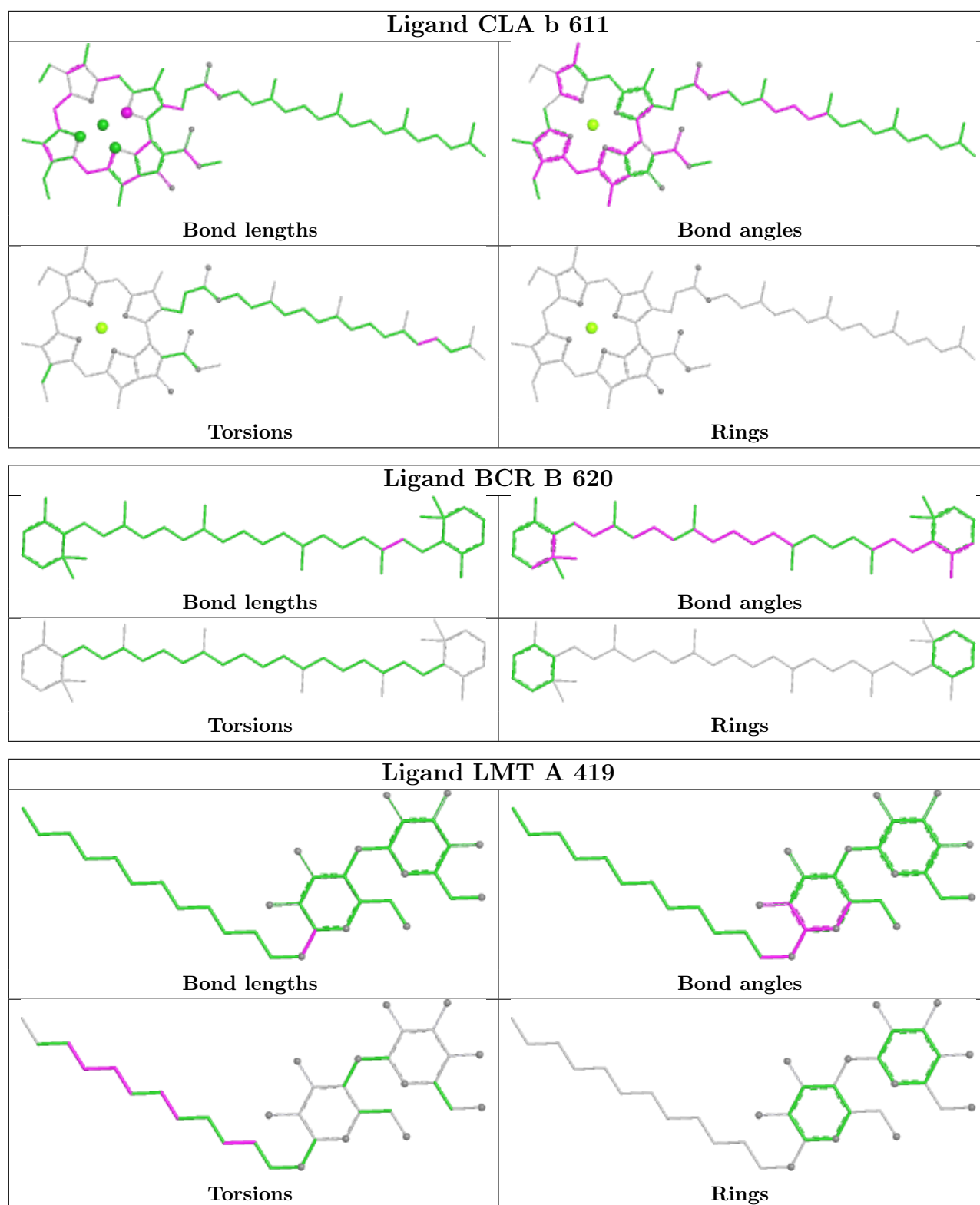


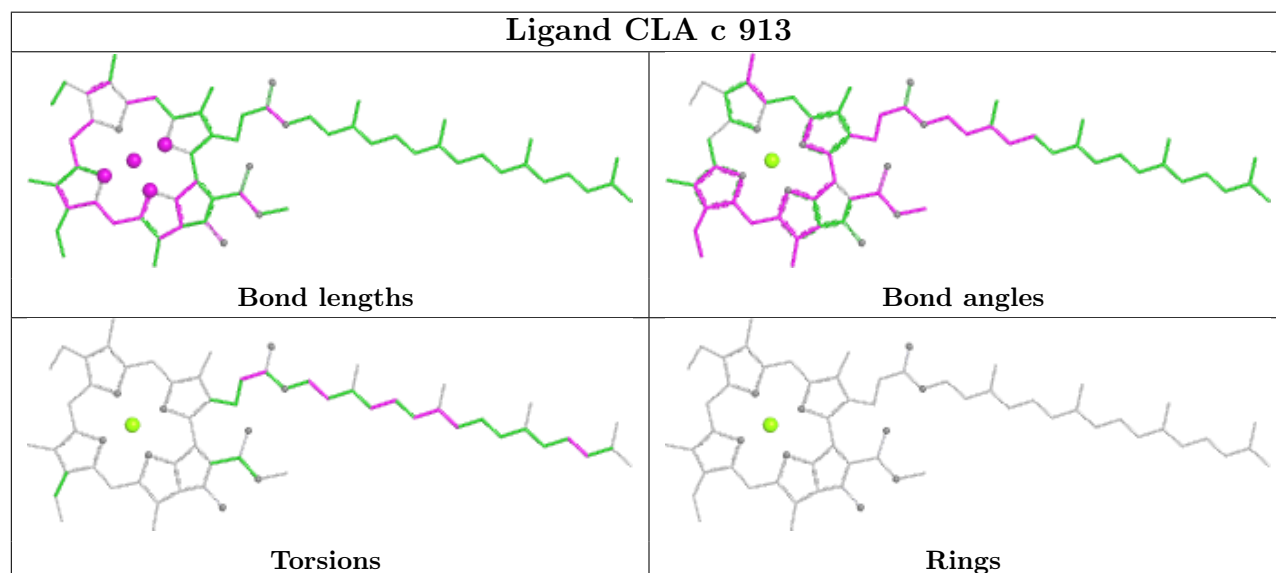
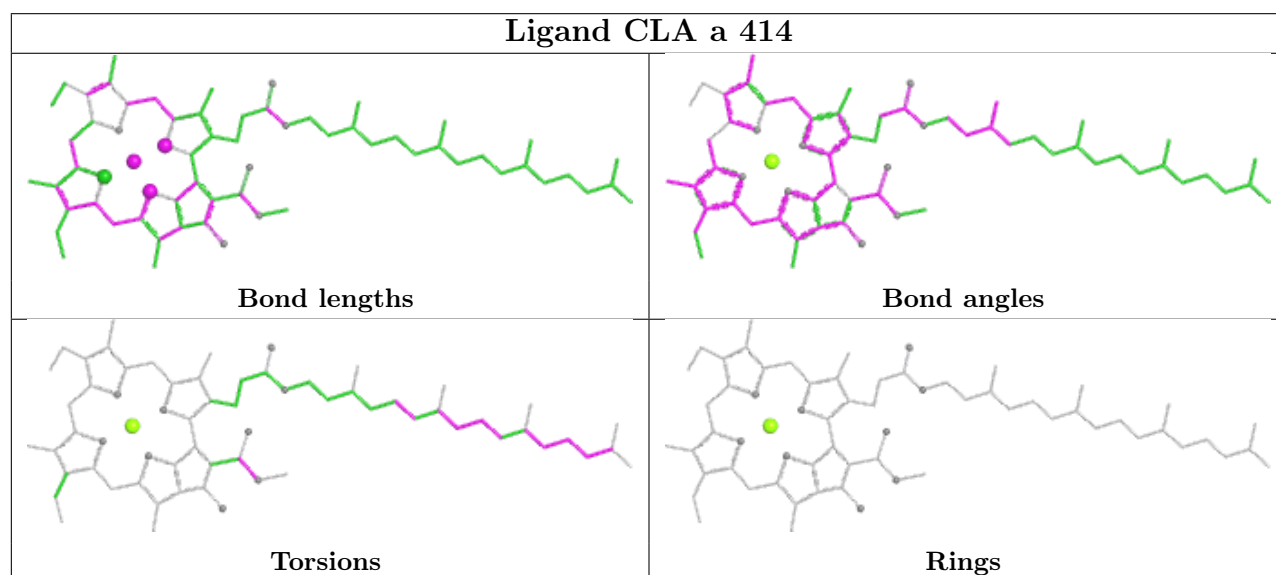
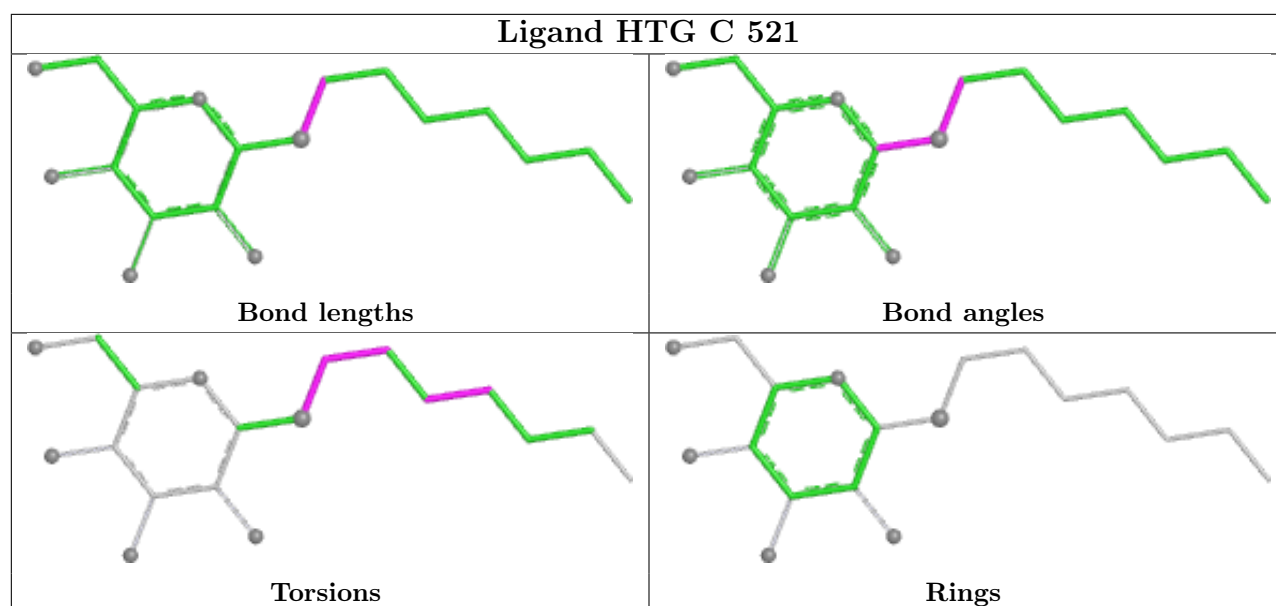


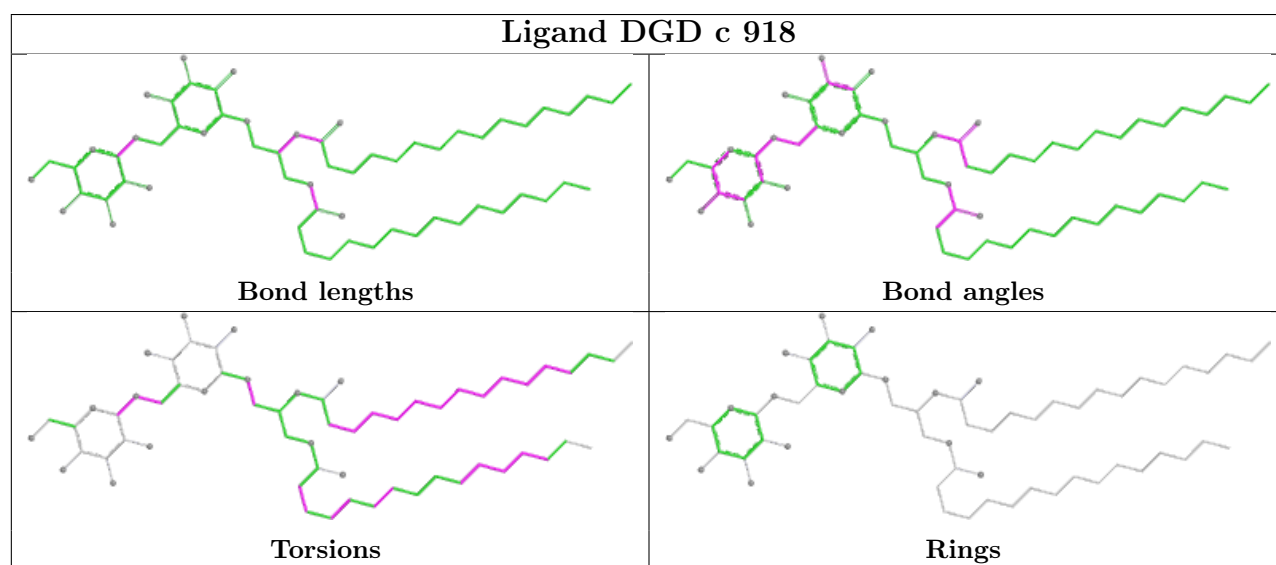
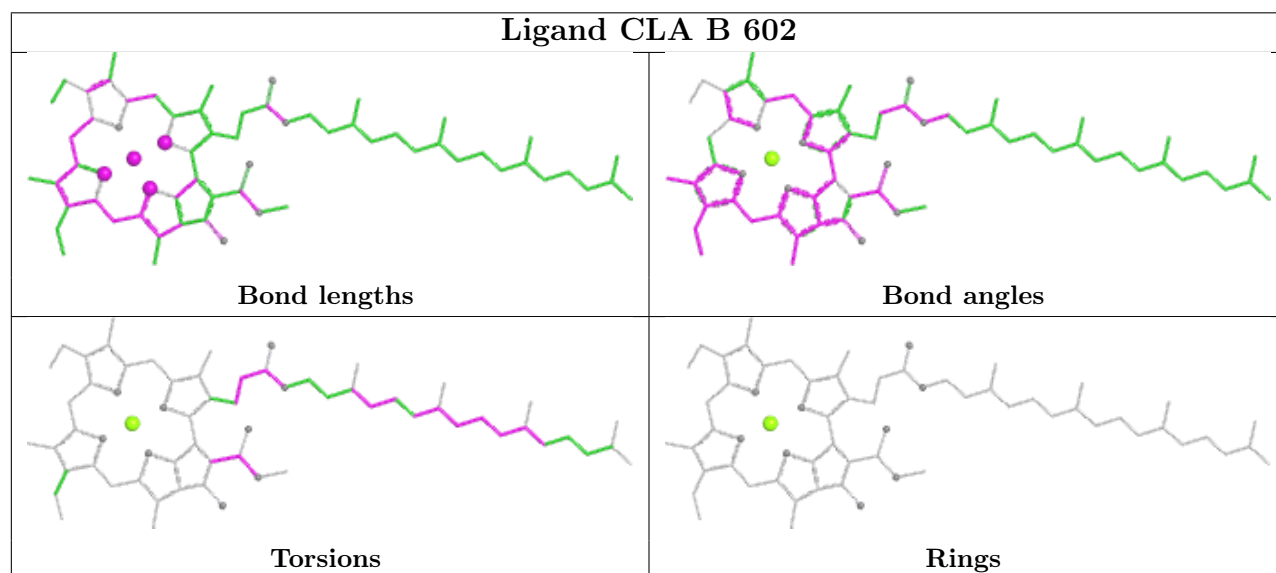
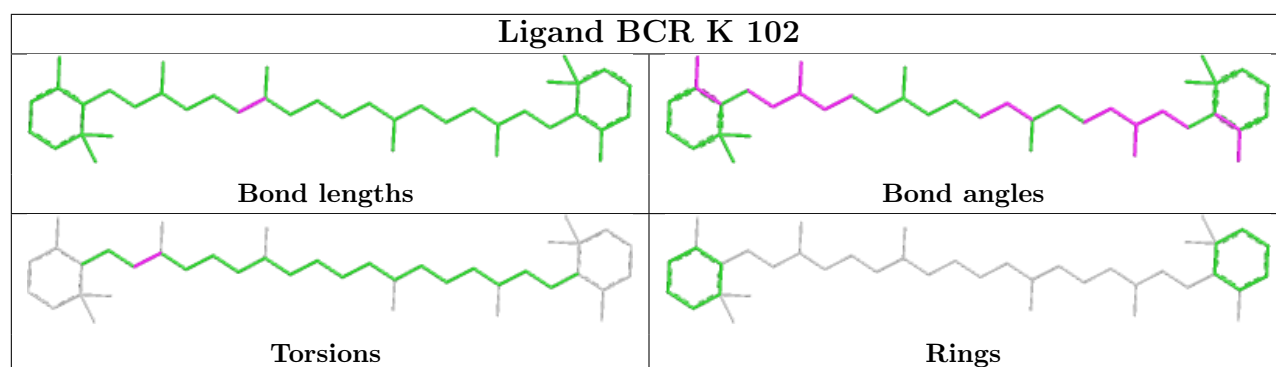


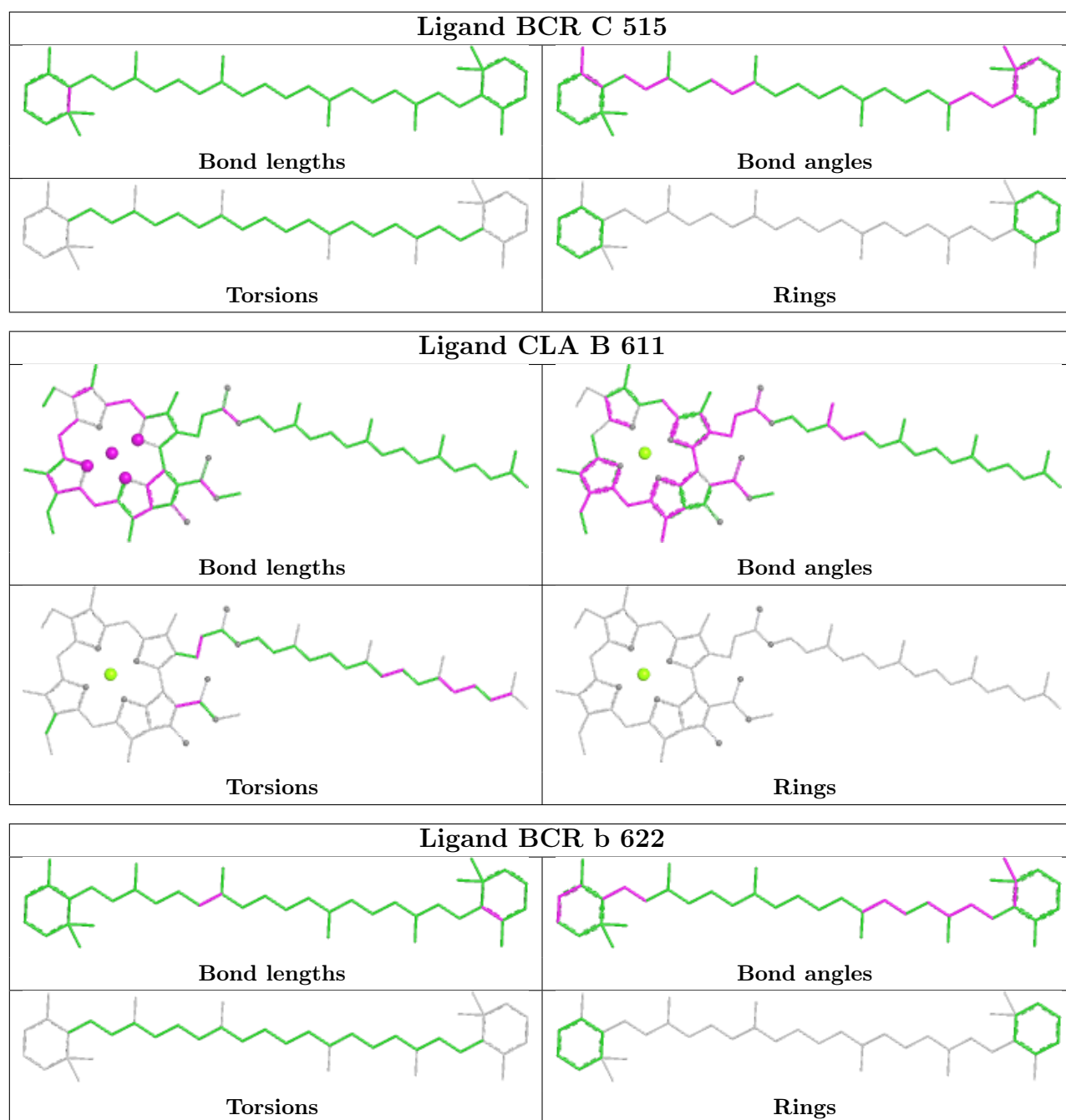


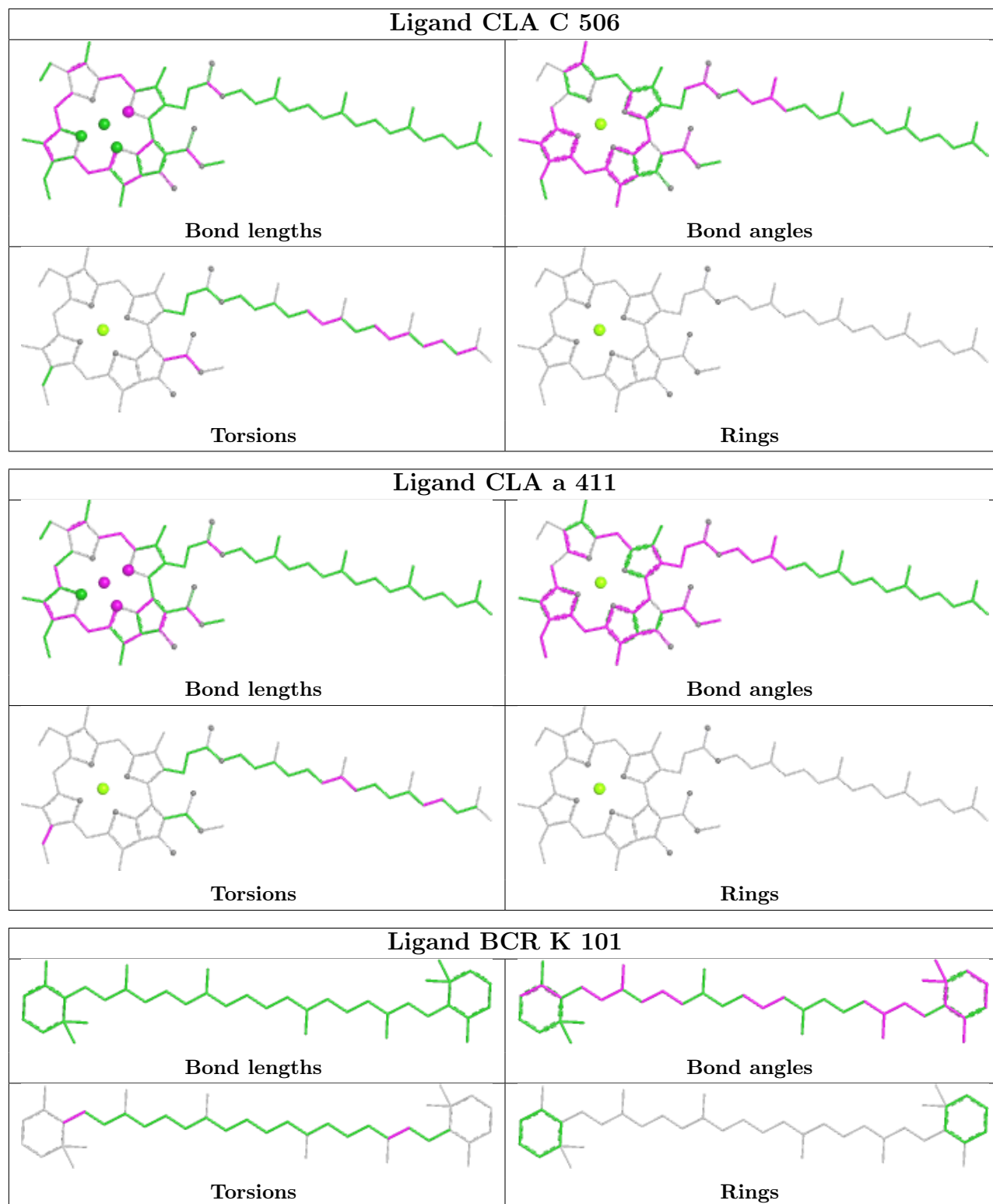


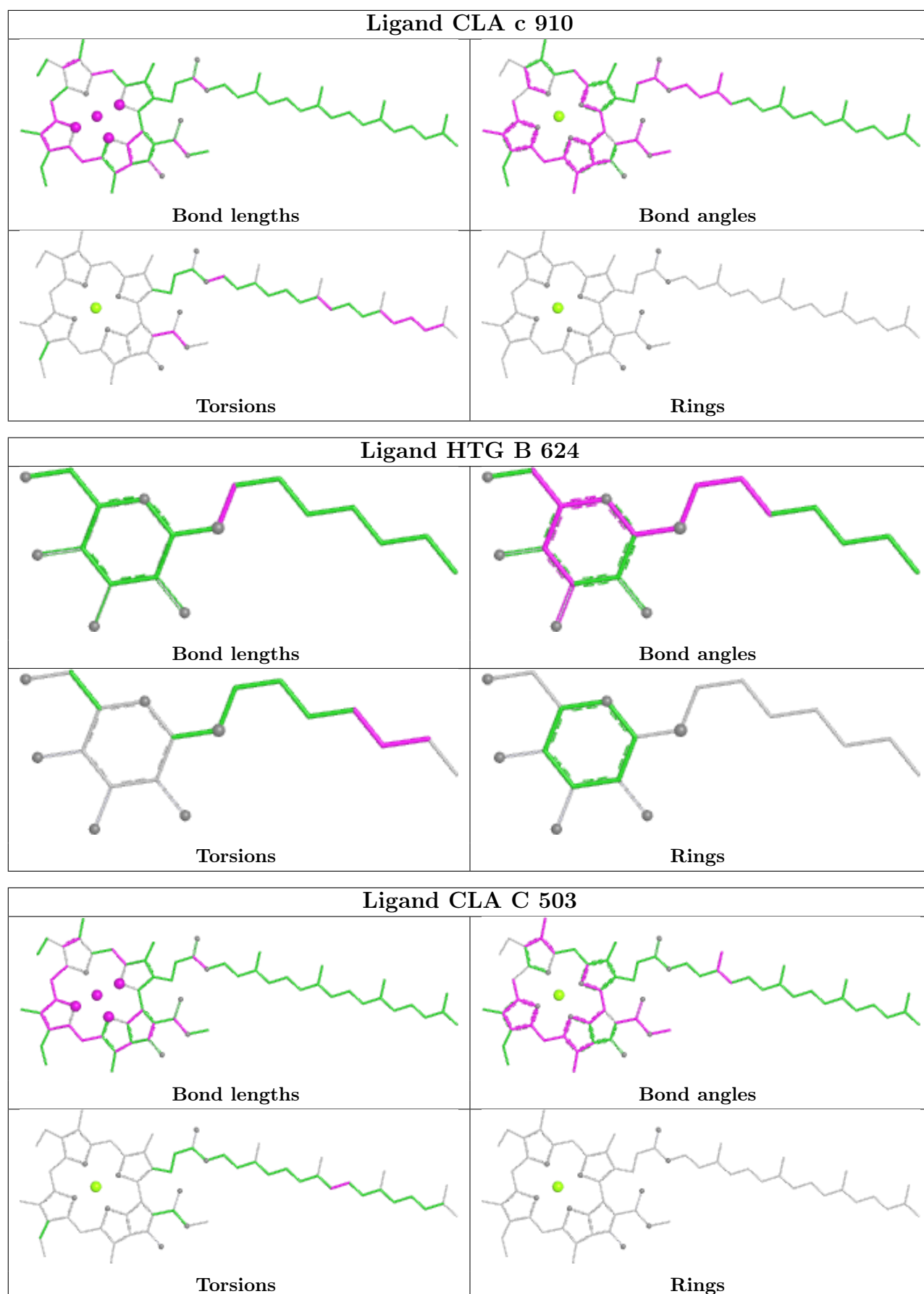


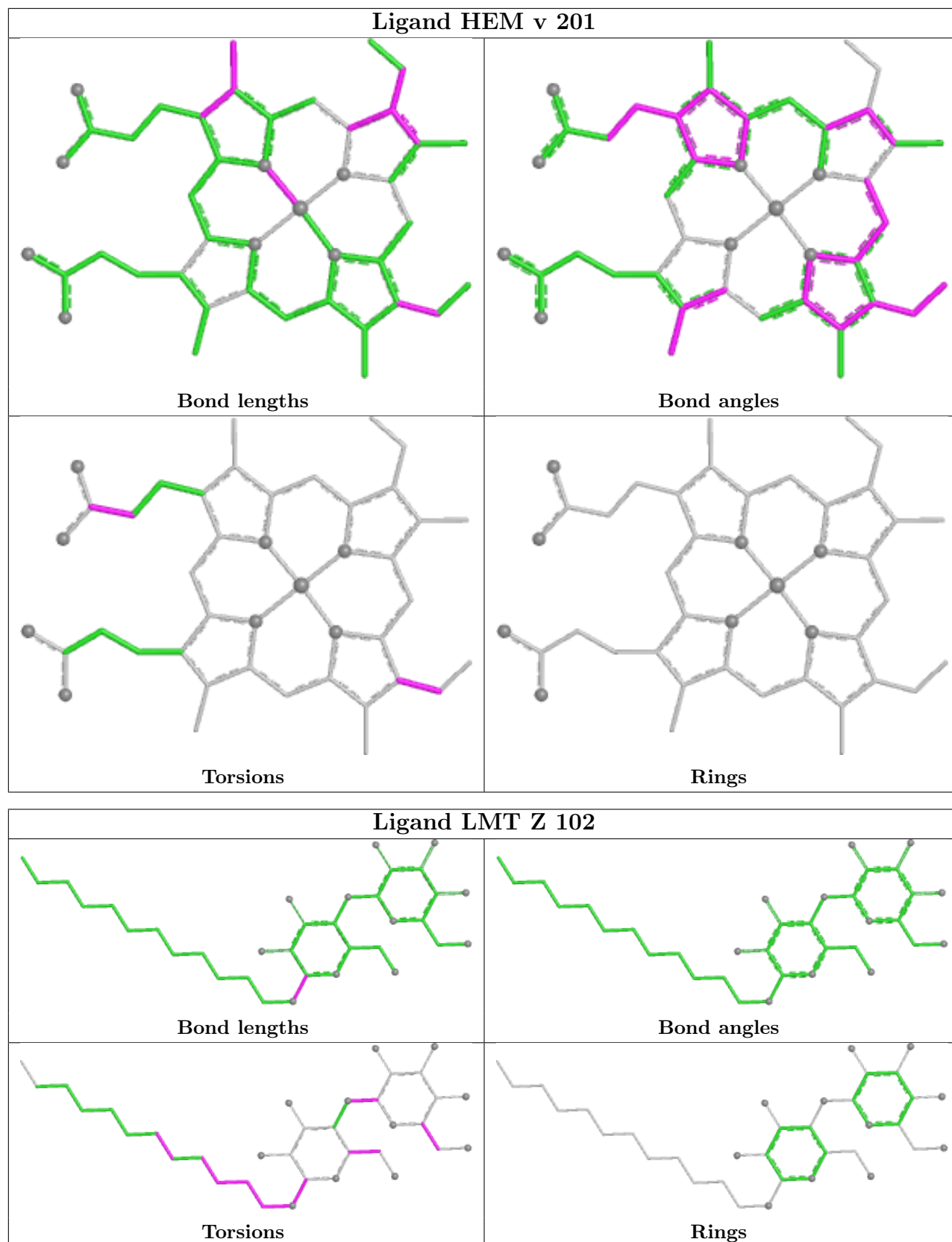


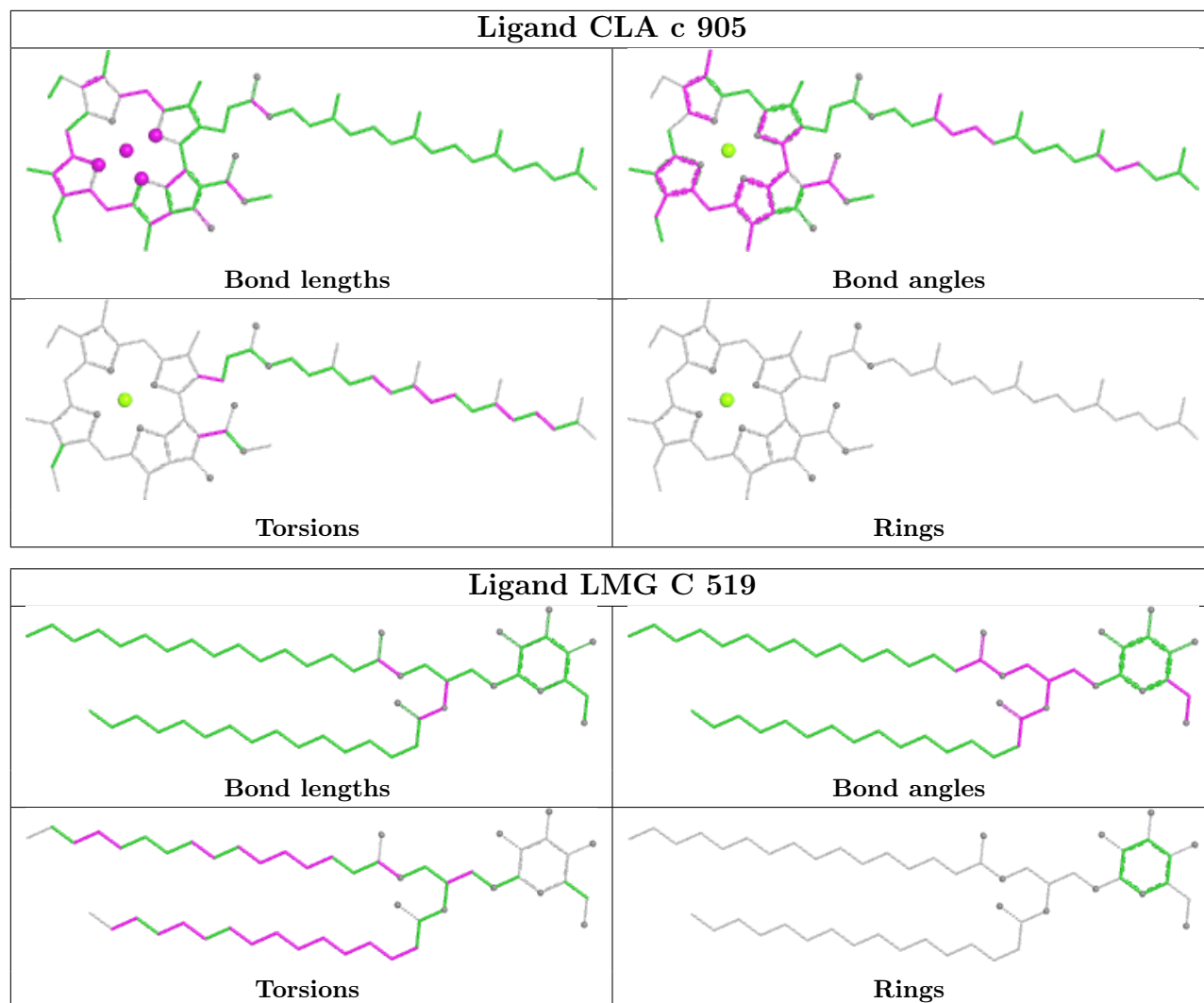


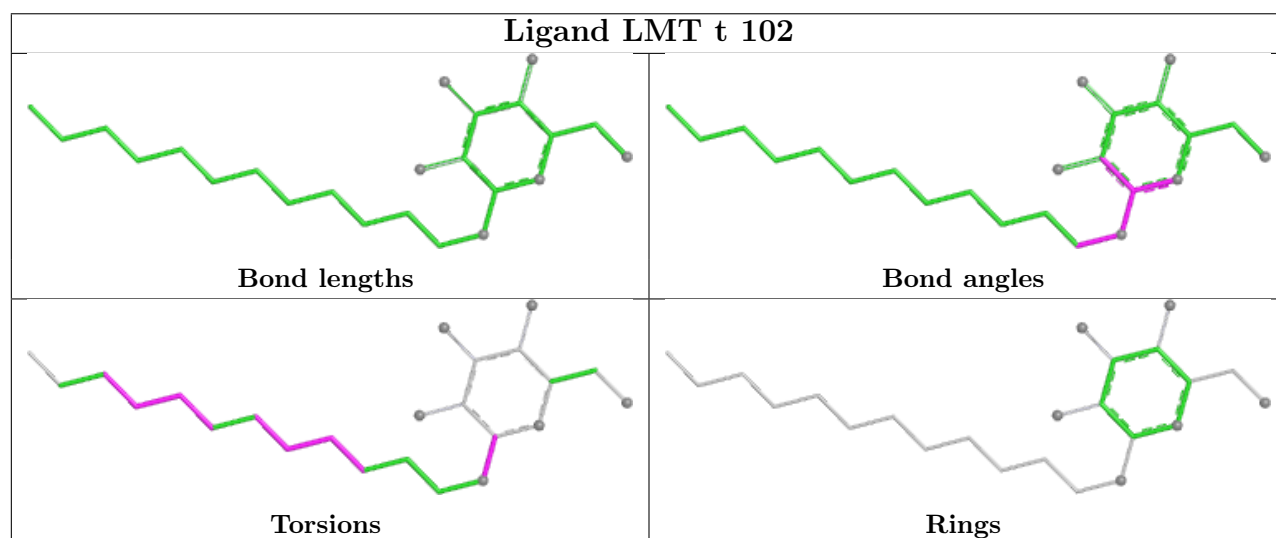
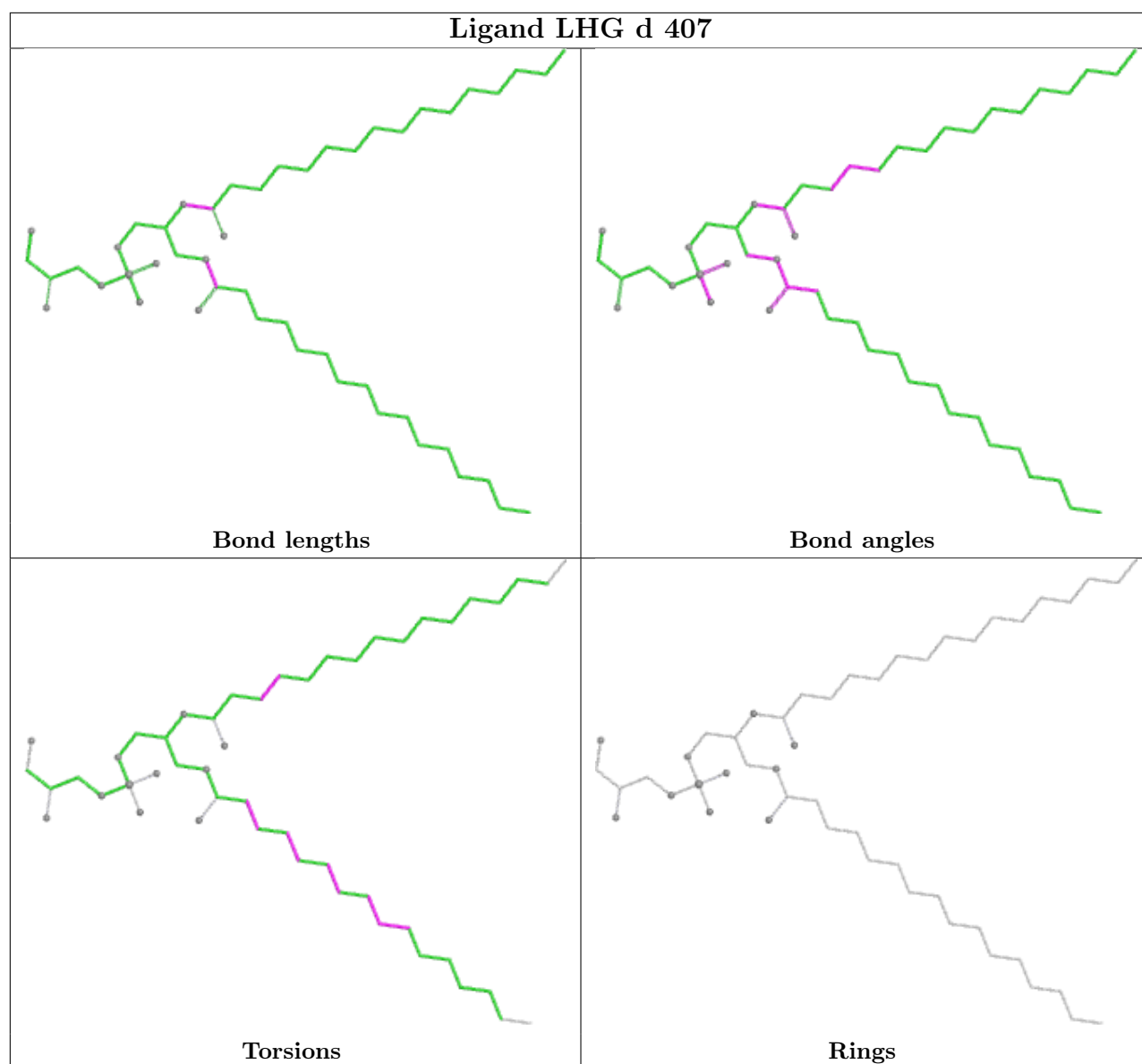


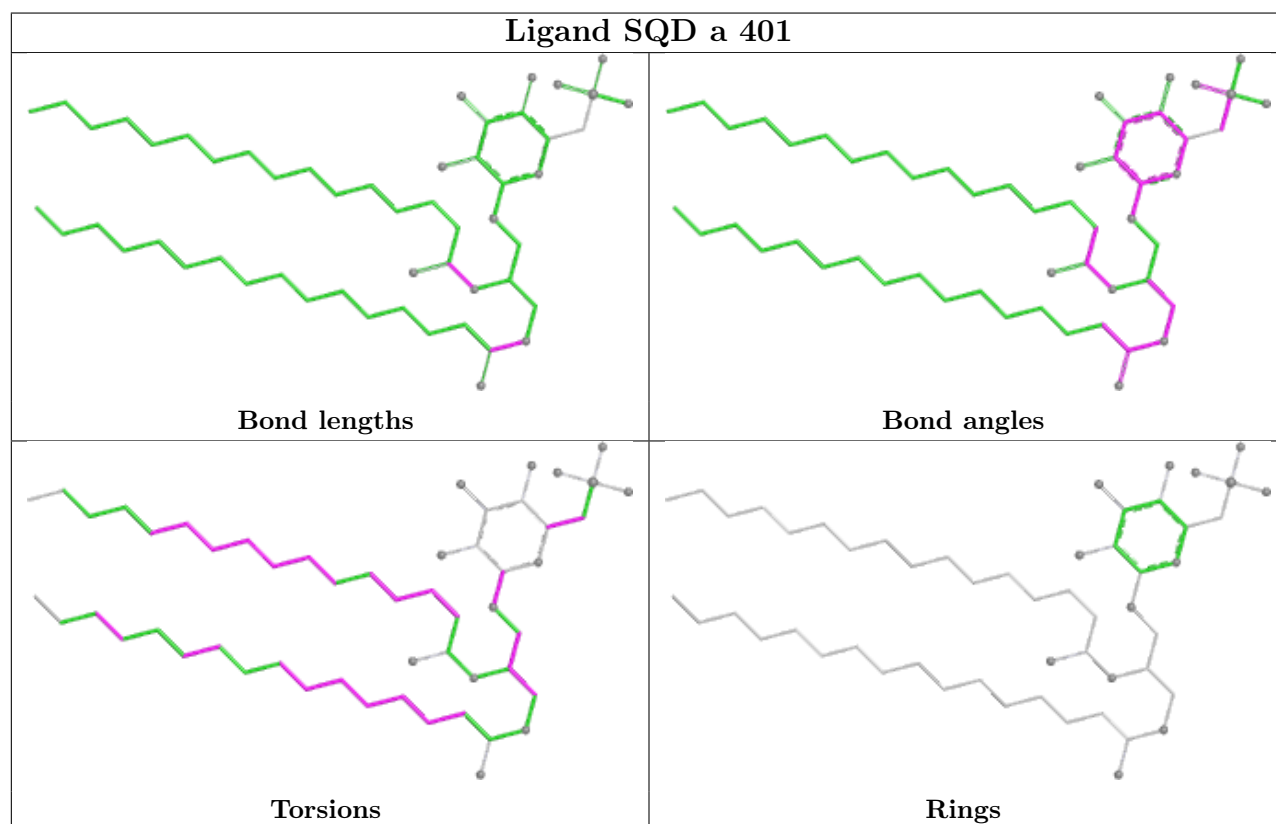
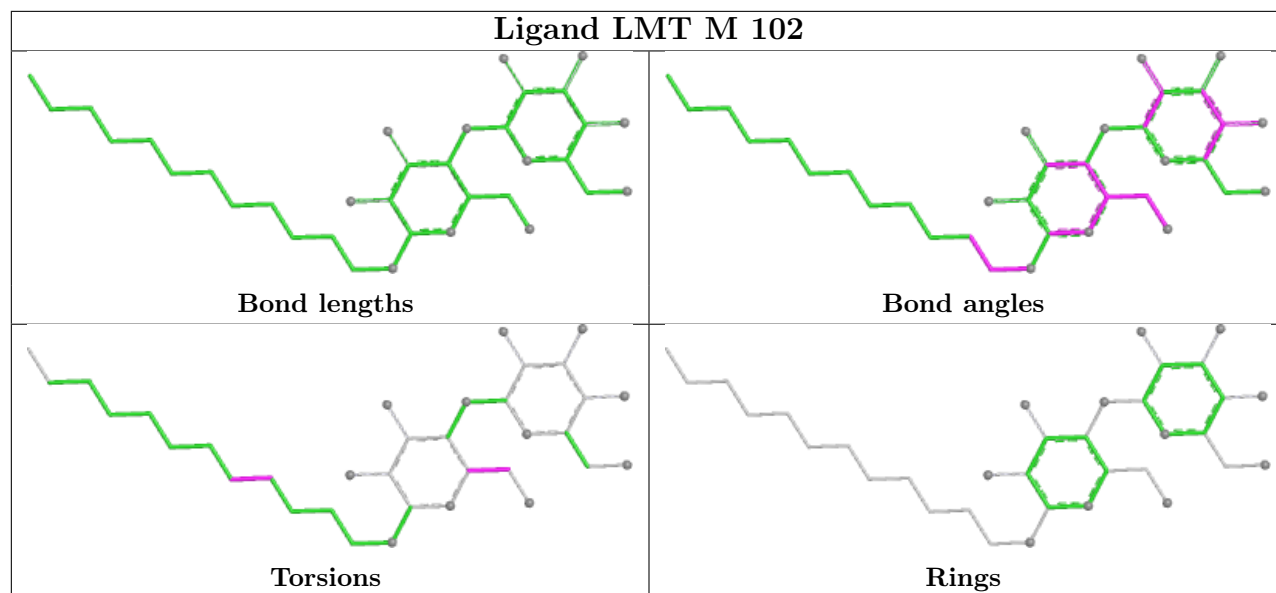


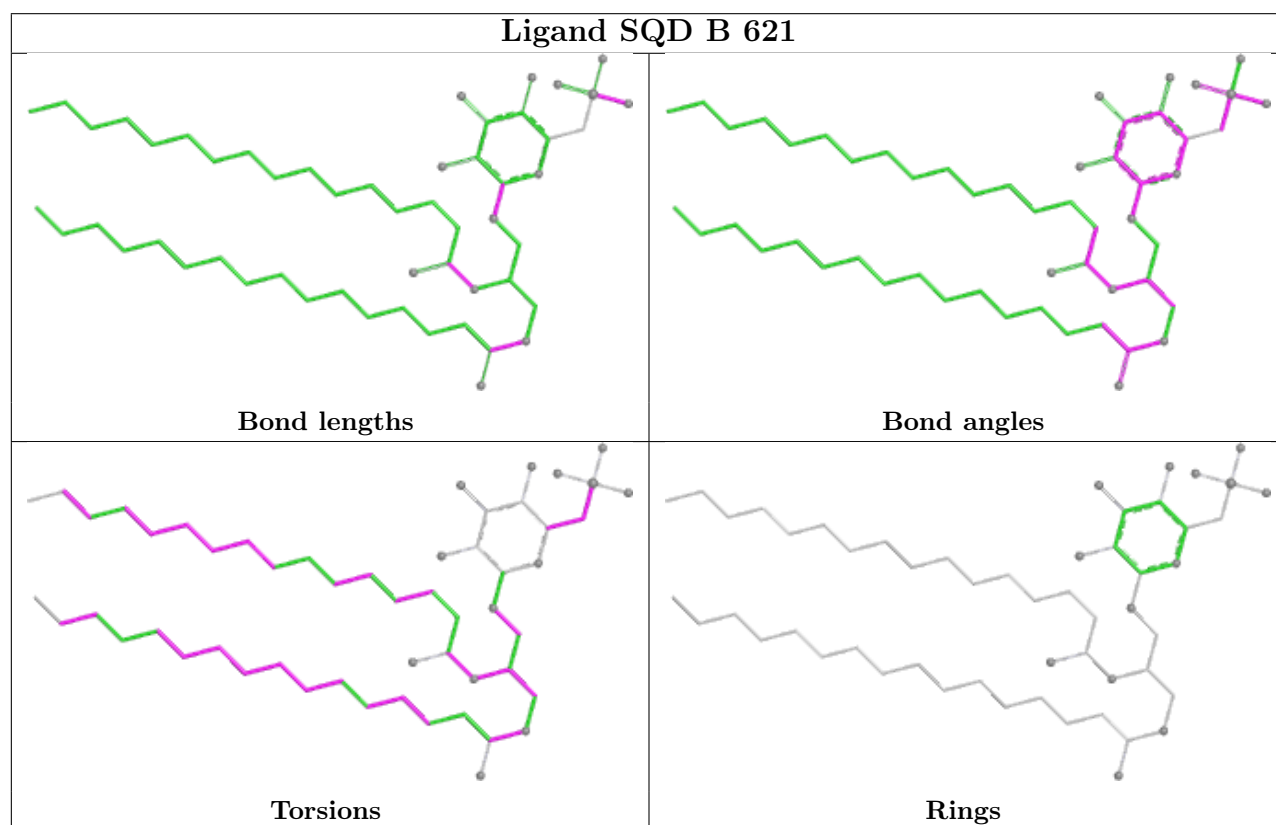
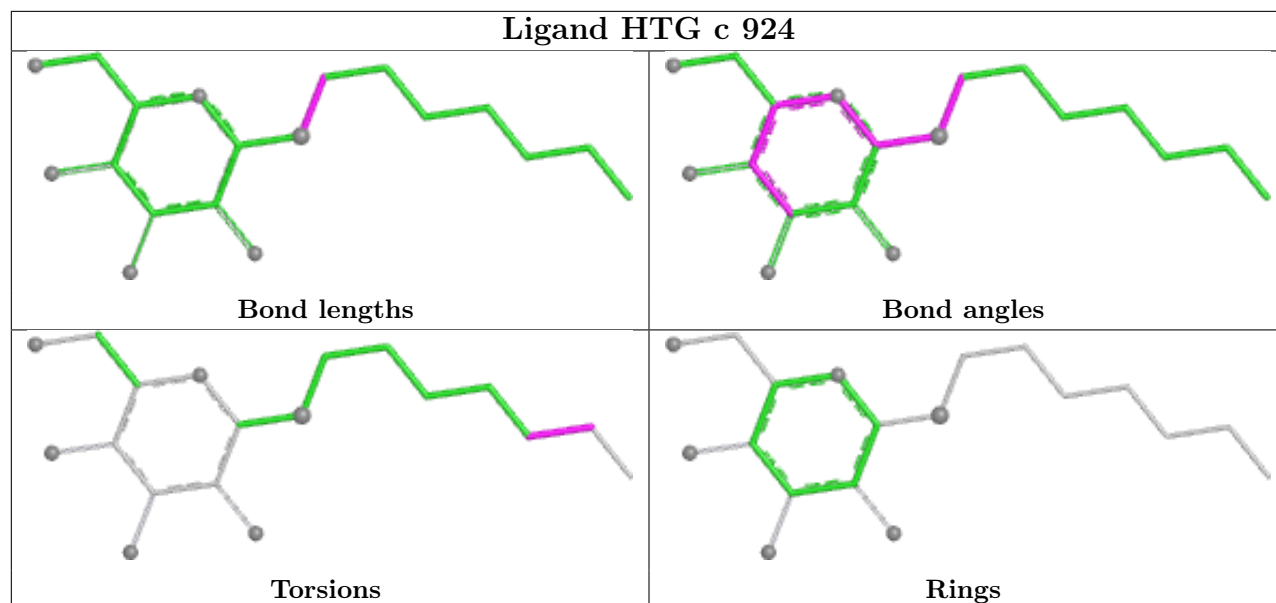


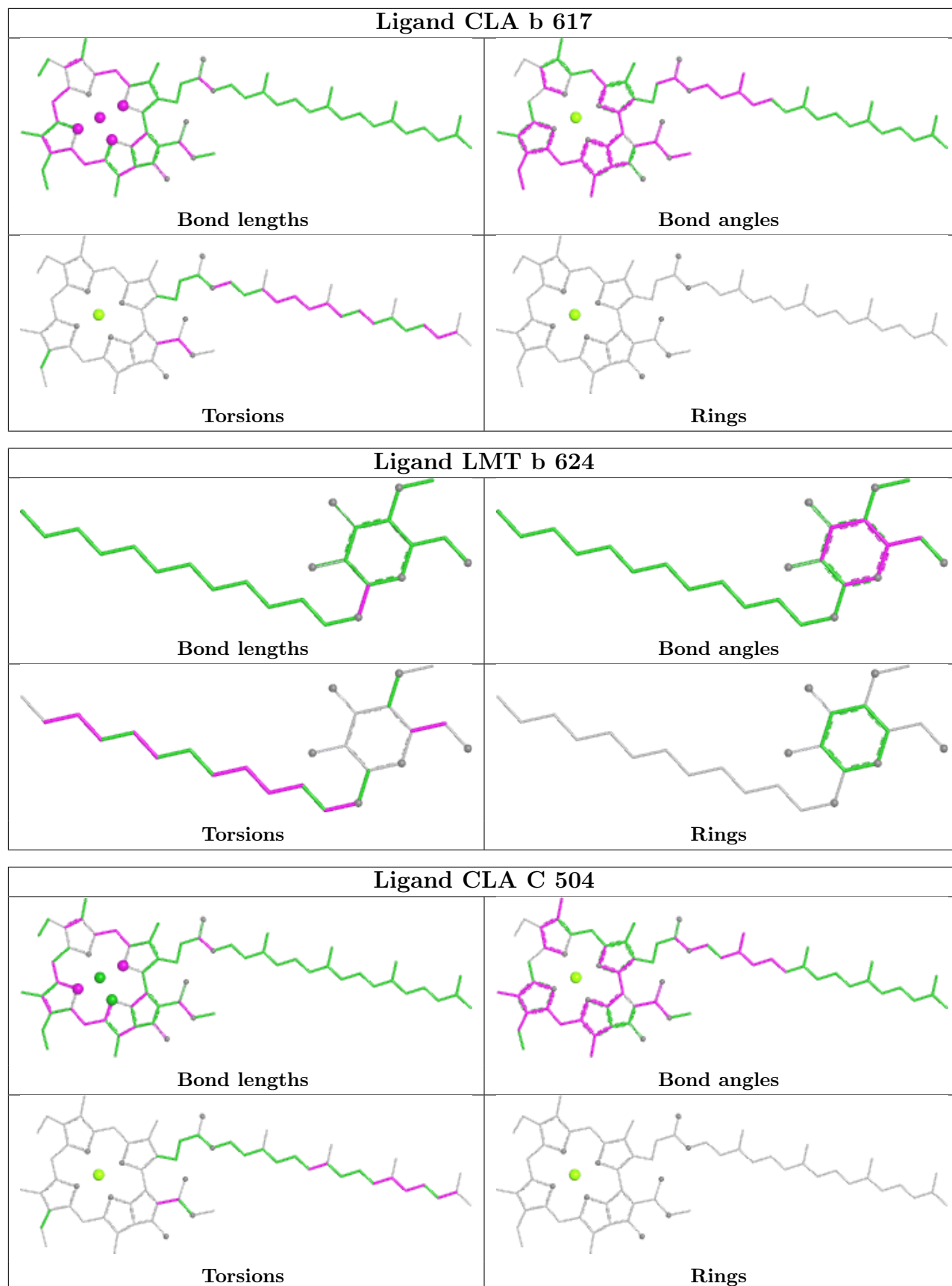


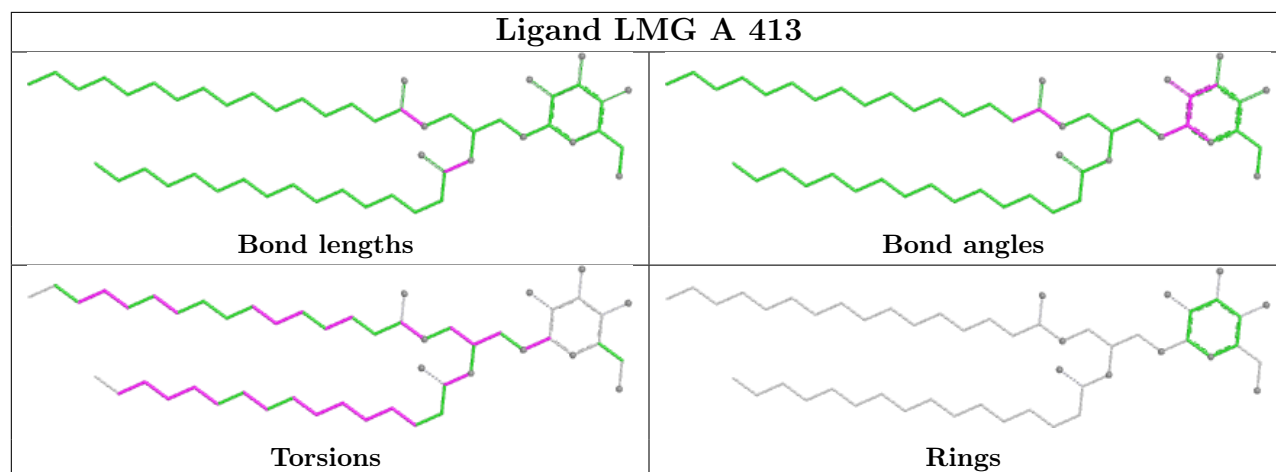
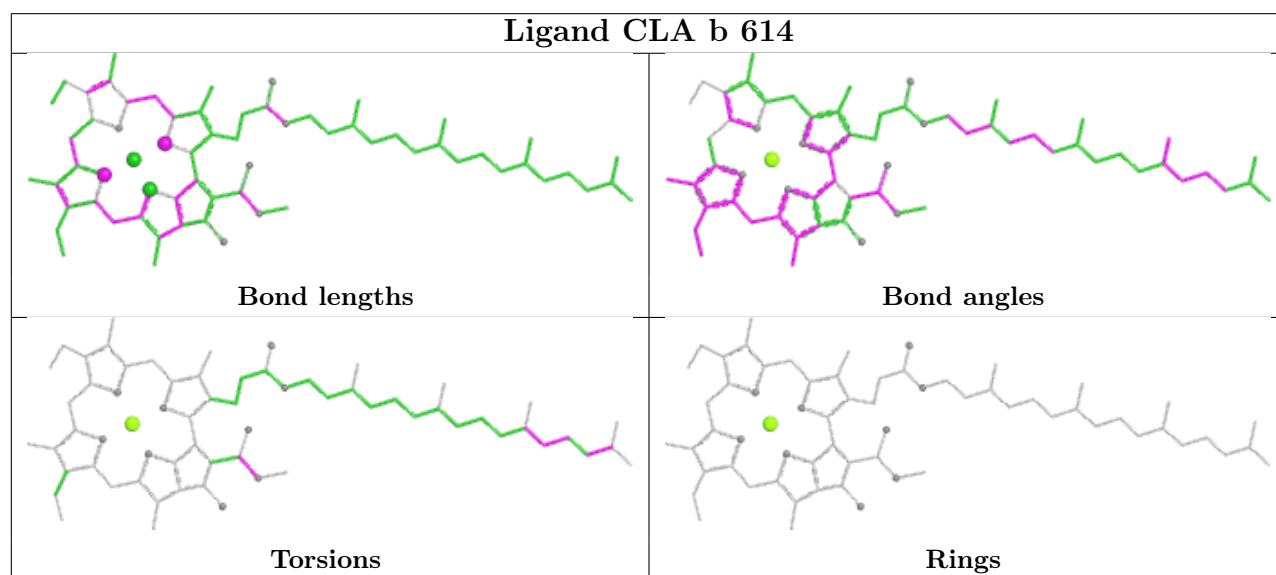
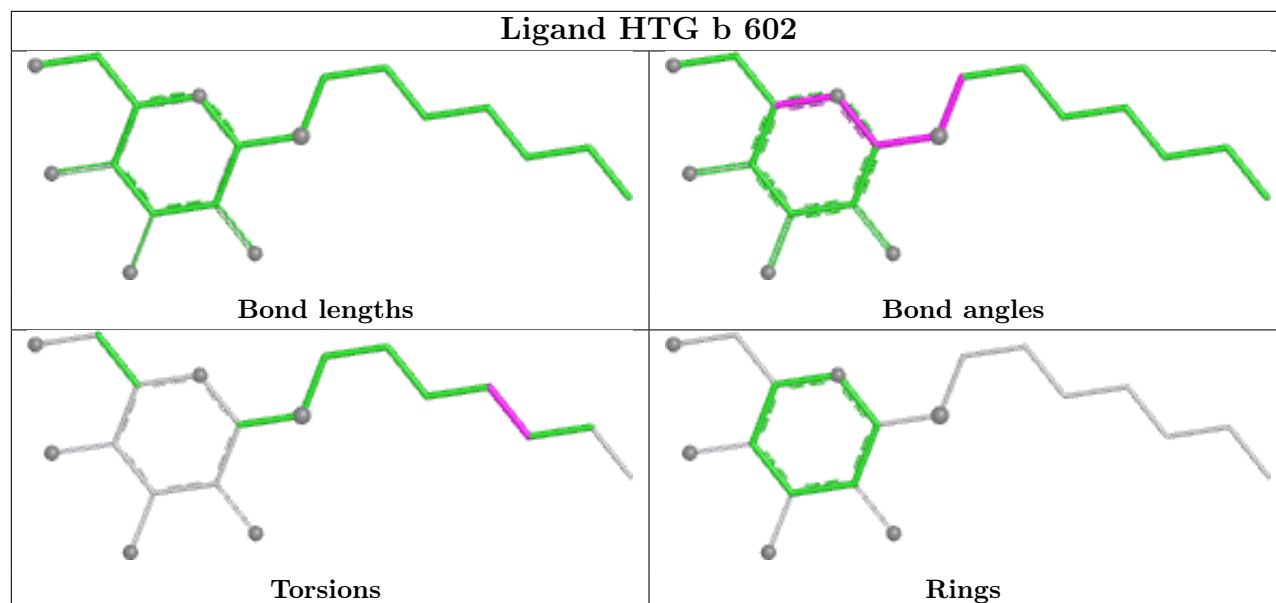


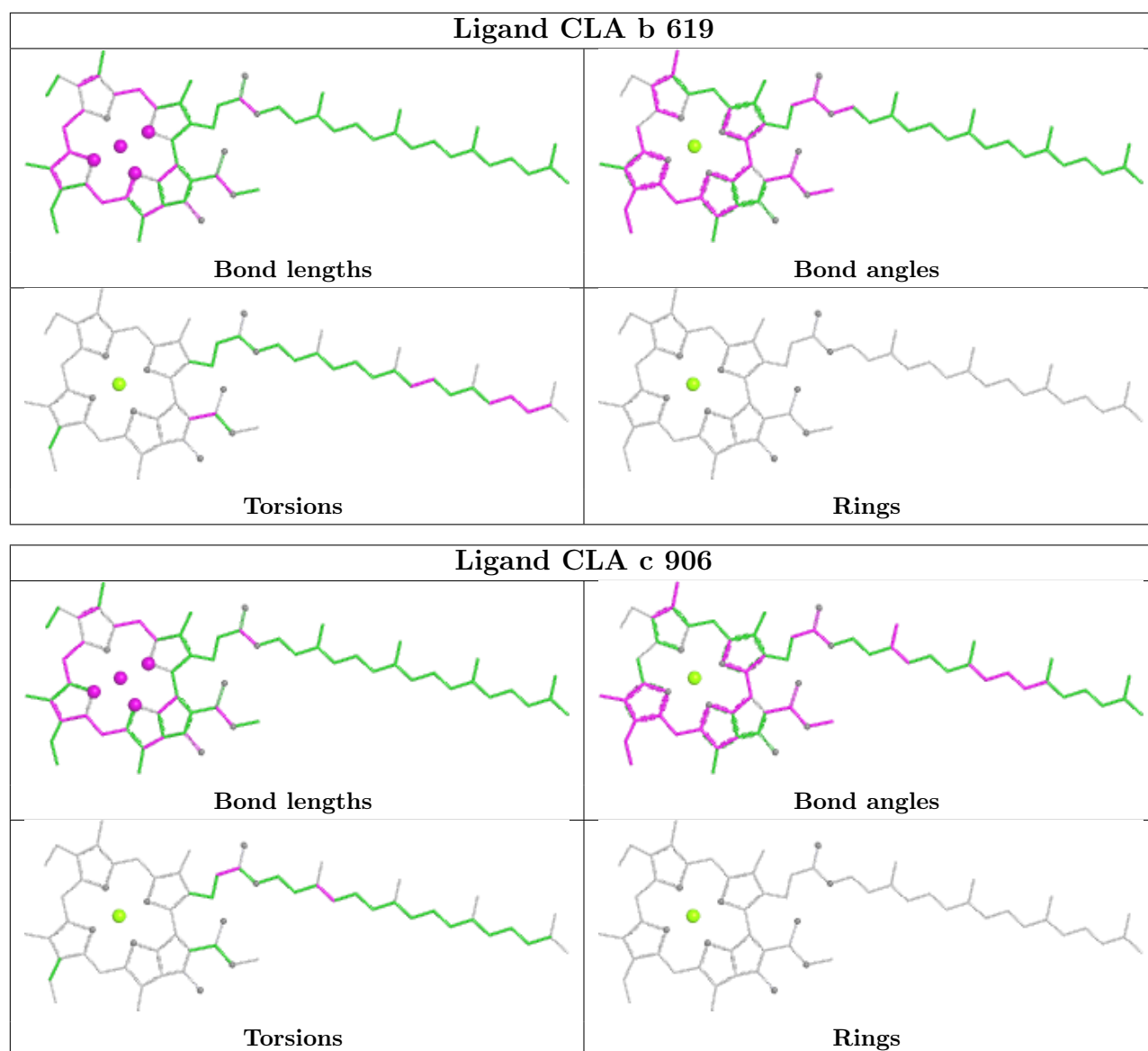


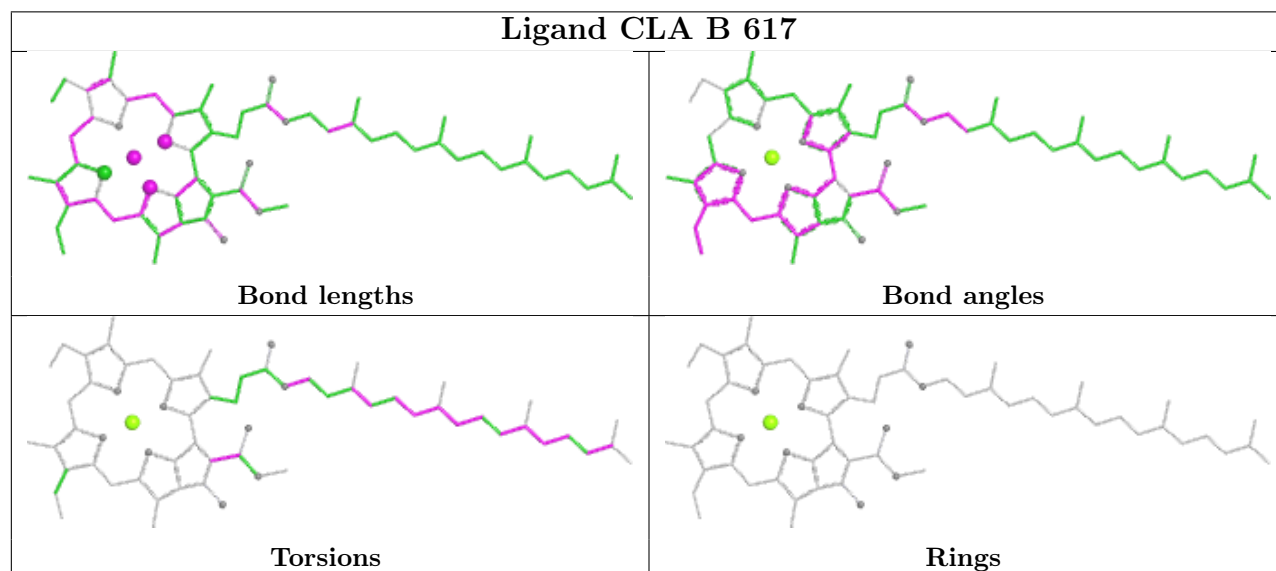
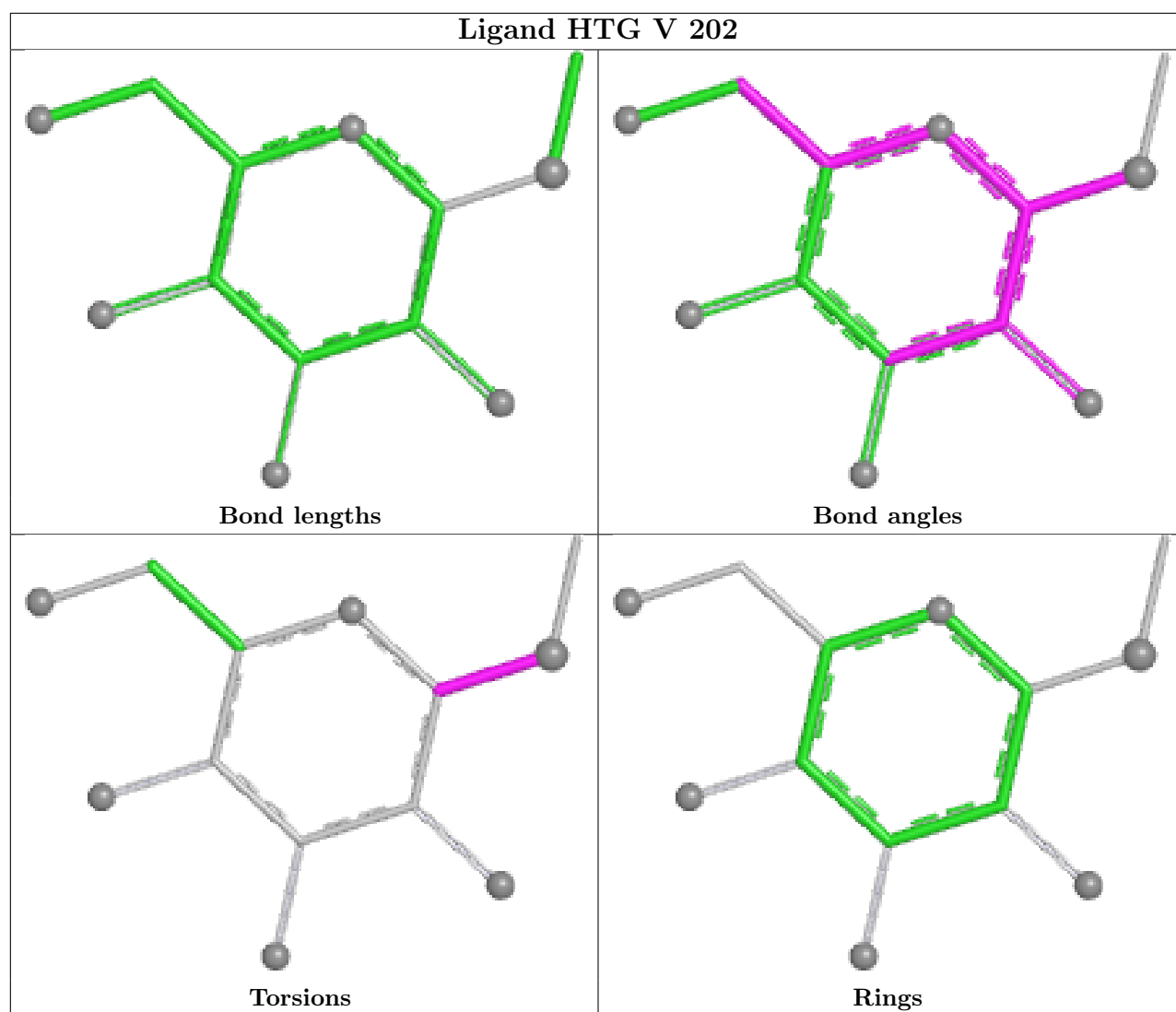


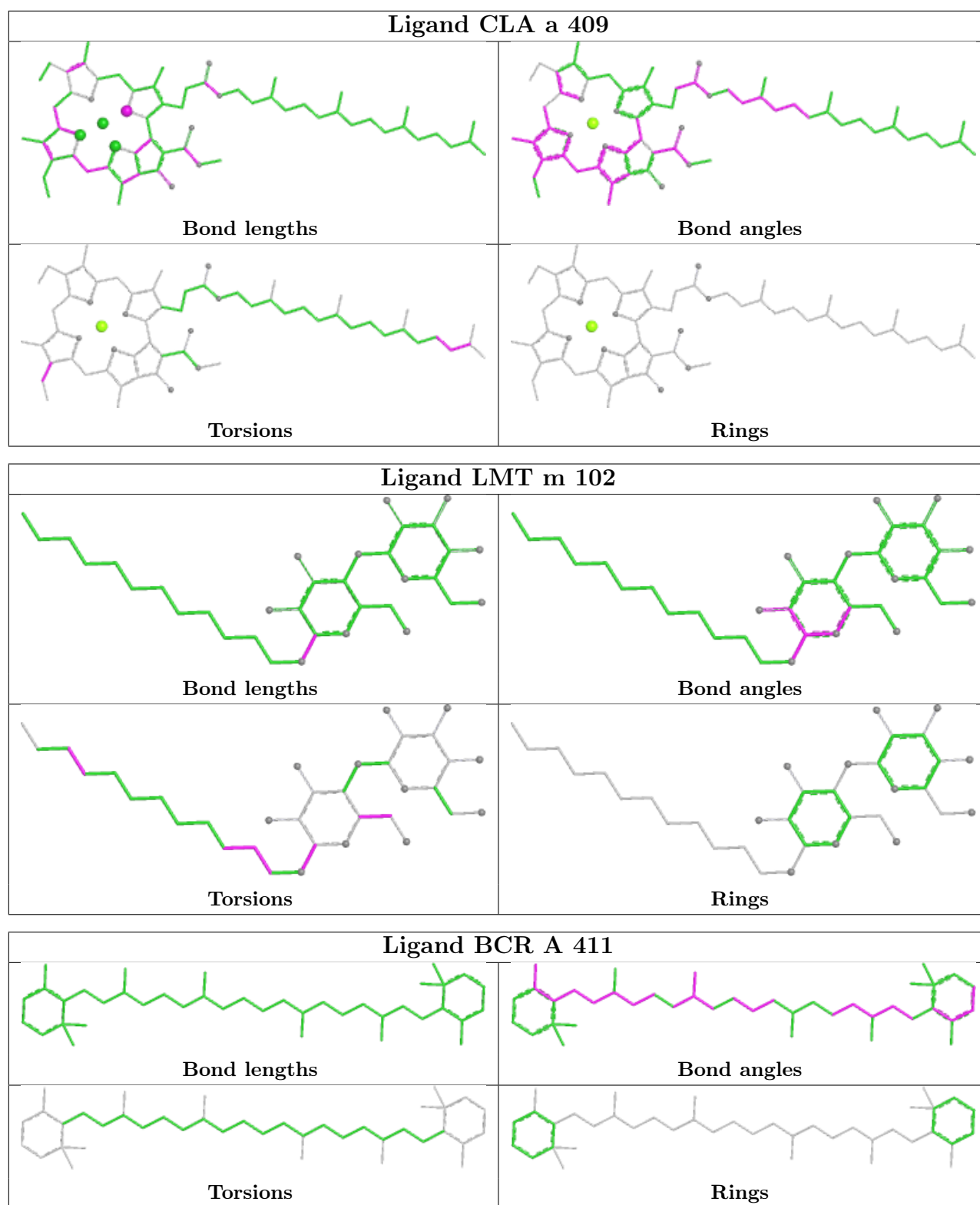


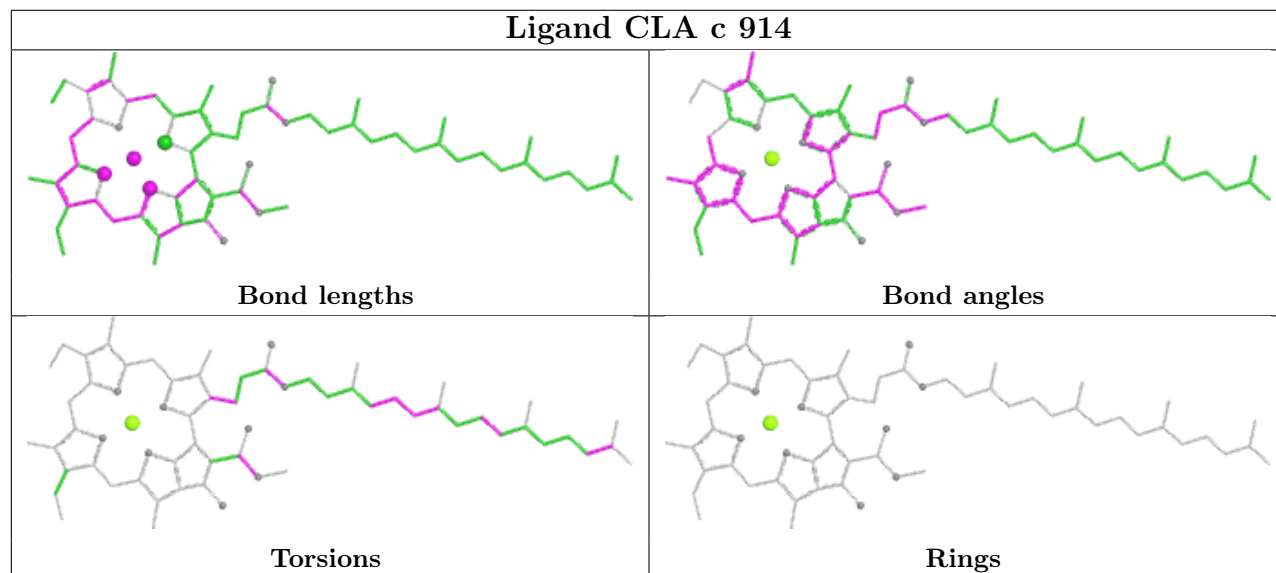
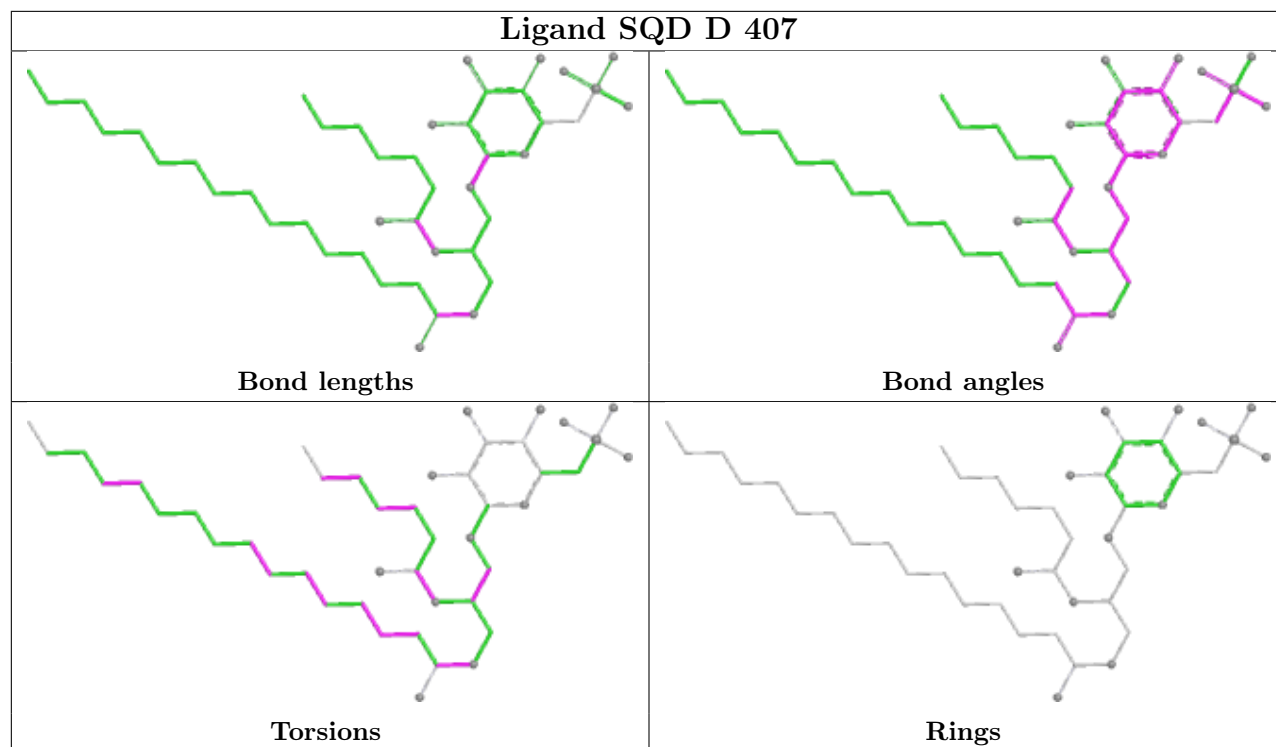


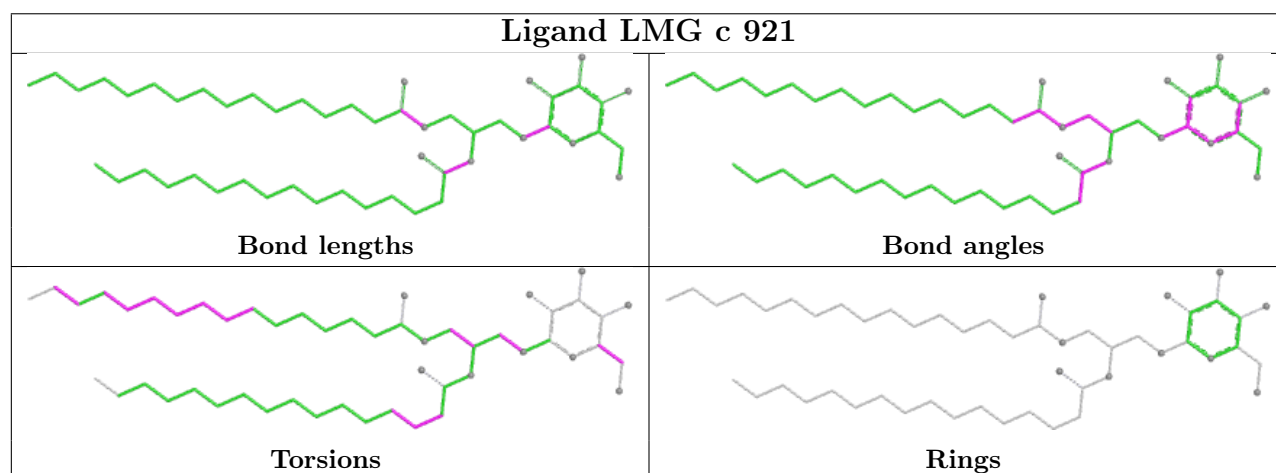
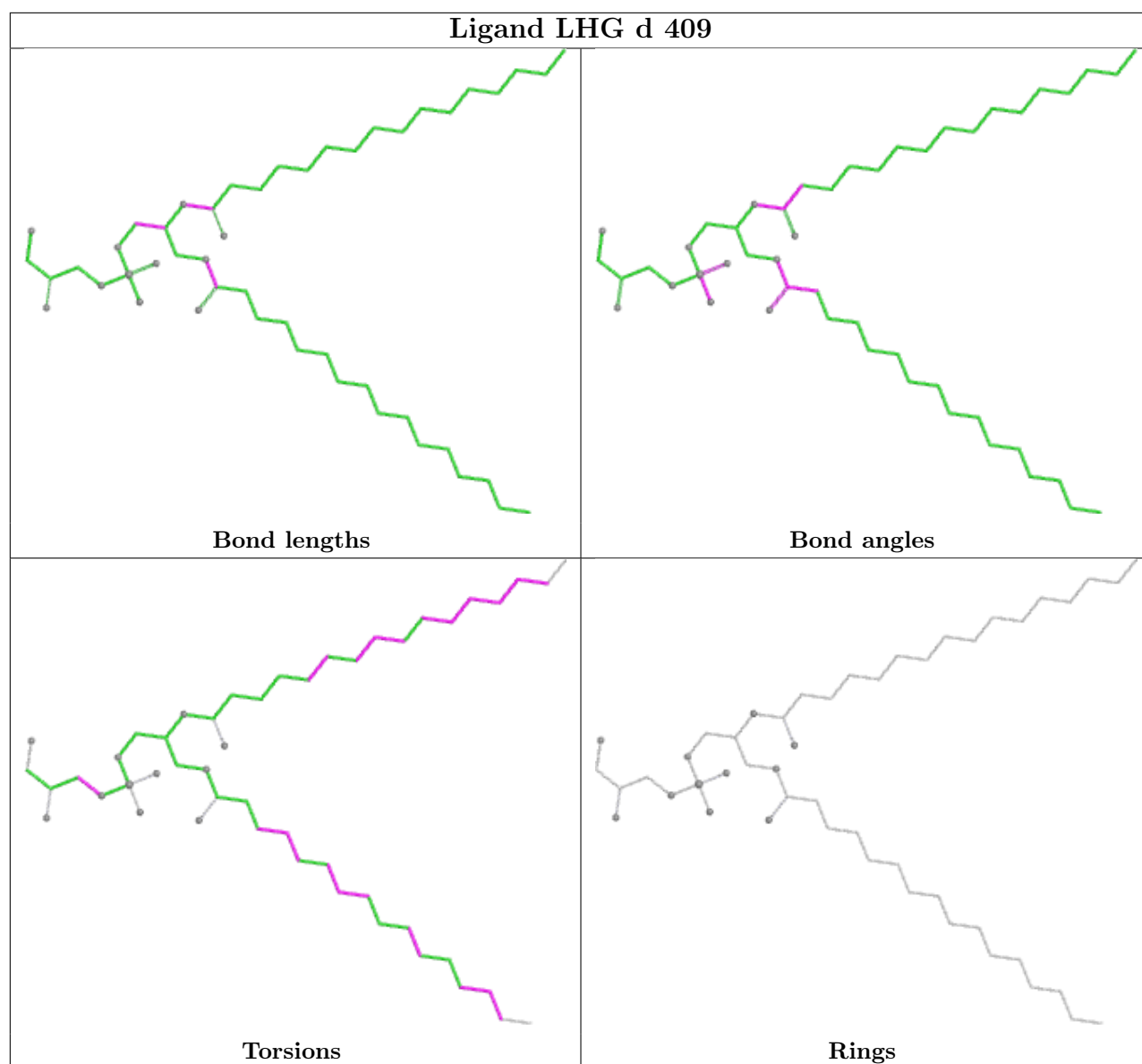


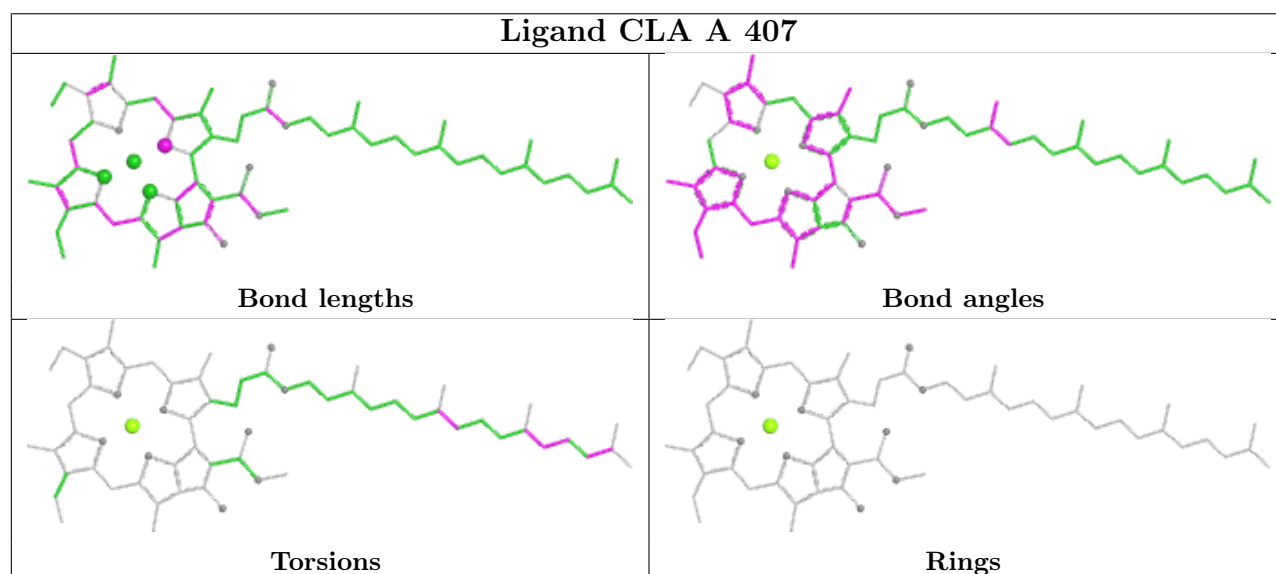
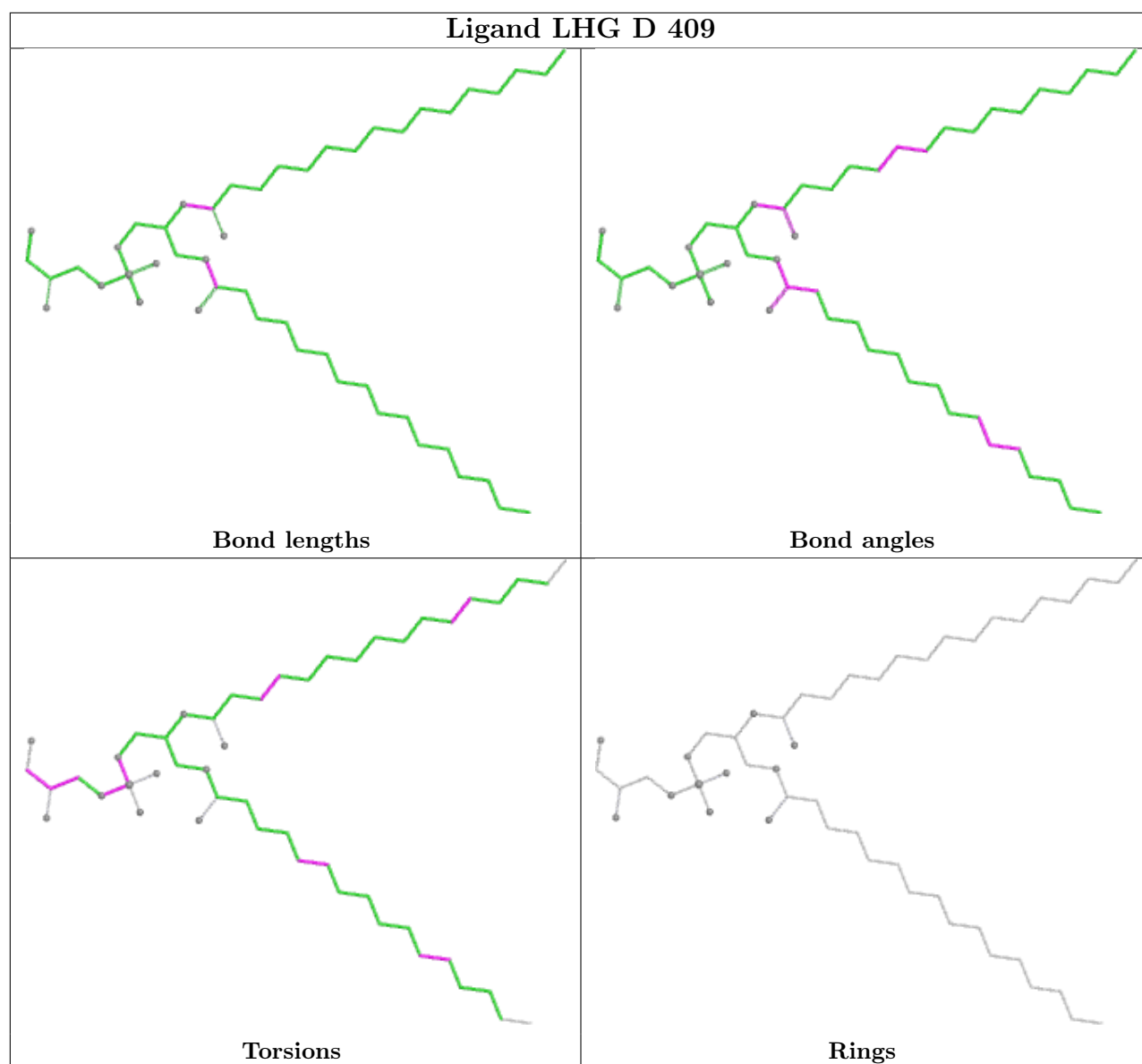


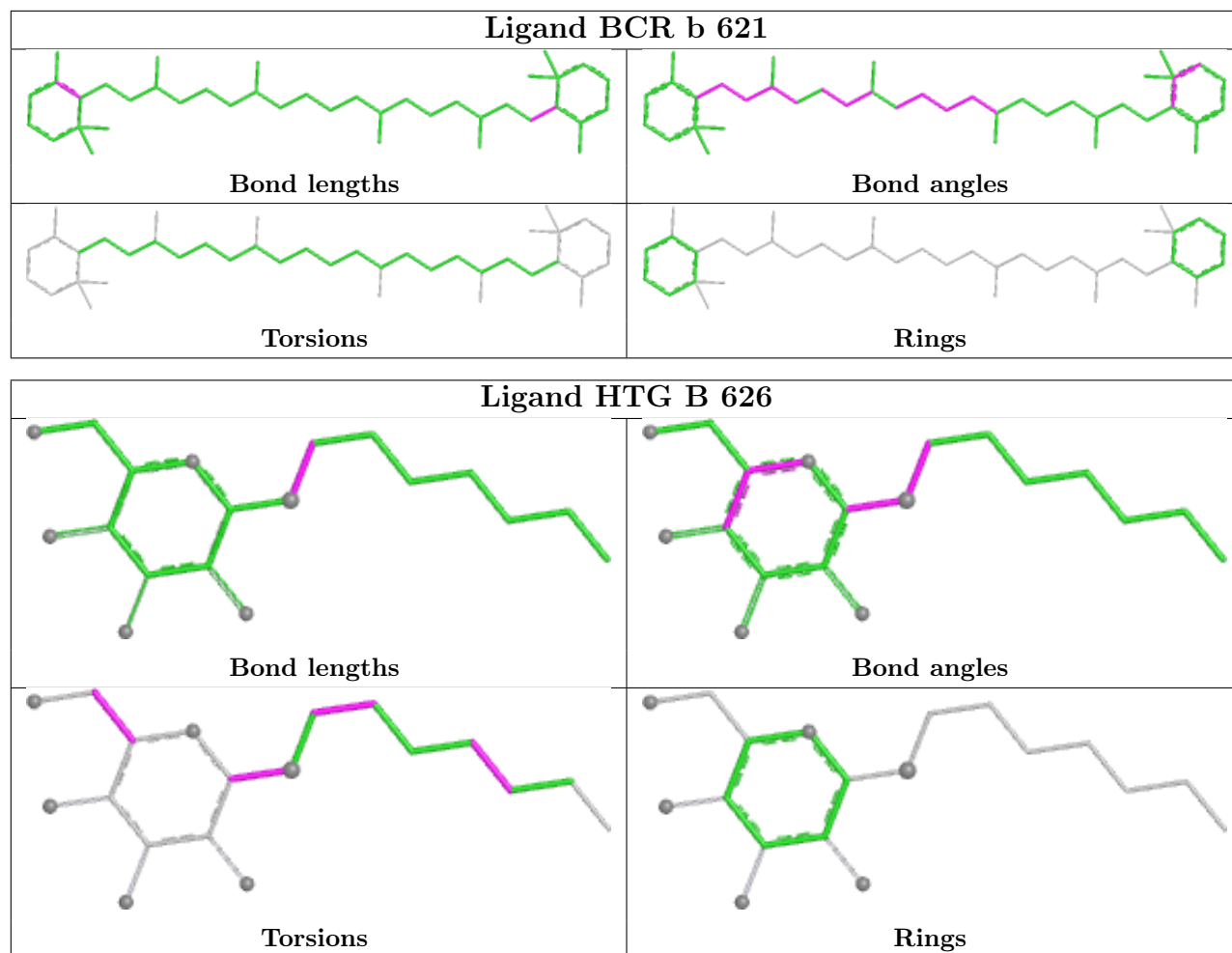


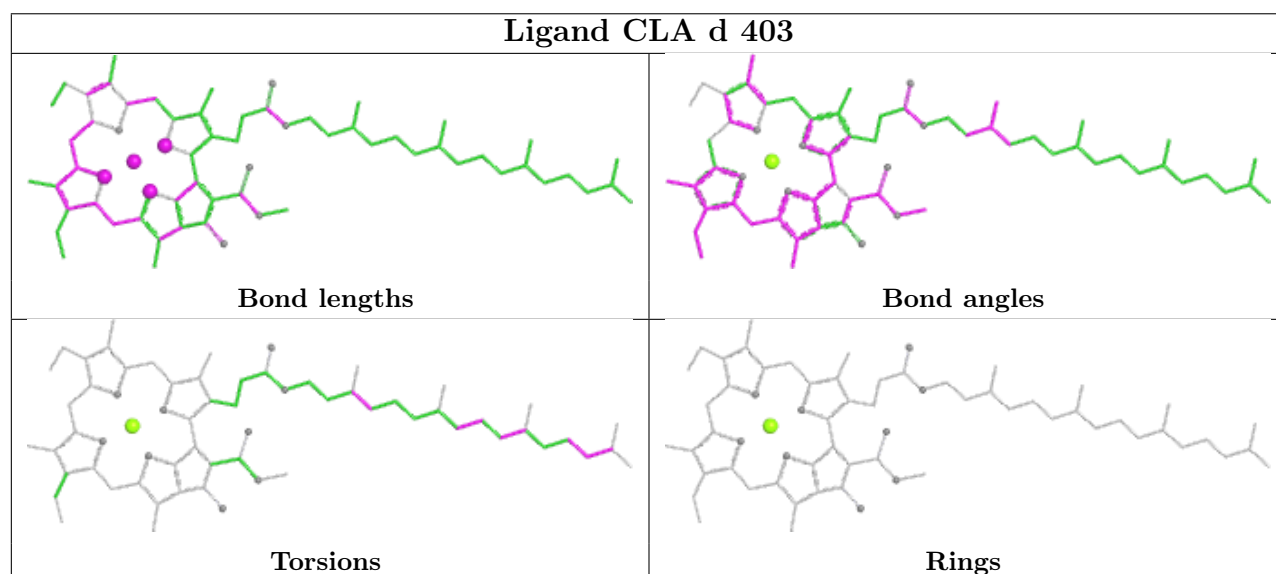
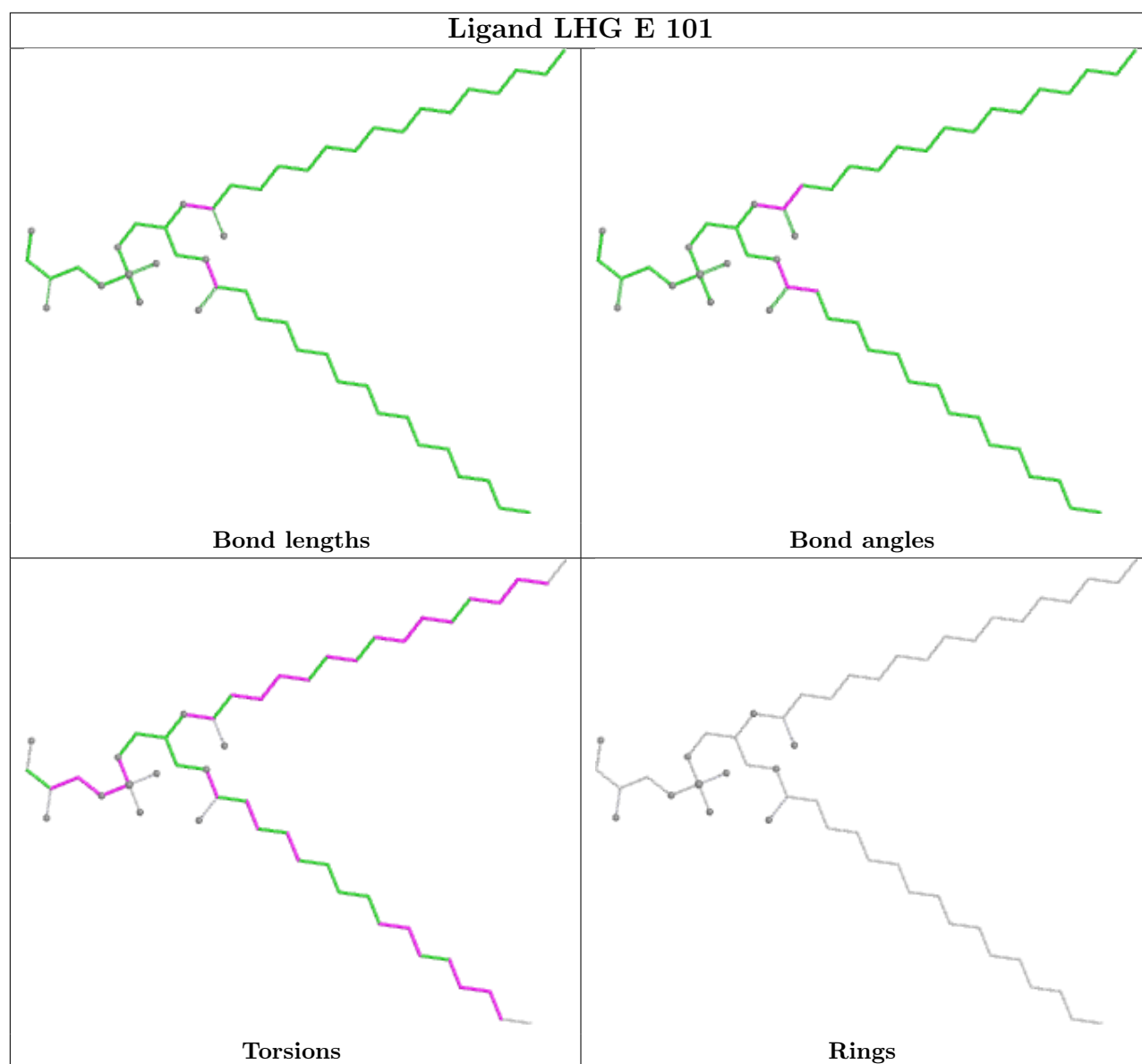


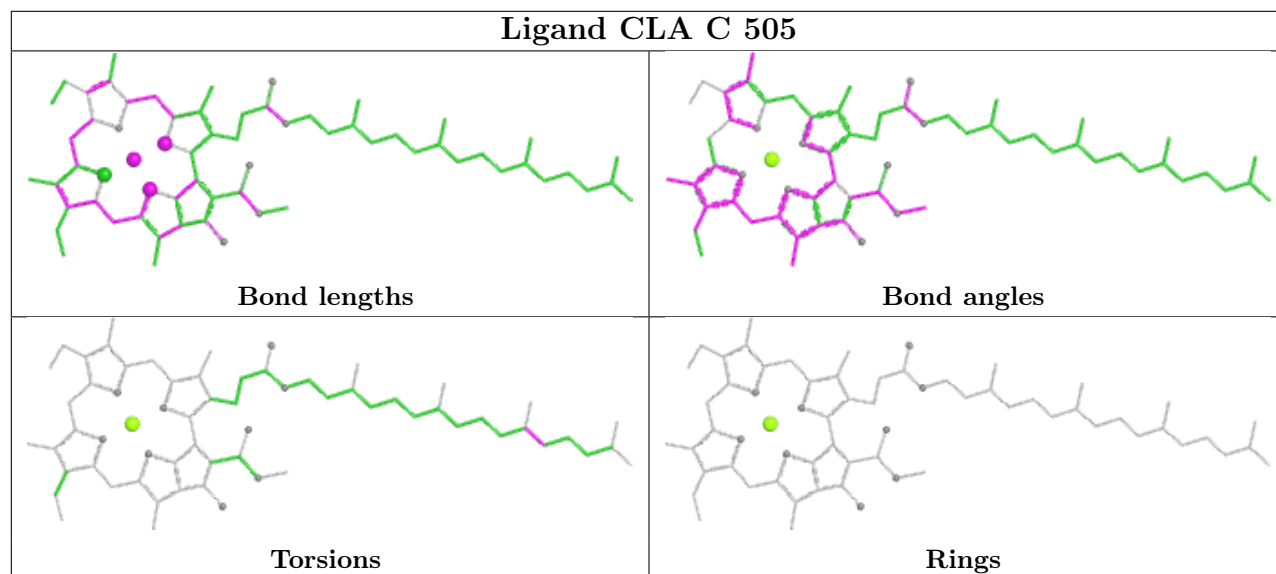
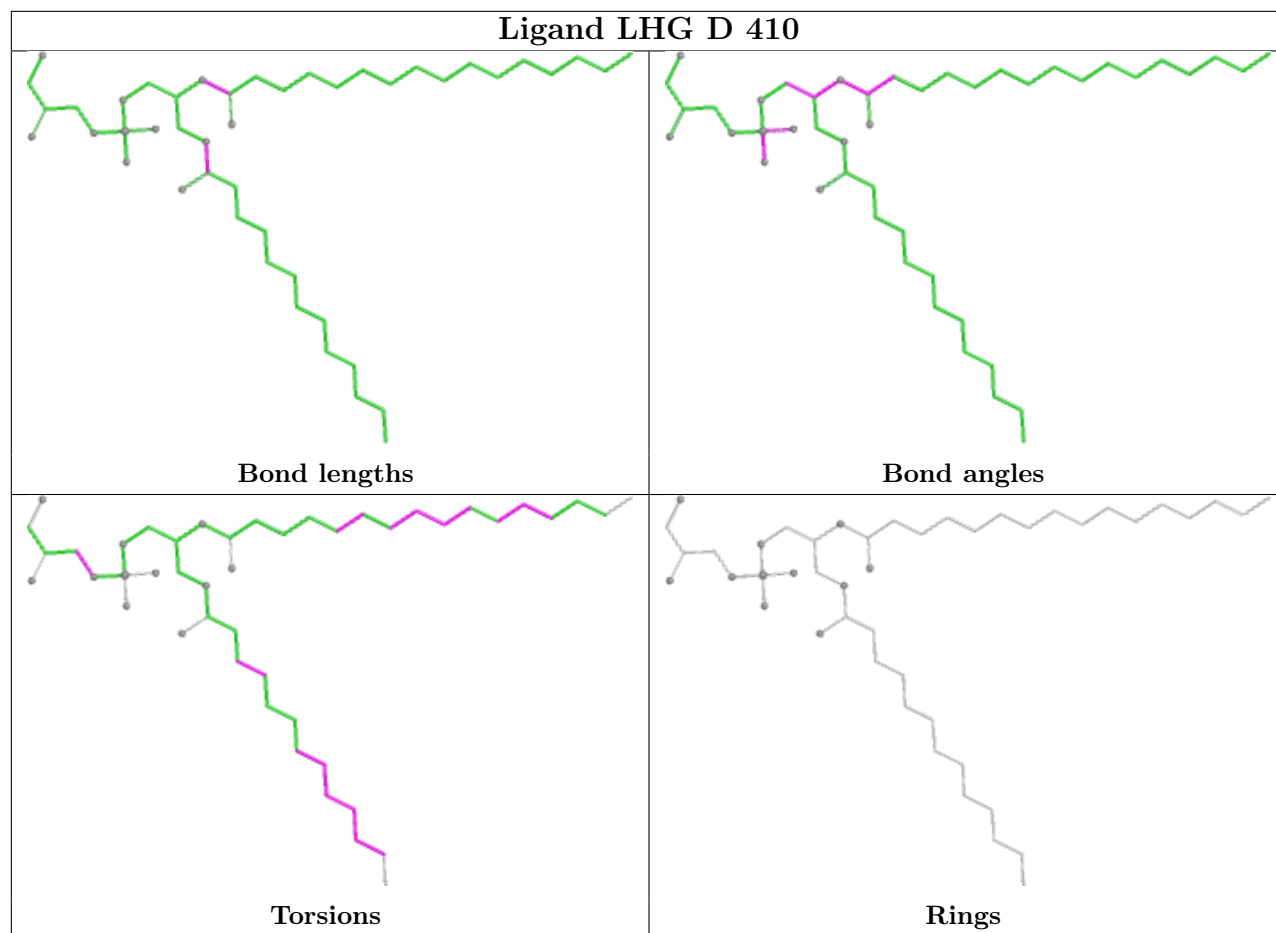


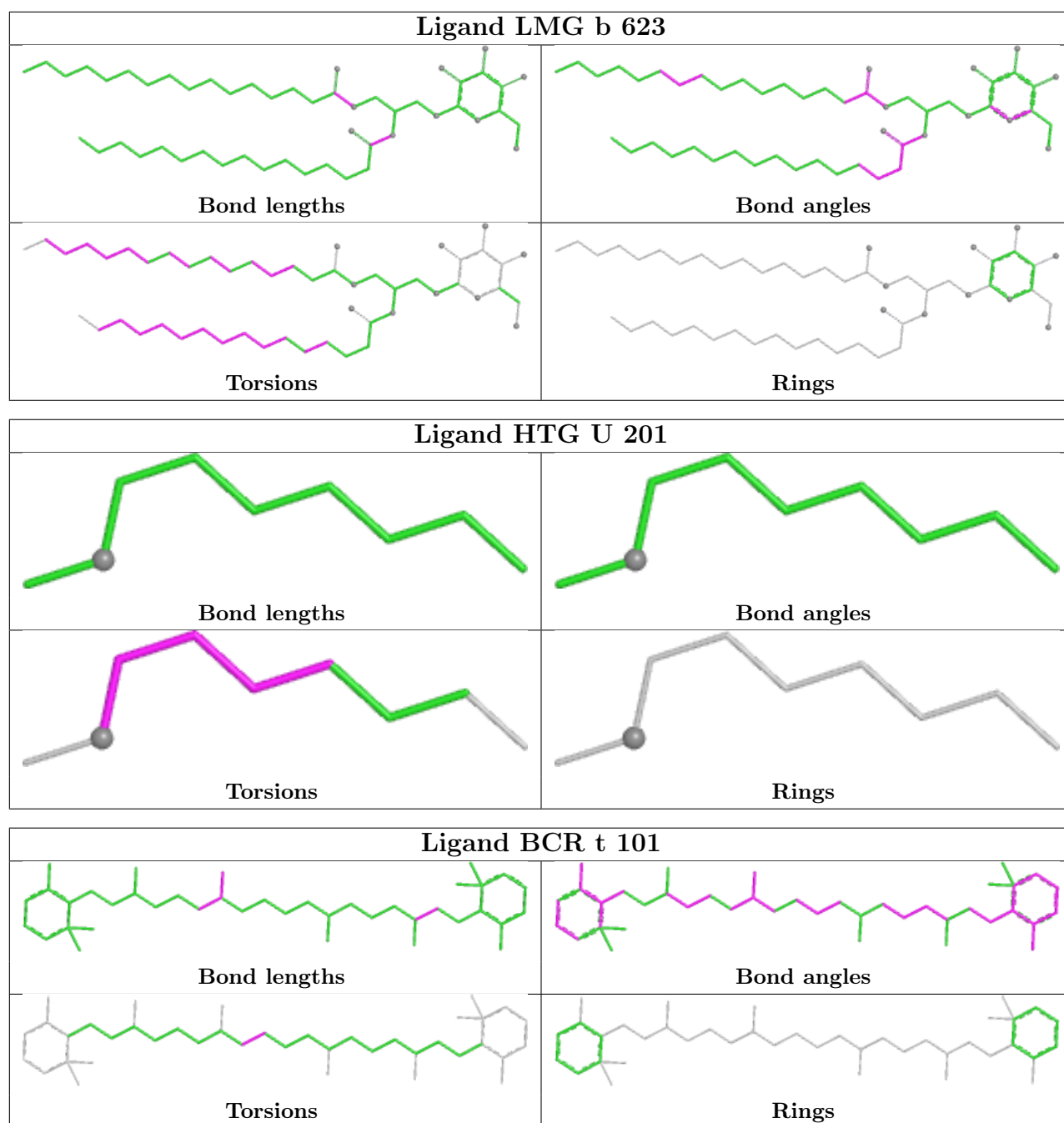


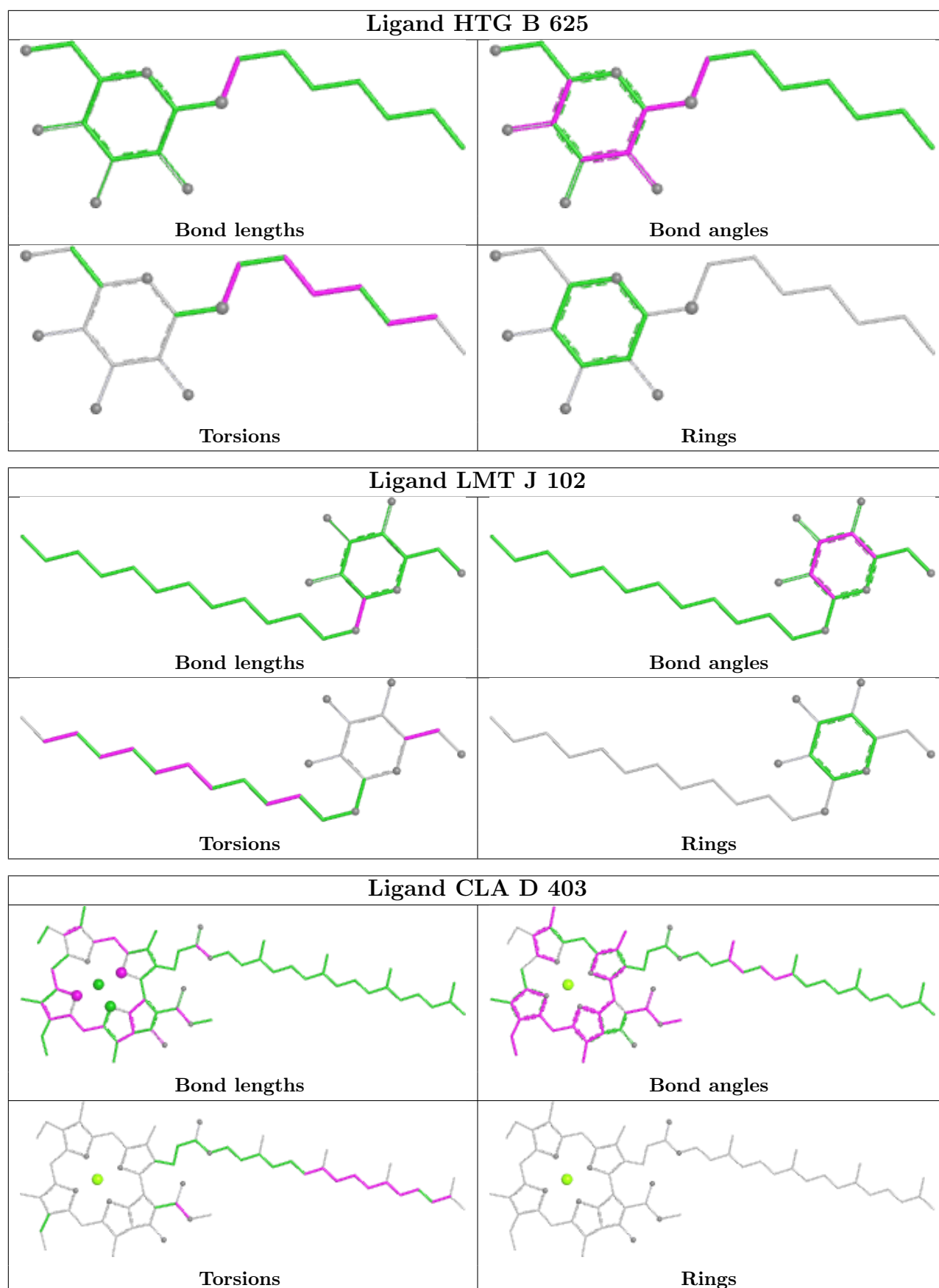


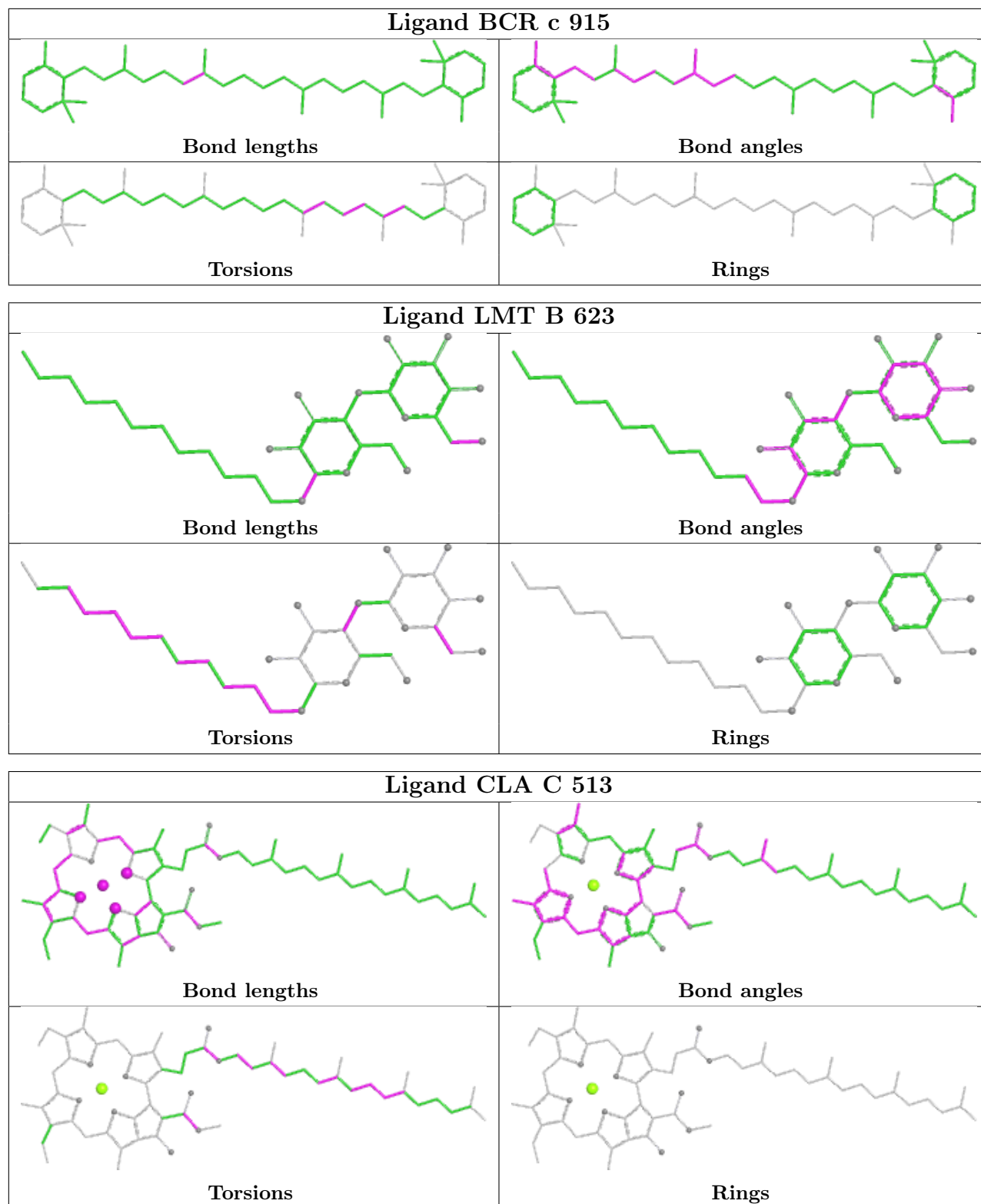


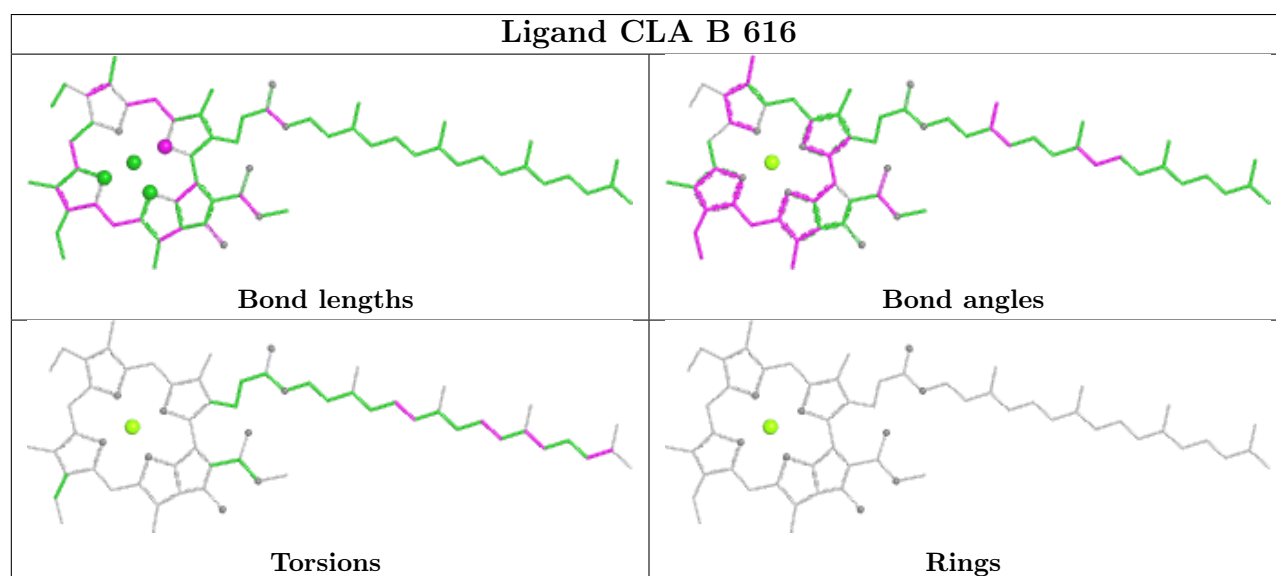
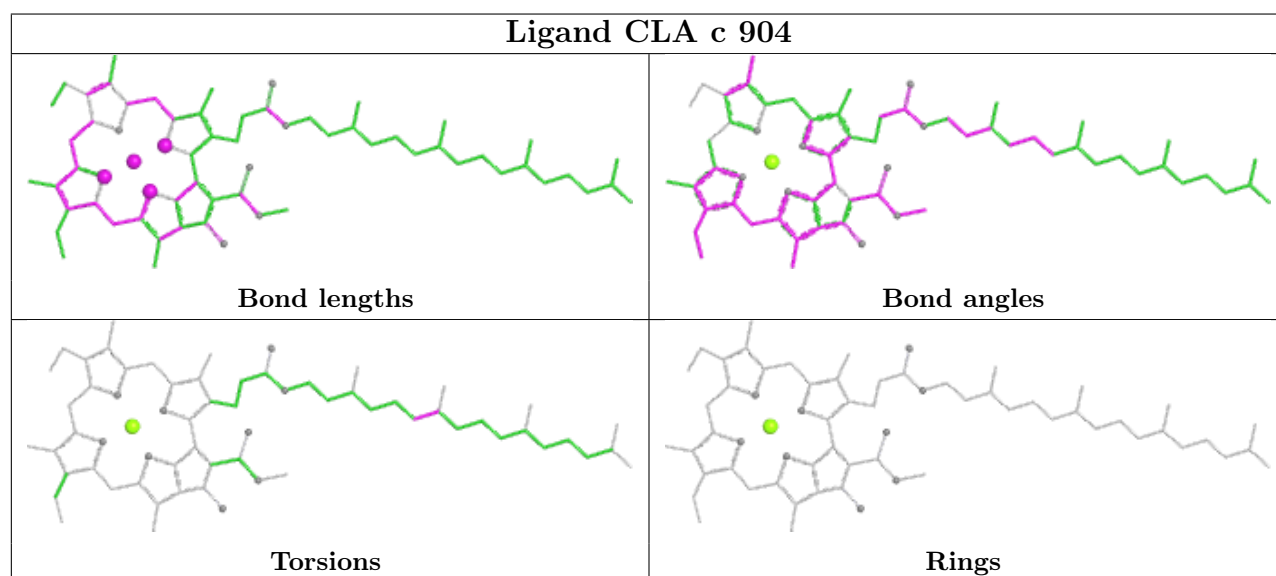
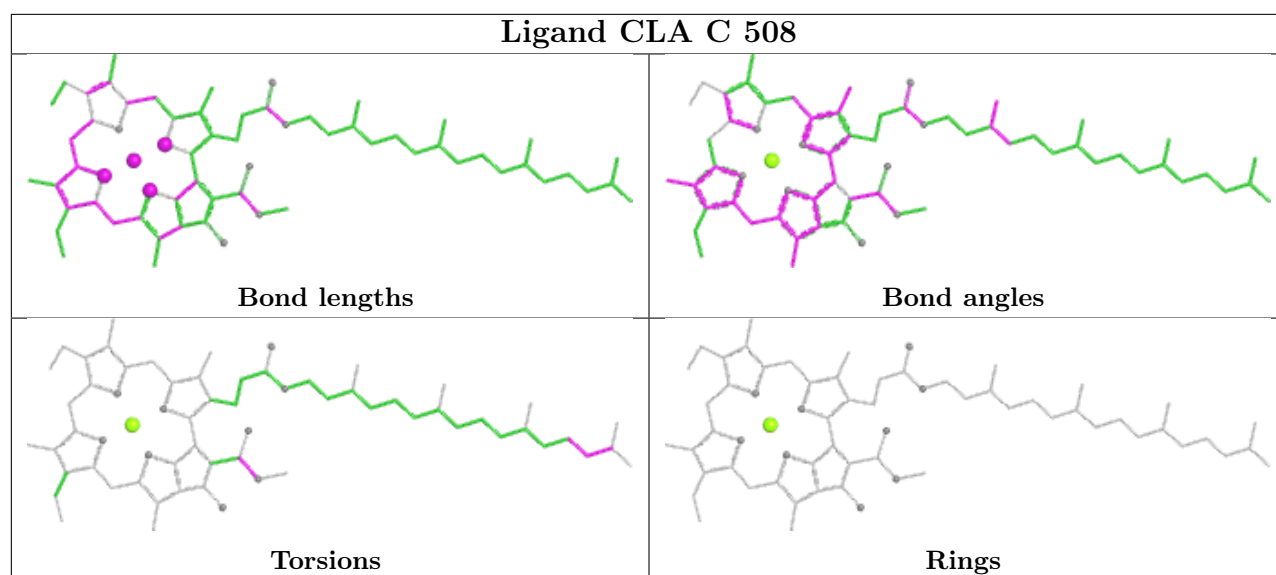


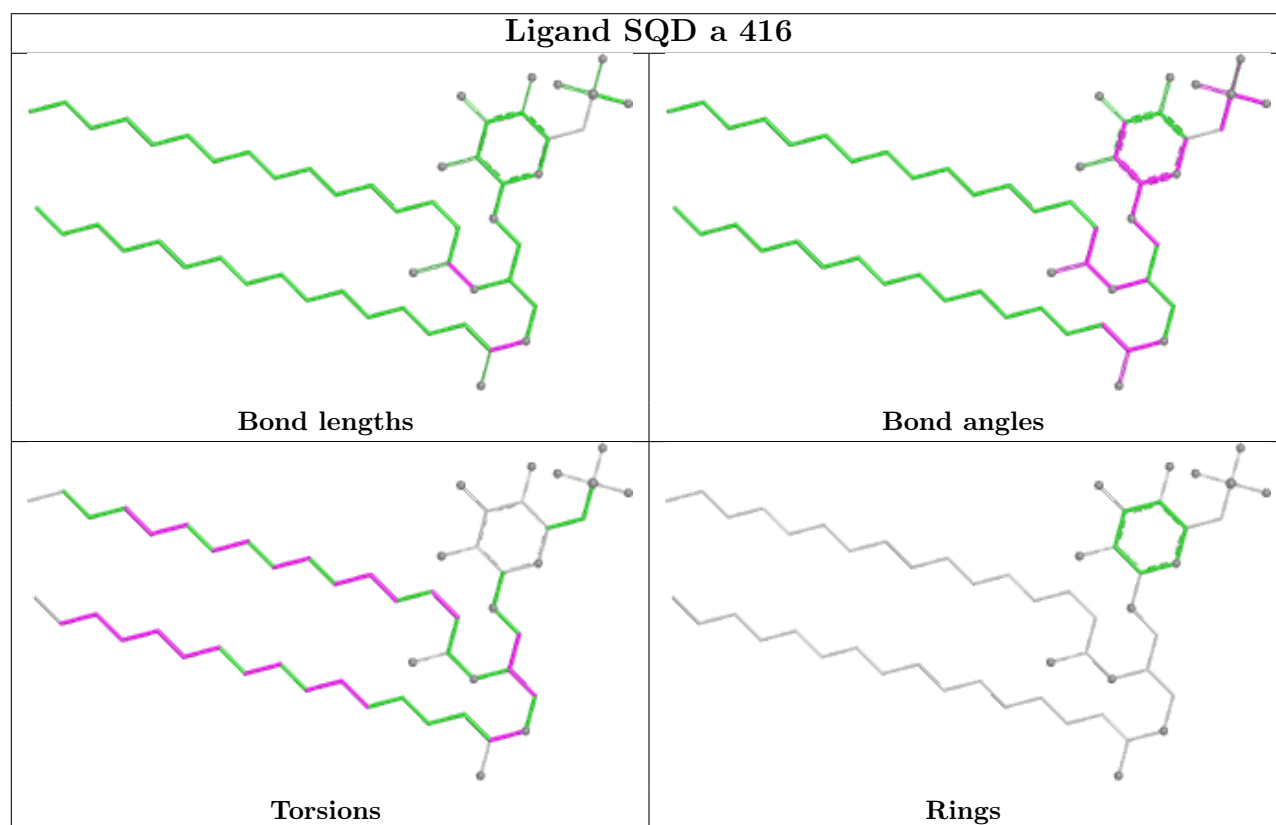
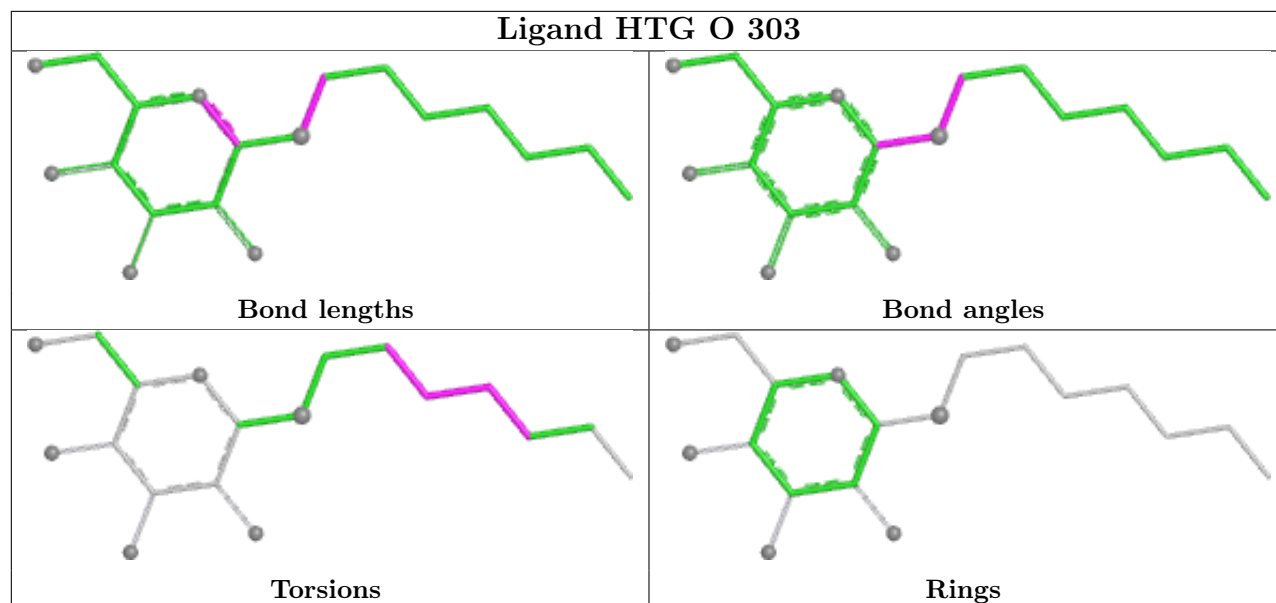


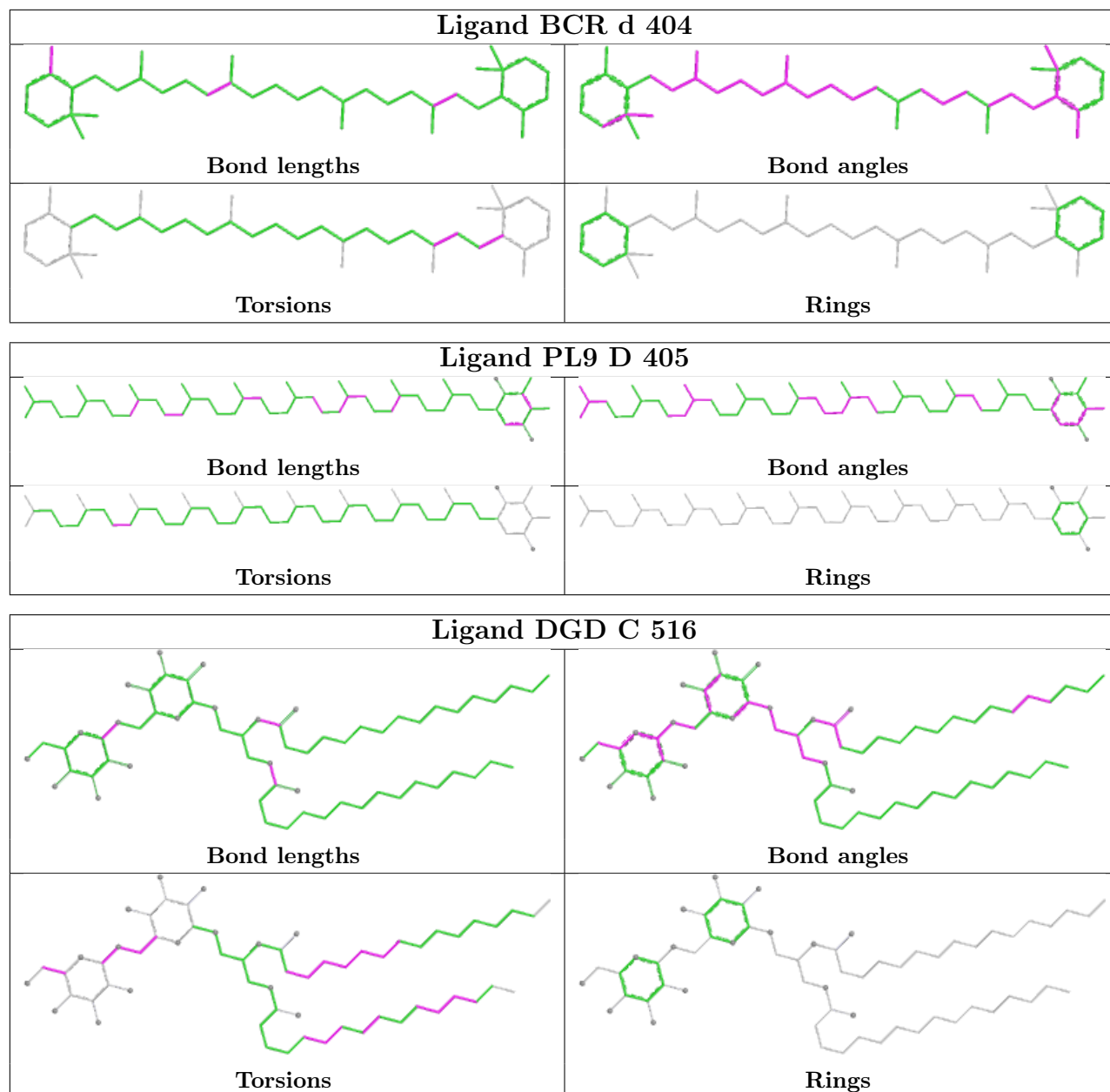


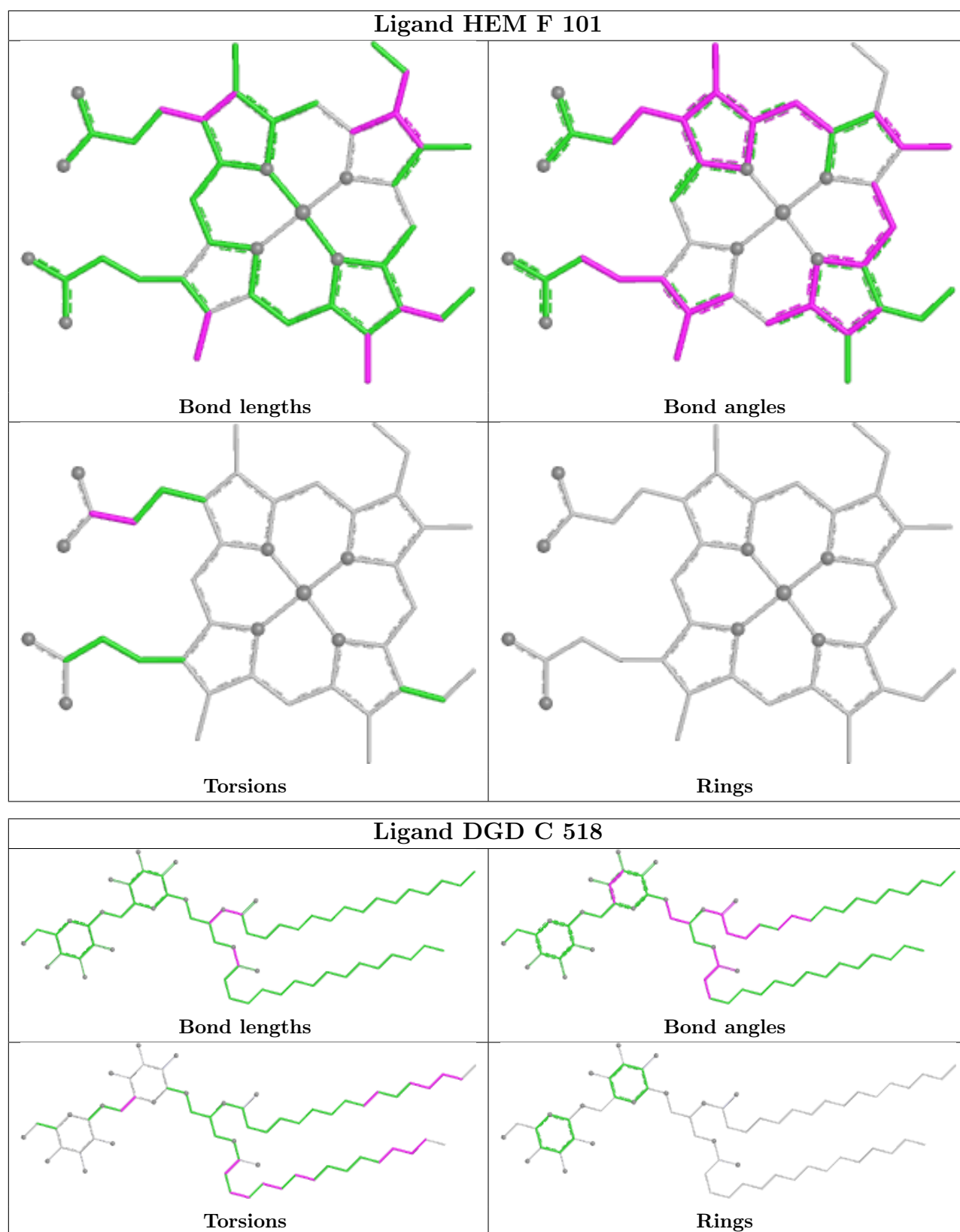


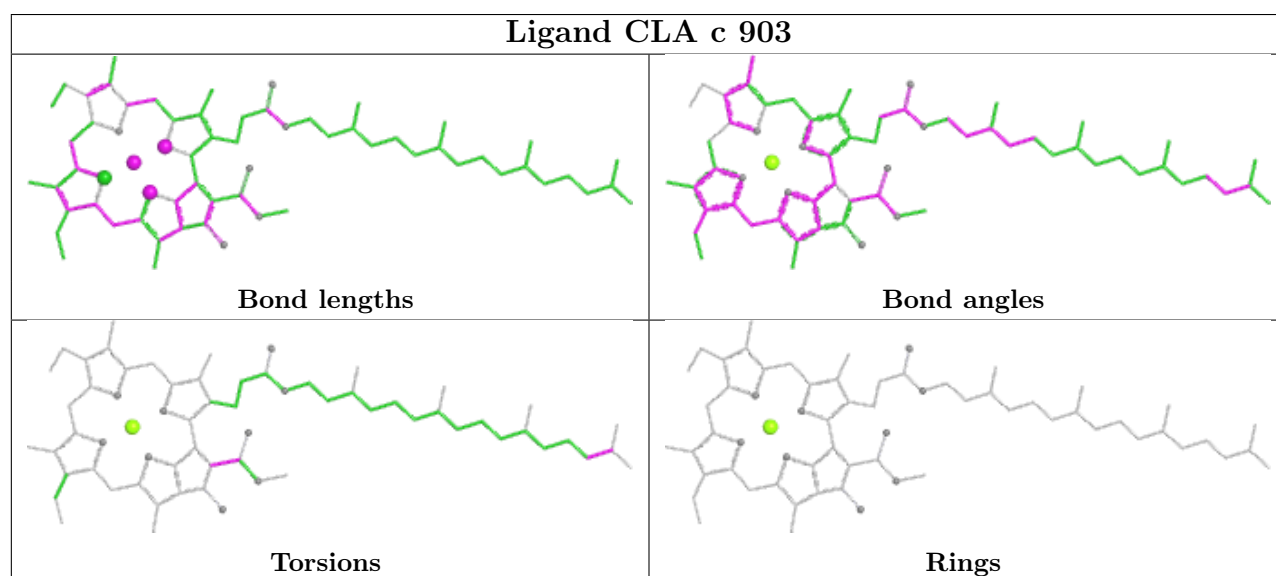
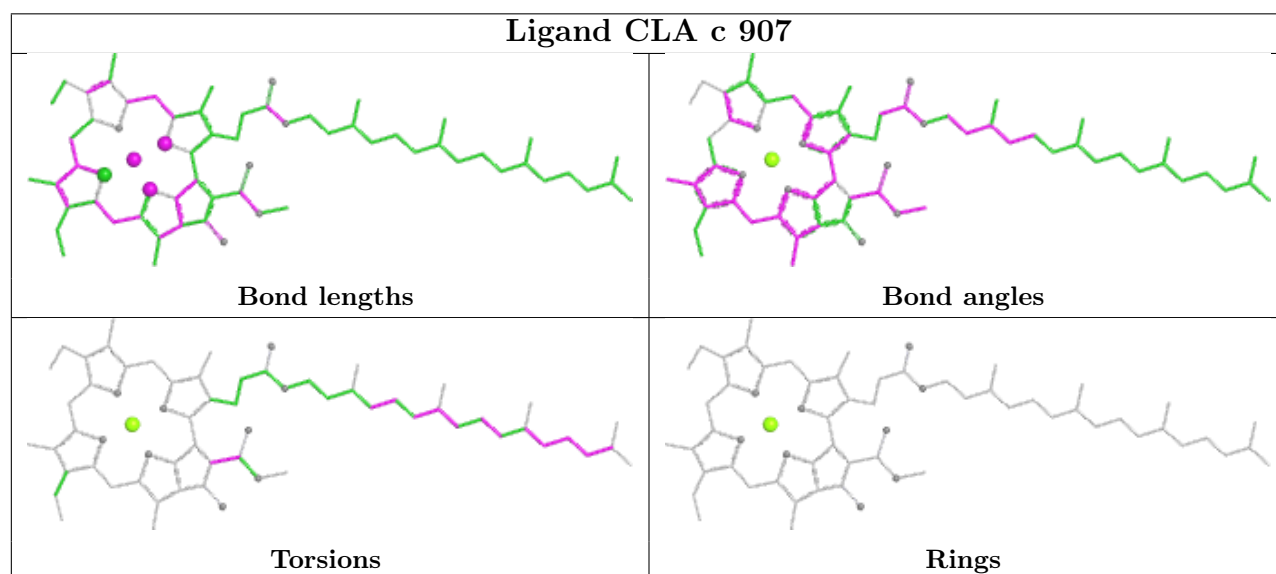
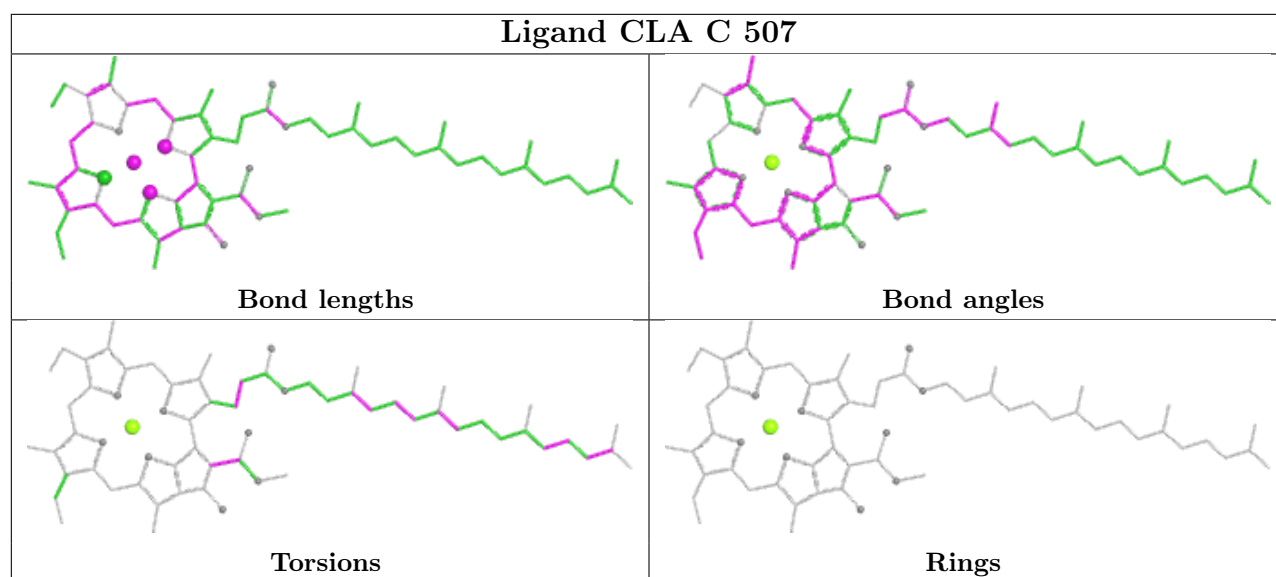


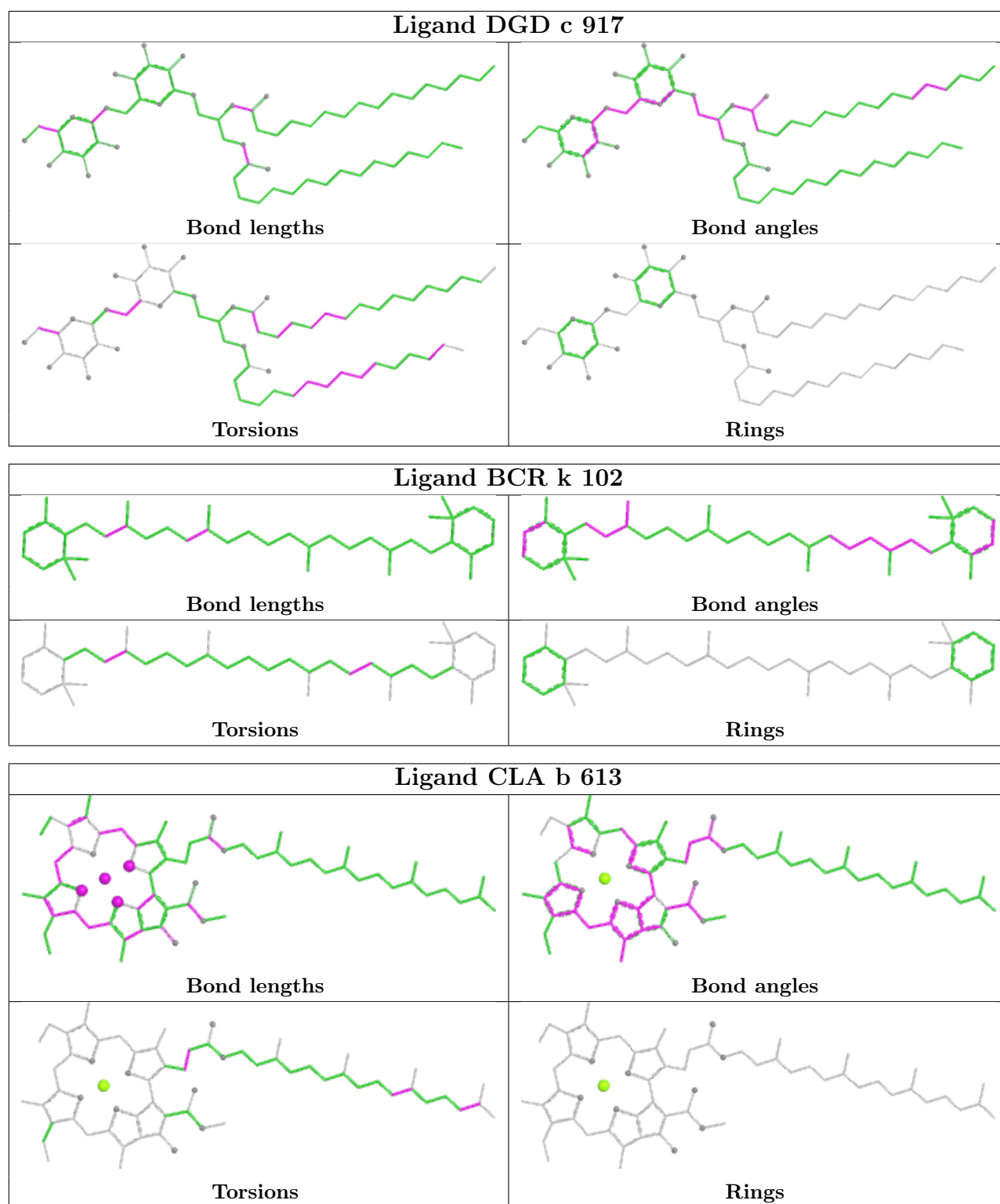


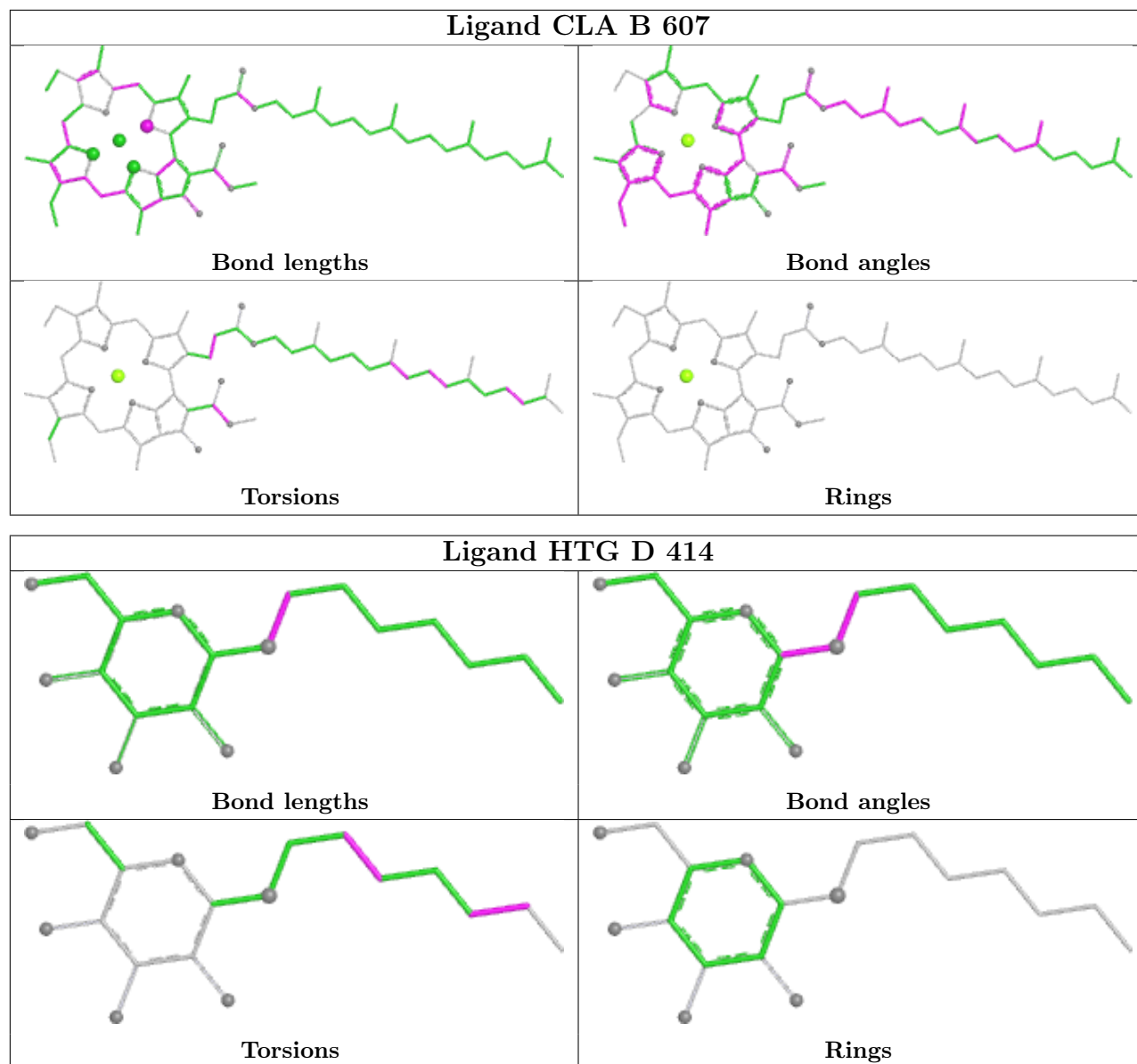


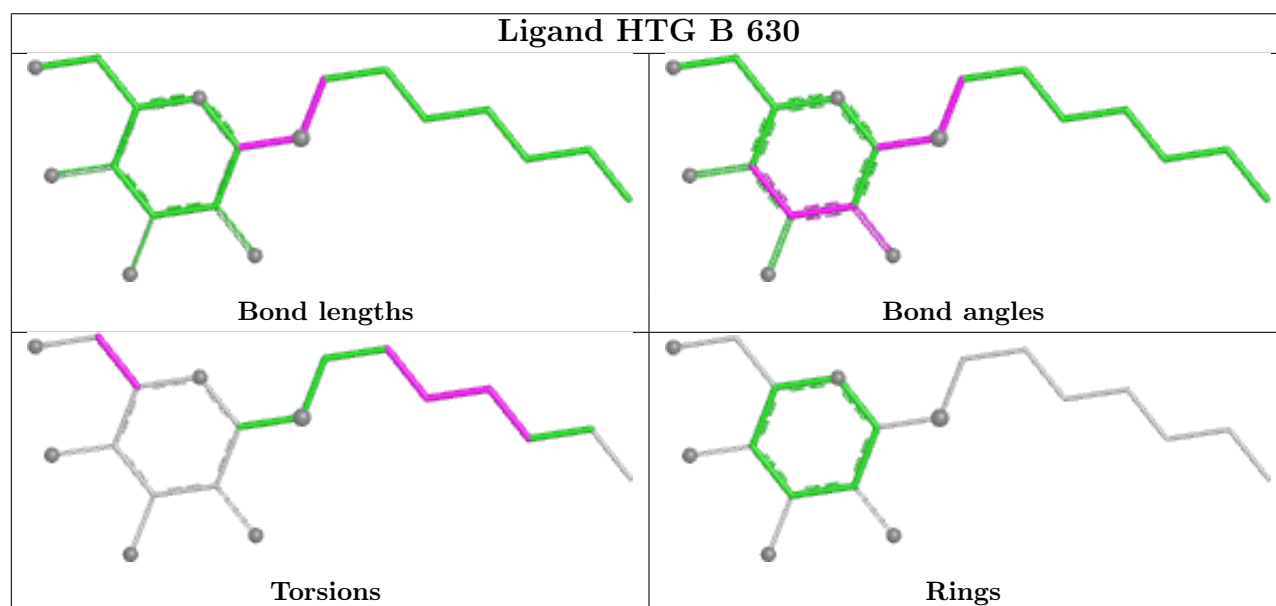
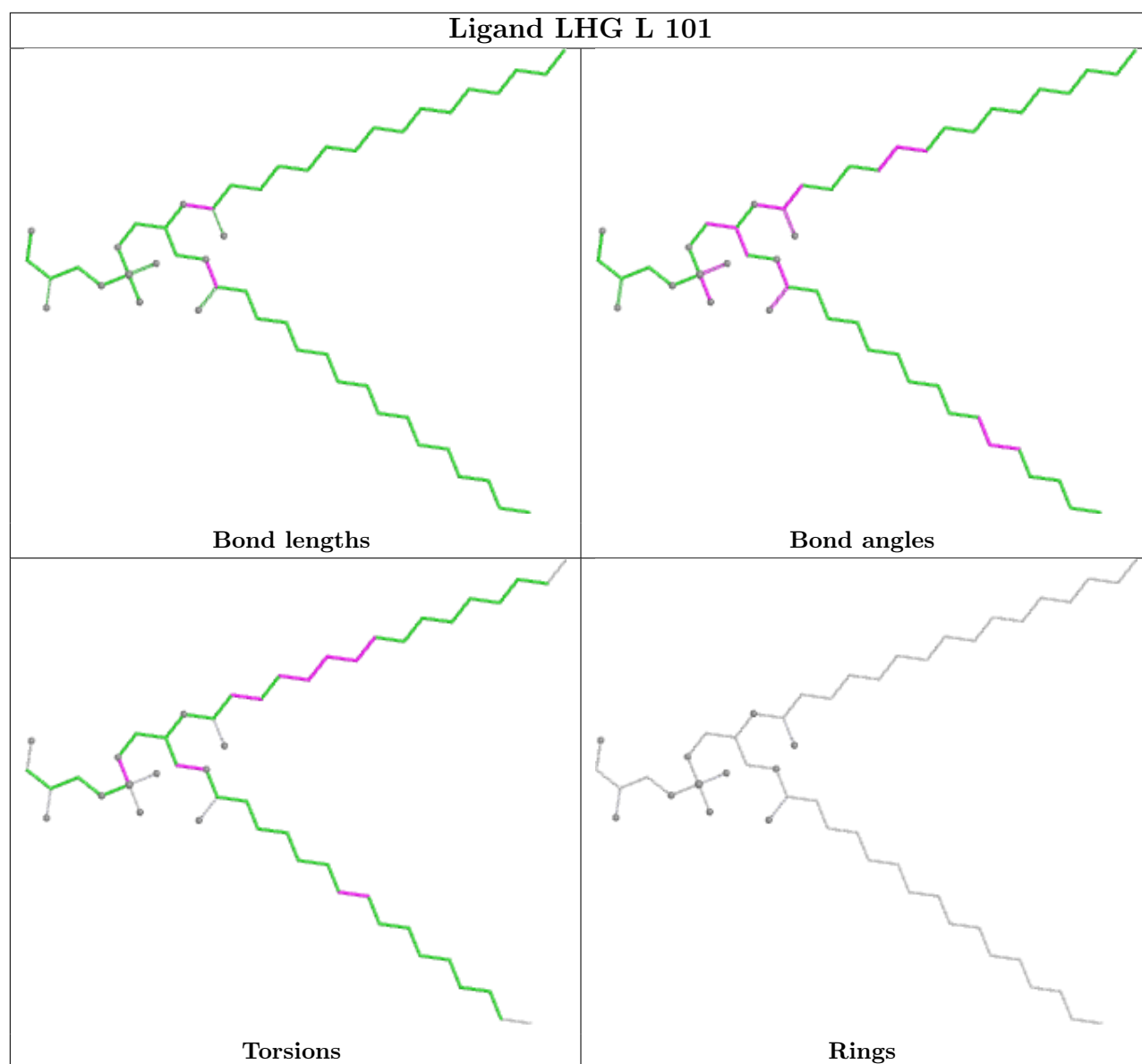


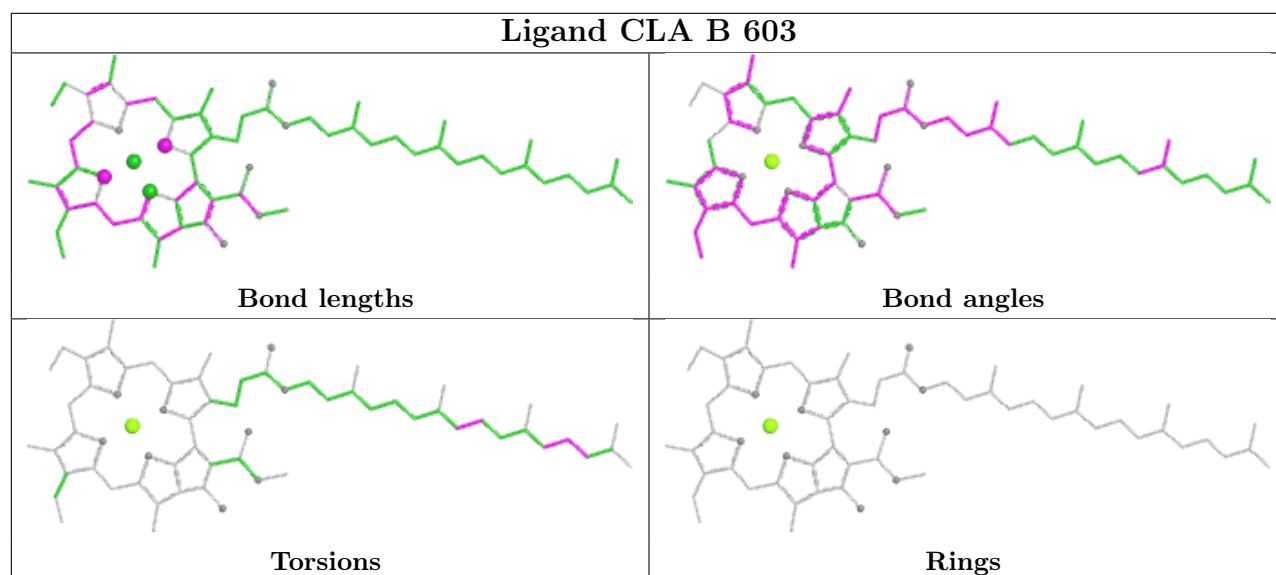
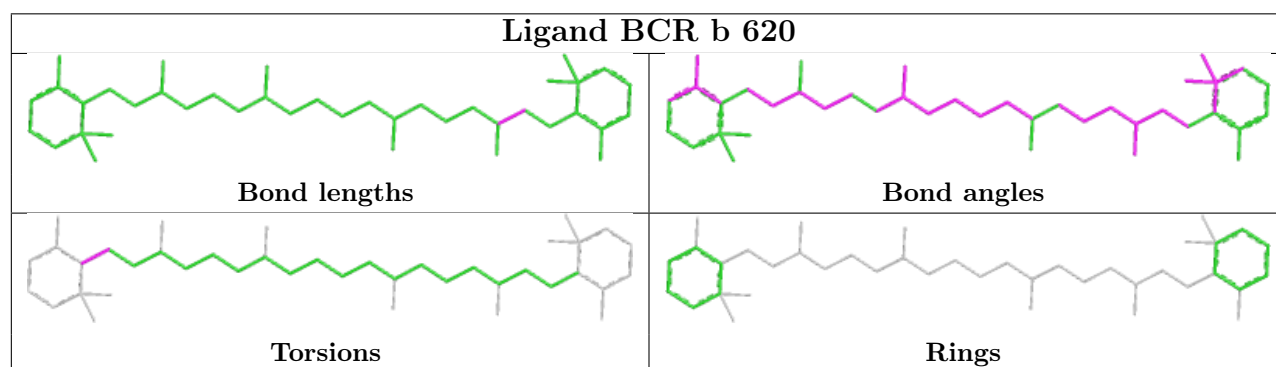
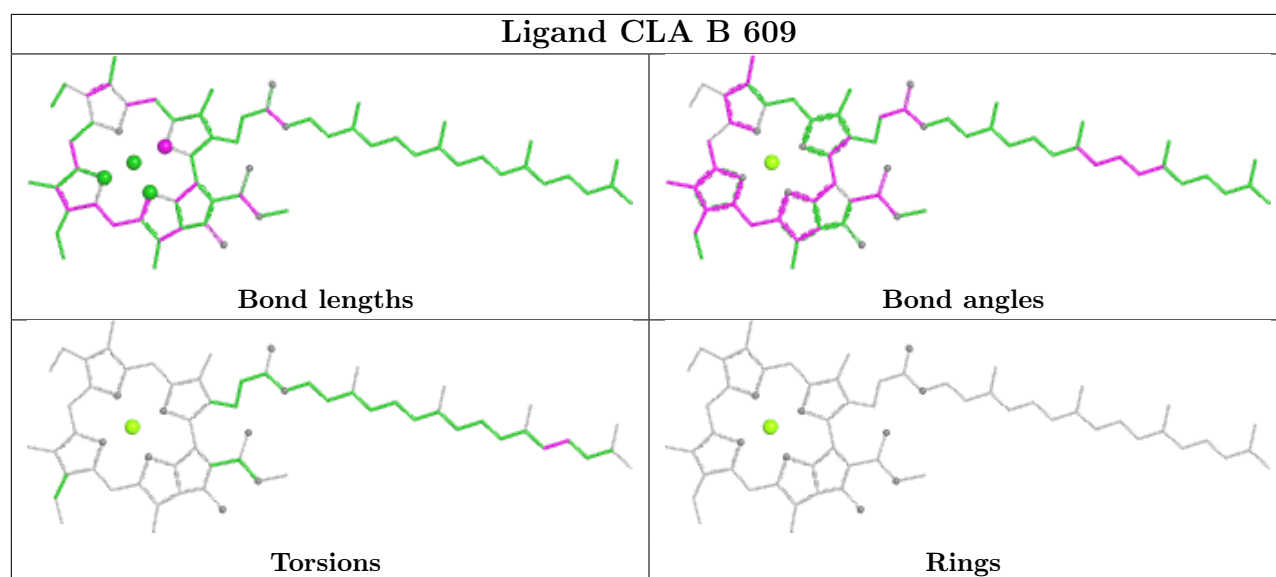


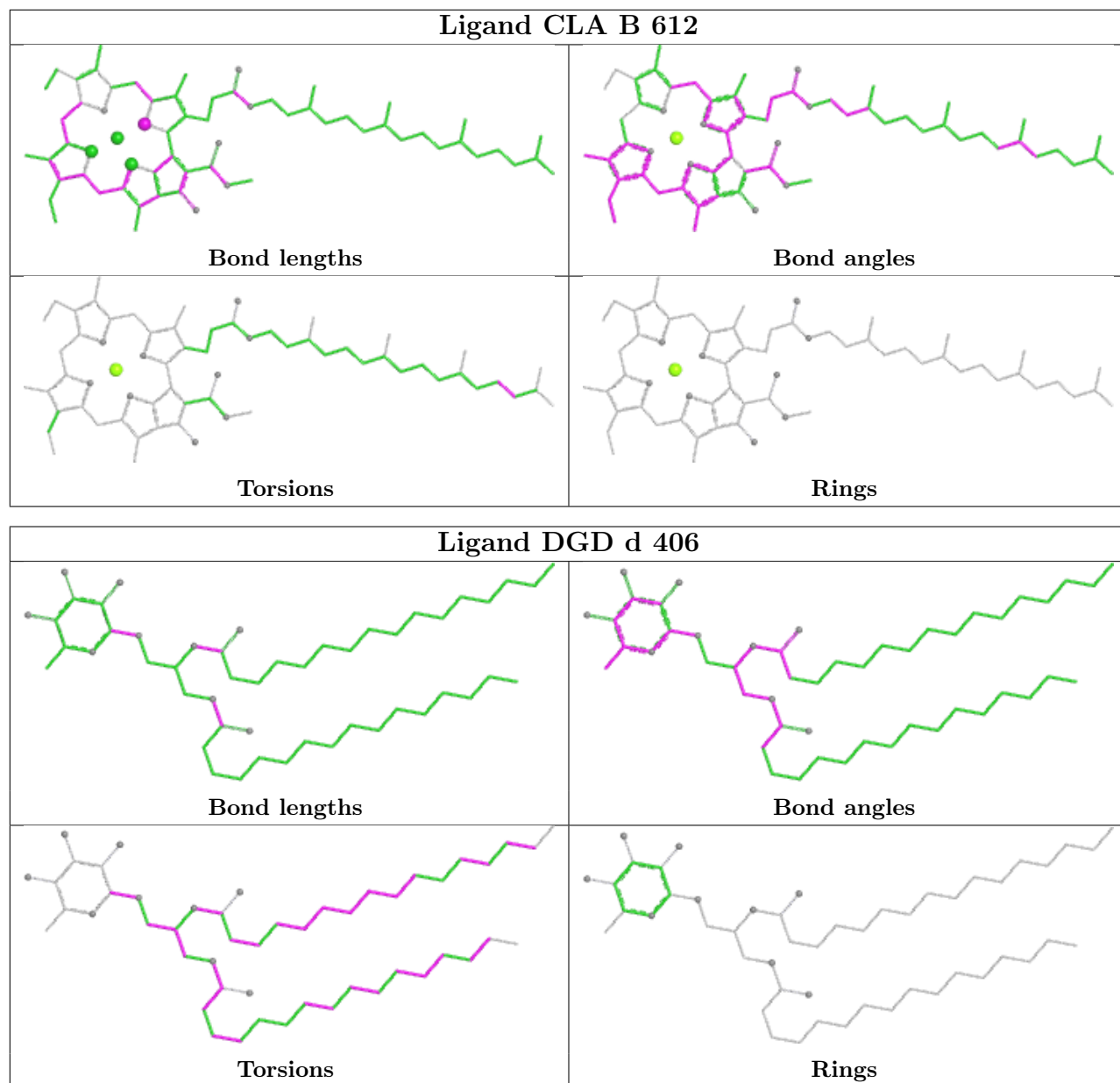


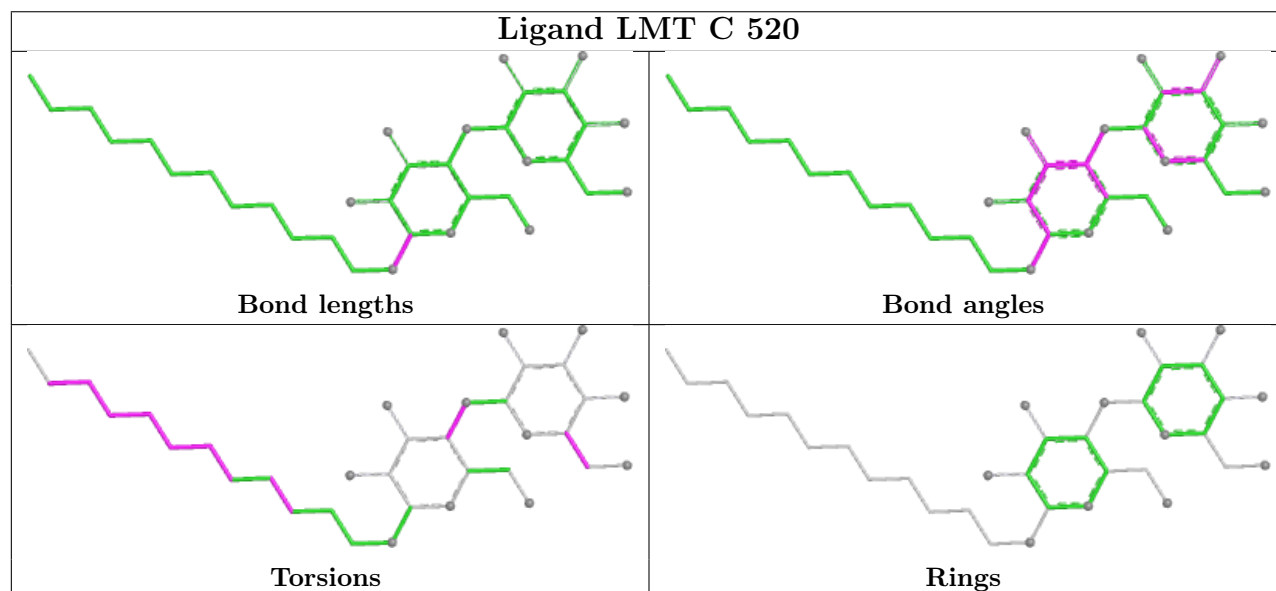
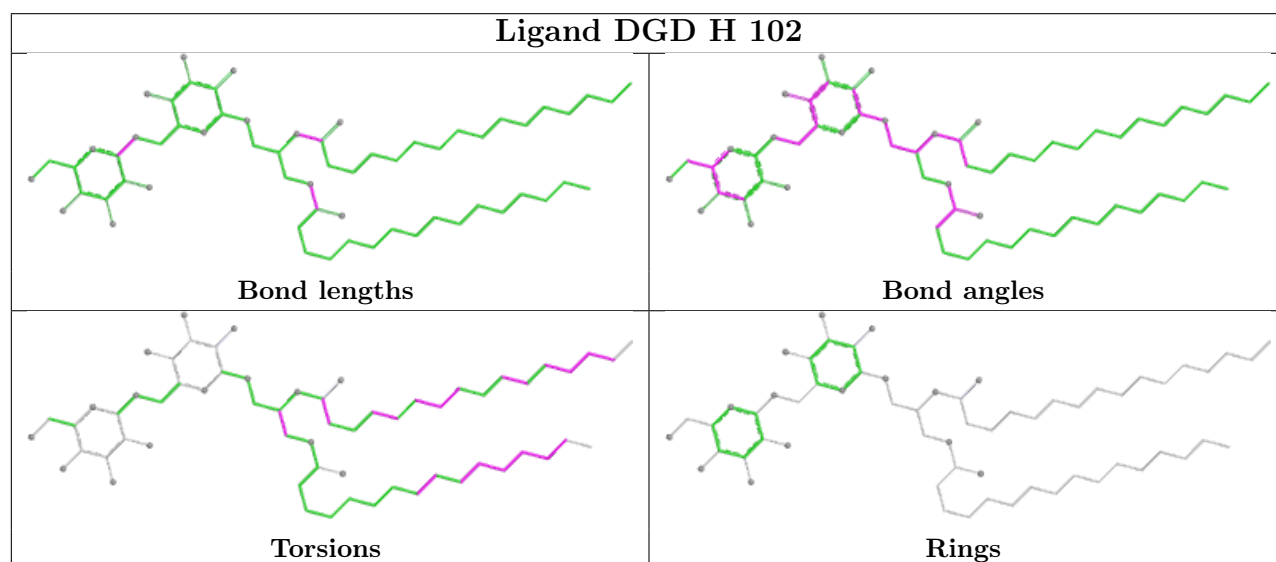
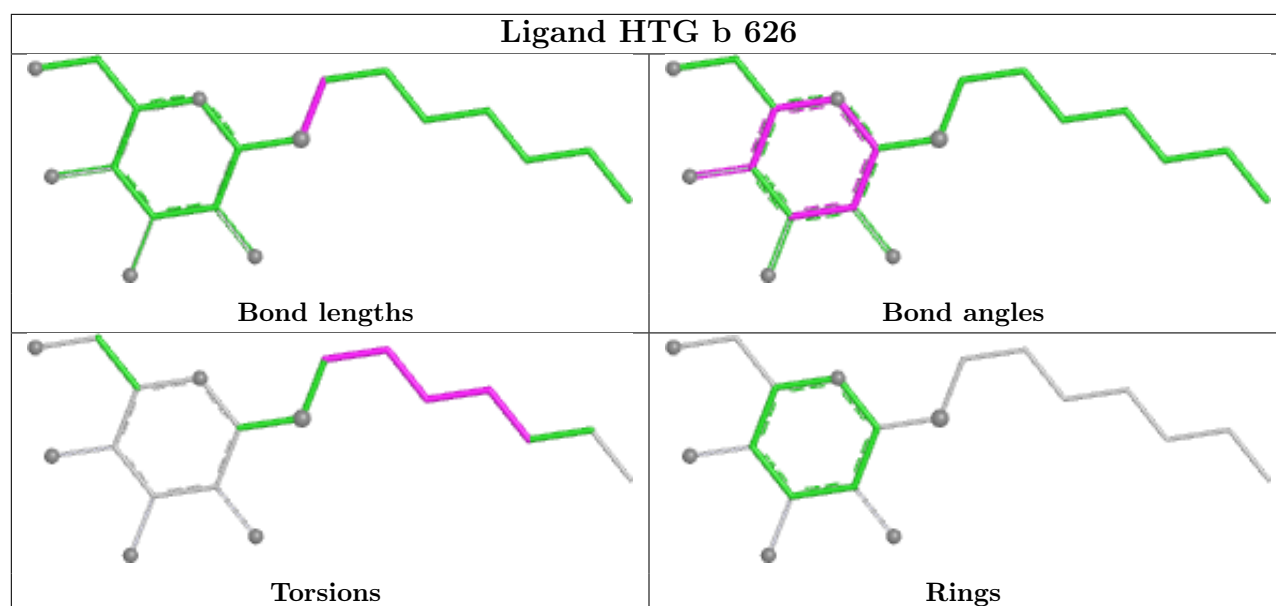


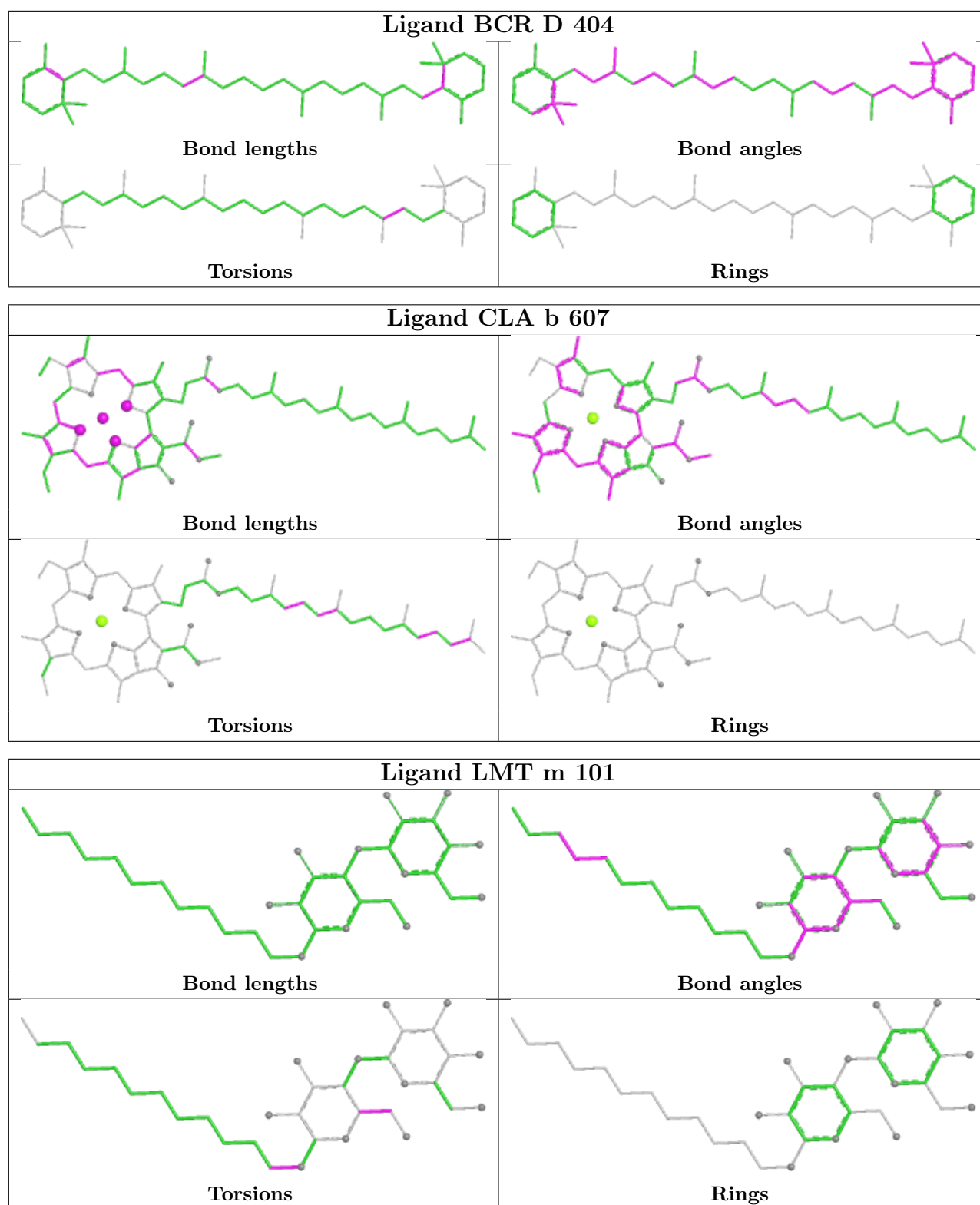


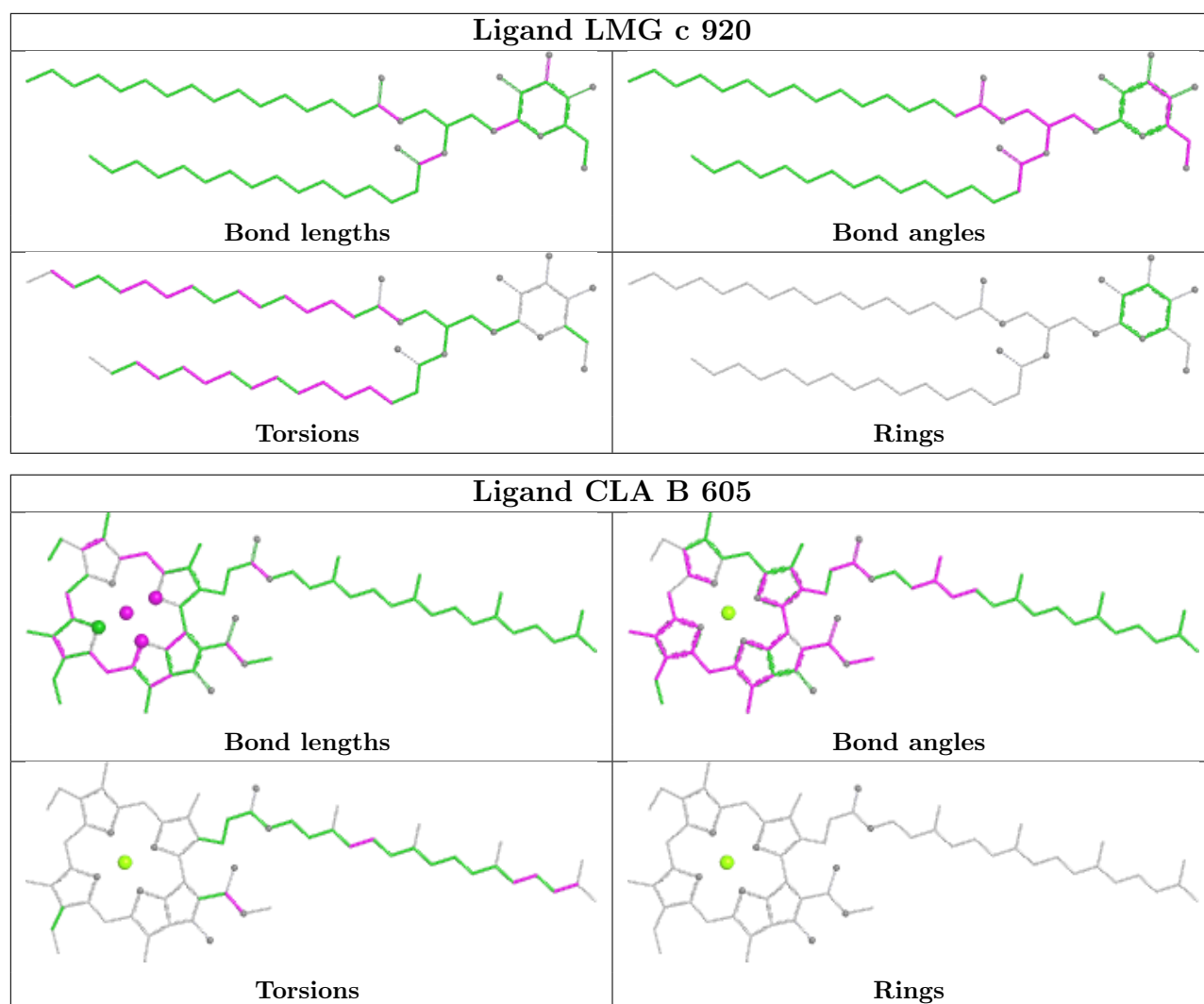


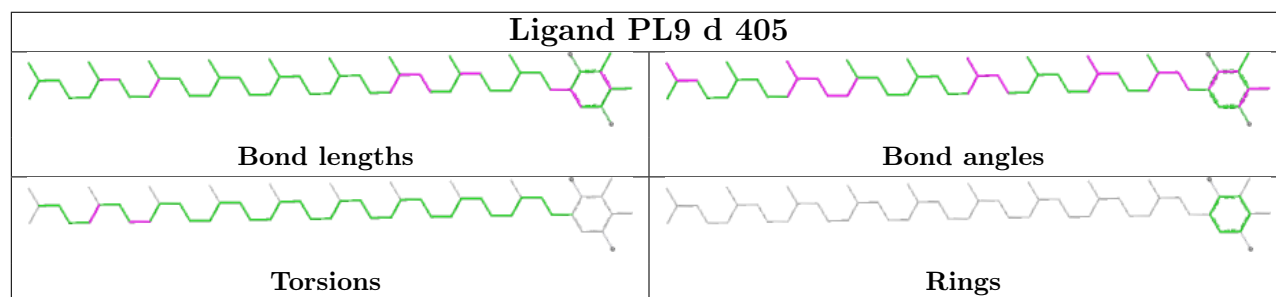
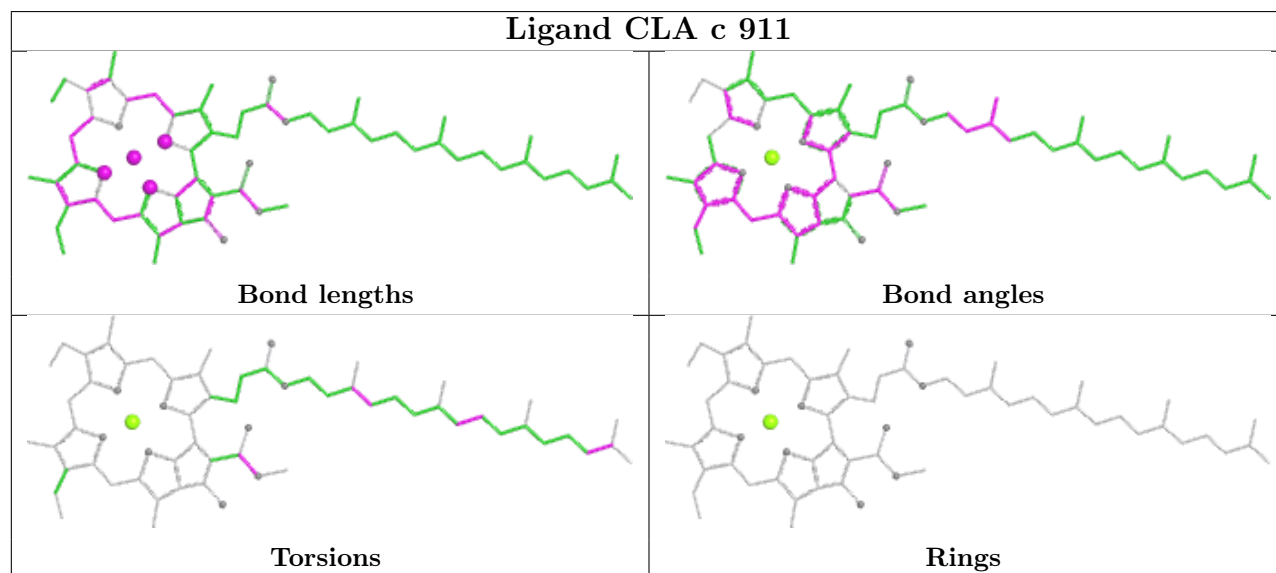
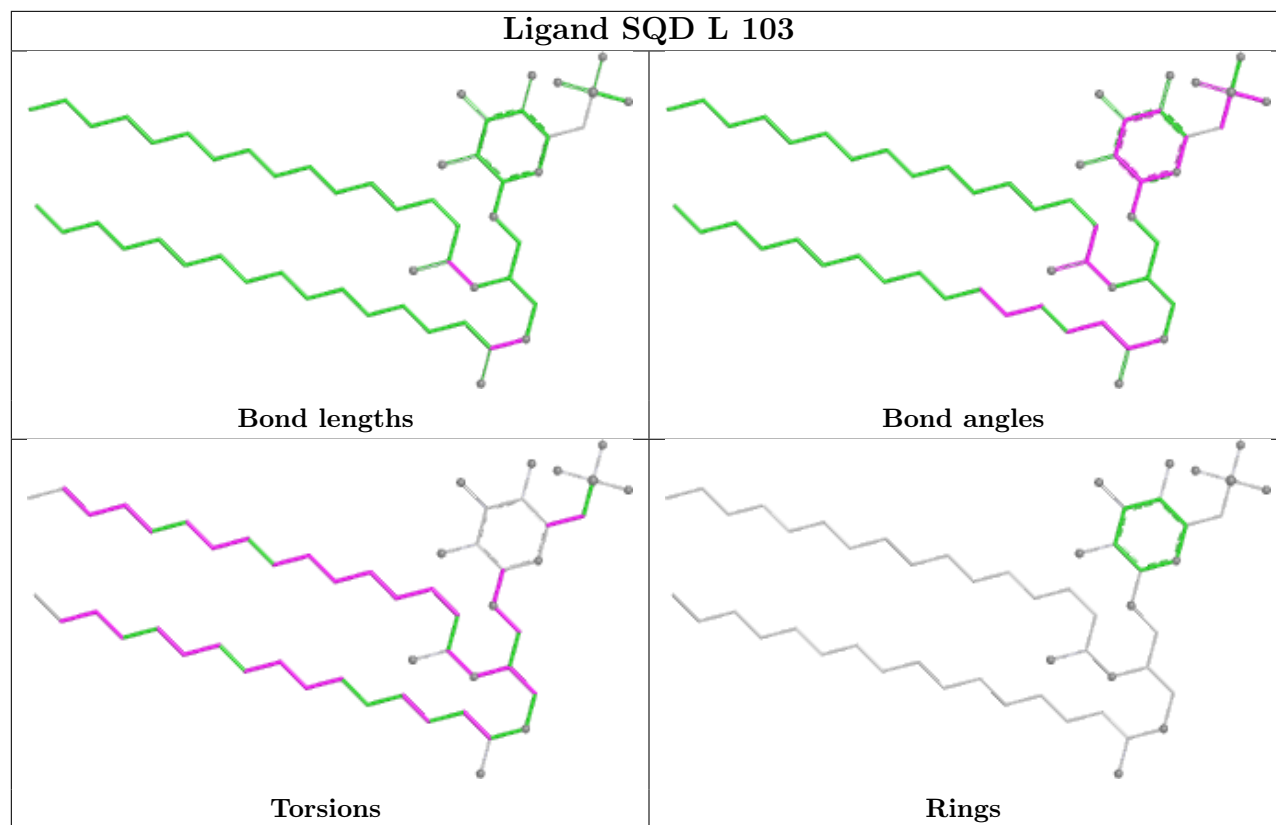


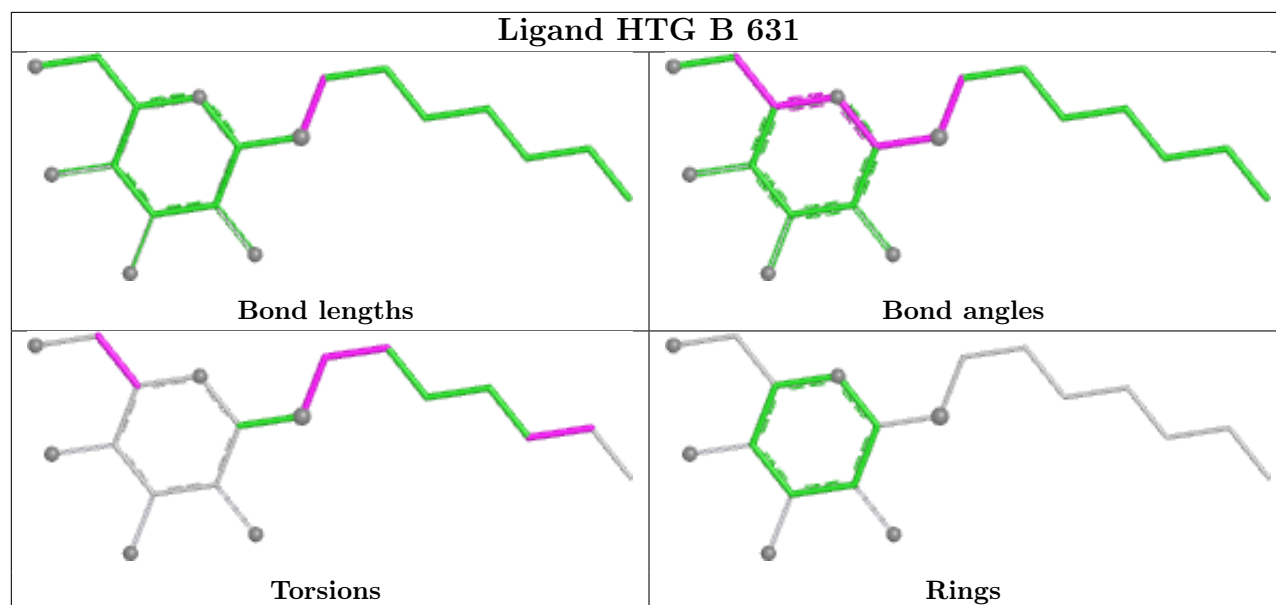
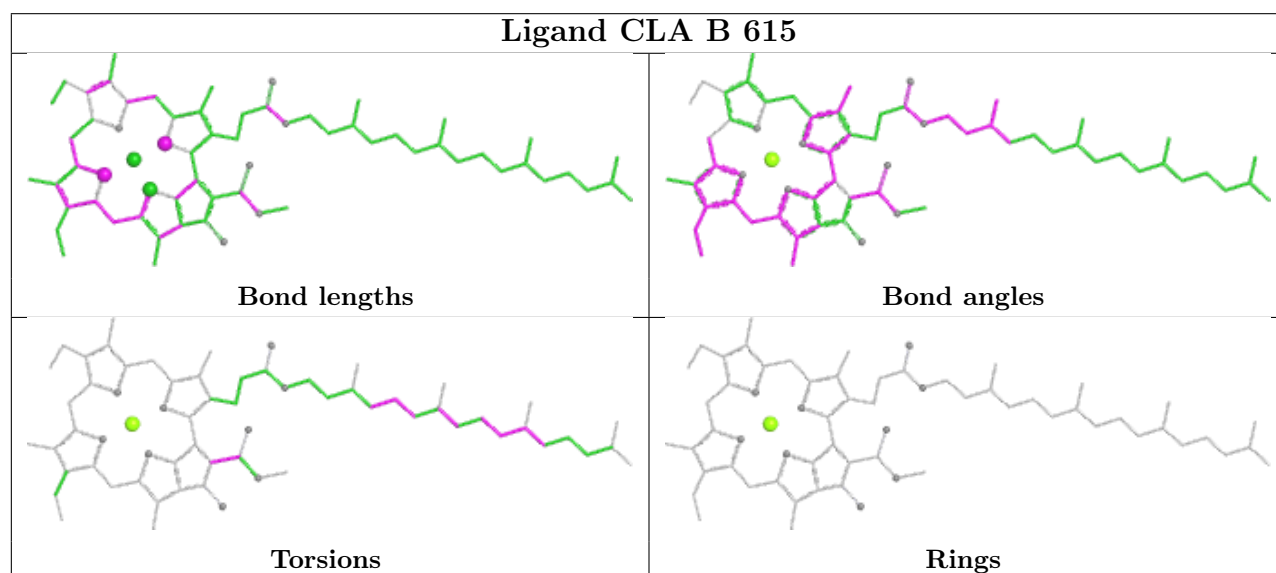
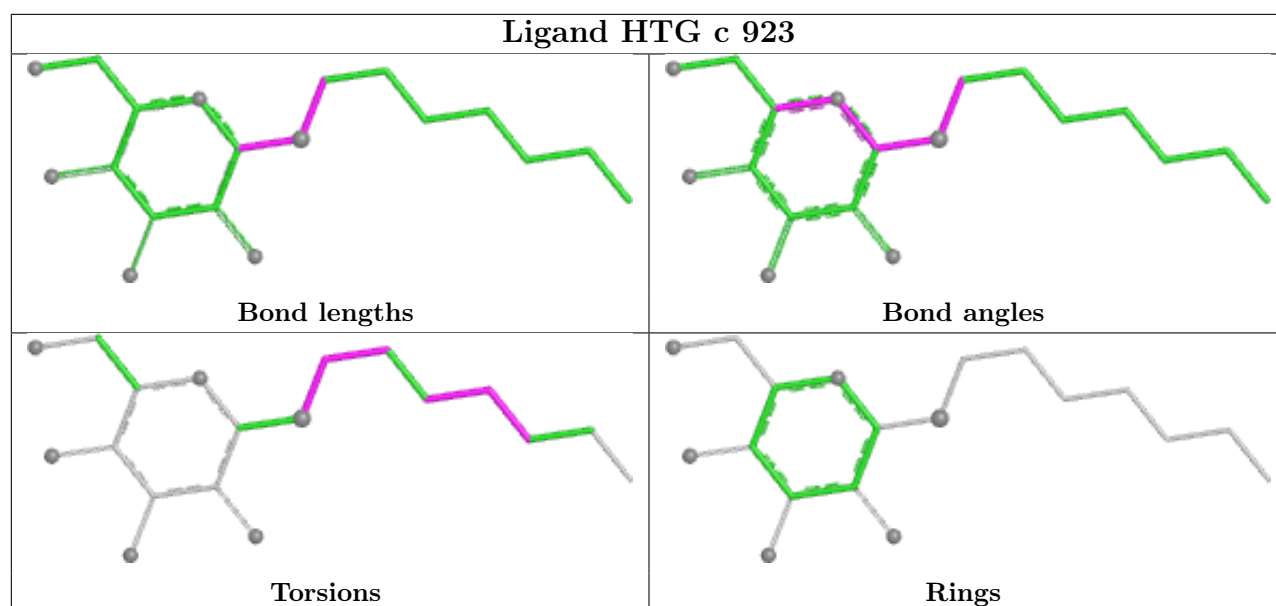


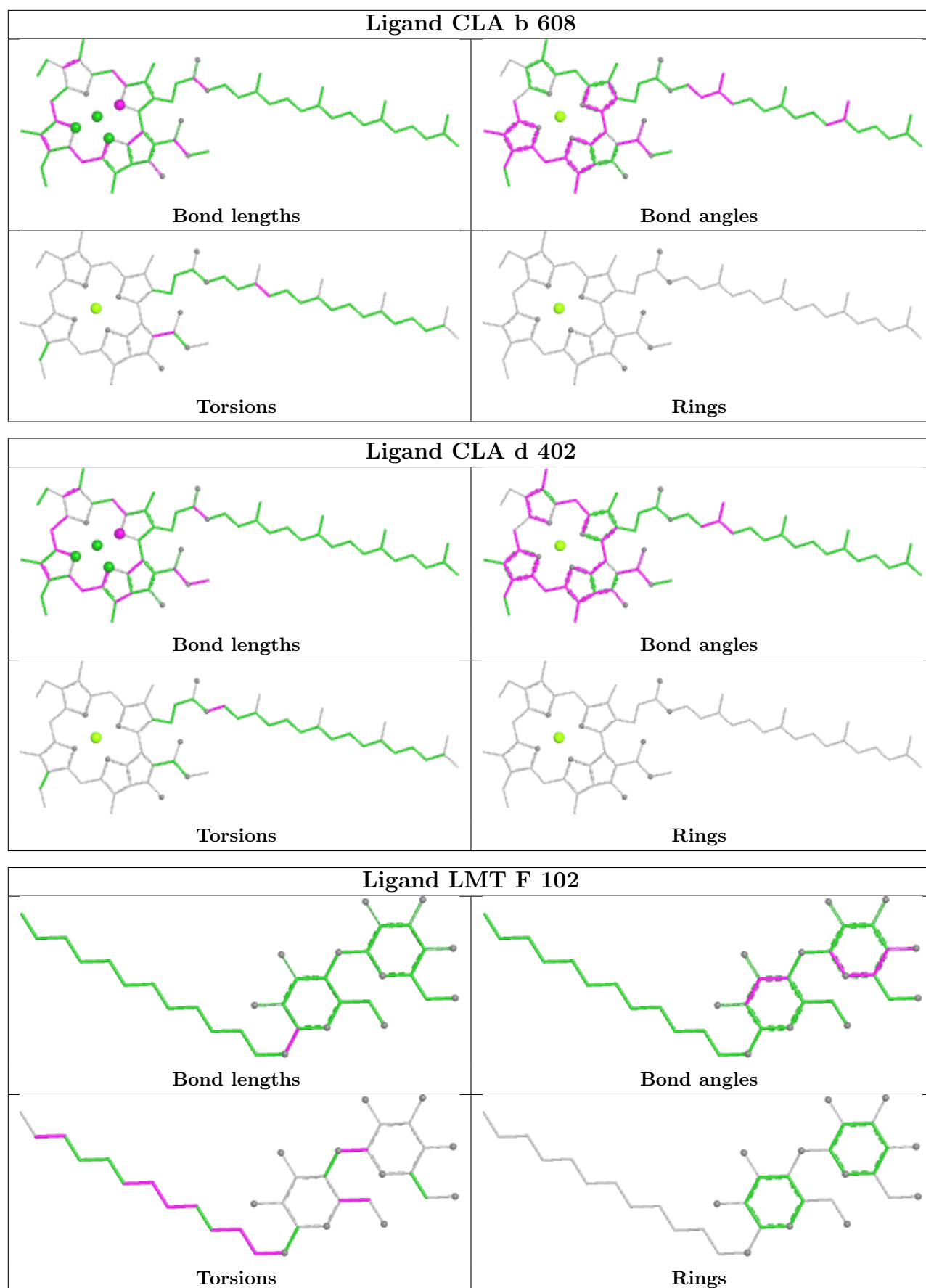


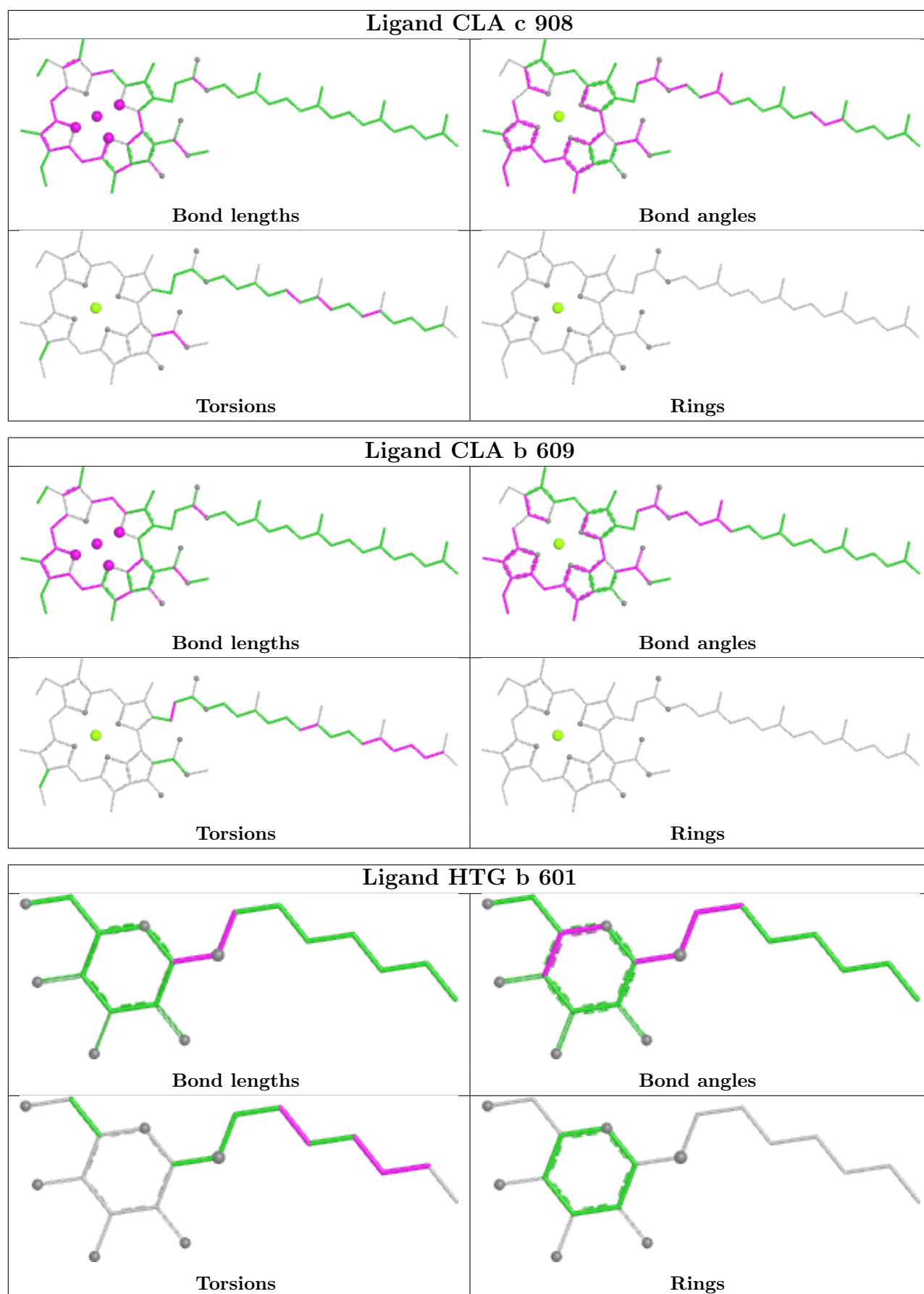


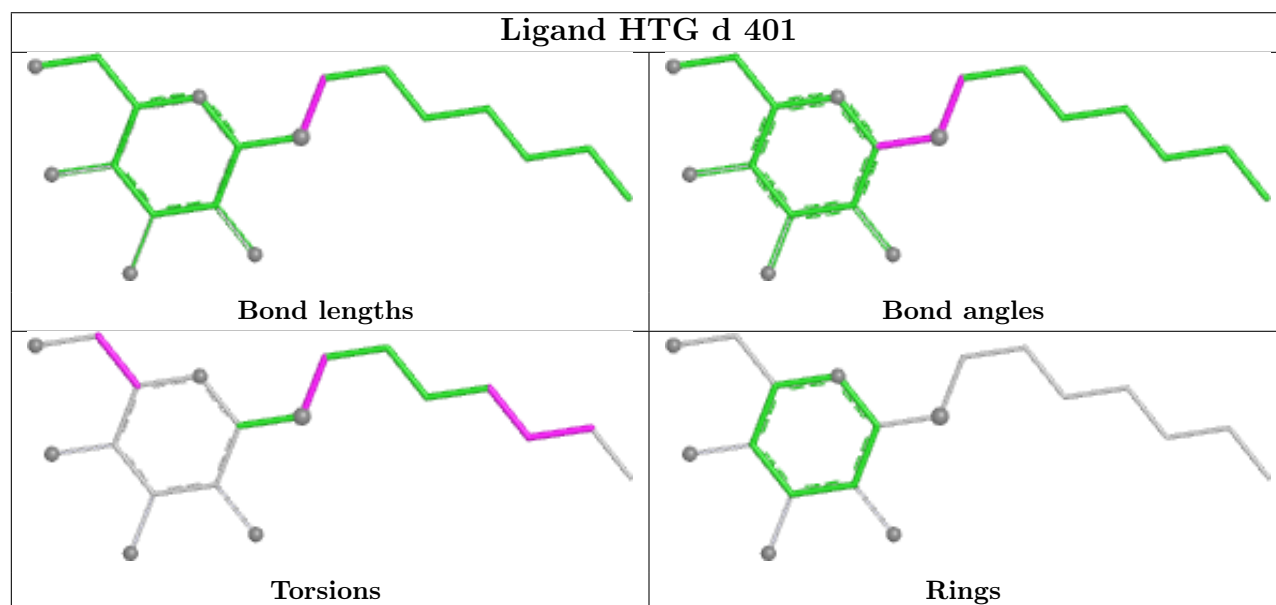
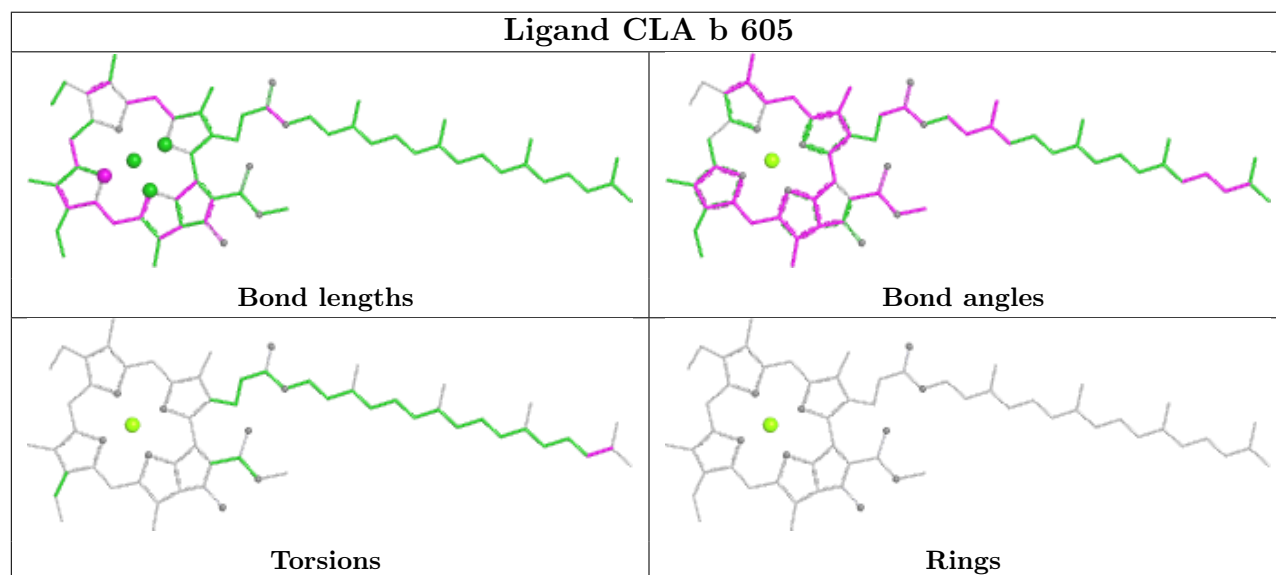
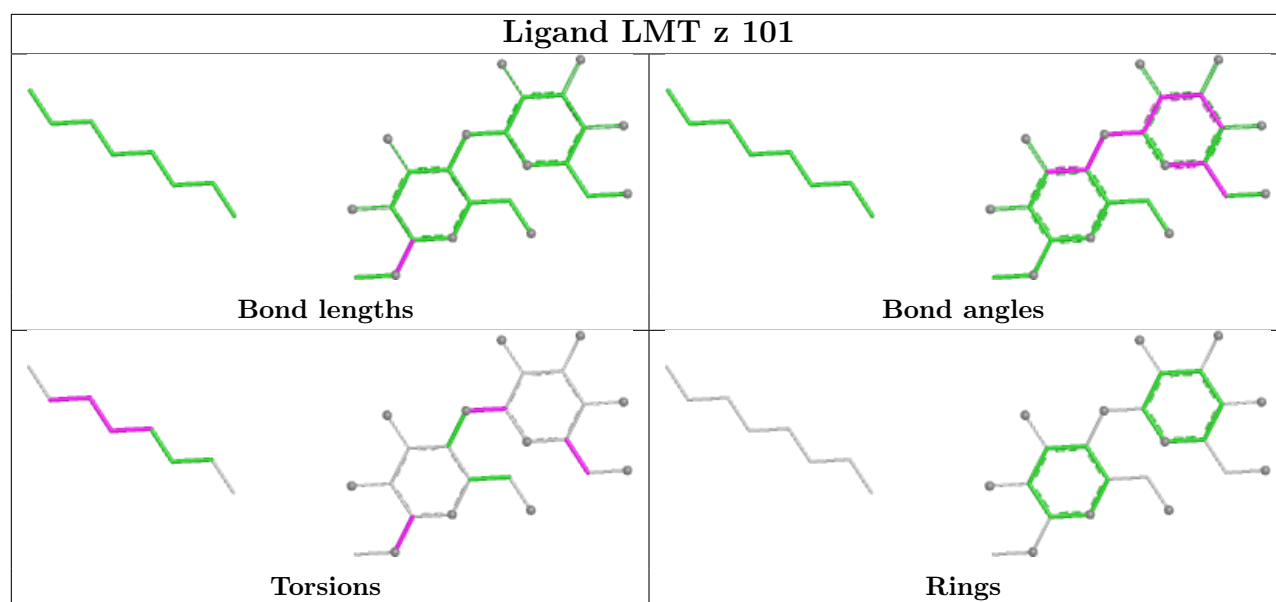


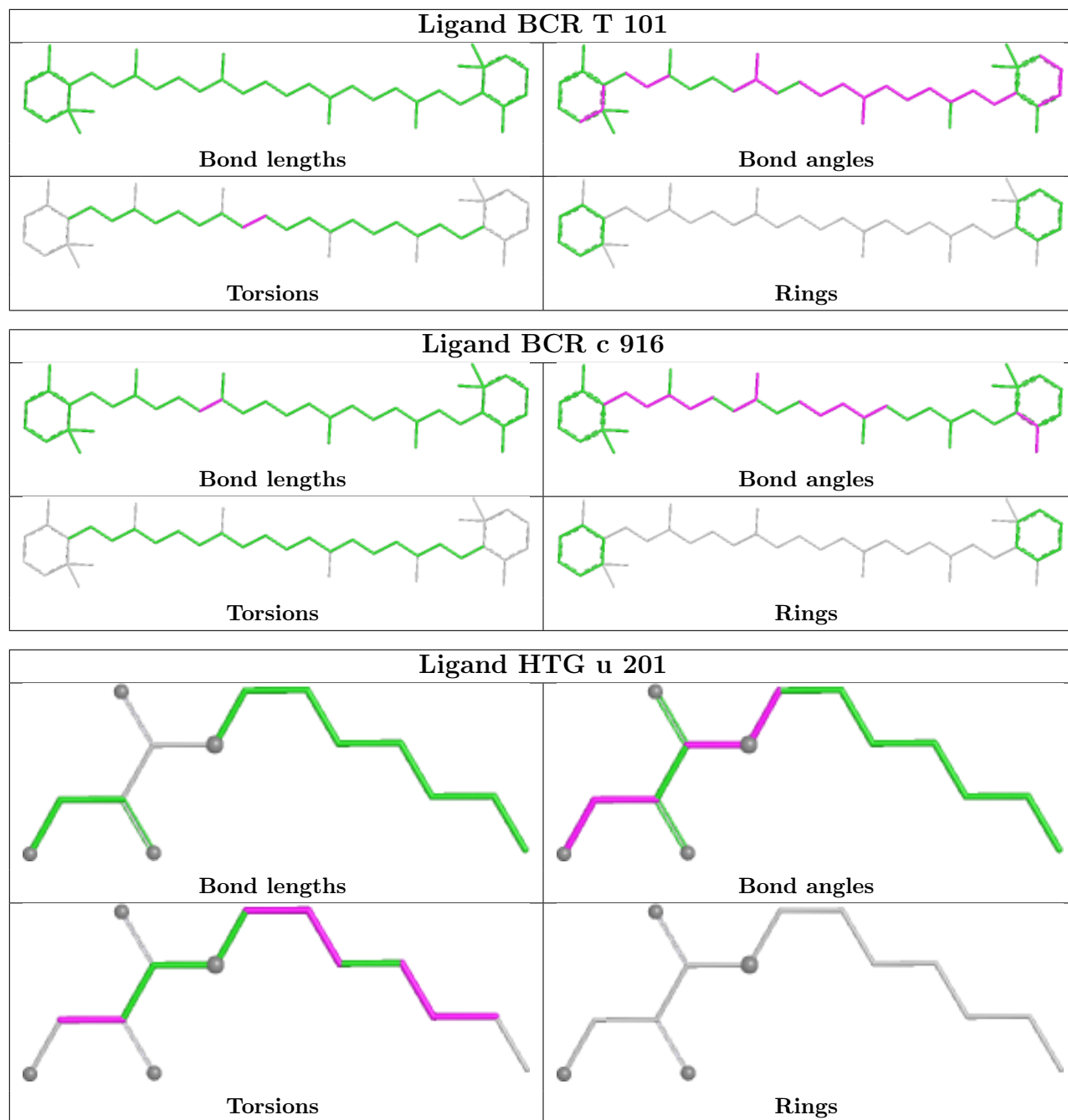


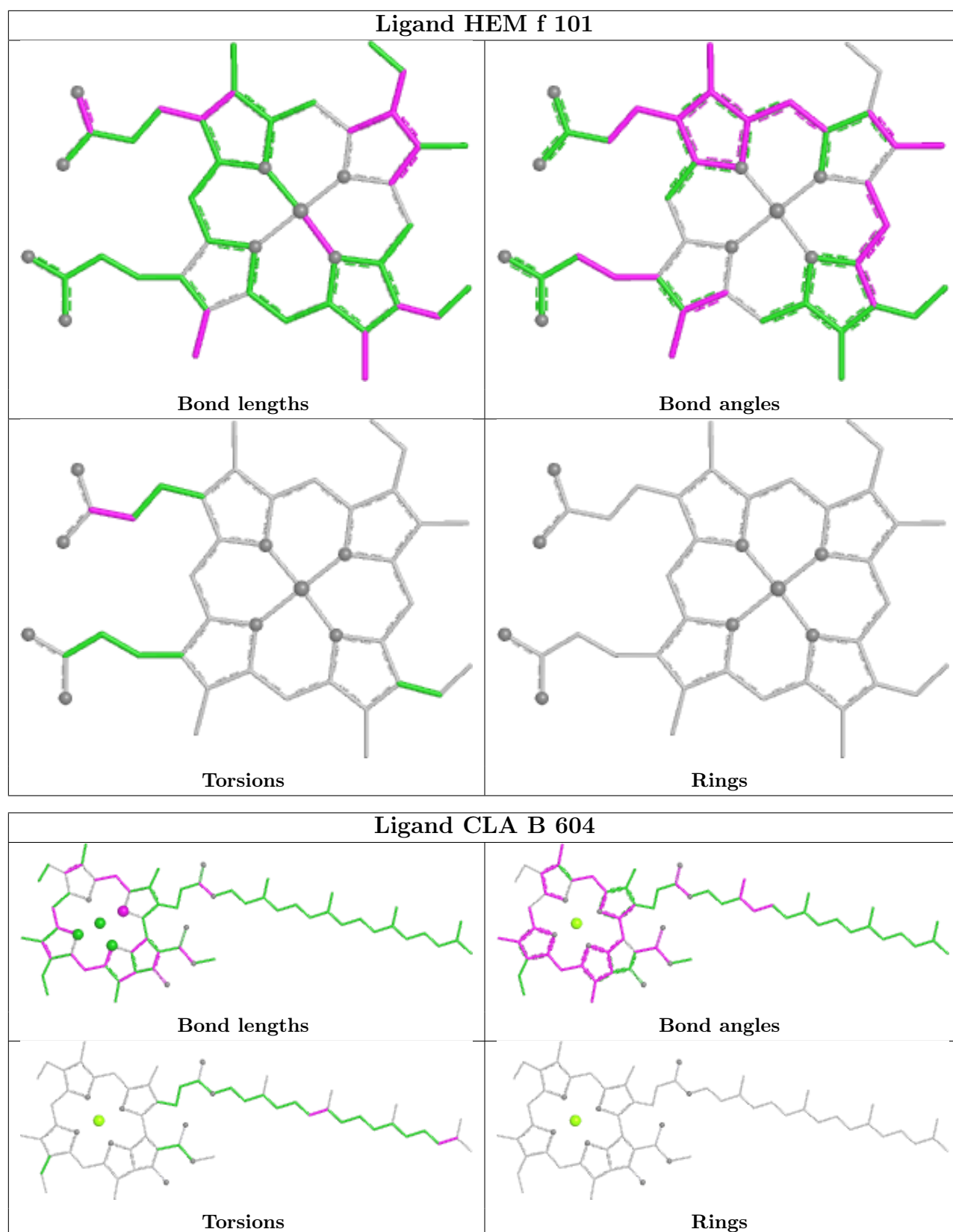


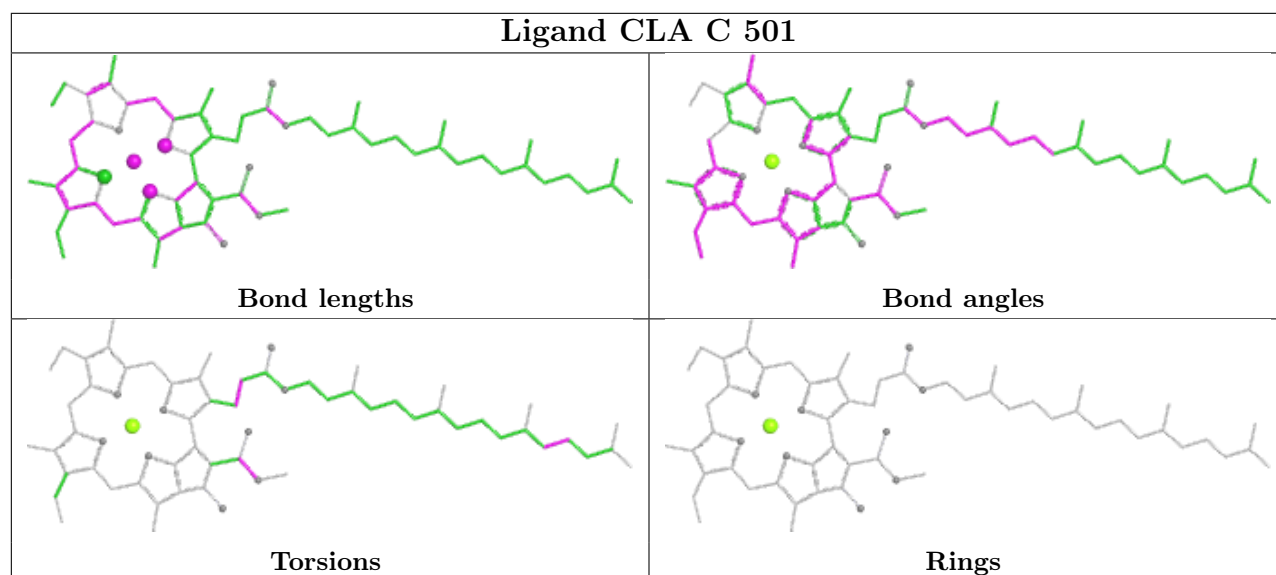
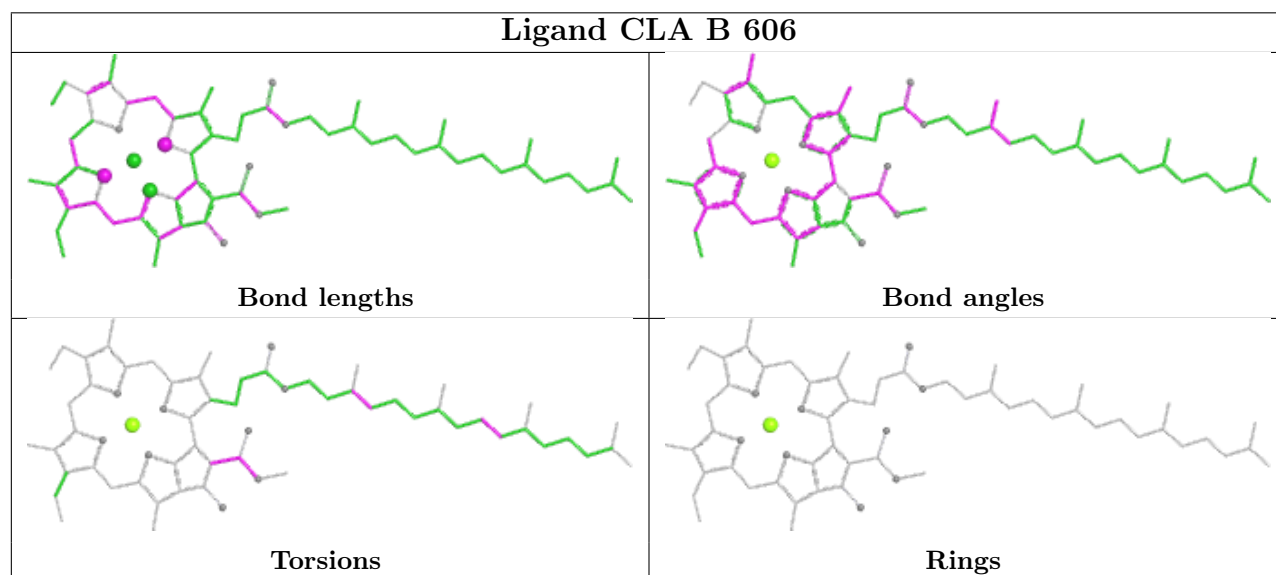
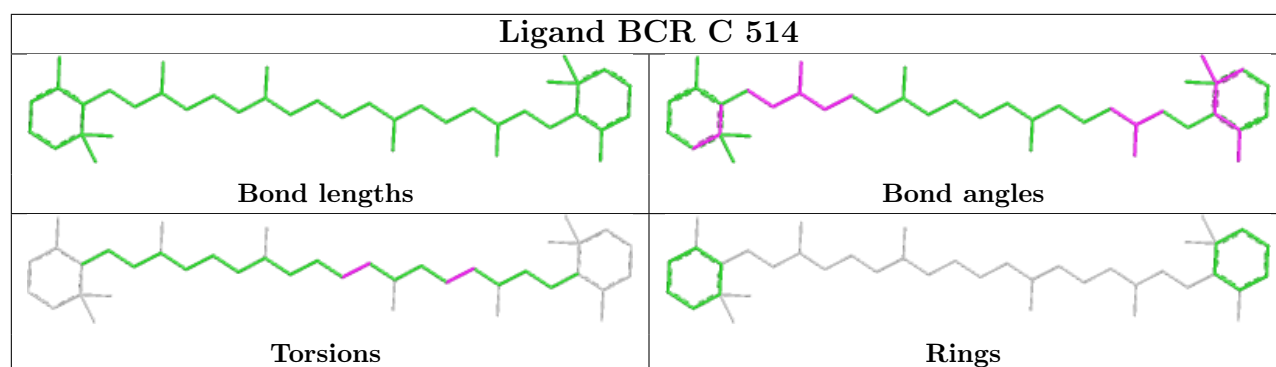


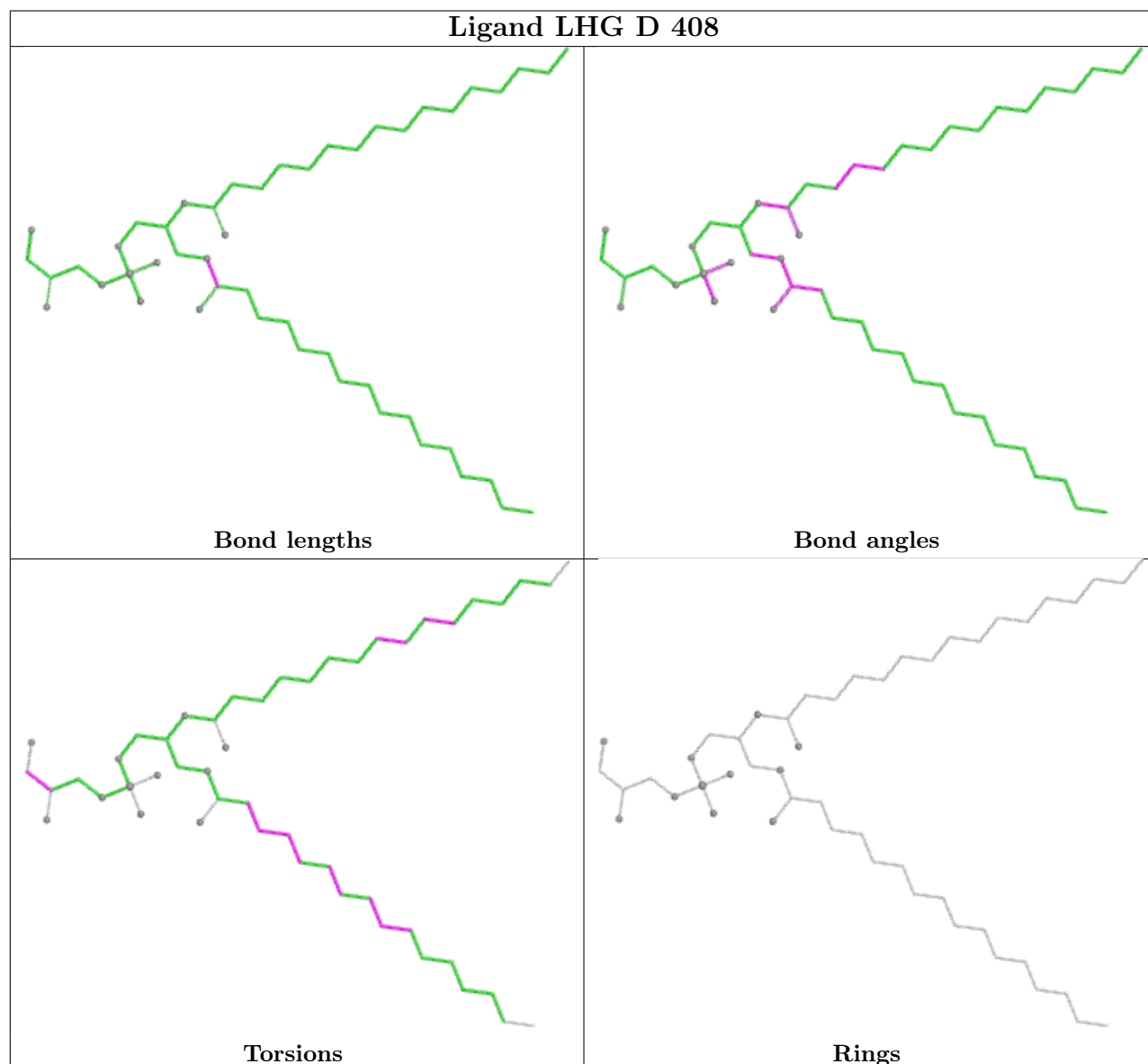
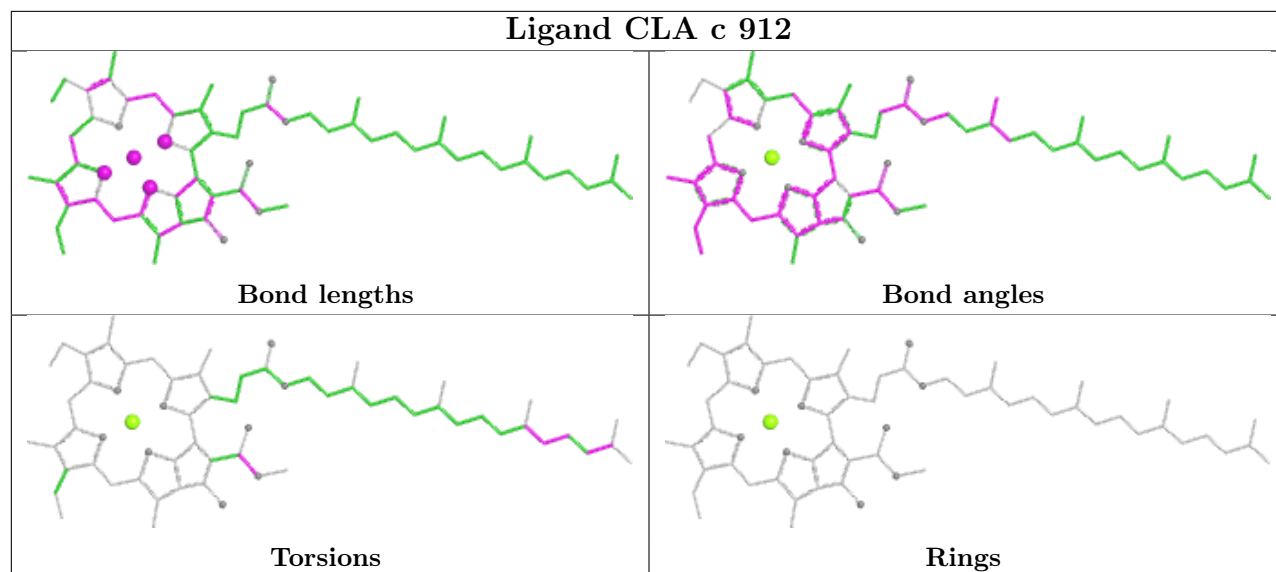












5.7 Other polymers [i](#)

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%)	-0.18	4 (1%) 79 81	16, 23, 46, 69	0
1	a	334/344 (97%)	-0.00	13 (3%) 39 42	18, 24, 50, 76	0
2	B	504/504 (100%)	0.07	39 (7%) 13 15	18, 27, 54, 88	0
2	b	501/504 (99%)	0.10	43 (8%) 10 12	20, 29, 58, 119	0
3	C	451/455 (99%)	-0.11	14 (3%) 49 51	21, 31, 46, 81	0
3	c	455/455 (100%)	0.14	25 (5%) 25 28	23, 34, 48, 79	0
4	D	340/342 (99%)	-0.23	7 (2%) 63 66	17, 24, 40, 70	0
4	d	340/342 (99%)	-0.19	6 (1%) 68 71	19, 26, 45, 80	0
5	E	81/83 (97%)	0.92	17 (20%) 1 1	27, 40, 62, 82	0
5	e	79/83 (95%)	1.19	22 (27%) 0 0	32, 44, 72, 82	0
6	F	34/44 (77%)	0.20	5 (14%) 2 2	26, 34, 63, 74	0
6	f	32/44 (72%)	0.35	3 (9%) 8 9	29, 37, 76, 86	0
7	H	63/63 (100%)	-0.08	1 (1%) 72 74	24, 33, 43, 70	0
7	h	63/63 (100%)	0.37	5 (7%) 12 14	27, 37, 51, 81	0
8	I	35/38 (92%)	-0.11	0 100 100	27, 34, 64, 86	0
8	i	37/38 (97%)	0.21	2 (5%) 25 29	26, 34, 71, 83	0
9	J	36/40 (90%)	0.14	4 (11%) 5 6	26, 38, 65, 79	0
9	j	39/40 (97%)	0.60	8 (20%) 1 1	30, 42, 68, 84	0
10	K	37/37 (100%)	-0.17	0 100 100	32, 38, 47, 63	0
10	k	37/37 (100%)	0.30	3 (8%) 12 13	36, 42, 55, 69	0
11	L	37/37 (100%)	-0.14	3 (8%) 12 13	17, 22, 65, 75	0
11	l	37/37 (100%)	0.14	2 (5%) 25 29	19, 23, 64, 95	0
12	M	32/36 (88%)	-0.17	1 (3%) 49 51	21, 24, 40, 56	0
12	m	33/36 (91%)	-0.01	2 (6%) 21 24	20, 25, 48, 68	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/244 (100%)	0.31	34 (13%) 2 3	18, 33, 66, 120	0
13	o	241/244 (98%)	0.38	39 (16%) 1 1	20, 35, 71, 87	0
14	T	29/32 (90%)	-0.01	1 (3%) 45 48	19, 23, 49, 85	0
14	t	29/32 (90%)	-0.01	1 (3%) 45 48	20, 23, 47, 72	0
15	U	97/104 (93%)	-0.13	0 100 100	23, 30, 52, 58	0
15	u	97/104 (93%)	-0.36	1 (1%) 82 84	24, 30, 40, 66	0
16	V	137/137 (100%)	-0.37	0 100 100	22, 28, 43, 51	0
16	v	137/137 (100%)	0.44	13 (9%) 8 9	26, 37, 52, 72	0
17	Y	27/30 (90%)	1.04	4 (14%) 2 2	37, 47, 70, 77	0
17	y	28/30 (93%)	1.15	7 (25%) 0 0	45, 55, 73, 77	0
18	X	38/40 (95%)	0.69	7 (18%) 1 1	32, 39, 65, 69	0
18	x	38/40 (95%)	0.93	9 (23%) 0 0	34, 42, 83, 94	0
19	Z	62/62 (100%)	1.46	19 (30%) 0 0	37, 46, 75, 92	0
19	z	60/62 (96%)	1.95	25 (41%) 0 0	47, 57, 88, 95	0
All	All	5235/5344 (97%)	0.11	389 (7%) 14 16	16, 30, 59, 120	0

The worst 5 of 389 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	494	GLY	8.3
2	b	496	TYR	8.1
18	x	37	VAL	7.9
13	o	246	ALA	7.4
13	O	60	ARG	7.4

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
12	FME	m	1	10/11	0.92	0.12	31,38,54,60	0
14	FME	t	1	10/11	0.95	0.09	20,23,41,50	0
4	HSK	d	336[B]	11/12	0.96	0.10	30,31,37,38	8

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	FME	M	1	10/11	0.96	0.11	27,34,51,59	0
4	HSK	d	336[A]	10/12	0.96	0.10	30,33,40,44	7
8	FME	I	1	10/11	0.97	0.13	27,34,38,39	0
14	FME	T	1	10/11	0.97	0.08	24,27,43,50	0
8	FME	i	1	10/11	0.98	0.11	30,32,37,39	0
4	HSK	D	336[B]	11/12	0.98	0.10	23,26,27,29	8
4	HSK	D	336[A]	10/12	0.98	0.10	26,28,31,34	7

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
34	DGD	D	406	53/66	0.54	0.29	53,77,92,103	0
31	GOL	h	103	6/6	0.56	0.28	78,83,83,84	0
29	UNL	a	420	40/-	0.56	0.33	53,72,88,94	0
33	HTG	d	401	19/19	0.57	0.30	55,101,111,114	0
29	UNL	E	103	12/-	0.59	0.29	65,73,83,88	0
29	UNL	A	415	36/-	0.60	0.25	58,67,75,79	0
34	DGD	d	406	50/66	0.62	0.26	56,75,94,97	0
29	UNL	E	102	15/-	0.63	0.23	57,64,83,83	0
30	LMT	M	102	35/35	0.63	0.24	35,52,60,63	0
26	SQD	B	621	54/54	0.63	0.27	48,65,108,109	0
29	UNL	i	103	13/-	0.66	0.29	58,65,76,78	0
29	UNL	B	629	14/-	0.66	0.27	61,70,89,90	0
33	HTG	b	602	19/19	0.67	0.28	50,93,111,117	0
30	LMT	M	101	35/35	0.68	0.24	43,61,77,90	0
33	HTG	B	631	19/19	0.68	0.26	49,111,120,125	0
29	UNL	C	523	34/-	0.69	0.28	52,77,88,93	0
36	LHG	a	417	40/49	0.69	0.26	60,109,148,151	0
30	LMT	b	624	25/35	0.70	0.21	51,71,94,98	0
30	LMT	F	102	35/35	0.70	0.36	53,84,91,96	0
29	UNL	j	103	12/-	0.71	0.25	55,65,70,71	0
29	UNL	t	103	16/-	0.71	0.46	63,74,94,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
33	HTG	D	414	19/19	0.71	0.31	66,93,106,107	0
26	SQD	L	103	54/54	0.71	0.24	43,64,89,96	0
29	UNL	b	631	16/-	0.72	0.23	59,66,77,79	0
27	LMG	Z	101	51/55	0.73	0.27	41,76,102,113	0
30	LMT	m	101	35/35	0.73	0.22	32,51,61,62	0
27	LMG	c	921	51/55	0.74	0.27	38,80,95,111	0
33	HTG	b	627	19/19	0.74	0.34	53,94,104,105	0
29	UNL	Z	103	16/-	0.74	0.21	48,63,81,81	0
33	HTG	B	626	19/19	0.74	0.42	48,87,92,93	0
29	UNL	c	925	30/-	0.74	0.18	59,72,89,95	0
30	LMT	B	623	35/35	0.74	0.24	43,79,117,129	0
29	UNL	H	103	10/-	0.75	0.23	60,69,74,76	0
33	HTG	C	522	19/19	0.75	0.34	50,79,92,94	0
30	LMT	J	102	24/35	0.75	0.19	45,55,79,83	0
29	UNL	c	926	10/-	0.75	0.17	65,67,71,72	0
28	PL9	a	419	55/55	0.75	0.23	52,74,98,109	0
29	UNL	i	104	10/-	0.75	0.28	67,72,77,78	0
27	LMG	a	418	51/55	0.75	0.22	43,60,68,73	0
29	UNL	b	630	16/-	0.75	0.39	51,62,73,74	0
26	SQD	a	401	54/54	0.75	0.18	45,59,85,90	0
30	LMT	m	102	35/35	0.76	0.19	41,54,72,84	0
29	UNL	e	800	11/-	0.76	0.29	53,60,68,68	0
28	PL9	A	414	55/55	0.76	0.26	47,66,93,96	0
29	UNL	I	101	13/-	0.77	0.22	44,53,61,63	0
29	UNL	z	102	16/-	0.77	0.22	51,70,89,92	0
29	UNL	J	103	14/-	0.77	0.16	61,66,73,76	0
30	LMT	c	922	35/35	0.78	0.32	61,73,85,90	0
33	HTG	c	924	19/19	0.78	0.41	53,85,97,100	0
29	UNL	B	632	16/-	0.78	0.32	50,59,73,73	0
29	UNL	T	102	13/-	0.78	0.54	66,70,83,87	0
30	LMT	t	102	24/35	0.78	0.26	33,55,94,95	0
30	LMT	b	625	24/35	0.78	0.25	35,61,99,100	0
30	LMT	Z	102	35/35	0.79	0.27	41,87,102,107	0
27	LMG	A	413	51/55	0.79	0.24	42,57,76,78	0
29	UNL	i	102	16/-	0.79	0.23	54,65,83,84	0
30	LMT	z	101	32/35	0.79	0.24	46,85,90,100	0
33	HTG	U	201	9/19	0.79	0.23	54,59,82,98	0
29	UNL	D	412	40/-	0.79	0.20	39,60,96,99	0
31	GOL	O	304	6/6	0.80	0.17	52,60,61,63	0
29	UNL	j	102	16/-	0.80	0.17	52,61,69,69	0
26	SQD	f	102	33/54	0.81	0.21	63,73,113,114	0
26	SQD	A	418	54/54	0.81	0.19	42,59,81,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	GOL	b	635	6/6	0.81	0.14	40,43,46,48	0
29	UNL	A	417	13/-	0.81	0.35	56,59,66,66	0
26	SQD	D	407	45/54	0.82	0.28	50,78,94,101	0
29	UNL	b	628	36/-	0.82	0.26	44,65,101,106	0
27	LMG	c	920	51/55	0.82	0.23	30,65,100,104	0
36	LHG	E	101	49/49	0.82	0.21	50,80,94,97	0
32	CA	B	601	1/1	0.82	0.09	81,81,81,81	0
29	UNL	B	627	16/-	0.83	0.14	43,47,69,69	0
33	HTG	u	201	14/19	0.83	0.25	46,64,90,96	0
30	LMT	C	520	35/35	0.83	0.31	52,71,83,89	0
40	SO4	O	302	5/5	0.83	0.29	78,87,95,105	0
33	HTG	B	630	19/19	0.84	0.15	39,52,66,79	0
29	UNL	I	102	11/-	0.84	0.22	62,65,66,68	0
30	LMT	a	402	35/35	0.84	0.17	37,54,69,80	0
33	HTG	c	923	19/19	0.85	0.24	64,75,82,83	0
31	GOL	a	424	6/6	0.85	0.20	42,56,59,74	0
29	UNL	M	103	16/-	0.85	0.23	49,58,77,79	0
31	GOL	c	927	6/6	0.86	0.13	43,53,60,68	0
29	UNL	J	104	12/-	0.86	0.17	53,65,72,74	0
29	UNL	d	411	16/-	0.86	0.32	39,49,63,66	0
27	LMG	C	519	51/55	0.86	0.19	29,59,97,105	0
29	UNL	B	628	10/-	0.86	0.27	52,56,70,74	0
33	HTG	b	601	19/19	0.87	0.15	43,51,62,68	0
27	LMG	B	622	51/55	0.87	0.18	28,37,53,63	0
30	LMT	A	419	35/35	0.87	0.15	37,56,73,94	0
31	GOL	b	636	6/6	0.87	0.12	45,56,58,60	0
34	DGD	h	102	62/66	0.88	0.18	27,35,45,52	0
23	CLA	B	610	65/65	0.88	0.13	23,28,33,35	0
31	GOL	A	422	6/6	0.88	0.13	42,55,58,67	0
38	RRX	H	101	41/41	0.88	0.14	25,30,44,47	0
38	RRX	h	101	41/41	0.88	0.12	27,35,49,54	0
27	LMG	b	623	51/55	0.88	0.19	30,39,52,63	0
29	UNL	b	629	16/-	0.89	0.11	43,48,56,60	0
31	GOL	l	102	6/6	0.89	0.38	37,55,57,57	0
31	GOL	C	526	6/6	0.89	0.14	38,43,51,57	0
29	UNL	D	413	16/-	0.89	0.26	39,47,65,65	0
23	CLA	b	612	65/65	0.89	0.13	26,30,36,38	0
29	UNL	L	102	14/-	0.89	0.22	52,58,66,69	0
29	UNL	a	421	10/-	0.89	0.29	53,57,61,64	0
25	BCR	k	102	40/40	0.89	0.13	29,41,48,50	0
23	CLA	C	506	65/65	0.90	0.13	25,38,94,97	0
23	CLA	c	914	65/65	0.90	0.15	38,53,90,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	CA	b	603	1/1	0.90	0.09	82,82,82,82	0
29	UNL	A	416	16/-	0.90	0.14	41,46,73,73	0
34	DGD	c	919	62/66	0.91	0.14	25,35,60,71	0
26	SQD	a	416	54/54	0.91	0.17	37,55,88,90	0
29	UNL	x	101	16/-	0.91	0.15	36,45,70,73	0
31	GOL	C	524	6/6	0.91	0.17	36,45,47,53	0
29	UNL	X	101	16/-	0.91	0.12	34,39,58,60	0
31	GOL	L	104	6/6	0.91	0.26	44,52,54,55	0
31	GOL	f	104	6/6	0.91	0.33	46,51,51,54	0
34	DGD	H	102	62/66	0.91	0.20	24,31,40,45	0
33	HTG	V	202	13/19	0.92	0.26	43,48,76,84	0
34	DGD	c	918	62/66	0.92	0.15	27,35,79,91	0
27	LMG	d	410	51/55	0.92	0.12	29,36,80,91	0
23	CLA	b	609	65/65	0.92	0.11	23,31,57,63	0
23	CLA	B	602	65/65	0.92	0.18	29,41,78,95	0
23	CLA	B	603	65/65	0.92	0.14	23,26,34,37	0
33	HTG	C	521	19/19	0.92	0.18	56,63,76,80	0
36	LHG	l	101	49/49	0.92	0.17	22,31,47,57	0
29	UNL	i	101	16/-	0.92	0.13	40,46,56,62	0
25	BCR	c	915	40/40	0.92	0.10	44,51,59,60	0
29	UNL	a	403	6/-	0.92	0.42	57,62,66,66	0
31	GOL	b	633	6/6	0.93	0.23	41,46,49,52	0
23	CLA	c	913	65/65	0.93	0.12	33,45,67,72	0
31	GOL	B	637	6/6	0.93	0.13	36,38,45,54	0
31	GOL	B	638	6/6	0.93	0.10	35,47,49,53	0
23	CLA	b	605	65/65	0.93	0.12	24,29,36,39	0
27	LMG	D	411	51/55	0.93	0.17	23,35,91,99	0
23	CLA	C	513	65/65	0.93	0.13	35,46,78,83	0
29	UNL	A	420	4/-	0.93	0.53	64,66,66,66	0
23	CLA	b	604	65/65	0.93	0.17	34,47,73,81	0
33	HTG	B	625	19/19	0.94	0.15	31,38,71,75	0
25	BCR	c	916	40/40	0.94	0.10	28,36,45,47	0
34	DGD	C	516	62/66	0.94	0.20	22,32,85,87	0
34	DGD	C	517	62/66	0.94	0.14	22,31,78,92	0
25	BCR	d	404	40/40	0.94	0.10	25,33,56,58	0
25	BCR	k	101	40/40	0.94	0.09	33,39,47,49	0
34	DGD	c	917	62/66	0.94	0.15	24,33,77,80	0
23	CLA	c	904	65/65	0.94	0.15	24,37,42,42	0
26	SQD	A	412	54/54	0.94	0.14	35,54,71,74	0
23	CLA	c	905	65/65	0.94	0.18	24,31,64,66	0
23	CLA	c	907	65/65	0.94	0.09	28,36,76,80	0
36	LHG	D	408	49/49	0.94	0.16	26,35,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	GOL	c	928	6/6	0.94	0.22	42,51,54,54	0
36	LHG	L	101	49/49	0.94	0.14	22,31,44,49	0
31	GOL	B	635	6/6	0.94	0.12	38,47,49,50	0
36	LHG	d	407	49/49	0.94	0.23	27,36,46,49	0
23	CLA	c	908	65/65	0.94	0.12	26,32,52,55	0
23	CLA	C	512	65/65	0.94	0.10	34,41,69,74	0
23	CLA	B	607	65/65	0.94	0.10	21,27,55,61	0
23	CLA	c	902	65/65	0.94	0.13	27,34,46,50	0
28	PL9	d	405	55/55	0.95	0.16	19,25,30,34	0
31	GOL	B	633	6/6	0.95	0.13	34,39,47,52	0
31	GOL	c	930	6/6	0.95	0.21	49,54,57,59	0
23	CLA	b	618	65/65	0.95	0.08	24,30,49,53	0
31	GOL	B	636	6/6	0.95	0.14	33,43,47,56	0
25	BCR	t	101	40/40	0.95	0.14	23,30,42,44	0
31	GOL	v	203	6/6	0.95	0.15	31,35,41,43	0
31	GOL	v	204	6/6	0.95	0.25	46,50,61,62	0
25	BCR	B	619	40/40	0.95	0.19	19,26,42,45	0
32	CA	O	301	1/1	0.95	0.14	49,49,49,49	0
25	BCR	B	620	40/40	0.95	0.09	22,31,41,44	0
32	CA	o	301	1/1	0.95	0.11	51,51,51,51	0
25	BCR	C	514	40/40	0.95	0.08	33,42,46,46	0
25	BCR	K	101	40/40	0.95	0.10	30,35,40,43	0
25	BCR	b	622	40/40	0.95	0.10	25,33,43,45	0
31	GOL	V	203	6/6	0.95	0.15	26,32,36,38	0
31	GOL	V	204	6/6	0.95	0.26	39,52,59,59	0
31	GOL	a	422	6/6	0.95	0.10	30,38,44,45	0
23	CLA	C	507	65/65	0.95	0.10	26,33,56,61	0
36	LHG	d	408	49/49	0.95	0.14	22,27,42,47	0
31	GOL	b	632	6/6	0.95	0.11	35,42,46,47	0
23	CLA	c	903	65/65	0.95	0.19	22,29,42,55	0
23	CLA	c	912	65/65	0.95	0.09	29,37,45,50	0
23	CLA	C	511	65/65	0.95	0.09	27,34,40,42	0
23	CLA	b	615	65/65	0.96	0.14	19,27,33,38	0
33	HTG	B	624	19/19	0.96	0.09	27,33,41,51	0
23	CLA	b	617	65/65	0.96	0.14	20,25,71,83	0
31	GOL	B	634	6/6	0.96	0.10	29,29,34,37	0
23	CLA	A	410	65/65	0.96	0.11	20,24,99,105	0
23	CLA	b	619	65/65	0.96	0.12	25,32,89,97	0
23	CLA	B	611	65/65	0.96	0.14	19,25,34,39	0
23	CLA	C	508	65/65	0.96	0.14	24,29,73,81	0
23	CLA	C	509	65/65	0.96	0.13	27,31,47,51	0
23	CLA	C	510	65/65	0.96	0.15	22,28,38,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	GOL	D	415	6/6	0.96	0.20	35,36,42,46	0
23	CLA	c	906	65/65	0.96	0.10	26,31,46,50	0
23	CLA	B	612	65/65	0.96	0.13	18,21,34,37	0
33	HTG	b	626	19/19	0.96	0.17	29,40,73,75	0
23	CLA	B	615	65/65	0.96	0.11	19,24,67,74	0
23	CLA	B	617	65/65	0.96	0.10	20,28,79,83	0
23	CLA	D	402	65/65	0.96	0.11	13,18,36,39	0
31	GOL	a	423	6/6	0.96	0.14	33,34,35,45	0
23	CLA	D	403	65/65	0.96	0.11	22,28,73,79	0
25	BCR	B	618	40/40	0.96	0.15	20,26,29,30	0
23	CLA	C	501	65/65	0.96	0.14	25,32,46,53	0
34	DGD	C	518	62/66	0.96	0.15	20,30,68,75	0
31	GOL	b	634	6/6	0.96	0.12	32,39,44,46	0
23	CLA	C	503	65/65	0.96	0.12	26,31,38,39	0
23	CLA	b	606	65/65	0.96	0.12	20,26,37,42	0
25	BCR	C	515	40/40	0.96	0.14	28,34,41,44	0
25	BCR	D	404	40/40	0.96	0.16	24,29,55,57	0
23	CLA	b	607	65/65	0.96	0.16	20,25,54,59	0
25	BCR	K	102	40/40	0.96	0.08	28,31,39,42	0
35	BCT	a	408	4/4	0.96	0.10	30,32,37,46	0
25	BCR	T	101	40/40	0.96	0.16	24,32,47,53	0
36	LHG	D	409	49/49	0.96	0.12	22,28,40,44	0
25	BCR	a	415	40/40	0.96	0.07	21,25,30,31	0
31	GOL	v	202	6/6	0.96	0.10	35,36,40,41	0
25	BCR	b	621	40/40	0.96	0.20	21,28,43,46	0
23	CLA	C	504	65/65	0.96	0.15	23,28,62,68	0
23	CLA	C	505	65/65	0.96	0.14	26,31,47,51	0
36	LHG	d	409	49/49	0.96	0.16	27,32,85,91	0
32	CA	F	103	1/1	0.96	0.15	55,55,55,55	0
23	CLA	b	613	65/65	0.96	0.13	24,28,35,40	0
31	GOL	A	421	6/6	0.96	0.13	30,37,38,41	0
32	CA	c	901	1/1	0.96	0.07	46,46,46,46	0
23	CLA	B	616	65/65	0.97	0.10	23,28,48,50	0
23	CLA	B	606	65/65	0.97	0.15	17,23,35,40	0
23	CLA	A	405	65/65	0.97	0.10	14,19,25,42	0
23	CLA	C	502	65/65	0.97	0.14	21,26,39,48	0
23	CLA	B	608	65/65	0.97	0.14	17,20,34,37	0
23	CLA	a	414	65/65	0.97	0.09	19,25,99,104	0
23	CLA	B	609	65/65	0.97	0.16	18,24,31,34	0
23	CLA	A	406	65/65	0.97	0.09	13,18,29,39	0
23	CLA	A	407	65/65	0.97	0.16	18,21,80,92	0
25	BCR	b	620	40/40	0.97	0.16	23,27,33,33	0

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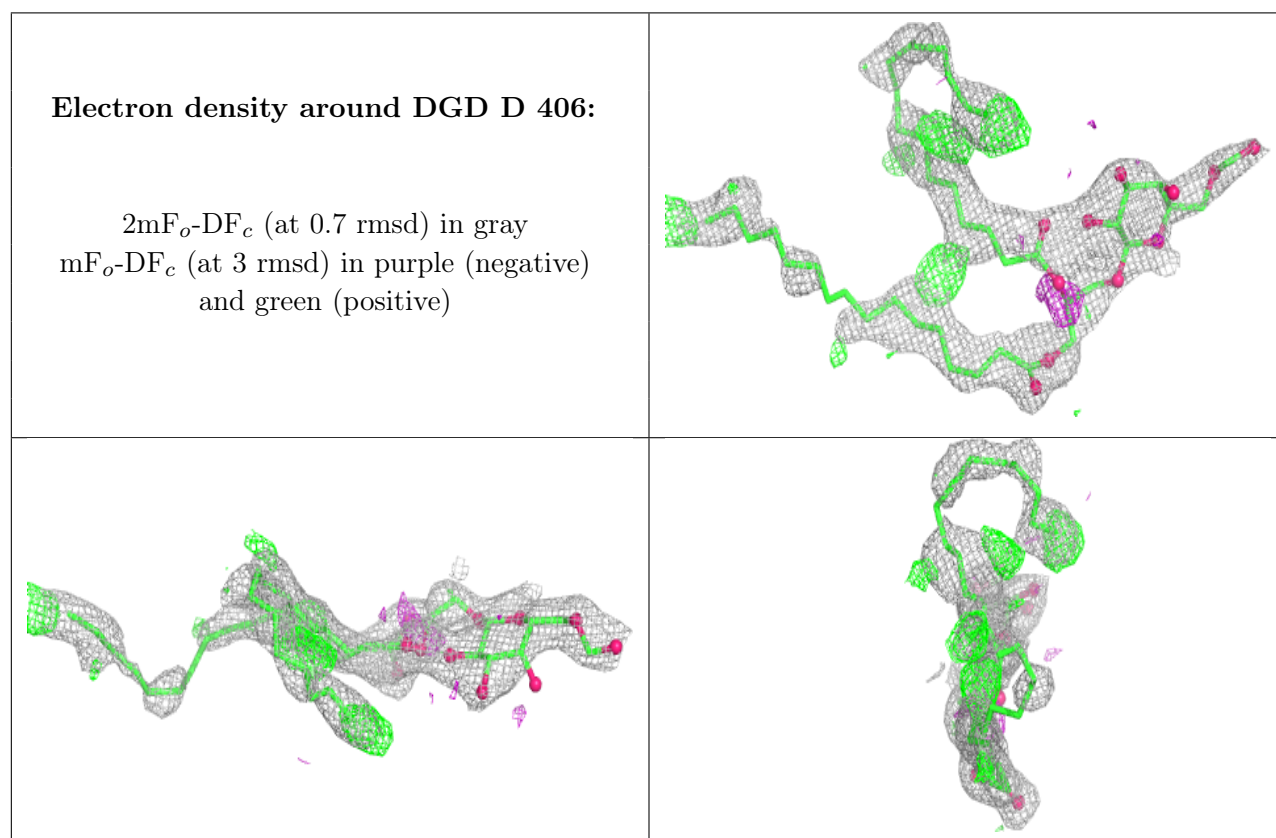
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	B	604	65/65	0.97	0.14	17,22,34,41	0
23	CLA	B	613	65/65	0.97	0.14	19,24,31,34	0
32	CA	f	103	1/1	0.97	0.18	56,56,56,56	0
23	CLA	c	909	65/65	0.97	0.18	25,30,82,98	0
28	PL9	D	405	55/55	0.97	0.10	18,23,31,38	0
23	CLA	c	910	65/65	0.97	0.18	25,31,49,52	0
31	GOL	V	205	6/6	0.97	0.23	33,36,37,41	0
23	CLA	c	911	65/65	0.97	0.22	24,30,41,45	0
36	LHG	D	410	46/49	0.97	0.14	24,32,82,87	0
23	CLA	b	610	65/65	0.97	0.15	18,23,32,35	0
23	CLA	B	614	65/65	0.97	0.17	18,23,48,54	0
23	CLA	B	605	65/65	0.97	0.18	19,22,53,55	0
23	CLA	d	403	65/65	0.97	0.08	25,32,83,90	0
33	HTG	O	303	19/19	0.97	0.09	27,32,50,52	0
24	PHO	A	408	64/64	0.97	0.11	16,21,25,27	0
24	PHO	A	409	64/64	0.97	0.14	19,22,29,37	0
37	HEM	F	101	43/43	0.97	0.12	36,42,49,52	0
24	PHO	a	413	64/64	0.97	0.13	19,25,30,35	0
25	BCR	A	411	40/40	0.97	0.12	21,26,33,36	0
23	CLA	b	614	65/65	0.97	0.17	20,24,36,45	0
23	CLA	a	411	65/65	0.98	0.14	18,23,106,117	0
23	CLA	d	402	65/65	0.98	0.12	18,21,39,44	0
23	CLA	a	409	65/65	0.98	0.12	18,21,31,43	0
23	CLA	b	616	65/65	0.98	0.20	20,24,46,50	0
23	CLA	b	611	65/65	0.98	0.18	22,27,39,43	0
31	GOL	C	525	6/6	0.98	0.15	26,26,27,29	0
35	BCT	D	401	4/4	0.98	0.08	32,35,41,51	0
24	PHO	a	412	64/64	0.98	0.12	17,22,26,27	0
37	HEM	f	101	43/43	0.98	0.19	39,47,61,77	0
37	HEM	v	201	43/43	0.98	0.08	25,31,35,38	0
31	GOL	A	423	6/6	0.98	0.25	39,43,45,53	0
23	CLA	a	410	65/65	0.98	0.13	17,20,28,34	0
23	CLA	b	608	65/65	0.98	0.11	20,24,33,34	0
37	HEM	V	201	43/43	0.99	0.07	22,24,28,33	0
21	FE2	a	405	1/1	0.99	0.06	27,27,27,27	0
22	CL	A	403	1/1	0.99	0.06	25,25,25,25	0
22	CL	A	404	1/1	0.99	0.13	22,22,22,22	0
31	GOL	c	929	6/6	0.99	0.15	25,27,30,30	0
39	MG	J	101	1/1	0.99	0.09	28,28,28,28	0
39	MG	j	101	1/1	0.99	0.17	35,35,35,35	0
22	CL	a	407	1/1	0.99	0.12	27,27,27,27	0
20	OEX	a	404	10/10	1.00	0.07	22,26,28,29	0

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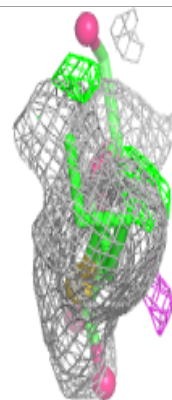
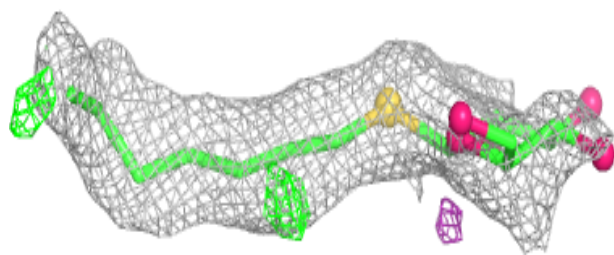
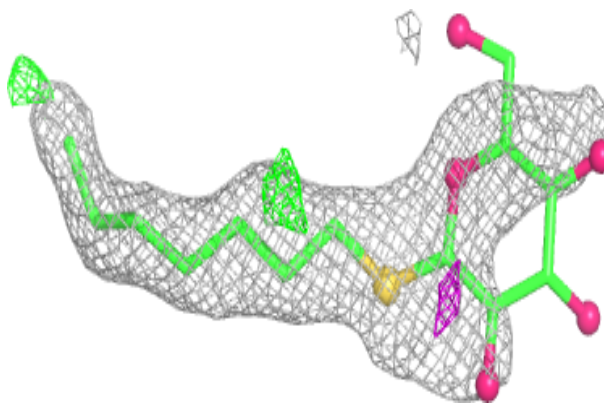
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	FE2	A	402	1/1	1.00	0.06	26,26,26,26	0
22	CL	a	406	1/1	1.00	0.04	29,29,29,29	0
20	OEX	A	401	10/10	1.00	0.07	21,23,27,28	0

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.

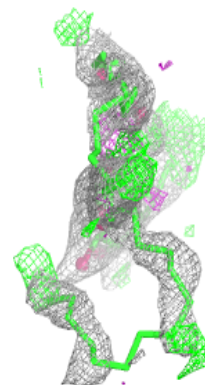
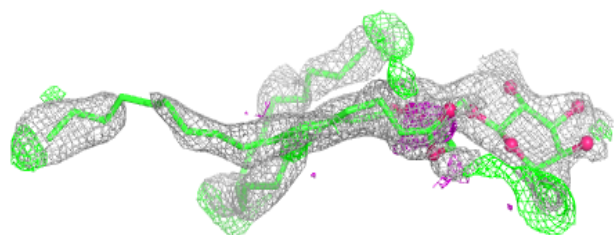
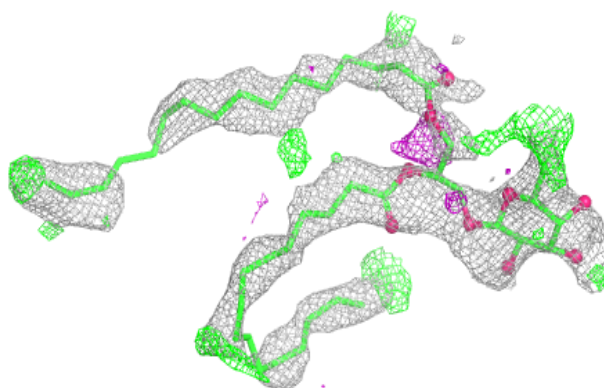


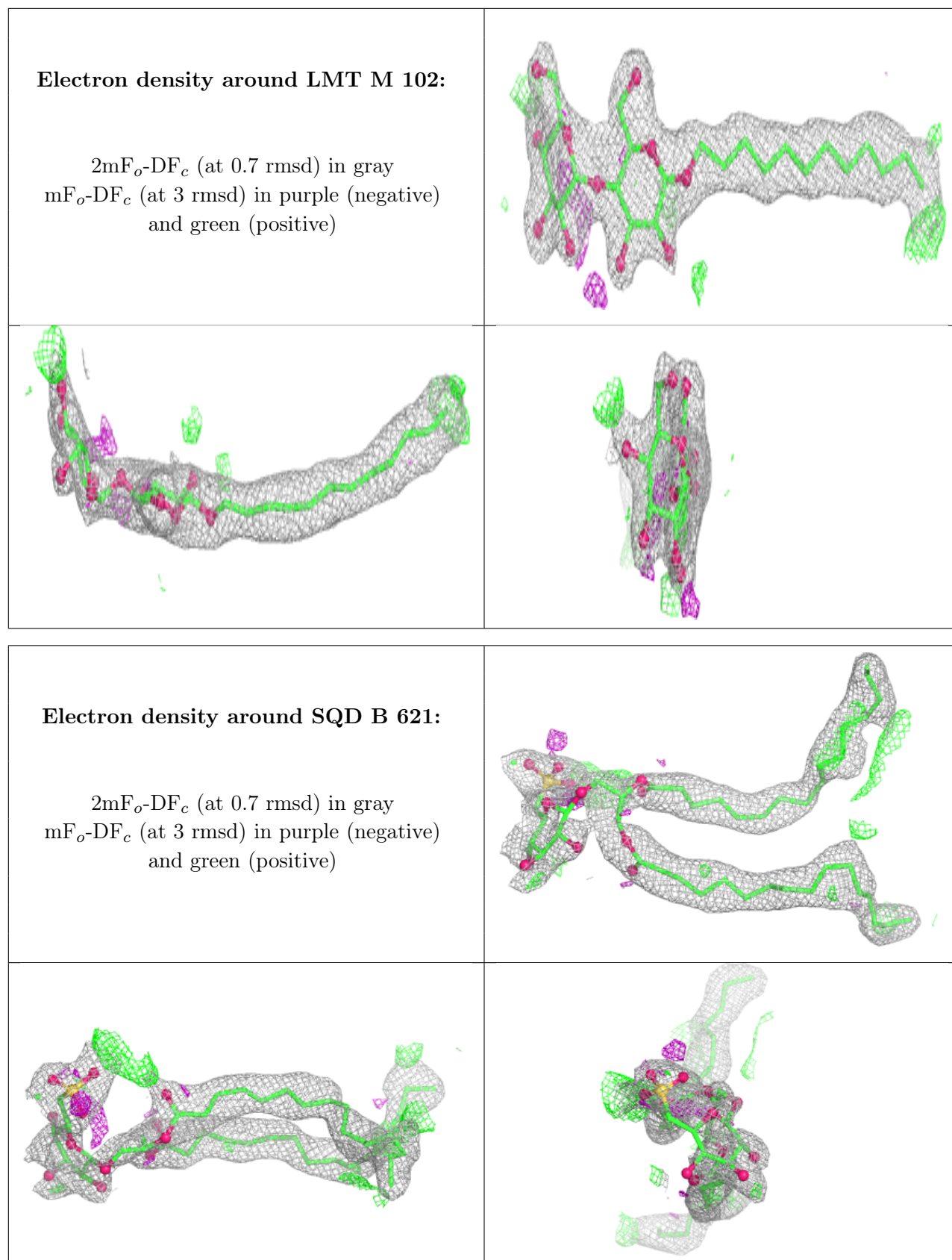
Electron density around HTG d 401:

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

**Electron density around DGD d 406:**

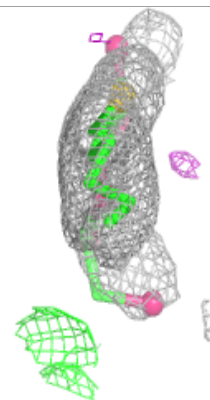
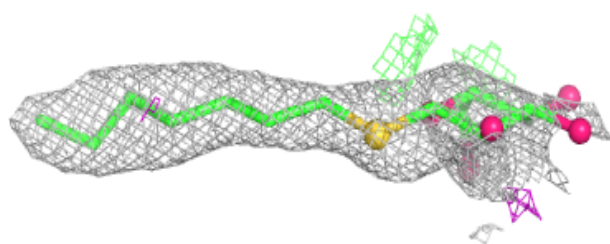
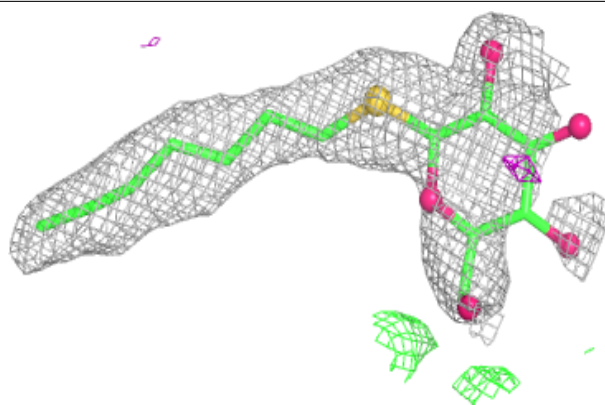
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



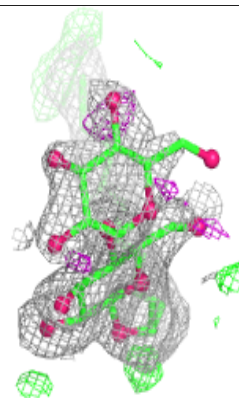
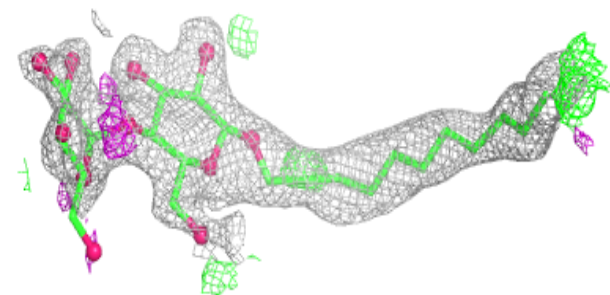
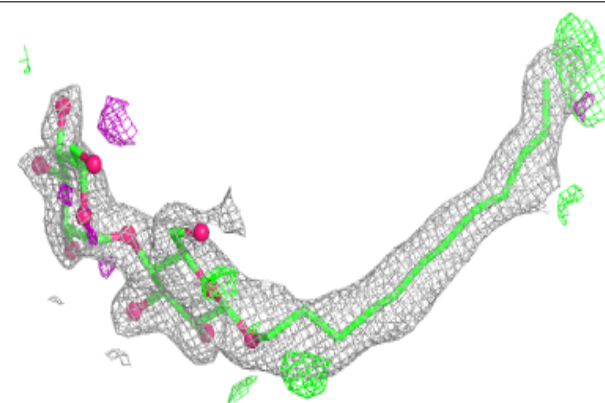


Electron density around HTG b 602:

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

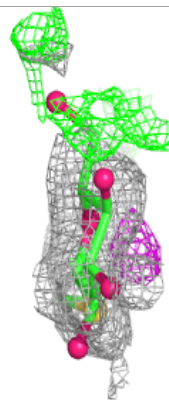
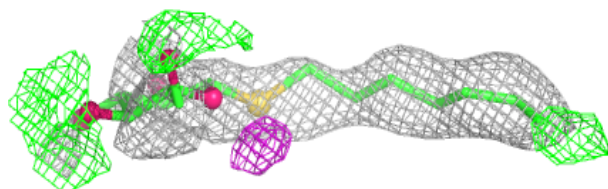
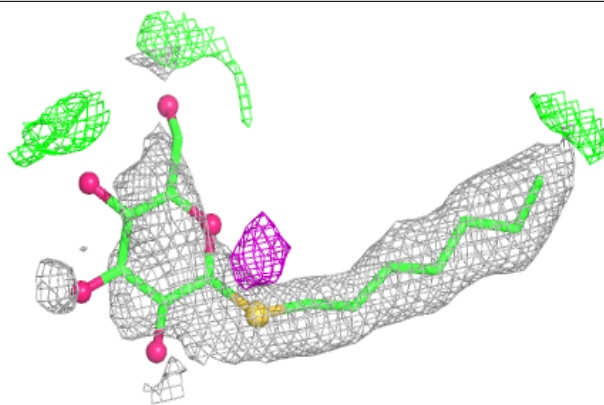
**Electron density around LMT M 101:**

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

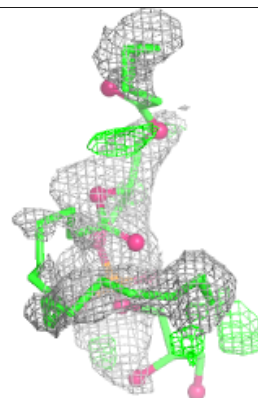
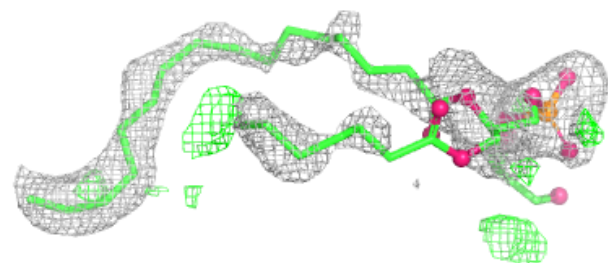
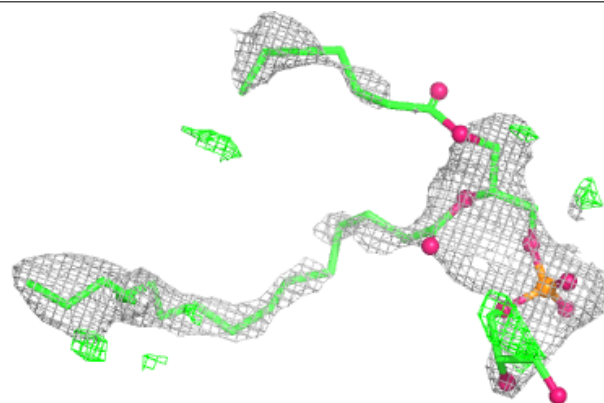


Electron density around HTG B 631:

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

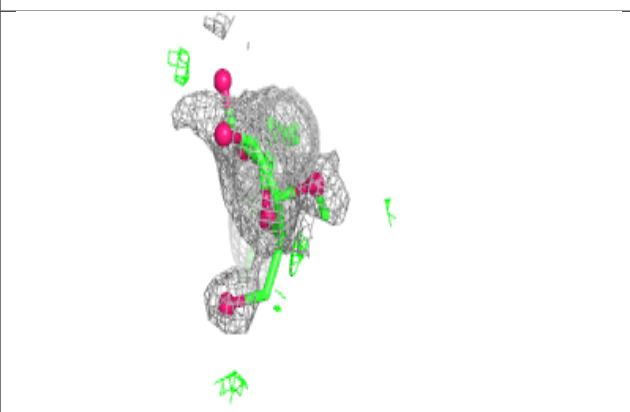
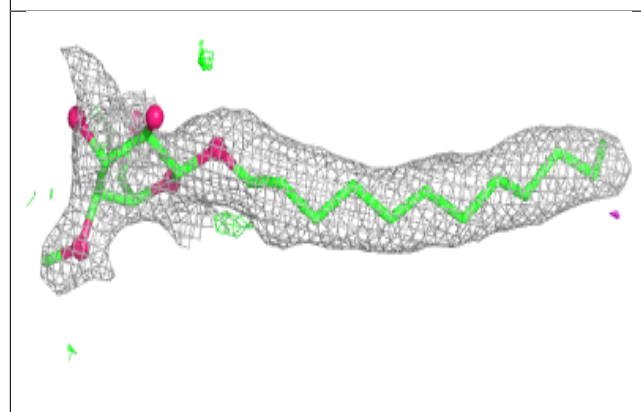
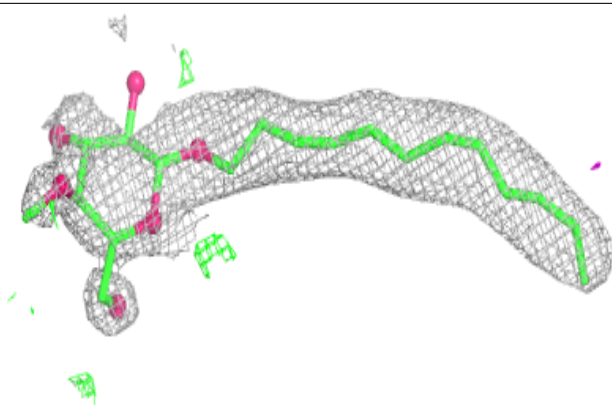
**Electron density around LHG a 417:**

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

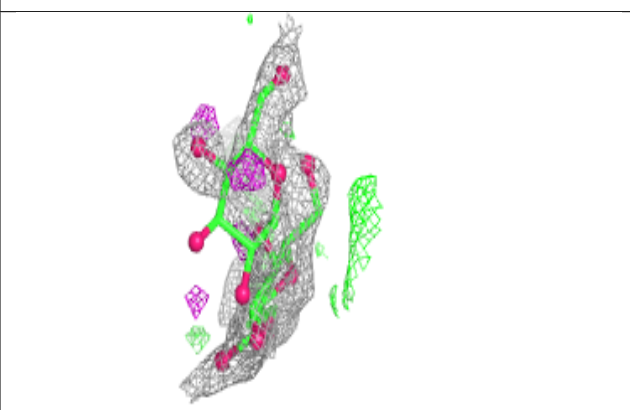
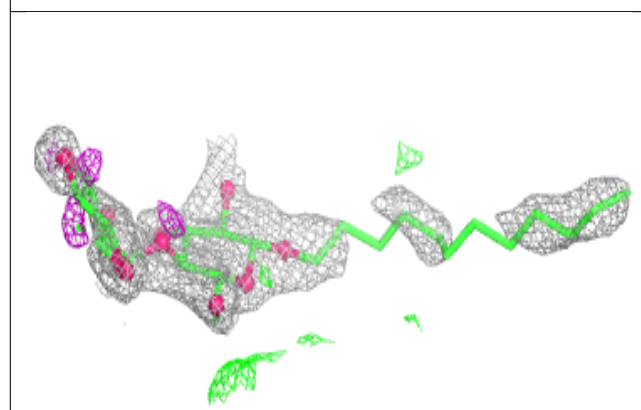
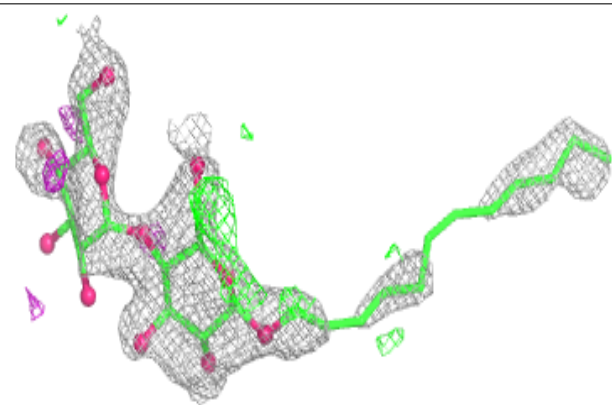


Electron density around LMT b 624:

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

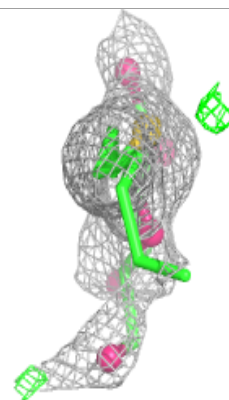
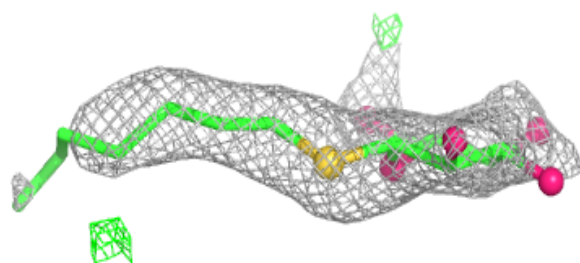
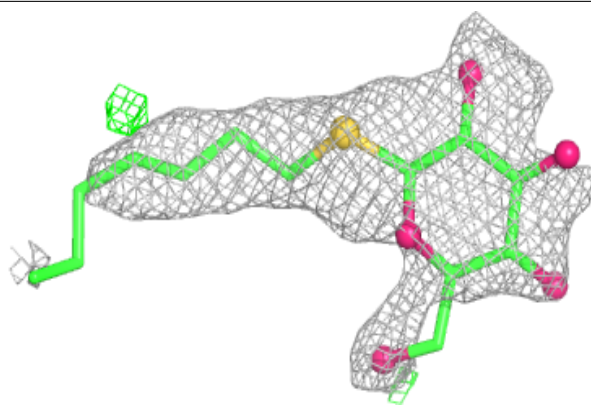
**Electron density around LMT F 102:**

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

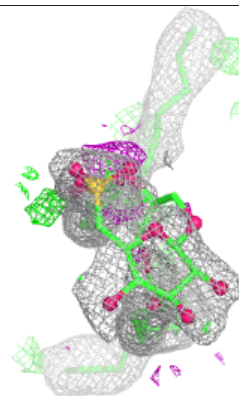
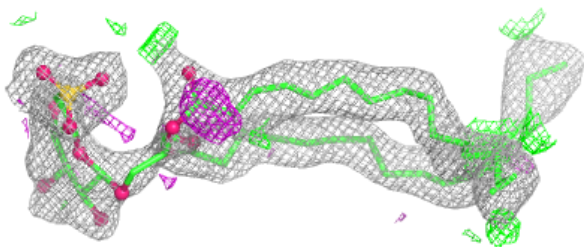
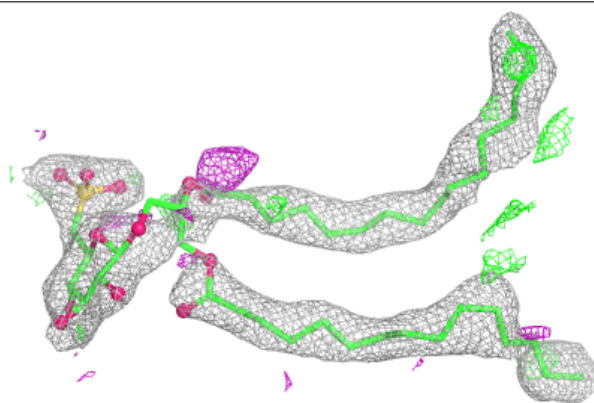


Electron density around HTG D 414:

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

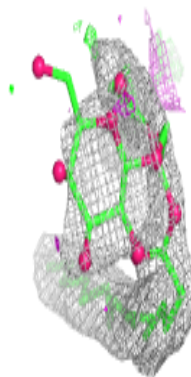
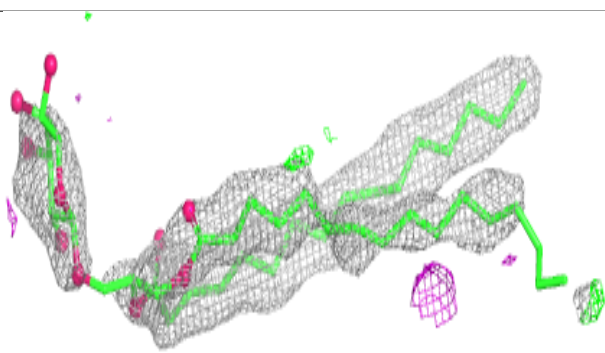
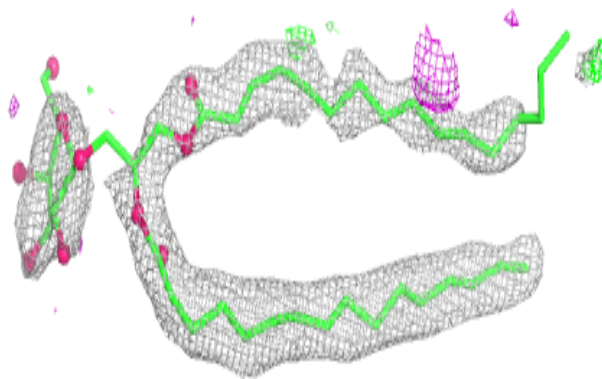
**Electron density around SQD L 103:**

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

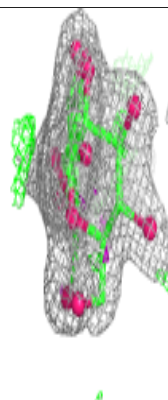
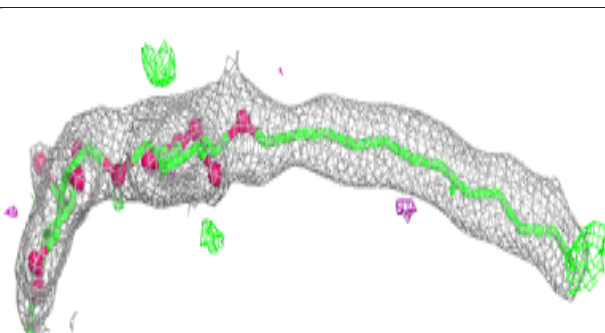
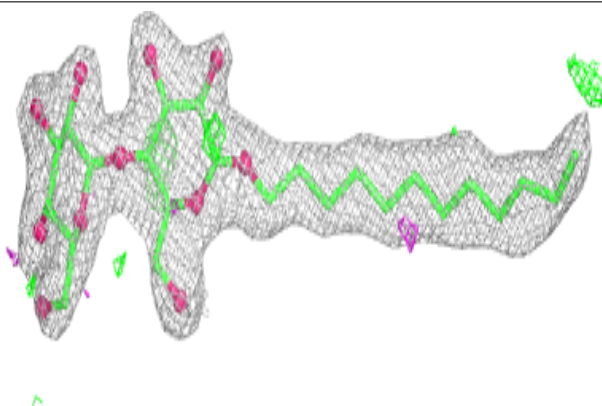


Electron density around LMG Z 101:

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

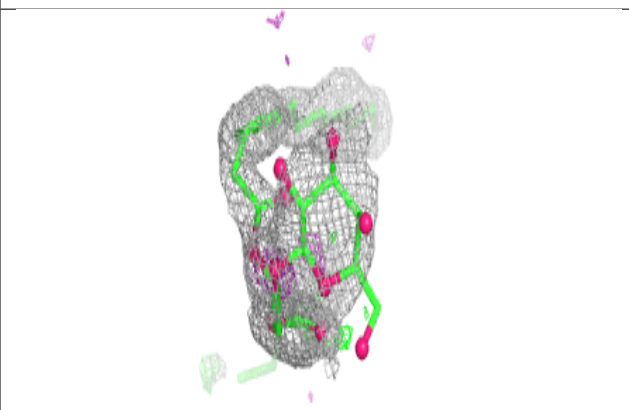
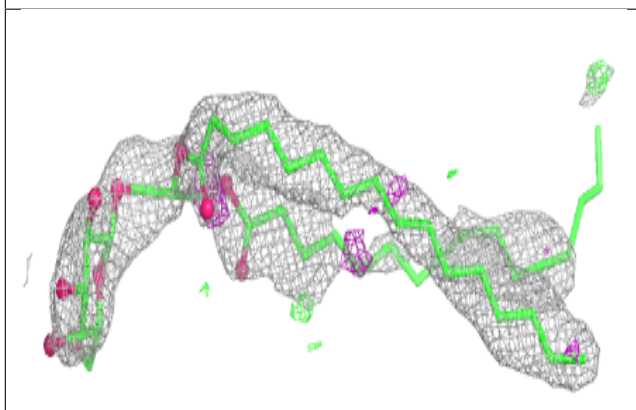
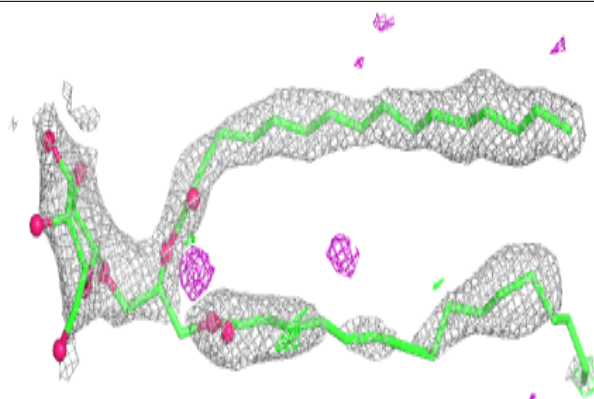
**Electron density around LMT m 101:**

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

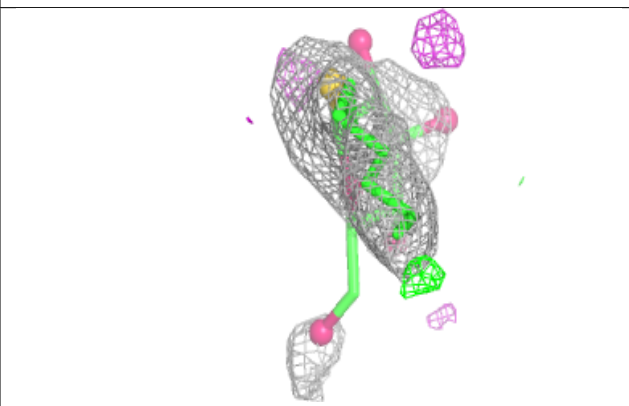
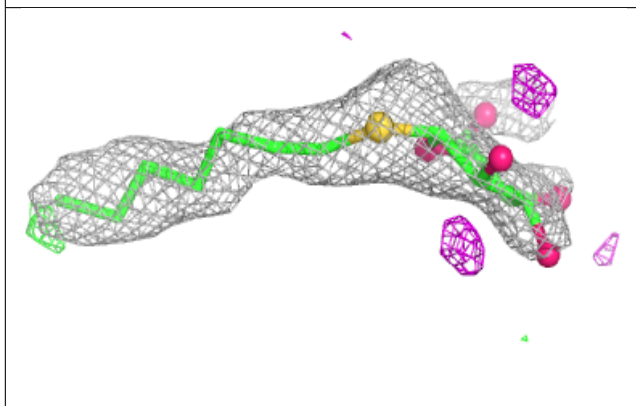


Electron density around LMG c 921:

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

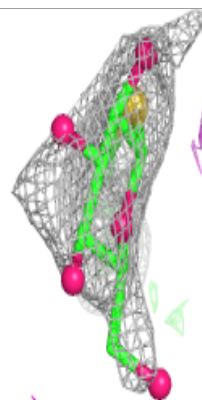
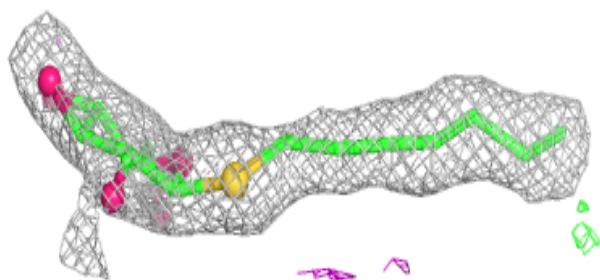
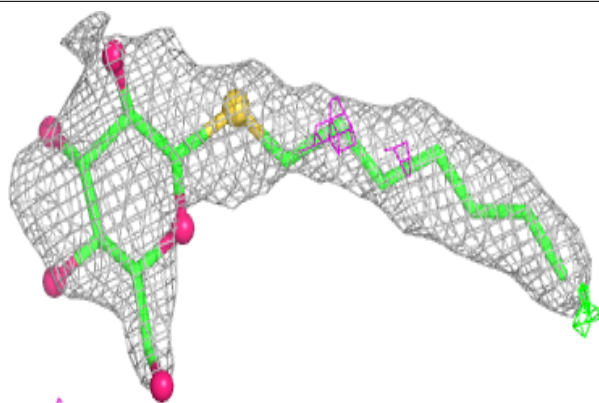
**Electron density around HTG b 627:**

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

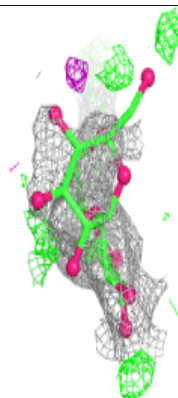
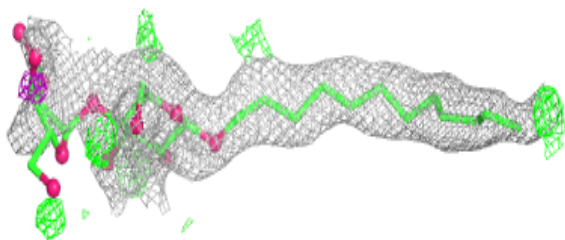
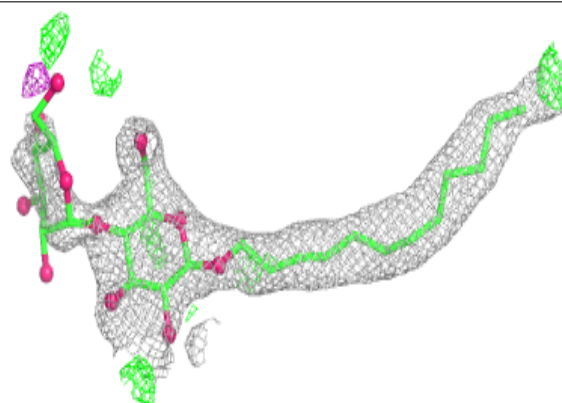


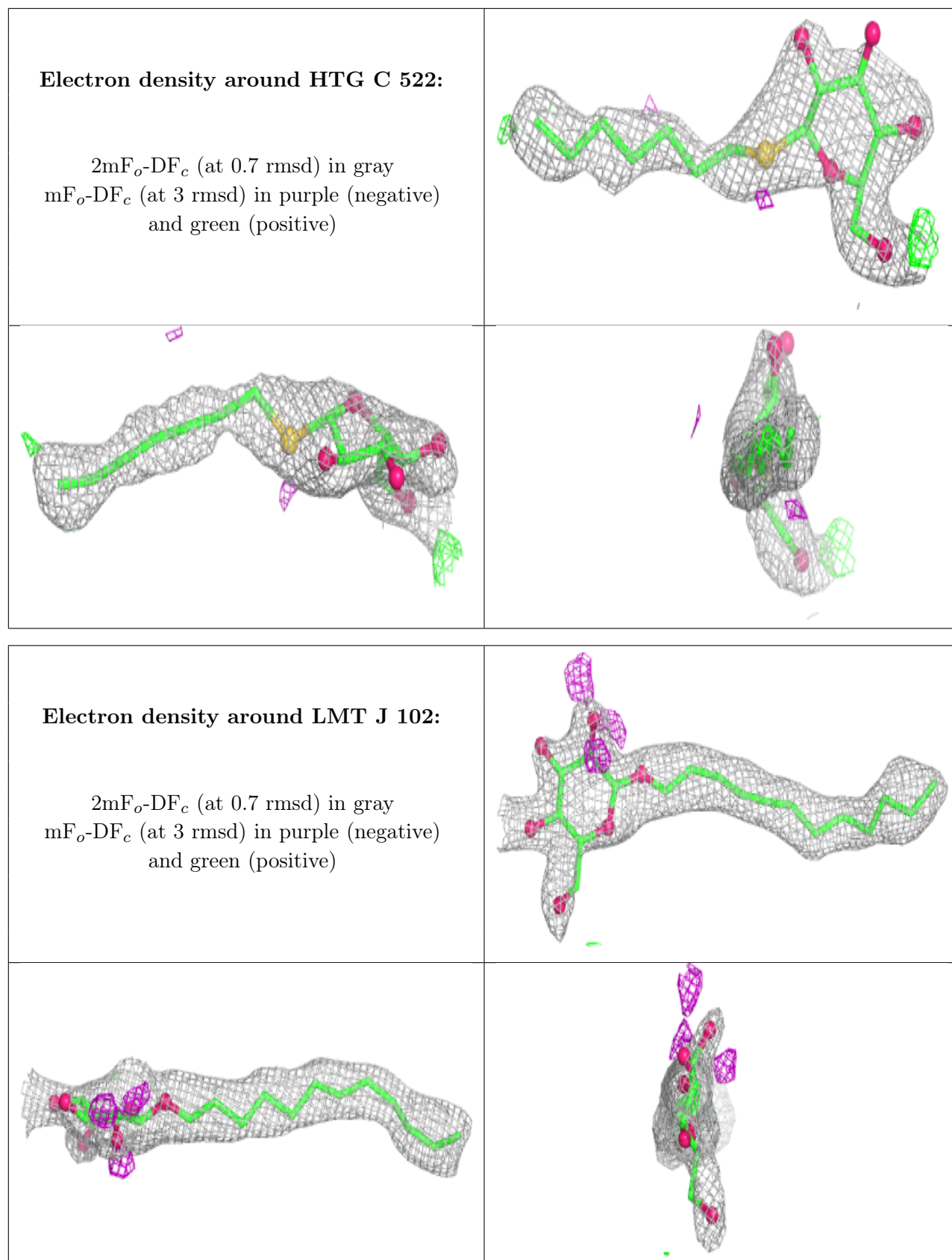
Electron density around HTG B 626:

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

**Electron density around LMT B 623:**

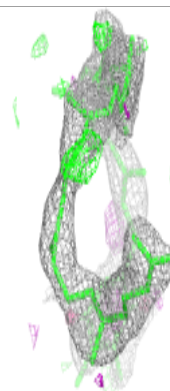
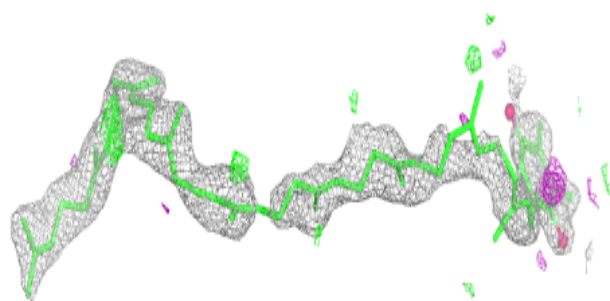
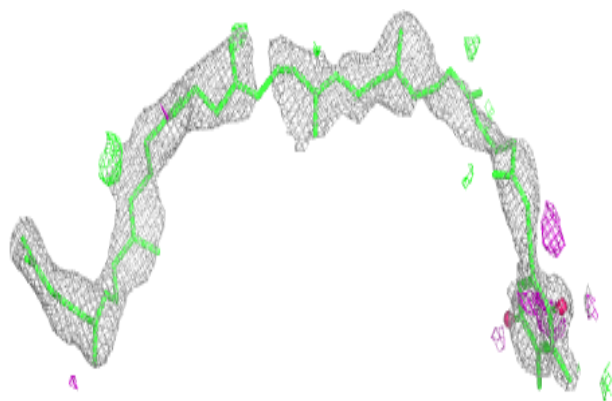
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



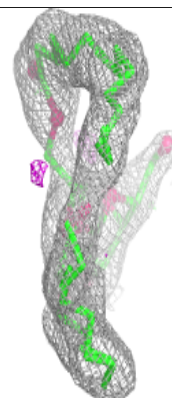
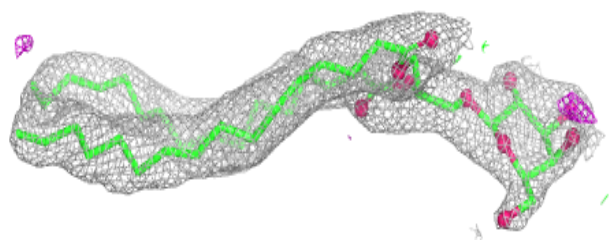
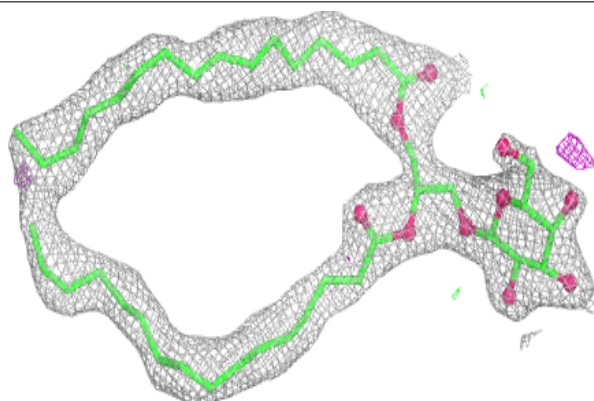


Electron density around PL9 a 419:

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

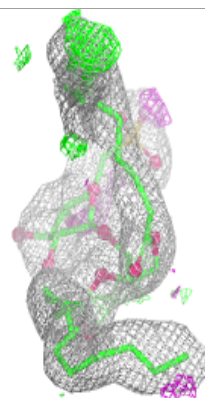
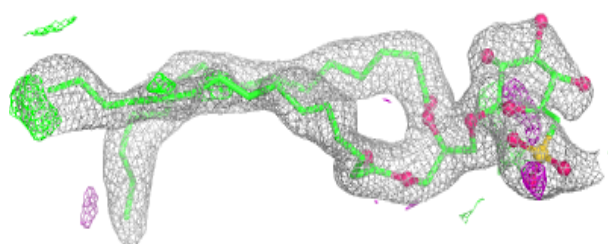
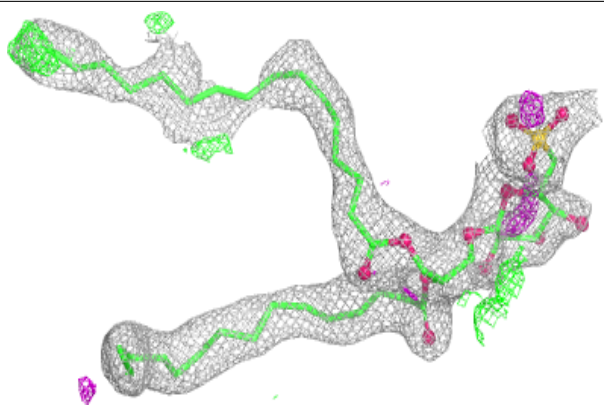
**Electron density around LMG a 418:**

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

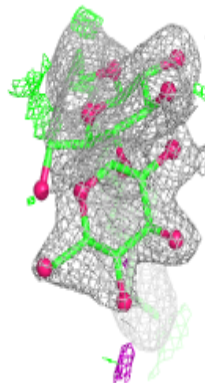
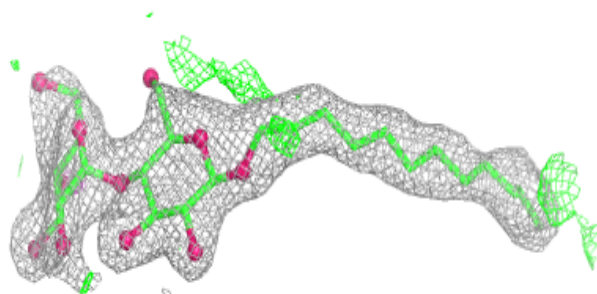
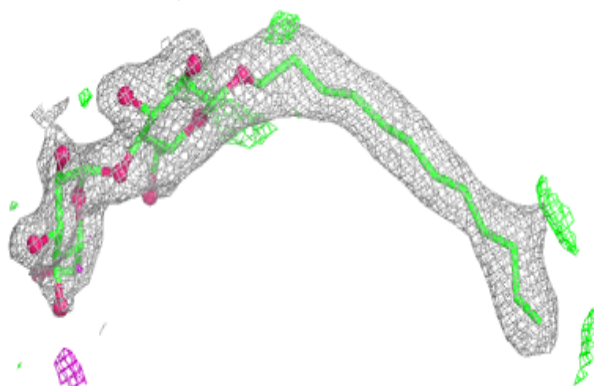


Electron density around SQD a 401:

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

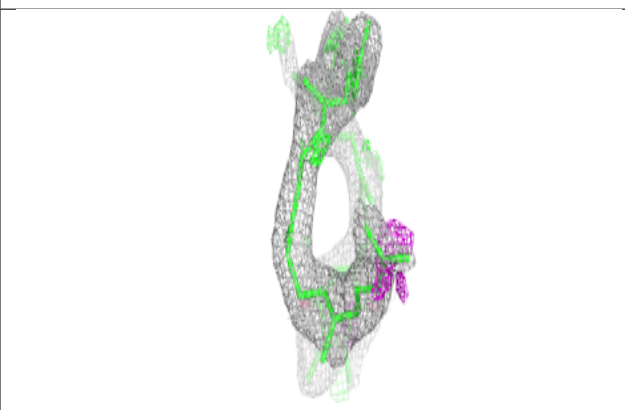
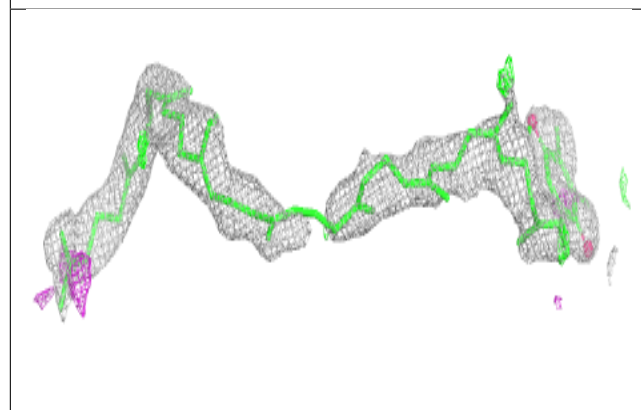
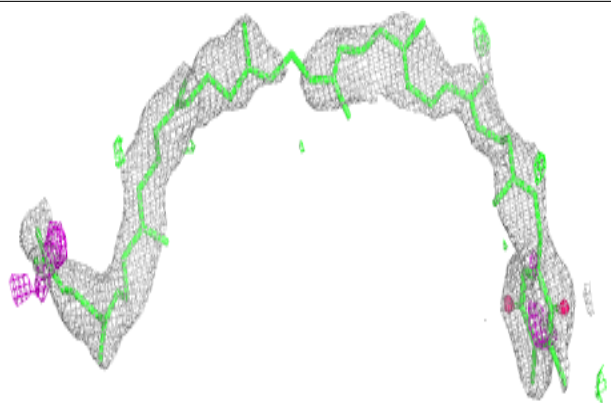
**Electron density around LMT m 102:**

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

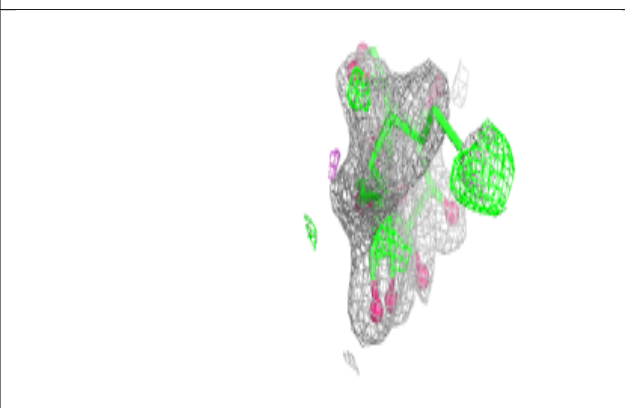
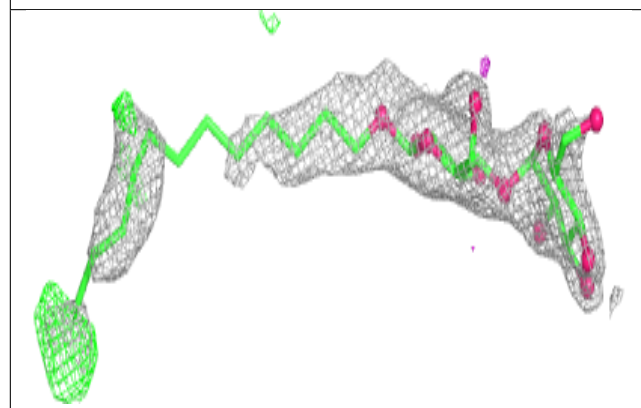
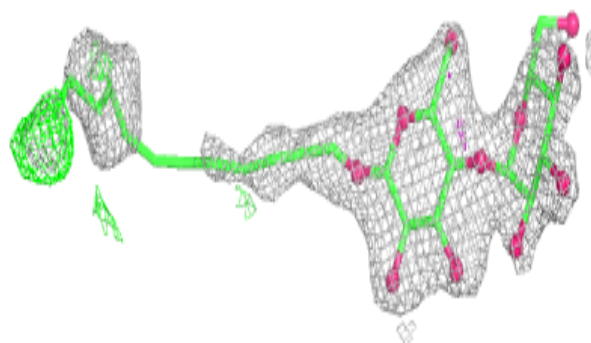


Electron density around PL9 A 414:

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

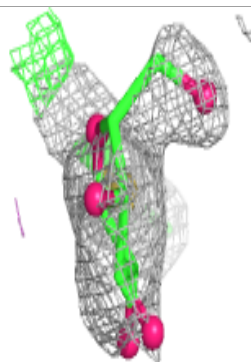
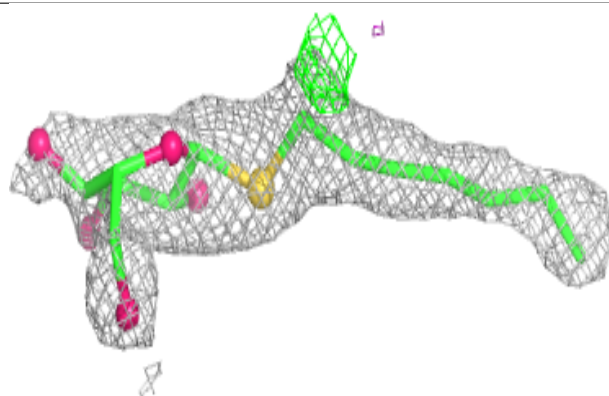
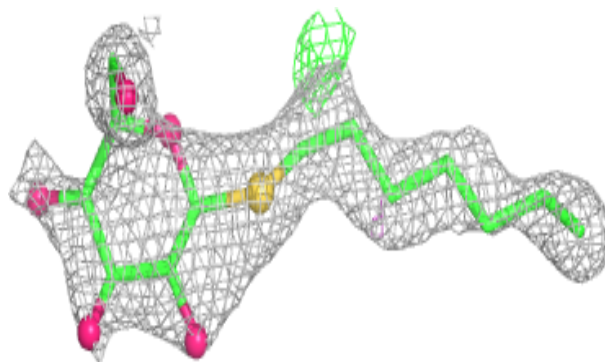
**Electron density around LMT c 922:**

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

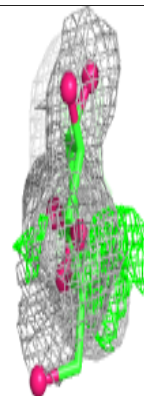
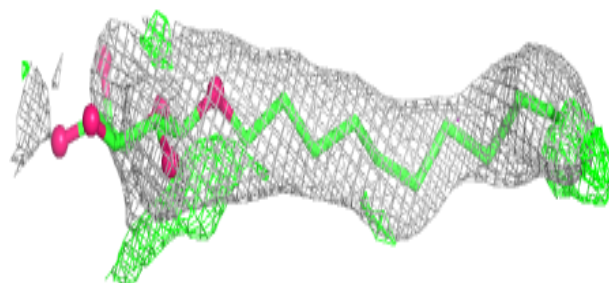
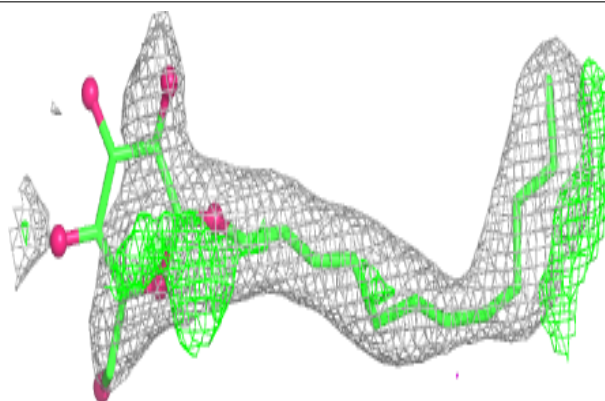


Electron density around HTG c 924:

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

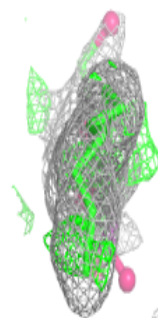
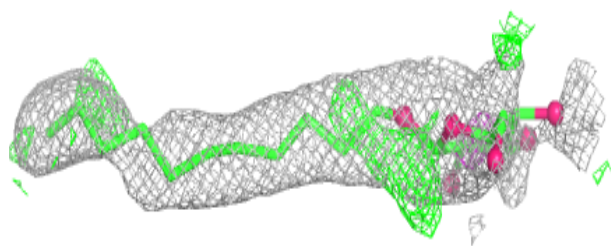
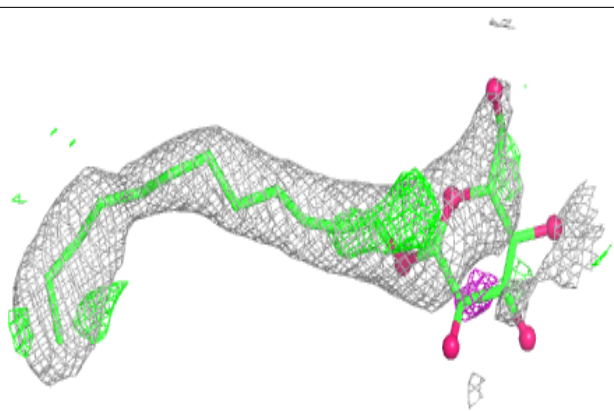
**Electron density around LMT t 102:**

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

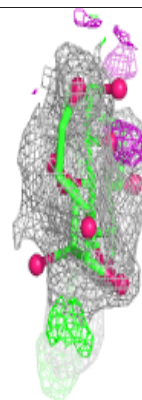
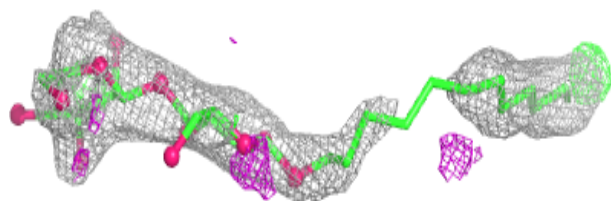
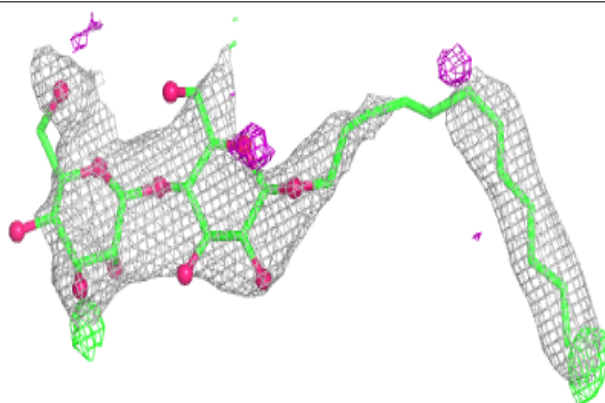


Electron density around LMT b 625:

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

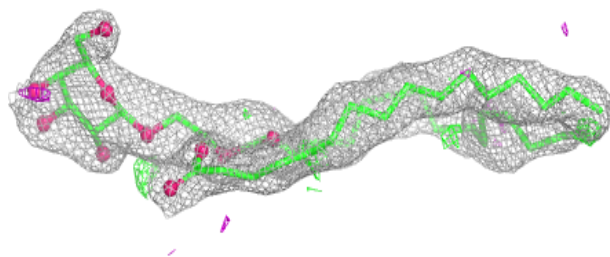
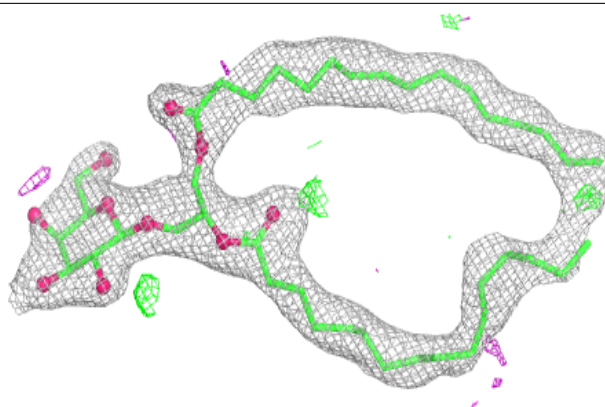
**Electron density around LMT Z 102:**

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

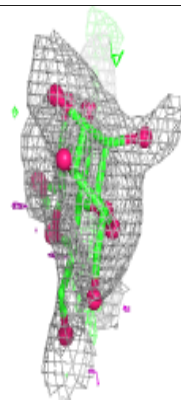
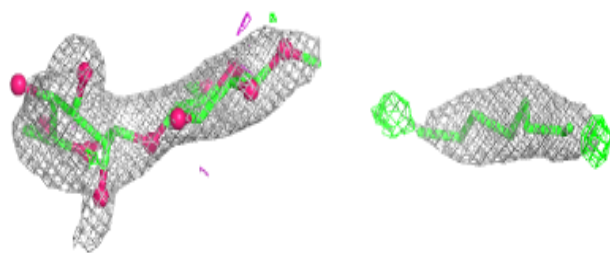
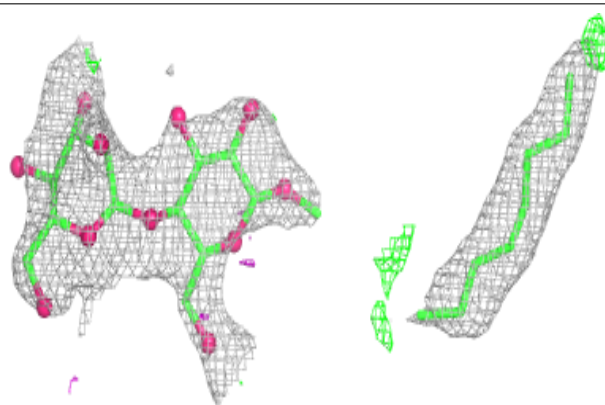


Electron density around LMG A 413:

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

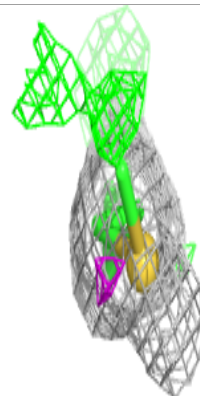
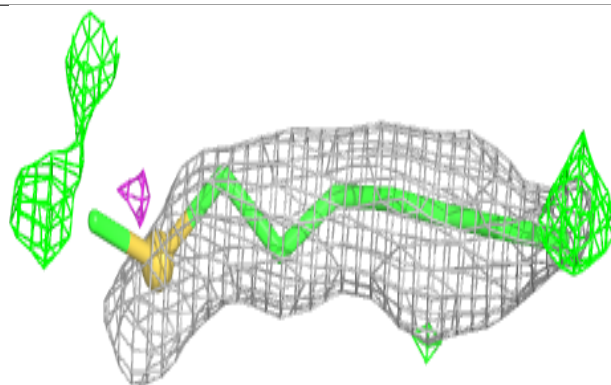
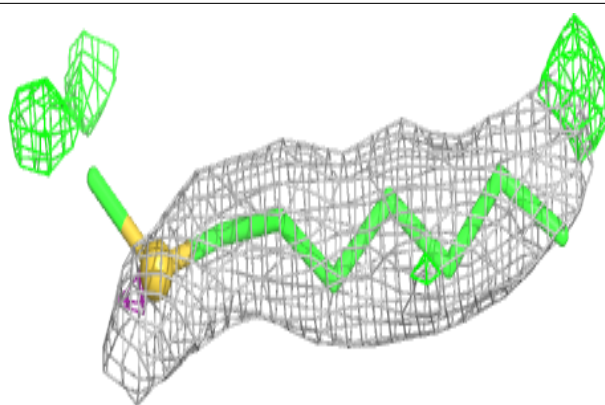
**Electron density around LMT z 101:**

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

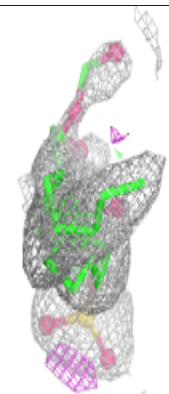
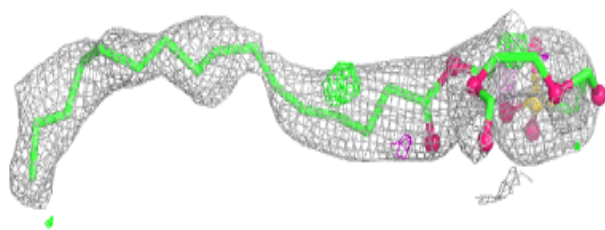
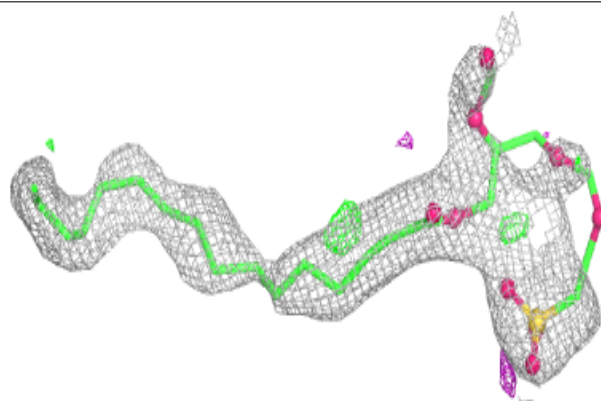


Electron density around HTG U 201:

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

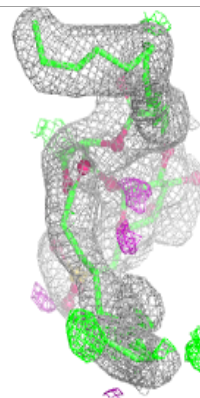
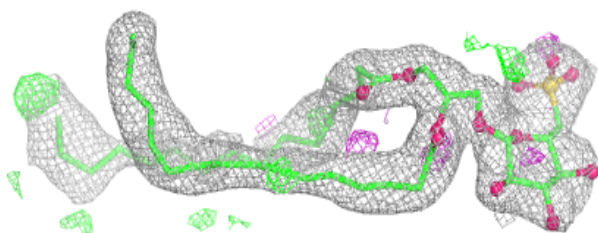
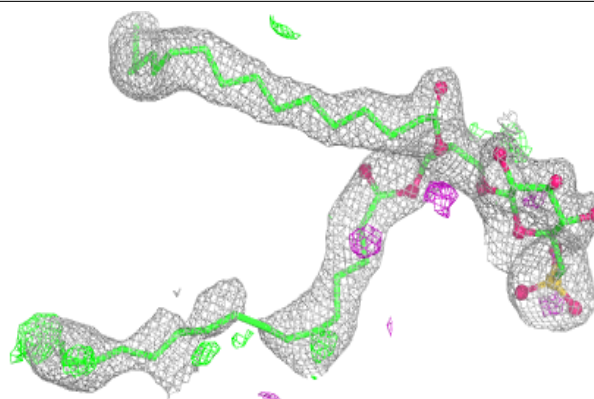
**Electron density around SQD f 102:**

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

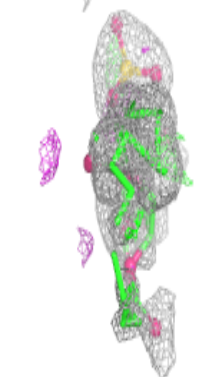
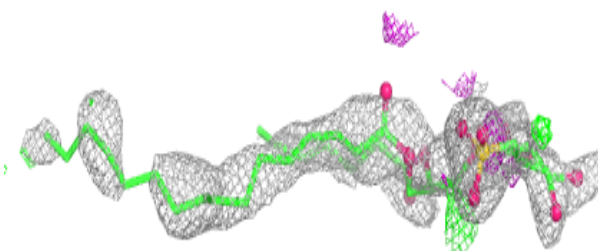
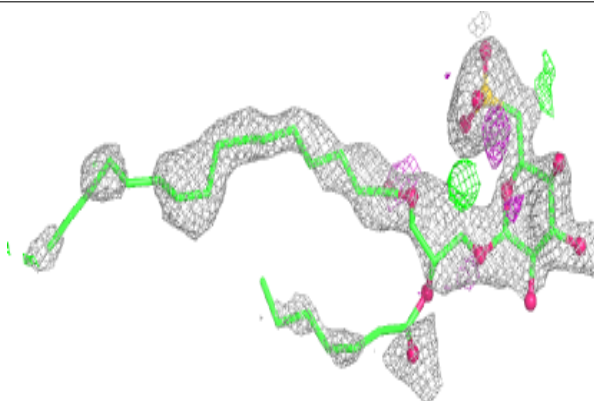


Electron density around SQD A 418:

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

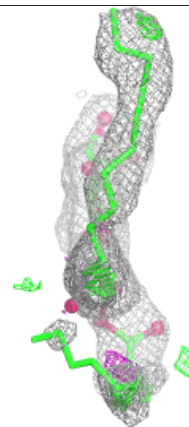
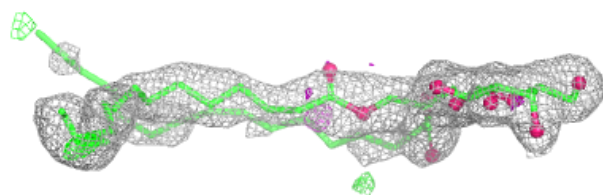
**Electron density around SQD D 407:**

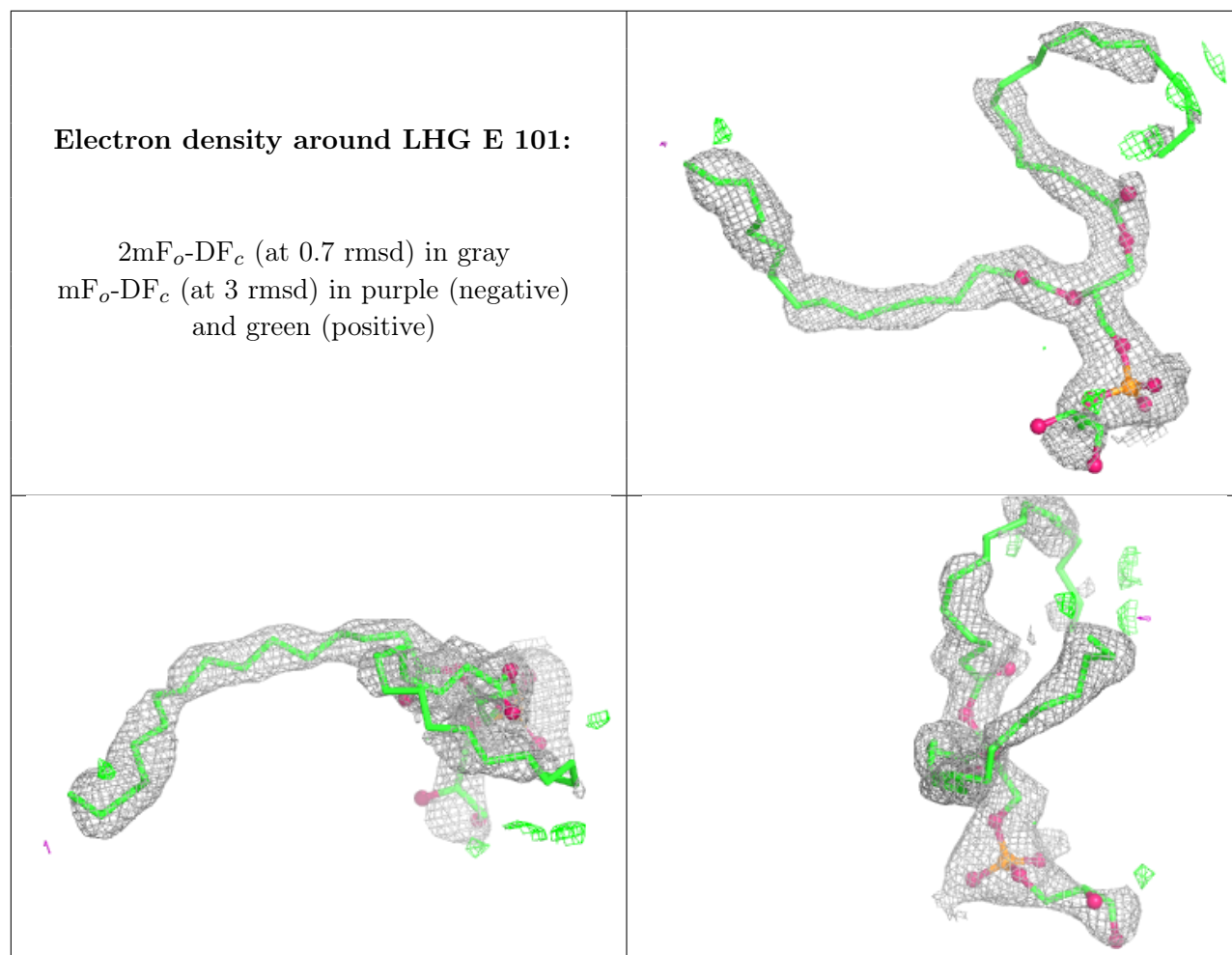
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LMG c 920:

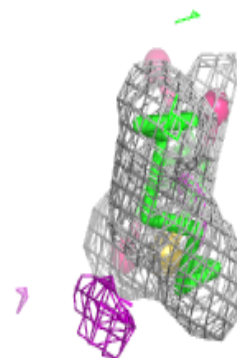
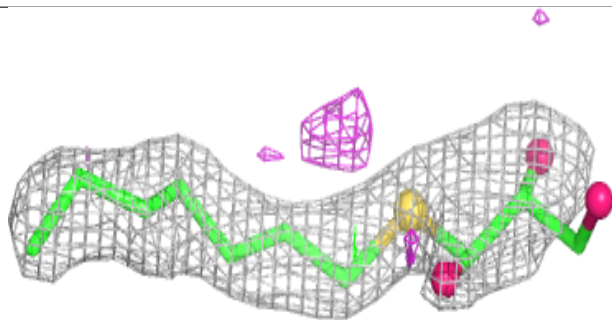
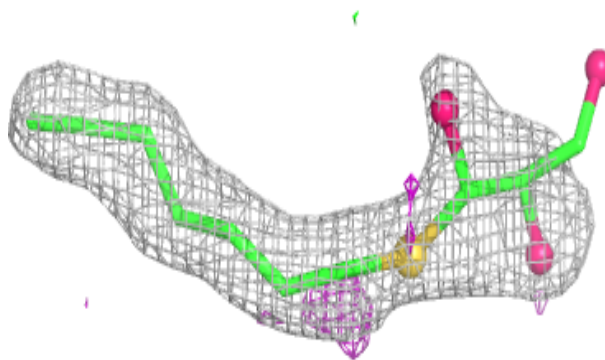
$2mF_o-DF_c$ (at 0.7 rnsd) in gray
 mF_o-DF_c (at 3 rnsd) in purple (negative)
and green (positive)



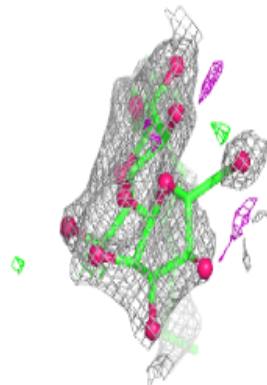
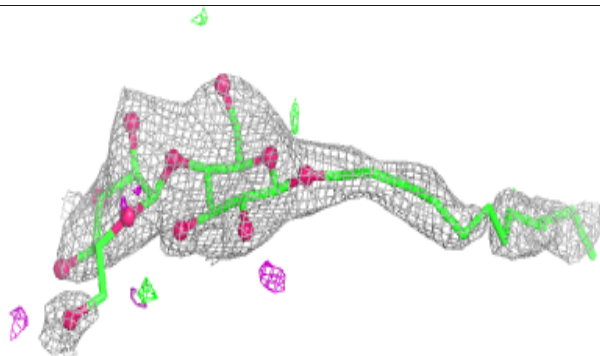
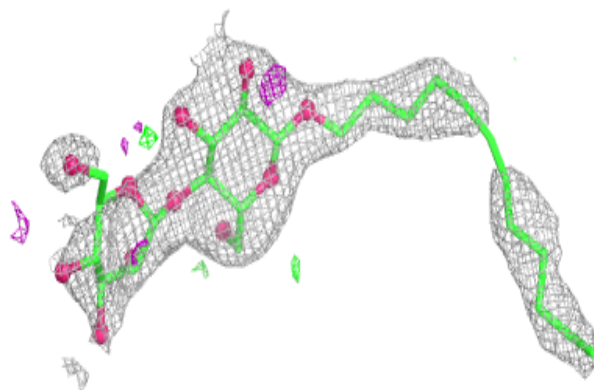


Electron density around HTG u 201:

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

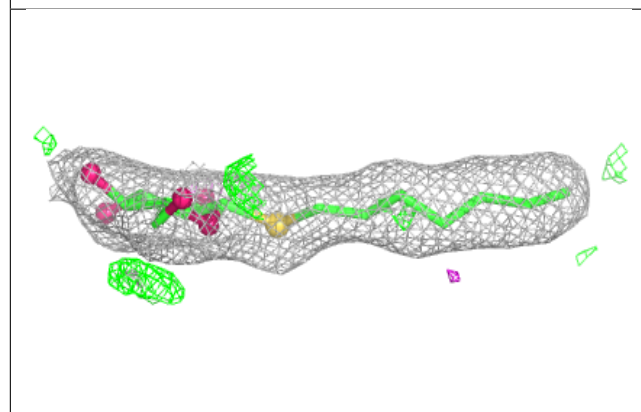
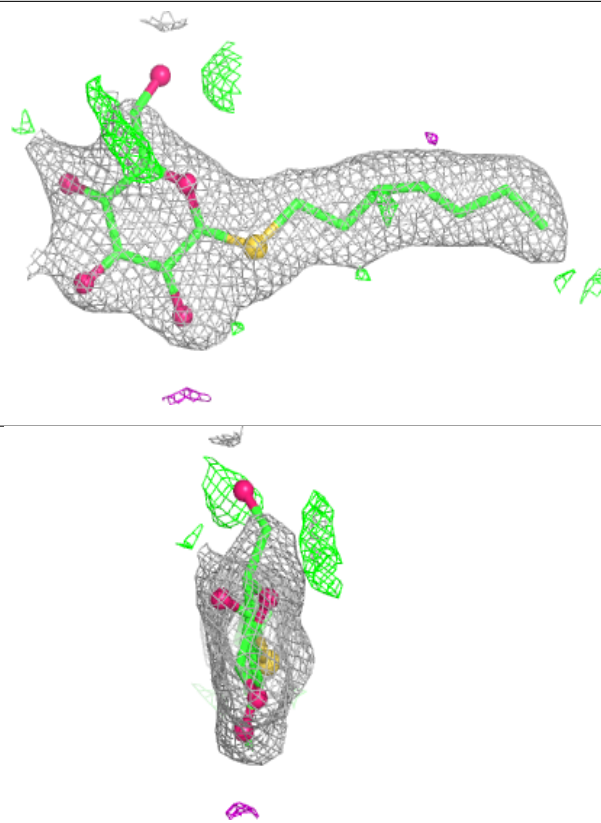
**Electron density around LMT C 520:**

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

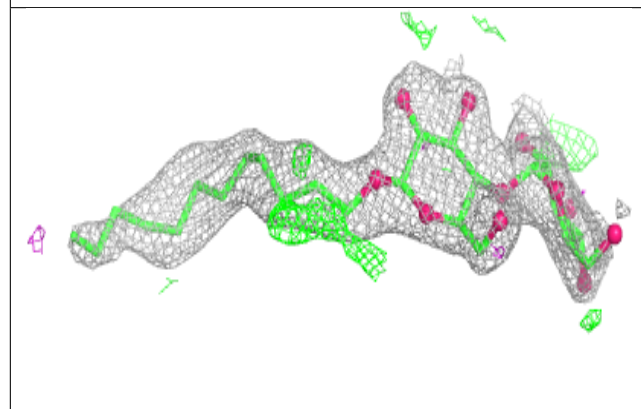
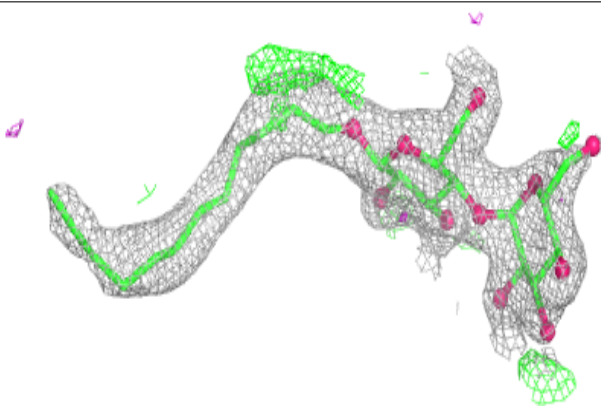


Electron density around HTG B 630:

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

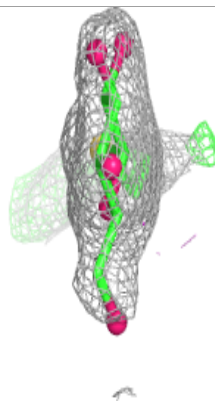
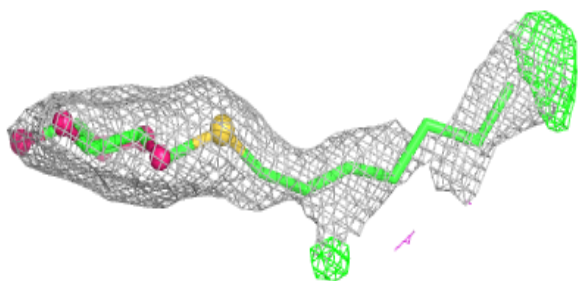
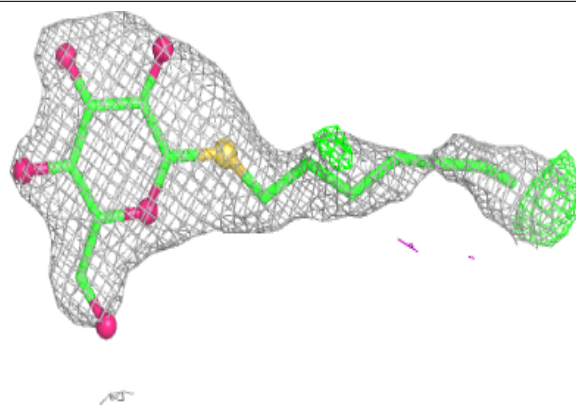
**Electron density around LMT a 402:**

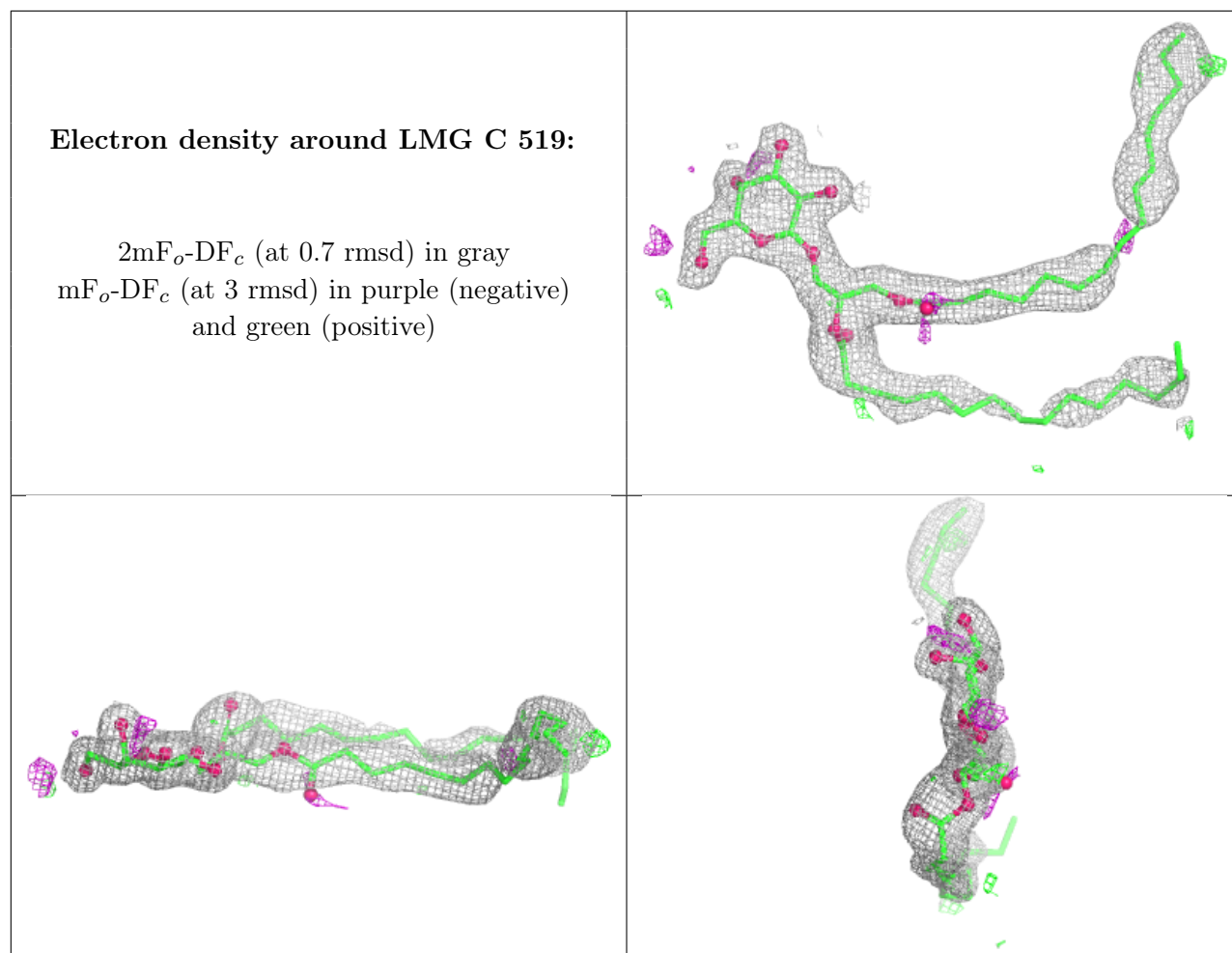
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HTG c 923:

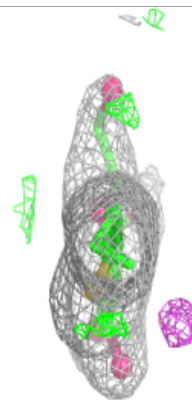
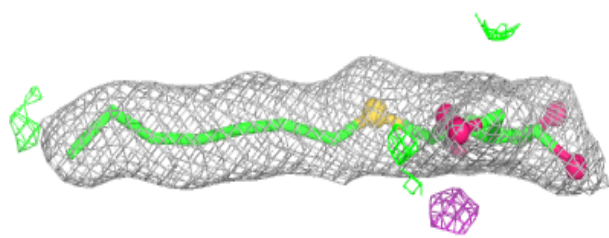
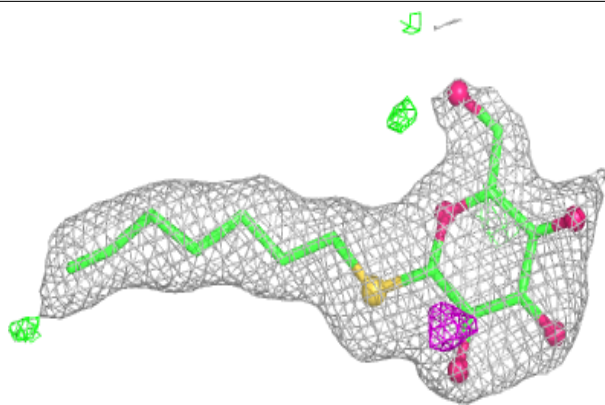
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



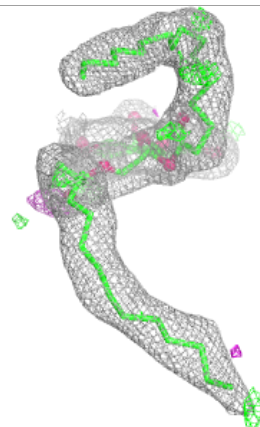
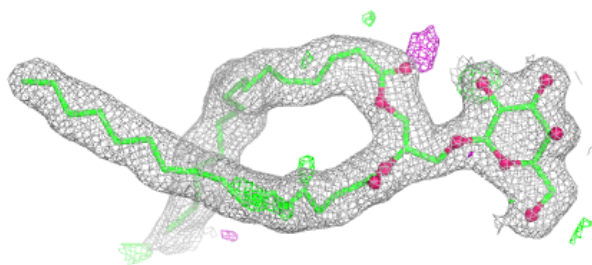
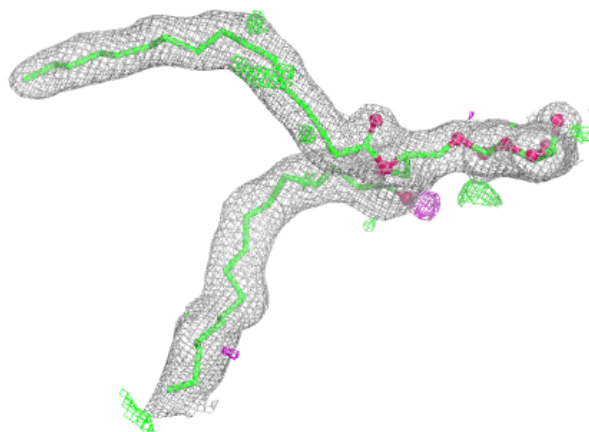


Electron density around HTG b 601:

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

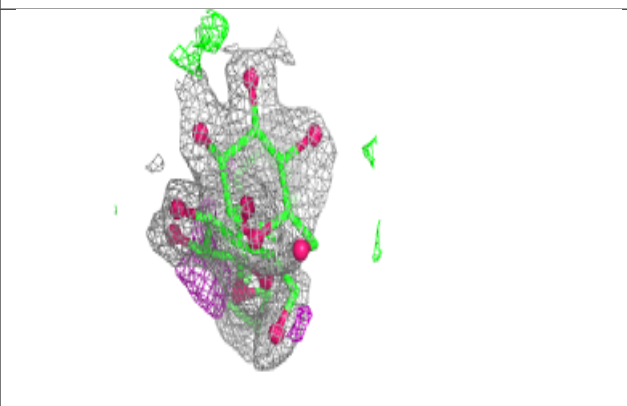
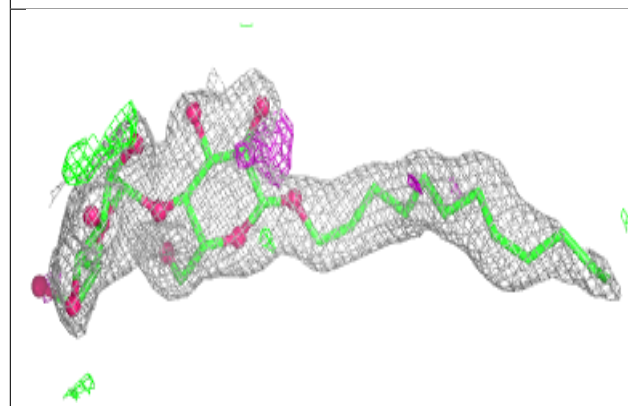
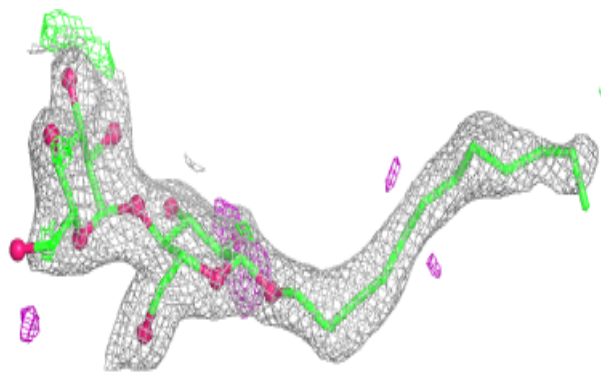
**Electron density around LMG B 622:**

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

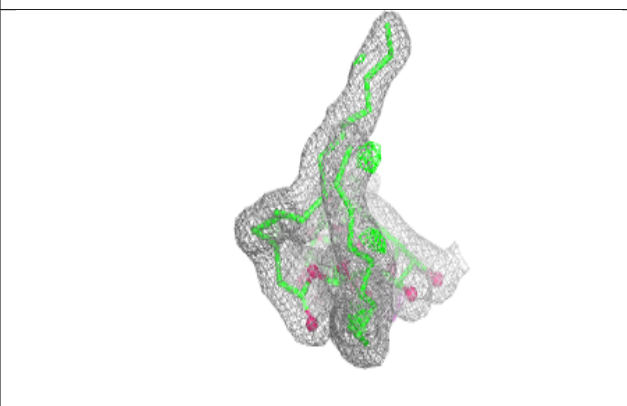
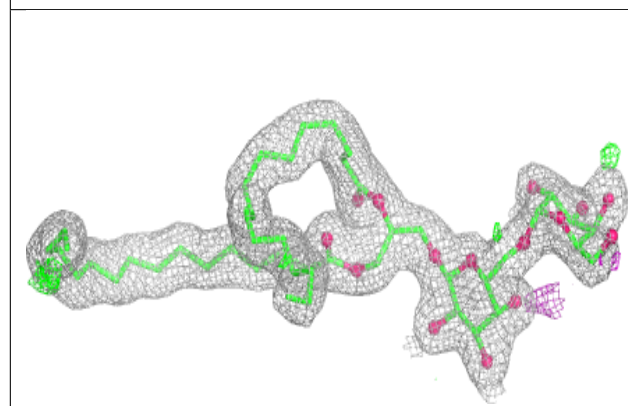
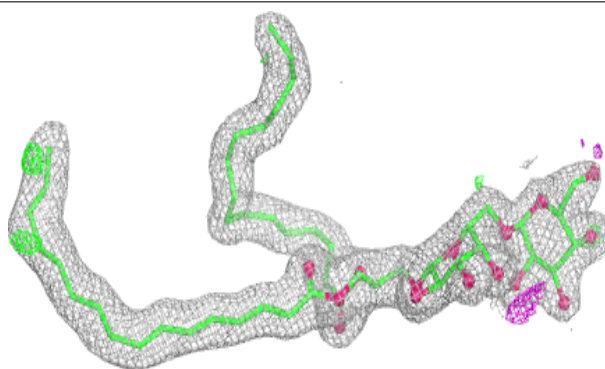


Electron density around LMT A 419:

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

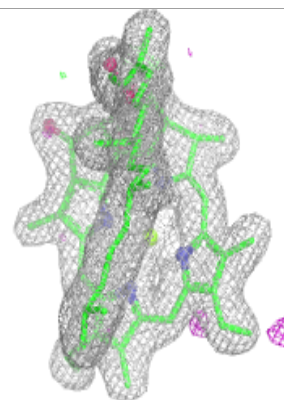
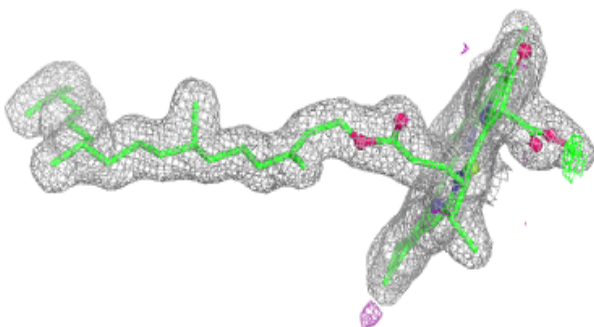
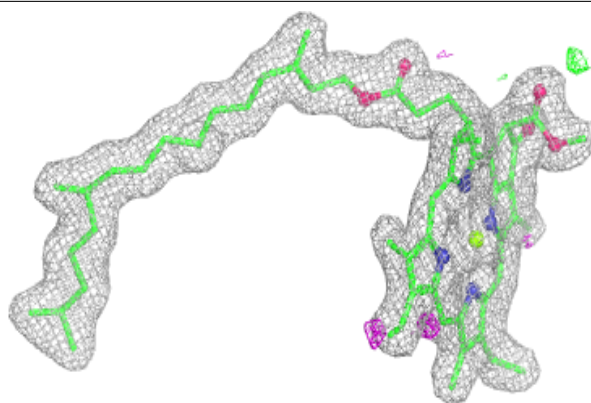
**Electron density around DGD h 102:**

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

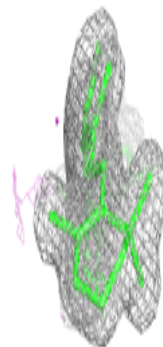
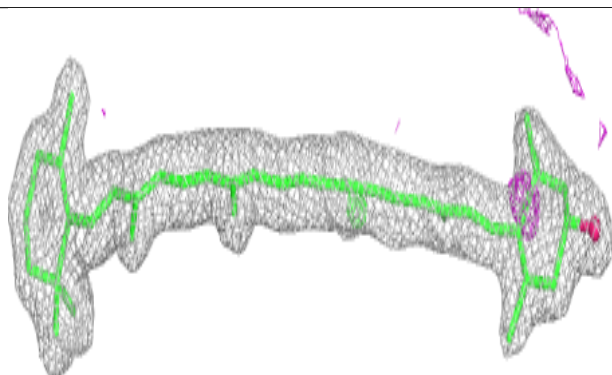
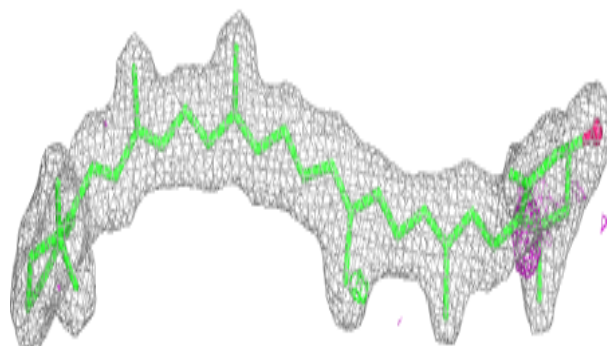


Electron density around CLA B 610:

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

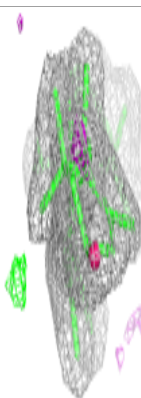
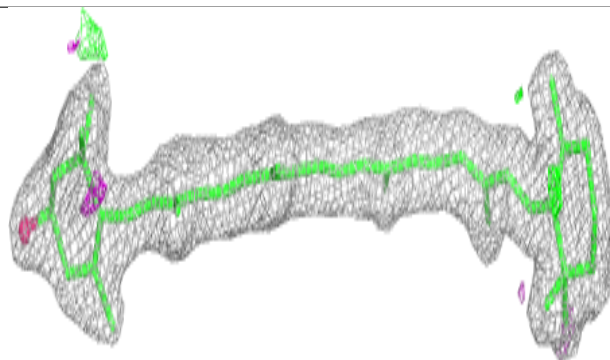
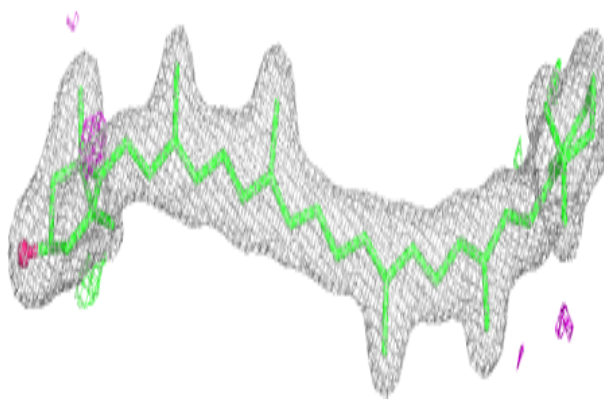
**Electron density around RRX H 101:**

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

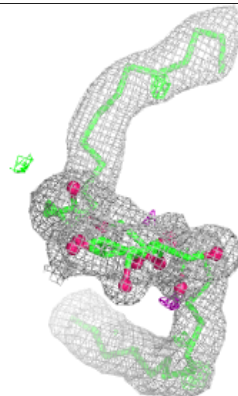
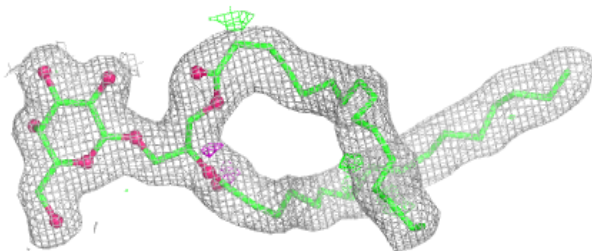
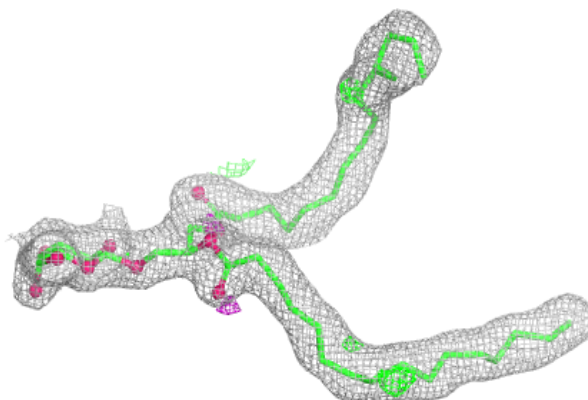


Electron density around RRX h 101:

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

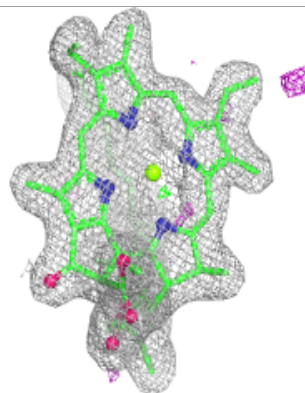
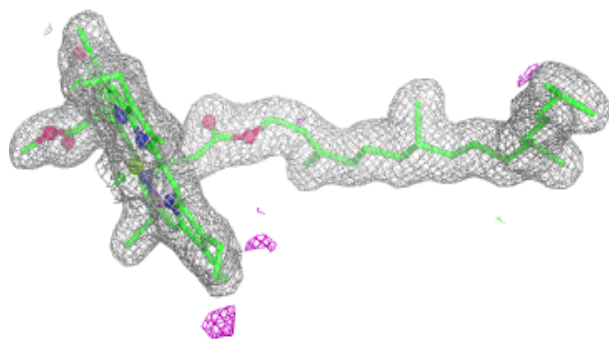
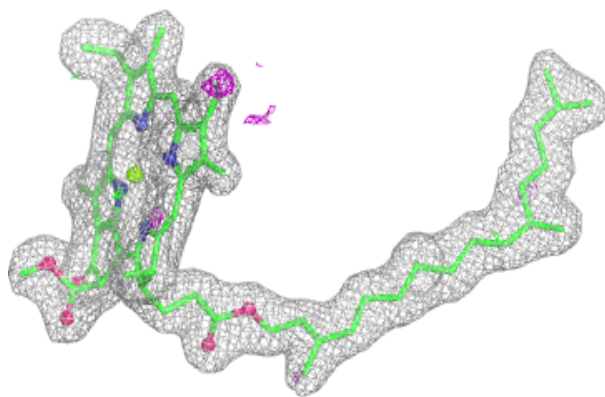
**Electron density around LMG b 623:**

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

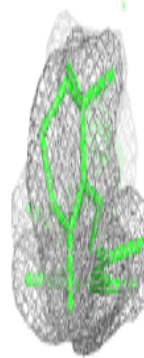
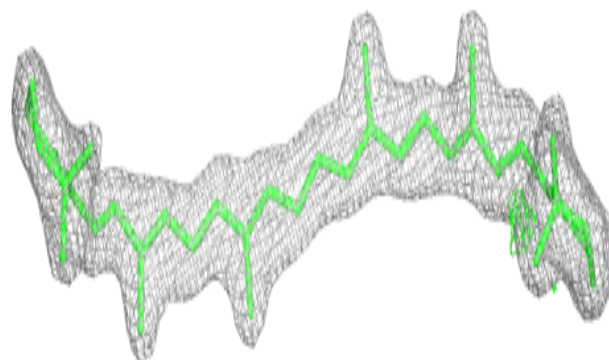
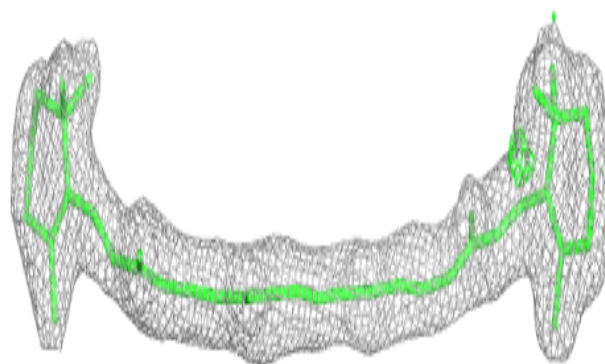


Electron density around CLA b 612:

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

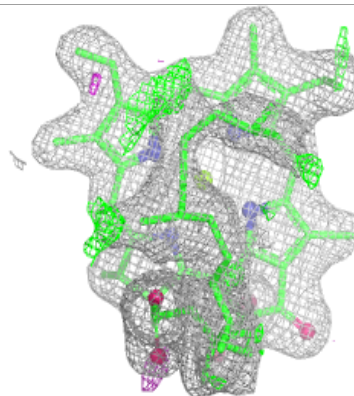
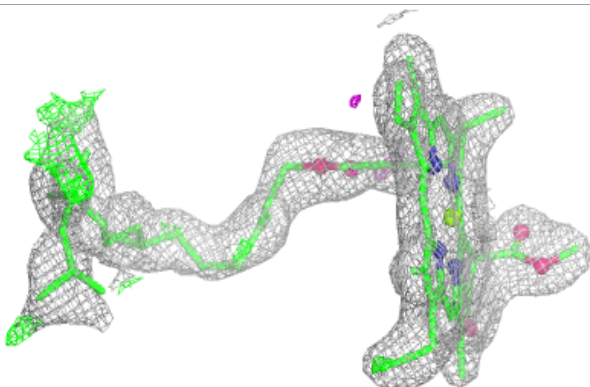
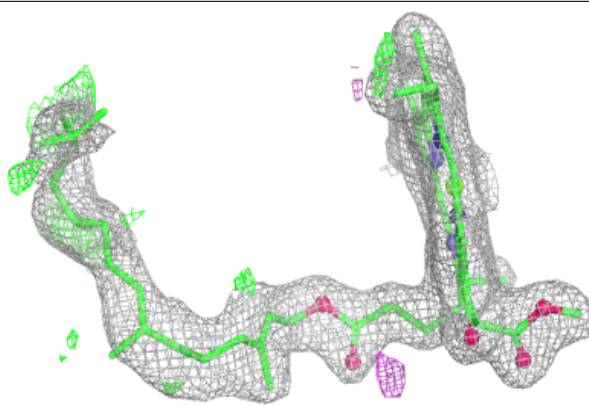
**Electron density around BCR k 102:**

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

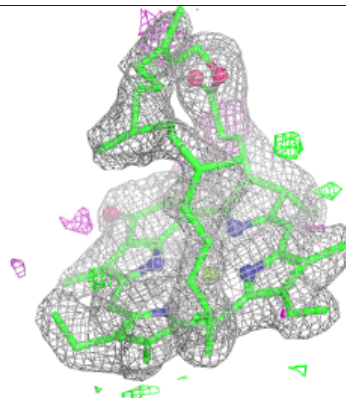
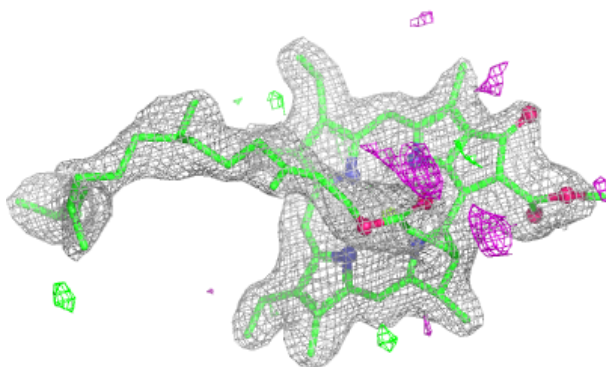
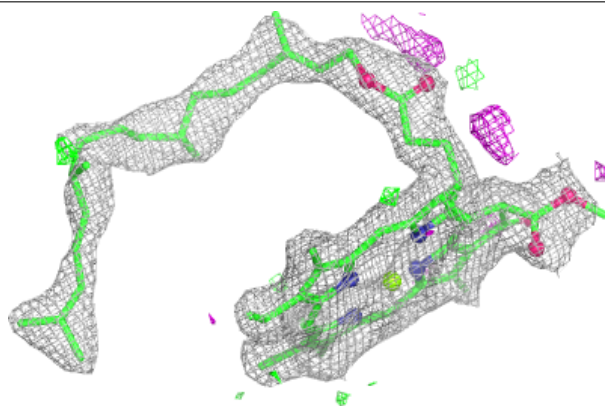


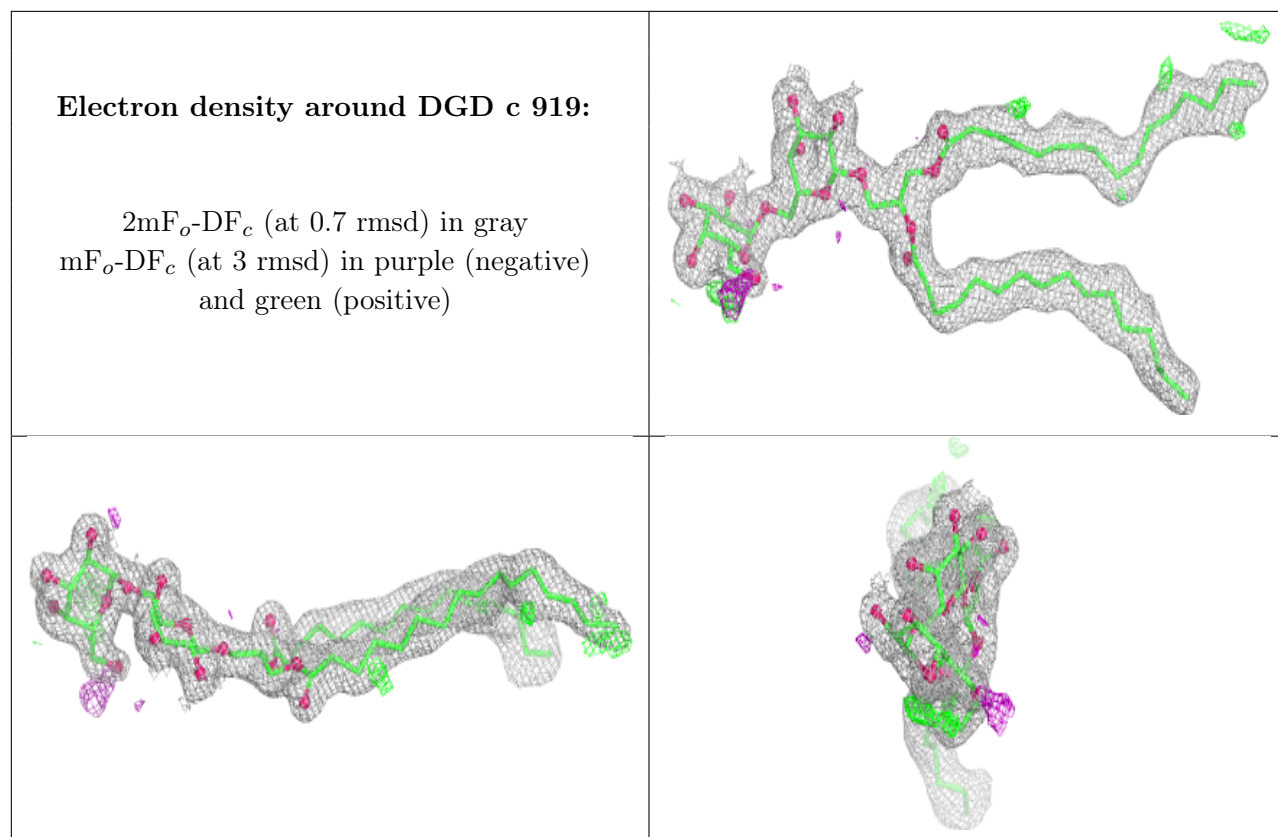
Electron density around CLA C 506:

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

**Electron density around CLA c 914:**

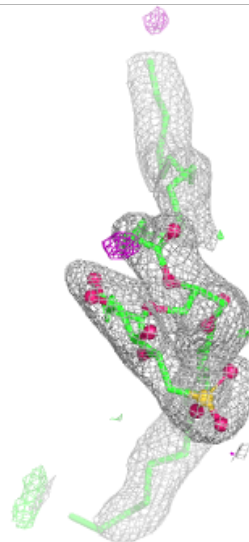
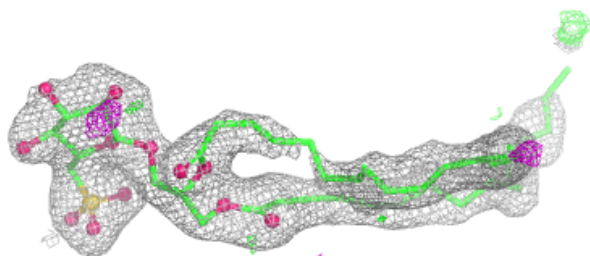
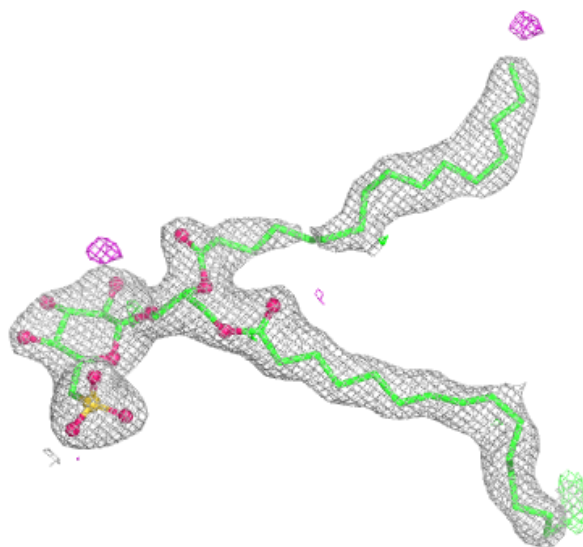
$2mF_o-DF_c$ (at 0.7 rnsd) in gray
 mF_o-DF_c (at 3 rnsd) in purple (negative)
and green (positive)

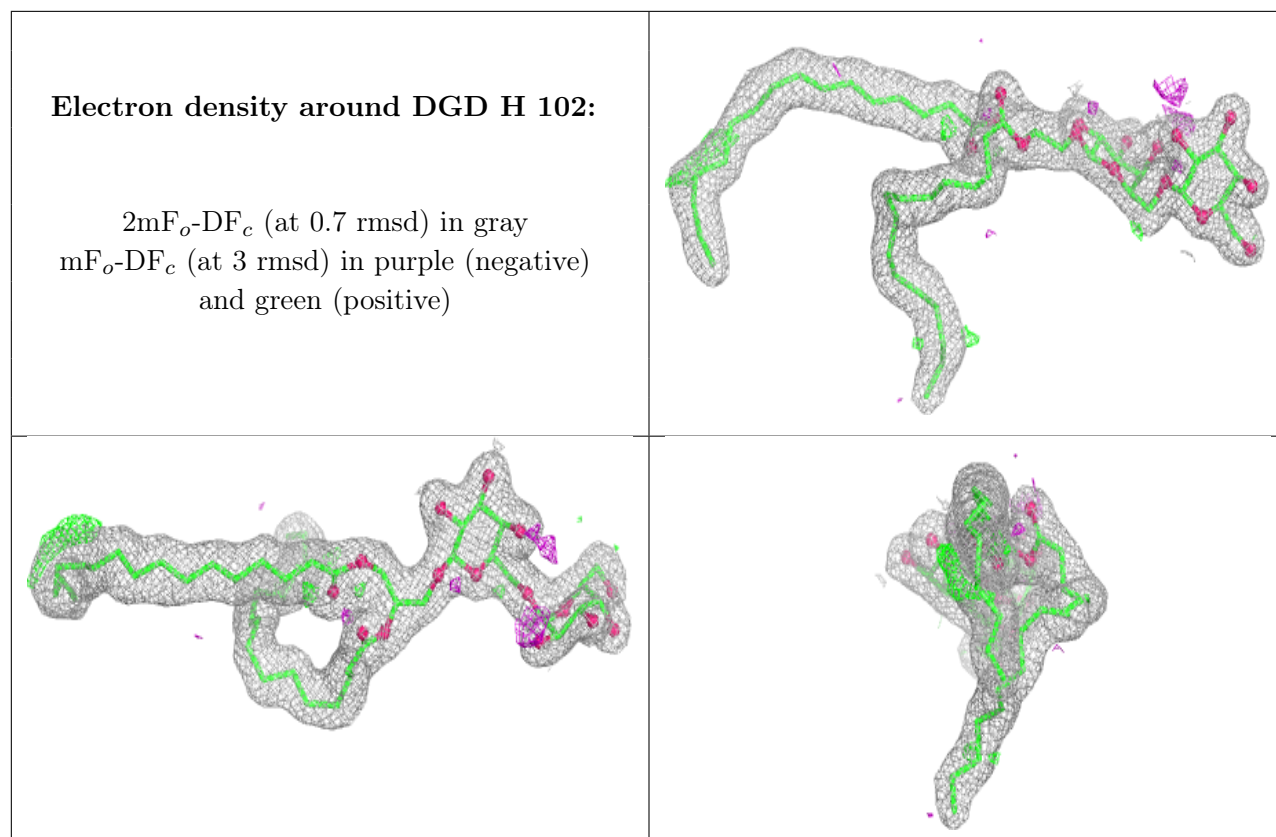




Electron density around SQD a 416:

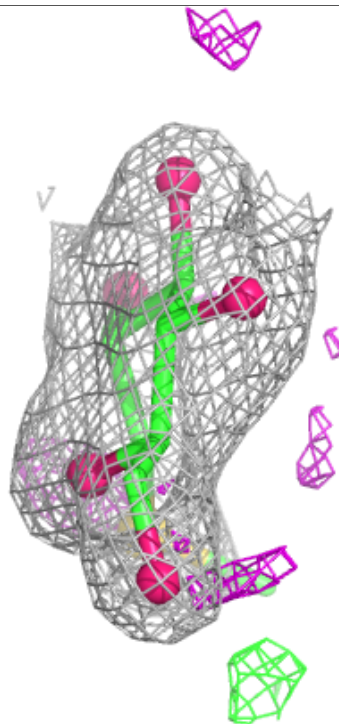
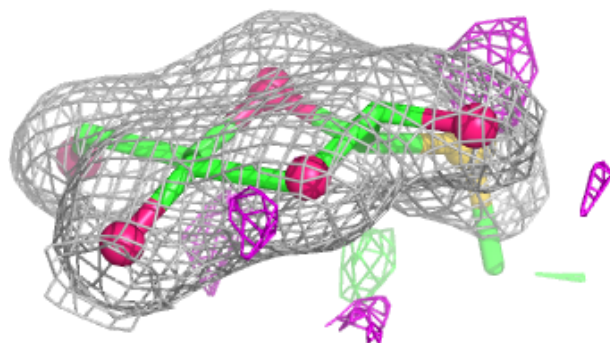
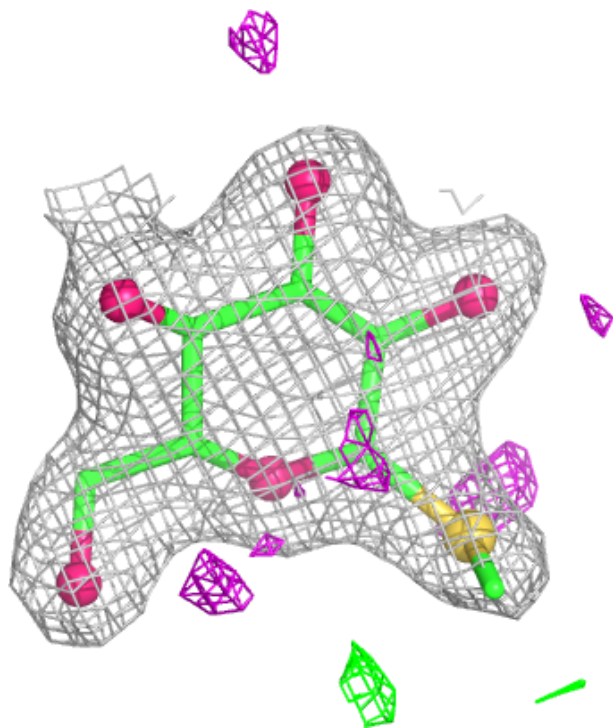
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





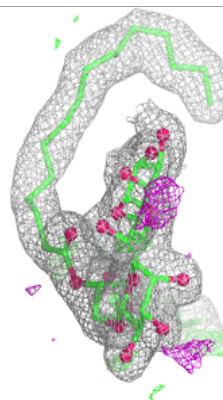
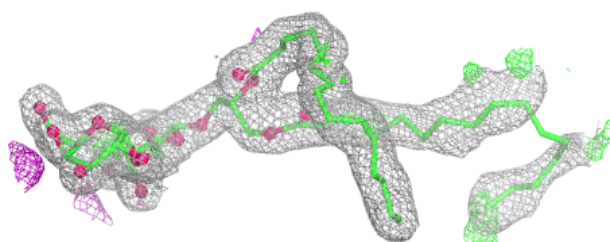
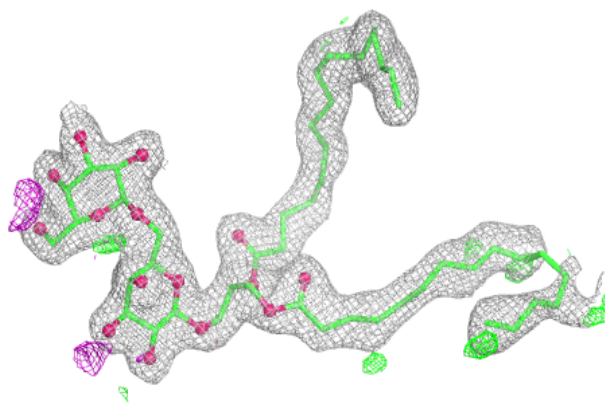
Electron density around HTG V 202:

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

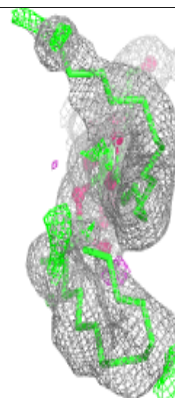
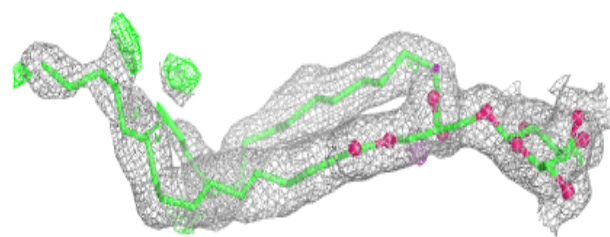
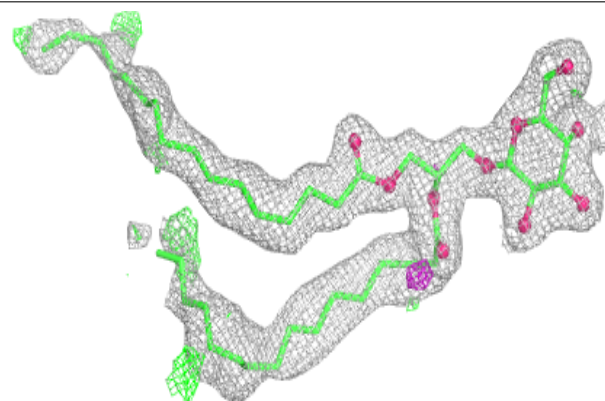


Electron density around DGD c 918:

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

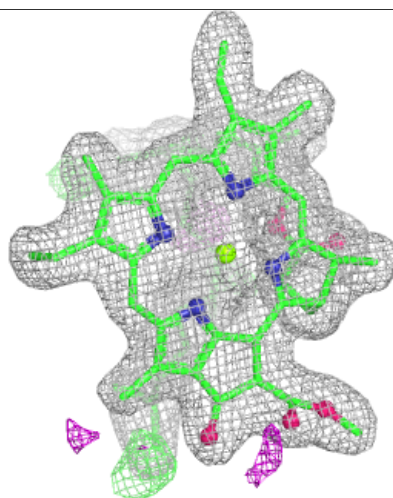
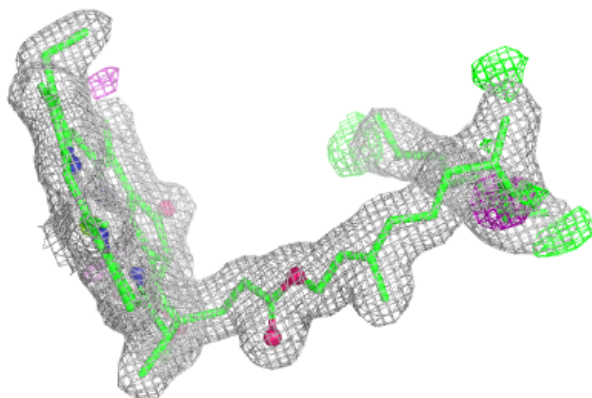
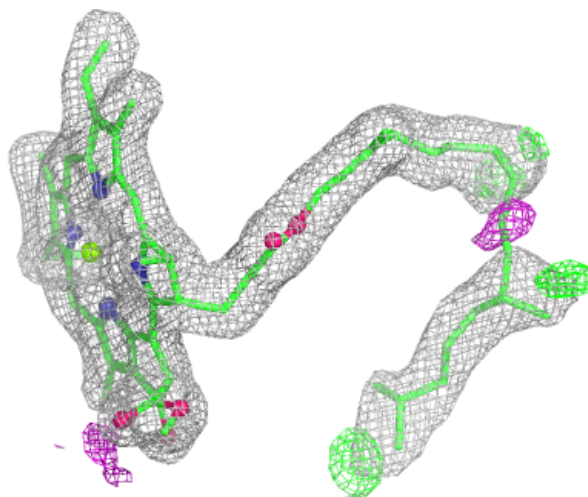
**Electron density around LMG d 410:**

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



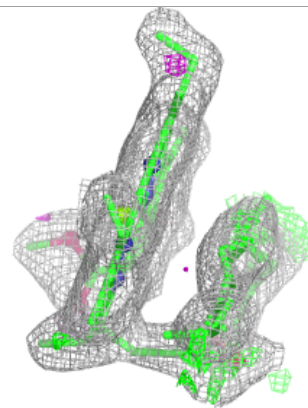
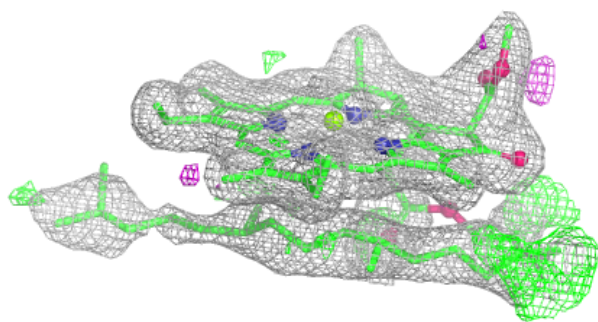
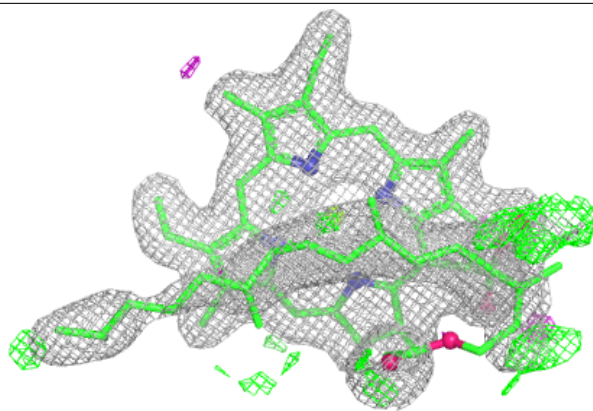
Electron density around CLA b 609:

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

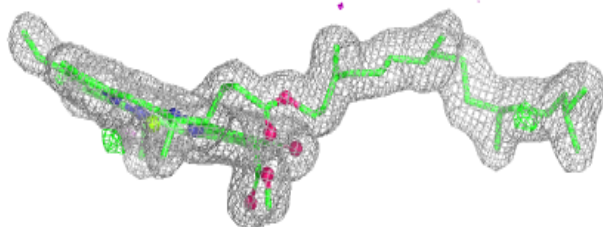
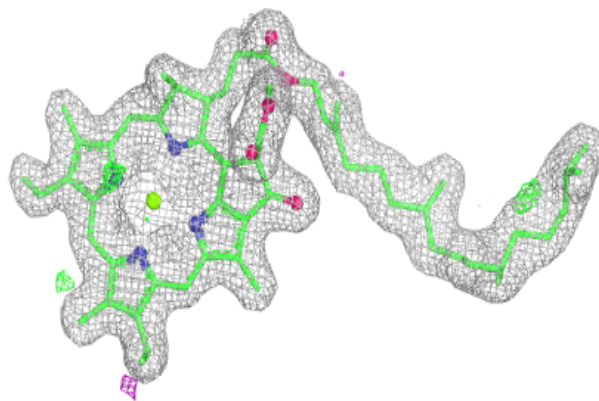


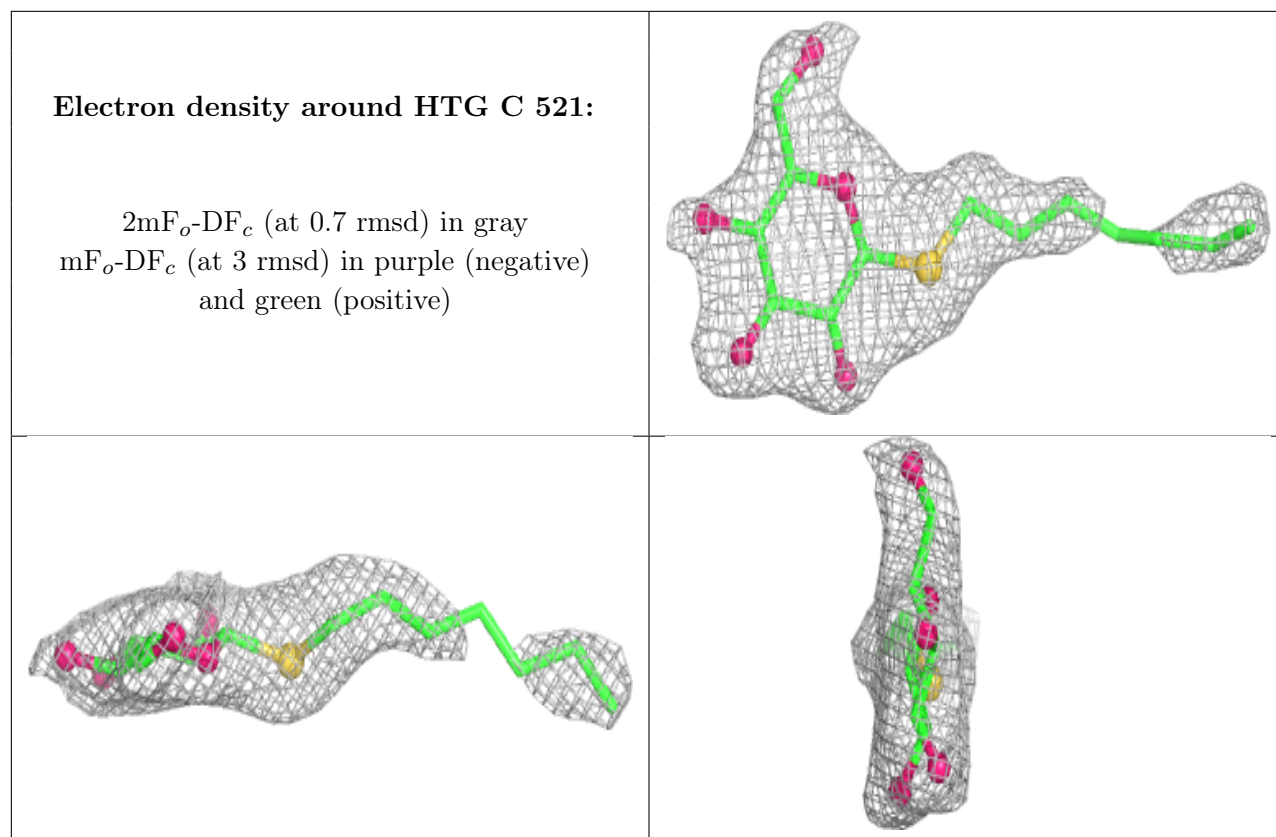
Electron density around CLA B 602:

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

**Electron density around CLA B 603:**

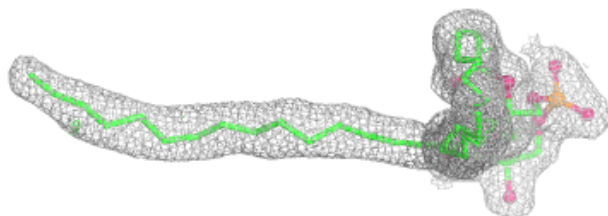
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





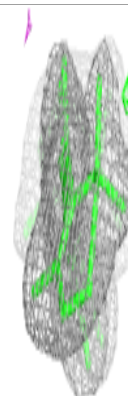
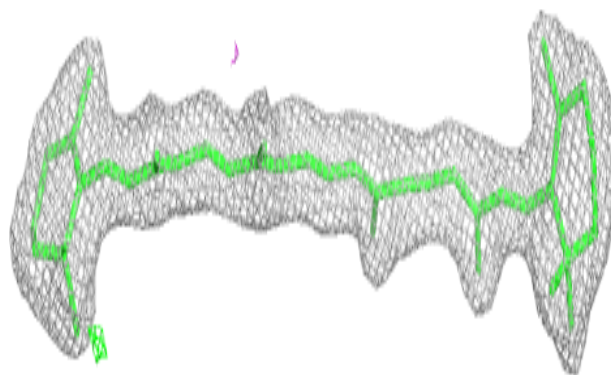
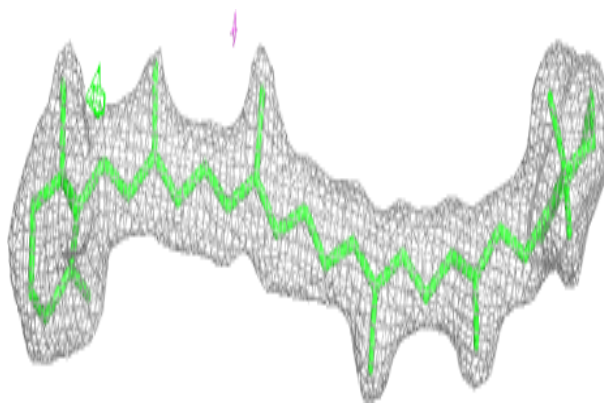
Electron density around LHG 1 101:

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



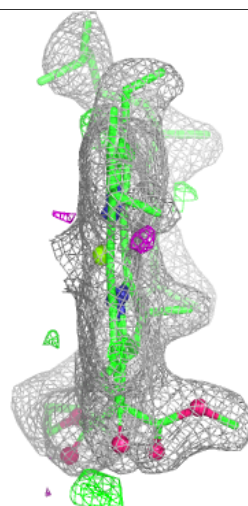
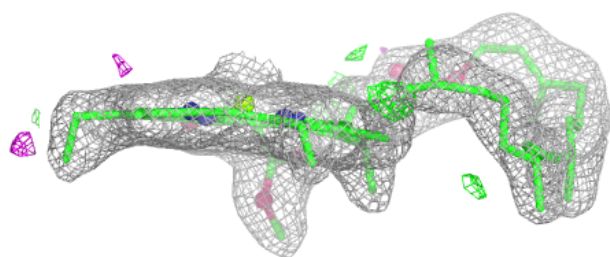
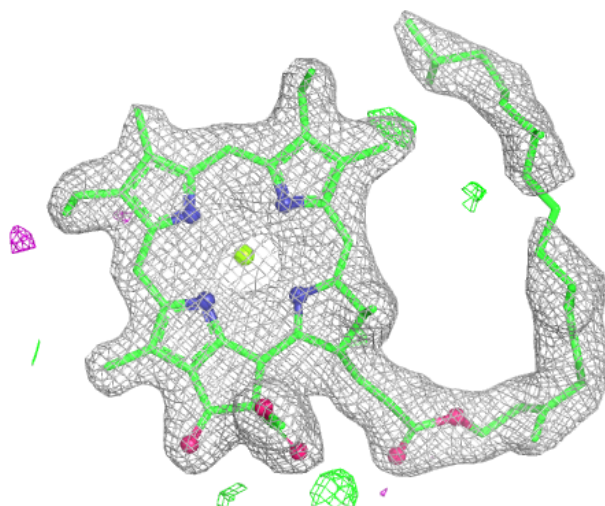
Electron density around BCR c 915:

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



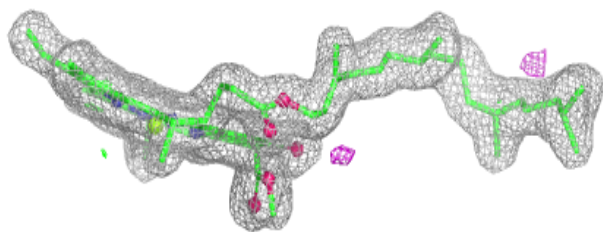
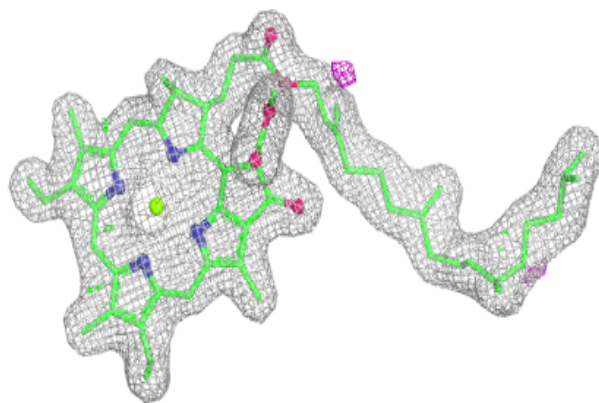
Electron density around CLA c 913:

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

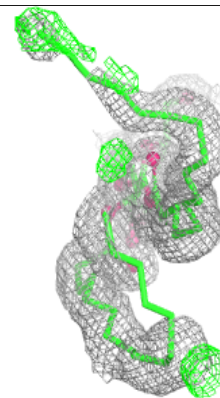
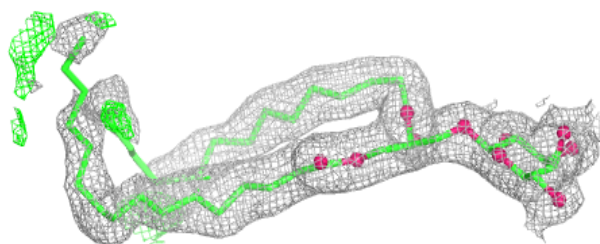
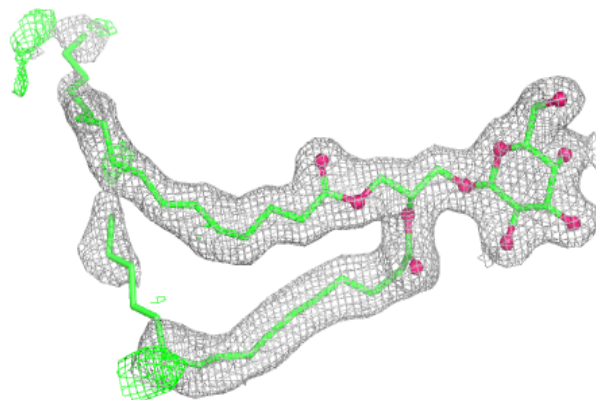


Electron density around CLA b 605:

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

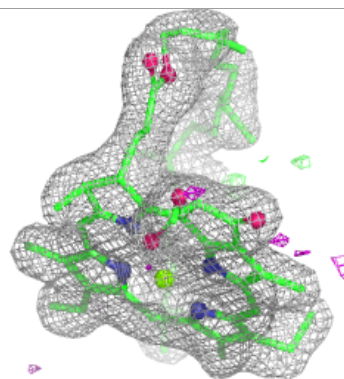
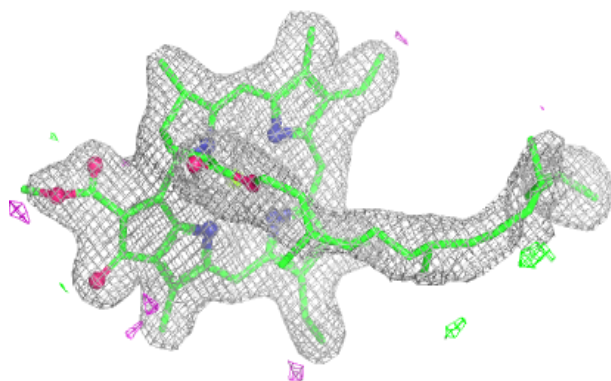
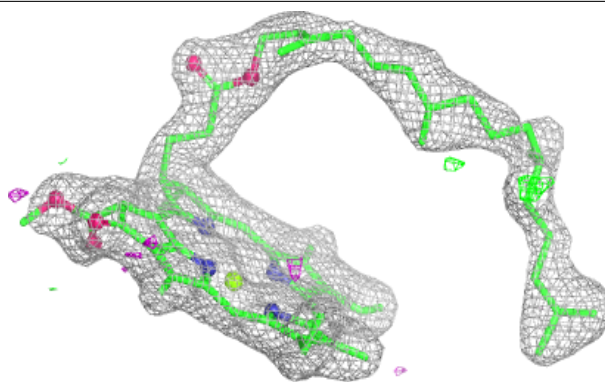
**Electron density around LMG D 411:**

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

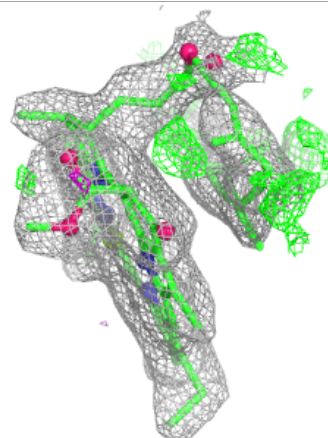
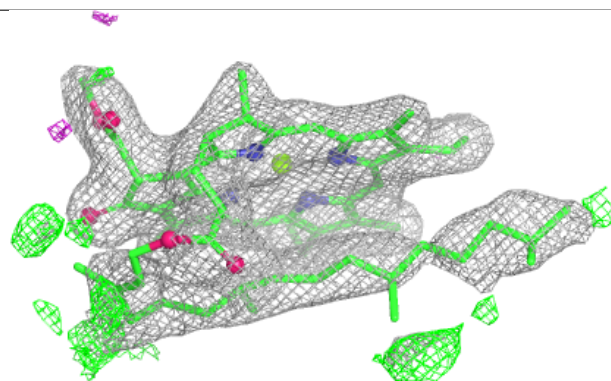
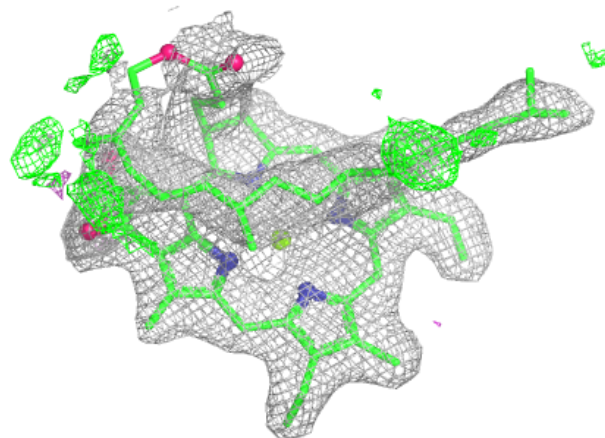


Electron density around CLA C 513:

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

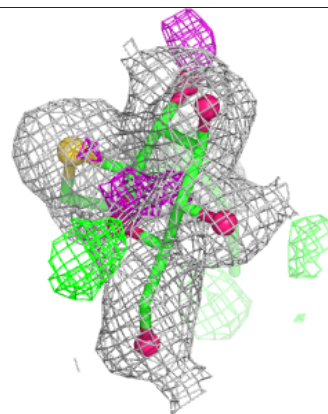
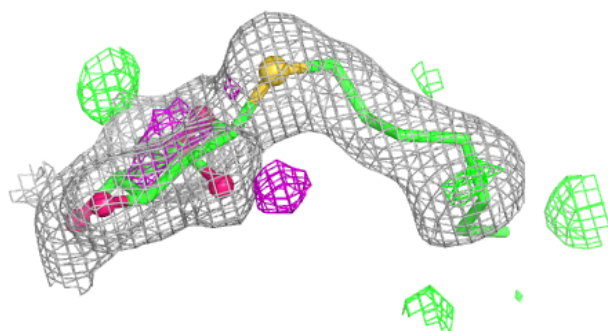
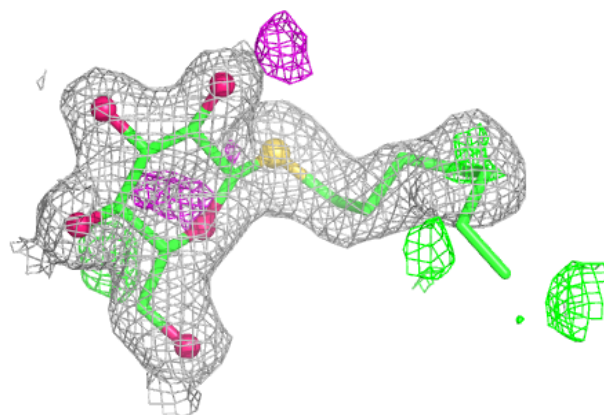
**Electron density around CLA b 604:**

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

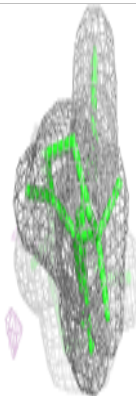
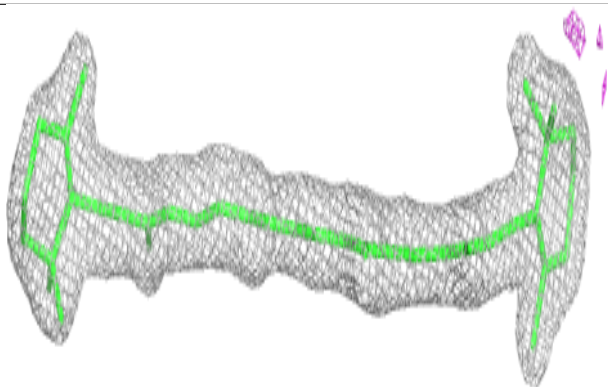
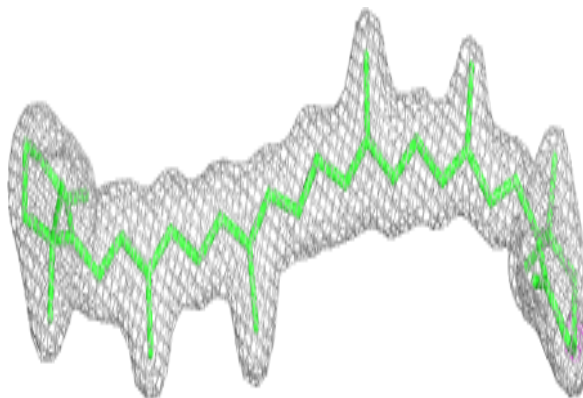


Electron density around HTG B 625:

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

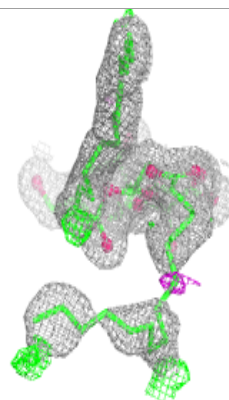
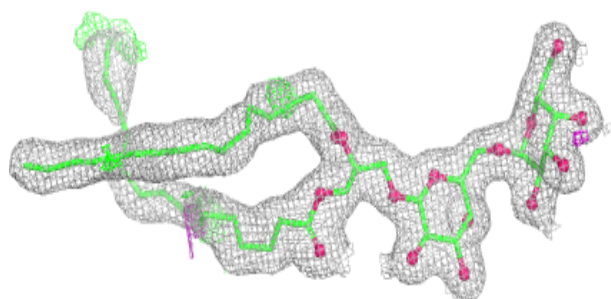
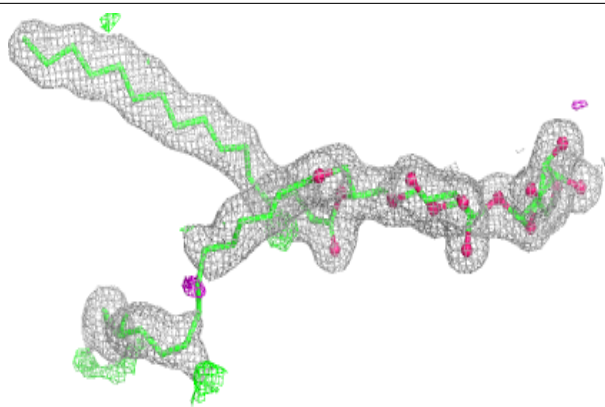
**Electron density around BCR c 916:**

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

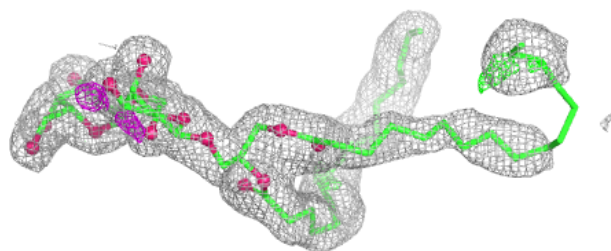
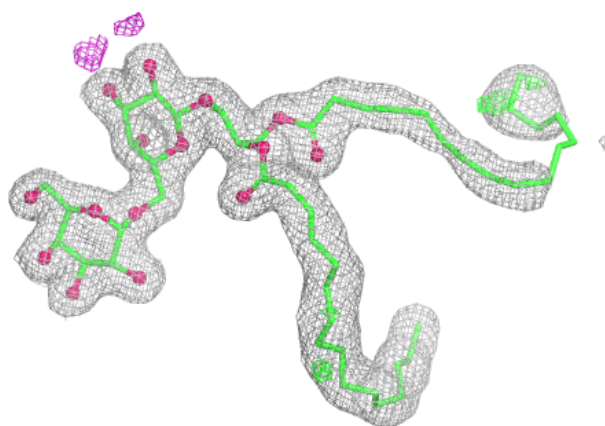


Electron density around DGD C 516:

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

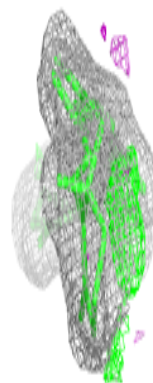
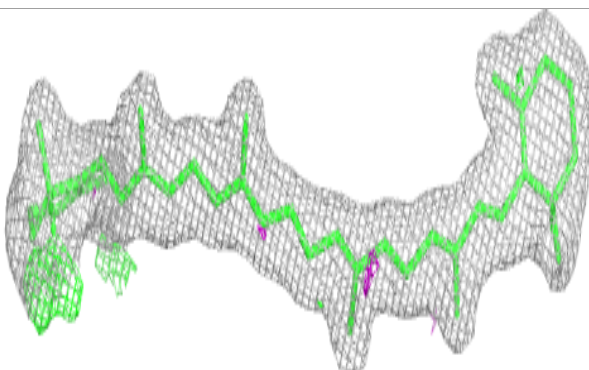
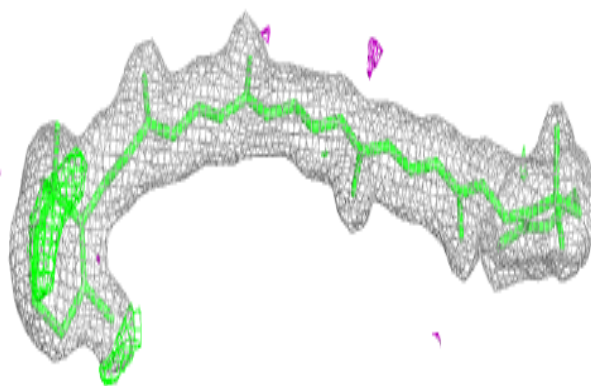
**Electron density around DGD C 517:**

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

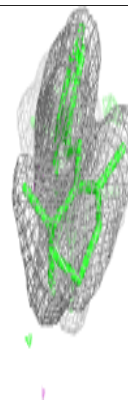
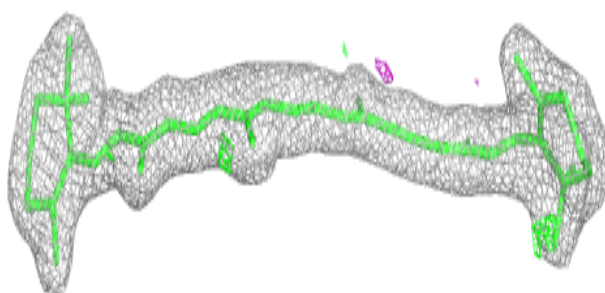
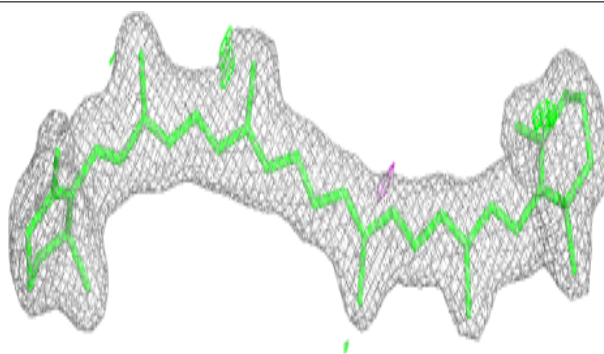


Electron density around BCR d 404:

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

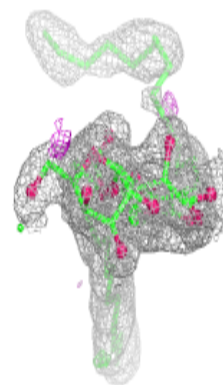
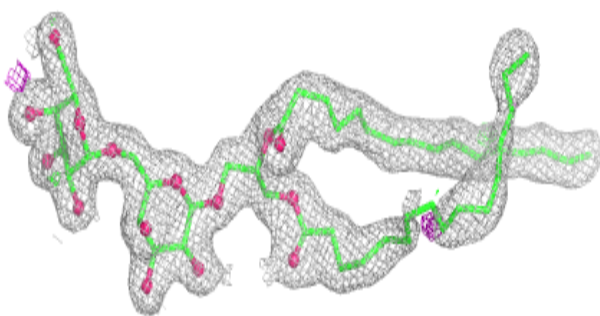
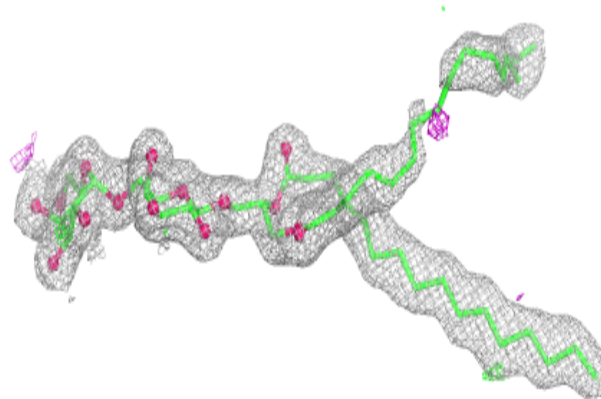
**Electron density around BCR k 101:**

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

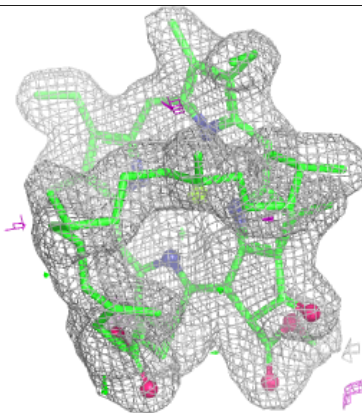
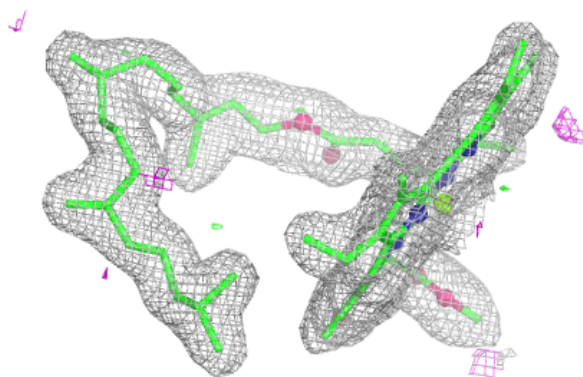
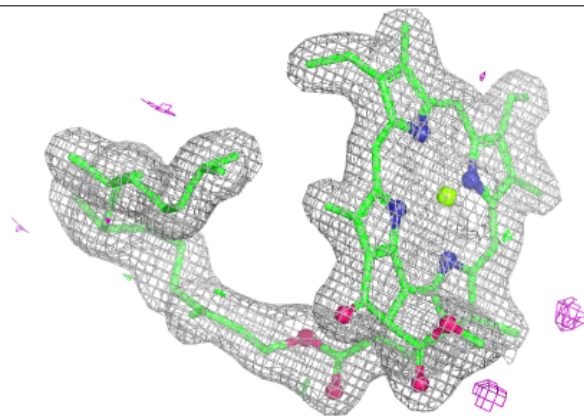


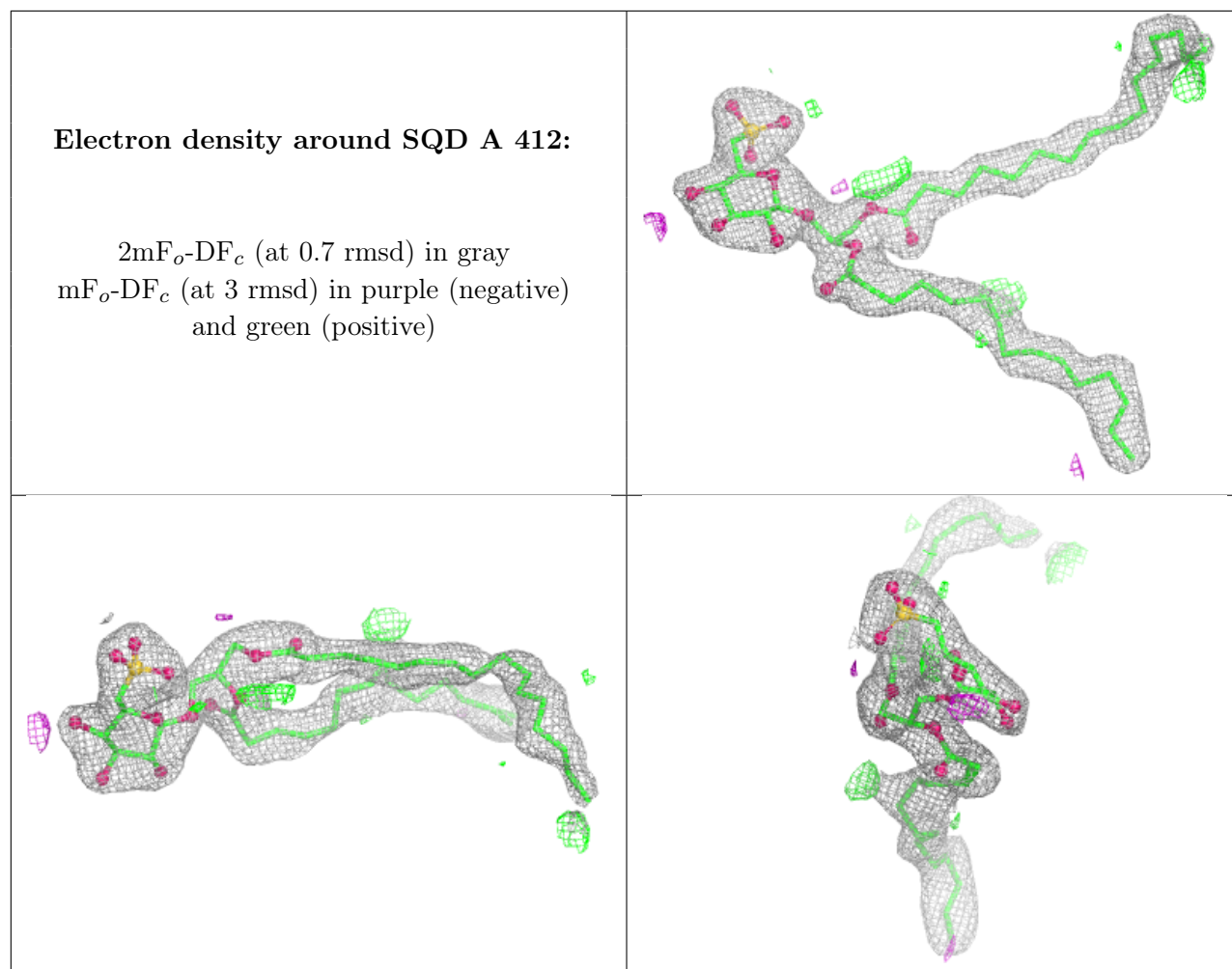
Electron density around DGD c 917:

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

**Electron density around CLA c 904:**

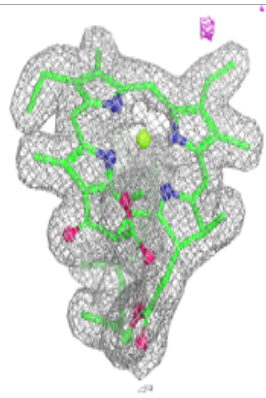
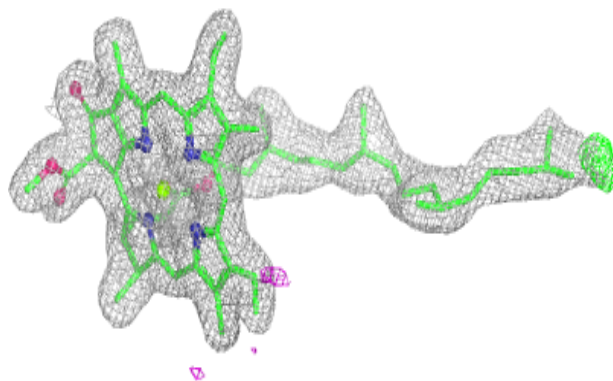
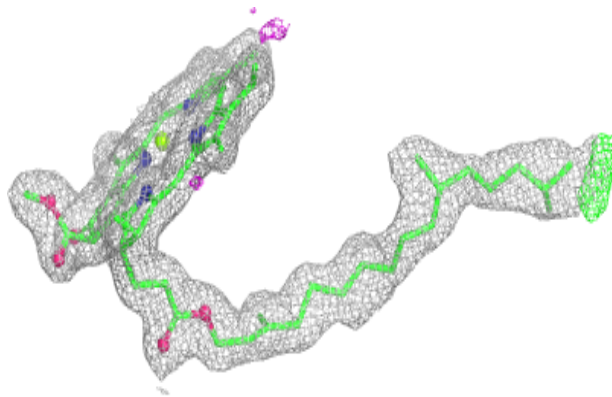
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



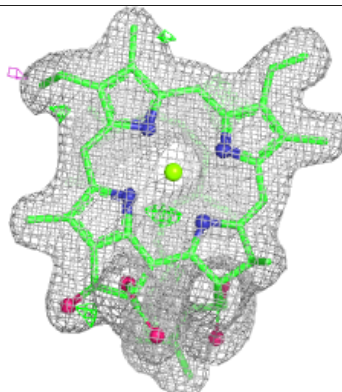
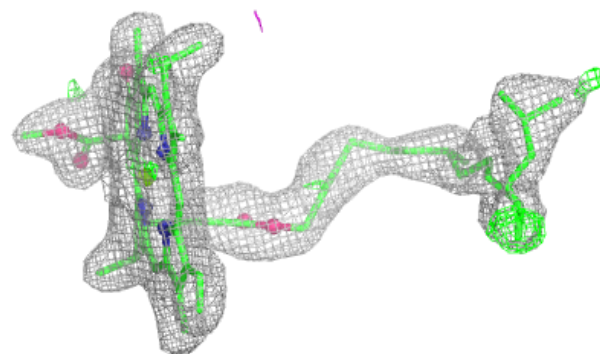
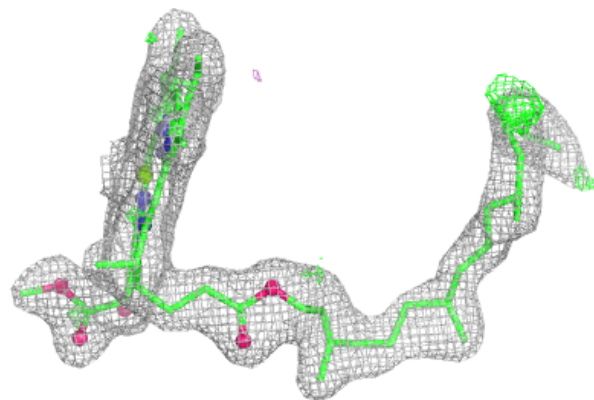


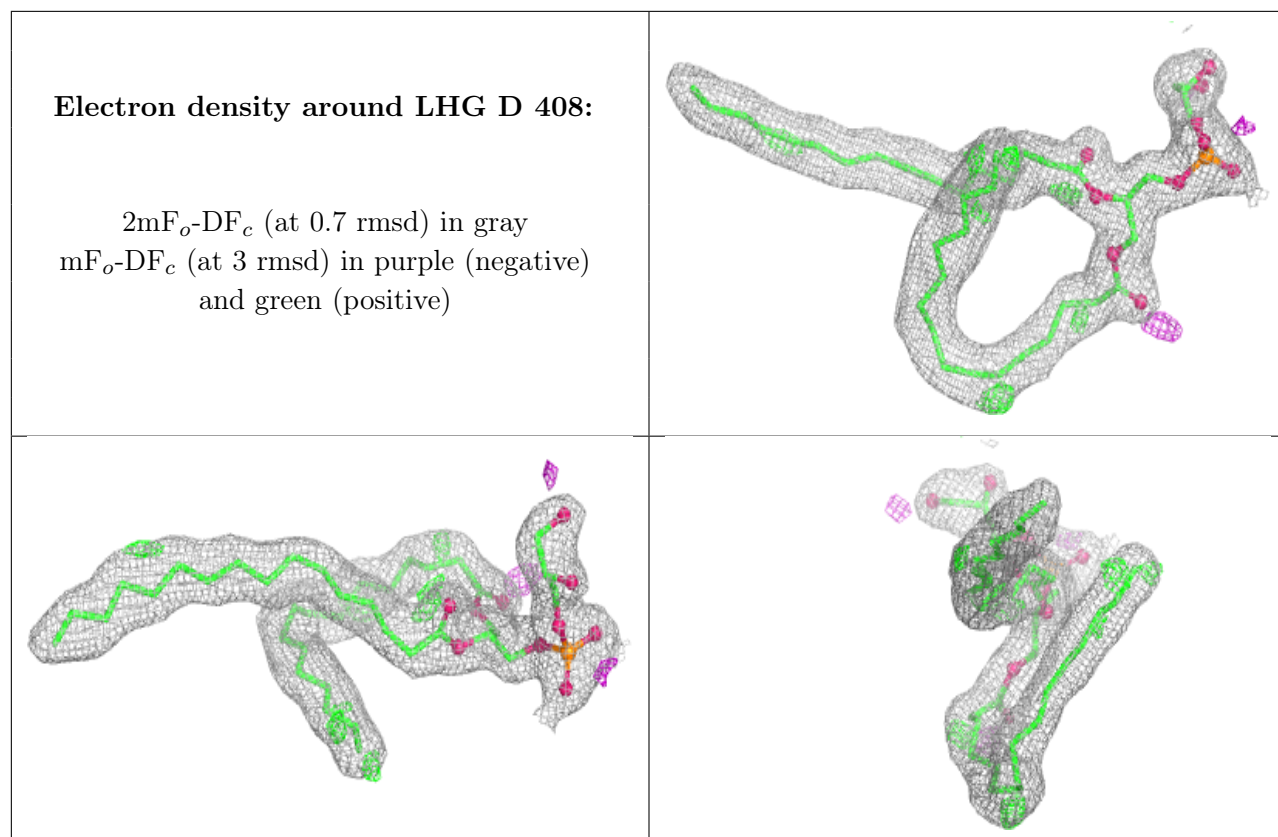
Electron density around CLA c 905:

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

**Electron density around CLA c 907:**

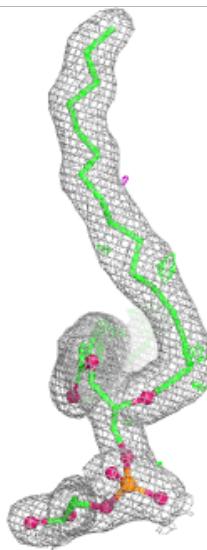
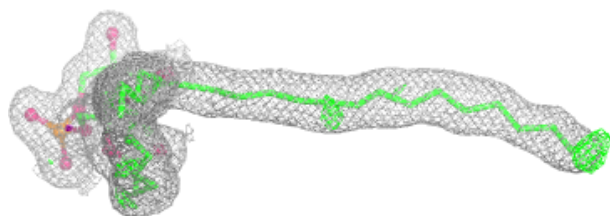
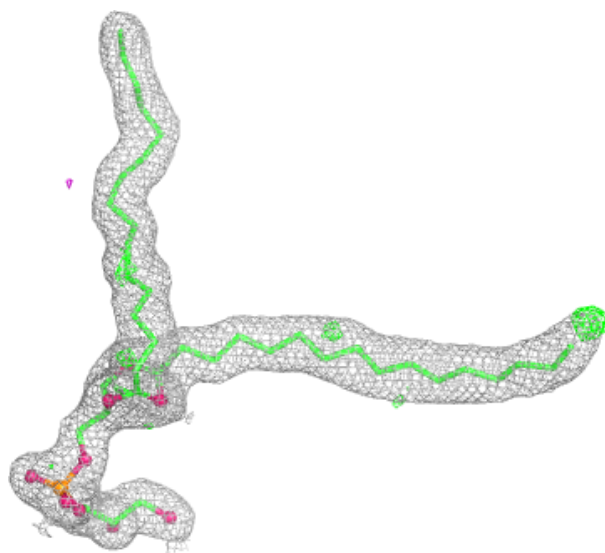
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





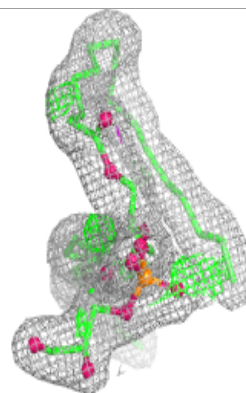
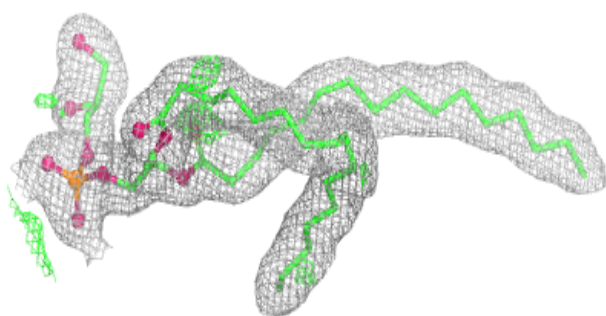
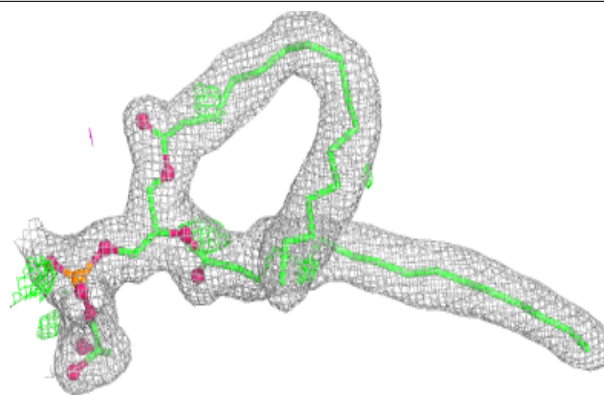
Electron density around LHG L 101:

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



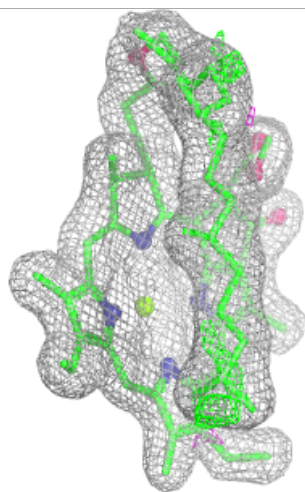
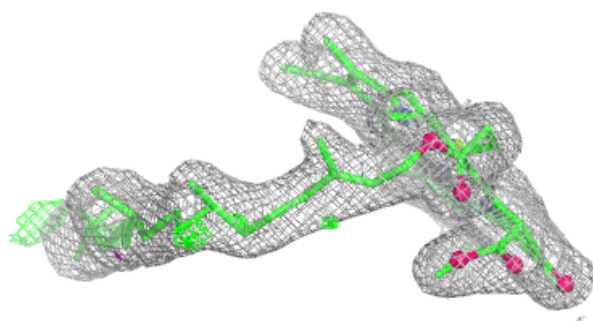
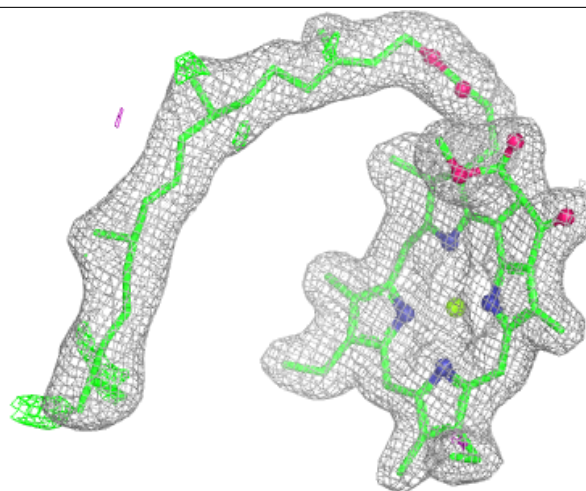
Electron density around LHG d 407:

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



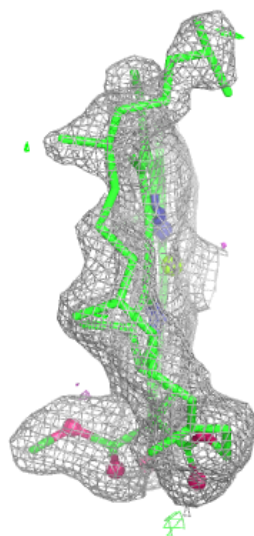
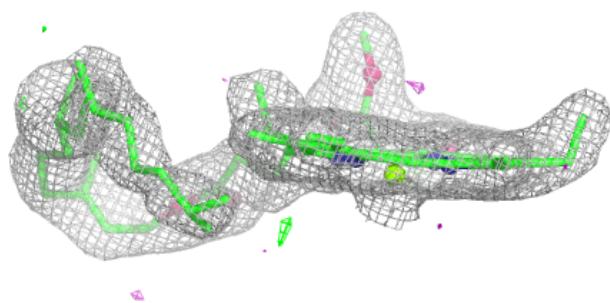
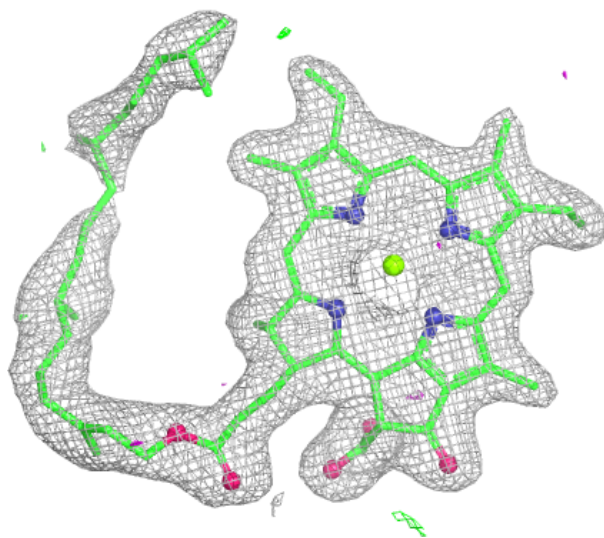
Electron density around CLA c 908:

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



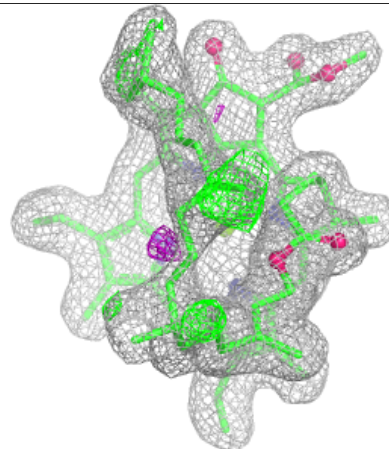
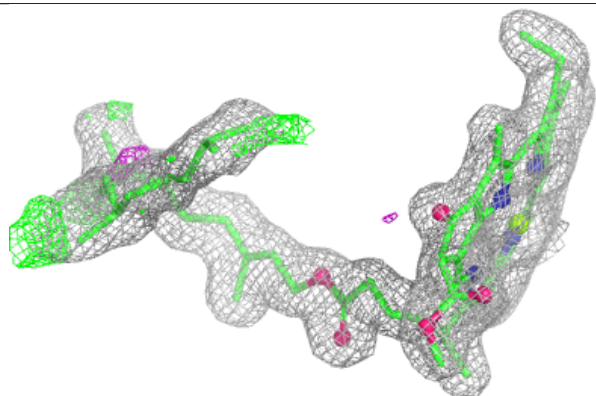
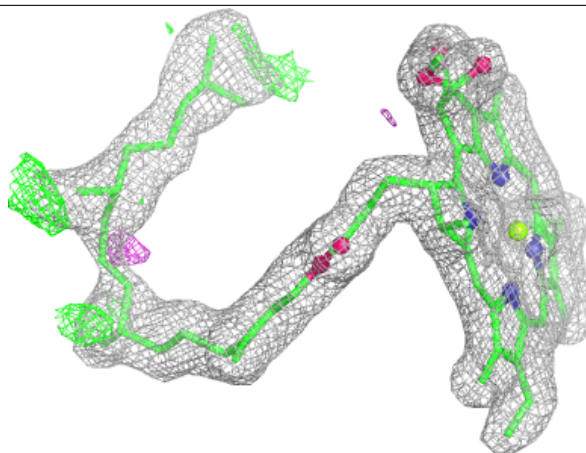
Electron density around CLA C 512:

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

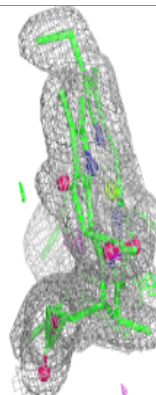
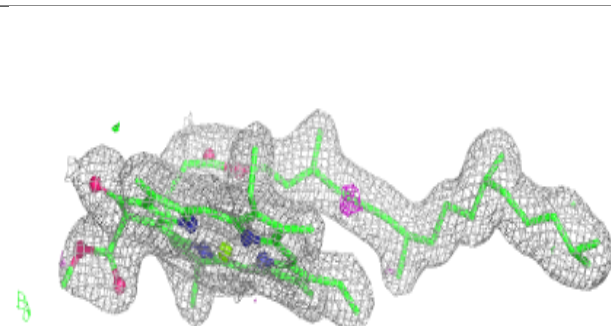
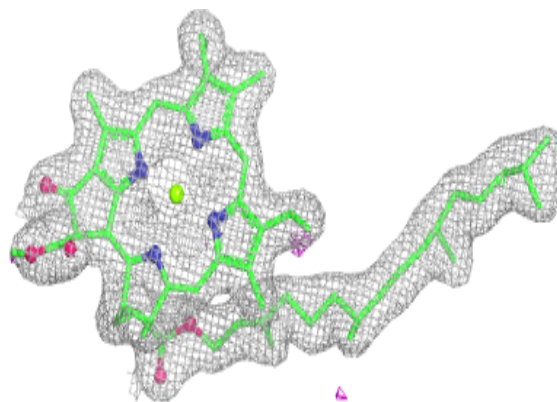


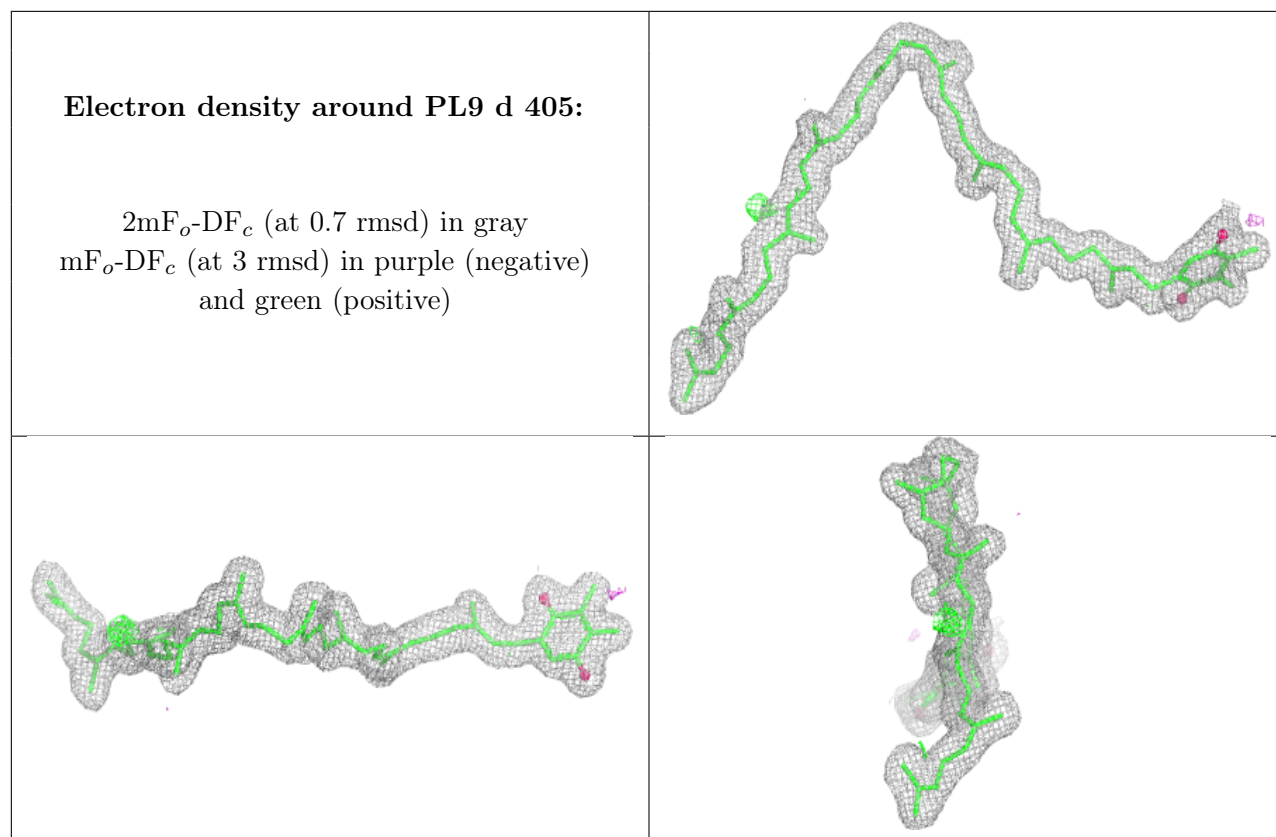
Electron density around CLA B 607:

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

**Electron density around CLA c 902:**

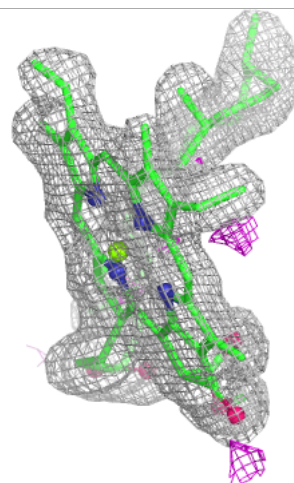
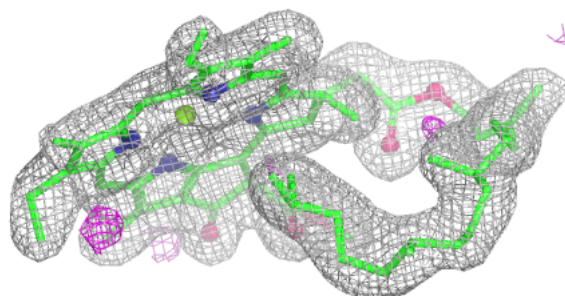
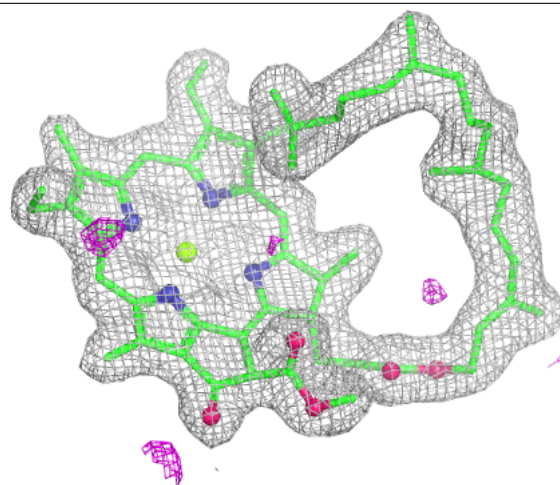
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





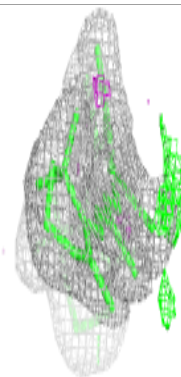
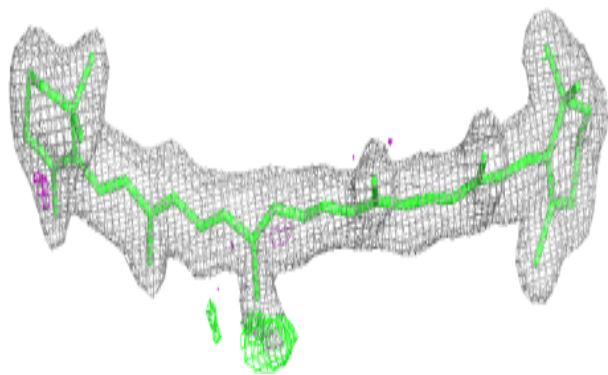
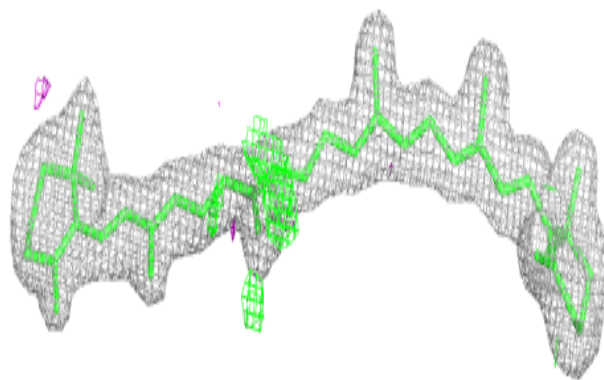
Electron density around CLA b 618:

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

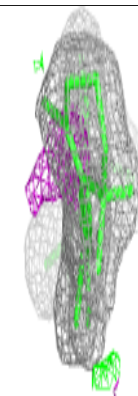
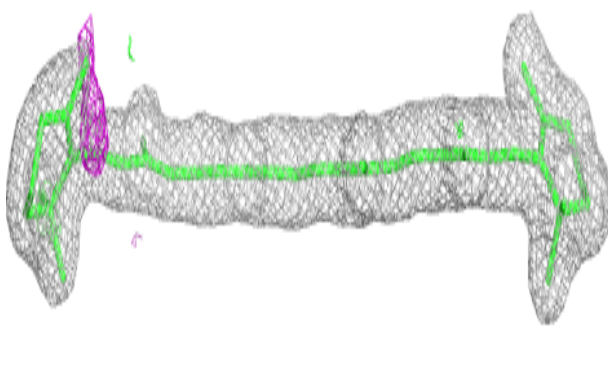
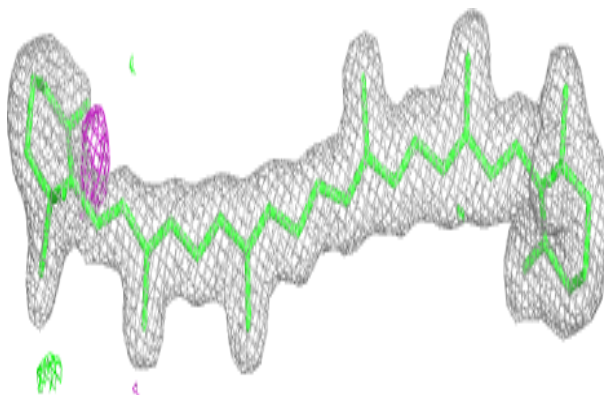


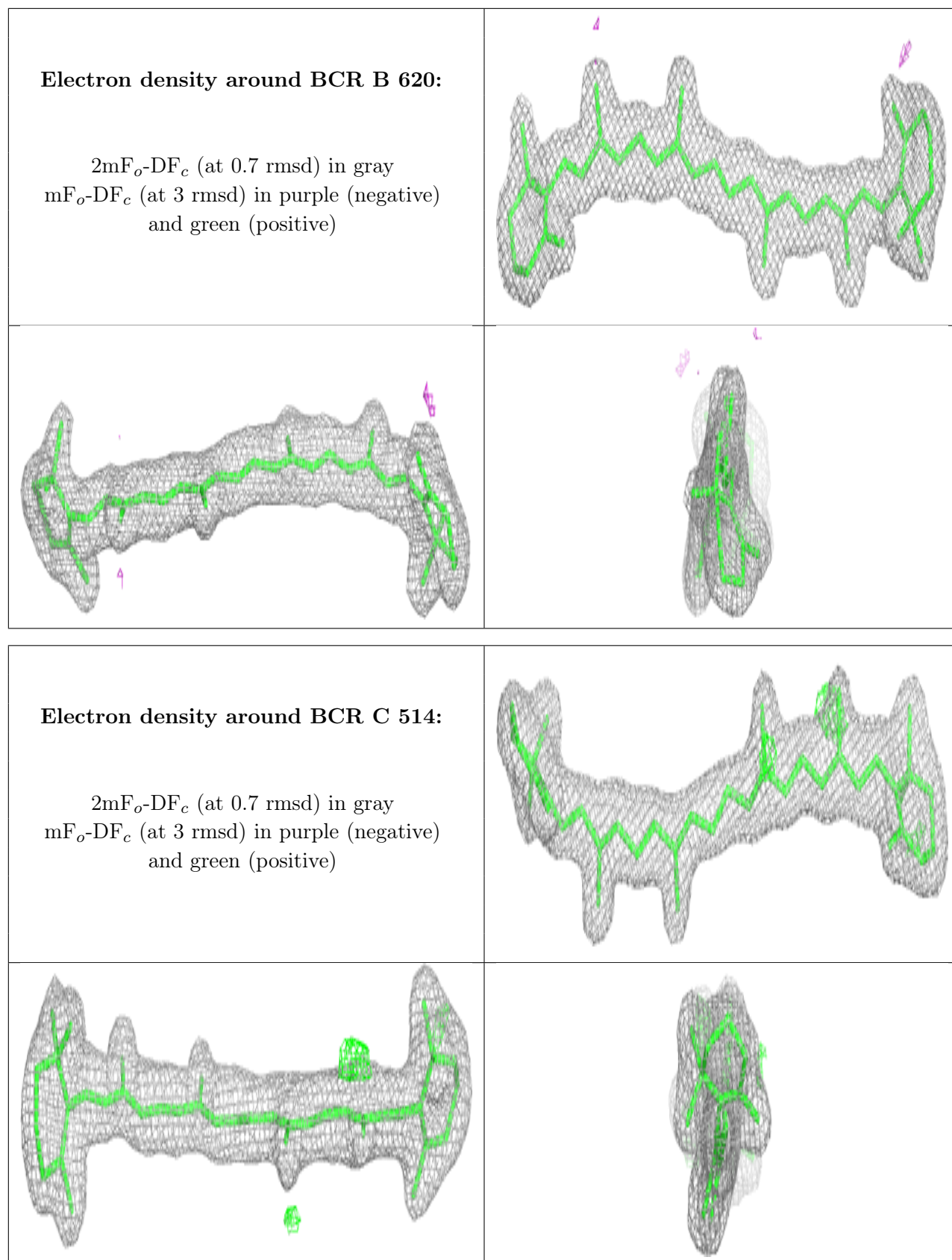
Electron density around BCR t 101:

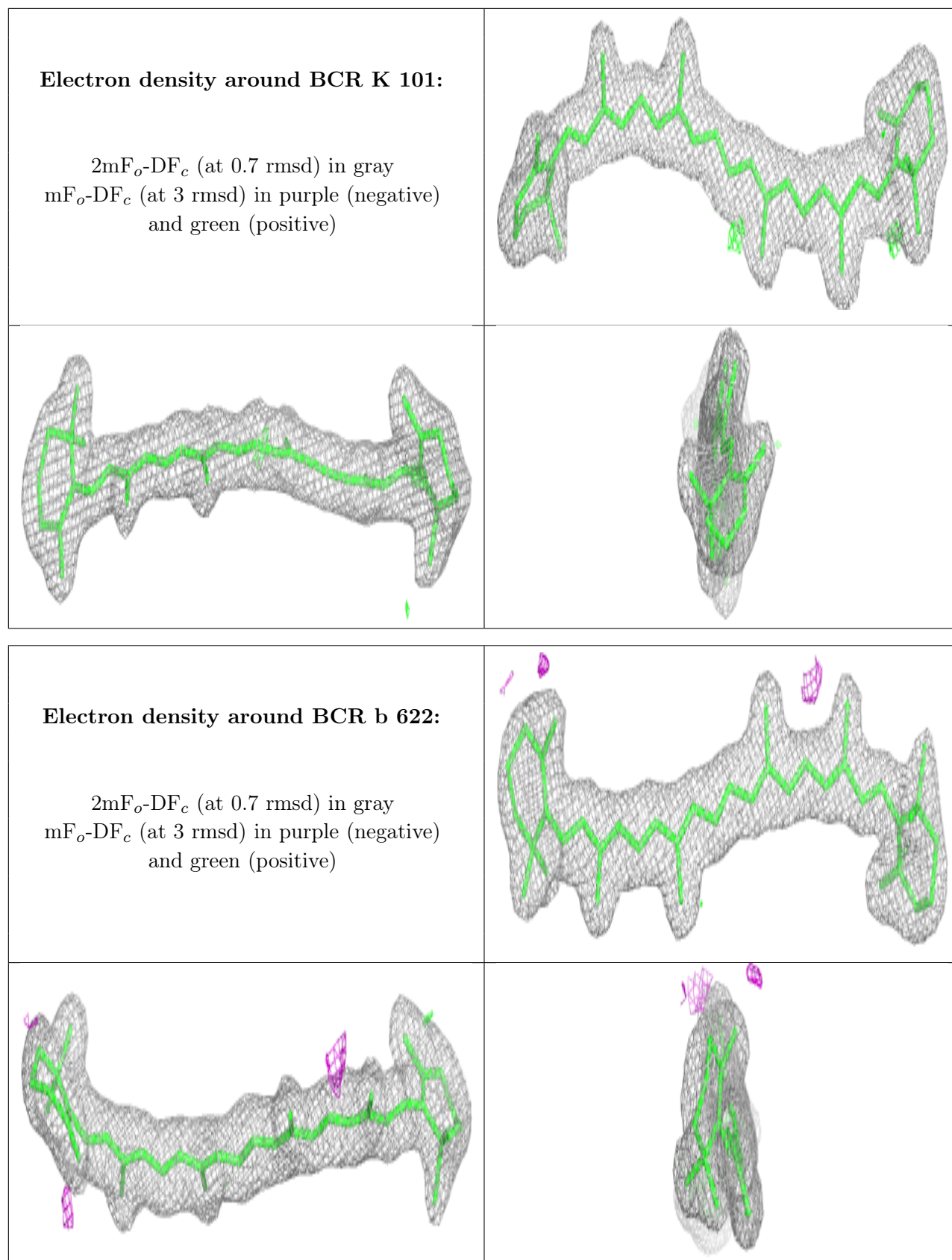
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around BCR B 619:**

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

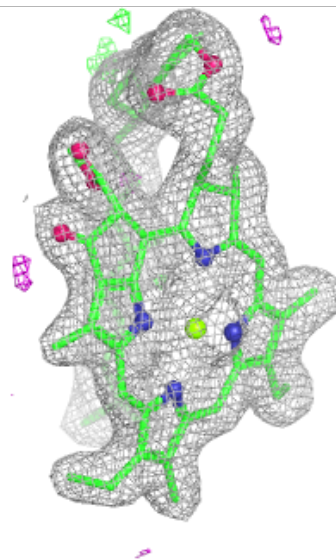
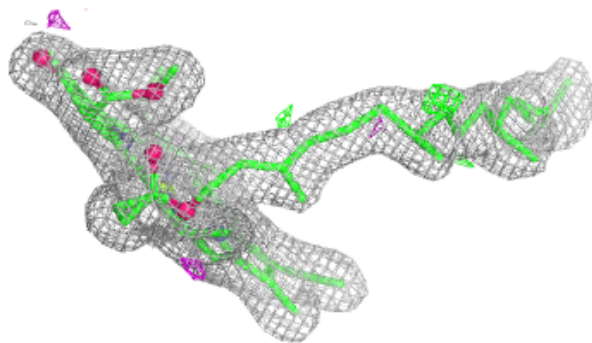
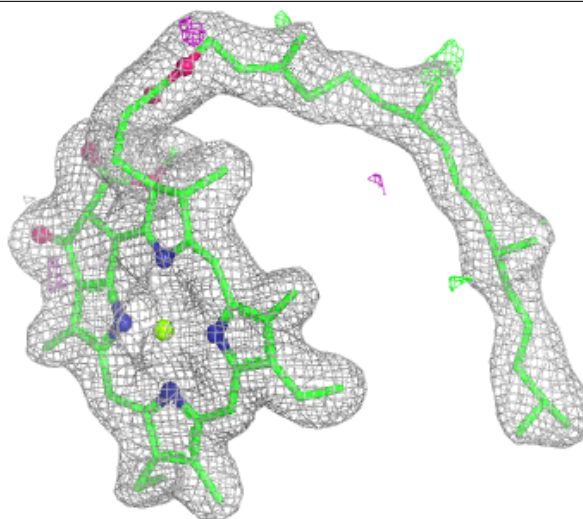






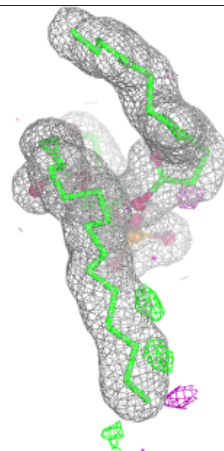
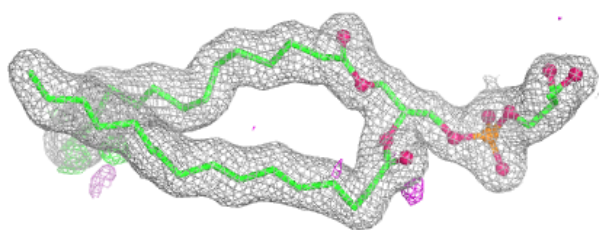
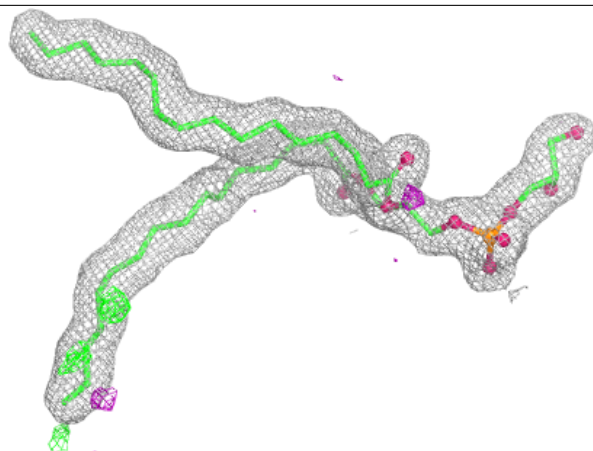
Electron density around CLA C 507:

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

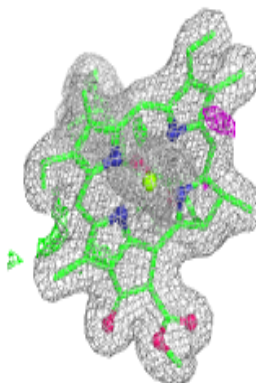
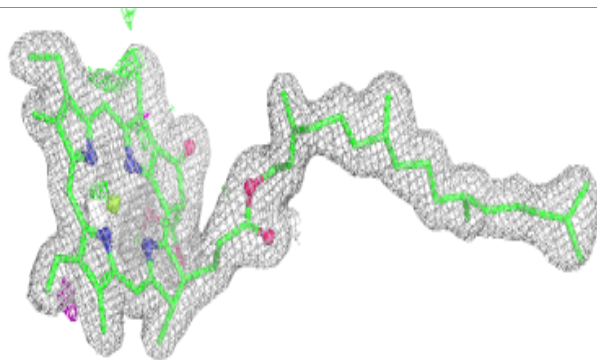
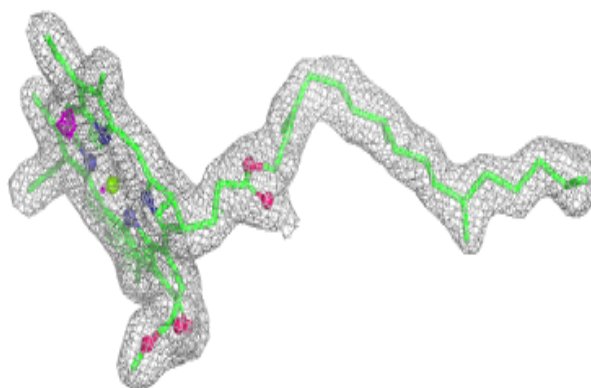


Electron density around LHG d 408:

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

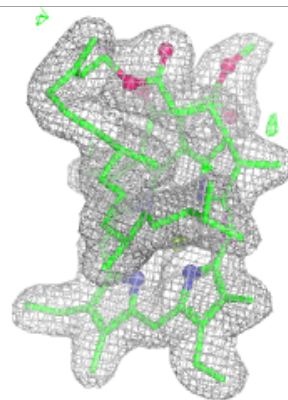
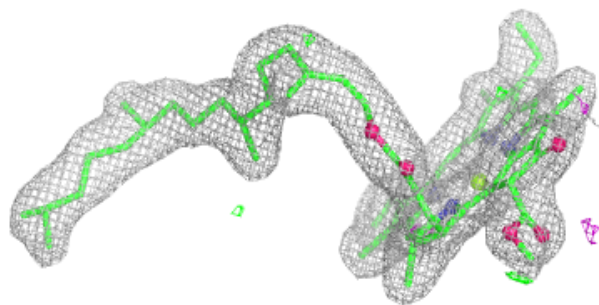
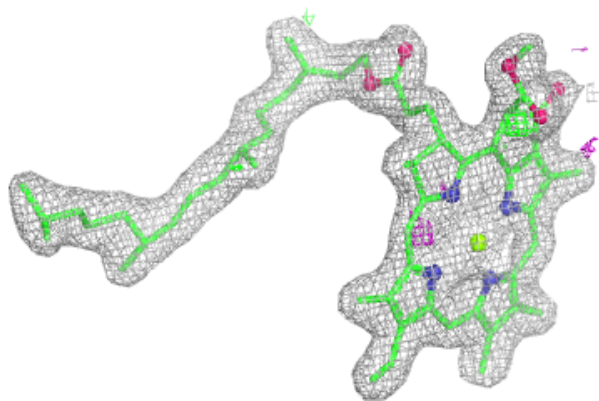
**Electron density around CLA c 903:**

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

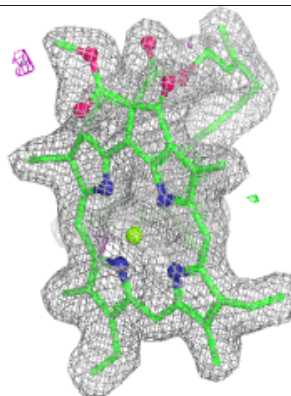
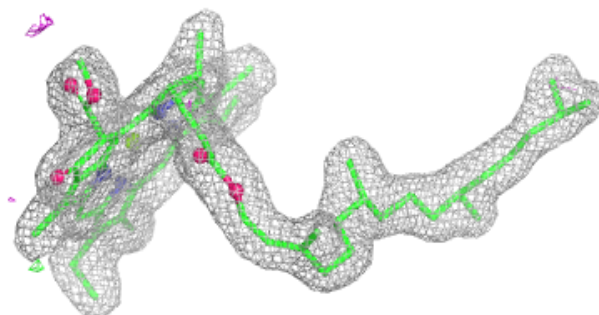
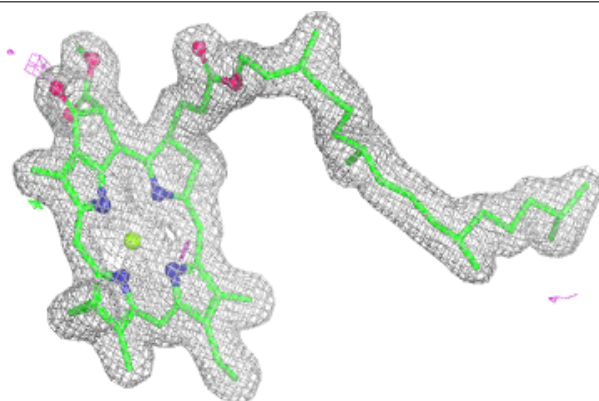


Electron density around CLA c 912:

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

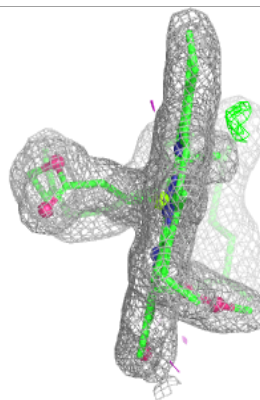
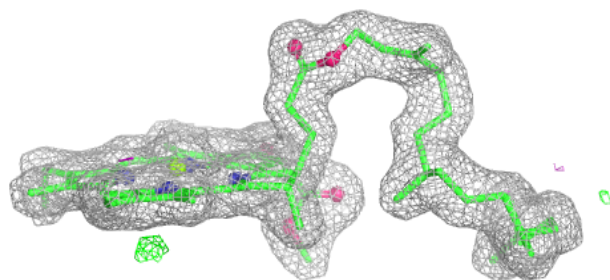
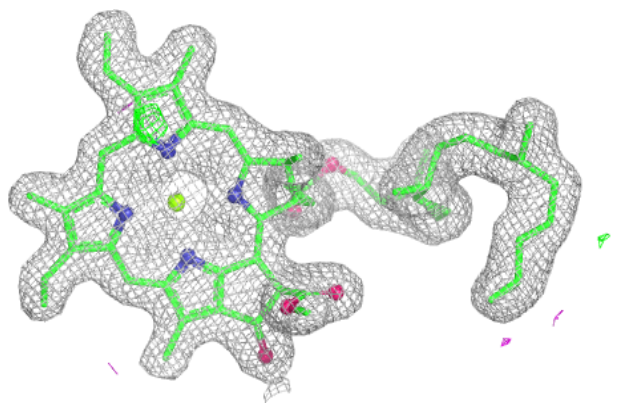
**Electron density around CLA C 511:**

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

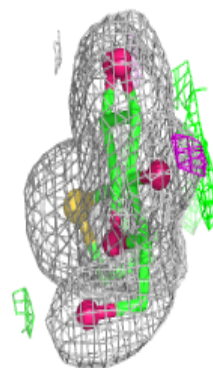
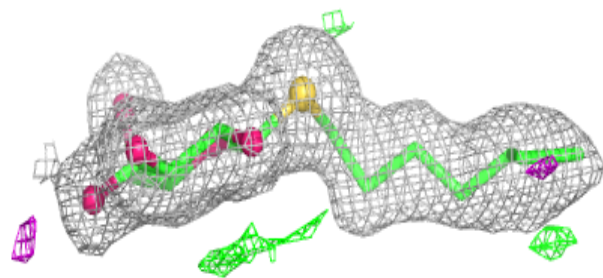
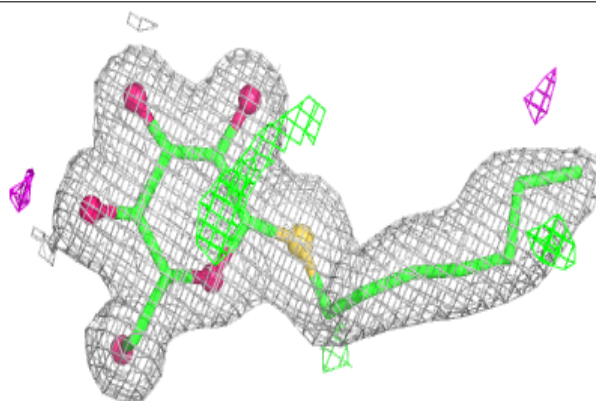


Electron density around CLA b 615:

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

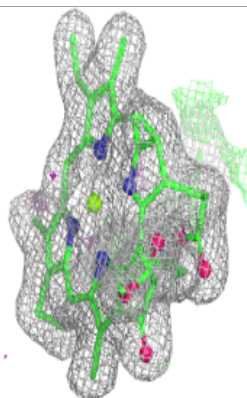
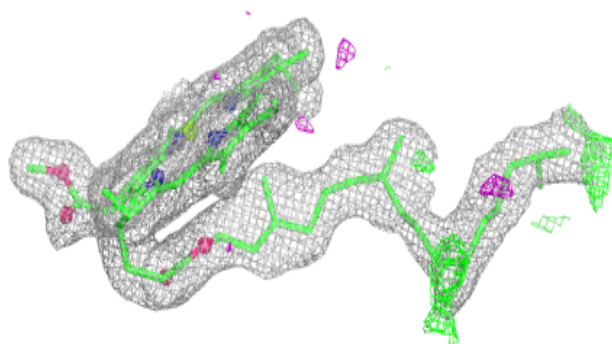
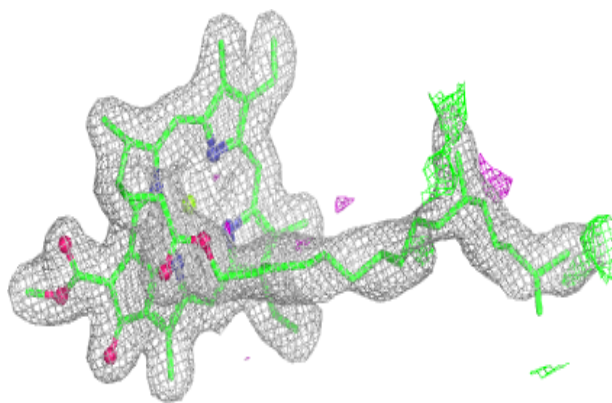
**Electron density around HTG B 624:**

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

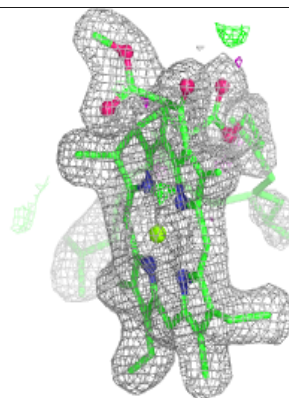
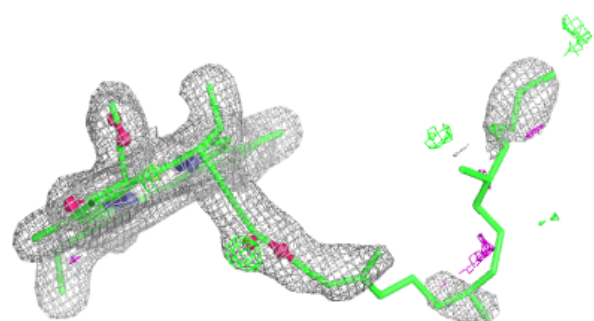
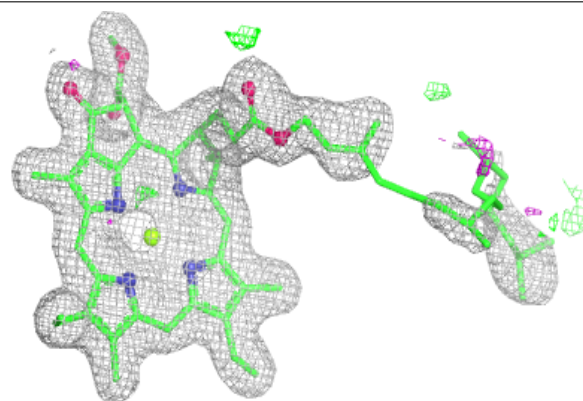


Electron density around CLA b 617:

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

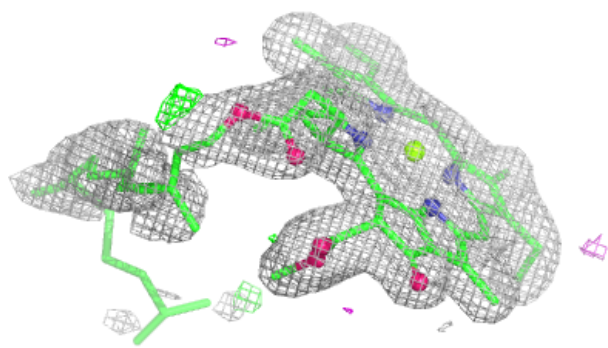
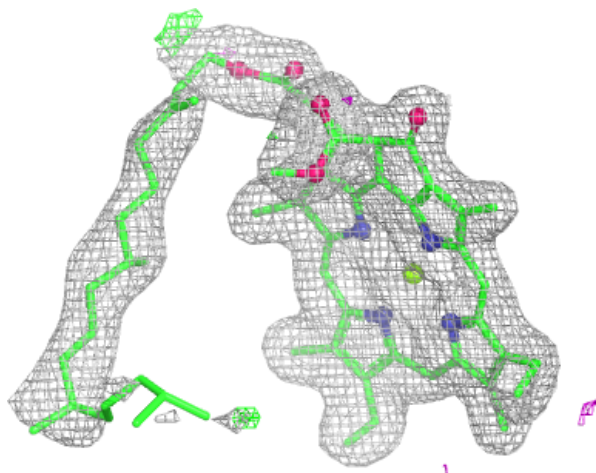
**Electron density around CLA A 410:**

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



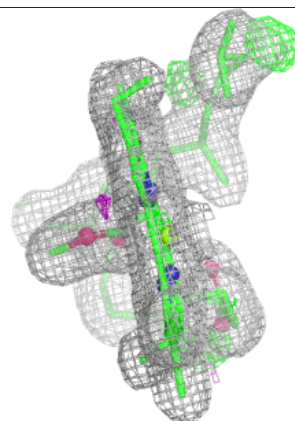
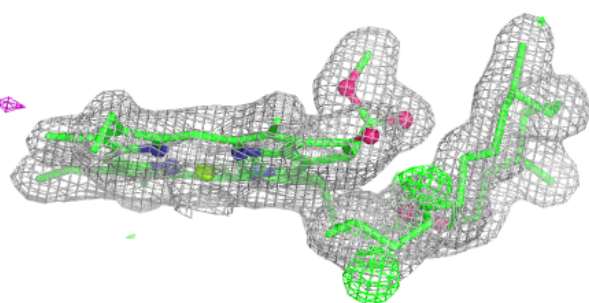
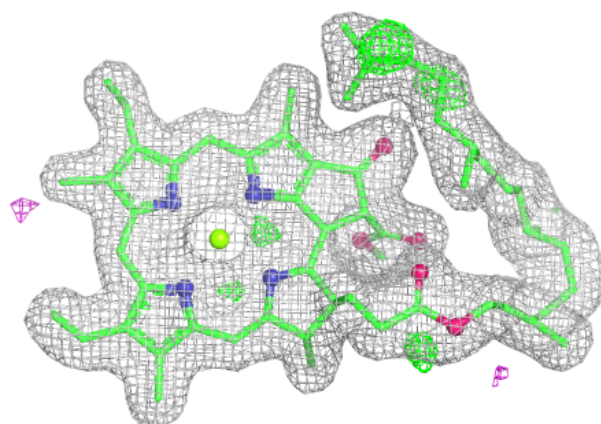
Electron density around CLA b 619:

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

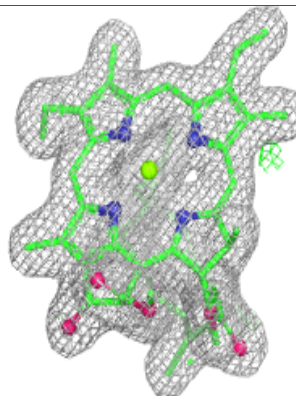
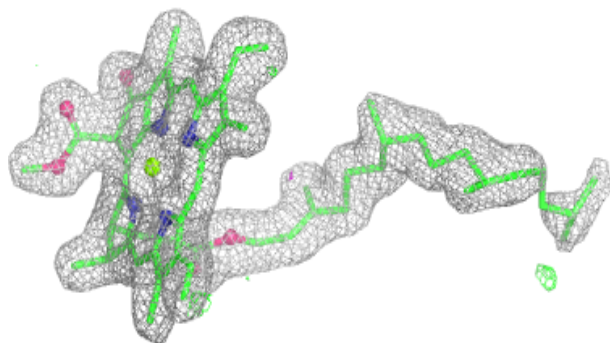
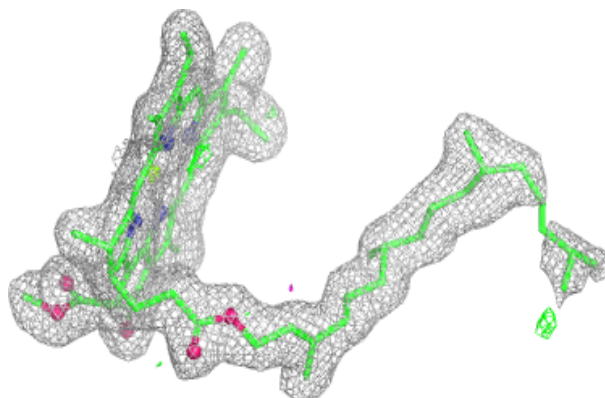


Electron density around CLA B 611:

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

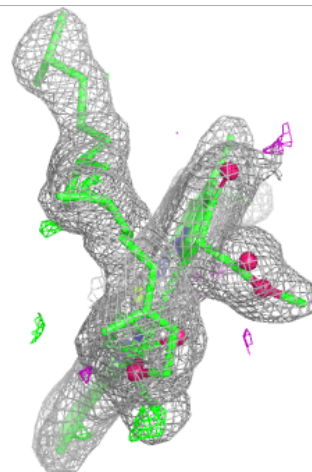
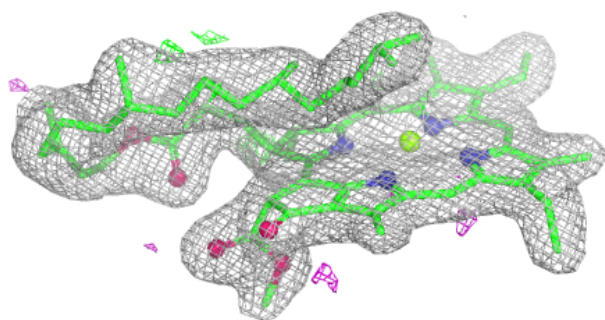
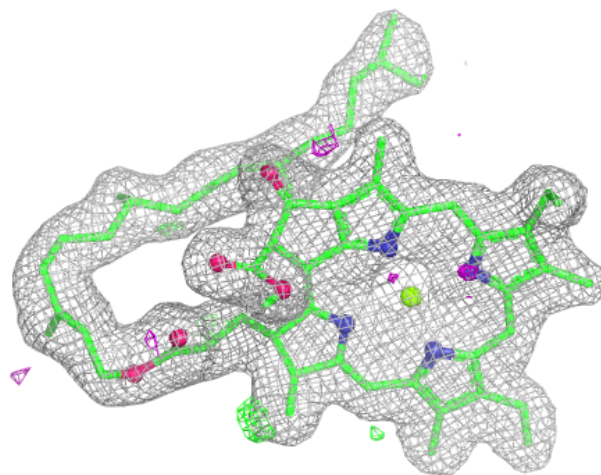
**Electron density around CLA C 508:**

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



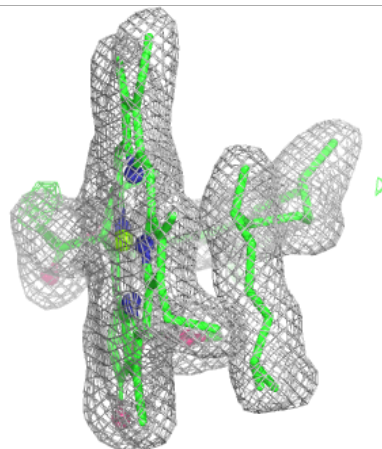
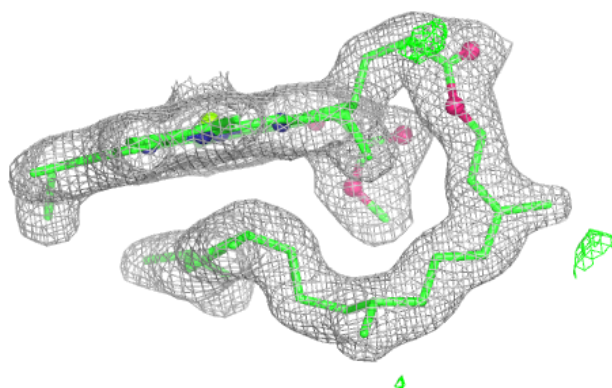
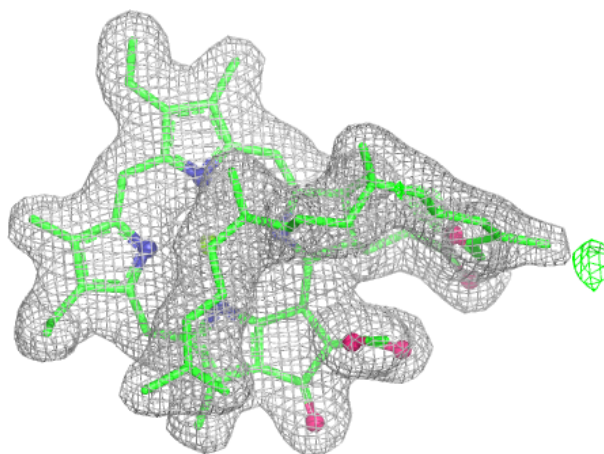
Electron density around CLA C 509:

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



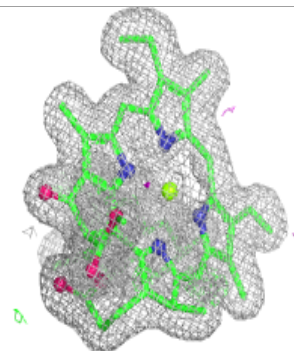
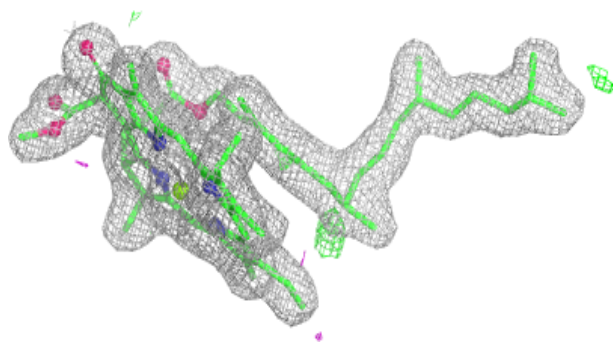
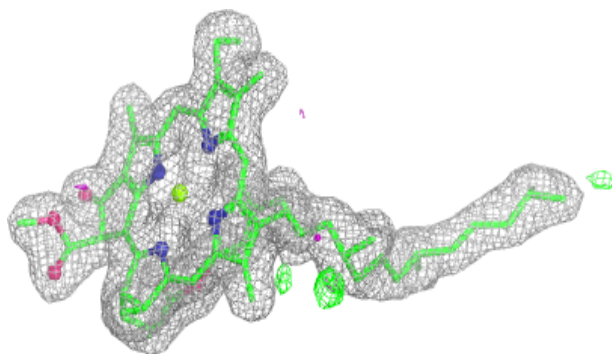
Electron density around CLA C 510:

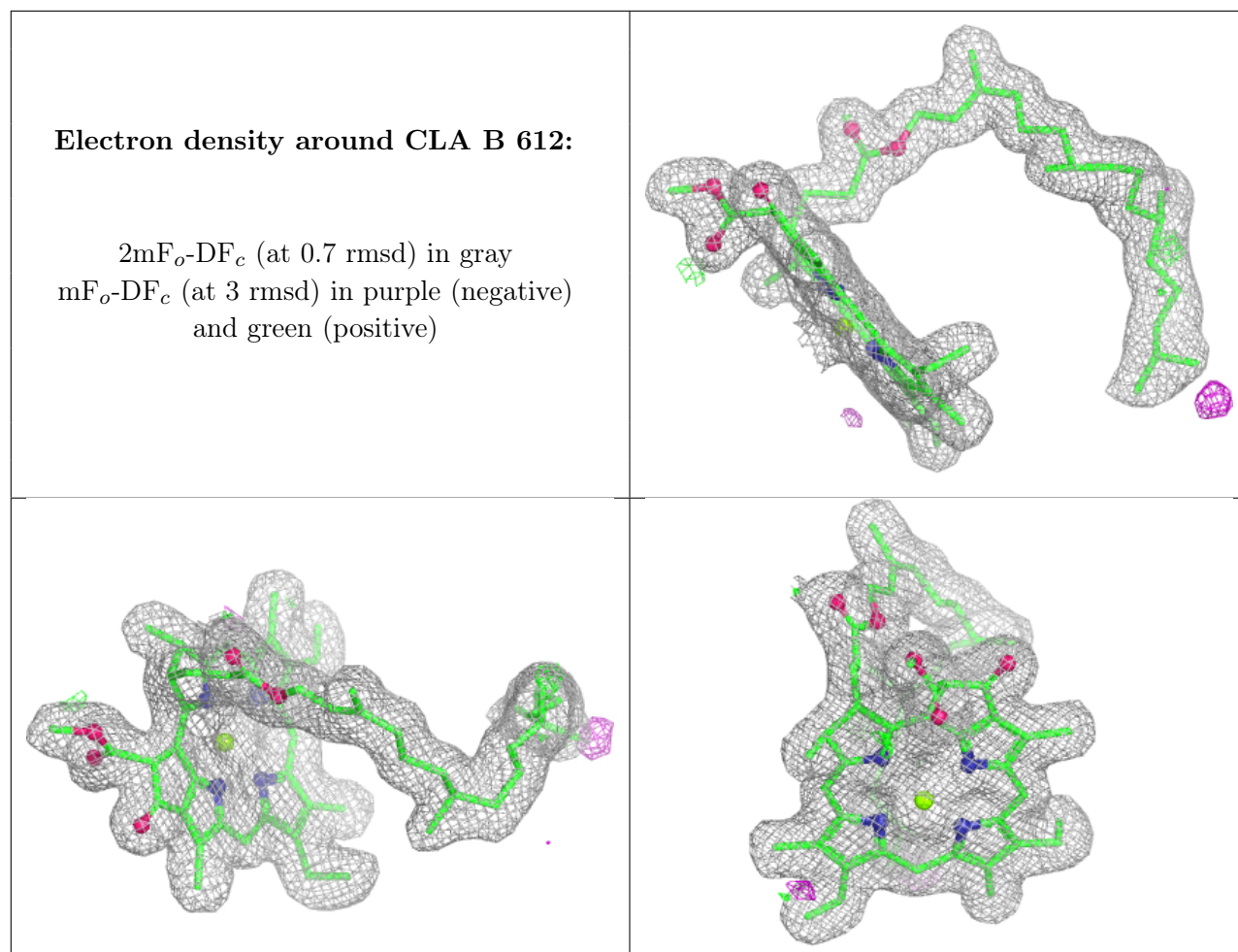
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

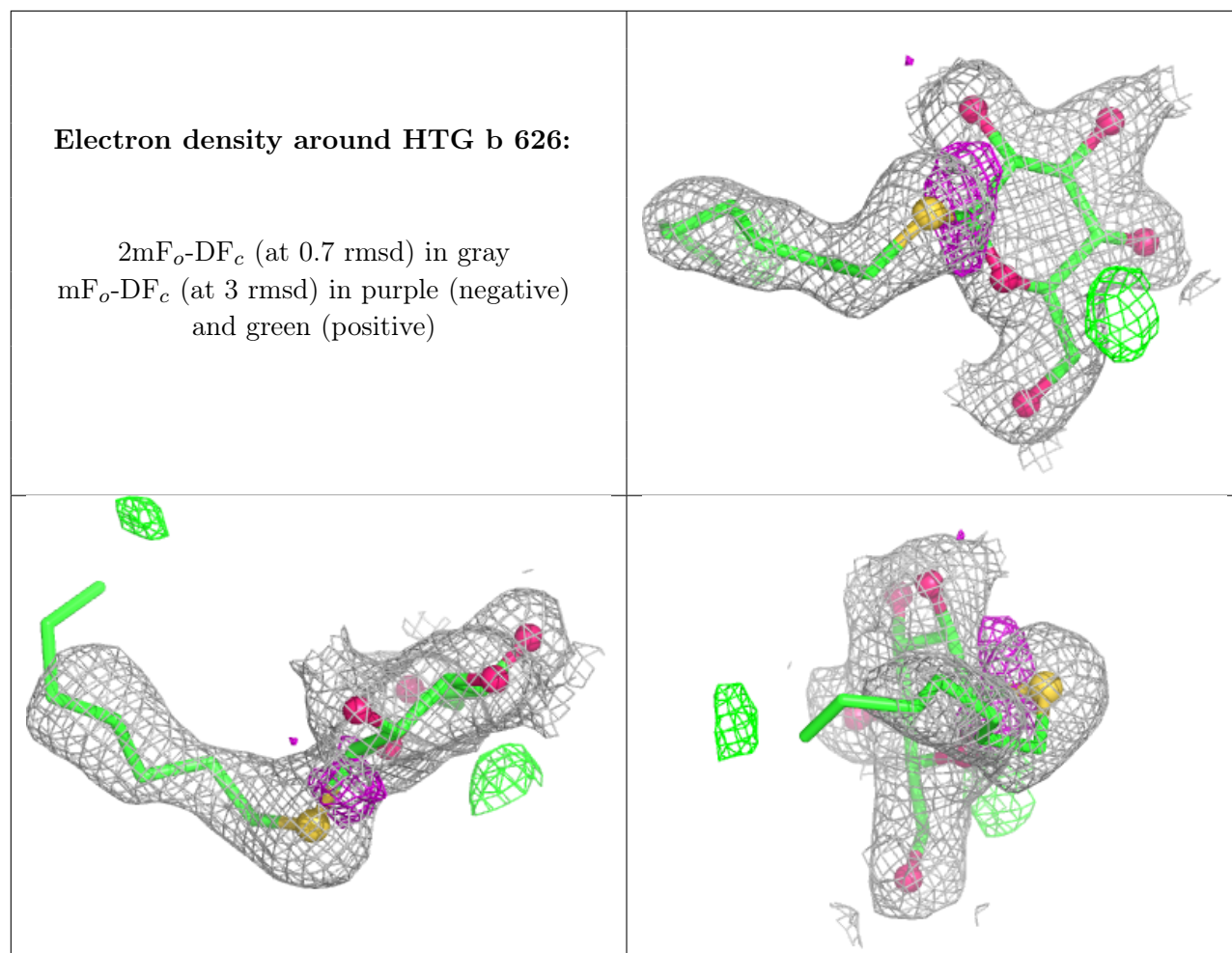


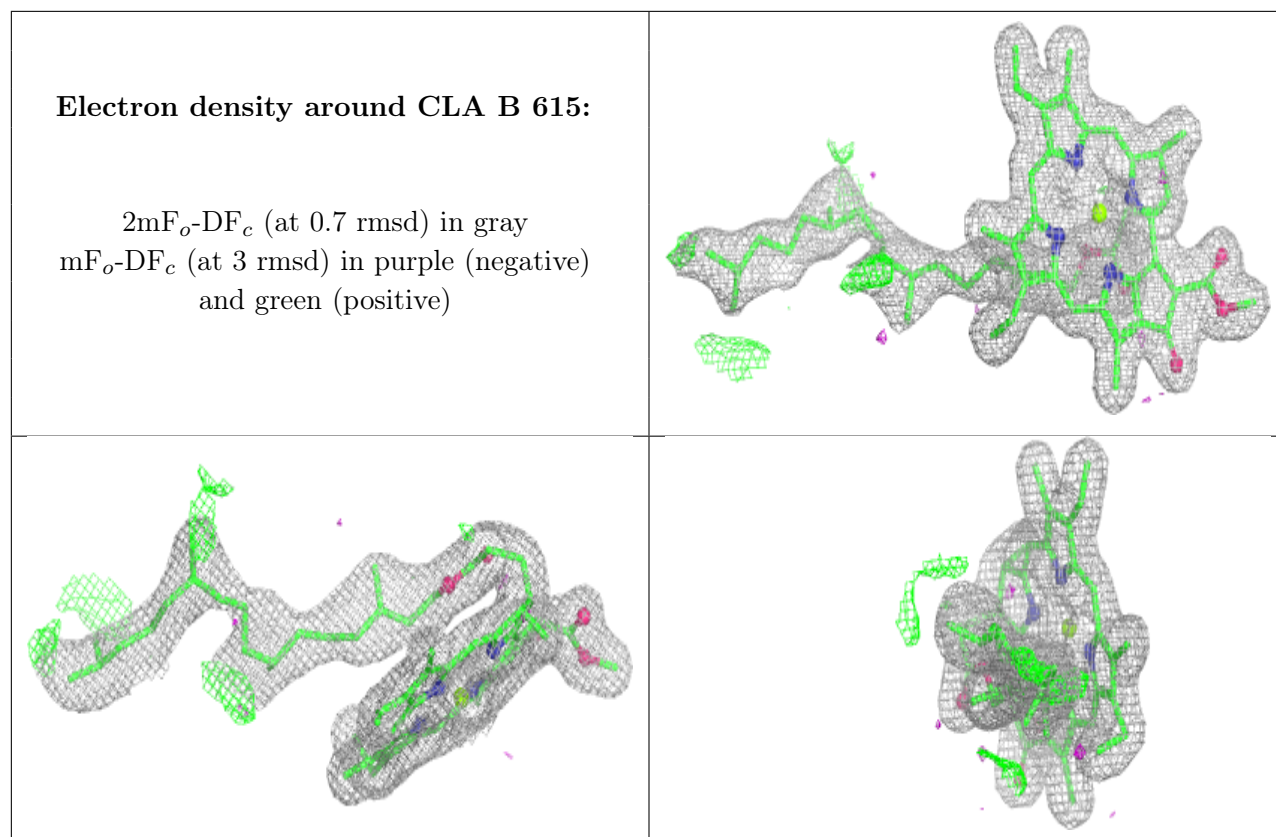
Electron density around CLA c 906:

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



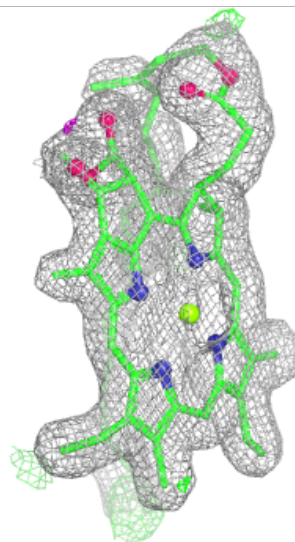
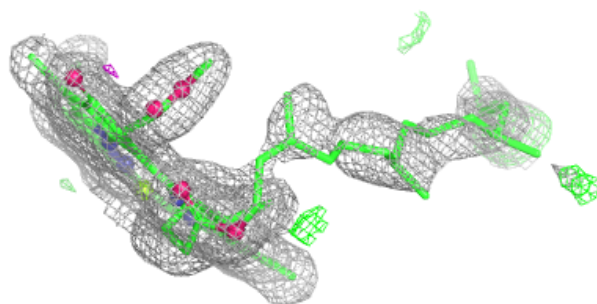
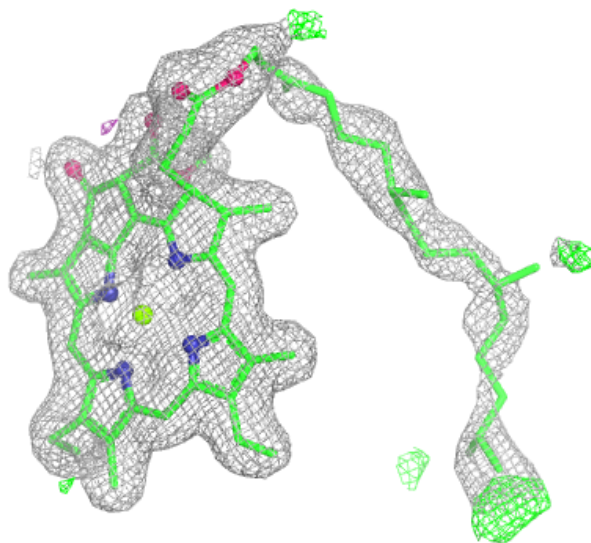






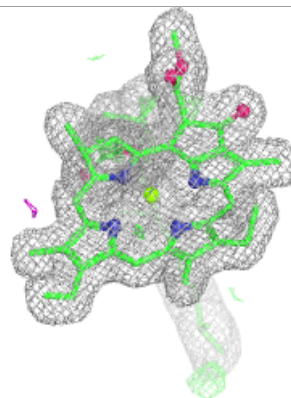
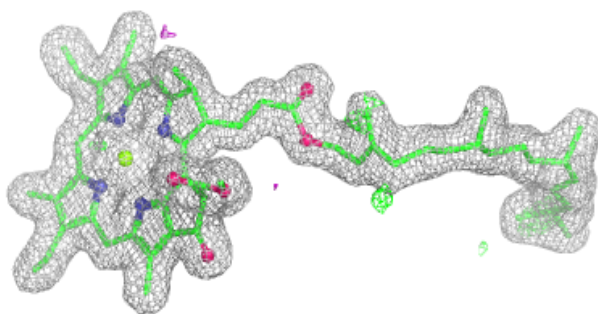
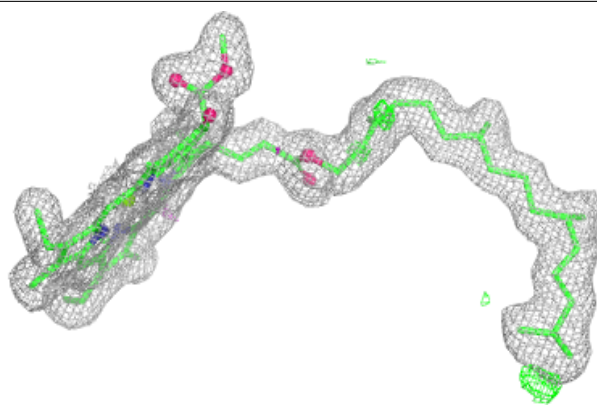
Electron density around CLA B 617:

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

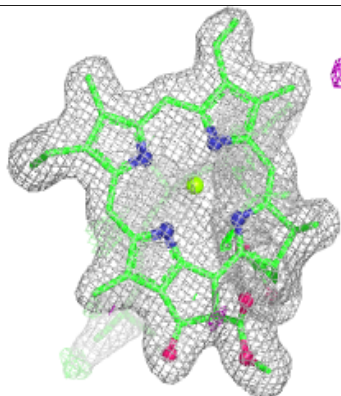
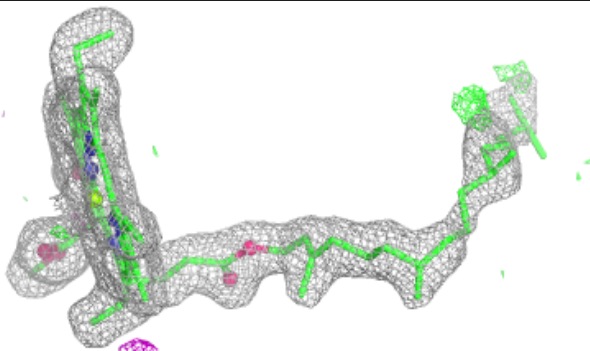
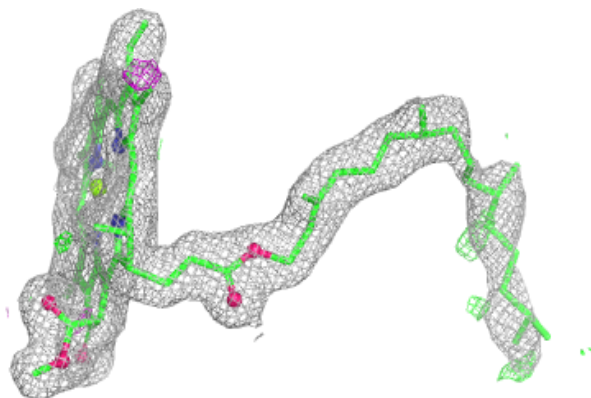


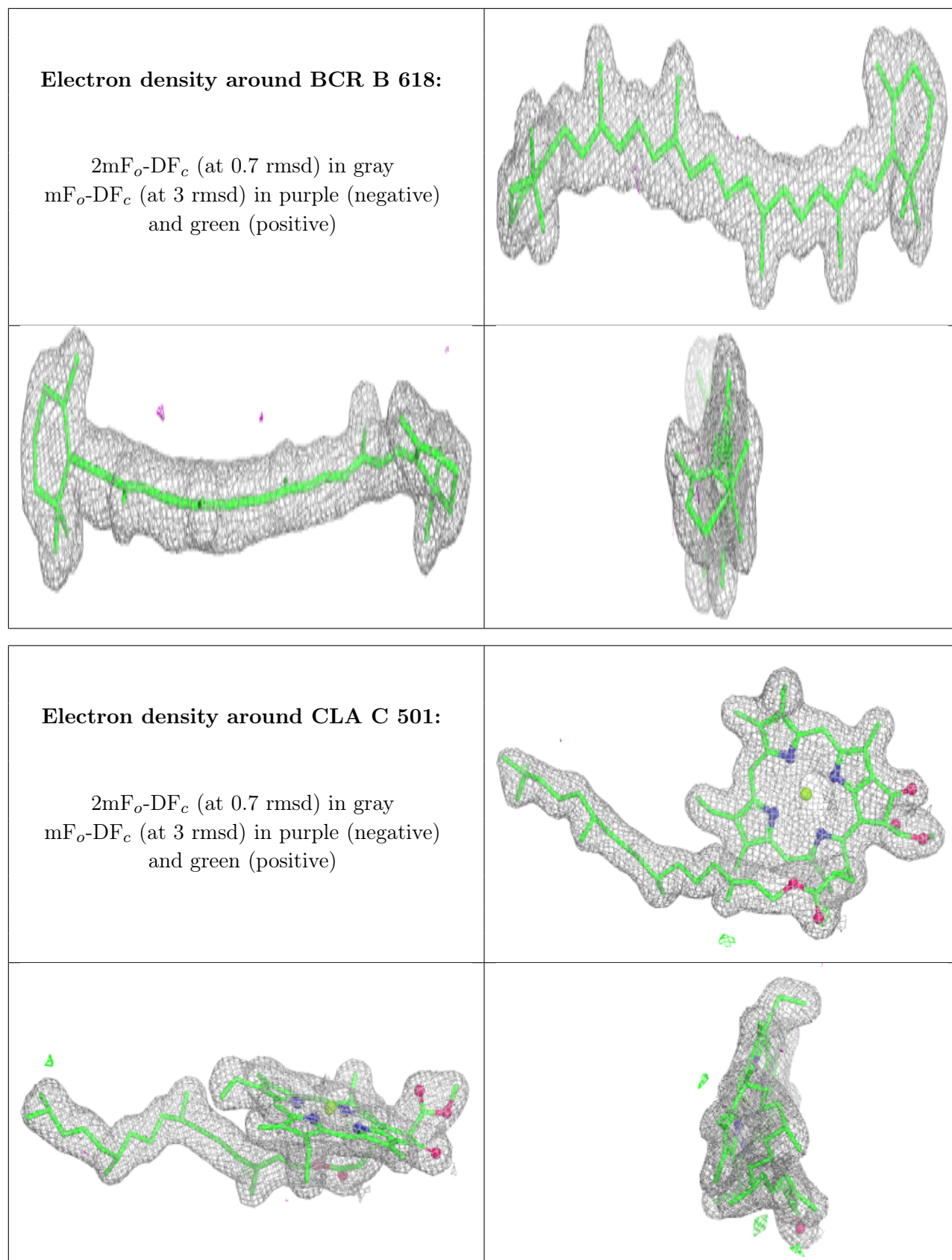
Electron density around CLA D 402:

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

**Electron density around CLA D 403:**

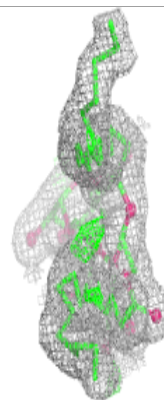
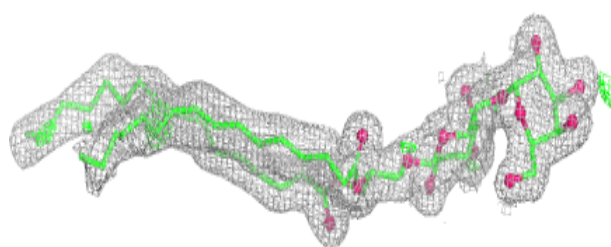
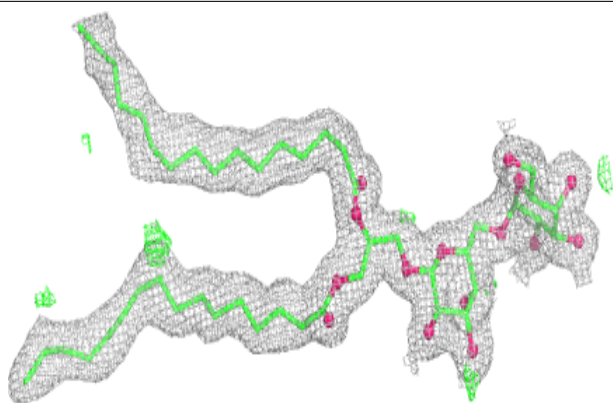
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



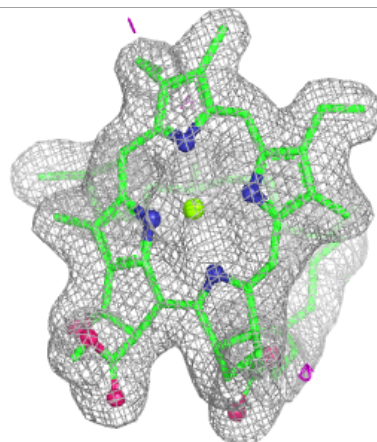
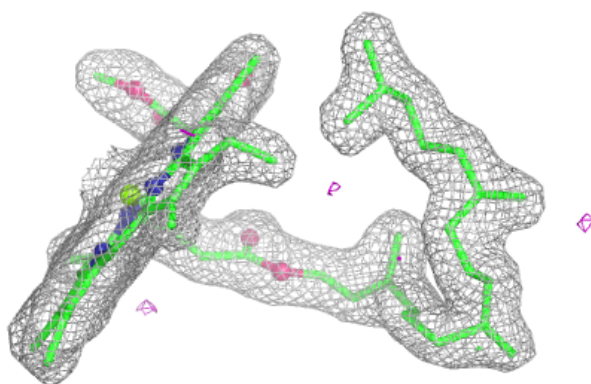
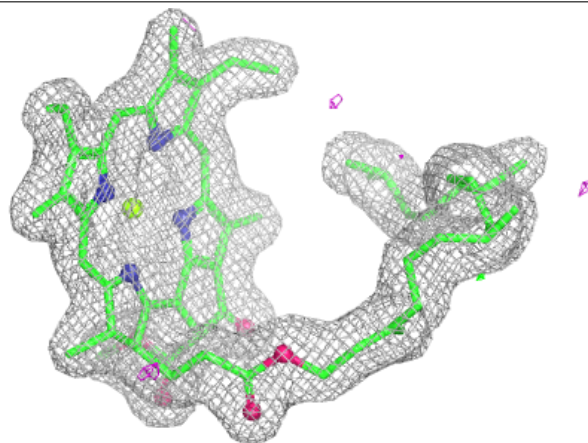


Electron density around DGD C 518:

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

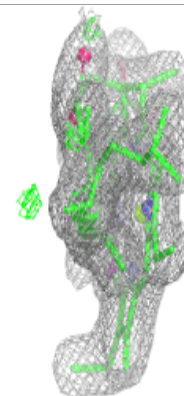
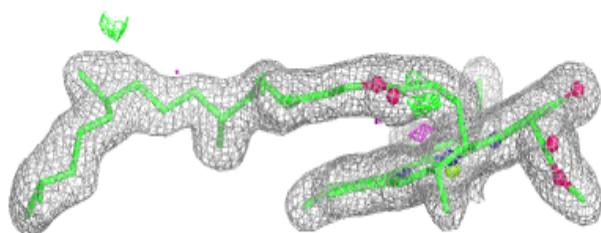
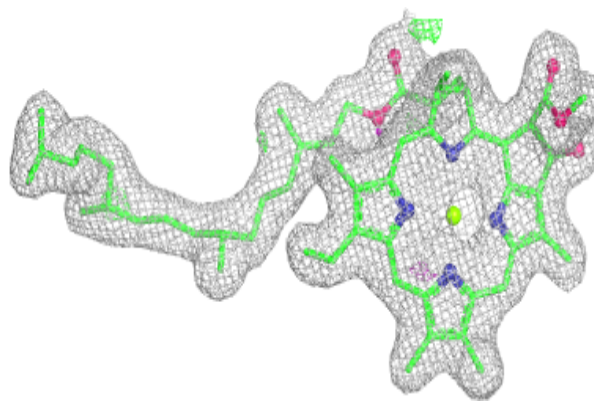
**Electron density around CLA C 503:**

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

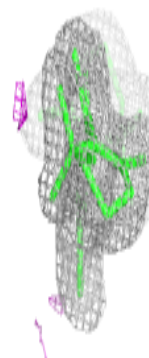
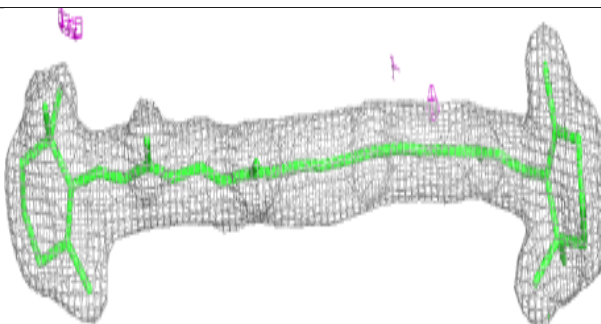
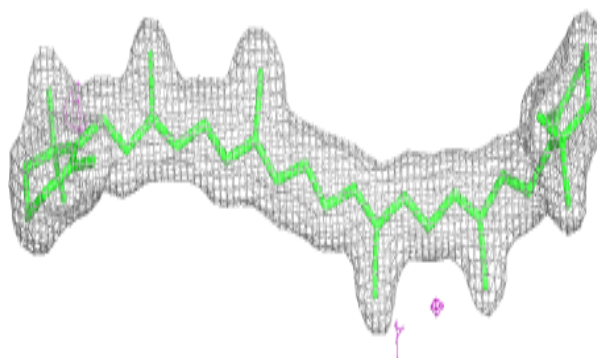


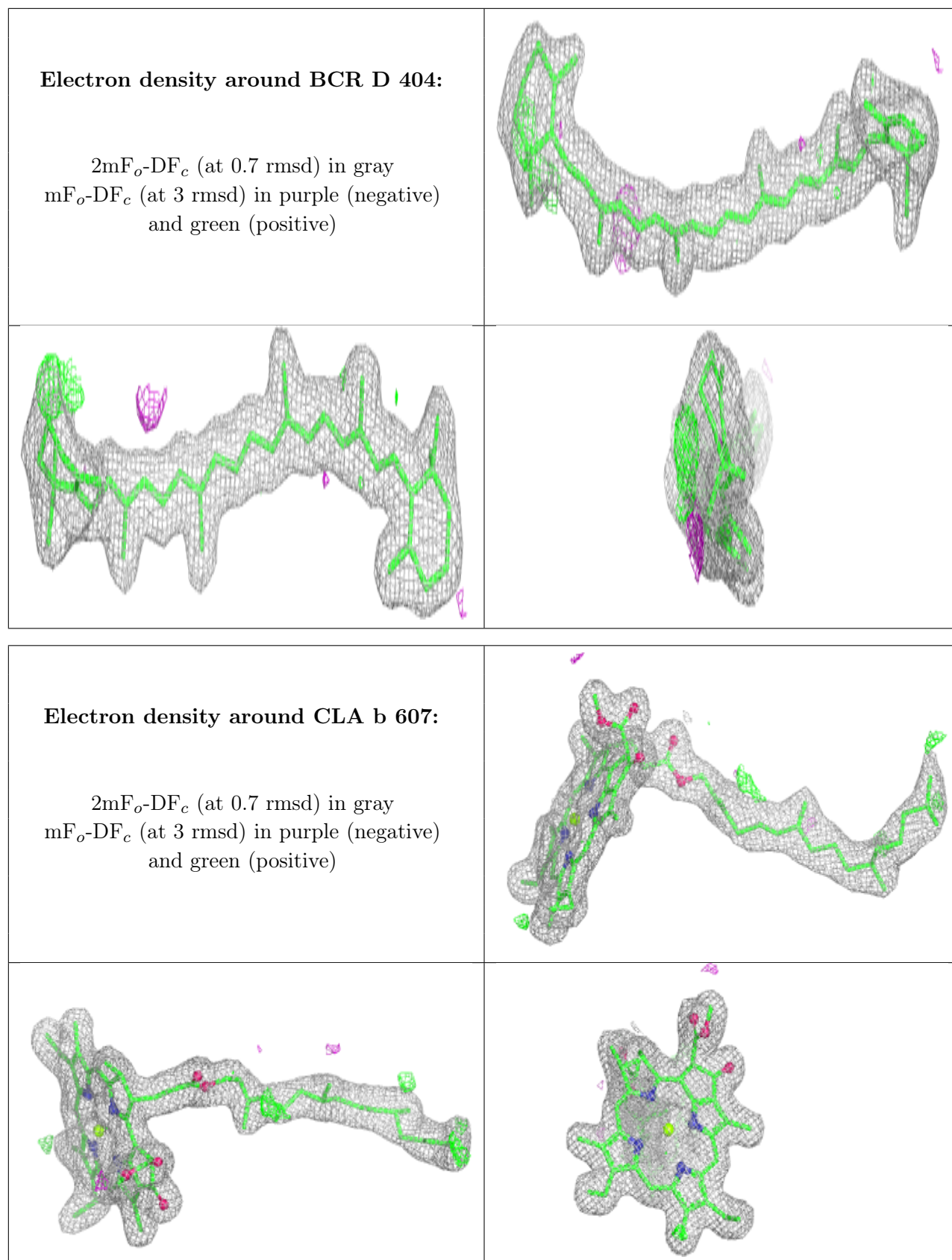
Electron density around CLA b 606:

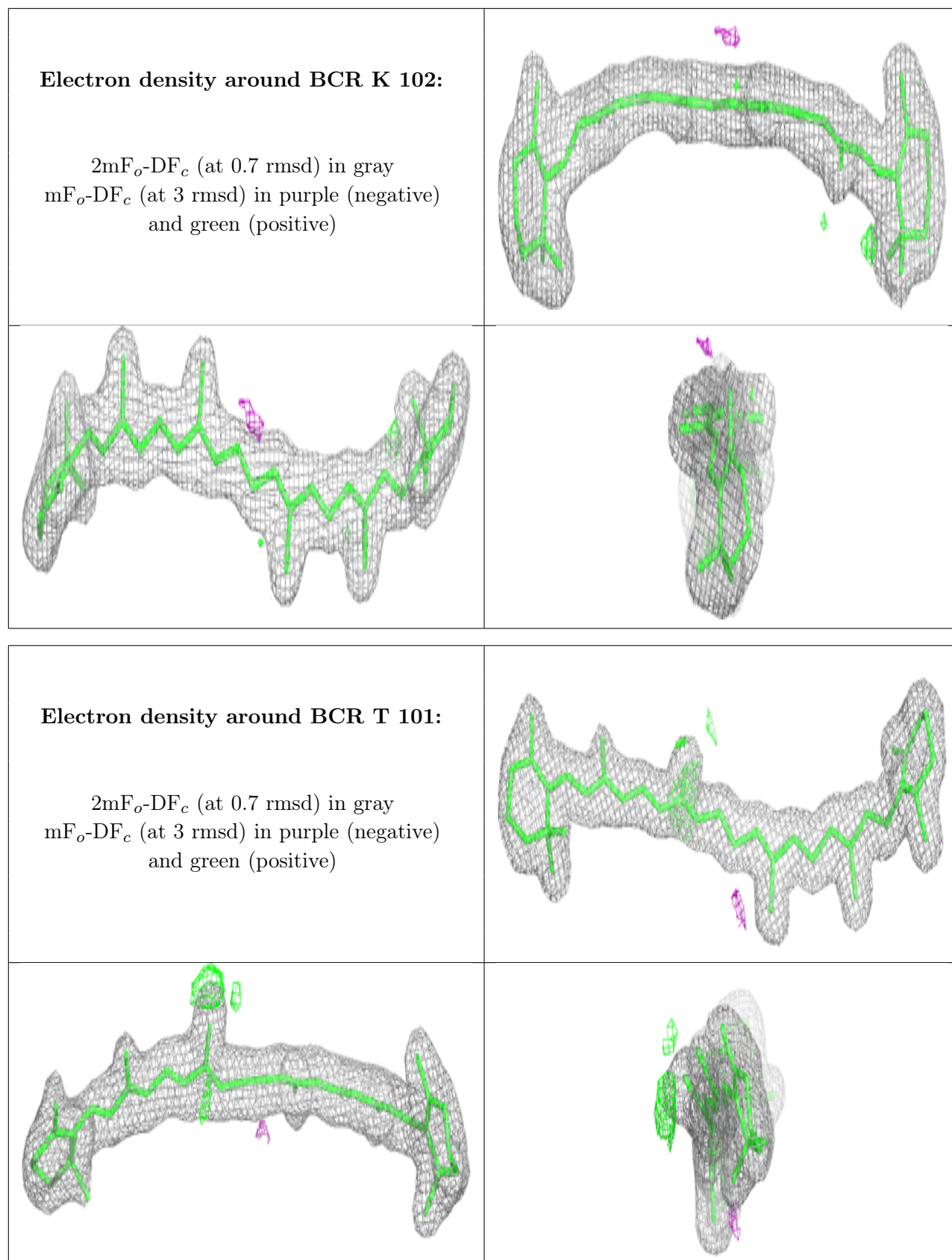
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around BCR 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)

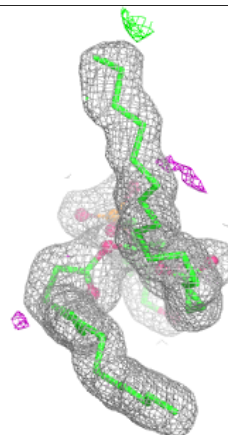
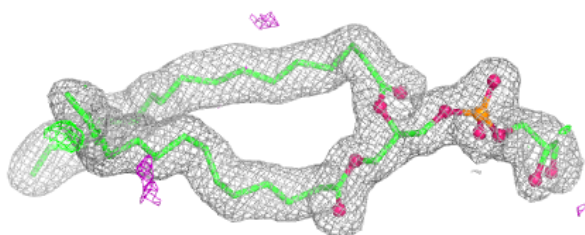
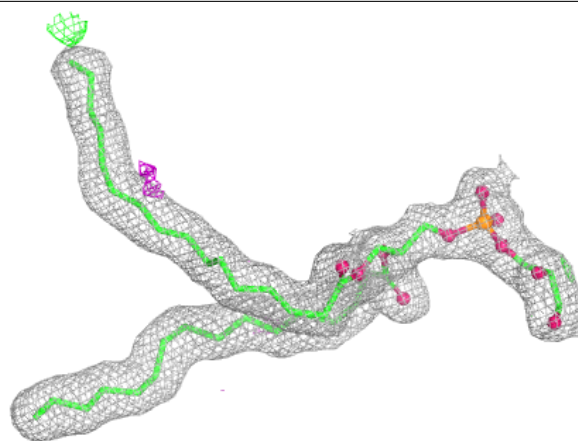




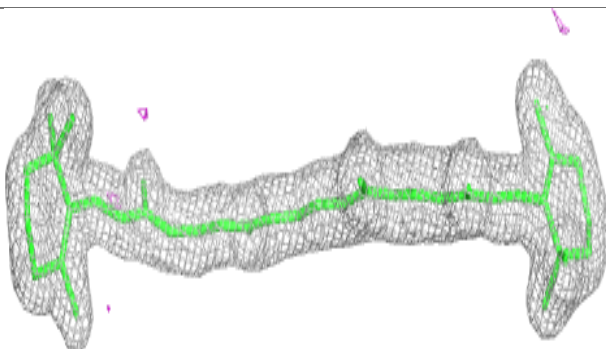
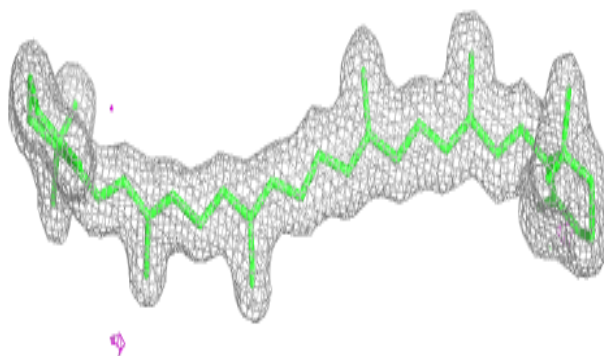


Electron density around LHG D 409:

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

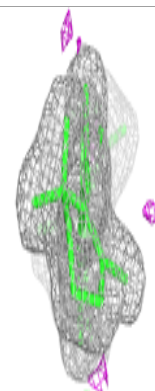
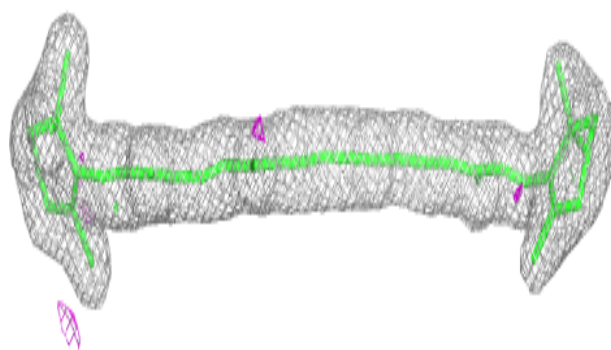
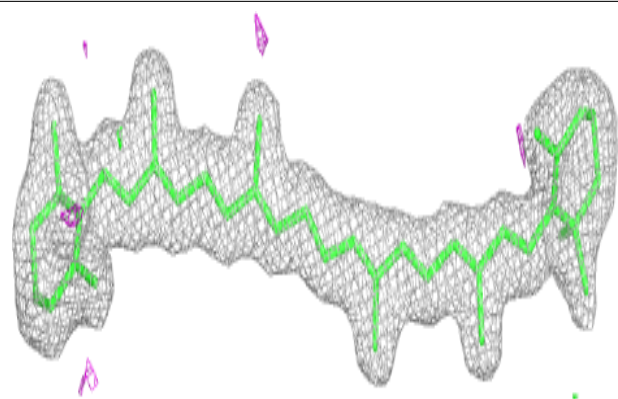
**Electron density around BCR a 415:**

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

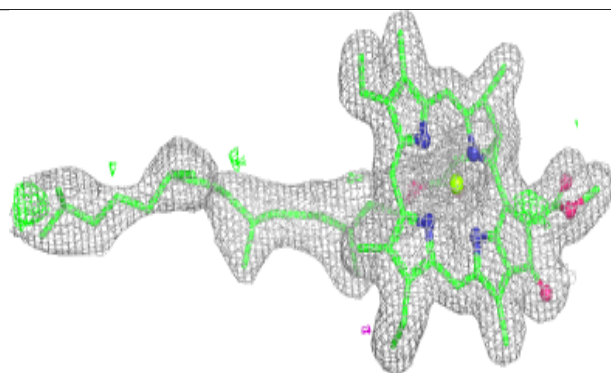
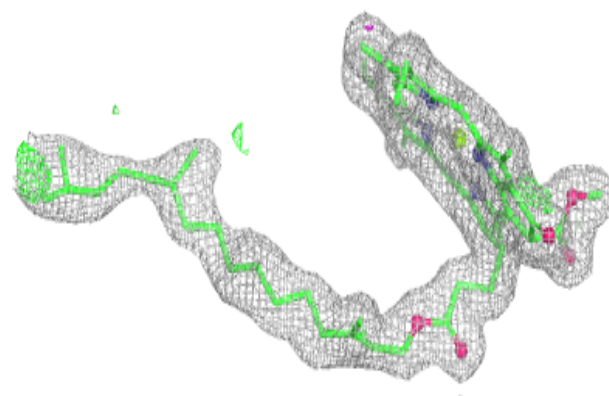


Electron density around BCR b 621:

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

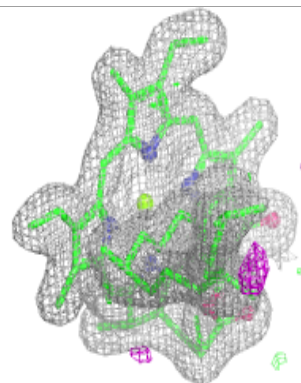
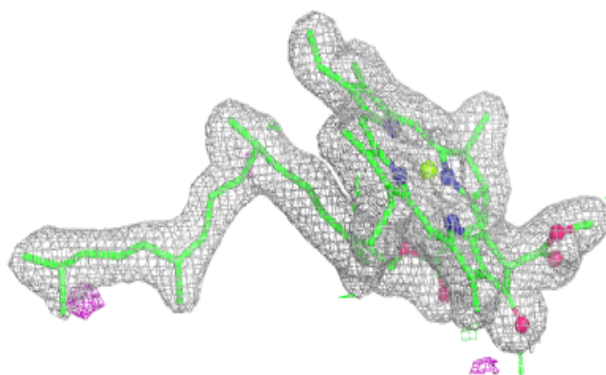
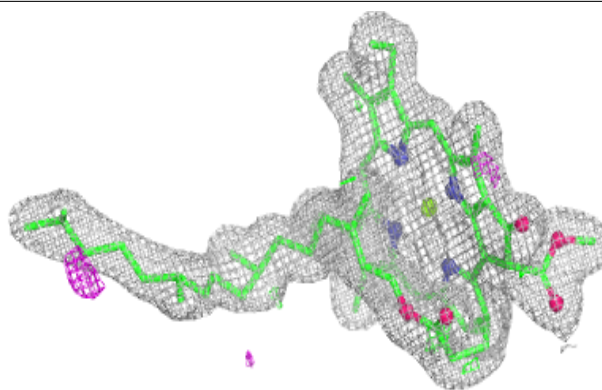
**Electron density around CLA C 504:**

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

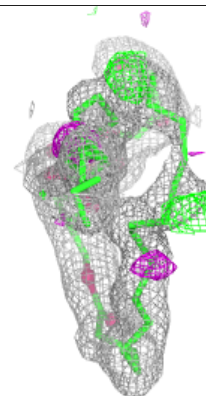
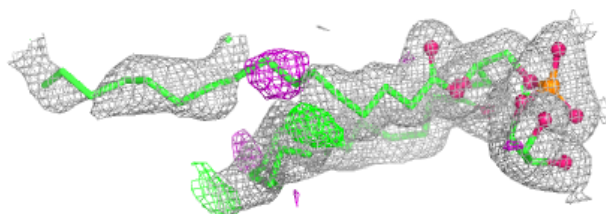
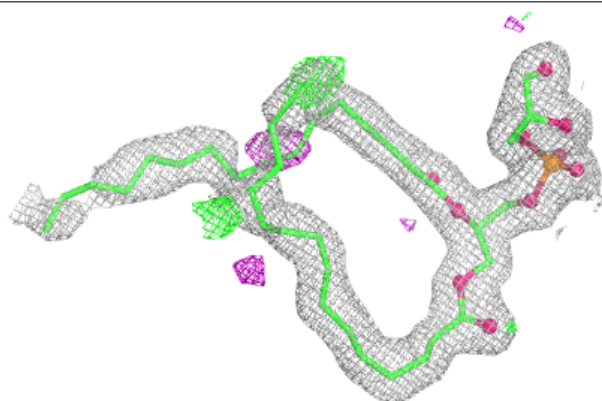


Electron density around CLA C 505:

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

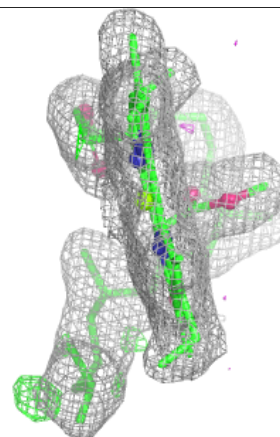
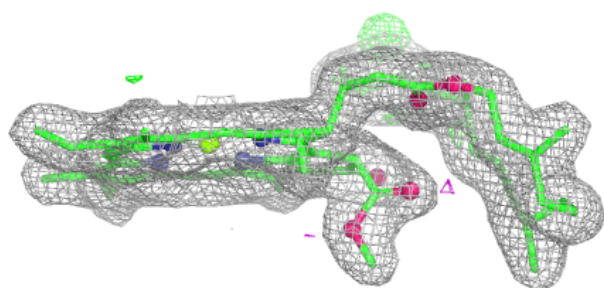
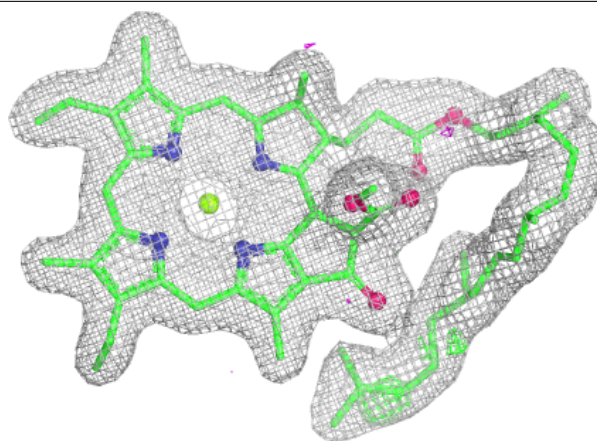
**Electron density around LHG d 409:**

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



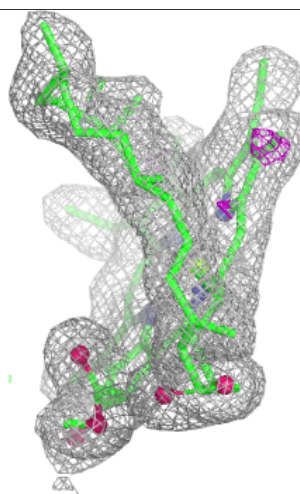
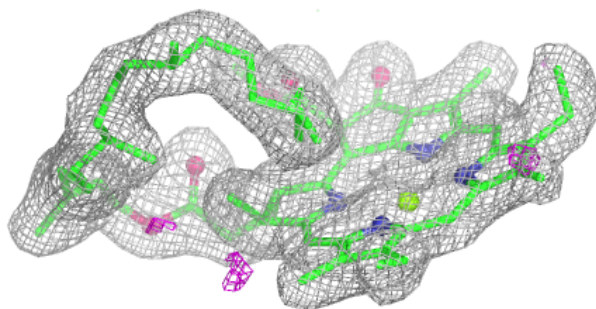
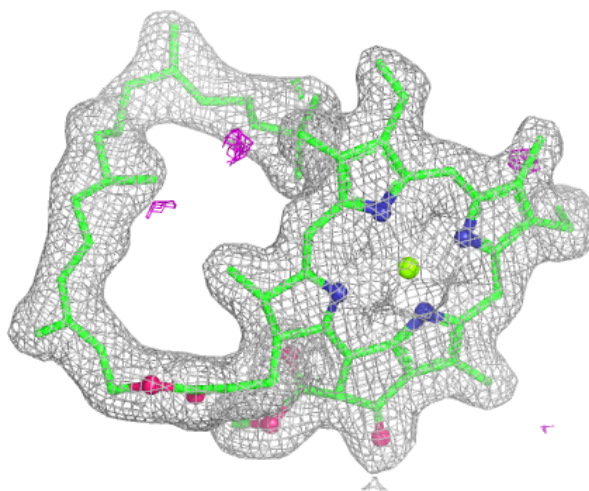
Electron density around CLA b 613:

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



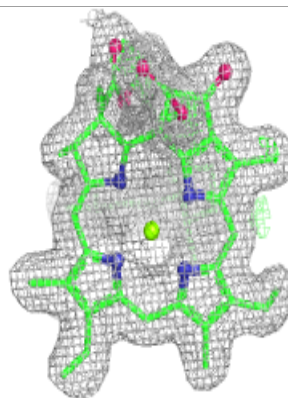
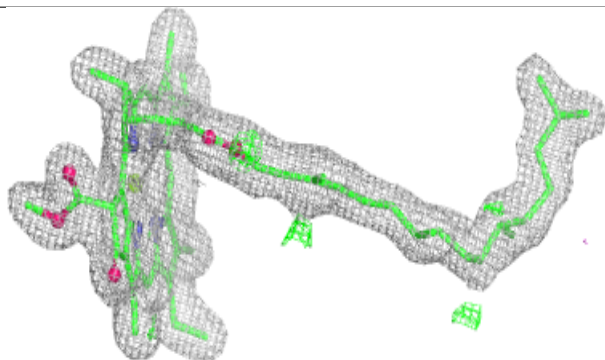
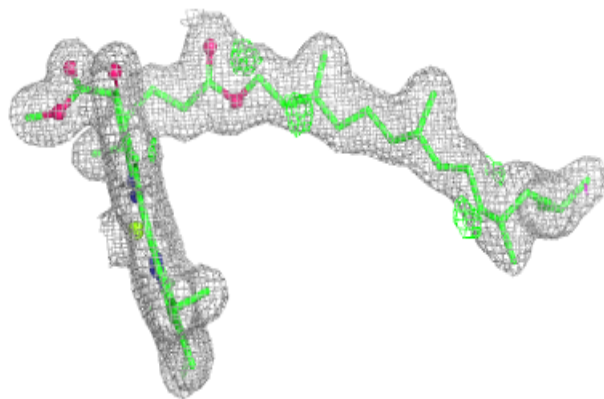
Electron density around CLA B 616:

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

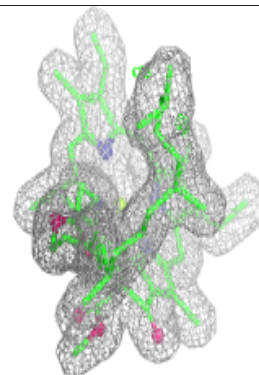
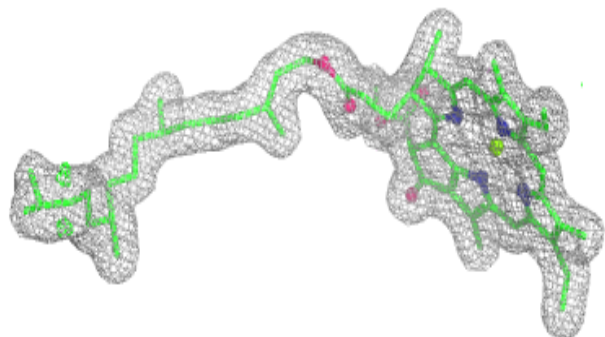
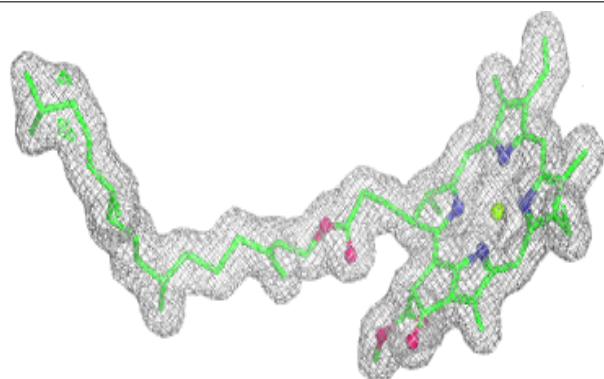


Electron density around CLA B 606:

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

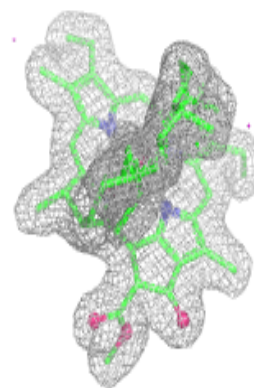
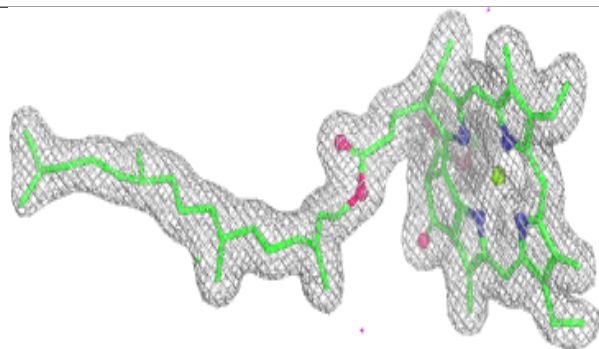
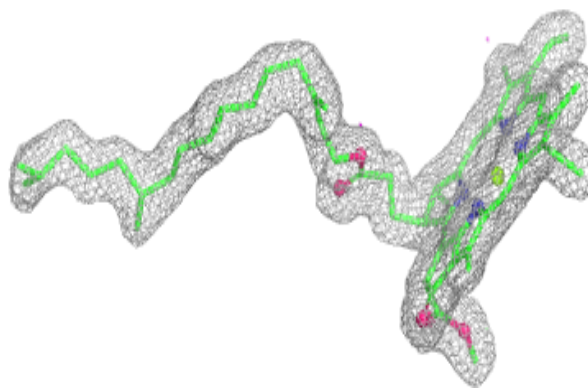
**Electron density around CLA A 405:**

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

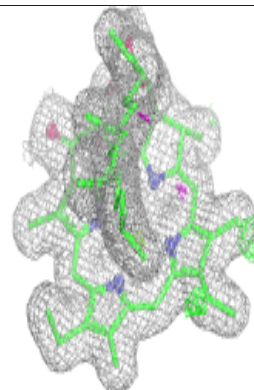
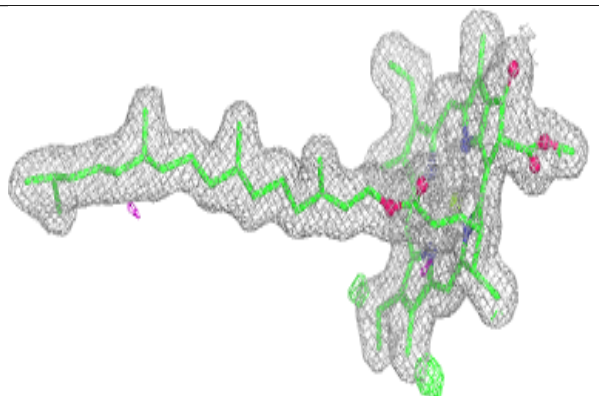
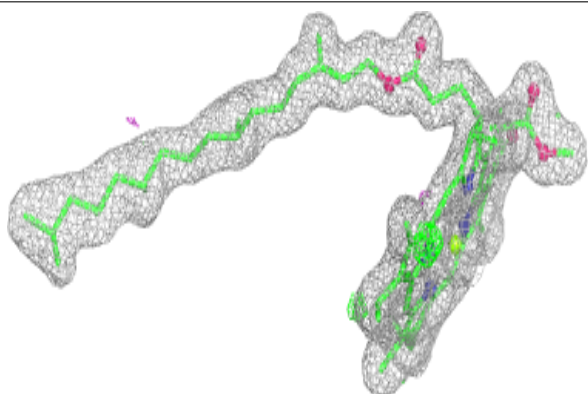


Electron density around CLA C 502:

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

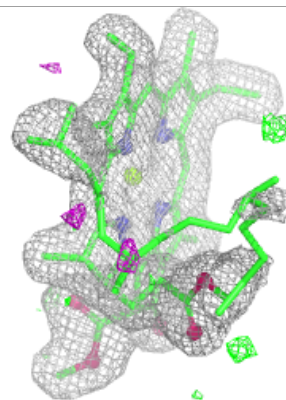
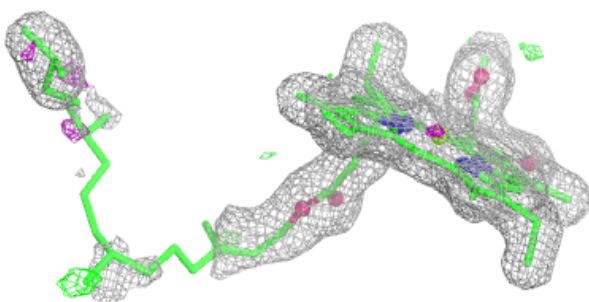
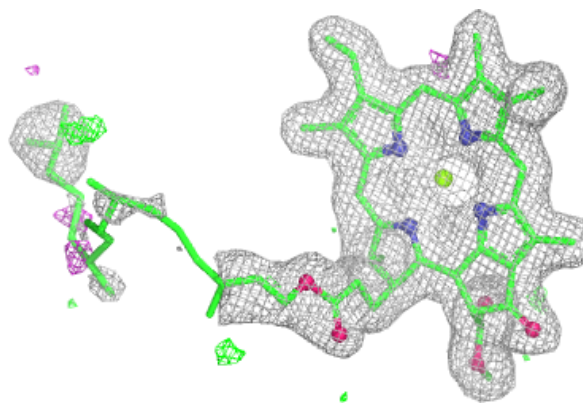
**Electron density around CLA B 608:**

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

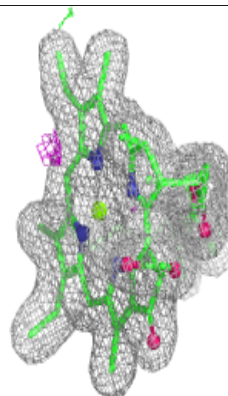
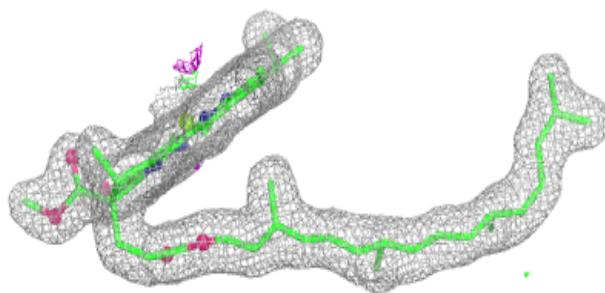
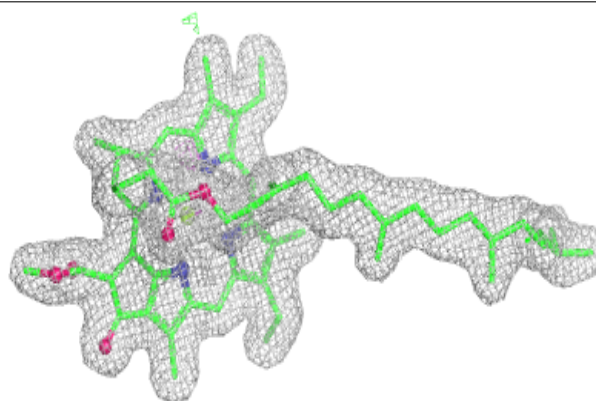


Electron density around CLA a 414:

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

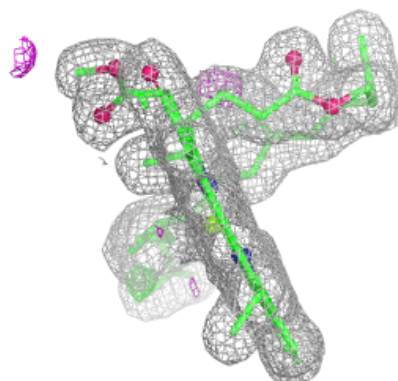
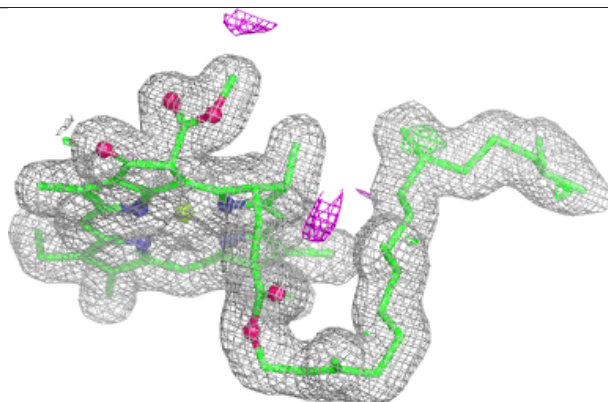
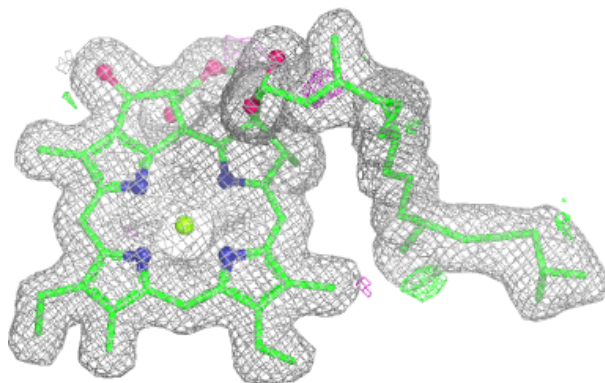
**Electron density around CLA B 609:**

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

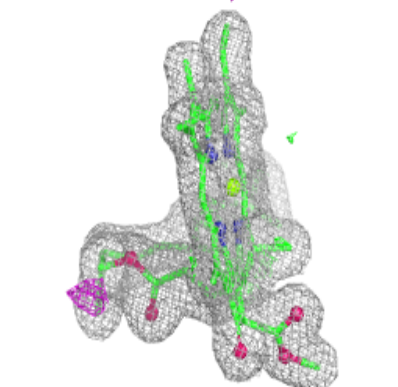
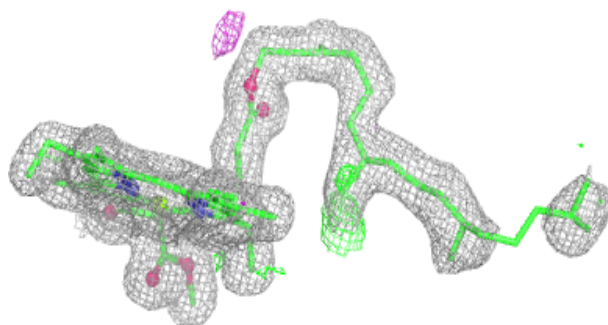
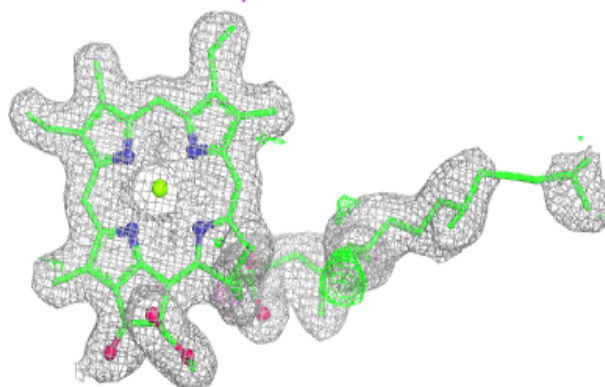


Electron density around CLA A 406:

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

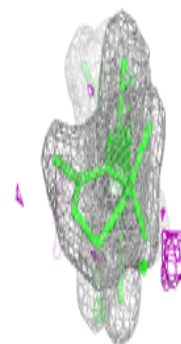
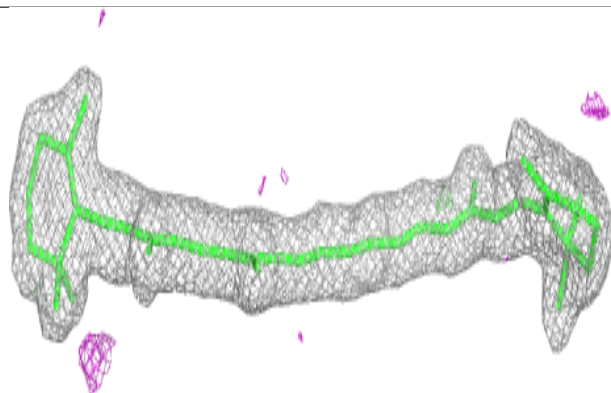
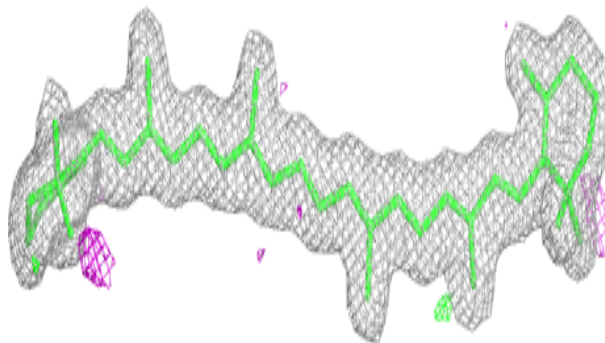
**Electron density around CLA A 407:**

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

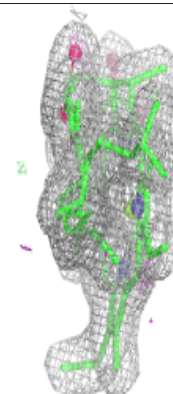
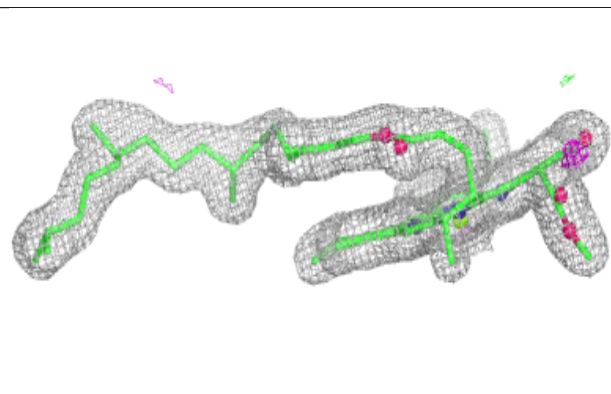
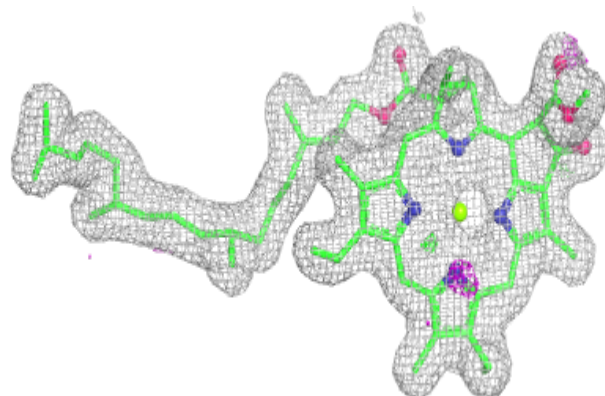


Electron density around BCR b 620:

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

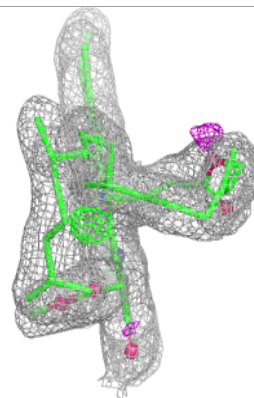
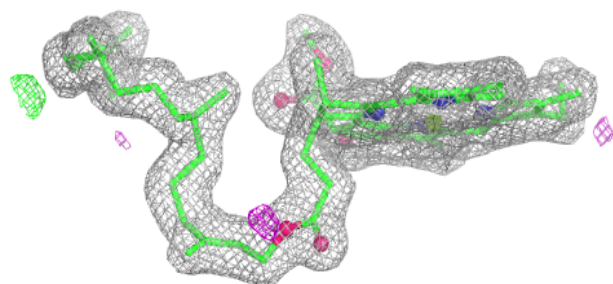
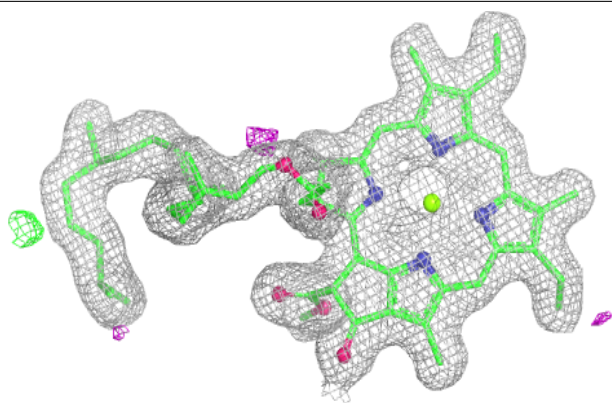
**Electron density around CLA B 604:**

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

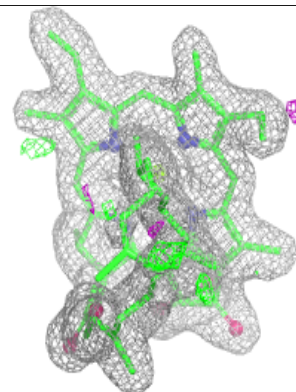
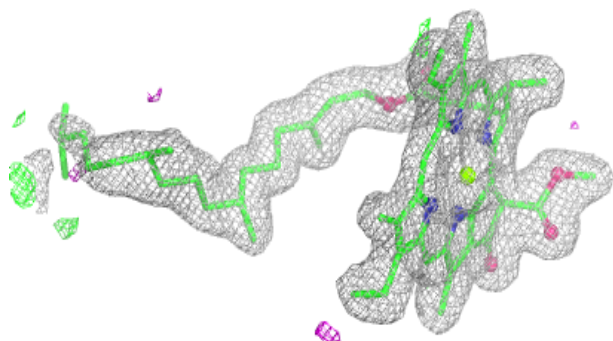
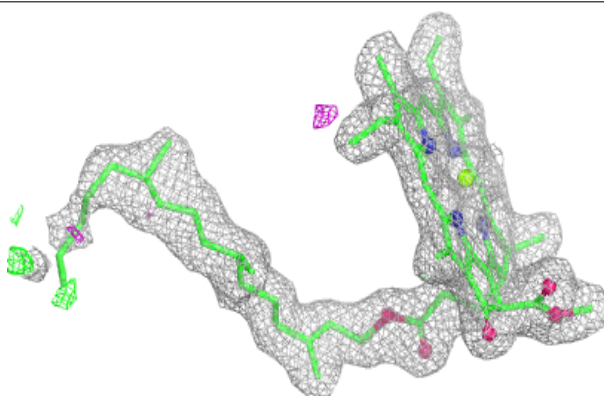


Electron density around CLA B 613:

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

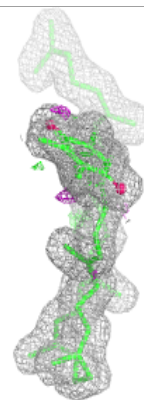
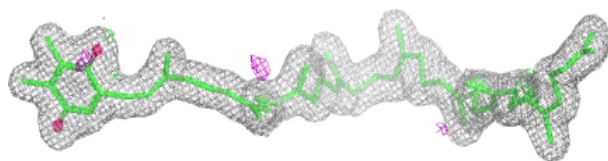
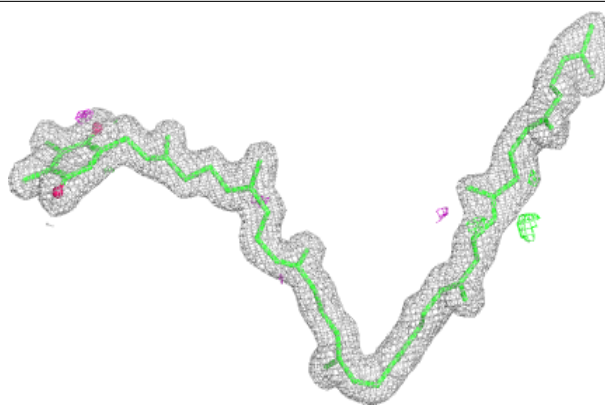
**Electron density around CLA c 909:**

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



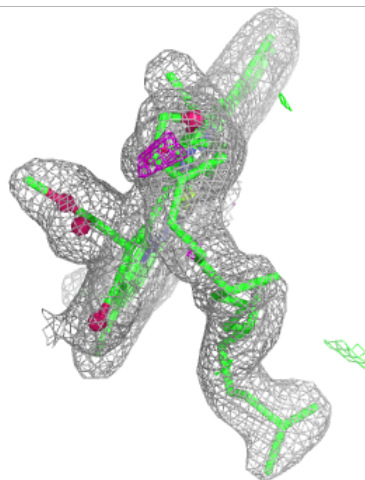
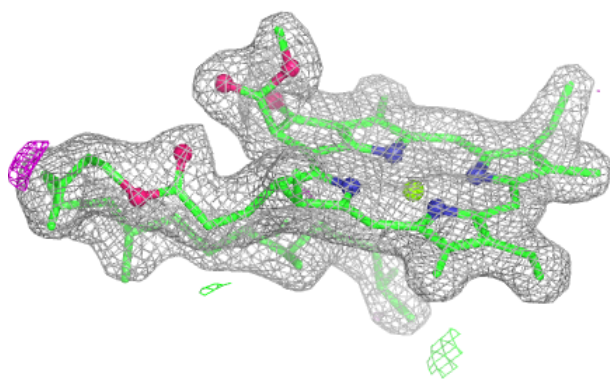
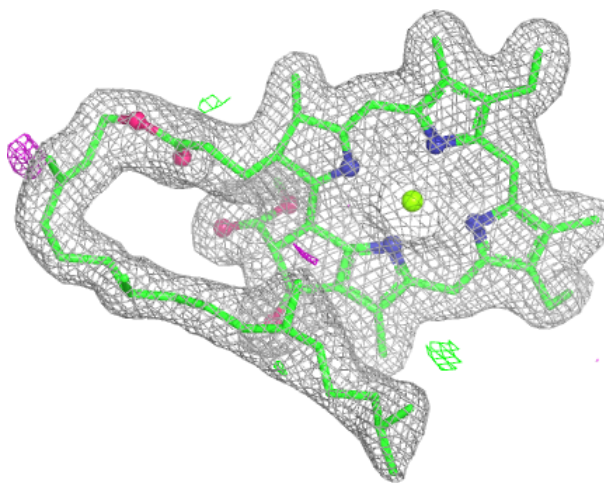
Electron density around PL9 D 405:

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



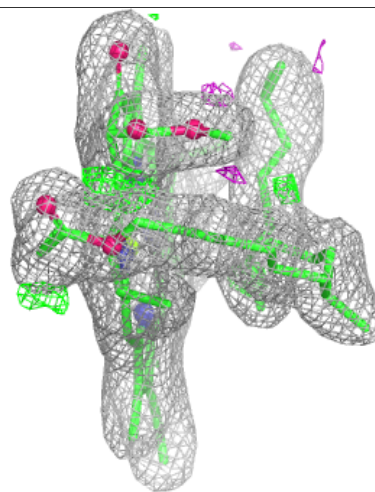
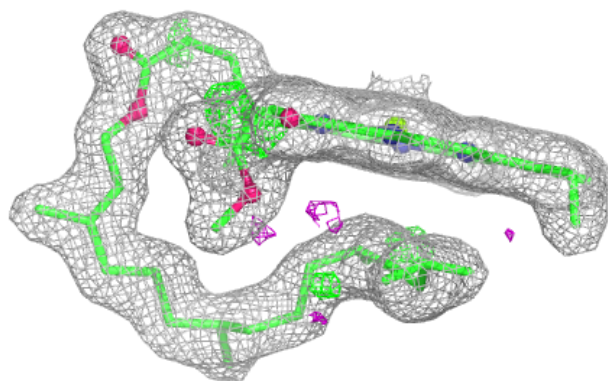
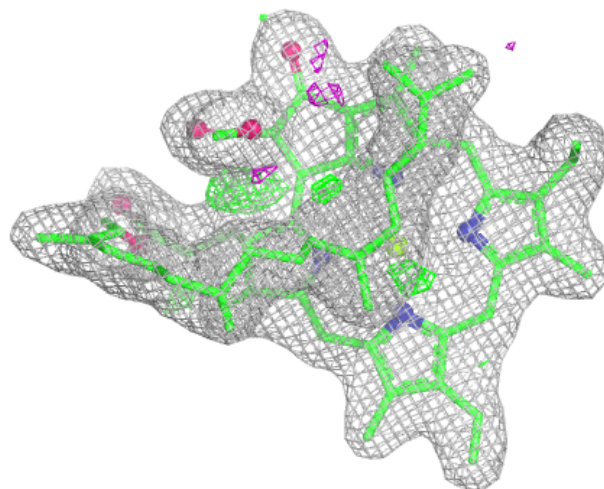
Electron density around CLA c 910:

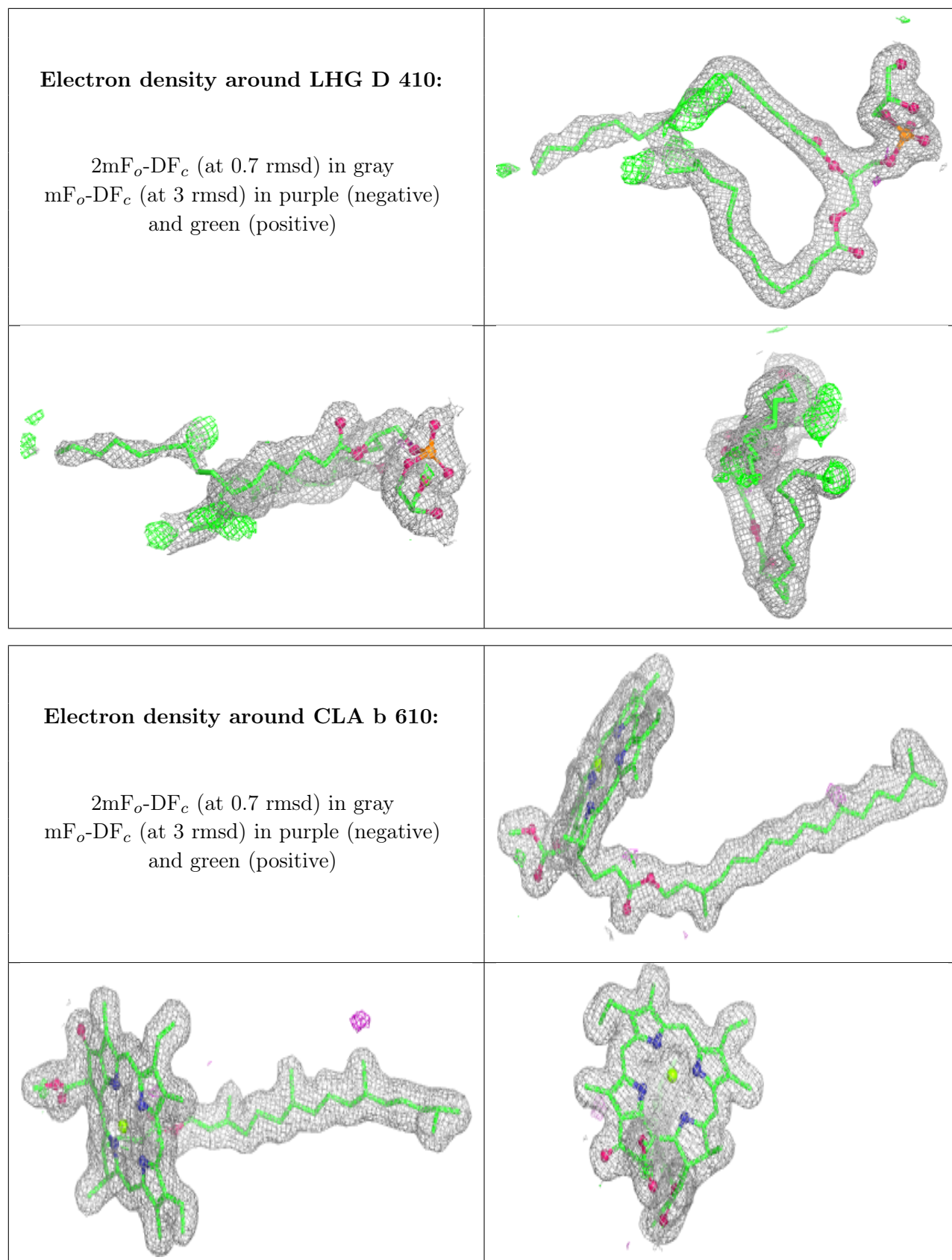
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA c 911:

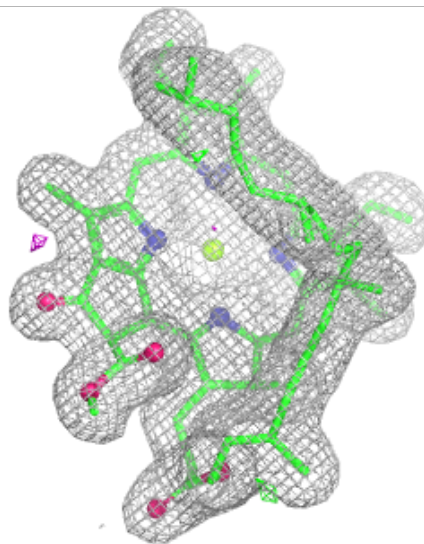
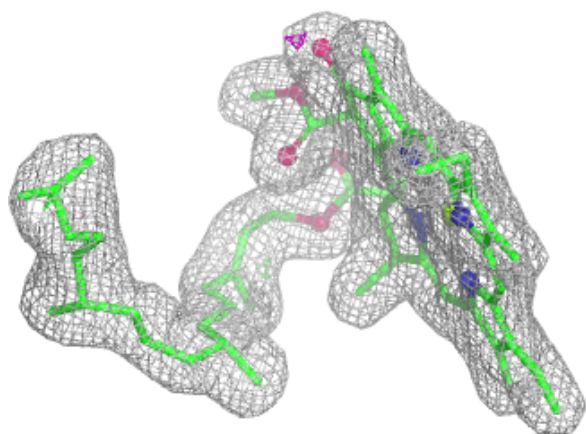
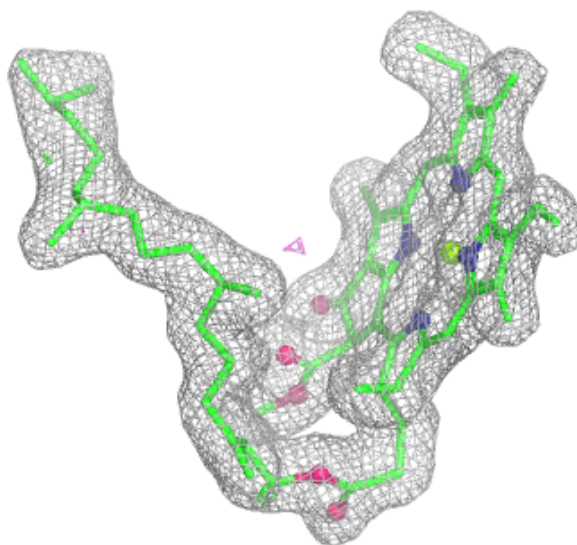
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





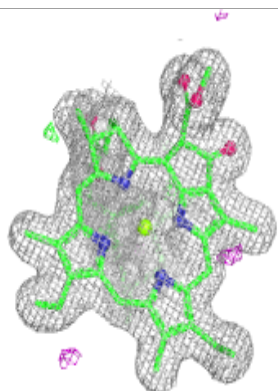
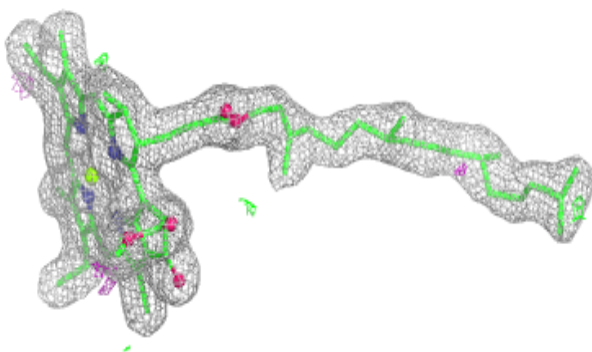
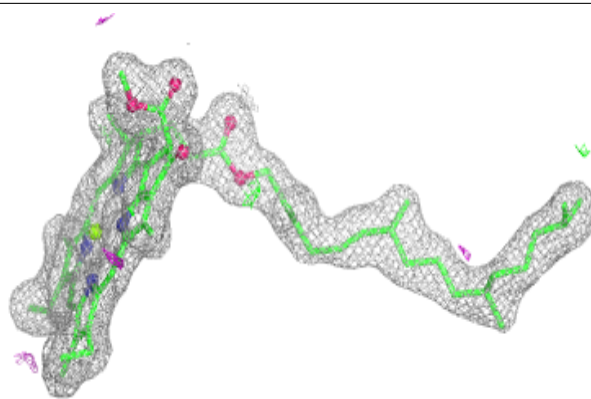
Electron density around CLA B 614:

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

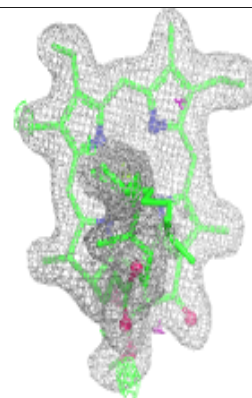
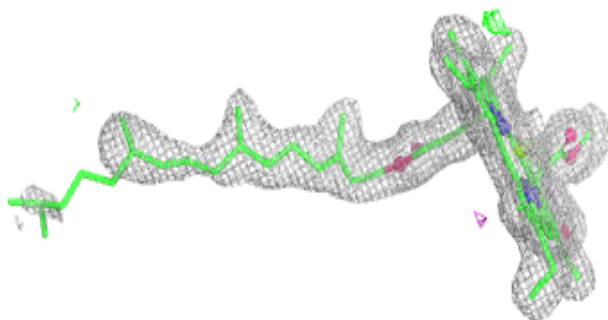
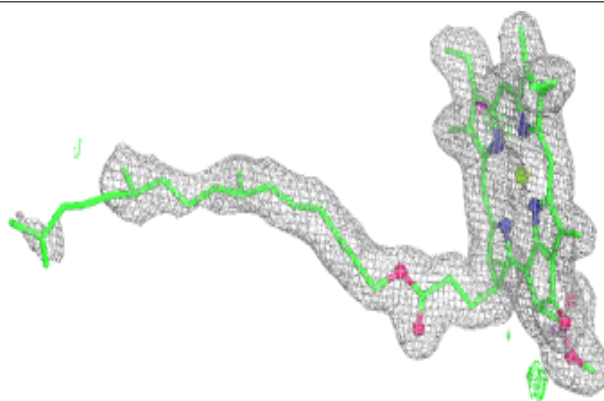


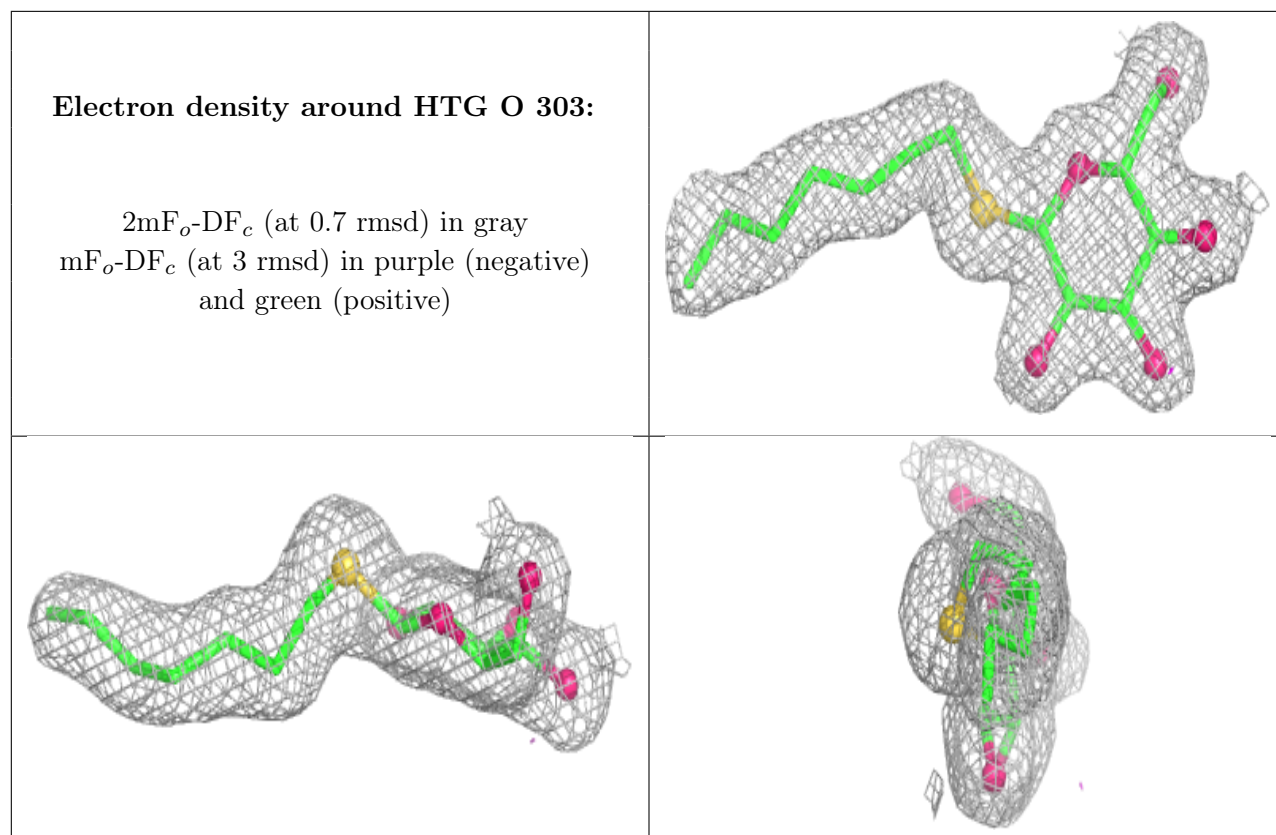
Electron density around CLA B 605:

$2mF_o-DF_c$ (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:**

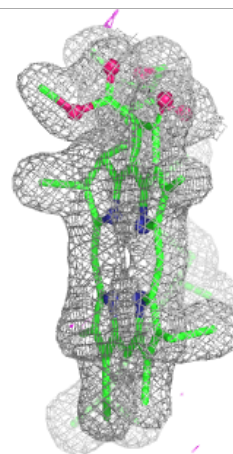
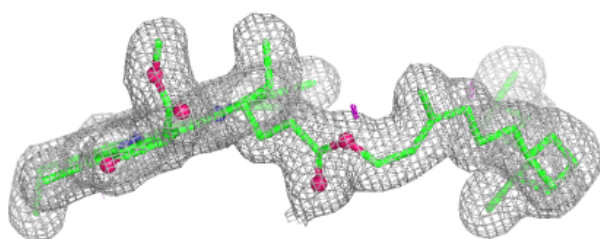
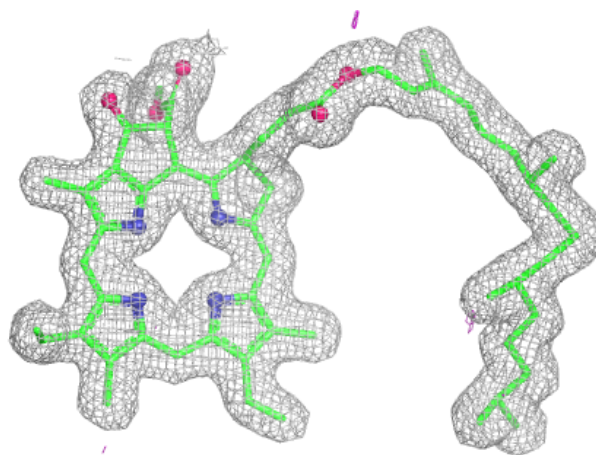
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





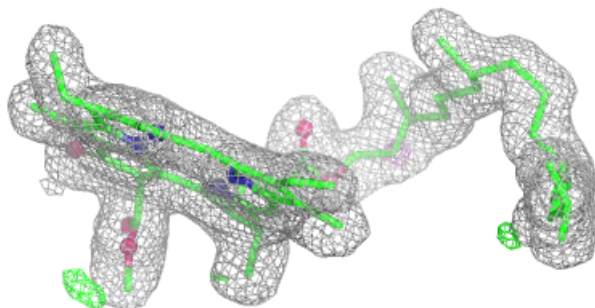
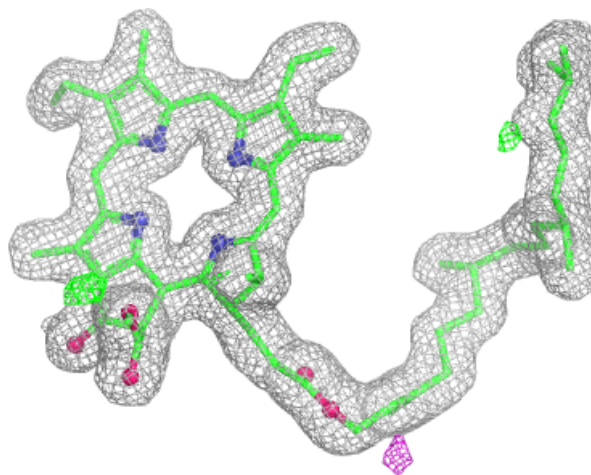
Electron density around PHO A 408:

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



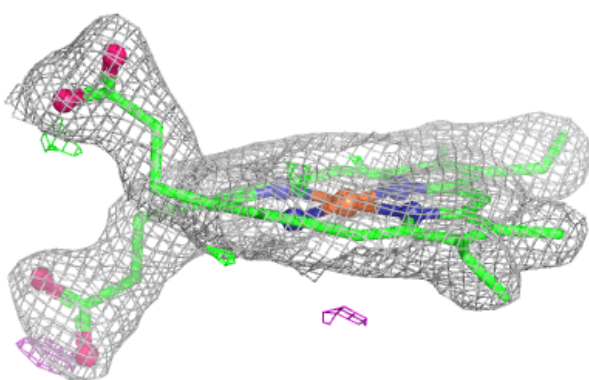
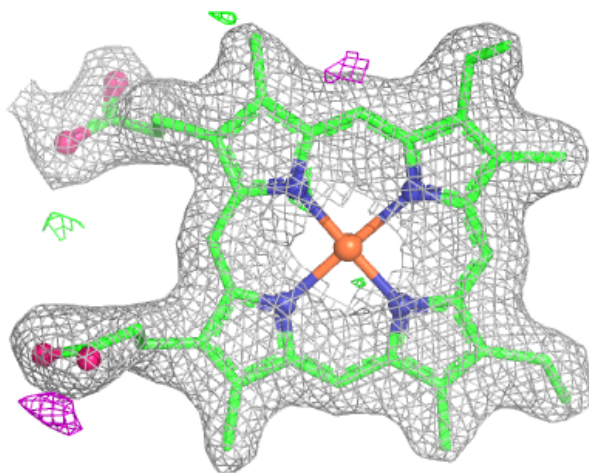
Electron density around PHO A 409:

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



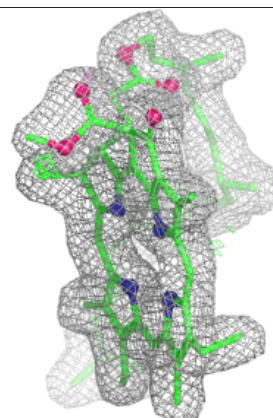
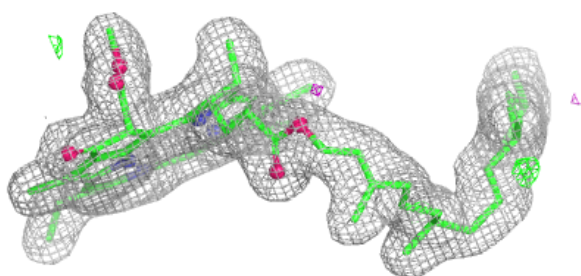
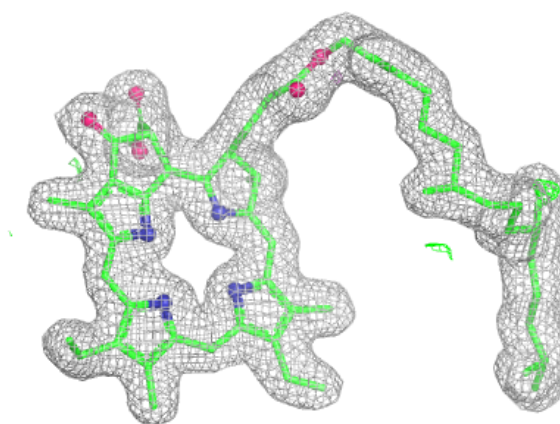
Electron density around HEM F 101:

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

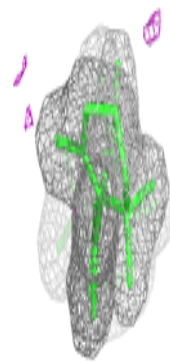
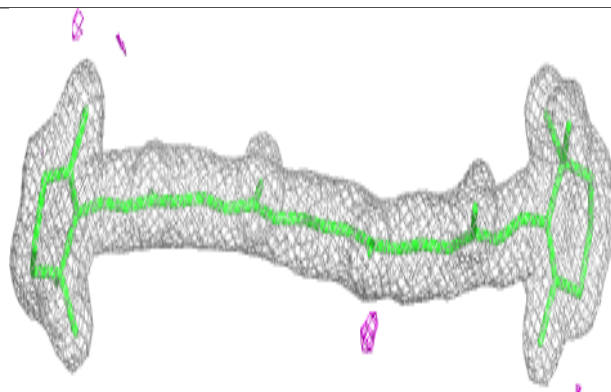
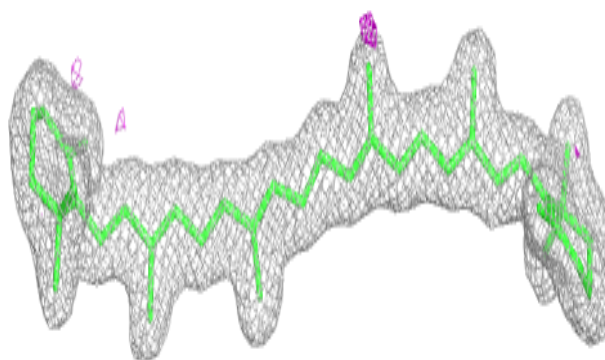


Electron density around PHO a 413:

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

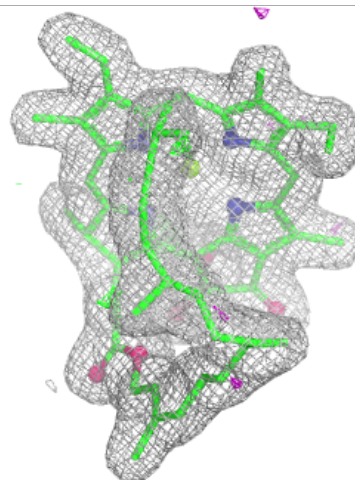
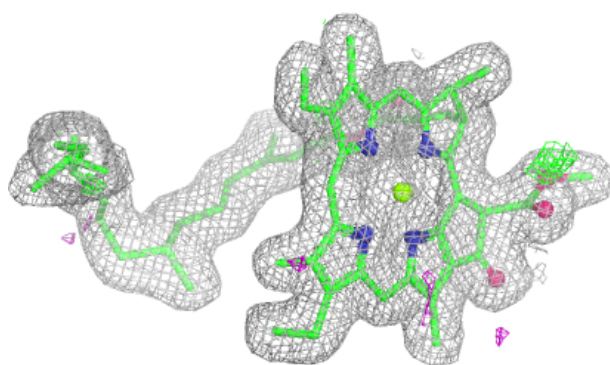
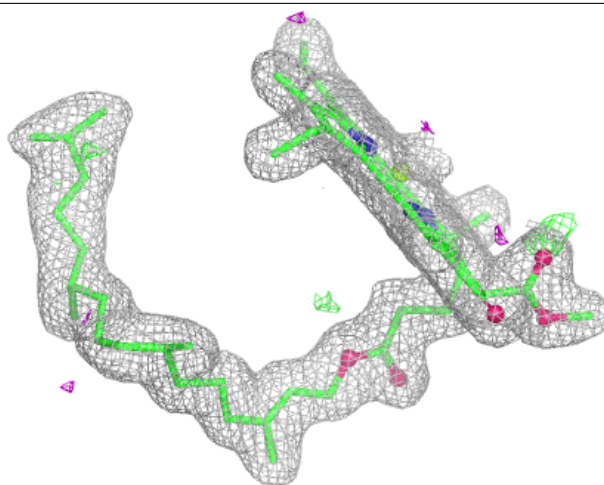
**Electron density around BCR A 411:**

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



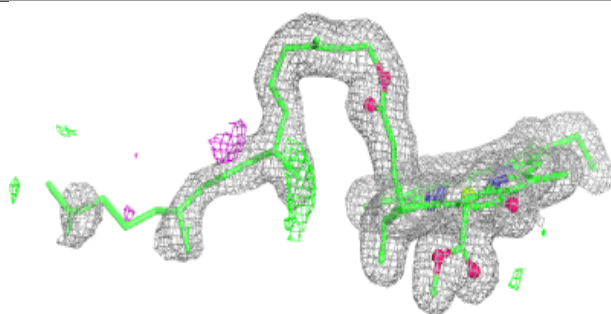
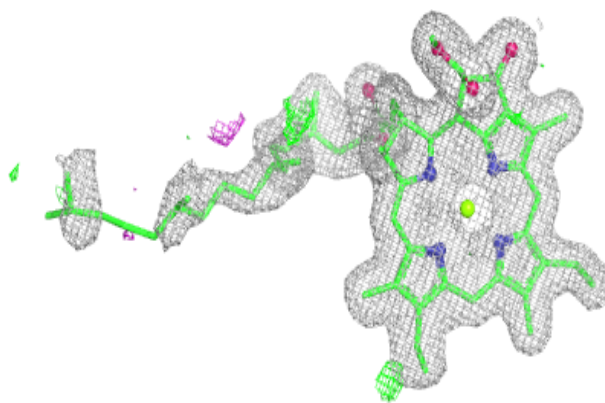
Electron density around CLA b 614:

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

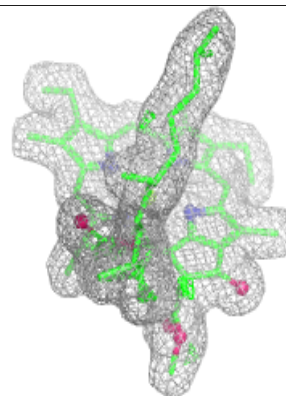
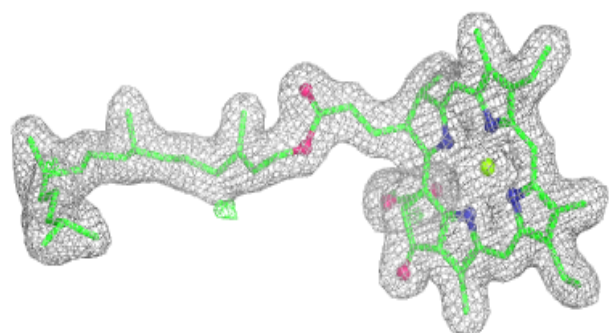
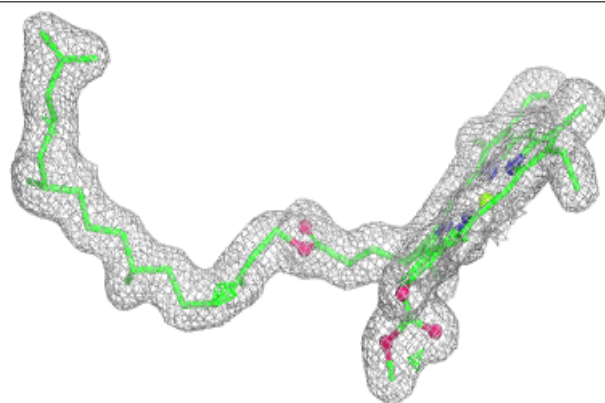


Electron density around CLA a 411:

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

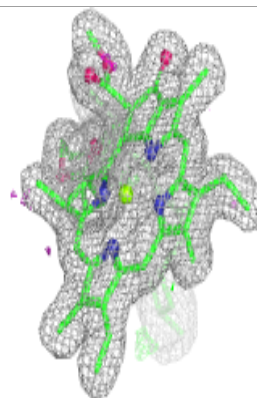
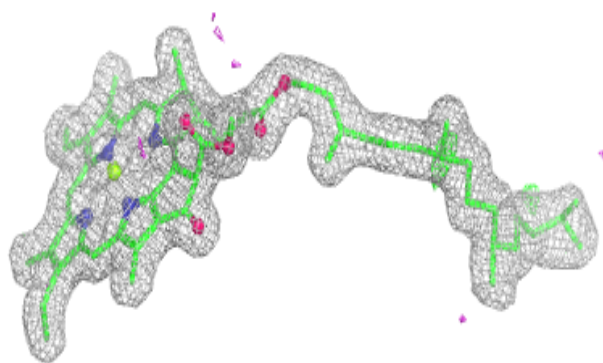
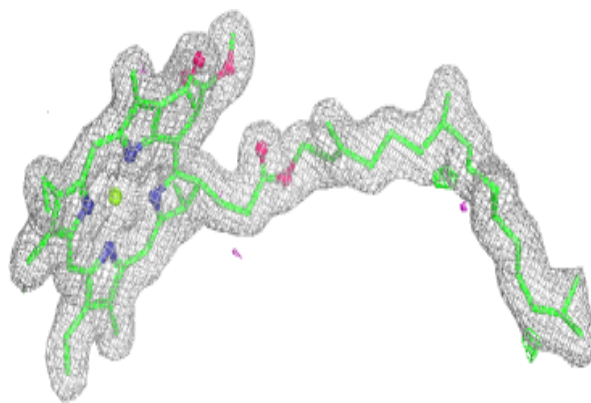
**Electron density around CLA d 402:**

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



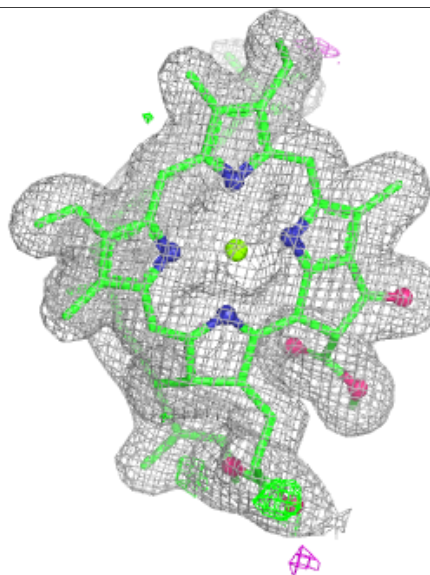
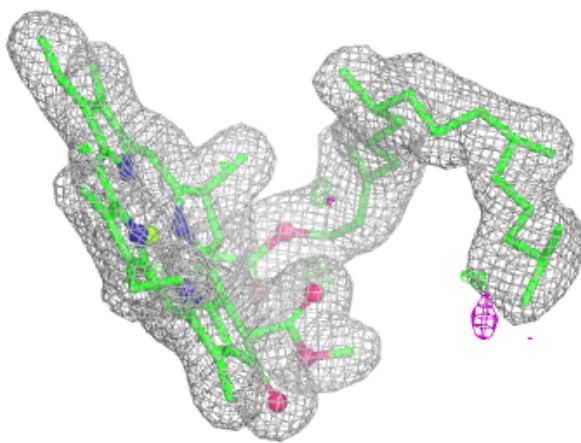
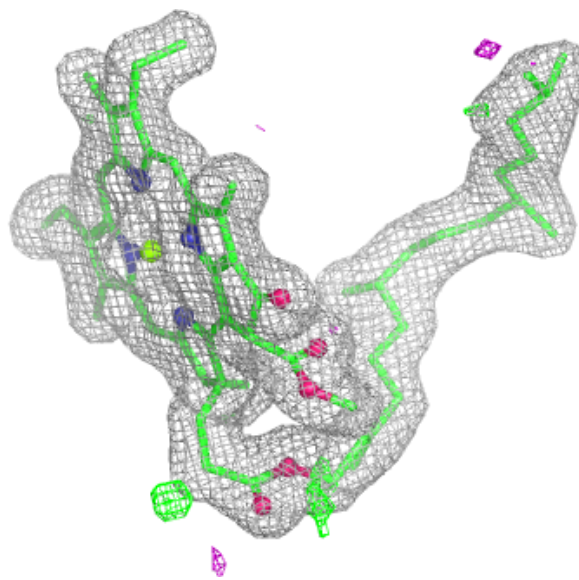
Electron density around CLA a 409:

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



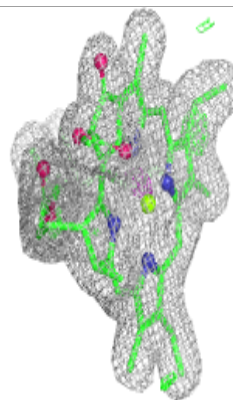
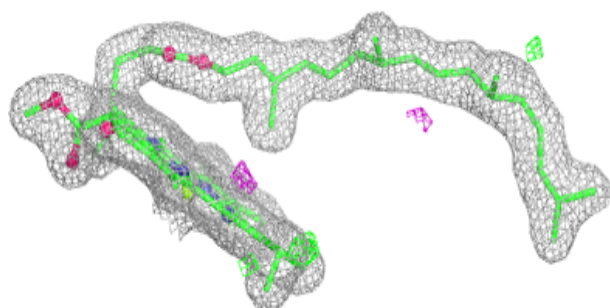
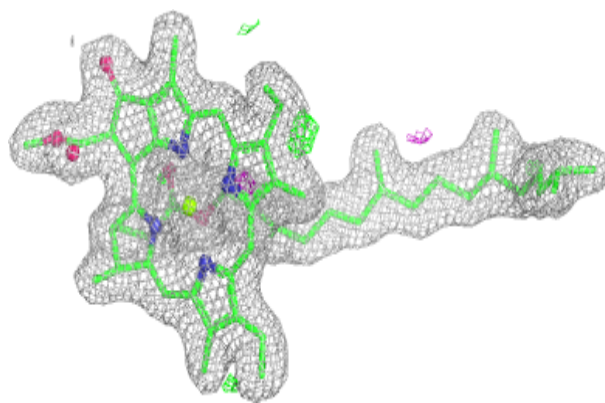
Electron density around CLA b 616:

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

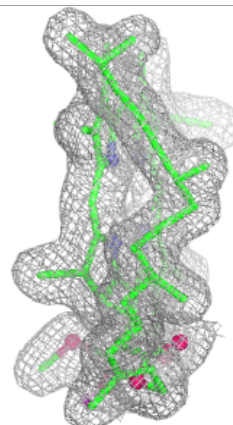
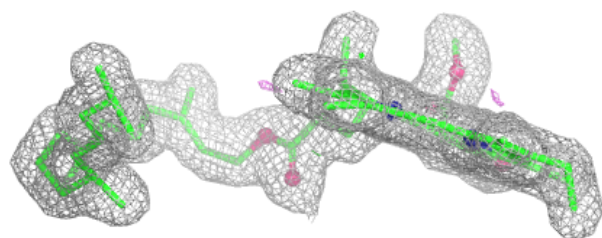
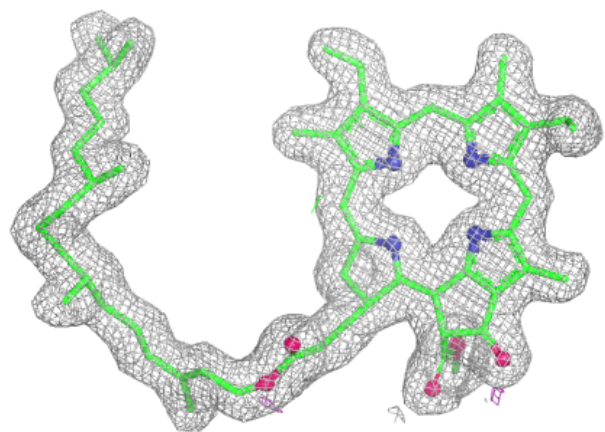


Electron density around CLA b 611:

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

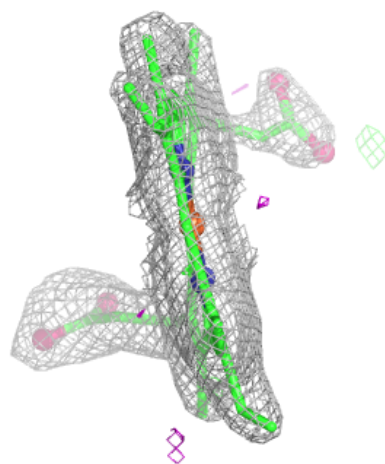
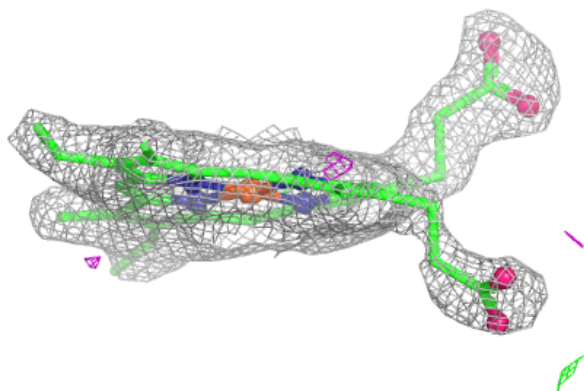
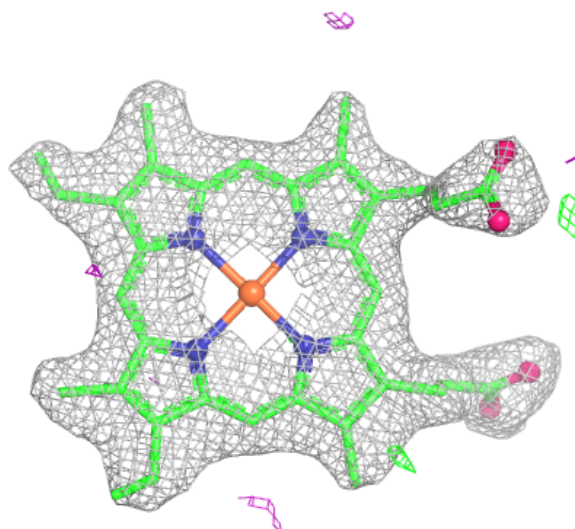
**Electron density around PHO a 412:**

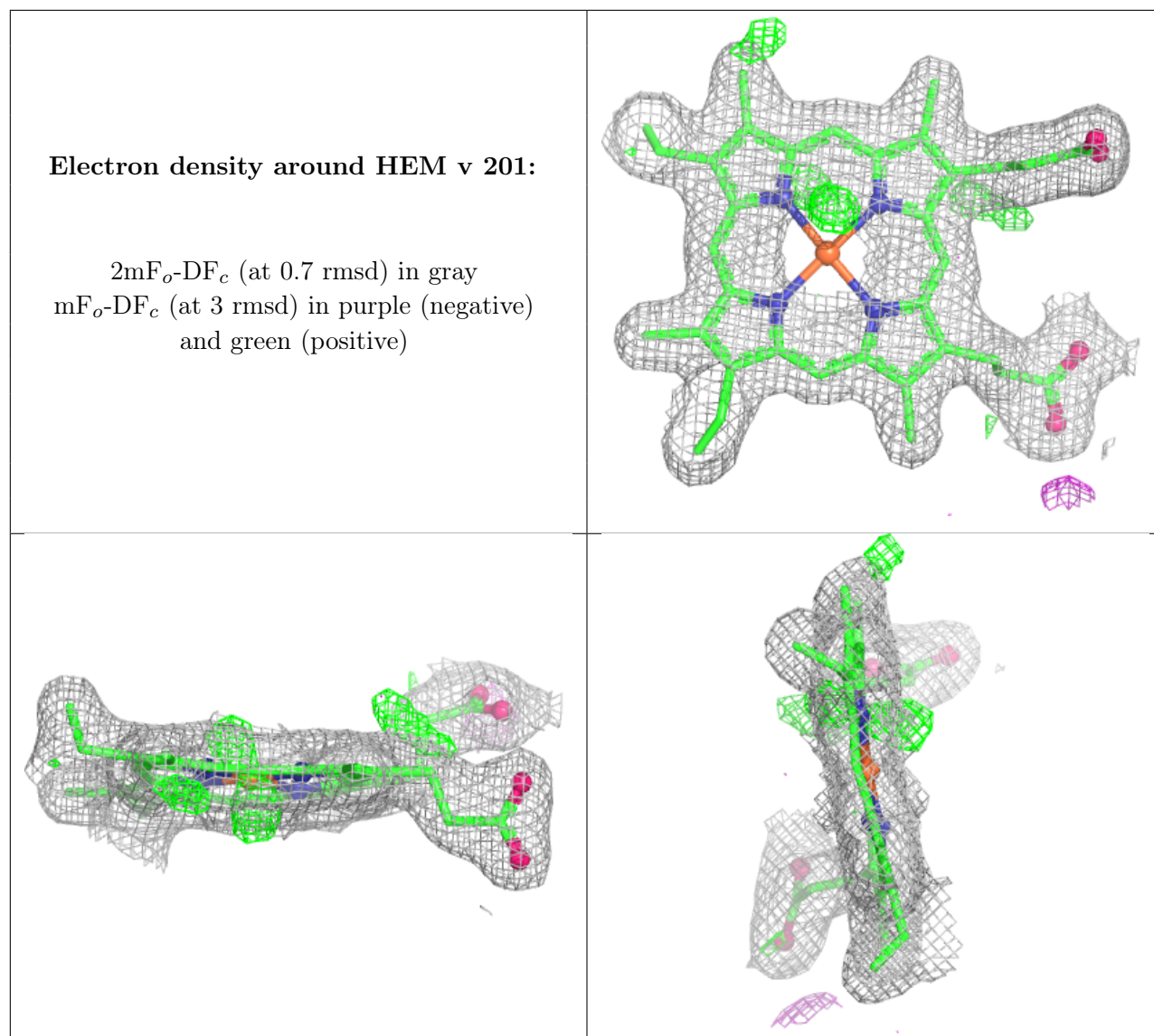
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM f 101:

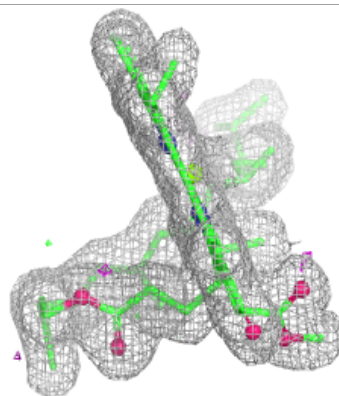
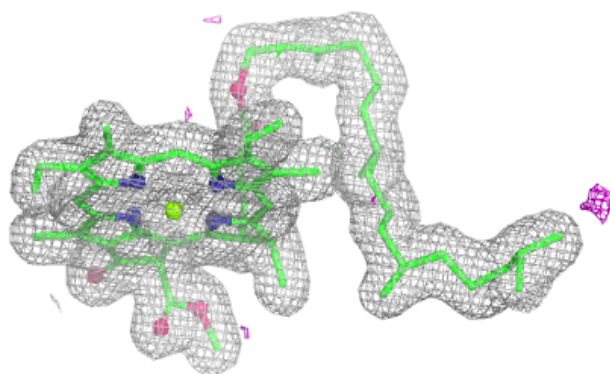
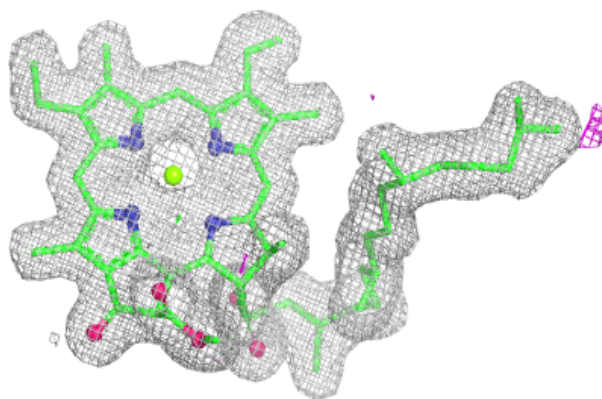
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



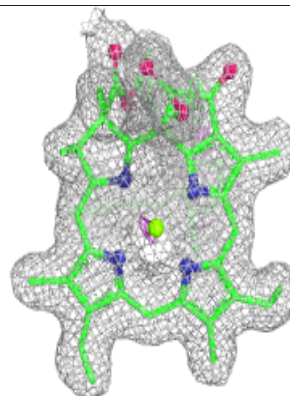
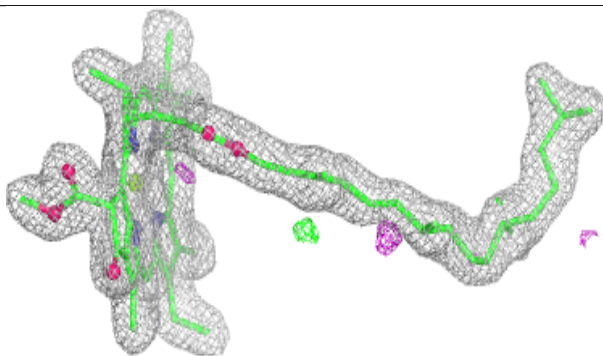
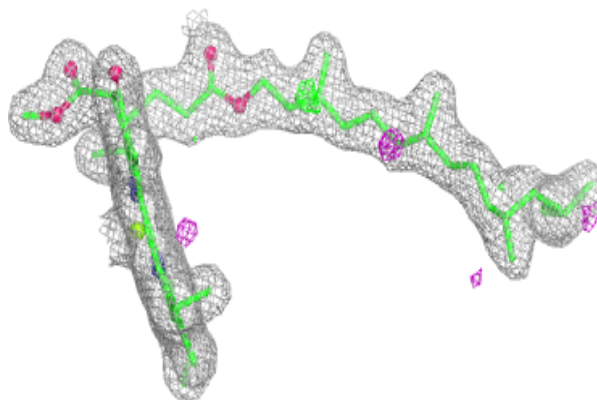


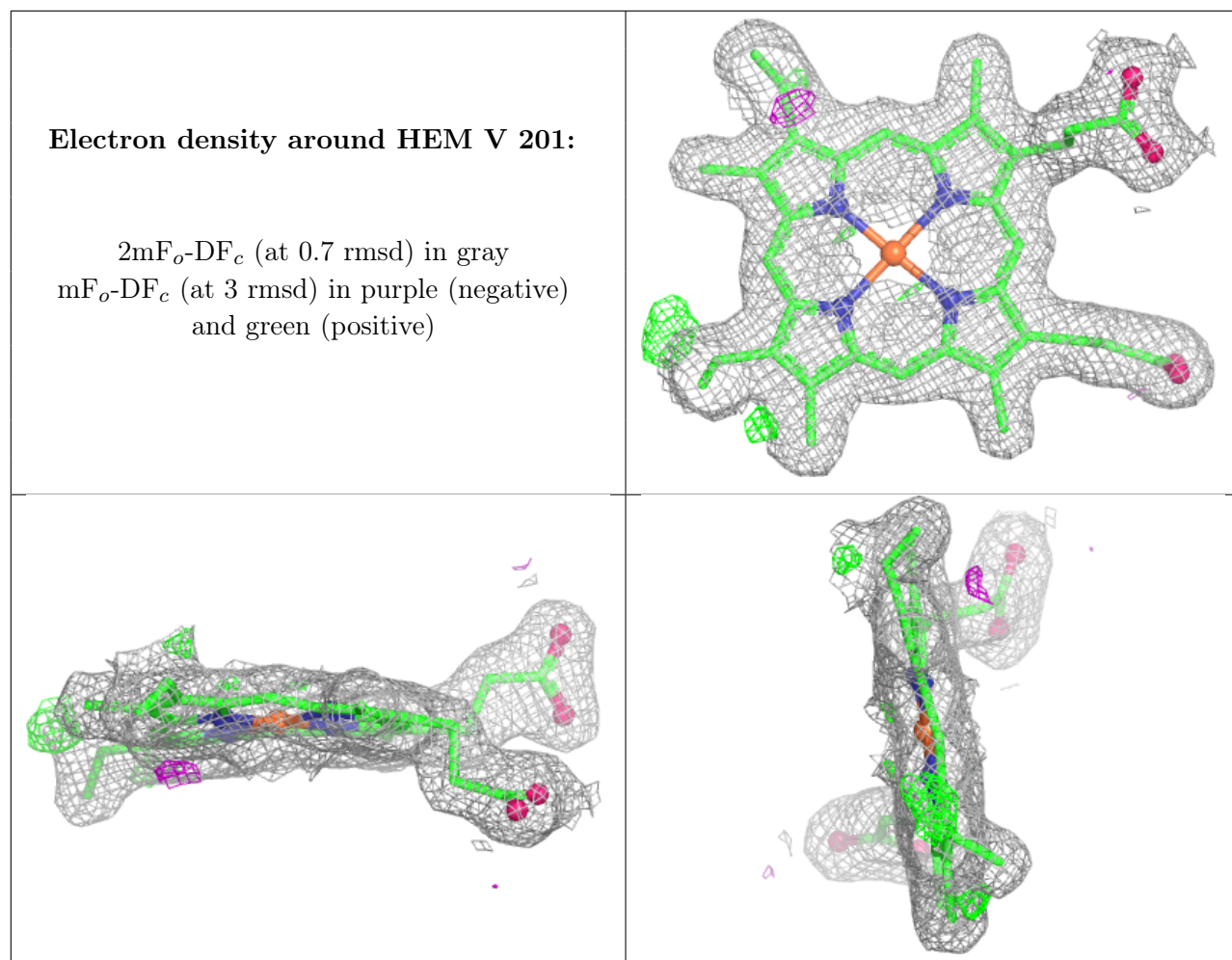
Electron density around CLA a 410:

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

**Electron density around CLA 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.