



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 12:44 AM UTC

PDB ID : 7COU / pdb_00007cou
Title : Structure of cyanobacterial photosystem II in the dark S1 state
Authors : Li, H.; Shen, J.-R.; Suga, M.
Deposited on : 2020-08-05
Resolution : 2.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

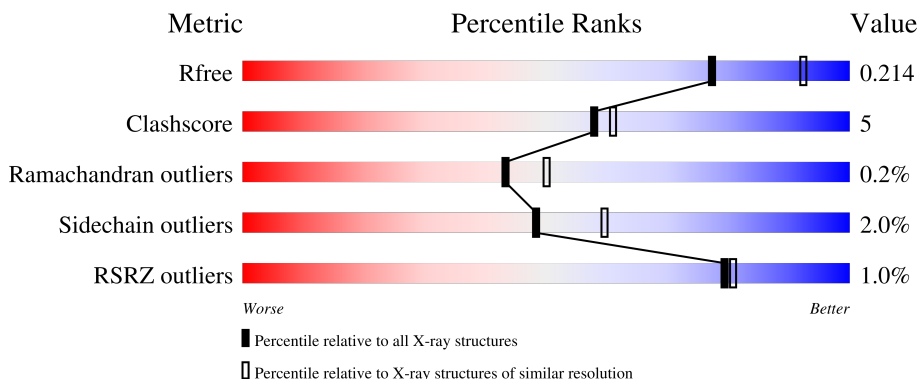
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 Å.

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




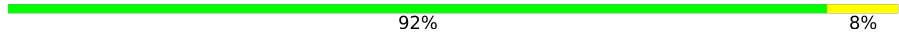





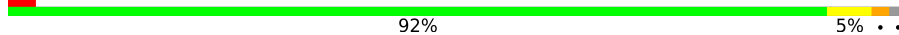

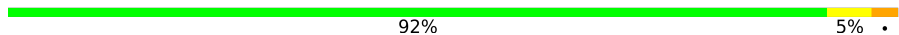
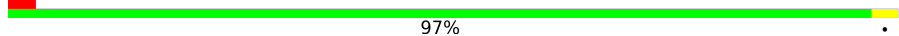














Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	344	 91% 6% .
1	a	344	 2% 89% 8% .
2	B	505	 91% 9%
2	b	505	 2% 90% 9% .
3	C	455	 91% 8% .

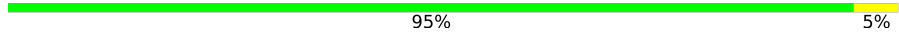
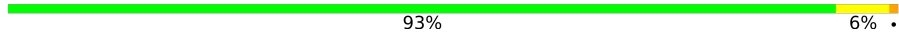




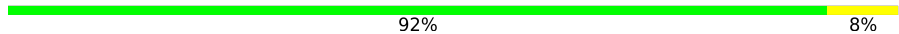


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Mol	Chain	Length	Quality of chain
3	c	455	 91% 8%
4	D	342	 92% 8%
4	d	342	 89% 10%
5	E	84	 69% 27%
5	e	84	 85% 7% 6%
6	F	44	 64% 14% 23%
6	f	44	 64% 7% 30%
7	H	65	 92% 5%
7	h	65	 89% 8%
8	I	38	 92% 5%
8	i	38	 97%
9	J	39	 82% 8% 8%
9	j	39	 85% 15%
10	K	37	 86% 14%
10	k	37	 84% 16%
11	L	37	 89% 8%
11	l	37	 92% 5%
12	M	36	 78% 14% 8%
12	m	36	 75% 17% 6%
13	O	244	 90% 9%
13	o	244	 91% 8%
14	T	32	 88% 6%
14	t	32	 88% 6% 6%
15	U	104	 85% 7% 8%
15	u	104	 90% 7%

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Mol	Chain	Length	Quality of chain
16	V	137	
16	v	137	
17	X	40	
17	x	40	
18	Y	30	
18	y	30	
19	Z	62	
19	z	62	
20	R	34	

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

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

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

2 Entry composition [i](#)

There are 40 unique types of molecules in this entry. The entry contains 53138 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	334	2634	1725	433	461	15	0	2	0
1	a	334	2642	1731	434	462	15	0	3	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	conflict	UNP P51765
a	279	PRO	ARG	conflict	UNP P51765

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	504	4050	2650	677	710	13	0	10	0
2	b	504	3998	2622	665	698	13	0	4	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	451	3513	2295	588	617	13	0	4	0
3	c	455	3534	2311	591	619	13	0	2	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	M	33	268	179	39	49	1	0	1	0
12	m	34	269	179	40	49	1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	conflict	UNP P12312
m	8	LEU	PHE	conflict	UNP P12312

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	O	243	1886	1177	318	386	5	0	3	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

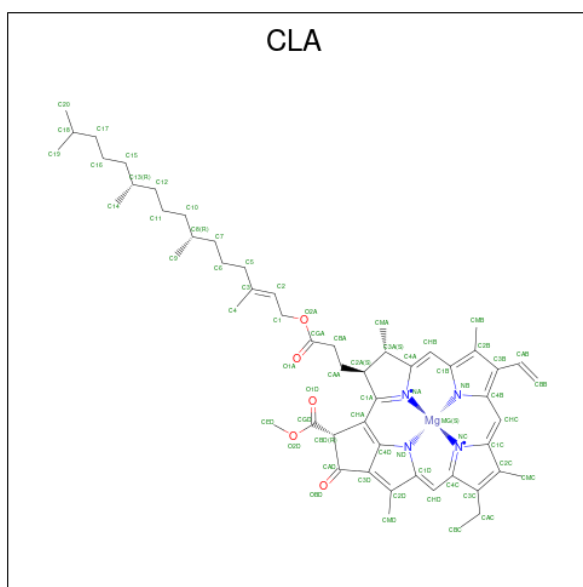
- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 22 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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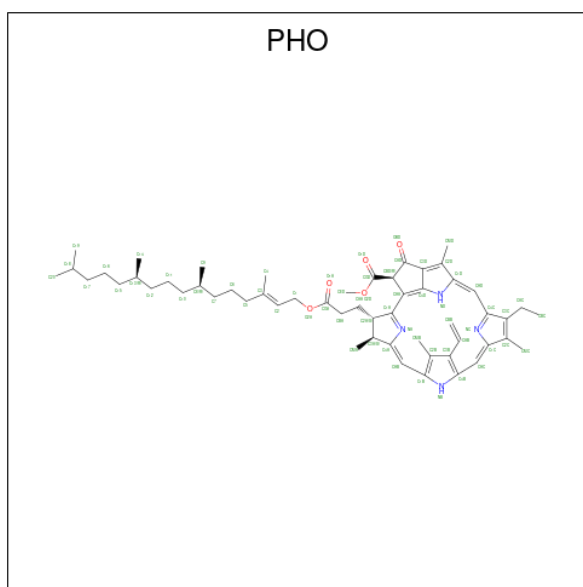
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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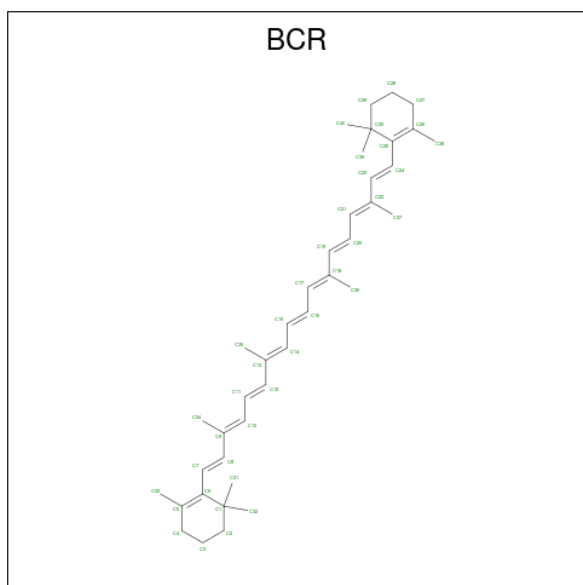
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	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 (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



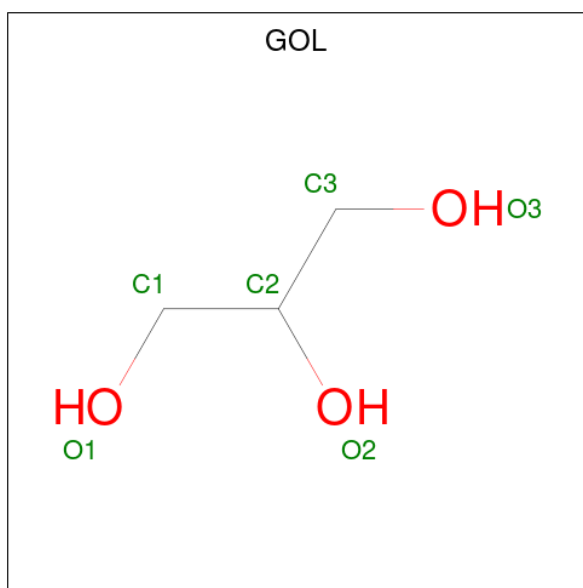
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			
24	A	1	Total	64	55	4	5	0	0
24	A	1	Total	64	55	4	5	0	0
24	a	1	Total	64	55	4	5	0	0
24	a	1	Total	64	55	4	5	0	0

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



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

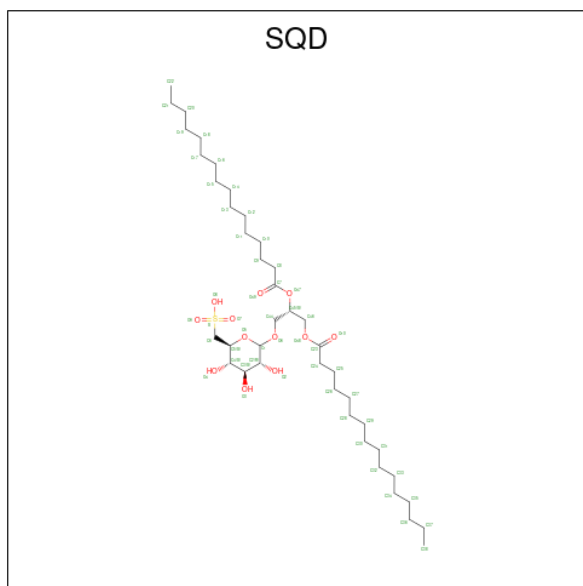
- Molecule 26 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

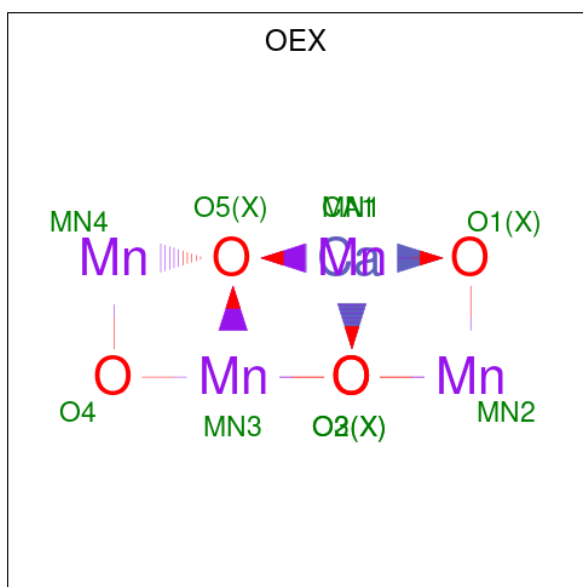
- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

LJ-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



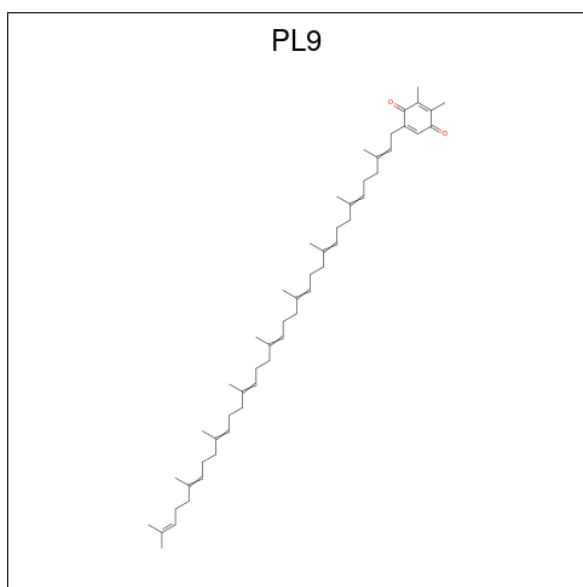
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
27	A	1	54	41	12	1	0	0
27	B	1	54	41	12	1	0	0
27	C	1	54	41	12	1	0	0
27	D	1	43	30	12	1	0	0
27	a	1	54	41	12	1	0	0
27	a	1	54	41	12	1	0	0
27	b	1	54	41	12	1	0	0
27	f	1	43	30	12	1	0	0

- Molecule 28 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn₄O₅).



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

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



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

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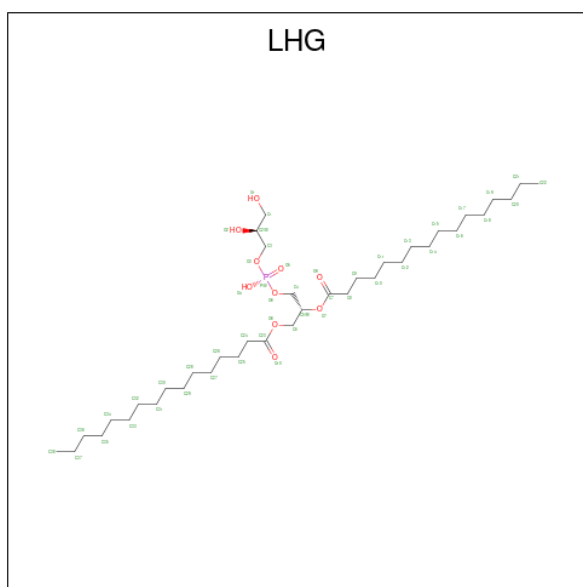
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	D	1	Total	C	O	0	0
			55	53	2		
29	a	1	Total	C	O	0	0
			55	53	2		
29	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 30 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

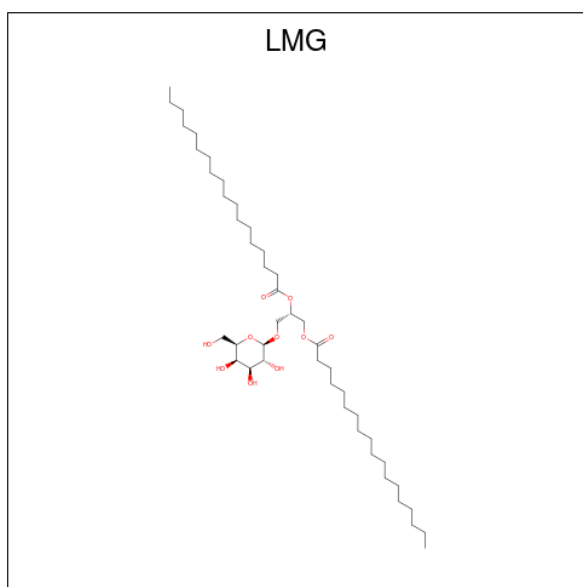
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			28	23	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	C	1	Total	C	O	0	0
			34	29	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	I	1	Total	C	O	0	0
			40	35	5		
30	J	1	Total	C		0	0
			10	10			
30	M	1	Total	C		0	0
			10	10			
30	X	1	Total	C	O	0	0
		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

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



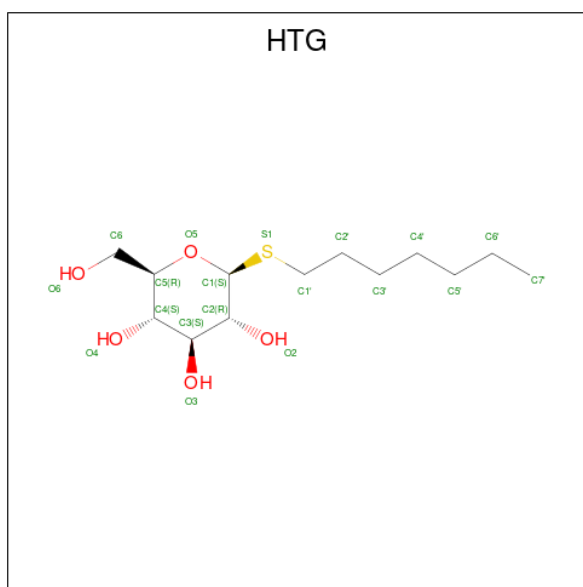
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
31	A	1	49	38	10	1	0	0
31	D	1	49	38	10	1	0	0
31	D	1	49	38	10	1	0	0
31	E	1	42	31	10	1	0	0
31	L	1	49	38	10	1	0	0
31	a	1	42	31	10	1	0	0
31	b	1	49	38	10	1	0	0
31	d	1	49	38	10	1	0	0
31	d	1	49	38	10	1	0	0
31	d	1	49	38	10	1	0	0

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



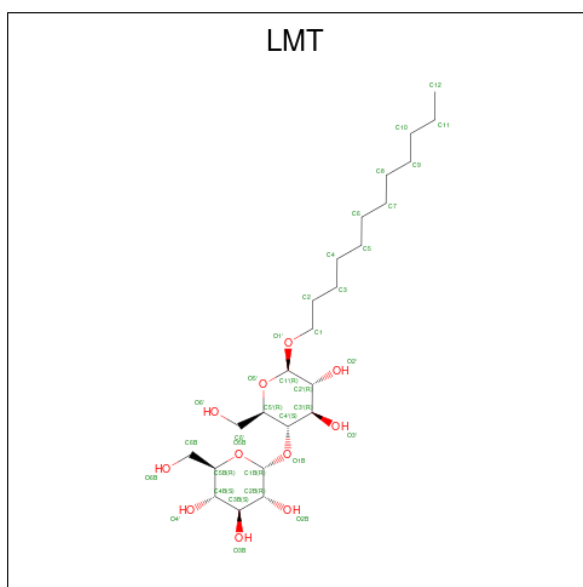
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	B	1	Total	C	O	0	0
			51	41	10		
32	C	1	Total	C	O	0	0
			51	41	10		
32	C	1	Total	C	O	0	0
			51	41	10		
32	C	1	Total	C	O	0	0
			51	41	10		
32	D	1	Total	C	O	0	0
			51	41	10		
32	Z	1	Total	C	O	0	0
			37	27	10		
32	c	1	Total	C	O	0	0
			51	41	10		
32	c	1	Total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

- Molecule 33 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C₁₃H₂₆O₅S).



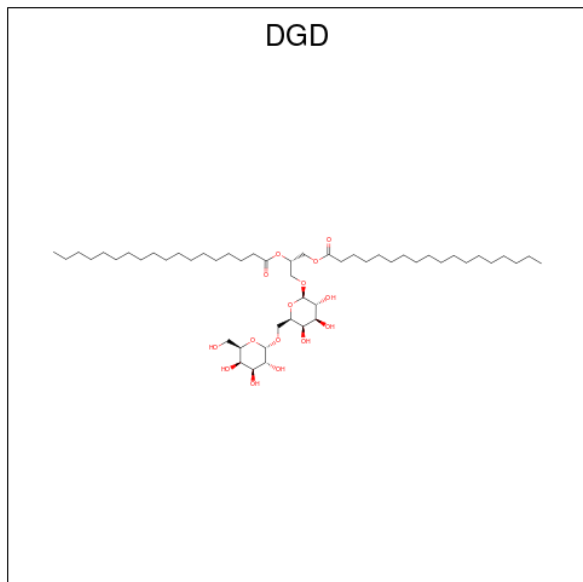
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	C	1	Total	C	O	S	0	0
			19	13	5	1		
33	D	1	Total	C	O	S	0	0
			16	10	5	1		
33	V	1	Total	C	O		0	0
			11	6	5			
33	b	1	Total	C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

- Molecule 34 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



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

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



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

- Molecule 36 is CALCIUM ION (CCD ID: CA) (formula: Ca).

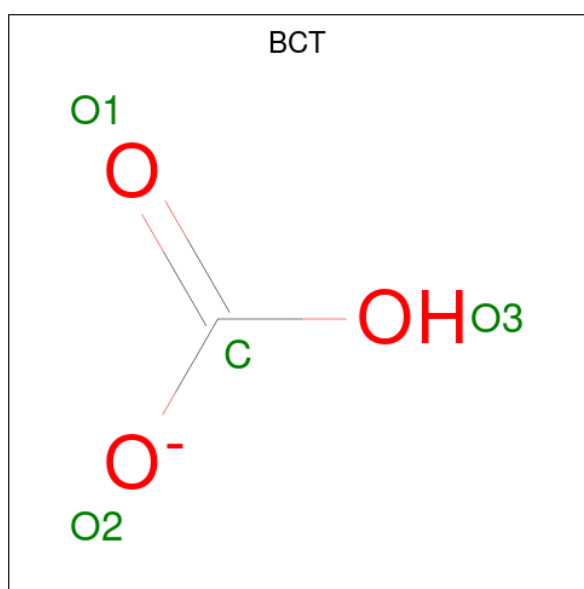
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	C	1	Total Ca 1 1	0	0
36	F	1	Total Ca 1 1	0	0

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

- Molecule 37 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

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

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

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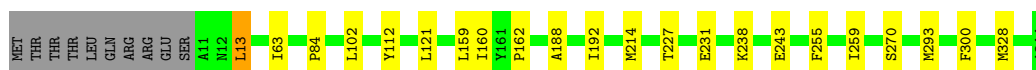
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	f	4	Total 4	O 4	0	0
40	h	23	Total 23	O 23	0	0
40	i	2	Total 2	O 2	0	0
40	j	3	Total 3	O 3	0	0
40	k	5	Total 5	O 5	0	0
40	l	7	Total 7	O 7	0	0
40	m	11	Total 11	O 11	0	0
40	o	99	Total 99	O 99	0	0
40	t	11	Total 11	O 11	0	0
40	u	71	Total 71	O 71	0	0
40	v	60	Total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

3 Residue-property plots [i](#)


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

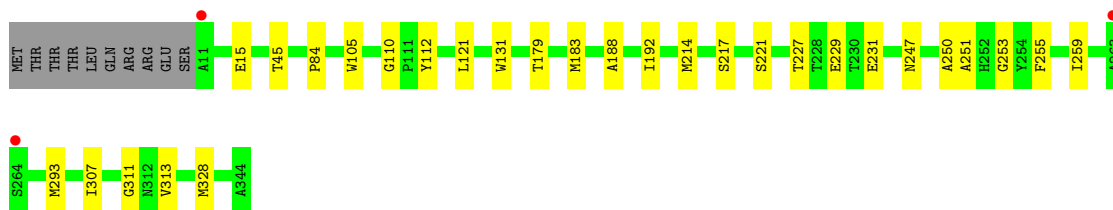
- Molecule 1: Photosystem II protein D1

Chain A:  91% 6%



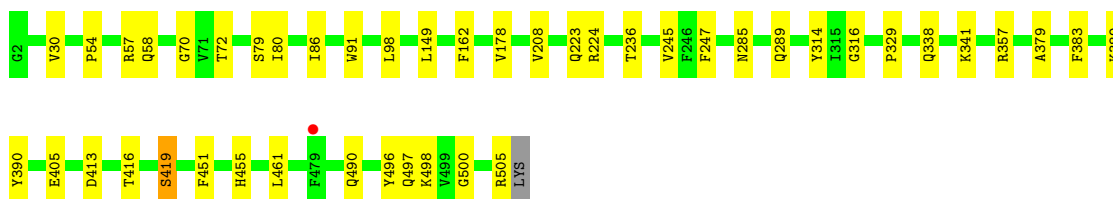
- Molecule 1: Photosystem II protein D1

Chain a:  89% 8%




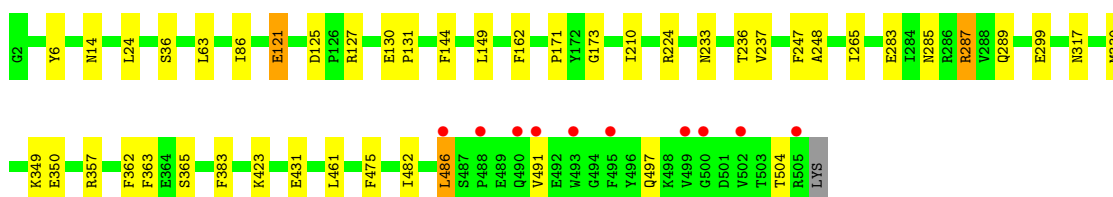
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  91% 9%



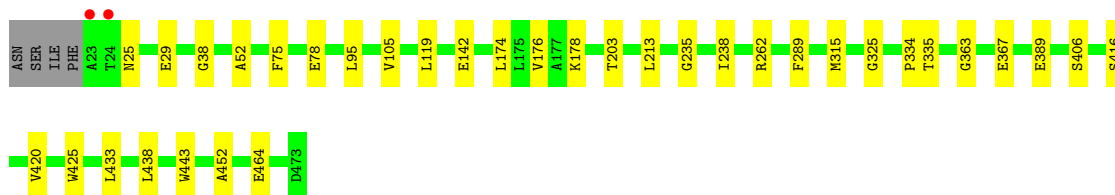
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  90% 9%



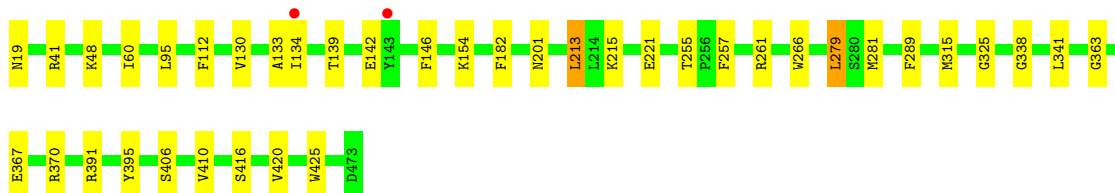
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C:  91% 8%



- Molecule 3: Photosystem II CP43 reaction center protein

Chain c:  91% 8%




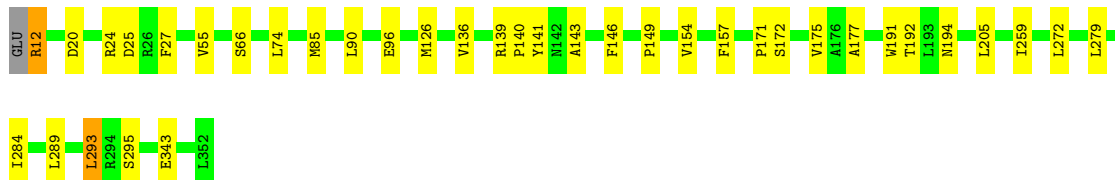
- Molecule 4: Photosystem II D2 protein

Chain D:  92% 8%



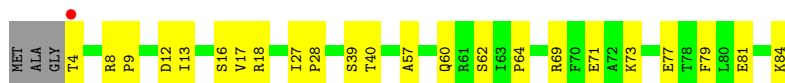
- Molecule 4: Photosystem II D2 protein

Chain d:  89% 10%




- Molecule 5: Cytochrome b559 subunit alpha

Chain E:  69% 27%

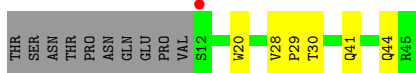


- Molecule 5: Cytochrome b559 subunit alpha

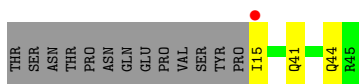
Chain e:  85% 7% 6%



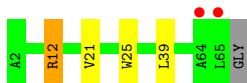
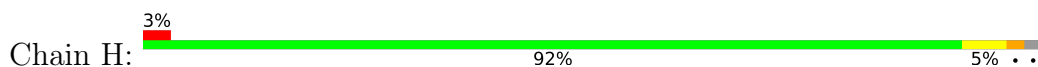
- Molecule 6: Cytochrome b559 subunit beta



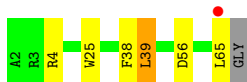
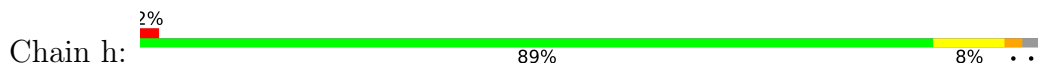
- Molecule 6: Cytochrome b559 subunit beta



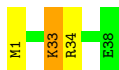
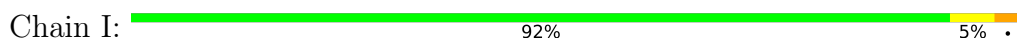
- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H



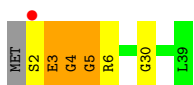
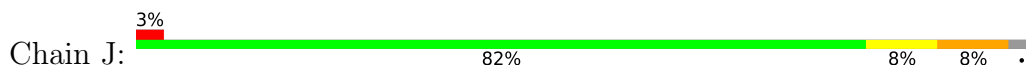
- Molecule 8: Photosystem II reaction center protein I



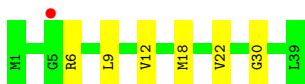
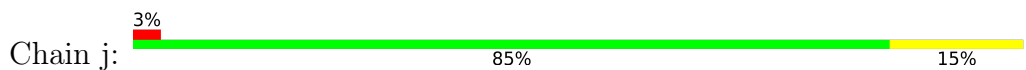
- Molecule 8: Photosystem II reaction center protein I



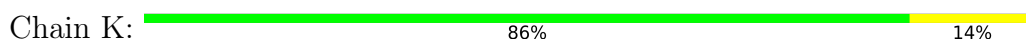
- Molecule 9: Photosystem II reaction center protein J



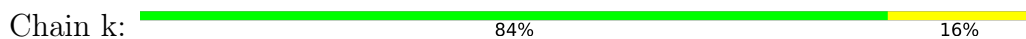
- Molecule 9: Photosystem II reaction center protein J



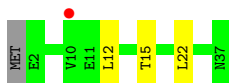
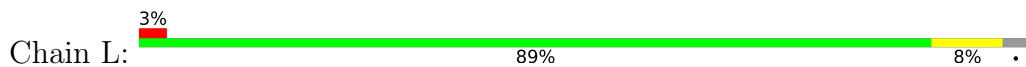
- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K



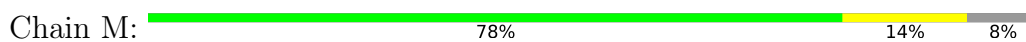
- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M



- Molecule 12: Photosystem II reaction center protein M

Chain m:  75% 17% 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  90% 9%




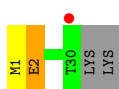
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  91% 8%




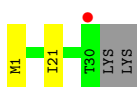
- Molecule 14: Photosystem II reaction center protein T

Chain T:  3% 88% 6% 6%




- Molecule 14: Photosystem II reaction center protein T

Chain t:  3% 88% 6% 6%




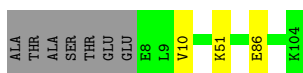
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  85% 7% 8%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  90% 7%



- Molecule 16: Cytochrome c-550

Chain V:  95% 5%




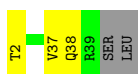
- Molecule 16: Cytochrome c-550

Chain v:  93% 6%




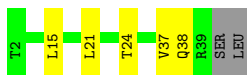
- Molecule 17: Photosystem II reaction center protein X

Chain X:  88% 8% 5%




- Molecule 17: Photosystem II reaction center protein X

Chain x:  82% 12% 5%




- Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:  7% 73% 23%



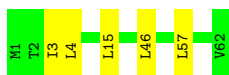
- Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:  77% 20%

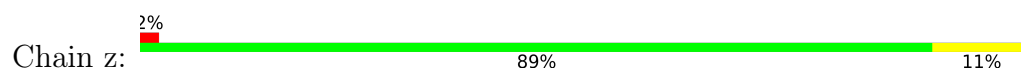


- Molecule 19: Photosystem II reaction center protein Z

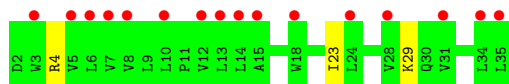
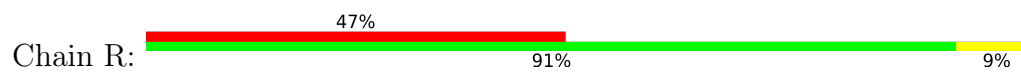
Chain Z:  92% 8%



- Molecule 19: Photosystem II reaction center protein Z



• Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	126.15Å 232.70Å 288.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.97 – 2.25 39.97 – 2.25	Depositor EDS
% Data completeness (in resolution range)	96.0 (39.97-2.25) 85.6 (39.97-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.25Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.169 , 0.211 0.171 , 0.214	Depositor DCC
R_{free} test set	20023 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	43.9	Xtrriage
Anisotropy	0.424	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 72.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	53138	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.37	0/2719	0.55	0/3708
1	a	0.34	0/2727	0.50	0/3719
2	B	0.34	0/4190	0.49	0/5708
2	b	0.31	0/4138	0.49	0/5640
3	C	0.29	0/3626	0.46	0/4936
3	c	0.27	0/3648	0.43	0/4966
4	D	0.36	0/2821	0.52	0/3844
4	d	0.33	0/2812	0.49	0/3832
5	E	0.26	0/687	0.45	0/936
5	e	0.24	0/667	0.40	0/908
6	F	0.25	0/284	0.39	0/387
6	f	0.22	0/257	0.43	0/349
7	H	0.27	0/530	0.50	0/723
7	h	0.25	0/519	0.48	0/708
8	I	0.24	0/311	0.36	0/419
8	i	0.26	0/311	0.41	0/419
9	J	0.23	0/278	0.37	0/376
9	j	0.23	0/283	0.39	0/383
10	K	0.25	0/303	0.46	0/416
10	k	0.24	0/303	0.44	0/416
11	L	0.40	0/311	0.47	0/423
11	l	0.33	0/311	0.50	0/423
12	M	0.35	0/261	0.51	0/357
12	m	0.35	0/262	0.50	0/357
13	O	0.30	0/1917	0.48	0/2599
13	o	0.28	0/1910	0.46	0/2589
14	T	0.36	0/257	0.42	0/349
14	t	0.35	0/257	0.41	0/349
15	U	0.33	0/776	0.53	0/1052
15	u	0.29	0/785	0.52	0/1064
16	V	0.29	0/1085	0.46	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.26	0/1085	0.41	0/1473
17	X	0.22	0/284	0.36	0/384
17	x	0.18	0/284	0.31	0/384
18	Y	0.20	0/216	0.37	0/289
18	y	0.18	0/216	0.38	0/289
19	Z	0.18	0/490	0.33	0/669
19	z	0.18	0/490	0.33	0/669
20	R	0.19	0/279	0.33	0/383
All	All	0.31	0/42890	0.47	0/58368

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2634	0	2531	14	0
1	a	2642	0	2541	23	0
2	B	4050	0	3894	31	0
2	b	3998	0	3852	36	0
3	C	3513	0	3424	23	0
3	c	3534	0	3446	26	0
4	D	2726	0	2627	23	0
4	d	2717	0	2621	25	0
5	E	668	0	652	16	0
5	e	648	0	634	7	0
6	F	275	0	282	5	0
6	f	250	0	261	3	0
7	H	517	0	542	4	0
7	h	506	0	529	5	0
8	I	314	0	328	2	0
8	i	314	0	328	0	0
9	J	272	0	279	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	277	0	284	4	0
10	K	293	0	305	1	0
10	k	293	0	305	3	0
11	L	304	0	314	2	0
11	l	304	0	314	2	0
12	M	268	0	285	4	0
12	m	269	0	288	5	0
13	O	1886	0	1856	14	0
13	o	1879	0	1850	11	0
14	T	258	0	261	1	0
14	t	258	0	261	1	0
15	U	765	0	767	4	0
15	u	774	0	773	1	0
16	V	1064	0	1073	4	0
16	v	1064	0	1073	6	0
17	X	281	0	312	2	0
17	x	281	0	312	4	0
18	Y	215	0	246	4	0
18	y	215	0	246	3	0
19	Z	479	0	516	2	0
19	z	479	0	516	2	0
20	R	273	0	305	2	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0
23	A	260	0	288	10	0
23	B	1040	0	1152	32	0
23	C	845	0	936	30	0
23	D	130	0	144	2	0
23	a	260	0	288	9	0
23	b	1040	0	1152	32	0
23	c	845	0	936	30	0
23	d	130	0	144	1	0
24	A	128	0	148	3	0
24	a	128	0	148	5	0
25	A	40	0	56	2	0
25	B	120	0	168	7	0
25	C	80	0	112	1	0
25	D	40	0	56	0	0
25	H	40	0	56	3	0
25	K	40	0	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	T	40	0	56	4	0
25	Y	40	0	56	1	0
25	a	40	0	56	2	0
25	b	120	0	168	9	0
25	c	80	0	112	5	0
25	d	40	0	56	1	0
25	h	40	0	56	3	0
25	k	40	0	56	1	0
25	t	40	0	56	5	0
25	y	40	0	56	2	0
26	A	6	0	8	0	0
26	B	18	0	24	0	0
26	C	6	0	8	0	0
26	O	6	0	8	0	0
26	a	6	0	8	0	0
26	b	12	0	16	1	0
26	c	6	0	8	1	0
26	o	6	0	8	0	0
26	v	6	0	8	1	0
27	A	54	0	78	1	0
27	B	54	0	78	0	0
27	C	54	0	77	3	0
27	D	43	0	53	0	0
27	a	108	0	155	2	0
27	b	54	0	78	1	0
27	f	43	0	53	2	0
28	A	10	0	0	0	0
28	a	10	0	0	0	0
29	A	55	0	80	5	0
29	D	55	0	80	2	0
29	a	55	0	80	6	0
29	d	55	0	80	1	0
30	A	28	0	0	0	0
30	B	33	0	0	1	0
30	C	34	0	0	0	0
30	D	57	0	0	0	0
30	I	40	0	0	0	0
30	J	10	0	0	0	0
30	M	10	0	0	0	0
30	X	18	0	0	0	0
30	a	30	0	0	0	0
30	b	33	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	c	32	0	0	0	0
30	d	71	0	0	0	0
30	i	40	0	0	0	0
30	j	10	0	0	0	0
30	m	10	0	0	0	0
31	A	49	0	74	2	0
31	D	98	0	148	6	0
31	E	42	0	57	2	0
31	L	49	0	74	2	0
31	a	42	0	57	5	0
31	b	49	0	74	0	0
31	d	147	0	222	10	0
32	B	51	0	72	3	0
32	C	153	0	216	4	0
32	D	51	0	72	1	0
32	Z	37	0	44	0	0
32	c	153	0	216	5	0
32	d	51	0	71	2	0
32	m	51	0	72	2	0
32	z	39	0	48	2	0
33	B	57	0	78	4	0
33	C	19	0	26	0	0
33	D	16	0	17	1	0
33	V	11	0	10	0	0
33	b	57	0	78	3	0
33	c	19	0	26	1	0
33	h	16	0	17	1	0
34	B	60	0	81	0	0
34	C	35	0	46	2	0
34	D	35	0	46	2	0
34	E	35	0	46	1	0
34	M	70	0	92	3	0
34	a	70	0	92	3	0
34	b	50	0	70	1	0
34	e	35	0	46	0	0
34	m	35	0	46	0	0
34	t	26	0	35	0	0
35	C	186	0	246	9	0
35	H	62	0	82	1	0
35	c	186	0	246	3	0
35	h	62	0	82	0	0
36	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	F	1	0	0	0	0
36	O	1	0	0	0	0
36	a	1	0	0	0	0
36	c	2	0	0	0	0
36	o	1	0	0	0	0
37	D	4	0	0	0	0
37	d	4	0	0	0	0
38	E	43	0	32	1	0
38	V	43	0	30	1	0
38	e	43	0	32	2	0
38	v	43	0	30	0	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	A	143	0	0	0	0
40	B	223	0	0	1	0
40	C	203	0	0	1	0
40	D	136	0	0	3	0
40	E	27	0	0	0	0
40	F	9	0	0	1	0
40	H	26	0	0	1	0
40	I	5	0	0	0	0
40	J	5	0	0	0	0
40	K	7	0	0	0	0
40	L	6	0	0	0	0
40	M	17	0	0	0	0
40	O	125	0	0	1	0
40	R	1	0	0	0	0
40	T	16	0	0	0	0
40	U	56	0	0	0	0
40	V	102	0	0	0	0
40	X	9	0	0	0	0
40	Y	1	0	0	0	0
40	a	143	0	0	0	0
40	b	234	0	0	1	0
40	c	174	0	0	3	0
40	d	125	0	0	0	0
40	e	16	0	0	0	0
40	f	4	0	0	1	0
40	h	23	0	0	0	0
40	i	2	0	0	0	0
40	j	3	0	0	0	0
40	k	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	l	7	0	0	0	0
40	m	11	0	0	0	0
40	o	99	0	0	0	0
40	t	11	0	0	0	0
40	u	71	0	0	0	0
40	v	60	0	0	1	0
40	x	9	0	0	0	0
40	y	4	0	0	0	0
All	All	53138	0	51938	468	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 468 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:c:515:CLA:HBB1	25:c:516:BCR:H24C	1.57	0.86
1:a:250:ALA:HA	2:b:491:VAL:HG11	1.58	0.83
4:D:85:MET:HE2	4:D:90:LEU:HD21	1.61	0.82
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.62	0.82
4:d:192:THR:HG23	23:d:402:CLA:HBC2	1.62	0.81

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	334/344 (97%)	330 (99%)	3 (1%)	1 (0%)	36	40
1	a	335/344 (97%)	328 (98%)	6 (2%)	1 (0%)	36	40
2	B	512/505 (101%)	505 (99%)	7 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	506/505 (100%)	497 (98%)	9 (2%)	0	100	100
3	C	453/455 (100%)	443 (98%)	8 (2%)	2 (0%)	30	31
3	c	455/455 (100%)	444 (98%)	10 (2%)	1 (0%)	43	50
4	D	340/342 (99%)	329 (97%)	11 (3%)	0	100	100
4	d	339/342 (99%)	331 (98%)	8 (2%)	0	100	100
5	E	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
5	e	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	29/44 (66%)	29 (100%)	0	0	100	100
7	H	63/65 (97%)	61 (97%)	2 (3%)	0	100	100
7	h	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
8	I	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
8	i	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
9	J	36/39 (92%)	33 (92%)	0	3 (8%)	0	0
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	32/36 (89%)	30 (94%)	2 (6%)	0	100	100
13	O	244/244 (100%)	237 (97%)	6 (2%)	1 (0%)	30	31
13	o	243/244 (100%)	236 (97%)	7 (3%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	94/104 (90%)	92 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
16	v	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
17	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
17	x	36/40 (90%)	35 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	Y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
18	y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	7	3
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	5246/5384 (97%)	5129 (98%)	107 (2%)	10 (0%)	43	50

5 of 10 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/279 (97%)	268 (99%)	3 (1%)	65	75
1	a	272/279 (98%)	271 (100%)	1 (0%)	84	89
2	B	412/403 (102%)	406 (98%)	6 (2%)	57	68
2	b	406/403 (101%)	399 (98%)	7 (2%)	53	65
3	C	356/356 (100%)	349 (98%)	7 (2%)	48	59
3	c	358/356 (101%)	352 (98%)	6 (2%)	53	65
4	D	277/277 (100%)	274 (99%)	3 (1%)	65	75
4	d	276/277 (100%)	271 (98%)	5 (2%)	51	63
5	E	73/73 (100%)	70 (96%)	3 (4%)	27	33
5	e	70/73 (96%)	67 (96%)	3 (4%)	26	31
6	F	28/38 (74%)	28 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	f	25/38 (66%)	25 (100%)	0	100	100
7	H	55/54 (102%)	52 (94%)	3 (6%)	19	20
7	h	54/54 (100%)	52 (96%)	2 (4%)	30	37
8	I	34/34 (100%)	33 (97%)	1 (3%)	37	47
8	i	34/34 (100%)	34 (100%)	0	100	100
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	26/27 (96%)	25 (96%)	1 (4%)	29	36
10	K	30/30 (100%)	26 (87%)	4 (13%)	4	2
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	5
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	47
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	30/32 (94%)	30 (100%)	0	100	100
12	m	30/32 (94%)	28 (93%)	2 (7%)	15	14
13	O	209/207 (101%)	206 (99%)	3 (1%)	59	70
13	o	208/207 (100%)	203 (98%)	5 (2%)	43	54
14	T	26/28 (93%)	25 (96%)	1 (4%)	29	36
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	83/89 (93%)	80 (96%)	3 (4%)	31	39
15	u	84/89 (94%)	82 (98%)	2 (2%)	43	54
16	V	117/117 (100%)	117 (100%)	0	100	100
16	v	117/117 (100%)	114 (97%)	3 (3%)	40	50
17	X	31/33 (94%)	30 (97%)	1 (3%)	34	43
17	x	31/33 (94%)	29 (94%)	2 (6%)	15	14
18	Y	22/23 (96%)	20 (91%)	2 (9%)	9	7
18	y	22/23 (96%)	20 (91%)	2 (9%)	9	7
19	Z	52/52 (100%)	51 (98%)	1 (2%)	50	61
19	z	52/52 (100%)	50 (96%)	2 (4%)	29	36
20	R	29/29 (100%)	28 (97%)	1 (3%)	32	40
All	All	4352/4403 (99%)	4263 (98%)	89 (2%)	48	59

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	d	12	ARG
12	m	5	GLN
4	d	154	VAL
7	h	39	LEU
13	o	69	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
3	c	19	ASN
13	o	80	GLN
4	D	186	GLN
13	O	231	HIS
15	U	78	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	I	1	8	8,9,10	0.70	0	8,9,11	1.04	1 (12%)
12	FME	m	1	12	8,9,10	0.59	0	8,9,11	1.50	2 (25%)
14	FME	t	1	14	8,9,10	0.67	0	8,9,11	1.66	2 (25%)
14	FME	T	1	14	8,9,10	0.73	0	8,9,11	1.36	2 (25%)
8	FME	i	1	8	8,9,10	0.60	0	8,9,11	0.97	1 (12%)
12	FME	M	1	12	8,9,10	0.64	0	8,9,11	1.58	3 (37%)

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

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

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	CA-N-CN	-3.25	117.82	122.82
12	M	1	FME	CA-N-CN	-3.08	118.08	122.82
14	t	1	FME	O-C-CA	-2.65	117.96	124.77
14	T	1	FME	O-C-CA	-2.52	118.29	124.77
14	T	1	FME	CA-N-CN	-2.36	119.19	122.82

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 216 ligands modelled in this entry, 15 are monoatomic and 18 are unknown - leaving 183 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	HTG	B	623	-	19,19,19	0.75	1 (5%)	23,24,24	1.67	4 (17%)
23	CLA	b	605	-	69,73,73	1.98	20 (28%)	82,113,113	2.82	27 (32%)
24	PHO	A	407	-	58,69,69	2.65	14 (24%)	55,99,99	2.90	17 (30%)
23	CLA	a	405	40	69,73,73	2.07	18 (26%)	82,113,113	2.74	32 (39%)
33	HTG	h	101	-	16,16,19	1.05	1 (6%)	20,21,24	2.01	5 (25%)
23	CLA	b	616	-	69,73,73	1.97	19 (27%)	82,113,113	2.78	34 (41%)
25	BCR	B	617	-	41,41,41	1.08	1 (2%)	56,56,56	1.35	9 (16%)
32	LMG	C	502	-	51,51,55	0.93	2 (3%)	59,59,63	1.03	3 (5%)
23	CLA	c	505	-	69,73,73	2.04	19 (27%)	82,113,113	2.66	29 (35%)
34	LMT	M	103	-	36,36,36	0.46	0	47,47,47	1.04	2 (4%)
23	CLA	A	405	40	69,73,73	2.01	19 (27%)	82,113,113	2.73	33 (40%)
25	BCR	b	619	-	41,41,41	1.18	2 (4%)	56,56,56	1.51	12 (21%)
23	CLA	B	611	-	69,73,73	2.00	19 (27%)	82,113,113	2.81	34 (41%)
23	CLA	c	508	-	69,73,73	2.02	20 (28%)	82,113,113	2.65	31 (37%)
27	SQD	D	412	-	41,43,54	1.10	2 (4%)	51,54,65	1.76	10 (19%)
23	CLA	C	506	40	69,73,73	1.98	21 (30%)	82,113,113	2.65	32 (39%)
35	DGD	h	103	-	63,63,67	0.91	3 (4%)	77,77,81	1.01	3 (3%)
23	CLA	c	509	40	69,73,73	2.06	18 (26%)	82,113,113	2.75	30 (36%)
24	PHO	a	417	-	58,69,69	2.80	13 (22%)	55,99,99	3.08	14 (25%)
31	LHG	d	408	-	48,48,48	0.90	2 (4%)	51,54,54	1.08	3 (5%)
23	CLA	B	612	-	69,73,73	1.92	18 (26%)	82,113,113	2.81	31 (37%)
25	BCR	A	409	-	41,41,41	1.05	1 (2%)	56,56,56	1.47	10 (17%)
34	LMT	m	103	-	36,36,36	0.46	0	47,47,47	1.00	3 (6%)
31	LHG	E	101	-	41,41,48	1.05	2 (4%)	44,47,54	1.04	2 (4%)
32	LMG	c	522	-	51,51,55	0.96	2 (3%)	59,59,63	1.11	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	HTG	C	523	-	19,19,19	0.85	1 (5%)	23,24,24	1.24	1 (4%)
25	BCR	C	516	-	41,41,41	1.01	1 (2%)	56,56,56	1.62	9 (16%)
32	LMG	B	621	-	51,51,55	0.91	2 (3%)	59,59,63	1.16	3 (5%)
23	CLA	C	508	-	69,73,73	2.06	20 (28%)	82,113,113	2.66	33 (40%)
23	CLA	B	613	-	69,73,73	1.94	18 (26%)	82,113,113	2.66	29 (35%)
23	CLA	B	603	-	69,73,73	2.00	19 (27%)	82,113,113	2.78	30 (36%)
23	CLA	d	402	-	69,73,73	1.95	19 (27%)	82,113,113	2.63	33 (40%)
23	CLA	c	513	3	69,73,73	2.00	19 (27%)	82,113,113	2.72	31 (37%)
28	OEX	a	414	1,3,40	0,15,15	-	-	-	-	-
34	LMT	E	102	-	36,36,36	0.52	1 (2%)	47,47,47	0.86	1 (2%)
23	CLA	C	515	-	69,73,73	2.02	20 (28%)	82,113,113	2.69	31 (37%)
27	SQD	a	410	-	52,54,54	0.92	2 (3%)	62,65,65	1.63	11 (17%)
23	CLA	B	605	-	69,73,73	2.03	19 (27%)	82,113,113	2.68	30 (36%)
23	CLA	A	408	-	69,73,73	2.04	20 (28%)	82,113,113	2.65	33 (40%)
23	CLA	C	505	-	69,73,73	2.02	19 (27%)	82,113,113	2.72	28 (34%)
23	CLA	c	510	-	69,73,73	2.08	20 (28%)	82,113,113	2.72	30 (36%)
34	LMT	C	526	-	36,36,36	0.50	1 (2%)	47,47,47	1.06	3 (6%)
26	GOL	o	302	-	5,5,5	0.86	0	5,5,5	1.12	1 (20%)
23	CLA	c	514	-	69,73,73	2.03	19 (27%)	82,113,113	2.71	33 (40%)
23	CLA	b	609	-	69,73,73	2.00	21 (30%)	82,113,113	2.59	32 (39%)
23	CLA	C	503	-	69,73,73	1.97	20 (28%)	82,113,113	2.78	31 (37%)
23	CLA	b	602	-	69,73,73	2.05	20 (28%)	82,113,113	2.75	33 (40%)
25	BCR	b	617	-	41,41,41	1.12	1 (2%)	56,56,56	1.53	8 (14%)
27	SQD	b	620	-	52,54,54	0.98	2 (3%)	62,65,65	1.53	9 (14%)
26	GOL	a	411	-	5,5,5	0.91	0	5,5,5	1.12	1 (20%)
26	GOL	c	502	-	5,5,5	1.12	0	5,5,5	0.96	0
25	BCR	B	618	-	41,41,41	0.95	1 (2%)	56,56,56	1.41	6 (10%)
34	LMT	B	628	-	36,36,36	0.42	0	47,47,47	1.10	3 (6%)
26	GOL	B	629	-	5,5,5	1.06	0	5,5,5	0.94	0
33	HTG	b	622	-	19,19,19	1.03	1 (5%)	23,24,24	1.37	3 (13%)
33	HTG	V	202	-	11,11,19	0.21	0	15,15,24	1.22	2 (13%)
23	CLA	A	406	40	69,73,73	2.03	20 (28%)	82,113,113	2.66	29 (35%)
31	LHG	d	407	-	48,48,48	0.89	2 (4%)	51,54,54	1.02	4 (7%)
23	CLA	B	601	40	69,73,73	2.07	21 (30%)	82,113,113	2.69	30 (36%)
34	LMT	b	621	-	25,25,36	0.52	0	30,30,47	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	HTG	B	625	-	19,19,19	0.95	2 (10%)	23,24,24	1.04	1 (4%)
23	CLA	B	606	-	69,73,73	1.99	20 (28%)	82,113,113	2.73	31 (37%)
23	CLA	a	408	-	69,73,73	1.98	20 (28%)	82,113,113	2.69	31 (37%)
29	PL9	a	415	-	55,55,55	0.66	2 (3%)	68,69,69	2.00	21 (30%)
23	CLA	d	403	-	69,73,73	2.08	21 (30%)	82,113,113	2.74	32 (39%)
35	DGD	c	519	-	63,63,67	0.85	2 (3%)	77,77,81	1.01	4 (5%)
32	LMG	d	412	39	51,51,55	0.93	2 (3%)	59,59,63	0.87	2 (3%)
26	GOL	b	628	-	5,5,5	1.00	0	5,5,5	1.15	1 (20%)
38	HEC	v	202	16	46,50,50	1.88	6 (13%)	58,82,82	1.94	6 (10%)
25	BCR	a	409	-	41,41,41	1.09	1 (2%)	56,56,56	1.48	10 (17%)
29	PL9	D	406	-	55,55,55	0.69	2 (3%)	68,69,69	1.66	17 (25%)
35	DGD	C	519	-	63,63,67	0.90	3 (4%)	77,77,81	1.10	4 (5%)
35	DGD	c	520	-	63,63,67	0.89	3 (4%)	77,77,81	1.03	6 (7%)
23	CLA	c	506	40	69,73,73	2.03	20 (28%)	82,113,113	2.73	32 (39%)
26	GOL	b	624	-	5,5,5	1.00	0	5,5,5	1.14	0
23	CLA	b	607	40	69,73,73	2.02	18 (26%)	82,113,113	2.67	31 (37%)
26	GOL	B	624	-	5,5,5	0.91	0	5,5,5	1.10	0
24	PHO	A	415	-	58,69,69	2.71	14 (24%)	55,99,99	2.83	18 (32%)
25	BCR	C	517	-	41,41,41	1.02	1 (2%)	56,56,56	1.57	10 (17%)
25	BCR	h	102	-	41,41,41	1.08	1 (2%)	56,56,56	1.31	7 (12%)
23	CLA	B	610	40	69,73,73	2.03	20 (28%)	82,113,113	2.70	31 (37%)
23	CLA	B	602	-	69,73,73	2.05	20 (28%)	82,113,113	2.74	32 (39%)
27	SQD	C	501	-	52,54,54	0.88	2 (3%)	62,65,65	1.88	11 (17%)
29	PL9	A	413	-	55,55,55	0.68	2 (3%)	68,69,69	1.87	21 (30%)
32	LMG	c	521	-	51,51,55	0.92	2 (3%)	59,59,63	1.02	3 (5%)
23	CLA	C	510	-	69,73,73	2.01	20 (28%)	82,113,113	2.70	30 (36%)
23	CLA	D	403	-	69,73,73	1.97	19 (27%)	82,113,113	2.79	31 (37%)
25	BCR	T	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.59	12 (21%)
23	CLA	c	507	-	69,73,73	2.01	19 (27%)	82,113,113	2.61	30 (36%)
32	LMG	Z	101	-	37,37,55	1.02	3 (8%)	45,45,63	1.54	6 (13%)
23	CLA	A	404	-	69,73,73	2.01	19 (27%)	82,113,113	2.70	33 (40%)
26	GOL	A	410	-	5,5,5	1.17	0	5,5,5	0.88	0
23	CLA	b	601	40	69,73,73	2.10	20 (28%)	82,113,113	2.67	29 (35%)
32	LMG	z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.11	4 (8%)
34	LMT	D	402	-	36,36,36	0.53	1 (2%)	47,47,47	0.86	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LMG	C	522	-	51,51,55	1.01	3 (5%)	59,59,63	1.32	5 (8%)
23	CLA	B	616	-	69,73,73	1.95	20 (28%)	82,113,113	2.67	31 (37%)
31	LHG	D	408	-	48,48,48	0.90	2 (4%)	51,54,54	0.97	3 (5%)
34	LMT	e	101	-	36,36,36	0.53	1 (2%)	47,47,47	1.04	2 (4%)
35	DGD	C	520	-	63,63,67	0.84	2 (3%)	77,77,81	1.04	5 (6%)
23	CLA	D	404	-	69,73,73	2.04	18 (26%)	82,113,113	2.67	30 (36%)
34	LMT	a	418	-	36,36,36	0.45	0	47,47,47	0.94	1 (2%)
25	BCR	Y	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.85	16 (28%)
26	GOL	C	524	-	5,5,5	1.13	0	5,5,5	1.01	0
23	CLA	C	509	40	69,73,73	1.99	19 (27%)	82,113,113	2.63	28 (34%)
32	LMG	C	521	-	51,51,55	0.99	2 (3%)	59,59,63	1.04	3 (5%)
35	DGD	H	102	-	63,63,67	0.83	3 (4%)	77,77,81	1.05	7 (9%)
25	BCR	D	405	-	41,41,41	1.07	1 (2%)	56,56,56	1.66	13 (23%)
35	DGD	c	518	-	63,63,67	0.90	2 (3%)	77,77,81	1.05	6 (7%)
23	CLA	B	604	-	69,73,73	2.00	21 (30%)	82,113,113	2.61	31 (37%)
23	CLA	c	504	-	69,73,73	2.00	19 (27%)	82,113,113	2.61	29 (35%)
31	LHG	b	629	-	48,48,48	0.90	2 (4%)	51,54,54	1.05	3 (5%)
23	CLA	C	513	3	69,73,73	2.03	22 (31%)	82,113,113	2.65	30 (36%)
32	LMG	D	413	39	51,51,55	0.84	3 (5%)	59,59,63	0.96	3 (5%)
35	DGD	C	518	-	63,63,67	0.88	2 (3%)	77,77,81	1.00	3 (3%)
28	OEX	A	412	1,3,40	0,15,15	-	-	-	-	-
24	PHO	a	407	-	58,69,69	2.65	14 (24%)	55,99,99	2.97	16 (29%)
23	CLA	C	504	-	69,73,73	1.98	20 (28%)	82,113,113	2.62	30 (36%)
25	BCR	c	517	-	41,41,41	1.08	1 (2%)	56,56,56	1.44	13 (23%)
33	HTG	c	523	-	19,19,19	0.88	1 (5%)	23,24,24	1.30	1 (4%)
38	HEC	e	102	5,6	46,50,50	1.75	11 (23%)	58,82,82	1.69	13 (22%)
25	BCR	H	101	-	41,41,41	1.09	1 (2%)	56,56,56	1.36	7 (12%)
23	CLA	B	615	-	69,73,73	1.93	17 (24%)	82,113,113	2.71	31 (37%)
23	CLA	b	606	-	69,73,73	1.94	21 (30%)	82,113,113	2.83	32 (39%)
25	BCR	c	516	-	41,41,41	1.05	1 (2%)	56,56,56	1.44	8 (14%)
23	CLA	a	404	-	69,73,73	1.97	20 (28%)	82,113,113	2.73	32 (39%)
31	LHG	a	419	-	41,41,48	1.05	2 (4%)	44,47,54	0.98	2 (4%)
26	GOL	O	302	-	5,5,5	0.90	0	5,5,5	1.08	0
23	CLA	c	515	-	69,73,73	2.04	20 (28%)	82,113,113	2.67	32 (39%)
26	GOL	B	627	-	5,5,5	1.05	0	5,5,5	1.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	BCT	d	401	21	3,3,3	0.50	0	2,3,3	1.70	1 (50%)
33	HTG	B	622	-	19,19,19	0.93	1 (5%)	23,24,24	1.53	4 (17%)
34	LMT	t	101	-	26,26,36	0.56	1 (3%)	31,31,47	1.16	4 (12%)
23	CLA	B	614	-	69,73,73	1.96	19 (27%)	82,113,113	2.88	31 (37%)
23	CLA	c	503	-	69,73,73	2.01	19 (27%)	82,113,113	2.67	30 (36%)
34	LMT	b	627	-	25,25,36	0.46	0	30,30,47	0.90	1 (3%)
31	LHG	L	101	-	48,48,48	0.92	3 (6%)	51,54,54	1.12	4 (7%)
27	SQD	f	101	-	41,43,54	1.10	2 (4%)	51,54,65	1.27	8 (15%)
33	HTG	D	411	-	16,16,19	0.98	2 (12%)	20,21,24	1.15	1 (5%)
33	HTG	b	623	-	19,19,19	0.91	1 (5%)	23,24,24	1.41	2 (8%)
23	CLA	b	613	-	69,73,73	1.99	18 (26%)	82,113,113	2.69	31 (37%)
31	LHG	d	406	-	48,48,48	0.89	2 (4%)	51,54,54	1.14	5 (9%)
33	HTG	b	625	-	19,19,19	0.91	2 (10%)	23,24,24	1.23	3 (13%)
29	PL9	d	405	-	55,55,55	0.65	1 (1%)	68,69,69	1.61	13 (19%)
34	LMT	a	413	-	36,36,36	0.60	1 (2%)	47,47,47	1.16	4 (8%)
26	GOL	v	201	-	5,5,5	1.21	0	5,5,5	0.89	0
23	CLA	B	608	-	69,73,73	1.97	20 (28%)	82,113,113	2.68	32 (39%)
23	CLA	B	607	40	69,73,73	2.01	19 (27%)	82,113,113	2.64	32 (39%)
23	CLA	b	608	-	69,73,73	2.03	20 (28%)	82,113,113	2.67	32 (39%)
25	BCR	b	618	-	41,41,41	1.04	1 (2%)	56,56,56	1.30	8 (14%)
25	BCR	B	619	-	41,41,41	1.04	1 (2%)	56,56,56	1.31	8 (14%)
23	CLA	c	512	-	69,73,73	1.96	20 (28%)	82,113,113	2.61	31 (37%)
23	CLA	C	507	-	69,73,73	1.97	20 (28%)	82,113,113	2.62	29 (35%)
25	BCR	K	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.42	9 (16%)
38	HEC	V	201	16	46,50,50	1.92	7 (15%)	58,82,82	1.76	8 (13%)
23	CLA	b	615	-	69,73,73	1.98	18 (26%)	82,113,113	2.65	32 (39%)
25	BCR	d	404	-	41,41,41	1.15	1 (2%)	56,56,56	1.75	11 (19%)
32	LMG	c	501	-	51,51,55	0.93	2 (3%)	59,59,63	1.09	3 (5%)
23	CLA	C	512	-	69,73,73	2.03	20 (28%)	82,113,113	2.69	31 (37%)
27	SQD	a	412	-	52,54,54	0.98	2 (3%)	62,65,65	1.25	5 (8%)
23	CLA	b	603	-	69,73,73	2.03	20 (28%)	82,113,113	2.78	31 (37%)
37	BCT	D	401	21	3,3,3	0.44	0	2,3,3	1.20	0
31	LHG	A	416	-	48,48,48	0.89	2 (4%)	51,54,54	1.14	6 (11%)
25	BCR	y	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.63	10 (17%)
25	BCR	k	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.46	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LHG	D	407	-	48,48,48	0.89	3 (6%)	51,54,54	1.01	3 (5%)
23	CLA	b	610	40	69,73,73	2.02	20 (28%)	82,113,113	2.74	32 (39%)
23	CLA	b	612	-	69,73,73	1.98	19 (27%)	82,113,113	2.75	29 (35%)
23	CLA	b	604	-	69,73,73	2.00	19 (27%)	82,113,113	2.62	31 (37%)
23	CLA	a	406	40	69,73,73	1.92	18 (26%)	82,113,113	2.71	31 (37%)
23	CLA	C	514	-	69,73,73	2.02	20 (28%)	82,113,113	2.65	31 (37%)
23	CLA	c	511	-	69,73,73	2.07	20 (28%)	82,113,113	2.67	30 (36%)
34	LMT	M	101	-	36,36,36	0.45	0	47,47,47	0.99	3 (6%)
32	LMG	m	101	-	51,51,55	0.90	2 (3%)	59,59,63	1.12	5 (8%)
25	BCR	t	102	-	41,41,41	1.07	1 (2%)	56,56,56	1.44	9 (16%)
34	LMT	B	630	-	25,25,36	0.44	0	30,30,47	1.02	2 (6%)
23	CLA	b	614	-	69,73,73	1.97	20 (28%)	82,113,113	2.76	32 (39%)
27	SQD	B	620	-	52,54,54	0.98	2 (3%)	62,65,65	1.42	8 (12%)
38	HEC	E	103	5,6	46,50,50	1.75	10 (21%)	58,82,82	1.73	15 (25%)
23	CLA	B	609	-	69,73,73	1.97	18 (26%)	82,113,113	2.73	30 (36%)
23	CLA	b	611	-	69,73,73	1.95	20 (28%)	82,113,113	2.71	30 (36%)
23	CLA	C	511	-	69,73,73	2.08	19 (27%)	82,113,113	2.65	31 (37%)
27	SQD	A	411	-	52,54,54	0.99	2 (3%)	62,65,65	1.23	7 (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
33	HTG	B	623	-	-	4/10/30/30	0/1/1/1
23	CLA	b	605	-	1/1/15/20	6/39/115/115	-
24	PHO	A	407	-	-	0/37/103/103	0/5/6/6
23	CLA	a	405	40	1/1/15/20	9/39/115/115	-
33	HTG	h	101	-	-	1/7/27/30	0/1/1/1
23	CLA	b	616	-	1/1/15/20	6/39/115/115	-
25	BCR	B	617	-	-	0/29/63/63	0/2/2/2
32	LMG	C	502	-	-	25/46/66/70	0/1/1/1
23	CLA	c	505	-	1/1/15/20	1/39/115/115	-
34	LMT	M	103	-	-	9/21/61/61	0/2/2/2
23	CLA	A	405	40	1/1/15/20	3/39/115/115	-
25	BCR	b	619	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	611	-	1/1/15/20	3/39/115/115	-
23	CLA	c	508	-	1/1/15/20	11/39/115/115	-
27	SQD	D	412	-	-	15/38/58/69	0/1/1/1
23	CLA	C	506	40	1/1/15/20	7/39/115/115	-
35	DGD	h	103	-	-	14/51/91/95	0/2/2/2
23	CLA	c	509	40	1/1/15/20	7/39/115/115	-
24	PHO	a	417	-	-	2/37/103/103	0/5/6/6
31	LHG	d	408	-	-	10/53/53/53	-
23	CLA	B	612	-	1/1/15/20	2/39/115/115	-
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
34	LMT	m	103	-	-	7/21/61/61	0/2/2/2
31	LHG	E	101	-	-	14/46/46/53	-
32	LMG	c	522	-	-	9/46/66/70	0/1/1/1
33	HTG	C	523	-	-	1/10/30/30	0/1/1/1
25	BCR	C	516	-	-	2/29/63/63	0/2/2/2
32	LMG	B	621	-	-	11/46/66/70	0/1/1/1
23	CLA	C	508	-	1/1/15/20	10/39/115/115	-
23	CLA	B	613	-	1/1/15/20	8/39/115/115	-
23	CLA	B	603	-	1/1/15/20	6/39/115/115	-
23	CLA	c	513	3	1/1/15/20	8/39/115/115	-
23	CLA	d	402	-	1/1/15/20	3/39/115/115	-
34	LMT	E	102	-	-	7/21/61/61	0/2/2/2
23	CLA	C	515	-	-	14/39/115/115	-
27	SQD	a	410	-	-	14/49/69/69	0/1/1/1
23	CLA	B	605	-	1/1/15/20	3/39/115/115	-
23	CLA	A	408	-	1/1/15/20	9/39/115/115	-
23	CLA	C	505	-	1/1/15/20	4/39/115/115	-
23	CLA	c	510	-	1/1/15/20	8/39/115/115	-
34	LMT	C	526	-	-	8/21/61/61	0/2/2/2
26	GOL	o	302	-	-	2/4/4/4	-
23	CLA	c	514	-	1/1/15/20	14/39/115/115	-
23	CLA	b	609	-	1/1/15/20	7/39/115/115	-
23	CLA	C	503	-	1/1/15/20	4/39/115/115	-
23	CLA	b	602	-	1/1/15/20	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
27	SQD	b	620	-	-	26/49/69/69	0/1/1/1
26	GOL	a	411	-	-	4/4/4/4	-
26	GOL	c	502	-	-	0/4/4/4	-
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
34	LMT	B	628	-	-	9/21/61/61	0/2/2/2
26	GOL	B	629	-	-	0/4/4/4	-
33	HTG	b	622	-	-	2/10/30/30	0/1/1/1
33	HTG	V	202	-	-	1/2/19/30	0/1/1/1
23	CLA	A	406	40	-	6/39/115/115	-
31	LHG	d	407	-	-	19/53/53/53	-
23	CLA	B	601	40	1/1/15/20	9/39/115/115	-
34	LMT	b	621	-	-	7/17/37/61	0/1/1/2
33	HTG	B	625	-	-	3/10/30/30	0/1/1/1
23	CLA	B	606	-	1/1/15/20	9/39/115/115	-
23	CLA	a	408	-	1/1/15/20	16/39/115/115	-
29	PL9	a	415	-	-	13/53/73/73	0/1/1/1
23	CLA	d	403	-	1/1/15/20	7/39/115/115	-
35	DGD	c	519	-	-	17/51/91/95	0/2/2/2
32	LMG	d	412	39	-	8/46/66/70	0/1/1/1
26	GOL	b	628	-	-	0/4/4/4	-
38	HEC	v	202	16	-	6/14/54/54	-
25	BCR	a	409	-	-	1/29/63/63	0/2/2/2
29	PL9	D	406	-	-	8/53/73/73	0/1/1/1
35	DGD	C	519	-	-	16/51/91/95	0/2/2/2
35	DGD	c	520	-	-	10/51/91/95	0/2/2/2
23	CLA	c	506	40	1/1/15/20	5/39/115/115	-
26	GOL	b	624	-	-	3/4/4/4	-
23	CLA	b	607	40	1/1/15/20	0/39/115/115	-
26	GOL	B	624	-	-	2/4/4/4	-
24	PHO	A	415	-	-	2/37/103/103	0/5/6/6
25	BCR	C	517	-	-	0/29/63/63	0/2/2/2
25	BCR	h	102	-	-	0/29/63/63	0/2/2/2
23	CLA	B	610	40	1/1/15/20	5/39/115/115	-
23	CLA	B	602	-	1/1/15/20	5/39/115/115	-
27	SQD	C	501	-	-	12/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PL9	A	413	-	-	15/53/73/73	0/1/1/1
32	LMG	c	521	-	-	6/46/66/70	0/1/1/1
23	CLA	C	510	-	1/1/15/20	3/39/115/115	-
23	CLA	D	403	-	1/1/15/20	6/39/115/115	-
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
23	CLA	c	507	-	1/1/15/20	4/39/115/115	-
32	LMG	Z	101	-	-	9/31/51/70	0/1/1/1
23	CLA	A	404	-	1/1/15/20	3/39/115/115	-
26	GOL	A	410	-	-	2/4/4/4	-
23	CLA	b	601	40	1/1/15/20	16/39/115/115	-
32	LMG	z	101	-	-	8/34/54/70	0/1/1/1
34	LMT	D	402	-	-	8/21/61/61	0/2/2/2
32	LMG	C	522	-	-	12/46/66/70	0/1/1/1
23	CLA	B	616	-	1/1/15/20	10/39/115/115	-
31	LHG	D	408	-	-	13/53/53/53	-
34	LMT	e	101	-	-	8/21/61/61	0/2/2/2
35	DGD	C	520	-	-	10/51/91/95	0/2/2/2
23	CLA	D	404	-	1/1/15/20	9/39/115/115	-
34	LMT	a	418	-	-	4/21/61/61	0/2/2/2
25	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
26	GOL	C	524	-	-	0/4/4/4	-
23	CLA	C	509	40	1/1/15/20	7/39/115/115	-
32	LMG	C	521	-	-	10/46/66/70	0/1/1/1
35	DGD	H	102	-	-	13/51/91/95	0/2/2/2
25	BCR	D	405	-	-	6/29/63/63	0/2/2/2
35	DGD	c	518	-	-	19/51/91/95	0/2/2/2
23	CLA	B	604	-	1/1/15/20	9/39/115/115	-
23	CLA	c	504	-	1/1/15/20	7/39/115/115	-
31	LHG	b	629	-	-	14/53/53/53	-
23	CLA	C	513	3	1/1/15/20	2/39/115/115	-
32	LMG	D	413	39	-	8/46/66/70	0/1/1/1
35	DGD	C	518	-	-	15/51/91/95	0/2/2/2
24	PHO	a	407	-	-	3/37/103/103	0/5/6/6
23	CLA	C	504	-	-	9/39/115/115	-
25	BCR	c	517	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	HTG	c	523	-	-	3/10/30/30	0/1/1/1
38	HEC	e	102	5,6	-	7/14/54/54	-
25	BCR	H	101	-	-	1/29/63/63	0/2/2/2
23	CLA	B	615	-	1/1/15/20	9/39/115/115	-
23	CLA	b	606	-	1/1/15/20	11/39/115/115	-
25	BCR	c	516	-	-	0/29/63/63	0/2/2/2
23	CLA	a	404	-	1/1/15/20	6/39/115/115	-
31	LHG	a	419	-	-	18/46/46/53	-
26	GOL	O	302	-	-	4/4/4/4	-
23	CLA	c	515	-	1/1/15/20	9/39/115/115	-
26	GOL	B	627	-	-	0/4/4/4	-
33	HTG	B	622	-	-	4/10/30/30	0/1/1/1
34	LMT	t	101	-	-	6/17/38/61	0/1/1/2
23	CLA	B	614	-	1/1/15/20	12/39/115/115	-
23	CLA	c	503	-	1/1/15/20	4/39/115/115	-
34	LMT	b	627	-	-	9/17/37/61	0/1/1/2
31	LHG	L	101	-	-	13/53/53/53	-
27	SQD	f	101	-	-	19/38/58/69	0/1/1/1
33	HTG	D	411	-	-	2/7/27/30	0/1/1/1
33	HTG	b	623	-	-	2/10/30/30	0/1/1/1
23	CLA	b	613	-	1/1/15/20	5/39/115/115	-
31	LHG	d	406	-	-	14/53/53/53	-
33	HTG	b	625	-	-	4/10/30/30	0/1/1/1
29	PL9	d	405	-	-	6/53/73/73	0/1/1/1
34	LMT	a	413	-	-	7/21/61/61	0/2/2/2
26	GOL	v	201	-	-	2/4/4/4	-
23	CLA	B	608	-	-	1/39/115/115	-
23	CLA	B	607	40	1/1/15/20	3/39/115/115	-
23	CLA	b	608	-	-	2/39/115/115	-
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
23	CLA	c	512	-	1/1/15/20	6/39/115/115	-
23	CLA	C	507	-	1/1/15/20	8/39/115/115	-
25	BCR	K	101	-	-	0/29/63/63	0/2/2/2
38	HEC	V	201	16	-	6/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	615	-	1/1/15/20	8/39/115/115	-
25	BCR	d	404	-	-	4/29/63/63	0/2/2/2
32	LMG	c	501	-	-	18/46/66/70	0/1/1/1
23	CLA	C	512	-	1/1/15/20	10/39/115/115	-
27	SQD	a	412	-	-	17/49/69/69	0/1/1/1
23	CLA	b	603	-	1/1/15/20	3/39/115/115	-
31	LHG	A	416	-	-	16/53/53/53	-
25	BCR	y	101	-	-	5/29/63/63	0/2/2/2
25	BCR	k	101	-	-	2/29/63/63	0/2/2/2
31	LHG	D	407	-	-	11/53/53/53	-
23	CLA	b	610	40	1/1/15/20	8/39/115/115	-
23	CLA	b	612	-	1/1/15/20	4/39/115/115	-
23	CLA	b	604	-	1/1/15/20	10/39/115/115	-
23	CLA	a	406	40	-	8/39/115/115	-
23	CLA	C	514	-	1/1/15/20	11/39/115/115	-
23	CLA	c	511	-	1/1/15/20	15/39/115/115	-
34	LMT	M	101	-	-	6/21/61/61	0/2/2/2
32	LMG	m	101	-	-	11/46/66/70	0/1/1/1
25	BCR	t	102	-	-	4/29/63/63	0/2/2/2
34	LMT	B	630	-	-	5/17/37/61	0/1/1/2
23	CLA	b	614	-	1/1/15/20	10/39/115/115	-
27	SQD	B	620	-	-	17/49/69/69	0/1/1/1
38	HEC	E	103	5,6	-	8/14/54/54	-
23	CLA	B	609	-	1/1/15/20	4/39/115/115	-
23	CLA	b	611	-	1/1/15/20	4/39/115/115	-
23	CLA	C	511	-	1/1/15/20	5/39/115/115	-
27	SQD	A	411	-	-	11/49/69/69	0/1/1/1

The worst 5 of 1587 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	417	PHO	C1B-C2B	9.19	1.49	1.39
24	A	407	PHO	C1D-C2D	9.02	1.49	1.39
24	a	417	PHO	C1D-C2D	8.87	1.49	1.39
24	a	407	PHO	C1B-C2B	8.80	1.49	1.39
24	A	415	PHO	C1D-C2D	8.39	1.48	1.39

The worst 5 of 2810 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	407	PHO	C2D-C1D-ND	11.72	117.90	109.43
24	a	417	PHO	C2D-C1D-ND	11.38	117.66	109.43
24	A	415	PHO	C2D-C1D-ND	10.59	117.08	109.43
24	A	407	PHO	C2D-C1D-ND	10.53	117.04	109.43
23	c	513	CLA	C1D-ND-C4D	-10.46	98.97	106.31

5 of 64 chirality outliers are listed below:

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

5 of 1261 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	C	504	CLA	C2B-C3B-CAB-CBB
23	C	504	CLA	C4B-C3B-CAB-CBB
23	C	504	CLA	C14-C13-C15-C16

There are no ring outliers.

138 monomers are involved in 270 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	B	623	HTG	2	0
23	b	605	CLA	6	0
24	A	407	PHO	2	0
23	a	405	CLA	5	0
33	h	101	HTG	1	0
23	b	616	CLA	5	0
25	B	617	BCR	2	0
32	C	502	LMG	3	0
23	c	505	CLA	5	0
23	A	405	CLA	2	0
25	b	619	BCR	5	0
23	c	508	CLA	1	0
23	C	506	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	c	509	CLA	3	0
24	a	417	PHO	3	0
31	d	408	LHG	5	0
23	B	612	CLA	1	0
25	A	409	BCR	2	0
31	E	101	LHG	2	0
32	B	621	LMG	3	0
23	C	508	CLA	6	0
23	B	613	CLA	3	0
23	B	603	CLA	1	0
23	d	402	CLA	1	0
23	c	513	CLA	3	0
34	E	102	LMT	1	0
23	C	515	CLA	1	0
27	a	410	SQD	2	0
23	B	605	CLA	4	0
23	A	408	CLA	4	0
23	C	505	CLA	4	0
23	c	510	CLA	2	0
34	C	526	LMT	2	0
23	c	514	CLA	4	0
23	b	609	CLA	2	0
23	C	503	CLA	5	0
25	b	617	BCR	1	0
27	b	620	SQD	1	0
26	c	502	GOL	1	0
25	B	618	BCR	4	0
33	b	622	HTG	2	0
23	A	406	CLA	2	0
31	d	407	LHG	2	0
23	B	601	CLA	1	0
34	b	621	LMT	1	0
23	B	606	CLA	2	0
23	a	408	CLA	2	0
29	a	415	PL9	6	0
35	c	519	DGD	1	0
32	d	412	LMG	2	0
26	b	628	GOL	1	0
25	a	409	BCR	2	0
29	D	406	PL9	2	0
35	C	519	DGD	2	0
35	c	520	DGD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	c	506	CLA	2	0
24	A	415	PHO	1	0
25	C	517	BCR	1	0
25	h	102	BCR	3	0
23	B	610	CLA	2	0
23	B	602	CLA	3	0
27	C	501	SQD	3	0
29	A	413	PL9	5	0
32	c	521	LMG	1	0
23	C	510	CLA	3	0
23	D	403	CLA	2	0
25	T	101	BCR	4	0
23	c	507	CLA	6	0
23	A	404	CLA	3	0
23	b	601	CLA	1	0
32	z	101	LMG	2	0
34	D	402	LMT	2	0
23	B	616	CLA	5	0
31	D	408	LHG	5	0
35	C	520	DGD	3	0
34	a	418	LMT	2	0
25	Y	101	BCR	1	0
23	C	509	CLA	3	0
32	C	521	LMG	1	0
35	H	102	DGD	1	0
35	c	518	DGD	1	0
23	B	604	CLA	4	0
23	C	513	CLA	2	0
32	D	413	LMG	1	0
35	C	518	DGD	4	0
24	a	407	PHO	2	0
23	C	504	CLA	5	0
25	c	517	BCR	1	0
33	c	523	HTG	1	0
38	e	102	HEC	2	0
25	H	101	BCR	3	0
23	B	615	CLA	5	0
23	b	606	CLA	7	0
25	c	516	BCR	4	0
23	a	404	CLA	1	0
31	a	419	LHG	5	0
23	c	515	CLA	4	0

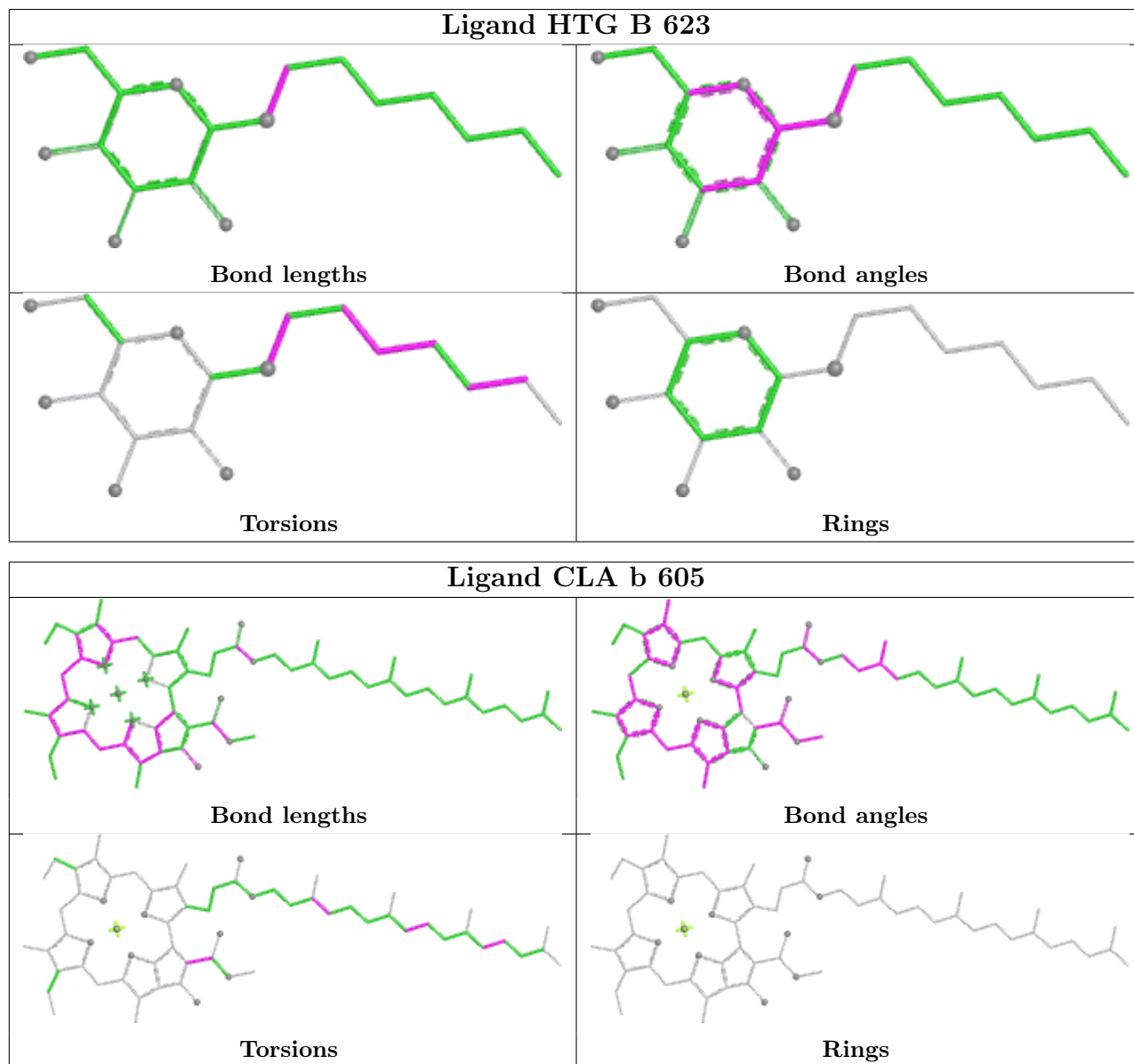
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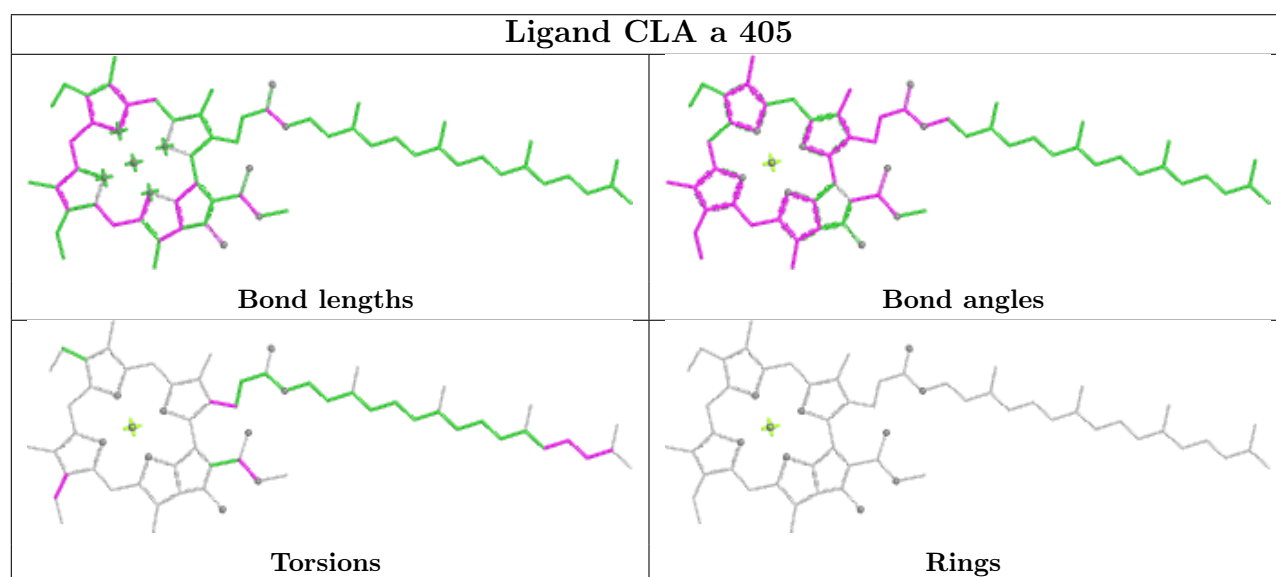
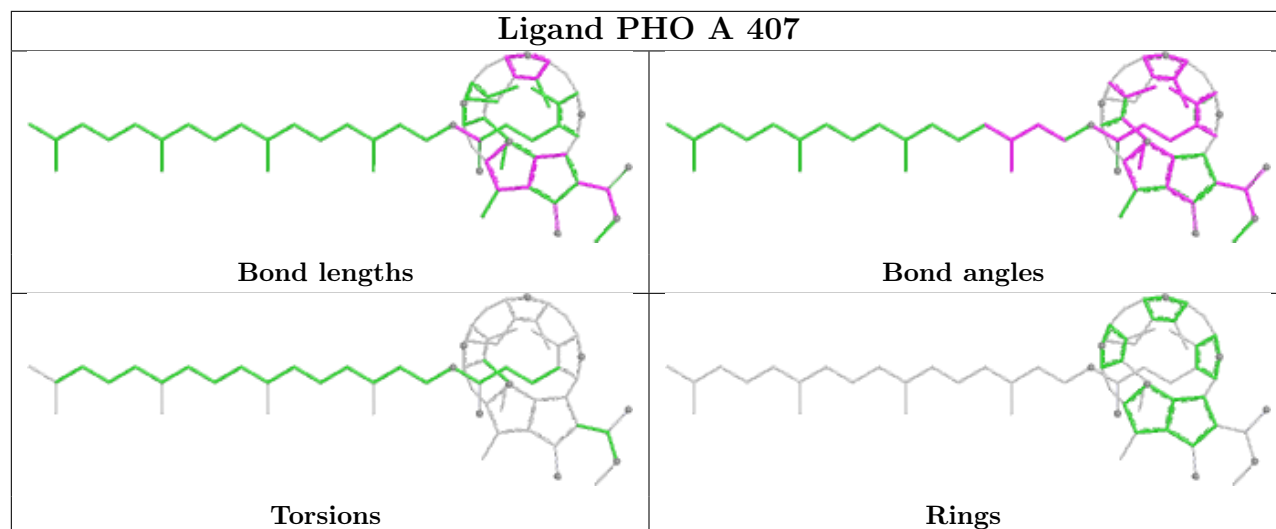
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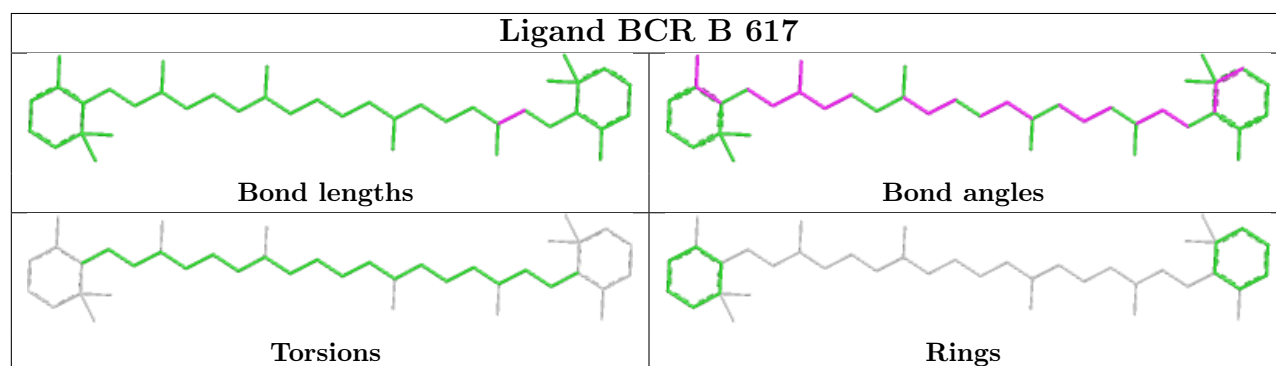
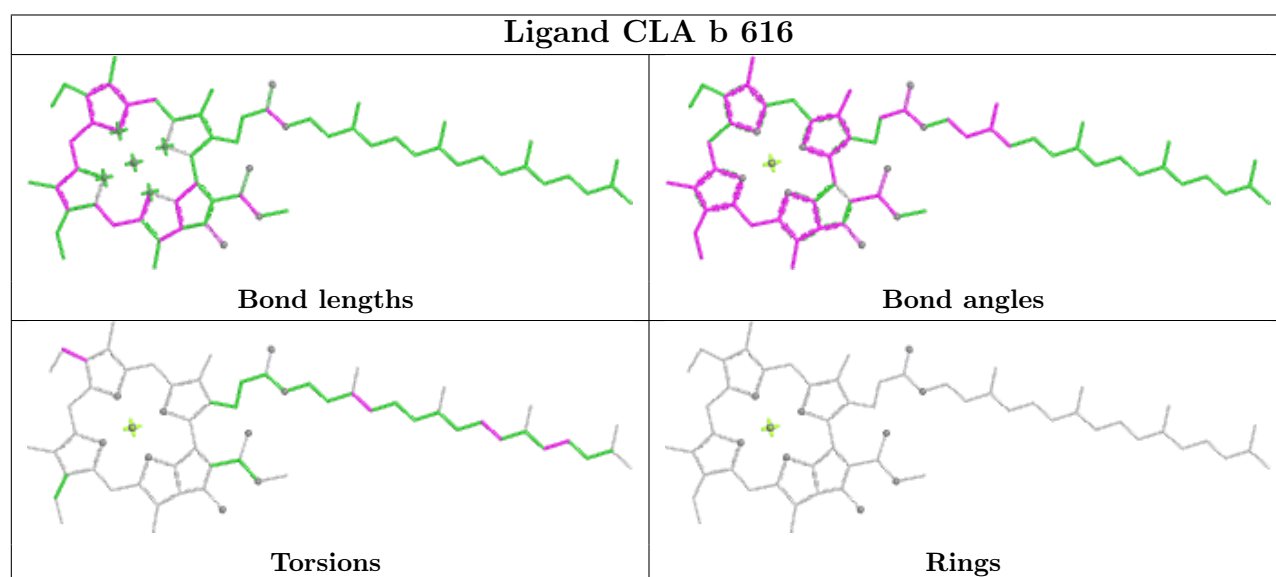
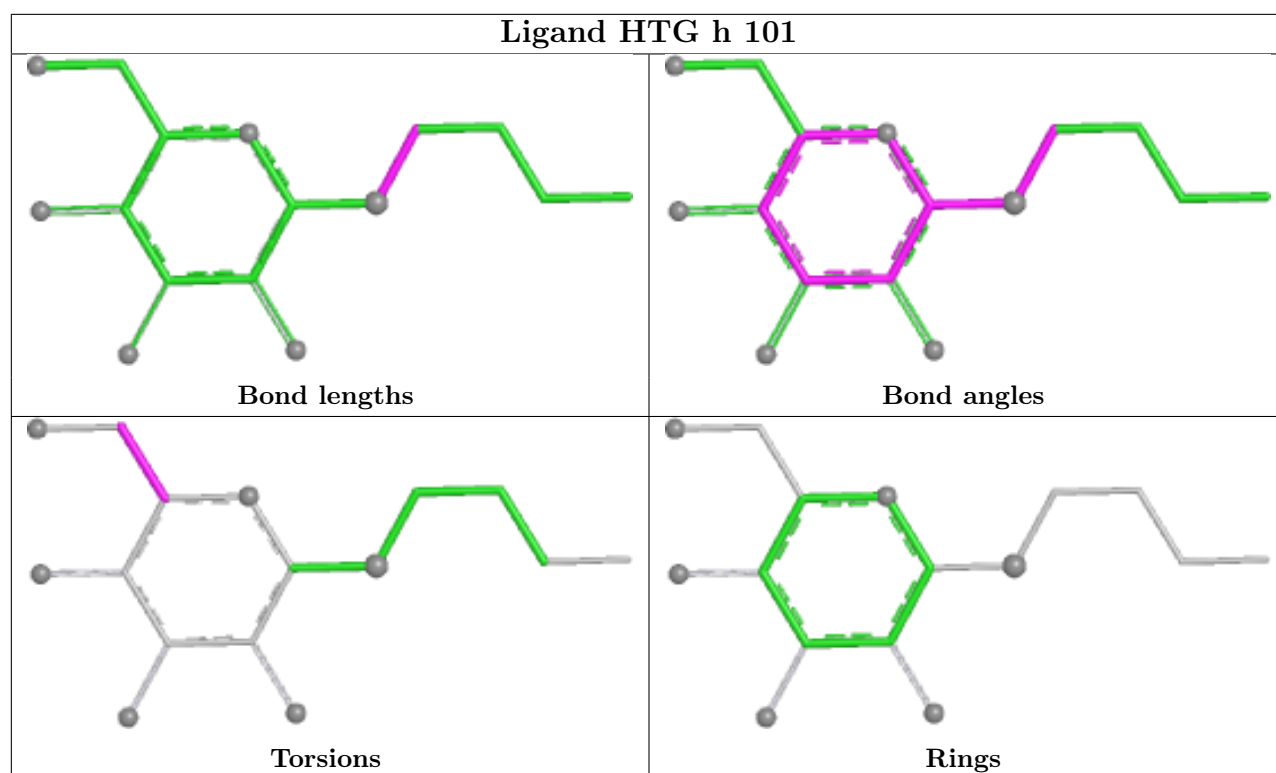
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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23	B	614	CLA	3	0
23	c	503	CLA	3	0
31	L	101	LHG	2	0
27	f	101	SQD	2	0
33	D	411	HTG	1	0
23	b	613	CLA	3	0
31	d	406	LHG	3	0
33	b	625	HTG	1	0
29	d	405	PL9	1	0
34	a	413	LMT	1	0
26	v	201	GOL	1	0
23	B	607	CLA	2	0
23	b	608	CLA	3	0
25	b	618	BCR	3	0
25	B	619	BCR	1	0
23	c	512	CLA	1	0
23	C	507	CLA	2	0
25	K	101	BCR	1	0
38	V	201	HEC	1	0
23	b	615	CLA	2	0
25	d	404	BCR	1	0
32	c	501	LMG	4	0
23	C	512	CLA	2	0
23	b	603	CLA	3	0
31	A	416	LHG	2	0
25	y	101	BCR	2	0
25	k	101	BCR	1	0
31	D	407	LHG	1	0
23	b	610	CLA	1	0
23	b	604	CLA	2	0
23	a	406	CLA	1	0
23	C	514	CLA	1	0
23	c	511	CLA	3	0
34	M	101	LMT	3	0
32	m	101	LMG	2	0
25	t	102	BCR	5	0
23	b	614	CLA	1	0
38	E	103	HEC	1	0
23	B	609	CLA	1	0
27	A	411	SQD	1	0

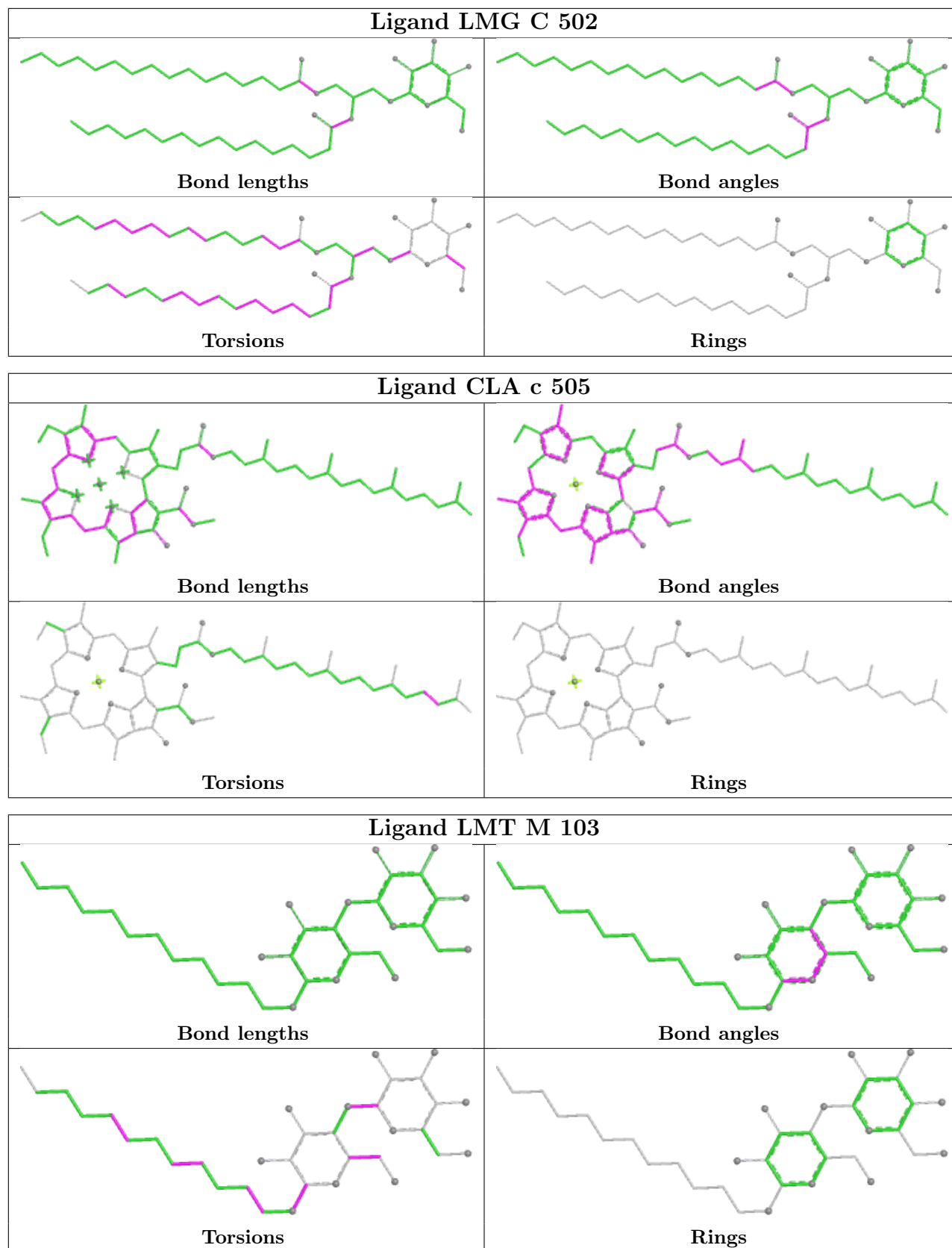
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

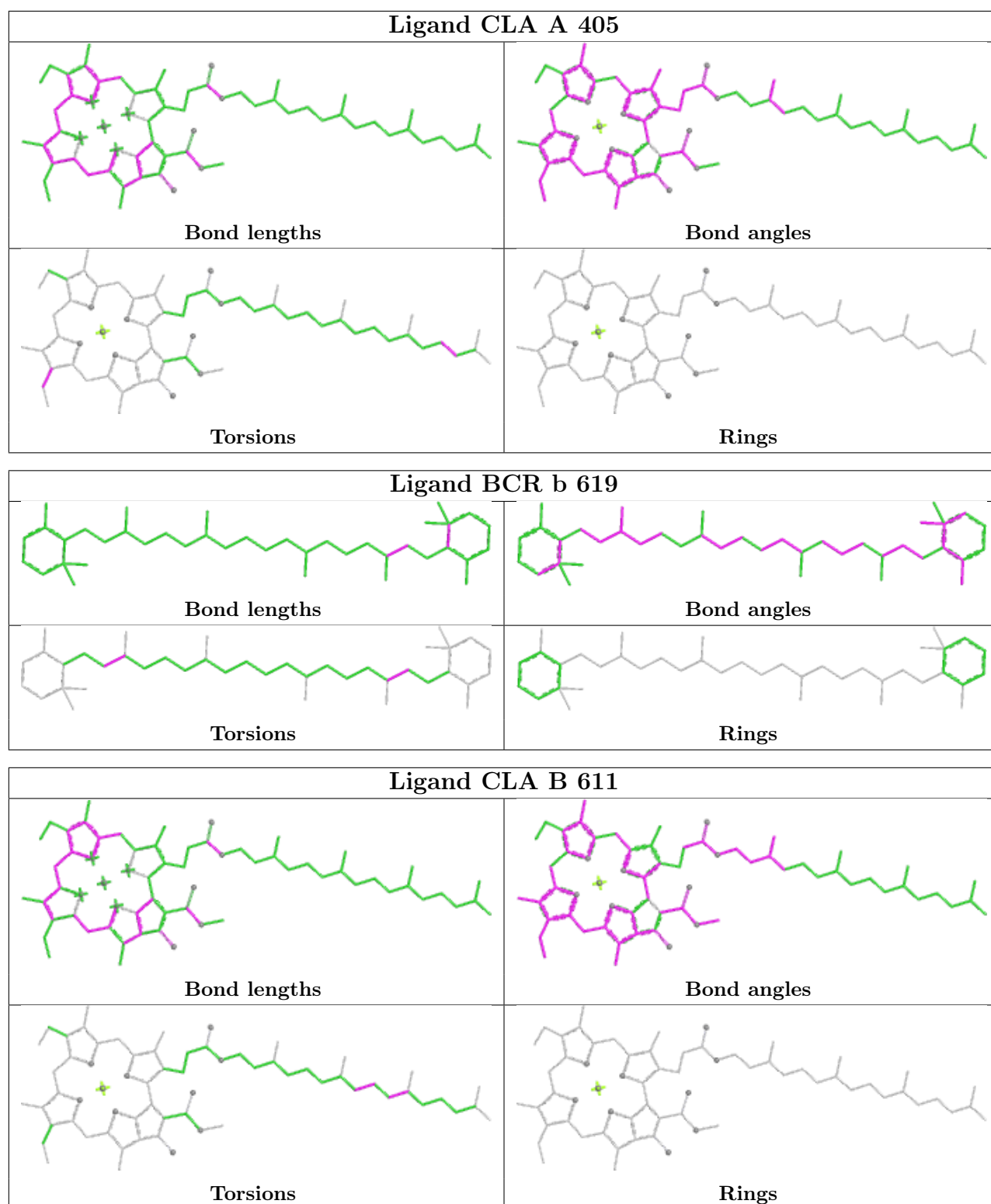
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

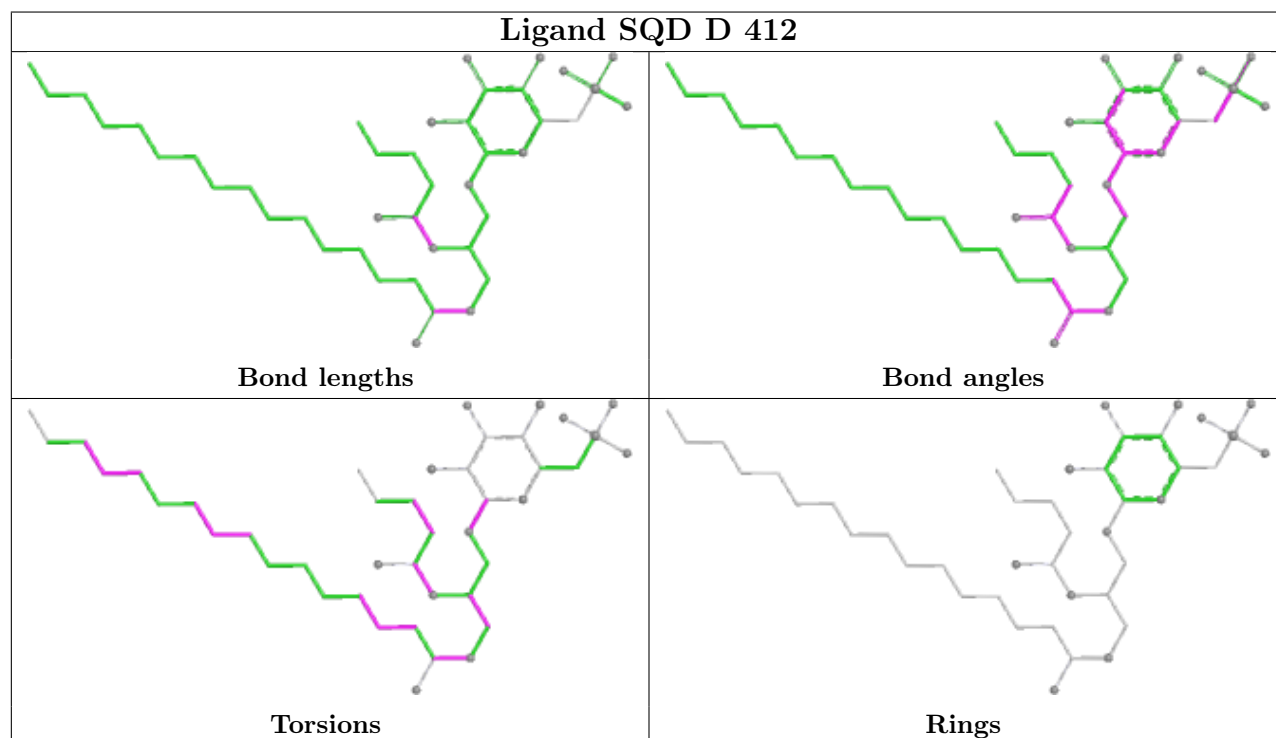
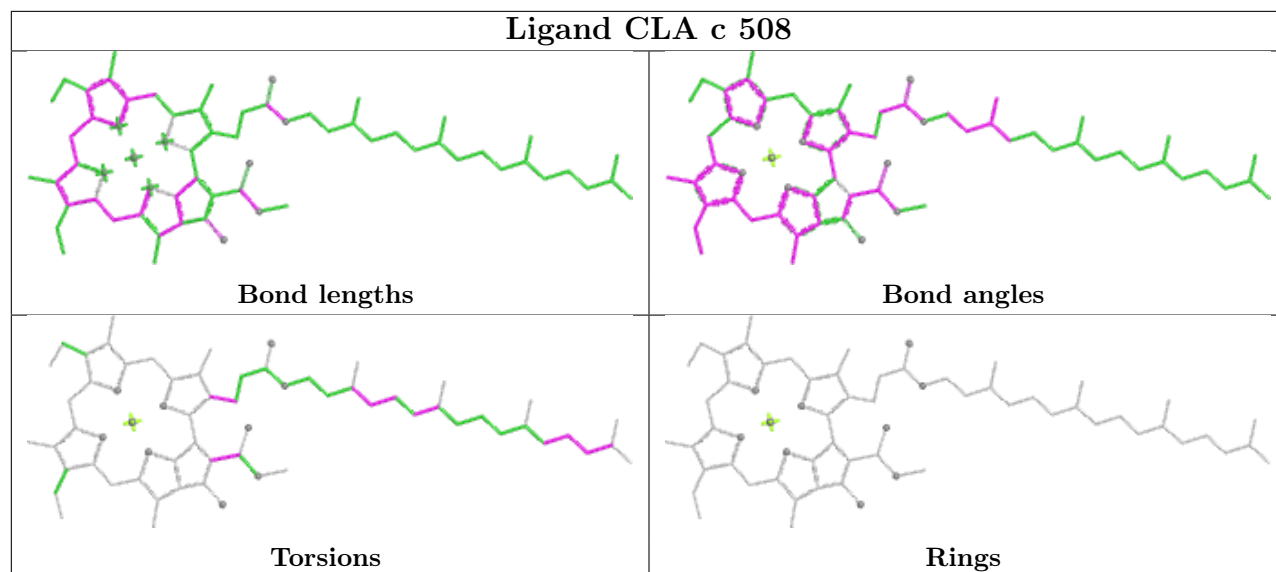


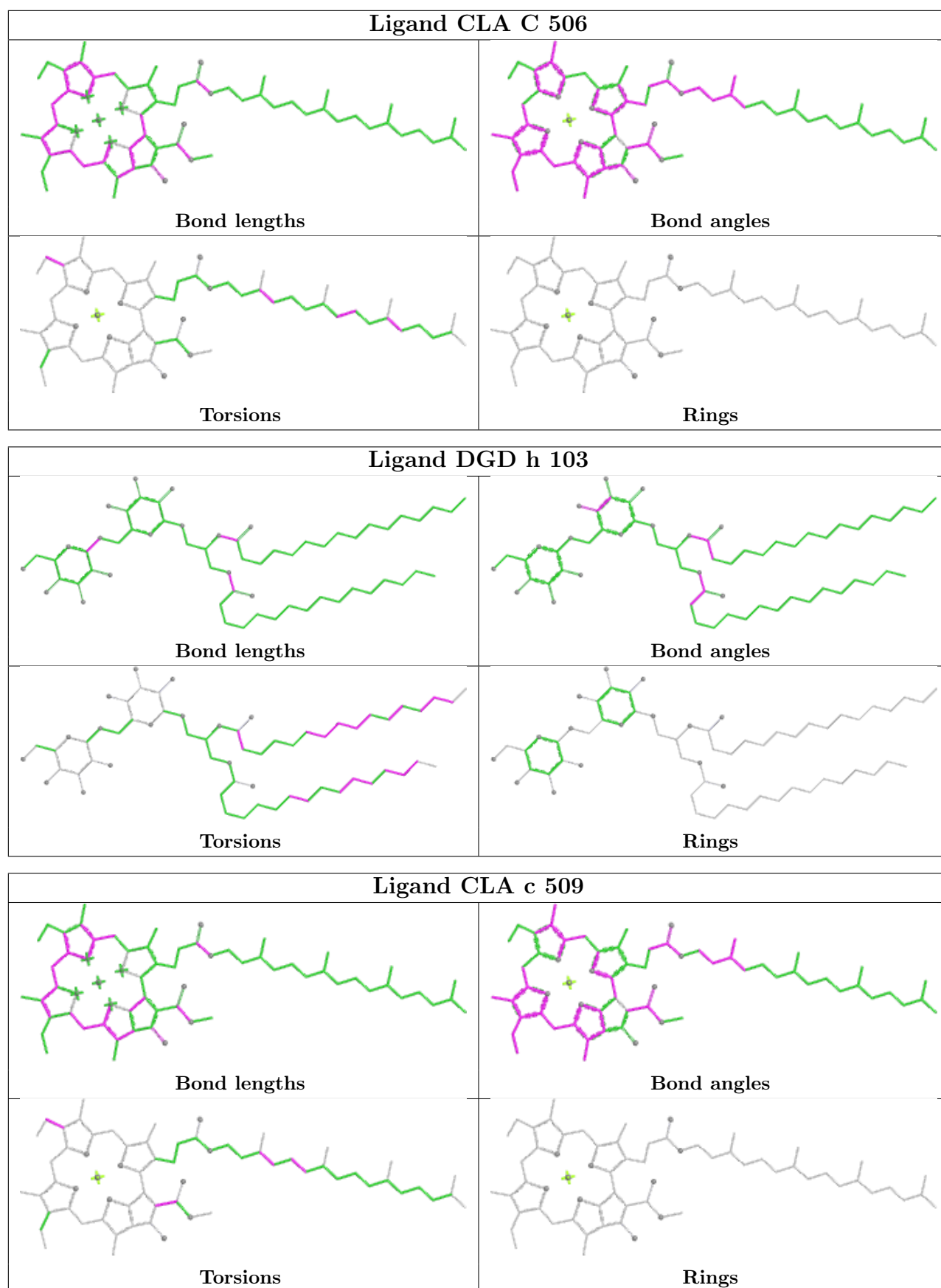


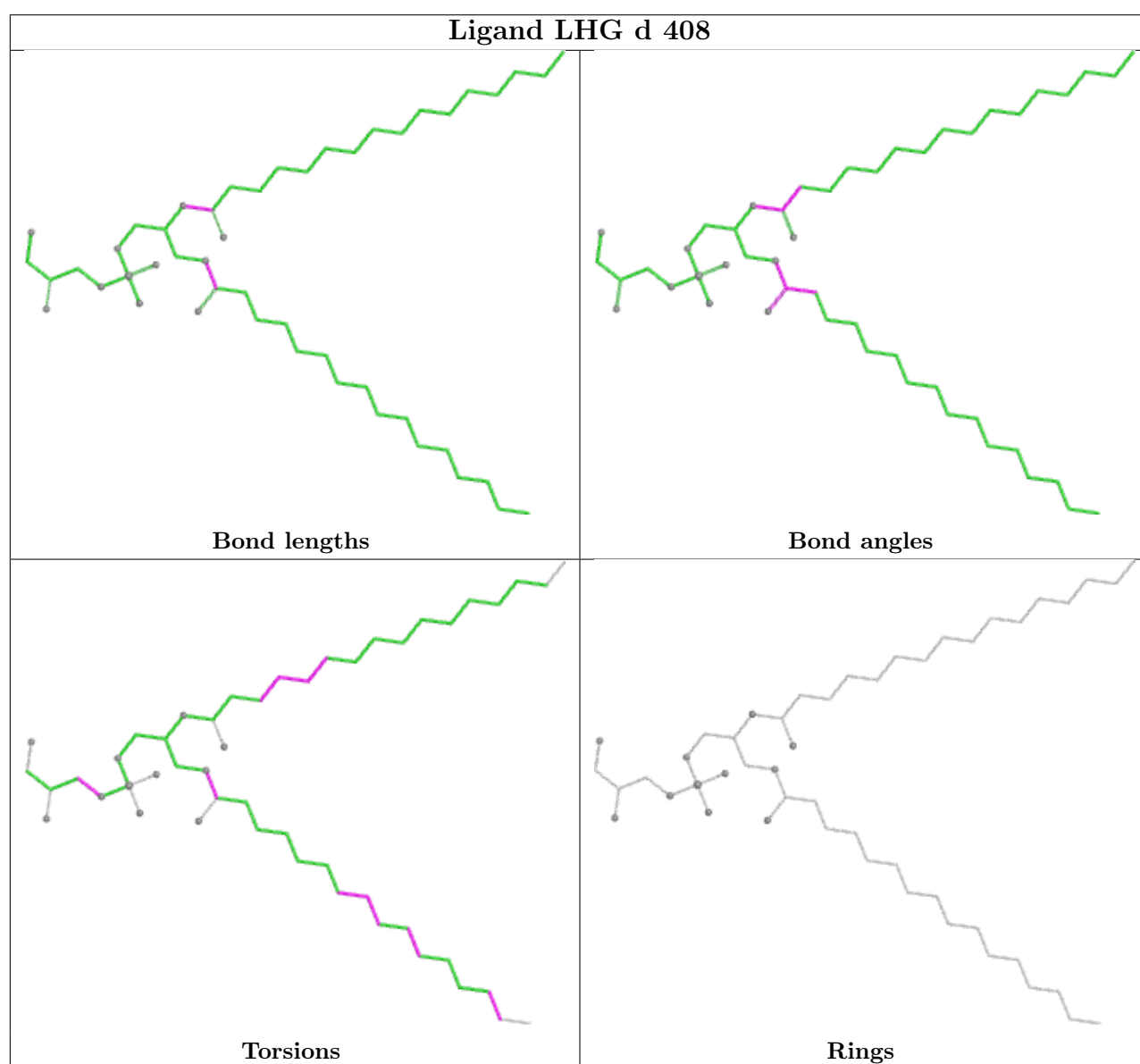
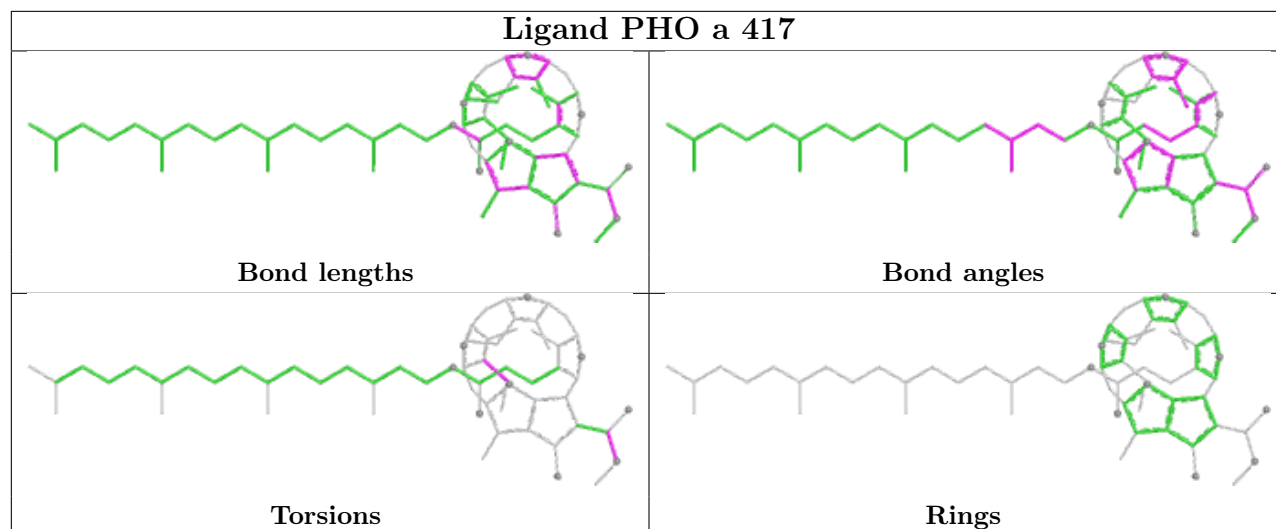


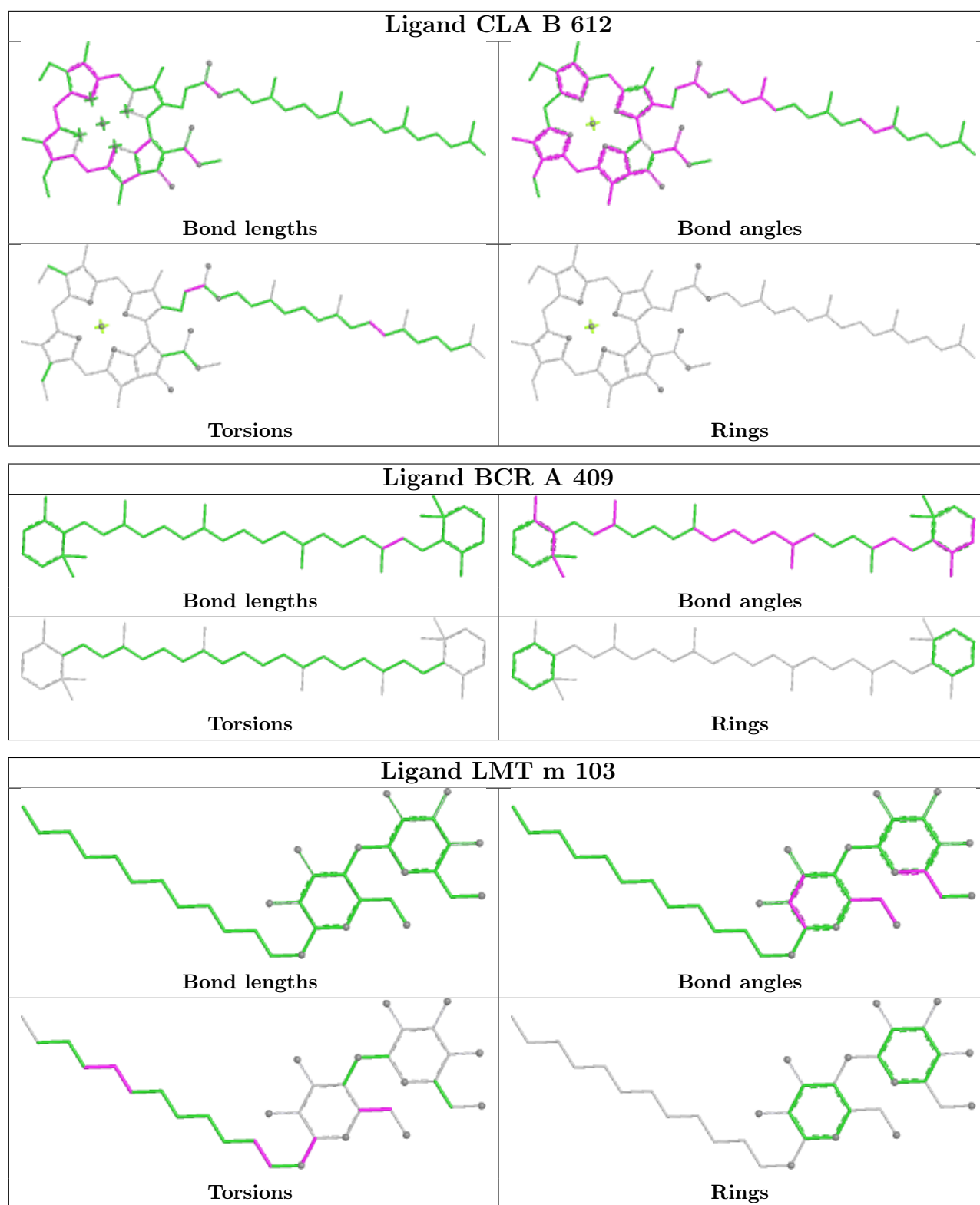


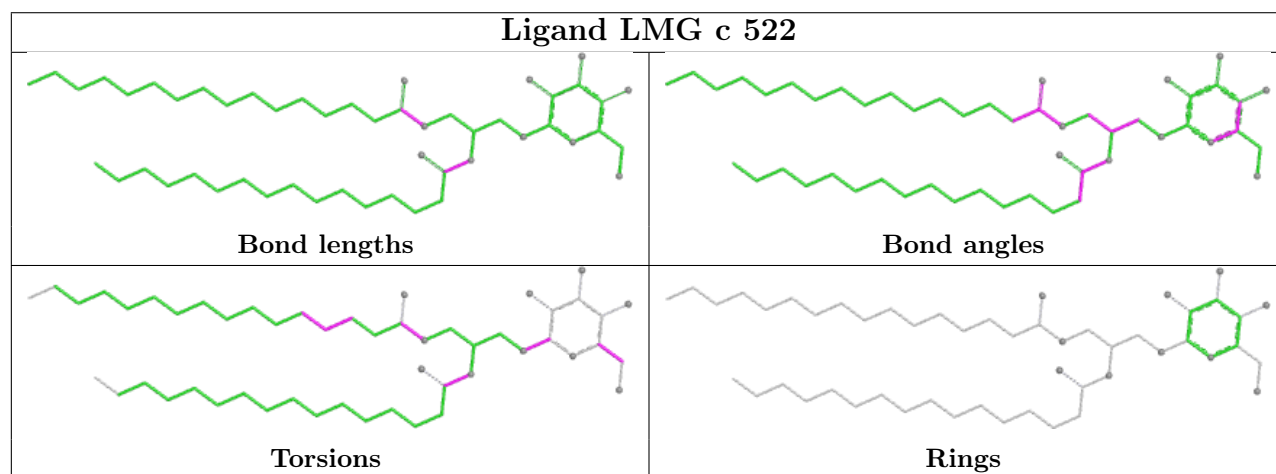
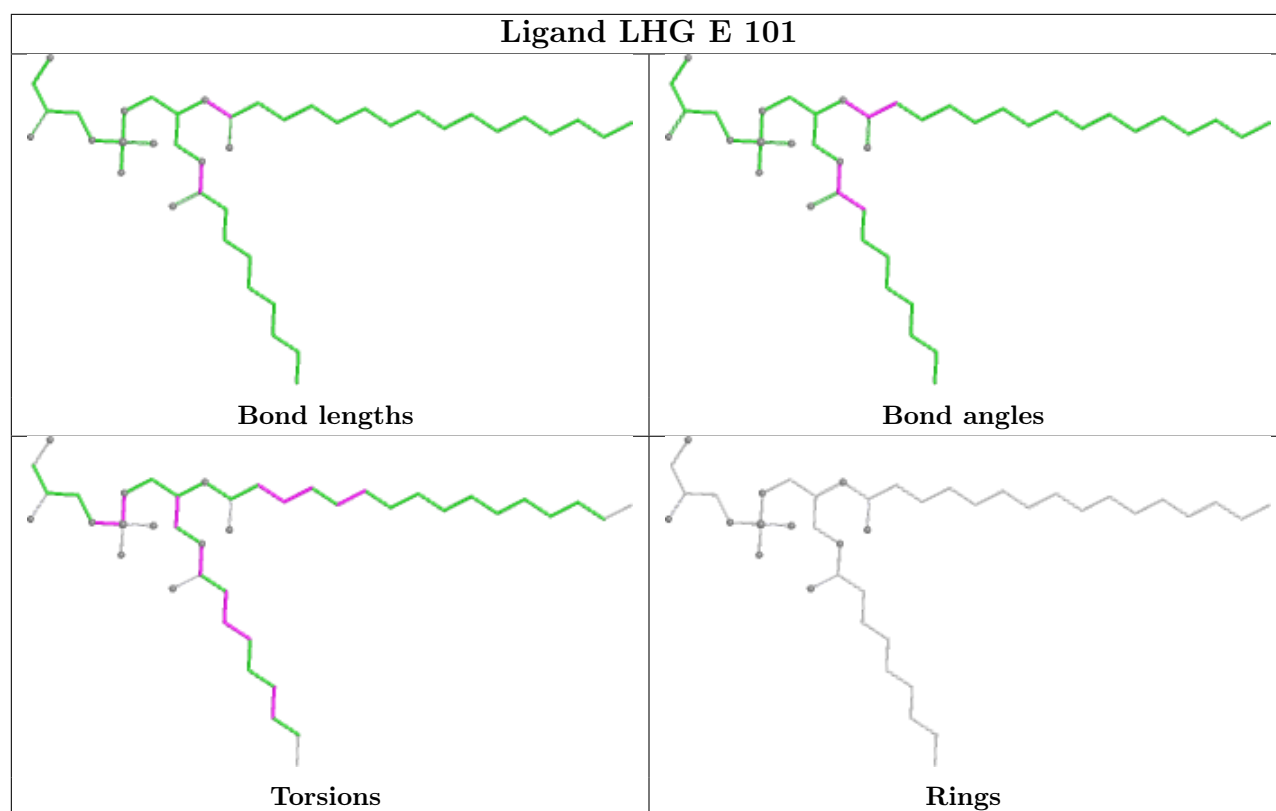


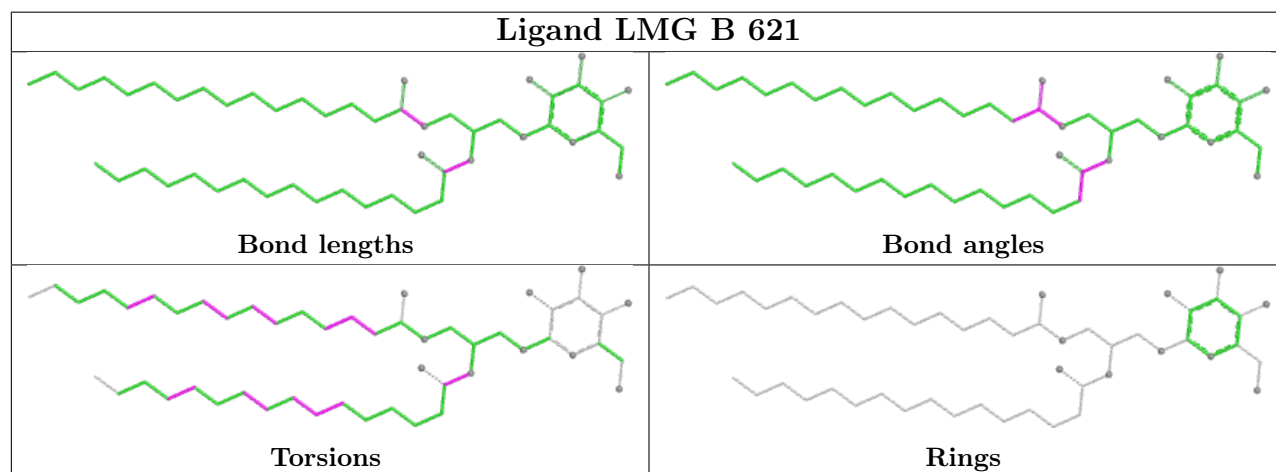
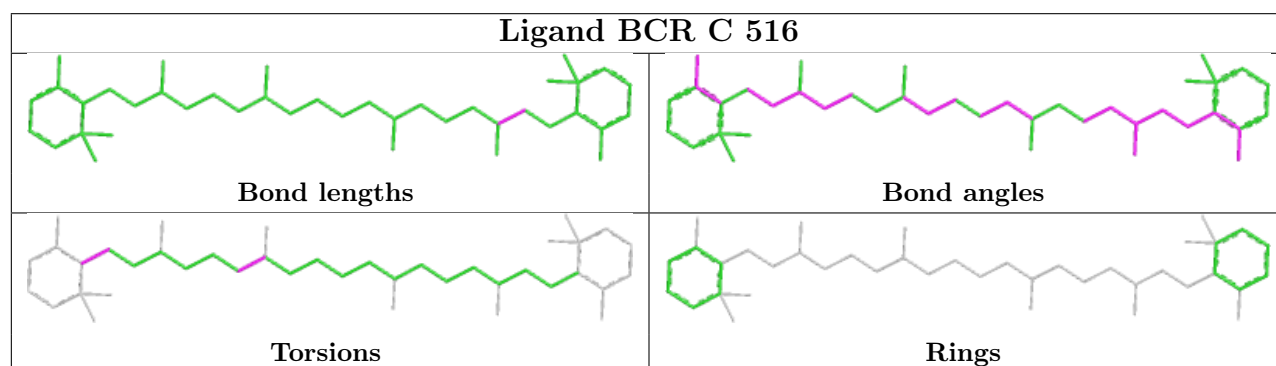
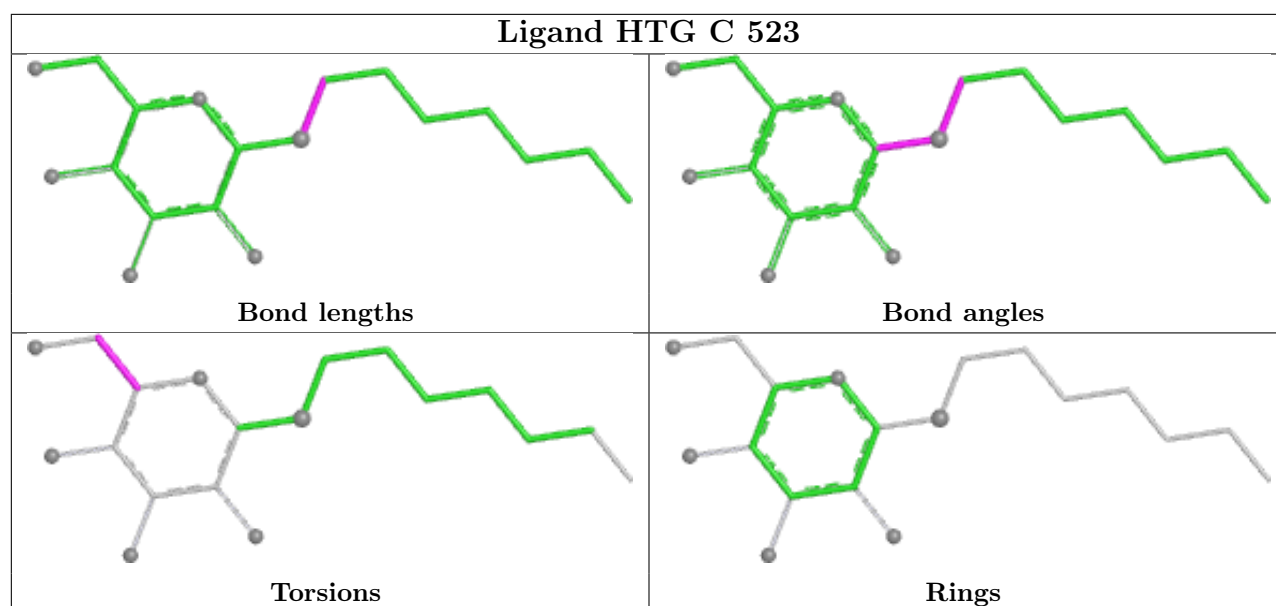


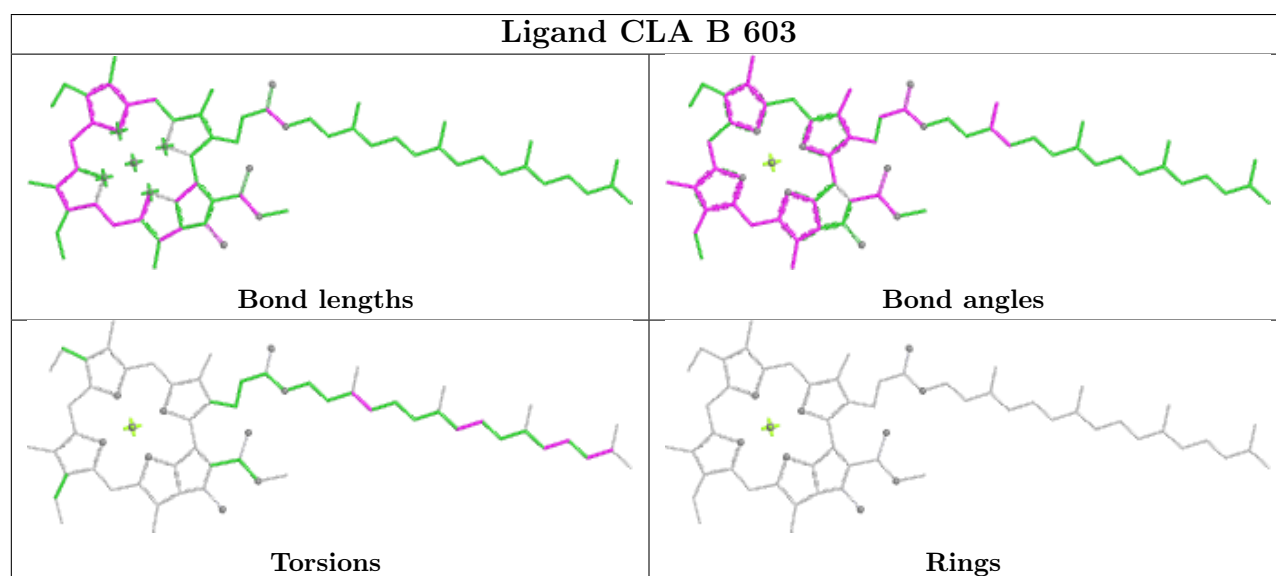
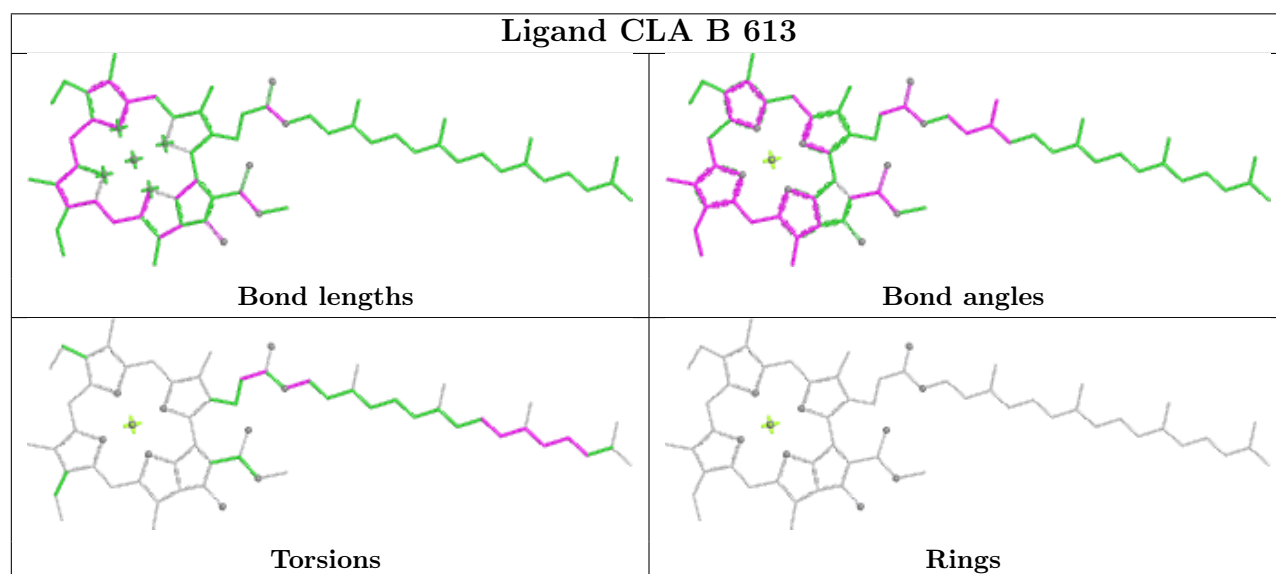
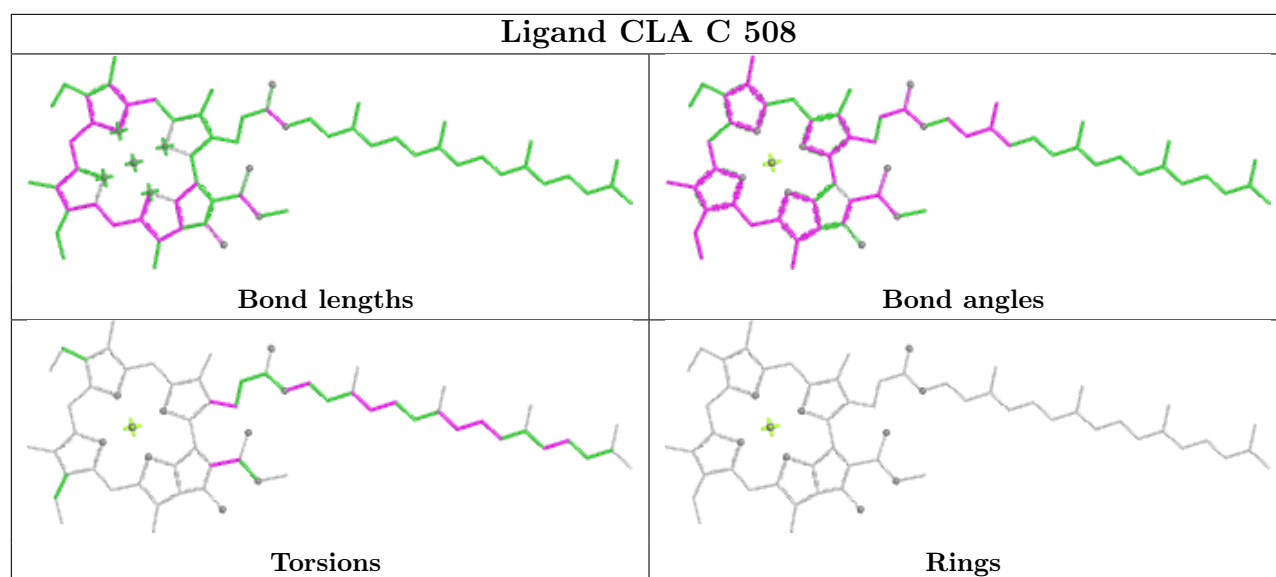


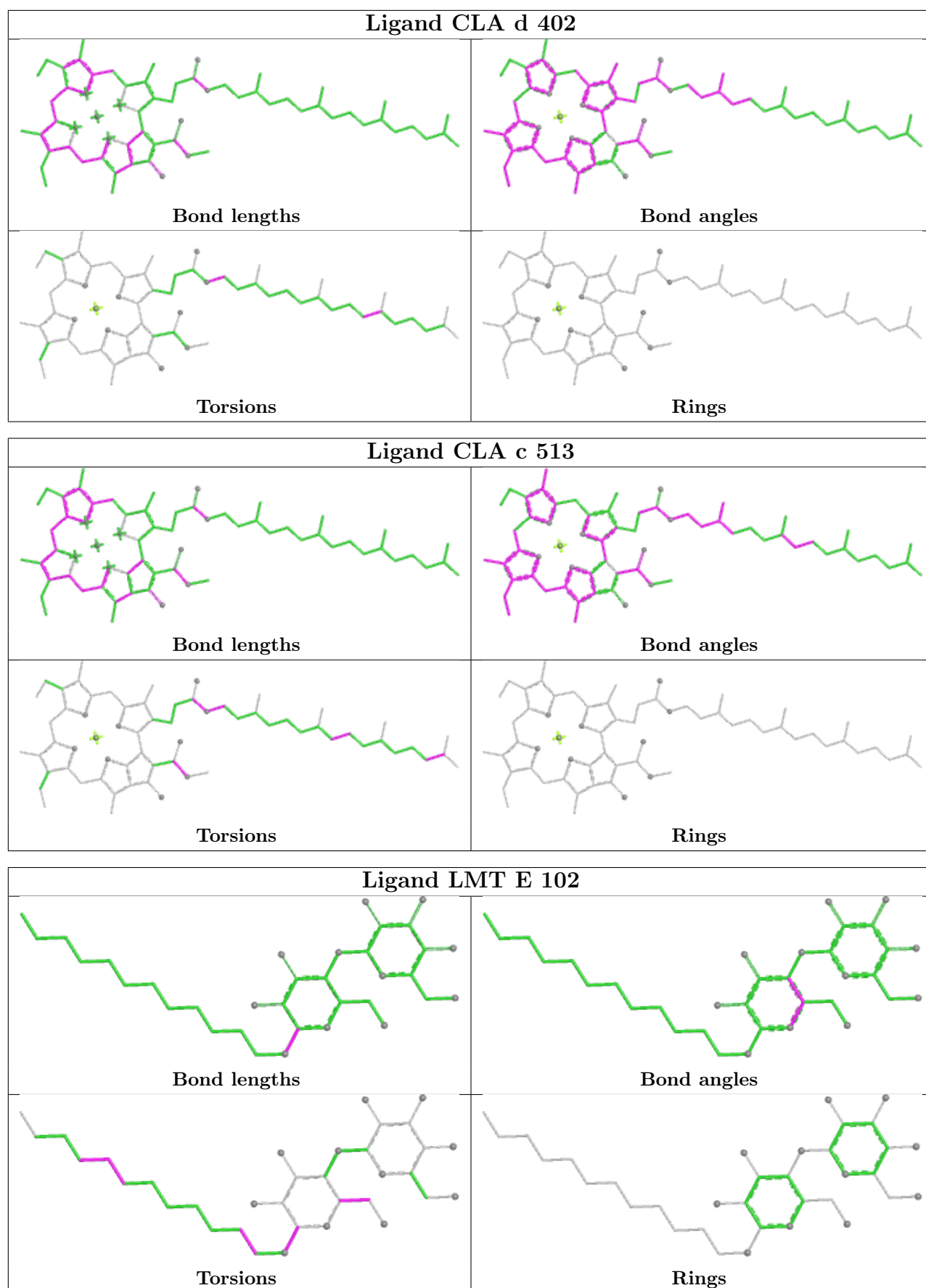


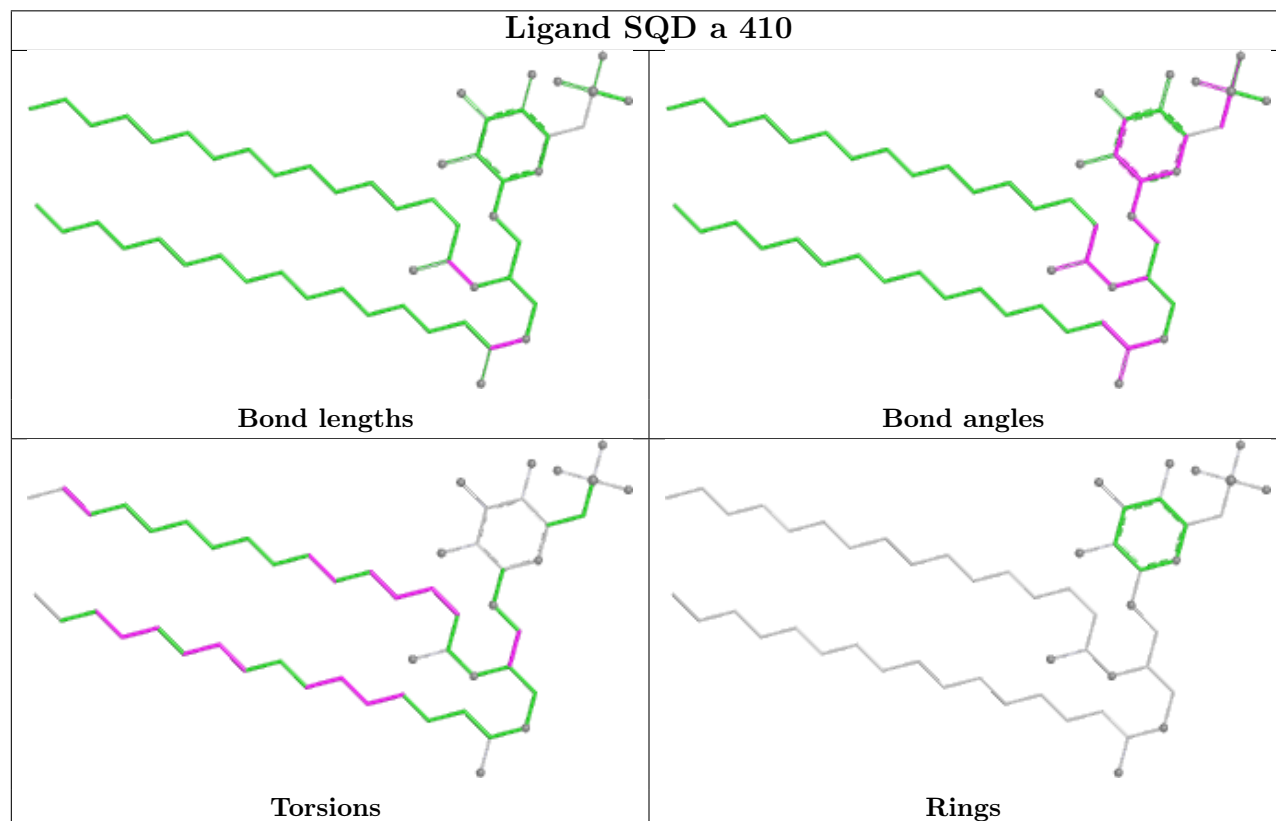
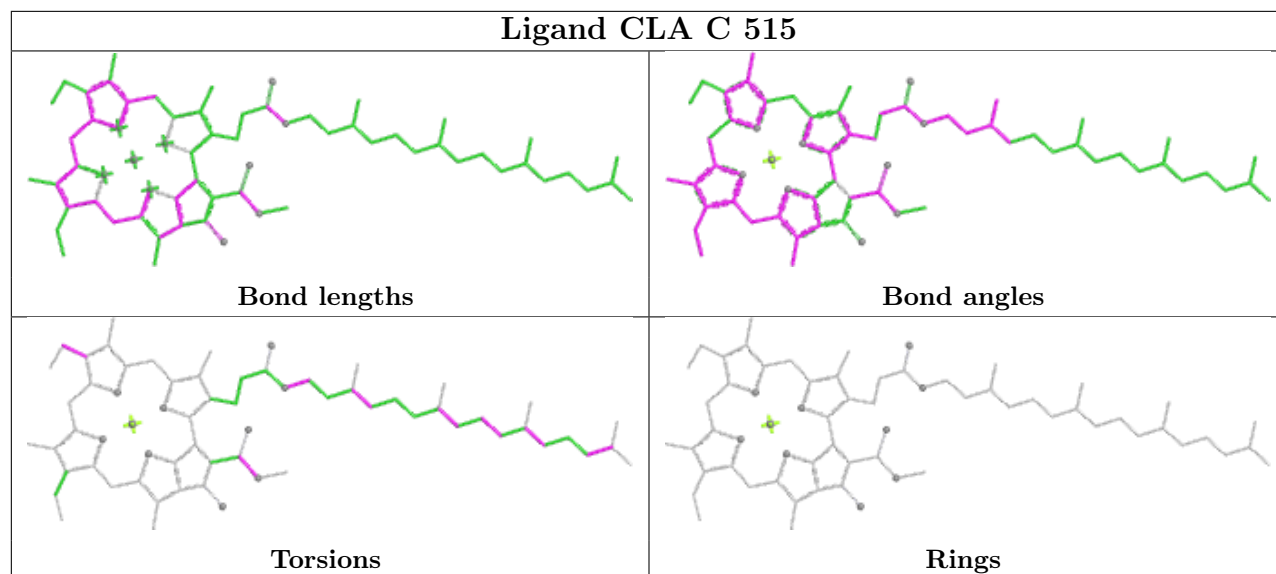


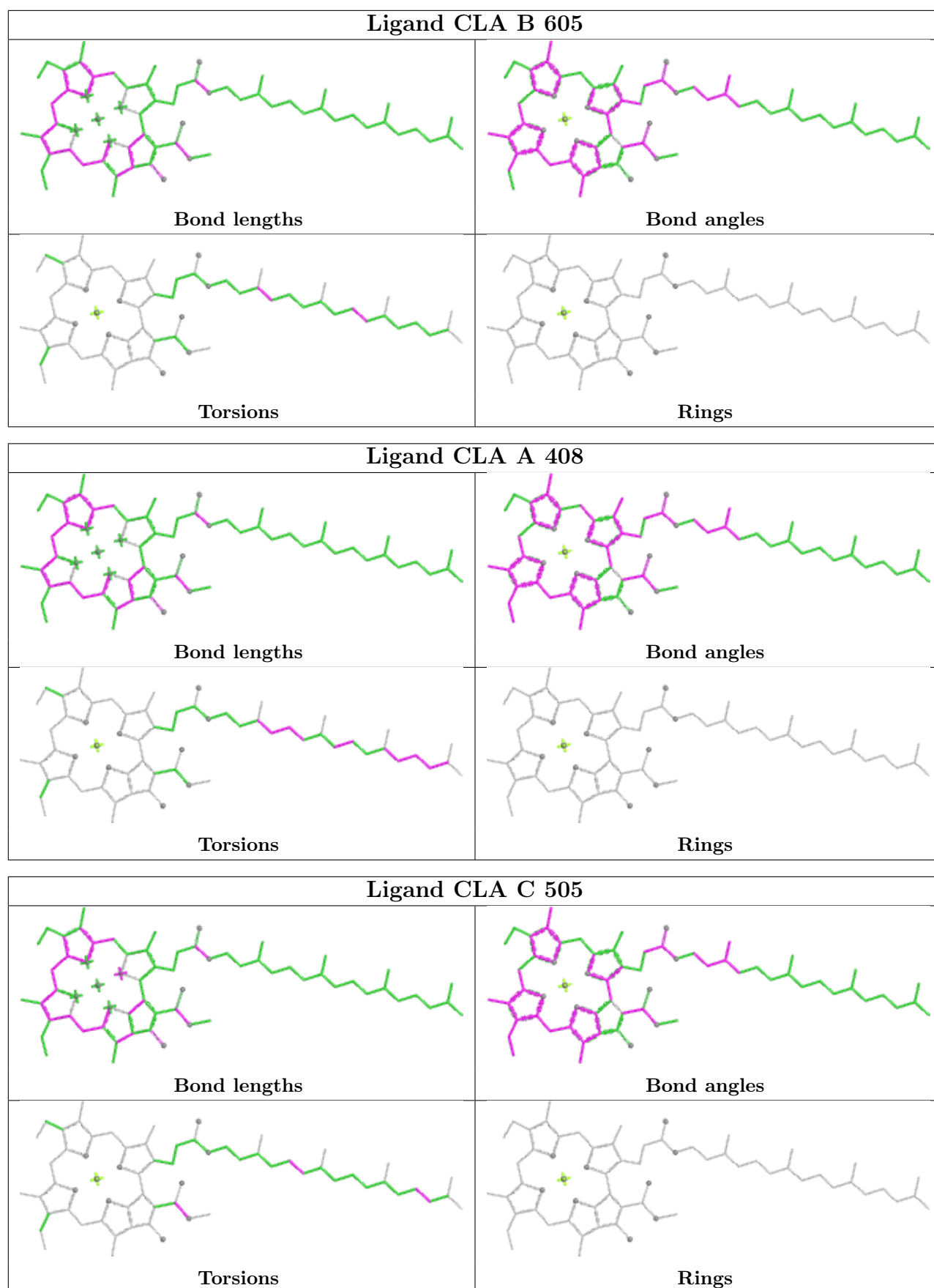


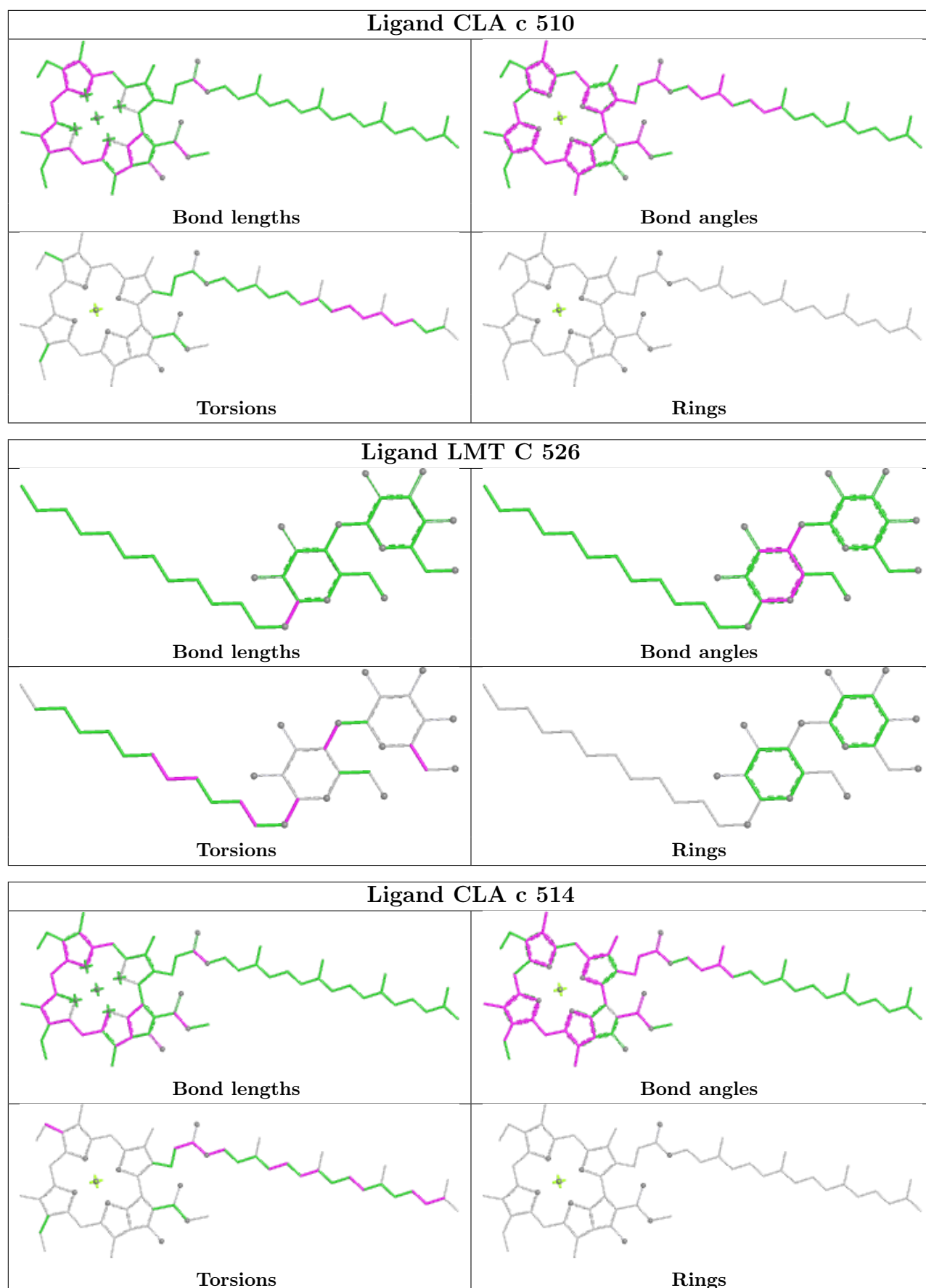


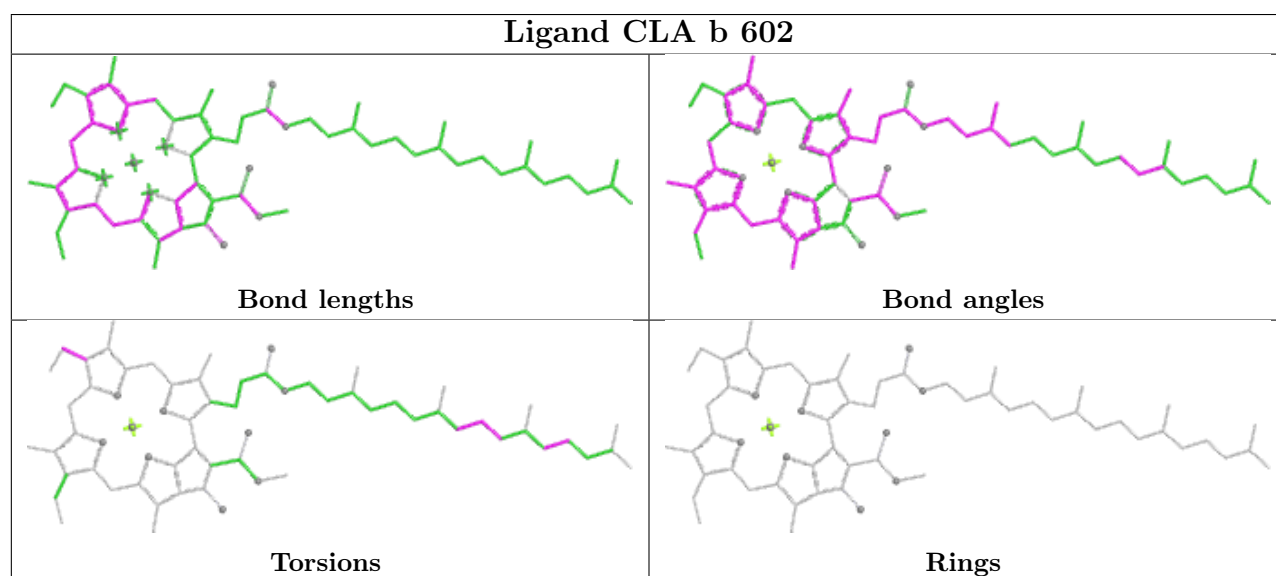
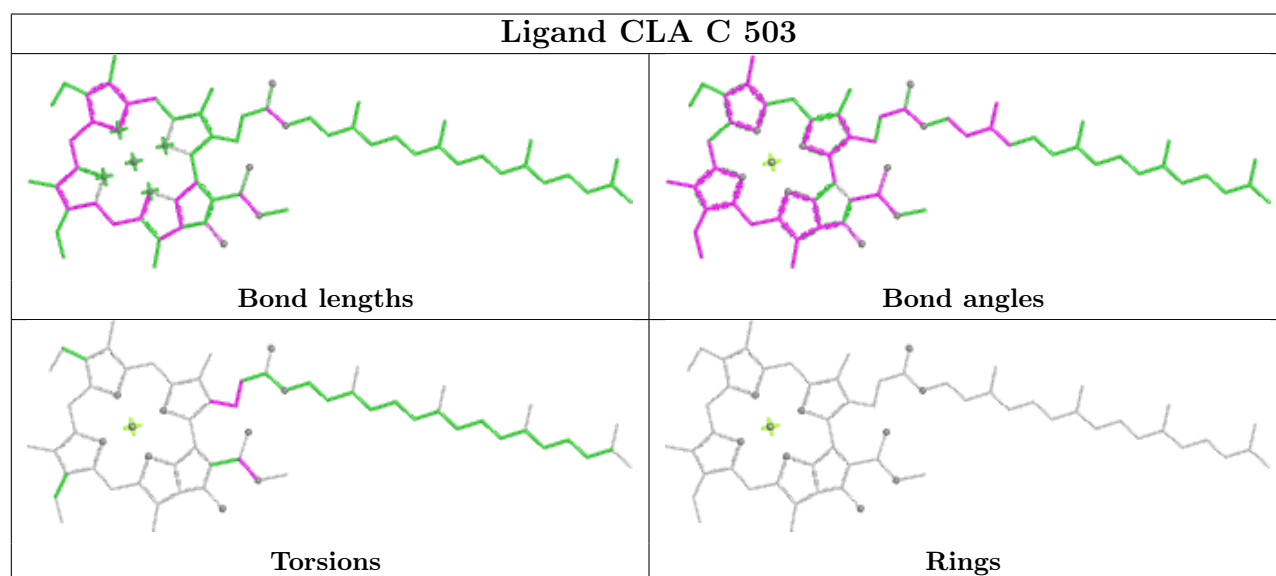
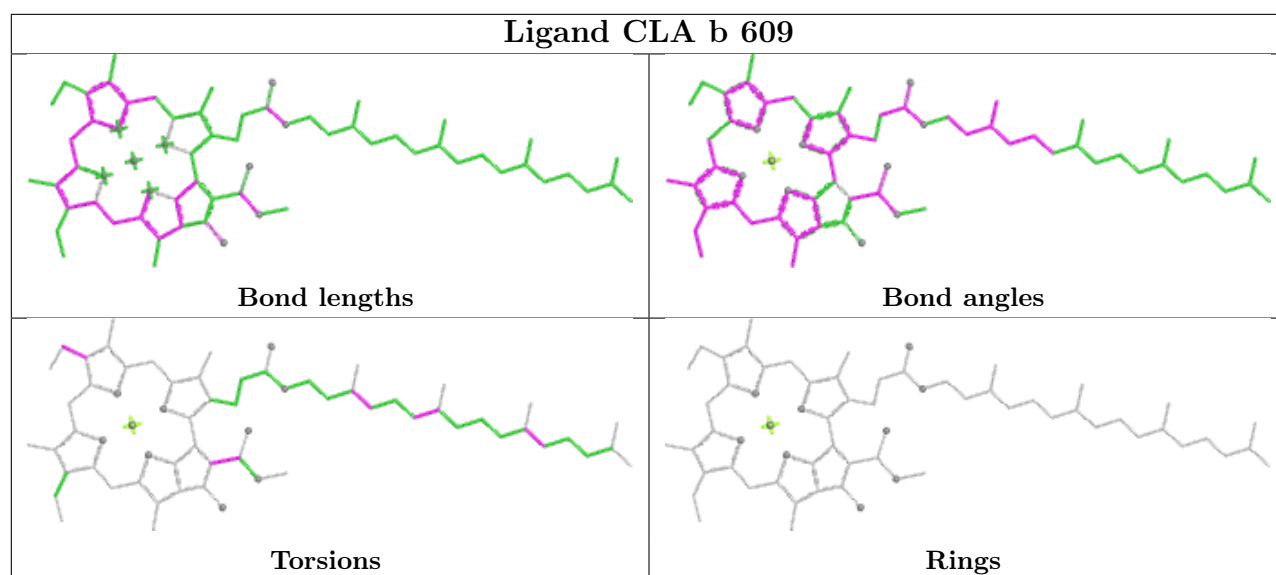


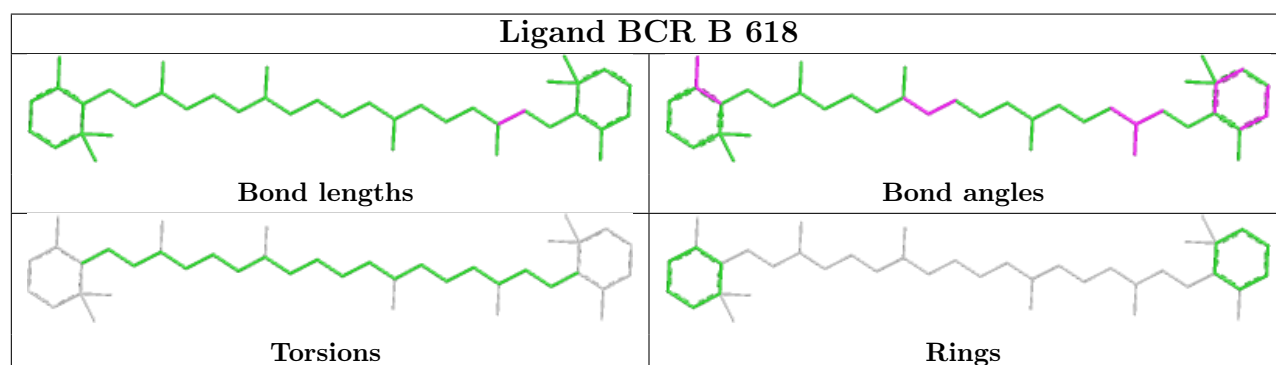
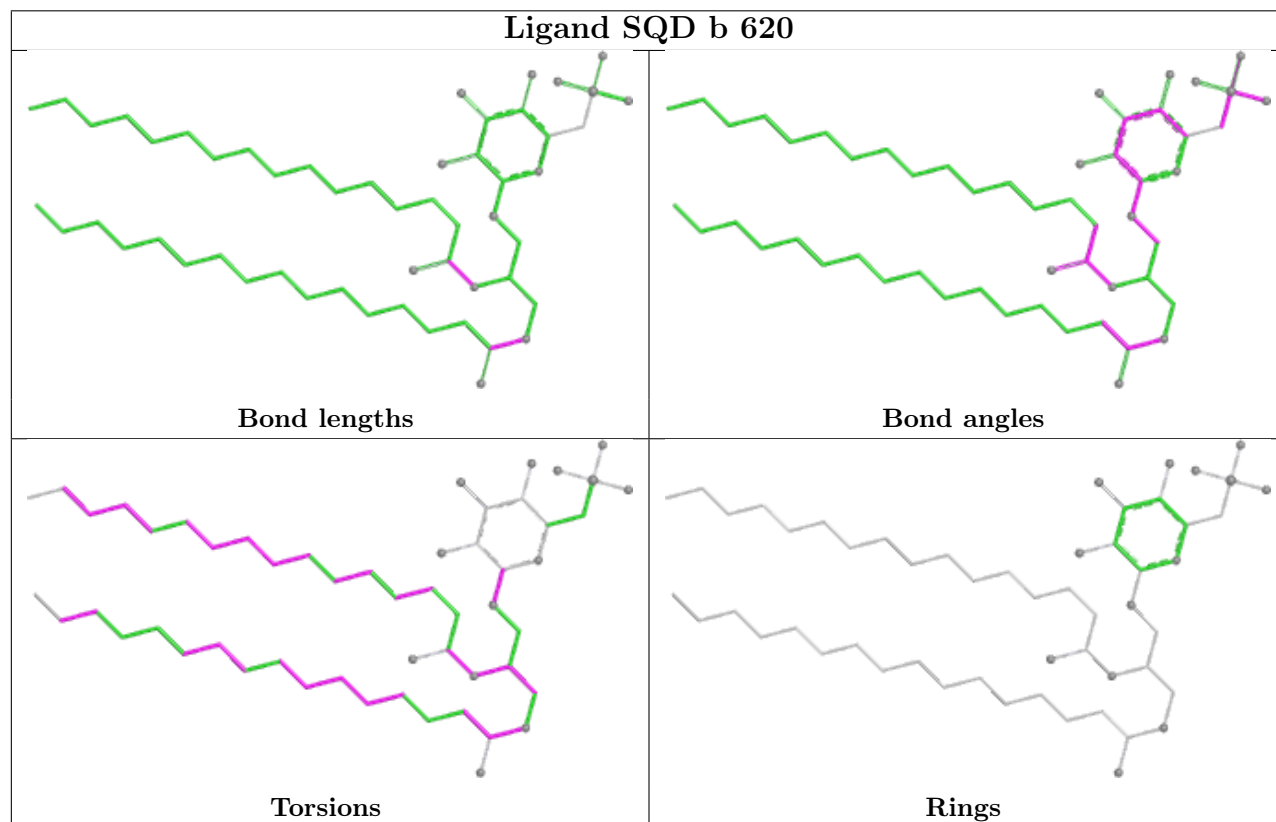
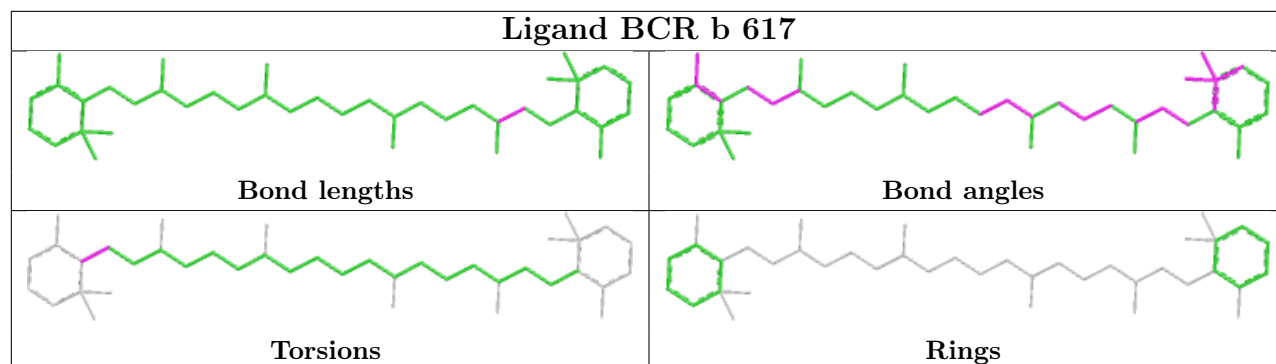


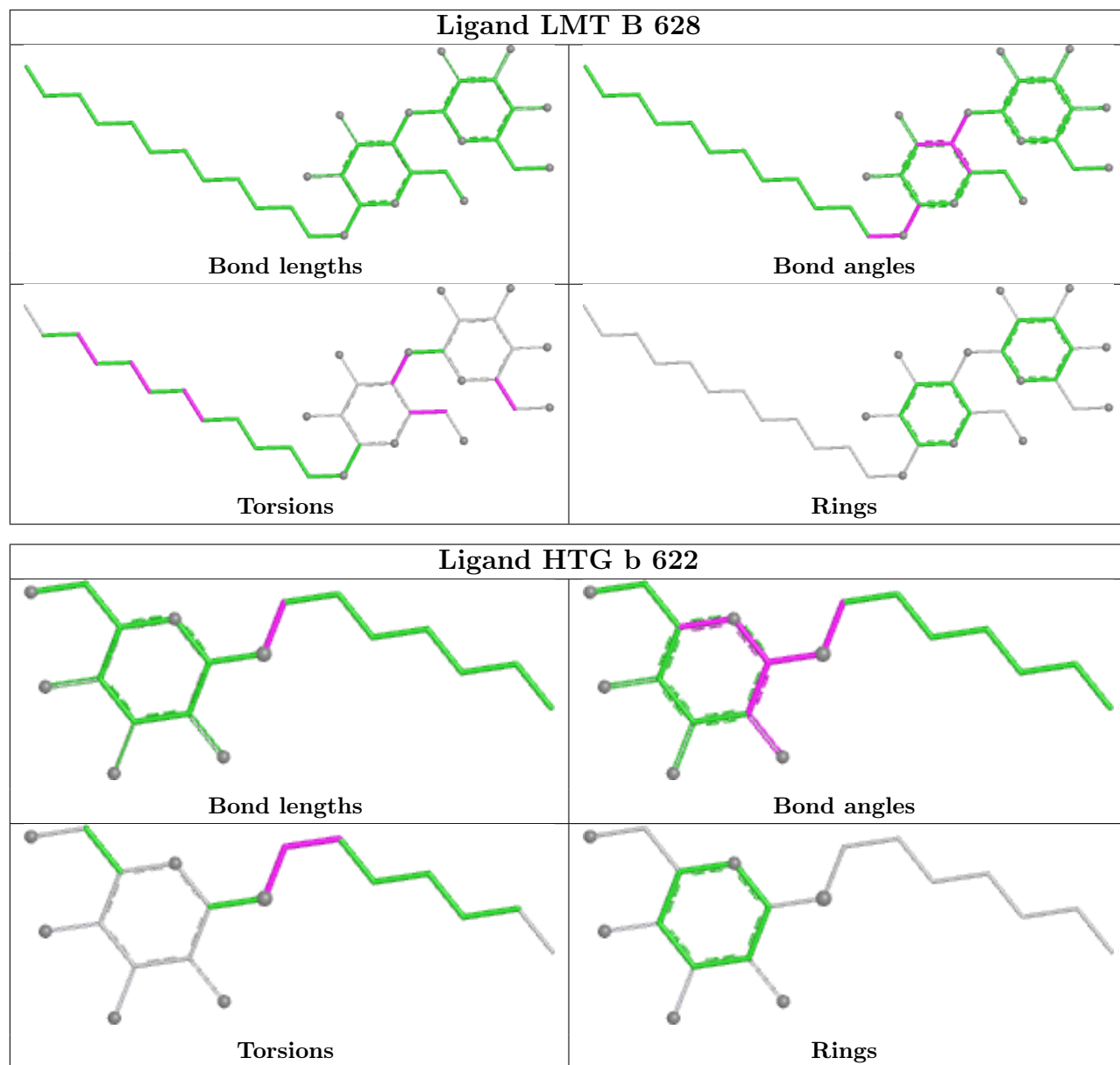


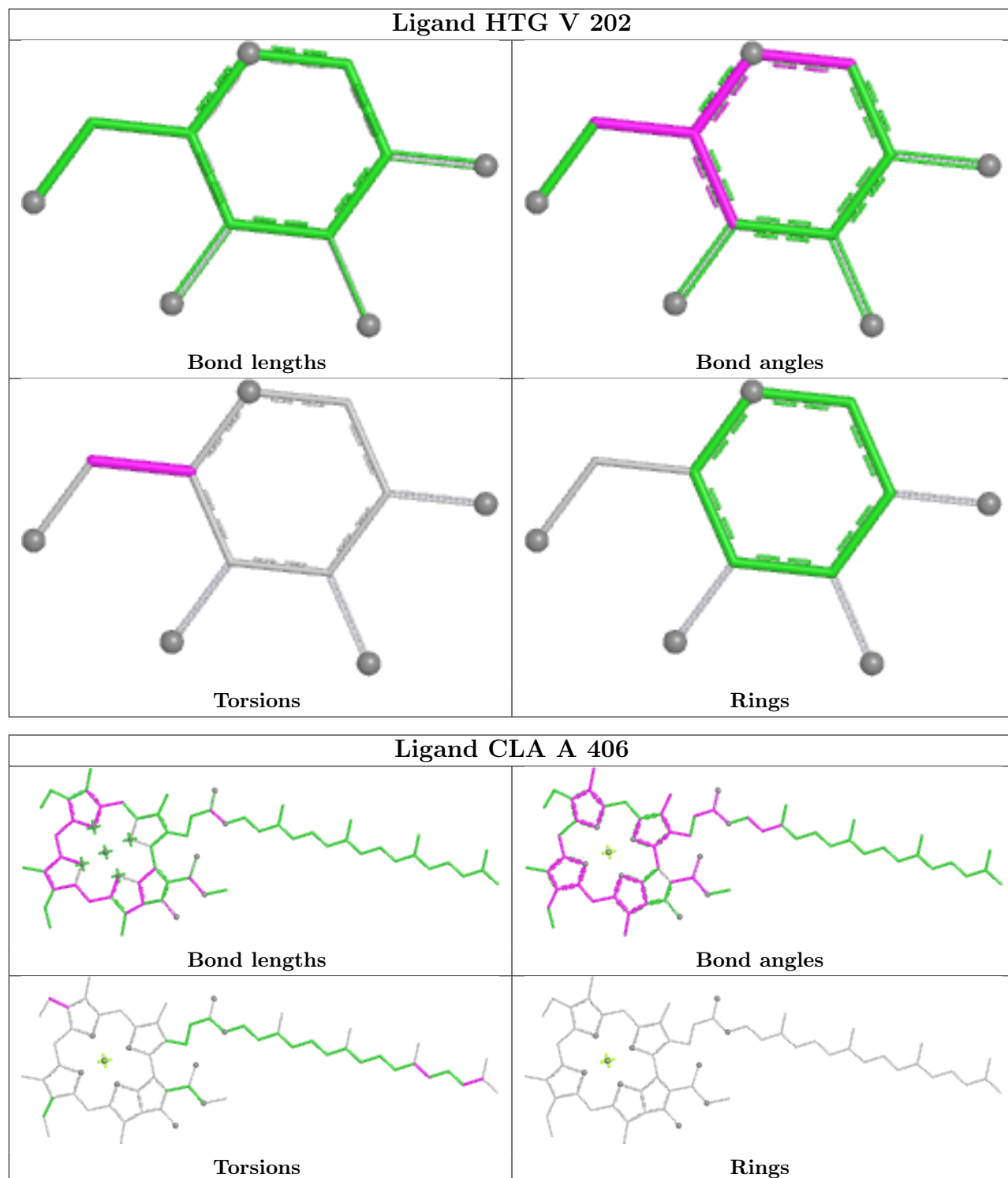


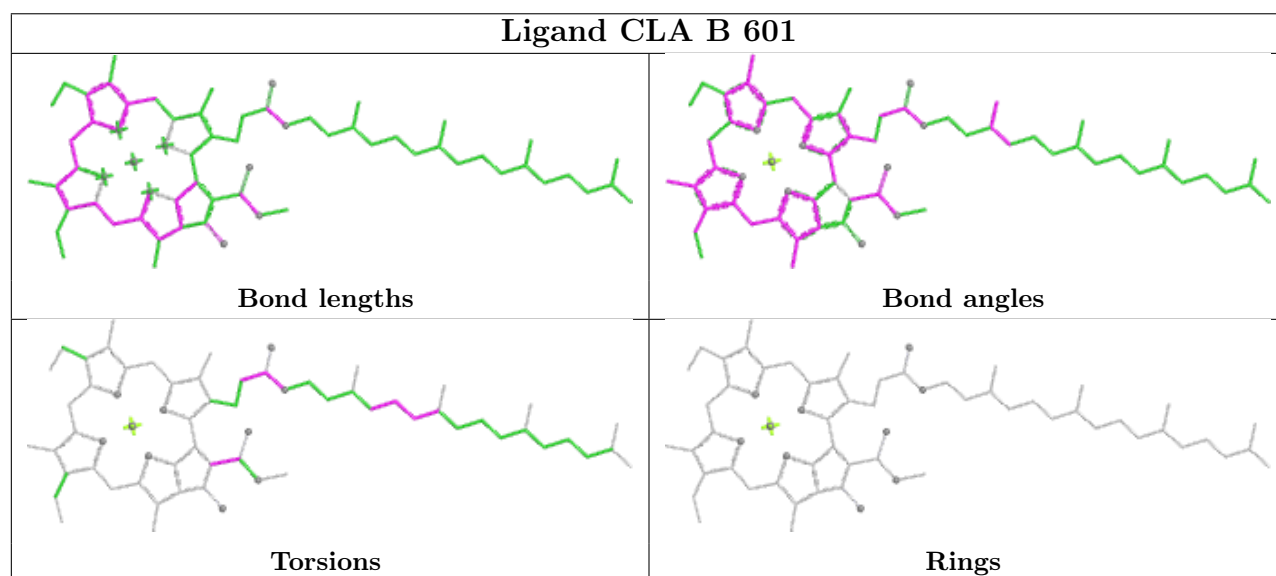
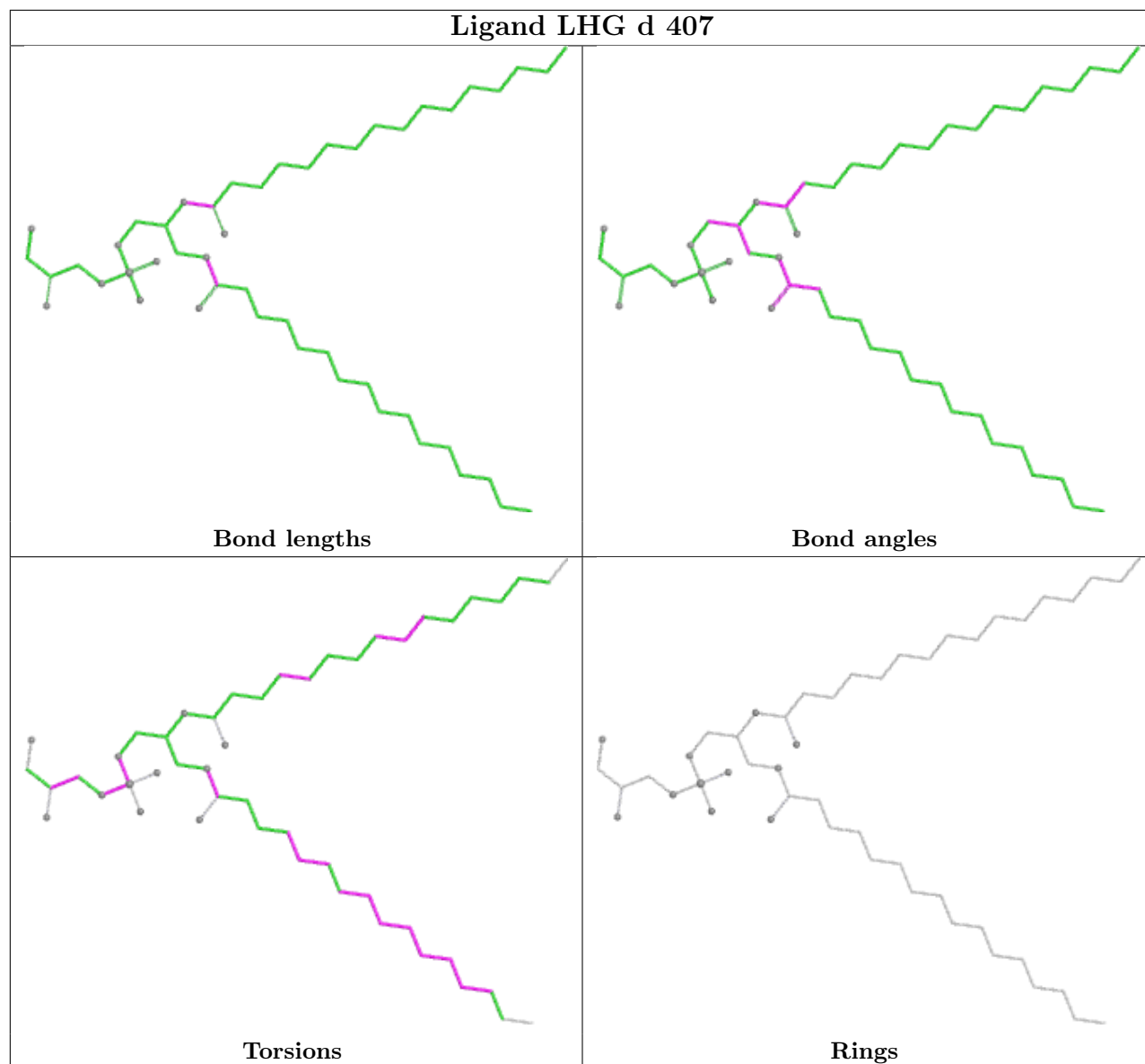


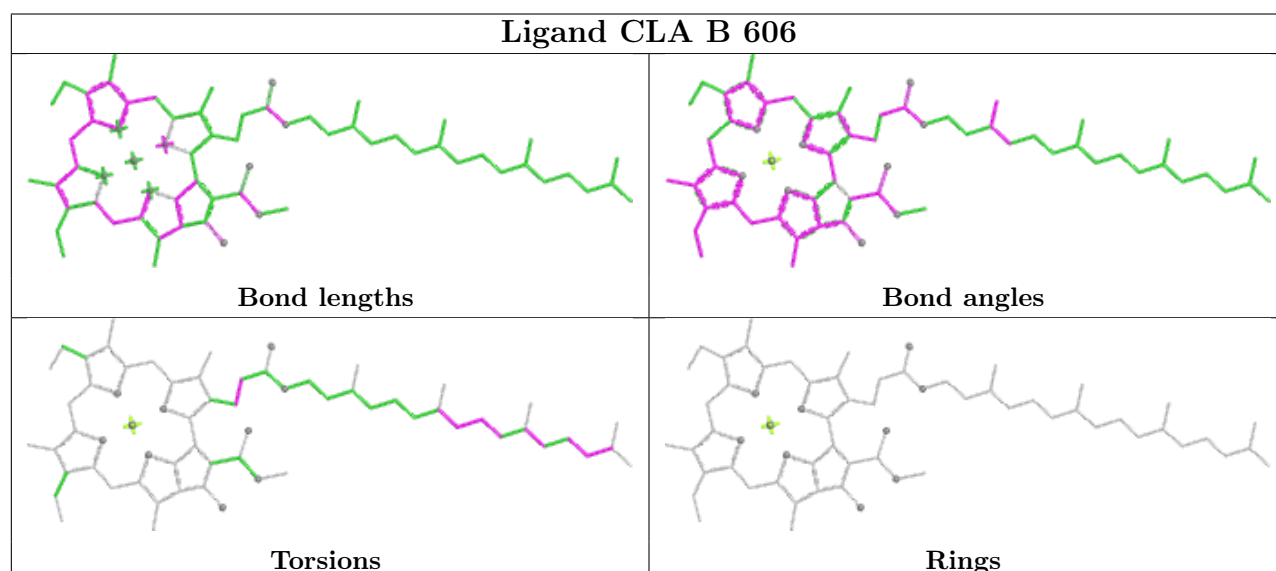
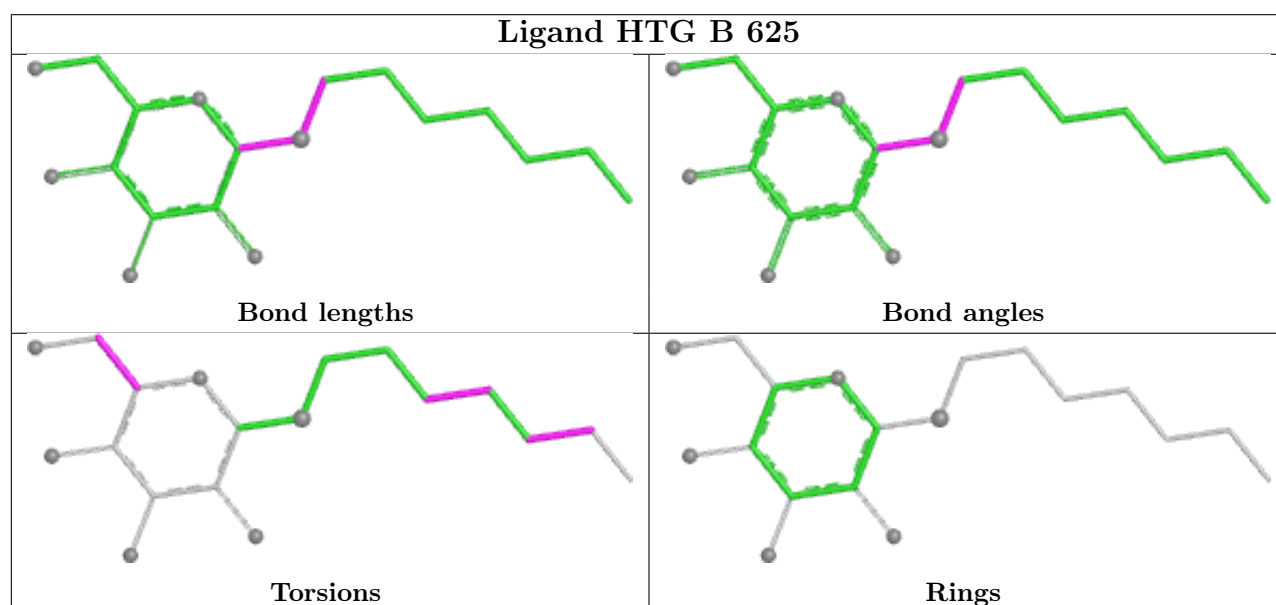
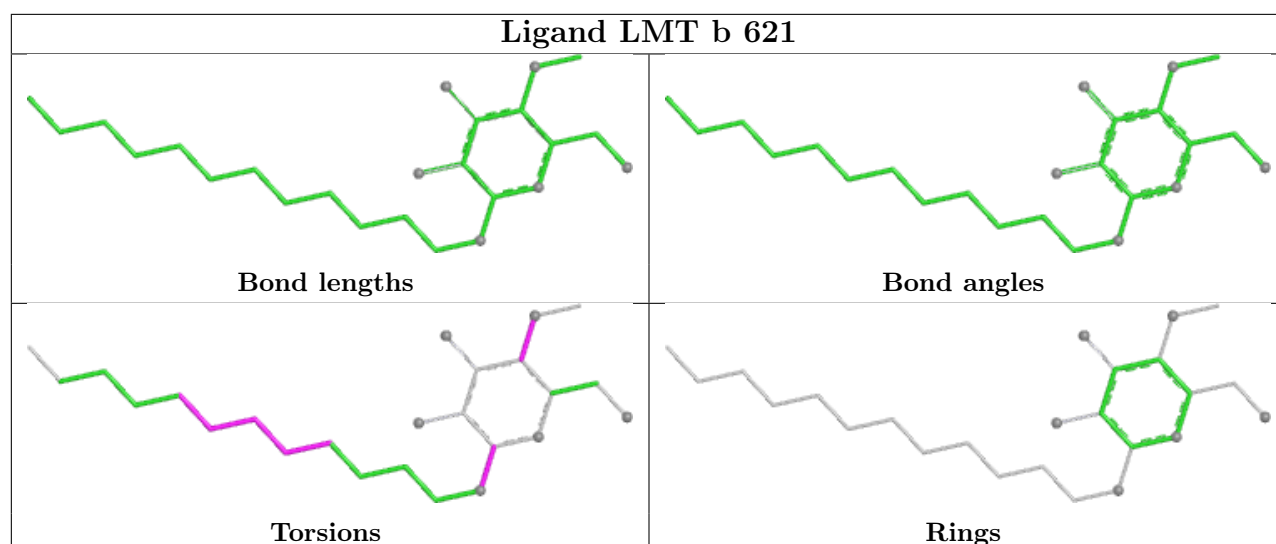


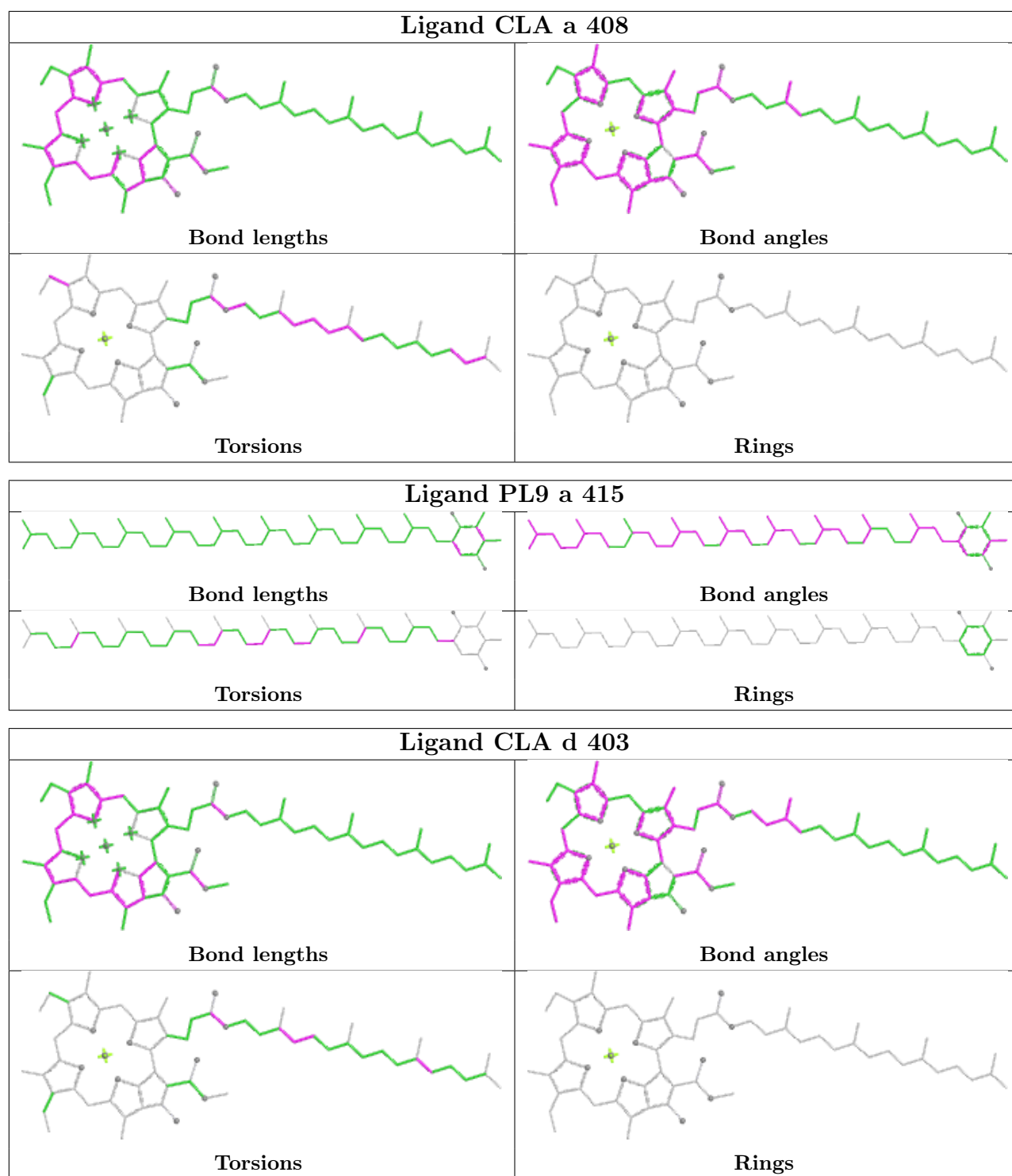


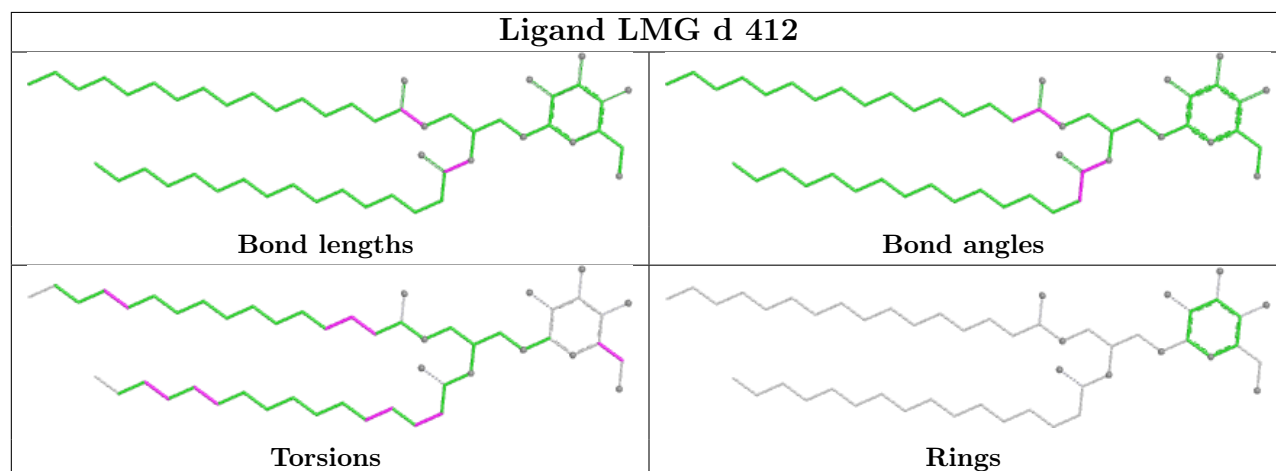
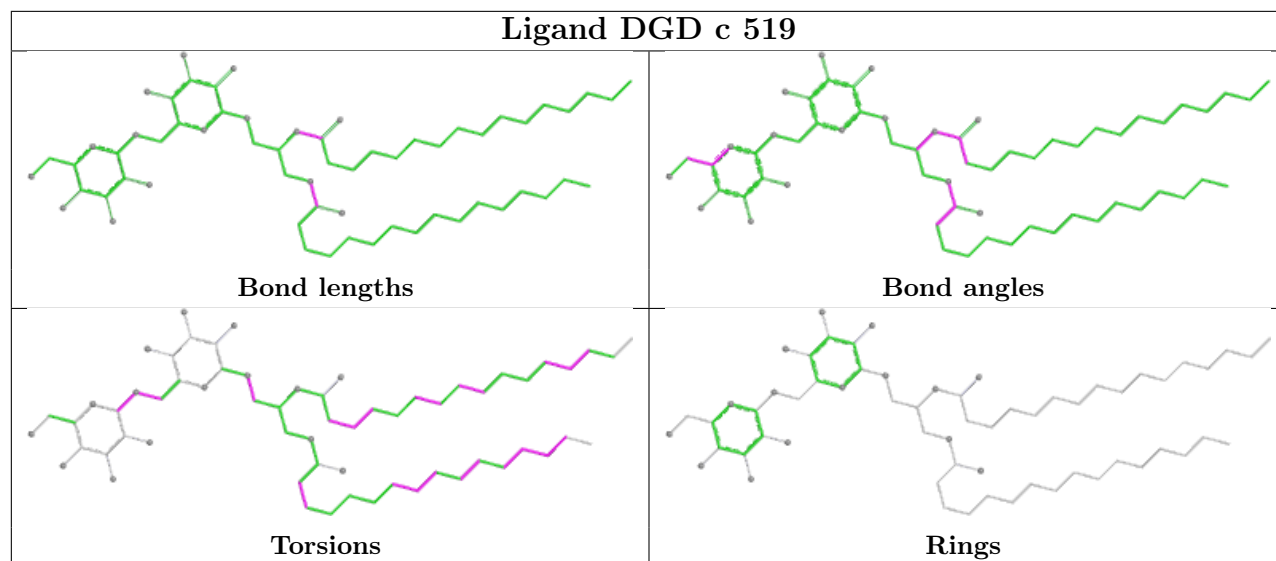


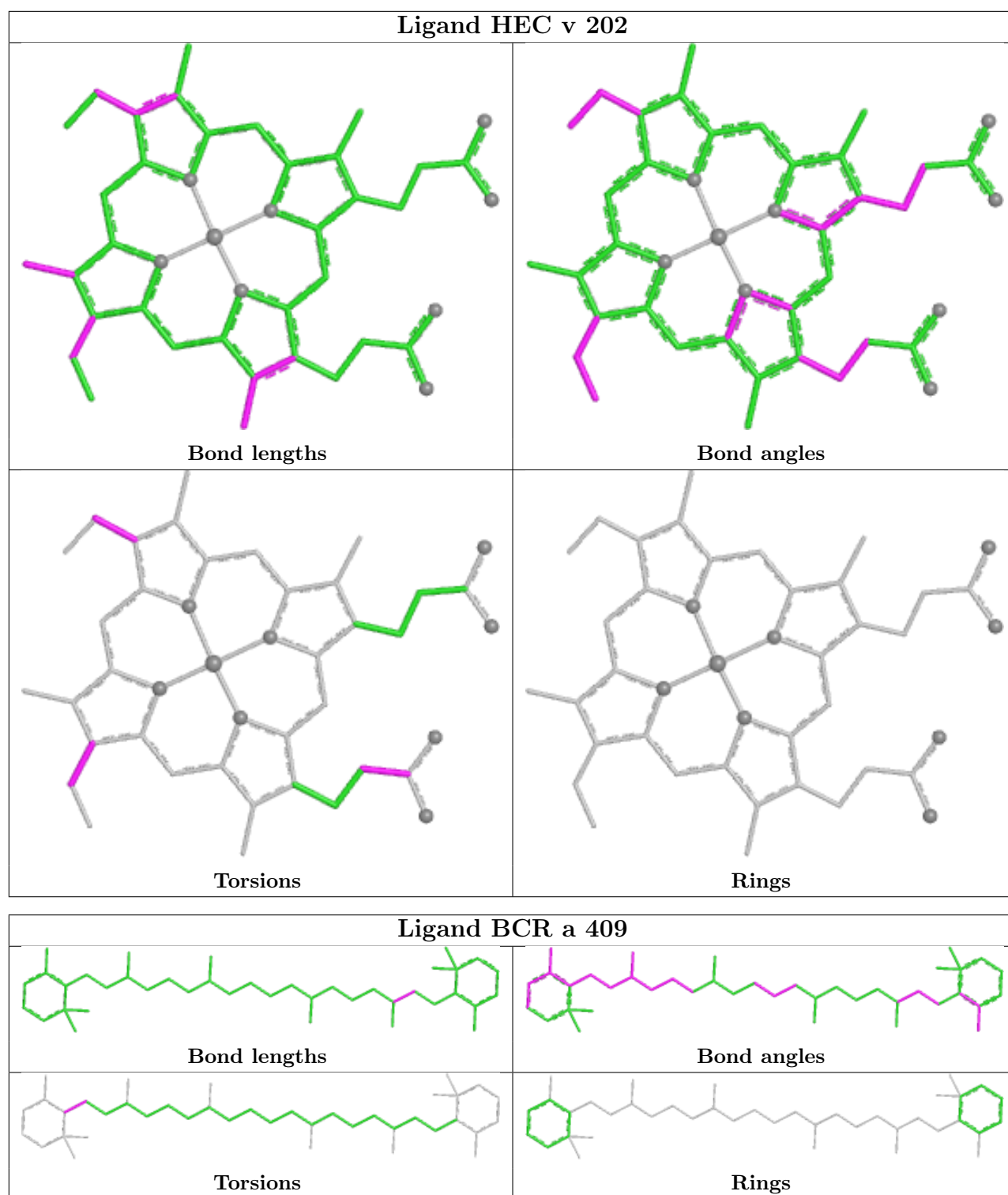


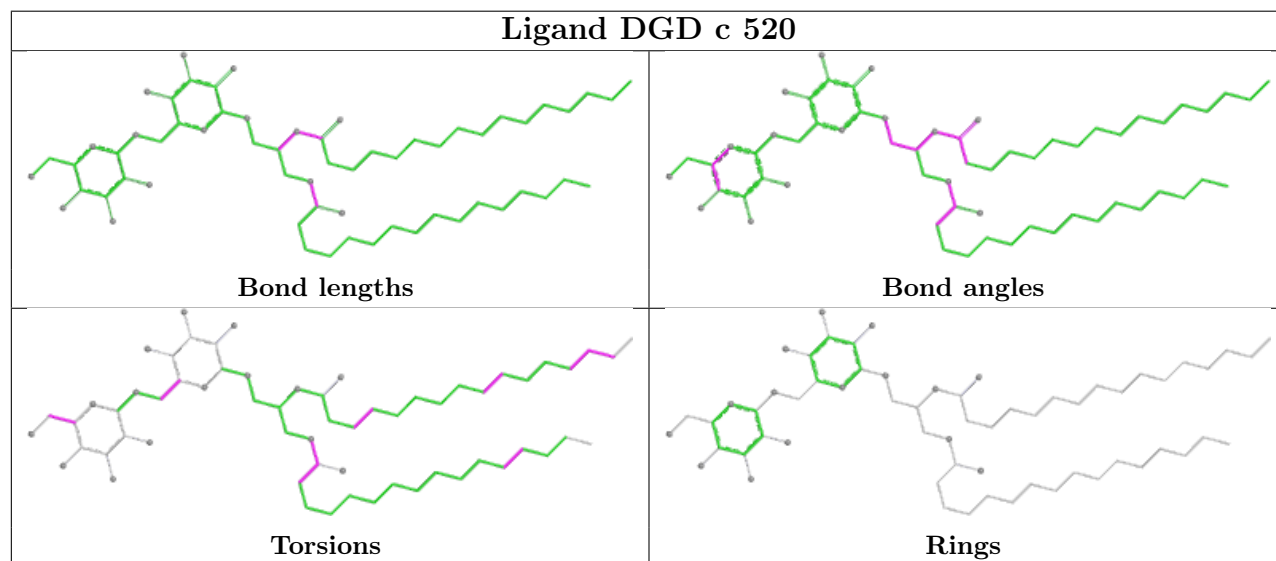
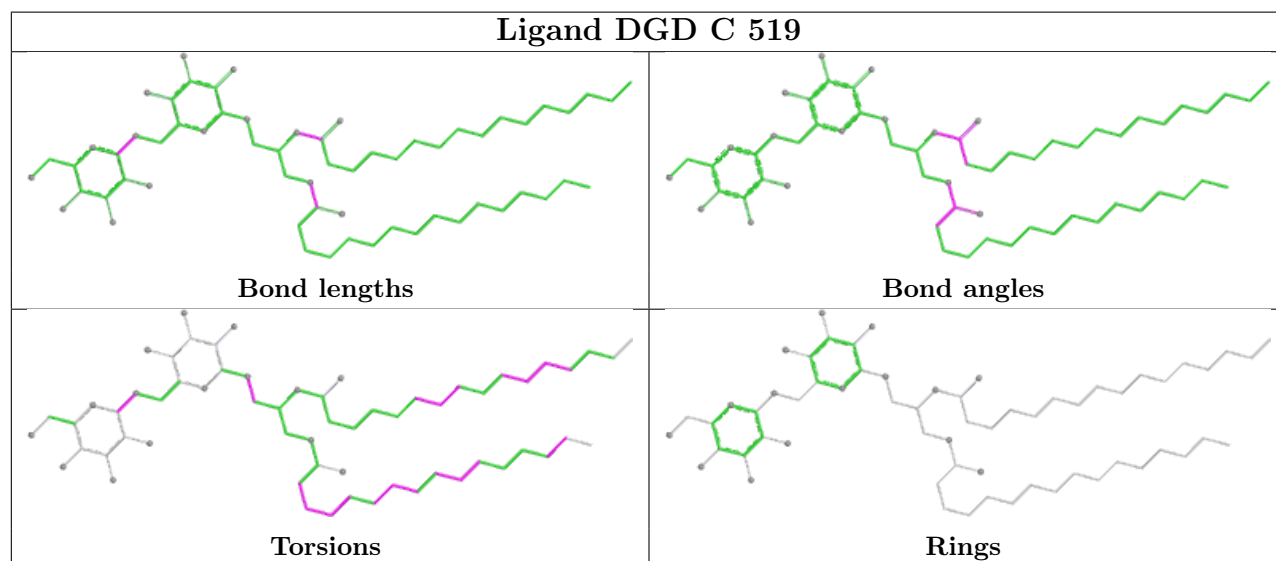
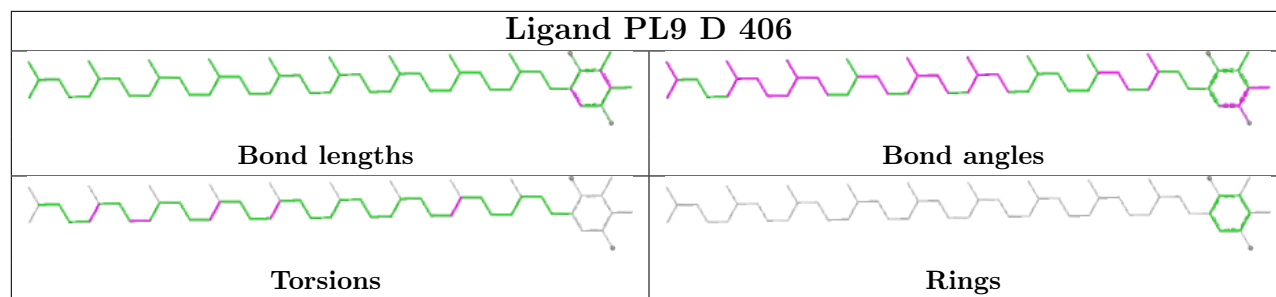


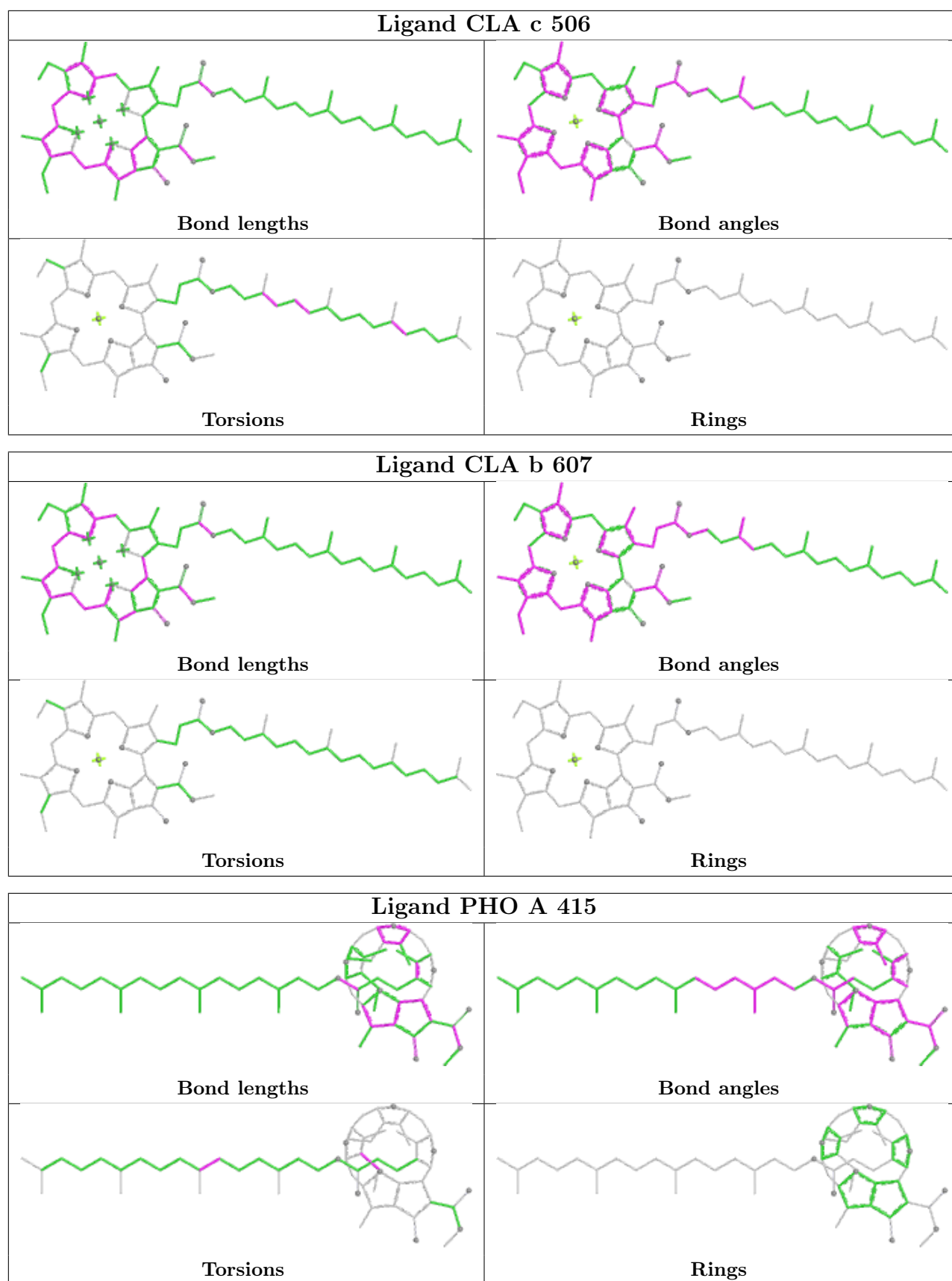


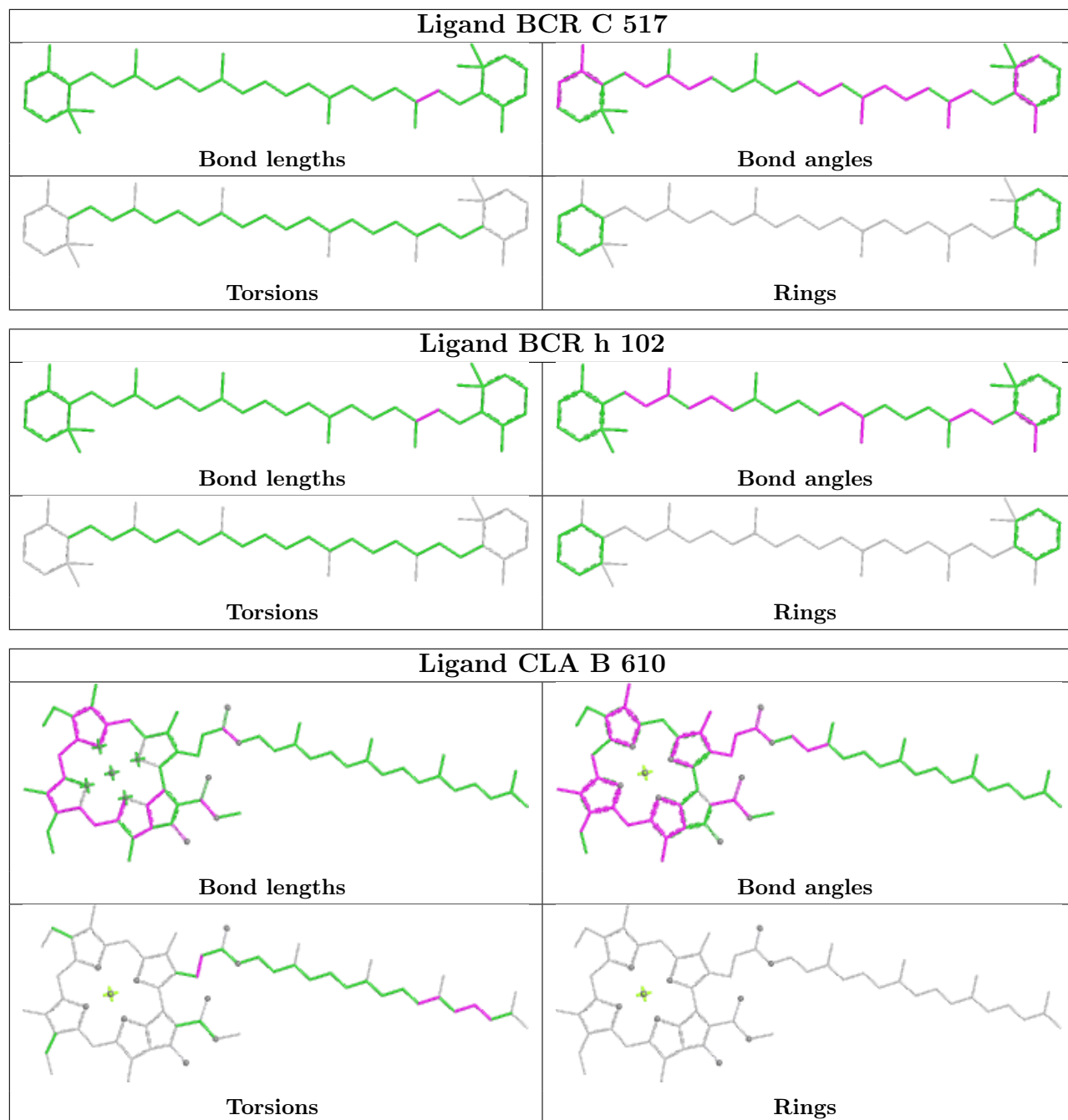


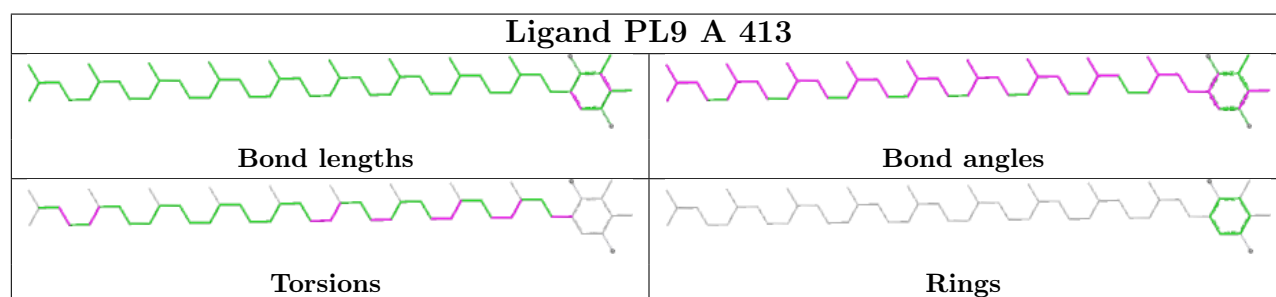
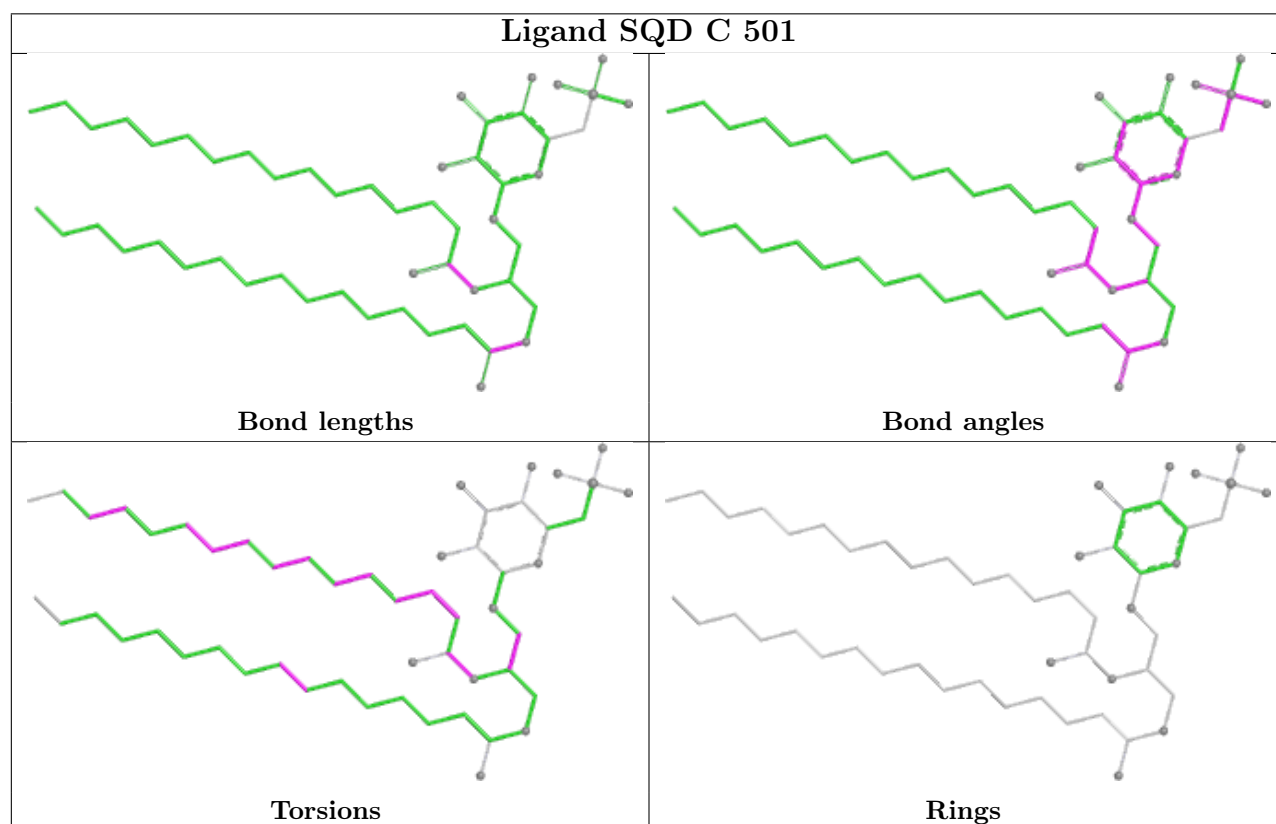
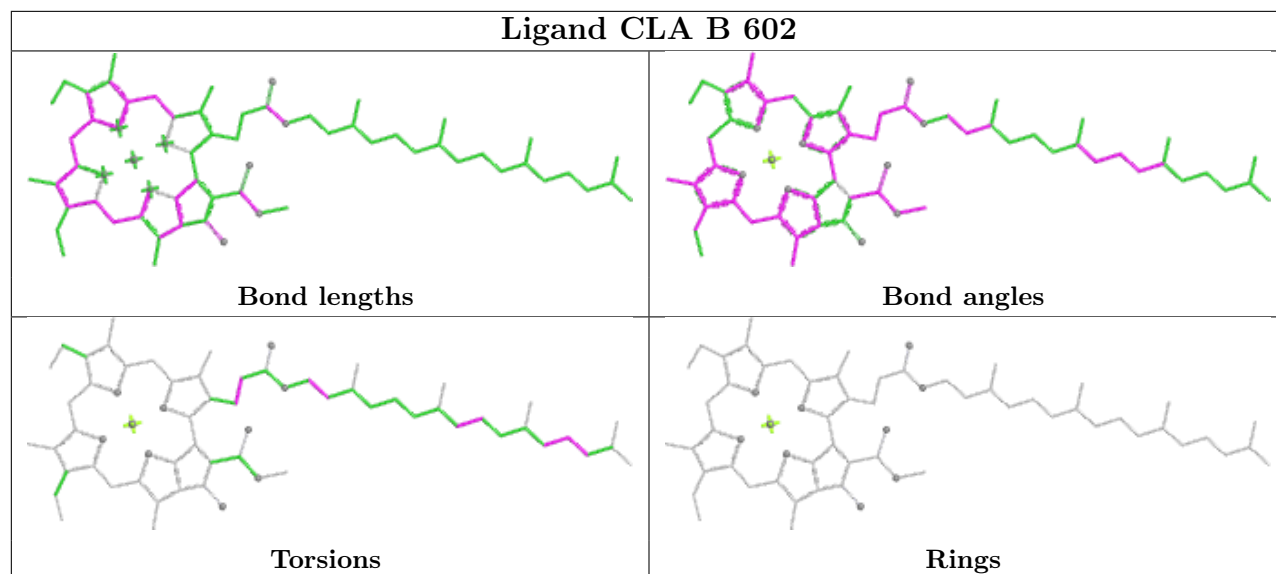


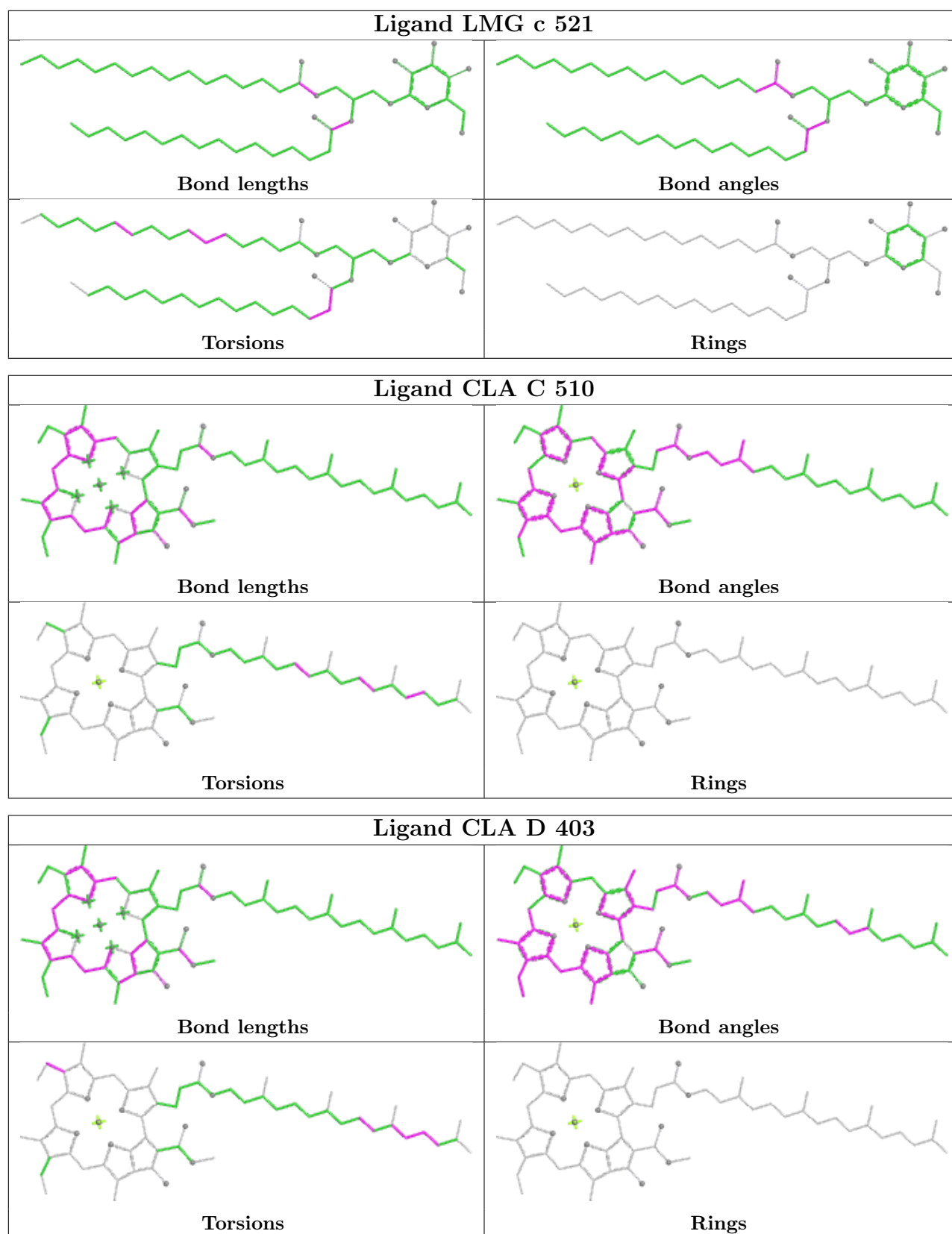


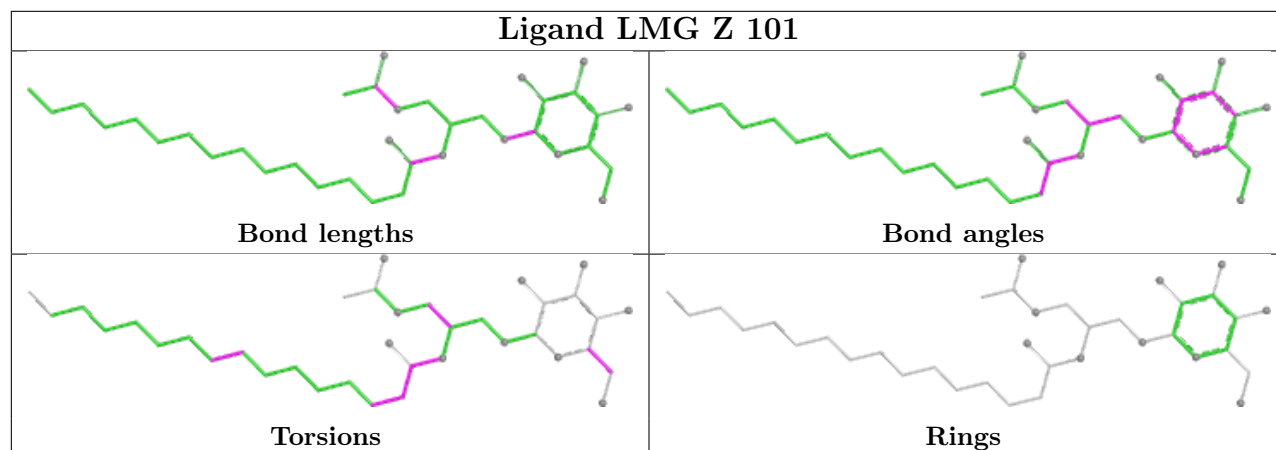
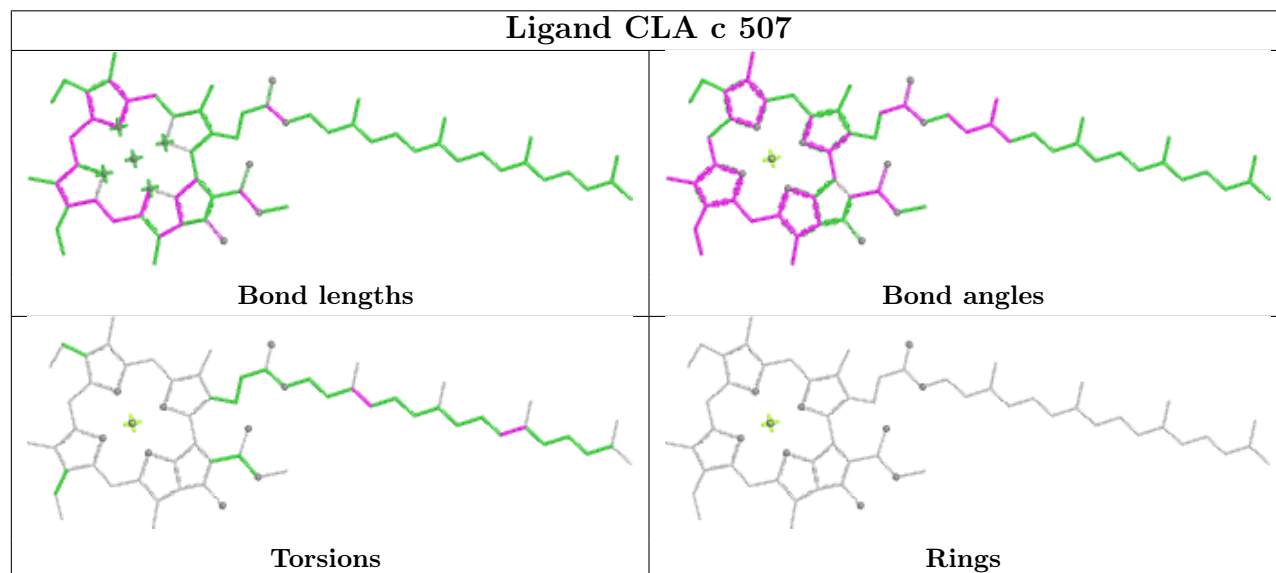
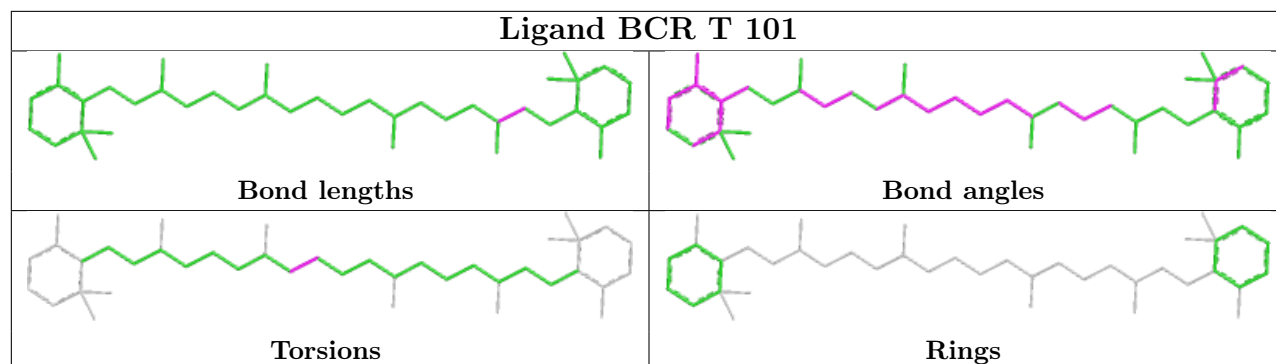


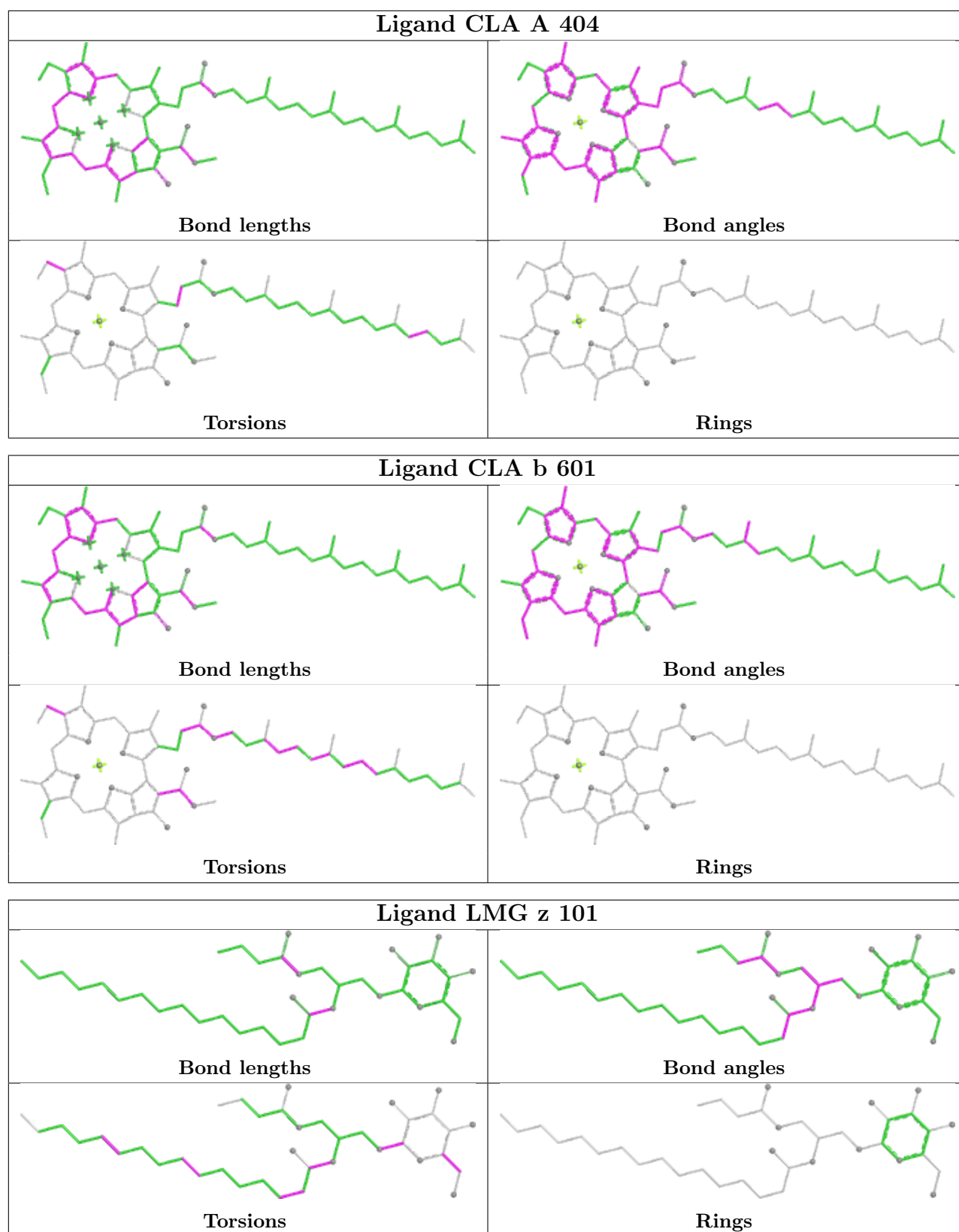


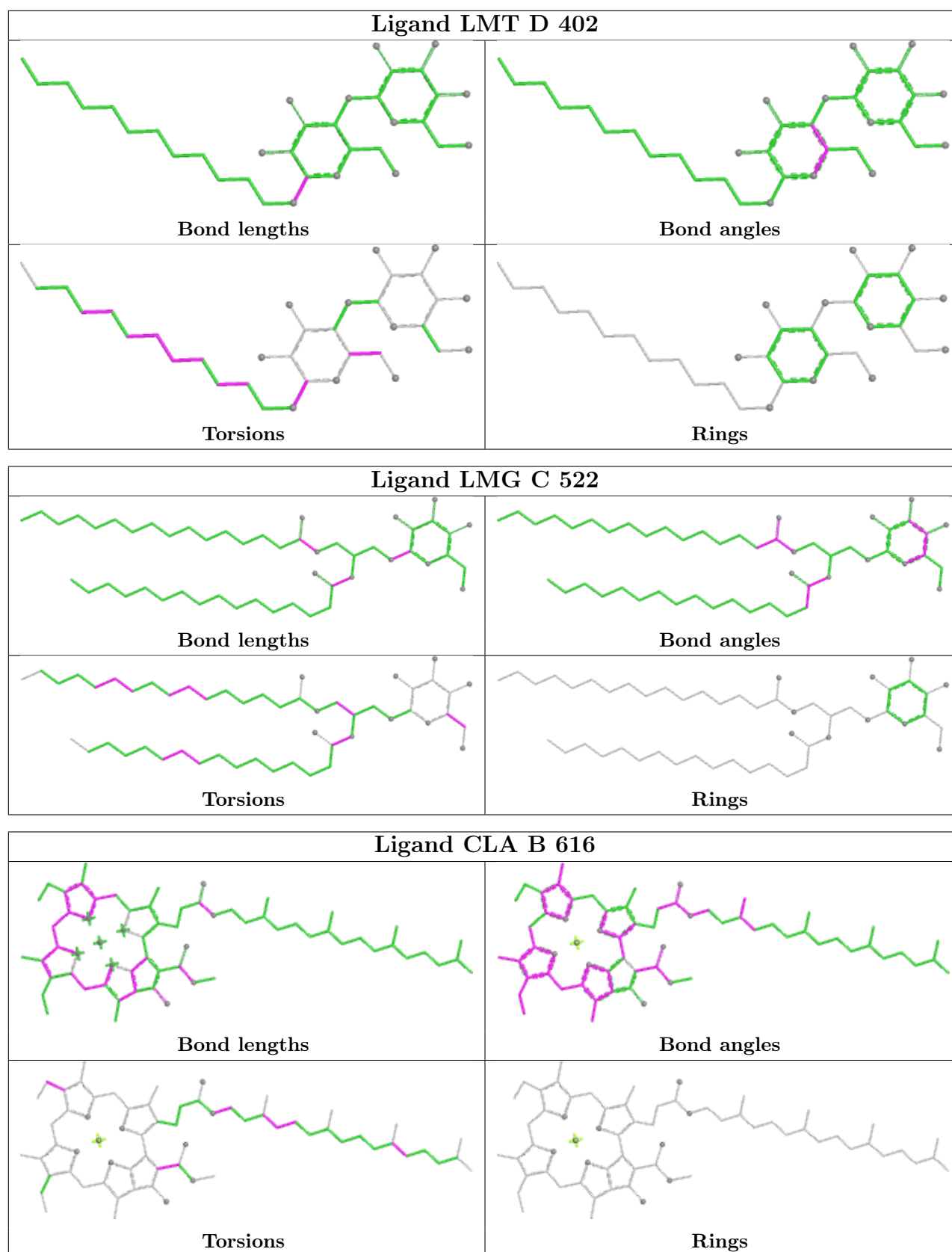


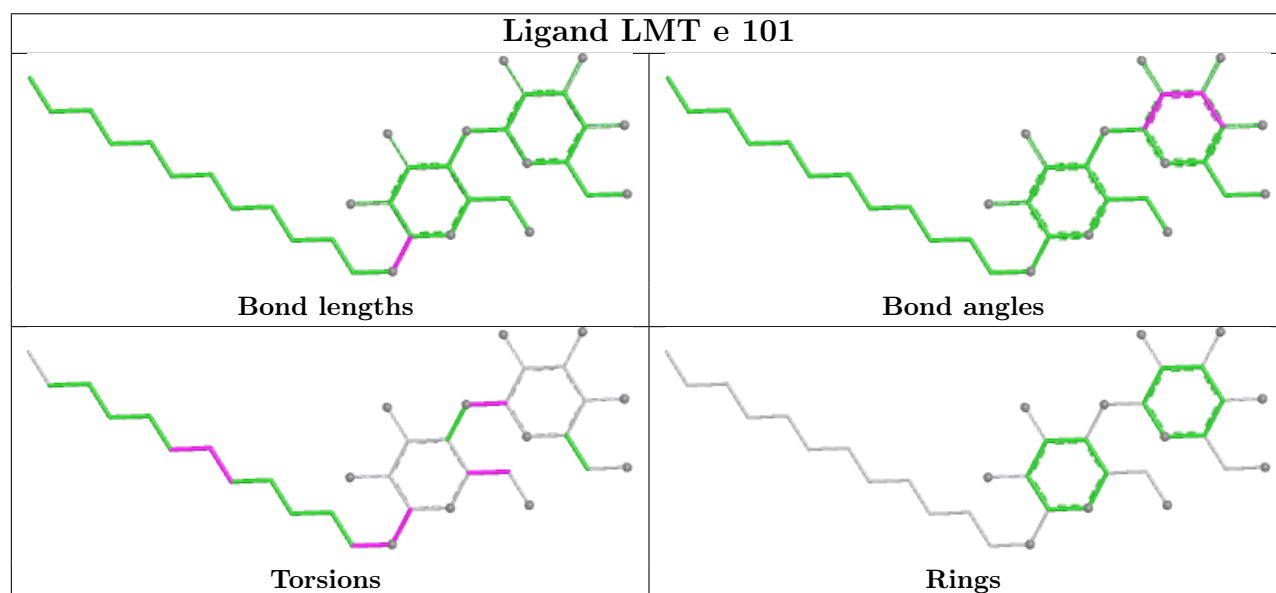
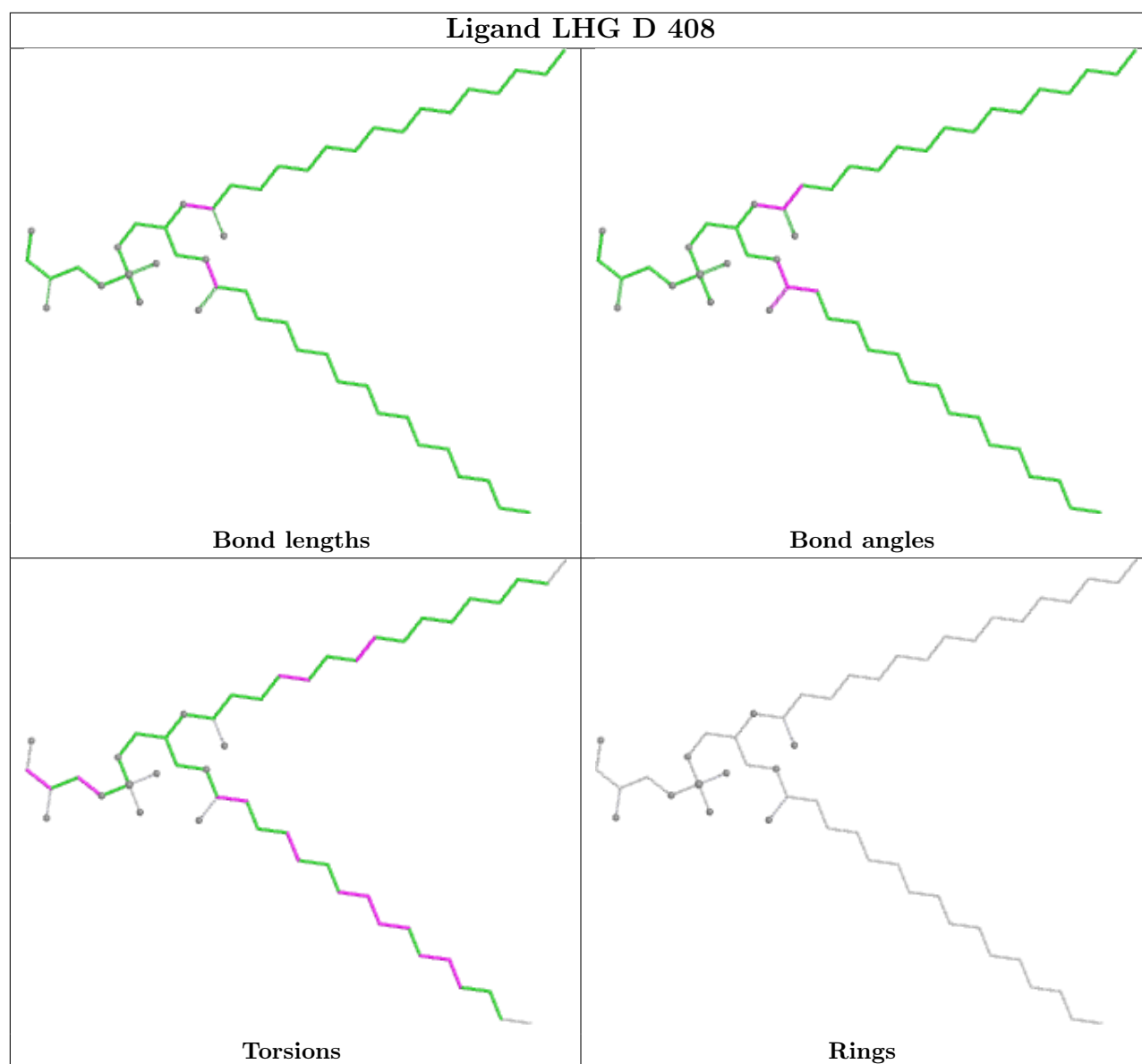


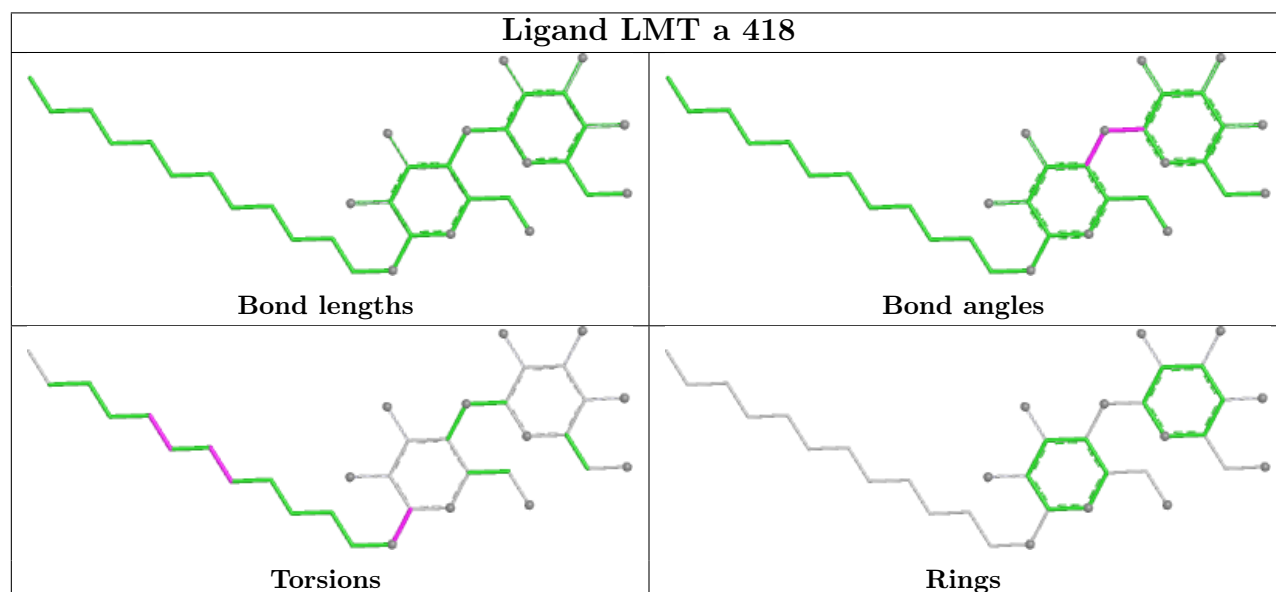
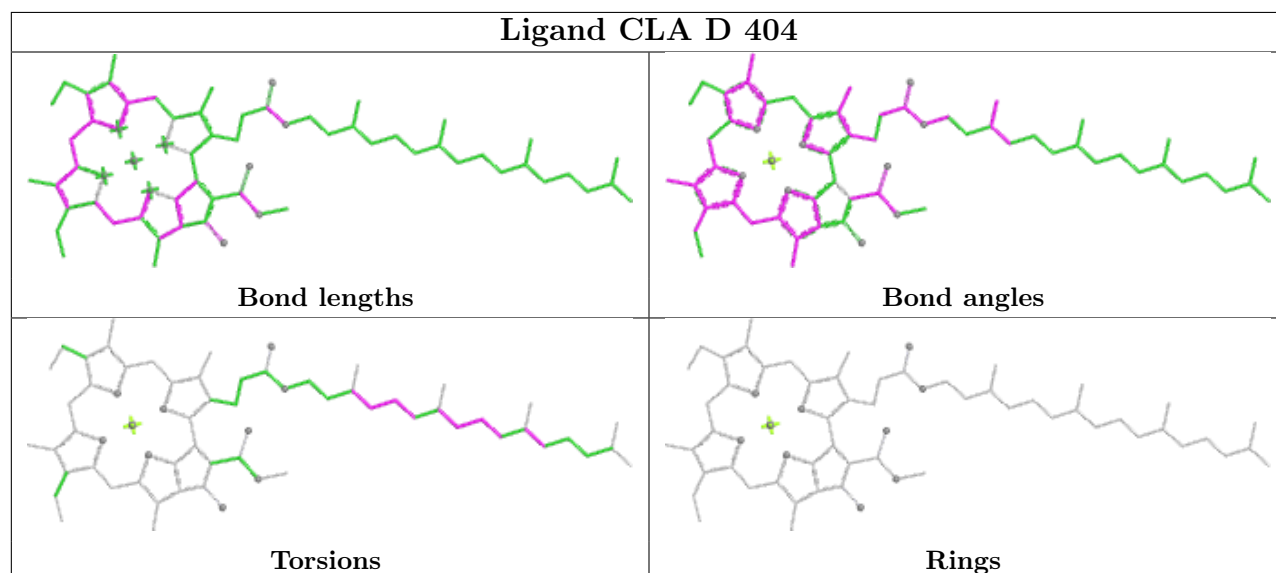
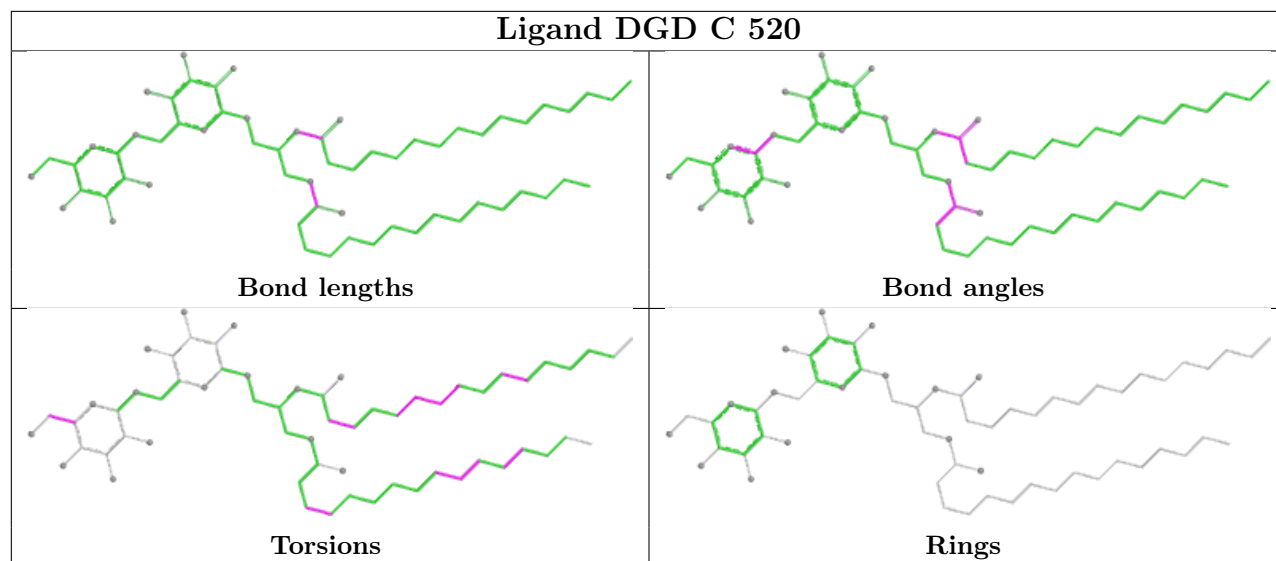


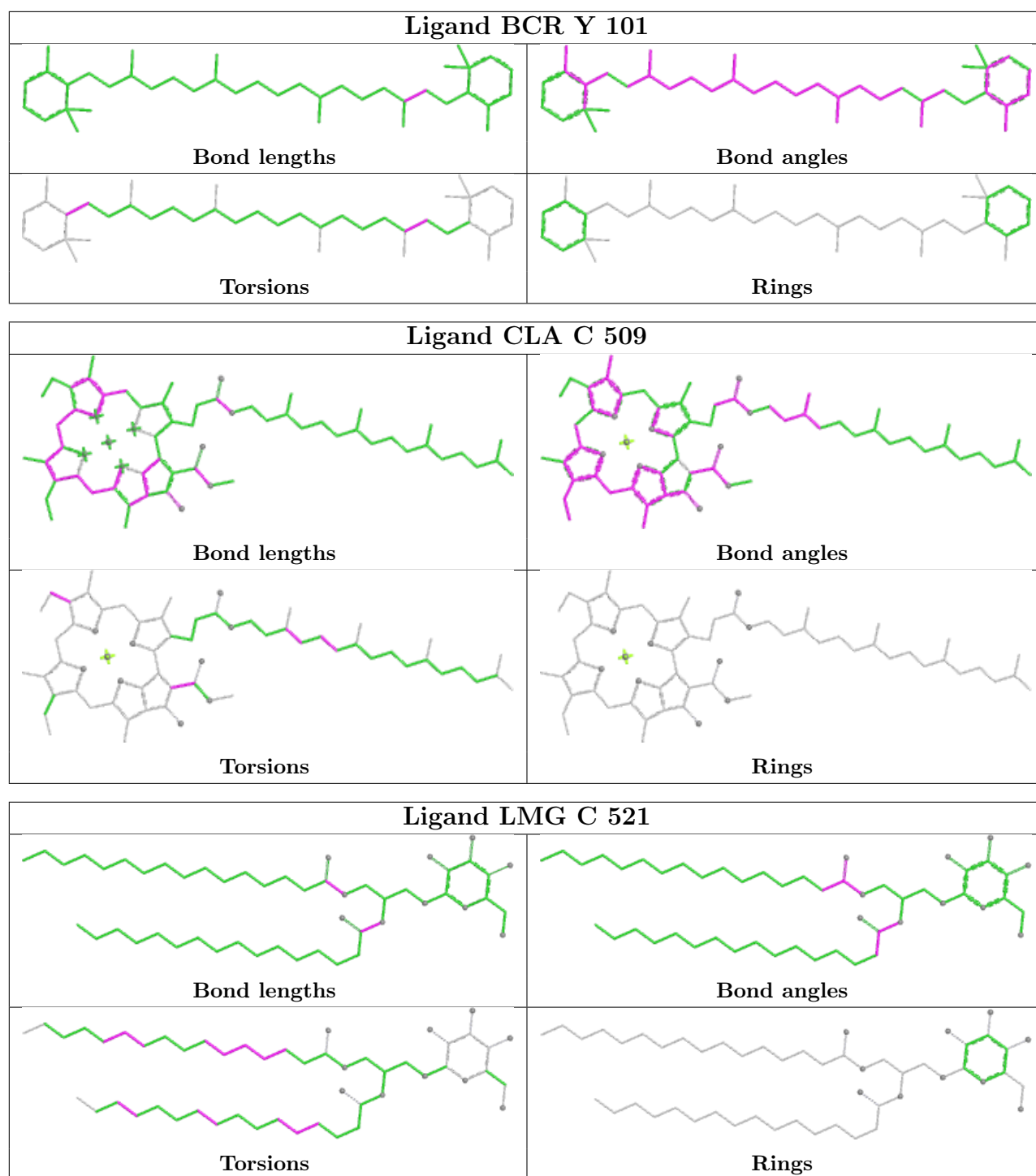


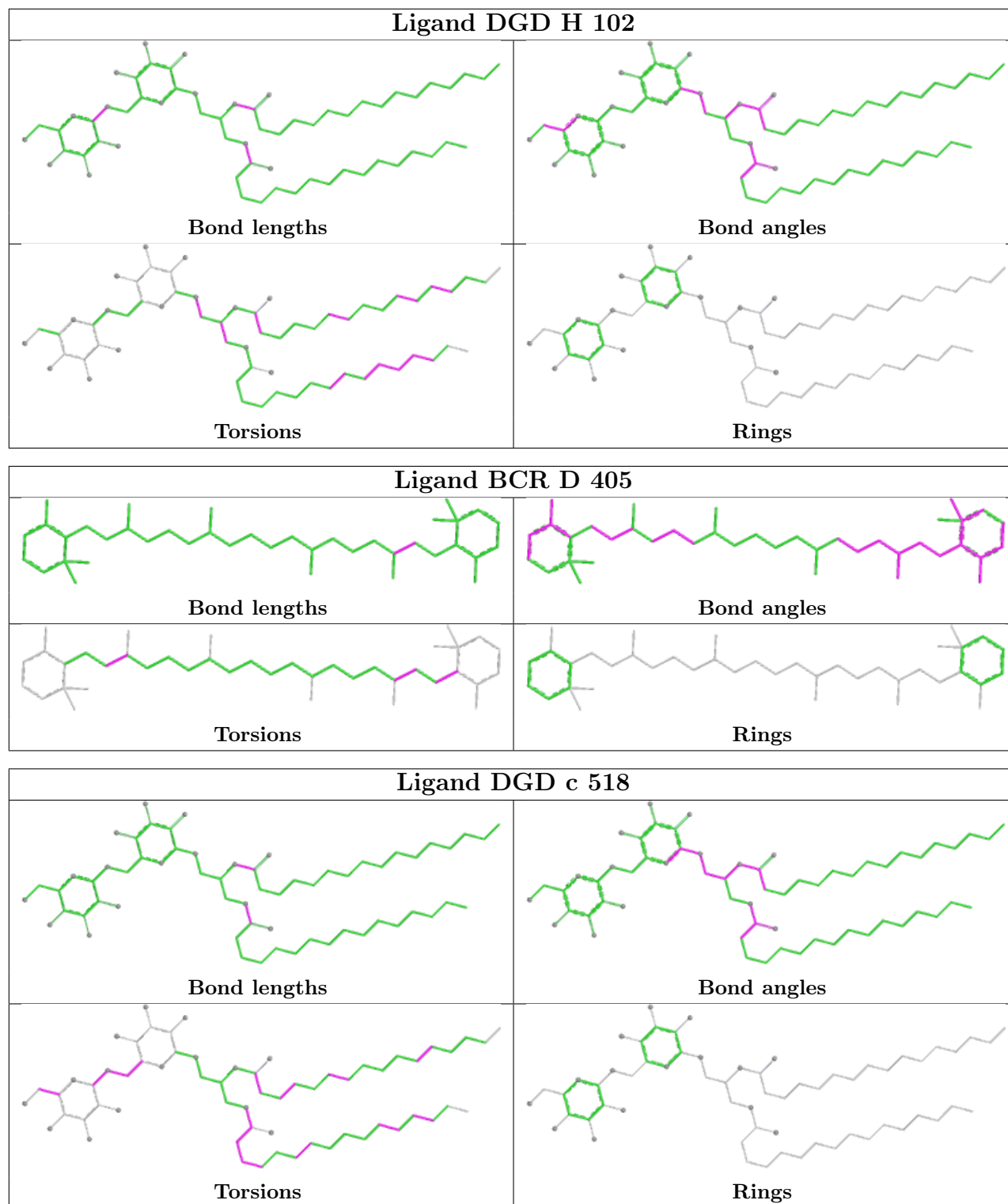


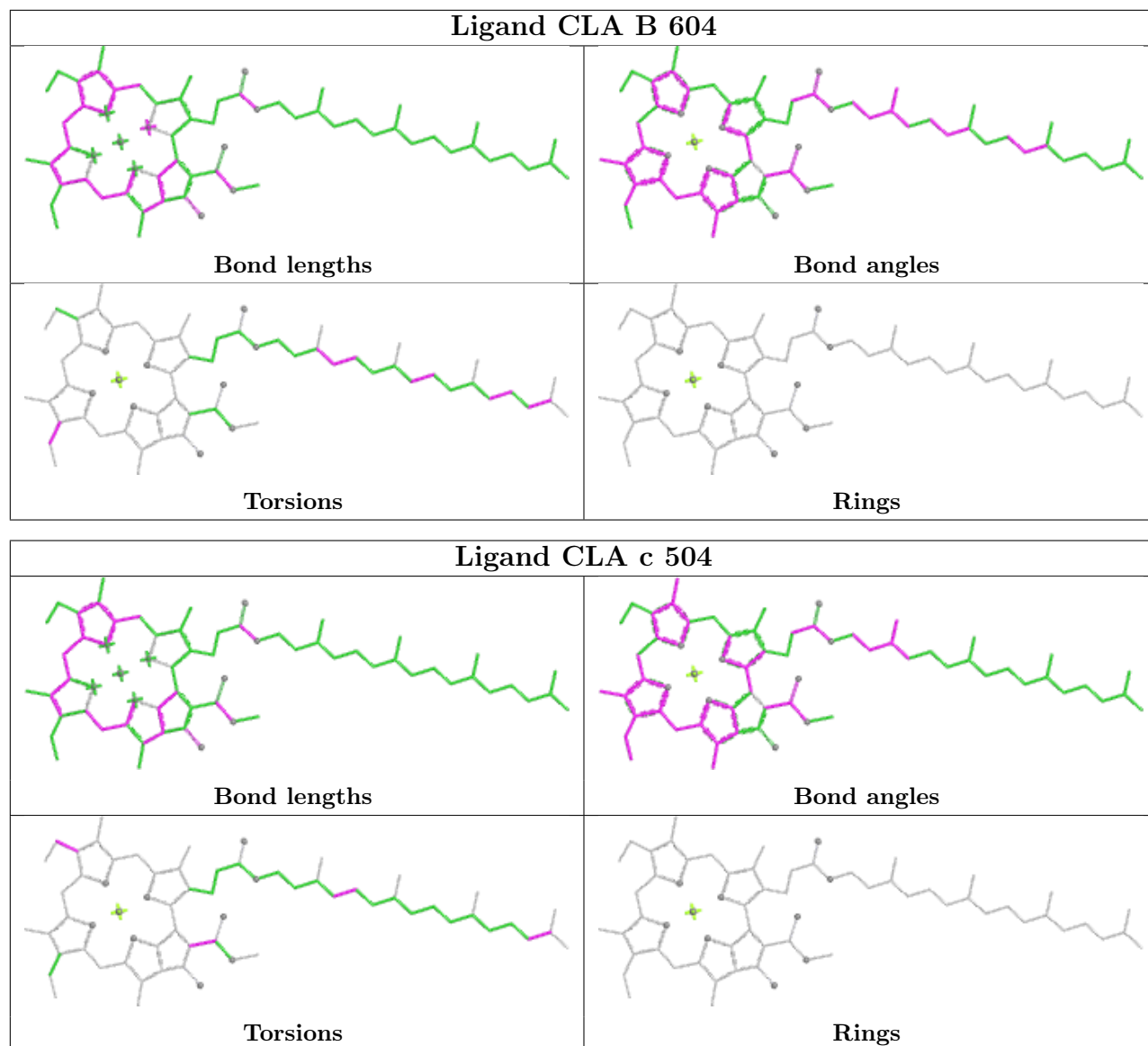


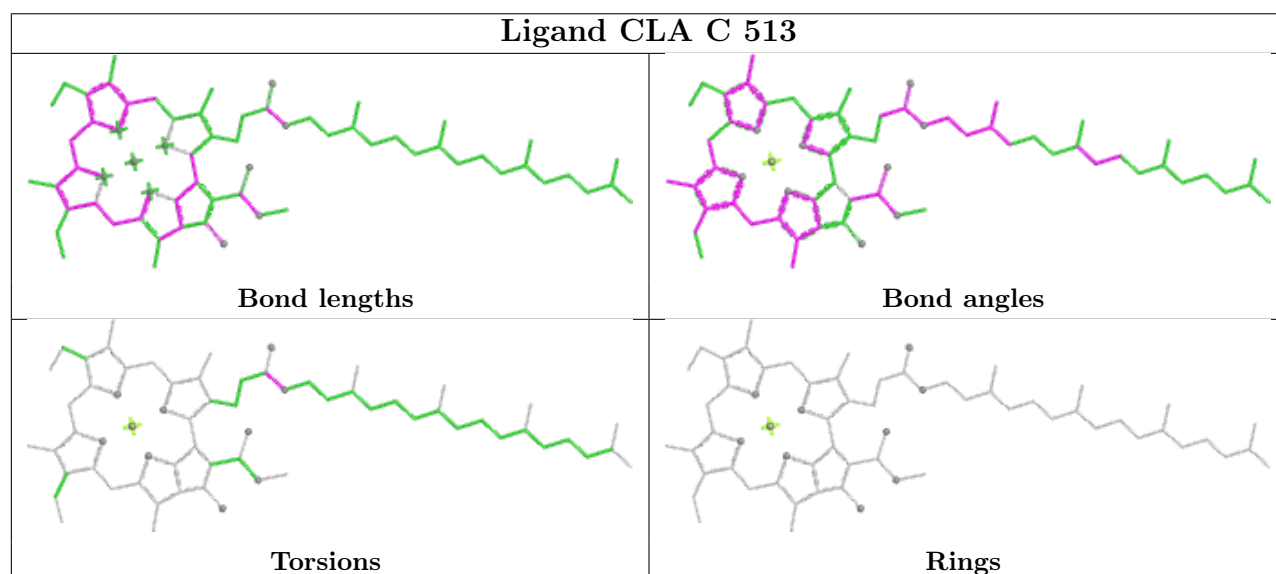
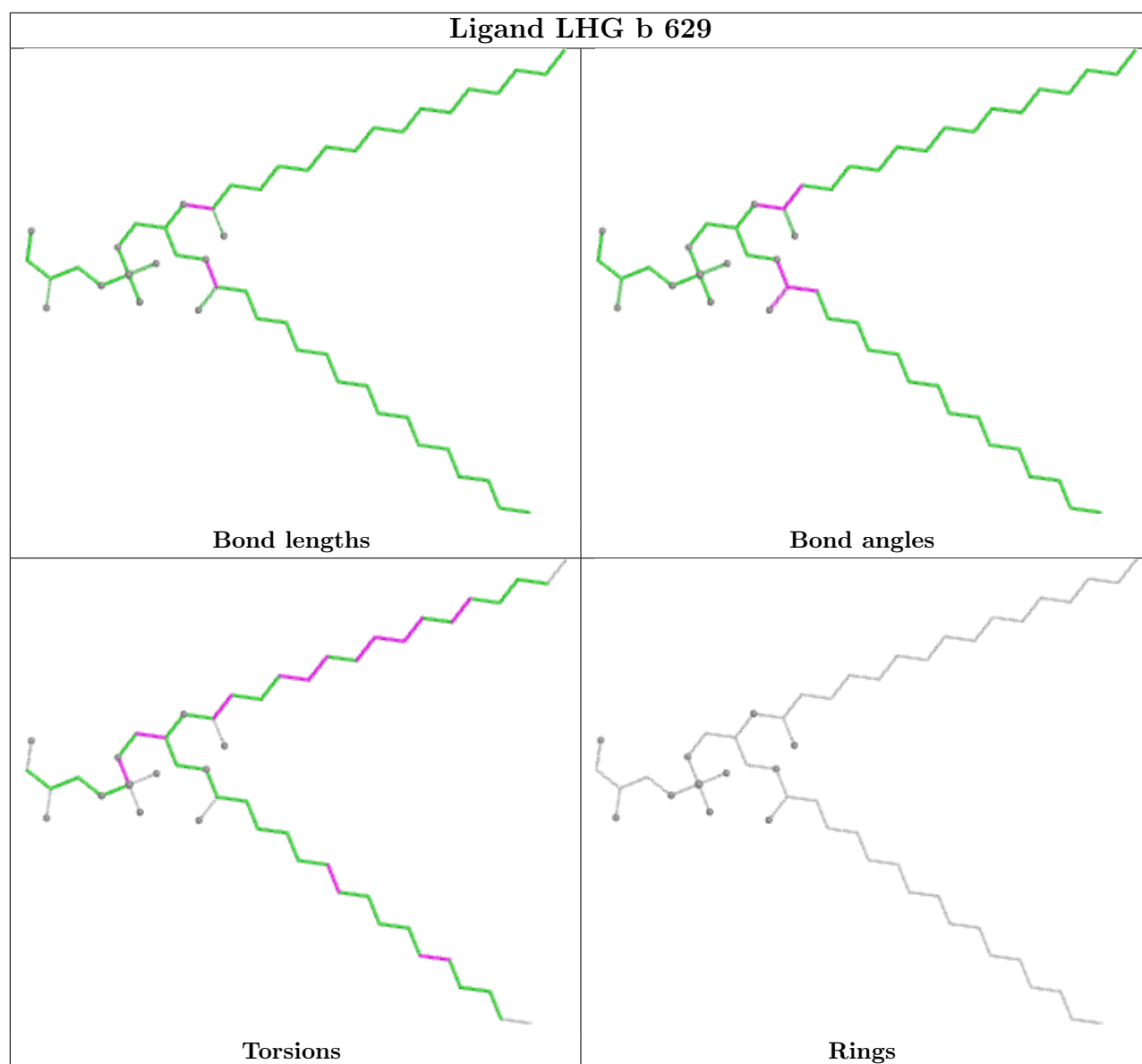


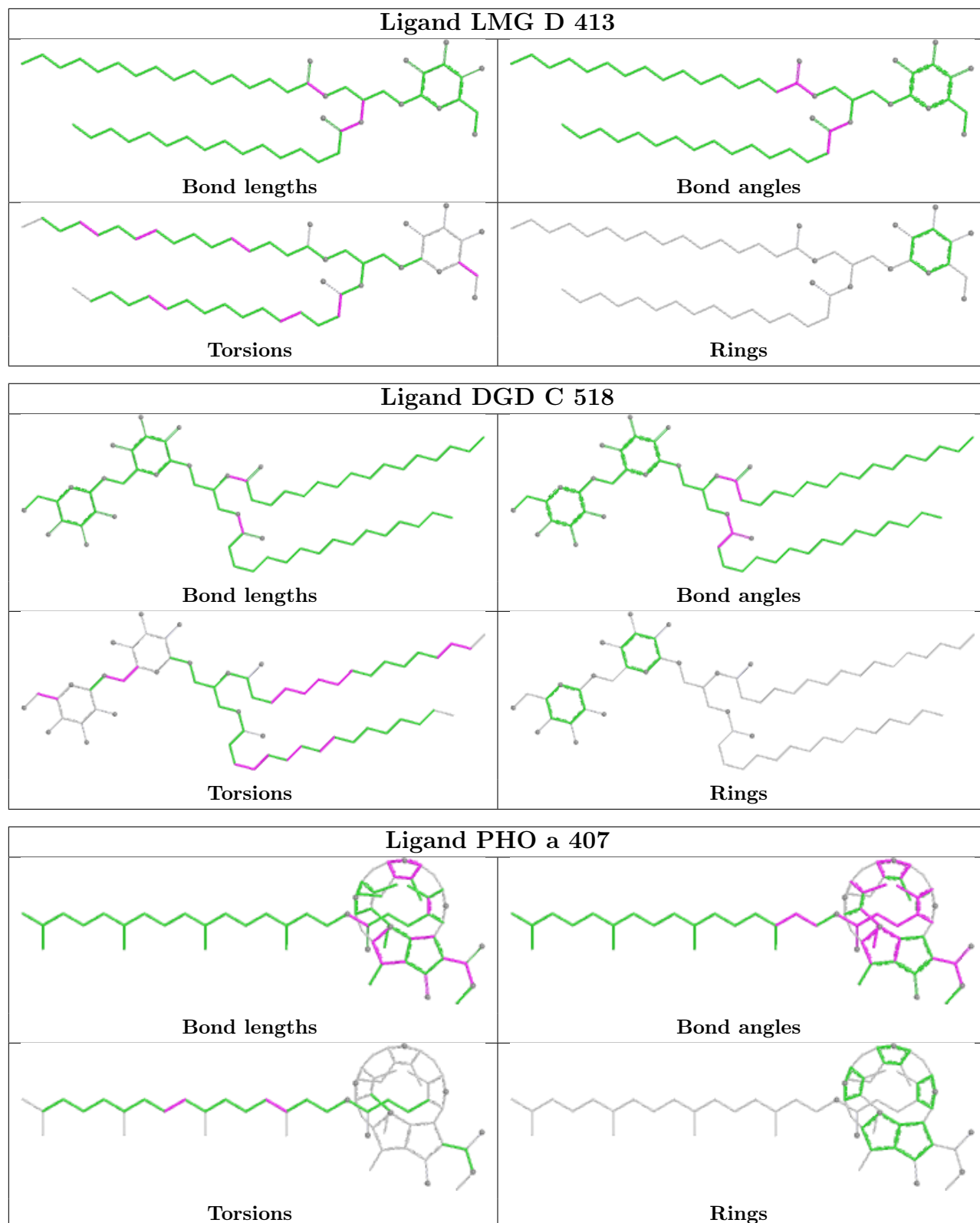


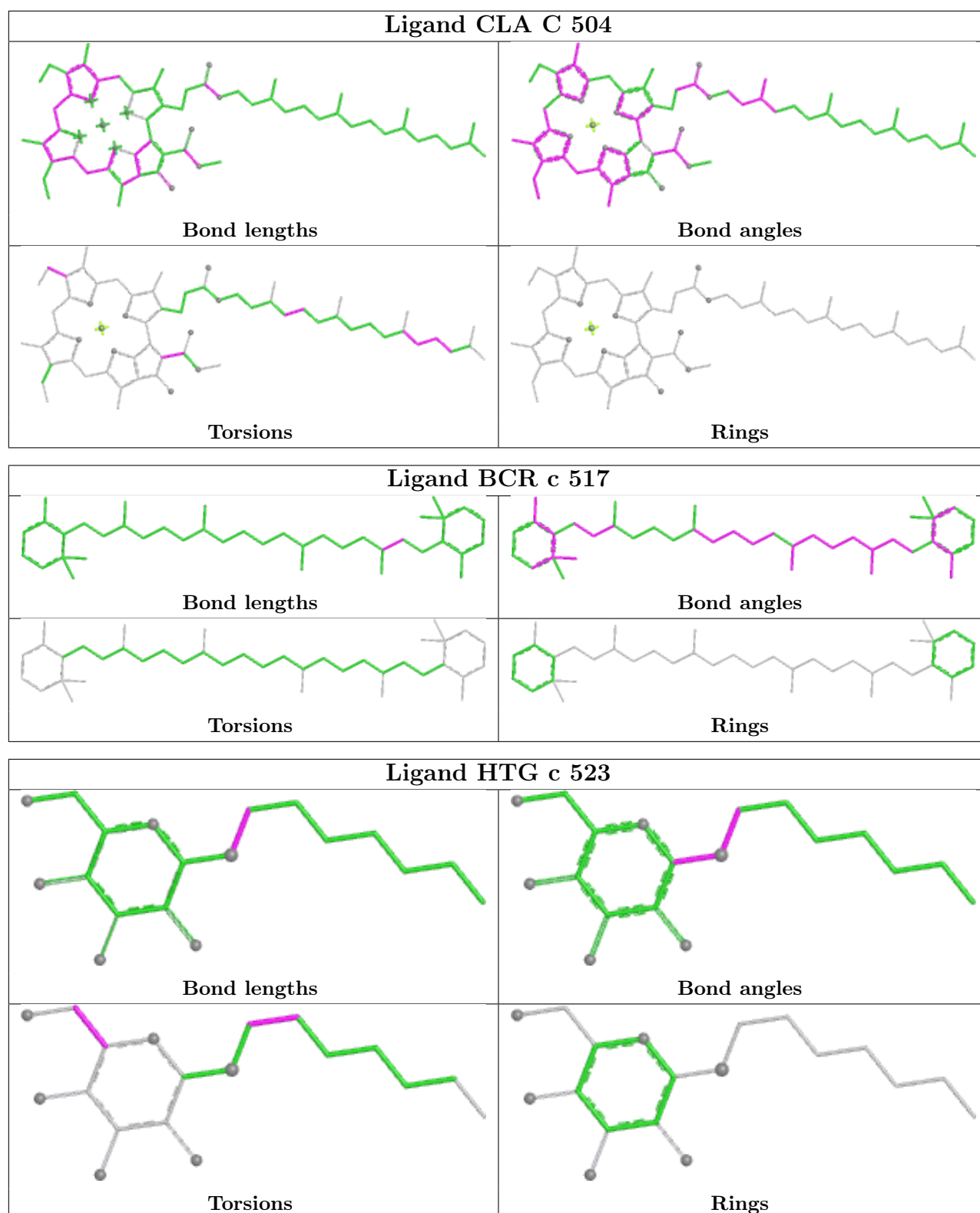


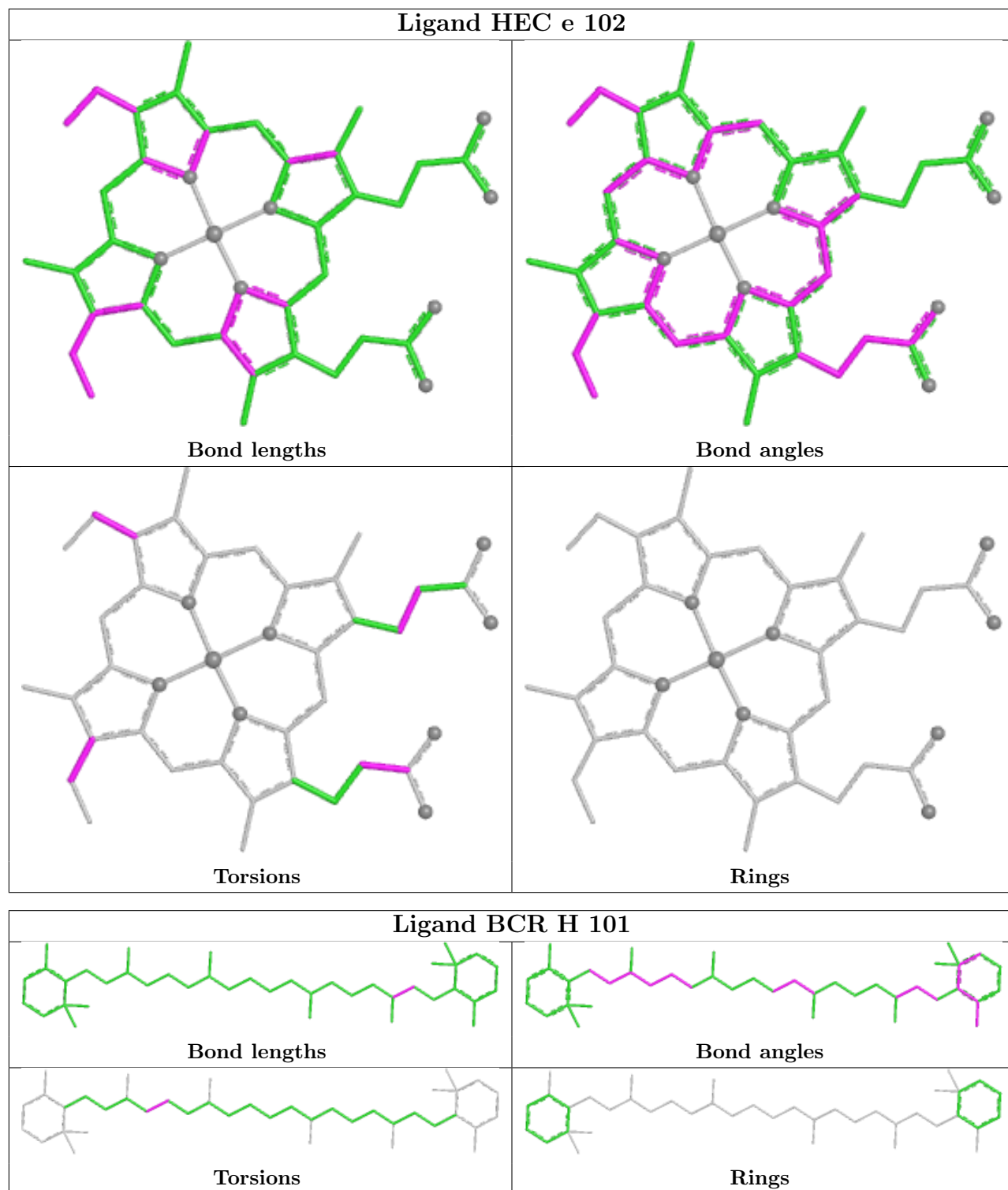


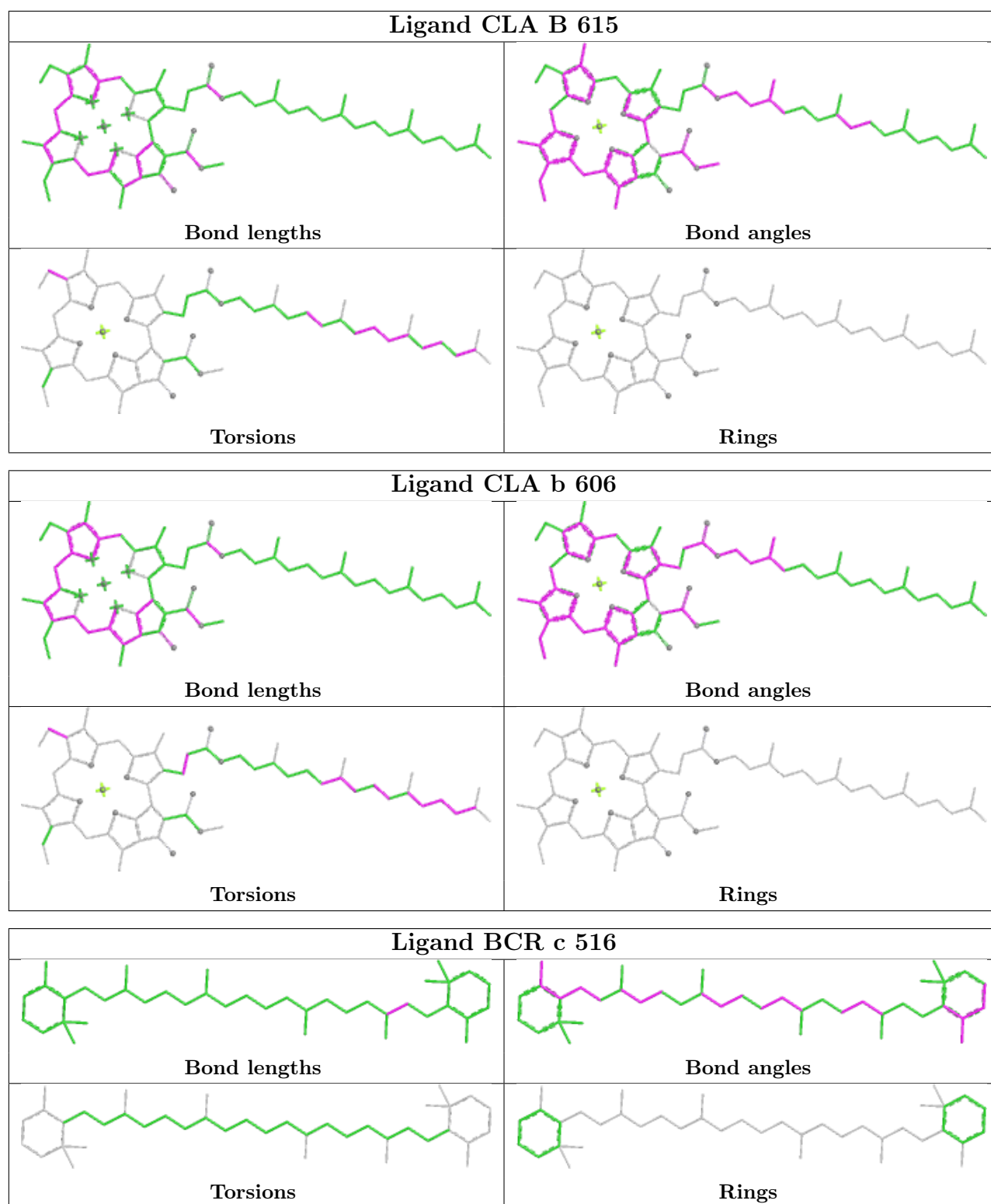


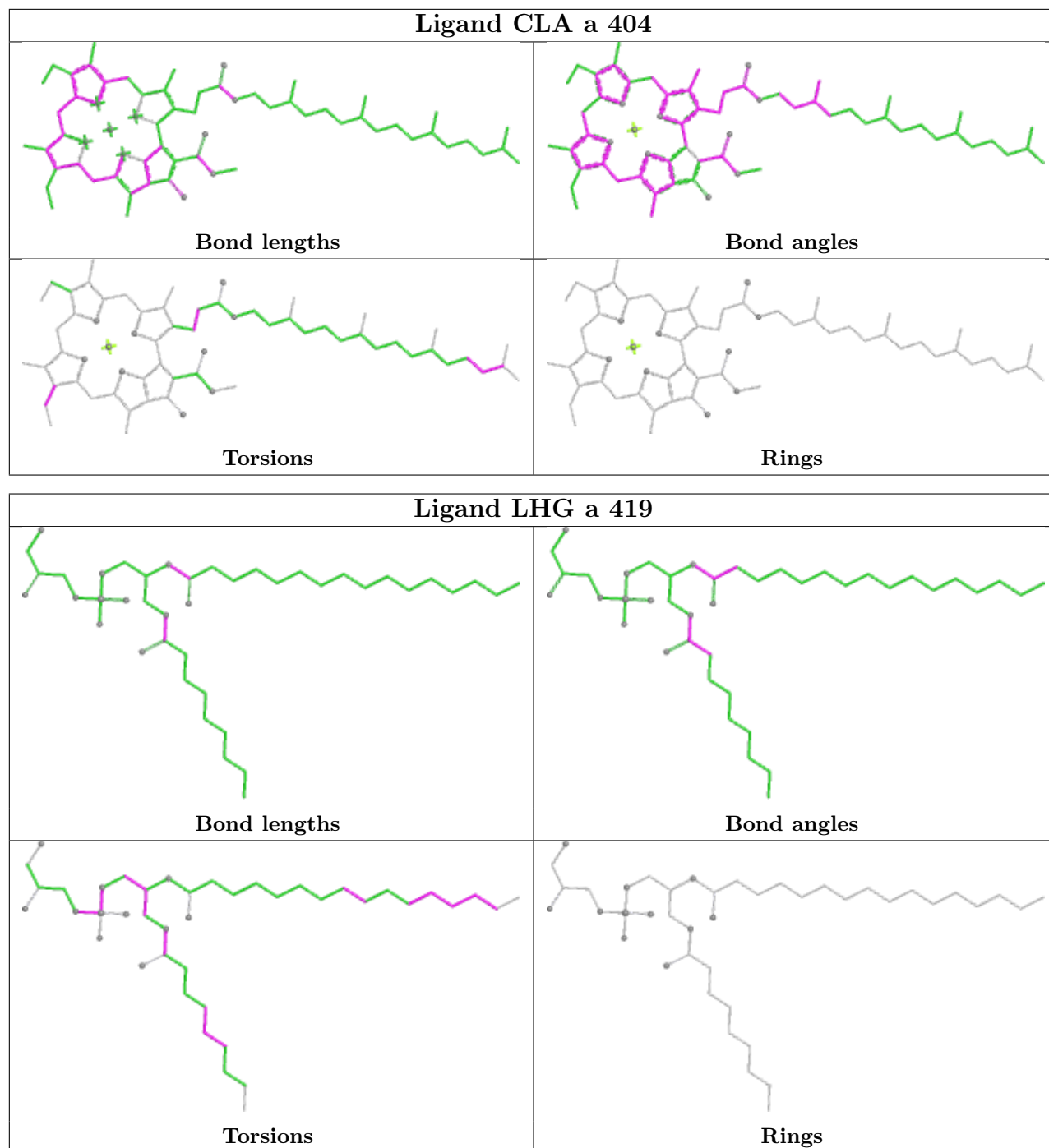


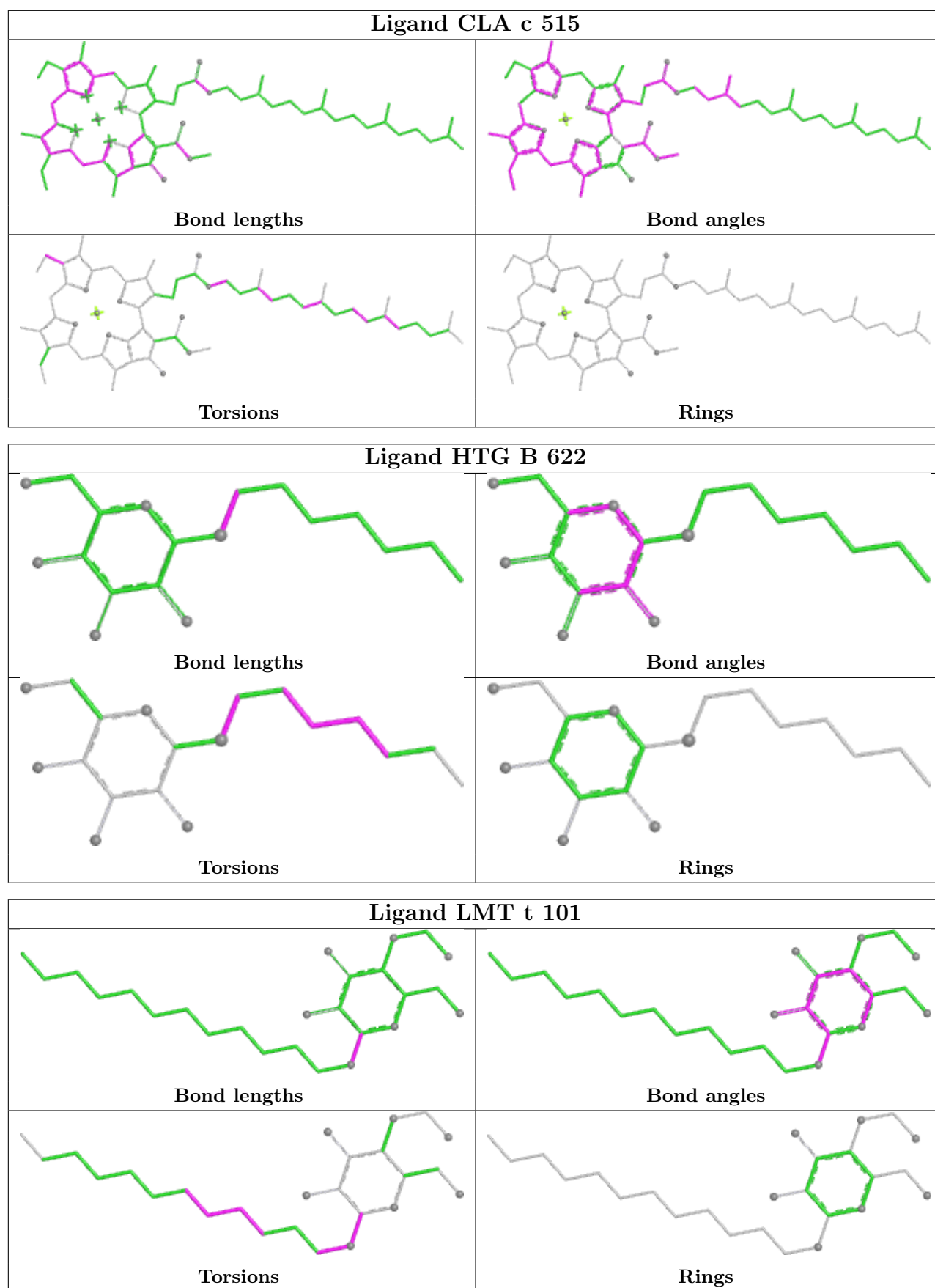


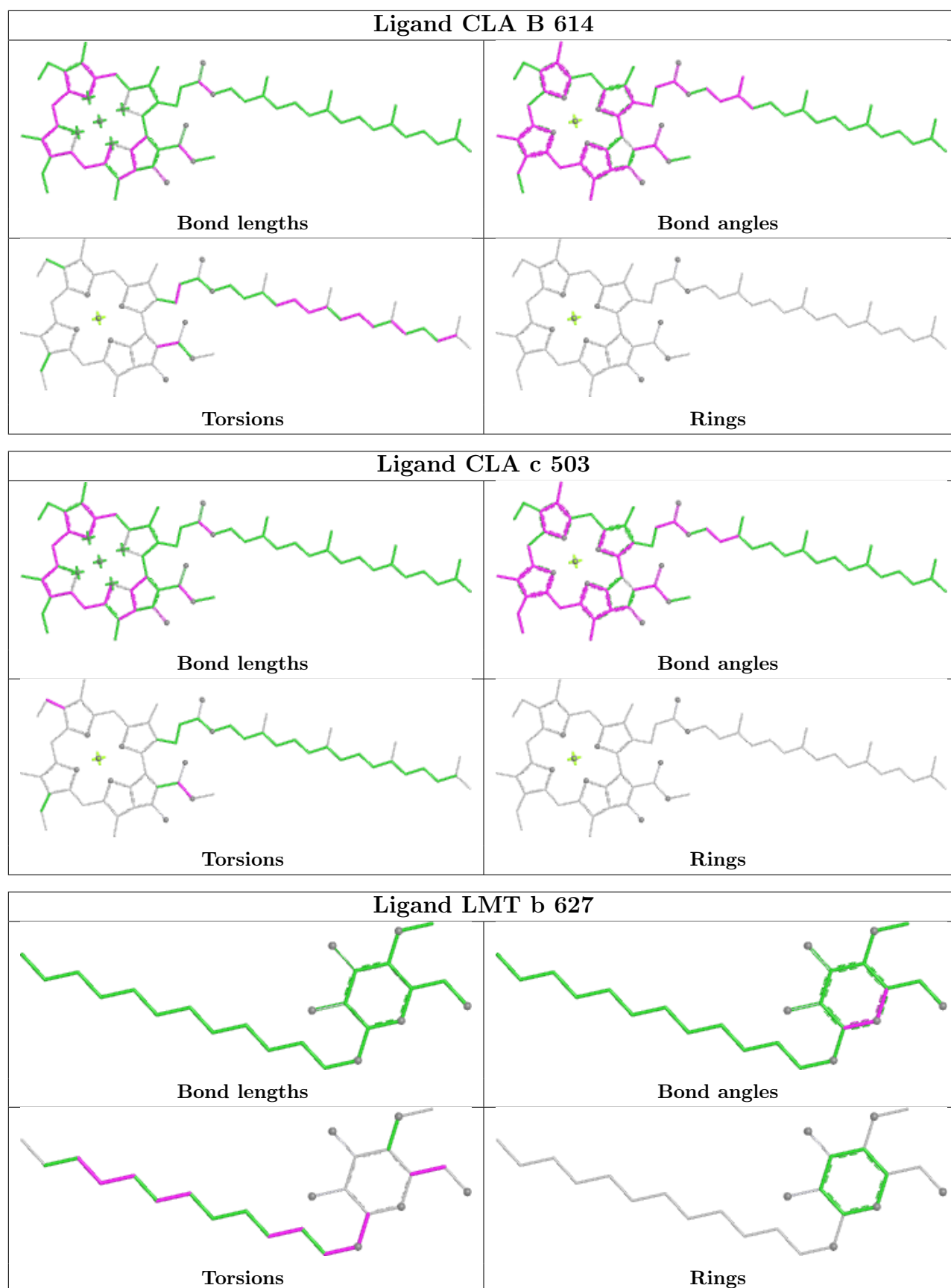


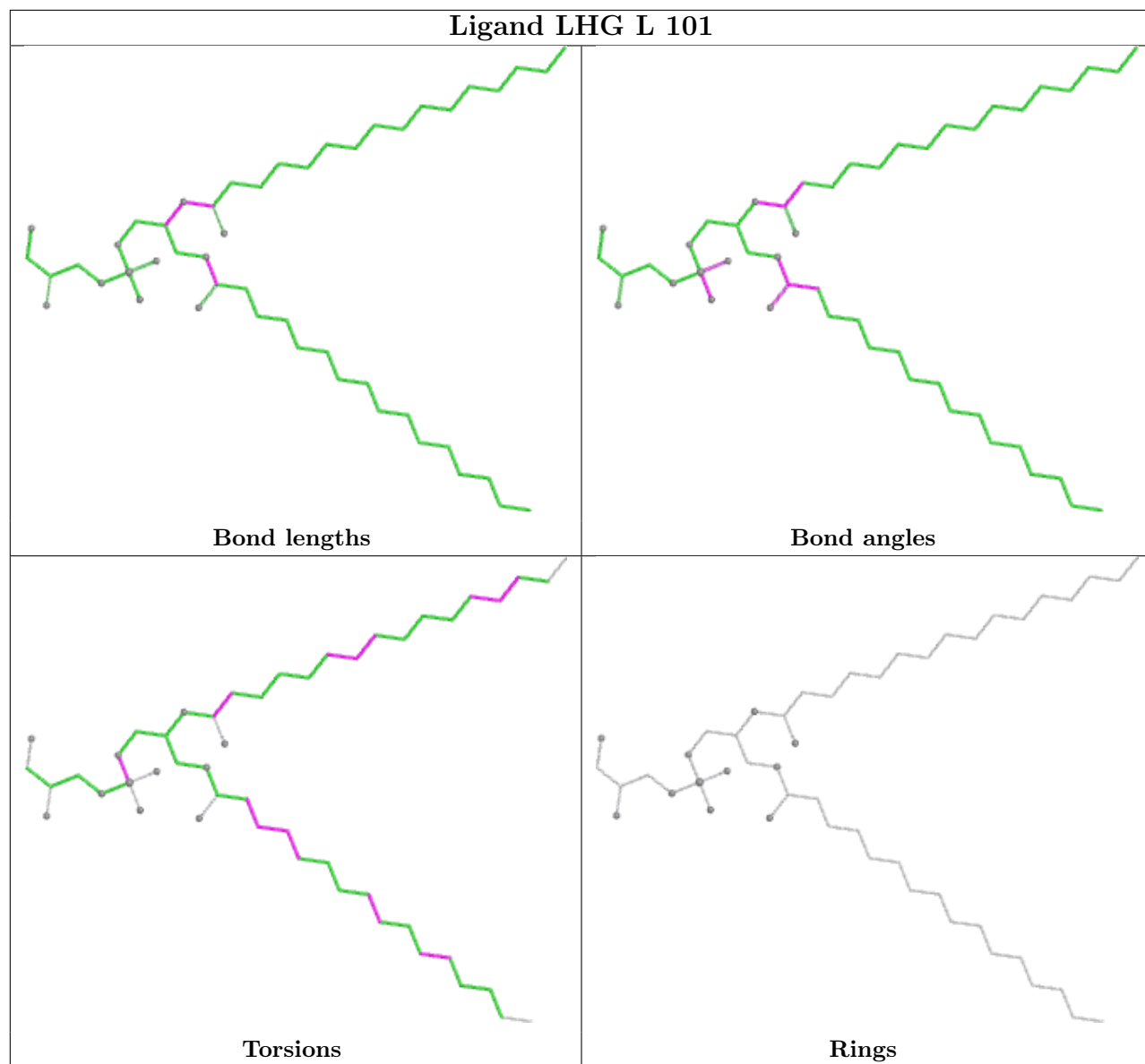


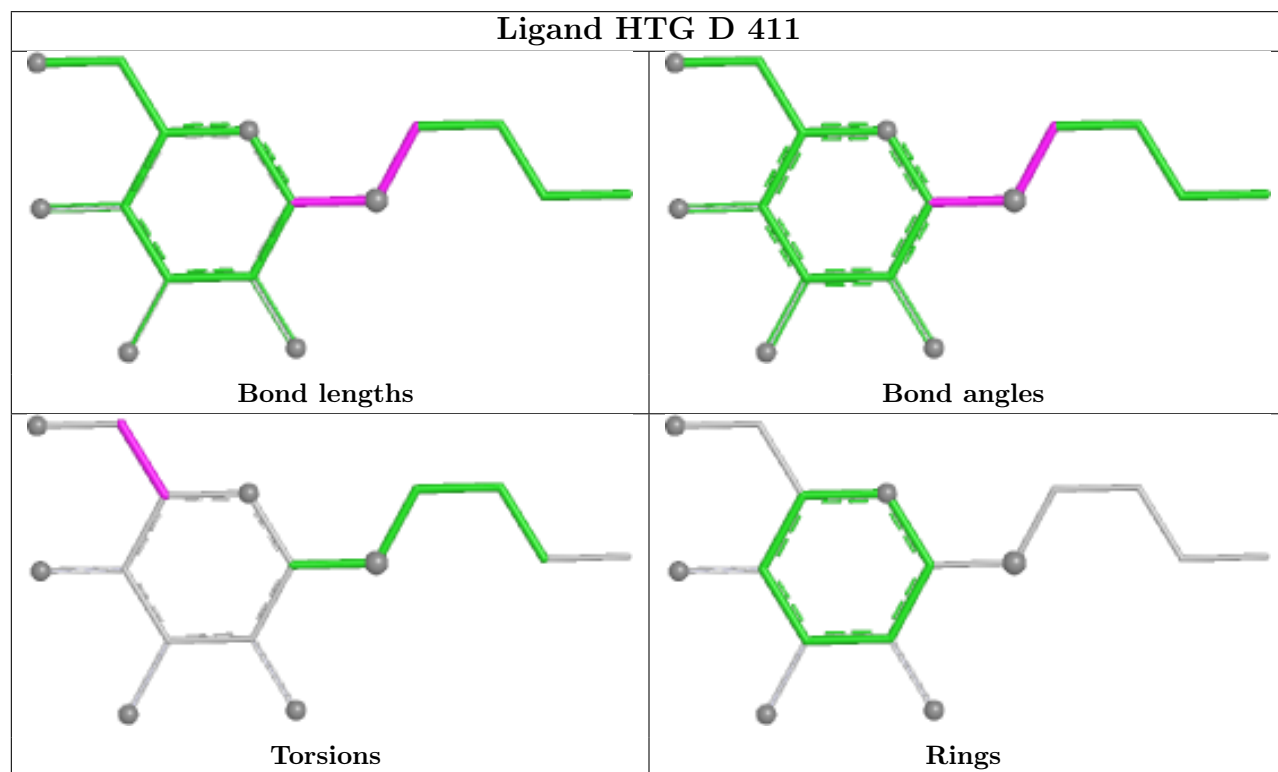
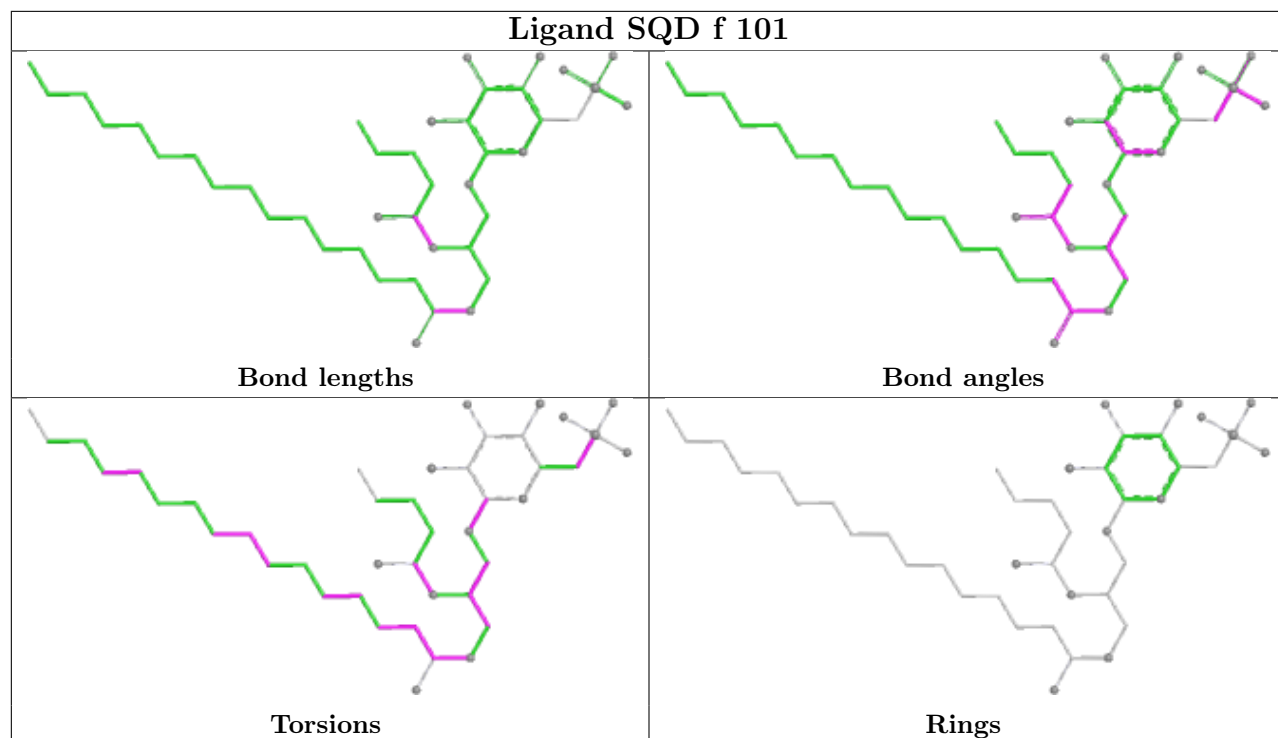


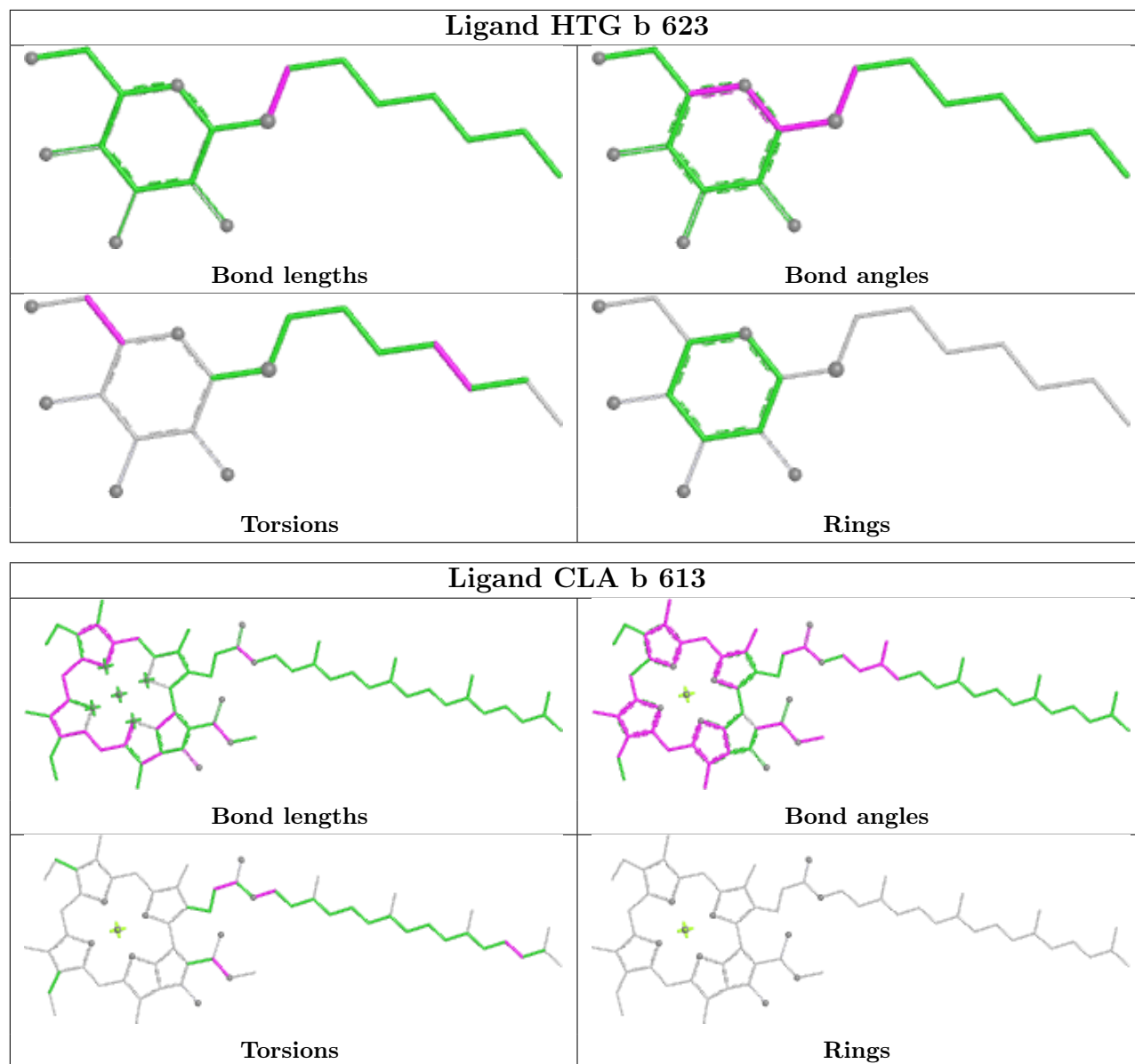


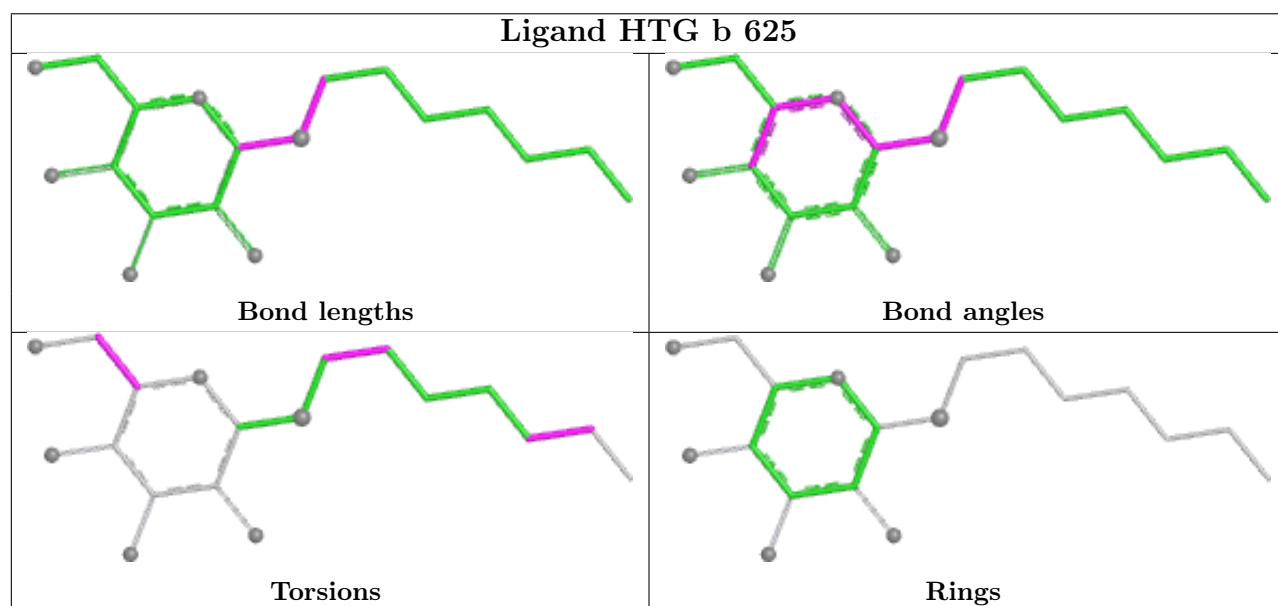
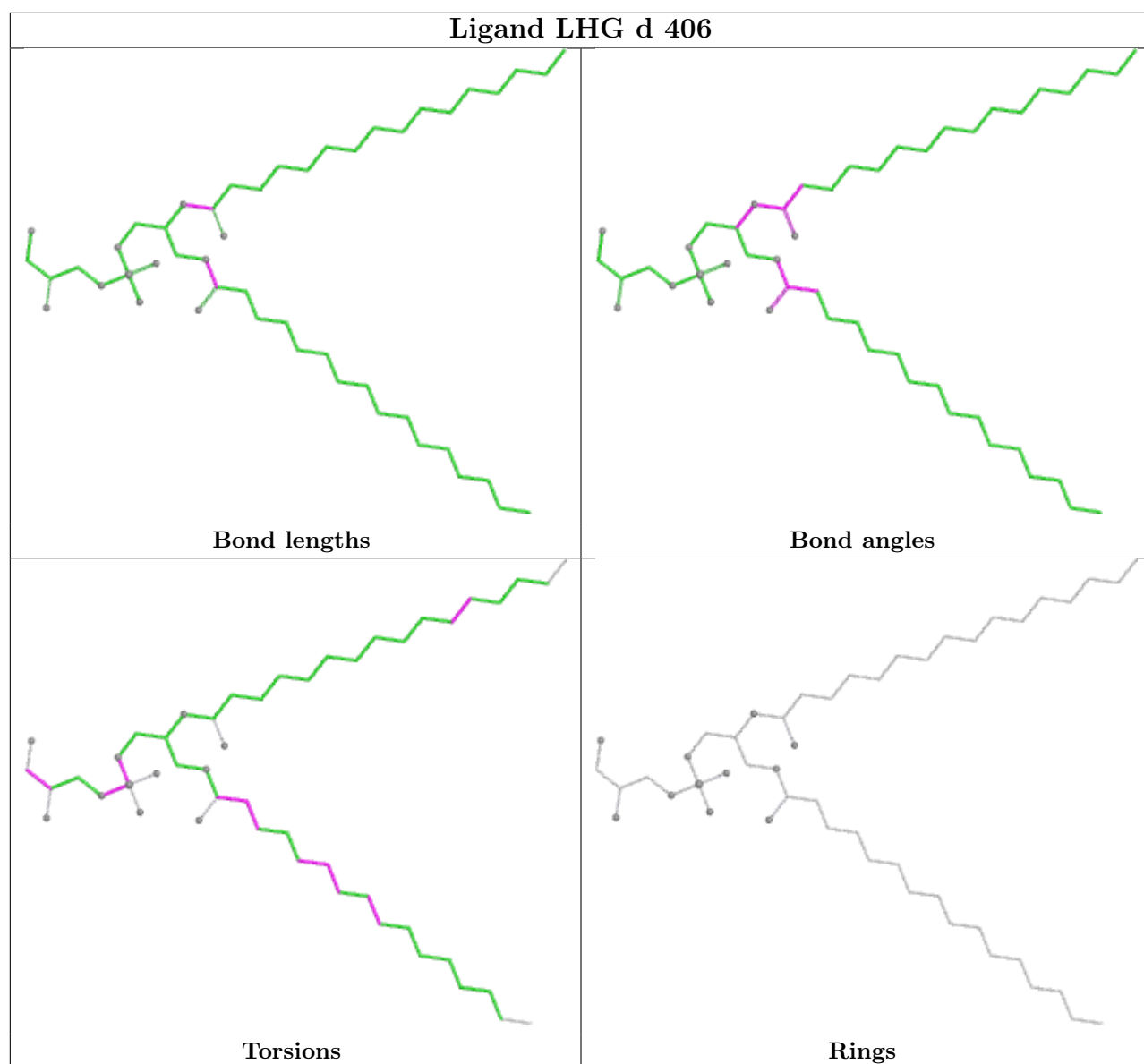


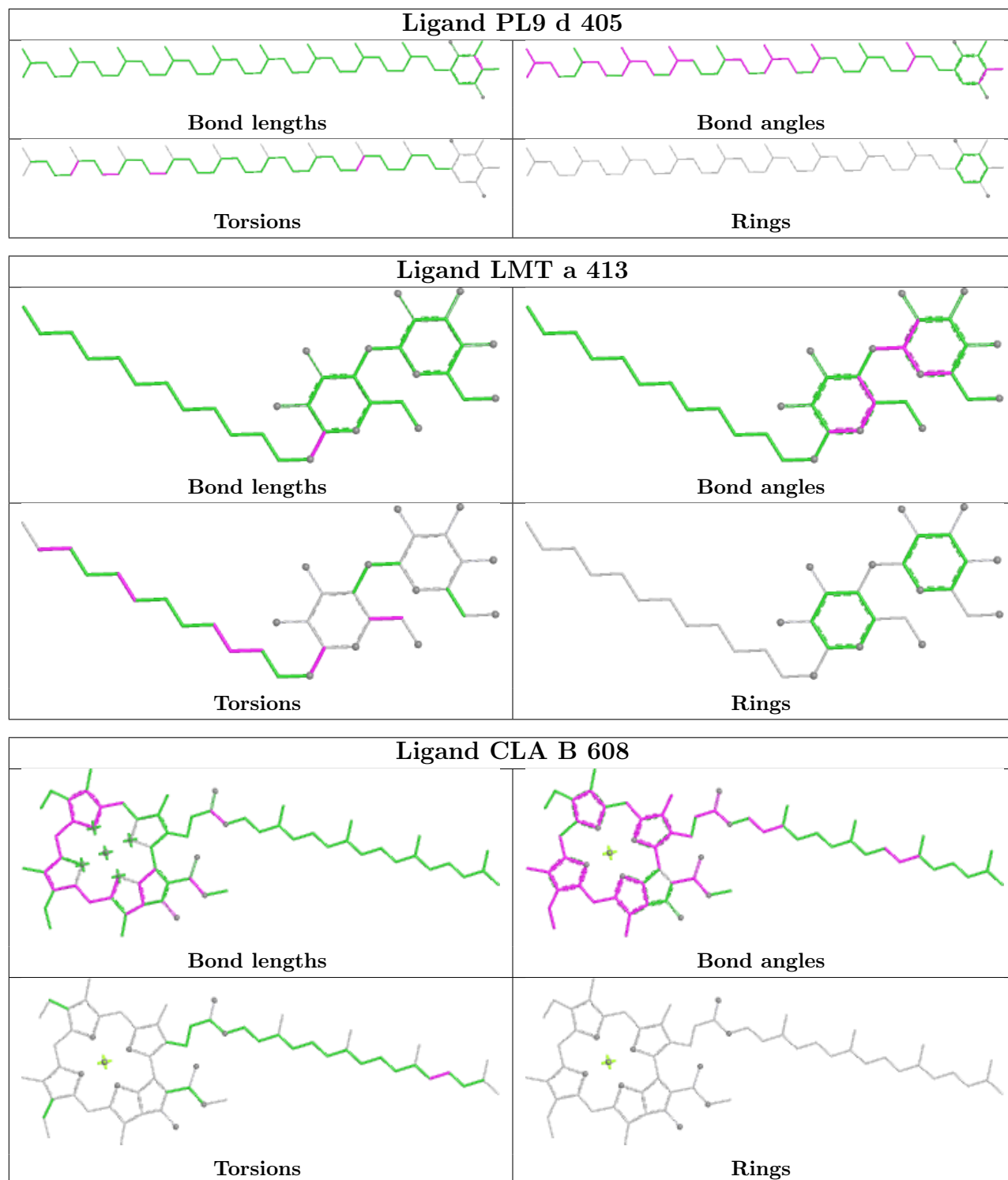


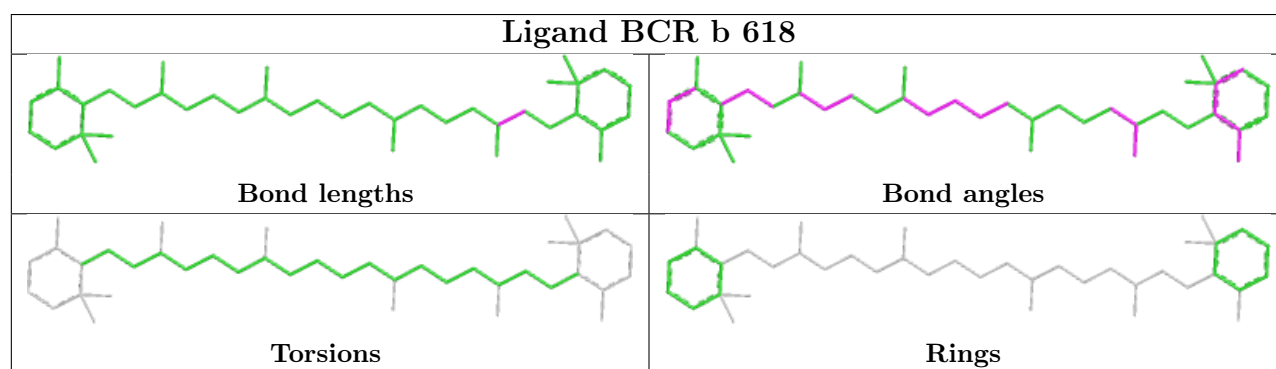
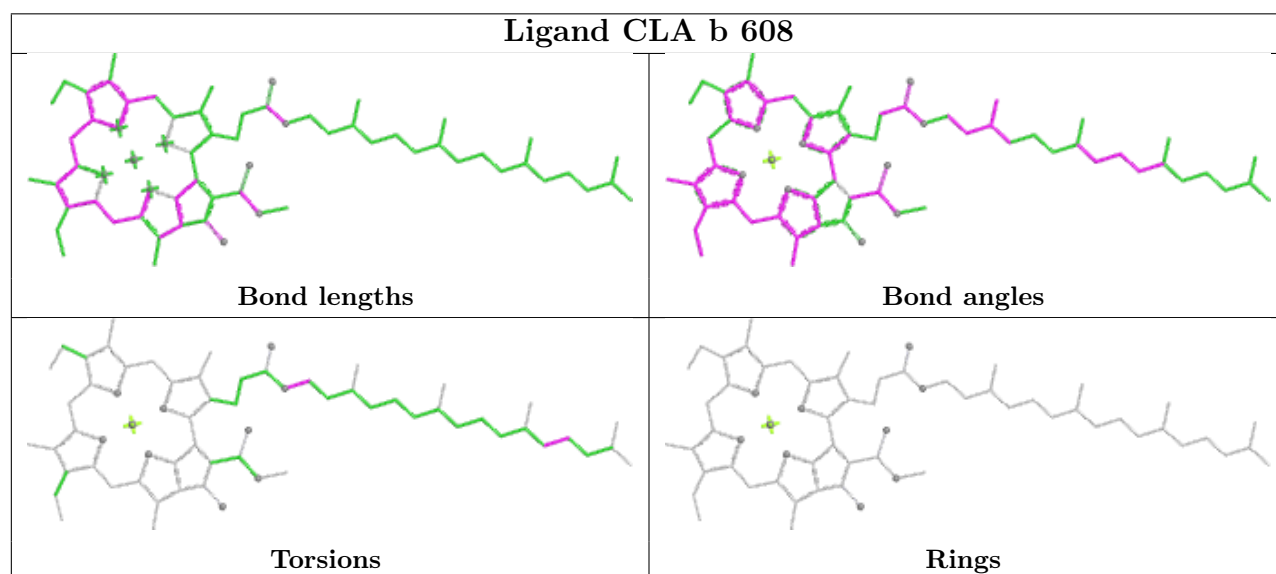
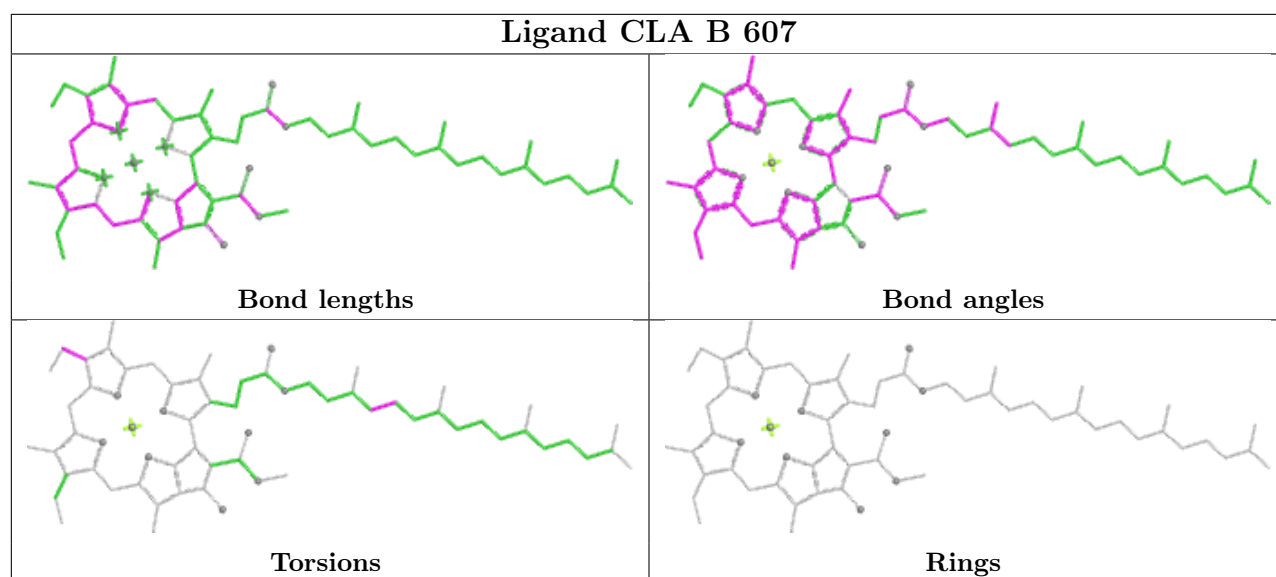


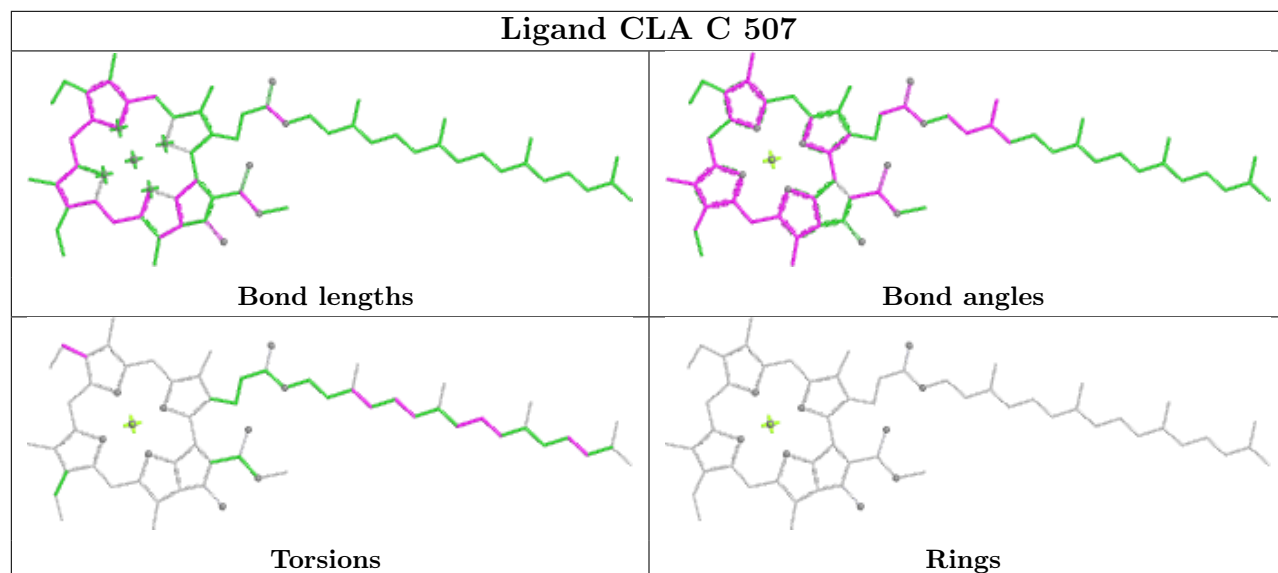
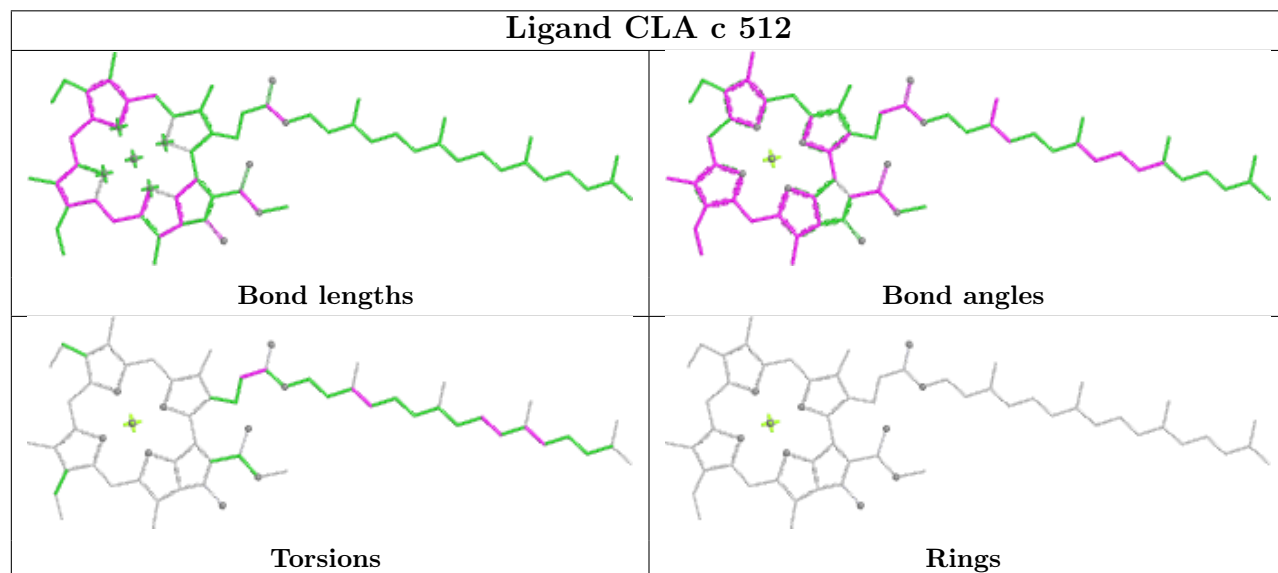
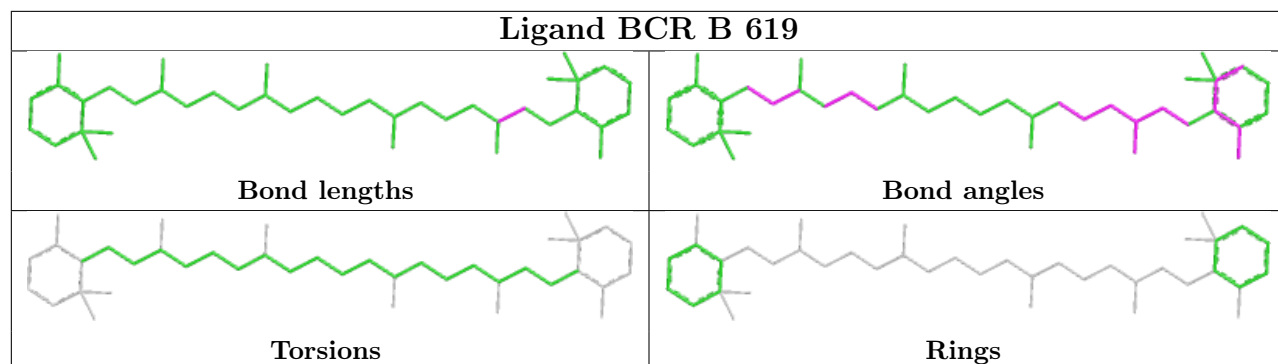


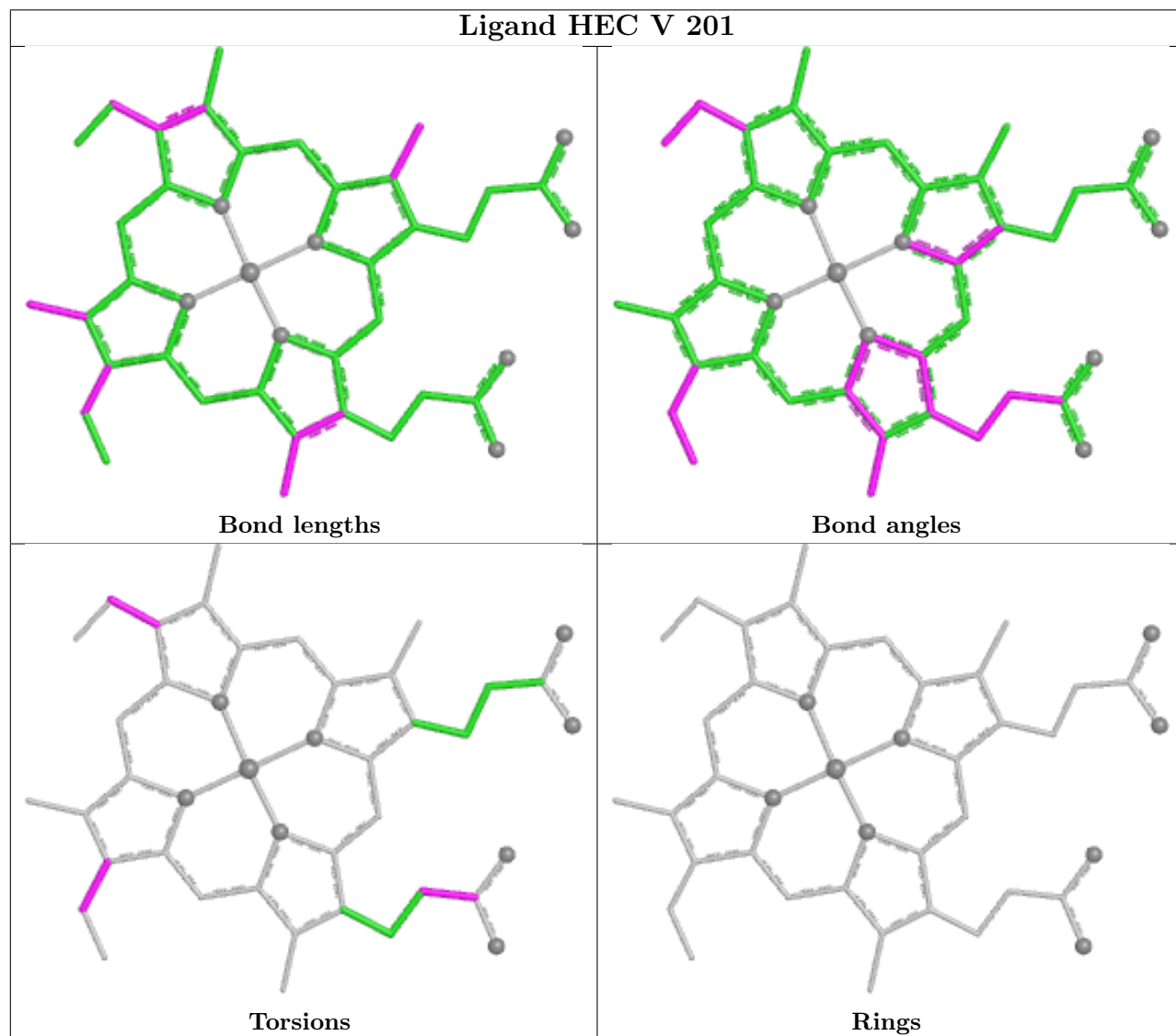
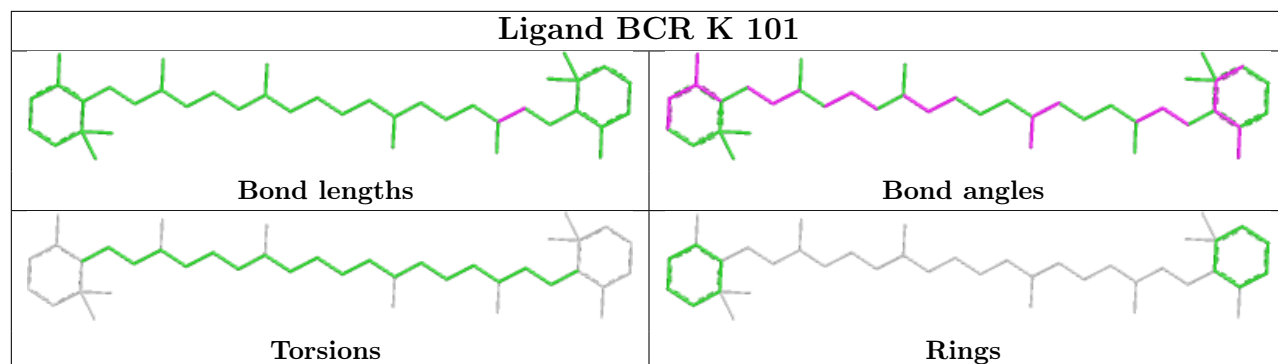


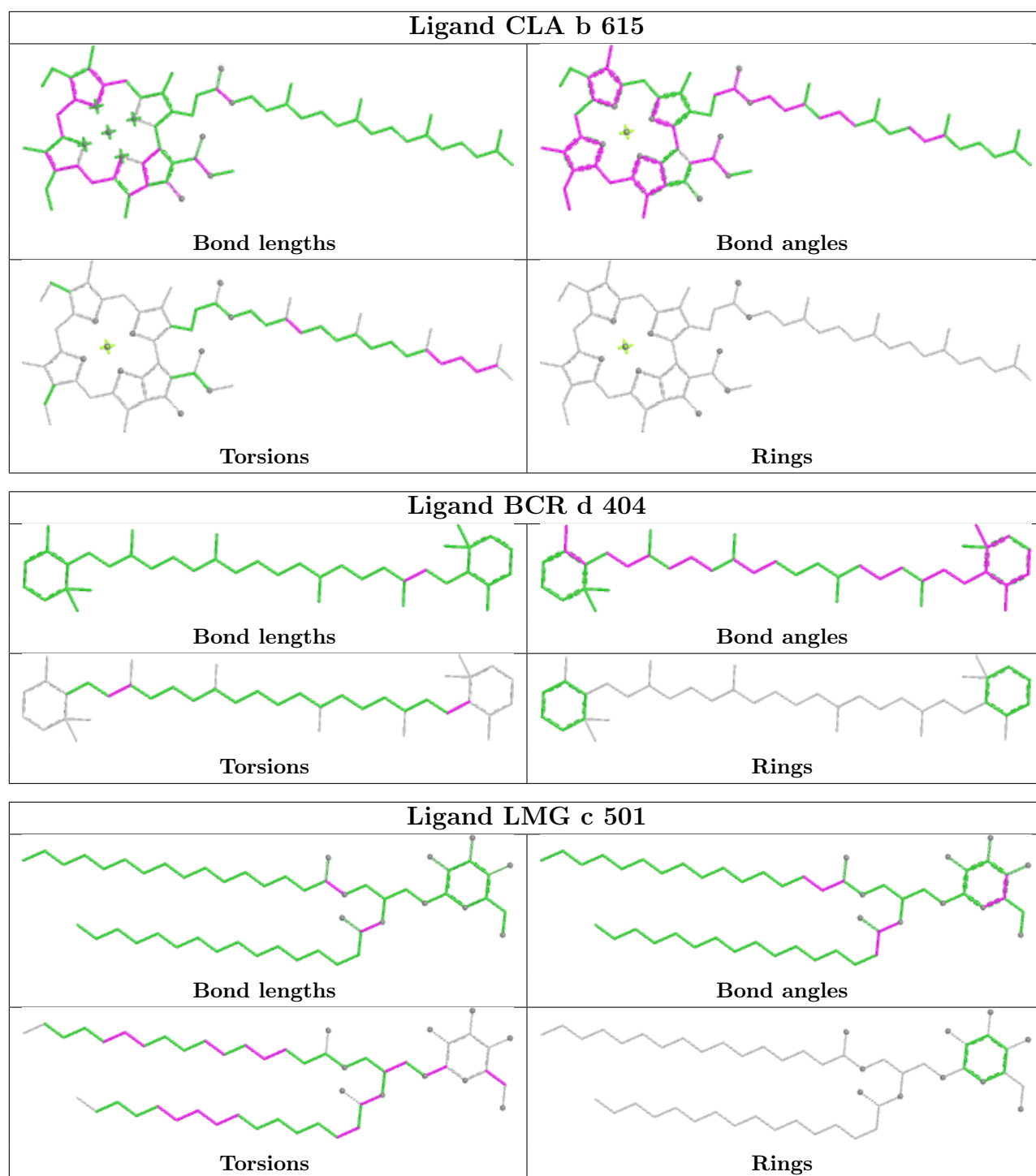


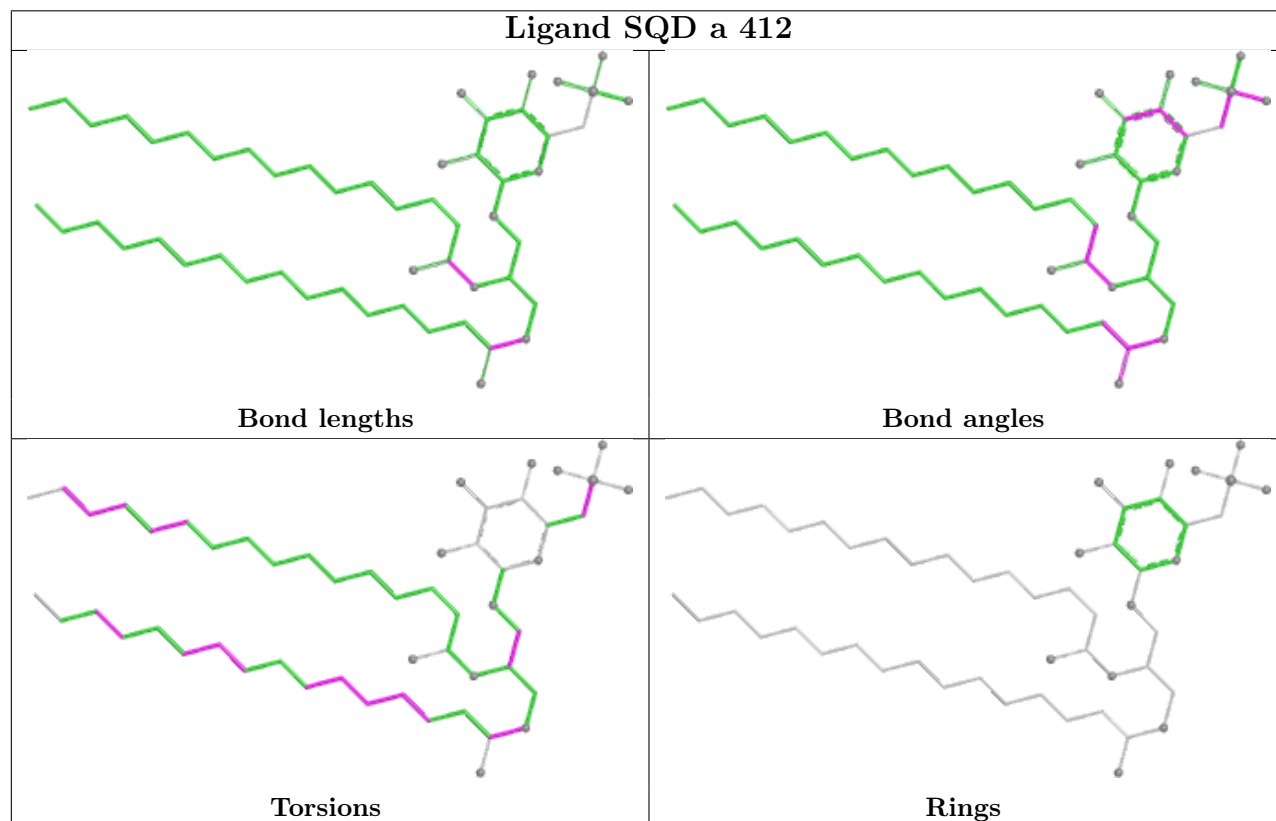
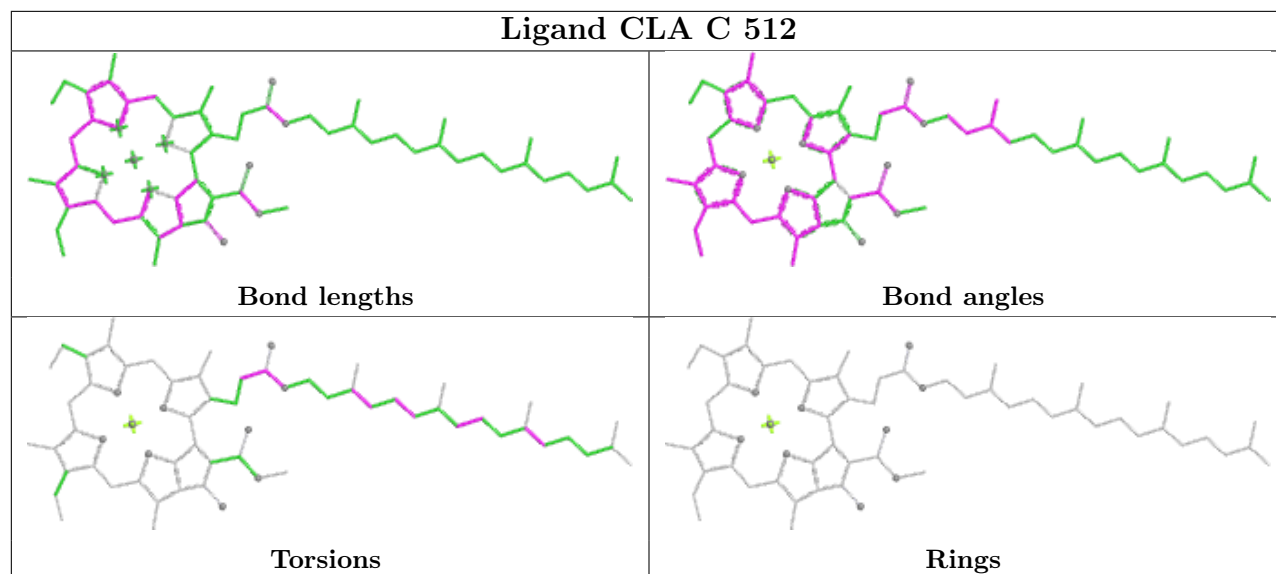


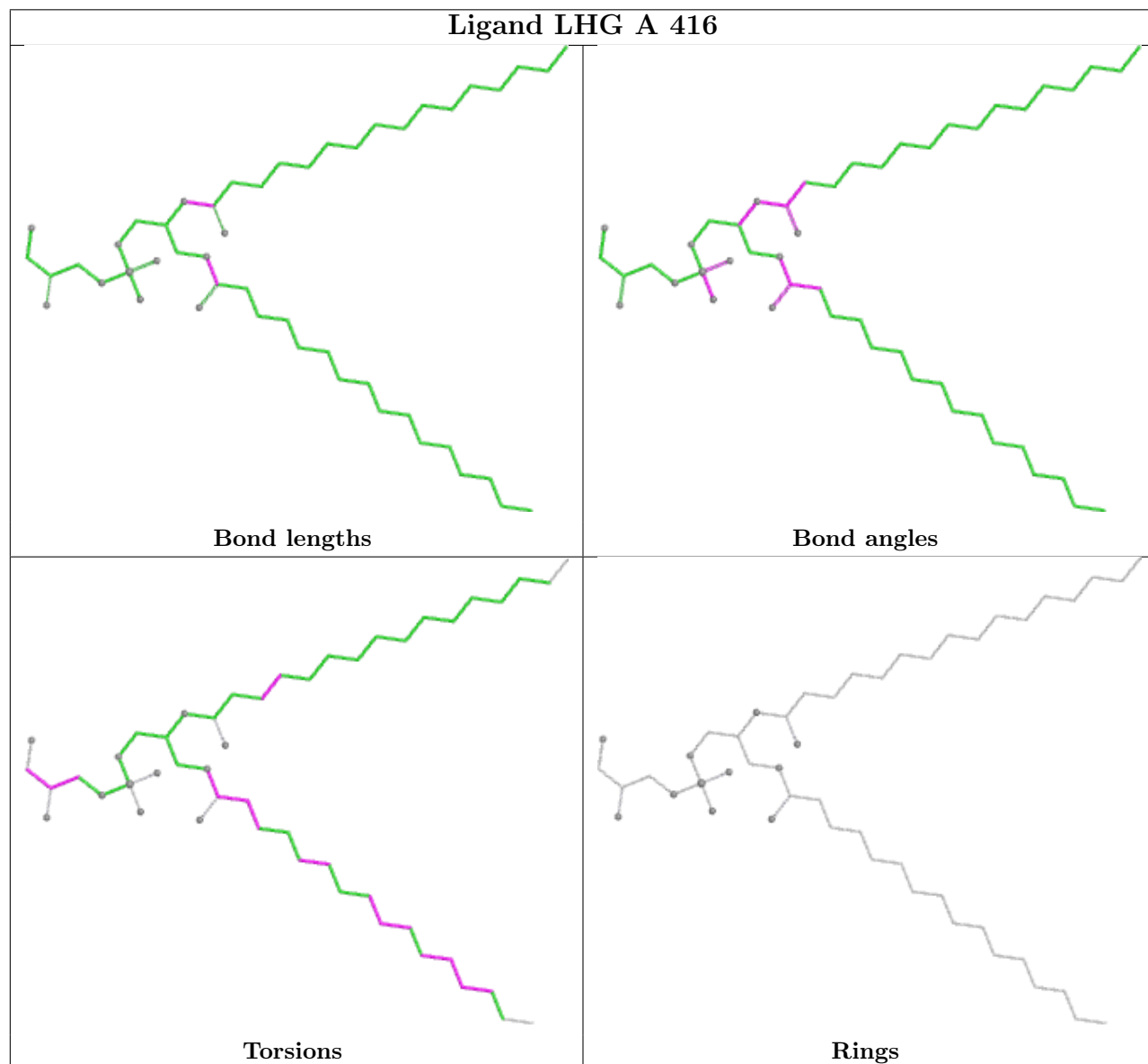
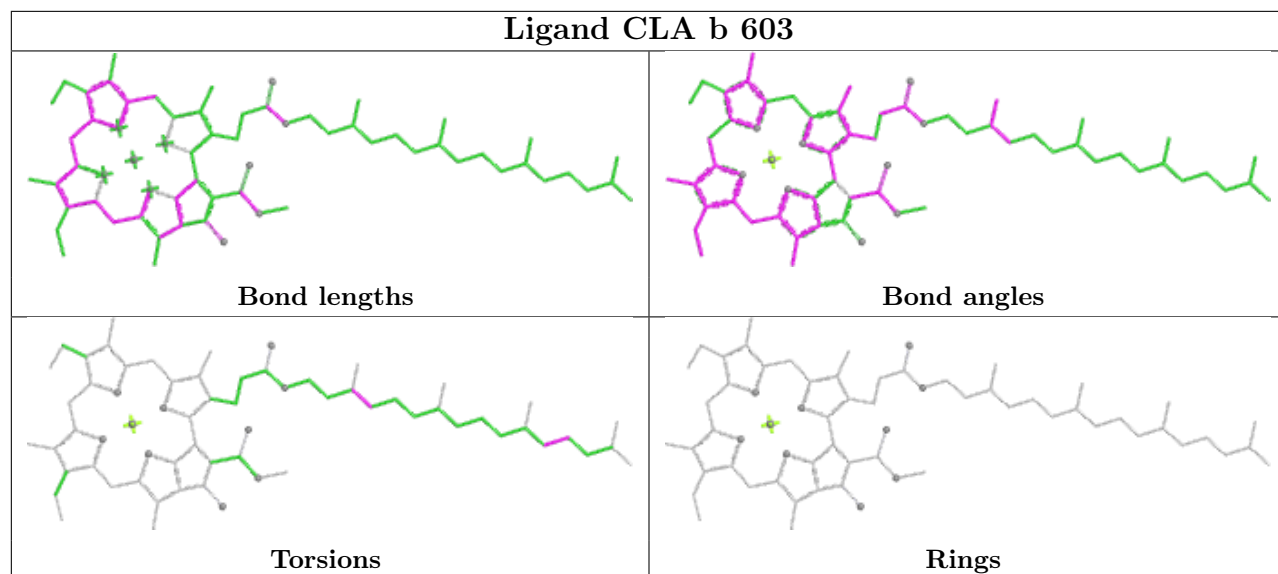


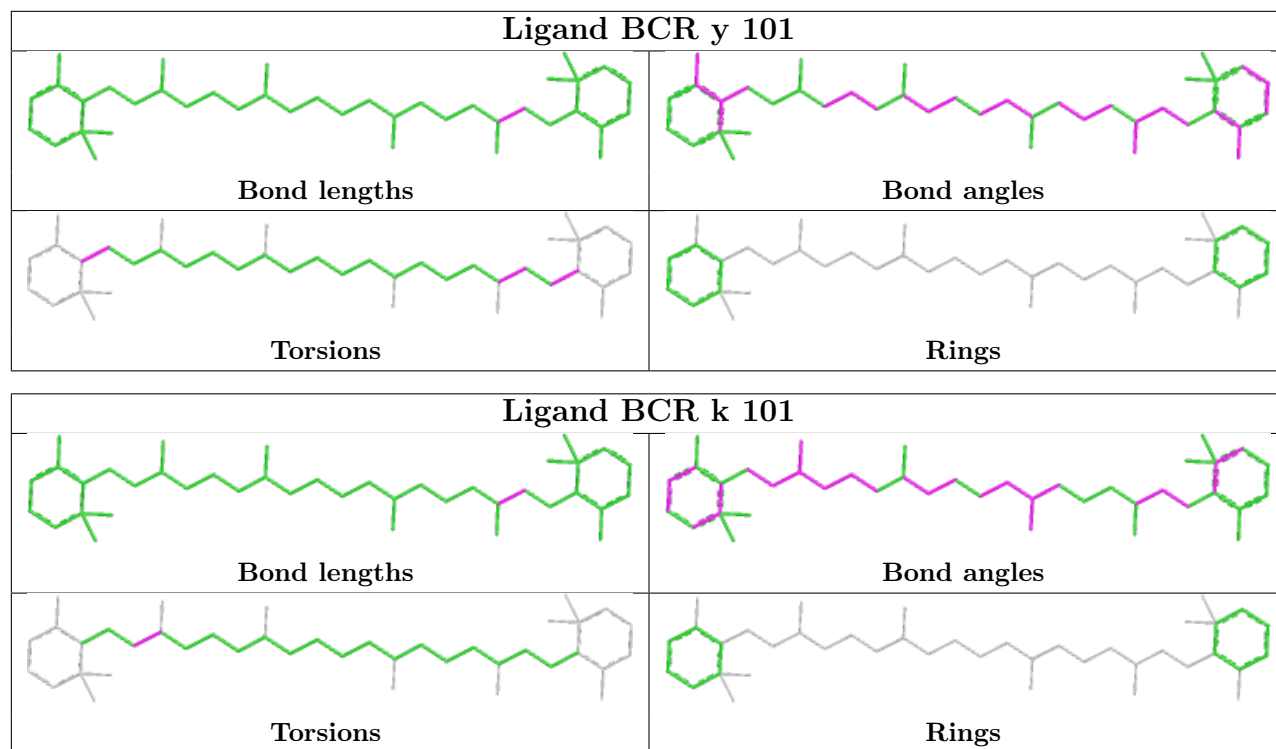


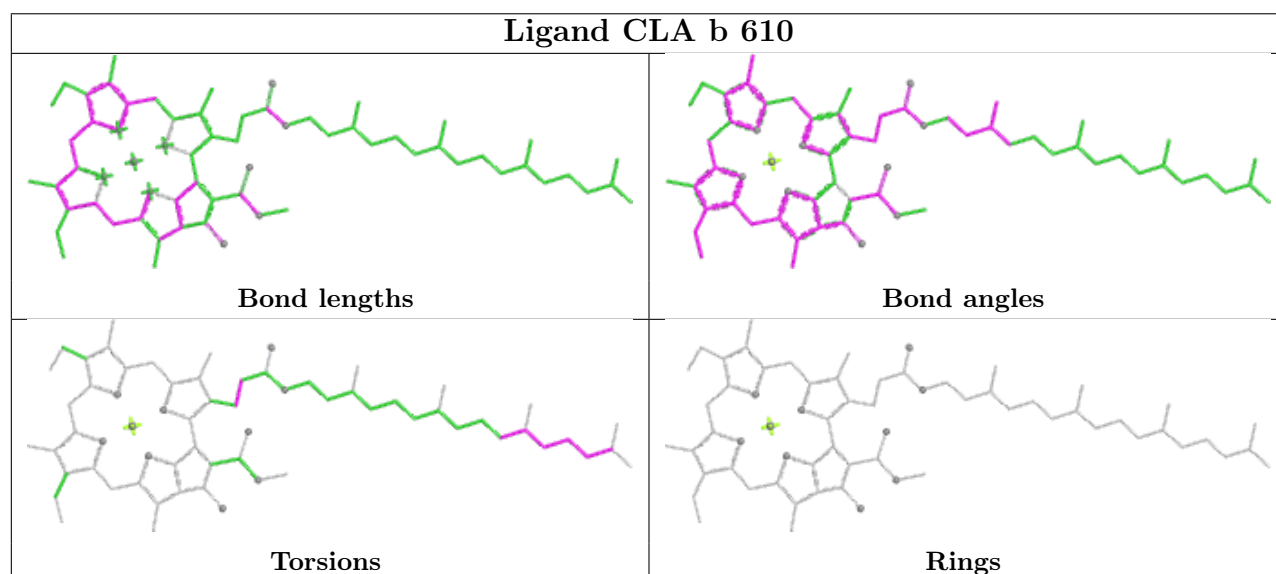
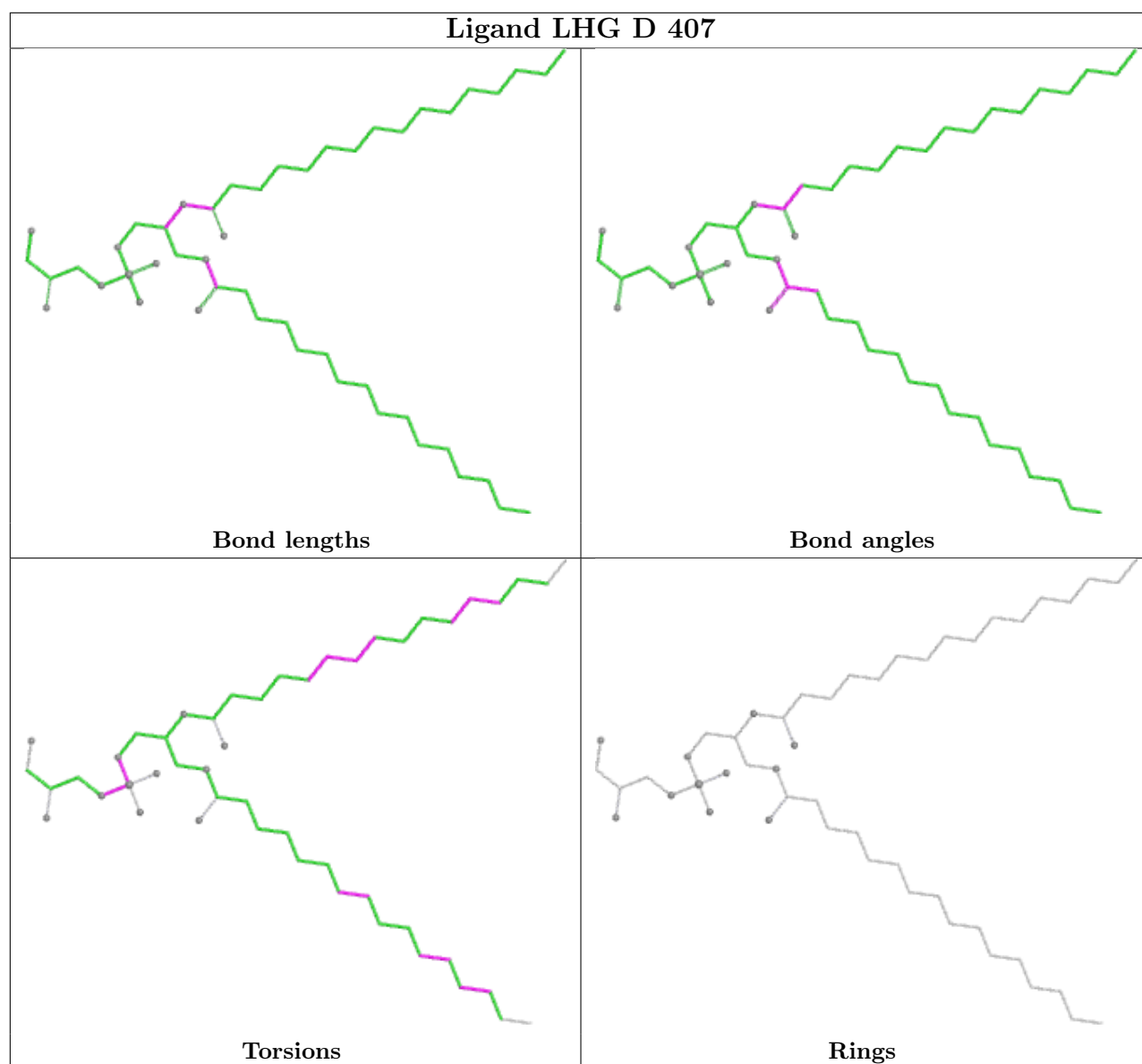


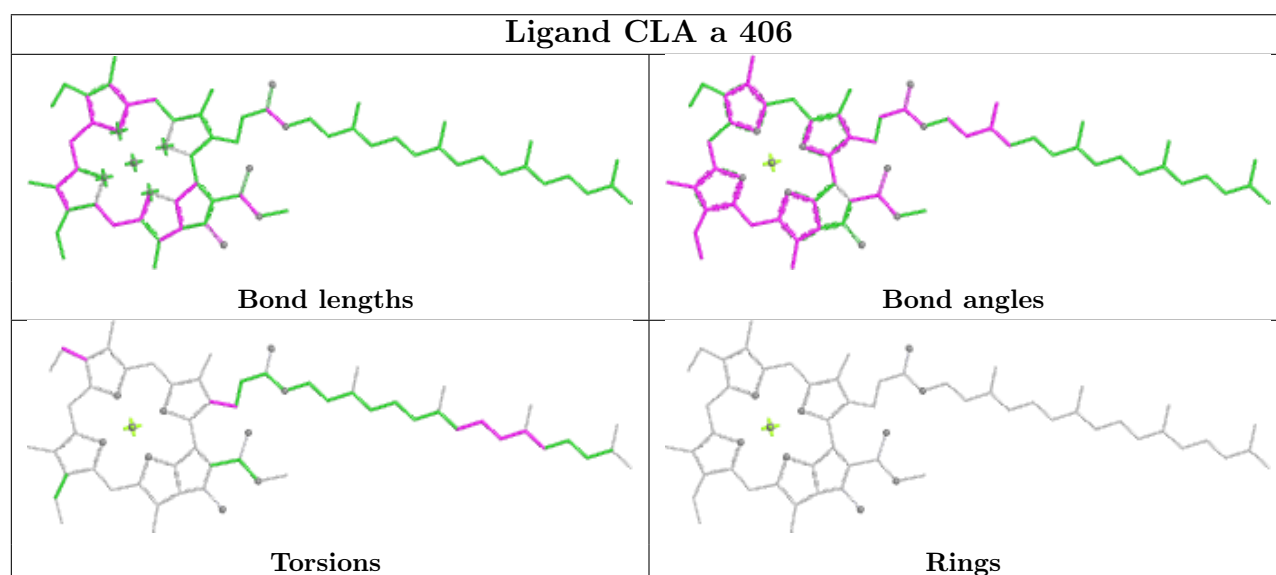
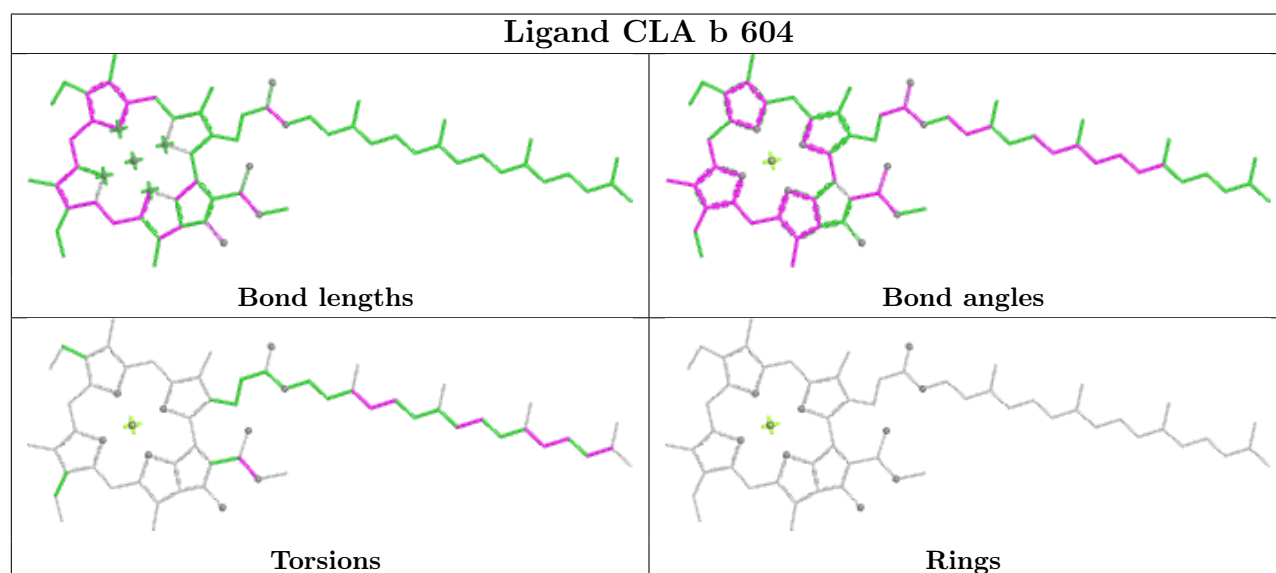
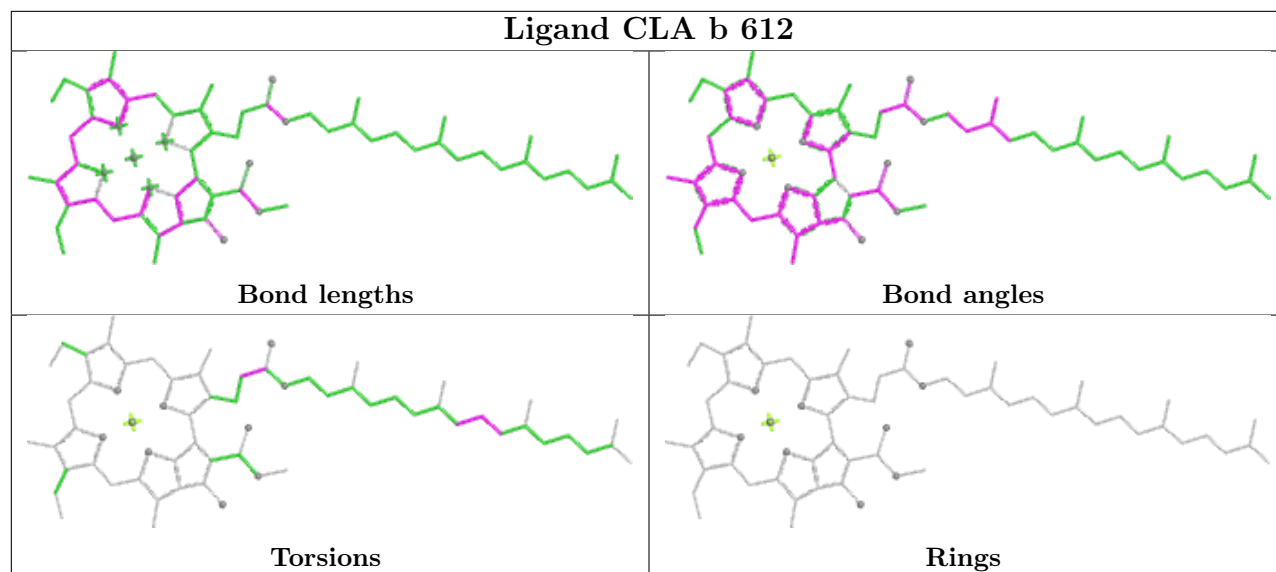


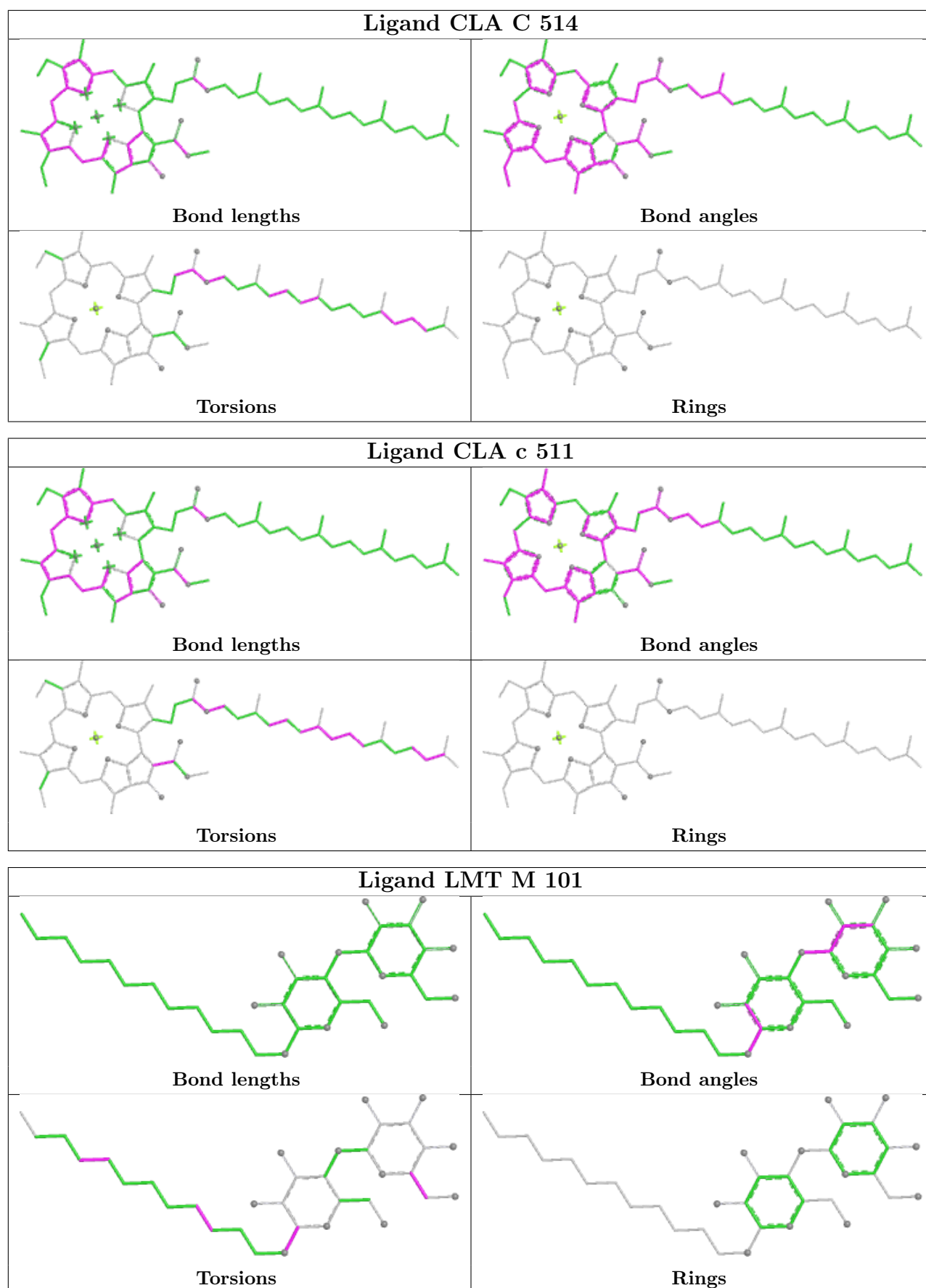


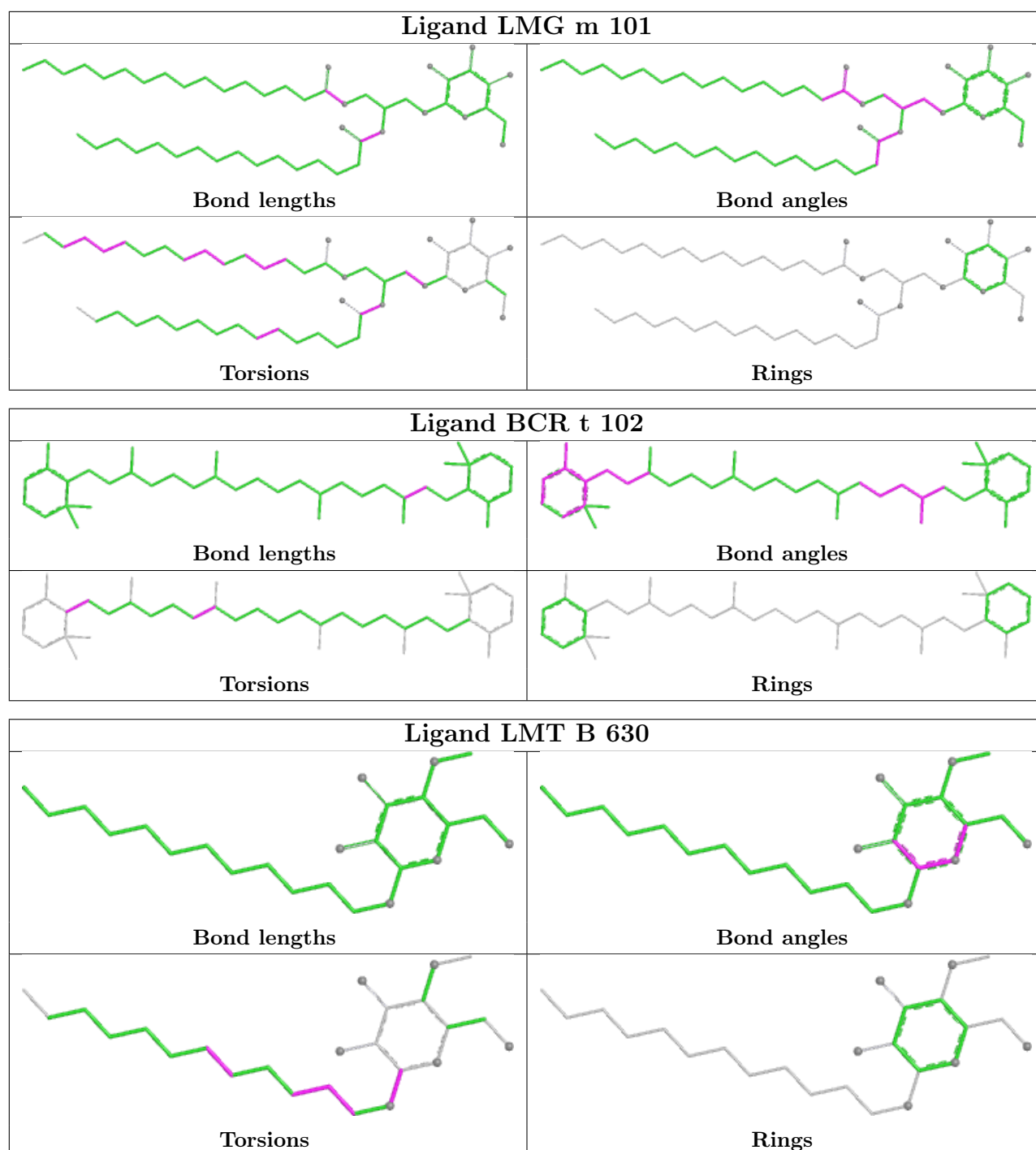


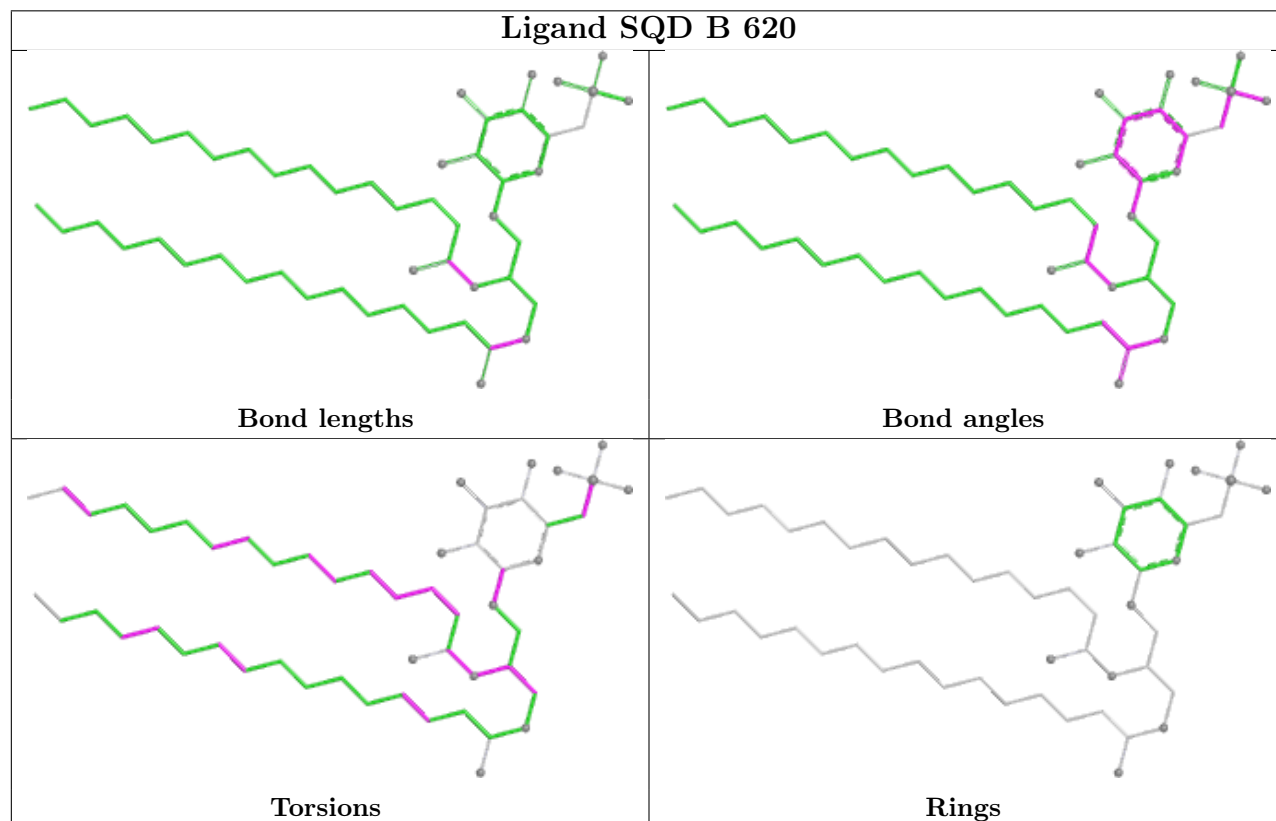
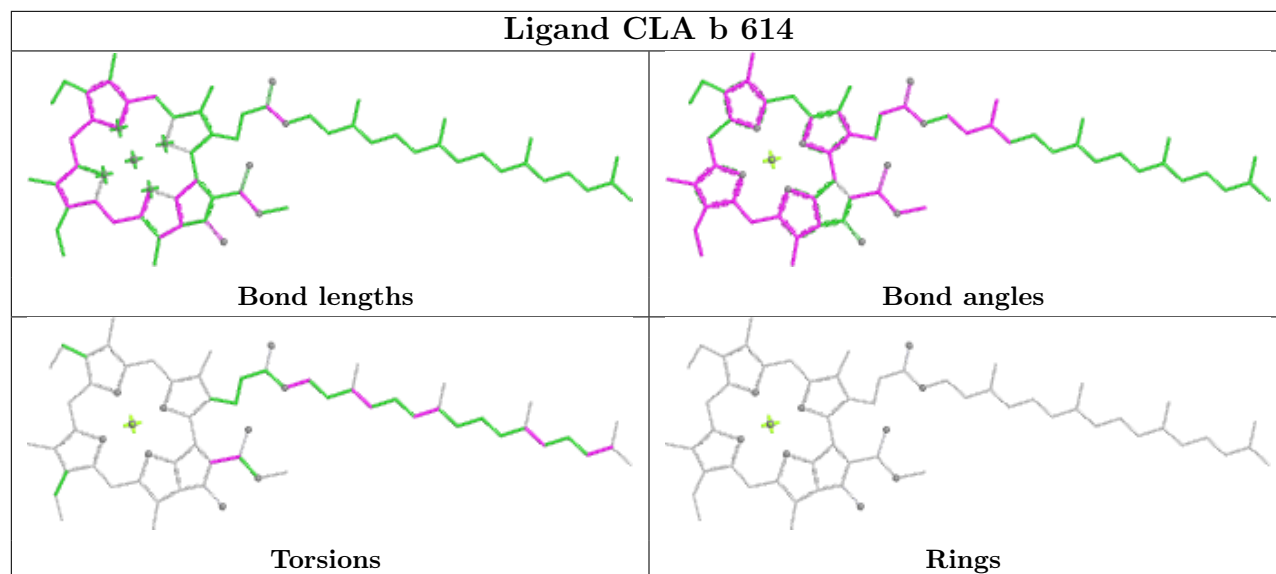


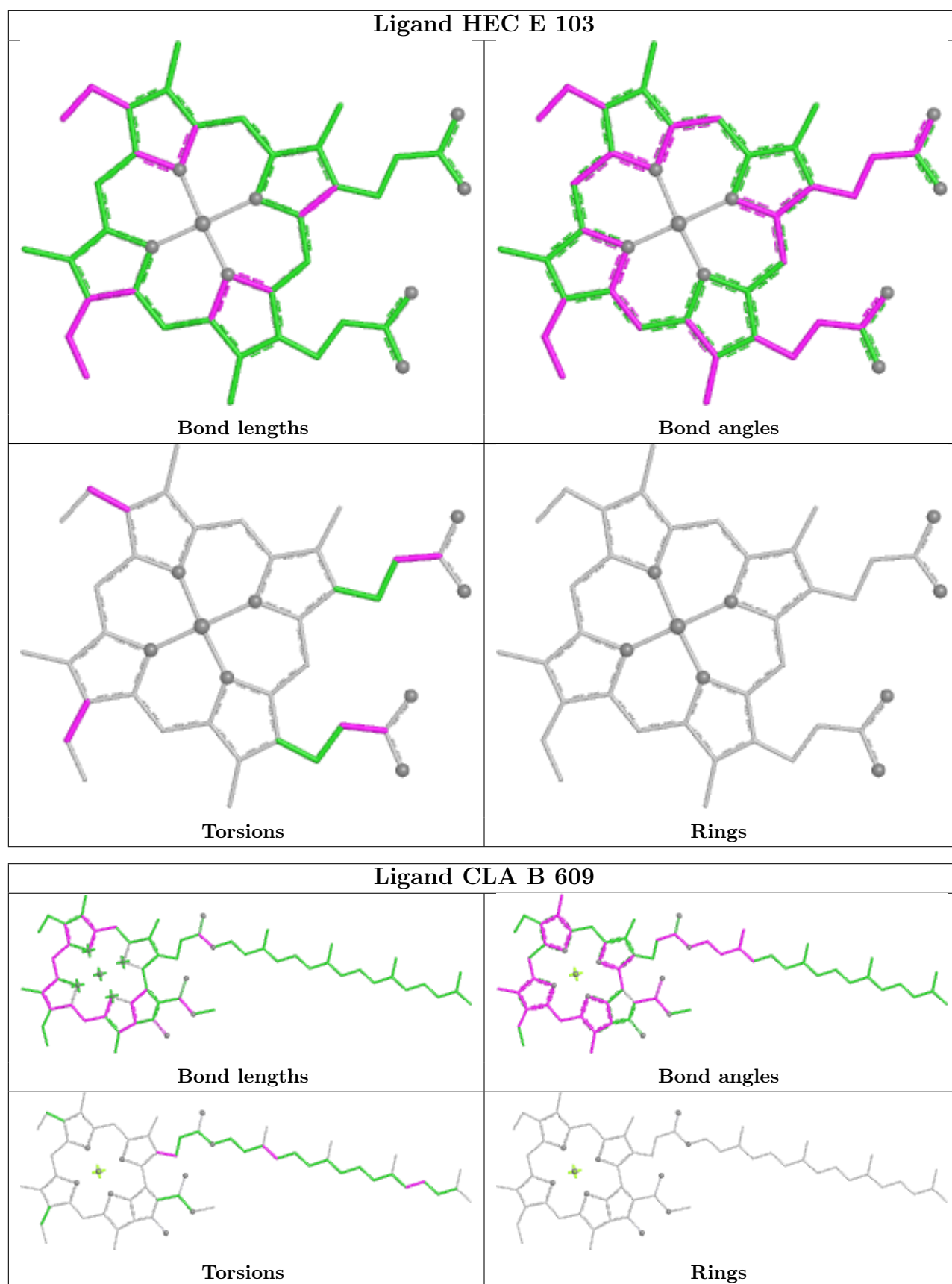


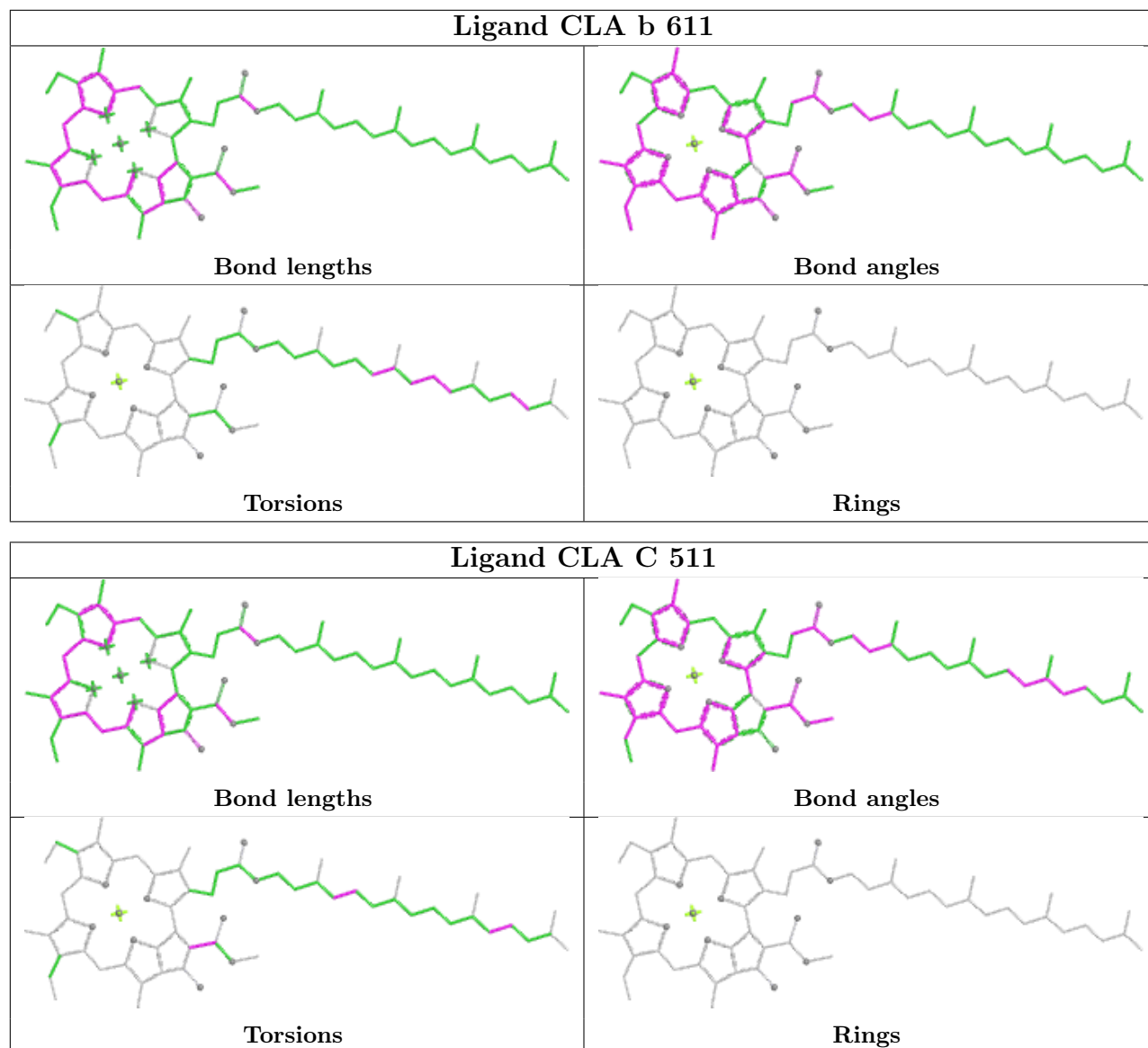


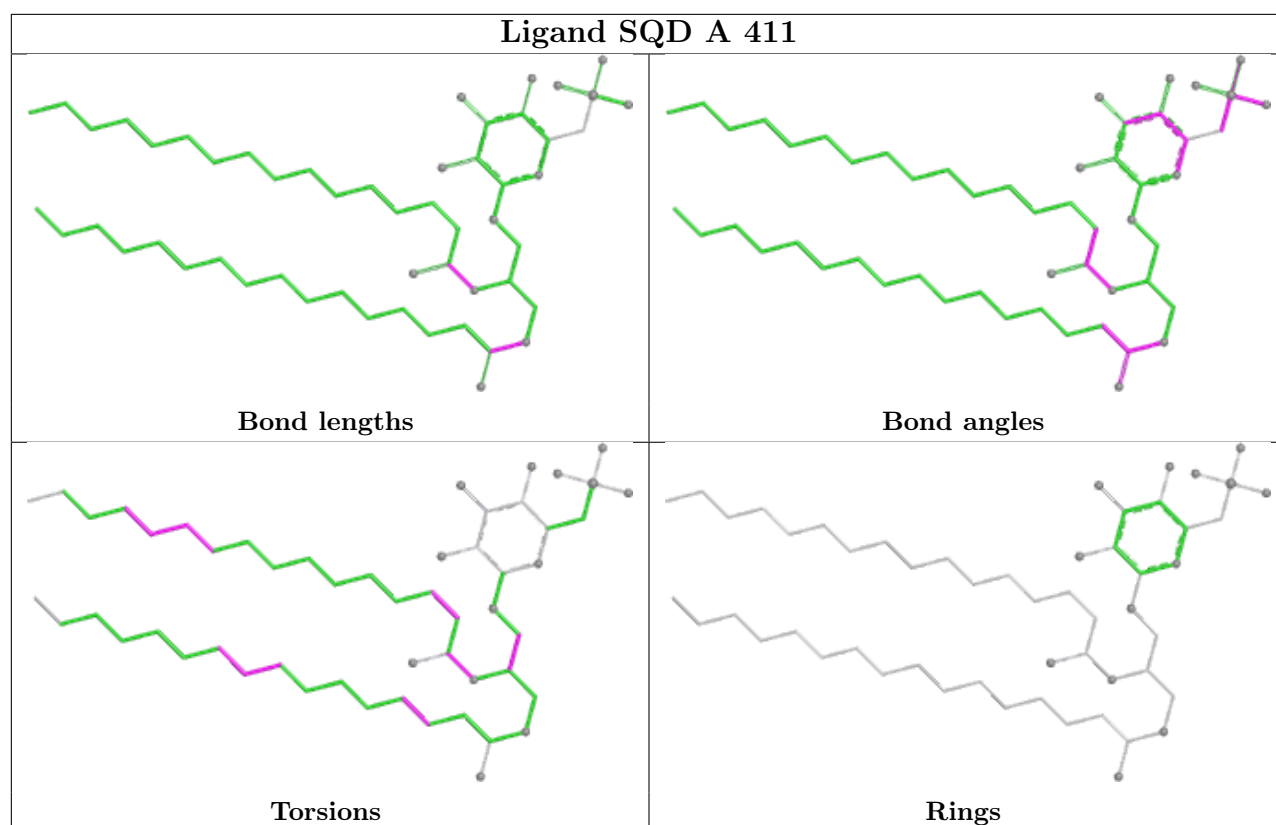












5.7 Other polymers [i](#)

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%)	-0.38	0 100 100	22, 41, 67, 126	2 (0%)
1	a	334/344 (97%)	-0.36	3 (0%) 81 82	23, 46, 80, 122	3 (0%)
2	B	504/505 (99%)	-0.31	1 (0%) 91 92	19, 46, 79, 129	10 (1%)
2	b	504/505 (99%)	-0.19	10 (1%) 65 65	22, 50, 92, 164	4 (0%)
3	C	451/455 (99%)	-0.19	2 (0%) 88 89	23, 54, 77, 144	4 (0%)
3	c	455/455 (100%)	-0.18	2 (0%) 88 89	31, 62, 84, 127	2 (0%)
4	D	342/342 (100%)	-0.35	0 100 100	33, 43, 65, 134	0
4	d	341/342 (99%)	-0.39	0 100 100	35, 49, 74, 136	0
5	E	81/84 (96%)	-0.02	1 (1%) 76 77	32, 66, 95, 140	1 (1%)
5	e	79/84 (94%)	-0.02	0 100 100	57, 74, 117, 150	0
6	F	34/44 (77%)	-0.04	1 (2%) 53 54	48, 58, 92, 113	0
6	f	31/44 (70%)	0.04	1 (3%) 50 50	57, 66, 93, 154	0
7	H	64/65 (98%)	0.08	2 (3%) 51 51	29, 58, 77, 105	1 (1%)
7	h	64/65 (98%)	0.08	1 (1%) 70 71	51, 63, 85, 108	0
8	I	37/38 (97%)	0.08	0 100 100	47, 58, 120, 144	0
8	i	37/38 (97%)	-0.11	1 (2%) 56 57	49, 59, 117, 145	0
9	J	38/39 (97%)	-0.01	1 (2%) 57 58	47, 66, 127, 181	0
9	j	39/39 (100%)	0.16	1 (2%) 57 58	55, 74, 135, 179	0
10	K	37/37 (100%)	-0.27	0 100 100	53, 65, 88, 102	0
10	k	37/37 (100%)	-0.16	0 100 100	66, 72, 94, 109	0
11	L	36/37 (97%)	-0.18	1 (2%) 55 55	18, 39, 95, 137	1 (2%)
11	l	36/37 (97%)	-0.19	1 (2%) 55 55	19, 40, 96, 132	1 (2%)
12	M	32/36 (88%)	-0.33	0 100 100	19, 42, 66, 135	1 (3%)
12	m	33/36 (91%)	-0.42	0 100 100	36, 43, 78, 125	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.22	0 100 100	23, 57, 110, 186	3 (1%)
13	o	243/244 (99%)	-0.12	1 (0%) 88 89	24, 59, 124, 166	2 (0%)
14	T	29/32 (90%)	-0.31	1 (3%) 48 48	36, 40, 78, 109	0
14	t	29/32 (90%)	-0.30	1 (3%) 48 48	36, 43, 70, 137	0
15	U	96/104 (92%)	-0.37	0 100 100	41, 53, 85, 90	0
15	u	97/104 (93%)	-0.30	0 100 100	46, 58, 80, 132	0
16	V	137/137 (100%)	-0.39	0 100 100	40, 53, 79, 115	0
16	v	137/137 (100%)	-0.28	0 100 100	47, 68, 96, 138	0
17	X	38/40 (95%)	0.03	0 100 100	56, 68, 93, 110	0
17	x	38/40 (95%)	0.09	0 100 100	60, 74, 114, 163	0
18	Y	29/30 (96%)	0.31	2 (6%) 23 21	66, 82, 139, 159	0
18	y	29/30 (96%)	0.23	0 100 100	77, 89, 119, 120	0
19	Z	62/62 (100%)	0.06	0 100 100	66, 80, 132, 180	0
19	z	62/62 (100%)	0.39	1 (1%) 70 71	77, 94, 135, 178	0
20	R	34/34 (100%)	1.88	16 (47%) 0 0	102, 124, 154, 164	0
All	All	5283/5384 (98%)	-0.21	51 (0%) 79 81	18, 54, 98, 186	35 (0%)

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	5.3
14	t	30	THR	4.4
7	h	65	LEU	4.1
6	f	15	ILE	3.7
3	C	23	ALA	3.5

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	FME	I	1	10/11	0.95	0.08	44,65,72,73	0
14	FME	T	1	10/11	0.96	0.07	40,46,63,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	t	1	10/11	0.96	0.07	36,43,68,73	0
8	FME	i	1	10/11	0.97	0.06	49,58,67,73	0
12	FME	m	1	10/11	0.97	0.06	41,53,62,76	0
12	FME	M	1	10/11	0.97	0.09	37,50,80,87	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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	LMT	E	102	35/35	0.61	0.20	102,145,164,166	0
34	LMT	e	101	35/35	0.64	0.18	122,163,170,171	0
34	LMT	a	413	35/35	0.65	0.21	66,131,140,142	0
34	LMT	C	526	35/35	0.65	0.16	88,140,155,158	0
30	UNL	A	414	28/-	0.67	0.20	83,97,113,115	0
30	UNL	j	101	10/-	0.69	0.27	78,87,93,94	0
33	HTG	b	623	19/19	0.72	0.15	83,144,150,150	0
33	HTG	D	411	16/19	0.72	0.15	91,113,123,129	0
34	LMT	D	402	35/35	0.72	0.21	69,124,137,143	0
30	UNL	J	101	10/-	0.76	0.27	75,79,91,92	0
33	HTG	B	623	19/19	0.78	0.18	61,86,94,95	0
30	UNL	m	102	10/-	0.78	0.21	59,68,91,92	0
31	LHG	a	419	42/49	0.79	0.16	100,147,177,181	0
30	UNL	i	101	40/-	0.79	0.19	69,98,148,152	0
27	SQD	f	101	43/54	0.79	0.16	111,132,160,166	0
30	UNL	a	416	30/-	0.79	0.16	96,111,134,138	0
34	LMT	a	418	35/35	0.79	0.14	118,150,157,158	0
33	HTG	c	523	19/19	0.79	0.14	119,138,143,144	0
30	UNL	C	527	34/-	0.81	0.17	83,110,123,126	0
32	LMG	C	522	51/55	0.81	0.17	69,127,161,165	0
30	UNL	c	526	32/-	0.82	0.17	94,113,130,132	0
30	UNL	I	101	40/-	0.82	0.20	68,107,149,150	0
33	HTG	C	523	19/19	0.82	0.14	106,118,127,127	0
26	GOL	O	302	6/6	0.82	0.10	78,85,86,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
26	GOL	B	627	6/6	0.82	0.20	63,92,96,97	0
30	UNL	b	626	33/-	0.82	0.16	63,90,146,148	0
34	LMT	m	103	35/35	0.82	0.14	52,93,109,110	0
30	UNL	M	102	10/-	0.83	0.20	63,73,84,84	0
33	HTG	h	101	16/19	0.83	0.12	103,133,139,143	0
34	LMT	B	628	35/35	0.83	0.13	63,110,126,130	0
34	LMT	M	103	35/35	0.83	0.15	78,152,175,176	0
32	LMG	Z	101	37/55	0.84	0.16	72,123,156,161	0
34	LMT	b	621	25/35	0.84	0.16	89,129,154,154	0
26	GOL	c	502	6/6	0.84	0.18	61,75,77,81	0
33	HTG	V	202	11/19	0.84	0.13	110,119,121,121	0
31	LHG	E	101	42/49	0.85	0.16	72,126,138,141	0
32	LMG	c	522	51/55	0.85	0.15	72,129,152,157	0
33	HTG	b	622	19/19	0.85	0.16	64,71,105,109	0
26	GOL	b	624	6/6	0.85	0.21	86,95,99,105	0
26	GOL	v	201	6/6	0.85	0.20	51,70,78,80	0
34	LMT	M	101	35/35	0.85	0.12	53,98,131,139	0
36	CA	F	101	1/1	0.85	0.12	115,115,115,115	0
27	SQD	A	411	54/54	0.86	0.13	60,82,123,130	0
30	UNL	d	410	36/-	0.86	0.17	70,94,127,130	0
34	LMT	b	627	25/35	0.86	0.15	50,75,135,136	0
30	UNL	B	626	33/-	0.86	0.15	52,108,152,156	0
26	GOL	B	629	6/6	0.86	0.20	103,111,114,116	0
29	PL9	a	415	55/55	0.86	0.23	87,111,124,126	0
32	LMG	z	101	39/55	0.87	0.15	80,128,136,139	0
30	UNL	D	410	40/-	0.87	0.17	56,85,125,129	0
27	SQD	a	412	54/54	0.87	0.12	59,85,125,127	0
26	GOL	A	410	6/6	0.87	0.14	68,68,74,81	0
27	SQD	D	412	43/54	0.87	0.15	74,111,131,138	0
34	LMT	B	630	25/35	0.87	0.14	55,84,135,139	0
23	CLA	b	601	65/65	0.88	0.12	58,80,120,129	0
33	HTG	B	622	19/19	0.88	0.17	61,83,110,111	0
26	GOL	o	302	6/6	0.88	0.16	110,113,118,120	0
27	SQD	b	620	54/54	0.88	0.13	59,88,112,115	0
27	SQD	B	620	54/54	0.88	0.13	54,88,124,129	0
29	PL9	A	413	55/55	0.88	0.20	72,102,112,115	0
32	LMG	C	521	51/55	0.90	0.14	52,87,119,120	0
34	LMT	t	101	26/35	0.90	0.15	77,117,136,140	0
23	CLA	B	601	65/65	0.90	0.11	52,72,115,121	0
26	GOL	a	411	6/6	0.91	0.12	57,68,80,81	0
33	HTG	B	625	19/19	0.91	0.11	65,75,82,87	0
32	LMG	C	502	51/55	0.92	0.12	57,84,104,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
32	LMG	c	501	51/55	0.92	0.14	60,88,109,117	0
32	LMG	c	521	51/55	0.92	0.14	68,92,125,127	0
23	CLA	c	515	65/65	0.92	0.12	64,83,117,119	0
23	CLA	C	515	65/65	0.92	0.12	59,70,111,114	0
32	LMG	D	413	51/55	0.92	0.12	44,64,111,123	0
30	UNL	D	409	17/-	0.93	0.16	56,77,114,114	0
25	BCR	t	102	40/40	0.93	0.08	37,51,66,70	0
32	LMG	m	101	51/55	0.93	0.11	51,68,96,98	0
26	GOL	b	628	6/6	0.93	0.17	94,100,102,103	0
31	LHG	A	416	49/49	0.93	0.13	41,57,80,87	0
23	CLA	C	506	65/65	0.93	0.11	42,51,85,95	0
25	BCR	B	619	40/40	0.93	0.10	43,53,72,75	0
32	LMG	B	621	51/55	0.93	0.11	49,65,92,114	0
25	BCR	K	101	40/40	0.93	0.10	54,63,69,71	0
26	GOL	C	524	6/6	0.93	0.17	53,56,60,61	0
25	BCR	T	101	40/40	0.93	0.08	37,48,57,61	0
30	UNL	d	409	17/-	0.93	0.13	67,82,97,97	0
33	HTG	b	625	19/19	0.93	0.10	66,72,92,98	0
25	BCR	h	102	40/40	0.93	0.10	50,61,74,75	0
35	DGD	C	519	62/66	0.93	0.12	42,62,116,121	0
30	UNL	d	411	18/-	0.93	0.13	74,78,109,112	0
36	CA	a	420	1/1	0.93	0.10	105,105,105,105	0
27	SQD	C	501	54/54	0.94	0.11	59,79,105,107	0
25	BCR	d	404	40/40	0.94	0.10	52,63,87,92	0
27	SQD	a	410	54/54	0.94	0.12	64,83,117,118	0
23	CLA	b	612	65/65	0.94	0.09	38,46,61,70	0
23	CLA	b	614	65/65	0.94	0.09	35,44,102,105	0
25	BCR	y	101	40/40	0.94	0.09	57,70,83,86	0
23	CLA	b	616	65/65	0.94	0.10	43,55,114,116	0
29	PL9	D	406	55/55	0.94	0.09	32,42,54,60	0
31	LHG	b	629	49/49	0.94	0.11	40,55,71,78	0
26	GOL	B	624	6/6	0.94	0.12	76,87,95,97	0
29	PL9	d	405	55/55	0.94	0.10	35,46,56,61	0
23	CLA	c	509	65/65	0.94	0.10	53,63,73,83	0
23	CLA	c	514	65/65	0.94	0.11	64,77,112,122	0
23	CLA	C	508	65/65	0.94	0.12	51,63,123,130	0
25	BCR	B	618	40/40	0.94	0.08	35,50,63,72	0
23	CLA	B	614	65/65	0.94	0.10	33,43,93,97	0
25	BCR	D	405	40/40	0.94	0.11	45,58,95,103	0
25	BCR	H	101	40/40	0.94	0.09	44,61,71,74	0
23	CLA	a	408	65/65	0.94	0.11	40,48,128,132	0
30	UNL	X	101	18/-	0.94	0.12	60,68,98,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	B	610	65/65	0.94	0.10	41,48,59,77	0
25	BCR	b	617	40/40	0.94	0.08	35,43,56,58	0
25	BCR	b	618	40/40	0.94	0.08	37,50,67,72	0
25	BCR	c	516	40/40	0.94	0.11	68,83,90,94	0
23	CLA	b	605	65/65	0.95	0.09	35,43,66,75	0
23	CLA	b	606	65/65	0.95	0.09	38,49,110,115	0
25	BCR	c	517	40/40	0.95	0.10	53,65,71,71	0
23	CLA	b	610	65/65	0.95	0.09	43,50,62,73	0
32	LMG	d	412	51/55	0.95	0.11	53,67,111,119	0
23	CLA	C	503	65/65	0.95	0.09	45,53,68,78	0
23	CLA	C	505	65/65	0.95	0.08	47,55,67,72	0
23	CLA	B	606	65/65	0.95	0.09	38,46,101,108	0
23	CLA	c	505	65/65	0.95	0.09	53,63,73,77	0
23	CLA	c	506	65/65	0.95	0.10	49,58,103,110	0
23	CLA	c	507	65/65	0.95	0.09	43,56,83,86	0
23	CLA	c	508	65/65	0.95	0.10	56,69,121,126	0
23	CLA	A	408	65/65	0.95	0.10	38,45,111,119	0
23	CLA	c	510	65/65	0.95	0.09	47,57,127,132	0
23	CLA	C	509	65/65	0.95	0.09	50,57,76,80	0
23	CLA	C	510	65/65	0.95	0.09	43,51,117,130	0
23	CLA	d	403	65/65	0.95	0.09	48,58,115,123	0
24	PHO	A	415	64/64	0.95	0.07	35,43,52,54	0
25	BCR	A	409	40/40	0.95	0.07	33,42,54,58	0
23	CLA	C	513	65/65	0.95	0.09	49,62,77,78	0
23	CLA	C	514	65/65	0.95	0.11	55,65,114,119	0
25	BCR	C	516	40/40	0.95	0.10	59,74,81,83	0
31	LHG	D	407	49/49	0.95	0.09	40,48,64,76	0
31	LHG	D	408	49/49	0.95	0.13	45,57,124,134	0
25	BCR	C	517	40/40	0.95	0.08	49,56,64,73	0
31	LHG	L	101	49/49	0.95	0.10	39,51,65,84	0
23	CLA	B	611	65/65	0.95	0.08	34,39,61,68	0
23	CLA	D	404	65/65	0.95	0.10	44,54,126,133	0
31	LHG	d	406	49/49	0.95	0.11	50,61,76,81	0
31	LHG	d	408	49/49	0.95	0.12	53,65,117,122	0
23	CLA	a	406	65/65	0.95	0.10	39,49,114,118	0
23	CLA	B	603	65/65	0.95	0.09	38,46,62,66	0
35	DGD	C	518	62/66	0.95	0.10	40,54,93,96	0
25	BCR	Y	101	40/40	0.95	0.09	53,64,73,77	0
35	DGD	C	520	62/66	0.95	0.10	40,53,95,108	0
35	DGD	H	102	62/66	0.95	0.10	40,55,67,69	0
35	DGD	c	518	62/66	0.95	0.10	45,58,90,95	0
35	DGD	c	519	62/66	0.95	0.09	50,70,107,118	0

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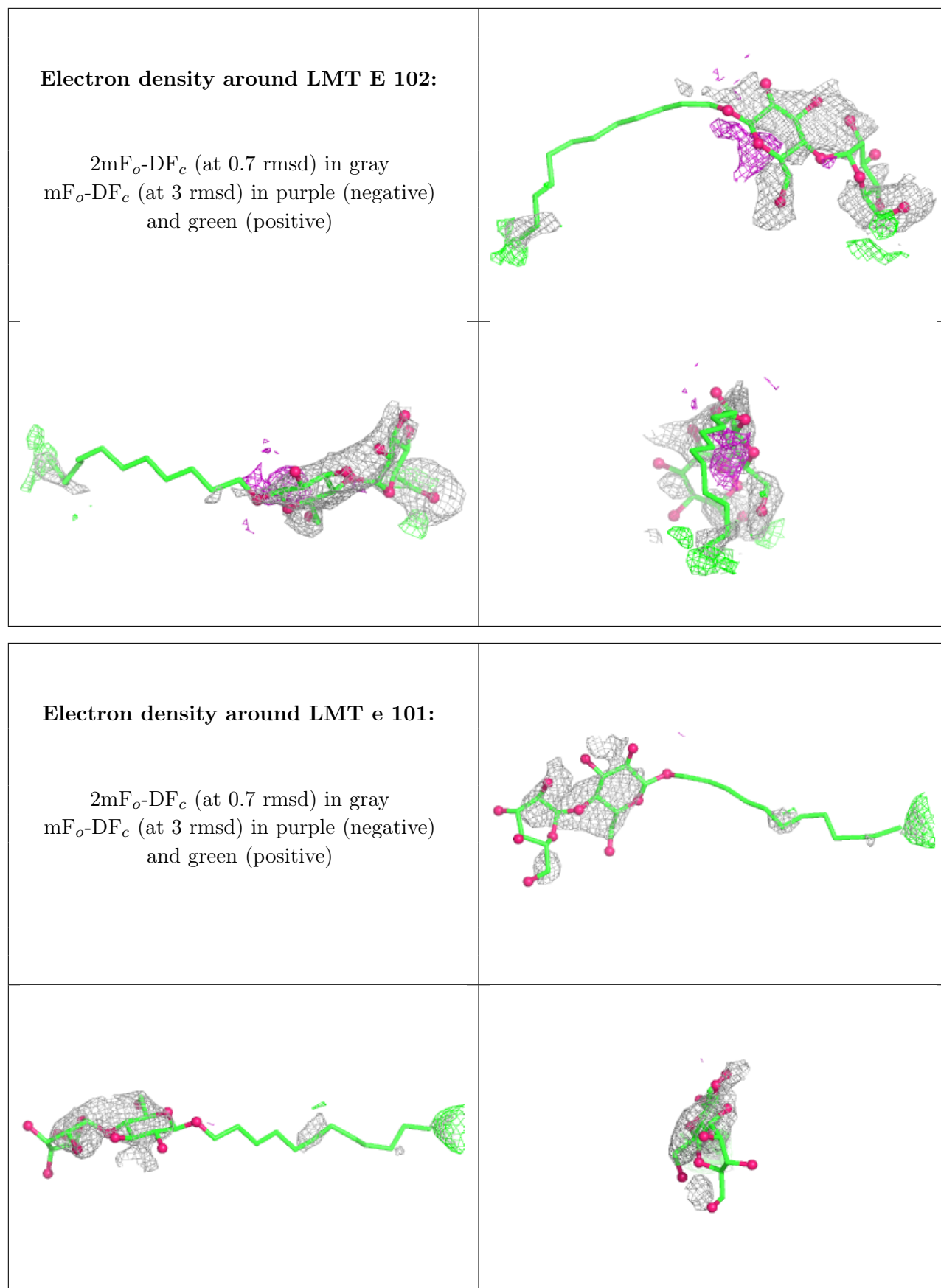
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	DGD	c	520	62/66	0.95	0.10	48,60,98,111	0
35	DGD	h	103	62/66	0.95	0.09	50,59,68,71	0
25	BCR	a	409	40/40	0.95	0.07	36,45,56,59	0
23	CLA	B	616	65/65	0.95	0.11	41,52,136,137	0
36	CA	o	301	1/1	0.95	0.05	100,100,100,100	0
37	BCT	d	401	4/4	0.95	0.07	52,54,62,64	0
23	CLA	A	406	65/65	0.96	0.09	34,42,114,117	0
23	CLA	b	611	65/65	0.96	0.08	36,44,70,76	0
23	CLA	B	607	65/65	0.96	0.07	31,40,64,69	0
23	CLA	B	609	65/65	0.96	0.07	43,51,74,81	0
23	CLA	D	403	65/65	0.96	0.07	32,37,53,62	0
23	CLA	c	503	65/65	0.96	0.09	53,61,74,82	0
23	CLA	c	504	65/65	0.96	0.08	48,56,73,83	0
23	CLA	B	602	65/65	0.96	0.08	39,48,72,77	0
23	CLA	a	404	65/65	0.96	0.07	37,41,64,73	0
31	LHG	d	407	49/49	0.96	0.09	41,51,68,78	0
25	BCR	b	619	40/40	0.96	0.08	46,53,74,84	0
23	CLA	a	405	65/65	0.96	0.07	34,40,57,62	0
23	CLA	A	404	65/65	0.96	0.08	33,36,61,75	0
23	CLA	B	613	65/65	0.96	0.08	34,41,89,94	0
23	CLA	B	605	65/65	0.96	0.08	35,41,61,73	0
25	BCR	k	101	40/40	0.96	0.09	58,70,81,81	0
23	CLA	c	511	65/65	0.96	0.09	54,62,86,88	0
23	CLA	c	512	65/65	0.96	0.08	52,59,73,76	0
23	CLA	c	513	65/65	0.96	0.08	55,65,81,85	0
23	CLA	b	602	65/65	0.96	0.08	43,54,70,80	0
23	CLA	b	603	65/65	0.96	0.08	41,50,70,88	0
23	CLA	b	604	65/65	0.96	0.09	34,43,111,119	0
24	PHO	A	407	64/64	0.96	0.07	32,37,47,52	0
23	CLA	C	511	65/65	0.96	0.09	48,56,77,79	0
24	PHO	a	417	64/64	0.96	0.07	39,47,55,60	0
23	CLA	C	512	65/65	0.96	0.08	46,56,78,87	0
25	BCR	B	617	40/40	0.96	0.07	34,45,55,58	0
36	CA	O	301	1/1	0.96	0.06	103,103,103,103	0
23	CLA	b	607	65/65	0.96	0.08	32,40,73,80	0
23	CLA	b	608	65/65	0.96	0.07	45,52,69,76	0
37	BCT	D	401	4/4	0.96	0.08	51,57,61,62	0
23	CLA	b	609	65/65	0.96	0.08	49,57,78,100	0
38	HEC	e	102	43/43	0.96	0.08	64,78,119,130	0
39	MG	J	102	1/1	0.96	0.08	50,50,50,50	0
23	CLA	B	612	65/65	0.97	0.07	35,44,54,59	0
36	CA	C	525	1/1	0.97	0.10	66,66,66,66	0

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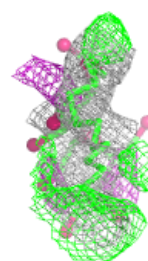
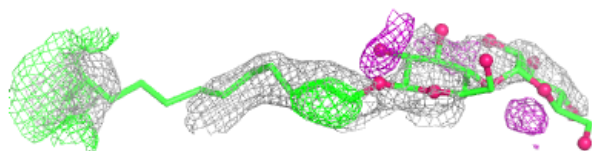
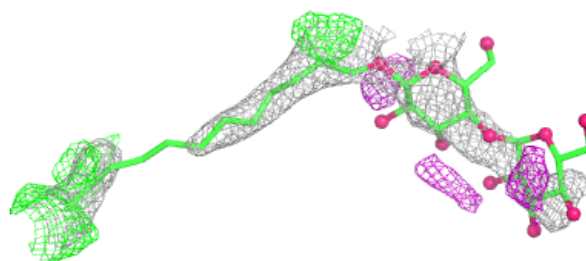
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	B	608	65/65	0.97	0.07	39,47,62,65	0
23	CLA	b	613	65/65	0.97	0.07	33,42,84,88	0
23	CLA	C	504	65/65	0.97	0.07	43,50,71,82	0
36	CA	c	524	1/1	0.97	0.07	73,73,73,73	0
23	CLA	b	615	65/65	0.97	0.08	42,50,74,79	0
23	CLA	A	405	65/65	0.97	0.07	31,37,52,56	0
24	PHO	a	407	64/64	0.97	0.06	35,42,47,50	0
38	HEC	E	103	43/43	0.97	0.07	57,65,80,93	0
38	HEC	V	201	43/43	0.97	0.07	43,46,51,54	0
23	CLA	B	615	65/65	0.97	0.07	40,46,77,83	0
38	HEC	v	202	43/43	0.97	0.08	52,58,63,64	0
23	CLA	C	507	65/65	0.97	0.08	43,52,86,93	0
23	CLA	d	402	65/65	0.98	0.06	36,40,68,77	0
22	CL	A	403	1/1	0.98	0.04	40,40,40,40	0
23	CLA	B	604	65/65	0.98	0.08	32,39,110,116	0
39	MG	j	102	1/1	0.98	0.04	60,60,60,60	0
22	CL	a	403	1/1	0.99	0.05	44,44,44,44	0
22	CL	A	402	1/1	0.99	0.04	35,35,35,35	0
36	CA	c	525	1/1	0.99	0.04	80,80,80,80	0
22	CL	a	402	1/1	0.99	0.04	42,42,42,42	0
28	OEX	A	412	10/10	0.99	0.04	35,38,45,46	0
28	OEX	a	414	10/10	0.99	0.03	39,45,49,49	0
21	FE2	A	401	1/1	1.00	0.04	53,53,53,53	0
21	FE2	a	401	1/1	1.00	0.04	57,57,57,57	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.

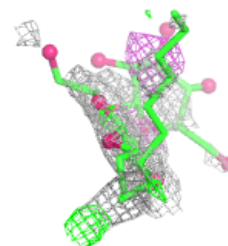
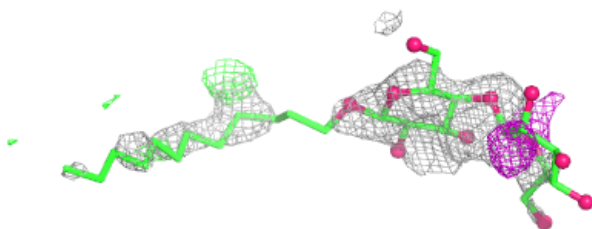
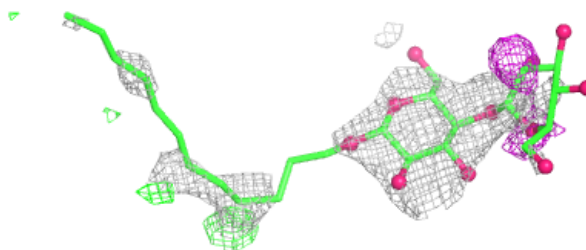


Electron density around LMT a 413:

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

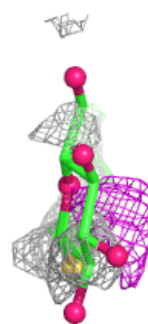
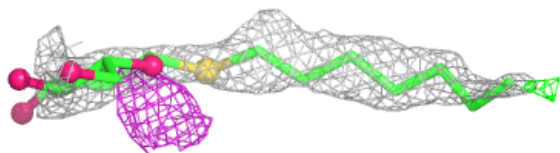
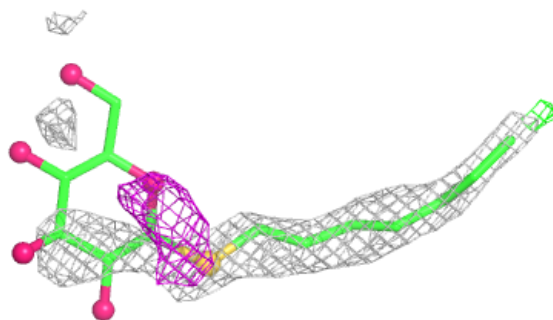
**Electron density around LMT C 526:**

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

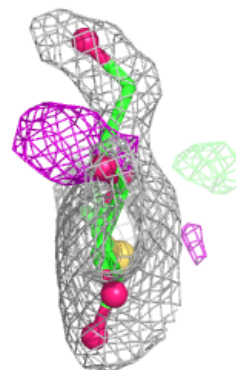
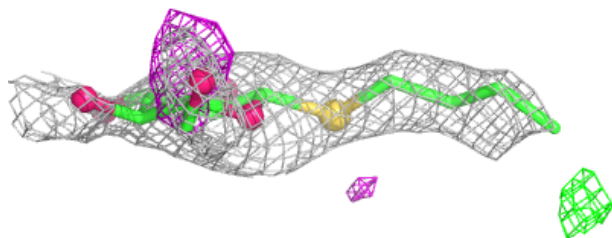
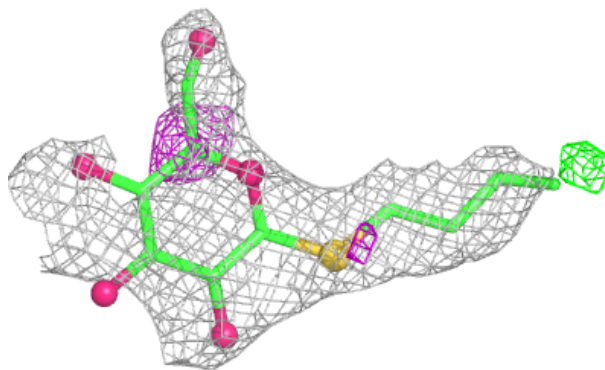


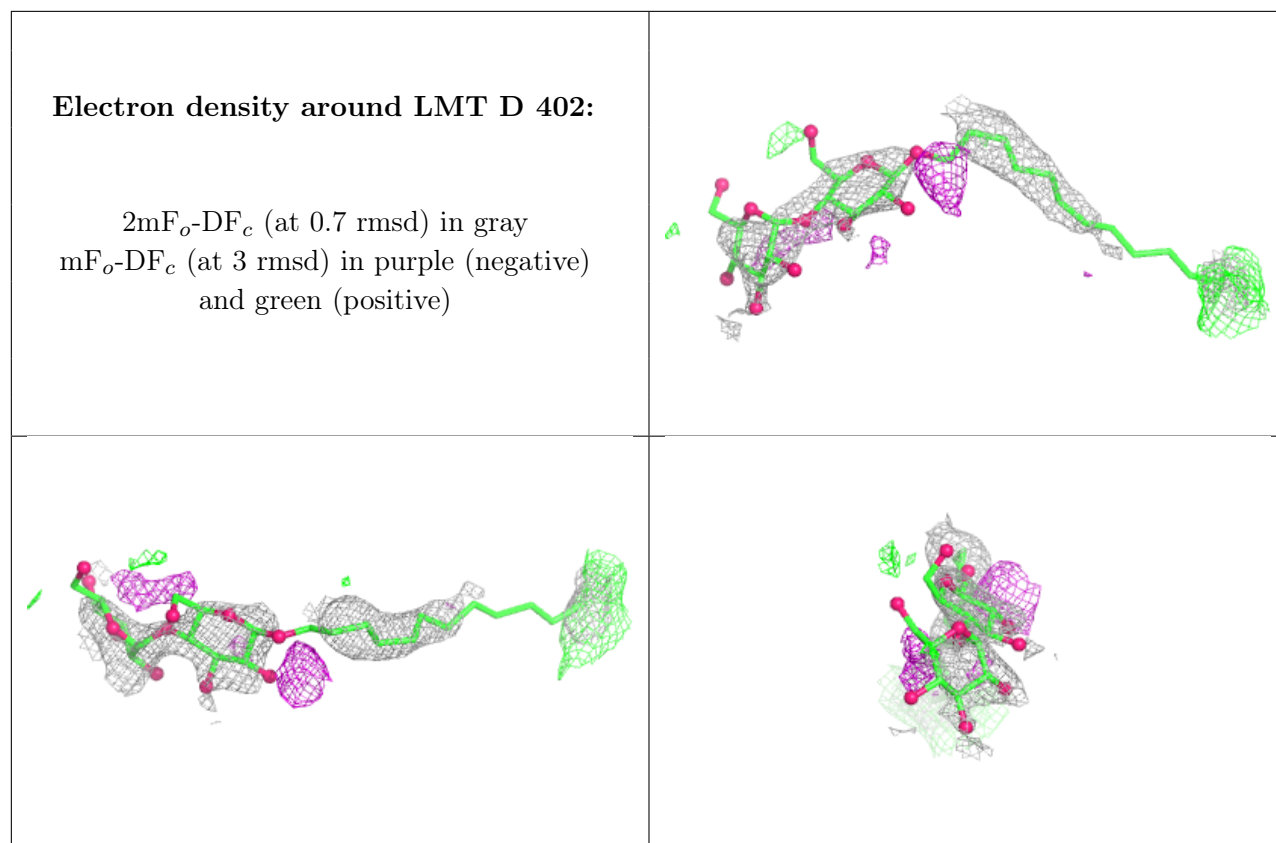
Electron density around HTG b 623:

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

**Electron density around HTG D 411:**

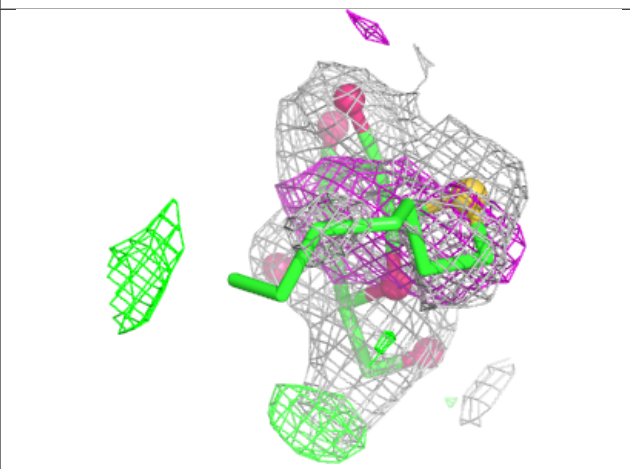
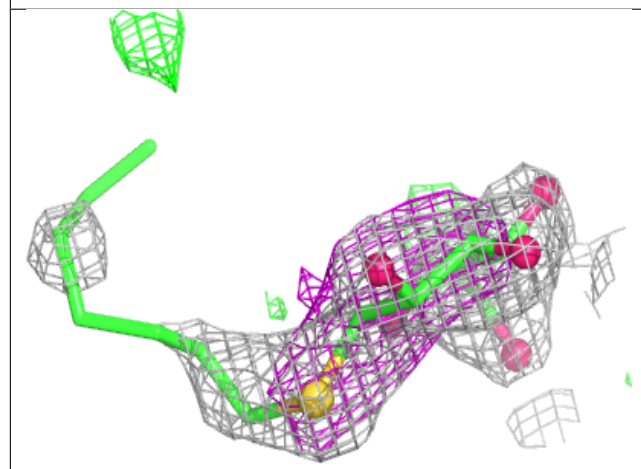
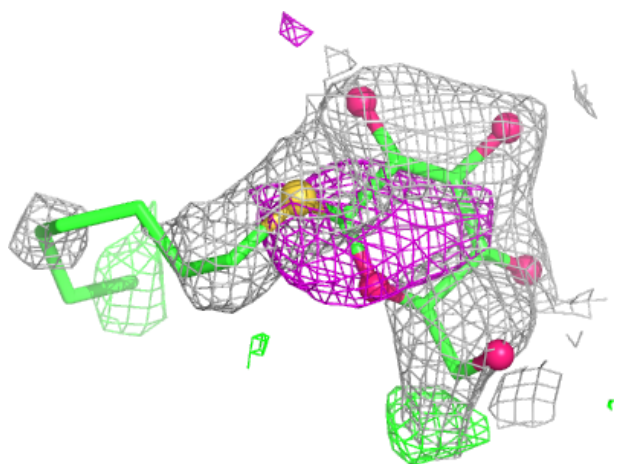
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





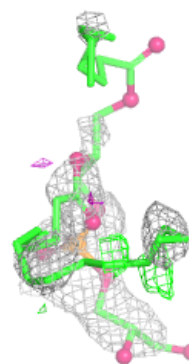
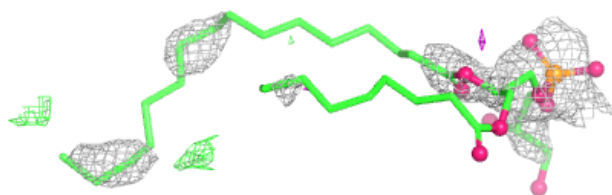
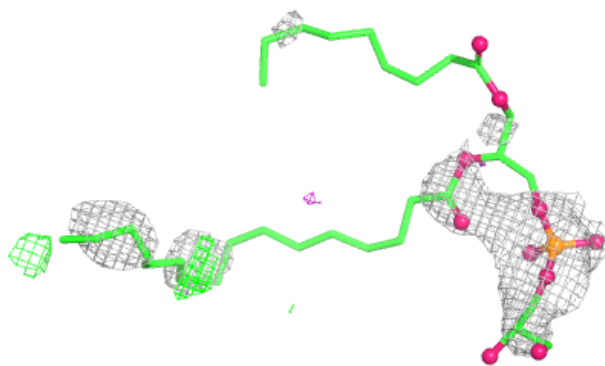
Electron density around HTG B 623:

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

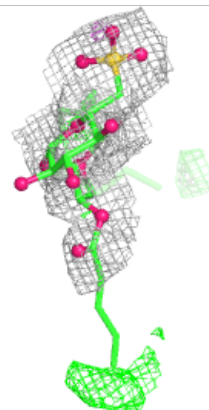
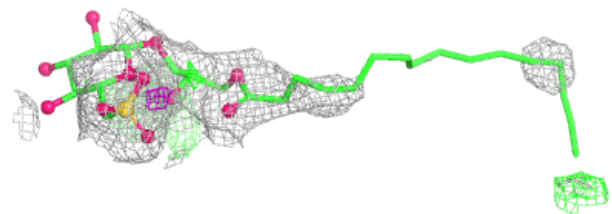
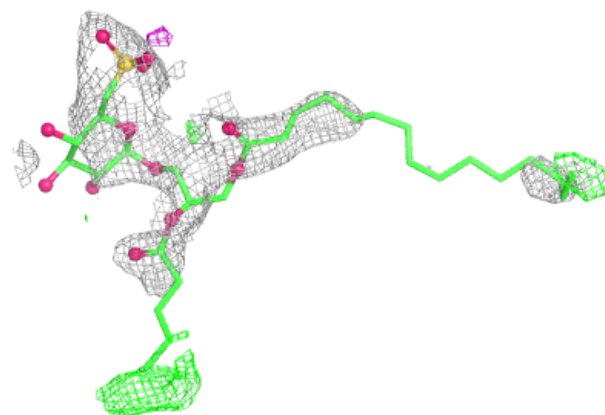


Electron density around LHG a 419:

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

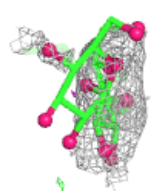
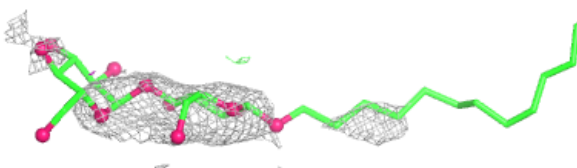
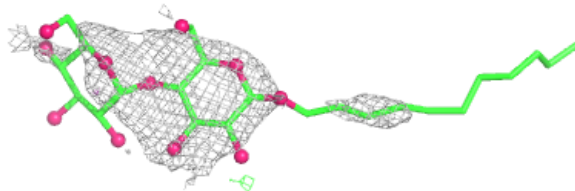
**Electron density around SQD f 101:**

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

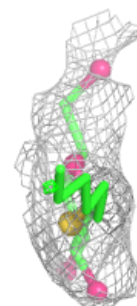
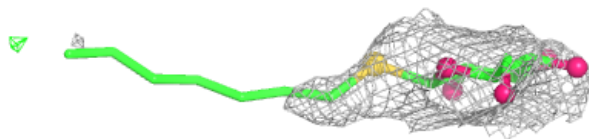
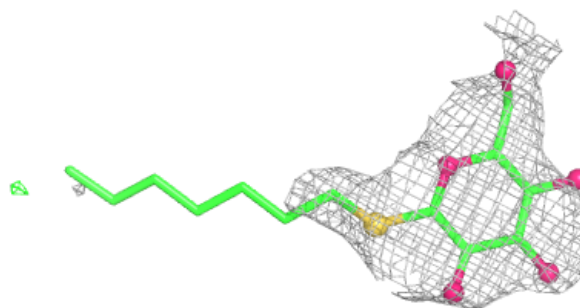


Electron density around LMT a 418:

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

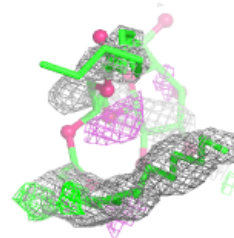
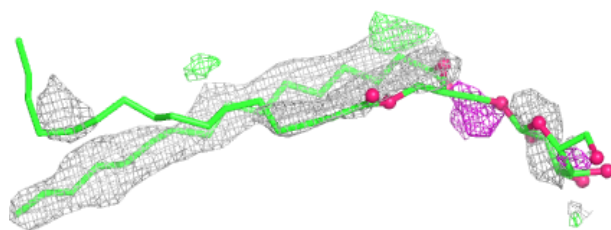
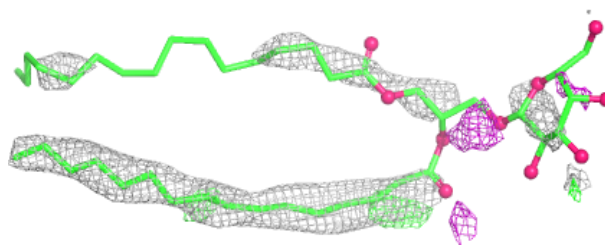
**Electron density around HTG c 523:**

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

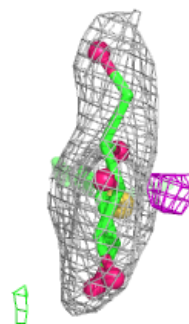
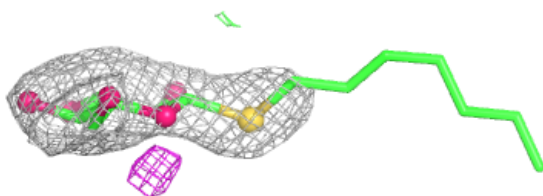
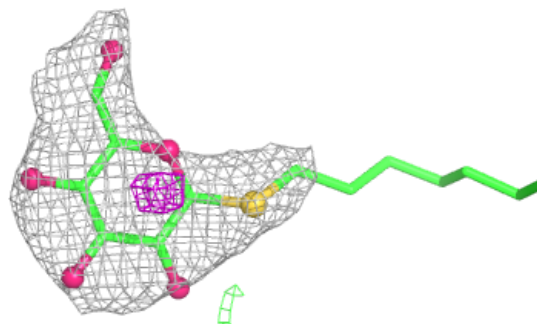


Electron density around LMG C 522:

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

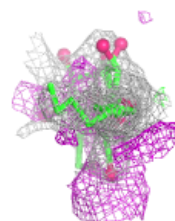
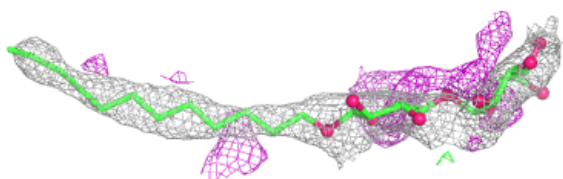
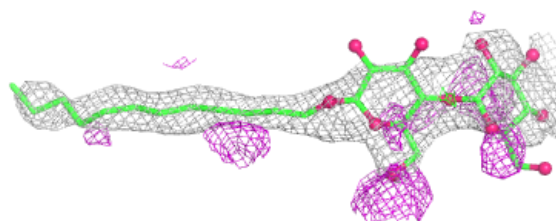
**Electron density around HTG C 523:**

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

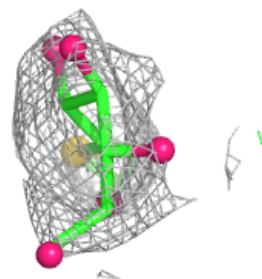
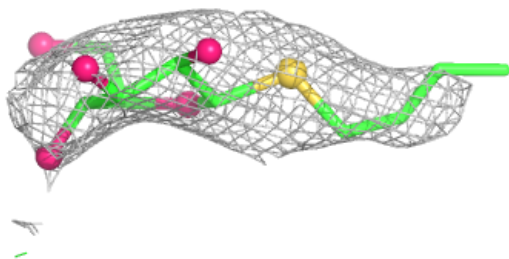
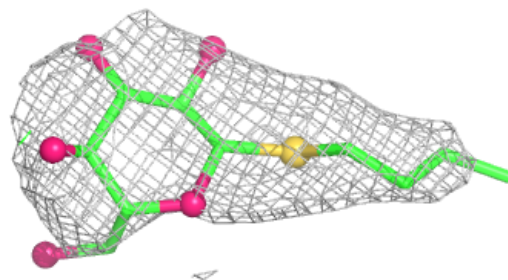


Electron density around LMT m 103:

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

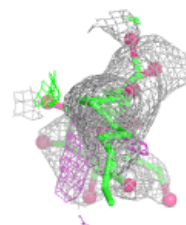
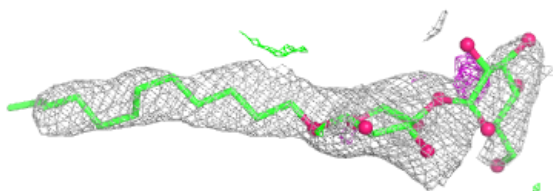
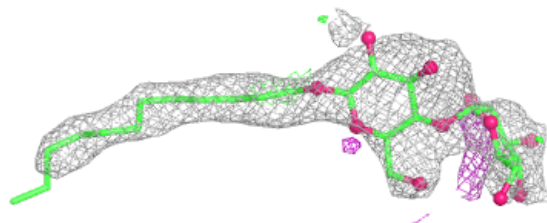
**Electron density around HTG h 101:**

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

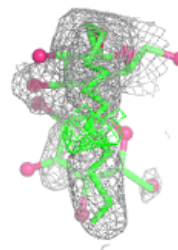
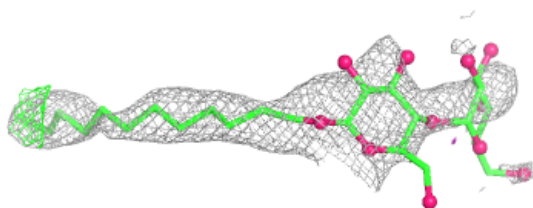
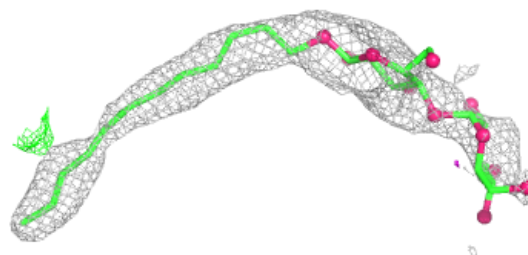


Electron density around LMT B 628:

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

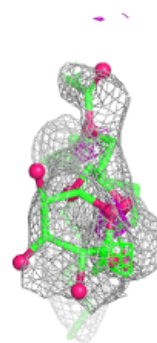
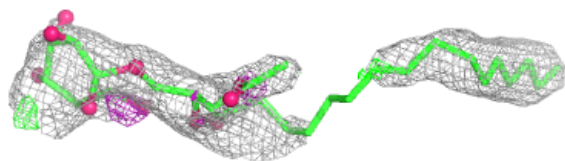
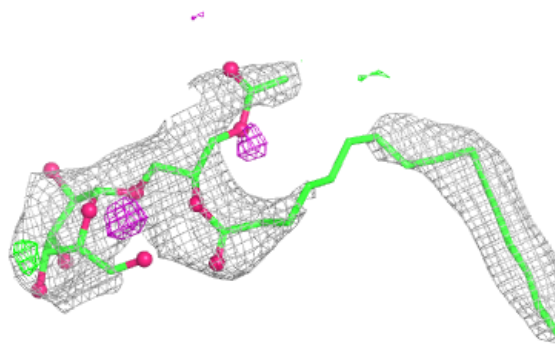
**Electron density around LMT M 103:**

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

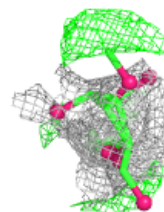
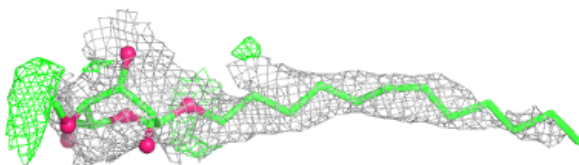
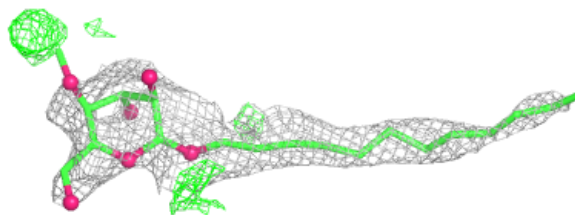


Electron density around LMG Z 101:

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

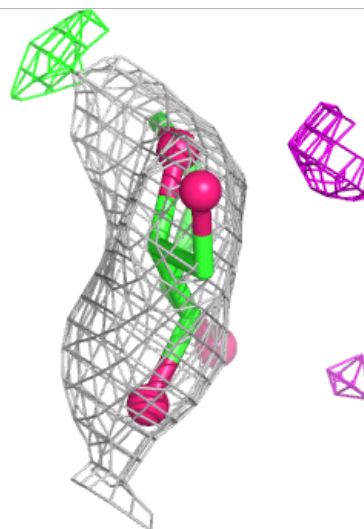
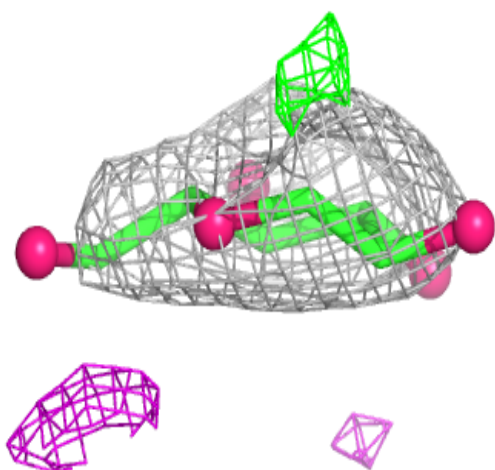
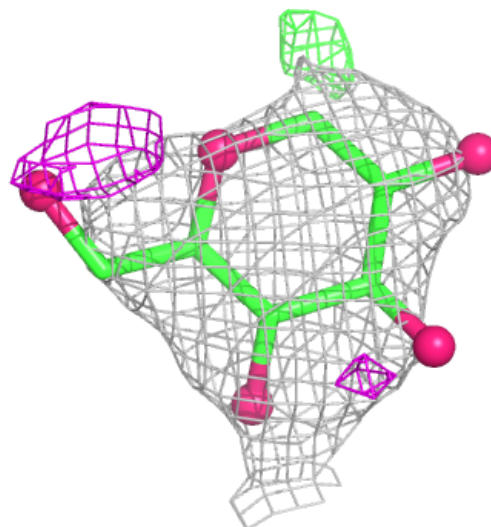
**Electron density around LMT b 621:**

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



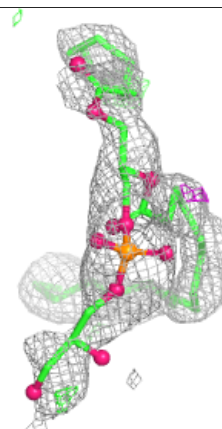
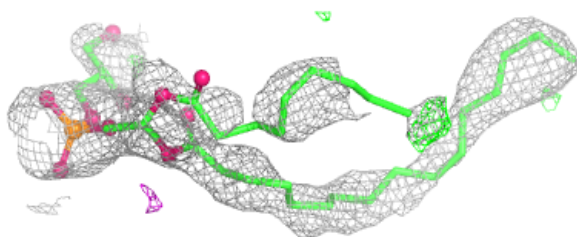
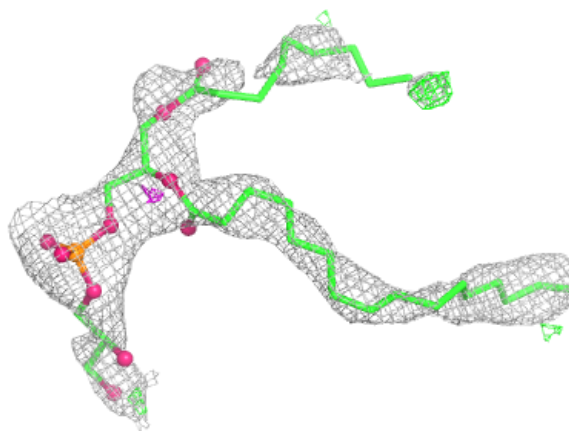
Electron density around HTG V 202:

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

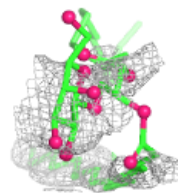
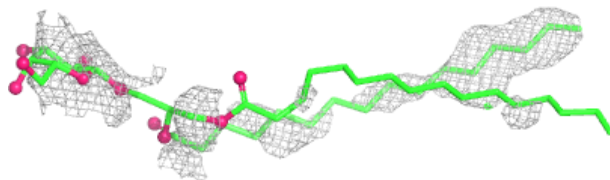
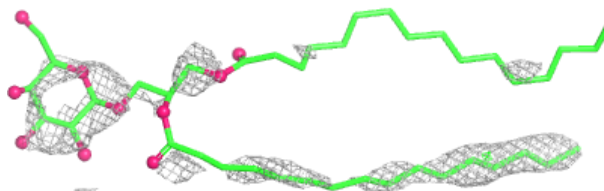


Electron density around LHG E 101:

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

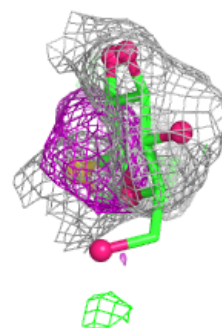
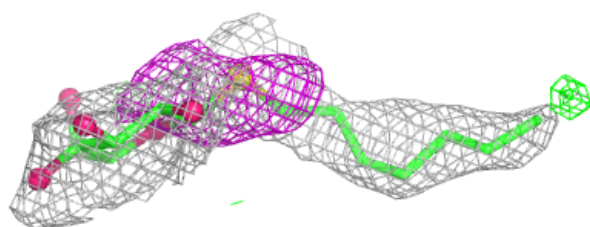
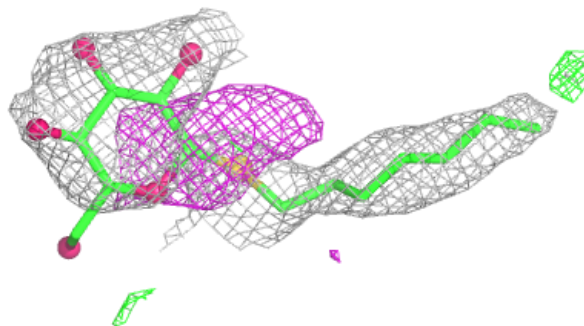
**Electron density around LMG c 522:**

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

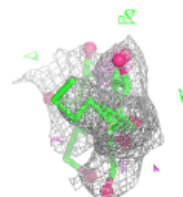
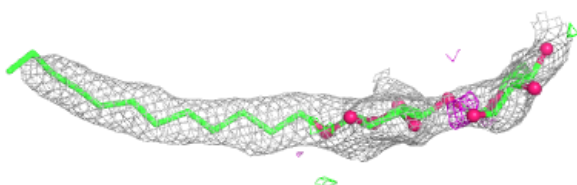
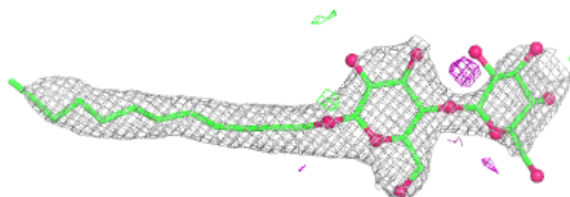


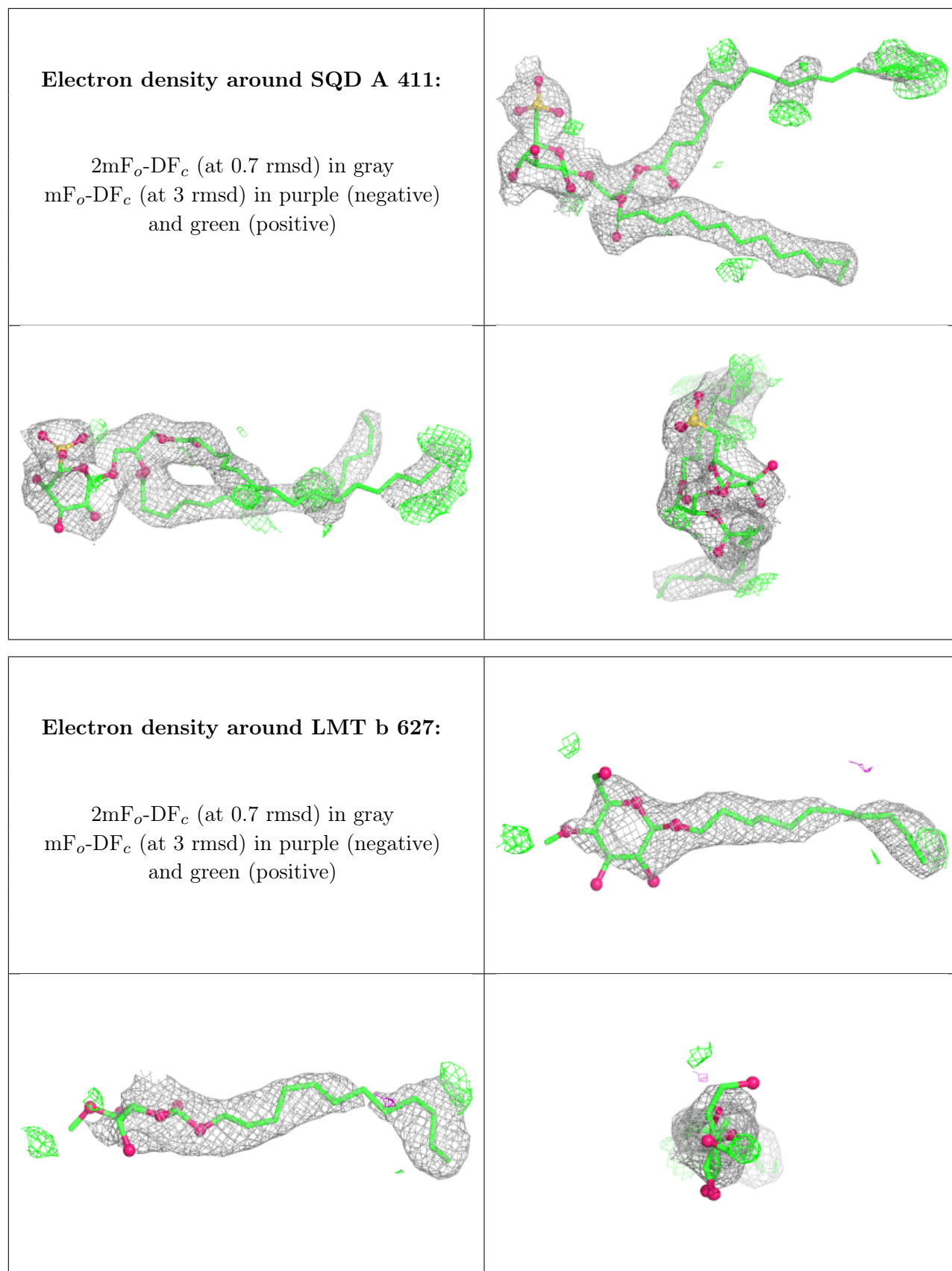
Electron density around HTG b 622:

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

**Electron density around LMT M 101:**

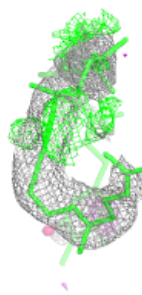
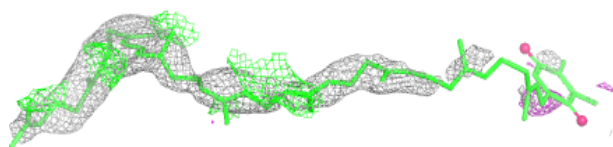
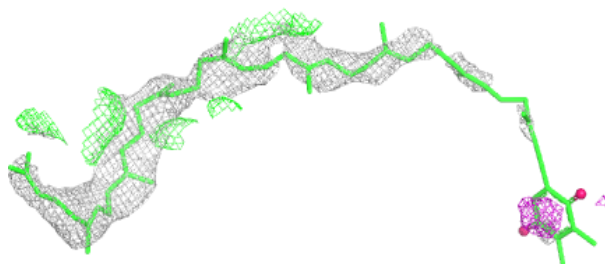
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



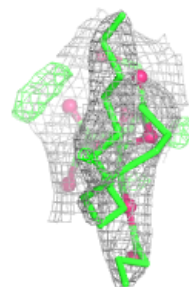
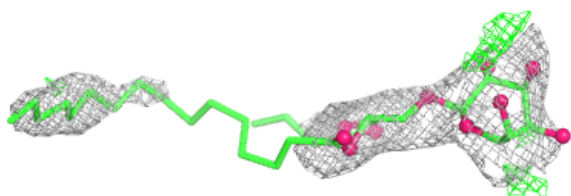
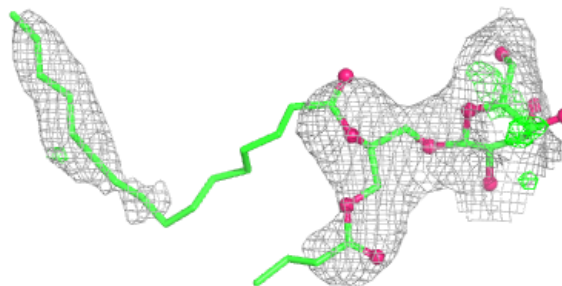


Electron density around PL9 a 415:

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

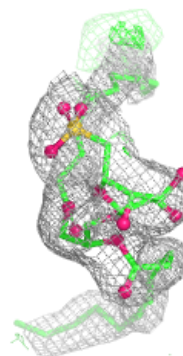
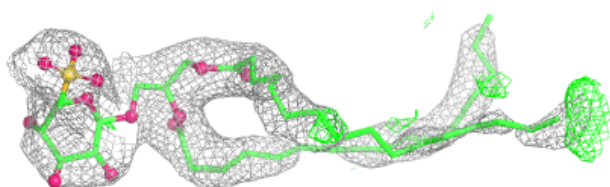
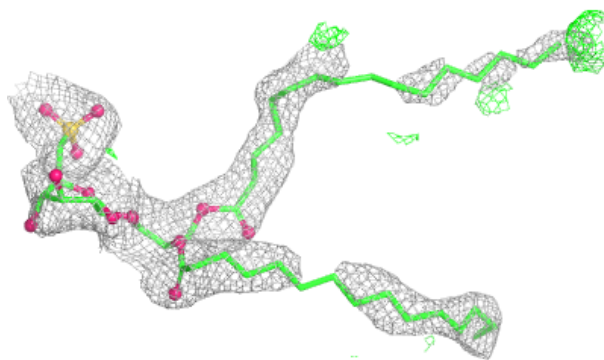
**Electron density around LMG z 101:**

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

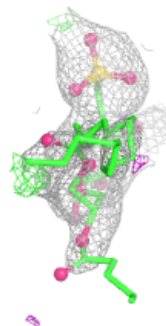
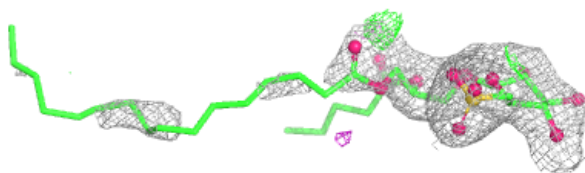
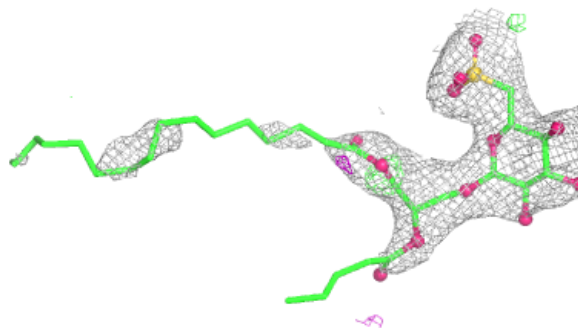


Electron density around SQD a 412:

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

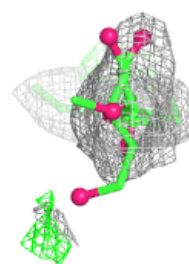
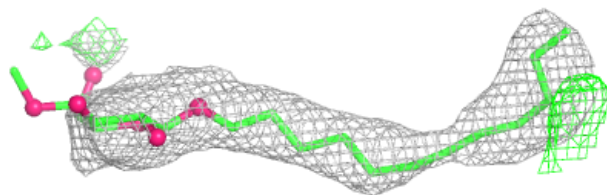
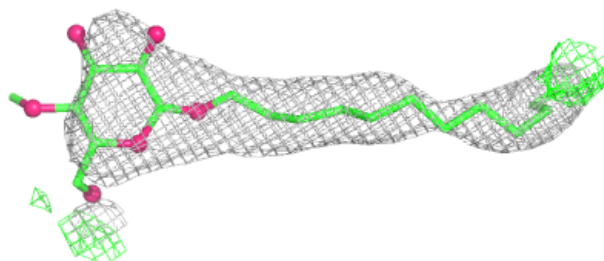
**Electron density around SQD D 412:**

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

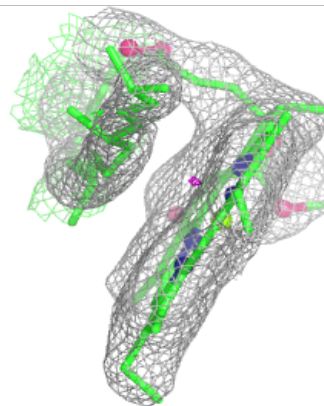
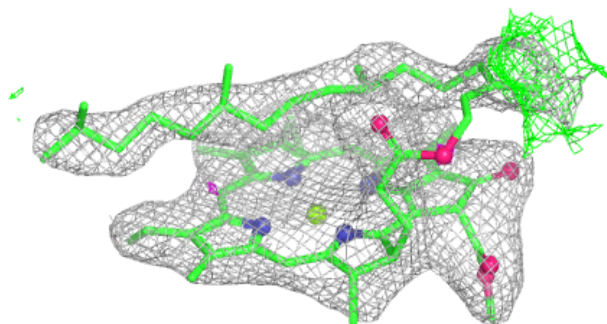
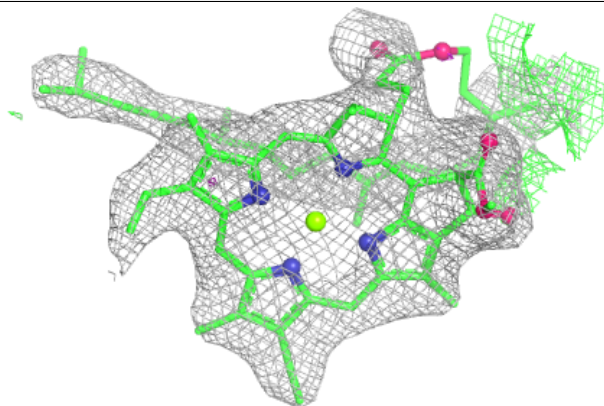


Electron density around LMT B 630:

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

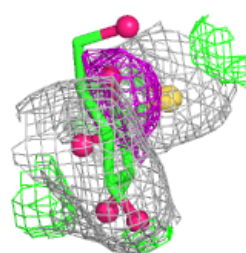
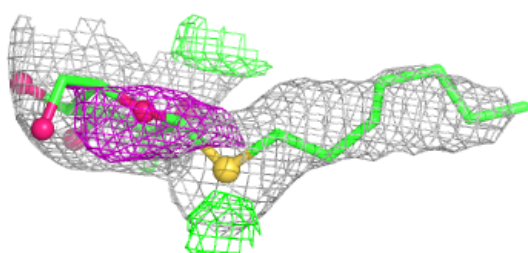
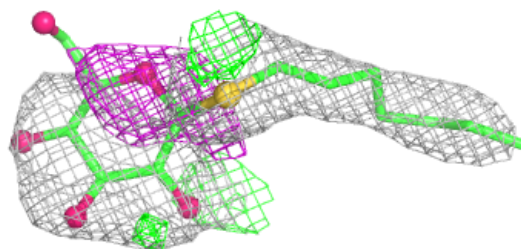
**Electron density around CLA b 601:**

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

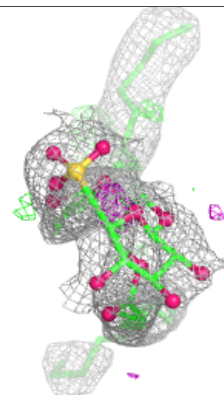
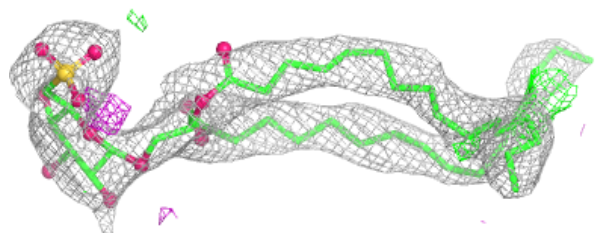
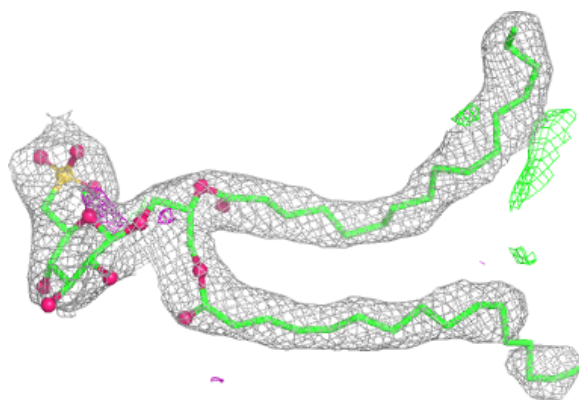


Electron density around HTG B 622:

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

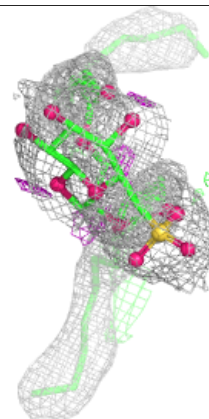
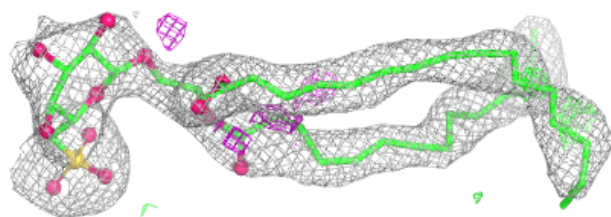
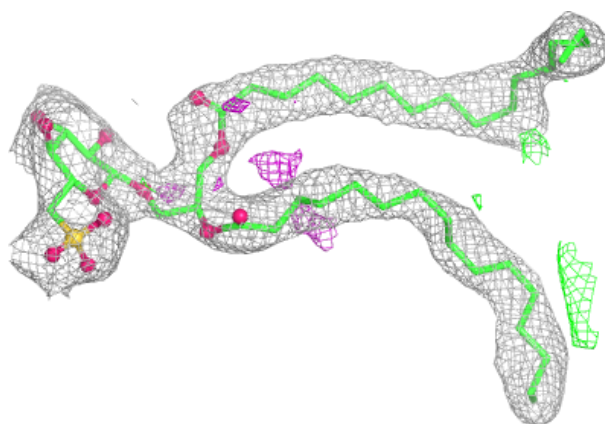
**Electron density around SQD b 620:**

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

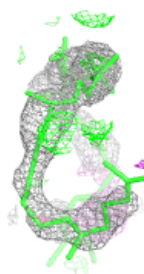
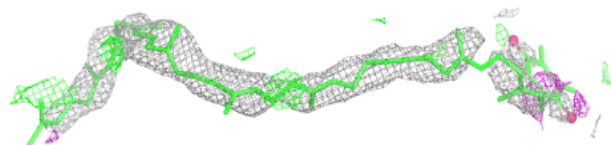
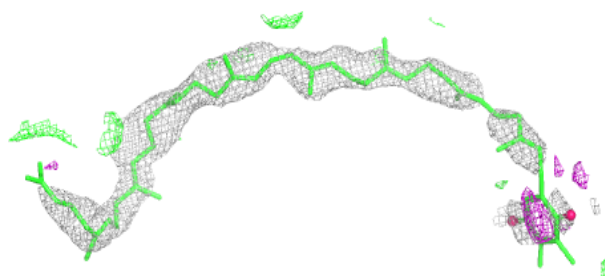


Electron density around SQD B 620:

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

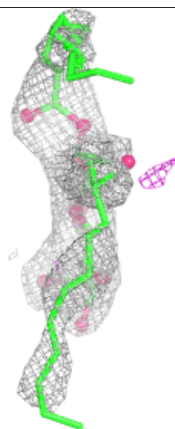
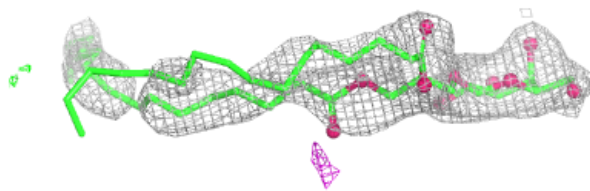
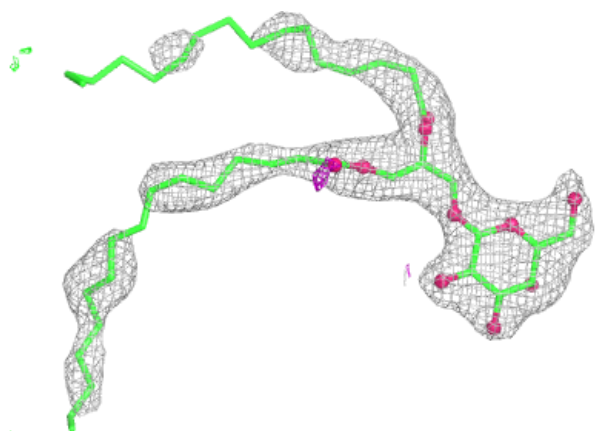
**Electron density around PL9 A 413:**

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

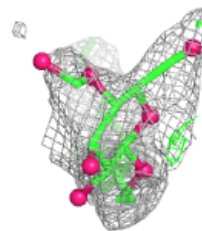
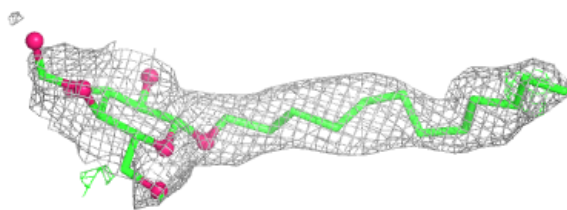
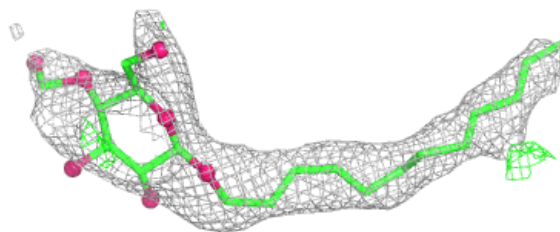


Electron density around LMG C 521:

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

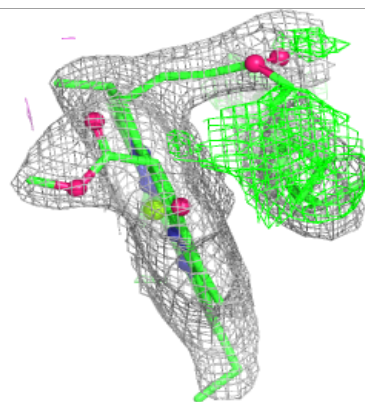
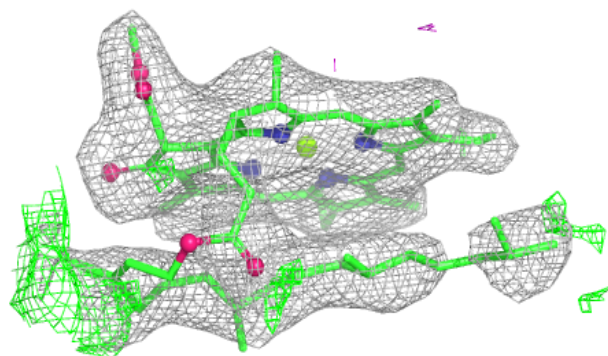
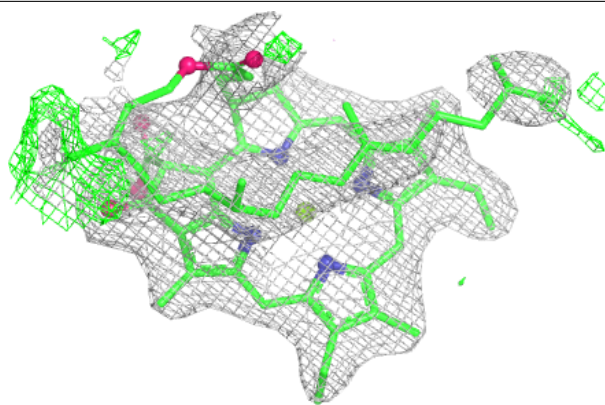
**Electron density around LMT t 101:**

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

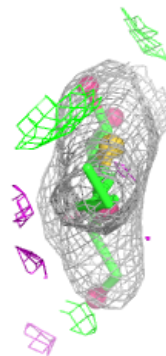
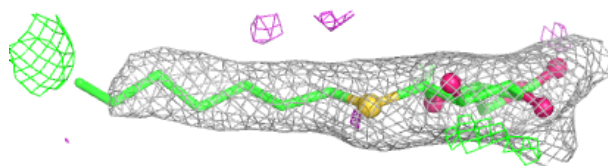
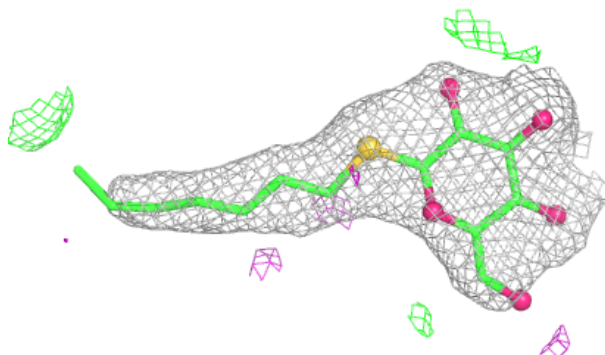


Electron density around CLA B 601:

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

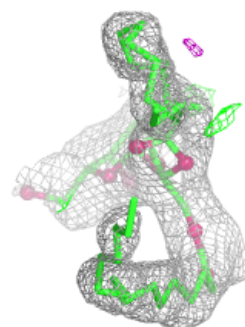
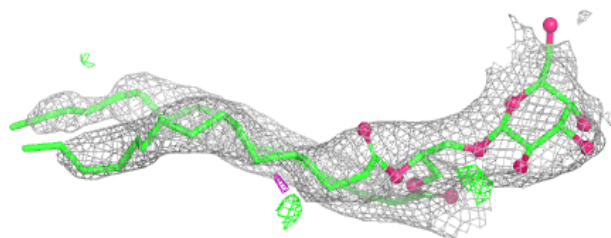
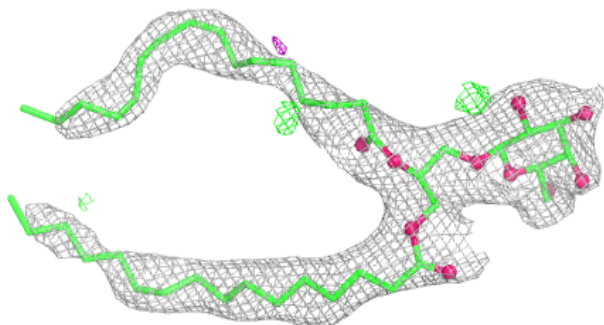
**Electron density around HTG B 625:**

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

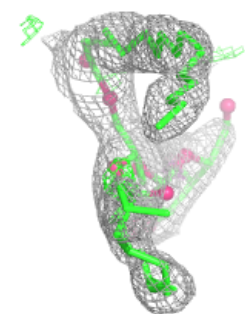
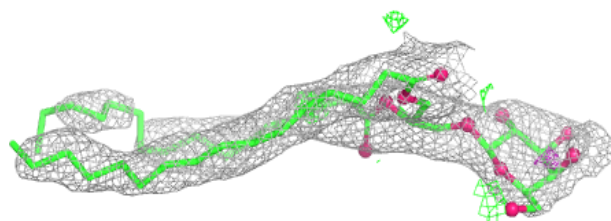
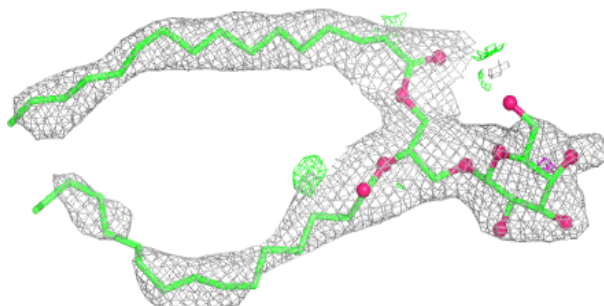


Electron density around LMG C 502:

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

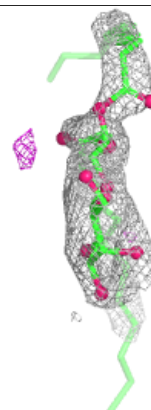
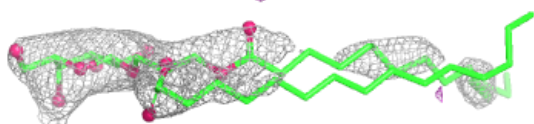
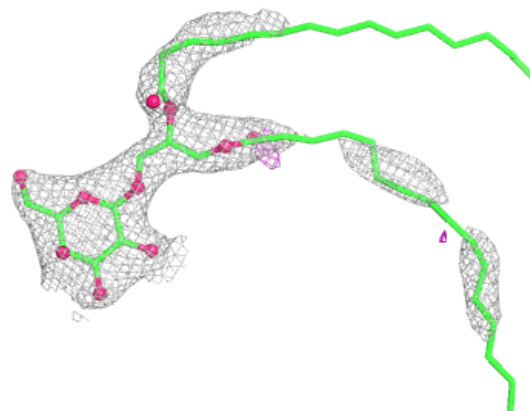
**Electron density around LMG c 501:**

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

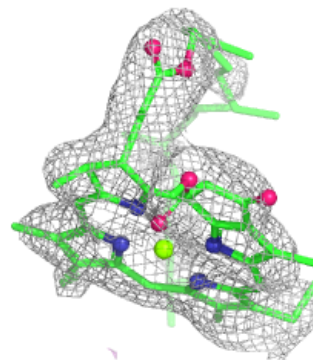
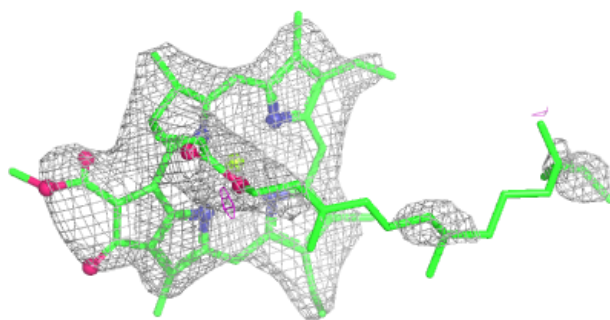
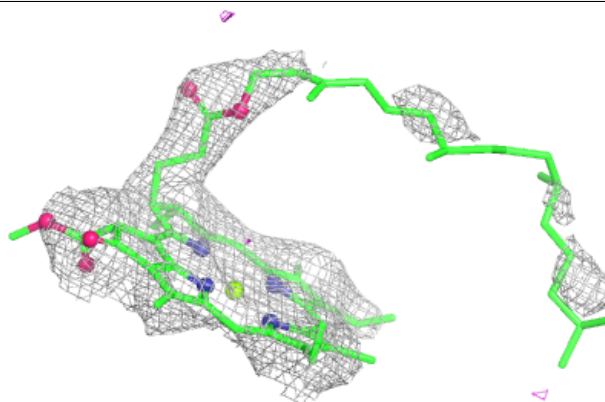


Electron density around LMG c 521:

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

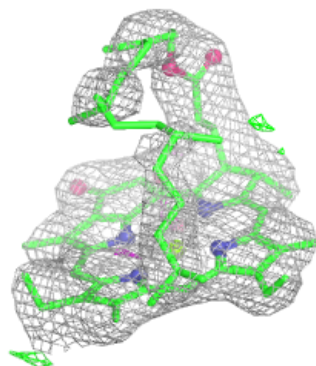
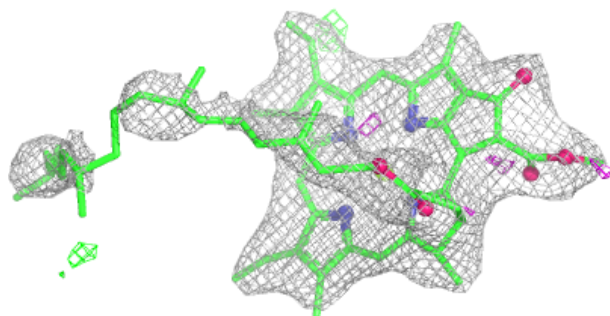
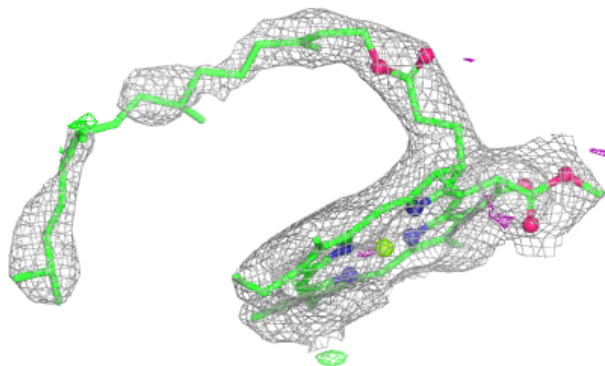
**Electron density around CLA c 515:**

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

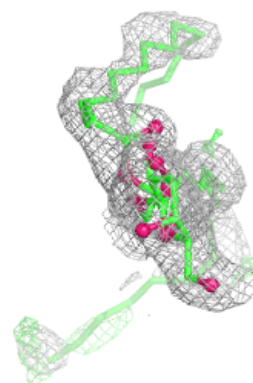
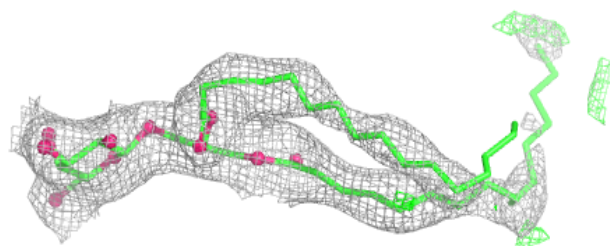
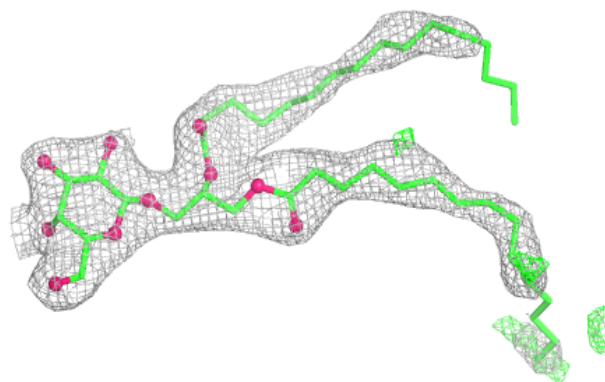


Electron density around CLA C 515:

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

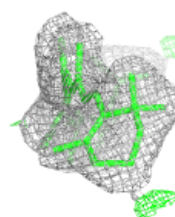
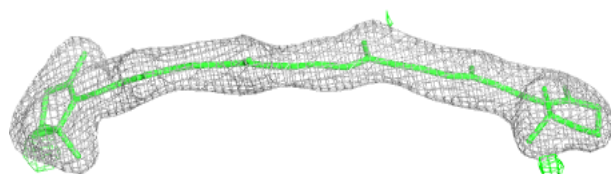
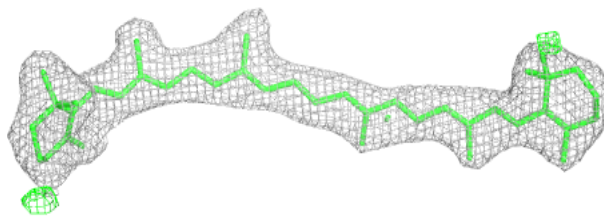
**Electron density around LMG D 413:**

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

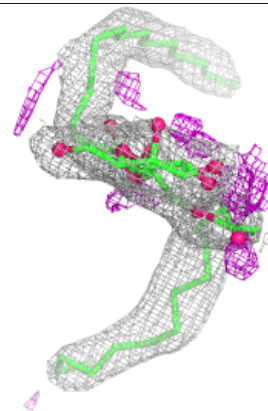
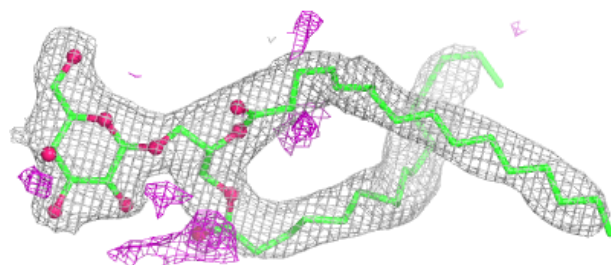
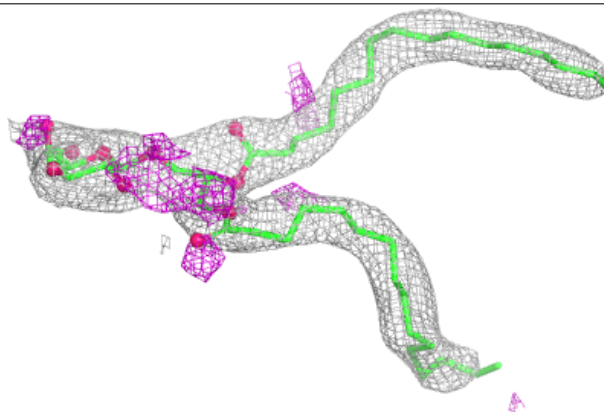


Electron density around BCR t 102:

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

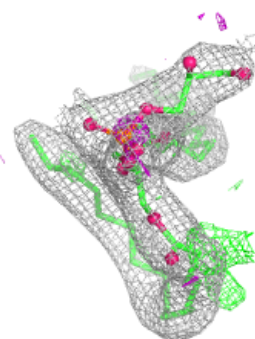
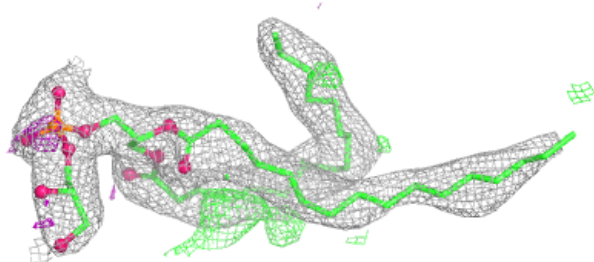
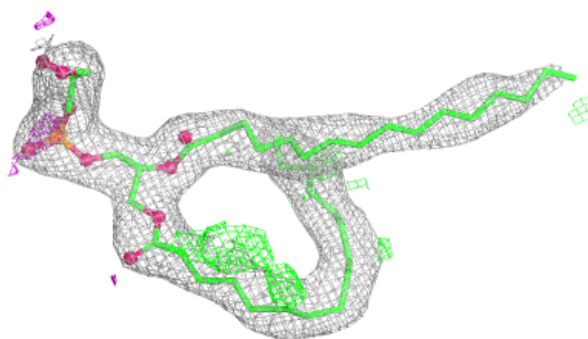
**Electron density around LMG m 101:**

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

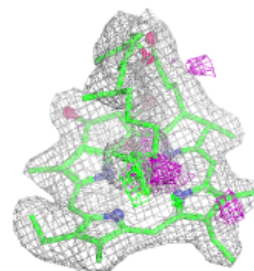
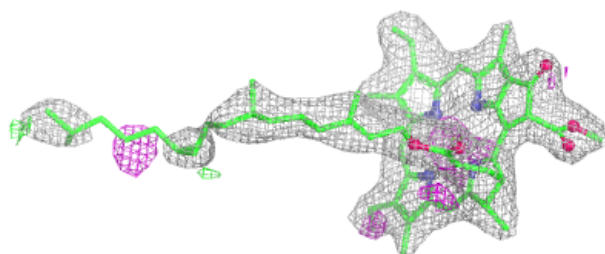
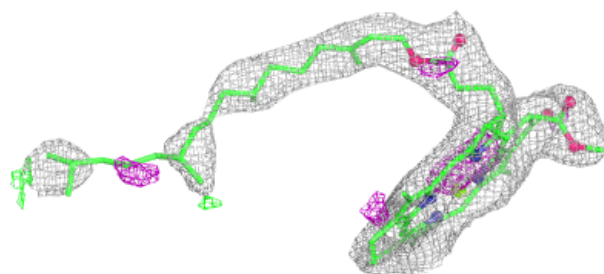


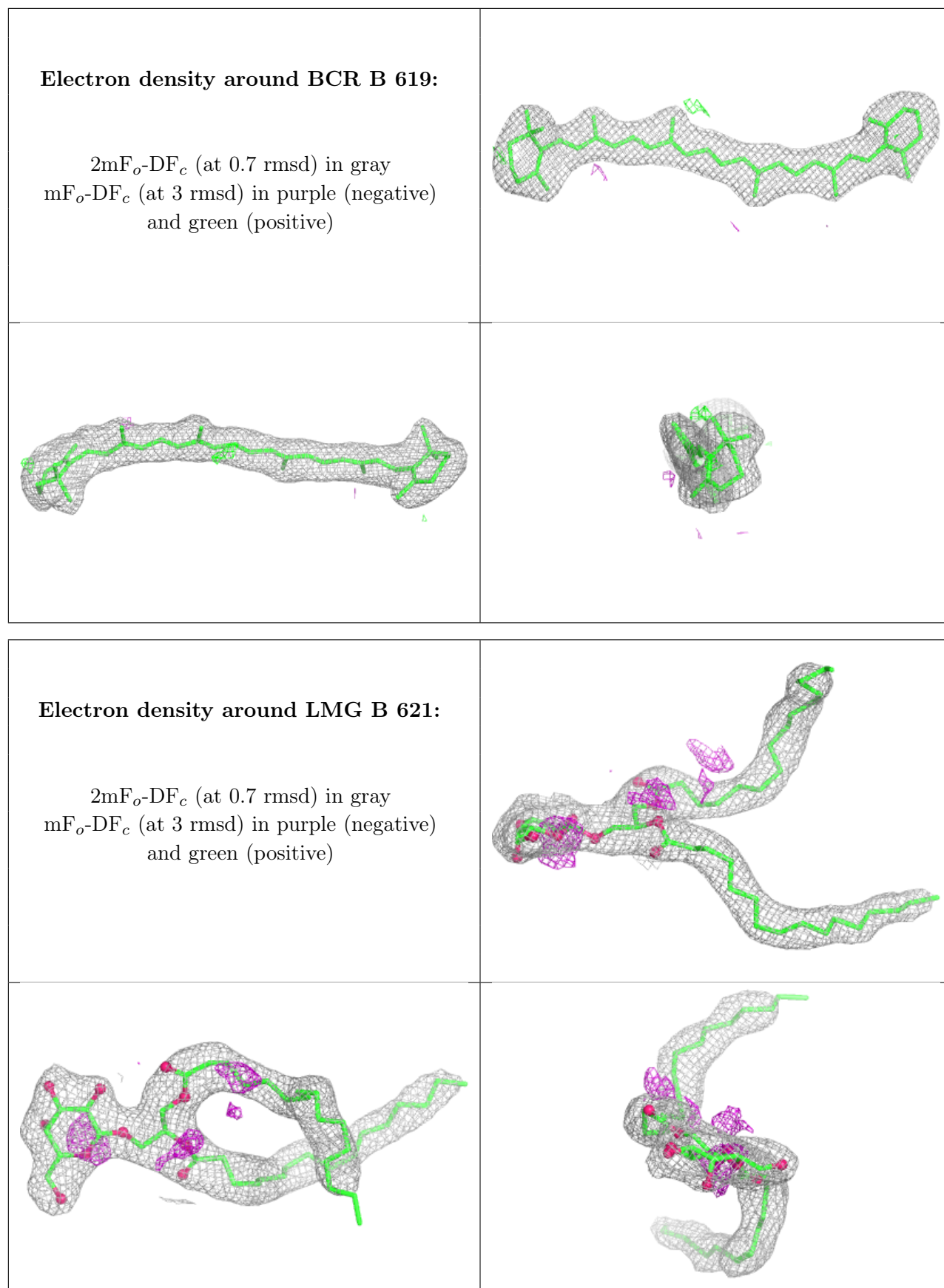
Electron density around LHG A 416:

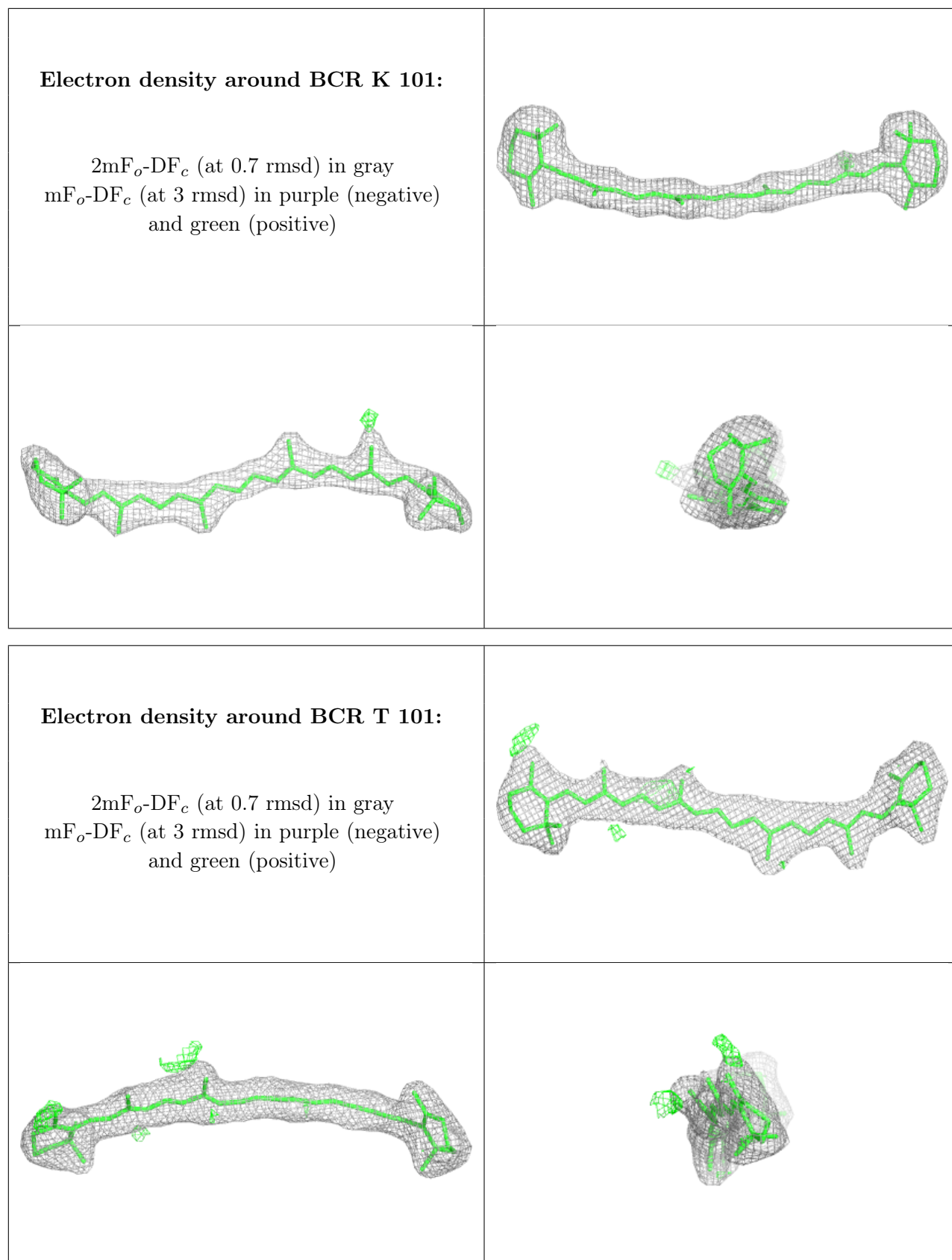
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around CLA C 506:**

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

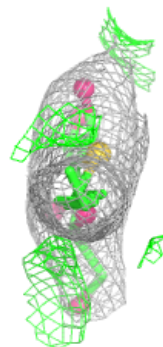
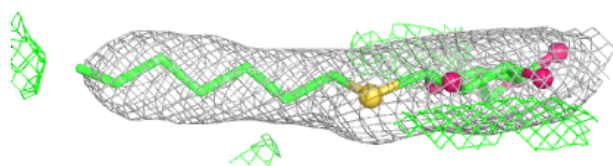
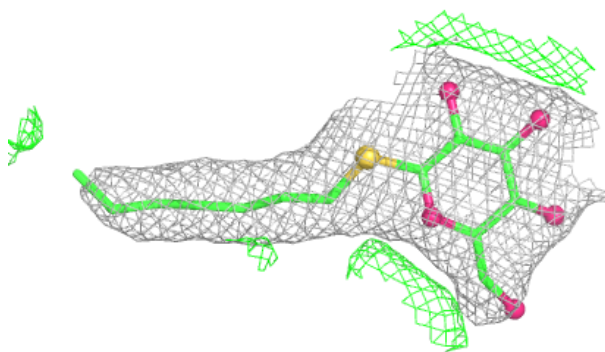




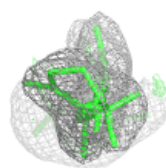
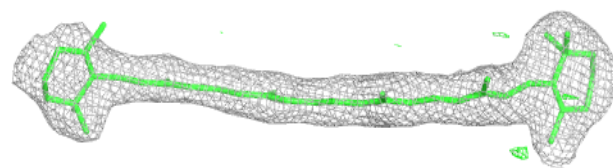


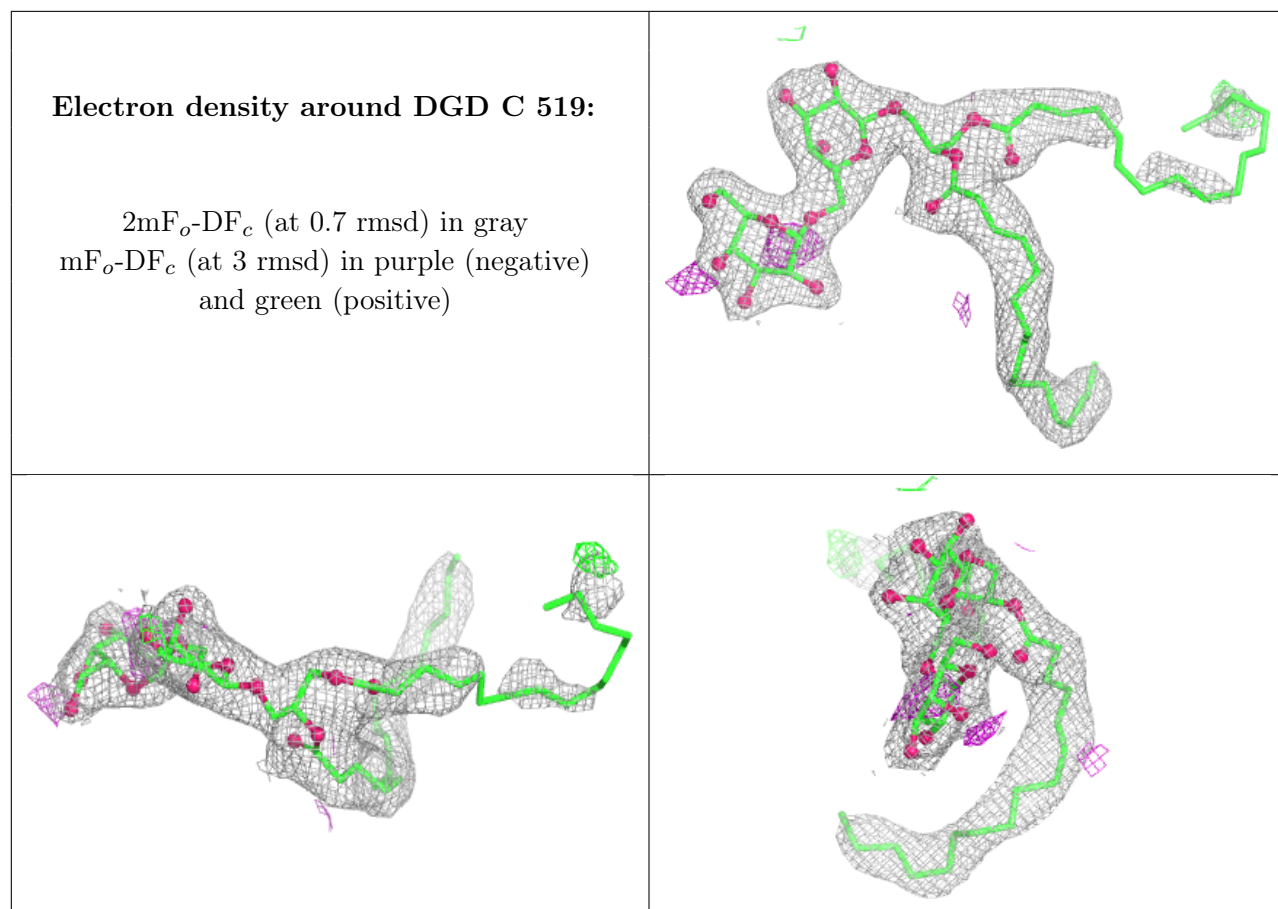
Electron density around HTG b 625:

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

**Electron density around BCR h 102:**

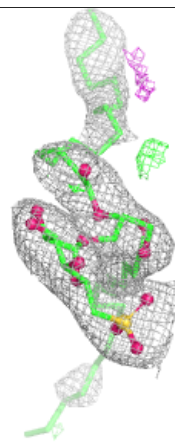
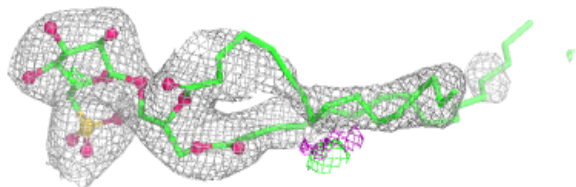
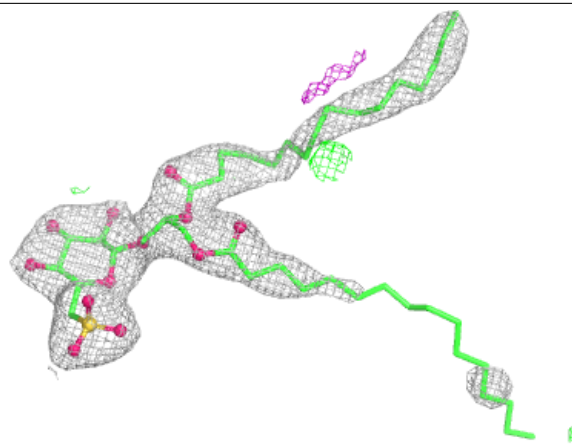
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



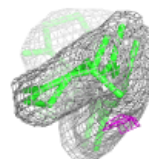
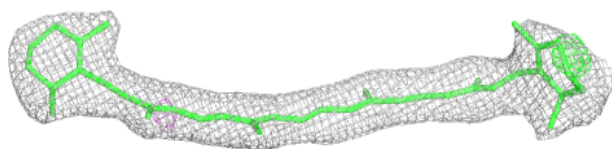
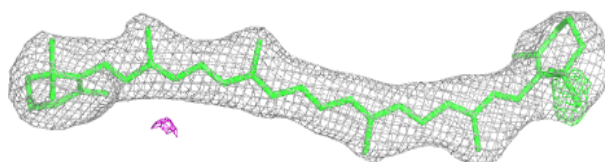


Electron density around SQD C 501:

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

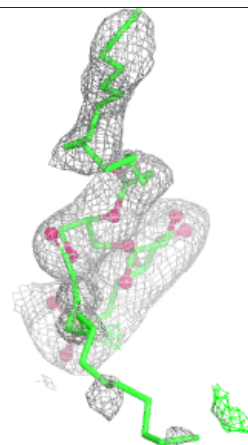
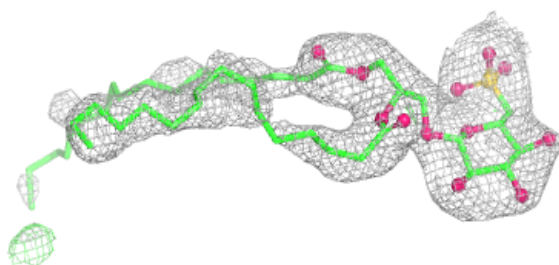
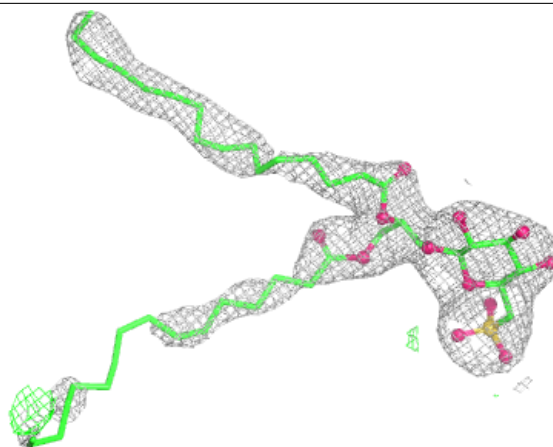
**Electron density around BCR d 404:**

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

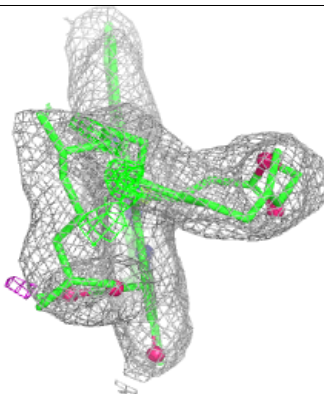
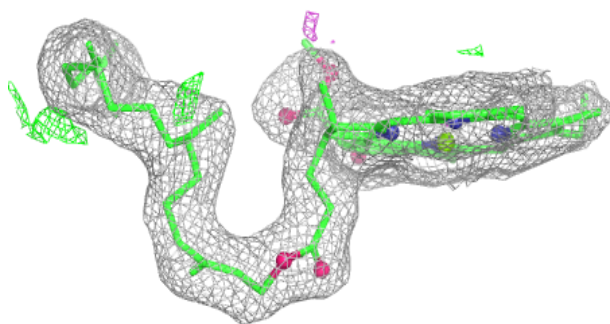
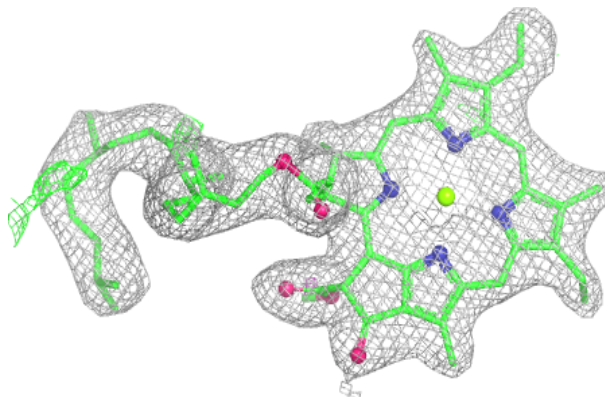


Electron density around SQD a 410:

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

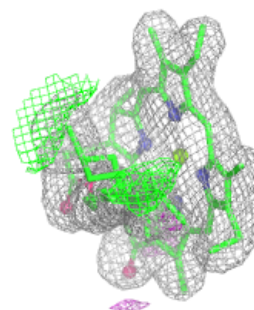
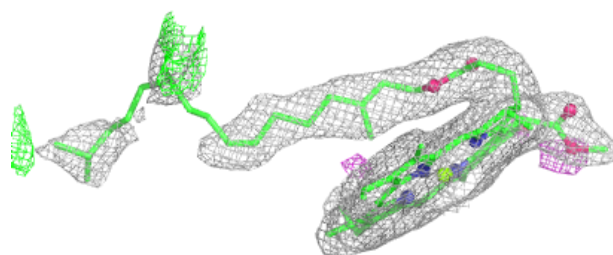
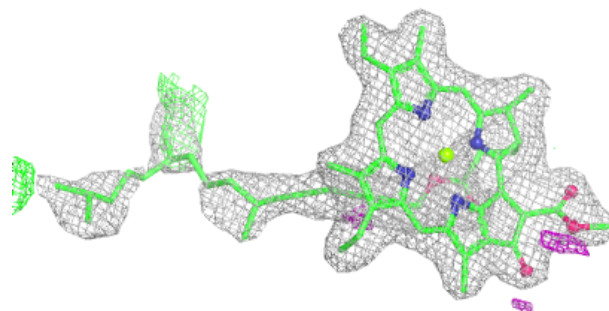
**Electron density around CLA b 612:**

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

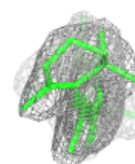
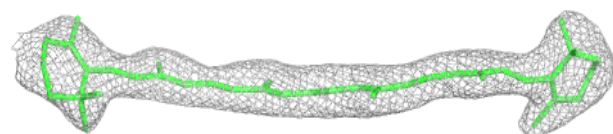
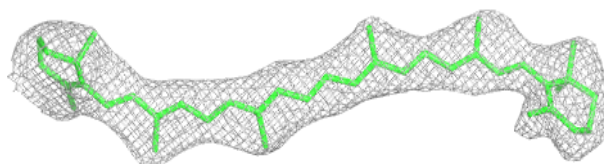


Electron density around CLA b 614:

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

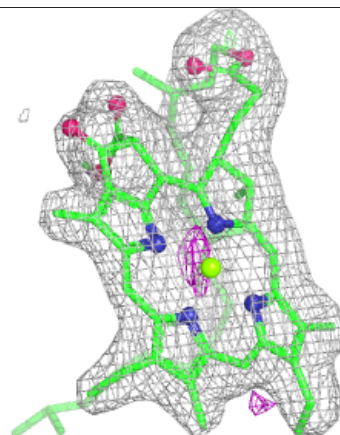
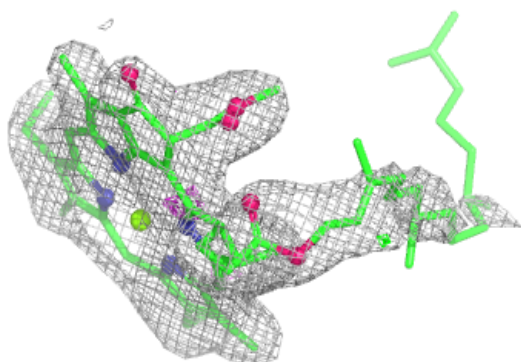
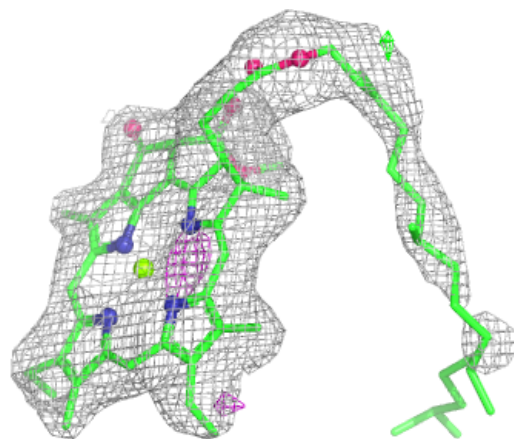
**Electron density around BCR y 101:**

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

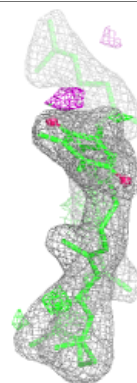
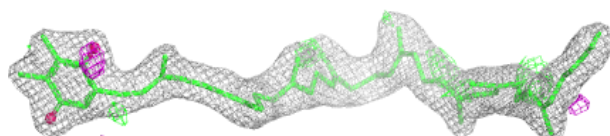
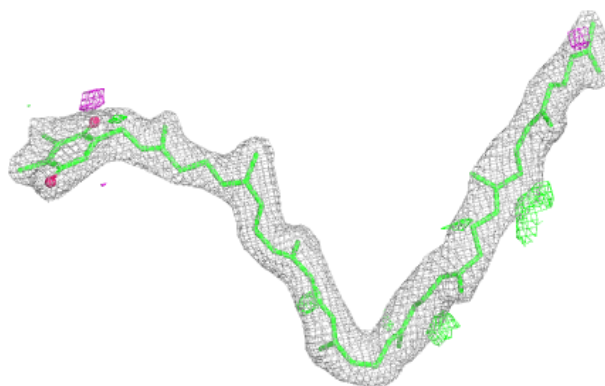


Electron density around CLA b 616:

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

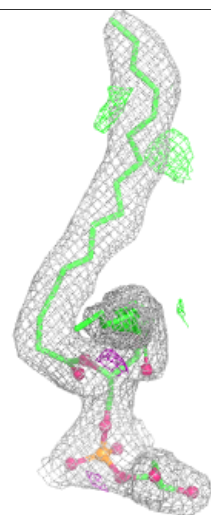
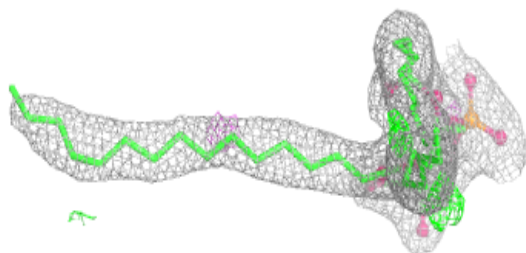
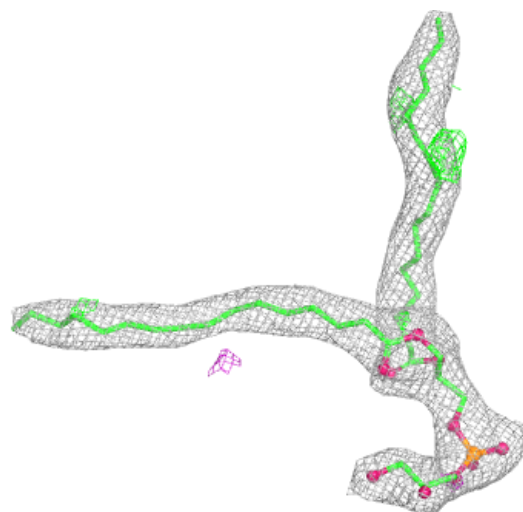
**Electron density around PL9 D 406:**

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



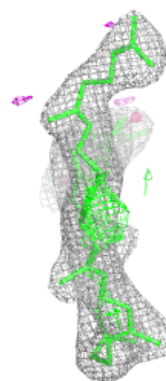
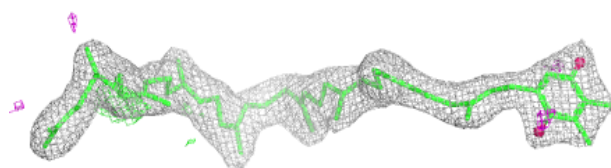
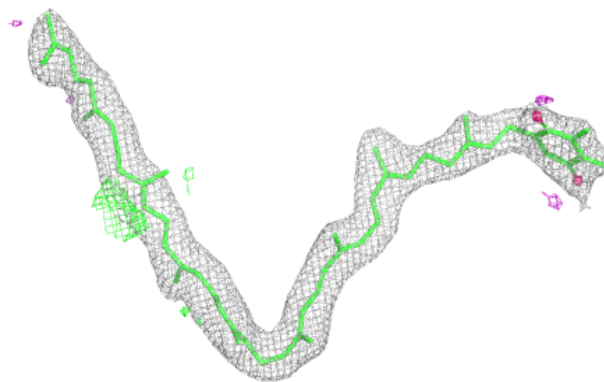
Electron density around LHG b 629:

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



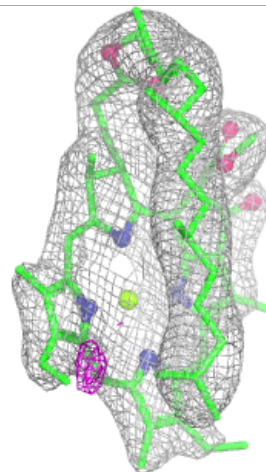
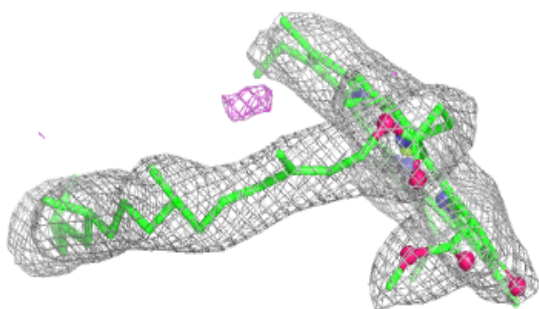
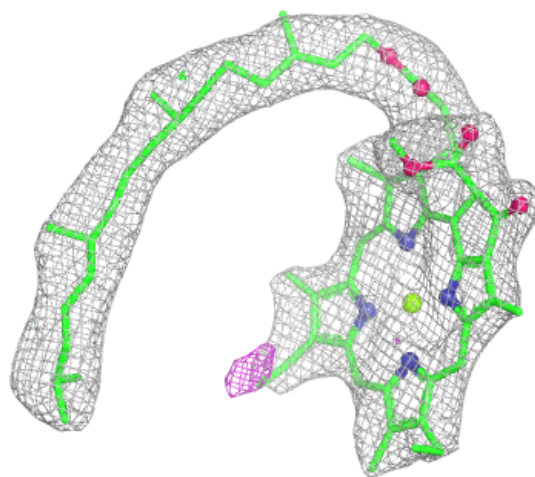
Electron density around PL9 d 405:

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



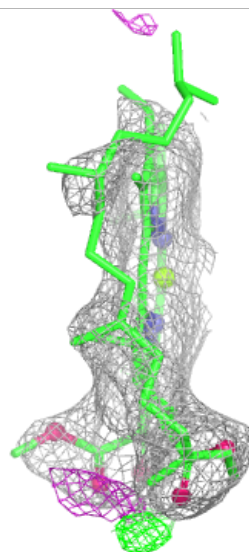
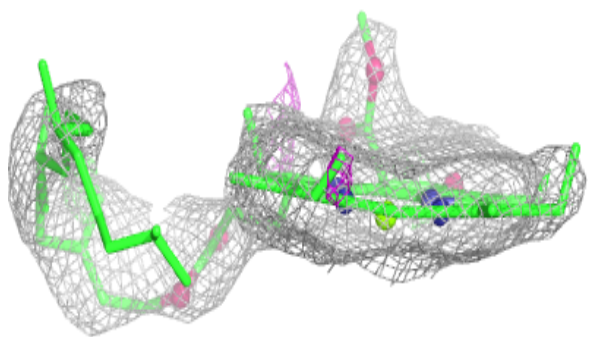
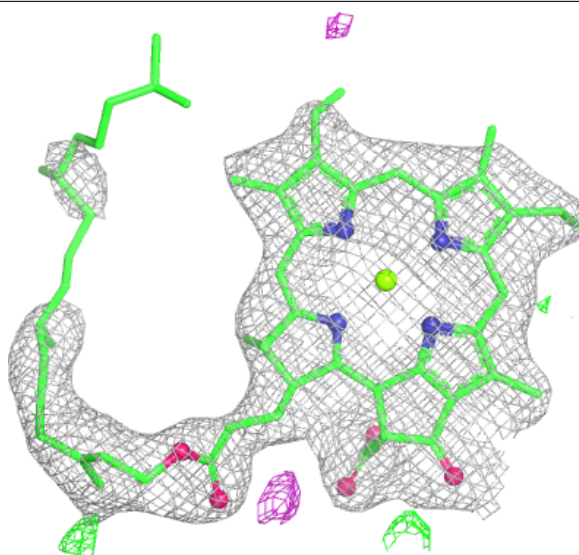
Electron density around CLA c 509:

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



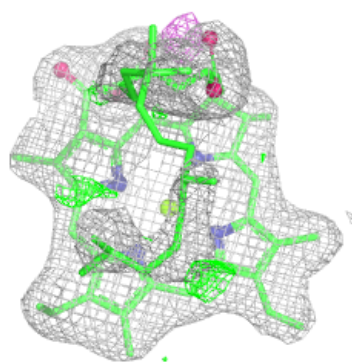
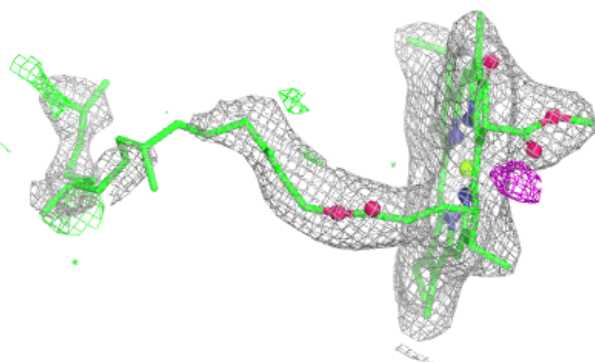
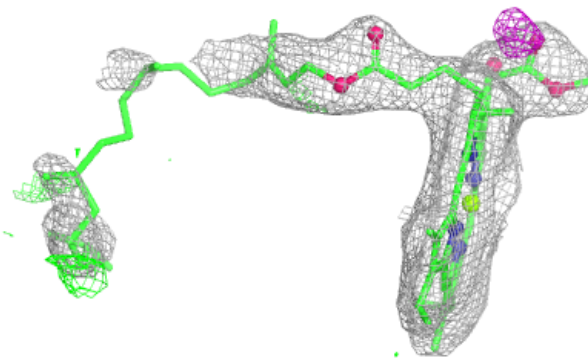
Electron density around CLA c 514:

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

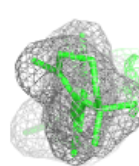
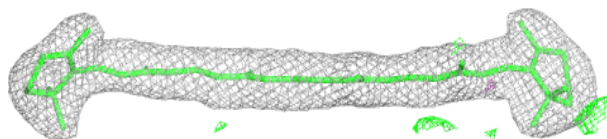
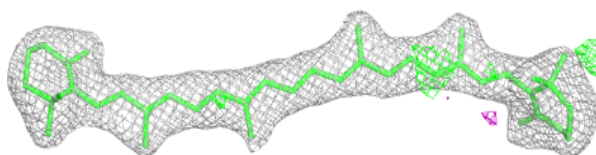


Electron density around CLA C 508:

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

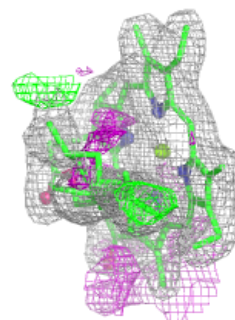
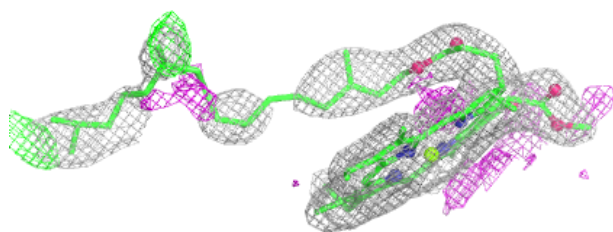
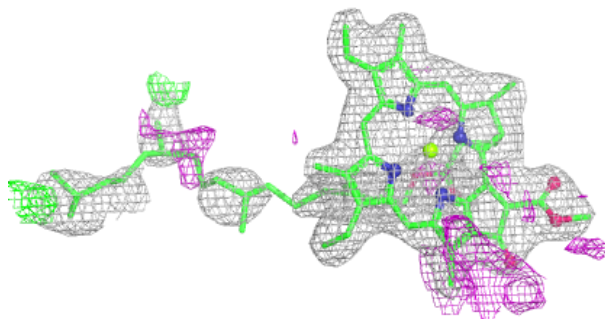
**Electron density around BCR B 618:**

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

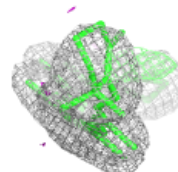
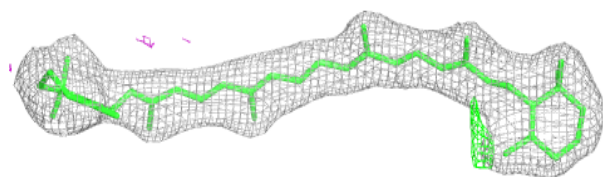
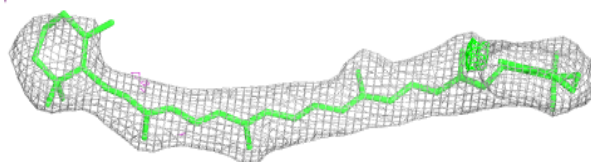


Electron density around CLA B 614:

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

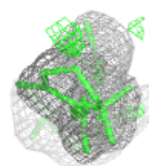
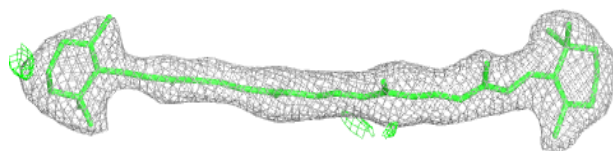
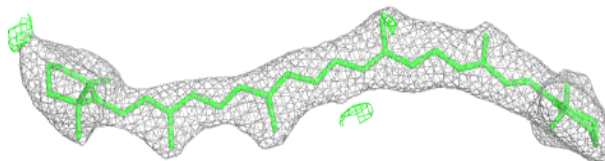
**Electron density around BCR D 405:**

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

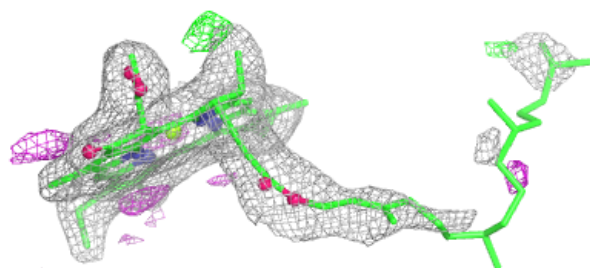
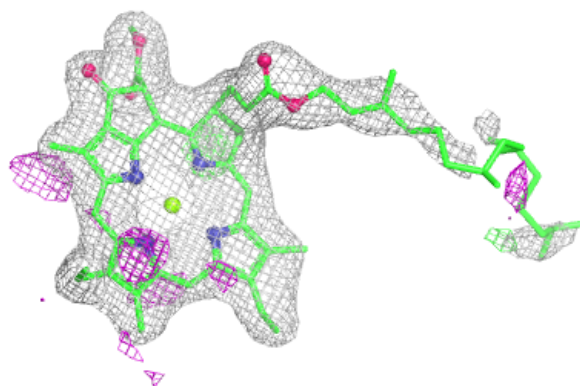


Electron density around BCR H 101:

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

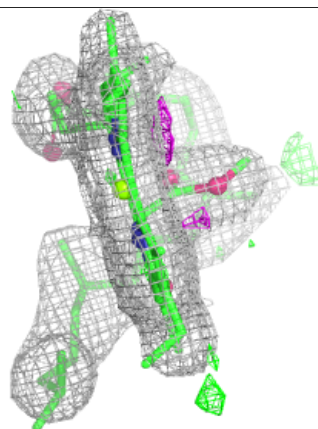
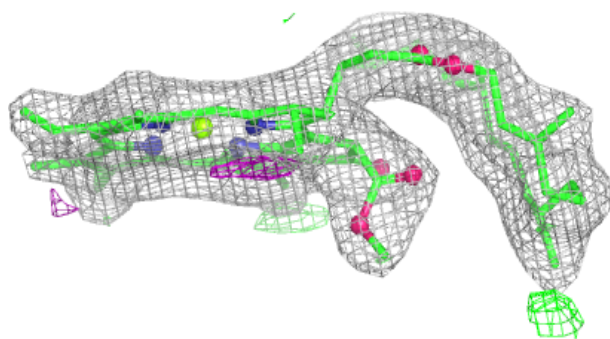
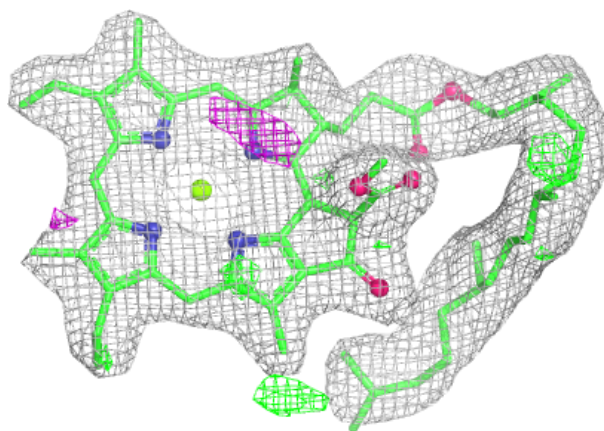
**Electron density around CLA a 408:**

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

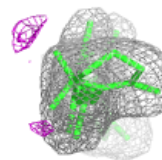
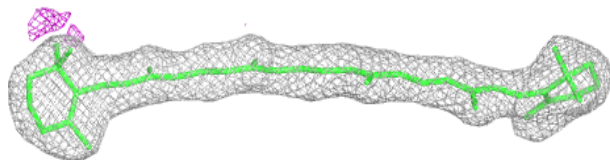
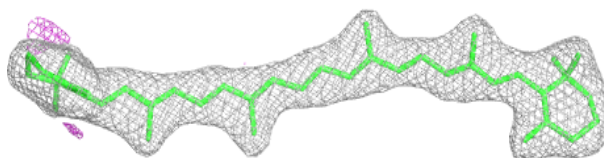


Electron density around CLA B 610:

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

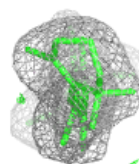
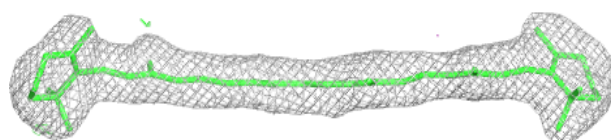
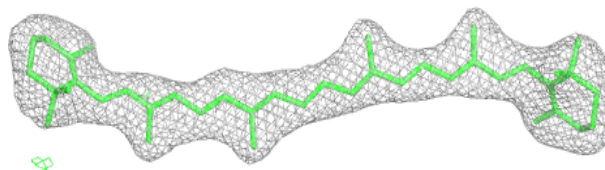
**Electron density around BCR b 617:**

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

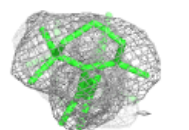
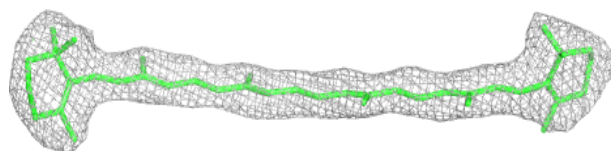
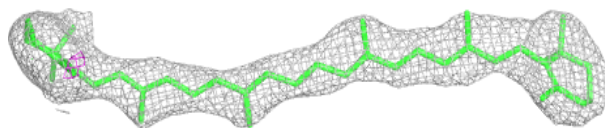


Electron density around BCR b 618:

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

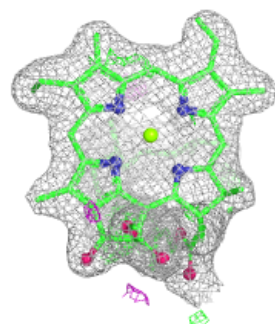
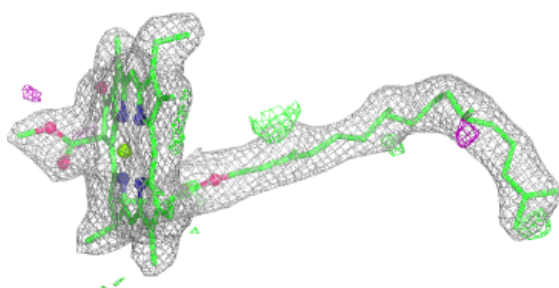
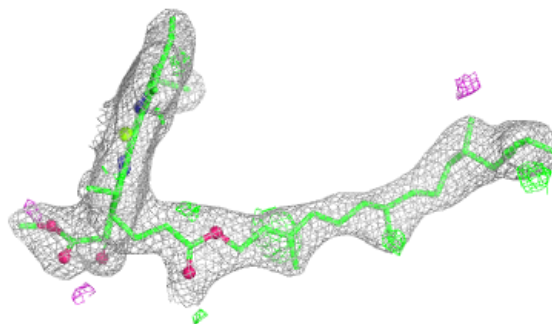
**Electron density around BCR c 516:**

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

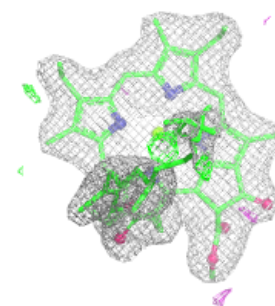
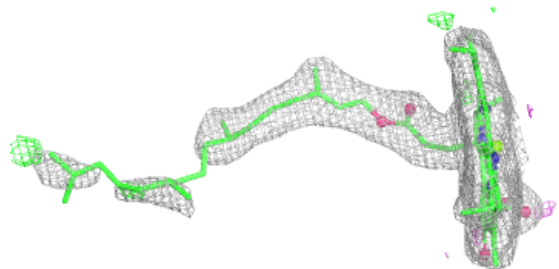
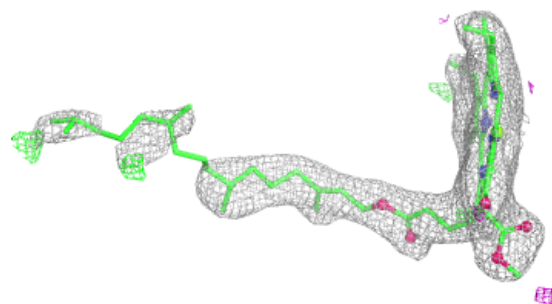


Electron density around CLA b 605:

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

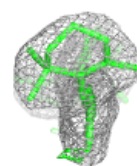
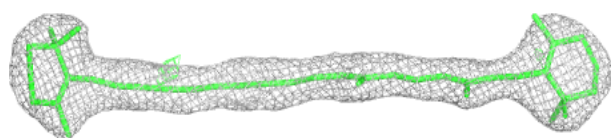
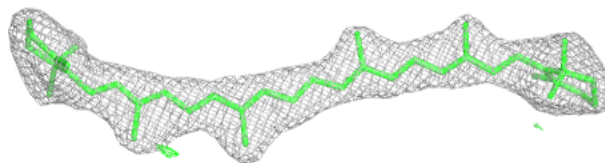
**Electron density around CLA b 606:**

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

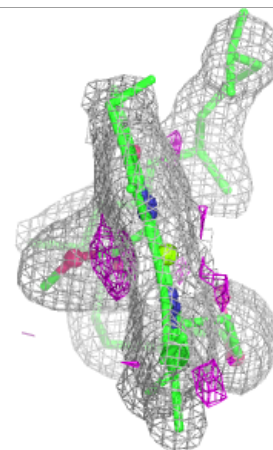
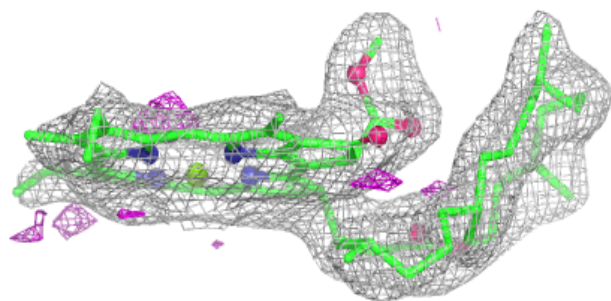
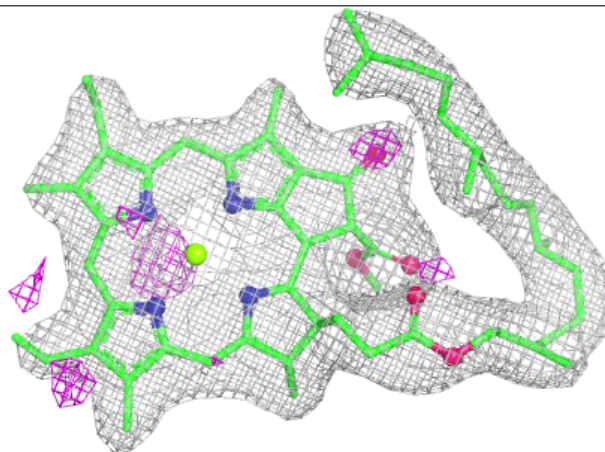


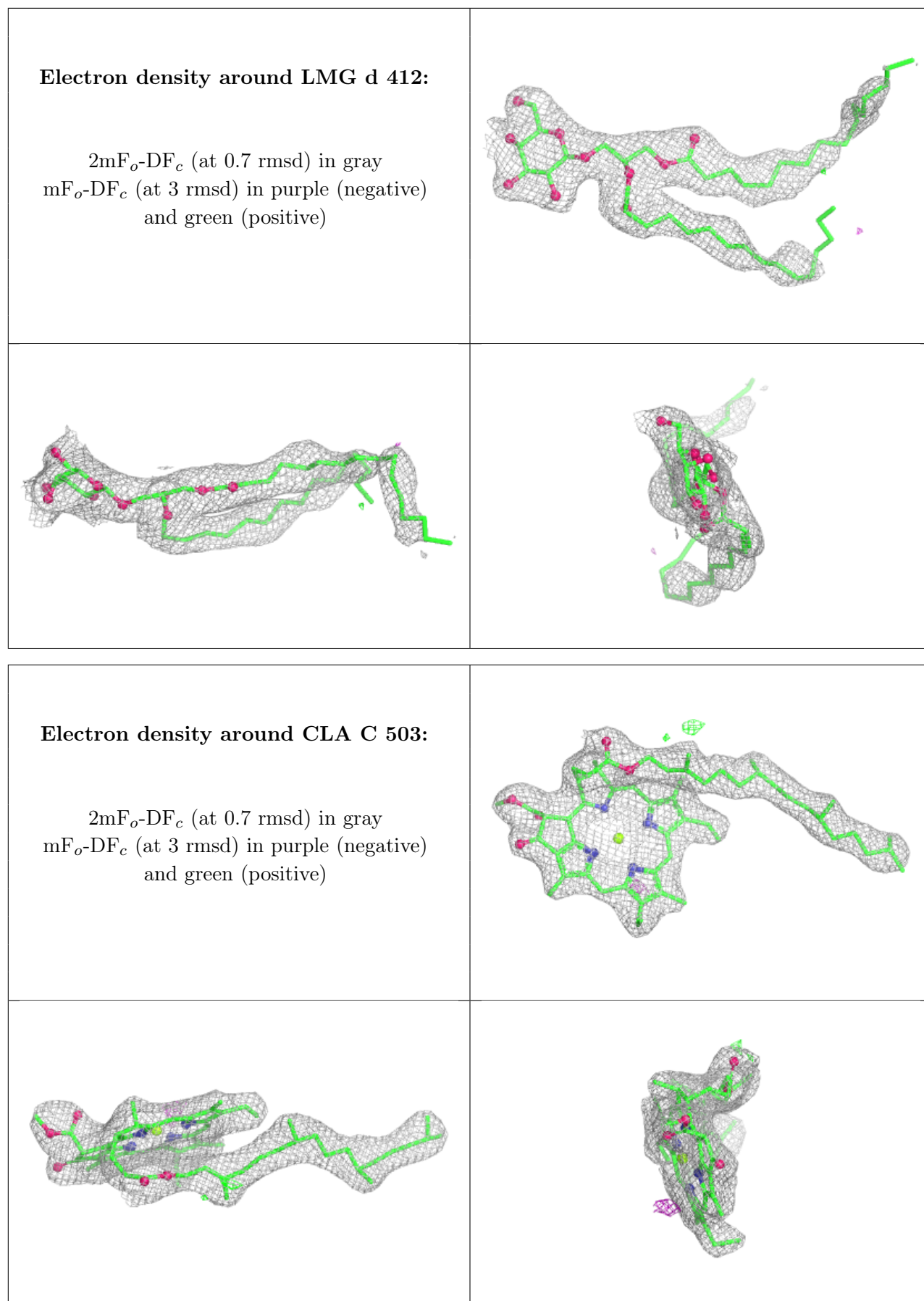
Electron density around BCR c 517:

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

**Electron density around CLA b 610:**

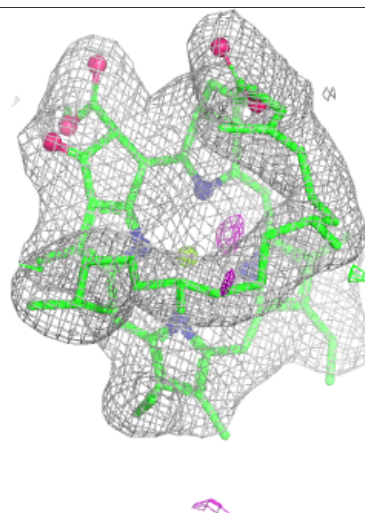
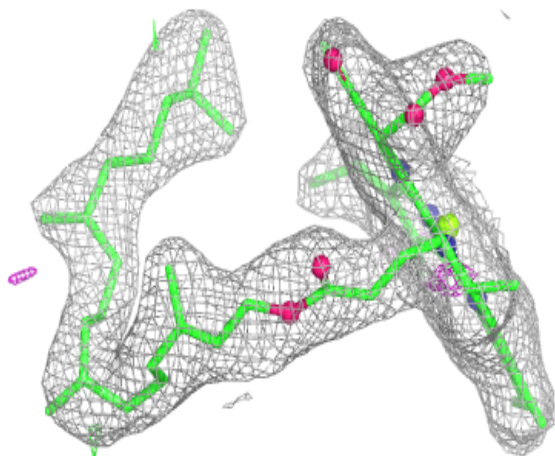
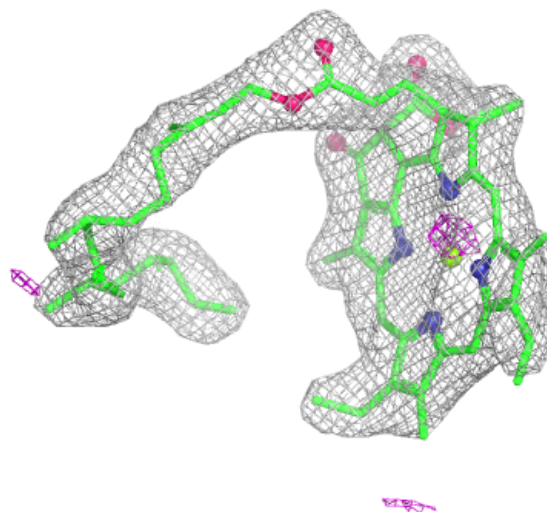
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





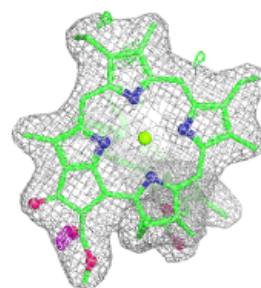
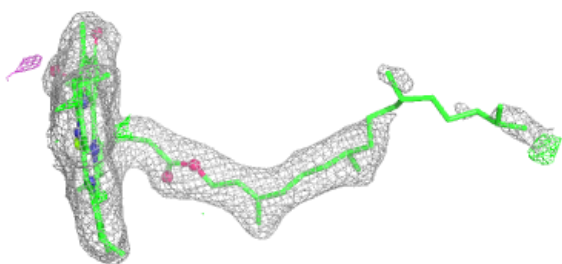
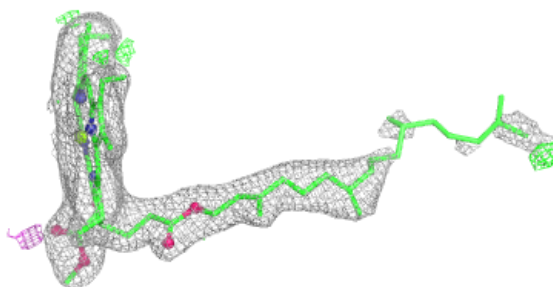
Electron density around CLA C 505:

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

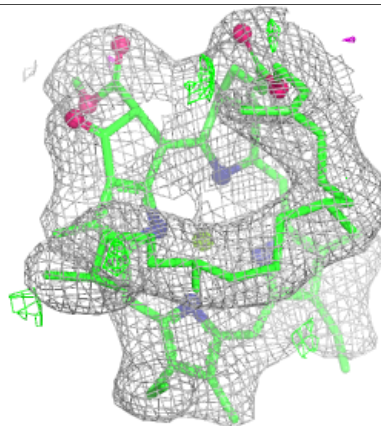
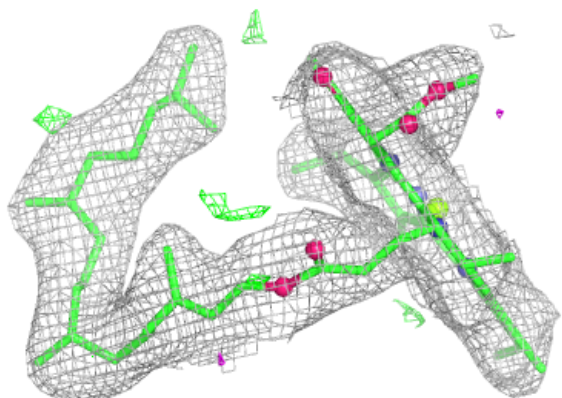
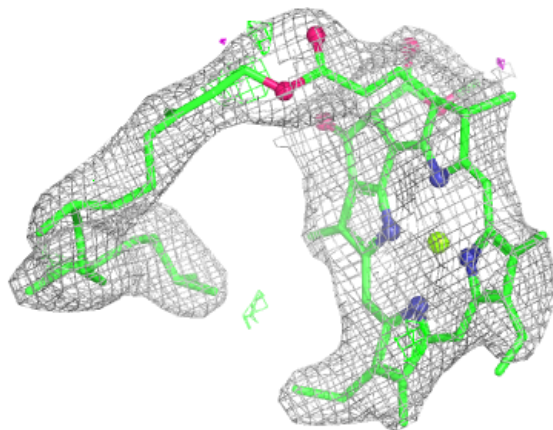


Electron density around CLA B 606:

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

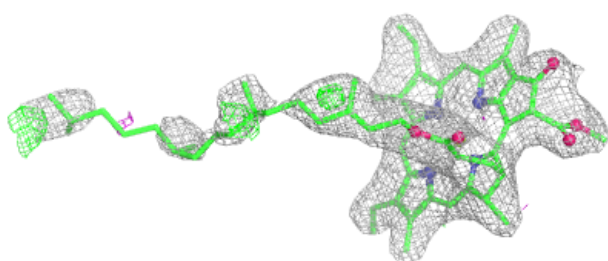
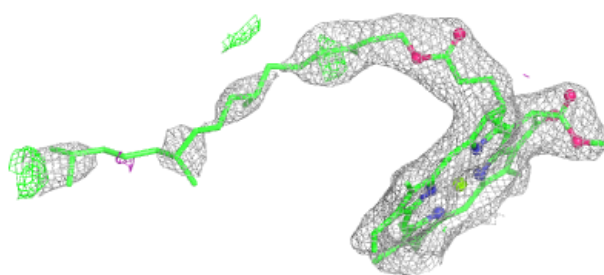
**Electron density around CLA c 505:**

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

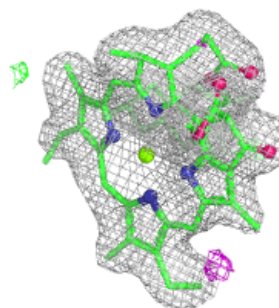
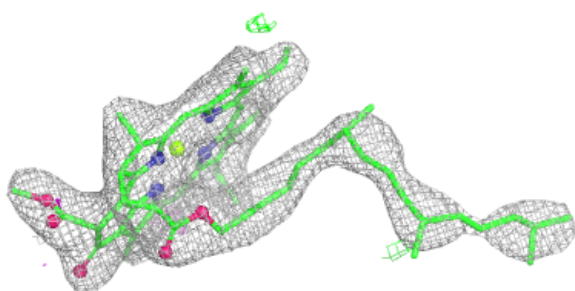
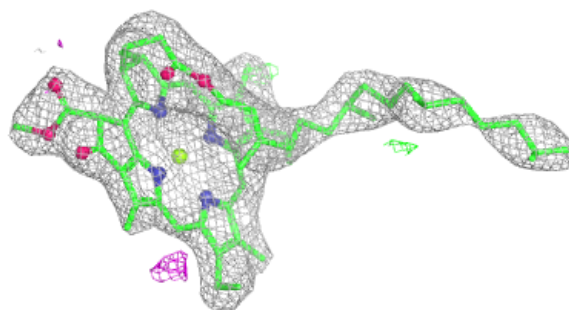


Electron density around CLA c 506:

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

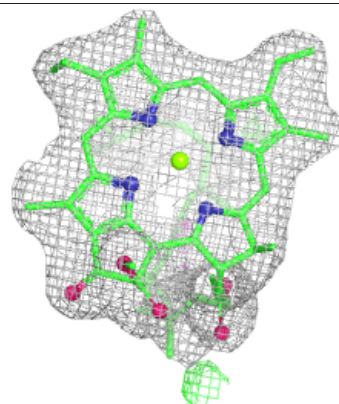
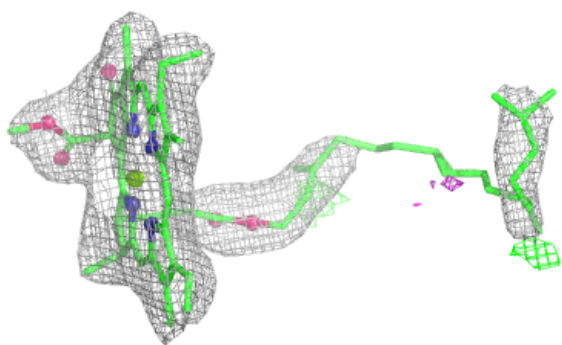
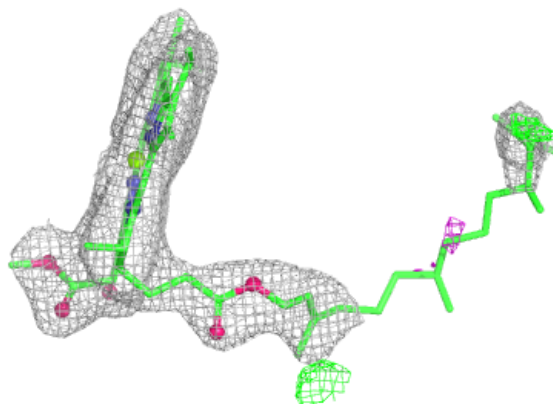
**Electron density around CLA c 507:**

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

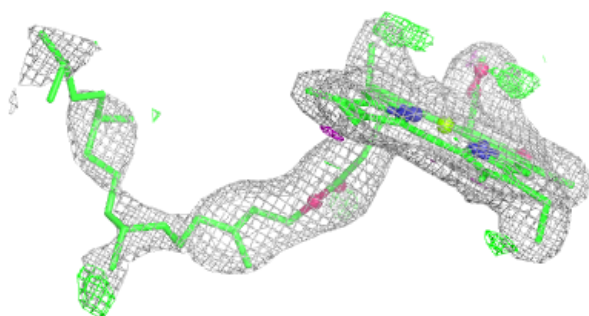
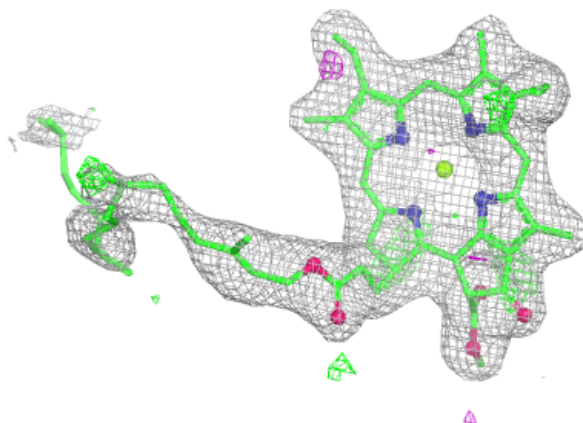


Electron density around CLA c 508:

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

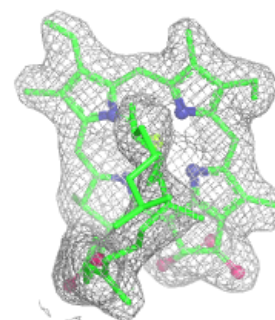
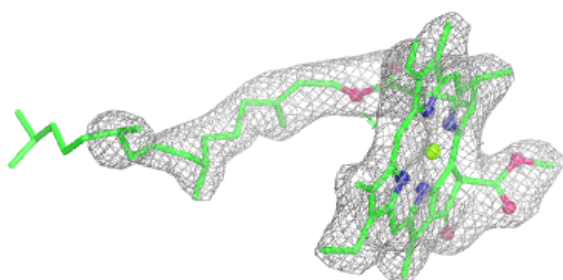
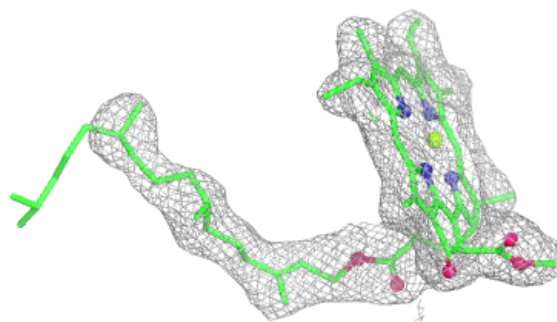
**Electron density around CLA A 408:**

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



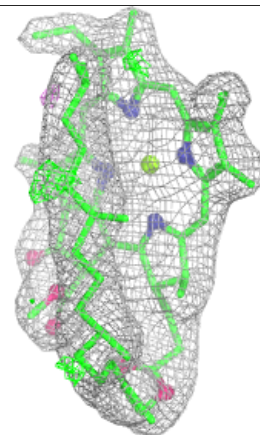
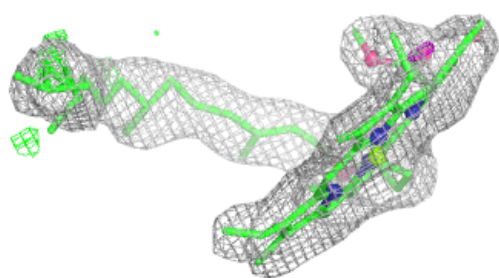
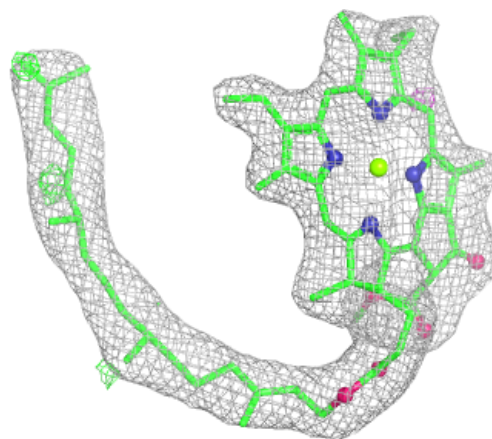
Electron density around CLA c 510:

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



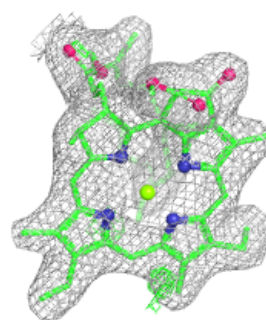
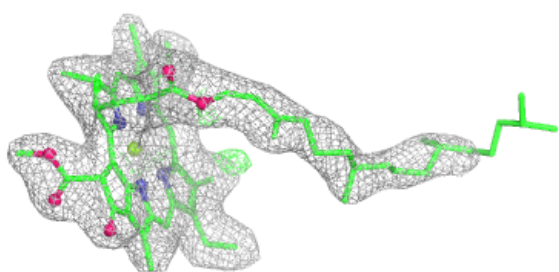
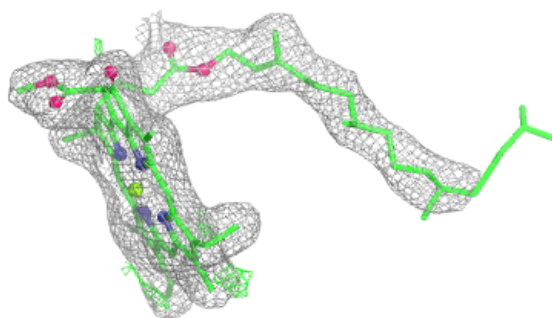
Electron density around CLA C 509:

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

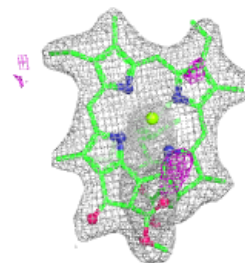
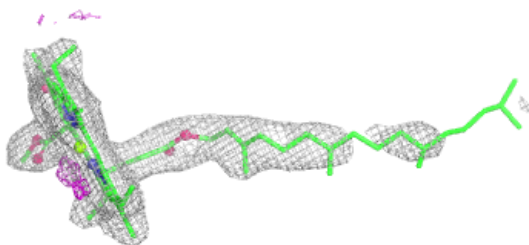
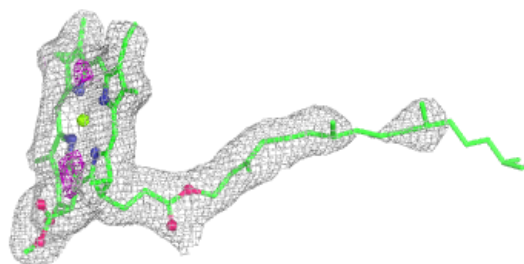


Electron density around CLA C 510:

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

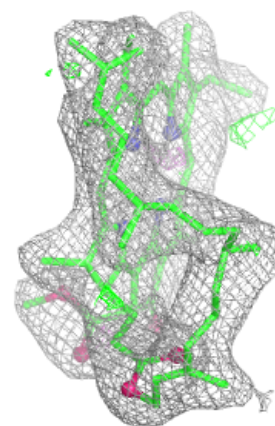
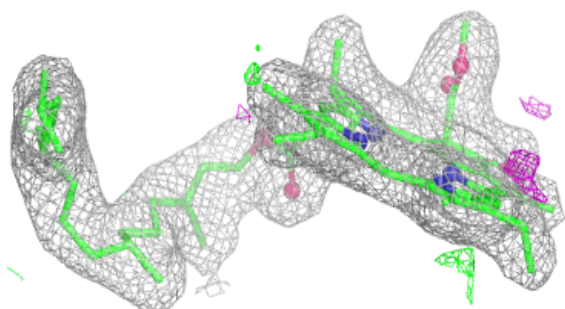
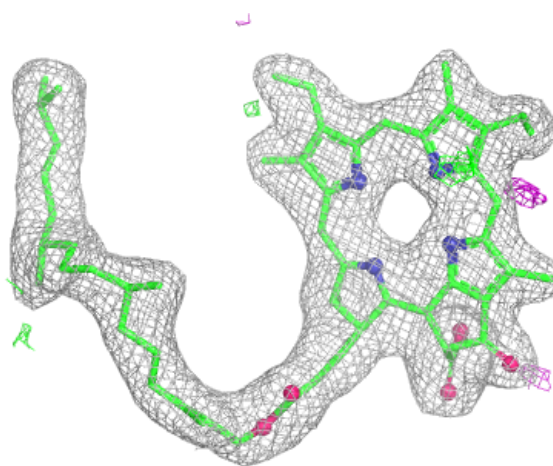
**Electron density around CLA d 403:**

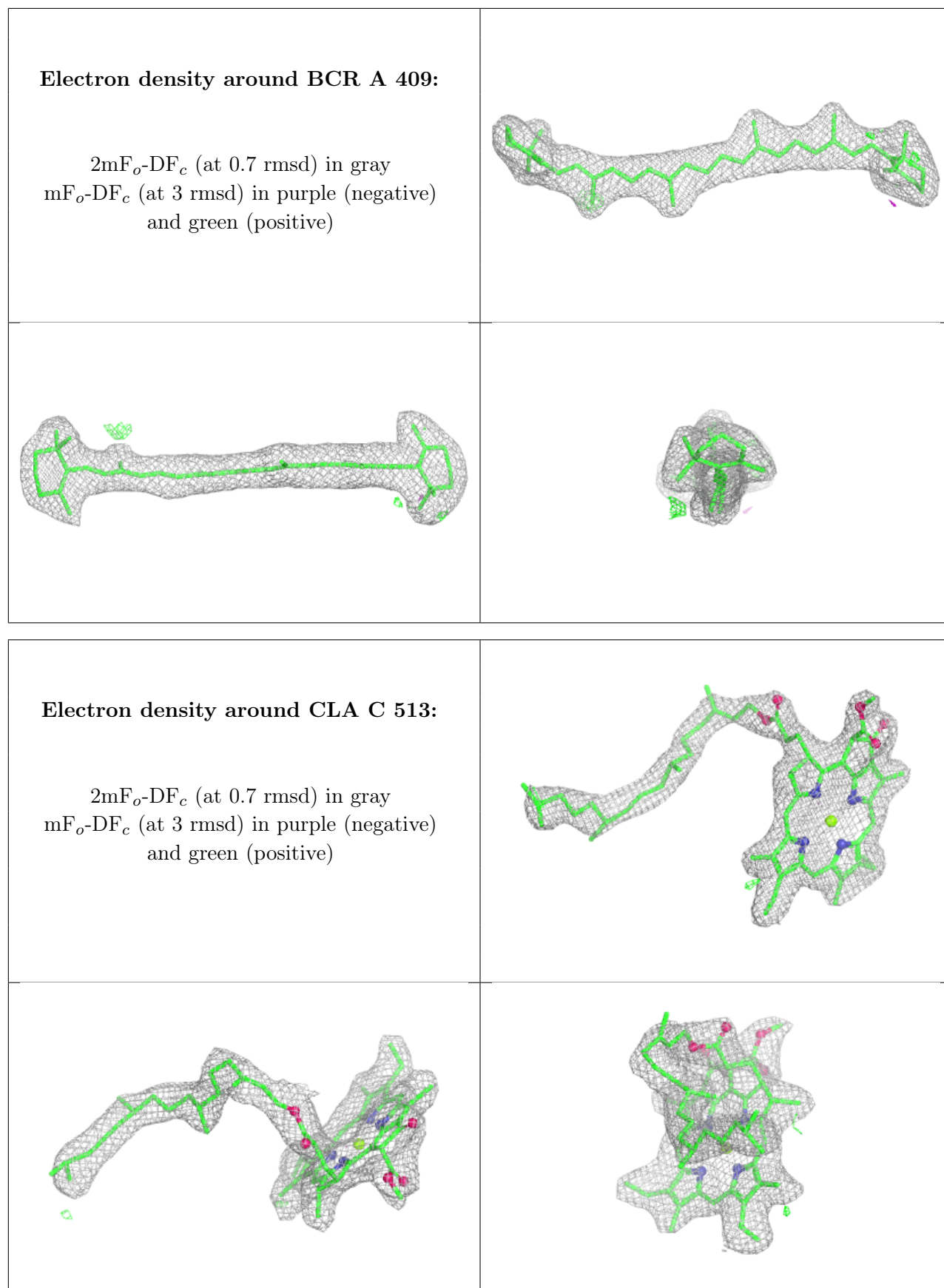
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PHO A 415:

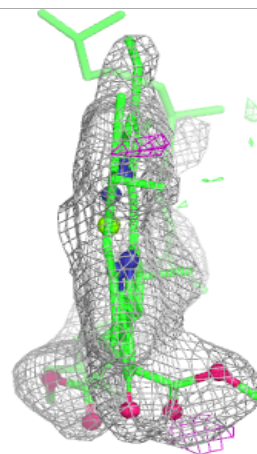
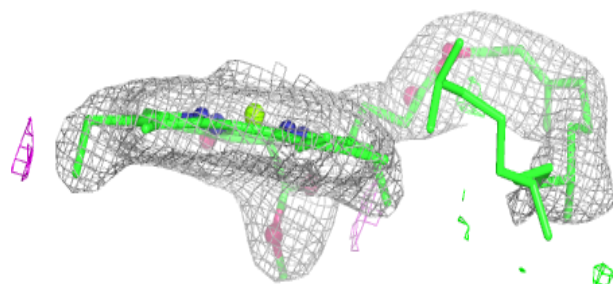
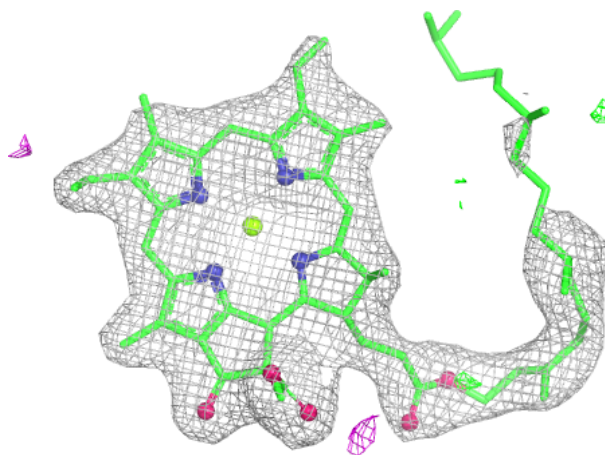
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

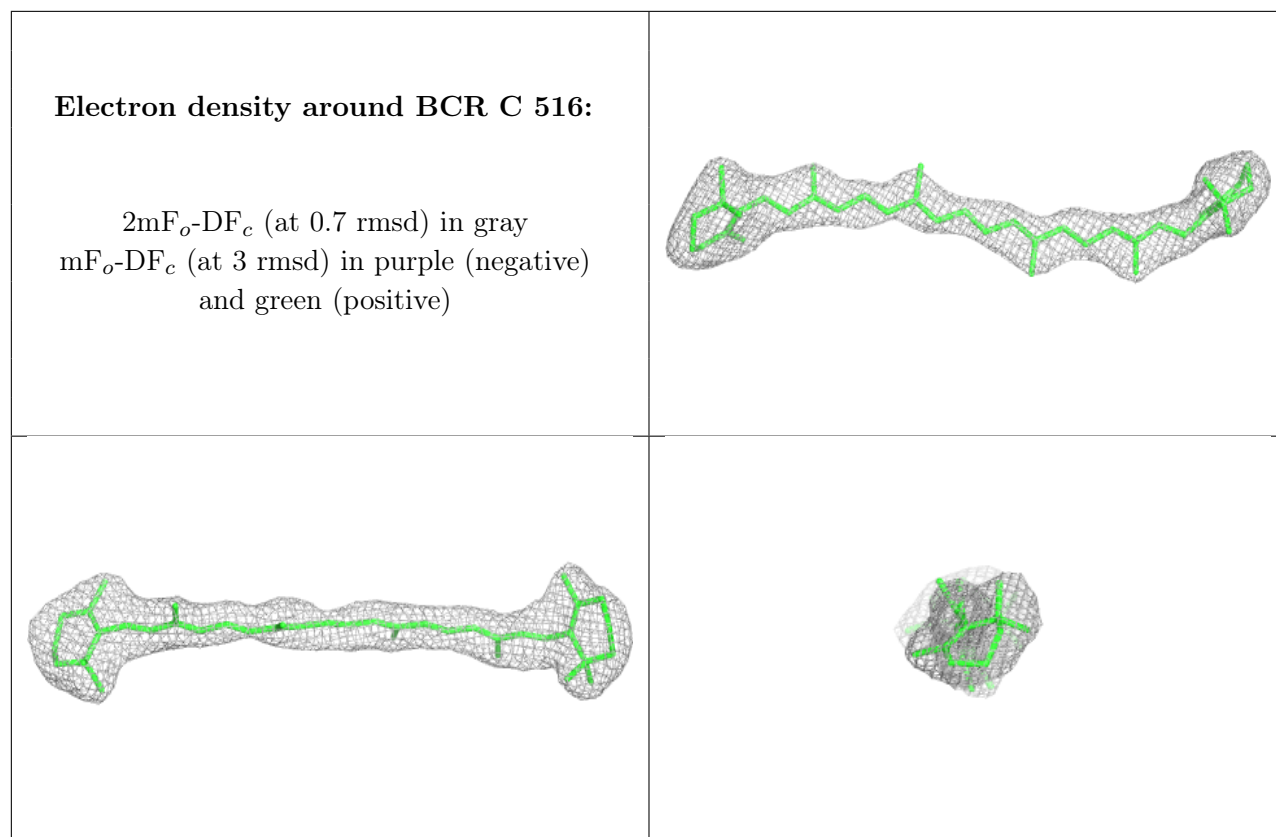




Electron density around CLA C 514:

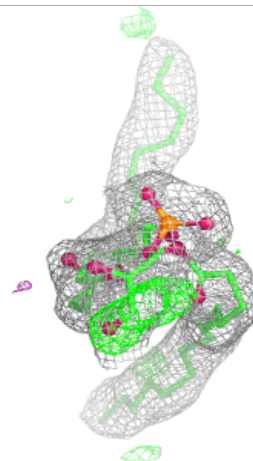
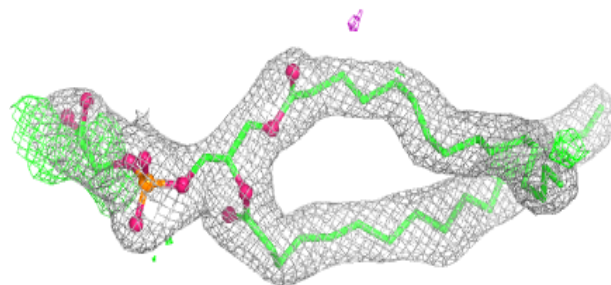
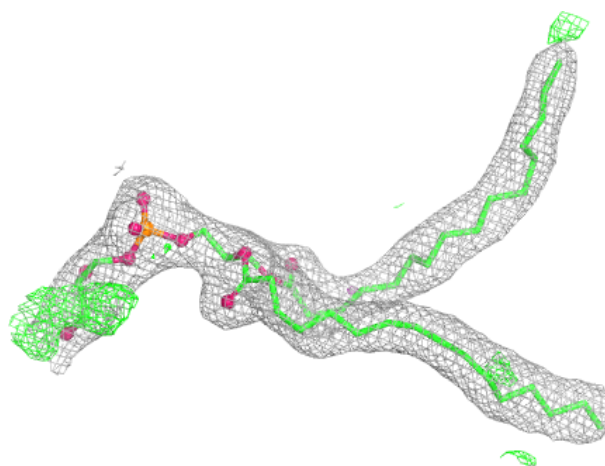
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

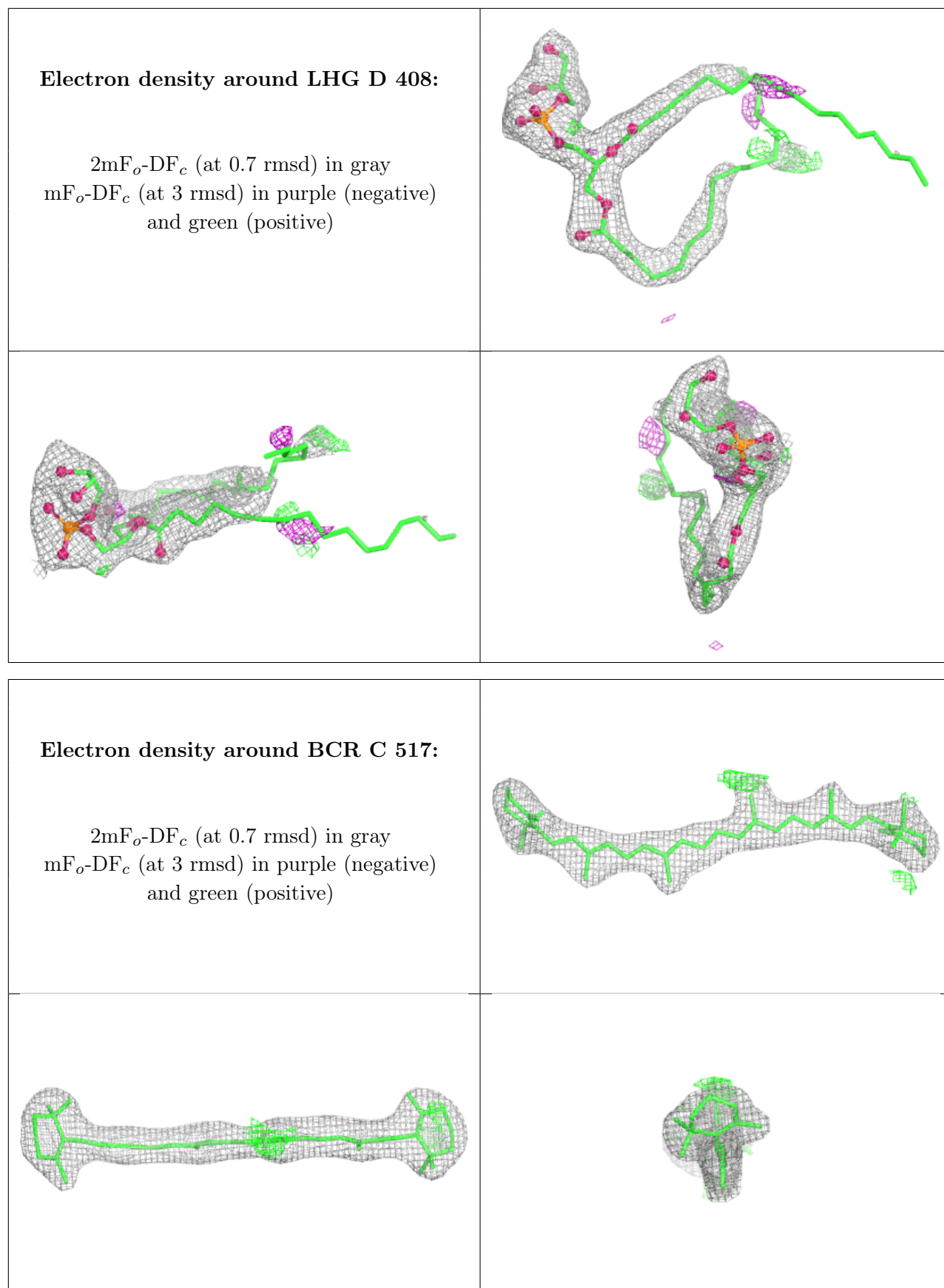




Electron density around LHG D 407:

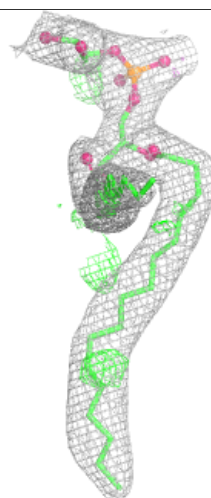
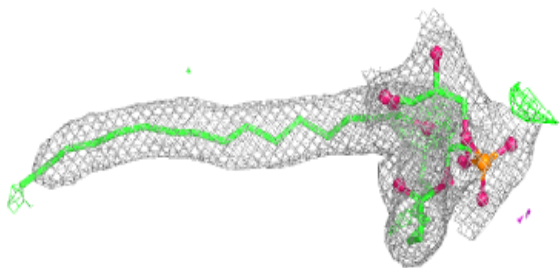
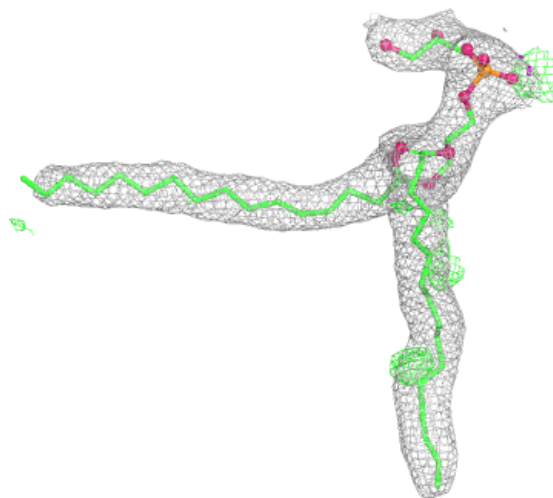
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





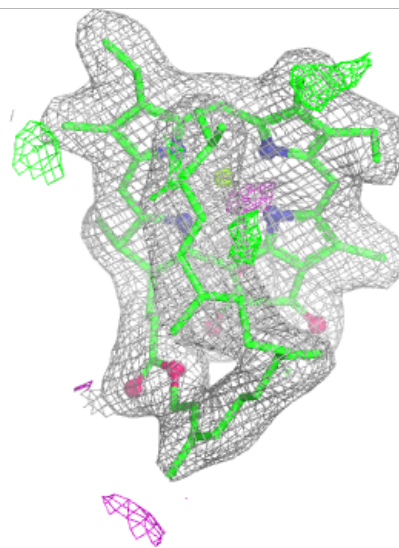
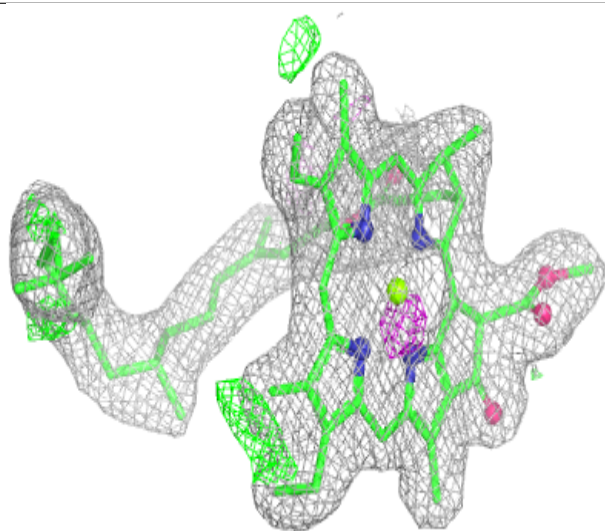
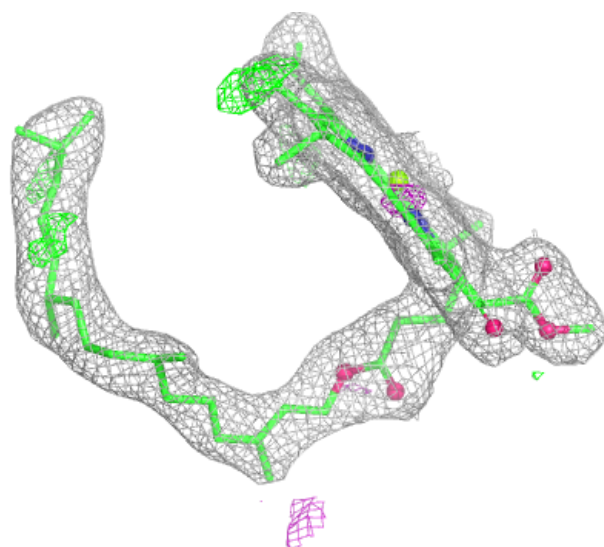
Electron density around LHG L 101:

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



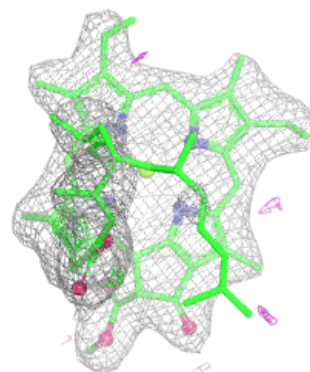
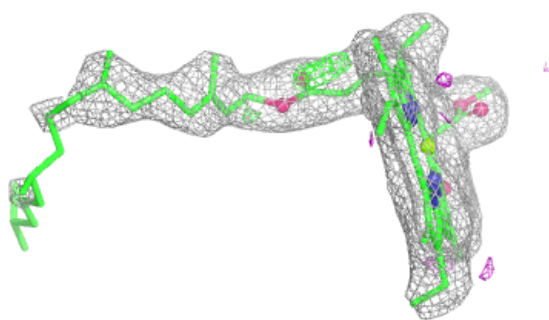
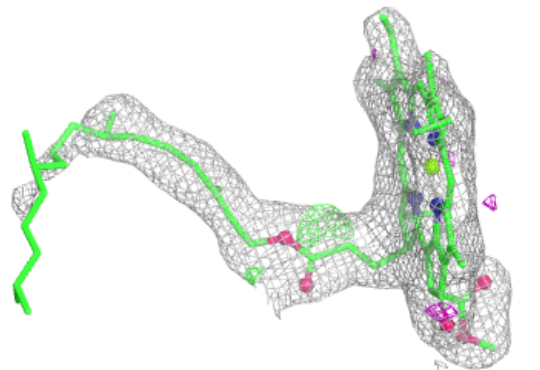
Electron density around CLA B 611:

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

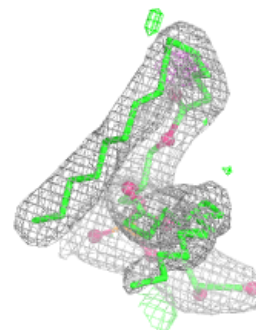
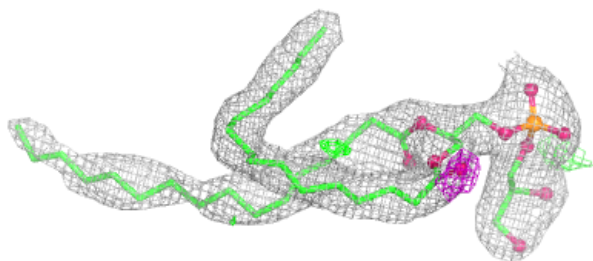
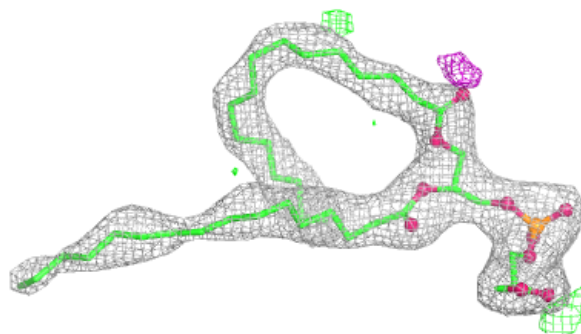


Electron density around CLA D 404:

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

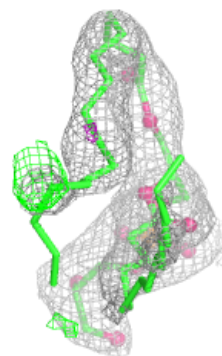
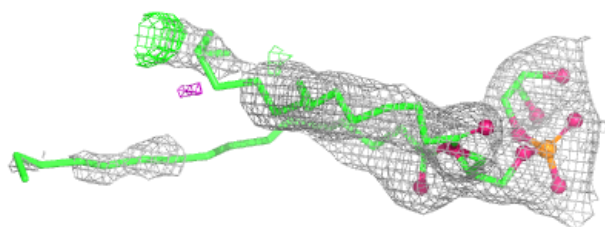
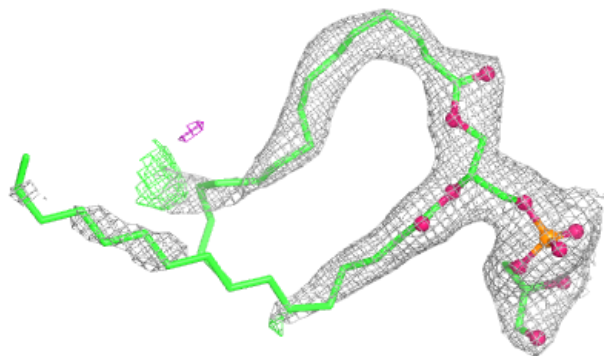
**Electron density around LHG d 406:**

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

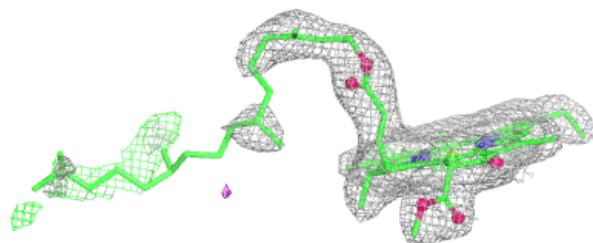
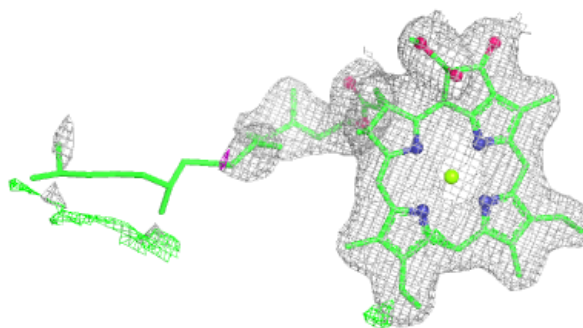


Electron density around LHG d 408:

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

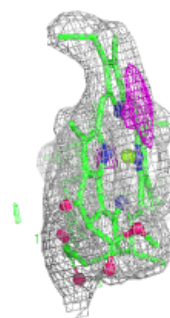
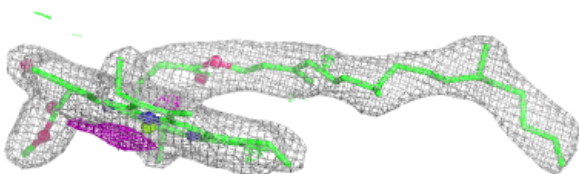
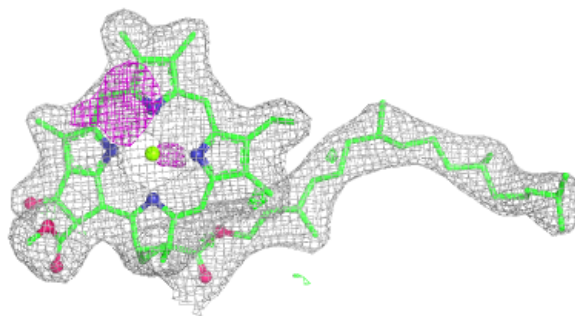
**Electron density around CLA a 406:**

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

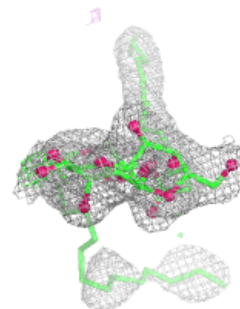
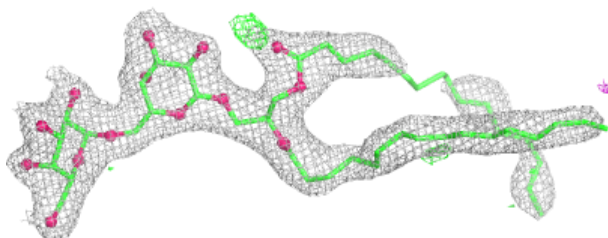
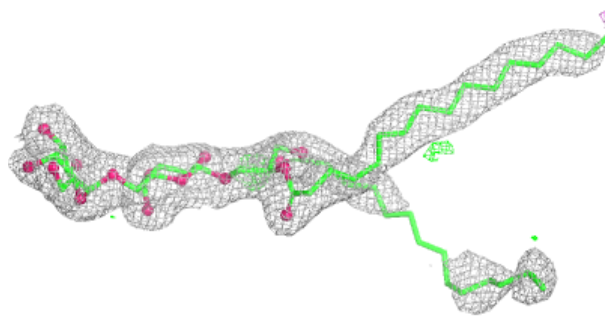


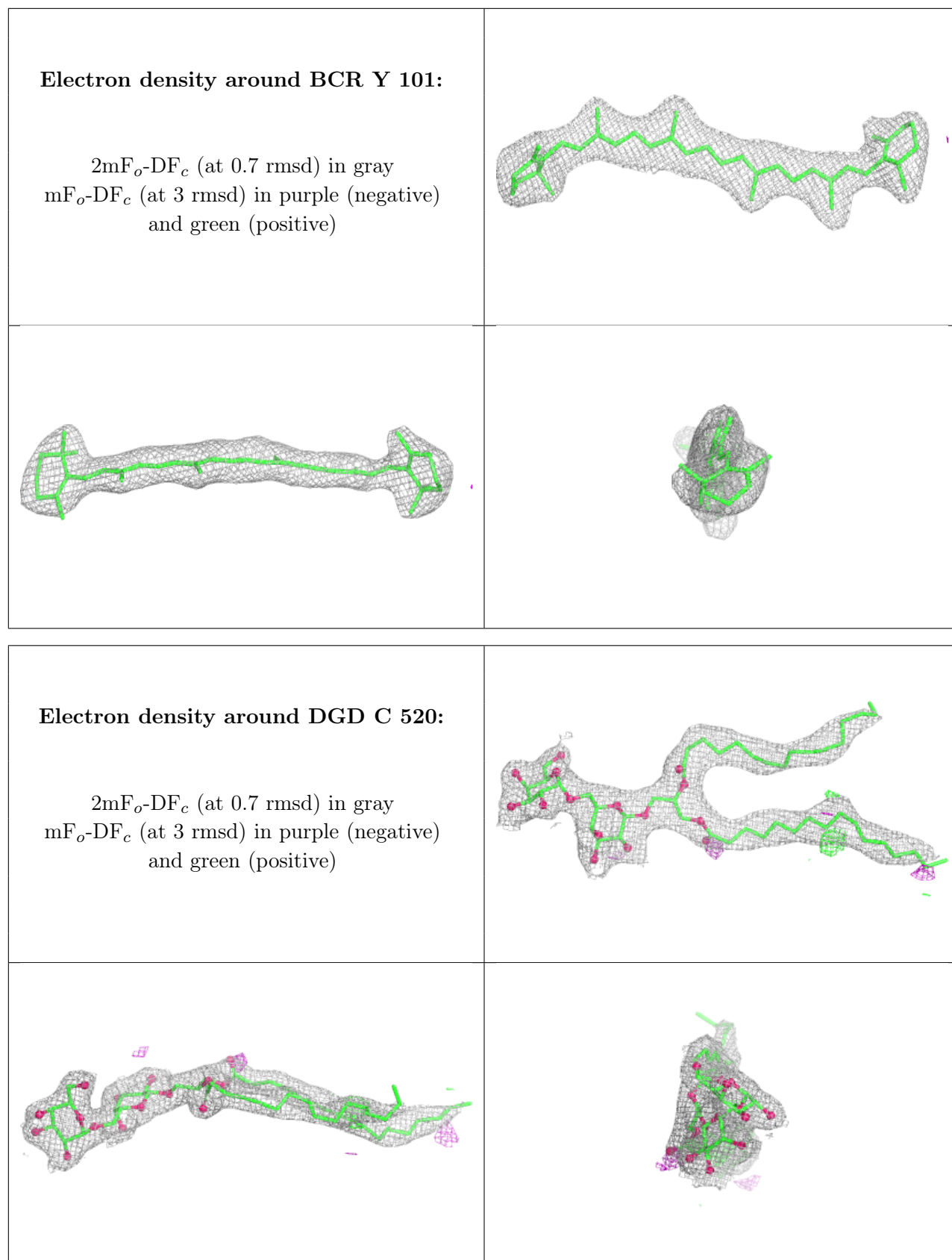
Electron density around CLA B 603:

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

**Electron density around DGD C 518:**

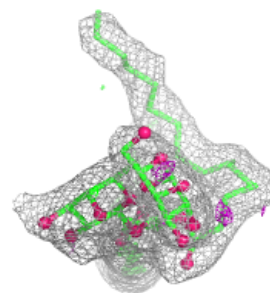
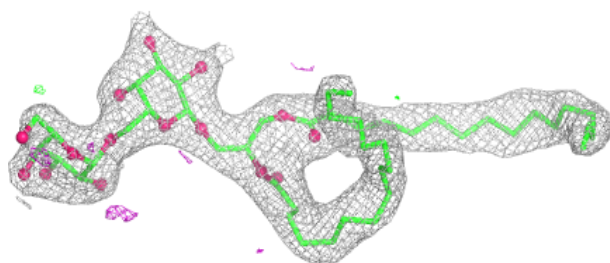
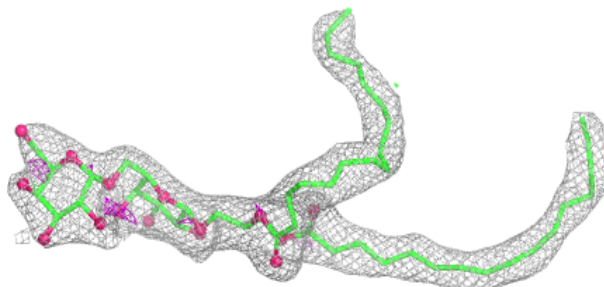
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



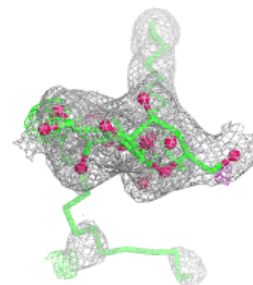
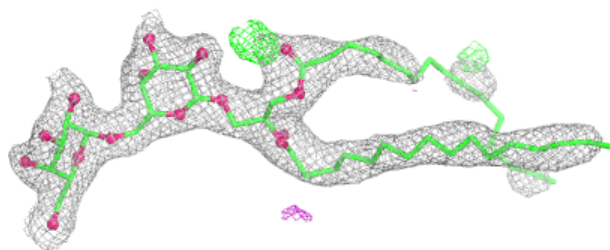
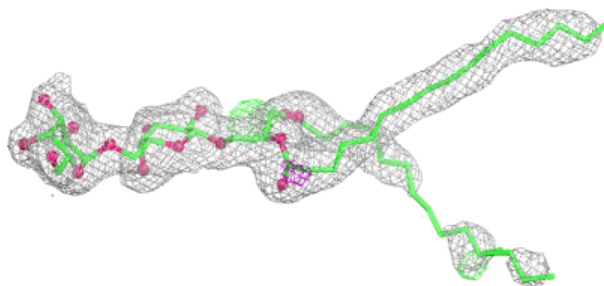


Electron density around DGD H 102:

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

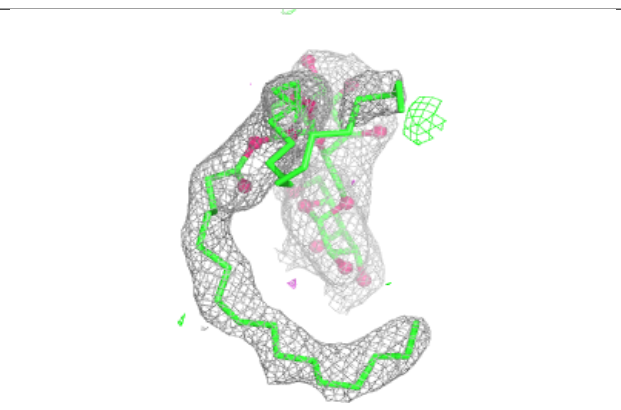
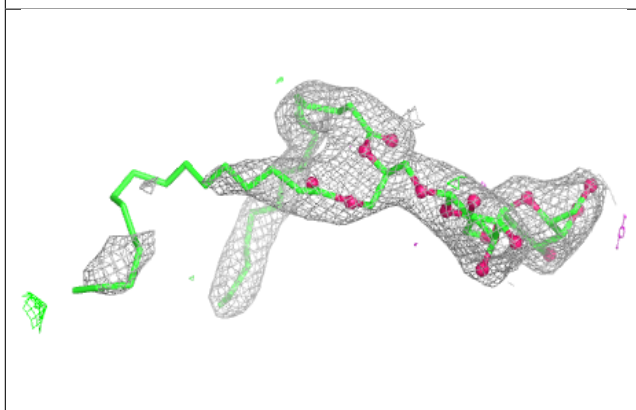
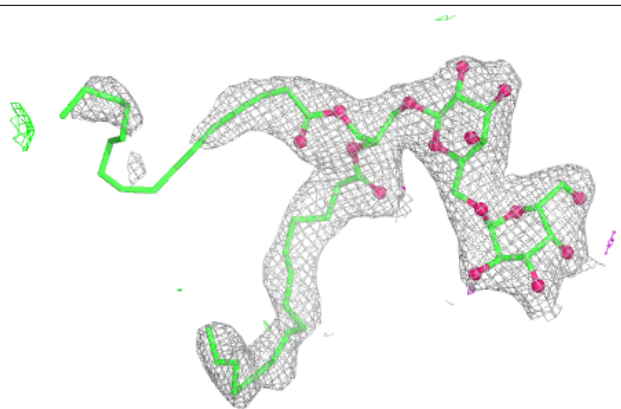
**Electron density around DGD c 518:**

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

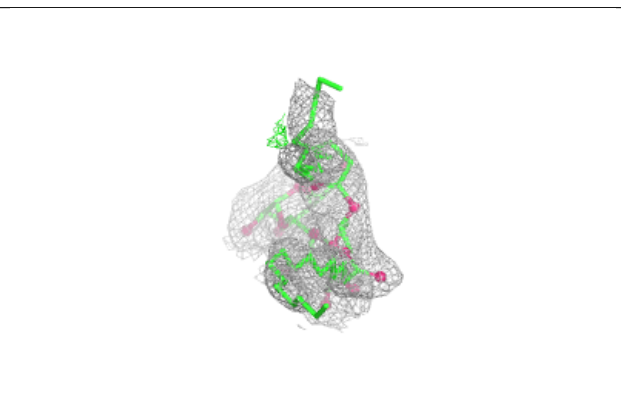
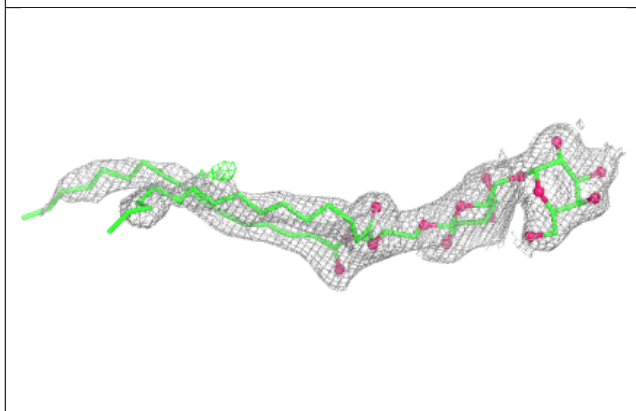
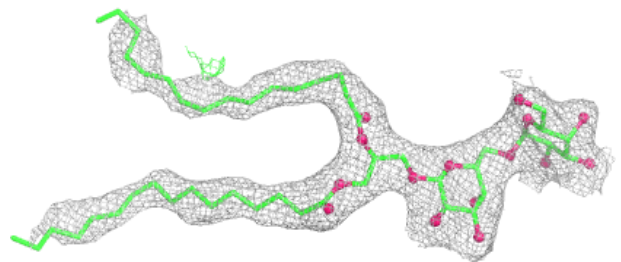


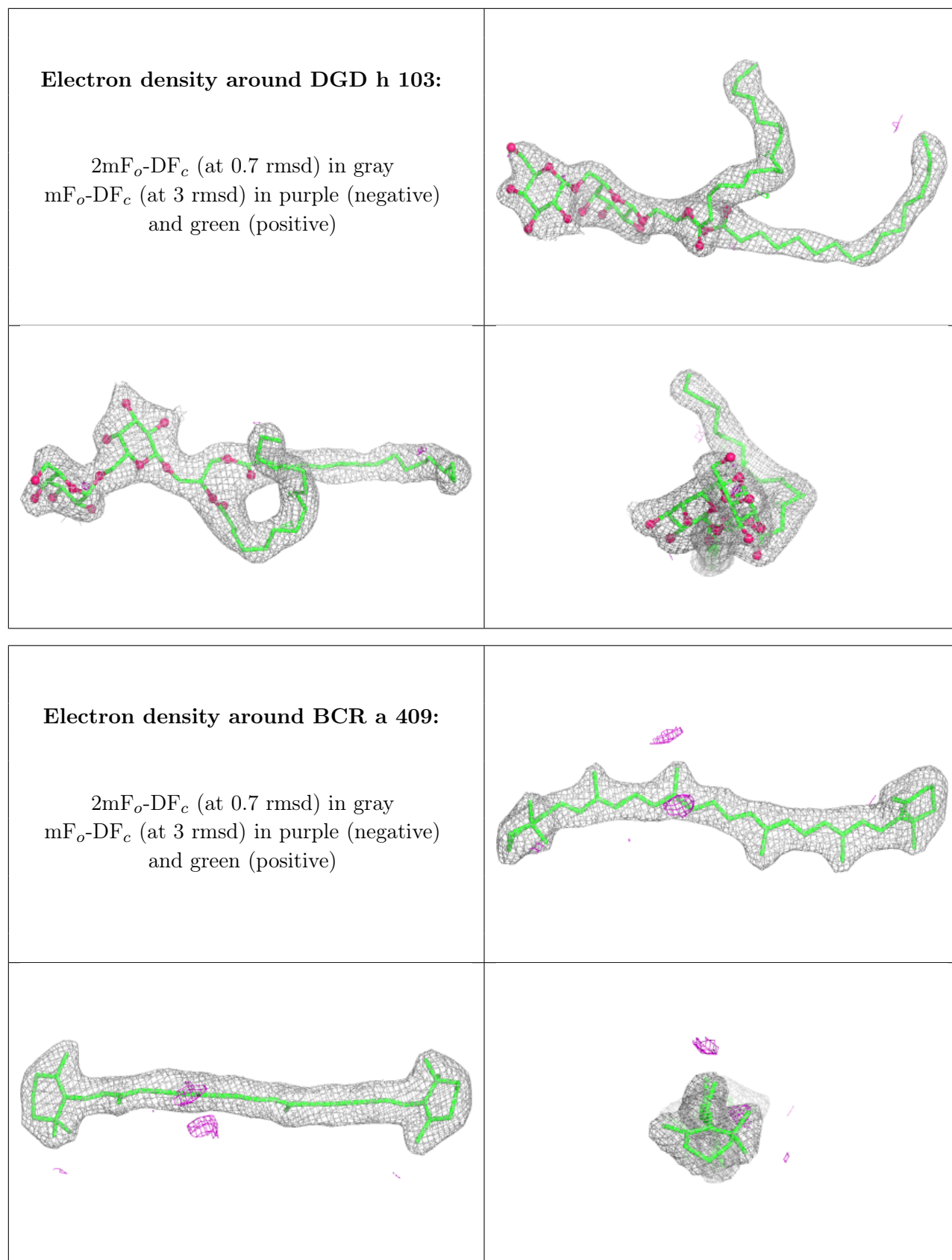
Electron density around DGD c 519:

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

**Electron density around DGD c 520:**

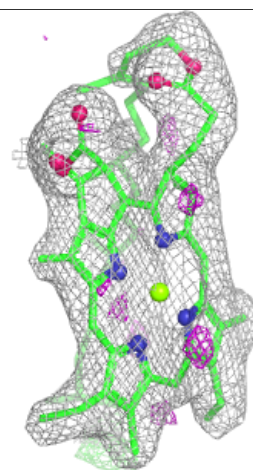
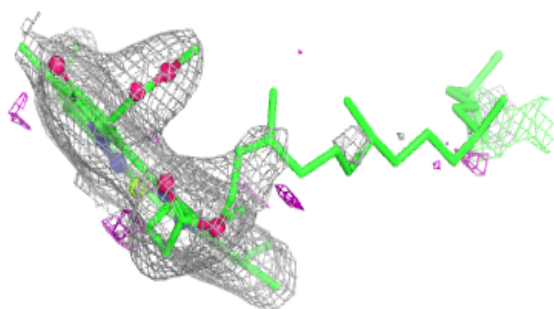
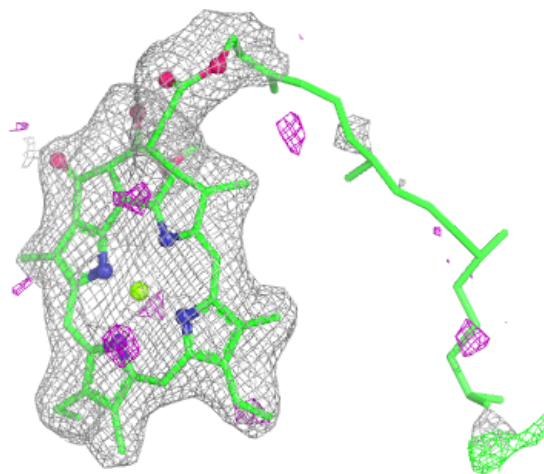
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

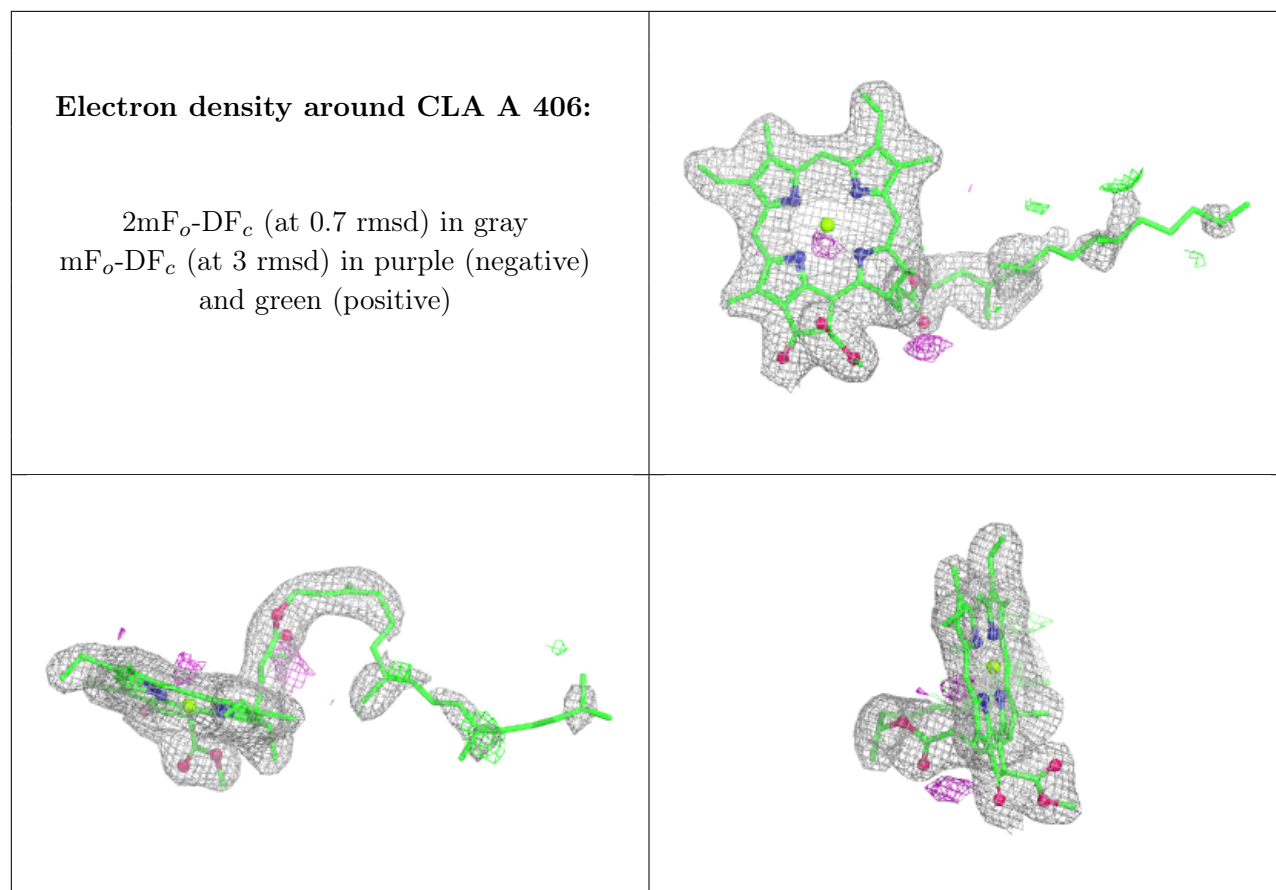




Electron density around CLA B 616:

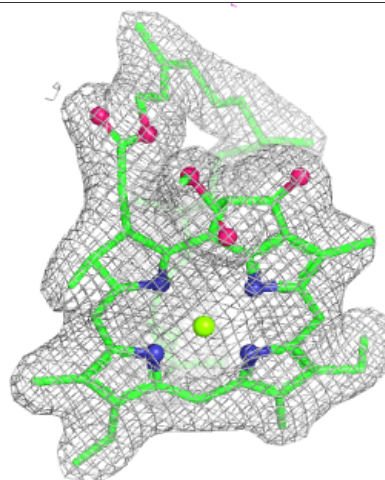
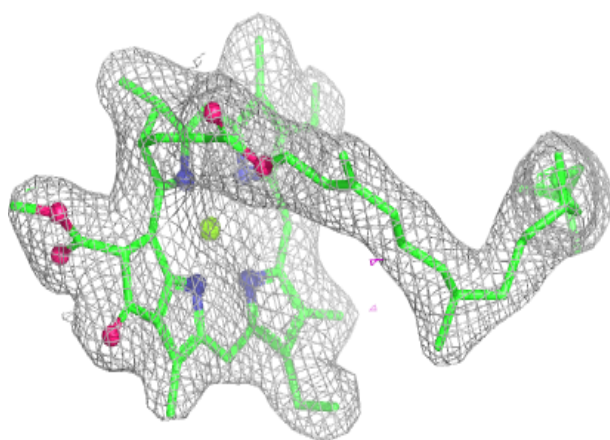
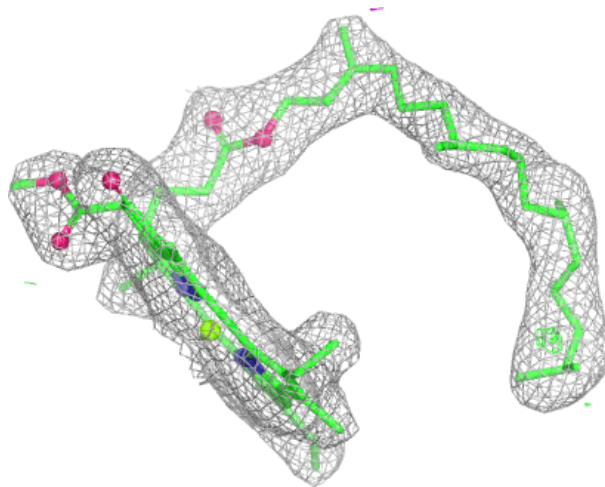
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





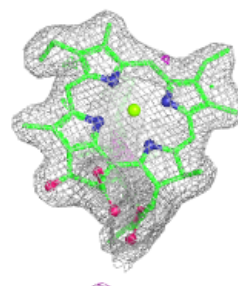
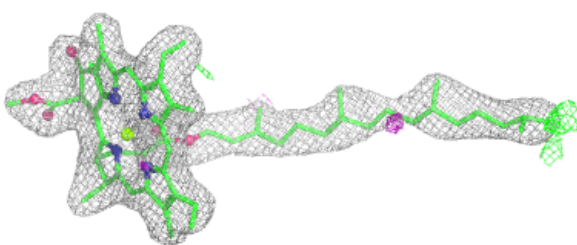
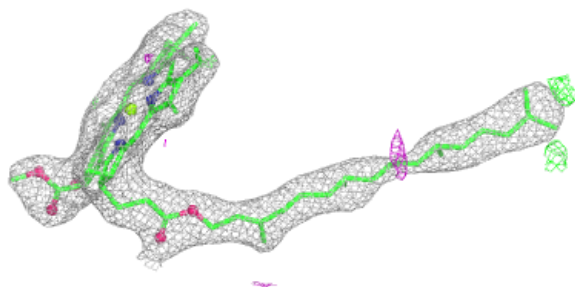
Electron density around CLA b 611:

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

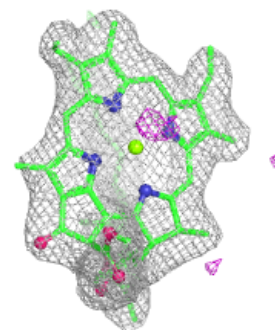
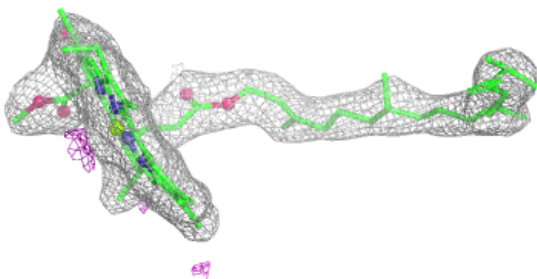
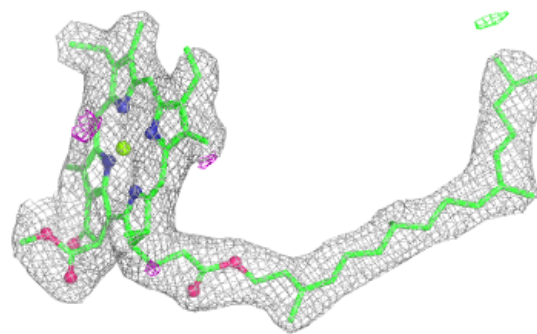


Electron density around CLA B 607:

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

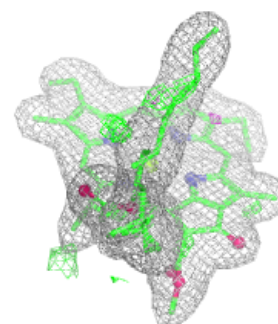
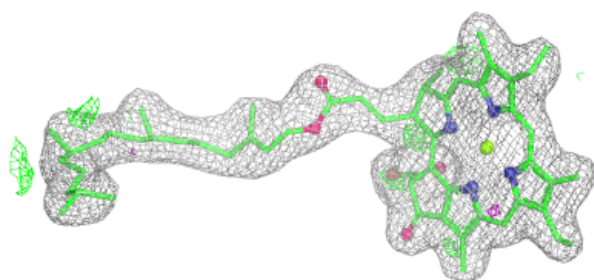
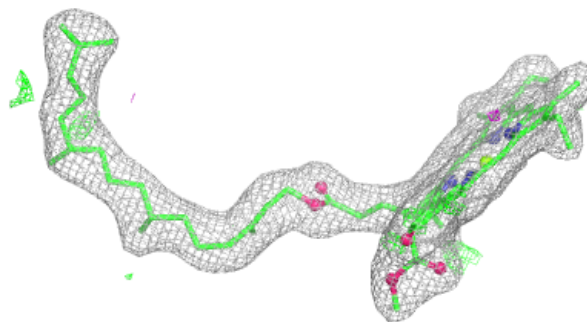
**Electron density around CLA B 609:**

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

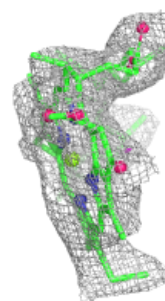
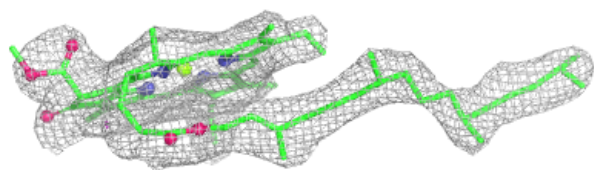
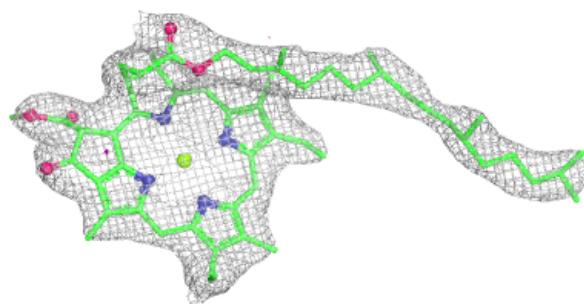


Electron density around CLA D 403:

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

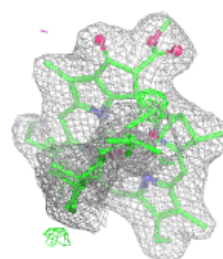
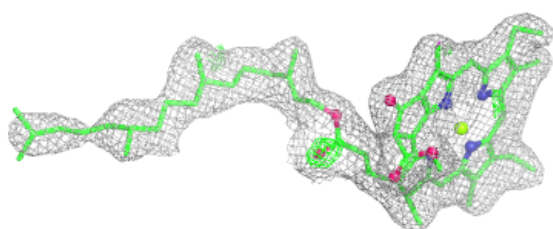
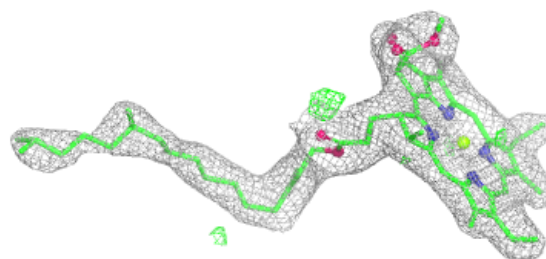
**Electron density around CLA c 503:**

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

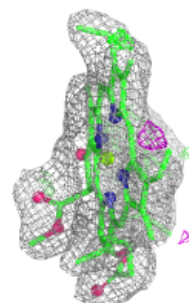
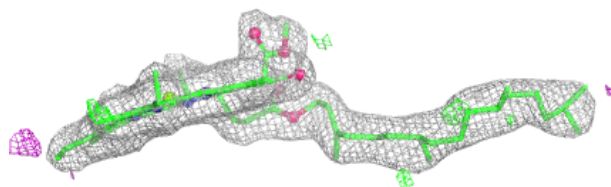
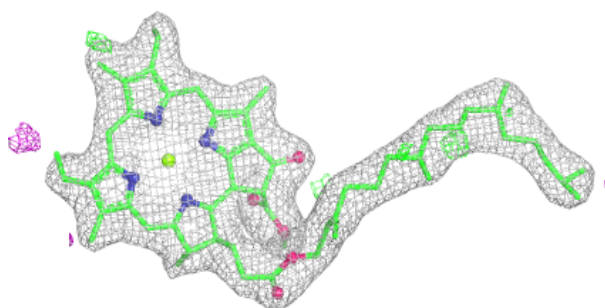


Electron density around CLA c 504:

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

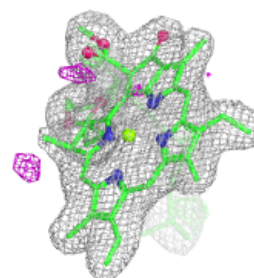
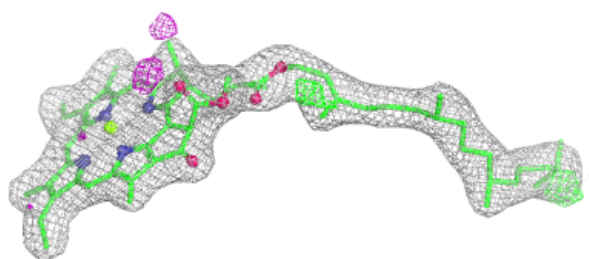
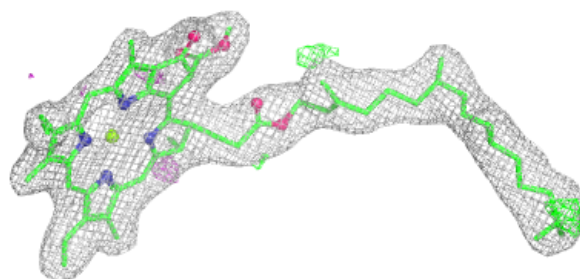
**Electron density around CLA B 602:**

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



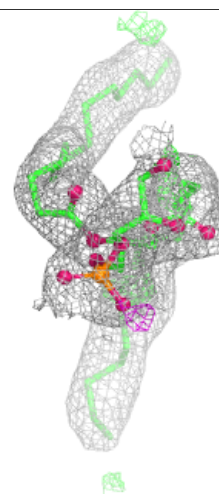
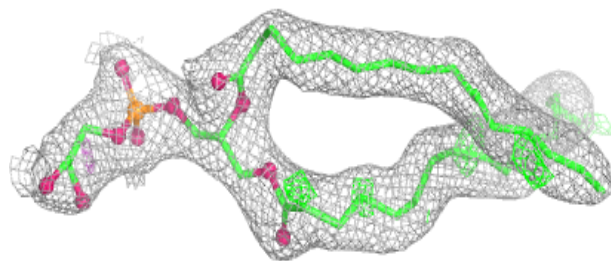
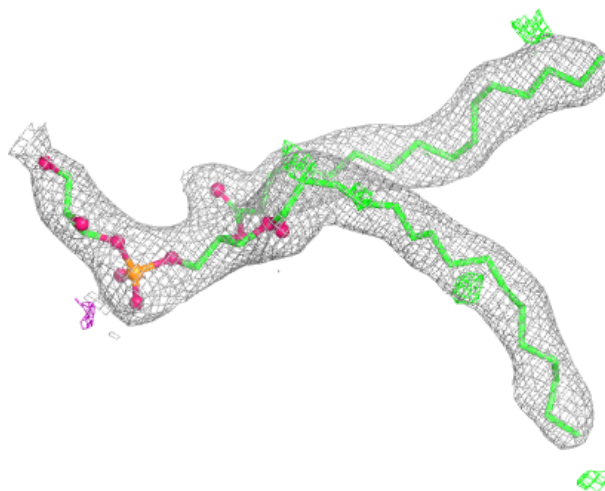
Electron density around CLA a 404:

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



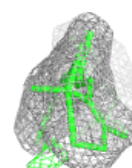
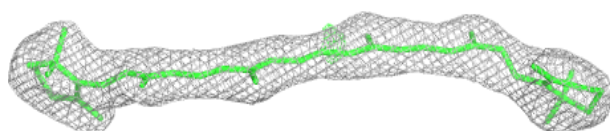
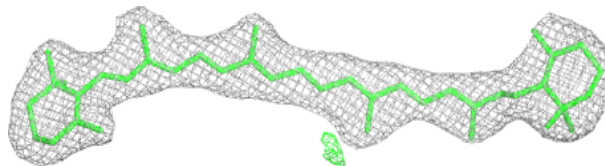
Electron density around LHG d 407:

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

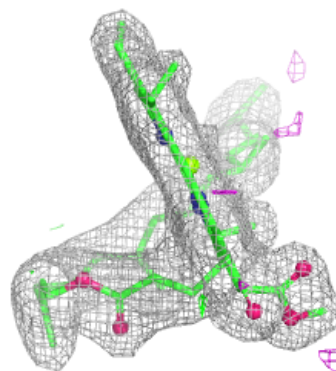
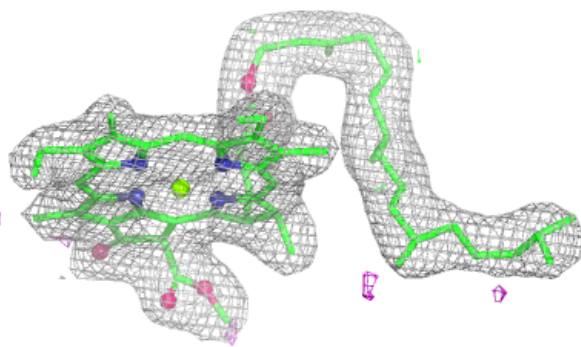
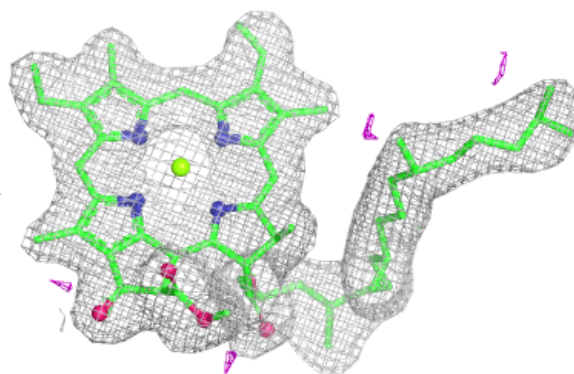


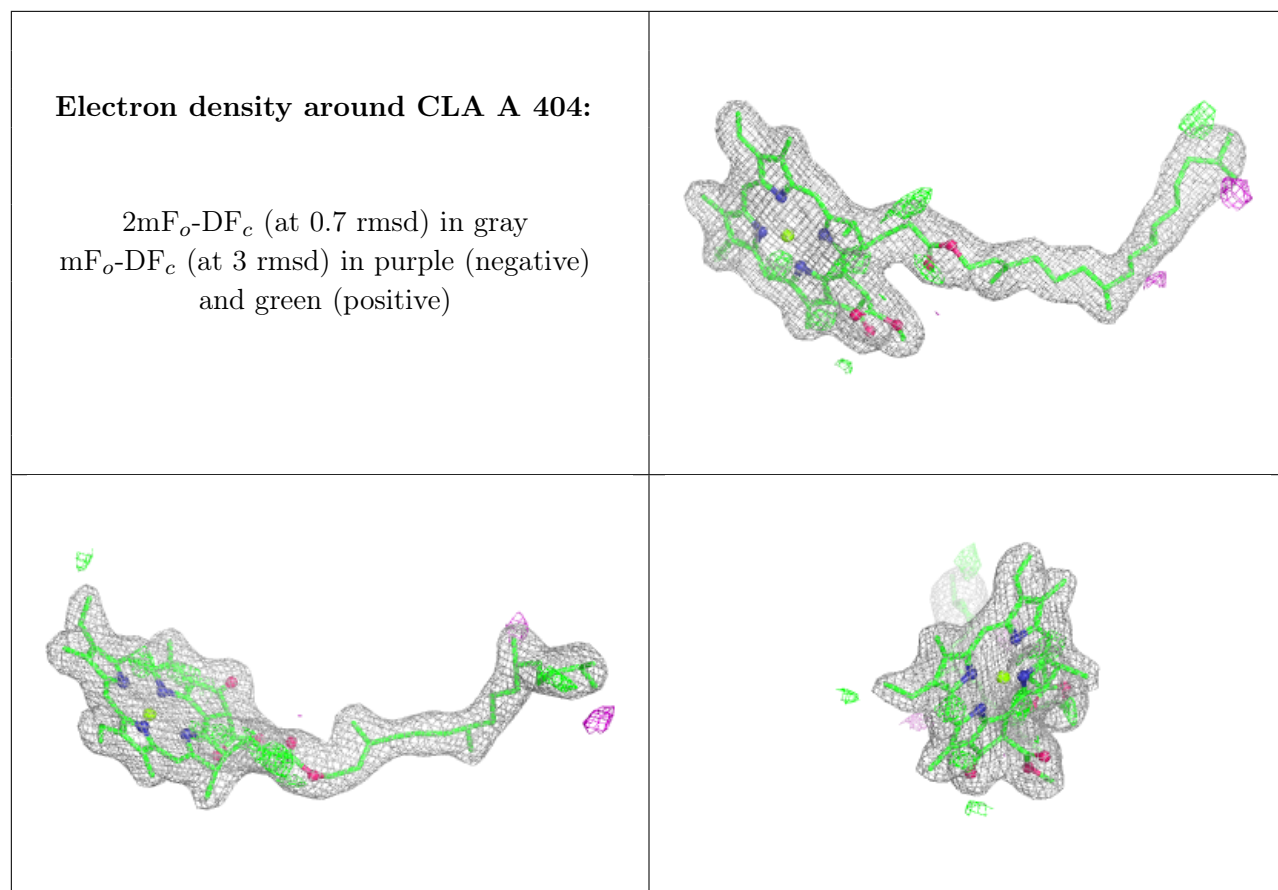
Electron density around BCR b 619:

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

**Electron density around CLA a 405:**

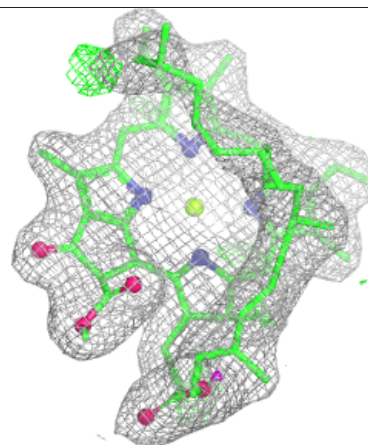
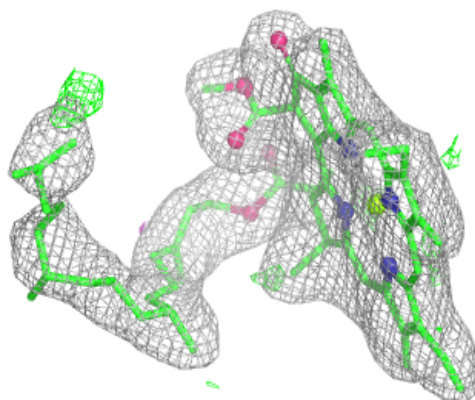
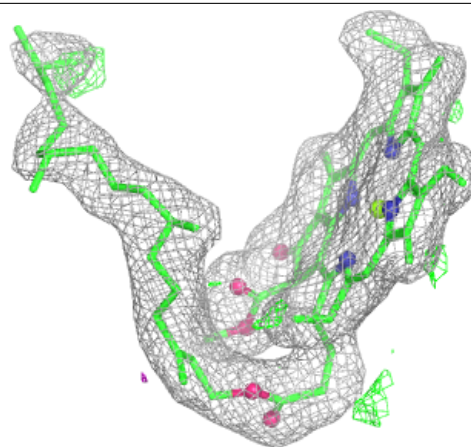
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





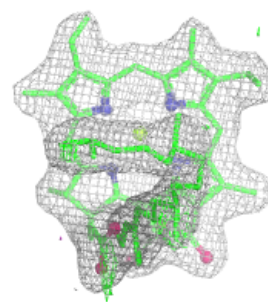
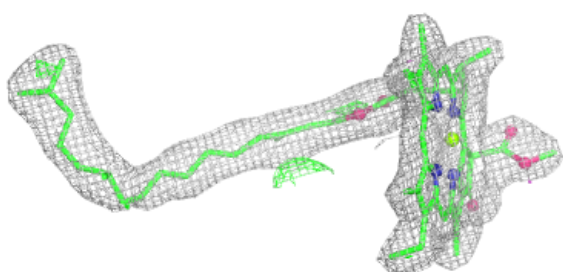
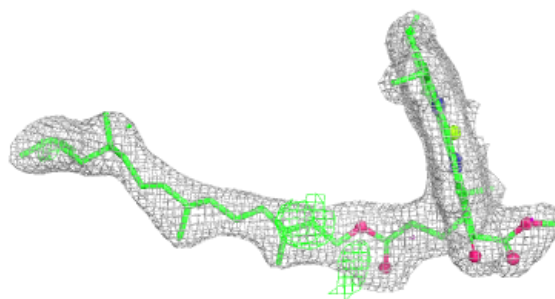
Electron density around CLA B 613:

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

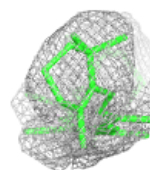
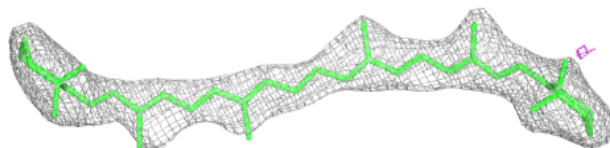
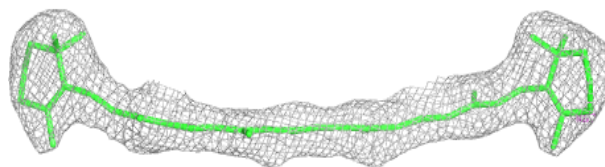


Electron density around CLA B 605:

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

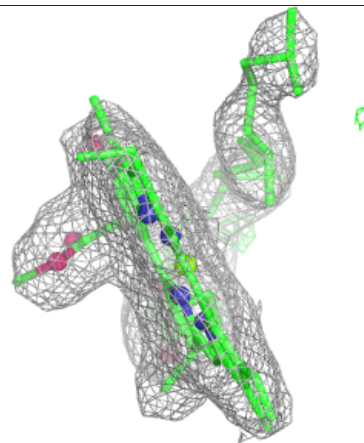
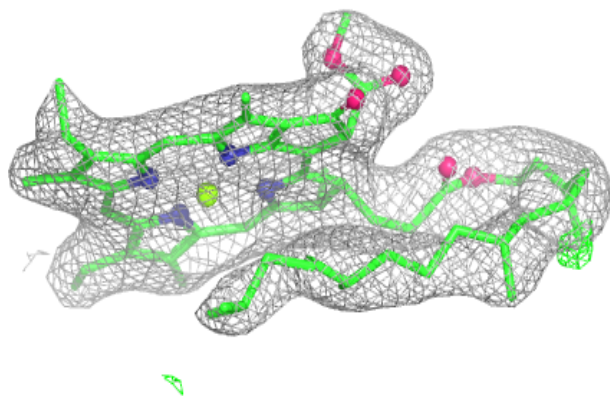
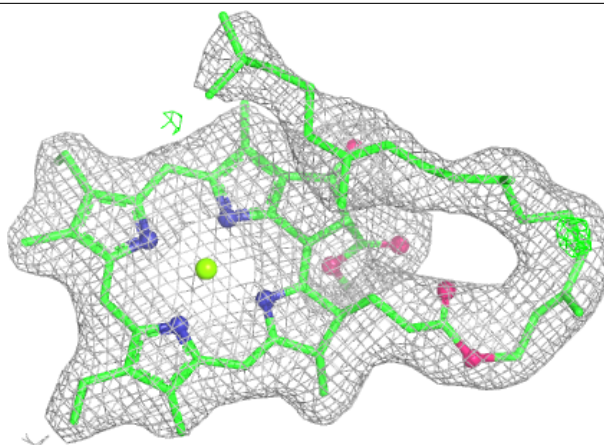
**Electron density around BCR k 101:**

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



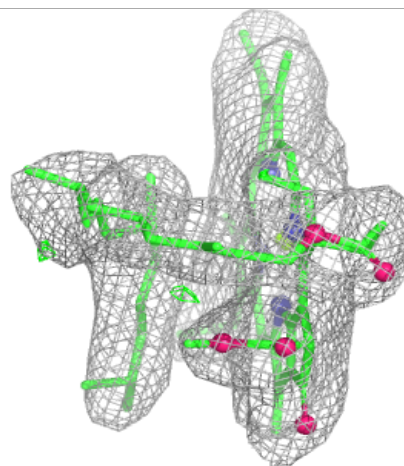
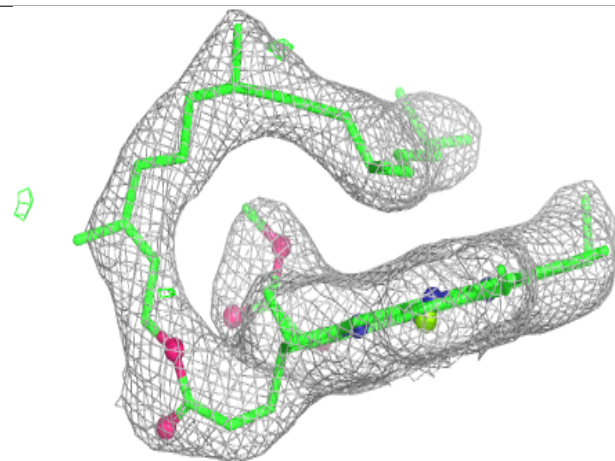
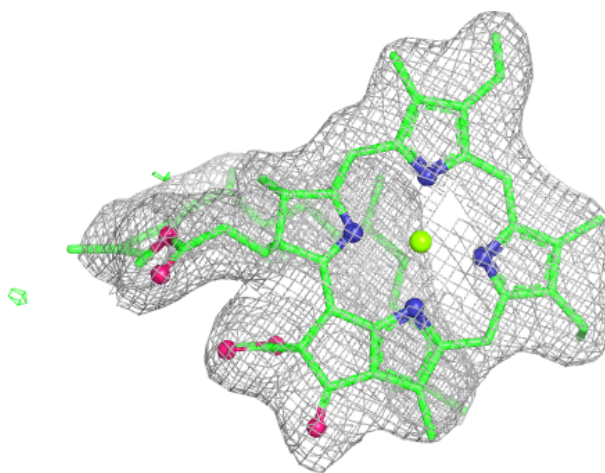
Electron density around CLA c 511:

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



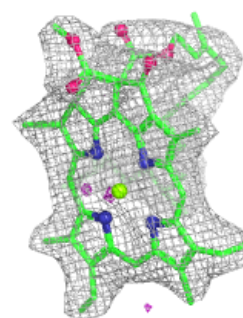
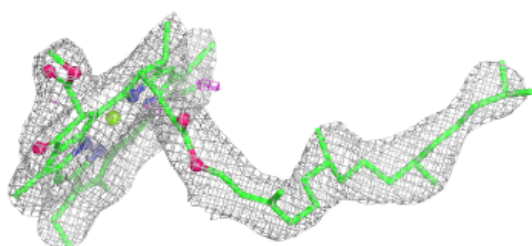
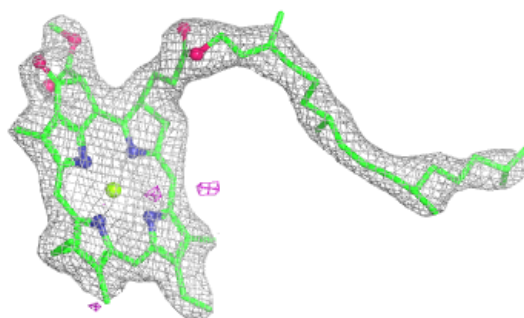
Electron density around CLA c 512:

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

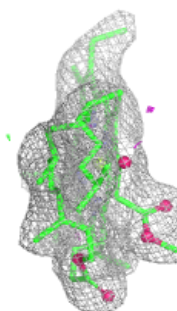
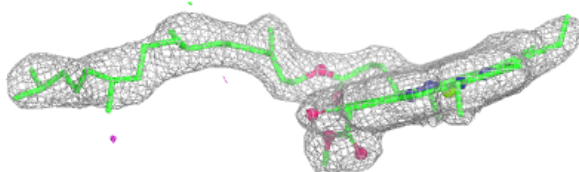
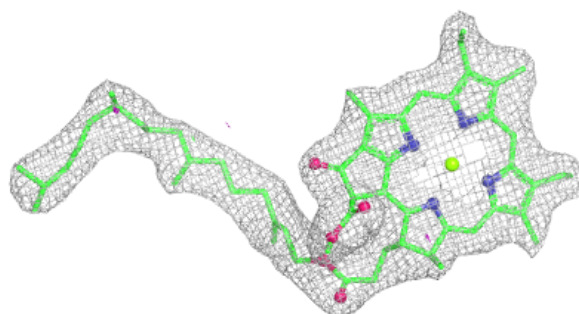


Electron density around CLA c 513:

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

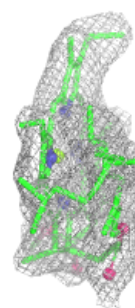
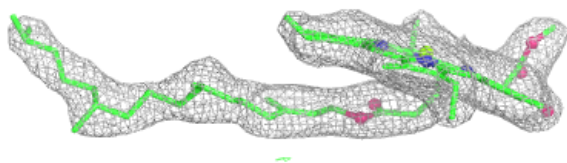
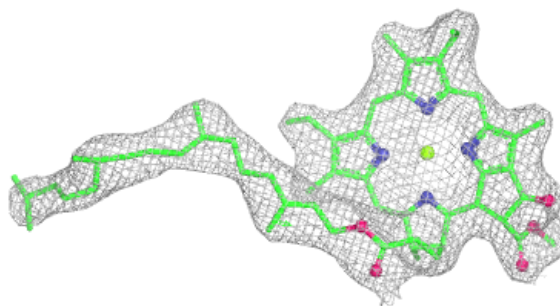
**Electron density around CLA b 602:**

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

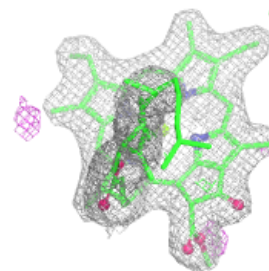
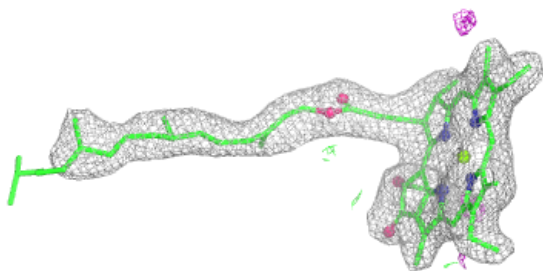
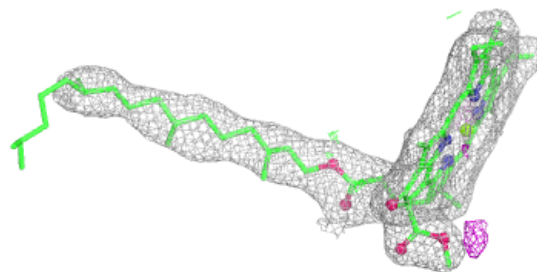


Electron density around CLA b 603:

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

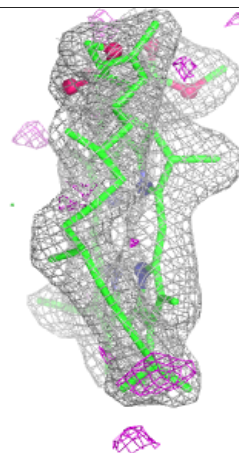
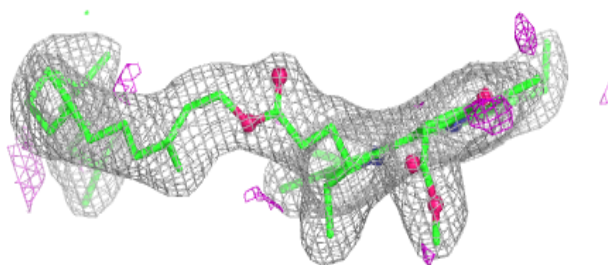
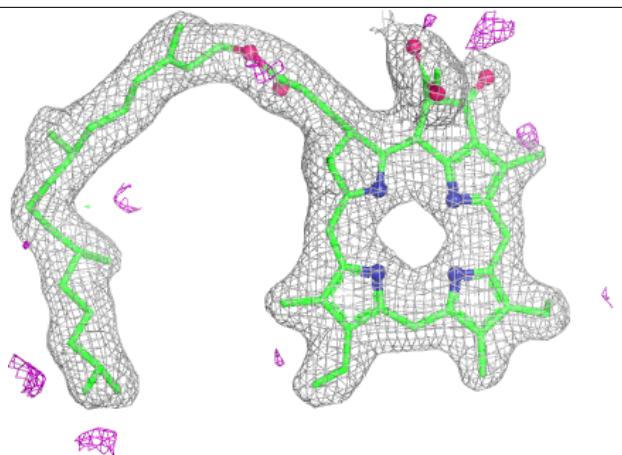
**Electron density around CLA b 604:**

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



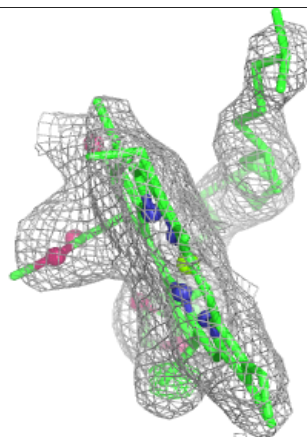
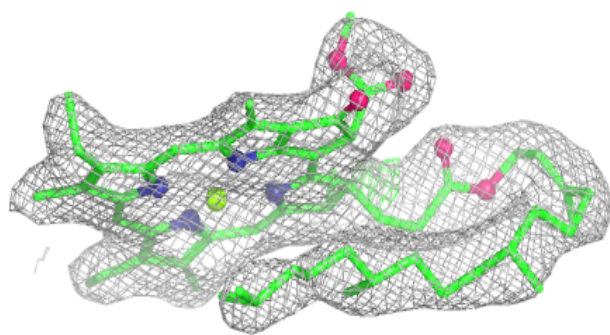
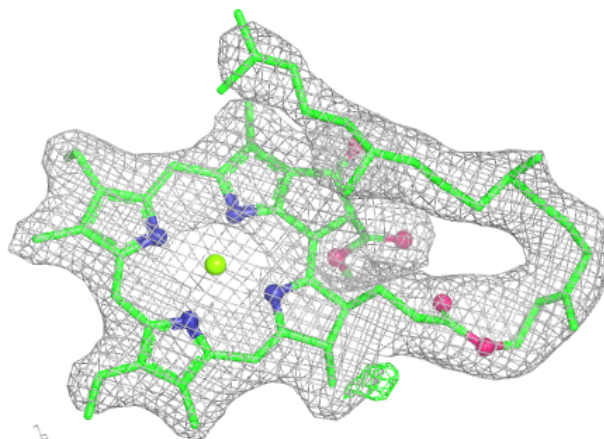
Electron density around PHO A 407:

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



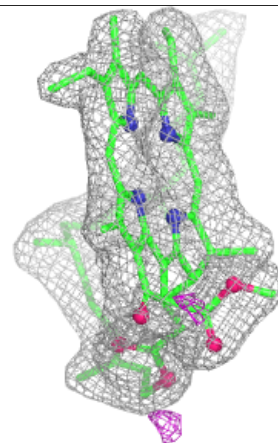
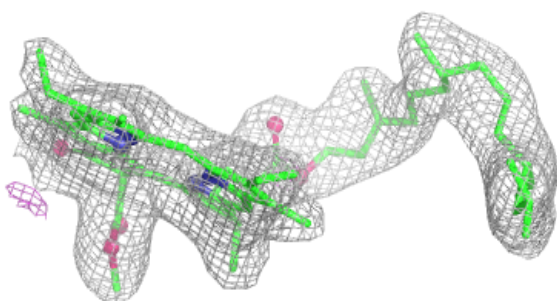
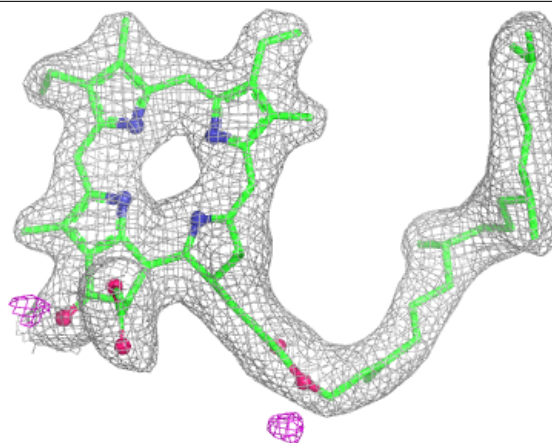
Electron density around CLA C 511:

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



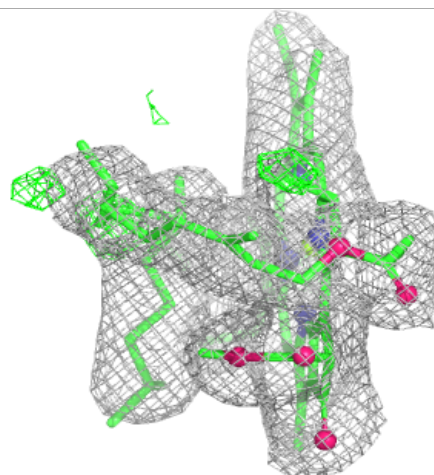
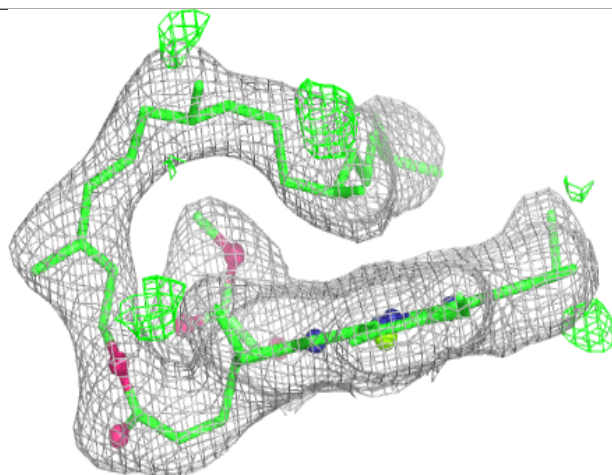
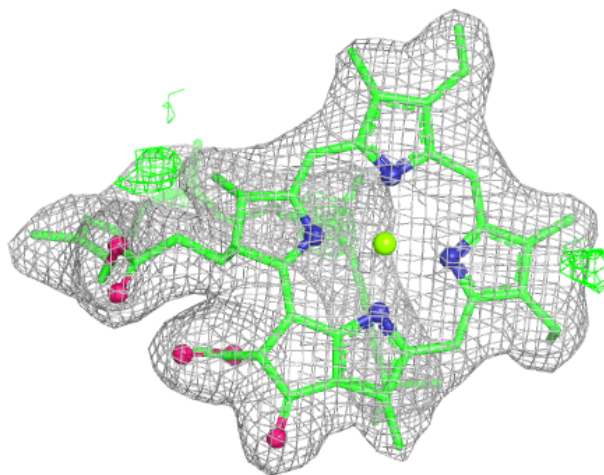
Electron density around PHO a 417:

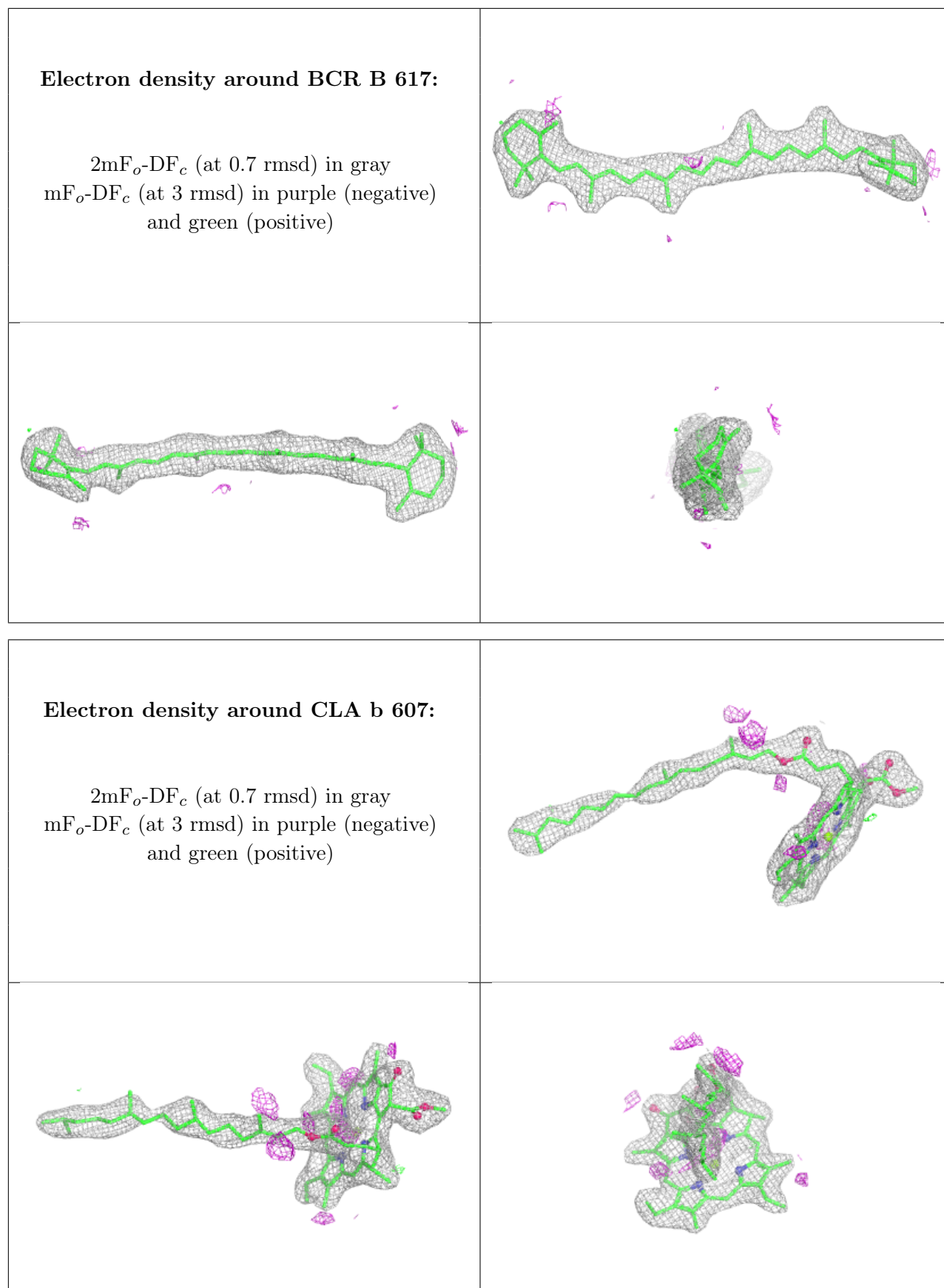
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA C 512:

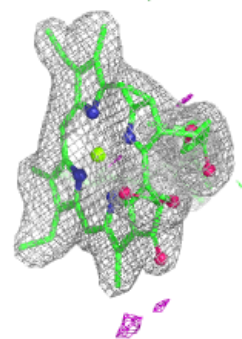
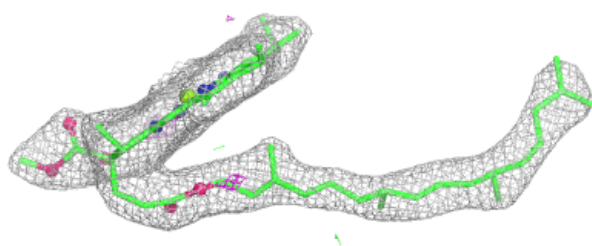
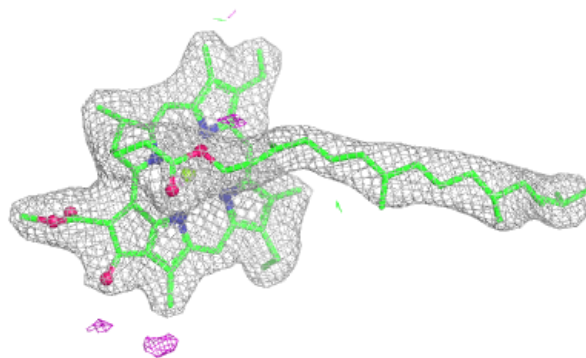
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



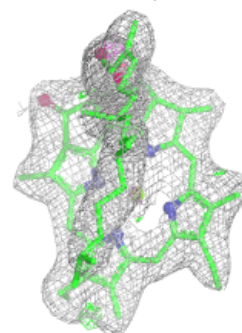
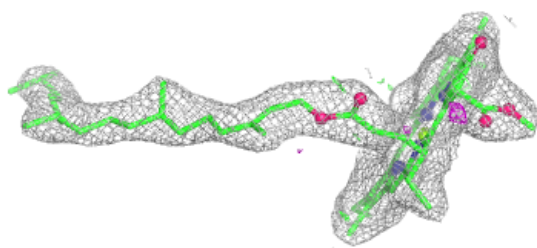
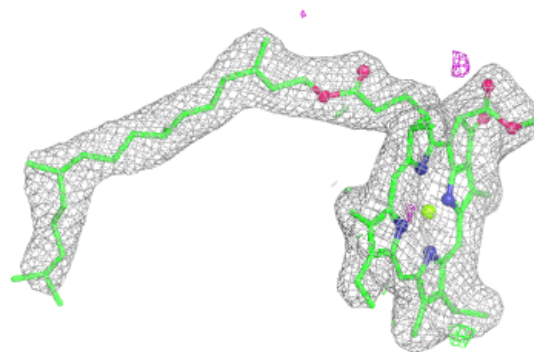


Electron density around CLA b 608:

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

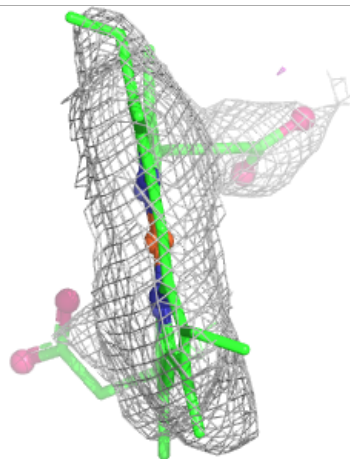
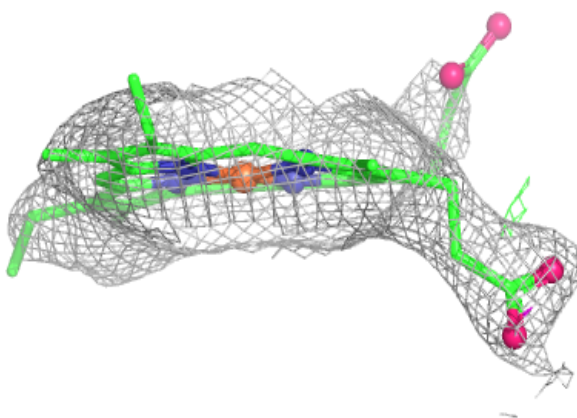
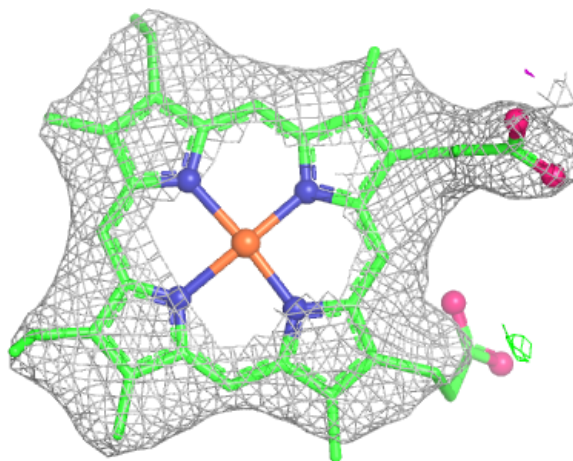
**Electron density around CLA b 609:**

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



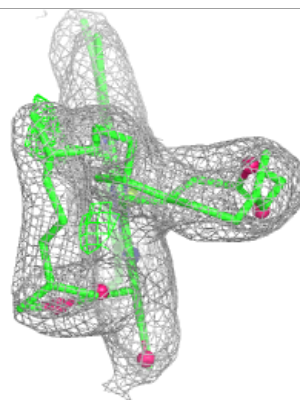
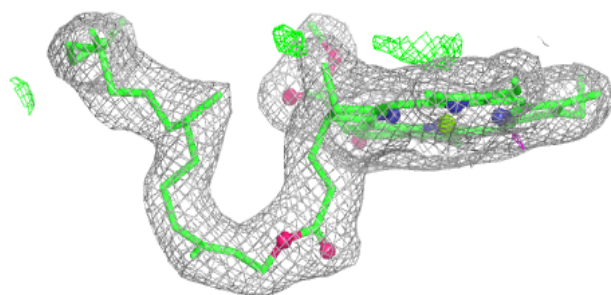
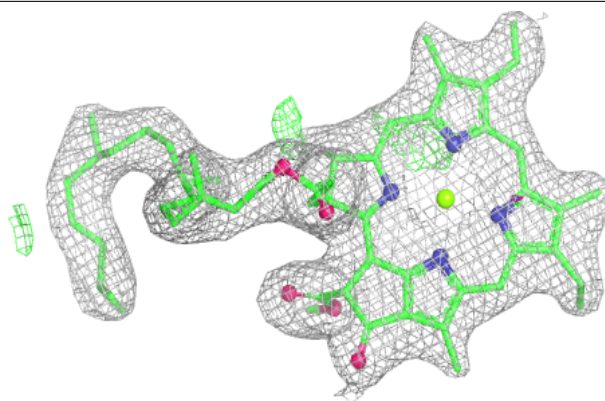
Electron density around HEC e 102:

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

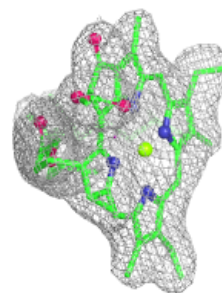
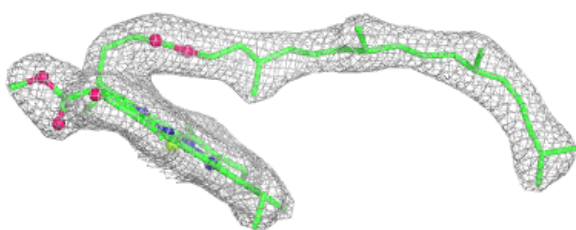
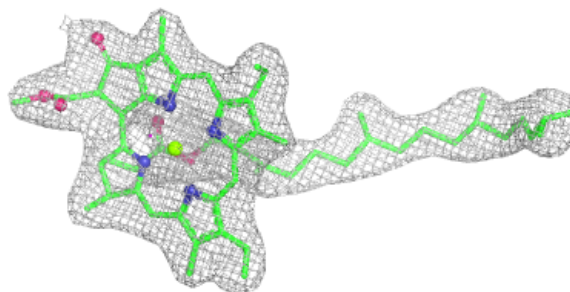


Electron density around CLA B 612:

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

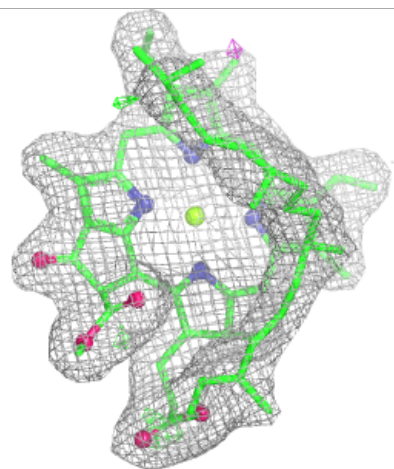
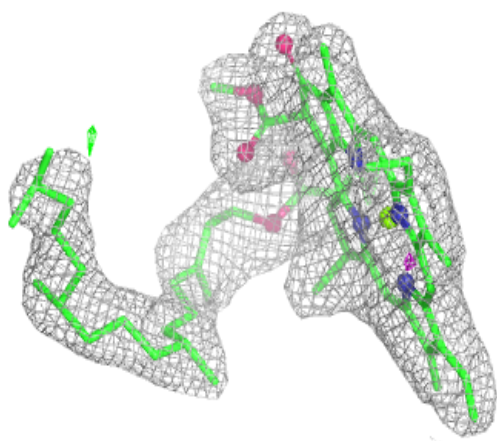
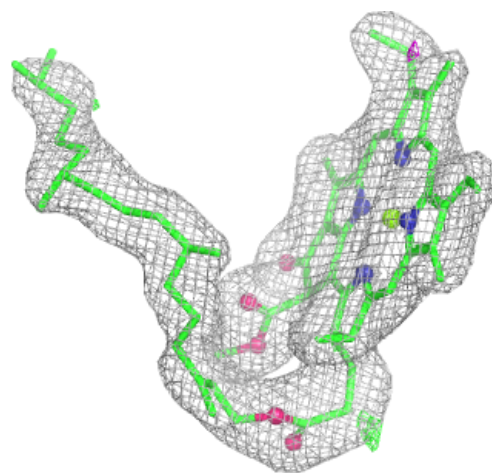
**Electron density around CLA B 608:**

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



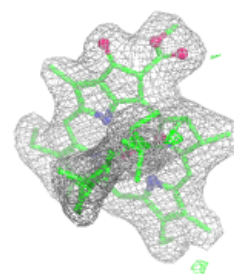
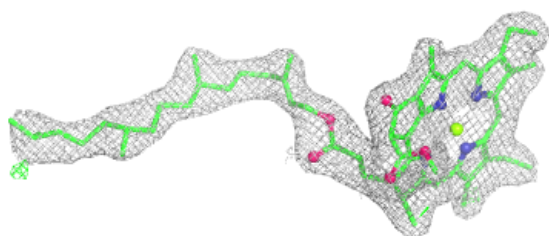
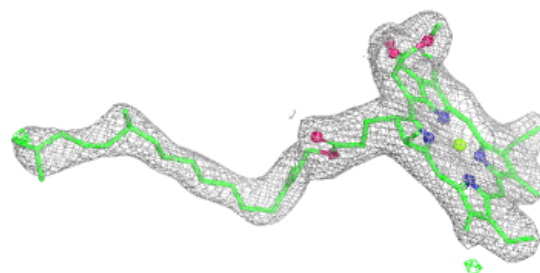
Electron density around CLA b 613:

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



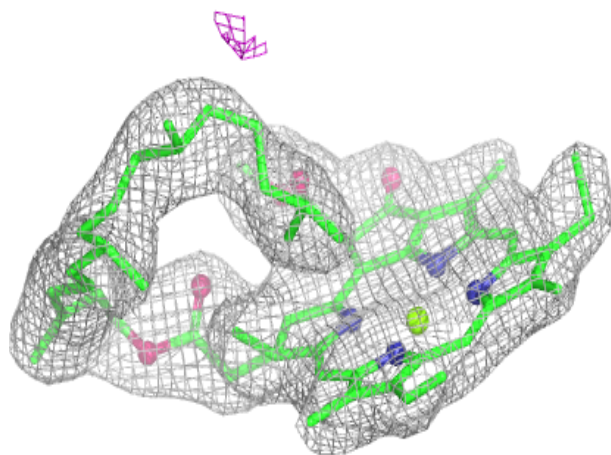
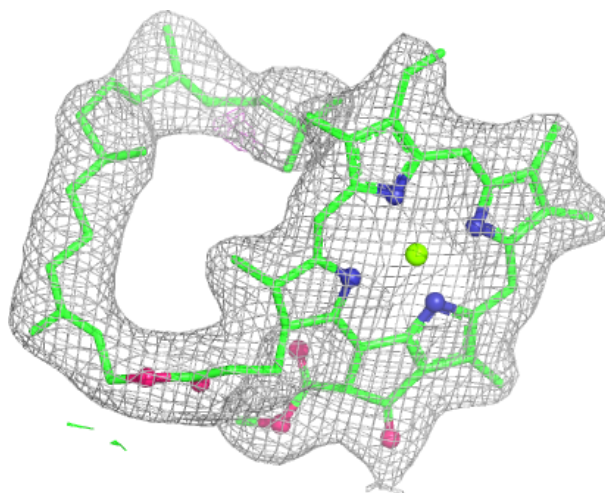
Electron density around CLA C 504:

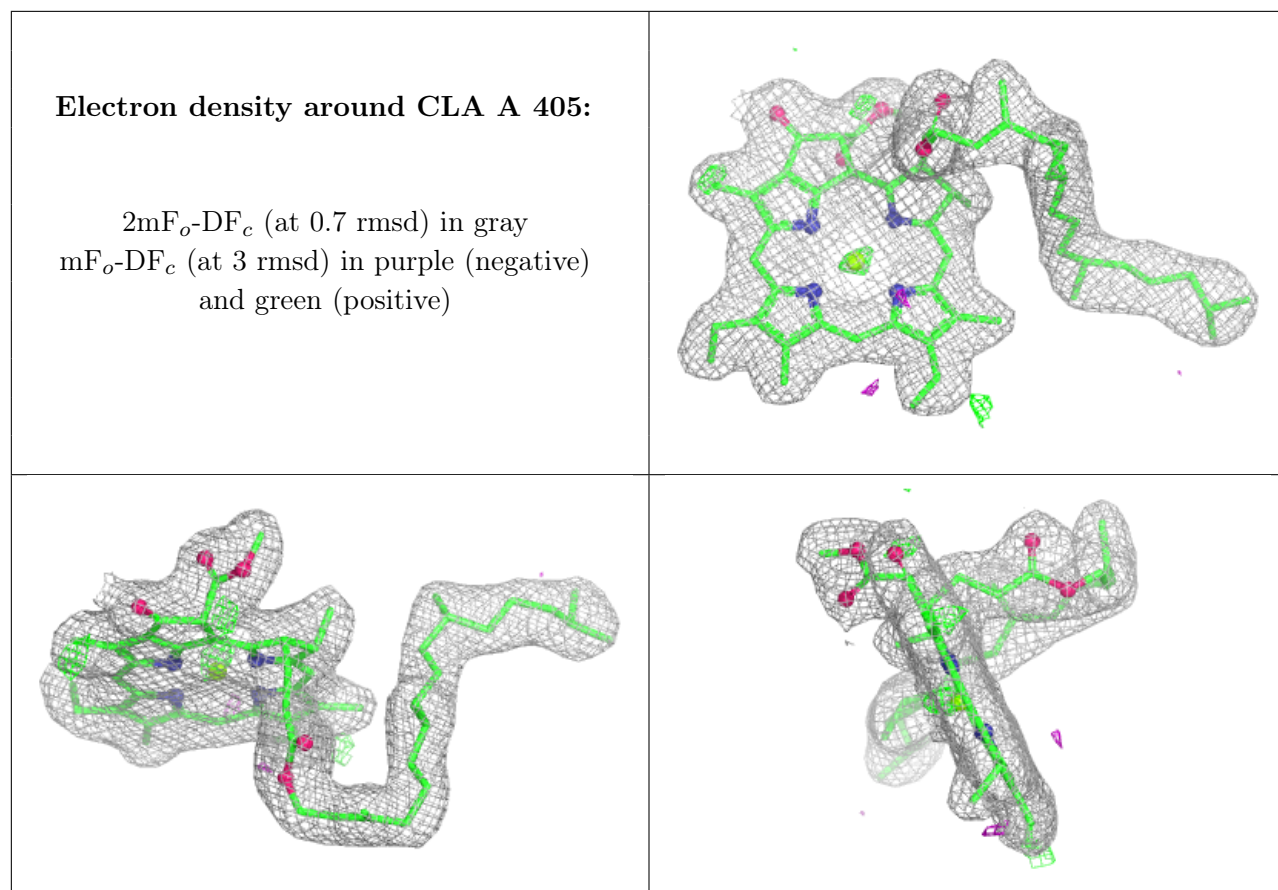
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA b 615:

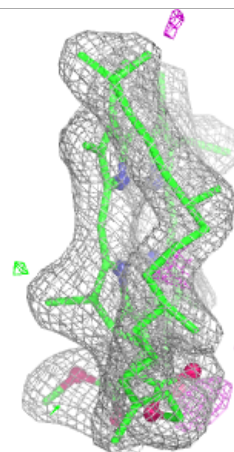
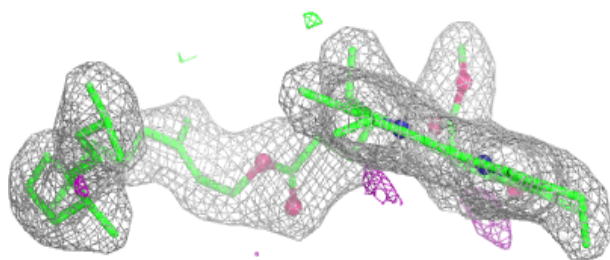
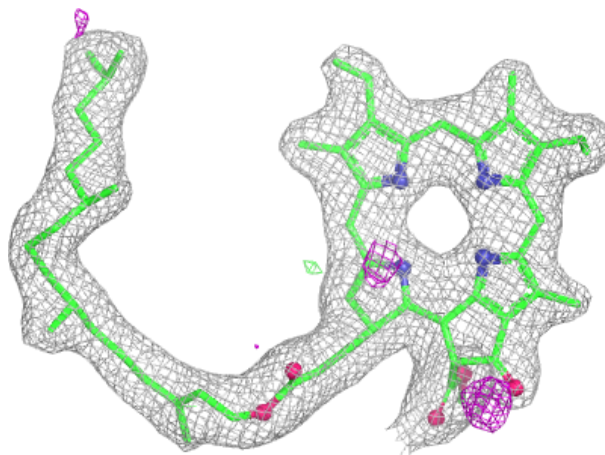
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

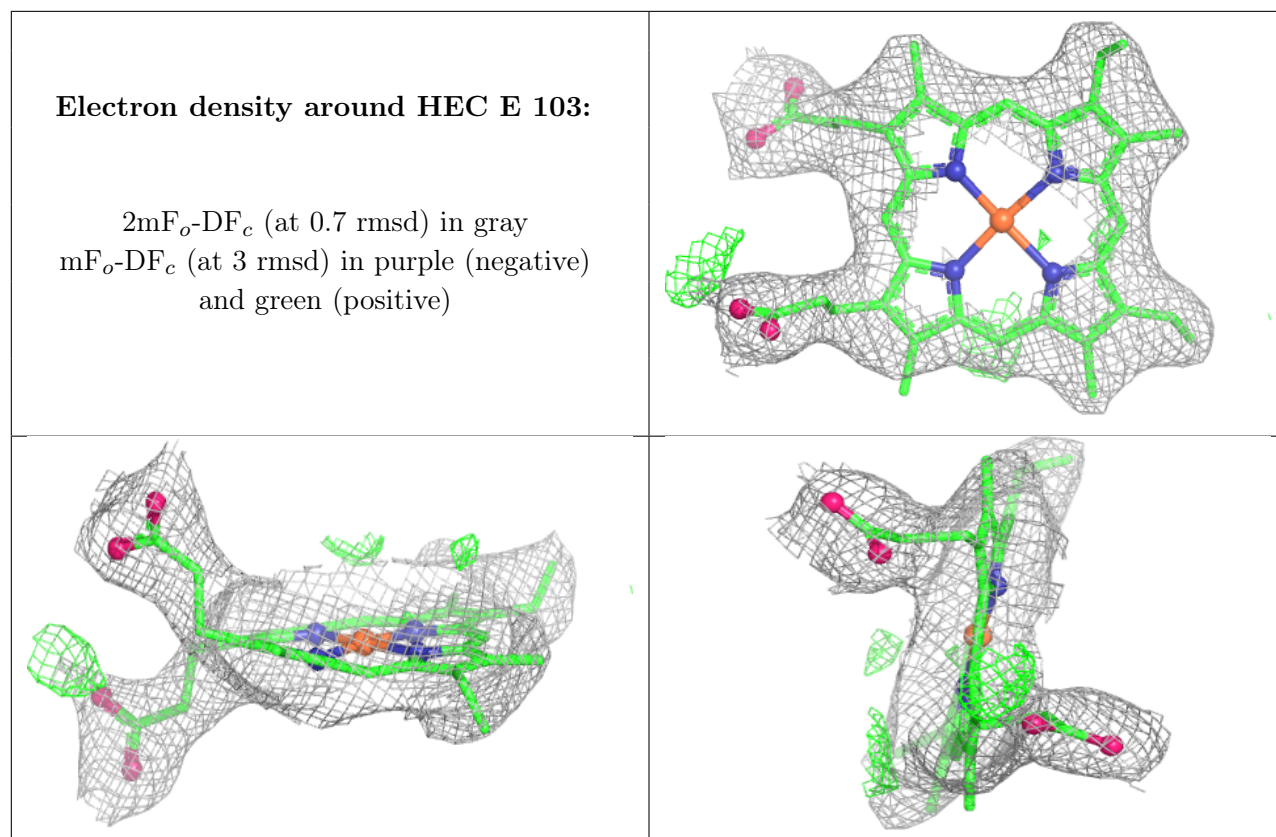




Electron density around PHO a 407:

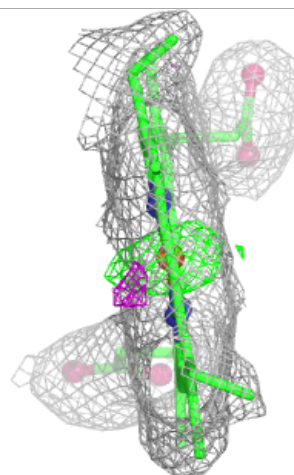
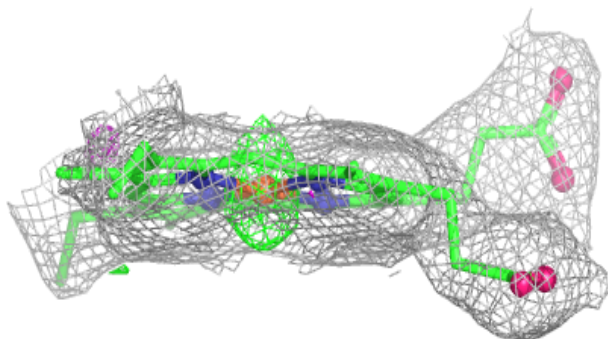
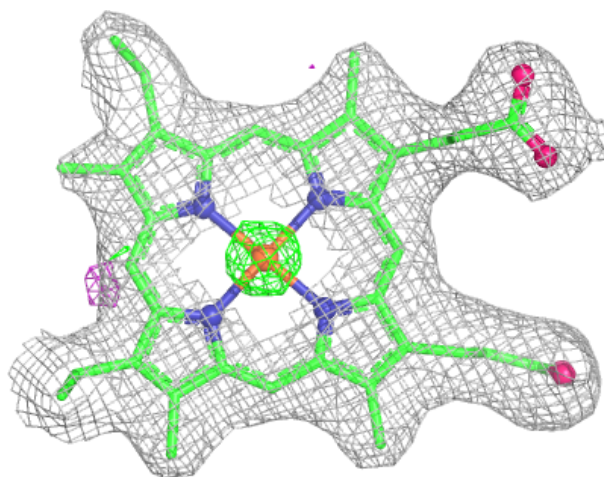
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





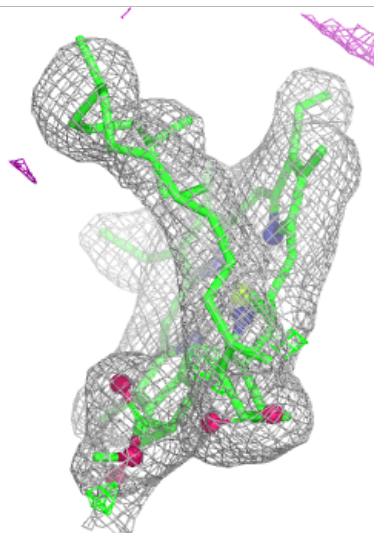
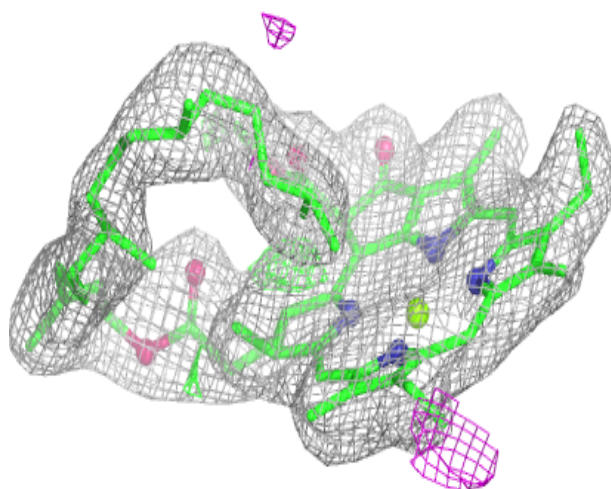
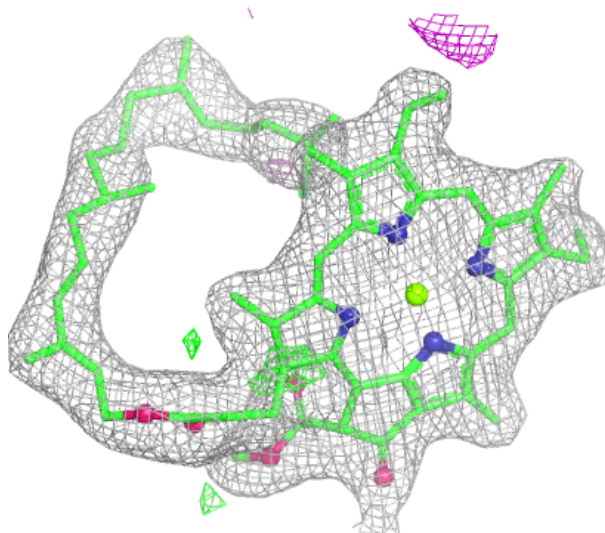
Electron density around HEC V 201:

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



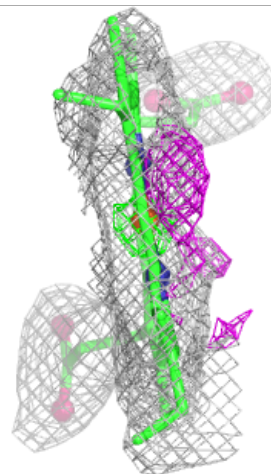
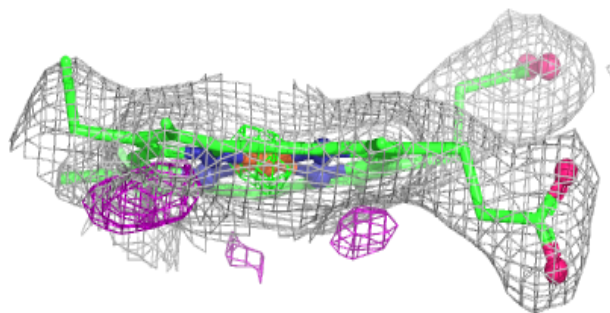
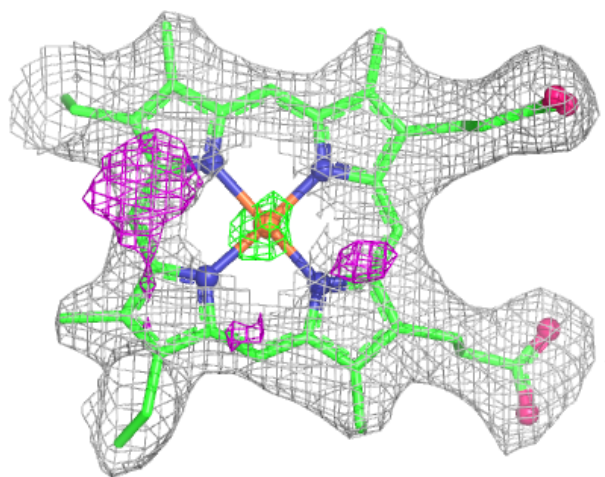
Electron density around CLA B 615:

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



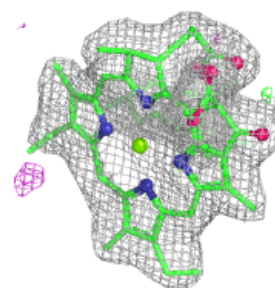
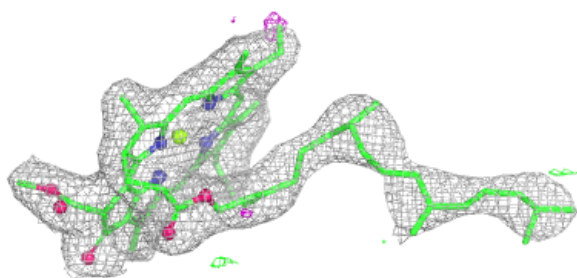
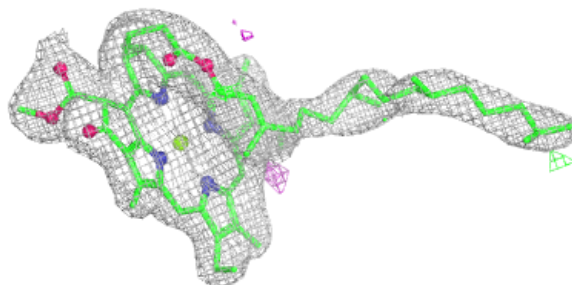
Electron density around HEC v 202:

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

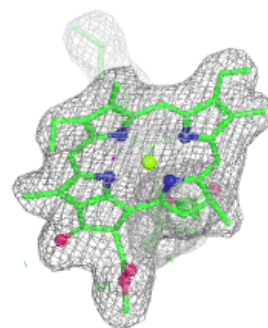
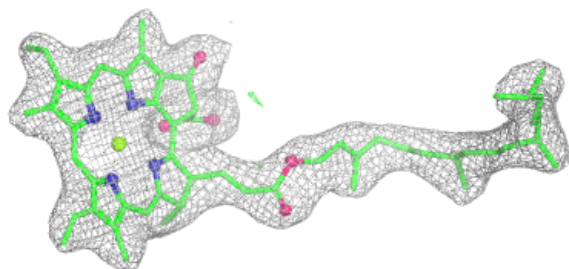
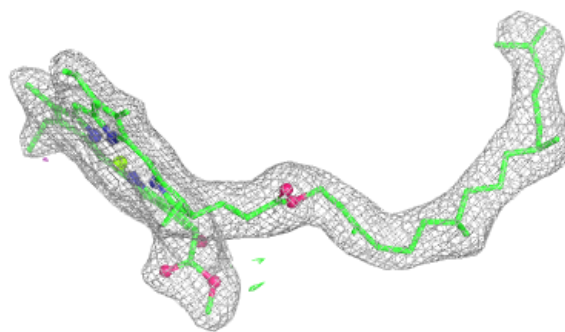


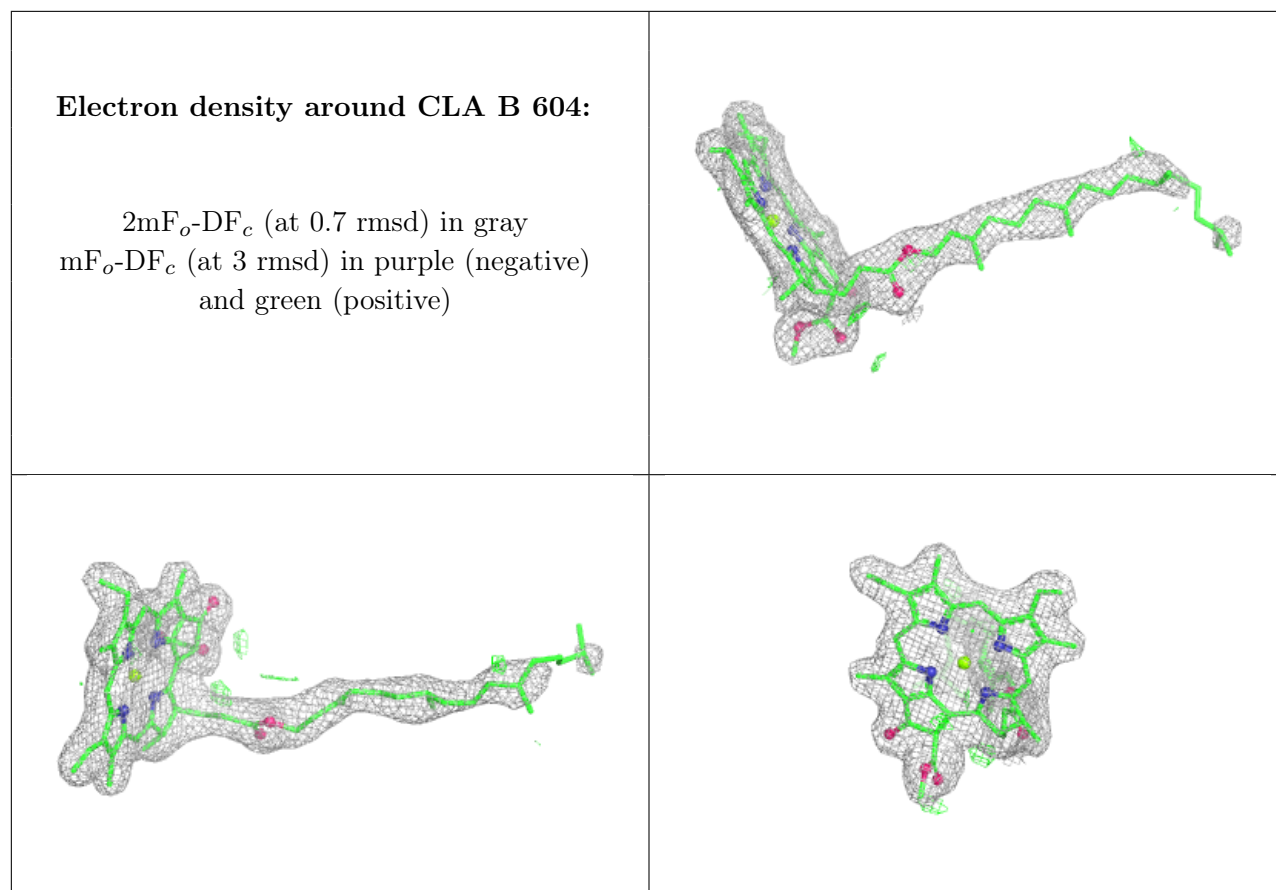
Electron density around CLA C 507:

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

**Electron density around CLA 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.