



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 16, 2026 – 07:56 PM UTC

PDB ID : 8IRD / pdb\_00008ird  
Title : XFEL structure of cyanobacterial photosystem II following two flashes (2F)  
with a 20-nanosecond delay  
Authors : Li, H.; Suga, M.; Shen, J.R.  
Deposited on : 2023-03-17  
Resolution : 2.30 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.48.1

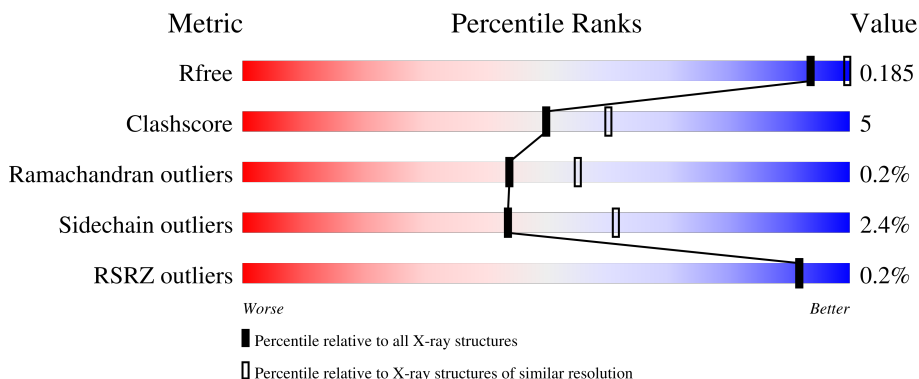
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

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





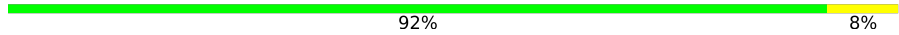




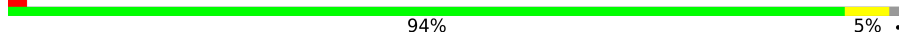

















Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	344	90% 7% .
1	a	344	85% 11% .
2	B	505	91% 9%
2	b	505	90% 8% .
3	C	455	91% 7% .

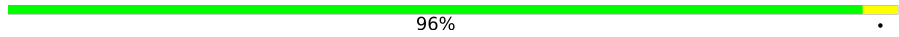







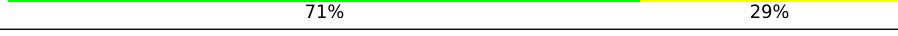
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Mol	Chain	Length	Quality of chain
3	c	455	 89% 10%
4	D	342	 90% 10%
4	d	342	 92% 8%
5	E	84	 79% 18%
5	e	84	 86% 8% 6%
6	F	44	 68% 9% 23%
6	f	44	 64% 7% 30%
7	H	65	 94% 5%
7	h	65	 83% 14%
8	I	38	 76% 21%
8	i	38	 87% 13%
9	J	39	 77% 21%
9	j	39	 92% 8%
10	K	37	 81% 16%
10	k	37	 78% 16% 5%
11	L	37	 92% 5%
11	l	37	 81% 16%
12	M	36	 78% 8% 6% 8%
12	m	36	 78% 14% 6%
13	O	244	 84% 16%
13	o	244	 89% 10%
14	T	32	 75% 16% 6%
14	t	32	 72% 22% 6%
15	U	104	 85% 8% 8%
15	u	104	 87% 6% 7%

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Mol	Chain	Length	Quality of chain
16	V	137	 96%
16	v	137	 90% 10%
17	X	40	 88% 8% 5%
17	x	40	 90% 5% 5%
18	Y	30	 80% 17%
18	y	30	 60% 37%
19	Z	62	 85% 13%
19	z	62	 74% 24%
20	R	34	 3% 71% 29%

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[A]	X	-	-	-
23	CLA	A	404[B]	X	-	-	-
23	CLA	A	405[A]	X	-	-	-
23	CLA	A	405[B]	X	-	-	-
23	CLA	A	407	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	502	X	-	-	-
23	CLA	C	503	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	D	403[A]	X	-	-	-
23	CLA	D	403[B]	X	-	-	-
23	CLA	D	404	X	-	-	-
23	CLA	a	404[A]	X	-	-	-
23	CLA	a	404[B]	X	-	-	-
23	CLA	a	407	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	502	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	-	-	-

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
23	CLA	c	513	X	-	-	-
23	CLA	d	402[A]	X	-	-	-
23	CLA	d	402[B]	X	-	-	-
23	CLA	d	403[A]	X	-	-	-
23	CLA	d	403[B]	X	-	-	-
23	CLA	d	404	X	-	-	-
26	GOL	D	402	-	-	X	-
26	GOL	D	413	-	X	-	-

## 2 Entry composition [i](#)

There are 41 unique types of molecules in this entry. The entry contains 62600 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	4338	2836	717	760	25	0	222	0
1	a	334	4330	2830	716	759	25	0	221	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	4146	2721	692	720	13	0	20	0
2	b	504	4134	2718	687	716	13	0	19	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	4260	2788	713	741	18	0	97	0
3	c	455	4308	2821	719	750	18	0	100	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	expression tag	UNP D0VWR7
C	20	SER	-	expression tag	UNP D0VWR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	expression tag	UNP D0VWR7
C	22	PHE	-	expression tag	UNP D0VWR7
c	19	ASN	-	expression tag	UNP D0VWR7
c	20	SER	-	expression tag	UNP D0VWR7
c	21	ILE	-	expression tag	UNP D0VWR7
c	22	PHE	-	expression tag	UNP D0VWR7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	114	0
			3620	2387	596	622	15			
4	d	341	Total	C	N	O	S	0	116	0
			3628	2391	599	623	15			

- 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	0	0
			662	432	107	123				
5	e	79	Total	C	N	O		0	2	0
			670	439	110	121				

- 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	1	0
			261	179	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	0	0
			506	339	81	84	2			
7	h	64	Total	C	N	O	S	0	1	0
			517	345	85	85	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
10	K	37	Total	C	N	O	0	0	0
			293	204	43	46			
10	k	37	Total	C	N	O	0	0	0
			293	204	43	46			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	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
11	L	36	Total	C	N	O	0	2	0
			311	207	49	55			
11	l	36	Total	C	N	O	0	2	0
			311	207	49	55			

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	2	0
			286	190	43	52	1			

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
13	O	243	Total	C	N	O	S	0	10	0
			1958	1221	335	398	4			
13	o	243	Total	C	N	O	S	0	8	0
			1933	1207	330	392	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	6	0
			311	213	48	48	2			
14	t	30	Total	C	N	O	S	0	5	0
			302	208	47	45	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	96	Total	C	N	O	0	4	0
			800	508	133	159			
15	u	97	Total	C	N	O	0	4	0
			807	513	134	160			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	6	0
			1120	711	185	220	4			
16	v	137	Total	C	N	O	S	0	6	0
			1117	712	185	216	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	38	Total	C	N	O	0	1	0
			289	194	46	49			
17	x	38	Total	C	N	O	0	0	0
			281	188	45	48			

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

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

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

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

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

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

- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 22 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

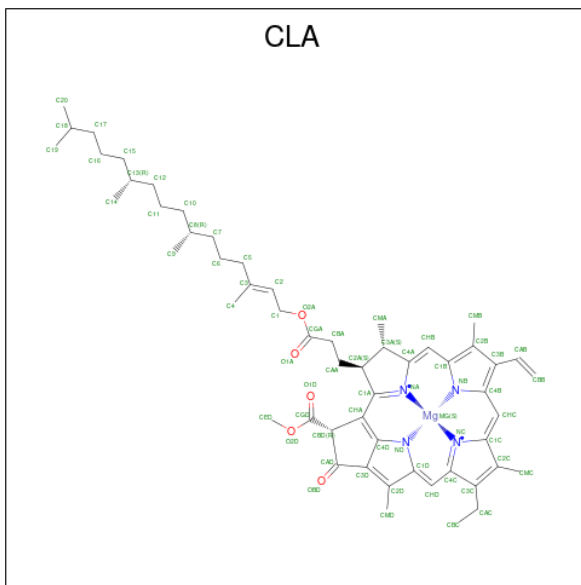
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	2
			4	4		

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

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
23	A	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	A	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	A	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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

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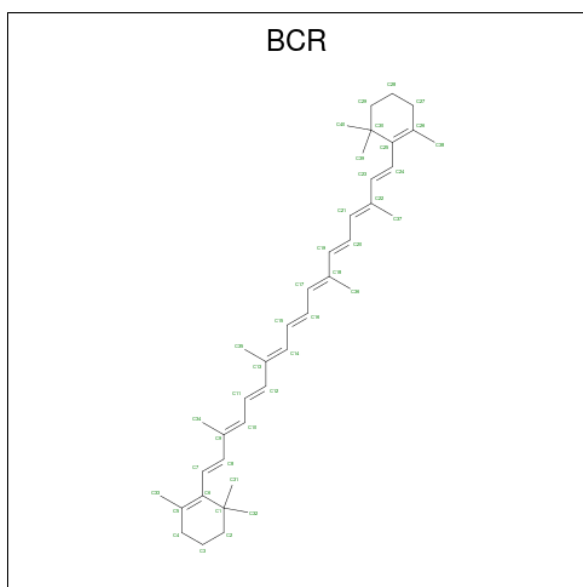
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	D	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	a	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
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	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	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	1
			130	110	2	8	10		
23	d	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



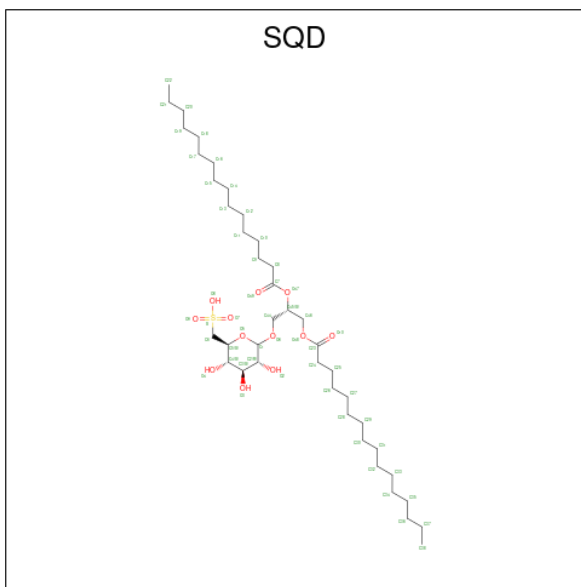
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	T	1	Total C 40 40	0	0
24	Y	1	Total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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	b	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	d	1	Total C 40 40	0	0
24	h	1	Total C 40 40	0	0
24	k	1	Total C 40 40	0	0
24	t	1	Total C 40 40	0	0
24	y	1	Total C 40 40	0	0

- Molecule 25 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



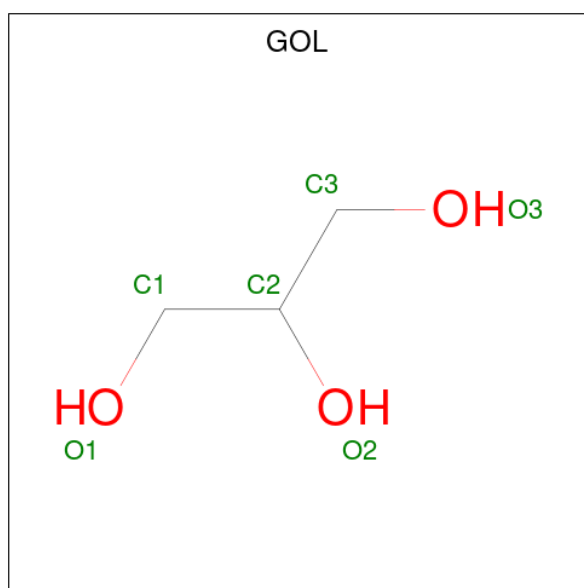
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O S 108 82 24 2	0	1
25	A	1	Total C O S 54 41 12 1	0	0
25	X	1	Total C O S 43 30 12 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	a	1	Total	C	O	S	0	1
			108	82	24	2		
25	a	1	Total	C	O	S	0	0
			54	41	12	1		
25	b	1	Total	C	O	S	0	0
			54	41	12	1		
25	f	1	Total	C	O	S	0	0
			43	30	12	1		
25	l	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 26 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



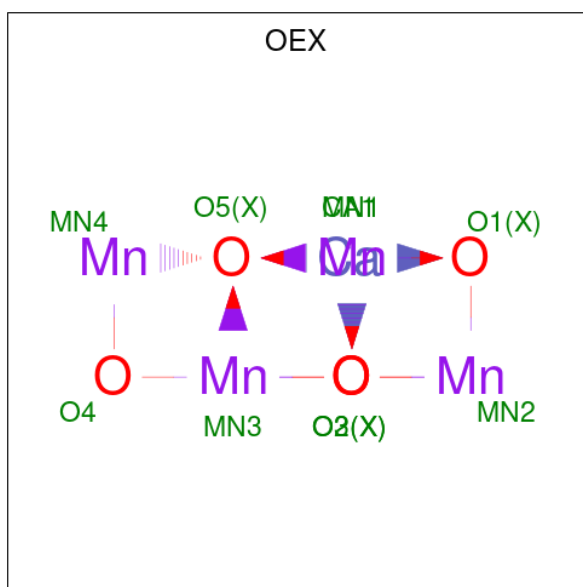
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	A	1	Total	C	O	0	0
			6	3	3		
26	B	1	Total	C	O	0	0
			6	3	3		
26	B	1	Total	C	O	0	0
			6	3	3		
26	C	1	Total	C	O	0	1
			12	6	6		
26	D	1	Total	C	O	0	0
			6	3	3		
26	D	1	Total	C	O	0	0
			6	3	3		

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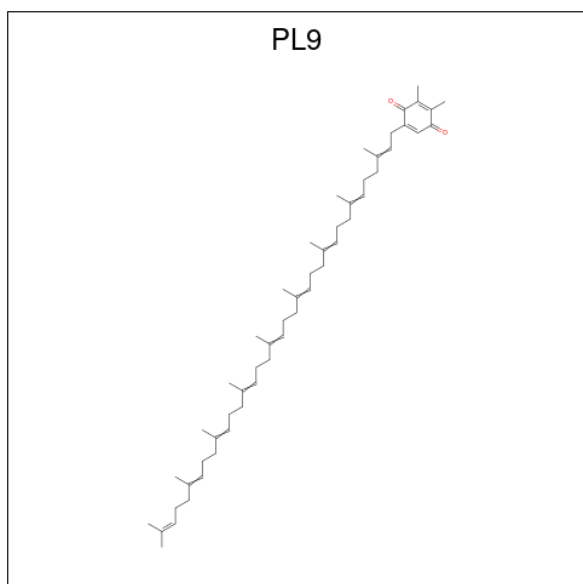
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	O	1	Total 6	C 3	O 3	0	0
26	O	1	Total 6	C 3	O 3	0	0
26	V	1	Total 12	C 6	O 6	0	1
26	a	1	Total 6	C 3	O 3	0	0
26	a	1	Total 6	C 3	O 3	0	0
26	a	1	Total 6	C 3	O 3	0	0
26	b	1	Total 6	C 3	O 3	0	0
26	b	1	Total 6	C 3	O 3	0	0
26	c	1	Total 12	C 6	O 6	0	1
26	c	1	Total 6	C 3	O 3	0	0
26	d	1	Total 6	C 3	O 3	0	0
26	l	1	Total 12	C 6	O 6	0	1
26	o	1	Total 6	C 3	O 3	0	0
26	o	1	Total 6	C 3	O 3	0	0
26	v	1	Total 12	C 6	O 6	0	1

- Molecule 27 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Ca	Mn	O		
27	A	1	20	2	8	10	0	1
27	a	1	20	2	8	10	0	1

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C<sub>53</sub>H<sub>80</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).

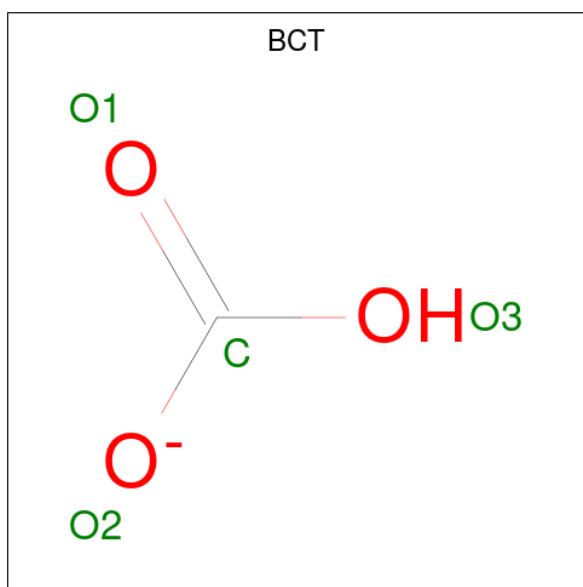


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	1
			110	106	4		
28	D	1	Total	C	O	0	1
			110	106	4		
28	a	1	Total	C	O	0	1
			110	106	4		
28	d	1	Total	C	O	0	1
			110	106	4		

- Molecule 29 is UNKNOWN LIGAND (CCD ID: UNL) (formula: ).

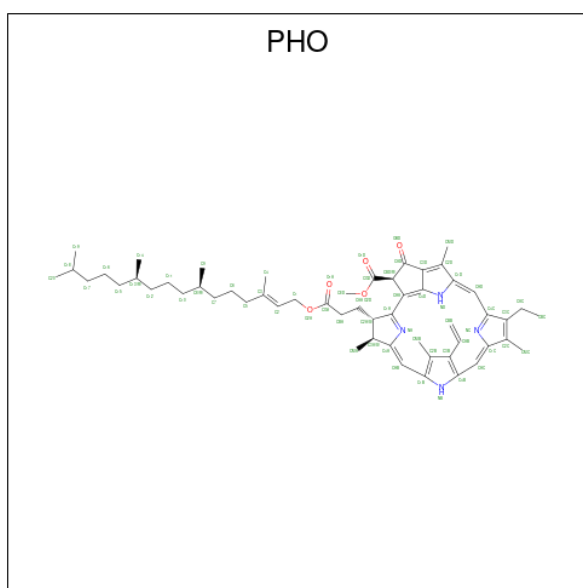
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			28	23	5		
29	B	2	Total	C	O	0	0
			73	63	10		
29	D	2	Total	C	O	0	0
			57	51	6		
29	I	1	Total	C	O	0	0
			40	35	5		
29	J	1	Total	C		0	0
			10	10			
29	K	1	Total	C	O	0	1
			68	58	10		
29	X	1	Total	C	O	0	0
			18	16	2		
29	a	1	Total	C	O	0	0
			30	25	5		
29	b	1	Total	C	O	0	0
			33	28	5		
29	c	1	Total	C	O	0	1
			64	54	10		
29	d	3	Total	C	O	0	0
			71	63	8		
29	j	1	Total	C		0	0
			10	10			
29	l	1	Total	C		0	0
			10	10			
29	m	1	Total	C		0	0
			10	10			

- Molecule 30 is BICARBONATE ION (CCD ID: BCT) (formula:  $\text{CHO}_3$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 31 is PHEOPHYTIN A (CCD ID: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



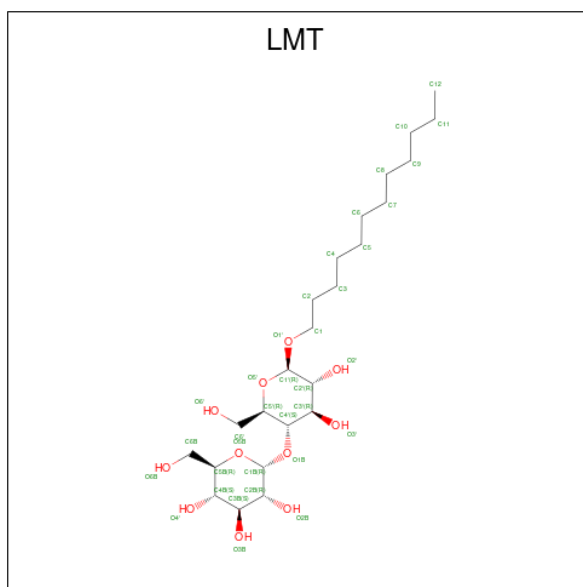
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	N	O	0	1
			128	110	8	10		
31	D	1	Total	C	N	O	0	1
			128	110	8	10		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	a	1	Total	C	N	O	0	1
			128	110	8	10		
31	a	1	Total	C	N	O	0	1
			128	110	8	10		

- Molecule 32 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



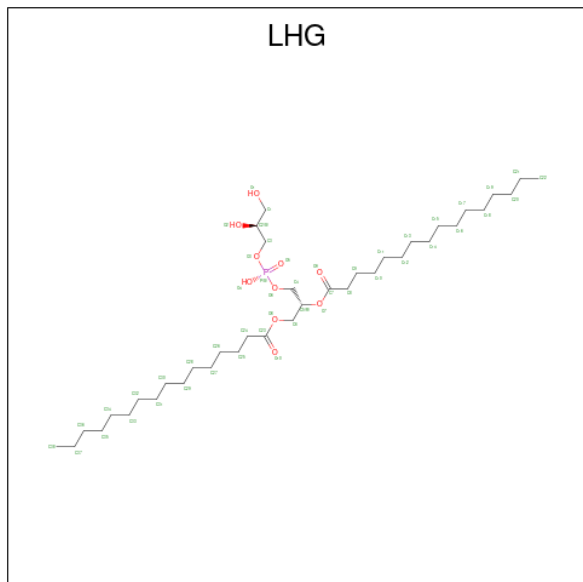
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			35	24	11		
32	A	1	Total	C	O	0	0
			35	24	11		
32	B	1	Total	C	O	0	0
			35	24	11		
32	B	1	Total	C	O	0	0
			35	24	11		
32	B	1	Total	C	O	0	0
			25	19	6		
32	F	1	Total	C	O	0	0
			35	24	11		
32	M	1	Total	C	O	0	0
			35	24	11		
32	T	1	Total	C	O	0	0
			35	24	11		
32	a	1	Total	C	O	0	0
			35	24	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	b	1	Total	C	O	0	0
			25	19	6		
32	b	1	Total	C	O	0	0
			25	19	6		
32	e	1	Total	C	O	0	0
			35	24	11		
32	m	1	Total	C	O	0	0
			35	24	11		
32	t	1	Total	C	O	0	0
			26	19	7		

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



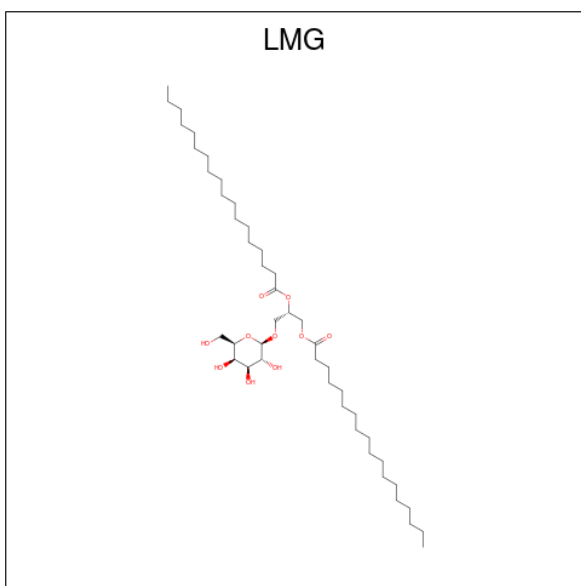
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	A	1	Total	C	O	P	0	1
			98	76	20	2		
33	D	1	Total	C	O	P	0	1
			98	76	20	2		
33	D	1	Total	C	O	P	0	1
			98	76	20	2		
33	E	1	Total	C	O	P	0	1
			84	62	20	2		
33	L	1	Total	C	O	P	0	1
			98	76	20	2		
33	a	1	Total	C	O	P	0	1
			84	62	20	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
33	b	1	98	76	20	2	0	1
33	d	1	98	76	20	2	0	1
33	d	1	98	76	20	2	0	1
33	d	1	98	76	20	2	0	1

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



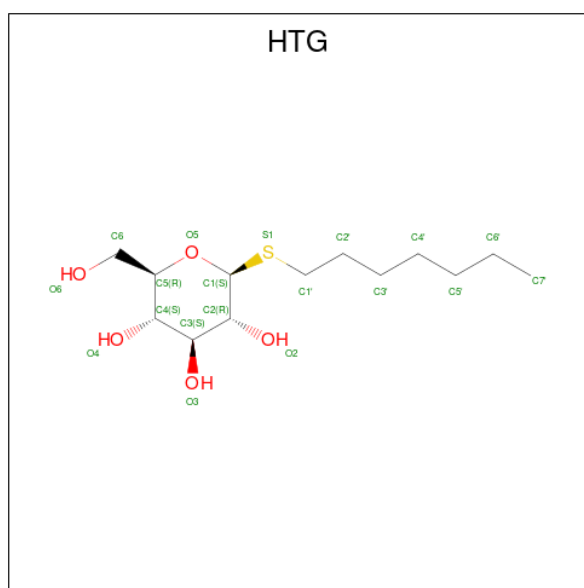
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
34	B	1	51	41	10	0	0
34	C	1	51	41	10	0	0
34	C	1	51	41	10	0	0
34	C	1	51	41	10	0	0
34	D	1	51	41	10	0	0
34	c	1	51	41	10	0	0
34	c	1	51	41	10	0	0

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

- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C<sub>13</sub>H<sub>26</sub>O<sub>5</sub>S).



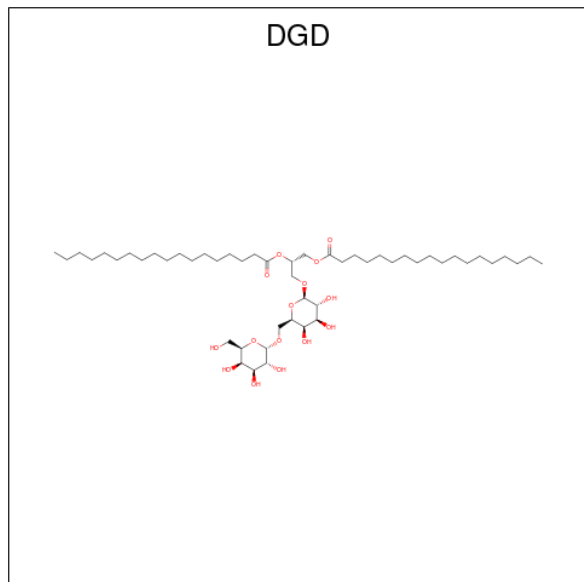
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	D	1	Total	C	O	S	0	0
			16	10	5	1		
35	V	1	Total	C	O		0	0
			11	6	5			
35	b	1	Total	C	O	S	0	0
			19	13	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			19	13	5	1		
35	d	1	Total	C	O	S	0	0
			16	10	5	1		
35	o	1	Total	C	O	S	0	0
			19	13	5	1		

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	C	1	Total	C	O	0	1
			124	94	30		
36	C	1	Total	C	O	0	1
			124	94	30		
36	C	1	Total	C	O	0	0
			62	47	15		
36	H	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	1
			124	94	30		
36	c	1	Total	C	O	0	1
			124	94	30		

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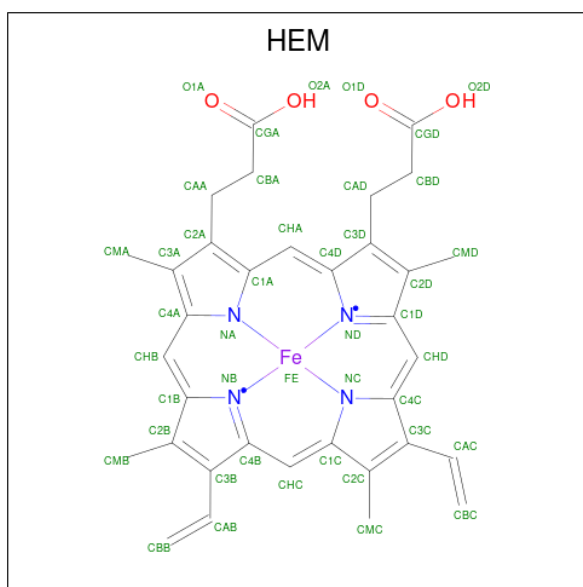
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	c	1	Total	C	O	0	0
			62	47	15		
36	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 37 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
38	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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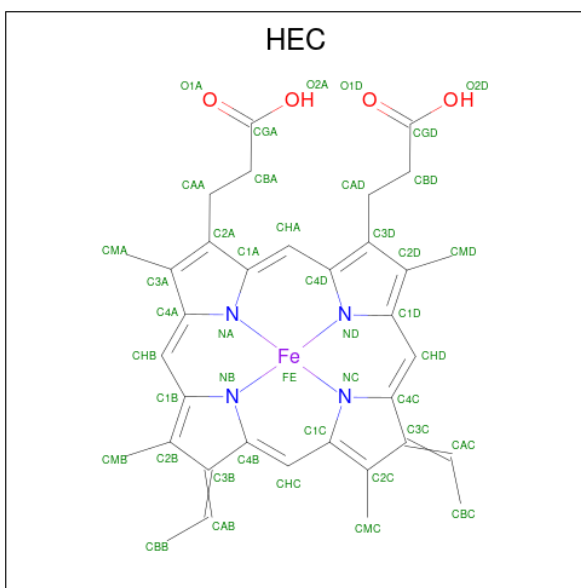
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
38	f	1	43	34	1	4	4	0	0

- Molecule 39 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 40 is HEME C (CCD ID: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
41	A	133	215	215	0	83
41	B	190	193	193	0	3

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	C	165	Total O 202 202	0	37
41	D	127	Total O 162 162	0	35
41	E	15	Total O 15 15	0	0
41	F	6	Total O 6 6	0	0
41	H	23	Total O 23 23	0	0
41	I	6	Total O 6 6	0	0
41	J	7	Total O 7 7	0	0
41	K	6	Total O 6 6	0	0
41	L	7	Total O 8 8	0	1
41	M	5	Total O 5 5	0	0
41	O	102	Total O 106 106	0	4
41	T	10	Total O 13 13	0	3
41	U	47	Total O 49 49	0	2
41	V	80	Total O 82 82	0	2
41	X	8	Total O 8 8	0	0
41	a	129	Total O 207 207	0	79
41	b	206	Total O 209 209	0	3
41	c	159	Total O 192 192	0	33
41	d	118	Total O 152 152	0	34
41	e	9	Total O 9 9	0	0
41	f	3	Total O 3 3	0	0

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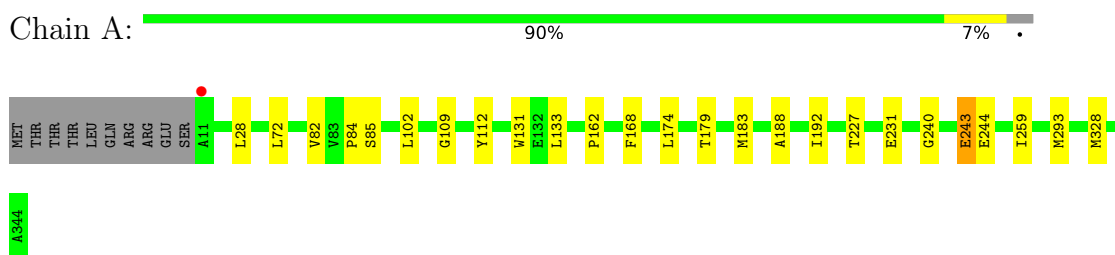
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	h	18	Total O 18 18	0	0
41	i	2	Total O 2 2	0	0
41	j	1	Total O 1 1	0	0
41	k	3	Total O 3 3	0	0
41	l	7	Total O 8 8	0	1
41	m	12	Total O 12 12	0	0
41	o	95	Total O 99 99	0	4
41	t	8	Total O 11 11	0	3
41	u	50	Total O 51 51	0	1
41	v	58	Total O 61 61	0	3
41	x	6	Total O 6 6	0	0
41	y	2	Total O 2 2	0	0

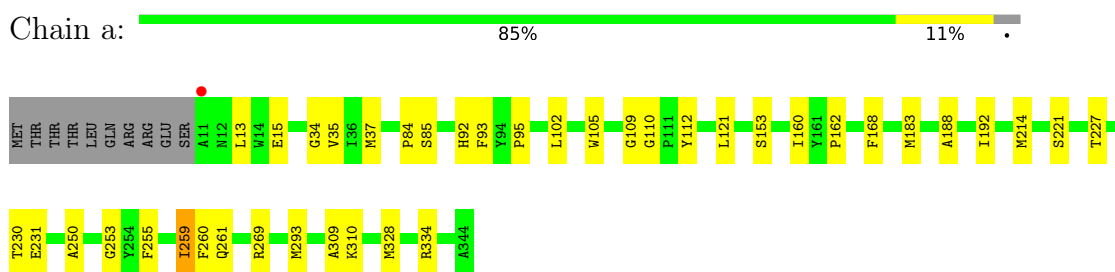
### 3 Residue-property plots [i](#)

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

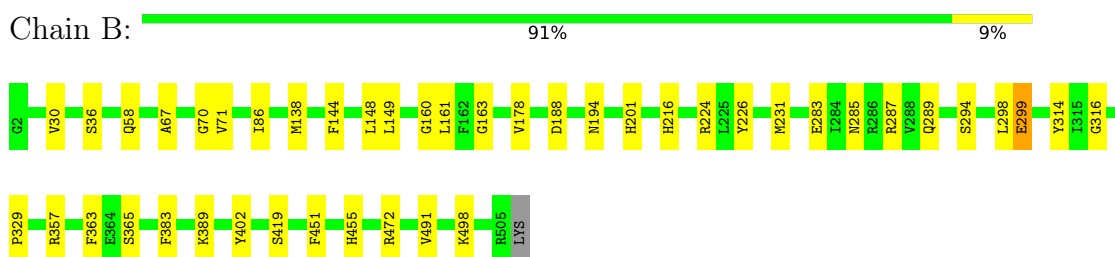
- Molecule 1: Photosystem II protein D1



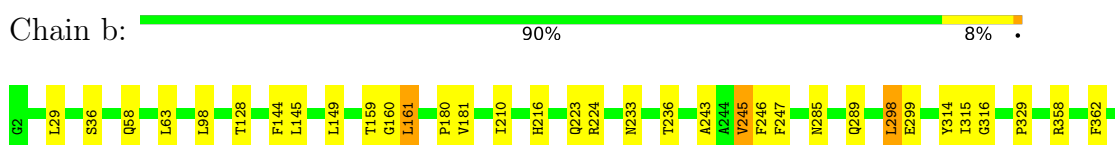
- Molecule 1: Photosystem II protein D1



- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein





- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 91% 7%



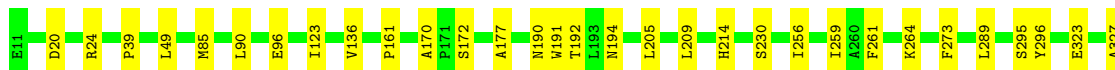
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 89% 10%



- Molecule 4: Photosystem II D2 protein

Chain D: 90% 10%



- Molecule 4: Photosystem II D2 protein

Chain d: 92% 8%

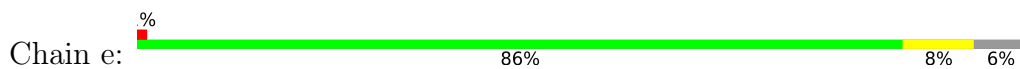


- Molecule 5: Cytochrome b559 subunit alpha

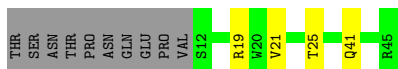
Chain E: 79% 18%



- Molecule 5: Cytochrome b559 subunit alpha



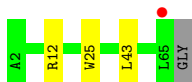
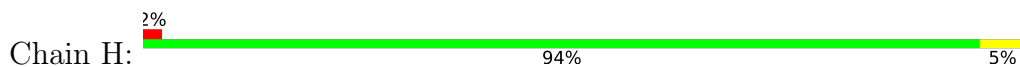
- Molecule 6: Cytochrome b559 subunit beta



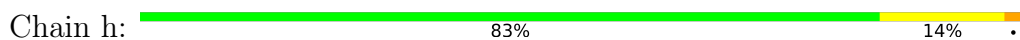
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H



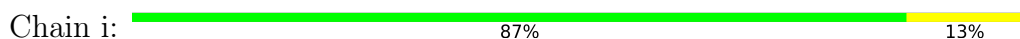
- Molecule 7: Photosystem II reaction center protein H




- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I




- Molecule 9: Photosystem II reaction center protein J

Chain J:  77% 21%




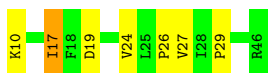
- Molecule 9: Photosystem II reaction center protein J

Chain j:  92% 8%




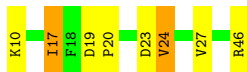
- Molecule 10: Photosystem II reaction center protein K

Chain K:  81% 16%



- Molecule 10: Photosystem II reaction center protein K

Chain k:  78% 16% 5%




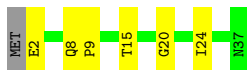
- Molecule 11: Photosystem II reaction center protein L

Chain L:  92% 5%




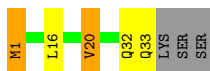
- Molecule 11: Photosystem II reaction center protein L

Chain l:  81% 16%




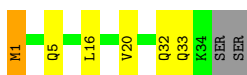
- Molecule 12: Photosystem II reaction center protein M

Chain M:  78% 8% 6% 8%




- Molecule 12: Photosystem II reaction center protein M

Chain m:  78% 14% 6%




- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  84% 16%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  89% 10%



- Molecule 14: Photosystem II reaction center protein T

Chain T:  75% 16% 6%




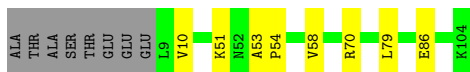
- Molecule 14: Photosystem II reaction center protein T

Chain t:  3% 72% 22% 6%




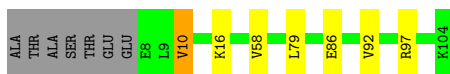
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  85% 8% 8%



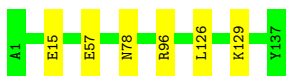
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  87% 6% 7%




- Molecule 16: Cytochrome c-550

Chain V:  96% .




- Molecule 16: Cytochrome c-550

Chain v:  90% 10% .




- Molecule 17: Photosystem II reaction center protein X

Chain X:  88% 8% 5% .




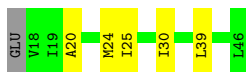
- Molecule 17: Photosystem II reaction center protein X

Chain x:  90% 5% 5% .



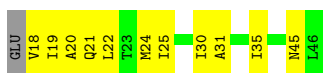
- Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:  80% 17% .




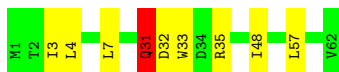
- Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:  60% 37% .



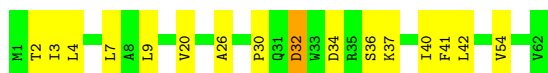
- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  85% 13% .




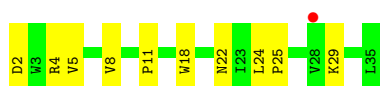
- Molecule 19: Photosystem II reaction center protein Z

Chain z:  74% 24%



● Molecule 20: Photosystem II protein Y

Chain R:  3% 71% 29%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.77Å 231.76Å 288.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.30 19.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.30) 99.7 (19.99-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 2.30Å)	Xtrriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, $R_{free}$	0.142 , 0.183 0.143 , 0.185	Depositor DCC
$R_{free}$ test set	18693 reflections (2.29%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.8	Xtrriage
Anisotropy	0.494	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 72.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	62600	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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

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	0.26	0/4478	0.42	0/6098
1	a	0.24	0/4470	0.40	0/6087
2	B	0.37	0/4293	0.50	0/5851
2	b	0.33	0/4285	0.49	0/5841
3	C	0.29	0/4404	0.43	0/5997
3	c	0.28	0/4459	0.43	0/6071
4	D	0.33	0/3741	0.46	0/5095
4	d	0.30	0/3749	0.46	0/5106
5	E	0.35	0/681	0.53	0/928
5	e	0.31	0/690	0.49	0/939
6	F	0.32	0/284	0.45	0/387
6	f	0.29	0/269	0.43	0/365
7	H	0.33	0/519	0.50	0/708
7	h	0.30	0/530	0.49	0/722
8	I	0.31	0/311	0.44	0/419
8	i	0.35	0/311	0.51	0/419
9	J	0.34	0/278	0.41	0/376
9	j	0.28	0/283	0.42	0/383
10	K	0.32	0/303	0.48	0/416
10	k	0.32	0/303	0.46	0/416
11	L	0.38	0/318	0.47	0/433
11	l	0.38	0/318	0.45	0/433
12	M	0.40	0/261	0.51	0/357
12	m	0.36	0/279	0.48	0/380
13	O	0.35	0/1991	0.51	0/2698
13	o	0.34	0/1966	0.52	0/2665
14	T	0.36	0/310	0.43	0/419
14	t	0.33	0/301	0.43	0/406
15	U	0.37	0/811	0.54	0/1095
15	u	0.36	0/818	0.57	0/1105
16	V	0.35	0/1142	0.48	0/1545

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	v	0.31	0/1139	0.47	0/1542
17	X	0.25	0/292	0.38	0/395
17	x	0.28	0/284	0.39	0/384
18	Y	0.25	0/216	0.43	0/289
18	y	0.25	0/216	0.41	0/289
19	Z	0.24	0/490	0.39	0/669
19	z	0.23	0/490	0.42	0/669
20	R	0.25	0/279	0.35	0/383
All	All	0.31	0/50562	0.46	0/68780

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	4338	0	4142	23	0
1	a	4330	0	4132	39	0
2	B	4146	0	3983	32	0
2	b	4134	0	3976	41	0
3	C	4260	0	4123	24	0
3	c	4308	0	4172	36	0
4	D	3620	0	3484	33	0
4	d	3628	0	3490	22	0
5	E	662	0	648	12	0
5	e	670	0	655	5	0
6	F	275	0	282	3	0
6	f	261	0	269	4	0
7	H	506	0	529	2	0
7	h	517	0	541	7	0
8	I	314	0	328	5	0
8	i	314	0	328	2	0
9	J	272	0	279	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	277	0	284	2	0
10	K	293	0	305	3	0
10	k	293	0	305	6	0
11	L	311	0	320	3	0
11	l	311	0	320	5	0
12	M	268	0	285	7	0
12	m	286	0	305	8	0
13	O	1958	0	1920	23	0
13	o	1933	0	1900	13	0
14	T	311	0	318	3	0
14	t	302	0	311	6	0
15	U	800	0	796	4	0
15	u	807	0	805	4	0
16	V	1120	0	1122	3	0
16	v	1117	0	1131	11	0
17	X	289	0	322	3	0
17	x	281	0	312	2	0
18	Y	215	0	246	3	0
18	y	215	0	246	6	0
19	Z	479	0	516	7	0
19	z	479	0	516	5	0
20	R	273	0	305	4	0
21	A	2	0	0	0	0
21	a	2	0	0	0	0
22	A	4	0	0	0	0
22	a	4	0	0	0	0
23	A	455	0	504	18	0
23	B	1040	0	1152	26	0
23	C	845	0	936	30	0
23	D	195	0	216	9	0
23	a	325	0	360	22	0
23	b	1040	0	1152	29	0
23	c	845	0	936	45	0
23	d	325	0	360	15	0
24	A	40	0	56	1	0
24	B	120	0	168	5	0
24	C	80	0	112	1	0
24	D	40	0	56	1	0
24	H	40	0	56	1	0
24	K	40	0	56	1	0
24	T	40	0	56	5	0
24	Y	40	0	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	40	0	56	1	0
24	b	120	0	168	8	0
24	c	80	0	112	3	0
24	d	40	0	56	2	0
24	h	40	0	56	5	0
24	k	40	0	56	1	0
24	t	40	0	56	7	0
24	y	40	0	56	1	0
25	A	162	0	234	3	0
25	X	43	0	53	1	0
25	a	162	0	233	10	0
25	b	54	0	78	2	0
25	f	43	0	53	1	0
25	l	54	0	78	2	0
26	A	6	0	8	0	0
26	B	12	0	16	2	0
26	C	12	0	16	0	0
26	D	12	0	16	7	0
26	O	12	0	16	3	0
26	V	12	0	16	0	0
26	a	18	0	24	5	0
26	b	12	0	16	2	0
26	c	18	0	24	0	0
26	d	6	0	8	0	0
26	l	12	0	16	2	0
26	o	12	0	16	0	0
26	v	12	0	16	3	0
27	A	20	0	0	0	0
27	a	20	0	0	0	0
28	A	110	0	160	21	0
28	D	110	0	160	2	0
28	a	110	0	160	8	0
28	d	110	0	160	0	0
29	A	28	0	0	0	0
29	B	73	0	0	0	0
29	D	57	0	0	0	0
29	I	40	0	0	0	0
29	J	10	0	0	0	0
29	K	68	0	0	0	0
29	X	18	0	0	0	0
29	a	30	0	0	1	0
29	b	33	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	c	64	0	0	0	0
29	d	71	0	0	0	0
29	j	10	0	0	0	0
29	l	10	0	0	0	0
29	m	10	0	0	0	0
30	A	8	0	0	0	0
30	d	8	0	0	0	0
31	A	128	0	148	2	0
31	D	128	0	148	3	0
31	a	256	0	296	4	0
32	A	70	0	91	2	0
32	B	95	0	127	3	0
32	F	35	0	46	0	0
32	M	35	0	45	2	0
32	T	35	0	46	0	0
32	a	35	0	46	1	0
32	b	50	0	70	1	0
32	e	35	0	46	1	0
32	m	35	0	46	2	0
32	t	26	0	34	3	0
33	A	98	0	148	2	0
33	D	196	0	296	11	0
33	E	84	0	114	6	0
33	L	98	0	148	1	0
33	a	84	0	114	8	0
33	b	98	0	148	0	0
33	d	294	0	444	22	0
34	B	51	0	72	2	0
34	C	153	0	216	3	0
34	D	51	0	72	0	0
34	Z	37	0	44	3	0
34	c	153	0	216	3	0
34	d	51	0	72	3	0
34	m	51	0	72	0	0
34	z	39	0	48	2	0
35	B	38	0	52	2	0
35	C	19	0	26	0	0
35	D	16	0	17	0	0
35	V	11	0	10	0	0
35	b	57	0	78	3	0
35	c	19	0	26	1	0
35	d	16	0	17	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	o	19	0	26	1	0
36	C	310	0	410	6	0
36	H	62	0	82	1	0
36	c	310	0	410	10	0
36	h	62	0	82	2	0
37	C	1	0	0	0	0
37	F	1	0	0	0	0
37	O	1	0	0	0	0
37	c	2	0	0	0	0
37	f	1	0	0	0	0
37	o	1	0	0	0	0
38	F	43	0	30	1	0
38	f	43	0	30	0	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	V	43	0	30	0	0
40	v	43	0	30	0	0
41	A	215	0	0	1	0
41	B	193	0	0	2	0
41	C	202	0	0	1	0
41	D	162	0	0	4	0
41	E	15	0	0	0	0
41	F	6	0	0	0	0
41	H	23	0	0	0	0
41	I	6	0	0	0	0
41	J	7	0	0	1	0
41	K	6	0	0	0	0
41	L	8	0	0	0	0
41	M	5	0	0	0	0
41	O	106	0	0	0	0
41	T	13	0	0	0	0
41	U	49	0	0	0	0
41	V	82	0	0	0	0
41	X	8	0	0	0	0
41	a	207	0	0	3	0
41	b	209	0	0	0	0
41	c	192	0	0	3	0
41	d	152	0	0	0	0
41	e	9	0	0	0	0
41	f	3	0	0	0	0
41	h	18	0	0	0	0
41	i	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	j	1	0	0	0	0
41	k	3	0	0	0	0
41	l	8	0	0	0	0
41	m	12	0	0	0	0
41	o	99	0	0	0	0
41	t	11	0	0	1	0
41	u	51	0	0	1	0
41	v	61	0	0	0	0
41	x	6	0	0	0	0
41	y	2	0	0	0	0
All	All	62600	0	61445	629	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 629 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:B:604:CLA:H42	23:B:605:CLA:H2	1.44	0.95
1:a:250[A]:ALA:HA	2:b:491[A]:VAL:HG11	1.51	0.93
1:a:250[B]:ALA:HA	2:b:491[B]:VAL:HG11	1.53	0.91
26:D:402:GOL:H11	12:M:1:FME:HG2	1.57	0.86
23:d:402[B]:CLA:HHC	23:d:402[B]:CLA:HBB1	1.64	0.80

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	553/344 (161%)	542 (98%)	9 (2%)	2 (0%)	30	39
1	a	552/344 (160%)	541 (98%)	9 (2%)	2 (0%)	30	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	522/505 (103%)	515 (99%)	7 (1%)	0	100	100
2	b	521/505 (103%)	510 (98%)	11 (2%)	0	100	100
3	C	546/455 (120%)	536 (98%)	9 (2%)	1 (0%)	44	55
3	c	553/455 (122%)	539 (98%)	13 (2%)	1 (0%)	44	55
4	D	453/342 (132%)	435 (96%)	18 (4%)	0	100	100
4	d	454/342 (133%)	439 (97%)	15 (3%)	0	100	100
5	E	79/84 (94%)	78 (99%)	1 (1%)	0	100	100
5	e	79/84 (94%)	79 (100%)	0	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
7	h	63/65 (97%)	59 (94%)	3 (5%)	1 (2%)	8	7
8	I	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	4	3
8	i	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	37 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	34/36 (94%)	34 (100%)	0	0	100	100
13	O	251/244 (103%)	242 (96%)	7 (3%)	2 (1%)	16	20
13	o	249/244 (102%)	243 (98%)	6 (2%)	0	100	100
14	T	33/32 (103%)	33 (100%)	0	0	100	100
14	t	32/32 (100%)	32 (100%)	0	0	100	100
15	U	97/104 (93%)	92 (95%)	5 (5%)	0	100	100
15	u	98/104 (94%)	93 (95%)	5 (5%)	0	100	100
16	V	140/137 (102%)	136 (97%)	4 (3%)	0	100	100
16	v	140/137 (102%)	134 (96%)	6 (4%)	0	100	100
17	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	x	36/40 (90%)	36 (100%)	0	0	100	100
18	Y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
18	y	27/30 (90%)	27 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	7
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	7	7
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	6171/5384 (115%)	6019 (98%)	140 (2%)	12 (0%)	44	55

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
8	I	36	ASP
13	O	26	ALA
3	c	416	SER
19	Z	31	GLN

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	444/279 (159%)	440 (99%)	4 (1%)	75	87
1	a	443/279 (159%)	441 (100%)	2 (0%)	86	93
2	B	421/403 (104%)	415 (99%)	6 (1%)	62	77
2	b	420/403 (104%)	408 (97%)	12 (3%)	37	54
3	C	430/356 (121%)	422 (98%)	8 (2%)	52	69
3	c	436/356 (122%)	426 (98%)	10 (2%)	45	63
4	D	368/277 (133%)	365 (99%)	3 (1%)	79	89
4	d	369/277 (133%)	362 (98%)	7 (2%)	52	69
5	E	72/73 (99%)	71 (99%)	1 (1%)	62	77
5	e	72/73 (99%)	71 (99%)	1 (1%)	62	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	26/38 (68%)	26 (100%)	0	100	100
7	H	54/54 (100%)	52 (96%)	2 (4%)	29	43
7	h	55/54 (102%)	53 (96%)	2 (4%)	30	44
8	I	34/34 (100%)	32 (94%)	2 (6%)	16	23
8	i	34/34 (100%)	33 (97%)	1 (3%)	37	54
9	J	26/27 (96%)	24 (92%)	2 (8%)	10	14
9	j	26/27 (96%)	25 (96%)	1 (4%)	28	42
10	K	30/30 (100%)	26 (87%)	4 (13%)	3	3
10	k	30/30 (100%)	27 (90%)	3 (10%)	6	8
11	L	36/35 (103%)	36 (100%)	0	100	100
11	l	36/35 (103%)	35 (97%)	1 (3%)	38	55
12	M	30/32 (94%)	27 (90%)	3 (10%)	6	8
12	m	32/32 (100%)	30 (94%)	2 (6%)	15	21
13	O	216/207 (104%)	211 (98%)	5 (2%)	45	63
13	o	213/207 (103%)	206 (97%)	7 (3%)	33	48
14	T	32/28 (114%)	28 (88%)	4 (12%)	3	4
14	t	31/28 (111%)	31 (100%)	0	100	100
15	U	86/89 (97%)	84 (98%)	2 (2%)	45	63
15	u	87/89 (98%)	85 (98%)	2 (2%)	45	63
16	V	123/117 (105%)	122 (99%)	1 (1%)	79	89
16	v	123/117 (105%)	119 (97%)	4 (3%)	33	48
17	X	32/33 (97%)	32 (100%)	0	100	100
17	x	31/33 (94%)	31 (100%)	0	100	100
18	Y	22/23 (96%)	21 (96%)	1 (4%)	23	34
18	y	22/23 (96%)	19 (86%)	3 (14%)	3	3
19	Z	52/52 (100%)	50 (96%)	2 (4%)	28	42
19	z	52/52 (100%)	44 (85%)	8 (15%)	2	2
20	R	29/29 (100%)	27 (93%)	2 (7%)	13	18
All	All	5103/4403 (116%)	4985 (98%)	118 (2%)	44	63

5 of 118 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	362	PHE
19	z	2	THR
3	c	416	SER
20	R	29	LYS
16	v	15	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
3	c	201	ASN
10	k	40	GLN
16	v	86	GLN
11	l	8	GLN
1	a	75	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	0.68	0	8,9,11	1.19	1 (12%)
8	FME	I	1	8	8,9,10	0.66	0	8,9,11	1.21	1 (12%)
14	FME	t	1	14	8,9,10	0.79	0	8,9,11	1.26	1 (12%)
12	FME	m	1	12	8,9,10	0.55	0	8,9,11	1.38	1 (12%)
12	FME	M	1	12	8,9,10	0.57	0	8,9,11	1.29	1 (12%)
14	FME	T	1	14	8,9,10	0.60	0	8,9,11	1.76	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. '-' means no outliers of that kind were identified.

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

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	CB-CA-N	-2.74	105.53	110.52
14	t	1	FME	O-C-CA	-2.41	118.58	124.77
12	m	1	FME	O1-CN-N	-2.40	119.12	125.32
14	T	1	FME	CA-N-CN	2.35	126.44	122.82
8	I	1	FME	O-C-CA	-2.23	119.03	124.77

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	m	1	FME	2	0
12	M	1	FME	3	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 274 ligands modelled in this entry, 21 are monoatomic and 20 are unknown - leaving 233 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
28	PL9	a	413[A]	-	55,55,55	0.68	2 (3%)	68,69,69	2.03	23 (33%)
23	CLA	B	611	-	63,73,73	2.64	17 (26%)	74,113,113	2.96	27 (36%)
23	CLA	A	406[A]	41	63,73,73	1.98	16 (25%)	74,113,113	2.67	30 (40%)
23	CLA	C	505	41	63,73,73	2.05	17 (26%)	74,113,113	2.73	30 (40%)
23	CLA	d	403[A]	-	63,73,73	1.99	16 (25%)	74,113,113	2.65	29 (39%)
26	GOL	l	103[A]	-	5,5,5	0.98	0	5,5,5	1.05	1 (20%)
23	CLA	B	614	-	63,73,73	2.00	15 (23%)	74,113,113	2.88	30 (40%)
24	BCR	c	516	-	41,41,41	1.03	1 (2%)	56,56,56	1.39	9 (16%)
25	SQD	b	620	-	52,54,54	1.00	2 (3%)	62,65,65	1.68	10 (16%)
24	BCR	B	617	-	41,41,41	1.06	1 (2%)	56,56,56	1.46	8 (14%)
26	GOL	c	526[B]	-	5,5,5	1.01	0	5,5,5	1.06	0
26	GOL	o	303	-	5,5,5	1.22	0	5,5,5	1.04	0
28	PL9	D	406[A]	-	55,55,55	0.65	1 (1%)	68,69,69	1.61	17 (25%)
32	LMT	a	416	-	36,36,36	0.98	2 (5%)	47,47,47	1.06	2 (4%)
23	CLA	b	614	-	63,73,73	2.02	16 (25%)	74,113,113	2.81	28 (37%)
35	HTG	o	301	-	19,19,19	1.04	2 (10%)	23,24,24	1.50	4 (17%)
32	LMT	t	101	-	26,26,36	0.91	2 (7%)	31,31,47	1.31	3 (9%)
35	HTG	b	623	-	19,19,19	0.96	1 (5%)	23,24,24	1.72	3 (13%)
23	CLA	D	404	-	63,73,73	2.12	16 (25%)	74,113,113	2.74	31 (41%)
23	CLA	c	514	-	63,73,73	2.14	17 (26%)	74,113,113	2.69	28 (37%)
23	CLA	D	403[B]	-	63,73,73	2.08	16 (25%)	74,113,113	2.79	28 (37%)
23	CLA	b	615	-	63,73,73	2.04	14 (22%)	74,113,113	2.67	28 (37%)
38	HEM	F	102	6,5	42,50,50	1.27	5 (11%)	46,82,82	1.99	14 (30%)
36	DGD	c	517[B]	-	63,63,67	0.87	2 (3%)	77,77,81	1.08	5 (6%)
23	CLA	B	616	-	63,73,73	2.14	17 (26%)	74,113,113	2.80	26 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	LHG	E	101[B]	-	41,41,48	1.06	2 (4%)	44,47,54	1.12	4 (9%)
25	SQD	a	411	-	52,54,54	1.02	2 (3%)	62,65,65	1.21	8 (12%)
25	SQD	a	409[B]	-	52,54,54	0.91	2 (3%)	62,65,65	1.58	11 (17%)
24	BCR	y	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.71	12 (21%)
31	PHO	a	415[B]	-	50,69,69	1.99	8 (16%)	48,99,99	2.00	11 (22%)
23	CLA	b	603	-	63,73,73	2.09	16 (25%)	74,113,113	2.75	30 (40%)
23	CLA	B	604	-	63,73,73	2.03	18 (28%)	74,113,113	2.55	30 (40%)
23	CLA	B	607	41	63,73,73	2.03	17 (26%)	74,113,113	2.82	29 (39%)
23	CLA	D	403[A]	-	63,73,73	2.08	16 (25%)	74,113,113	2.77	32 (43%)
23	CLA	B	613	-	63,73,73	1.97	15 (23%)	74,113,113	2.75	28 (37%)
34	LMG	z	101	-	39,39,55	1.11	2 (5%)	47,47,63	1.07	2 (4%)
23	CLA	C	514	-	63,73,73	2.09	16 (25%)	74,113,113	2.67	27 (36%)
23	CLA	b	607	41	63,73,73	2.03	17 (26%)	74,113,113	2.65	29 (39%)
26	GOL	D	402	-	5,5,5	1.42	2 (40%)	5,5,5	0.88	0
35	HTG	D	411	-	16,16,19	0.95	1 (6%)	20,21,24	1.31	1 (5%)
33	LHG	E	101[A]	-	41,41,48	1.08	2 (4%)	44,47,54	1.12	3 (6%)
36	DGD	C	517[B]	-	63,63,67	0.83	2 (3%)	77,77,81	1.11	5 (6%)
25	SQD	a	409[A]	-	52,54,54	0.89	2 (3%)	62,65,65	1.80	11 (17%)
35	HTG	d	411	-	16,16,19	0.87	1 (6%)	20,21,24	1.41	1 (5%)
24	BCR	k	101	-	41,41,41	1.08	1 (2%)	56,56,56	1.53	11 (19%)
23	CLA	B	609	-	63,73,73	2.06	15 (23%)	74,113,113	2.62	28 (37%)
23	CLA	c	510	-	63,73,73	2.04	15 (23%)	74,113,113	2.79	29 (39%)
25	SQD	A	409[B]	-	52,54,54	0.87	2 (3%)	62,65,65	1.69	11 (17%)
26	GOL	C	523[A]	-	5,5,5	1.16	0	5,5,5	0.94	0
23	CLA	C	512	3	63,73,73	2.11	18 (28%)	74,113,113	2.58	27 (36%)
23	CLA	c	505	41	63,73,73	2.14	16 (25%)	74,113,113	2.68	30 (40%)
23	CLA	B	602	-	63,73,73	2.08	16 (25%)	74,113,113	2.74	28 (37%)
36	DGD	C	517[A]	-	63,63,67	0.84	2 (3%)	77,77,81	1.20	6 (7%)
23	CLA	b	601	41	63,73,73	2.16	15 (23%)	74,113,113	2.70	28 (37%)
26	GOL	A	410	-	5,5,5	1.14	0	5,5,5	0.86	0
32	LMT	B	629	-	25,25,36	0.89	1 (4%)	30,30,47	1.21	3 (10%)
25	SQD	A	409[A]	-	52,54,54	0.86	2 (3%)	62,65,65	1.85	10 (16%)
24	BCR	b	618	-	41,41,41	1.02	1 (2%)	56,56,56	1.26	6 (10%)
28	PL9	D	406[B]	-	55,55,55	0.67	2 (3%)	68,69,69	1.65	17 (25%)
33	LHG	b	629[A]	-	48,48,48	0.84	3 (6%)	51,54,54	1.05	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	BCR	H	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.44	8 (14%)
24	BCR	K	102	-	41,41,41	1.09	1 (2%)	56,56,56	1.48	11 (19%)
24	BCR	b	617	-	41,41,41	1.05	1 (2%)	56,56,56	1.44	9 (16%)
25	SQD	f	102	-	41,43,54	1.15	2 (4%)	51,54,65	1.59	10 (19%)
23	CLA	C	506	-	63,73,73	2.02	16 (25%)	74,113,113	2.74	29 (39%)
35	HTG	B	623	-	19,19,19	0.97	2 (10%)	23,24,24	1.28	3 (13%)
23	CLA	c	504	-	63,73,73	2.04	17 (26%)	74,113,113	2.71	27 (36%)
24	BCR	D	405	-	41,41,41	1.12	1 (2%)	56,56,56	1.81	15 (26%)
23	CLA	c	507	-	63,73,73	2.07	16 (25%)	74,113,113	2.67	29 (39%)
35	HTG	V	202	-	11,11,19	0.31	0	15,15,24	1.25	1 (6%)
23	CLA	A	407	-	63,73,73	2.02	17 (26%)	74,113,113	2.78	32 (43%)
23	CLA	a	407	-	63,73,73	2.02	15 (23%)	74,113,113	2.83	29 (39%)
23	CLA	B	615	-	63,73,73	2.08	16 (25%)	74,113,113	2.80	30 (40%)
35	HTG	c	522	-	19,19,19	0.86	1 (5%)	23,24,24	1.40	1 (4%)
23	CLA	b	602	-	63,73,73	2.07	16 (25%)	74,113,113	2.87	34 (45%)
23	CLA	B	603	-	63,73,73	2.05	15 (23%)	74,113,113	2.85	29 (39%)
26	GOL	a	418	-	5,5,5	1.33	1 (20%)	5,5,5	1.03	0
26	GOL	B	622	-	5,5,5	0.88	0	5,5,5	1.24	1 (20%)
23	CLA	A	404[A]	-	63,73,73	2.06	15 (23%)	74,113,113	2.77	30 (40%)
23	CLA	d	402[B]	41	63,73,73	2.12	15 (23%)	74,113,113	2.69	28 (37%)
23	CLA	B	612	-	63,73,73	2.09	17 (26%)	74,113,113	2.72	29 (39%)
23	CLA	b	605	-	63,73,73	1.98	17 (26%)	74,113,113	2.80	27 (36%)
26	GOL	o	304	-	5,5,5	1.07	1 (20%)	5,5,5	1.16	0
26	GOL	b	624	-	5,5,5	1.25	1 (20%)	5,5,5	0.88	0
34	LMG	C	520	-	51,51,55	0.95	2 (3%)	59,59,63	1.13	4 (6%)
26	GOL	C	523[B]	-	5,5,5	1.29	0	5,5,5	0.83	0
32	LMT	A	419	-	36,36,36	1.02	2 (5%)	47,47,47	1.20	4 (8%)
23	CLA	b	612	-	63,73,73	2.06	16 (25%)	74,113,113	2.67	28 (37%)
24	BCR	T	102	-	41,41,41	1.06	1 (2%)	56,56,56	1.61	14 (25%)
26	GOL	v	202[B]	-	5,5,5	1.16	0	5,5,5	0.86	0
27	OEX	A	412[A]	1,3,41	0,15,15	-	-	-	-	-
23	CLA	C	503	-	63,73,73	2.13	16 (25%)	74,113,113	2.55	27 (36%)
24	BCR	d	405	-	41,41,41	1.17	2 (4%)	56,56,56	1.99	17 (30%)
35	HTG	B	621	-	19,19,19	0.78	1 (5%)	23,24,24	1.21	1 (4%)
23	CLA	c	509	-	63,73,73	2.22	16 (25%)	74,113,113	2.58	25 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	d	402[A]	41	63,73,73	2.02	14 (22%)	74,113,113	2.71	28 (37%)
32	LMT	b	627	-	25,25,36	0.88	0	30,30,47	1.07	2 (6%)
30	BCT	A	415[B]	21	3,3,3	0.54	0	2,3,3	0.83	0
24	BCR	A	408	-	41,41,41	1.04	1 (2%)	56,56,56	1.41	8 (14%)
23	CLA	b	609	-	63,73,73	2.08	15 (23%)	74,113,113	2.69	29 (39%)
33	LHG	A	418[B]	-	48,48,48	0.89	2 (4%)	51,54,54	1.16	5 (9%)
24	BCR	c	515	-	41,41,41	1.03	1 (2%)	56,56,56	1.62	11 (19%)
26	GOL	v	202[A]	-	5,5,5	1.26	0	5,5,5	0.88	0
23	CLA	B	610	41	63,73,73	2.05	16 (25%)	74,113,113	2.77	28 (37%)
33	LHG	b	629[B]	-	48,48,48	0.90	2 (4%)	51,54,54	1.05	3 (5%)
34	LMG	c	521	-	51,51,55	1.02	2 (3%)	59,59,63	1.36	7 (11%)
25	SQD	A	411	-	52,54,54	1.00	2 (3%)	62,65,65	1.21	7 (11%)
23	CLA	a	404[B]	-	63,73,73	2.12	16 (25%)	74,113,113	2.72	29 (39%)
26	GOL	V	203[B]	-	5,5,5	1.13	0	5,5,5	0.99	0
23	CLA	B	606	-	63,73,73	1.99	16 (25%)	74,113,113	2.91	29 (39%)
33	LHG	d	407[B]	-	48,48,48	0.88	2 (4%)	51,54,54	1.14	5 (9%)
24	BCR	a	408	-	41,41,41	1.05	1 (2%)	56,56,56	1.42	9 (16%)
25	SQD	X	101	-	41,43,54	1.17	3 (7%)	51,54,65	2.13	13 (25%)
34	LMG	d	412	39	51,51,55	0.90	2 (3%)	59,59,63	1.12	5 (8%)
30	BCT	A	415[A]	21	3,3,3	0.55	0	2,3,3	1.29	0
26	GOL	B	625	-	5,5,5	1.02	0	5,5,5	1.18	1 (20%)
23	CLA	c	511	-	63,73,73	2.12	16 (25%)	74,113,113	2.77	31 (41%)
32	LMT	B	626	-	36,36,36	1.18	4 (11%)	47,47,47	1.40	5 (10%)
24	BCR	B	618	-	41,41,41	1.00	2 (4%)	56,56,56	1.35	7 (12%)
33	LHG	A	418[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.29	6 (11%)
36	DGD	H	102	-	63,63,67	0.86	4 (6%)	77,77,81	1.07	7 (9%)
27	OEX	a	412[B]	1,3,41	0,15,15	-	-	-	-	-
23	CLA	a	404[A]	-	63,73,73	2.05	16 (25%)	74,113,113	2.79	32 (43%)
35	HTG	C	522	-	19,19,19	0.79	1 (5%)	23,24,24	1.22	2 (8%)
23	CLA	b	608	-	63,73,73	2.11	15 (23%)	74,113,113	2.69	29 (39%)
26	GOL	V	203[A]	-	5,5,5	1.41	1 (20%)	5,5,5	0.86	0
40	HEC	v	201	16	32,50,50	1.96	4 (12%)	30,82,82	2.51	9 (30%)
33	LHG	d	407[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.06	4 (7%)
23	CLA	C	504	-	63,73,73	2.01	16 (25%)	74,113,113	2.73	26 (35%)
33	LHG	d	414[B]	-	48,48,48	0.92	2 (4%)	51,54,54	1.09	4 (7%)
40	HEC	V	201	16	32,50,50	1.93	3 (9%)	30,82,82	2.61	9 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	LMT	M	101	-	36,36,36	1.09	2 (5%)	47,47,47	1.27	6 (12%)
23	CLA	A	404[B]	-	63,73,73	2.13	15 (23%)	74,113,113	2.72	31 (41%)
23	CLA	B	601	41	63,73,73	2.11	17 (26%)	74,113,113	2.70	26 (35%)
35	HTG	b	625	-	19,19,19	0.98	2 (10%)	23,24,24	1.49	3 (13%)
27	OEX	a	412[A]	1,3,41	0,15,15	-	-	-	-	-
32	LMT	A	417	-	36,36,36	0.91	0	47,47,47	1.07	2 (4%)
24	BCR	B	619	-	41,41,41	1.08	2 (4%)	56,56,56	1.47	11 (19%)
33	LHG	a	419[B]	-	41,41,48	1.04	2 (4%)	44,47,54	0.95	2 (4%)
23	CLA	C	502	-	63,73,73	2.00	16 (25%)	74,113,113	2.77	30 (40%)
36	DGD	h	102	-	63,63,67	0.86	4 (6%)	77,77,81	1.14	6 (7%)
23	CLA	c	503	-	63,73,73	2.13	16 (25%)	74,113,113	2.53	24 (32%)
23	CLA	c	506	-	63,73,73	2.07	17 (26%)	74,113,113	2.64	26 (35%)
33	LHG	d	414[A]	-	48,48,48	0.89	3 (6%)	51,54,54	1.13	4 (7%)
23	CLA	b	606	-	63,73,73	2.04	15 (23%)	74,113,113	2.70	27 (36%)
27	OEX	A	412[B]	1,3,41	0,15,15	-	-	-	-	-
23	CLA	c	513	-	63,73,73	2.08	15 (23%)	74,113,113	2.69	28 (37%)
23	CLA	C	507	-	63,73,73	2.02	17 (26%)	74,113,113	2.74	29 (39%)
23	CLA	c	512	3	63,73,73	2.17	16 (25%)	74,113,113	2.71	29 (39%)
32	LMT	b	621	-	25,25,36	0.95	1 (4%)	30,30,47	1.20	3 (10%)
36	DGD	C	519	-	63,63,67	0.86	3 (4%)	77,77,81	1.00	3 (3%)
36	DGD	c	518[A]	-	63,63,67	0.85	3 (4%)	77,77,81	0.98	4 (5%)
33	LHG	a	419[A]	-	41,41,48	1.06	2 (4%)	44,47,54	0.93	2 (4%)
28	PL9	A	413[B]	-	55,55,55	0.66	2 (3%)	68,69,69	1.97	25 (36%)
31	PHO	a	406[B]	-	50,69,69	1.90	7 (14%)	48,99,99	1.97	11 (22%)
31	PHO	D	401[B]	-	50,69,69	1.88	8 (16%)	48,99,99	1.98	9 (18%)
36	DGD	C	518[B]	-	63,63,67	0.86	2 (3%)	77,77,81	1.04	5 (6%)
32	LMT	B	627	-	36,36,36	1.00	3 (8%)	47,47,47	1.17	4 (8%)
34	LMG	c	501	-	51,51,55	0.92	2 (3%)	59,59,63	1.21	4 (6%)
23	CLA	c	508	41	63,73,73	2.06	15 (23%)	74,113,113	2.76	27 (36%)
26	GOL	D	413	-	5,5,5	1.59	2 (40%)	5,5,5	0.95	0
34	LMG	Z	101	-	37,37,55	1.02	3 (8%)	45,45,63	1.46	5 (11%)
33	LHG	d	408[B]	-	48,48,48	0.91	2 (4%)	51,54,54	1.12	5 (9%)
33	LHG	D	407[A]	-	48,48,48	0.88	3 (6%)	51,54,54	1.02	3 (5%)
26	GOL	c	527	-	5,5,5	1.21	1 (20%)	5,5,5	1.05	0
23	CLA	a	405[B]	41	63,73,73	2.07	15 (23%)	74,113,113	2.71	29 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	GOL	d	413	-	5,5,5	1.01	0	5,5,5	1.15	0
24	BCR	b	619	-	41,41,41	1.11	2 (4%)	56,56,56	1.34	8 (14%)
34	LMG	m	101	-	51,51,55	0.90	2 (3%)	59,59,63	1.29	6 (10%)
23	CLA	b	610	41	63,73,73	2.10	16 (25%)	74,113,113	2.84	29 (39%)
28	PL9	A	413[A]	-	55,55,55	0.71	3 (5%)	68,69,69	2.05	25 (36%)
31	PHO	a	406[A]	-	50,69,69	1.89	8 (16%)	48,99,99	2.00	9 (18%)
34	LMG	C	521	-	51,51,55	1.08	3 (5%)	59,59,63	1.42	8 (13%)
31	PHO	D	401[A]	-	50,69,69	1.82	8 (16%)	48,99,99	1.79	10 (20%)
36	DGD	C	518[A]	-	63,63,67	0.91	3 (4%)	77,77,81	1.04	5 (6%)
23	CLA	c	502	-	63,73,73	2.07	17 (26%)	74,113,113	2.75	28 (37%)
28	PL9	d	406[B]	-	55,55,55	0.66	1 (1%)	68,69,69	1.69	17 (25%)
33	LHG	d	408[A]	-	48,48,48	0.92	2 (4%)	51,54,54	1.02	3 (5%)
26	GOL	a	417	-	5,5,5	1.39	1 (20%)	5,5,5	1.13	1 (20%)
34	LMG	B	620	-	51,51,55	0.93	2 (3%)	59,59,63	1.29	4 (6%)
24	BCR	h	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.45	13 (23%)
23	CLA	a	405[A]	41	63,73,73	2.01	16 (25%)	74,113,113	2.67	28 (37%)
33	LHG	L	101[B]	-	48,48,48	0.93	3 (6%)	51,54,54	1.09	4 (7%)
32	LMT	T	101	-	36,36,36	1.05	3 (8%)	47,47,47	1.08	2 (4%)
25	SQD	l	101	-	52,54,54	1.03	3 (5%)	62,65,65	1.77	12 (19%)
26	GOL	b	628	-	5,5,5	0.57	0	5,5,5	1.48	1 (20%)
23	CLA	b	611	-	63,73,73	2.04	16 (25%)	74,113,113	2.73	30 (40%)
30	BCT	d	401[B]	21	3,3,3	0.51	0	2,3,3	1.18	0
24	BCR	C	516	-	41,41,41	1.05	1 (2%)	56,56,56	1.36	10 (17%)
31	PHO	A	416[B]	-	50,69,69	1.97	8 (16%)	48,99,99	2.02	12 (25%)
23	CLA	A	405[B]	41	63,73,73	2.07	16 (25%)	74,113,113	2.62	31 (41%)
23	CLA	b	616	-	63,73,73	2.02	15 (23%)	74,113,113	2.79	30 (40%)
33	LHG	D	408[B]	-	48,48,48	0.91	2 (4%)	51,54,54	1.10	3 (5%)
23	CLA	C	511	-	63,73,73	2.10	16 (25%)	74,113,113	2.76	28 (37%)
28	PL9	d	406[A]	-	55,55,55	0.72	1 (1%)	68,69,69	1.61	17 (25%)
34	LMG	c	520	-	51,51,55	0.90	2 (3%)	59,59,63	1.21	6 (10%)
26	GOL	c	526[A]	-	5,5,5	1.04	0	5,5,5	1.05	0
33	LHG	L	101[A]	-	48,48,48	0.89	3 (6%)	51,54,54	1.16	4 (7%)
26	GOL	a	410	-	5,5,5	0.97	0	5,5,5	1.04	0
34	LMG	D	412	39	51,51,55	0.81	3 (5%)	59,59,63	1.06	3 (5%)
36	DGD	c	518[B]	-	63,63,67	0.87	2 (3%)	77,77,81	1.01	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	PHO	A	416[A]	-	50,69,69	2.00	8 (16%)	48,99,99	1.97	10 (20%)
30	BCT	d	401[A]	21	3,3,3	0.49	0	2,3,3	1.49	0
23	CLA	b	613	-	63,73,73	2.07	16 (25%)	74,113,113	2.73	30 (40%)
23	CLA	A	405[A]	41	63,73,73	2.02	15 (23%)	74,113,113	2.70	31 (41%)
36	DGD	c	517[A]	-	63,63,67	0.86	2 (3%)	77,77,81	1.10	8 (10%)
33	LHG	D	408[A]	-	48,48,48	0.94	2 (4%)	51,54,54	1.04	4 (7%)
26	GOL	O	303	-	5,5,5	1.17	1 (20%)	5,5,5	1.18	1 (20%)
23	CLA	C	508	41	63,73,73	2.02	17 (26%)	74,113,113	2.60	25 (33%)
24	BCR	t	102	-	41,41,41	1.08	1 (2%)	56,56,56	1.63	12 (21%)
23	CLA	B	608	-	63,73,73	1.99	15 (23%)	74,113,113	2.72	34 (45%)
24	BCR	Y	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.77	15 (26%)
31	PHO	a	415[A]	-	50,69,69	1.95	8 (16%)	48,99,99	2.11	12 (25%)
23	CLA	B	605	-	63,73,73	2.06	16 (25%)	74,113,113	2.92	31 (41%)
33	LHG	D	407[B]	-	48,48,48	0.88	2 (4%)	51,54,54	1.07	4 (7%)
34	LMG	C	501	-	51,51,55	0.92	2 (3%)	59,59,63	1.53	8 (13%)
32	LMT	m	103	-	36,36,36	1.03	3 (8%)	47,47,47	1.09	3 (6%)
28	PL9	a	413[B]	-	55,55,55	0.66	2 (3%)	68,69,69	1.95	20 (29%)
26	GOL	O	302	-	5,5,5	0.98	0	5,5,5	0.97	0
35	HTG	b	622	-	19,19,19	1.12	2 (10%)	23,24,24	1.89	7 (30%)
23	CLA	C	509	-	63,73,73	2.17	17 (26%)	74,113,113	2.65	26 (35%)
23	CLA	A	406[B]	41	63,73,73	2.10	17 (26%)	74,113,113	2.67	28 (37%)
23	CLA	C	513	-	63,73,73	2.08	15 (23%)	74,113,113	2.74	30 (40%)
32	LMT	e	101	-	36,36,36	1.00	1 (2%)	47,47,47	0.99	1 (2%)
36	DGD	c	519	-	63,63,67	0.86	4 (6%)	77,77,81	1.09	5 (6%)
23	CLA	C	510	-	63,73,73	2.13	16 (25%)	74,113,113	2.72	27 (36%)
38	HEM	f	101	6,5	42,50,50	1.29	5 (11%)	46,82,82	1.80	11 (23%)
23	CLA	d	404	-	63,73,73	2.08	17 (26%)	74,113,113	2.72	30 (40%)
23	CLA	d	403[B]	-	63,73,73	2.08	14 (22%)	74,113,113	2.64	26 (35%)
32	LMT	F	101	-	36,36,36	1.03	1 (2%)	47,47,47	1.01	1 (2%)
24	BCR	C	515	-	41,41,41	1.08	1 (2%)	56,56,56	1.43	7 (12%)
26	GOL	l	103[B]	-	5,5,5	0.89	0	5,5,5	1.15	0
23	CLA	b	604	-	63,73,73	2.09	16 (25%)	74,113,113	2.67	28 (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.

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PL9	a	413[A]	-	-	14/53/73/73	0/1/1/1
23	CLA	B	611	-	1/1/15/20	3/37/115/115	-
23	CLA	A	406[A]	41	-	5/37/115/115	-
23	CLA	C	505	41	1/1/15/20	7/37/115/115	-
23	CLA	d	403[A]	-	1/1/15/20	4/37/115/115	-
26	GOL	l	103[A]	-	-	2/4/4/4	-
23	CLA	B	614	-	1/1/15/20	13/37/115/115	-
24	BCR	c	516	-	-	2/29/63/63	0/2/2/2
25	SQD	b	620	-	-	18/49/69/69	0/1/1/1
24	BCR	B	617	-	-	2/29/63/63	0/2/2/2
26	GOL	c	526[B]	-	-	0/4/4/4	-
26	GOL	o	303	-	-	2/4/4/4	-
28	PL9	D	406[A]	-	-	6/53/73/73	0/1/1/1
32	LMT	a	416	-	-	10/21/61/61	0/2/2/2
23	CLA	b	614	-	1/1/15/20	11/37/115/115	-
35	HTG	o	301	-	-	4/10/30/30	0/1/1/1
32	LMT	t	101	-	-	10/17/38/61	0/1/1/2
35	HTG	b	623	-	-	4/10/30/30	0/1/1/1
23	CLA	D	404	-	1/1/15/20	14/37/115/115	-
23	CLA	D	403[B]	-	1/1/15/20	0/37/115/115	-
23	CLA	b	615	-	1/1/15/20	8/37/115/115	-
23	CLA	c	514	-	-	9/37/115/115	-
38	HEM	F	102	6,5	-	3/12/54/54	-
36	DGD	c	517[B]	-	-	19/51/91/95	0/2/2/2
23	CLA	B	616	-	1/1/15/20	7/37/115/115	-
33	LHG	E	101[B]	-	-	19/46/46/53	-
25	SQD	a	411	-	-	16/49/69/69	0/1/1/1
25	SQD	a	409[B]	-	-	9/49/69/69	0/1/1/1
24	BCR	y	101	-	-	3/29/63/63	0/2/2/2
31	PHO	a	415[B]	-	-	4/37/103/103	0/5/6/6
23	CLA	b	603	-	1/1/15/20	2/37/115/115	-
23	CLA	B	604	-	1/1/15/20	1/37/115/115	-
23	CLA	B	607	41	1/1/15/20	3/37/115/115	-
23	CLA	D	403[A]	-	1/1/15/20	0/37/115/115	-
23	CLA	B	613	-	1/1/15/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMG	z	101	-	-	9/34/54/70	0/1/1/1
23	CLA	C	514	-	1/1/15/20	6/37/115/115	-
23	CLA	b	607	41	1/1/15/20	5/37/115/115	-
26	GOL	D	402	-	-	2/4/4/4	-
35	HTG	D	411	-	-	3/7/27/30	0/1/1/1
33	LHG	E	101[A]	-	-	21/46/46/53	-
36	DGD	C	517[B]	-	-	15/51/91/95	0/2/2/2
25	SQD	a	409[A]	-	-	9/49/69/69	0/1/1/1
35	HTG	d	411	-	-	1/7/27/30	0/1/1/1
24	BCR	k	101	-	-	0/29/63/63	0/2/2/2
23	CLA	B	609	-	1/1/15/20	0/37/115/115	-
23	CLA	c	510	-	1/1/15/20	16/37/115/115	-
25	SQD	A	409[B]	-	-	10/49/69/69	0/1/1/1
26	GOL	C	523[A]	-	-	0/4/4/4	-
23	CLA	C	512	3	1/1/15/20	5/37/115/115	-
23	CLA	c	505	41	1/1/15/20	5/37/115/115	-
23	CLA	B	602	-	1/1/15/20	8/37/115/115	-
36	DGD	C	517[A]	-	-	15/51/91/95	0/2/2/2
23	CLA	b	601	41	1/1/15/20	18/37/115/115	-
26	GOL	A	410	-	-	2/4/4/4	-
32	LMT	B	629	-	-	11/17/37/61	0/1/1/2
25	SQD	A	409[A]	-	-	12/49/69/69	0/1/1/1
24	BCR	b	618	-	-	0/29/63/63	0/2/2/2
28	PL9	D	406[B]	-	-	7/53/73/73	0/1/1/1
33	LHG	b	629[A]	-	-	15/53/53/53	-
24	BCR	H	101	-	-	3/29/63/63	0/2/2/2
24	BCR	K	102	-	-	2/29/63/63	0/2/2/2
24	BCR	b	617	-	-	2/29/63/63	0/2/2/2
25	SQD	f	102	-	-	11/38/58/69	0/1/1/1
23	CLA	C	506	-	1/1/15/20	6/37/115/115	-
35	HTG	B	623	-	-	4/10/30/30	0/1/1/1
23	CLA	c	504	-	1/1/15/20	0/37/115/115	-
24	BCR	D	405	-	-	4/29/63/63	0/2/2/2
23	CLA	c	507	-	1/1/15/20	8/37/115/115	-
35	HTG	V	202	-	-	0/2/19/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	A	407	-	1/1/15/20	7/37/115/115	-
23	CLA	a	407	-	1/1/15/20	9/37/115/115	-
23	CLA	B	615	-	1/1/15/20	7/37/115/115	-
35	HTG	c	522	-	-	2/10/30/30	0/1/1/1
23	CLA	b	602	-	1/1/15/20	3/37/115/115	-
23	CLA	B	603	-	1/1/15/20	3/37/115/115	-
26	GOL	a	418	-	-	2/4/4/4	-
26	GOL	B	622	-	-	4/4/4/4	-
23	CLA	A	404[A]	-	1/1/15/20	3/37/115/115	-
23	CLA	d	402[B]	41	1/1/15/20	2/37/115/115	-
23	CLA	B	612	-	1/1/15/20	5/37/115/115	-
23	CLA	b	605	-	1/1/15/20	6/37/115/115	-
26	GOL	o	304	-	-	4/4/4/4	-
26	GOL	b	624	-	-	2/4/4/4	-
34	LMG	C	520	-	-	12/46/66/70	0/1/1/1
26	GOL	C	523[B]	-	-	0/4/4/4	-
32	LMT	A	419	-	-	15/21/61/61	0/2/2/2
23	CLA	b	612	-	1/1/15/20	4/37/115/115	-
24	BCR	T	102	-	-	1/29/63/63	0/2/2/2
26	GOL	v	202[B]	-	-	2/4/4/4	-
23	CLA	C	503	-	1/1/15/20	9/37/115/115	-
24	BCR	d	405	-	-	4/29/63/63	0/2/2/2
35	HTG	B	621	-	-	2/10/30/30	0/1/1/1
23	CLA	c	509	-	1/1/15/20	2/37/115/115	-
23	CLA	d	402[A]	41	1/1/15/20	4/37/115/115	-
32	LMT	b	627	-	-	11/17/37/61	0/1/1/2
24	BCR	A	408	-	-	0/29/63/63	0/2/2/2
23	CLA	b	609	-	1/1/15/20	0/37/115/115	-
33	LHG	A	418[B]	-	-	16/53/53/53	-
24	BCR	c	515	-	-	0/29/63/63	0/2/2/2
26	GOL	v	202[A]	-	-	2/4/4/4	-
23	CLA	B	610	41	1/1/15/20	7/37/115/115	-
33	LHG	b	629[B]	-	-	18/53/53/53	-
34	LMG	c	521	-	-	10/46/66/70	0/1/1/1
25	SQD	A	411	-	-	14/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	a	404[B]	-	1/1/15/20	4/37/115/115	-
26	GOL	V	203[B]	-	-	2/4/4/4	-
23	CLA	B	606	-	1/1/15/20	6/37/115/115	-
33	LHG	d	407[B]	-	-	16/53/53/53	-
24	BCR	a	408	-	-	0/29/63/63	0/2/2/2
25	SQD	X	101	-	-	13/38/58/69	0/1/1/1
34	LMG	d	412	39	-	11/46/66/70	0/1/1/1
26	GOL	B	625	-	-	3/4/4/4	-
23	CLA	c	511	-	1/1/15/20	10/37/115/115	-
32	LMT	B	626	-	-	11/21/61/61	0/2/2/2
24	BCR	B	618	-	-	0/29/63/63	0/2/2/2
33	LHG	A	418[A]	-	-	14/53/53/53	-
36	DGD	H	102	-	-	10/51/91/95	0/2/2/2
23	CLA	a	404[A]	-	1/1/15/20	4/37/115/115	-
35	HTG	C	522	-	-	0/10/30/30	0/1/1/1
23	CLA	b	608	-	-	4/37/115/115	-
26	GOL	V	203[A]	-	-	2/4/4/4	-
40	HEC	v	201	16	-	2/10/54/54	-
33	LHG	d	407[A]	-	-	12/53/53/53	-
23	CLA	C	504	-	-	4/37/115/115	-
33	LHG	d	414[B]	-	-	8/53/53/53	-
40	HEC	V	201	16	-	2/10/54/54	-
32	LMT	M	101	-	-	4/21/61/61	0/2/2/2
23	CLA	A	404[B]	-	1/1/15/20	4/37/115/115	-
23	CLA	B	601	41	1/1/15/20	11/37/115/115	-
35	HTG	b	625	-	-	3/10/30/30	0/1/1/1
32	LMT	A	417	-	-	6/21/61/61	0/2/2/2
24	BCR	B	619	-	-	0/29/63/63	0/2/2/2
33	LHG	a	419[B]	-	-	16/46/46/53	-
23	CLA	C	502	-	1/1/15/20	4/37/115/115	-
36	DGD	h	102	-	-	16/51/91/95	0/2/2/2
23	CLA	c	503	-	1/1/15/20	3/37/115/115	-
23	CLA	c	506	-	1/1/15/20	6/37/115/115	-
33	LHG	d	414[A]	-	-	15/53/53/53	-
23	CLA	b	606	-	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	513	-	1/1/15/20	13/37/115/115	-
23	CLA	C	507	-	1/1/15/20	13/37/115/115	-
23	CLA	c	512	3	1/1/15/20	6/37/115/115	-
32	LMT	b	621	-	-	8/17/37/61	0/1/1/2
36	DGD	C	519	-	-	20/51/91/95	0/2/2/2
36	DGD	c	518[A]	-	-	16/51/91/95	0/2/2/2
33	LHG	a	419[A]	-	-	16/46/46/53	-
28	PL9	A	413[B]	-	-	13/53/73/73	0/1/1/1
31	PHO	a	406[B]	-	-	3/37/103/103	0/5/6/6
31	PHO	D	401[B]	-	-	2/37/103/103	0/5/6/6
36	DGD	C	518[B]	-	-	12/51/91/95	0/2/2/2
32	LMT	B	627	-	-	10/21/61/61	0/2/2/2
34	LMG	c	501	-	-	12/46/66/70	0/1/1/1
23	CLA	c	508	41	1/1/15/20	7/37/115/115	-
26	GOL	D	413	-	-	4/4/4/4	-
34	LMG	Z	101	-	-	11/31/51/70	0/1/1/1
33	LHG	d	408[B]	-	-	14/53/53/53	-
33	LHG	D	407[A]	-	-	17/53/53/53	-
26	GOL	c	527	-	-	2/4/4/4	-
23	CLA	a	405[B]	41	-	3/37/115/115	-
26	GOL	d	413	-	-	2/4/4/4	-
24	BCR	b	619	-	-	2/29/63/63	0/2/2/2
34	LMG	m	101	-	-	11/46/66/70	0/1/1/1
23	CLA	b	610	41	1/1/15/20	9/37/115/115	-
28	PL9	A	413[A]	-	-	14/53/73/73	0/1/1/1
31	PHO	a	406[A]	-	-	6/37/103/103	0/5/6/6
34	LMG	C	521	-	-	13/46/66/70	0/1/1/1
31	PHO	D	401[A]	-	-	0/37/103/103	0/5/6/6
36	DGD	C	518[A]	-	-	12/51/91/95	0/2/2/2
23	CLA	c	502	-	1/1/15/20	2/37/115/115	-
28	PL9	d	406[B]	-	-	8/53/73/73	0/1/1/1
33	LHG	d	408[A]	-	-	12/53/53/53	-
26	GOL	a	417	-	-	2/4/4/4	-
34	LMG	B	620	-	-	17/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	h	101	-	-	2/29/63/63	0/2/2/2
23	CLA	a	405[A]	41	-	4/37/115/115	-
33	LHG	L	101[B]	-	-	18/53/53/53	-
32	LMT	T	101	-	-	7/21/61/61	0/2/2/2
25	SQD	l	101	-	-	14/49/69/69	0/1/1/1
26	GOL	b	628	-	-	0/4/4/4	-
23	CLA	b	611	-	1/1/15/20	4/37/115/115	-
31	PHO	A	416[B]	-	-	0/37/103/103	0/5/6/6
24	BCR	C	516	-	-	1/29/63/63	0/2/2/2
23	CLA	A	405[B]	41	1/1/15/20	3/37/115/115	-
23	CLA	b	616	-	1/1/15/20	9/37/115/115	-
33	LHG	D	408[B]	-	-	12/53/53/53	-
23	CLA	C	511	-	1/1/15/20	13/37/115/115	-
28	PL9	d	406[A]	-	-	6/53/73/73	0/1/1/1
34	LMG	c	520	-	-	12/46/66/70	0/1/1/1
26	GOL	c	526[A]	-	-	0/4/4/4	-
33	LHG	L	101[A]	-	-	20/53/53/53	-
26	GOL	a	410	-	-	4/4/4/4	-
34	LMG	D	412	39	-	9/46/66/70	0/1/1/1
36	DGD	c	518[B]	-	-	13/51/91/95	0/2/2/2
31	PHO	A	416[A]	-	-	1/37/103/103	0/5/6/6
23	CLA	b	613	-	1/1/15/20	2/37/115/115	-
23	CLA	A	405[A]	41	1/1/15/20	1/37/115/115	-
36	DGD	c	517[A]	-	-	17/51/91/95	0/2/2/2
33	LHG	D	408[A]	-	-	13/53/53/53	-
26	GOL	O	303	-	-	2/4/4/4	-
23	CLA	C	508	41	1/1/15/20	8/37/115/115	-
24	BCR	t	102	-	-	0/29/63/63	0/2/2/2
23	CLA	B	608	-	-	3/37/115/115	-
24	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
31	PHO	a	415[A]	-	-	1/37/103/103	0/5/6/6
23	CLA	B	605	-	1/1/15/20	6/37/115/115	-
33	LHG	D	407[B]	-	-	19/53/53/53	-
34	LMG	C	501	-	-	11/46/66/70	0/1/1/1
32	LMT	m	103	-	-	8/21/61/61	0/2/2/2
28	PL9	a	413[B]	-	-	15/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	GOL	O	302	-	-	2/4/4/4	-
35	HTG	b	622	-	-	5/10/30/30	0/1/1/1
23	CLA	C	509	-	1/1/15/20	3/37/115/115	-
23	CLA	A	406[B]	41	-	4/37/115/115	-
23	CLA	C	513	-	1/1/15/20	6/37/115/115	-
32	LMT	e	101	-	-	15/21/61/61	0/2/2/2
36	DGD	c	519	-	-	9/51/91/95	0/2/2/2
23	CLA	C	510	-	1/1/15/20	7/37/115/115	-
38	HEM	f	101	6,5	-	6/12/54/54	-
23	CLA	d	404	-	1/1/15/20	8/37/115/115	-
23	CLA	d	403[B]	-	1/1/15/20	4/37/115/115	-
32	LMT	F	101	-	-	8/21/61/61	0/2/2/2
24	BCR	C	515	-	-	0/29/63/63	0/2/2/2
26	GOL	l	103[B]	-	-	2/4/4/4	-
23	CLA	b	604	-	1/1/15/20	9/37/115/115	-

The worst 5 of 1541 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	611	CLA	C3B-C2B	10.62	1.54	1.40
23	B	612	CLA	C3B-C2B	7.60	1.50	1.40
23	B	616	CLA	C3B-C2B	7.30	1.50	1.40
23	b	608	CLA	C3B-C2B	7.13	1.50	1.40
23	C	509	CLA	C3B-C2B	7.00	1.49	1.40

The worst 5 of 3139 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	407	CLA	C1D-ND-C4D	-11.00	98.60	106.31
23	B	611	CLA	C1D-ND-C4D	-10.88	98.68	106.31
23	a	404[B]	CLA	C1D-ND-C4D	-10.33	99.07	106.31
23	B	615	CLA	C1D-ND-C4D	-10.23	99.13	106.31
23	b	610	CLA	C1D-ND-C4D	-10.02	99.28	106.31

5 of 70 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404[A]	CLA	ND
23	A	404[B]	CLA	ND

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Mol	Chain	Res	Type	Atom
23	A	405[A]	CLA	ND
23	A	405[B]	CLA	ND
23	A	407	CLA	ND

5 of 1566 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	505	CLA	C2-C3-C5-C6
23	C	505	CLA	C4-C3-C5-C6
23	C	510	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

181 monomers are involved in 372 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	a	413[A]	PL9	4	0
23	A	406[A]	CLA	1	0
23	C	505	CLA	1	0
23	d	403[A]	CLA	1	0
26	l	103[A]	GOL	1	0
23	B	614	CLA	2	0
24	c	516	BCR	1	0
25	b	620	SQD	2	0
24	B	617	BCR	1	0
28	D	406[A]	PL9	1	0
32	a	416	LMT	1	0
23	b	614	CLA	1	0
35	o	301	HTG	1	0
32	t	101	LMT	3	0
23	D	404	CLA	1	0
23	c	514	CLA	2	0
23	D	403[B]	CLA	5	0
23	b	615	CLA	1	0
38	F	102	HEM	1	0
36	c	517[B]	DGD	2	0
23	B	616	CLA	3	0
33	E	101[B]	LHG	2	0
25	a	411	SQD	1	0
25	a	409[B]	SQD	4	0
24	y	101	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	a	415[B]	PHO	1	0
23	B	604	CLA	1	0
23	D	403[A]	CLA	3	0
23	B	613	CLA	4	0
34	z	101	LMG	2	0
23	C	514	CLA	1	0
23	b	607	CLA	2	0
26	D	402	GOL	4	0
33	E	101[A]	LHG	4	0
36	C	517[B]	DGD	1	0
25	a	409[A]	SQD	5	0
35	d	411	HTG	1	0
24	k	101	BCR	1	0
23	B	609	CLA	3	0
23	c	510	CLA	3	0
25	A	409[B]	SQD	1	0
23	C	512	CLA	2	0
23	c	505	CLA	2	0
23	B	602	CLA	1	0
36	C	517[A]	DGD	1	0
23	b	601	CLA	1	0
32	B	629	LMT	1	0
25	A	409[A]	SQD	1	0
24	b	618	BCR	3	0
28	D	406[B]	PL9	1	0
24	H	101	BCR	1	0
24	K	102	BCR	1	0
24	b	617	BCR	1	0
25	f	102	SQD	1	0
23	C	506	CLA	4	0
35	B	623	HTG	1	0
23	c	504	CLA	4	0
24	D	405	BCR	1	0
23	c	507	CLA	4	0
23	A	407	CLA	3	0
23	a	407	CLA	4	0
23	B	615	CLA	5	0
35	c	522	HTG	1	0
23	B	603	CLA	1	0
26	a	418	GOL	3	0
26	B	622	GOL	2	0
23	A	404[A]	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	d	402[B]	CLA	4	0
23	B	612	CLA	3	0
23	b	605	CLA	4	0
32	A	419	LMT	1	0
23	b	612	CLA	3	0
24	T	102	BCR	5	0
26	v	202[B]	GOL	2	0
23	C	503	CLA	2	0
24	d	405	BCR	2	0
35	B	621	HTG	1	0
23	c	509	CLA	9	0
23	d	402[A]	CLA	3	0
24	A	408	BCR	1	0
23	b	609	CLA	4	0
24	c	515	BCR	2	0
26	v	202[A]	GOL	1	0
23	B	610	CLA	2	0
34	c	521	LMG	1	0
25	A	411	SQD	1	0
23	a	404[B]	CLA	10	0
23	B	606	CLA	2	0
33	d	407[B]	LHG	2	0
24	a	408	BCR	1	0
25	X	101	SQD	1	0
34	d	412	LMG	3	0
23	c	511	CLA	2	0
32	B	626	LMT	1	0
24	B	618	BCR	2	0
33	A	418[A]	LHG	2	0
36	H	102	DGD	1	0
23	a	404[A]	CLA	2	0
23	b	608	CLA	1	0
33	d	407[A]	LHG	2	0
23	C	504	CLA	4	0
32	M	101	LMT	2	0
23	A	404[B]	CLA	6	0
23	B	601	CLA	1	0
35	b	625	HTG	1	0
32	A	417	LMT	1	0
24	B	619	BCR	2	0
33	a	419[B]	LHG	3	0
23	C	502	CLA	4	0

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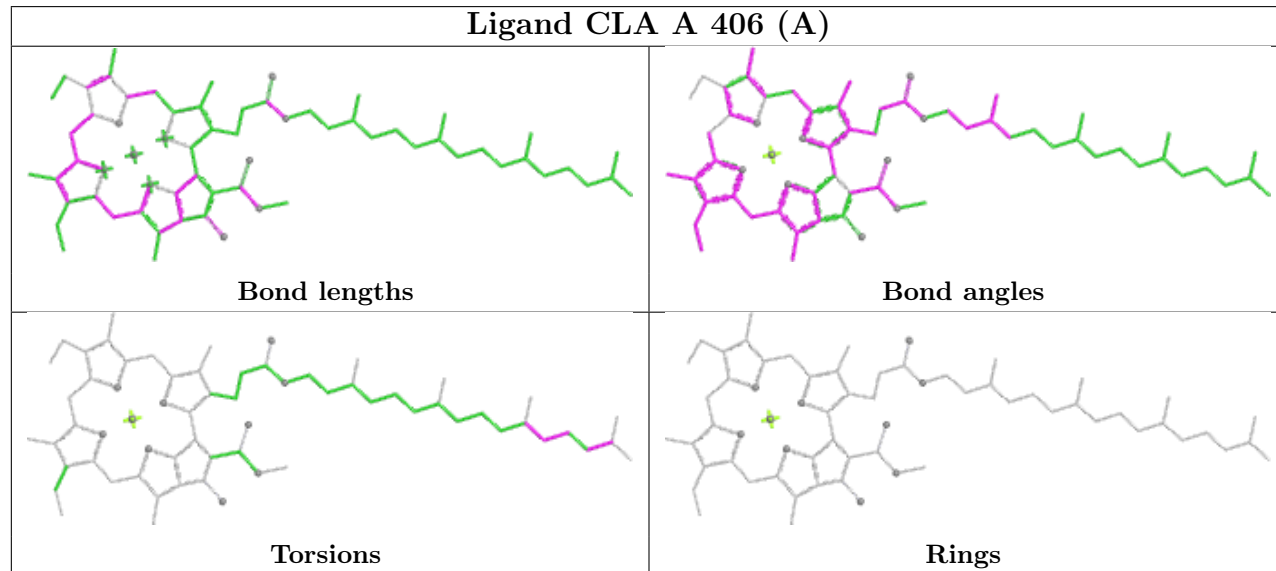
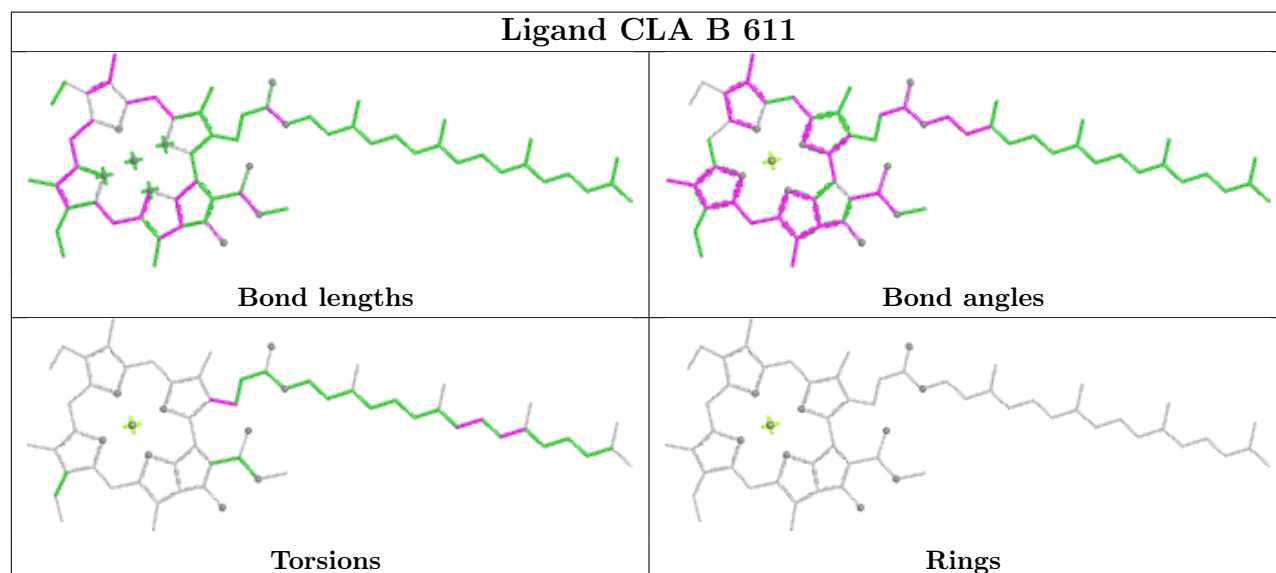
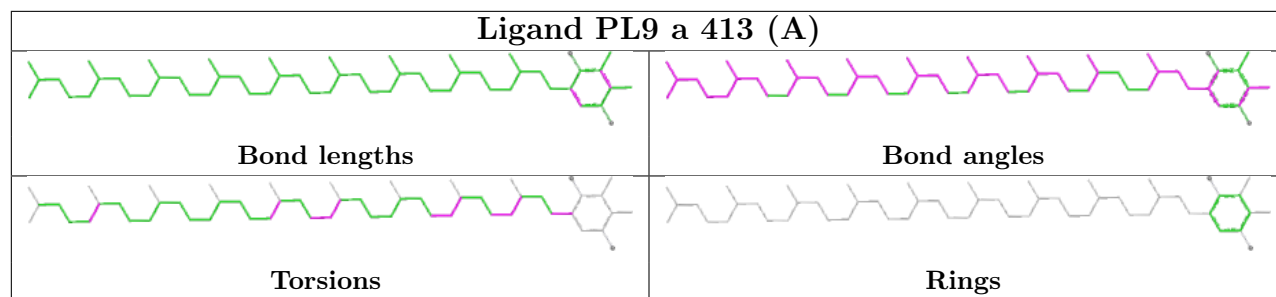
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	h	102	DGD	2	0
23	c	503	CLA	2	0
23	c	506	CLA	8	0
23	b	606	CLA	2	0
23	c	513	CLA	7	0
23	C	507	CLA	6	0
23	c	512	CLA	6	0
32	b	621	LMT	1	0
36	C	519	DGD	2	0
36	c	518[A]	DGD	3	0
33	a	419[A]	LHG	5	0
28	A	413[B]	PL9	10	0
31	a	406[B]	PHO	2	0
31	D	401[B]	PHO	2	0
36	C	518[B]	DGD	2	0
32	B	627	LMT	1	0
34	c	501	LMG	1	0
23	c	508	CLA	2	0
26	D	413	GOL	3	0
34	Z	101	LMG	3	0
33	d	408[B]	LHG	7	0
33	D	407[A]	LHG	2	0
23	a	405[B]	CLA	4	0
24	b	619	BCR	4	0
23	b	610	CLA	1	0
28	A	413[A]	PL9	11	0
34	C	521	LMG	3	0
31	D	401[A]	PHO	1	0
36	C	518[A]	DGD	1	0
23	c	502	CLA	2	0
33	d	408[A]	LHG	11	0
26	a	417	GOL	2	0
34	B	620	LMG	2	0
24	h	101	BCR	5	0
23	a	405[A]	CLA	2	0
33	L	101[B]	LHG	1	0
25	l	101	SQD	2	0
26	b	628	GOL	2	0
31	A	416[B]	PHO	1	0
23	A	405[B]	CLA	5	0
23	b	616	CLA	3	0
33	D	408[B]	LHG	3	0

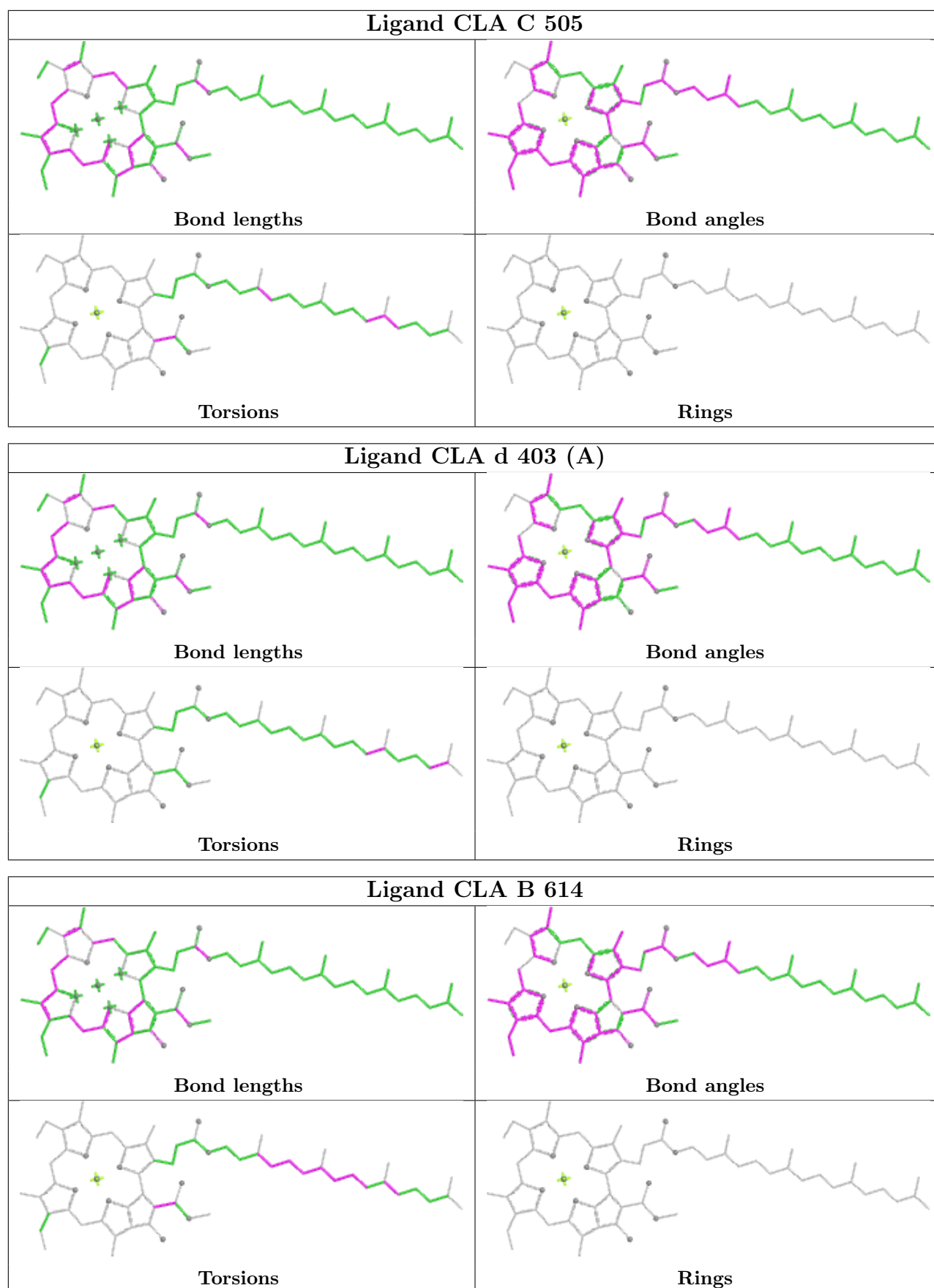
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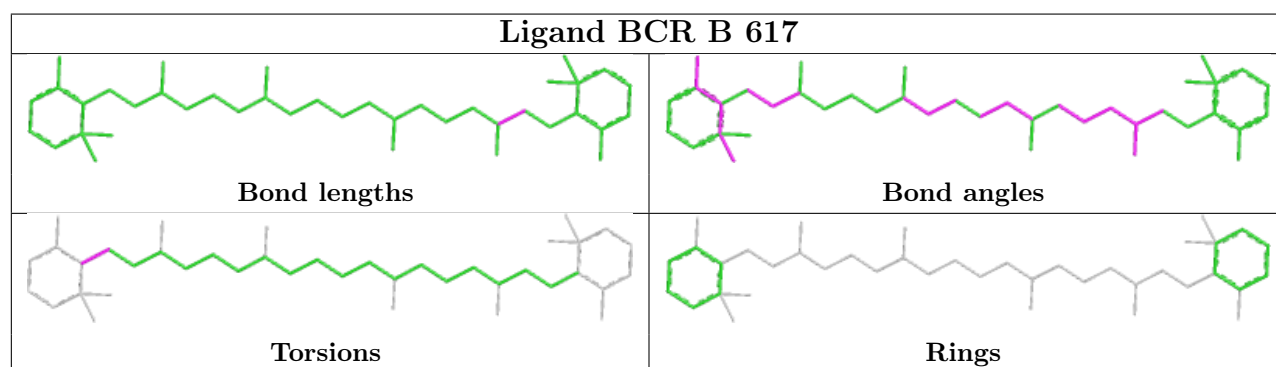
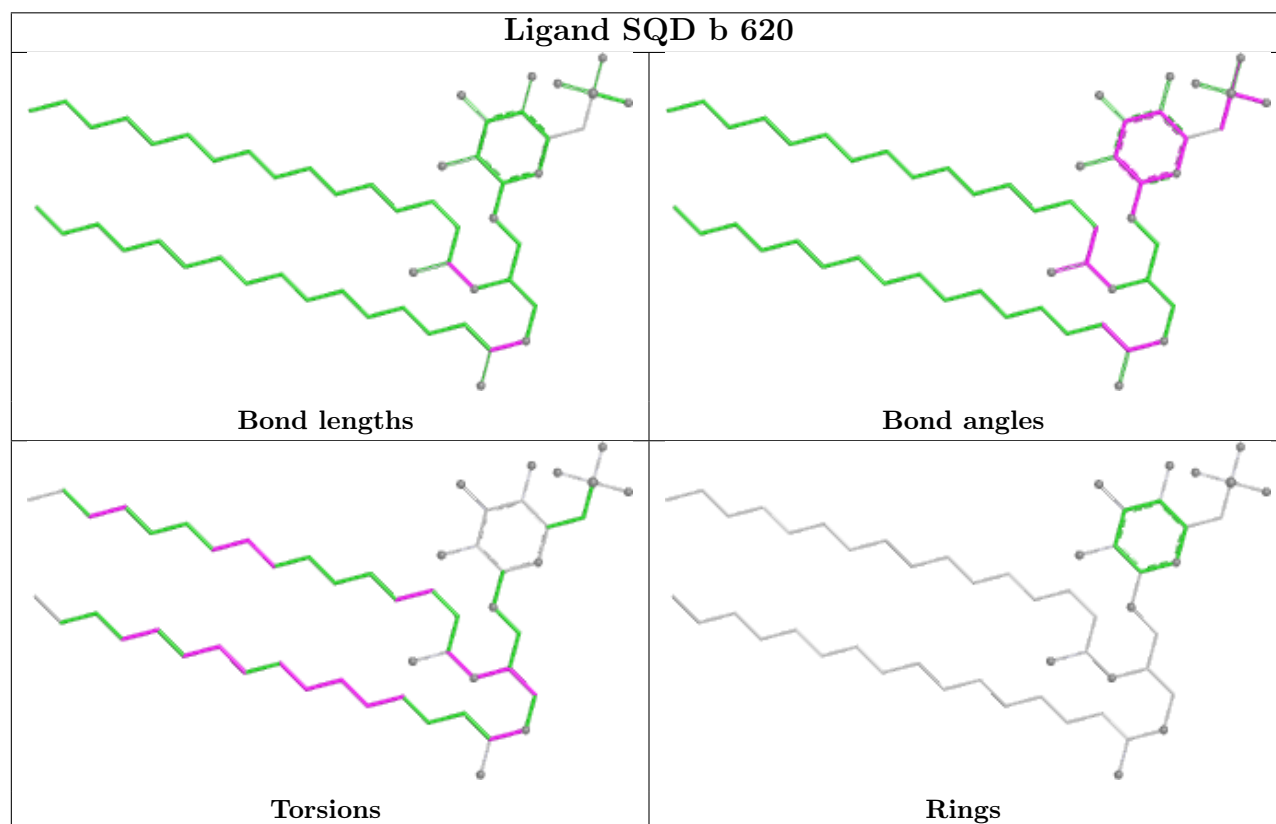
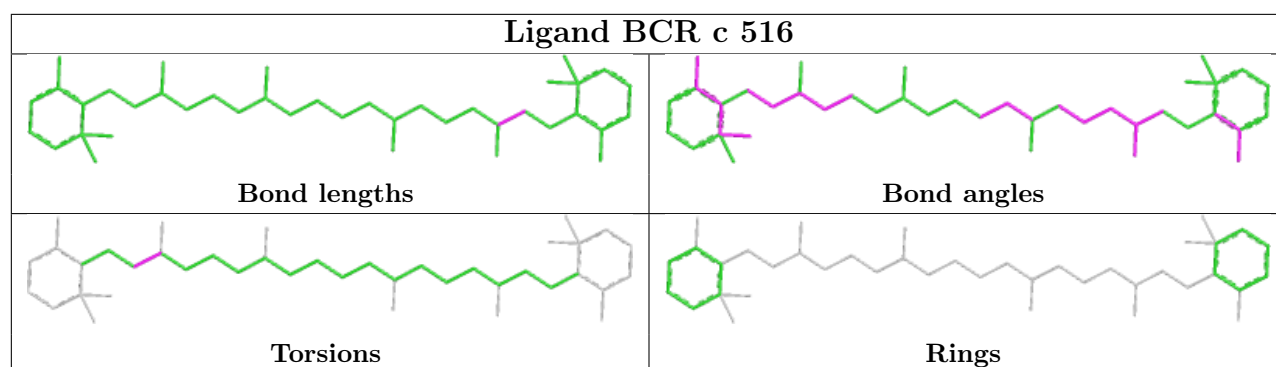
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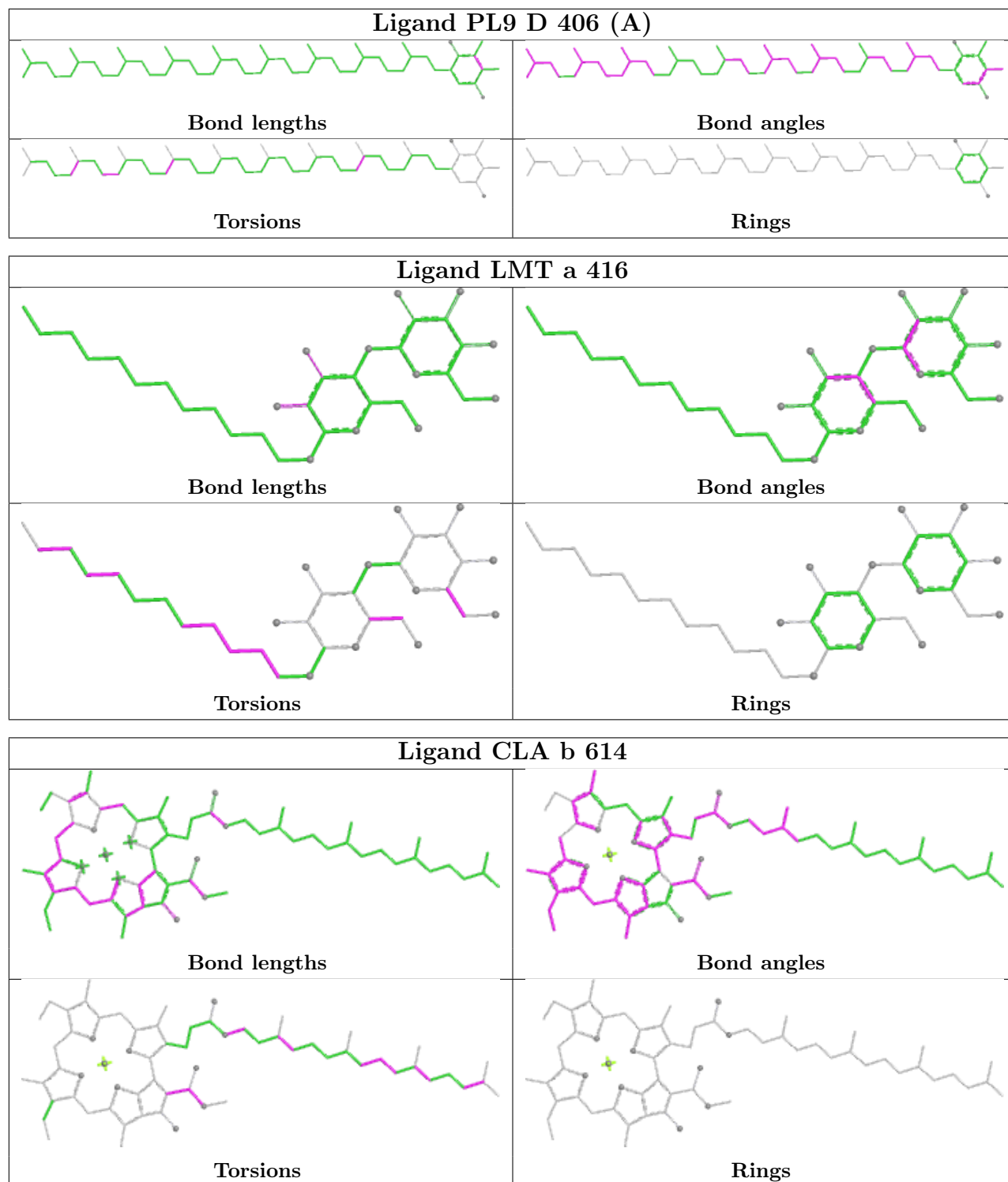
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	C	511	CLA	2	0
34	c	520	LMG	1	0
36	c	518[B]	DGD	2	0
31	A	416[A]	PHO	1	0
23	b	613	CLA	4	0
23	A	405[A]	CLA	1	0
36	c	517[A]	DGD	1	0
33	D	408[A]	LHG	4	0
26	O	303	GOL	2	0
23	C	508	CLA	2	0
24	t	102	BCR	7	0
24	Y	101	BCR	2	0
31	a	415[A]	PHO	1	0
23	B	605	CLA	3	0
33	D	407[B]	LHG	2	0
32	m	103	LMT	2	0
28	a	413[B]	PL9	4	0
26	O	302	GOL	1	0
35	b	622	HTG	2	0
23	C	509	CLA	4	0
23	A	406[B]	CLA	2	0
23	C	513	CLA	2	0
32	e	101	LMT	1	0
36	c	519	DGD	2	0
23	C	510	CLA	2	0
23	d	404	CLA	2	0
23	d	403[B]	CLA	5	0
24	C	515	BCR	1	0
26	l	103[B]	GOL	1	0
23	b	604	CLA	5	0

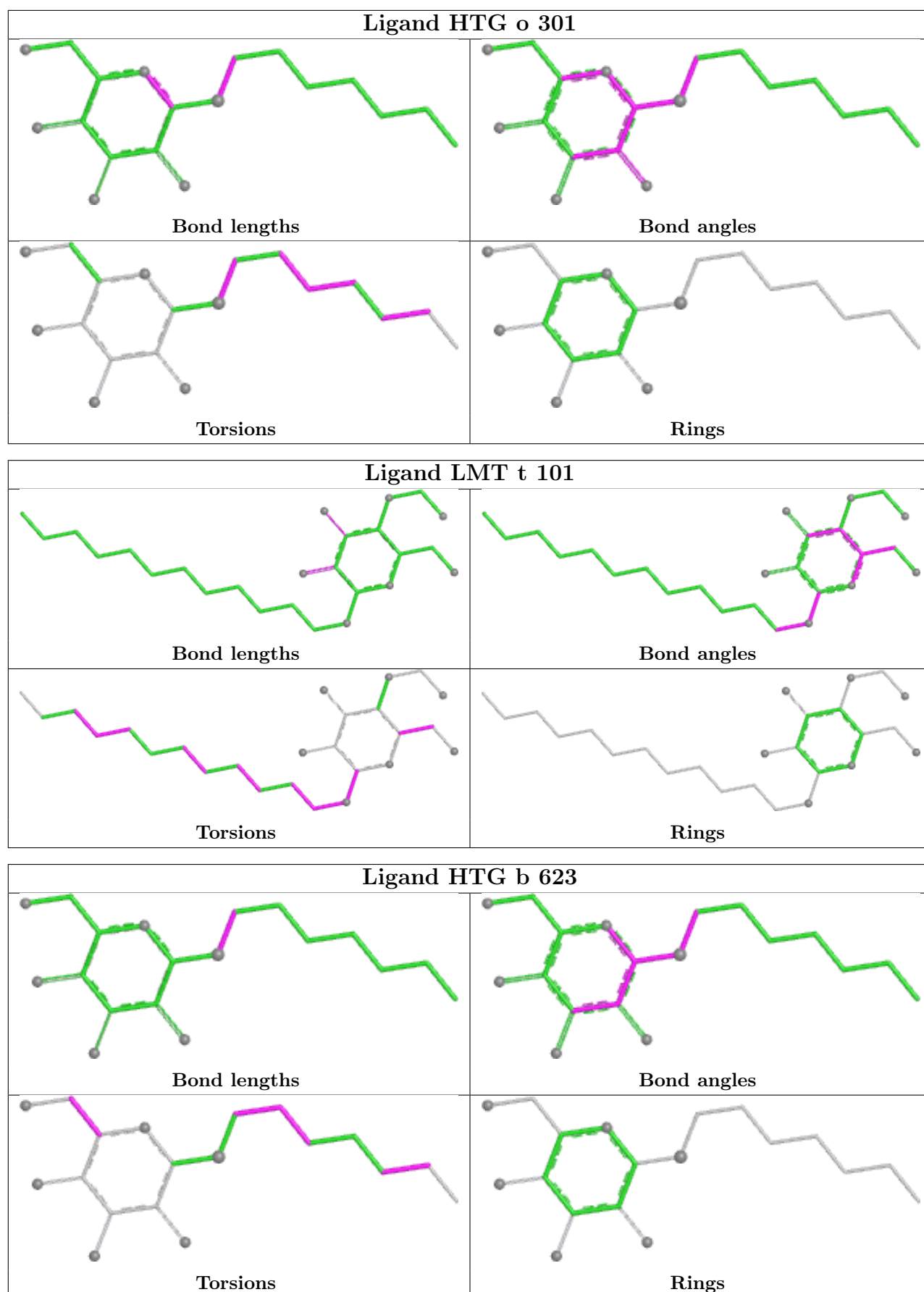
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

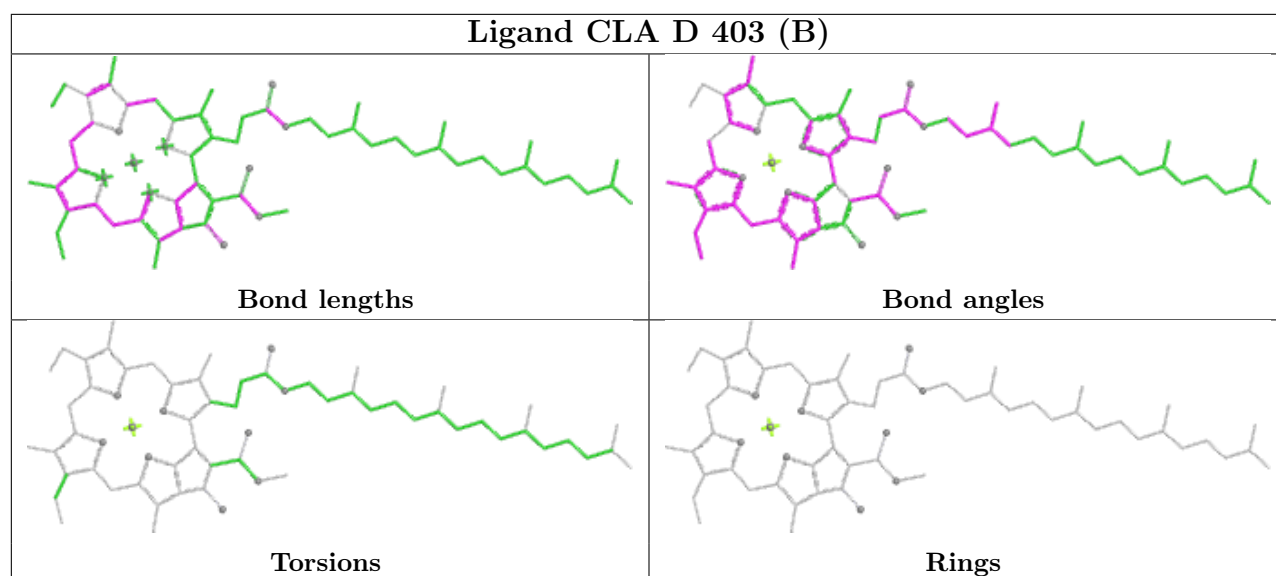
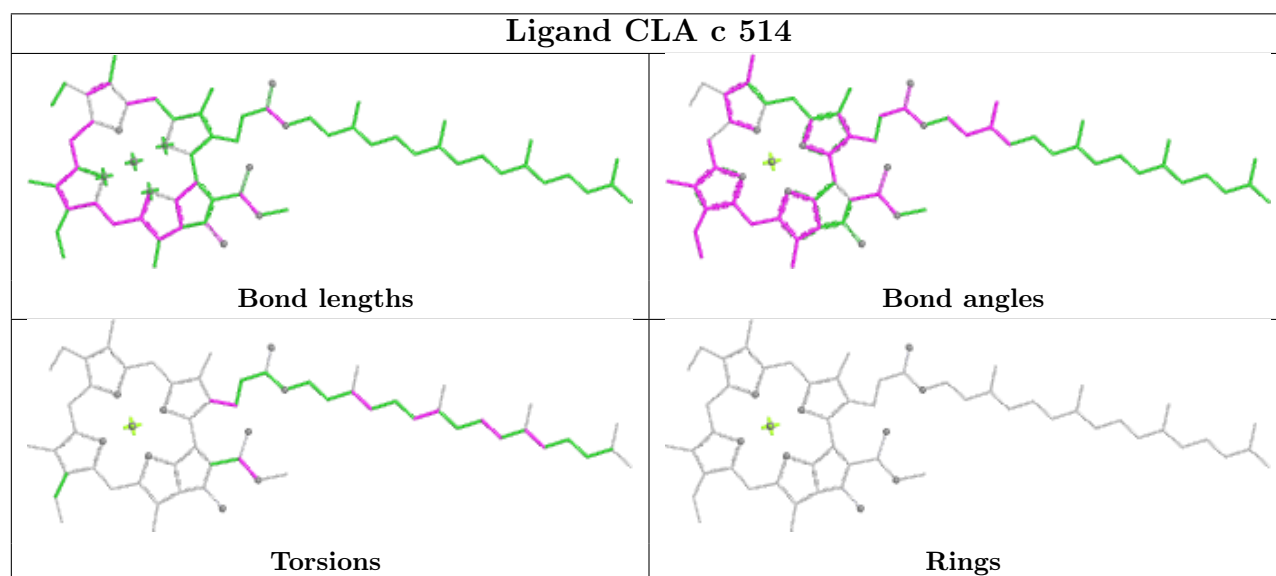
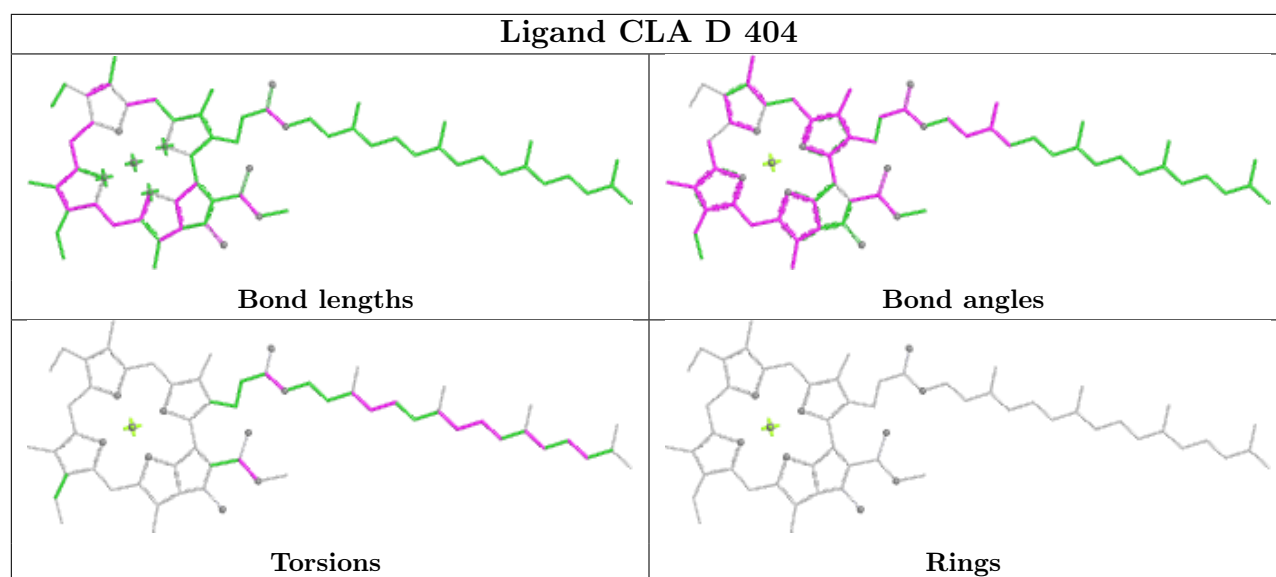


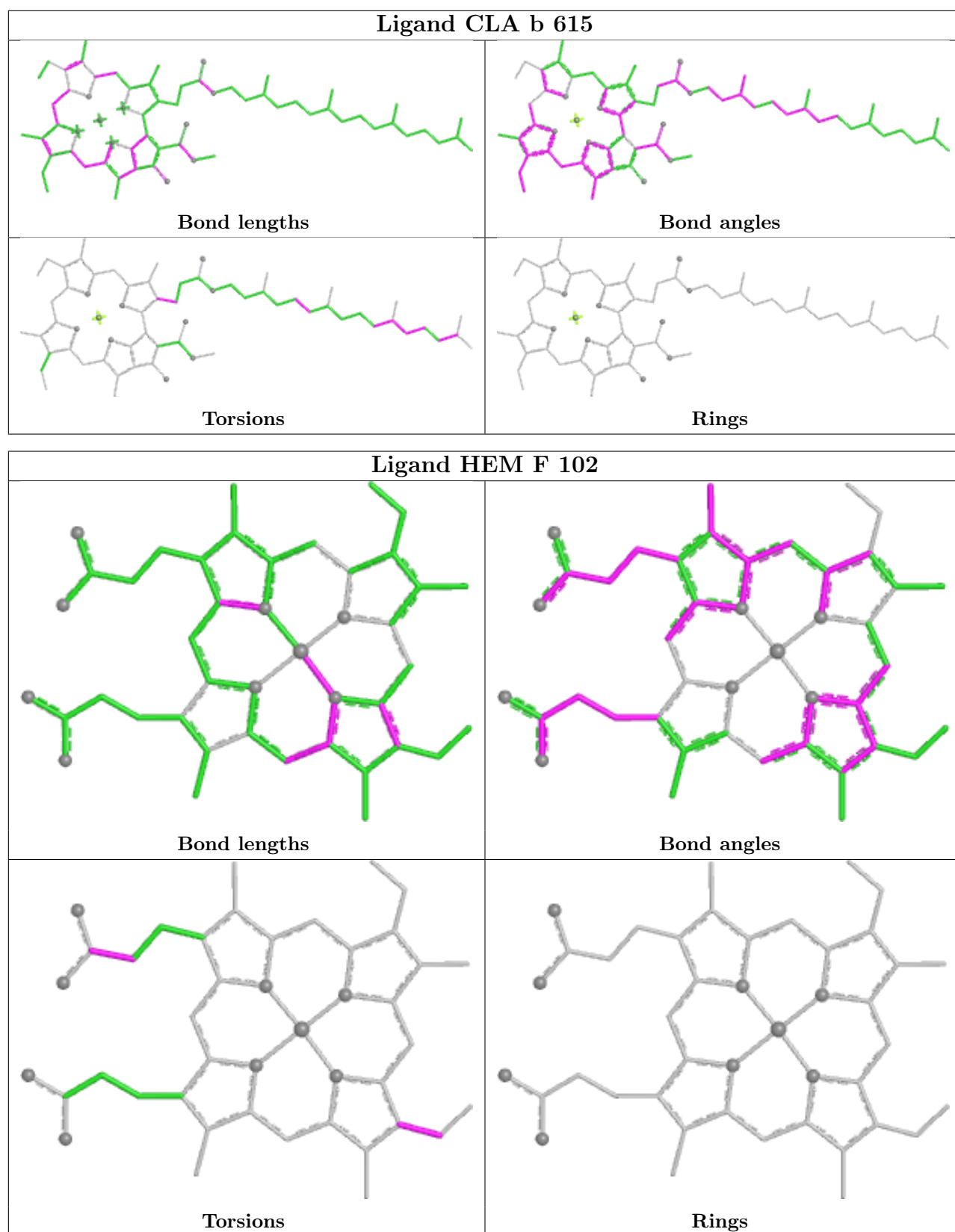


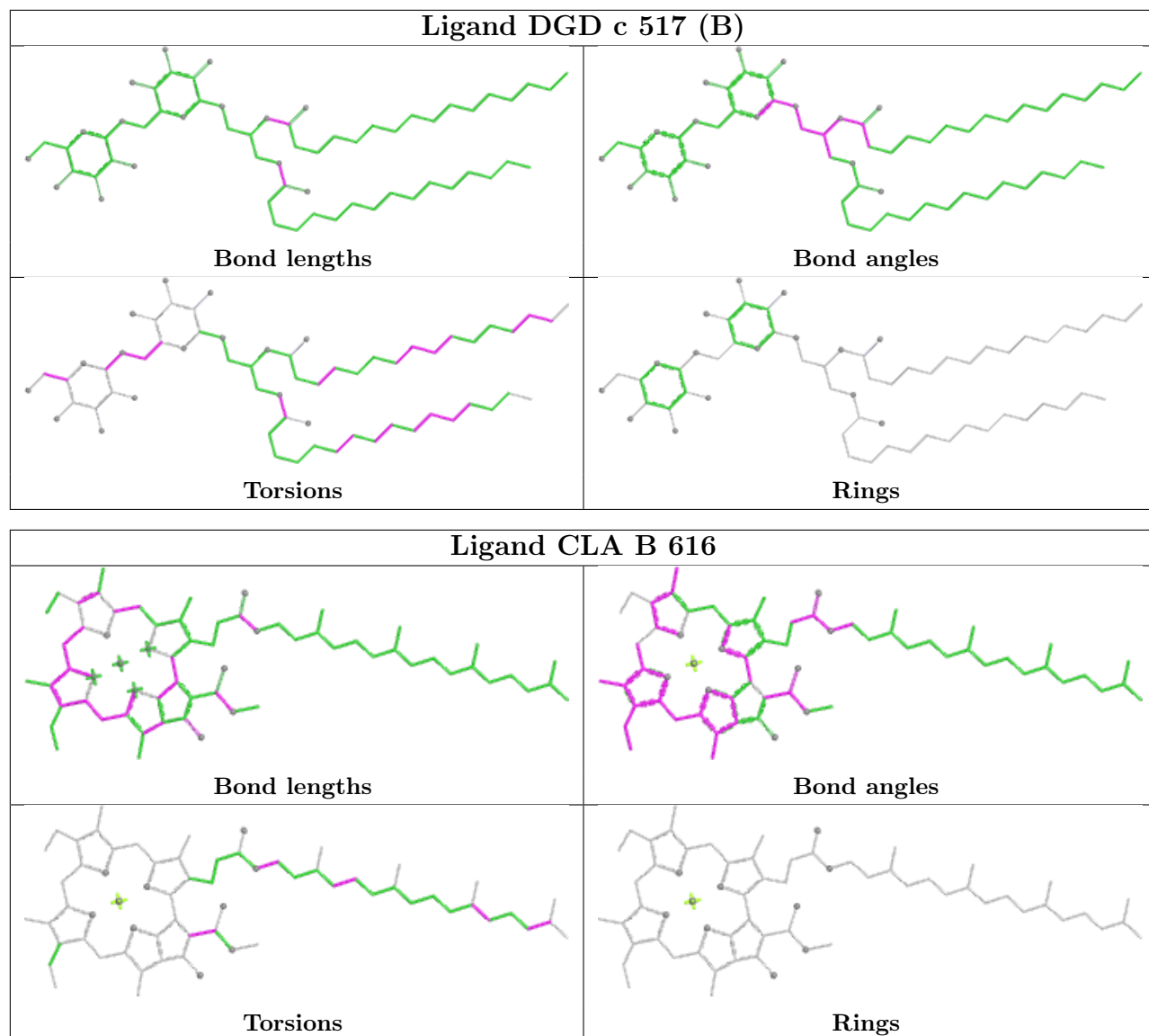


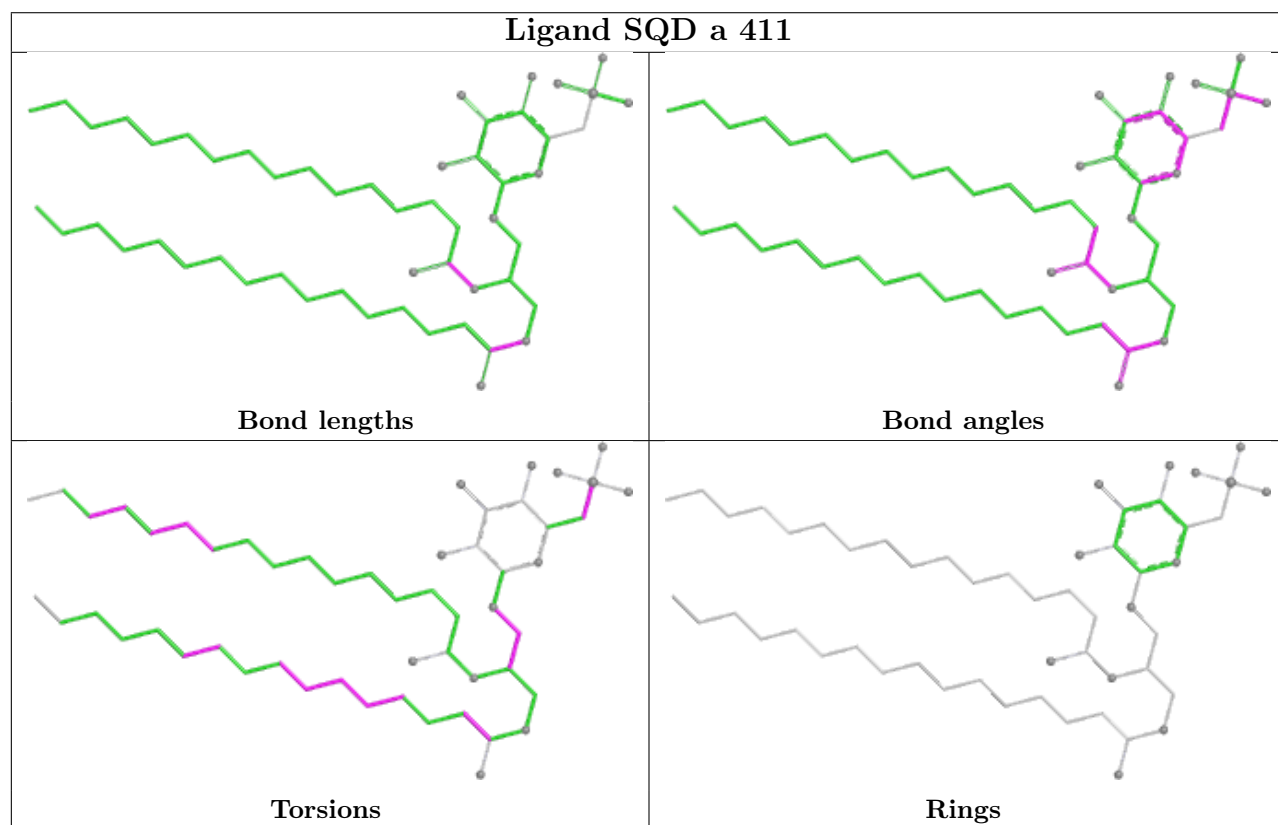
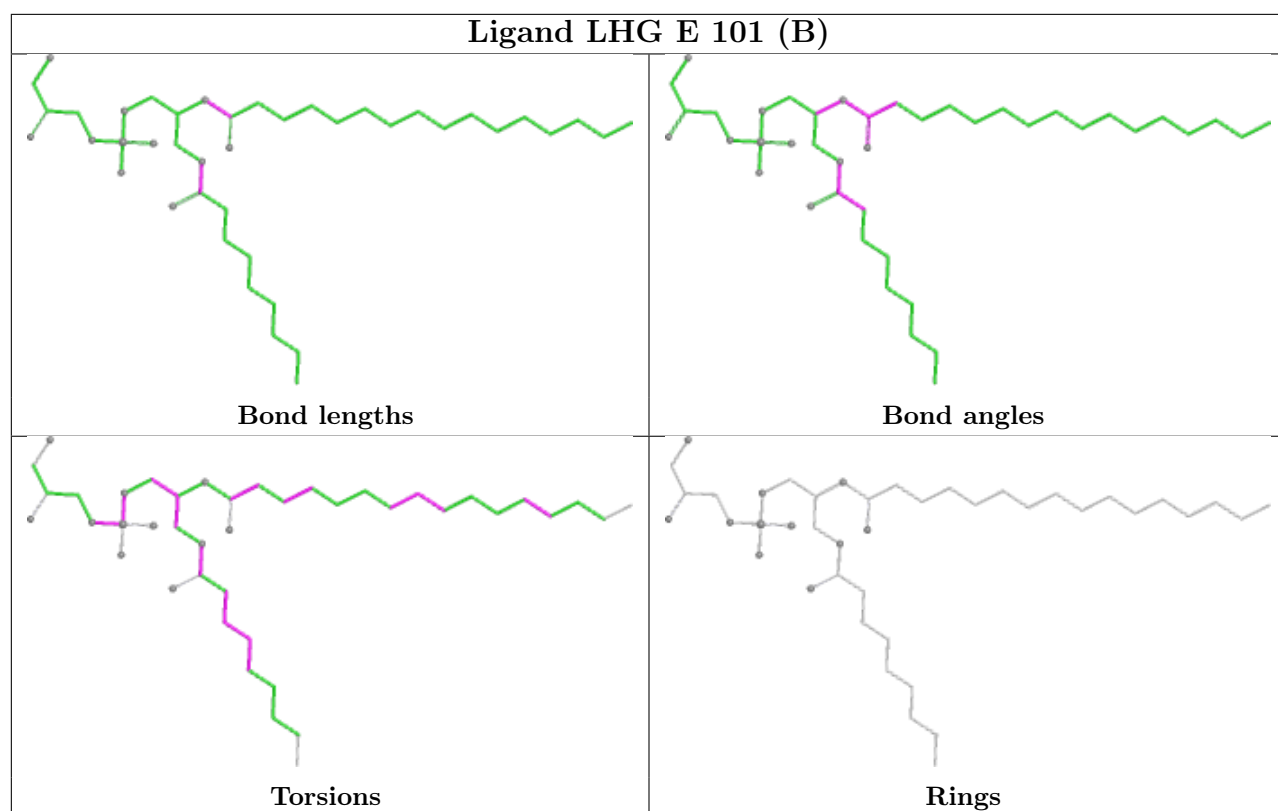


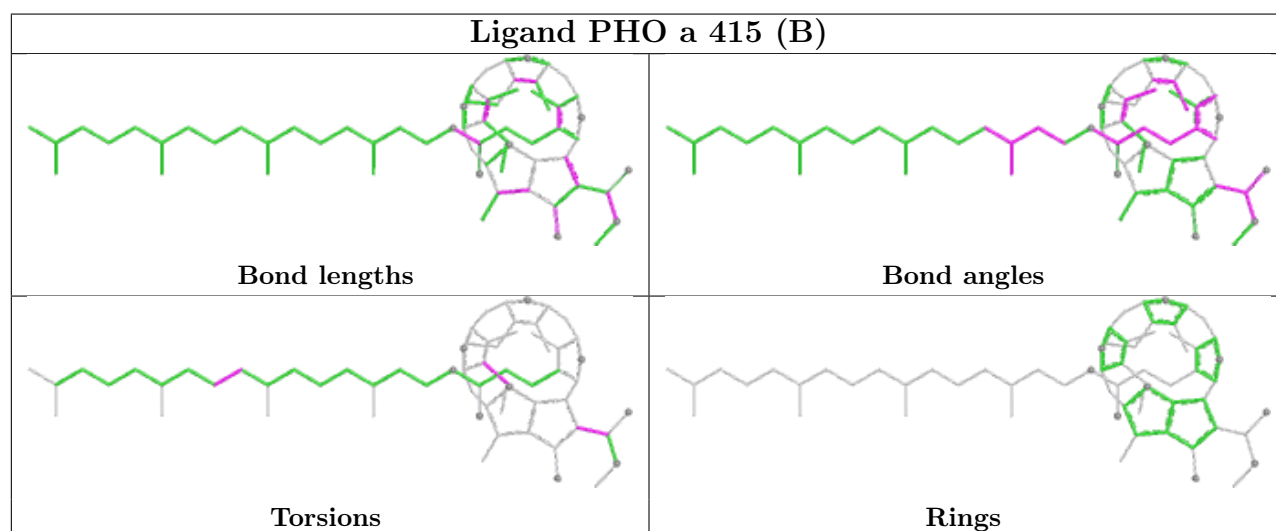
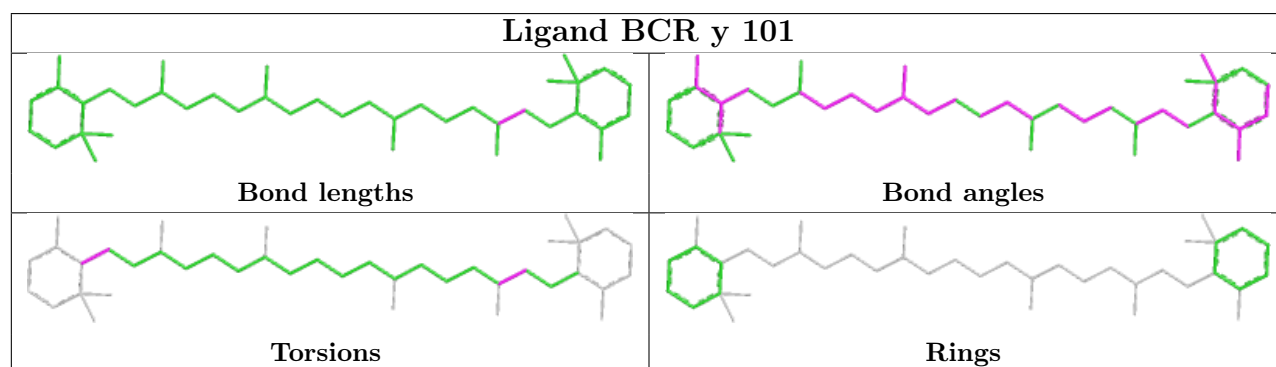
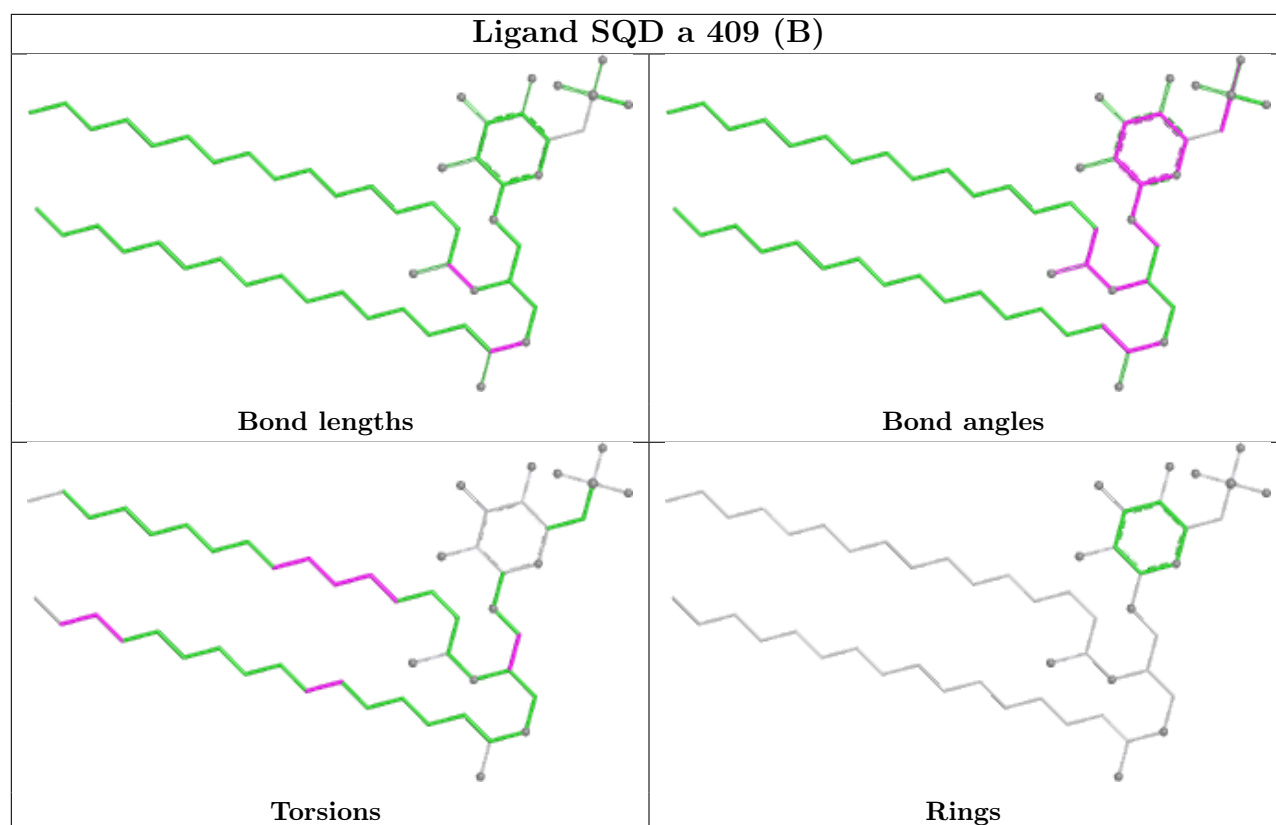


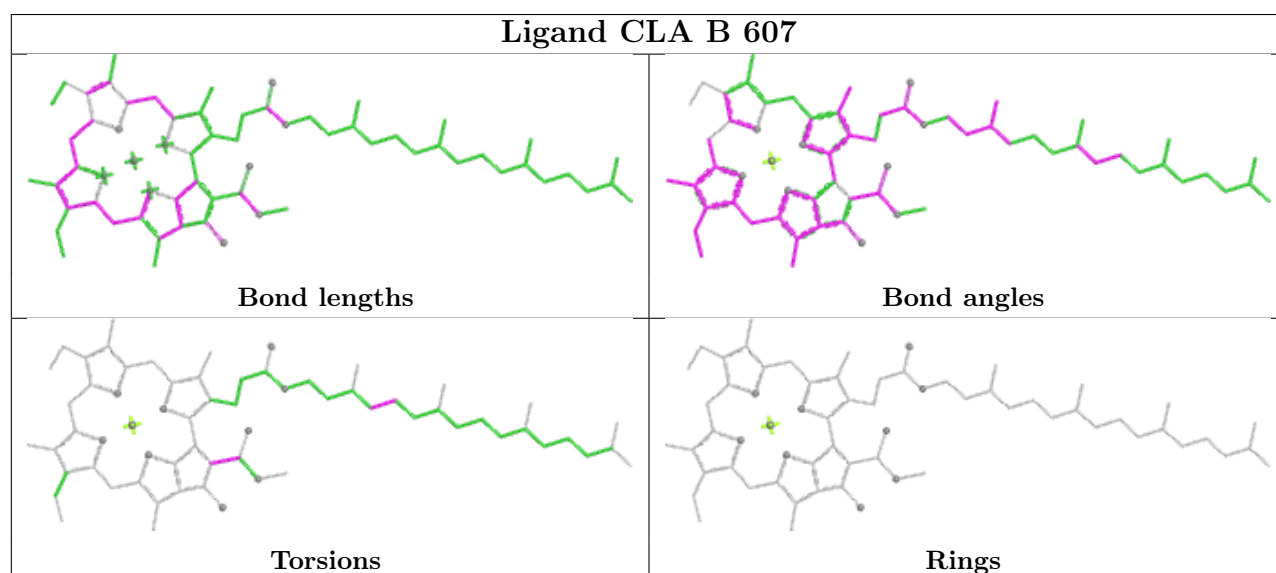
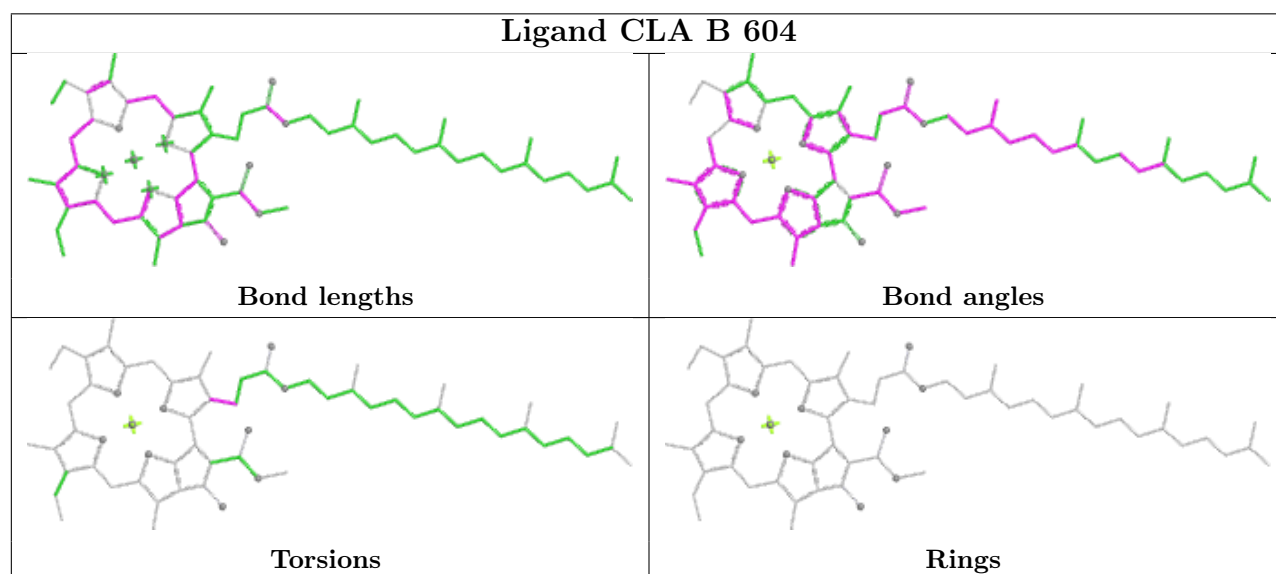
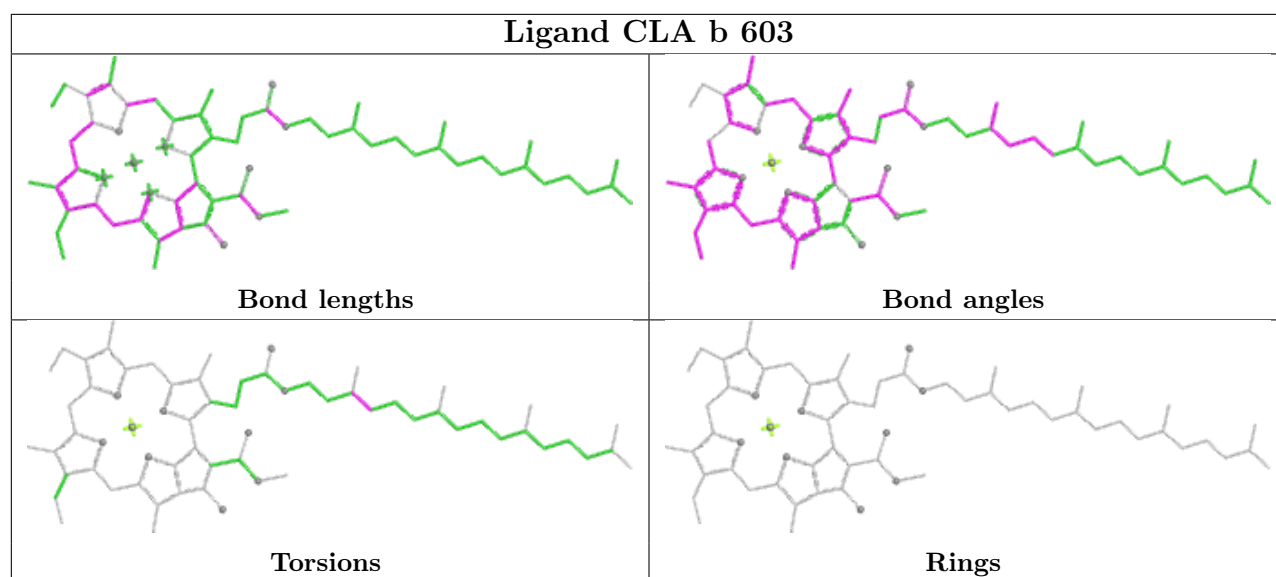


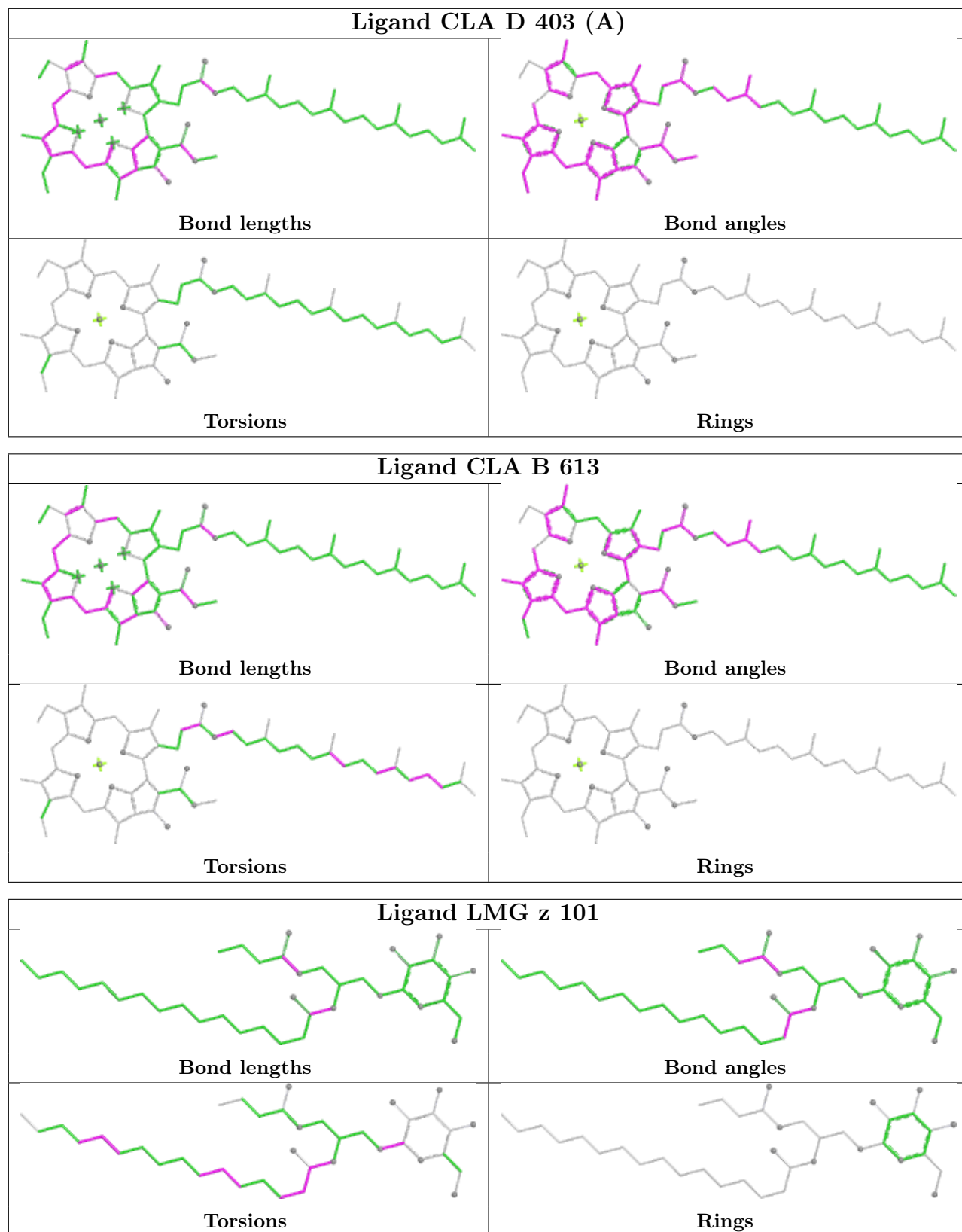


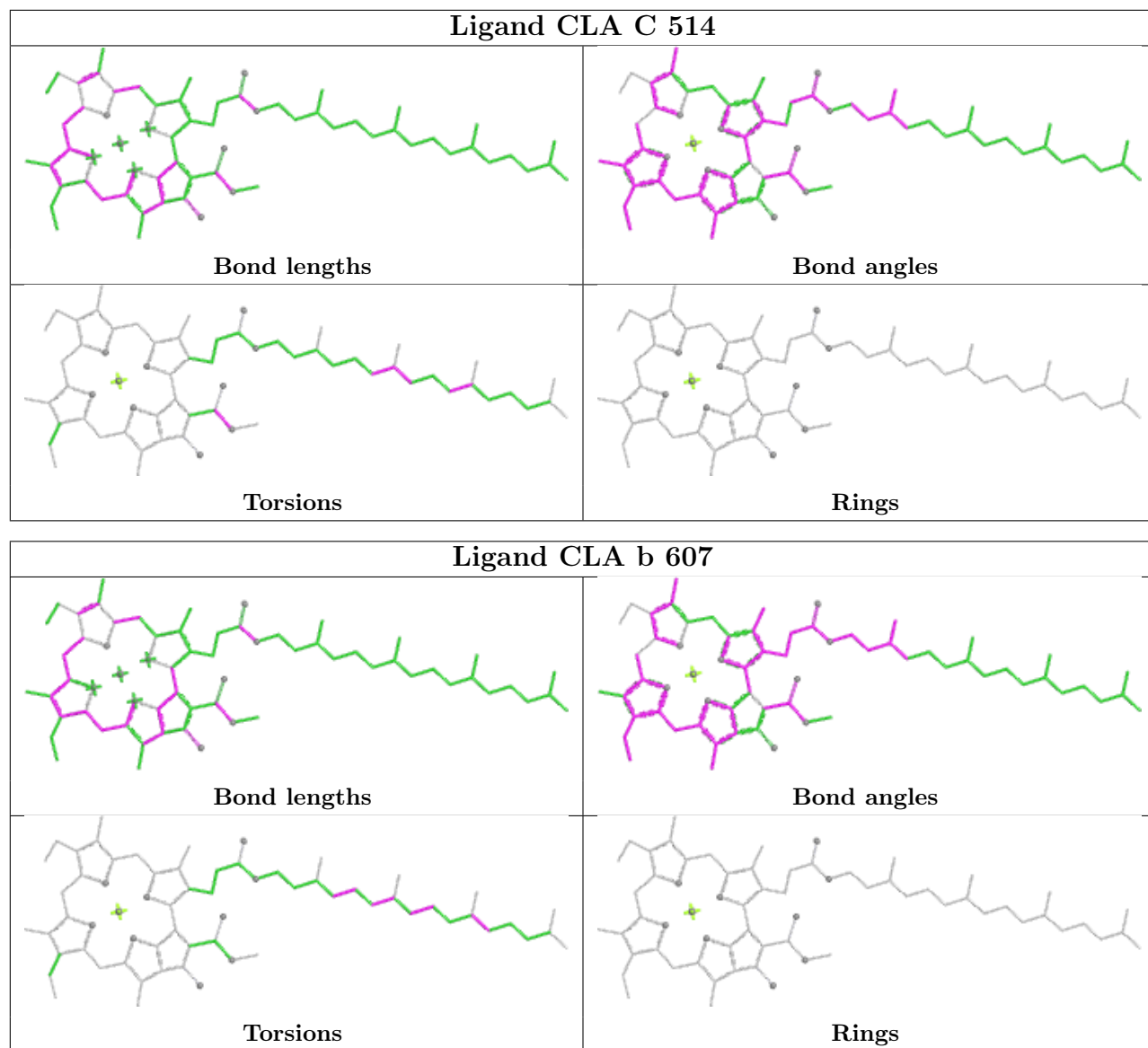


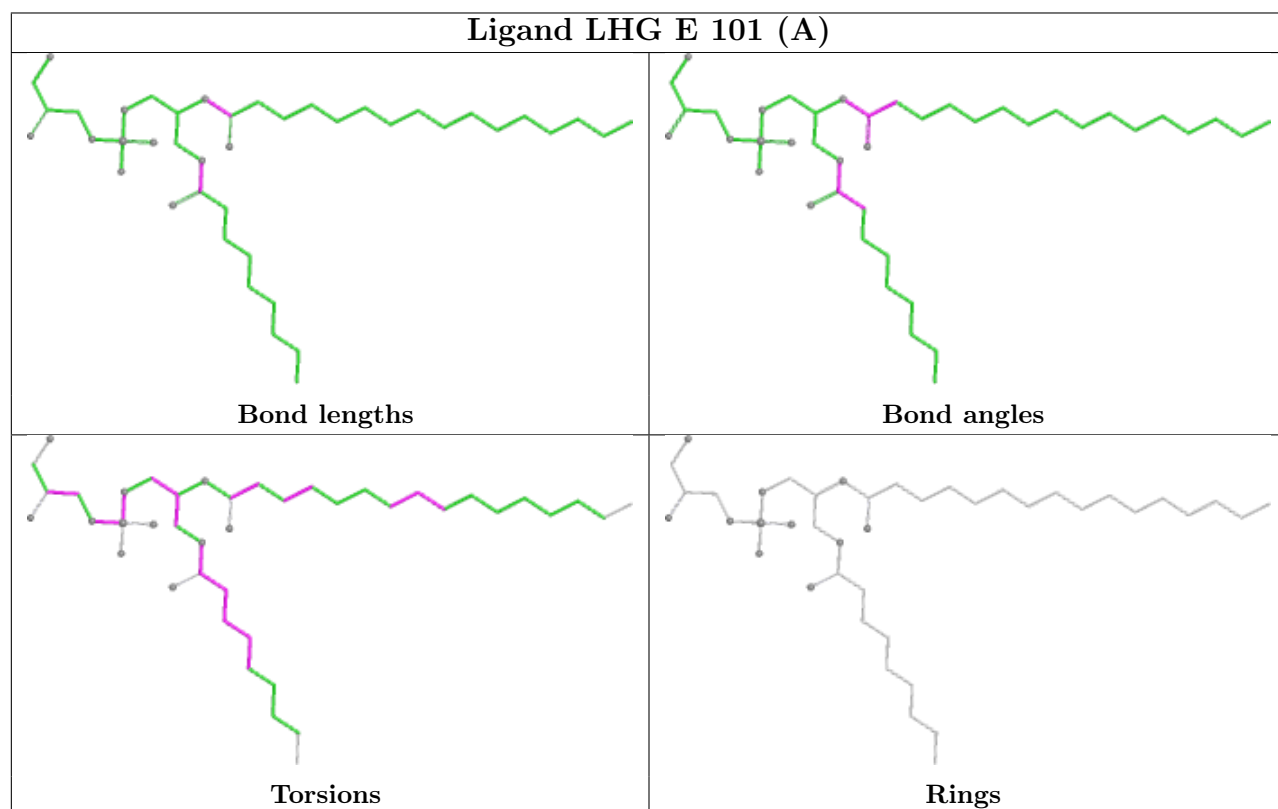
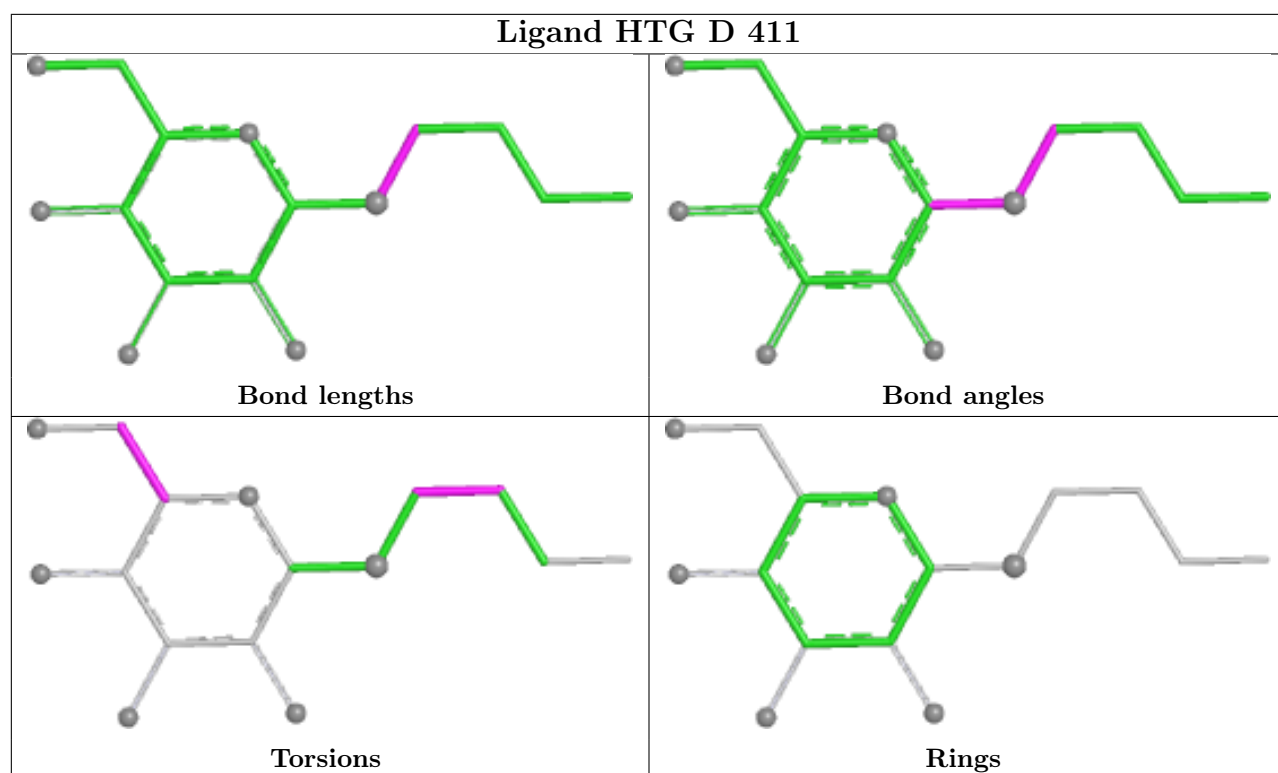


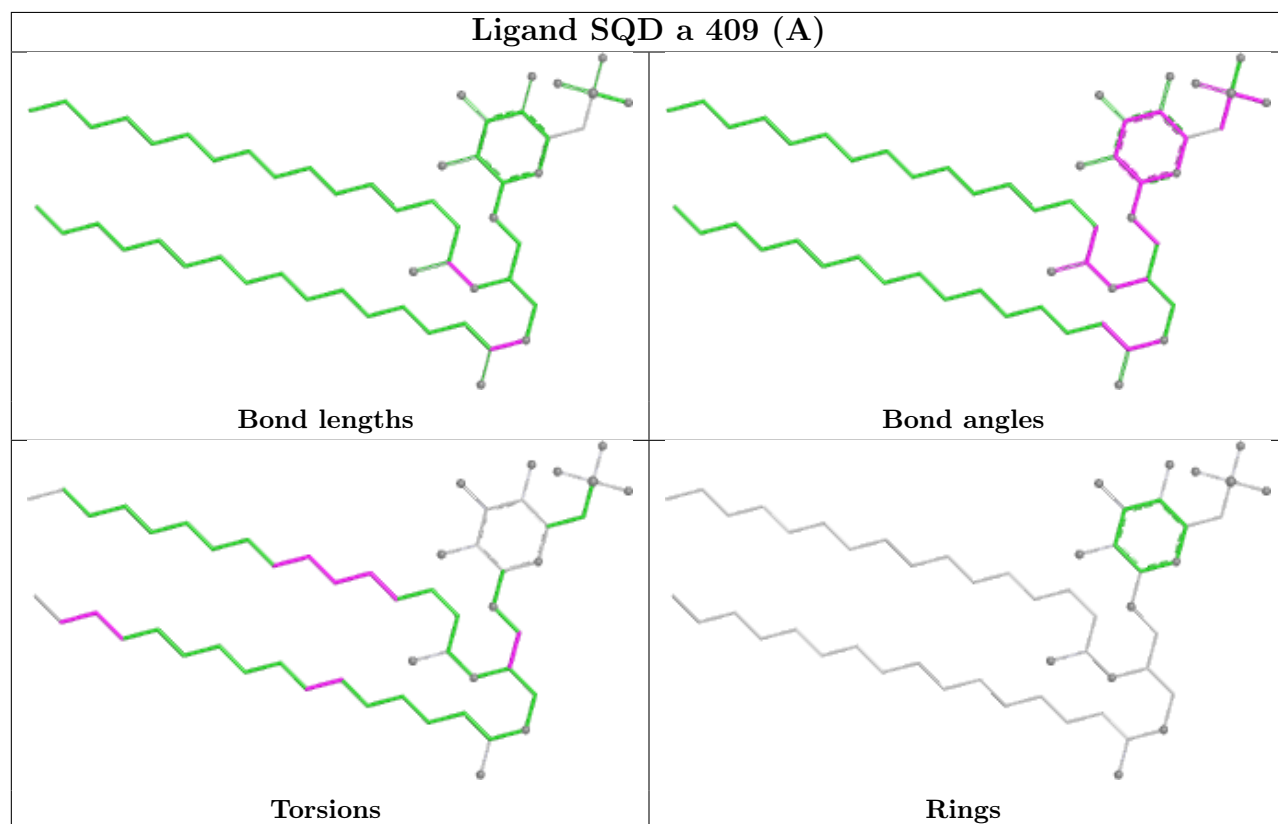
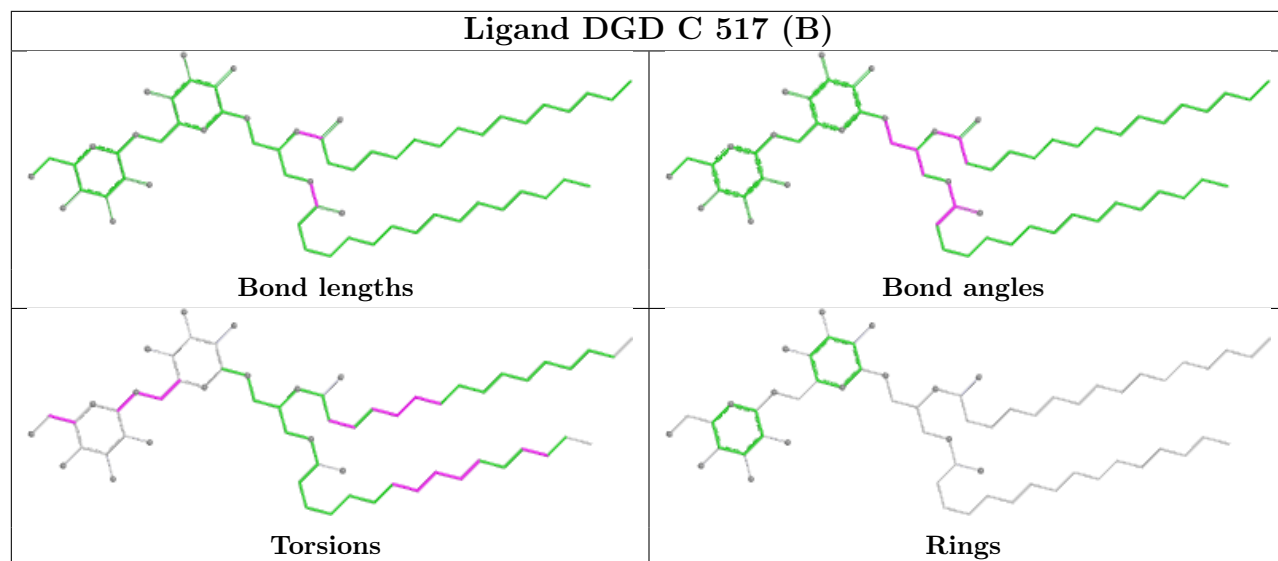


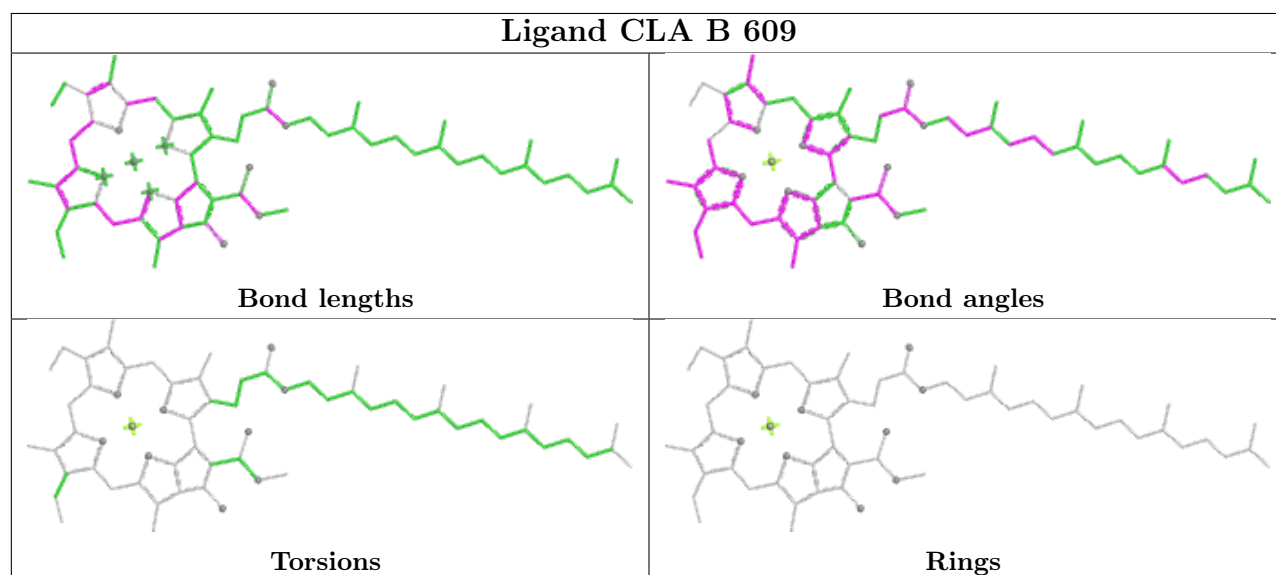
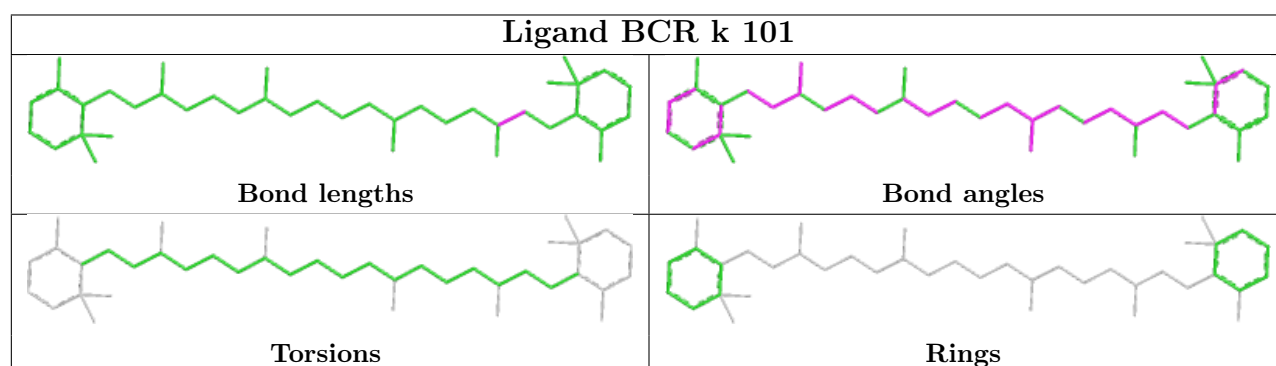
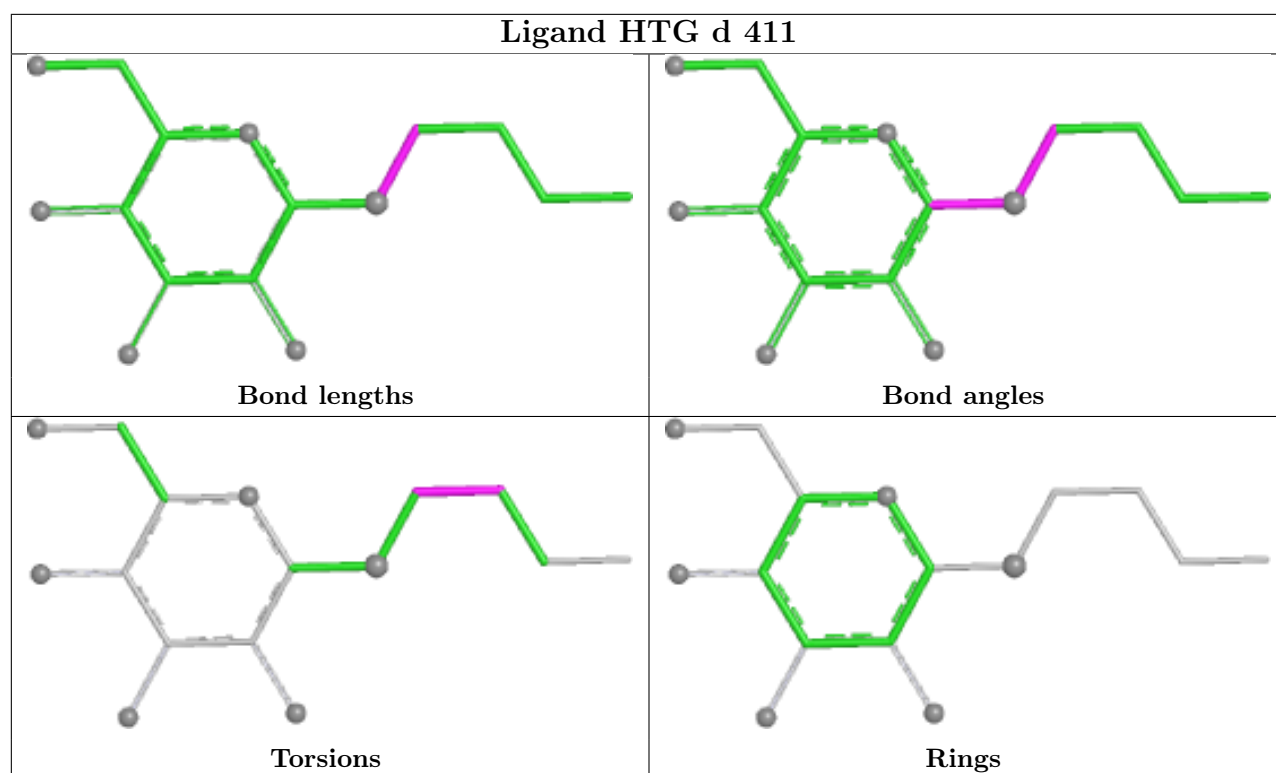


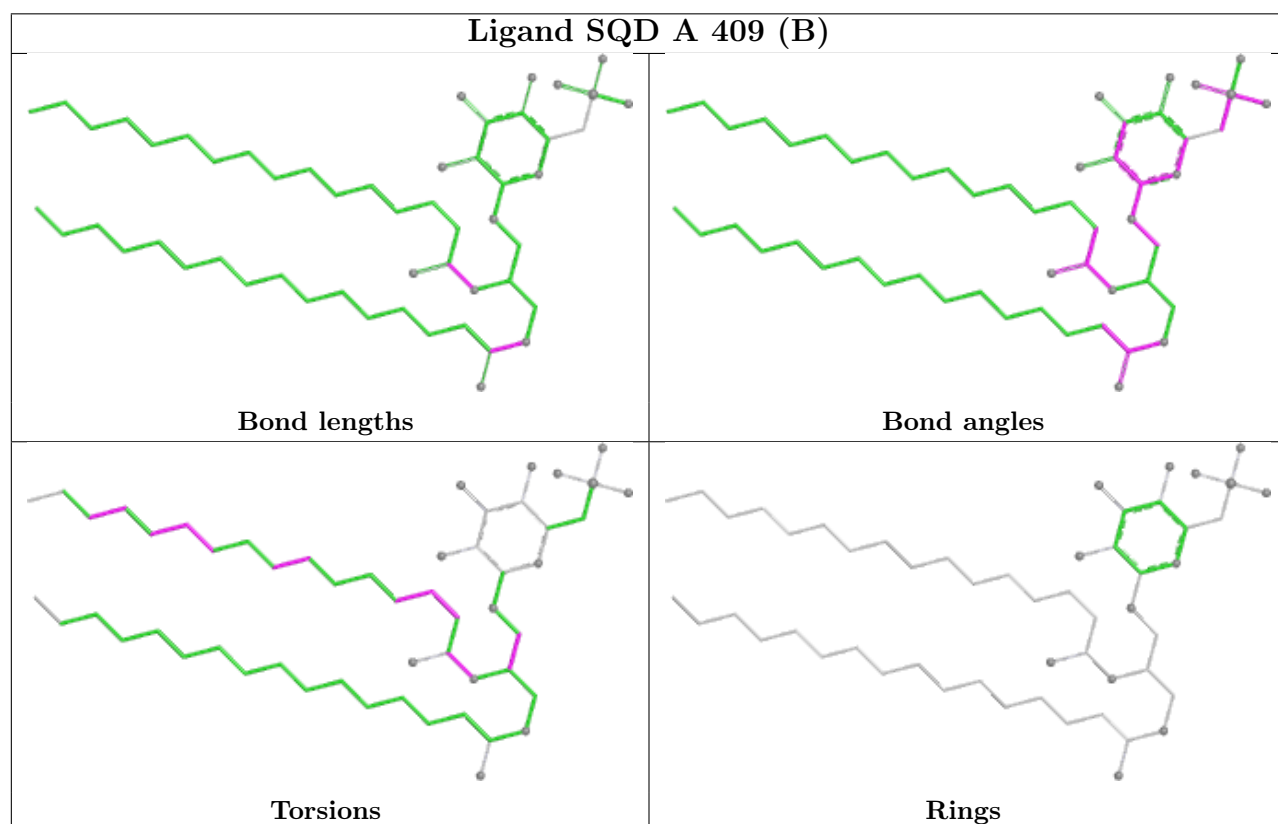
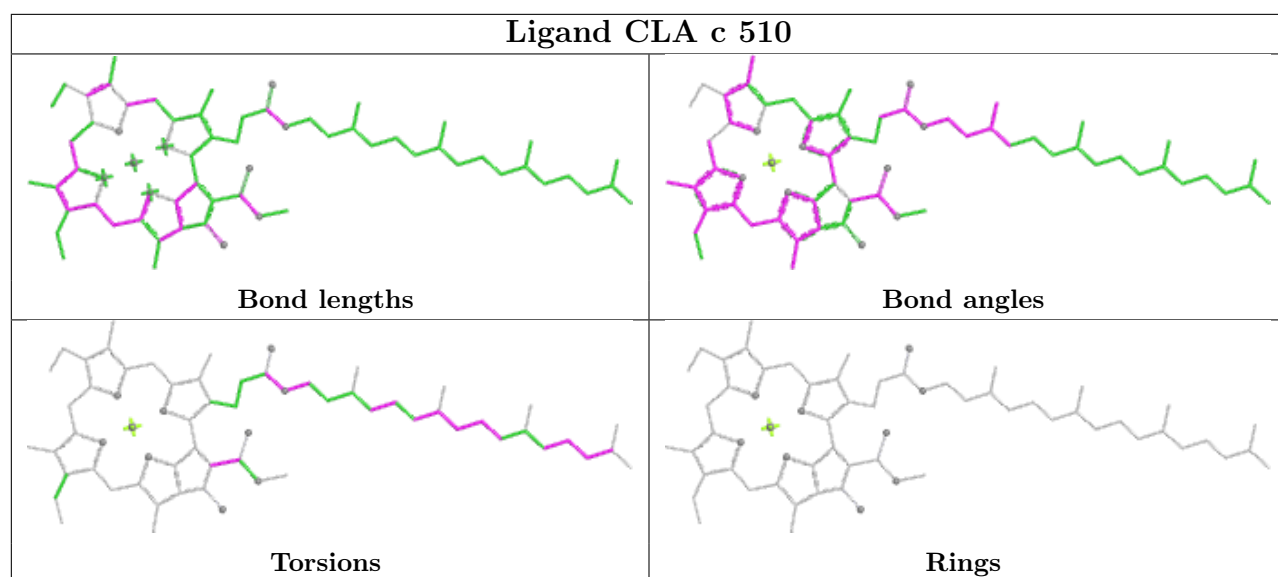


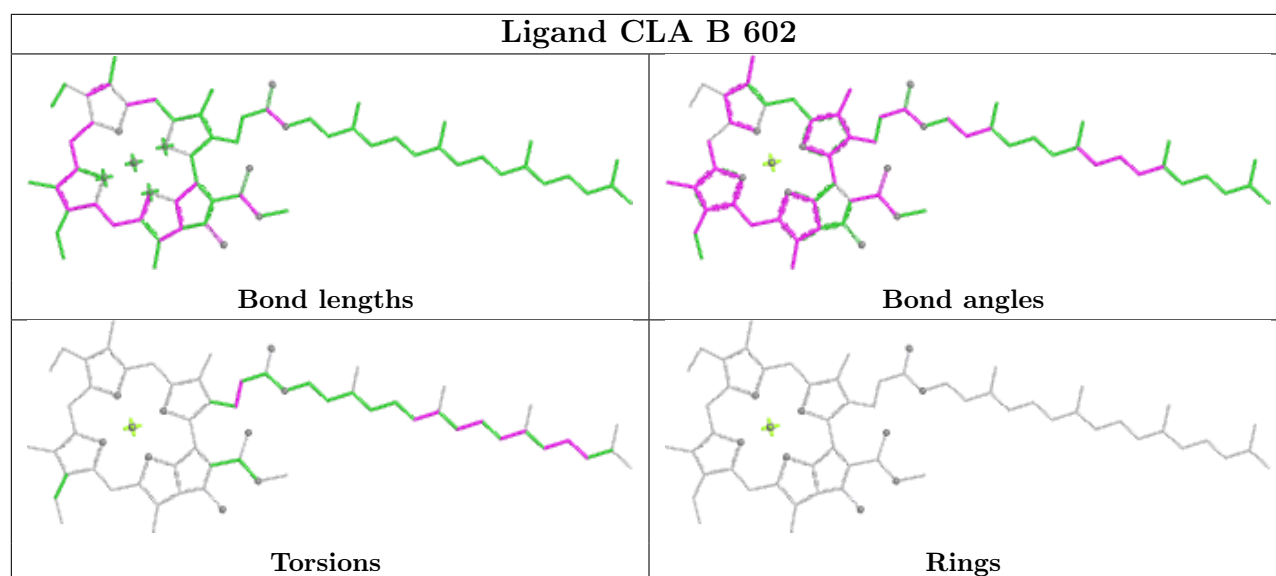
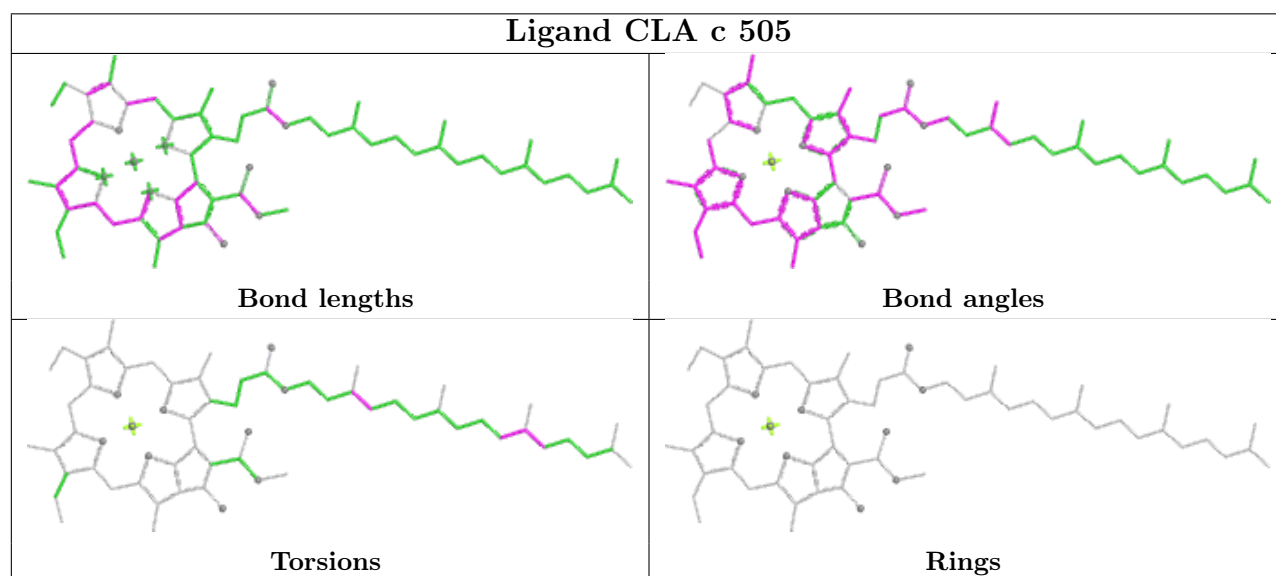
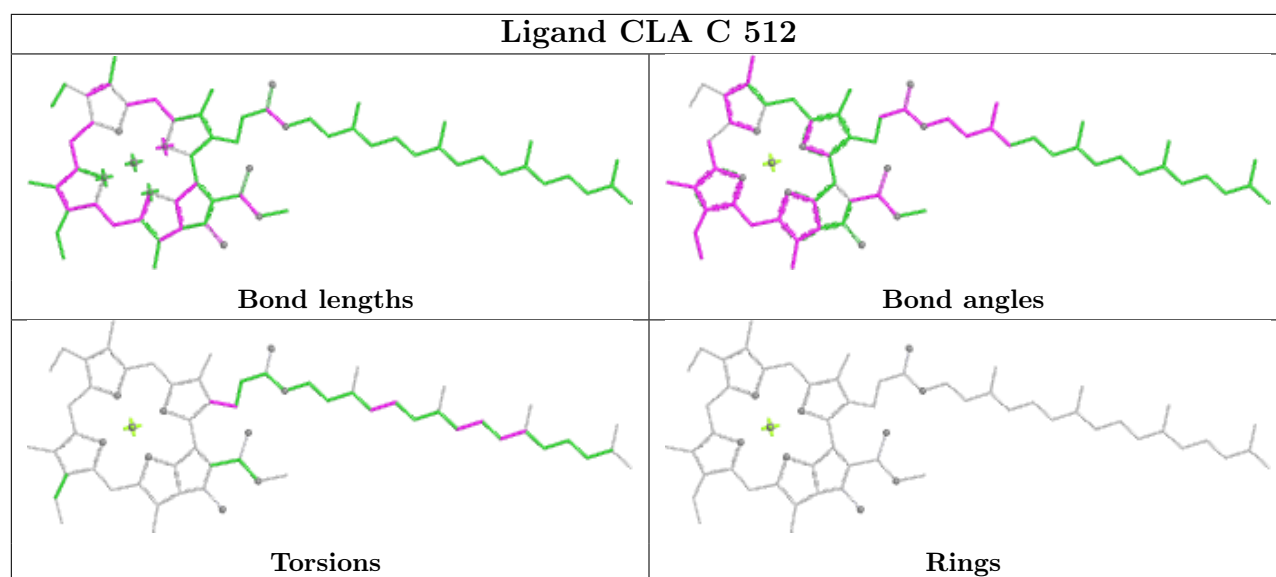


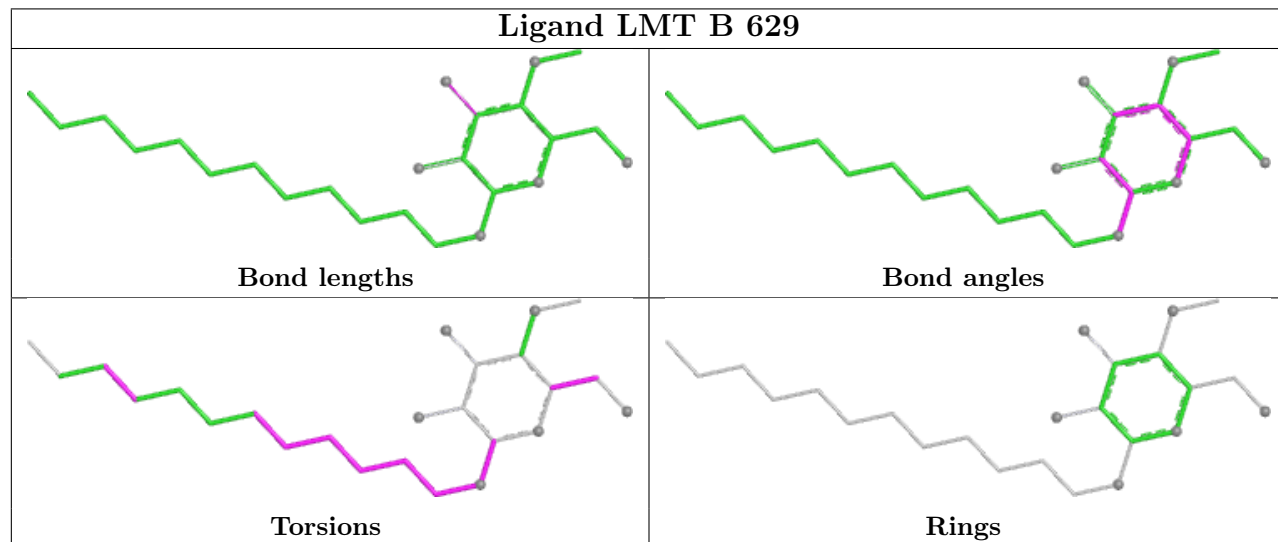
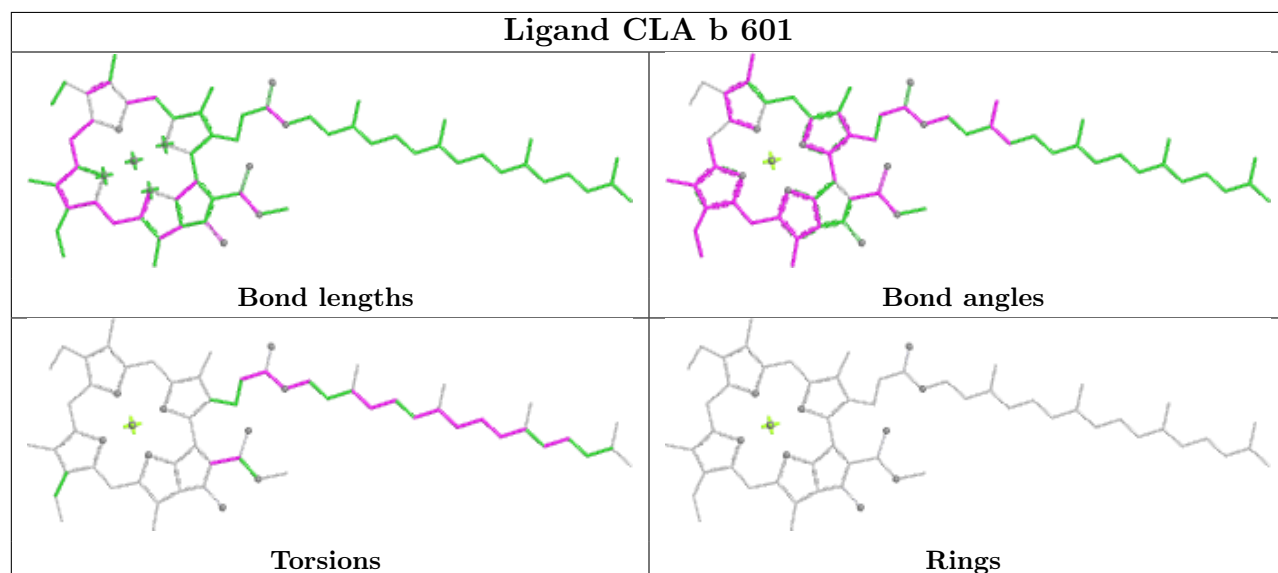
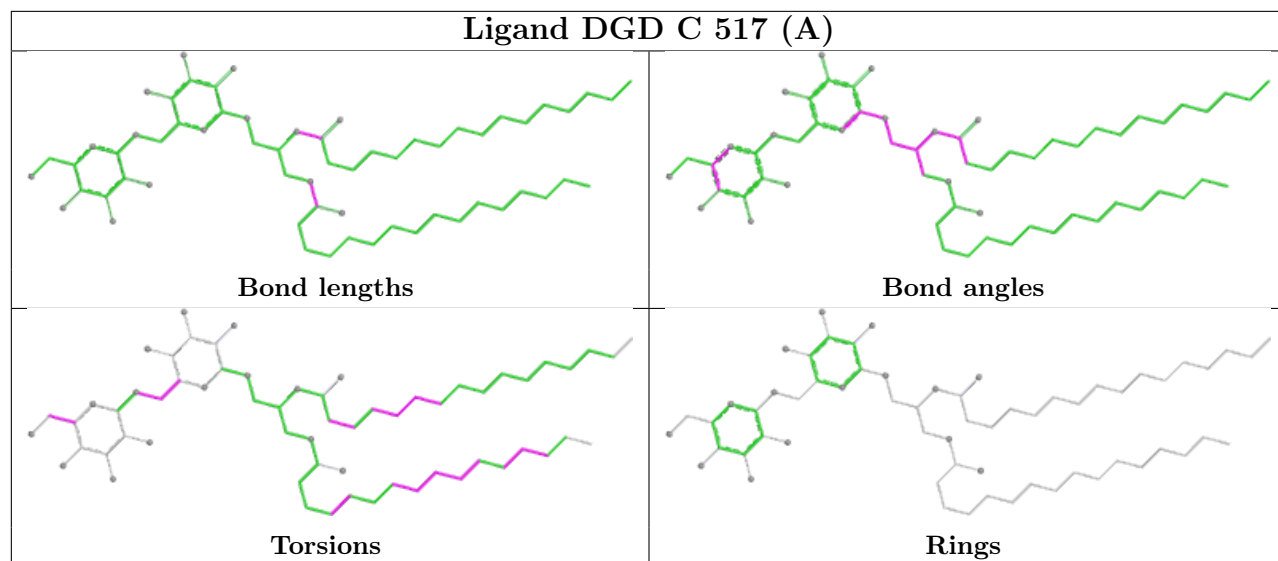


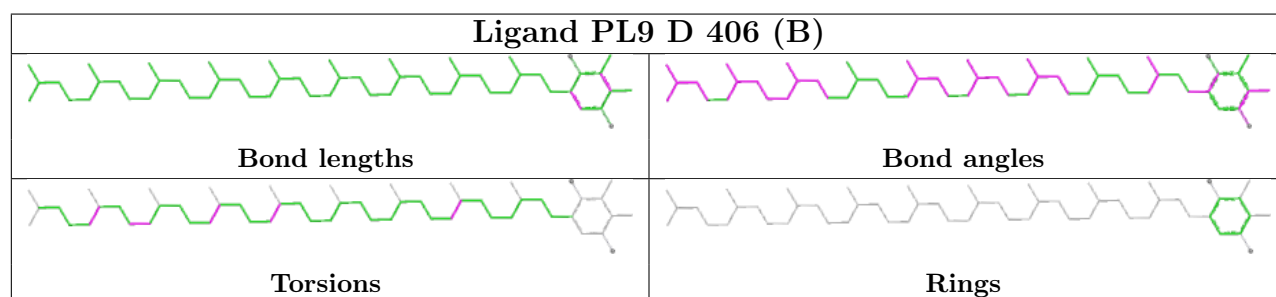
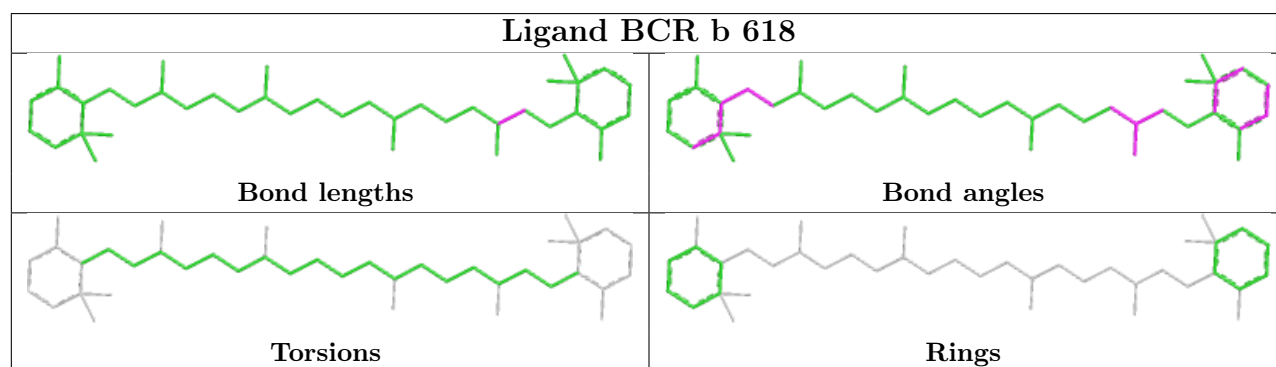
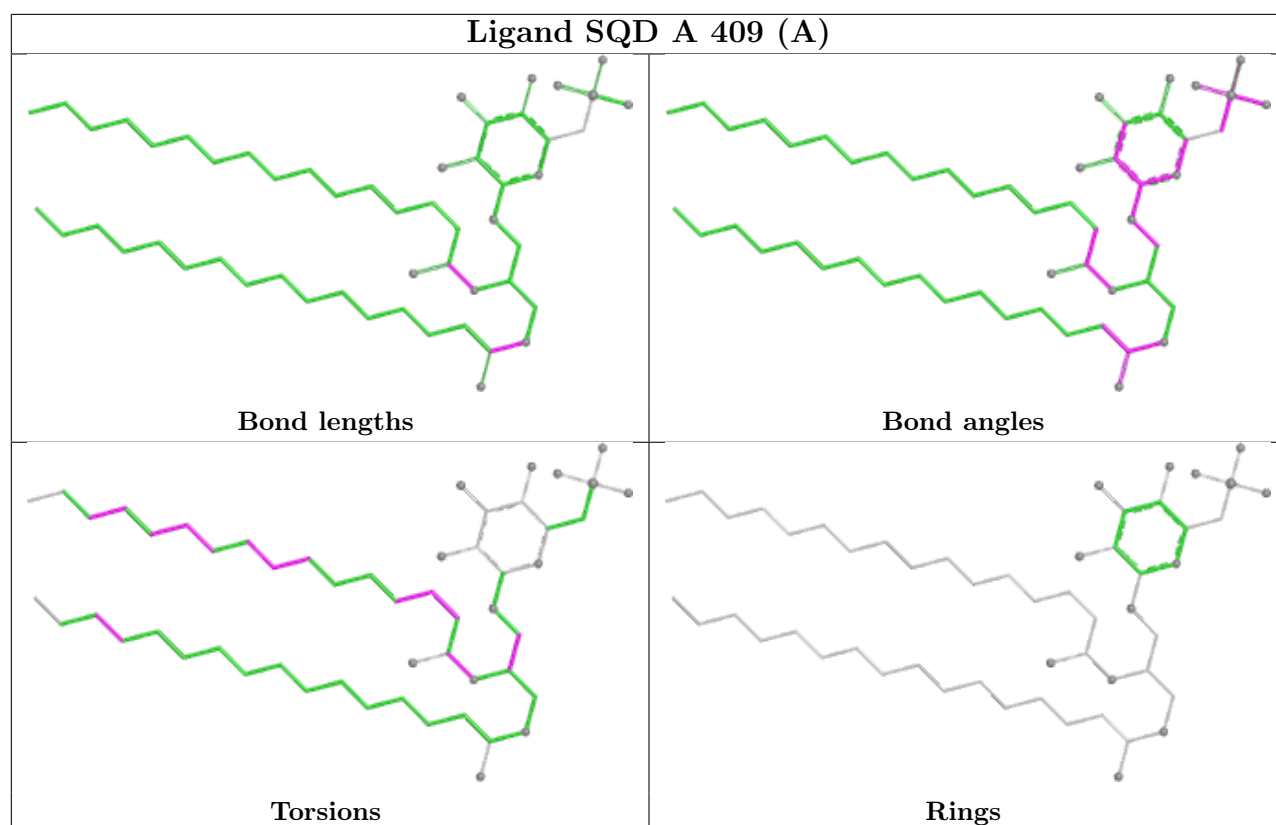


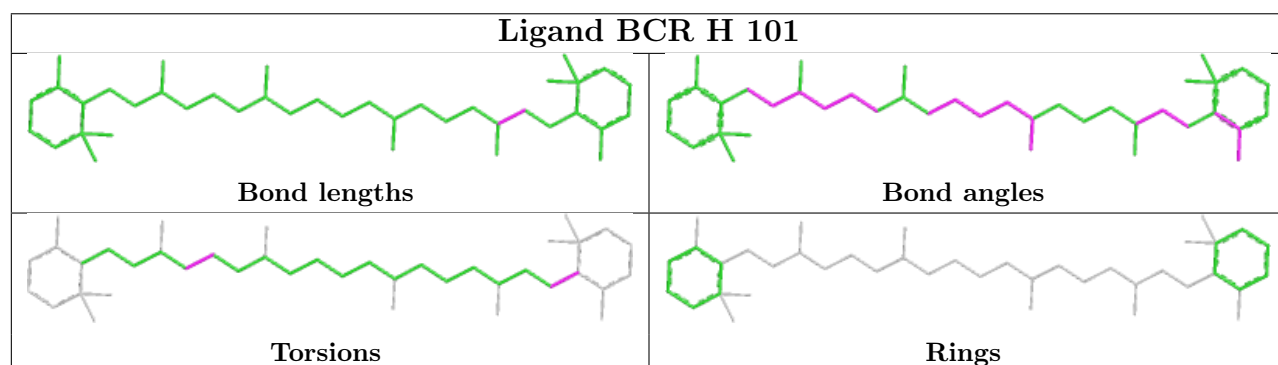
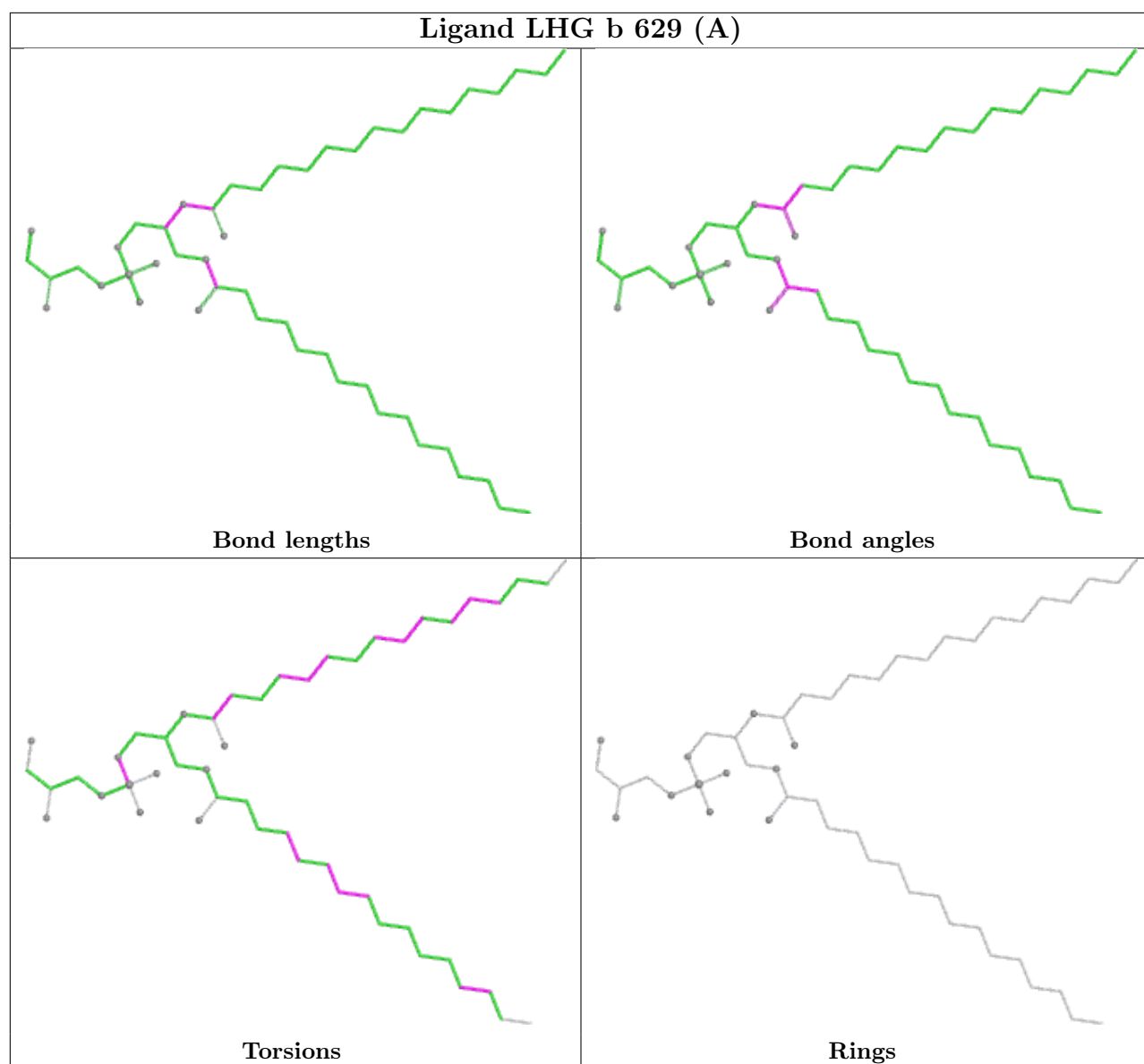


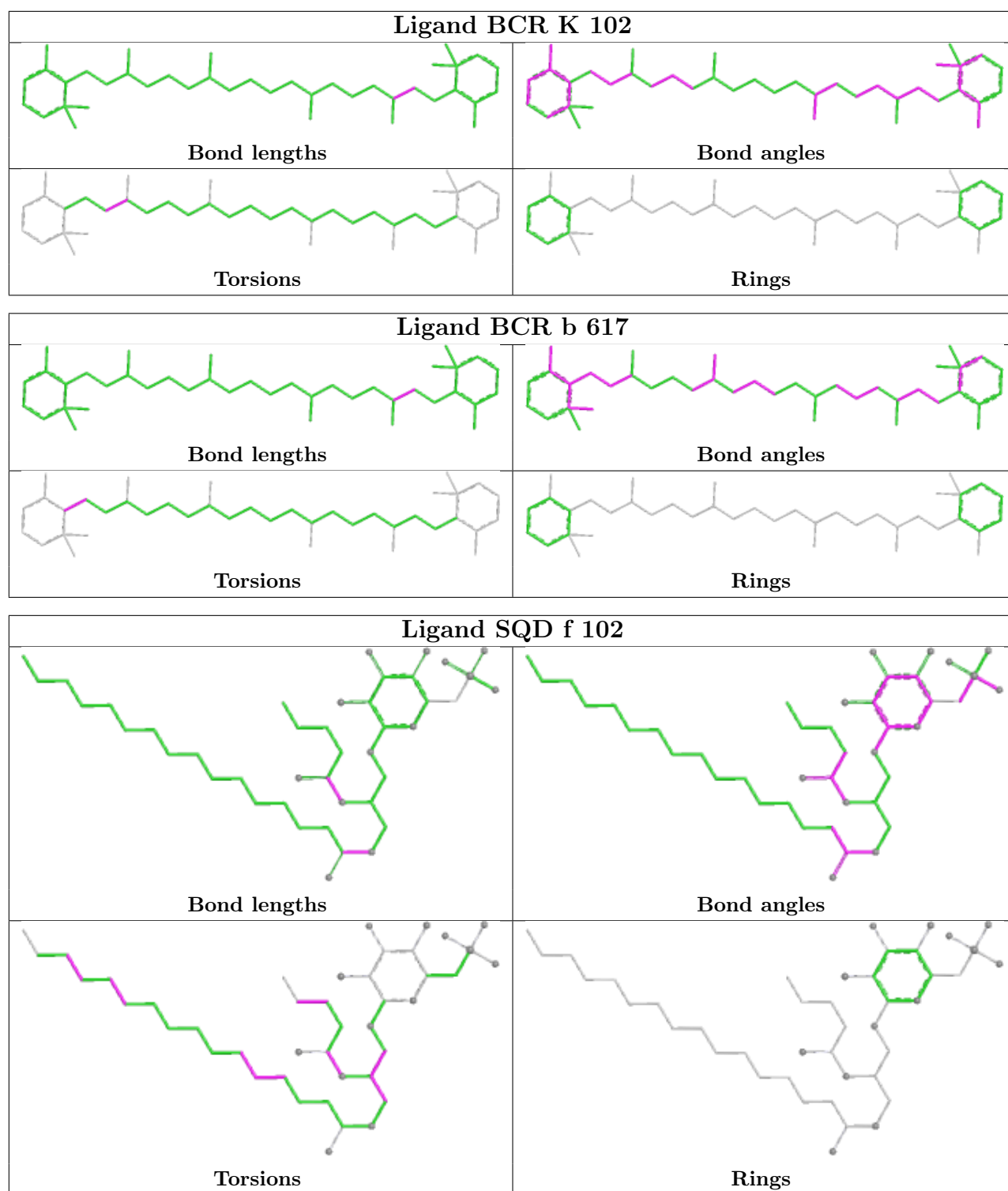


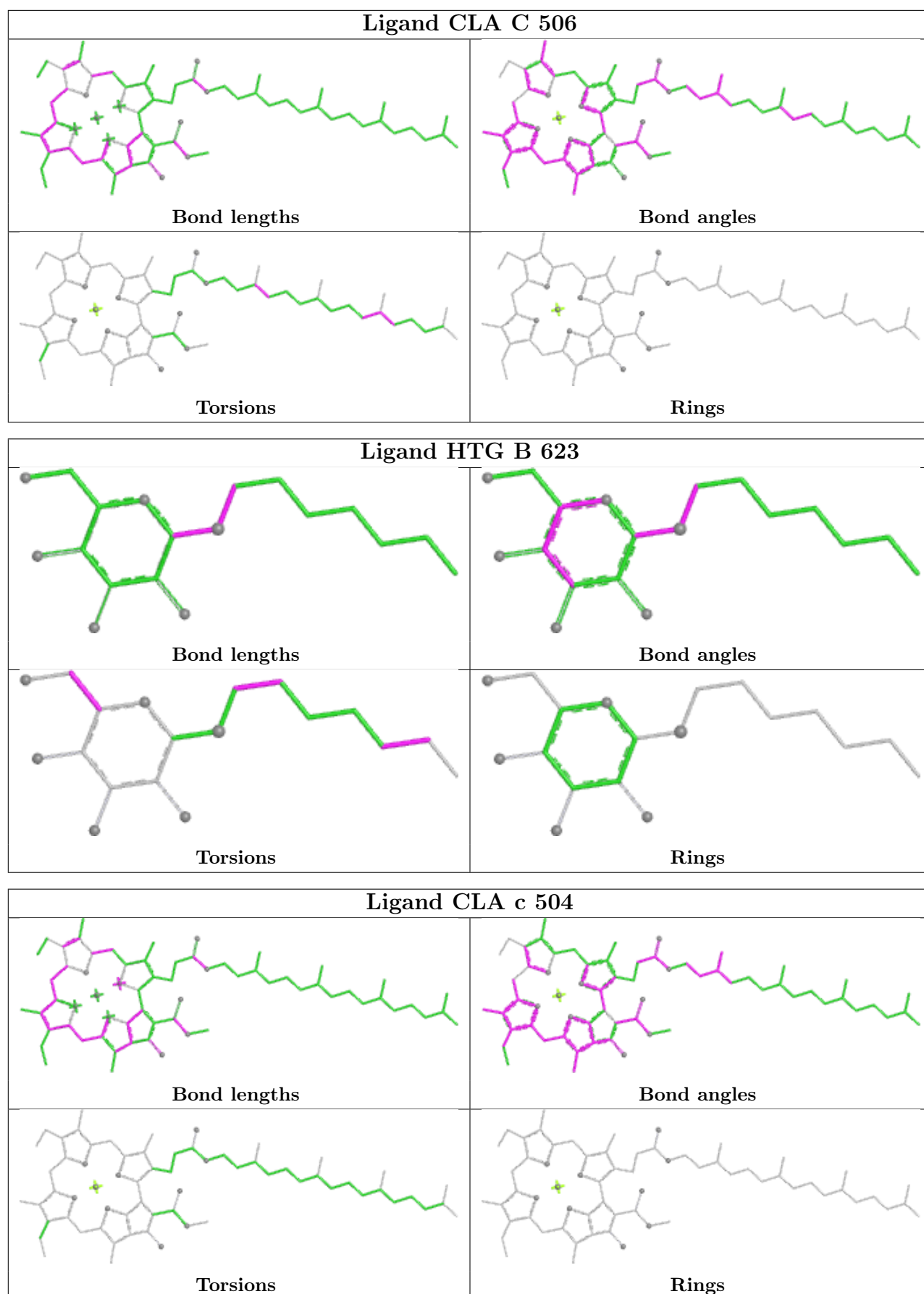


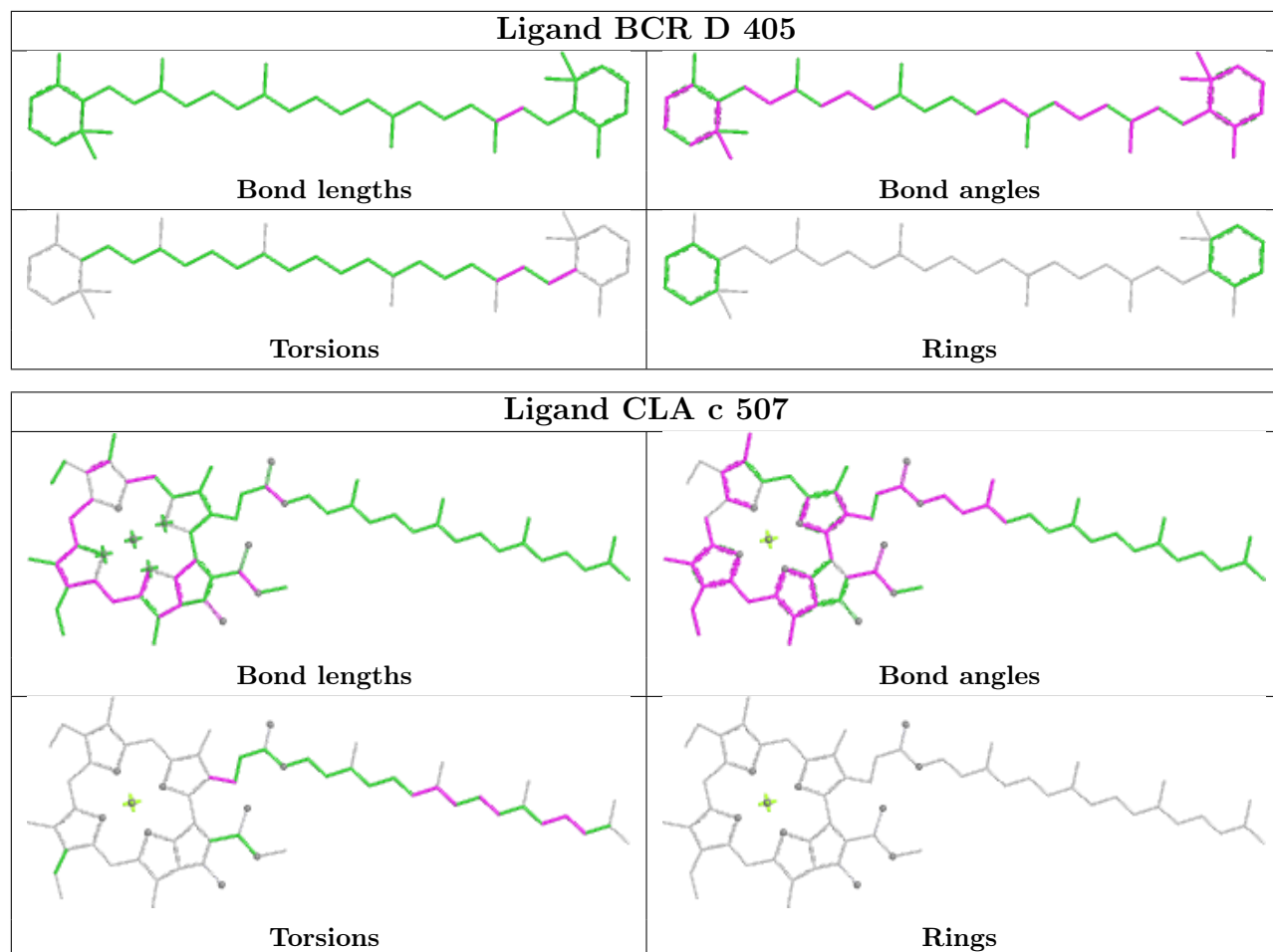


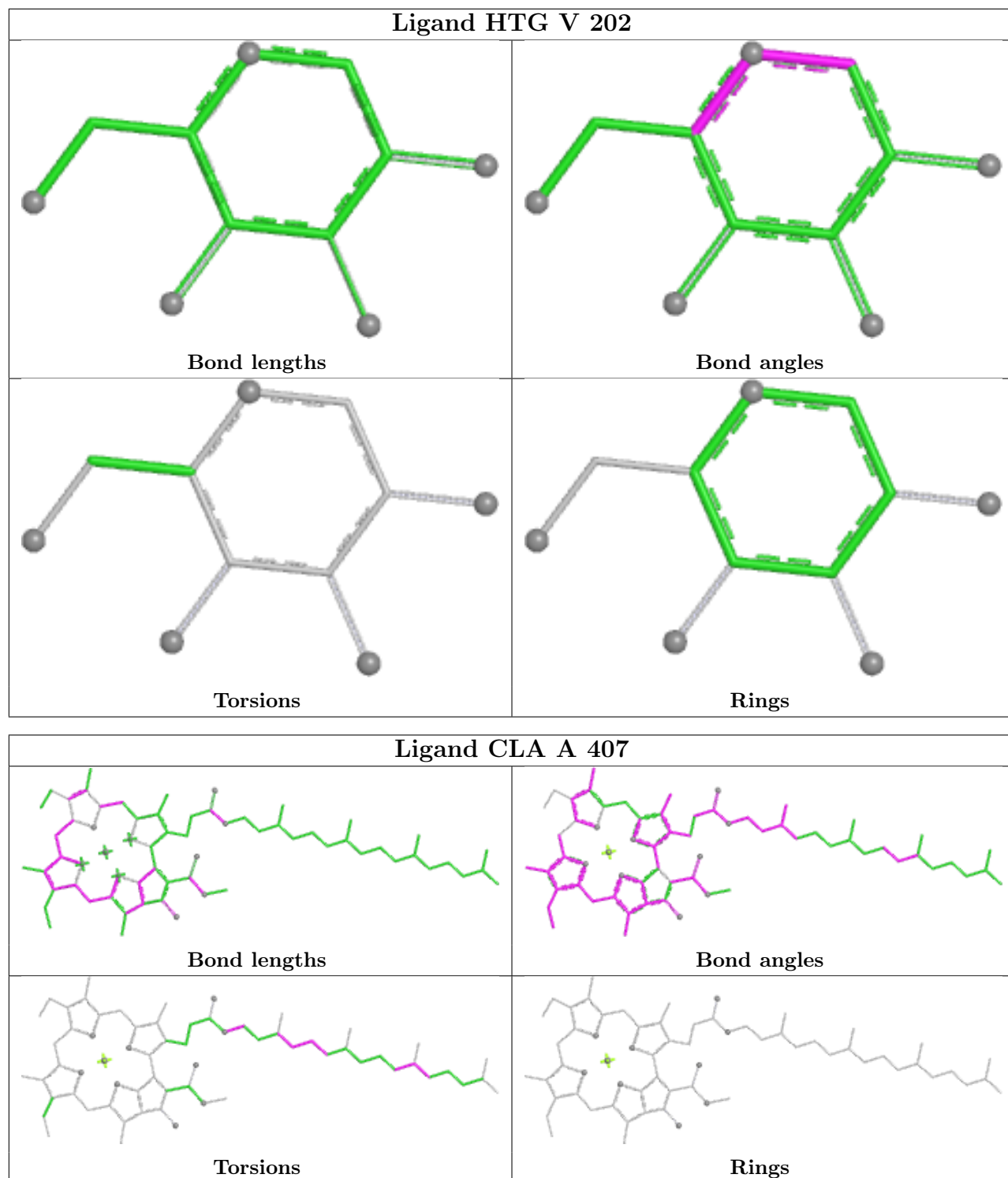


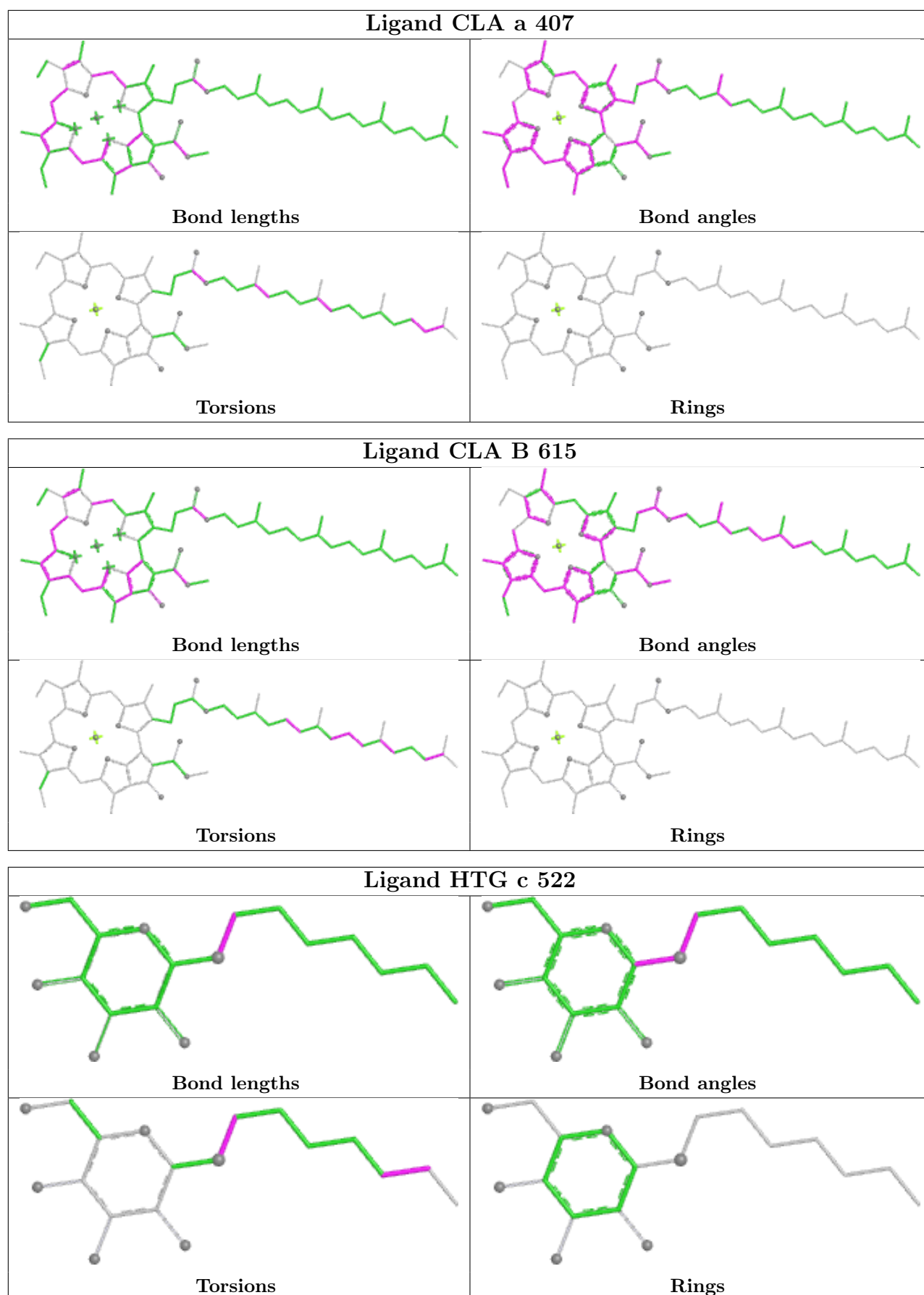


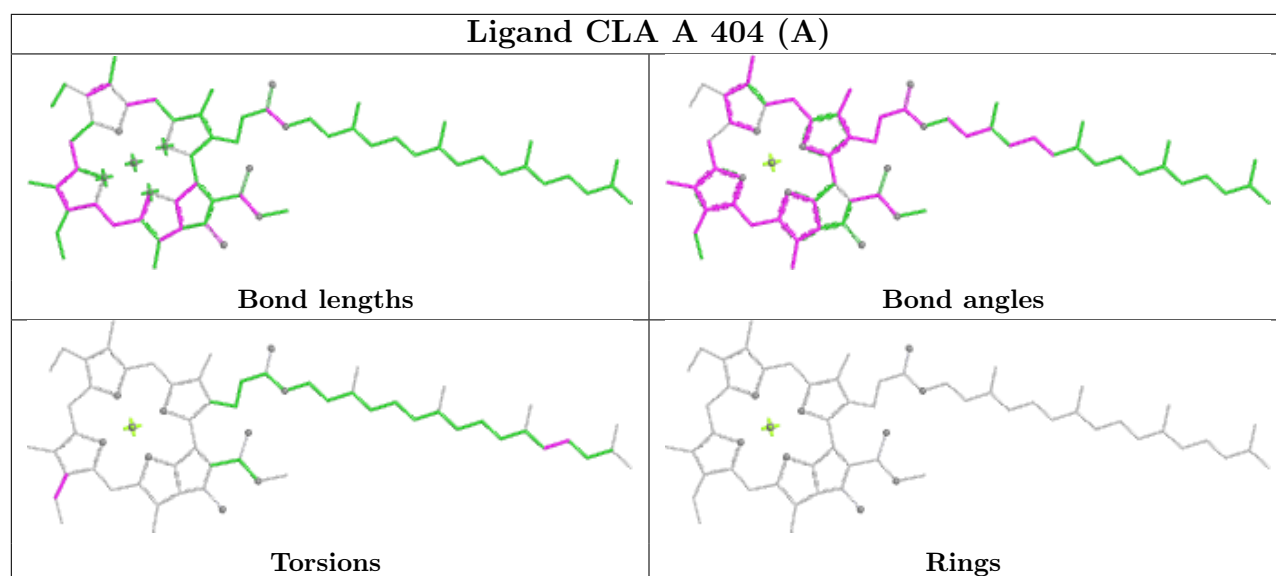
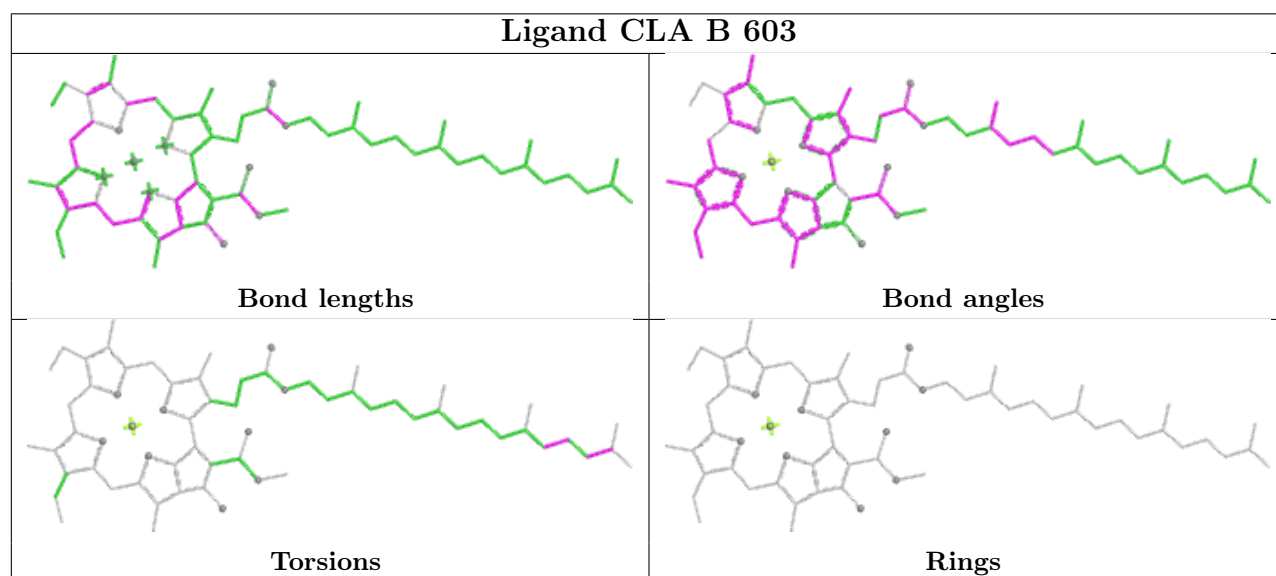
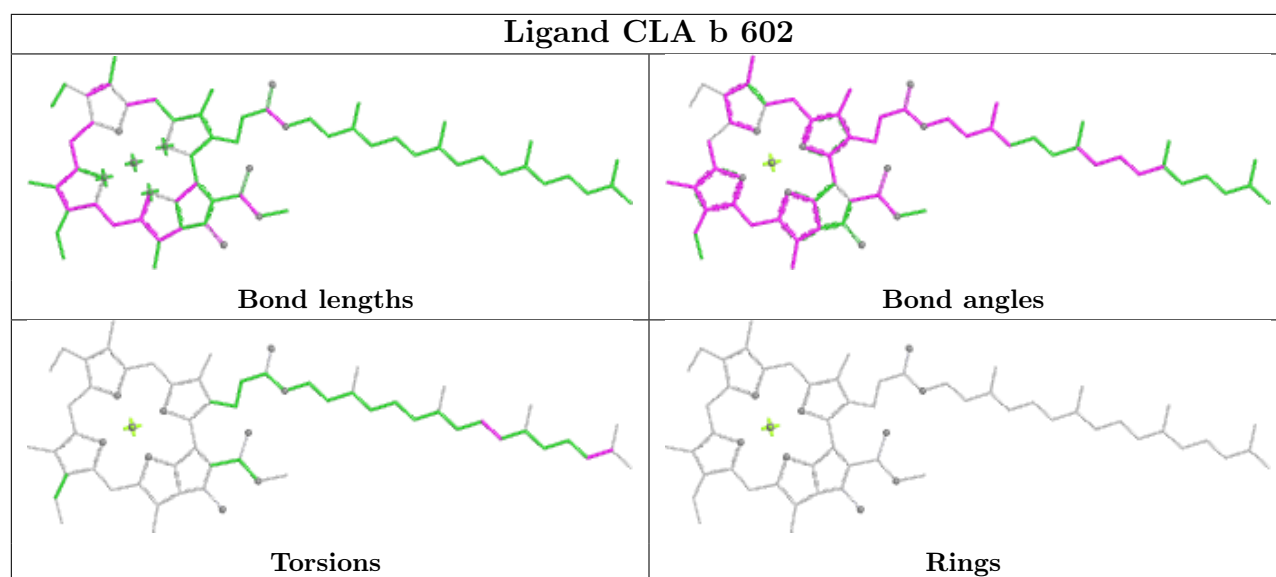


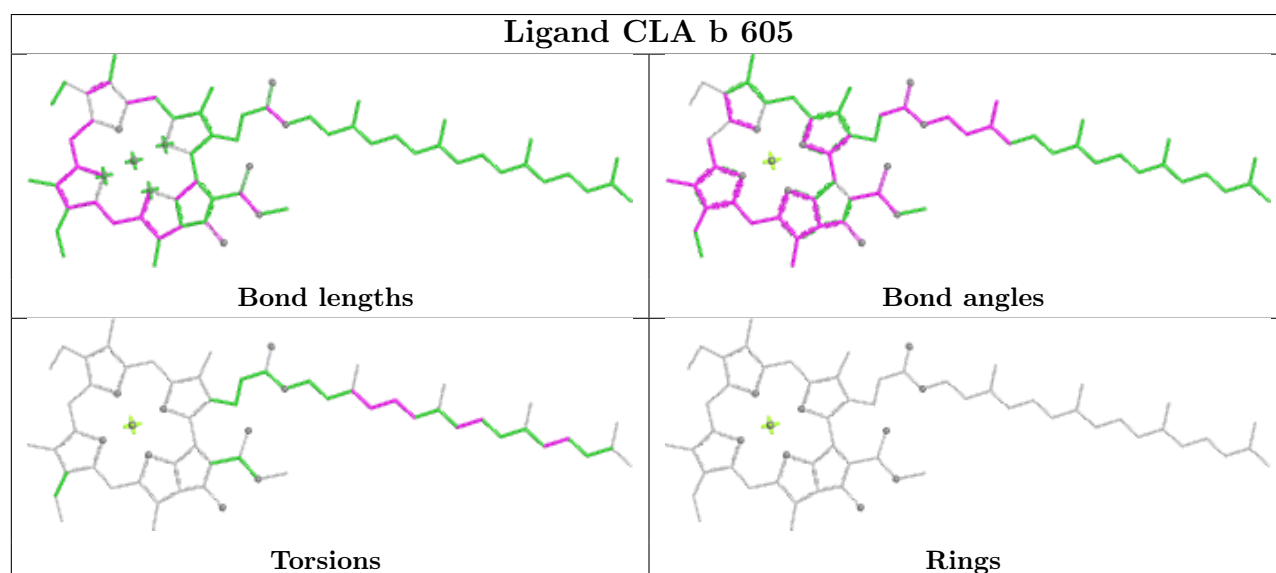
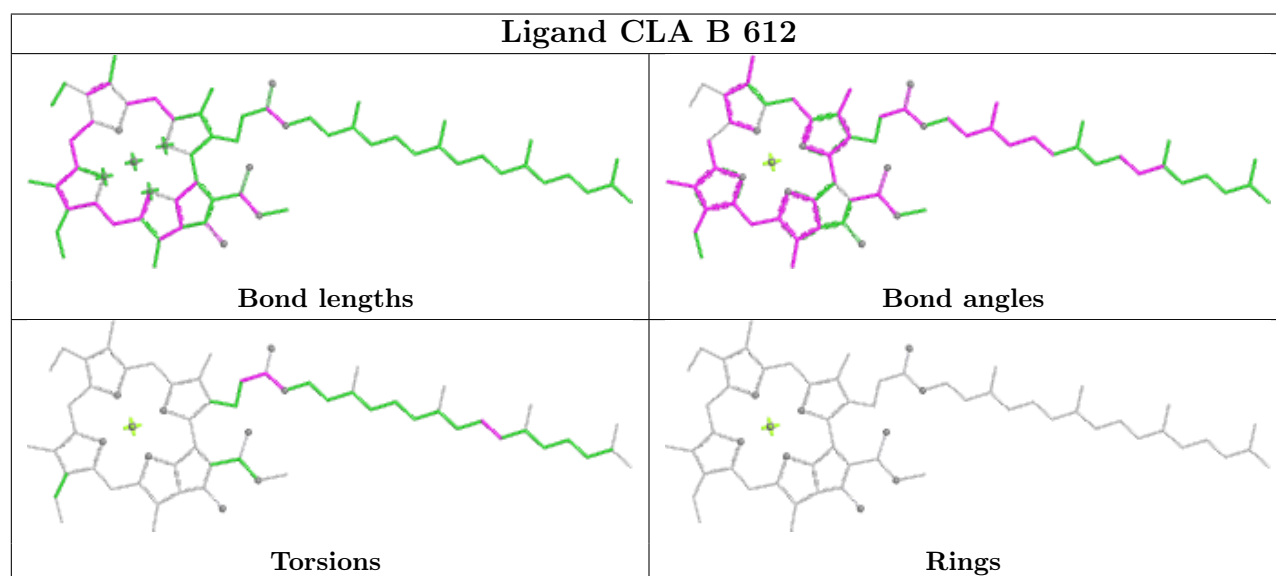
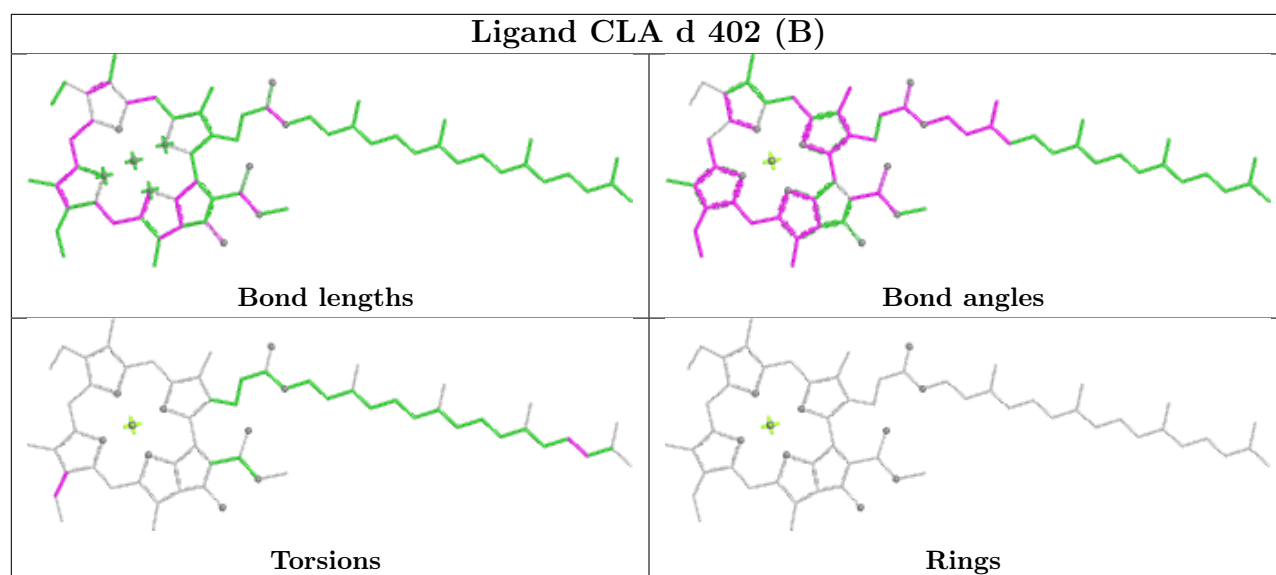


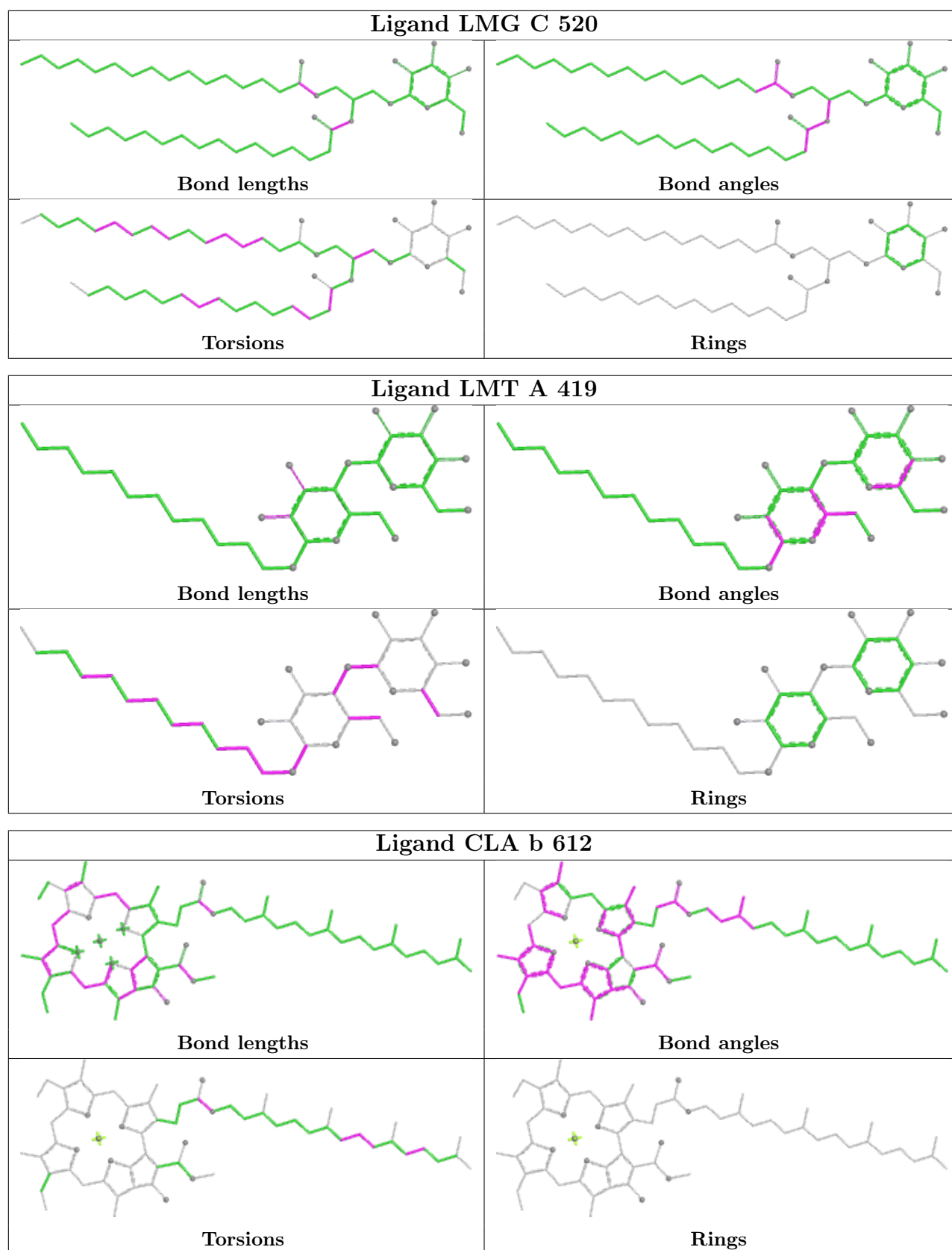


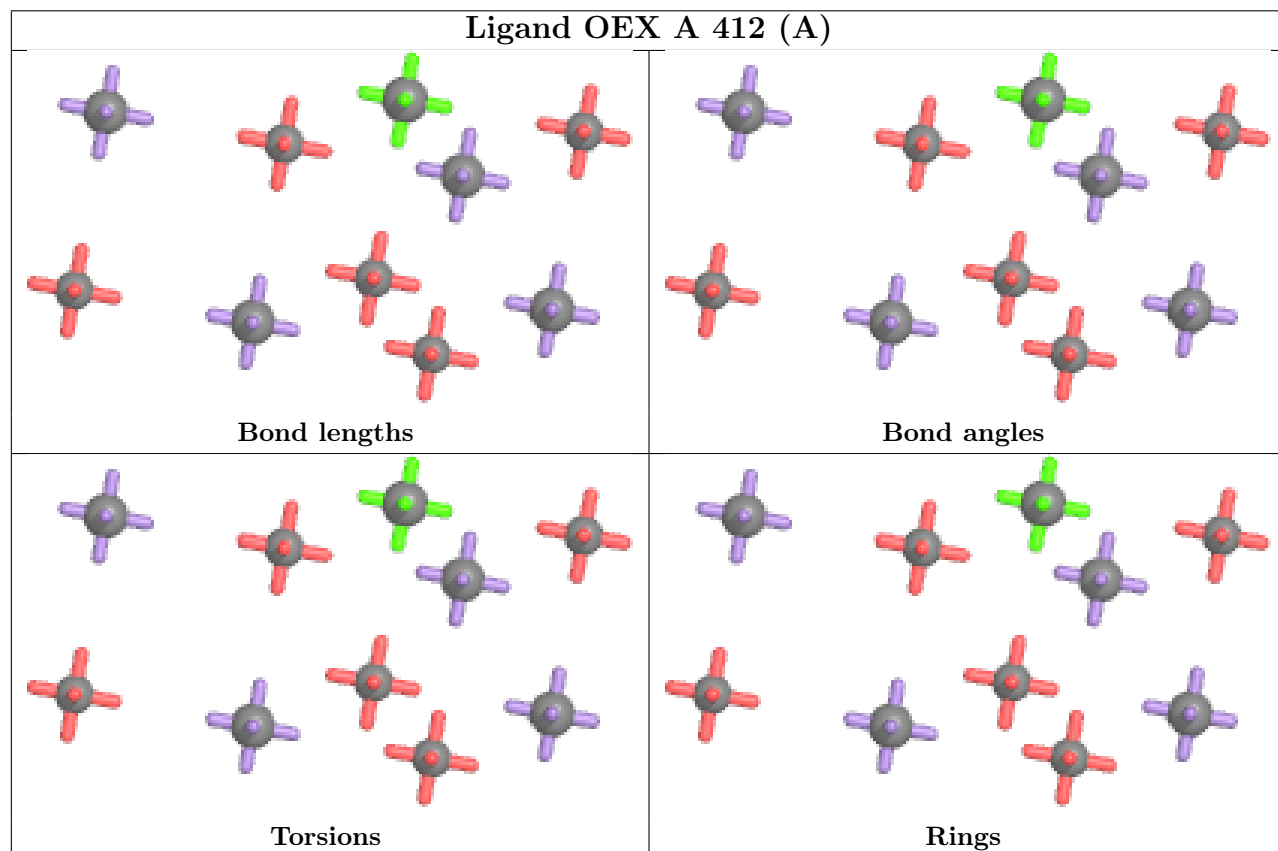
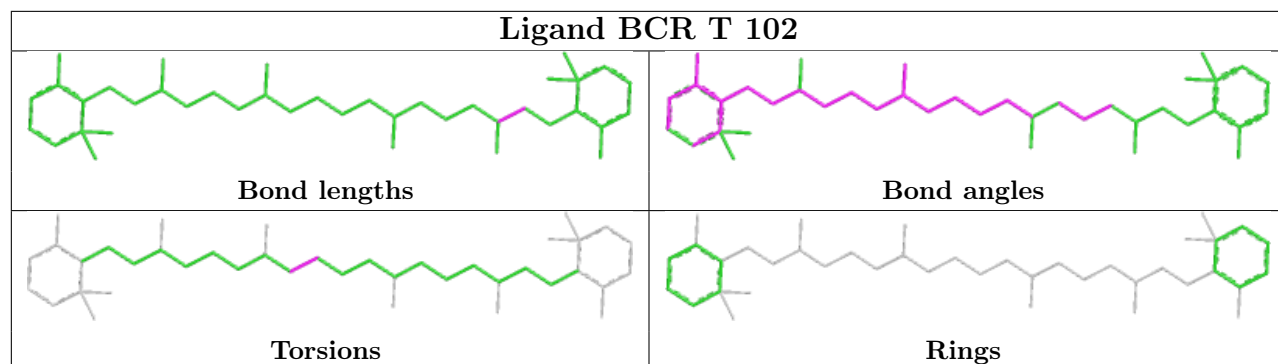


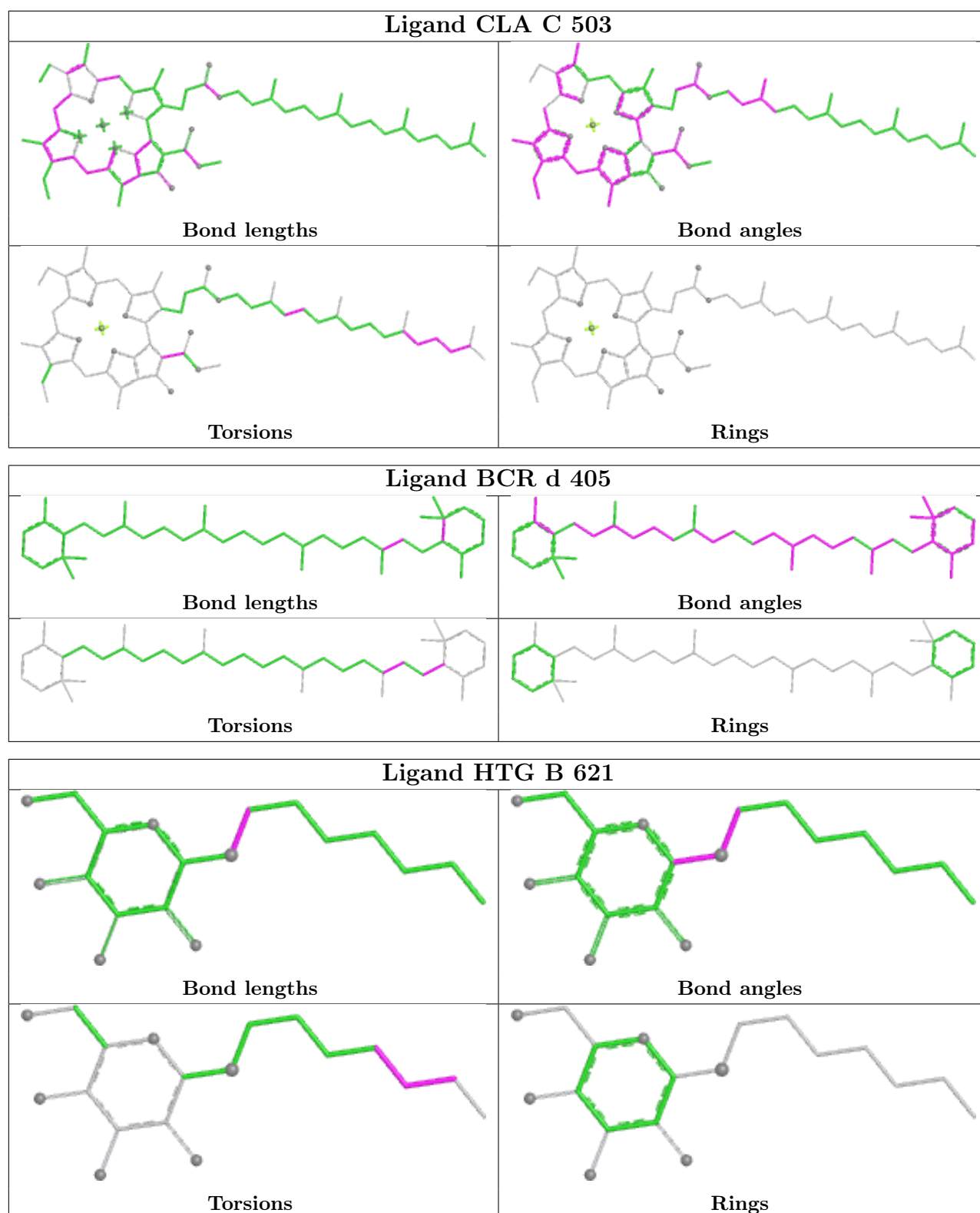


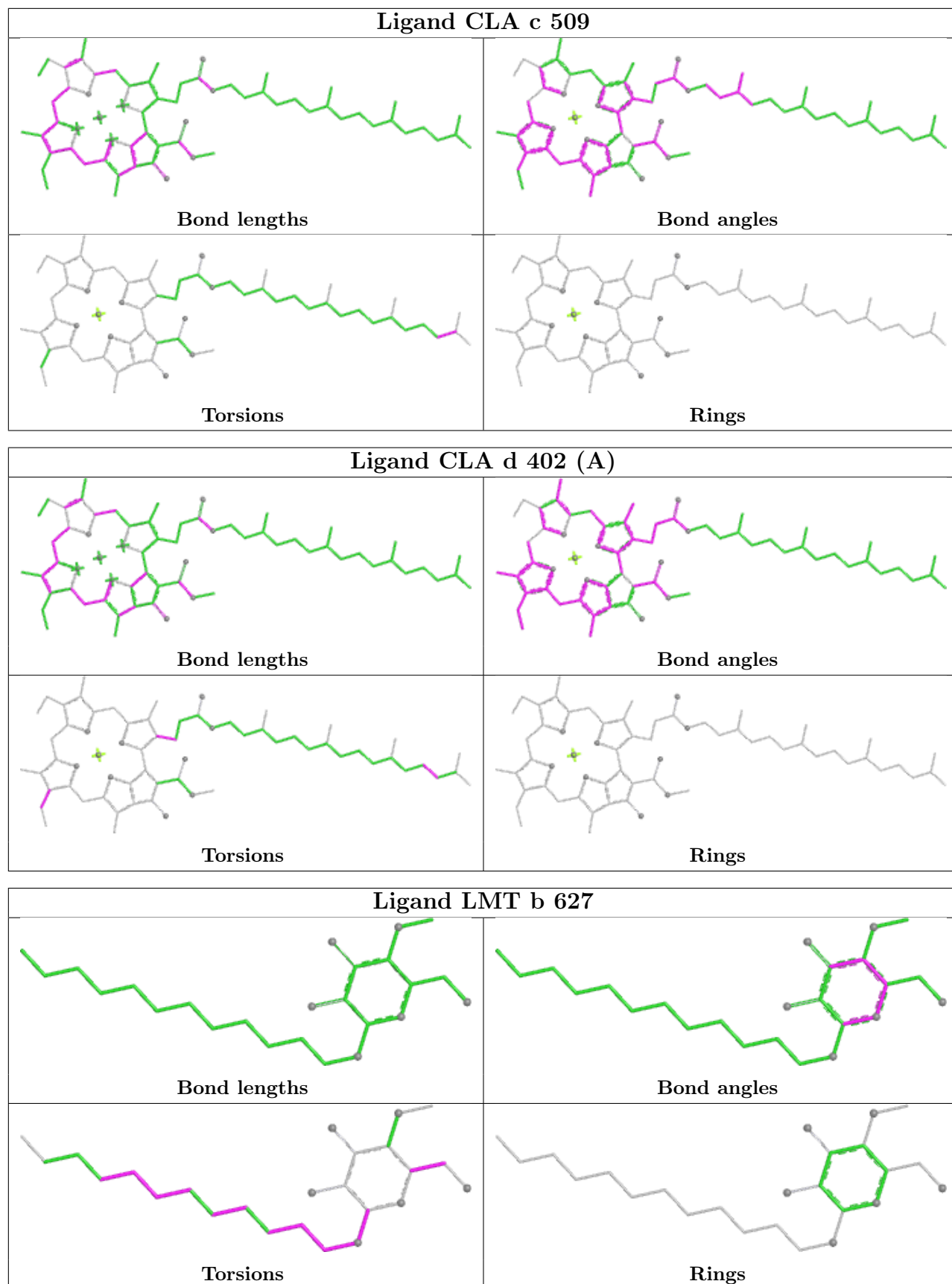


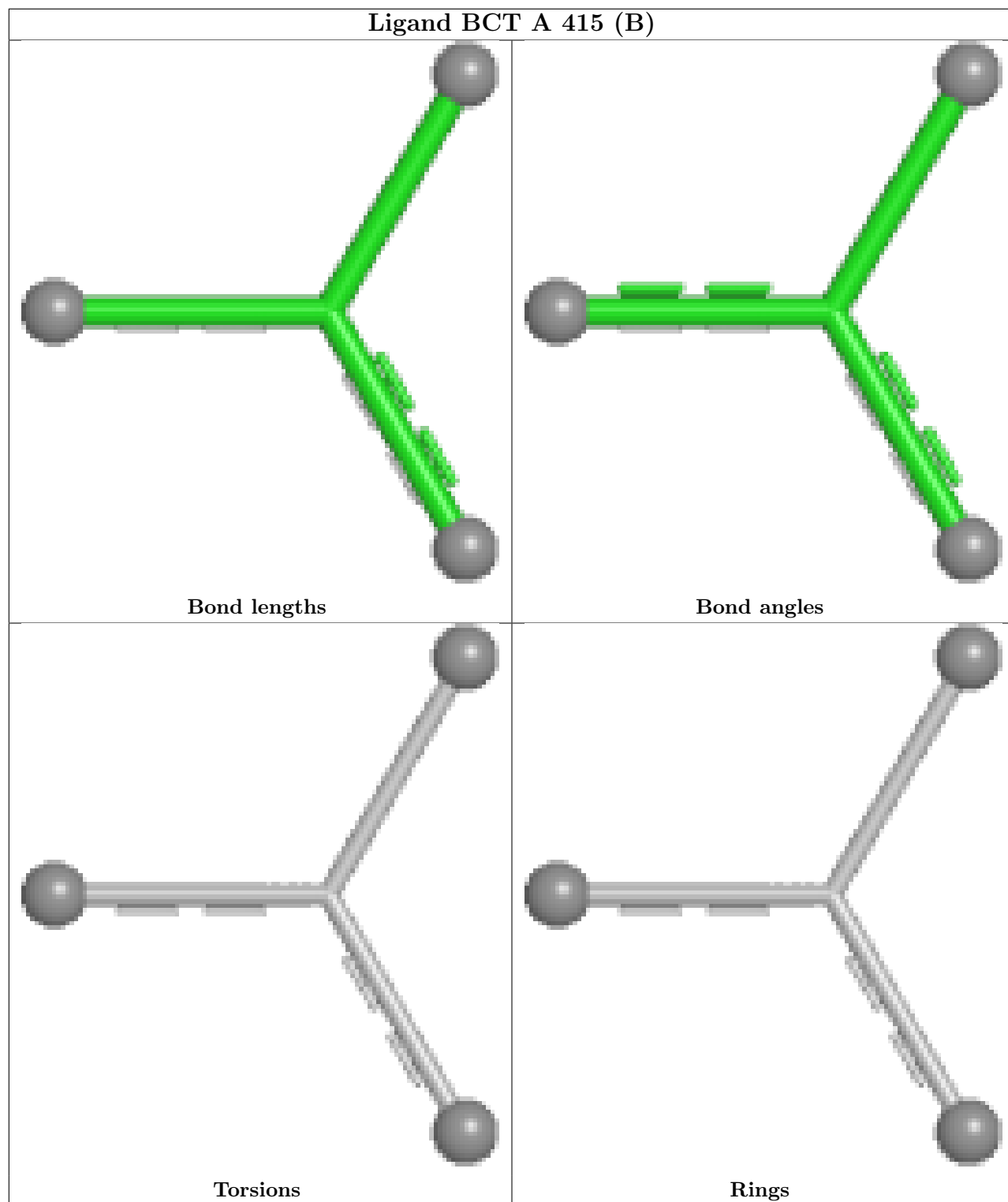


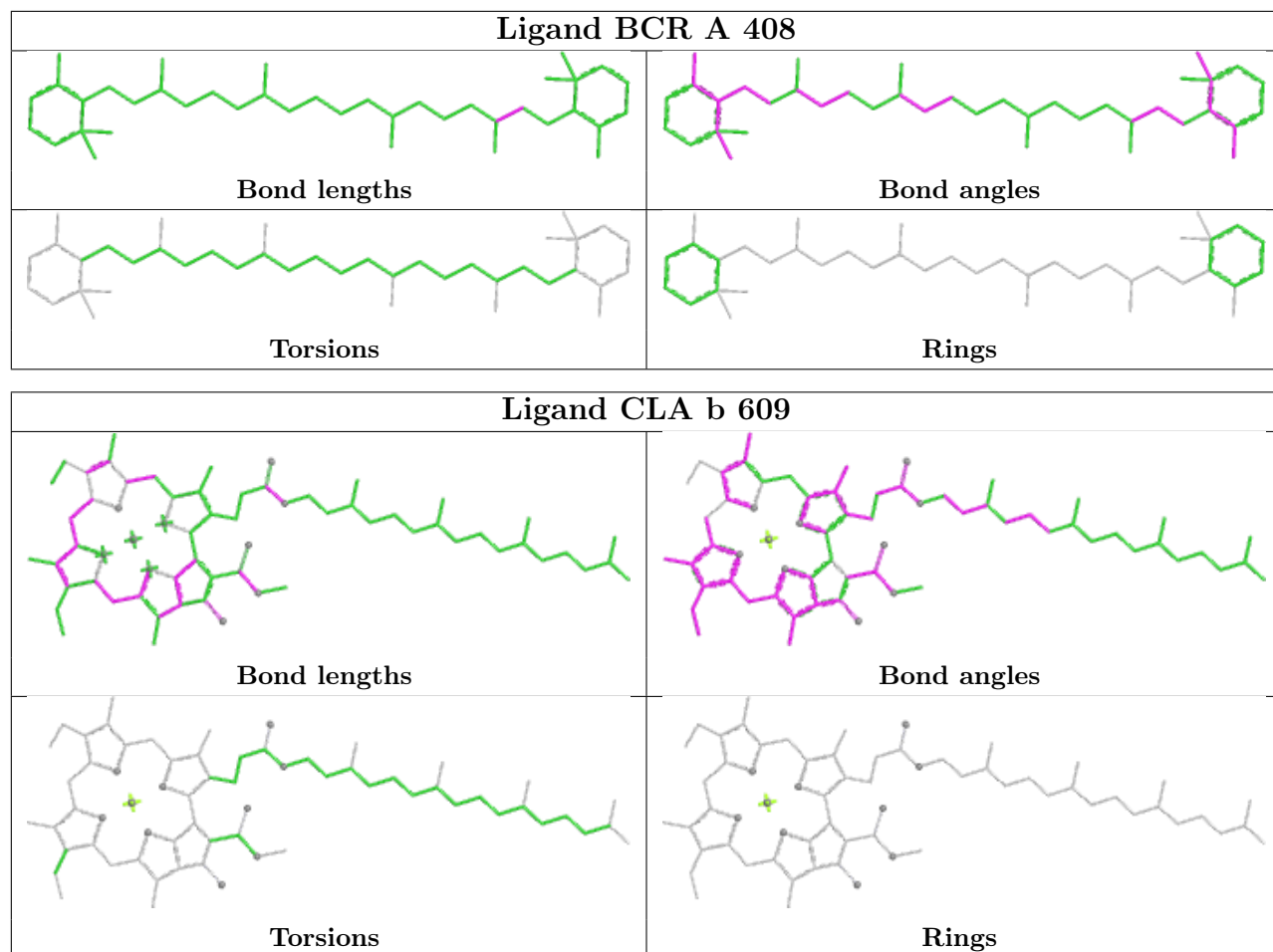


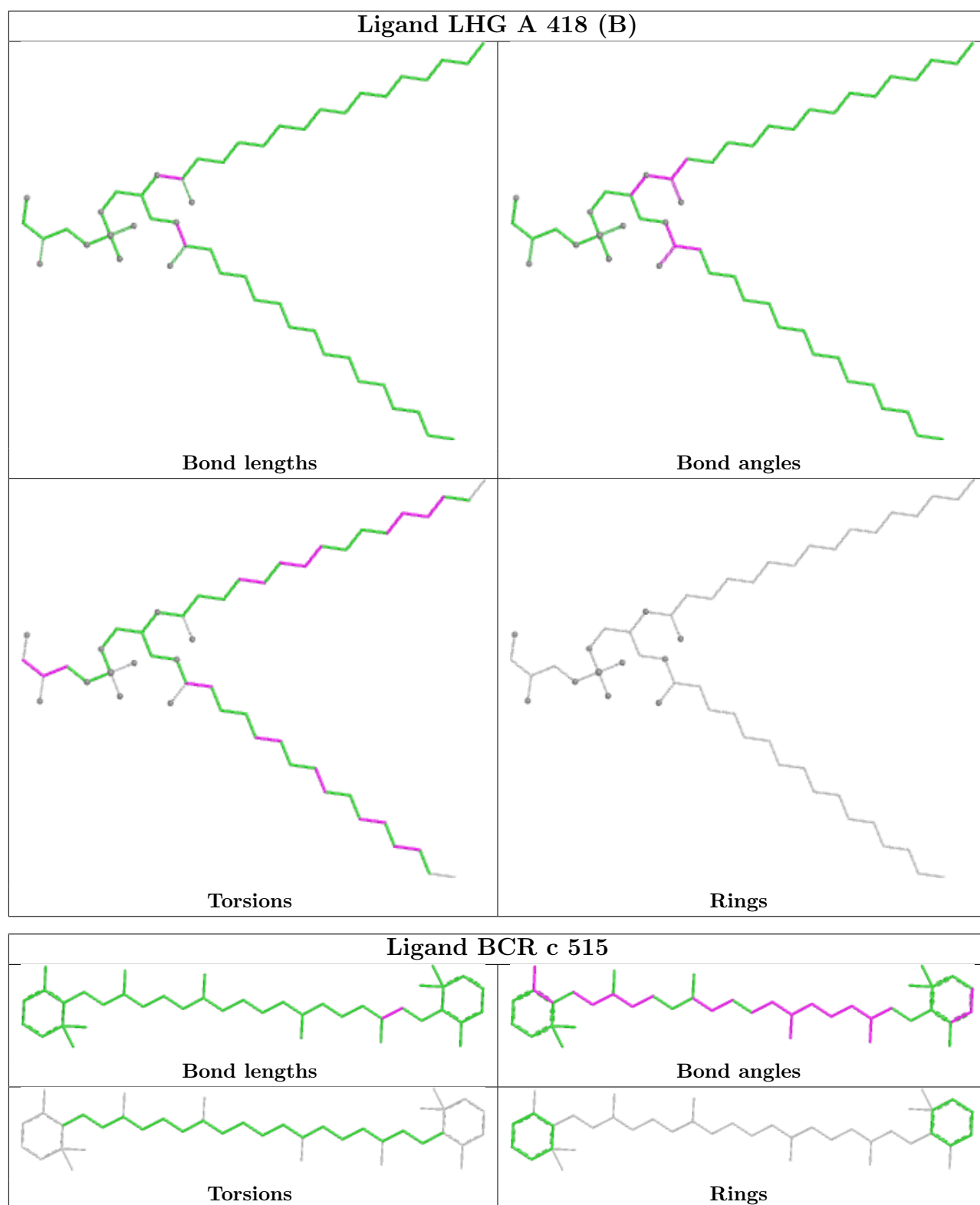


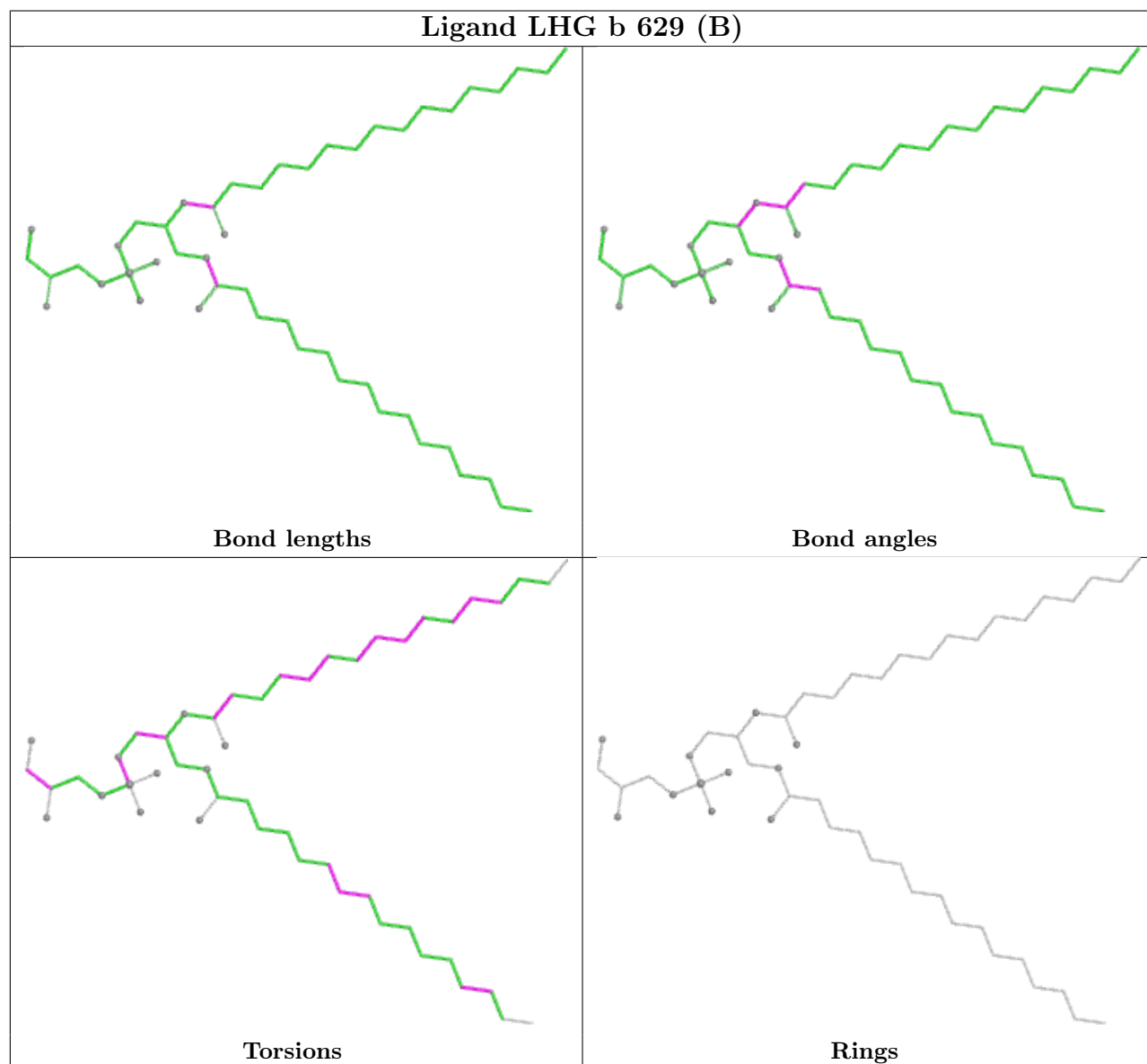
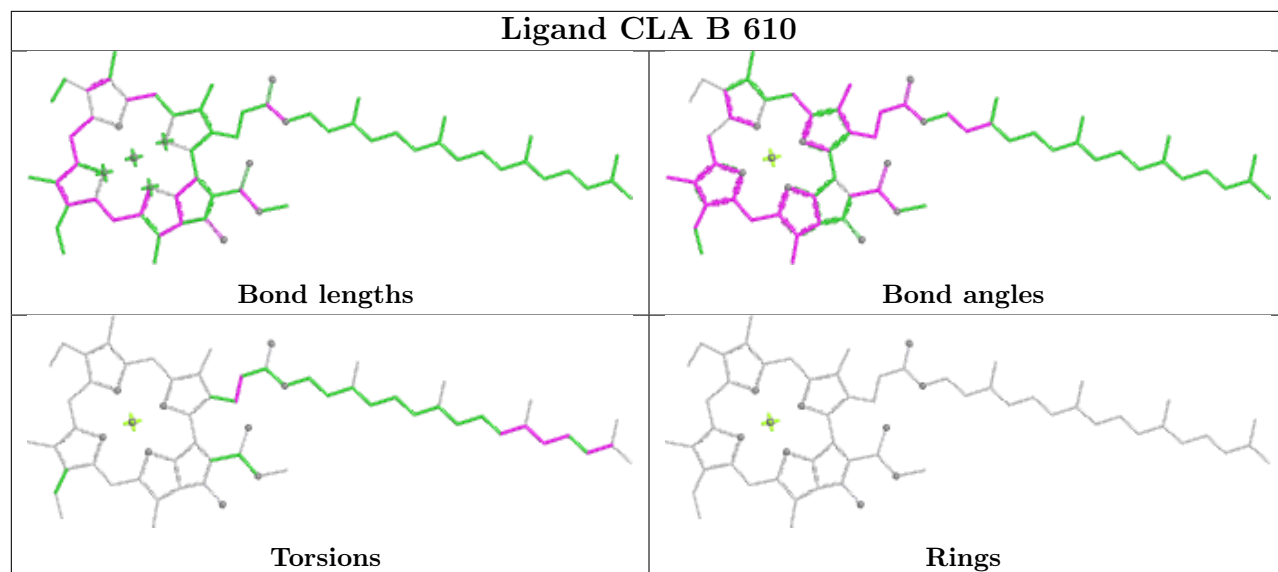


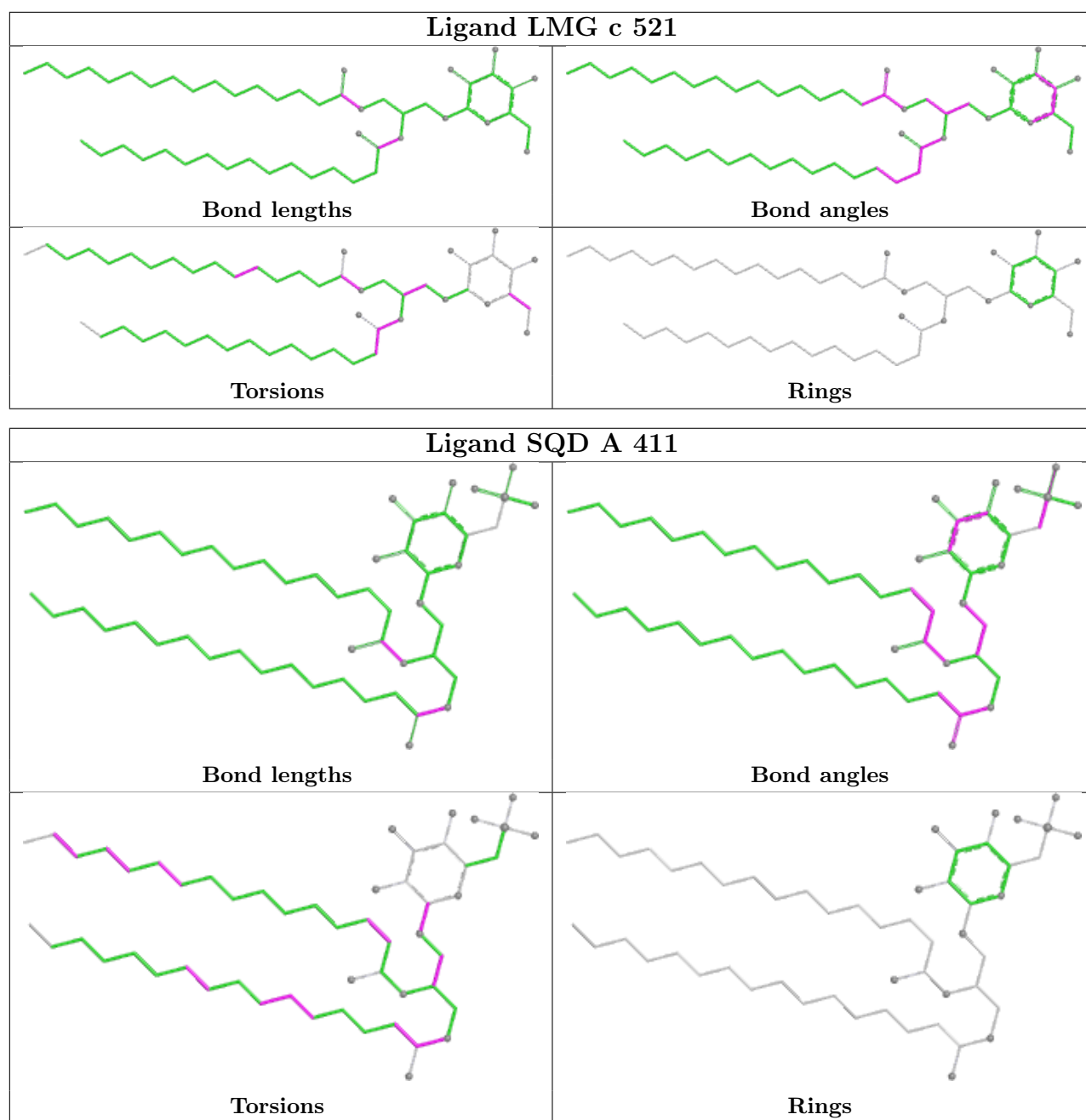


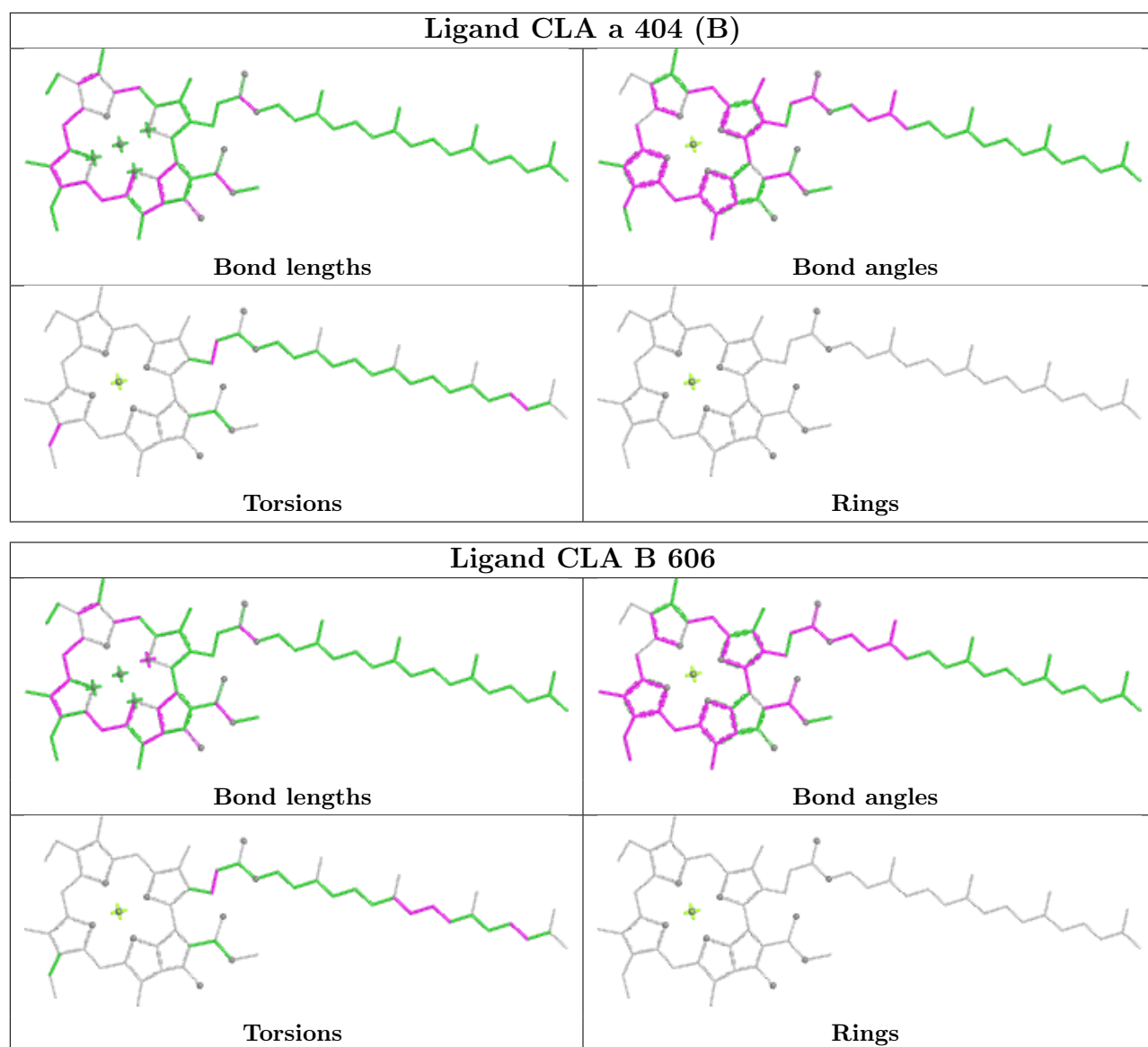


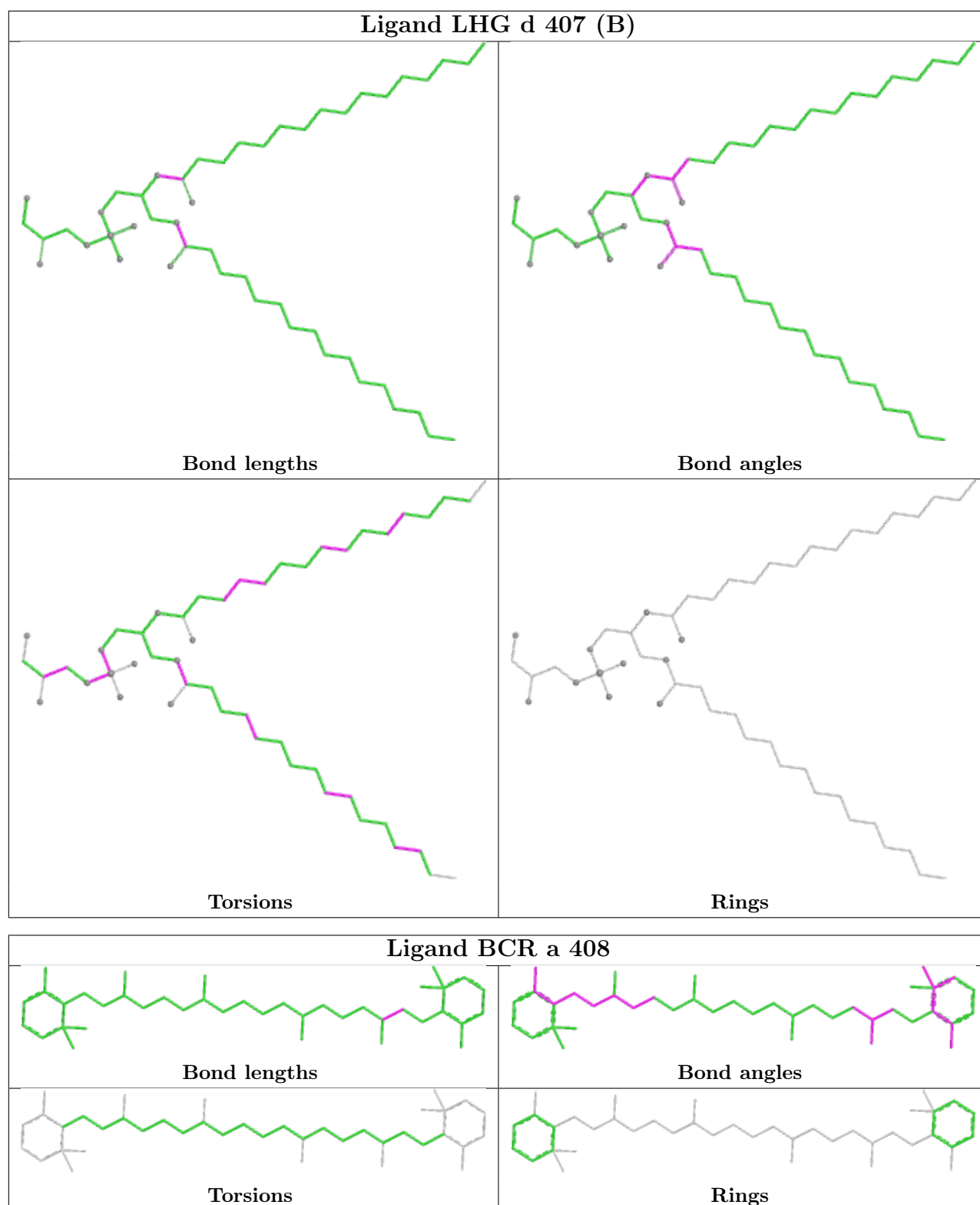


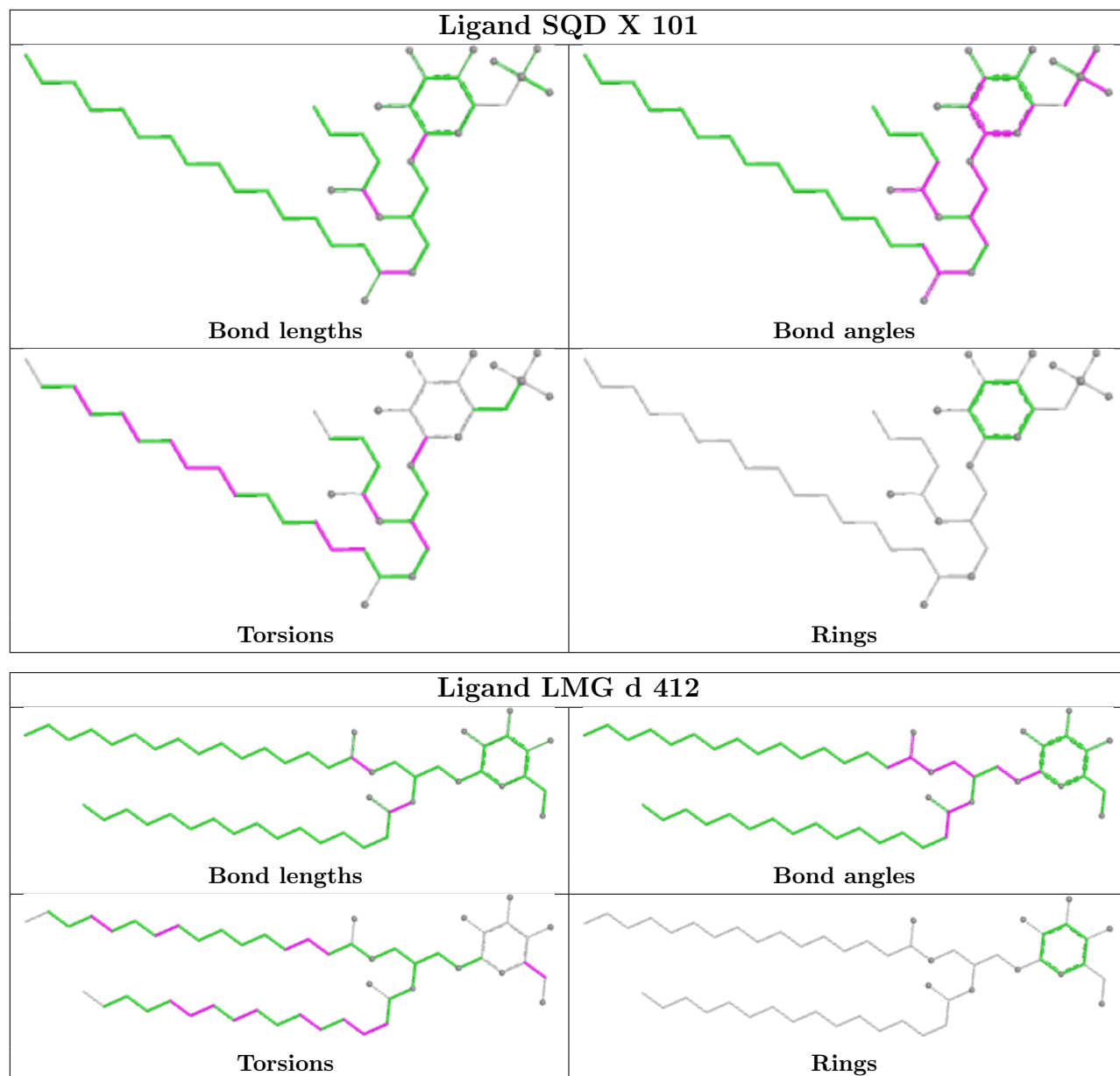


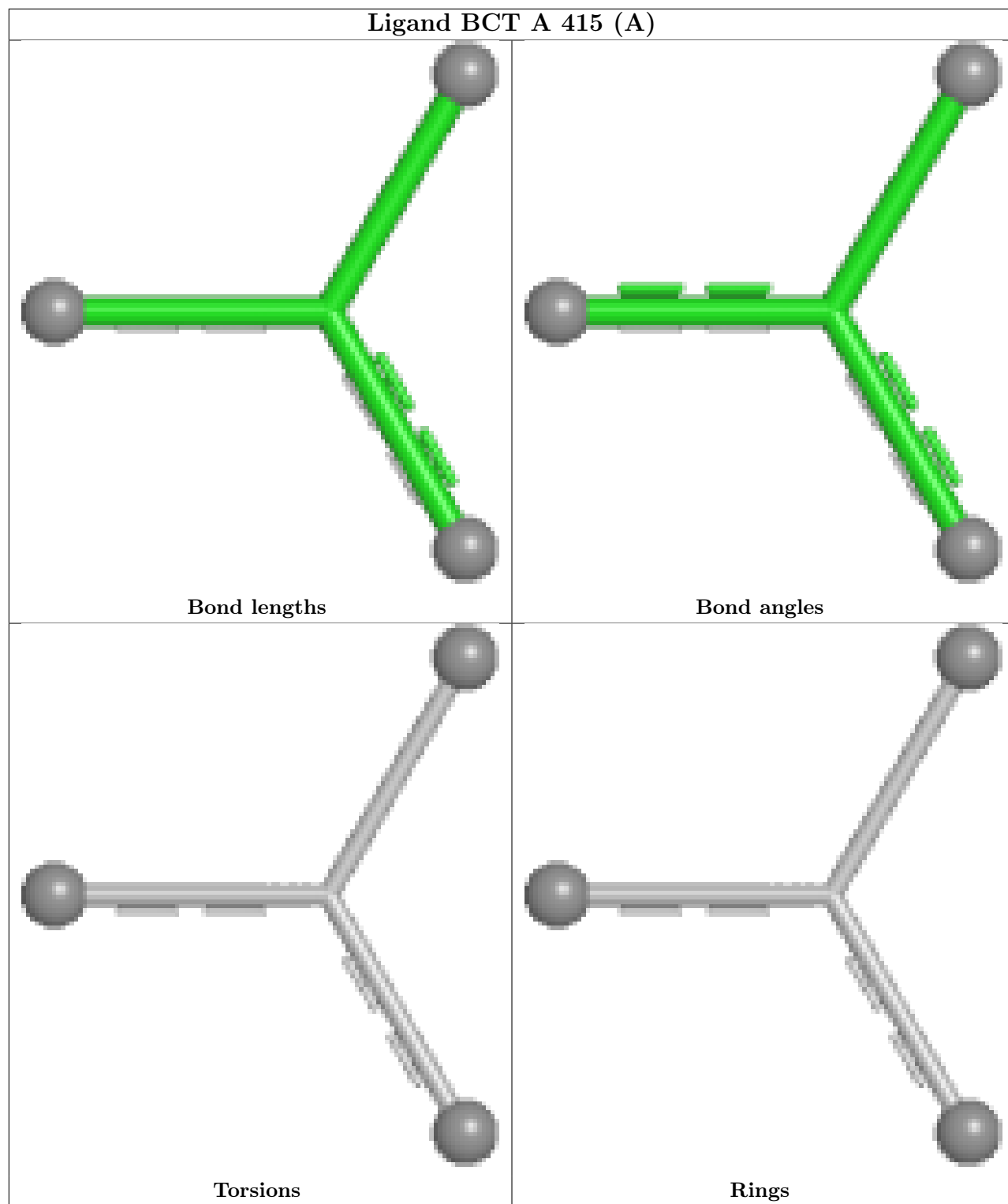


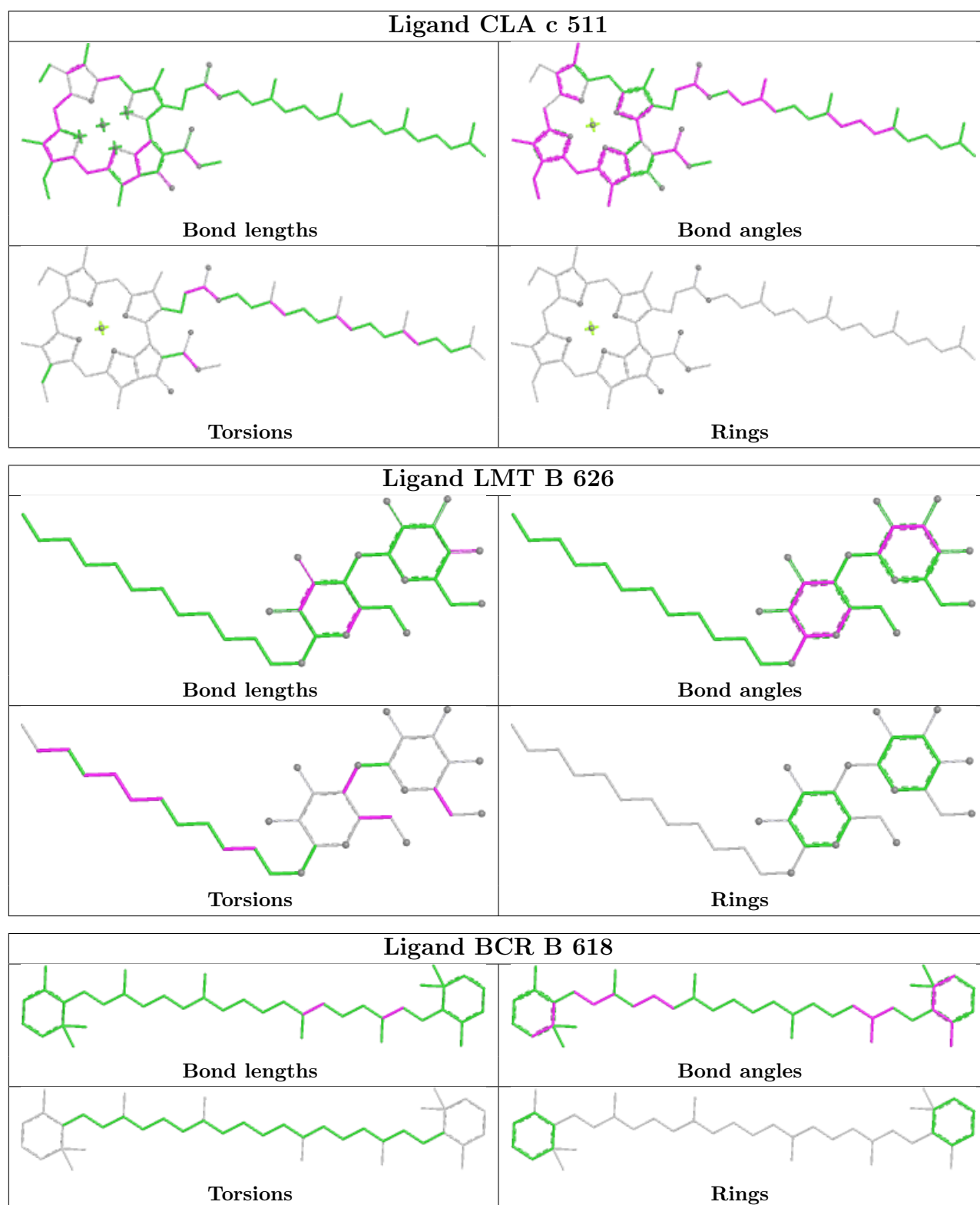


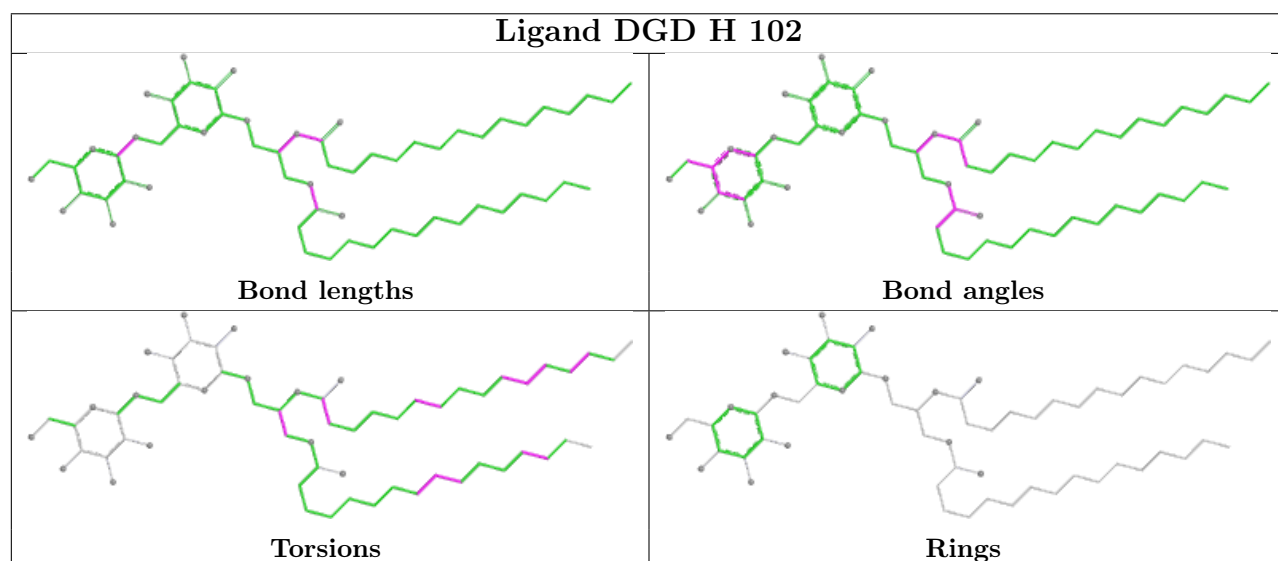
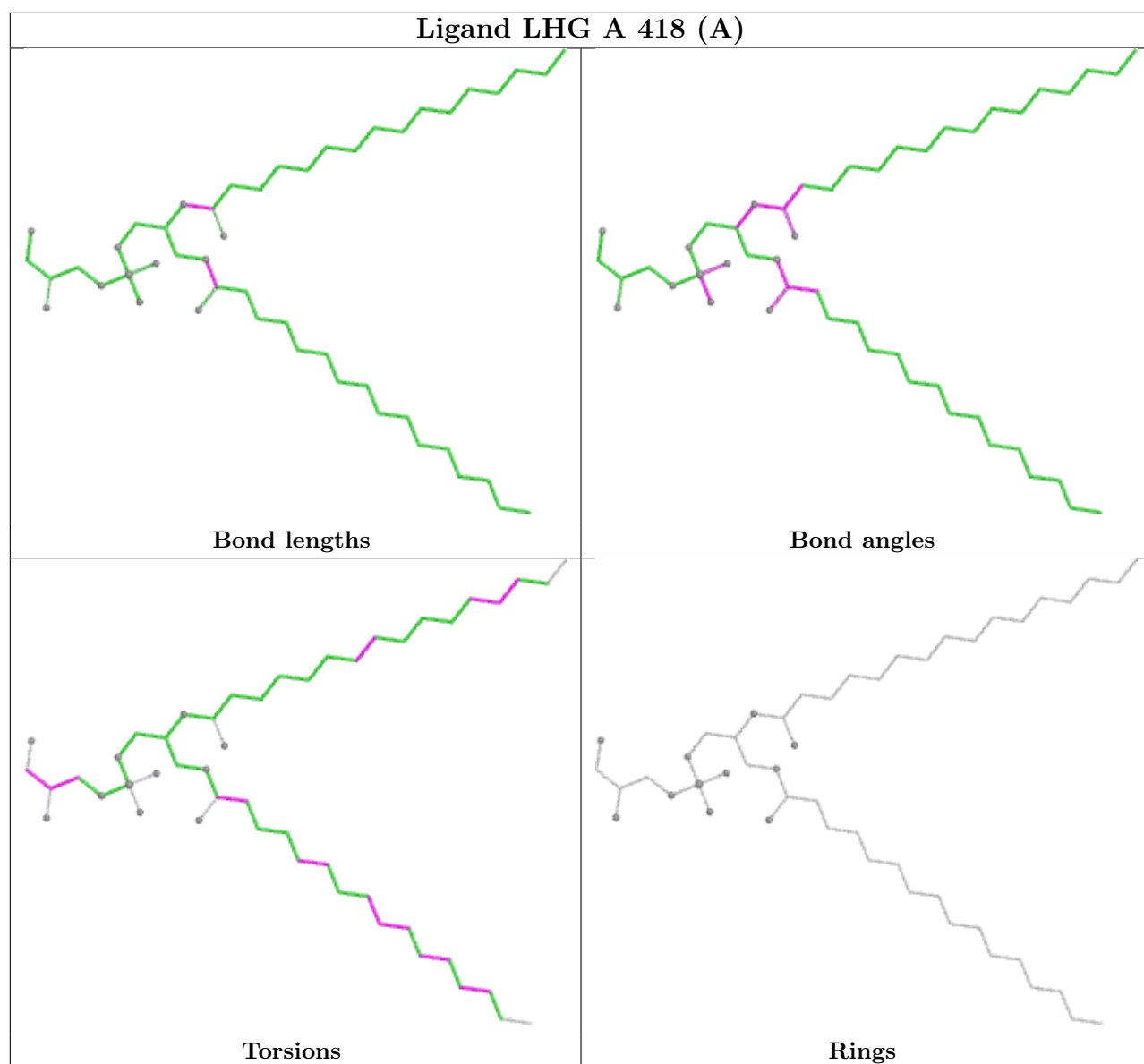


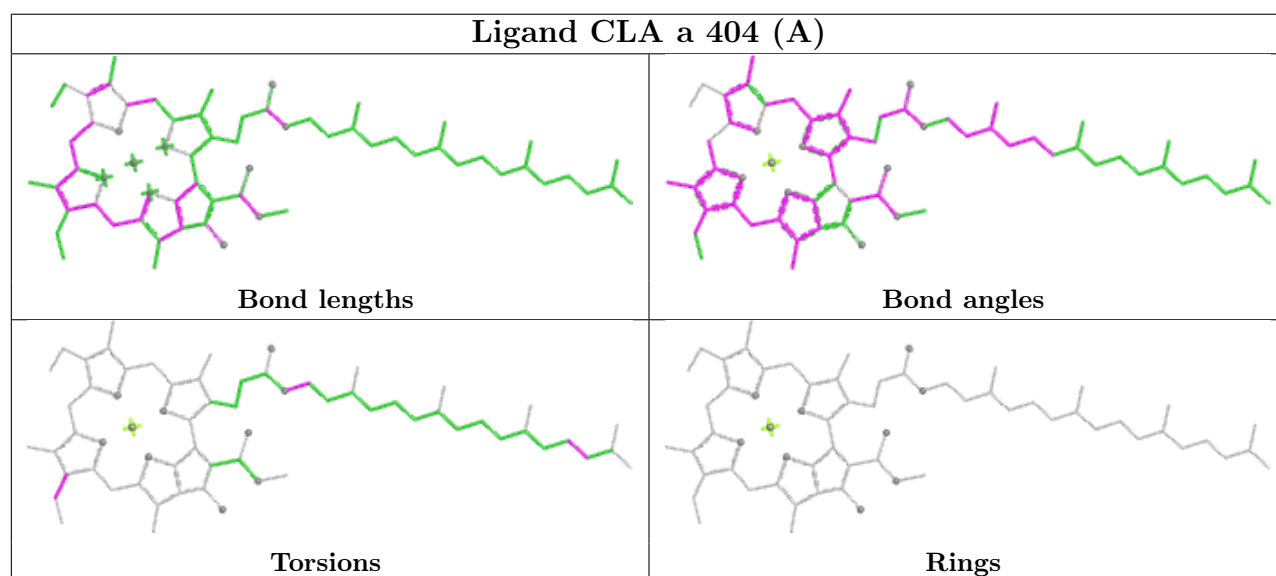
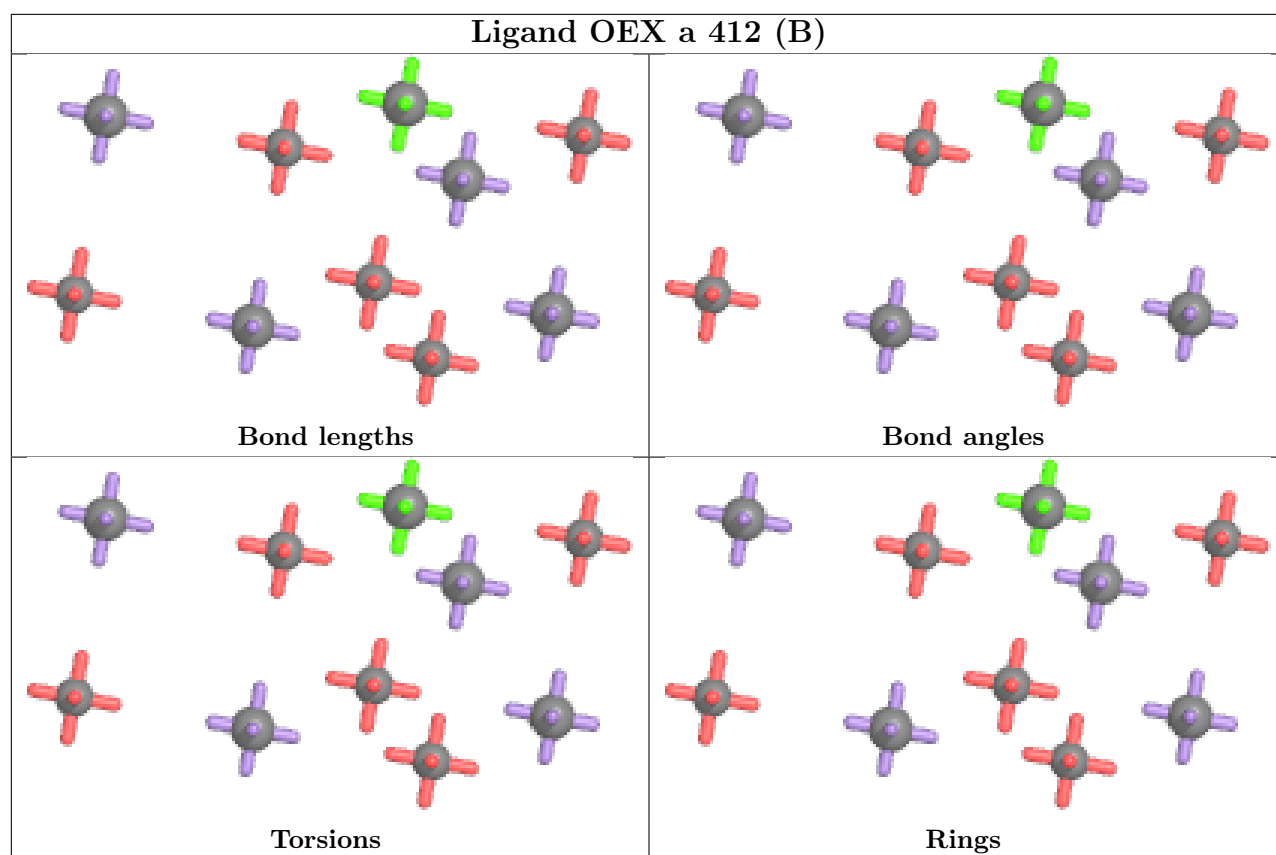


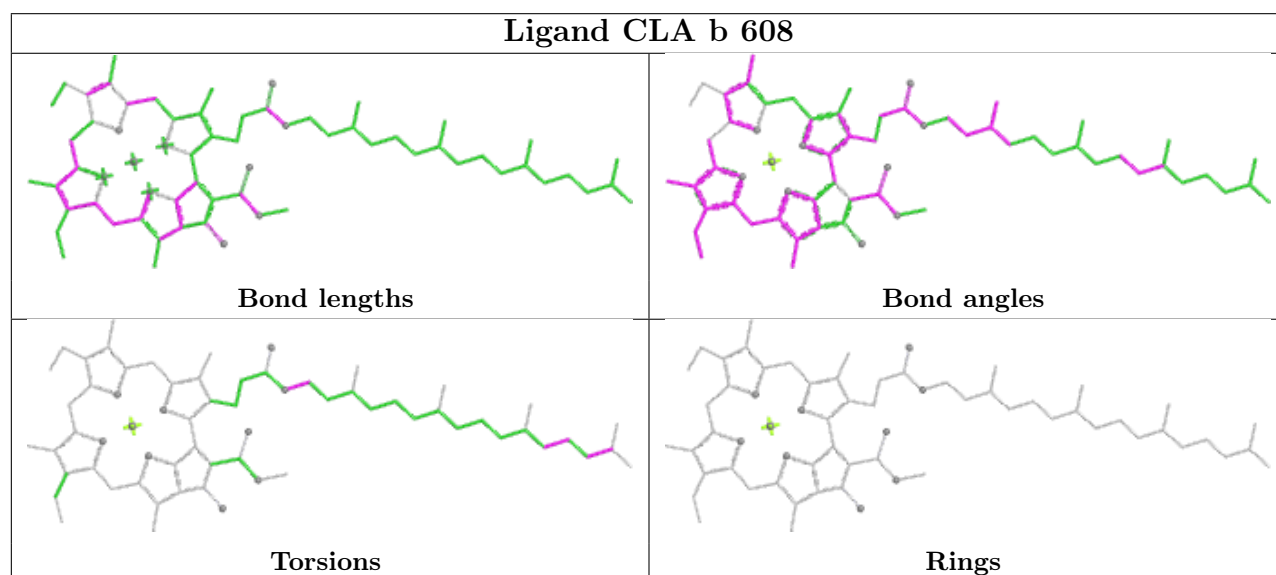
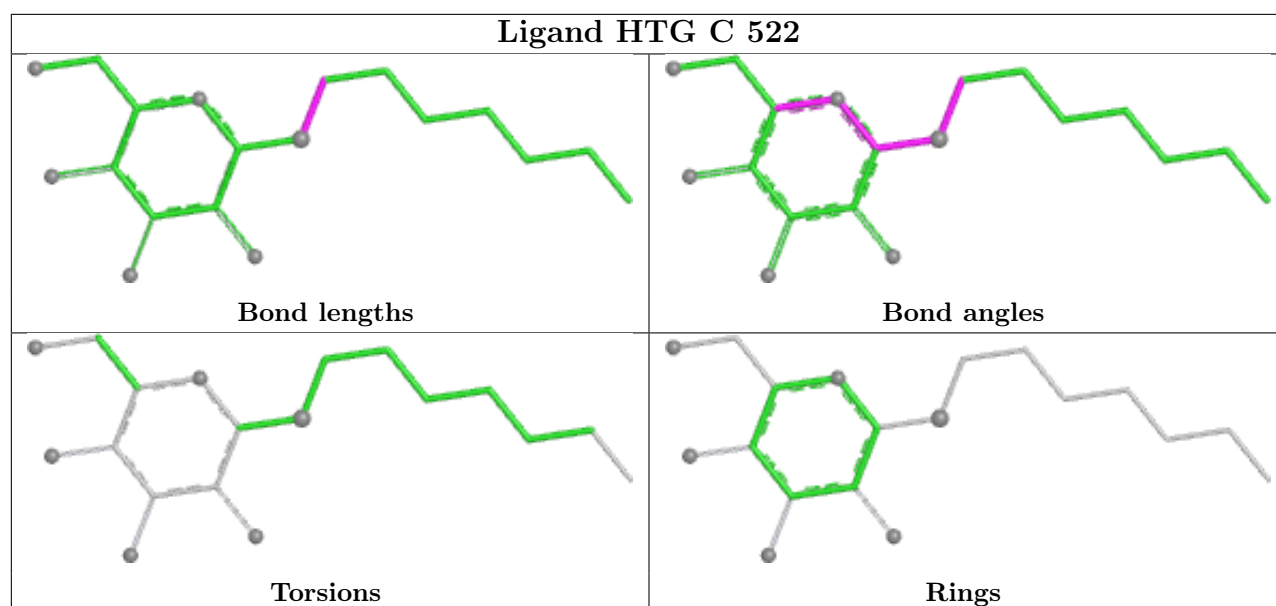


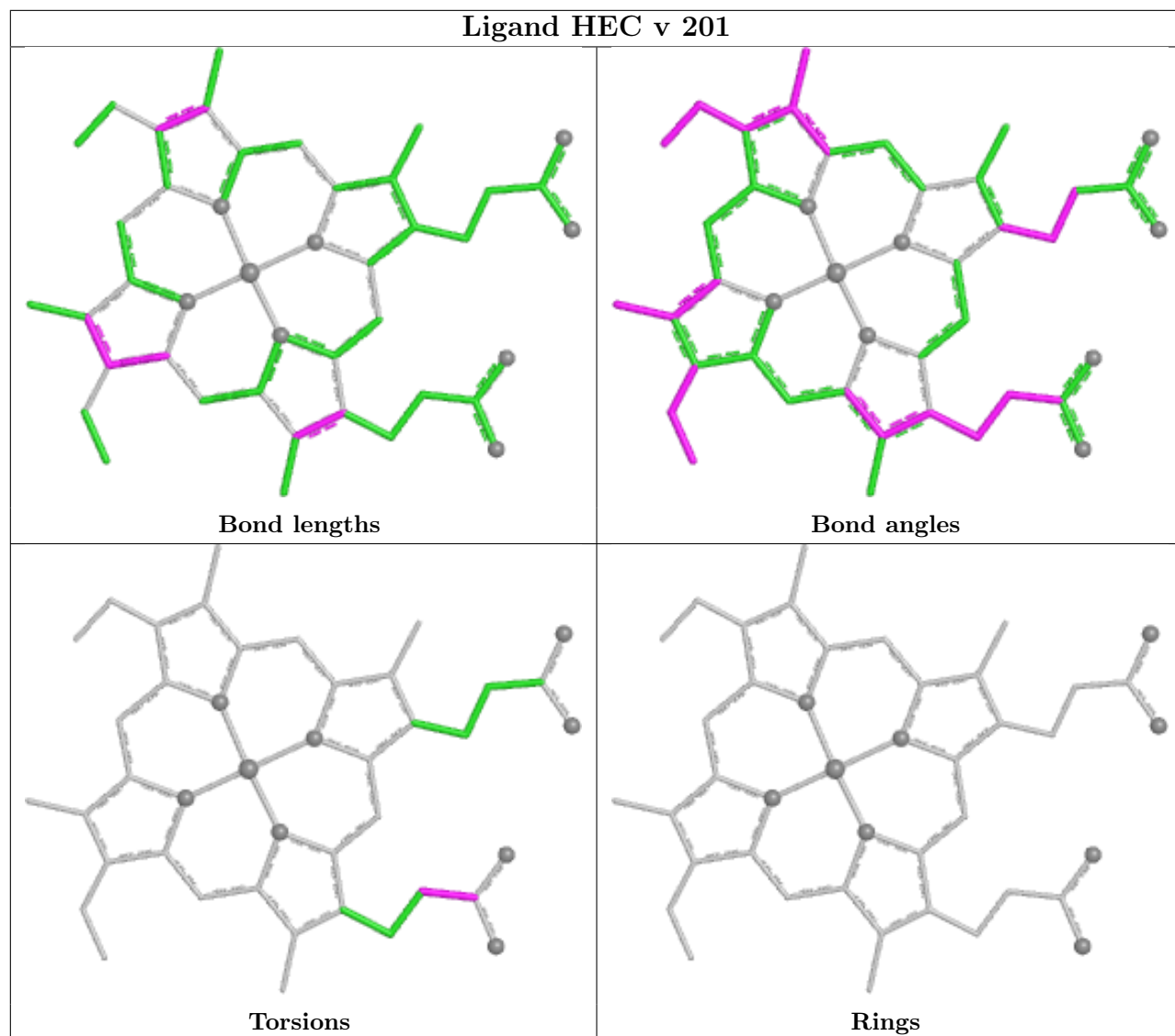


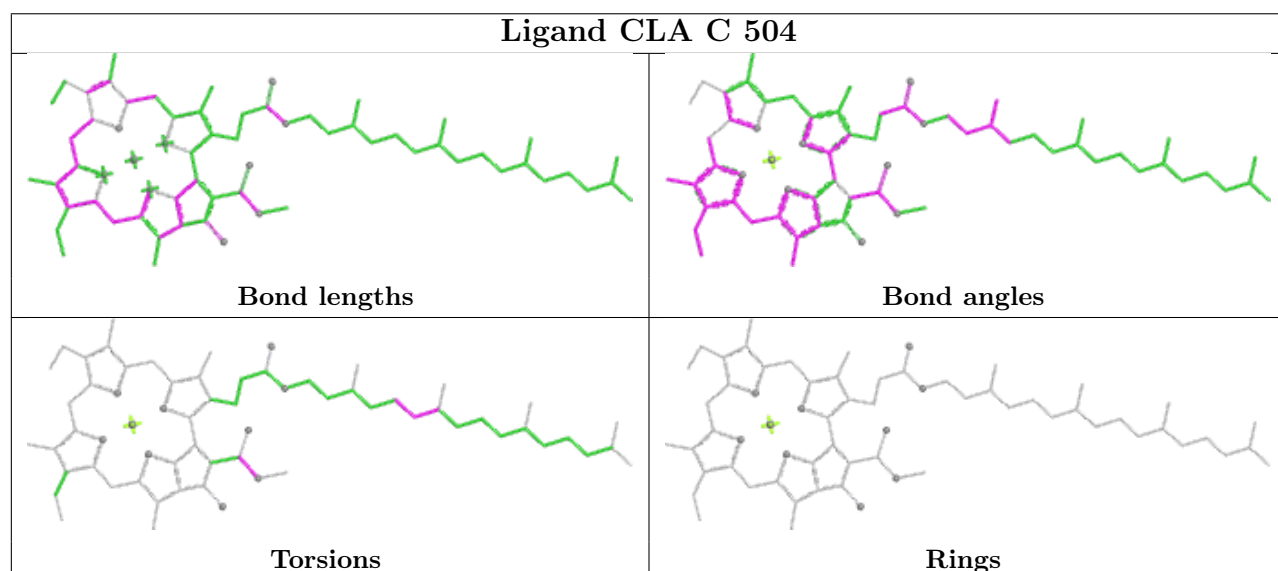
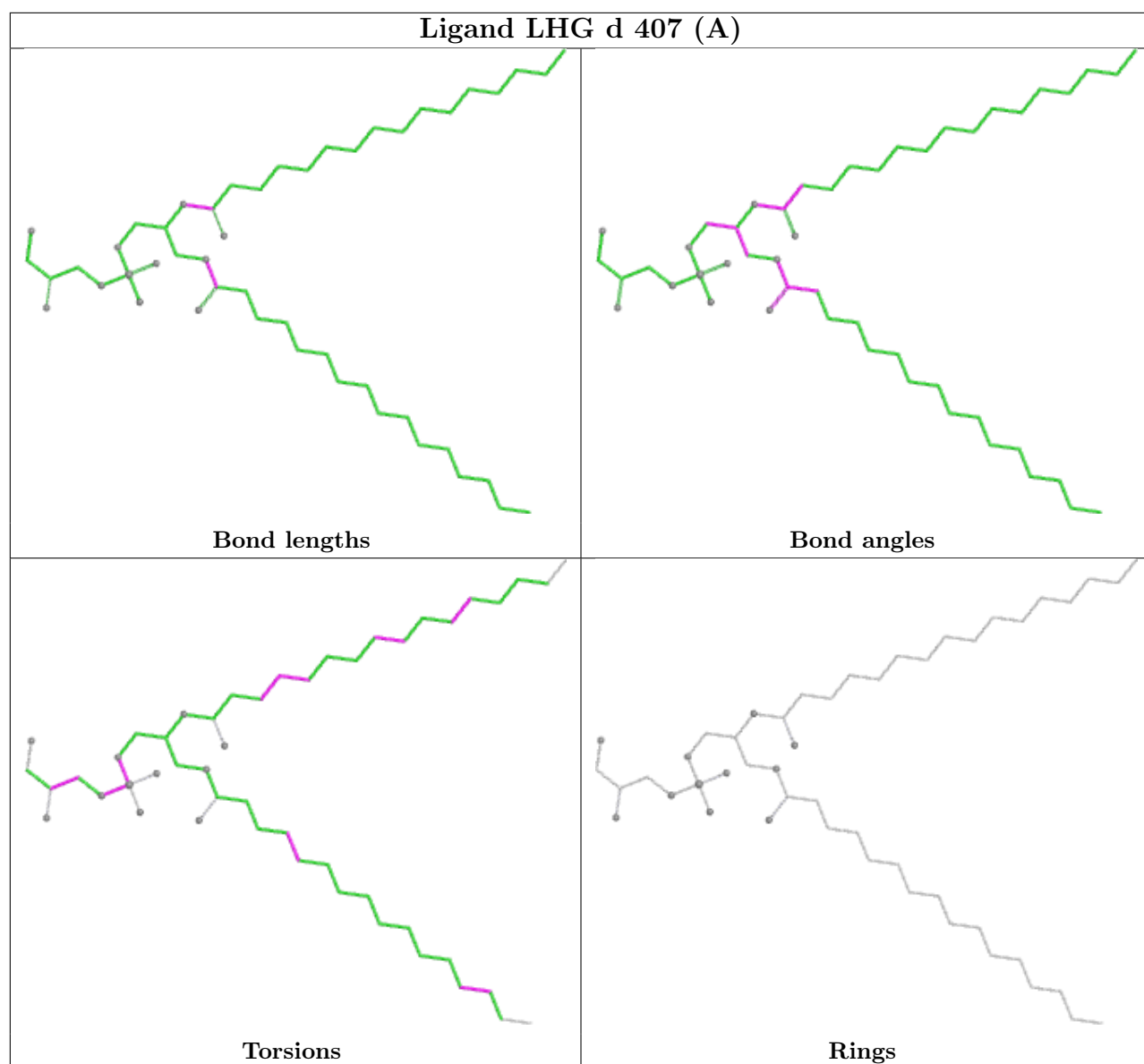


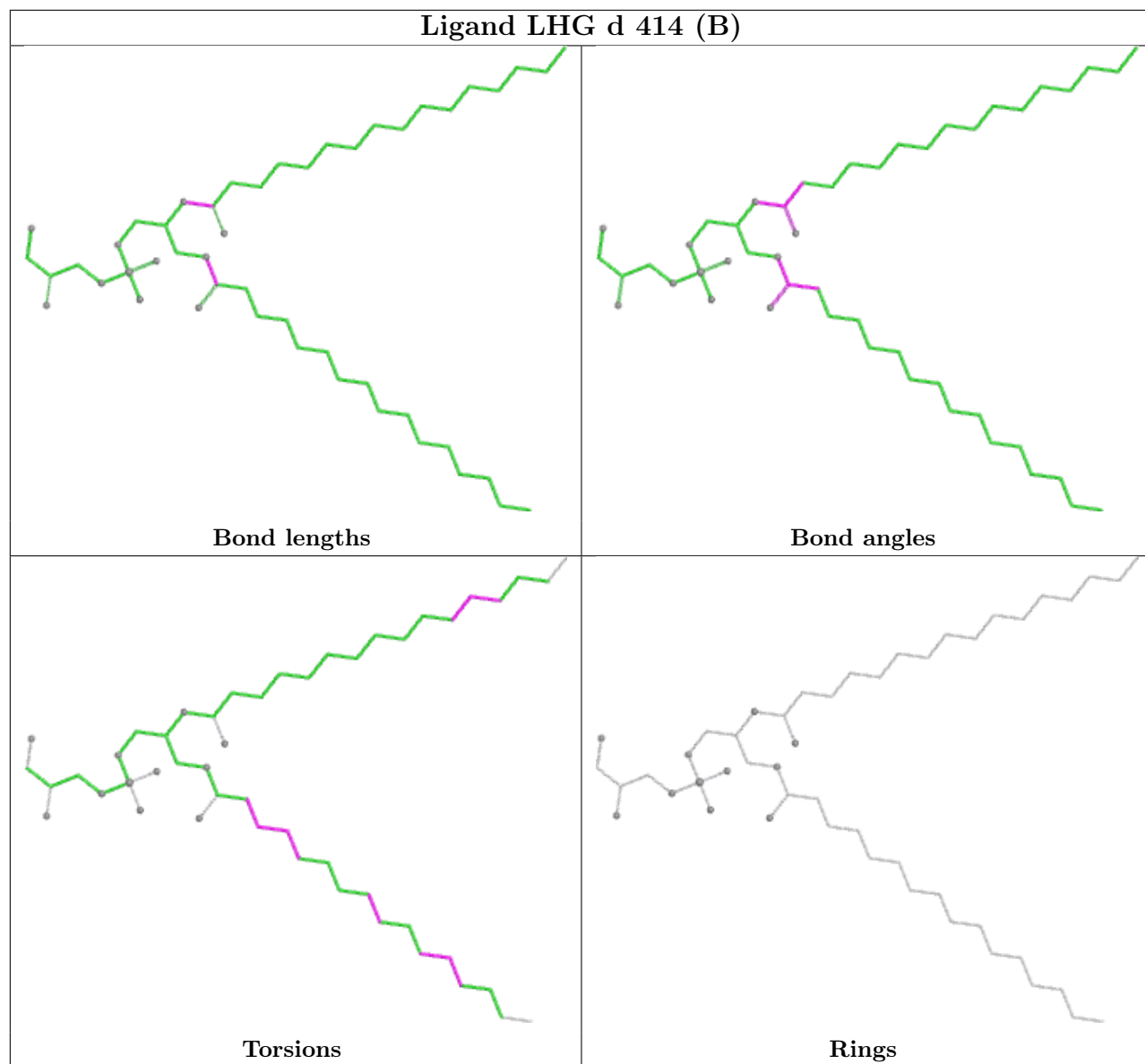


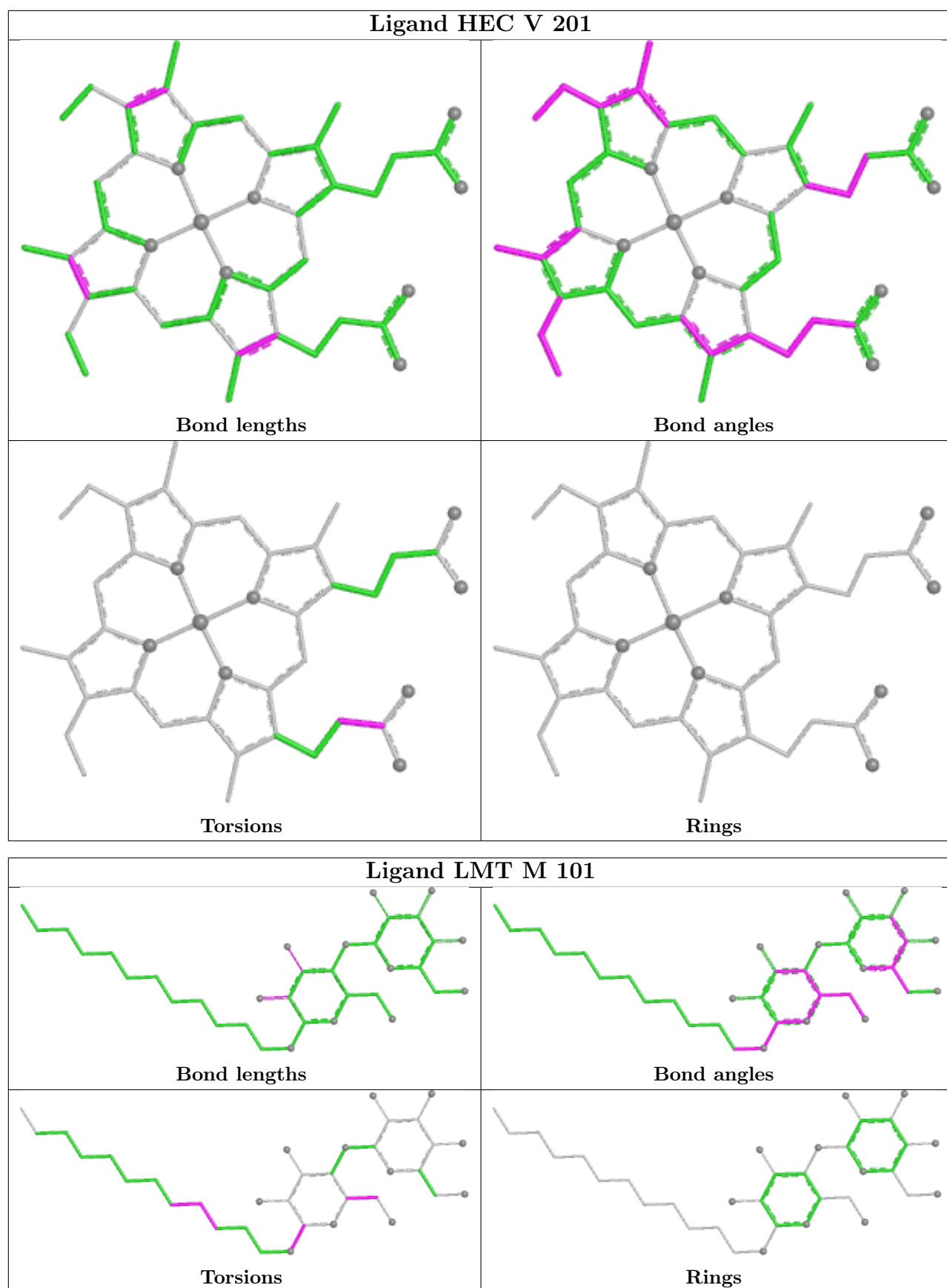


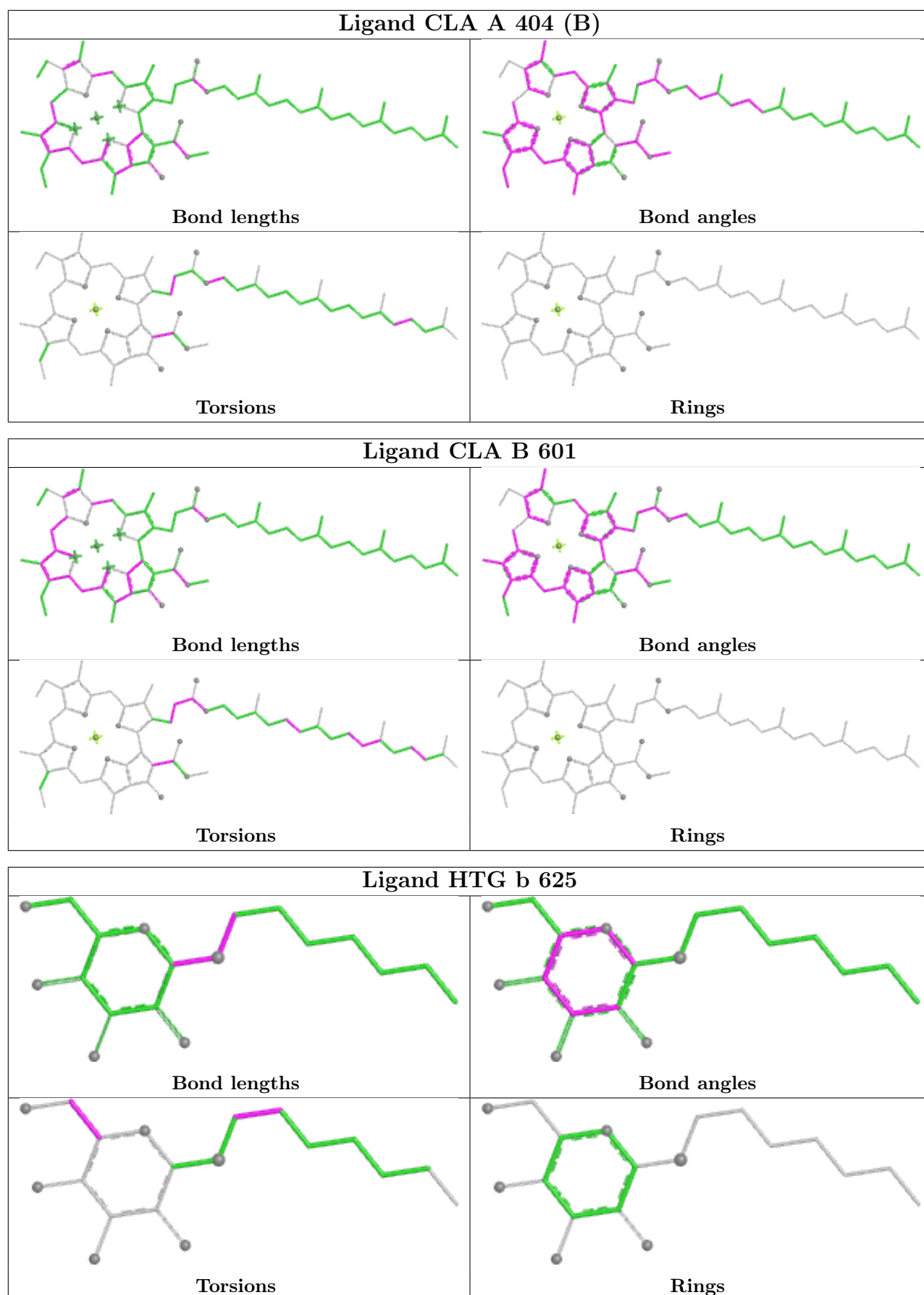


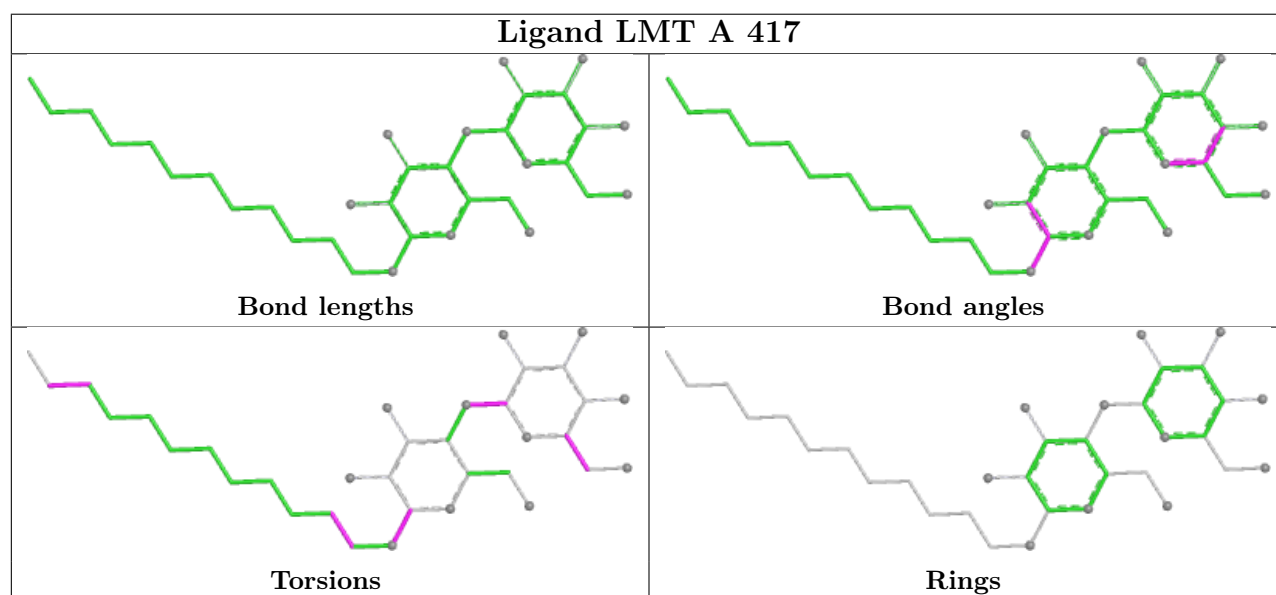
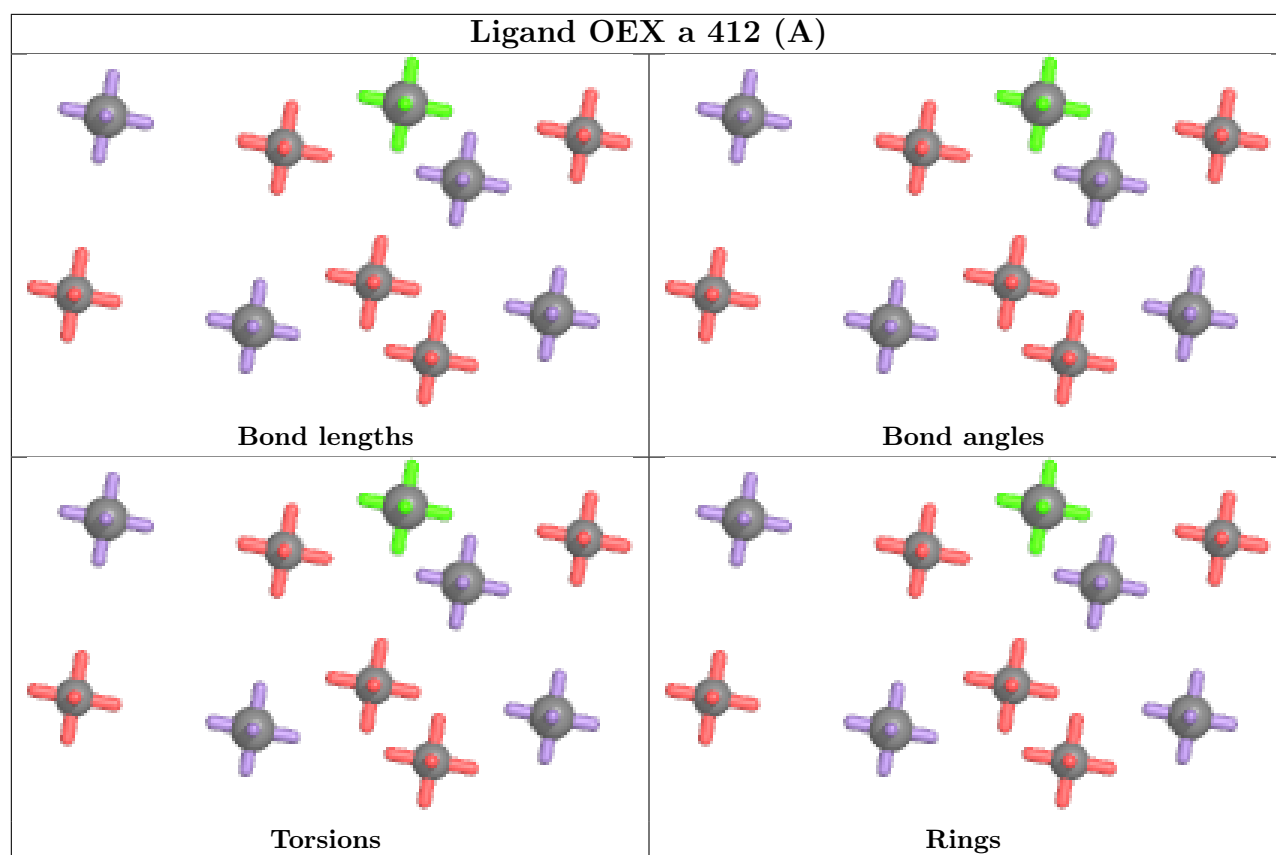


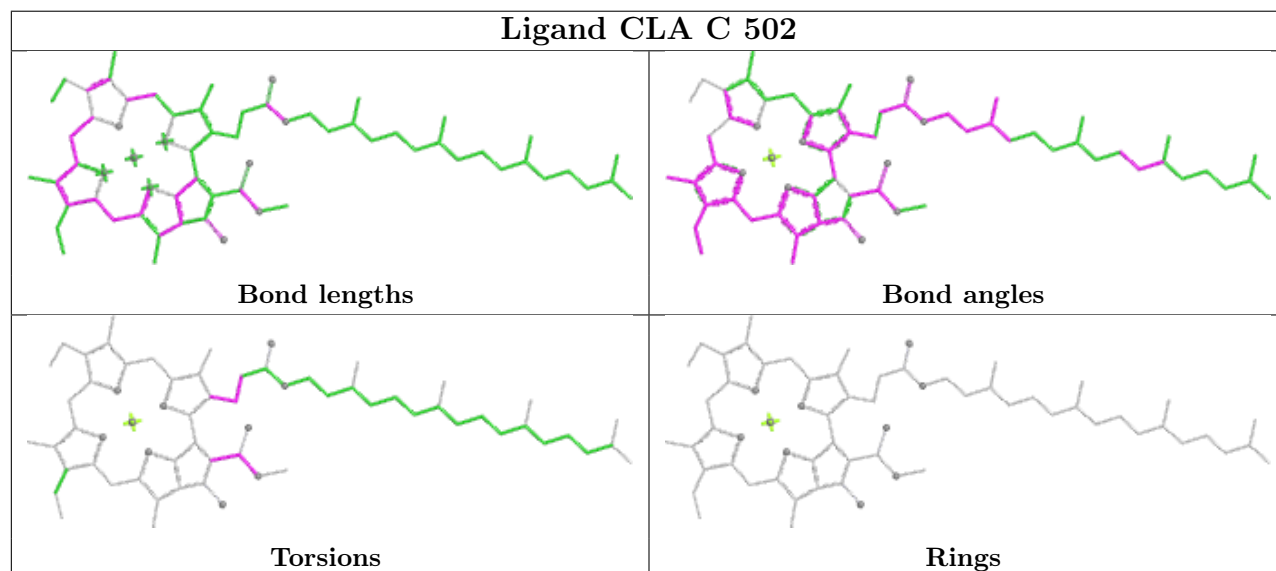
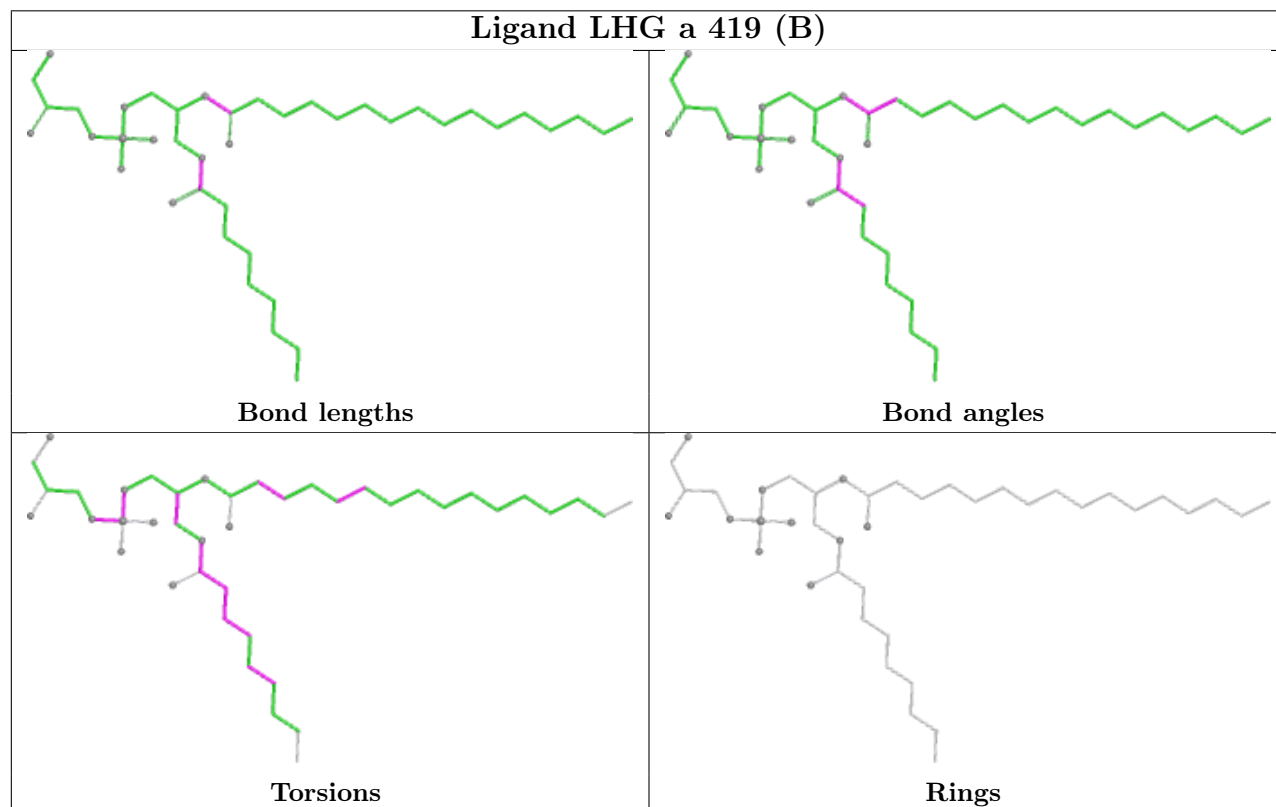
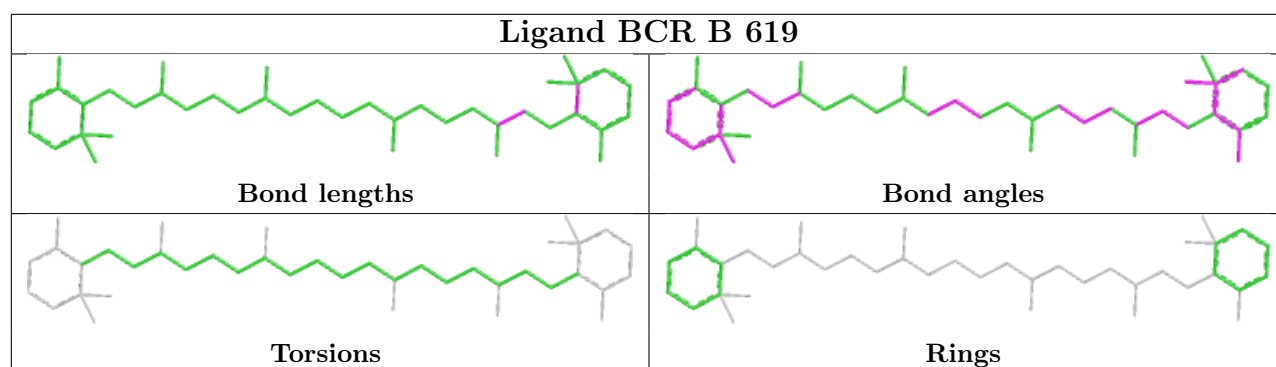


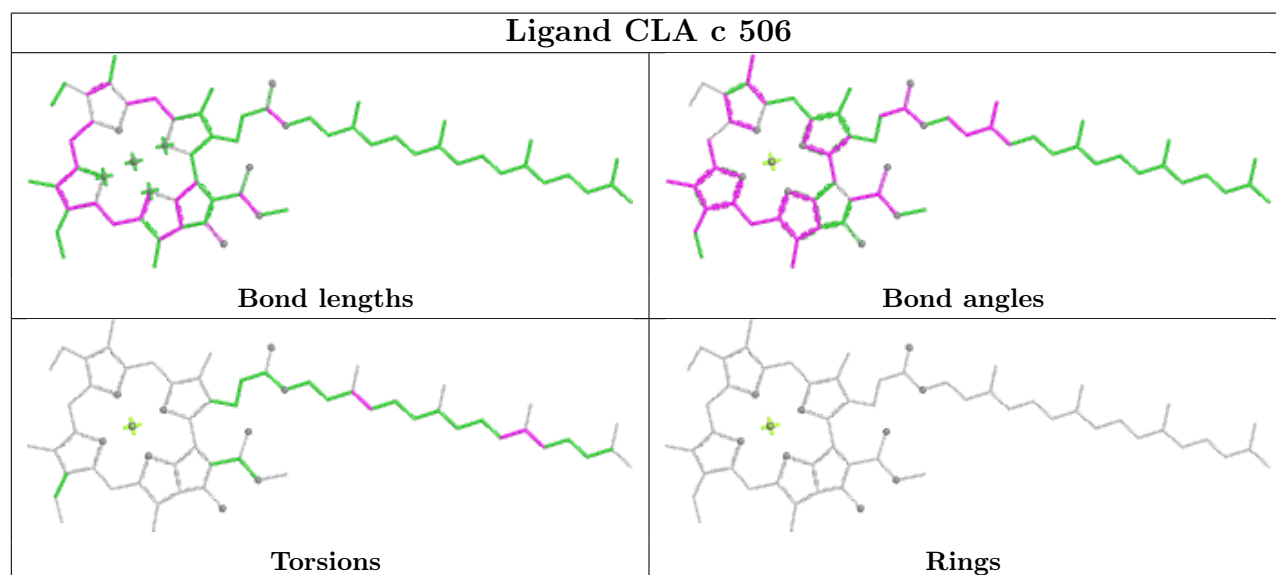
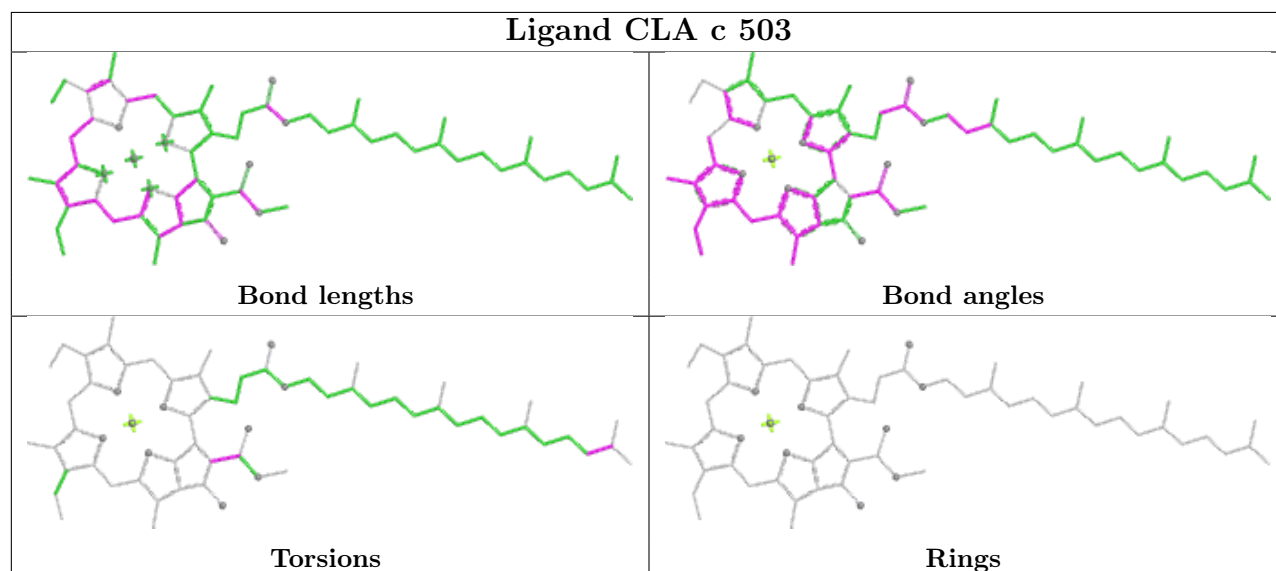
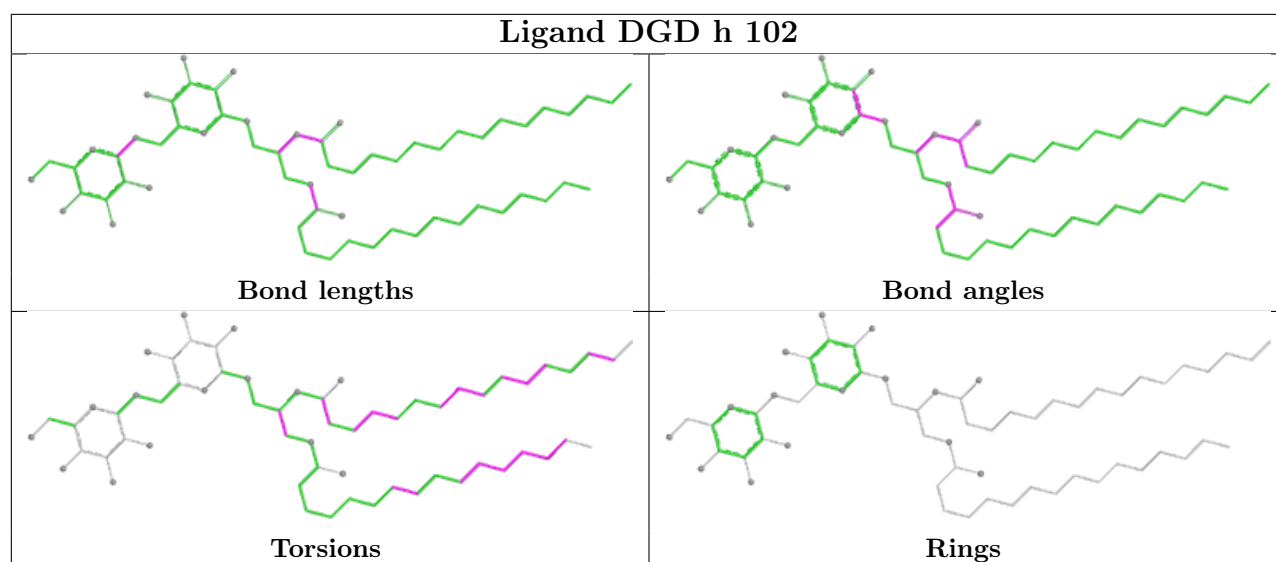


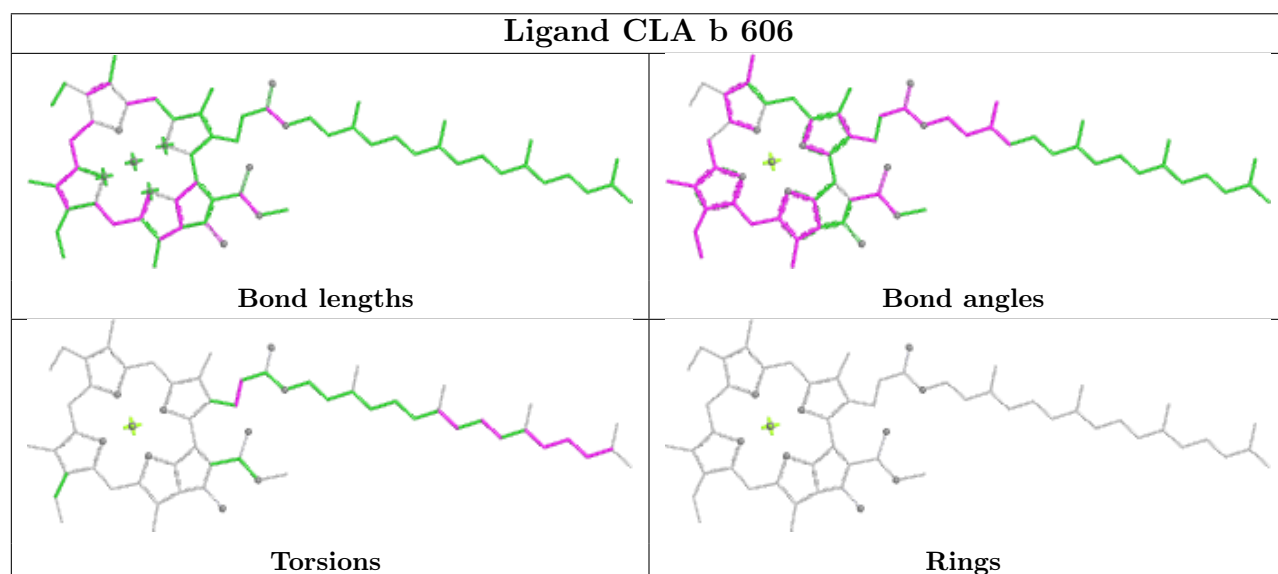
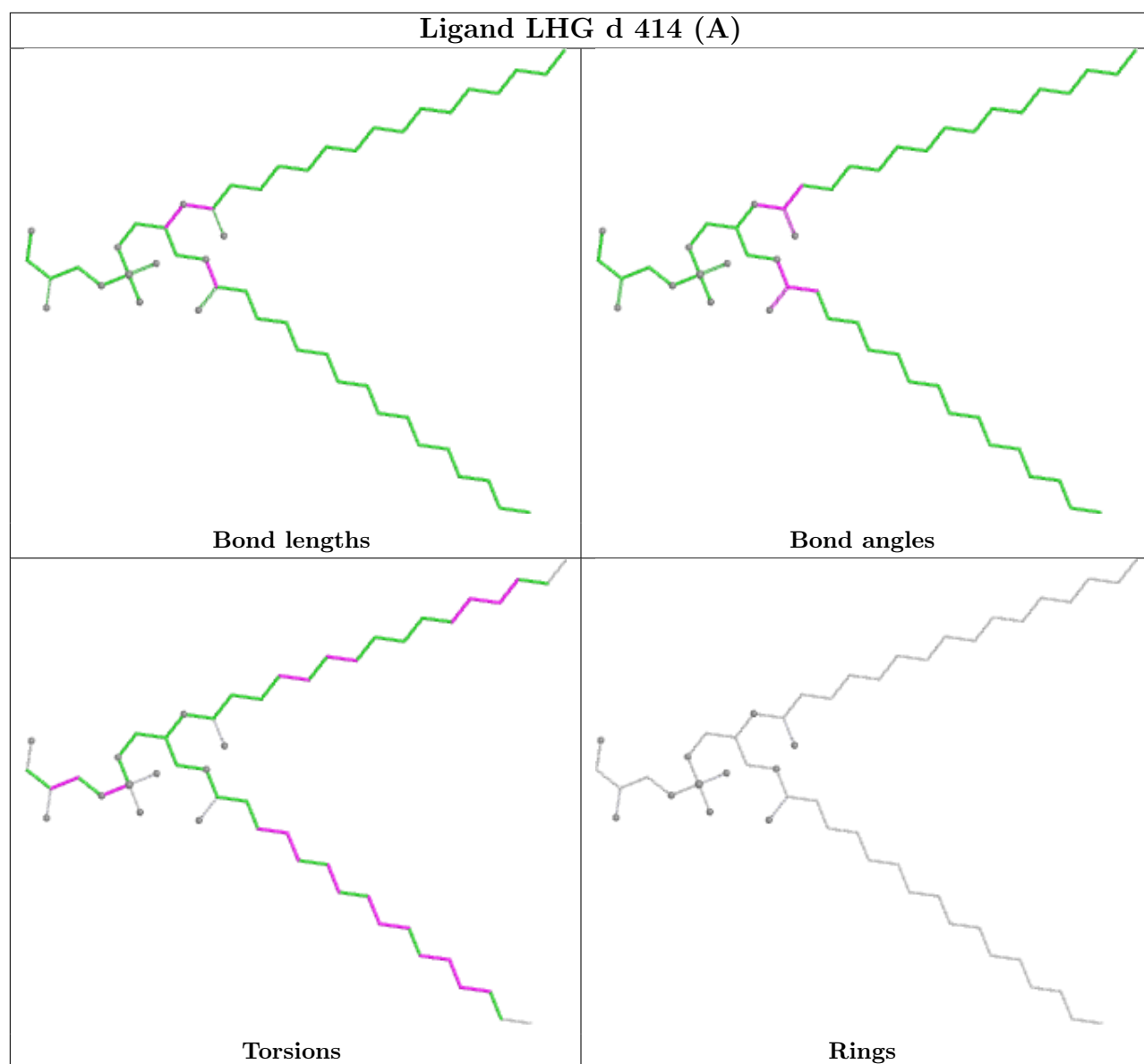


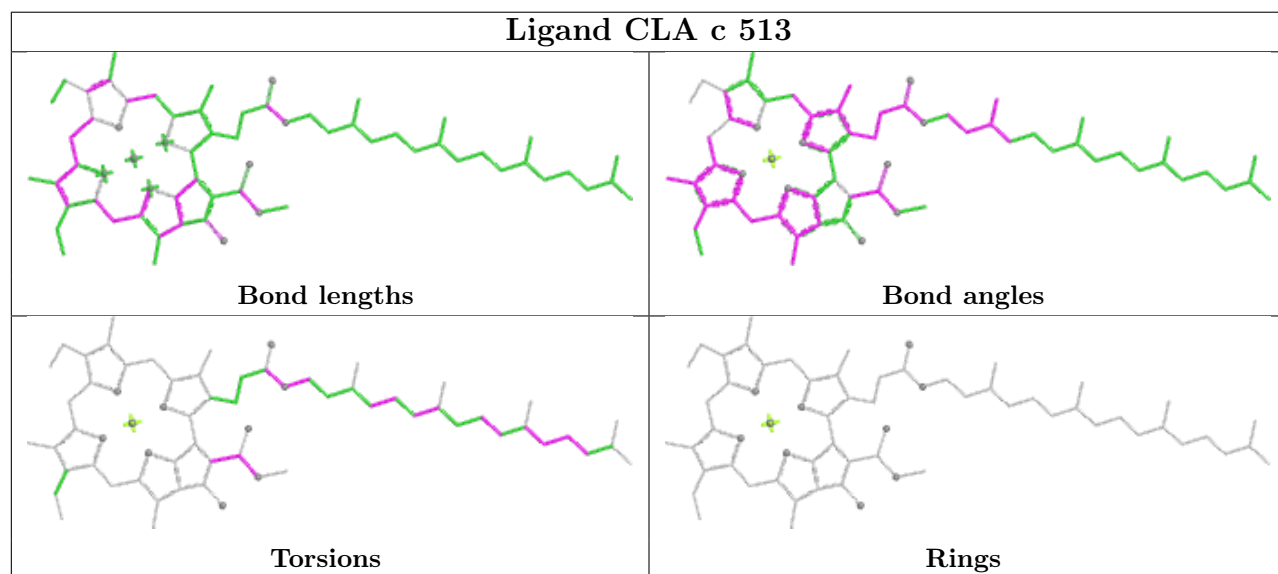
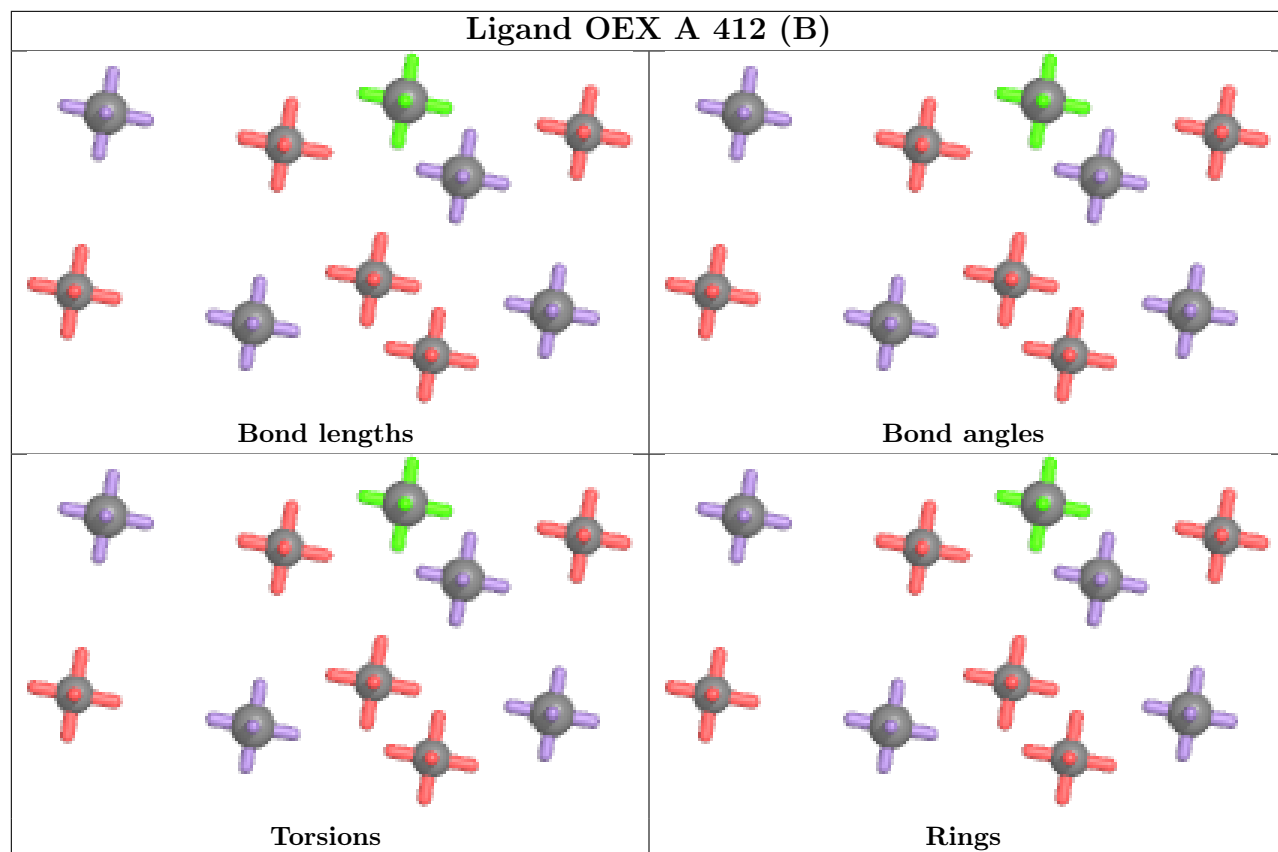


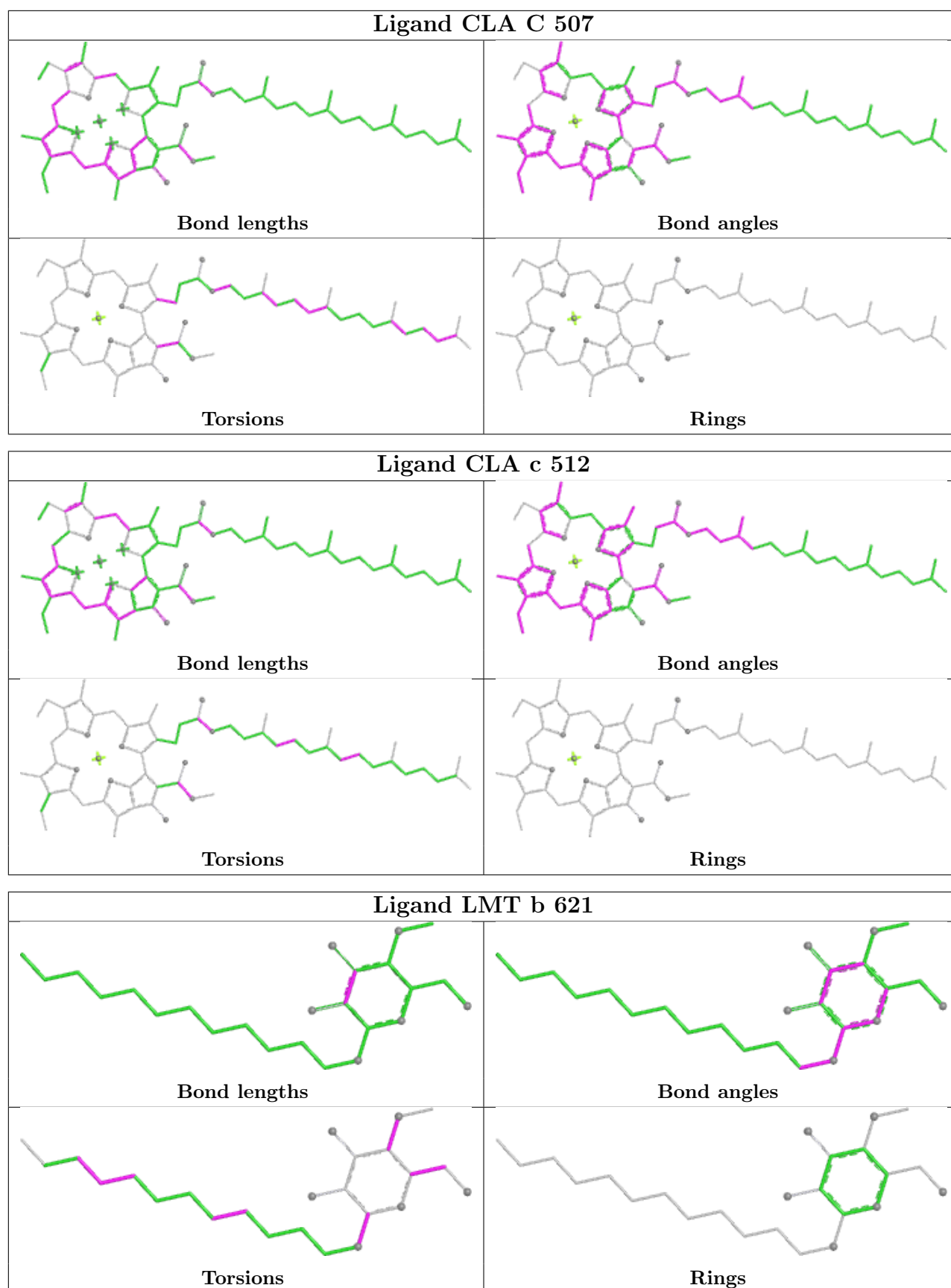


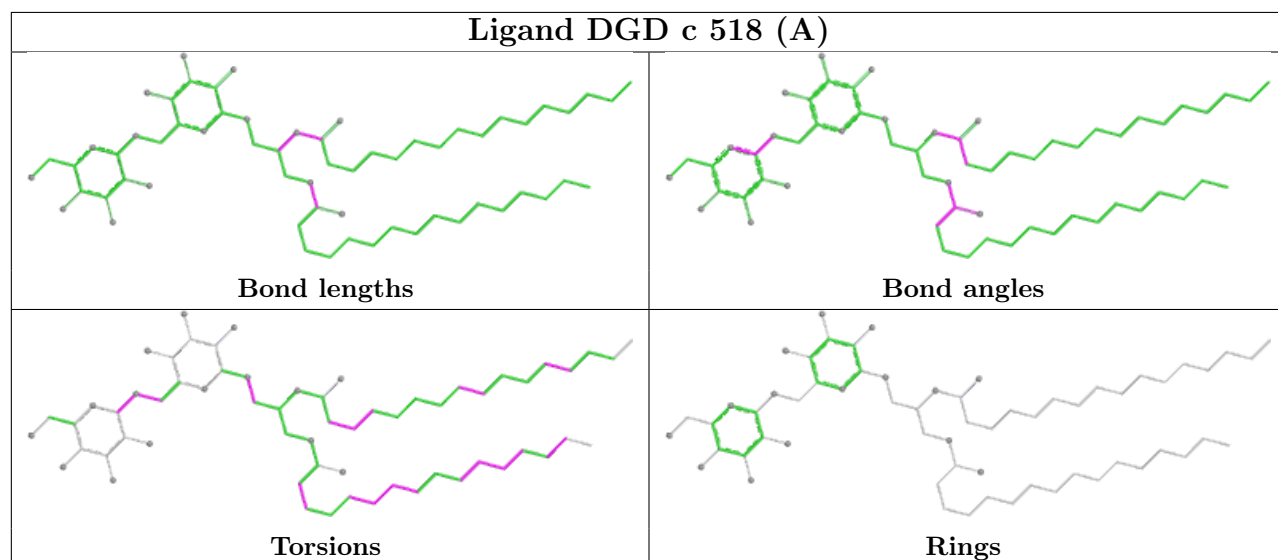
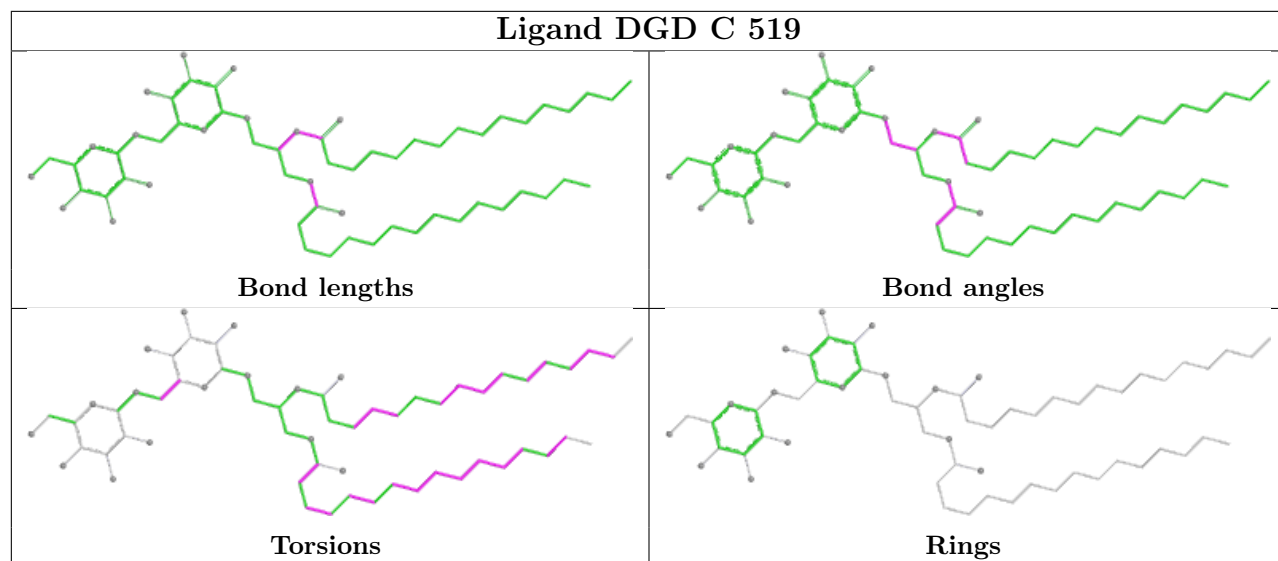


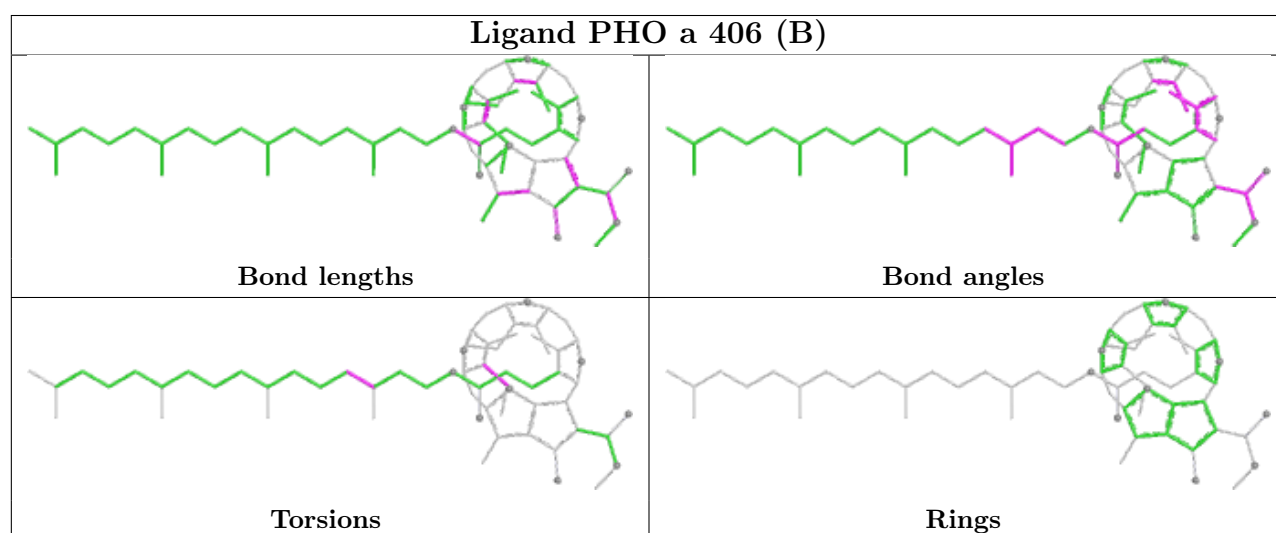
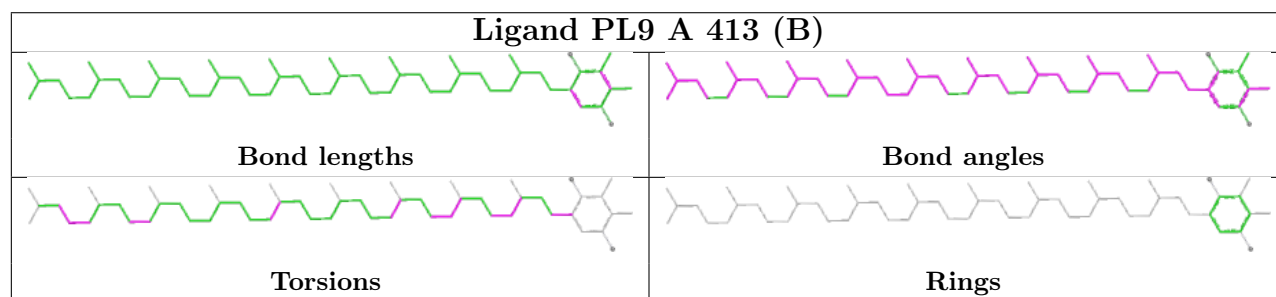
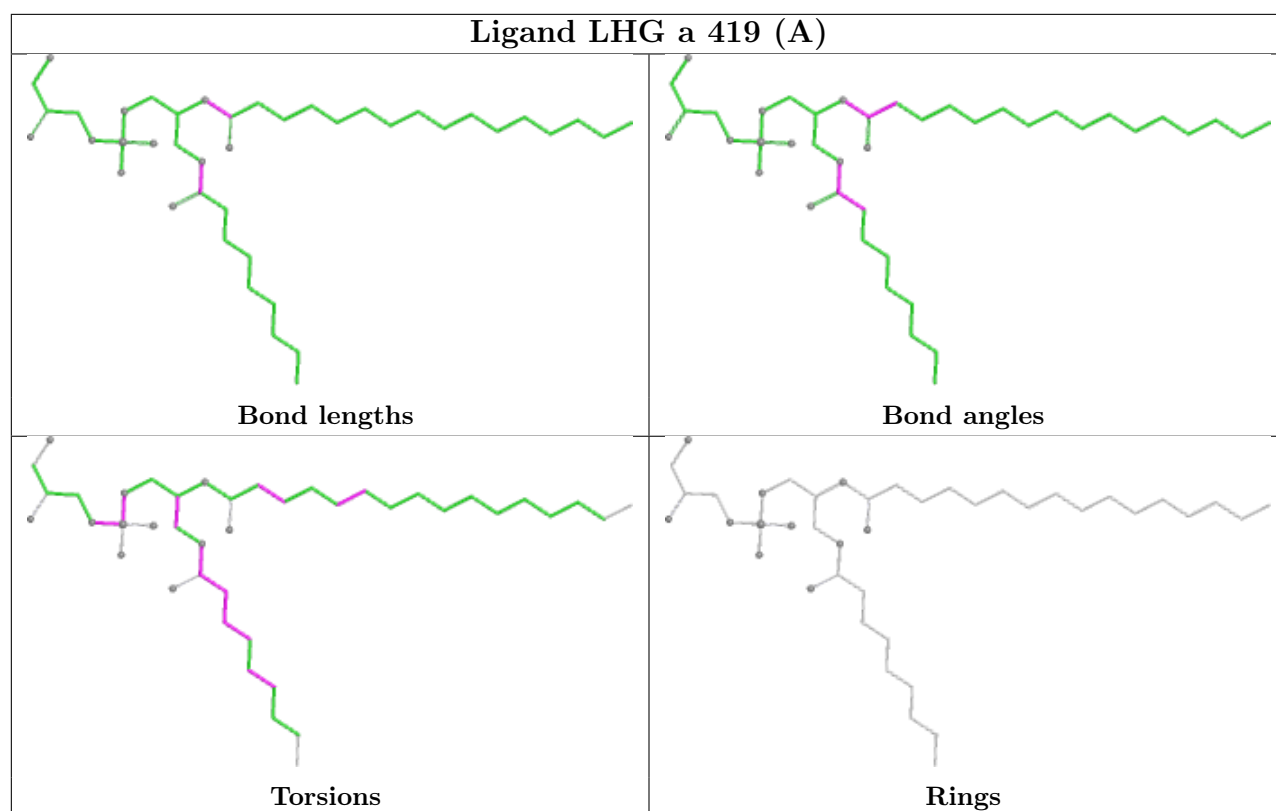


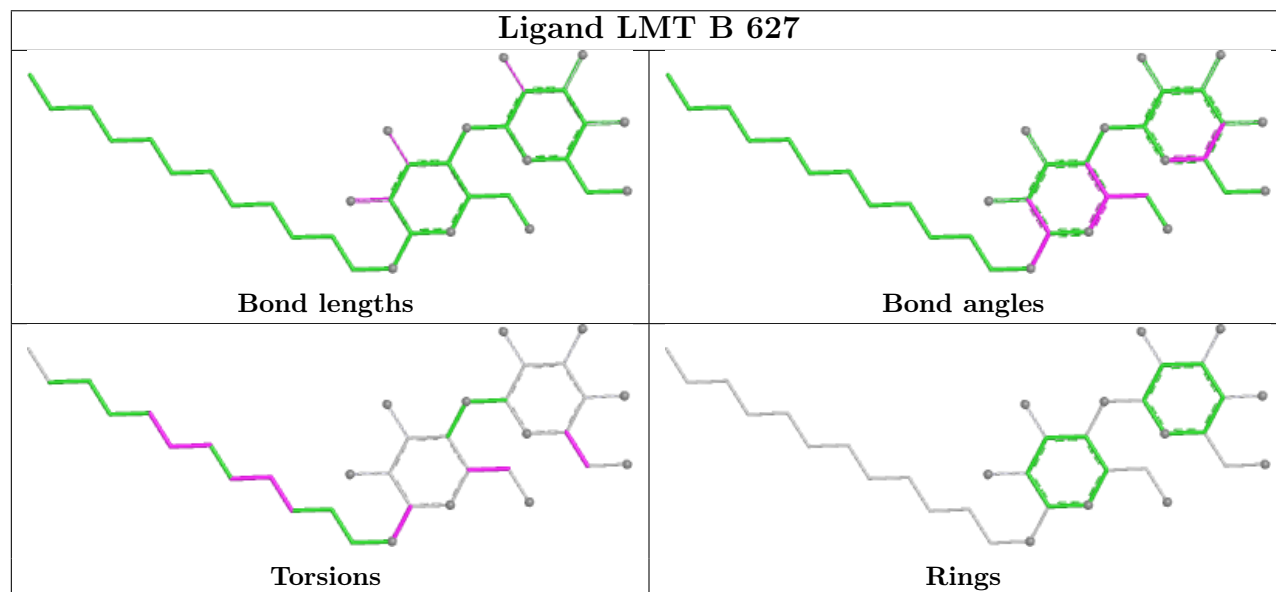
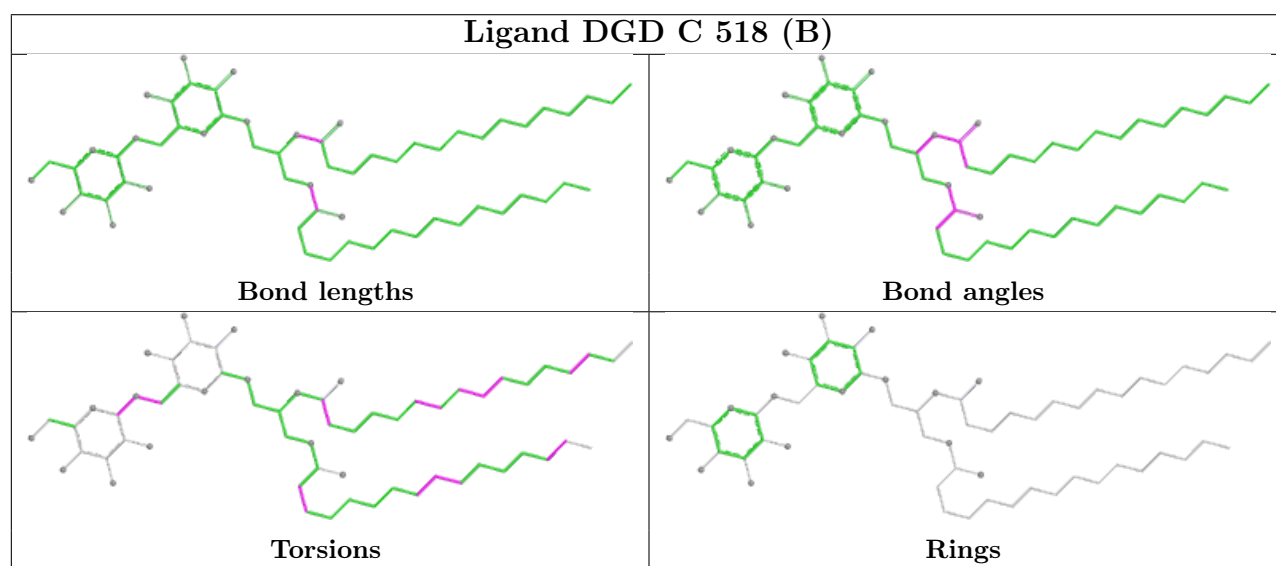
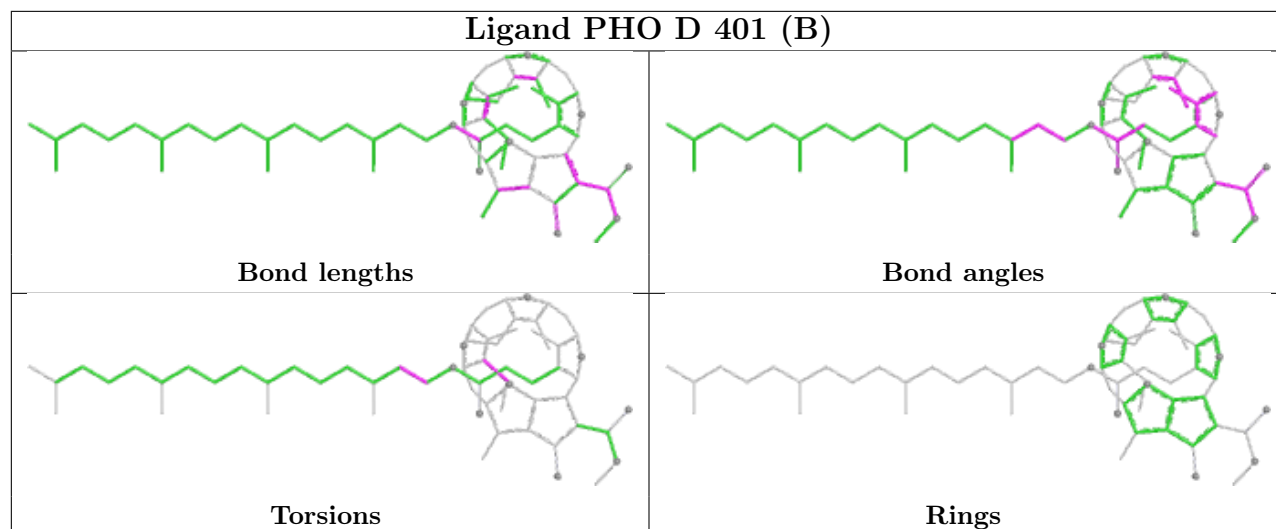


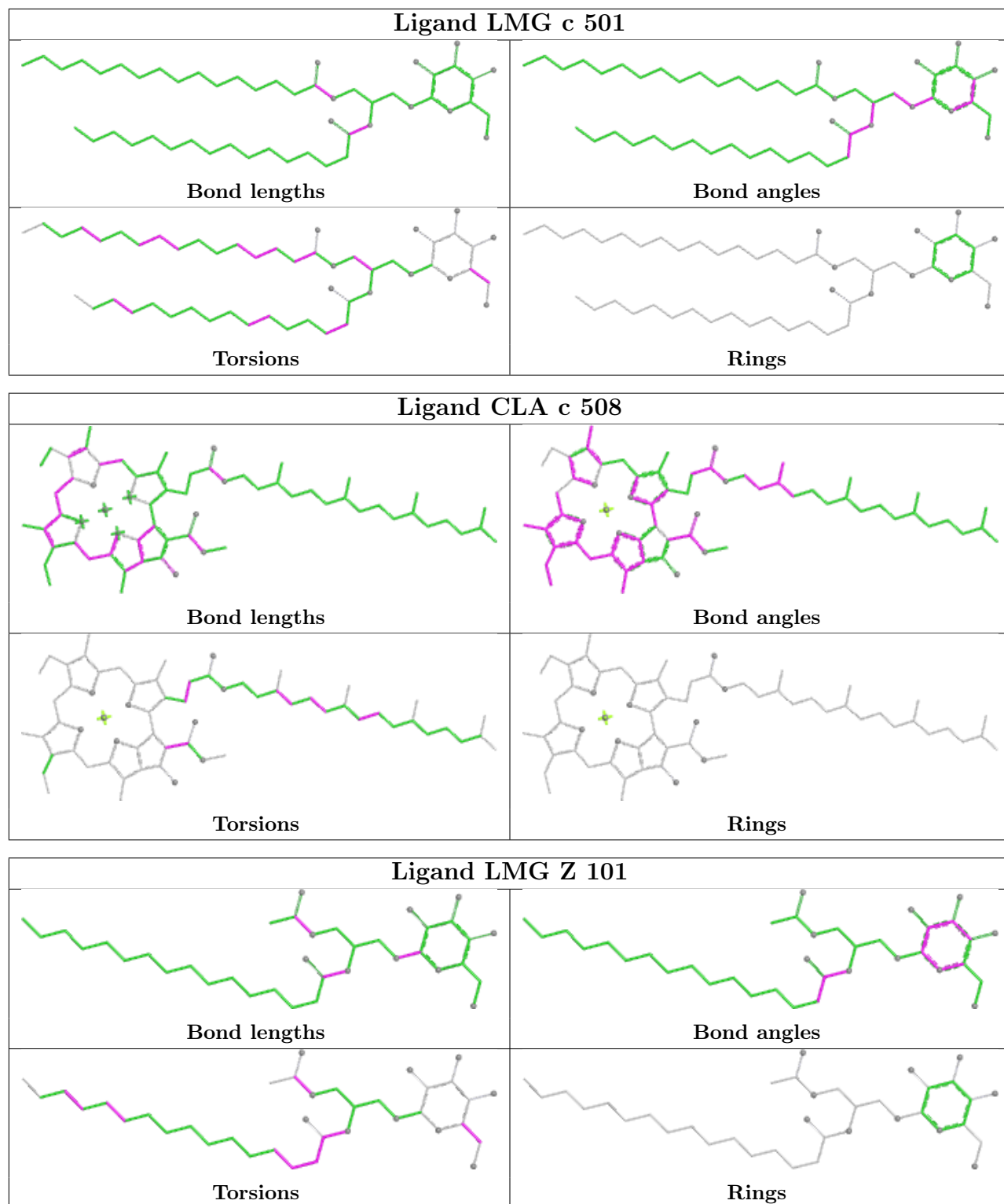


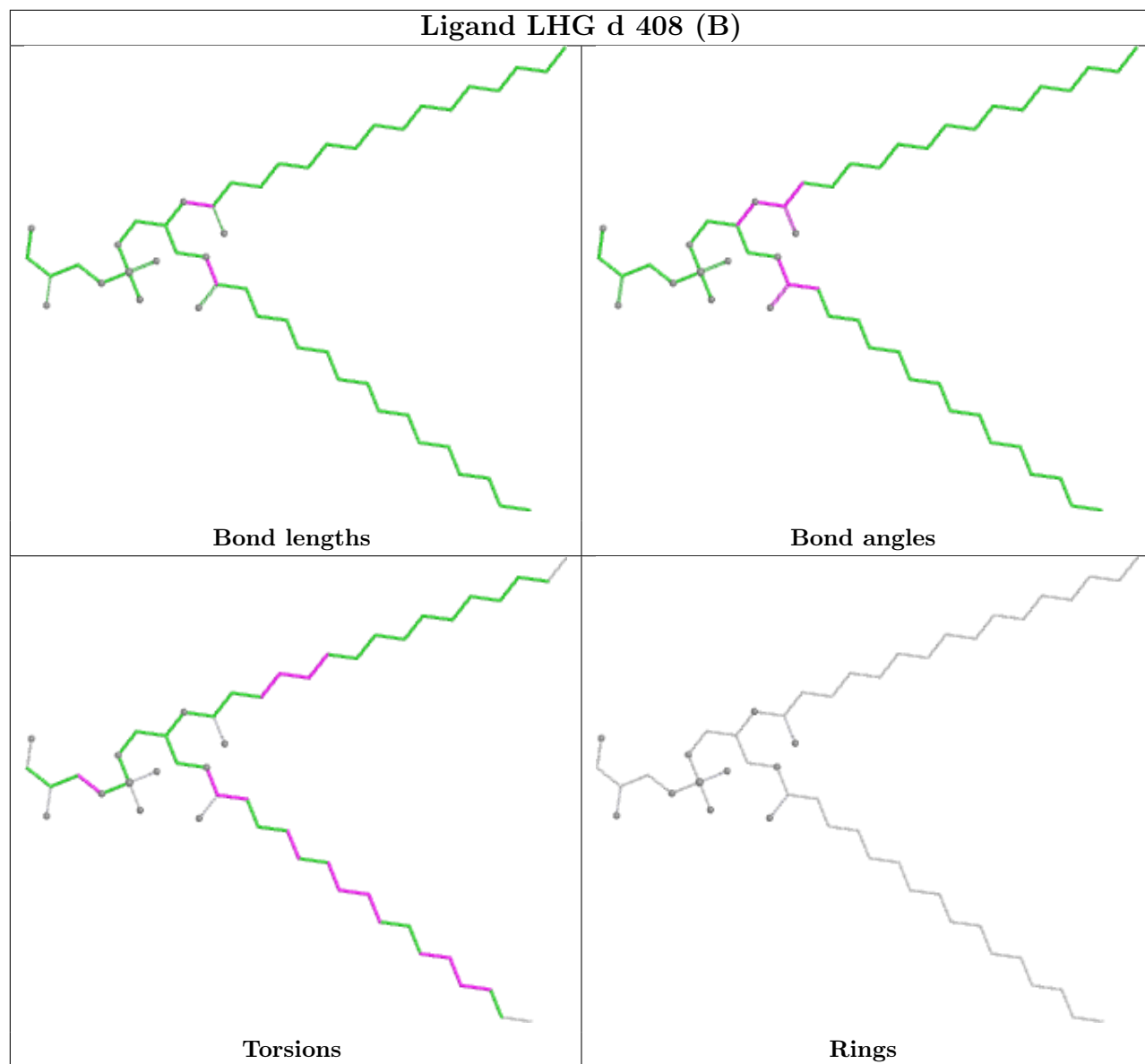


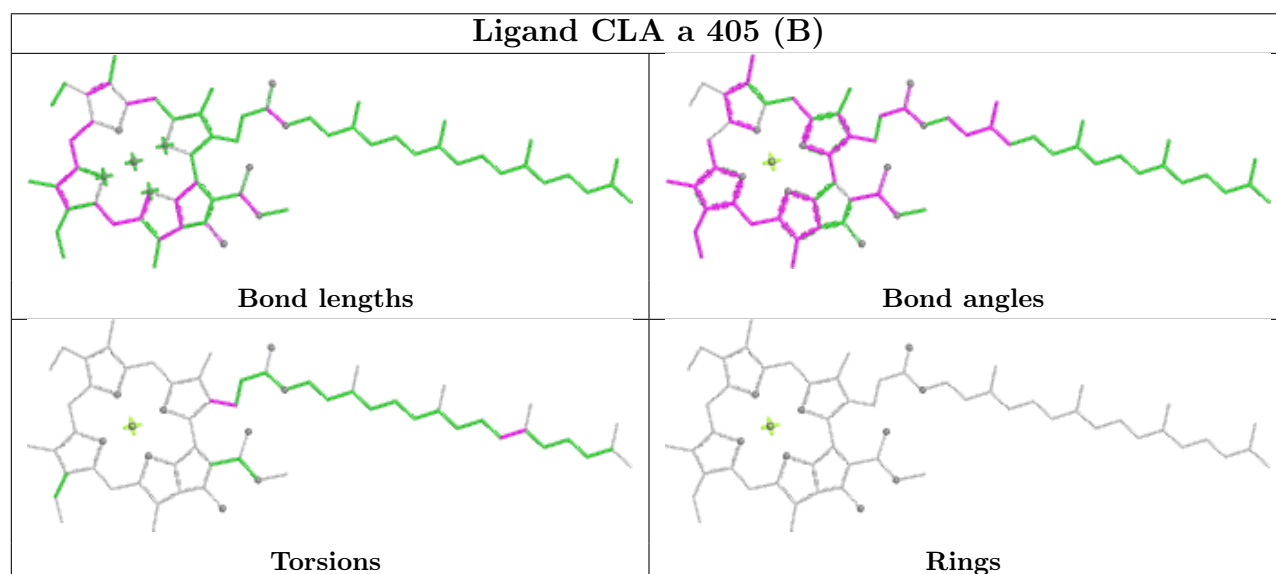
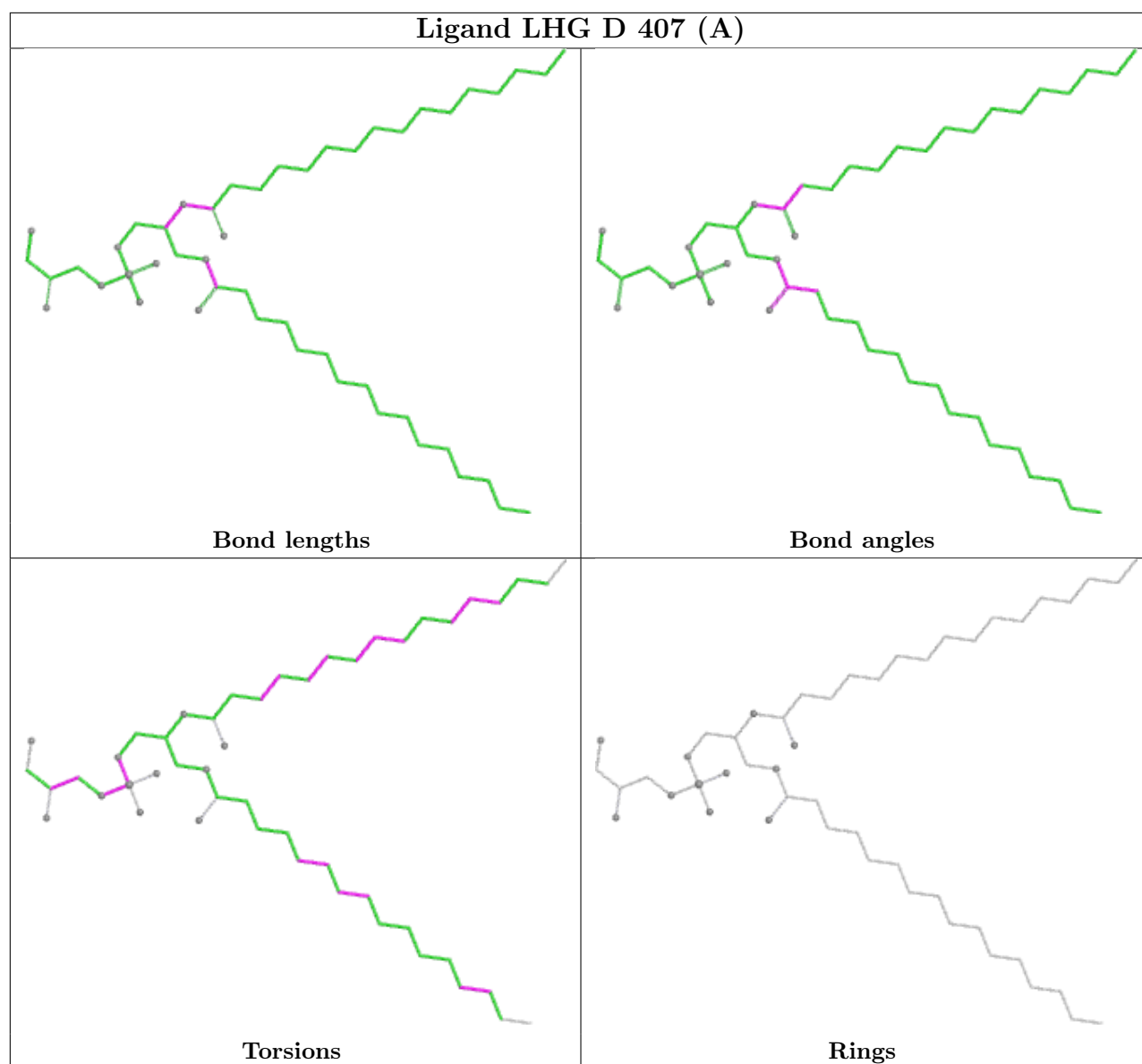


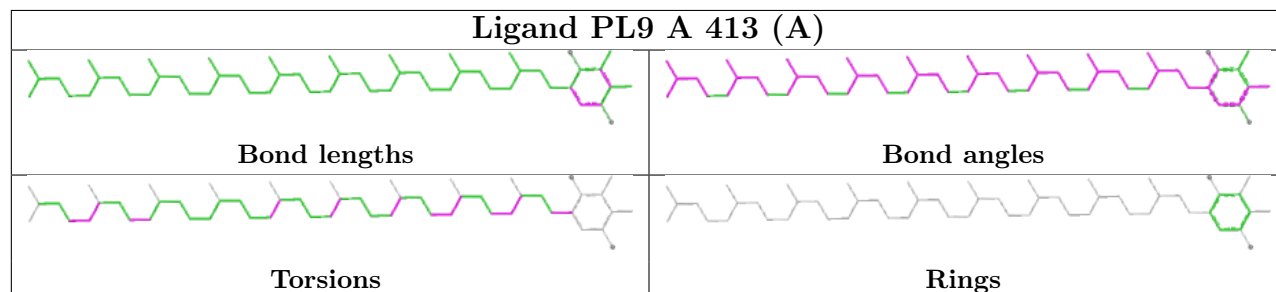
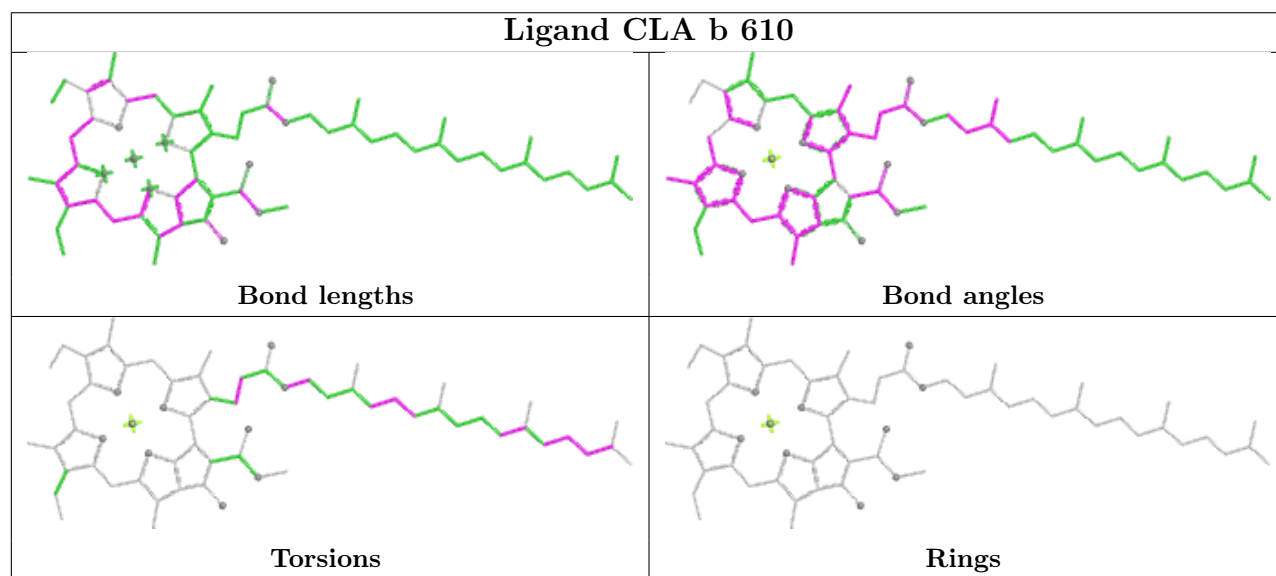
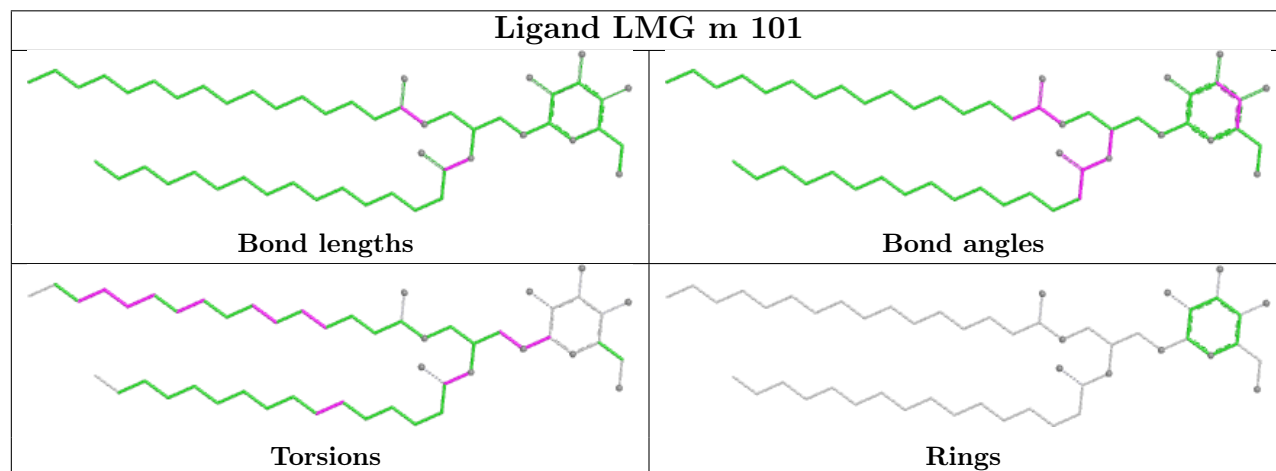
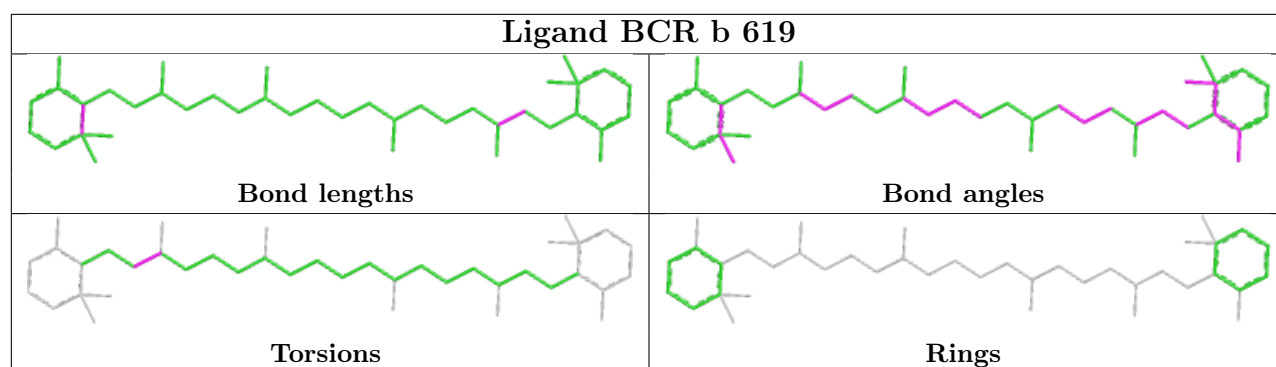


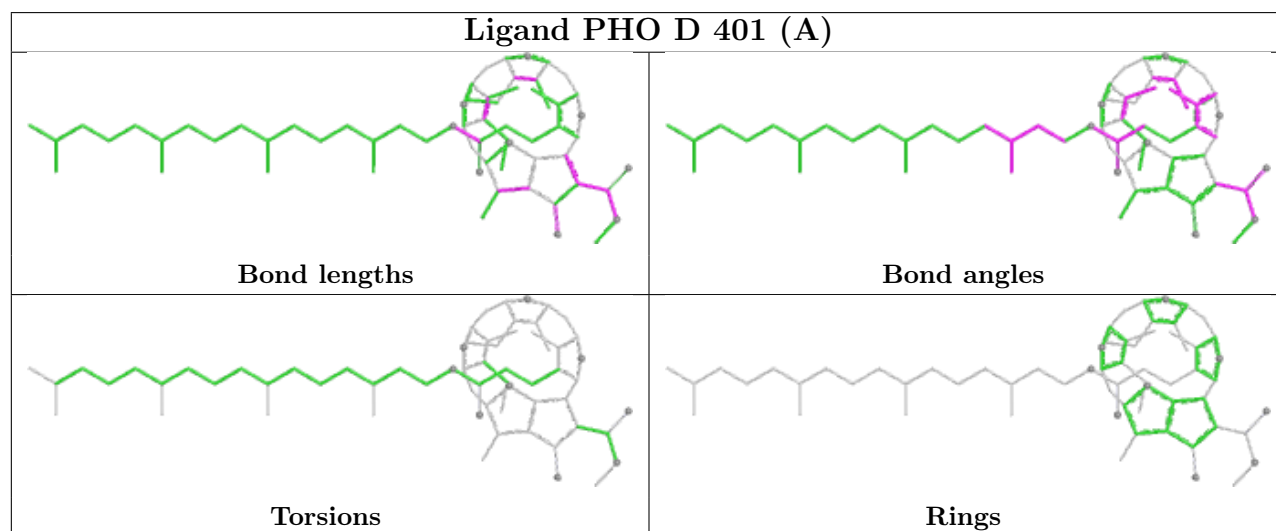
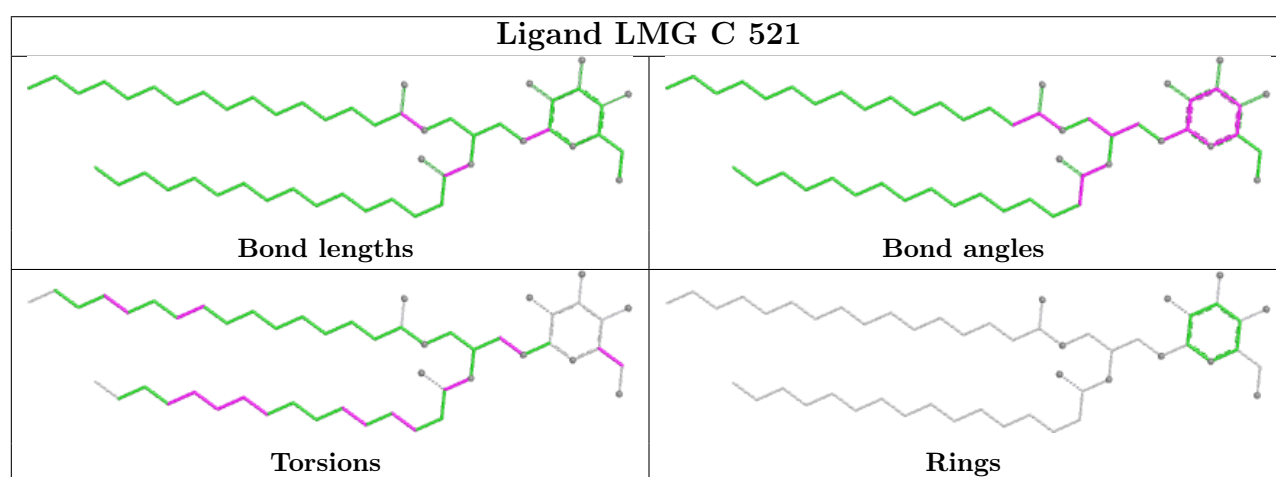
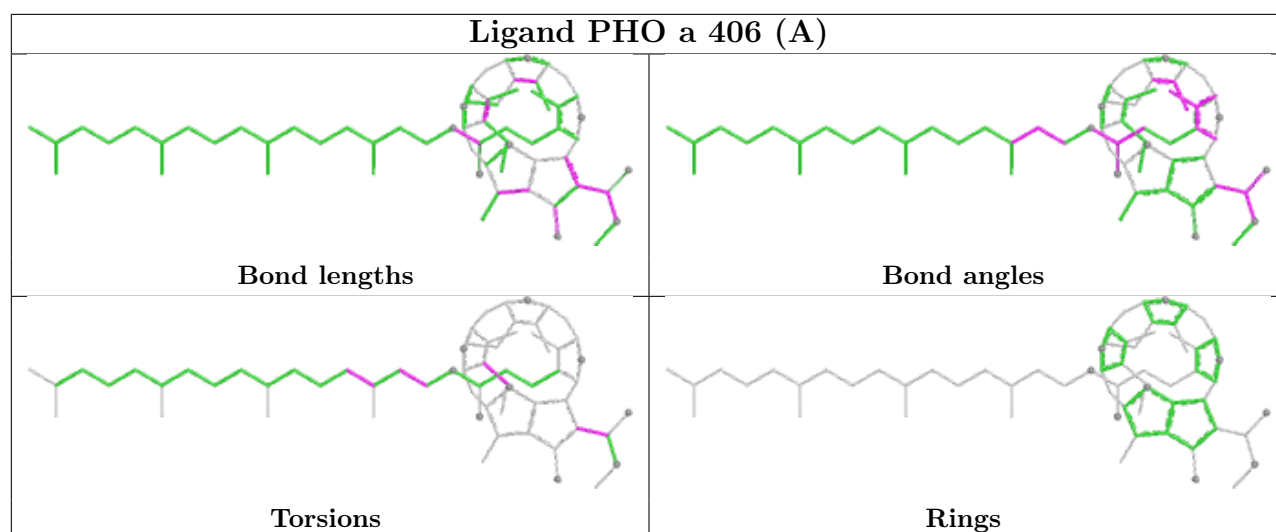


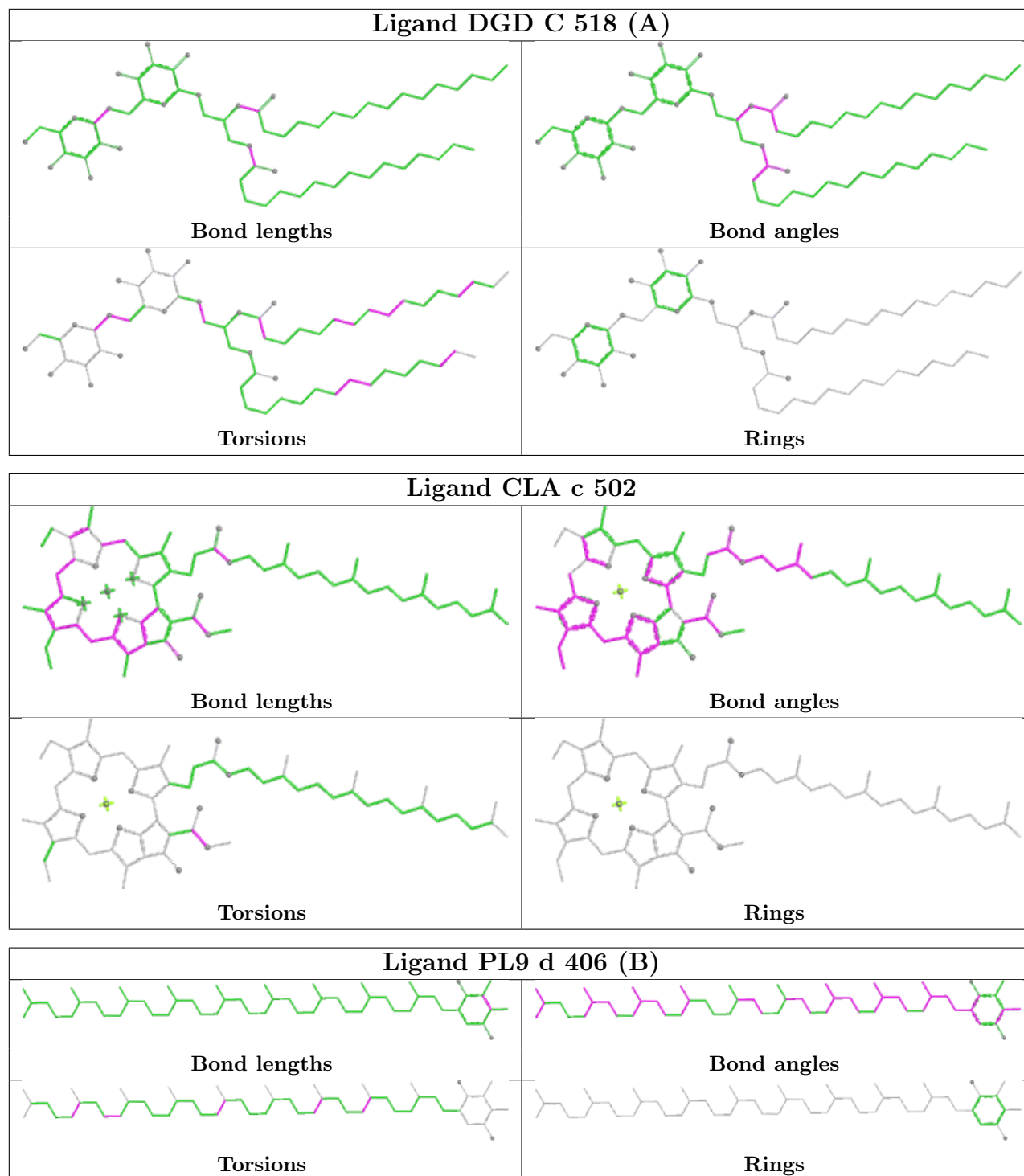


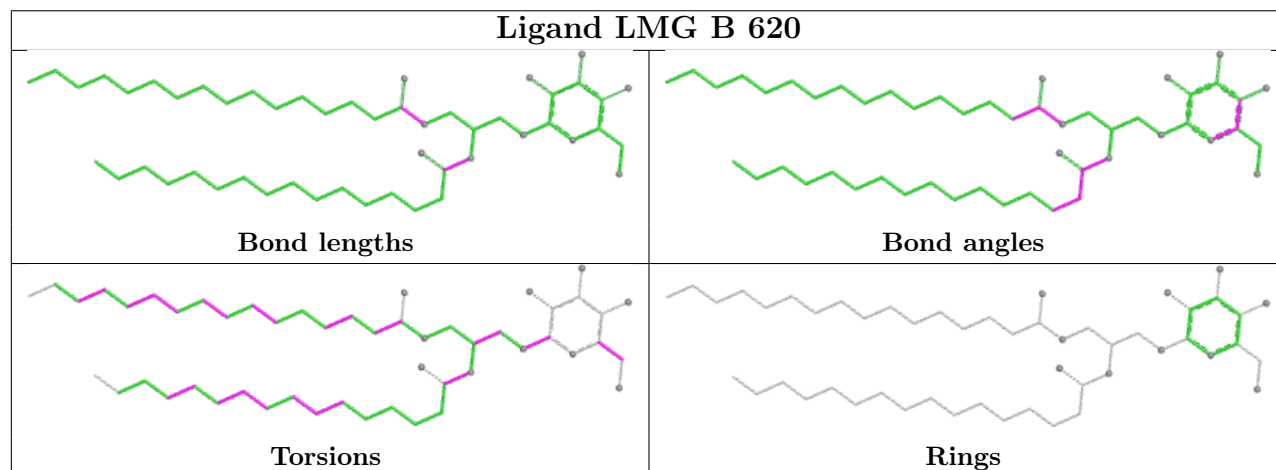
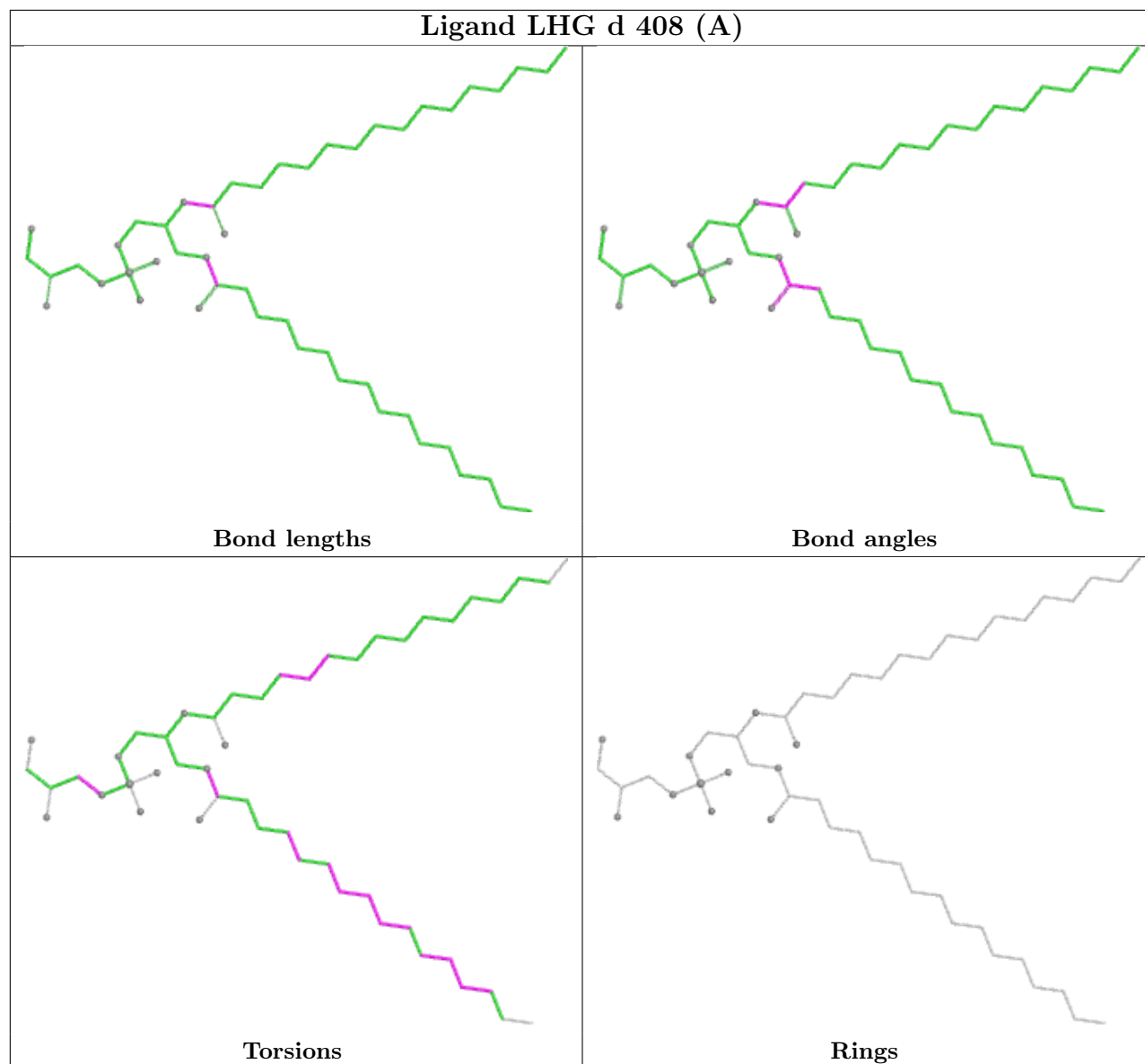


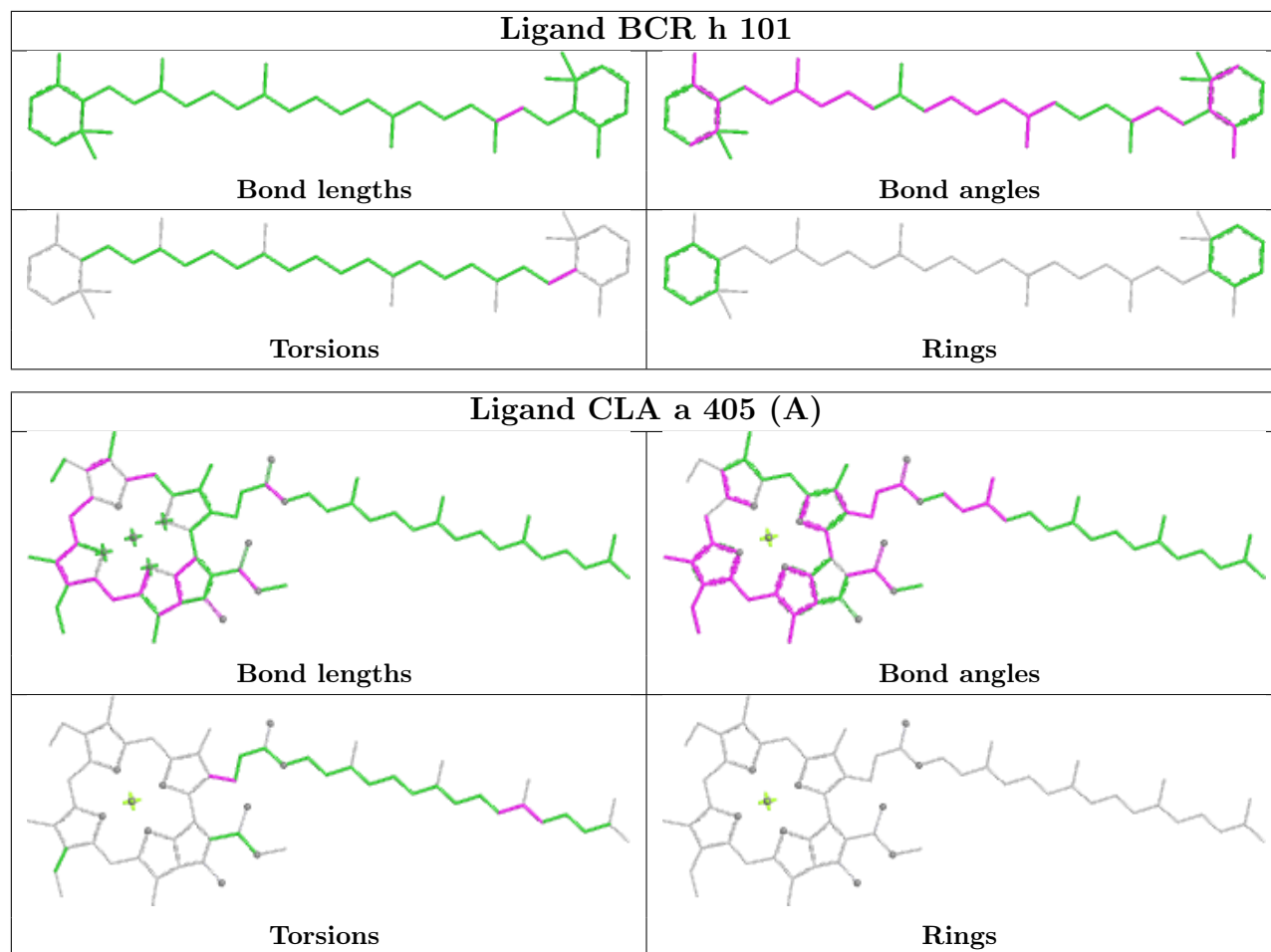


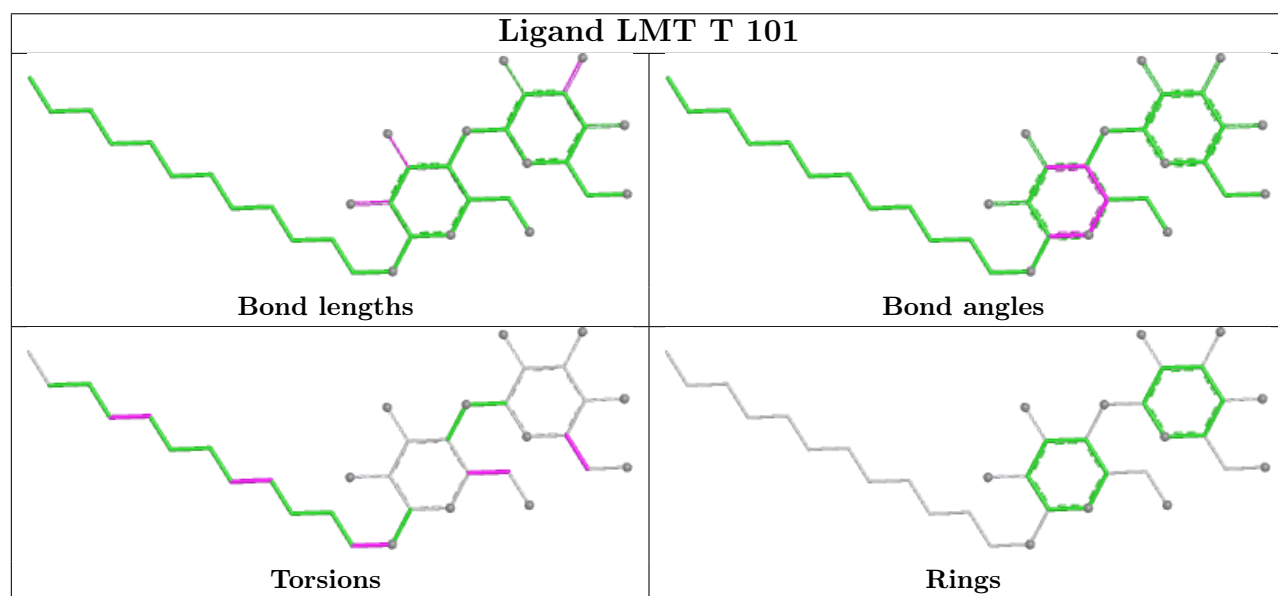
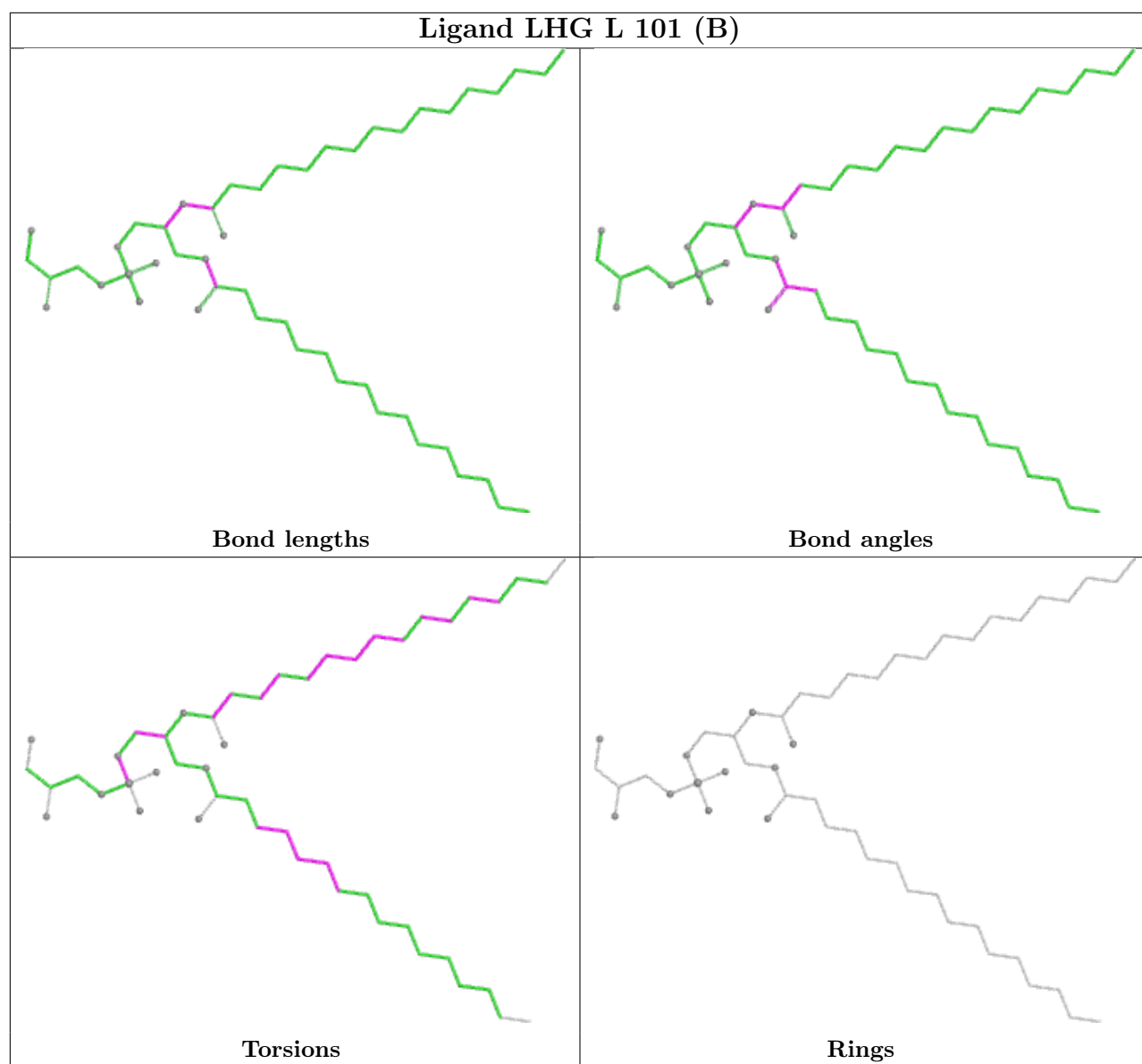


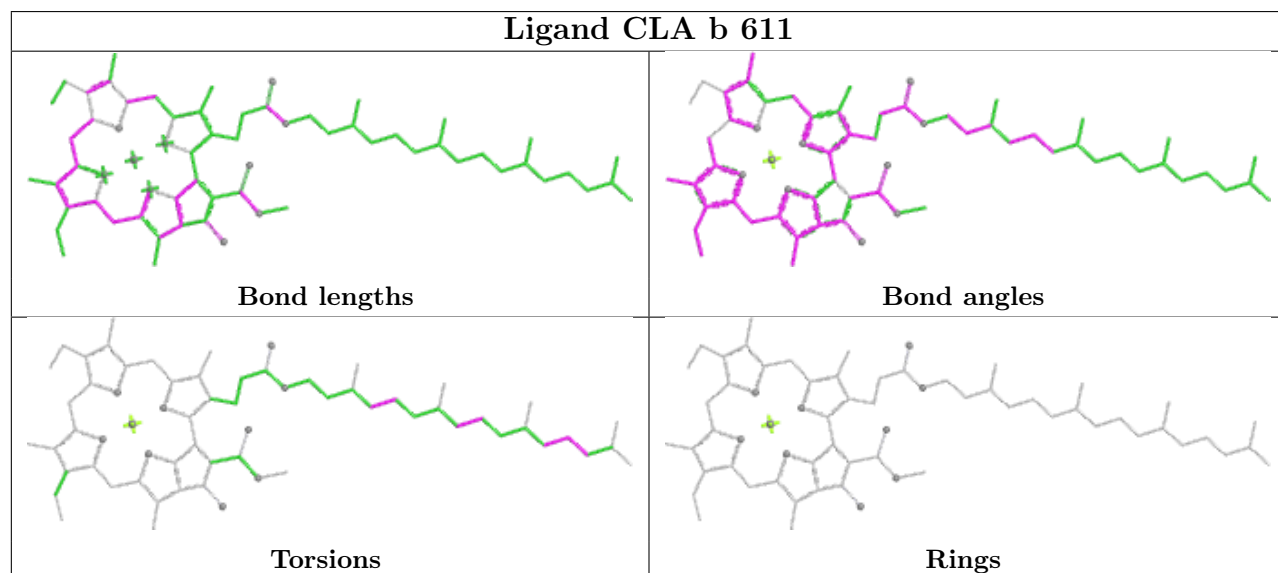
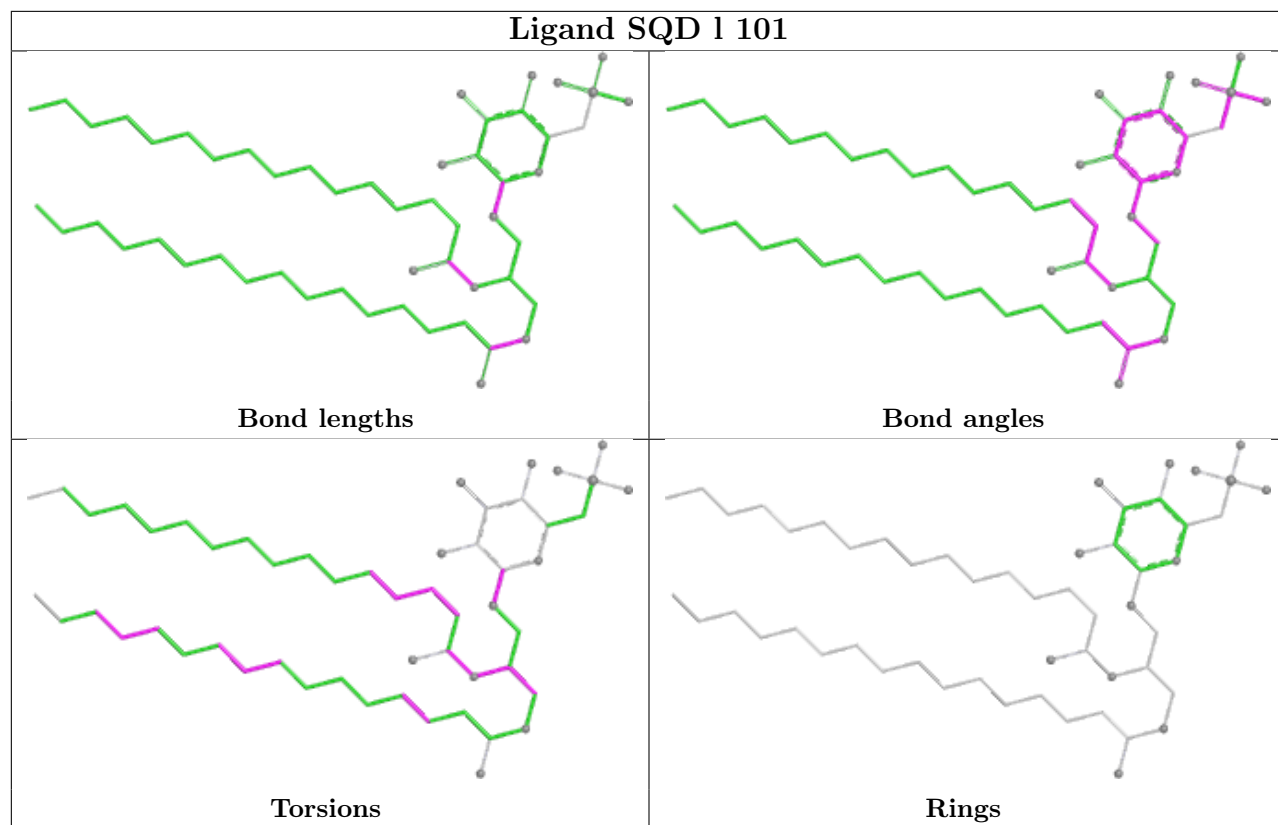


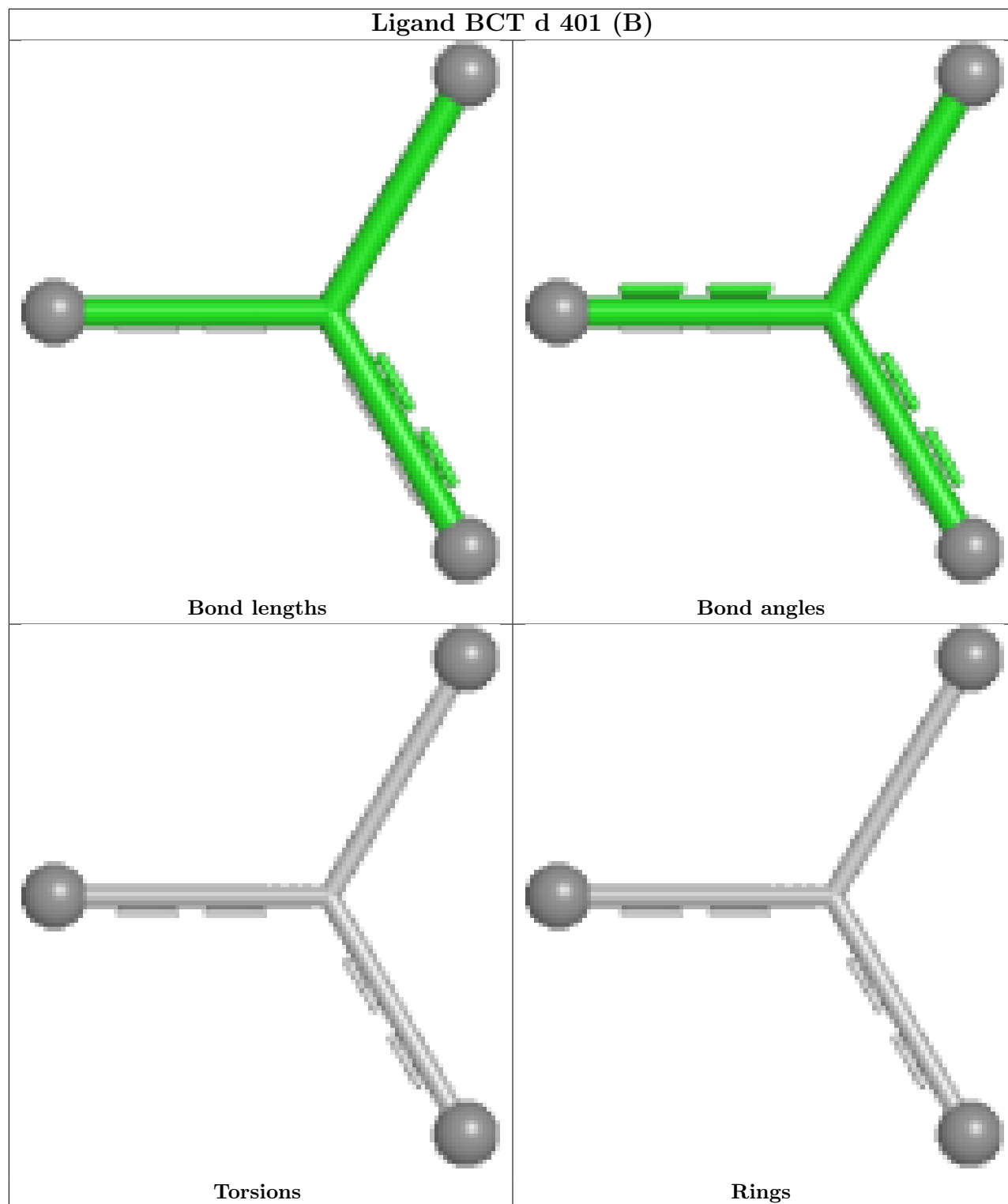


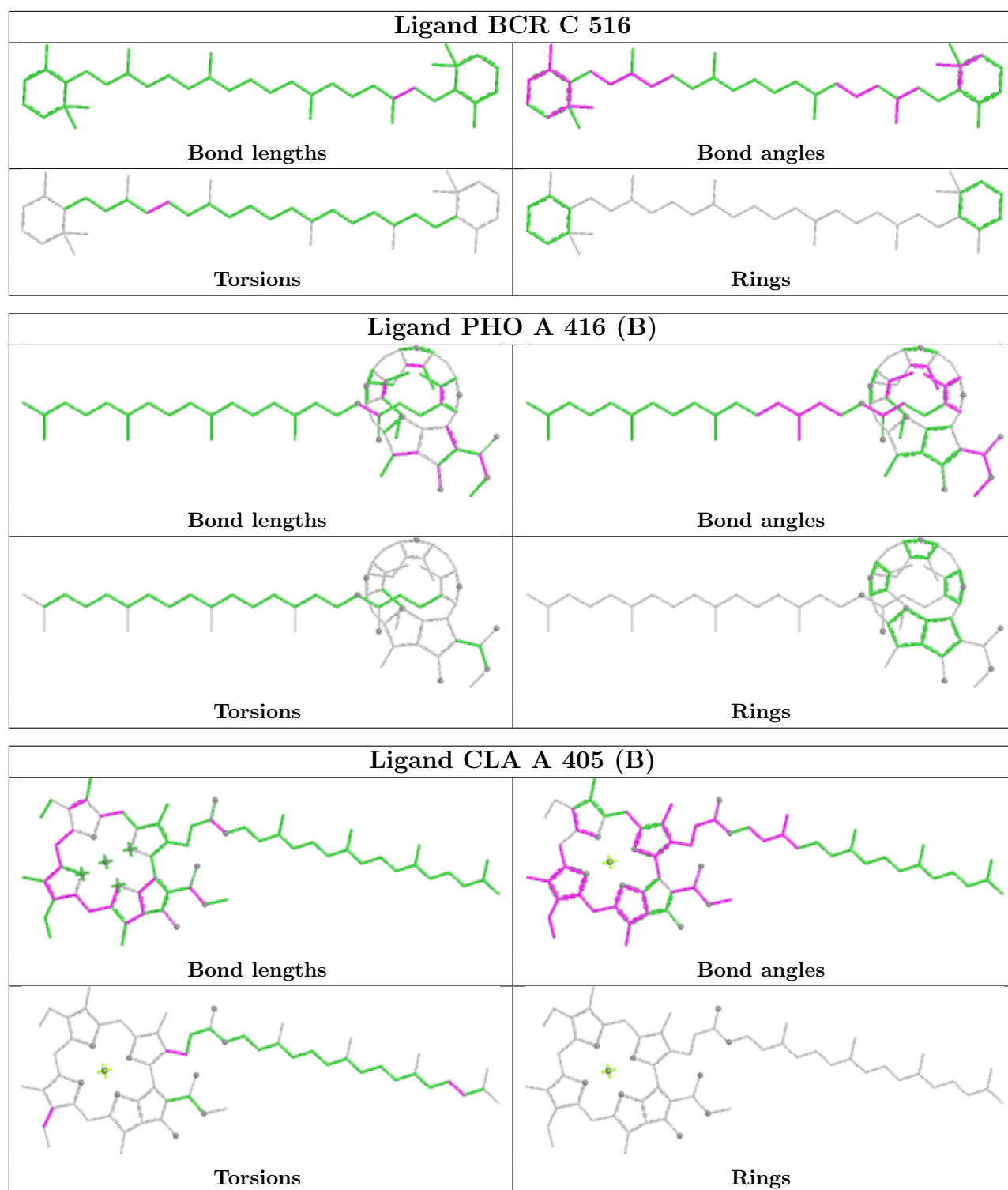


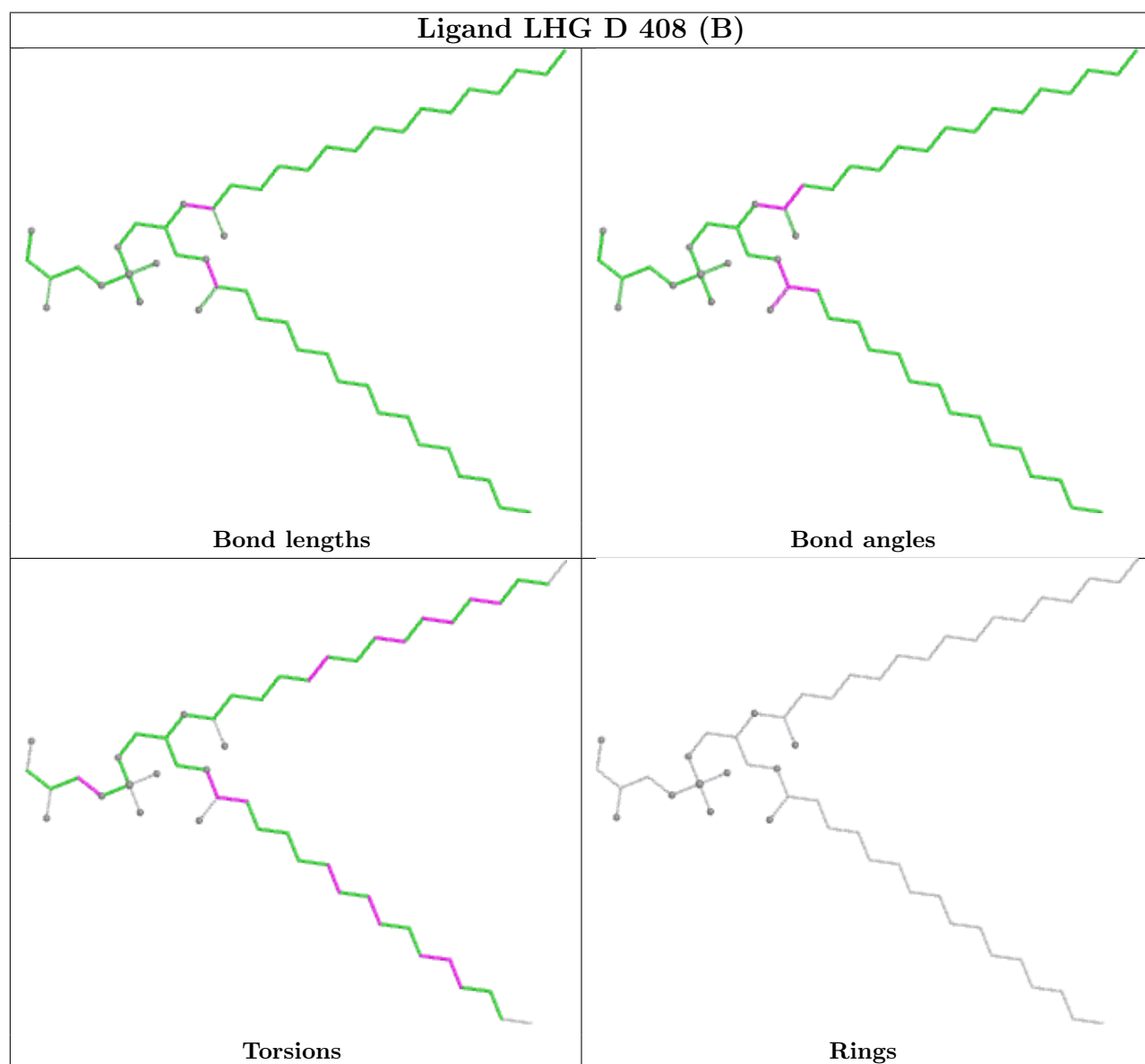
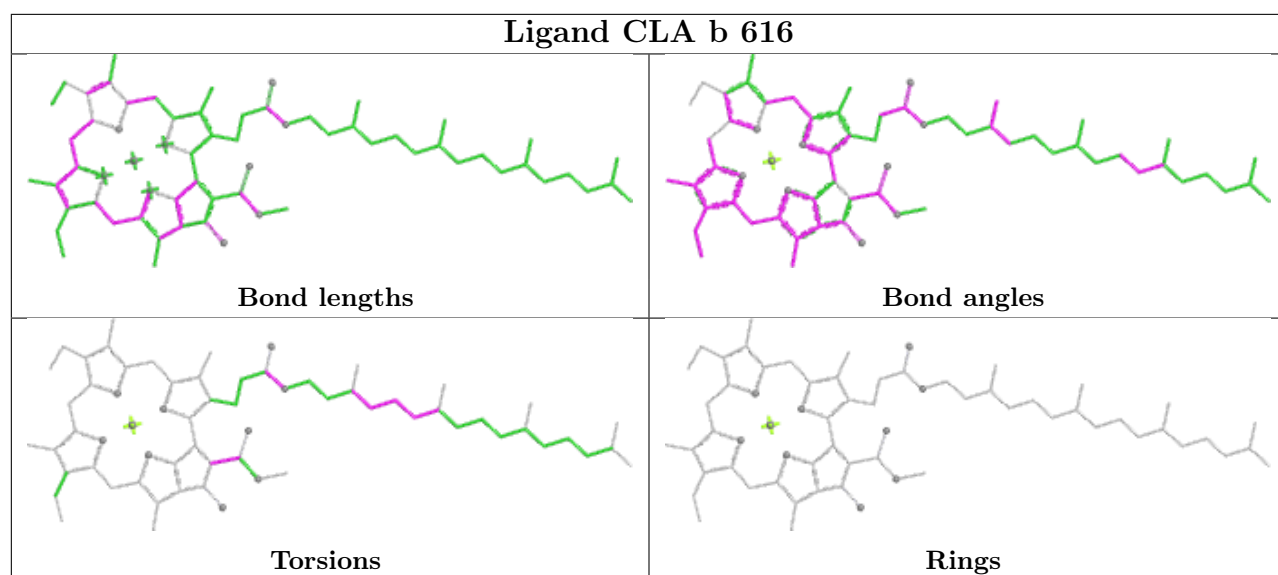


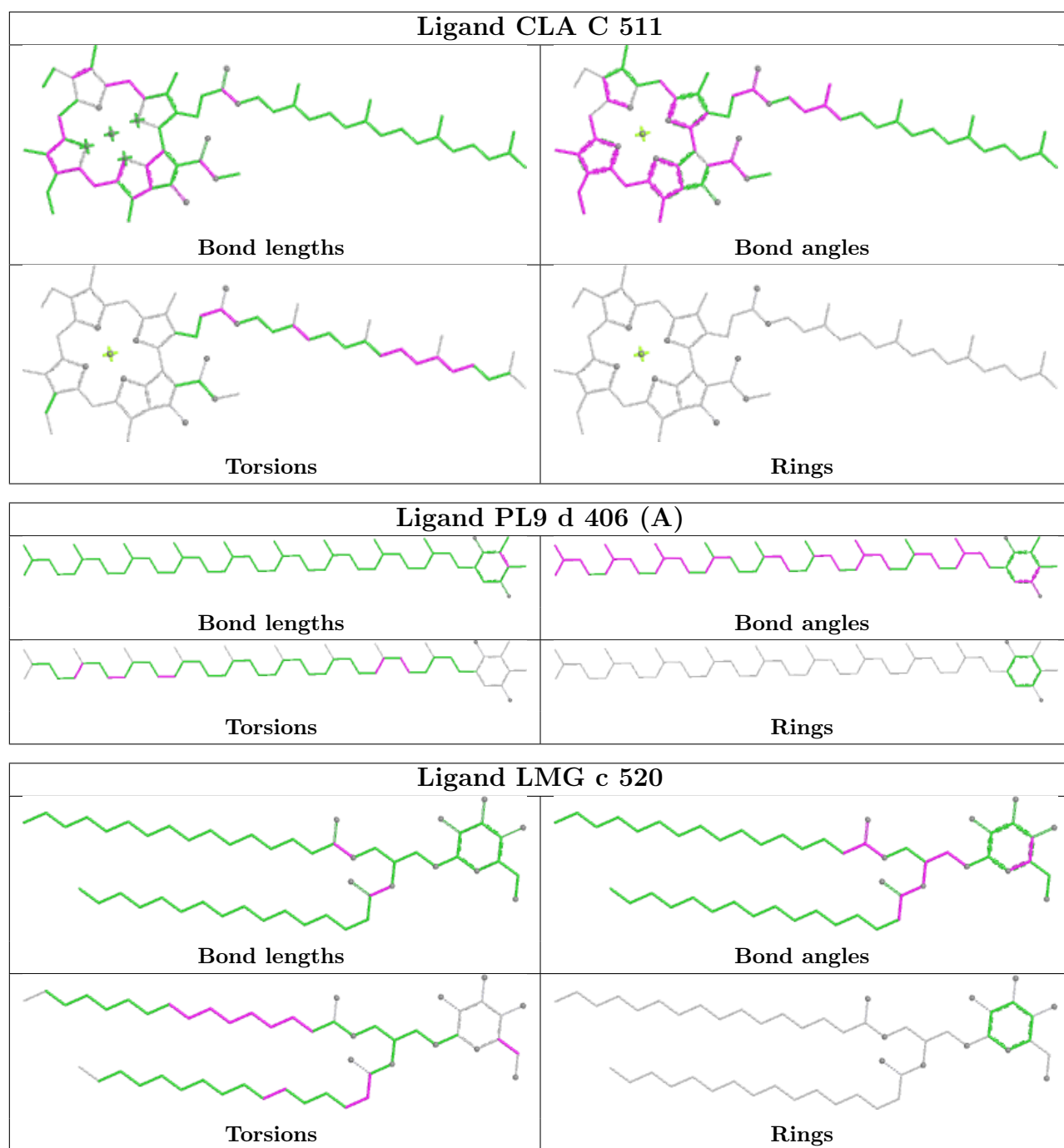


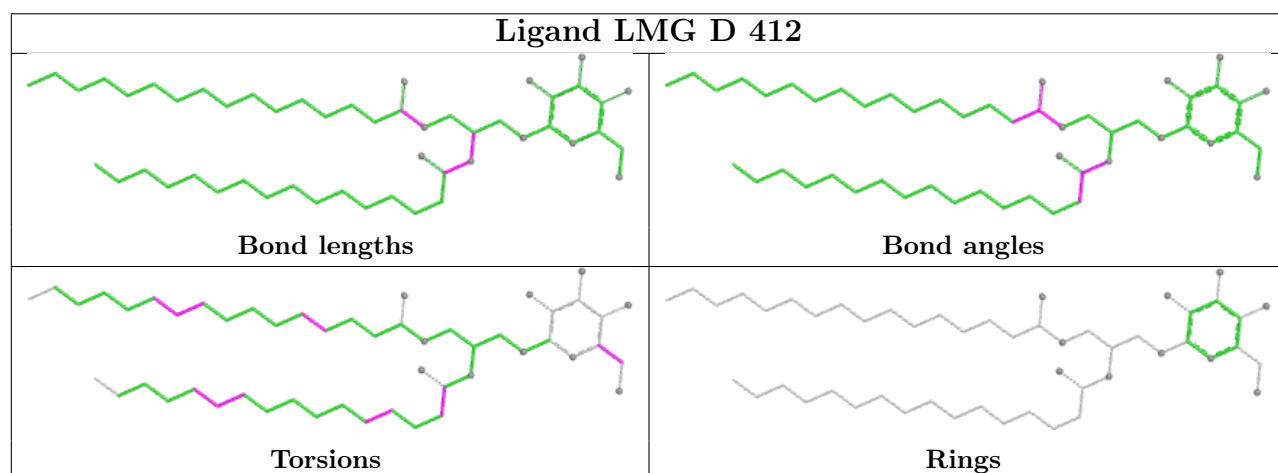
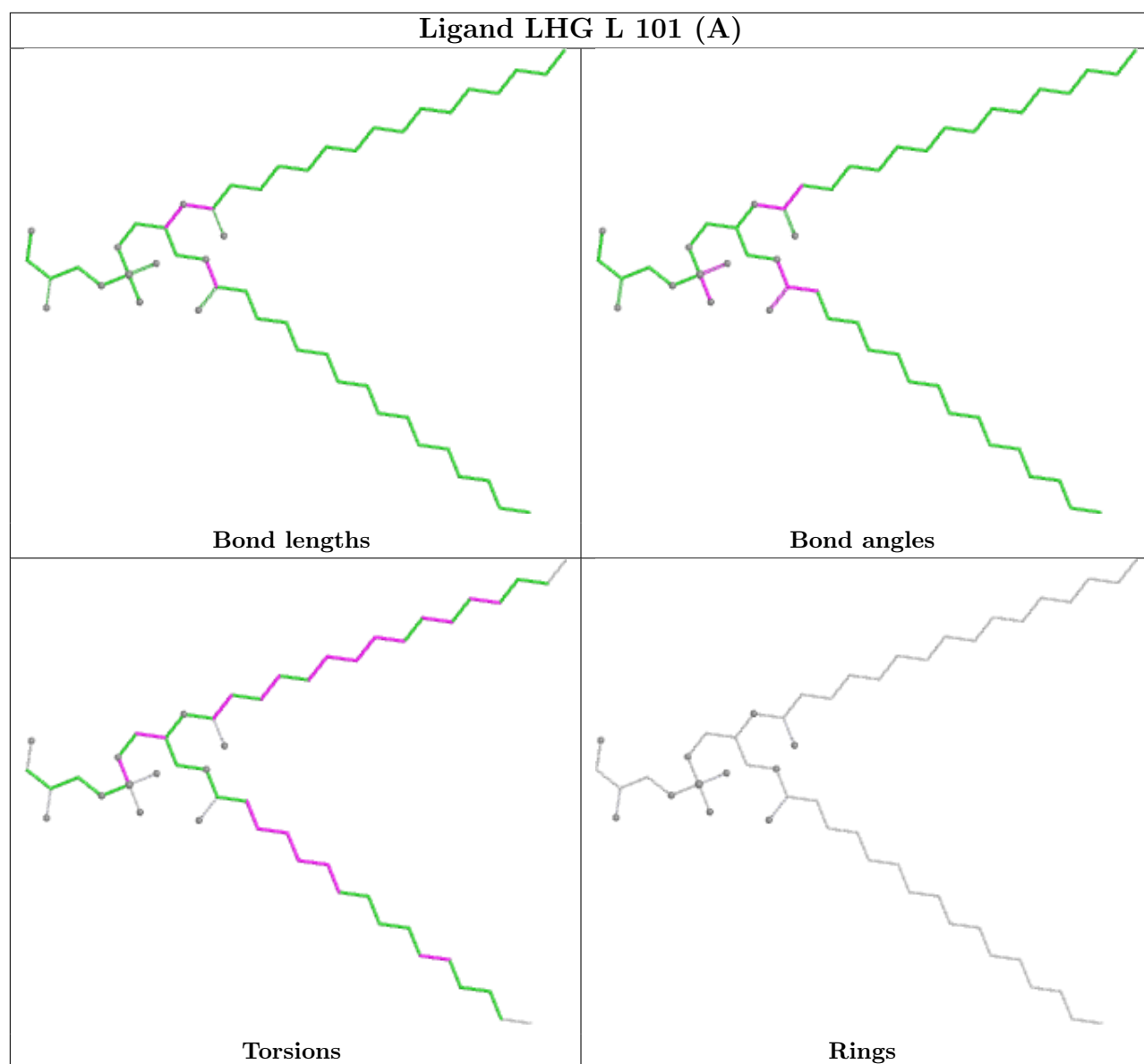


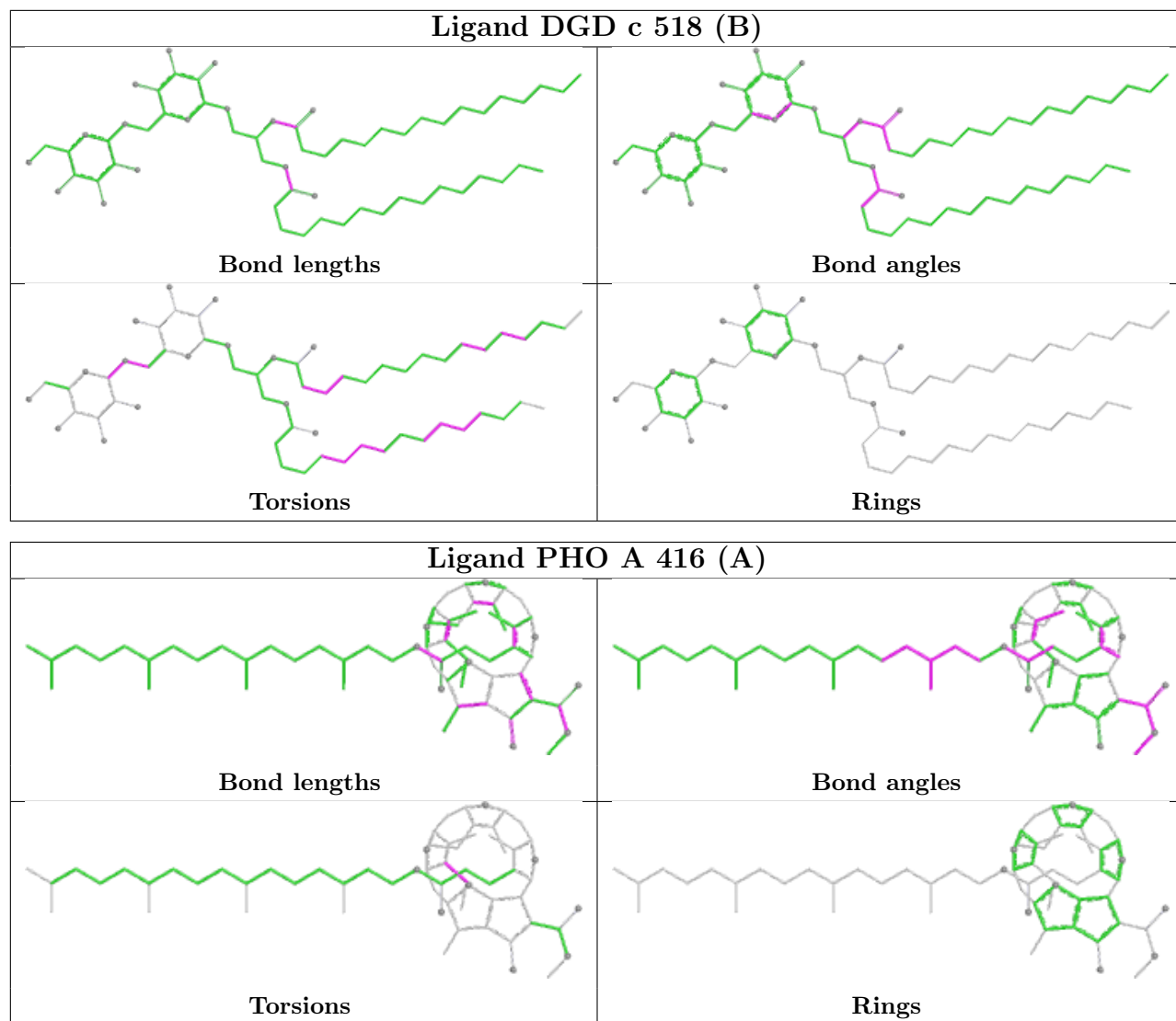


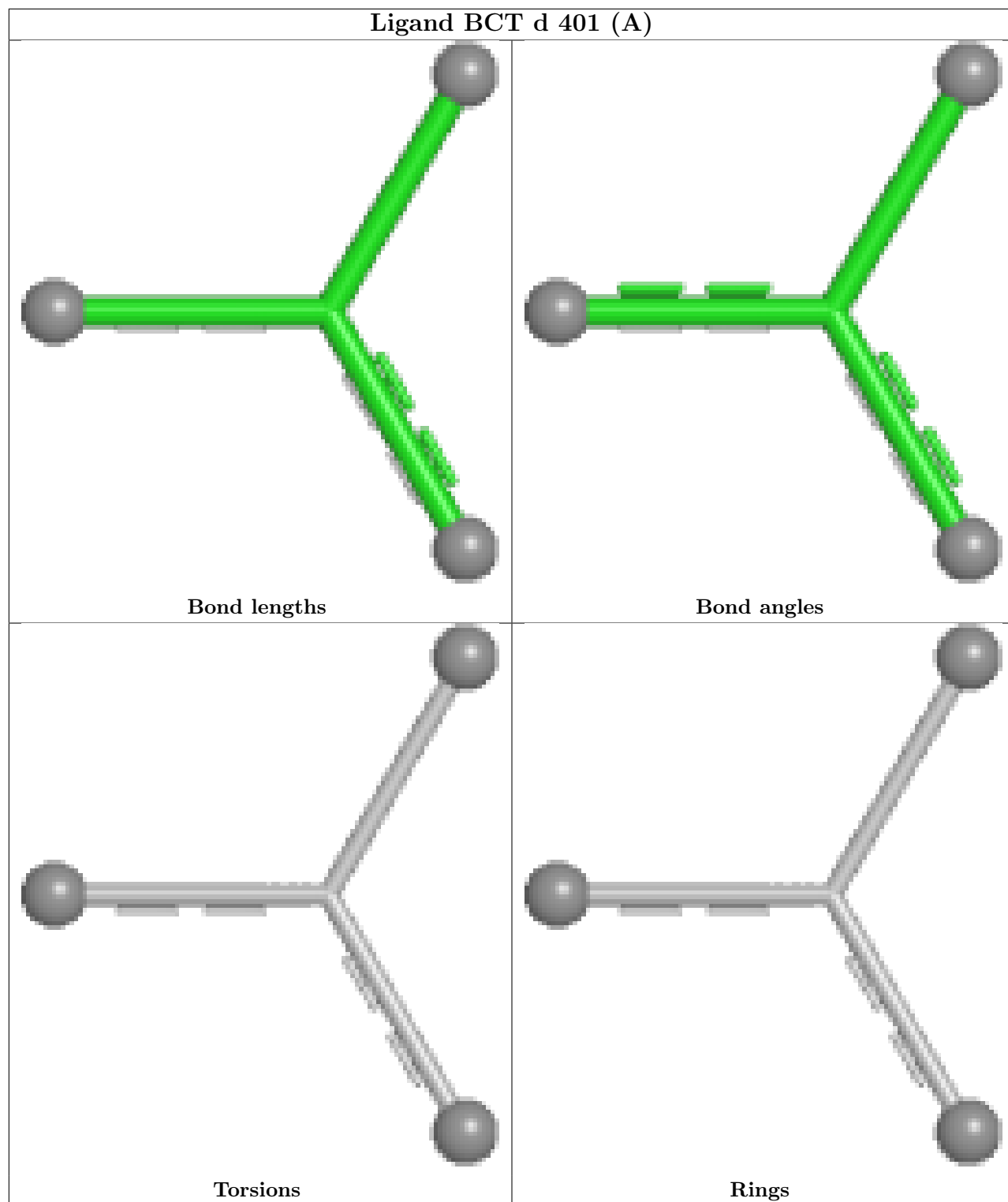


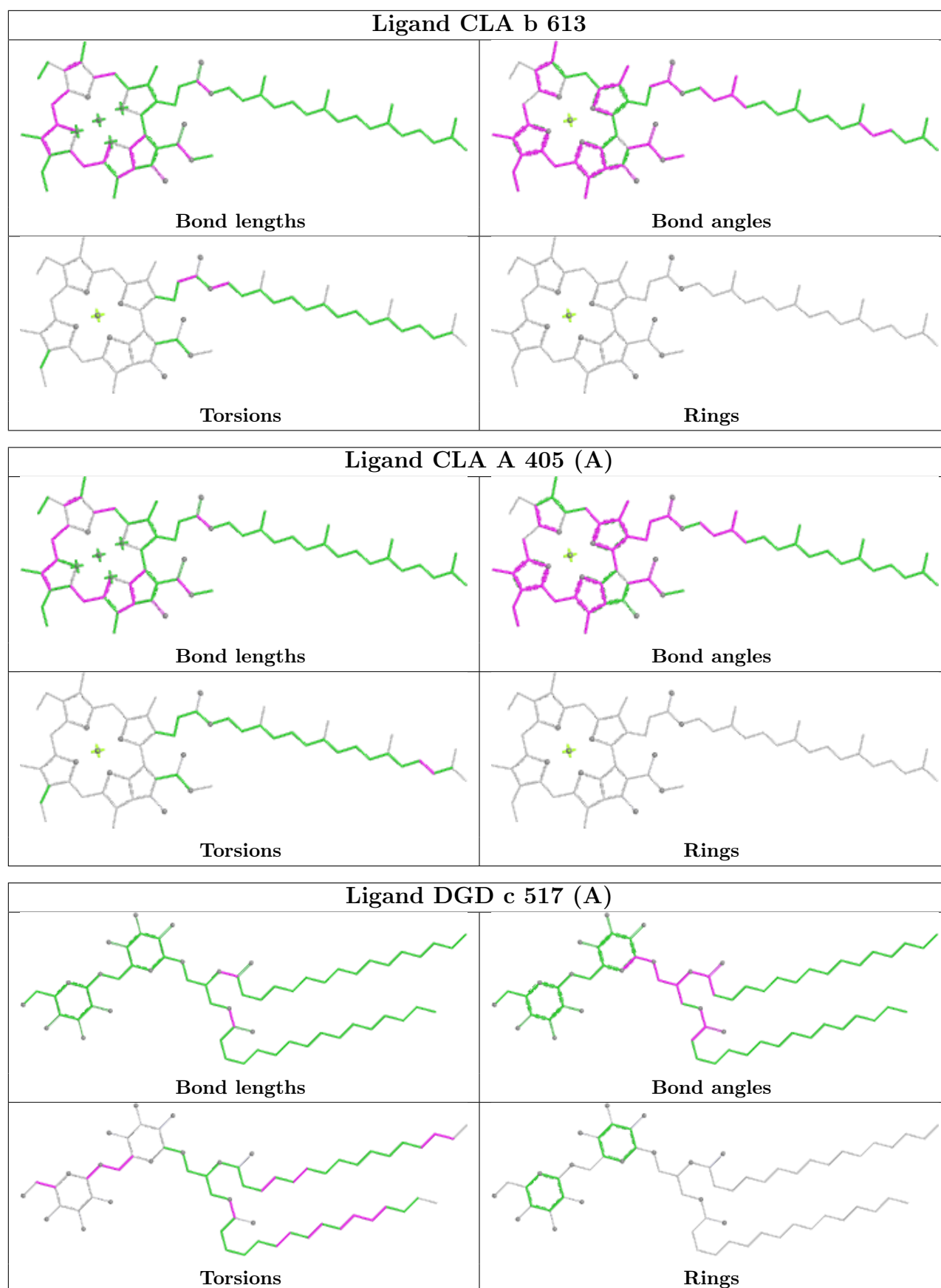


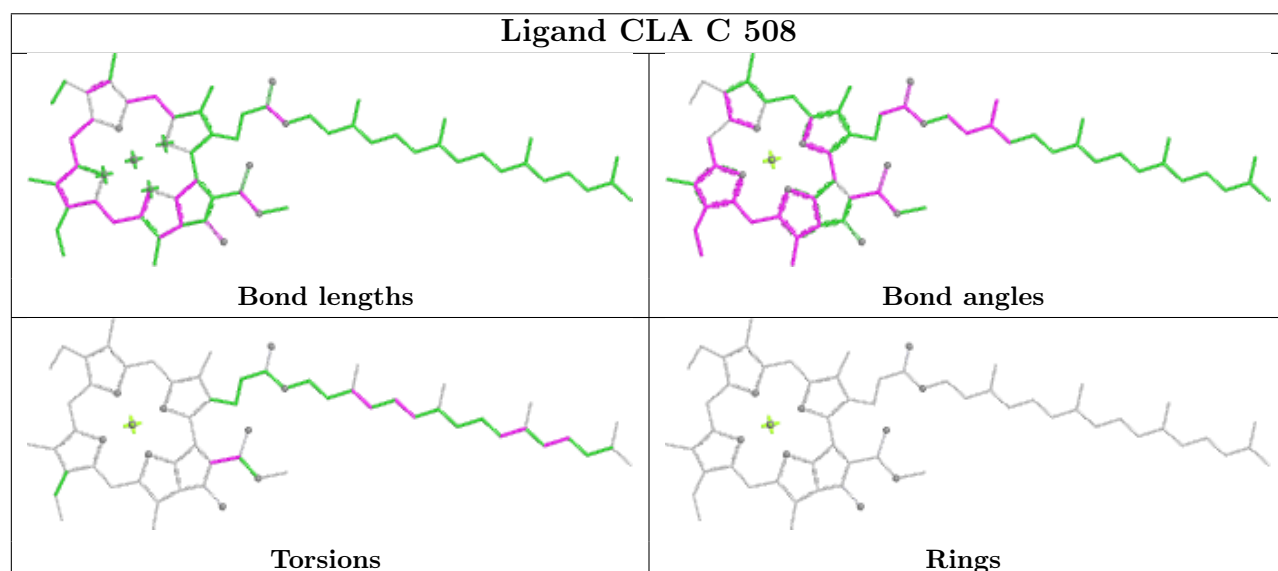
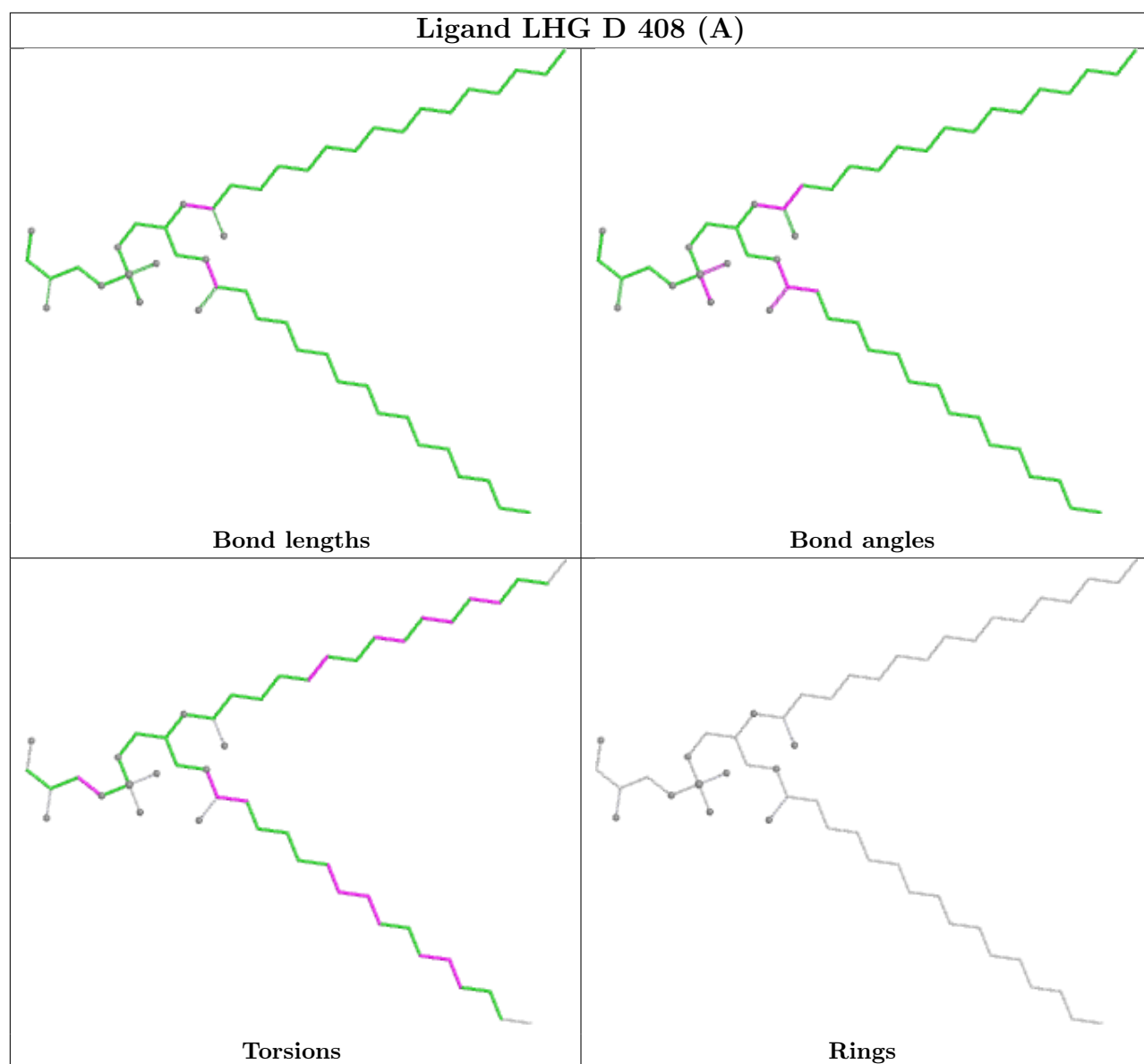


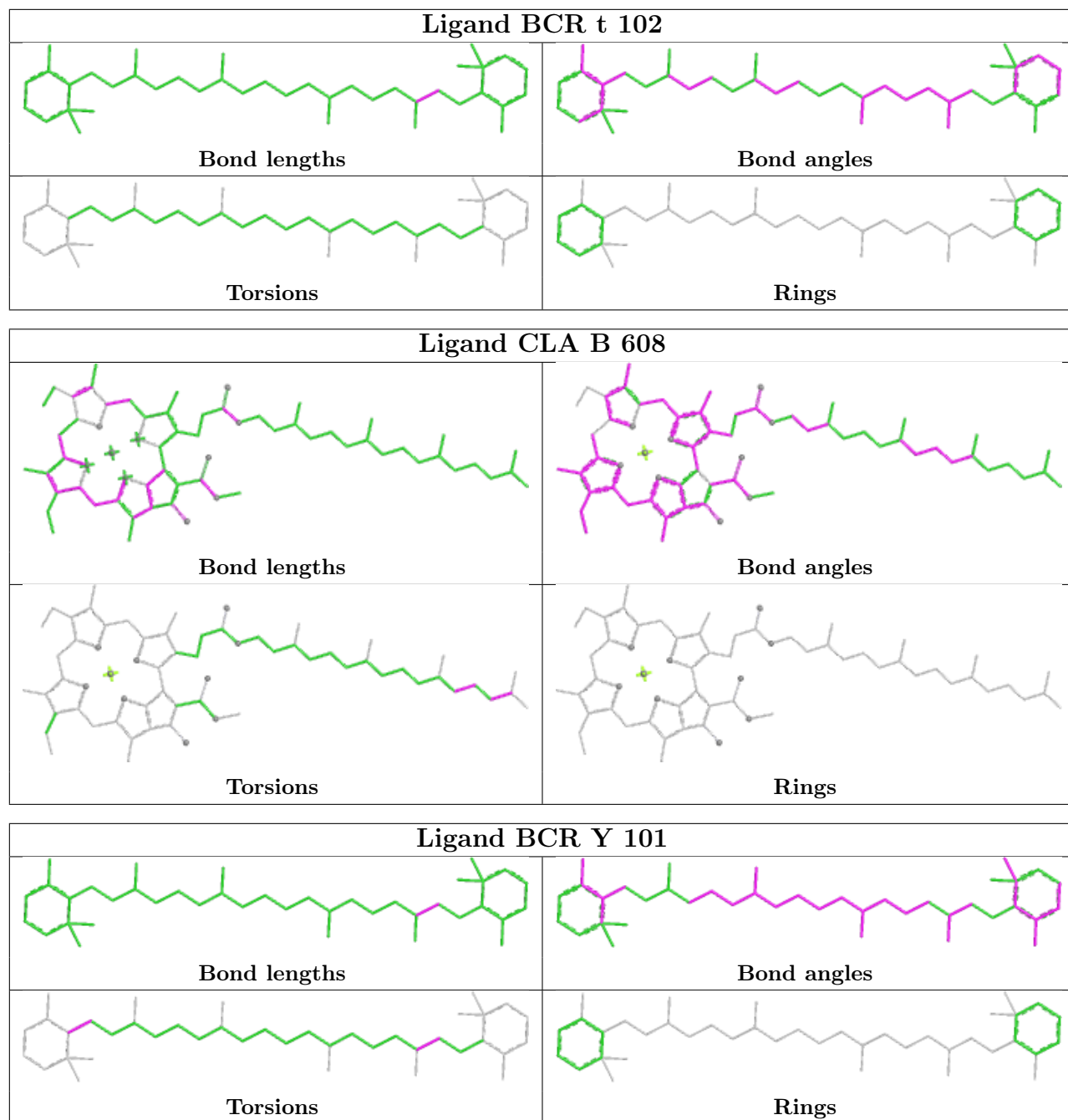


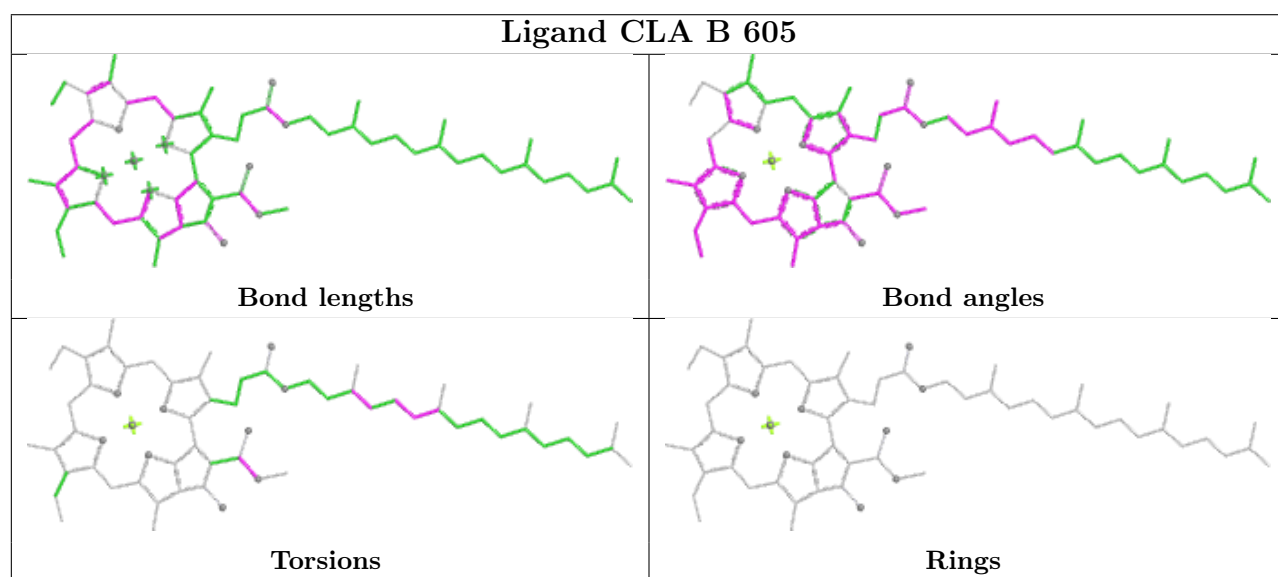
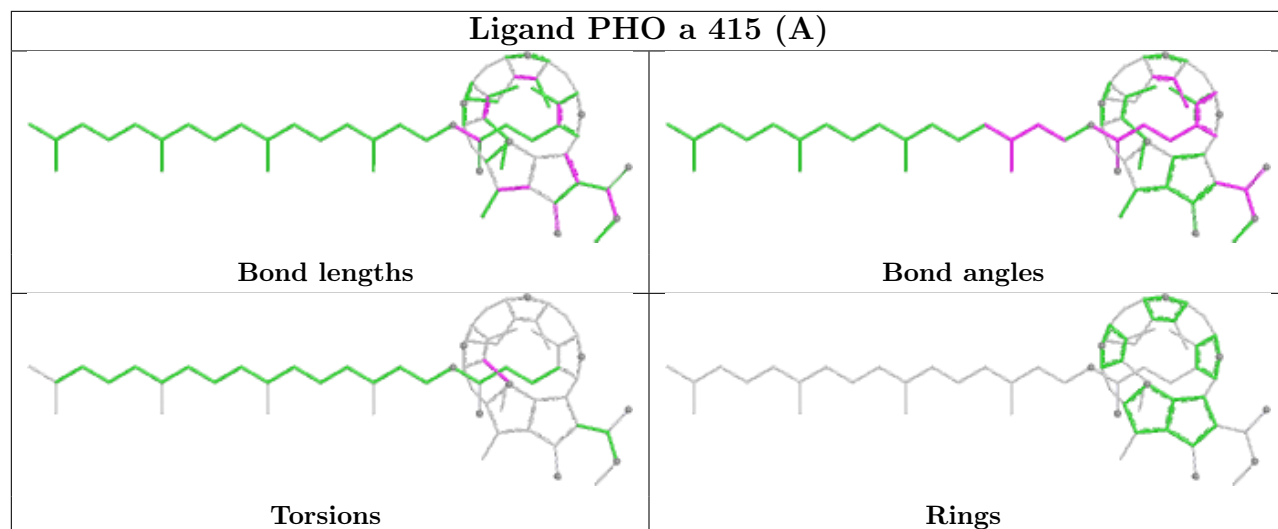


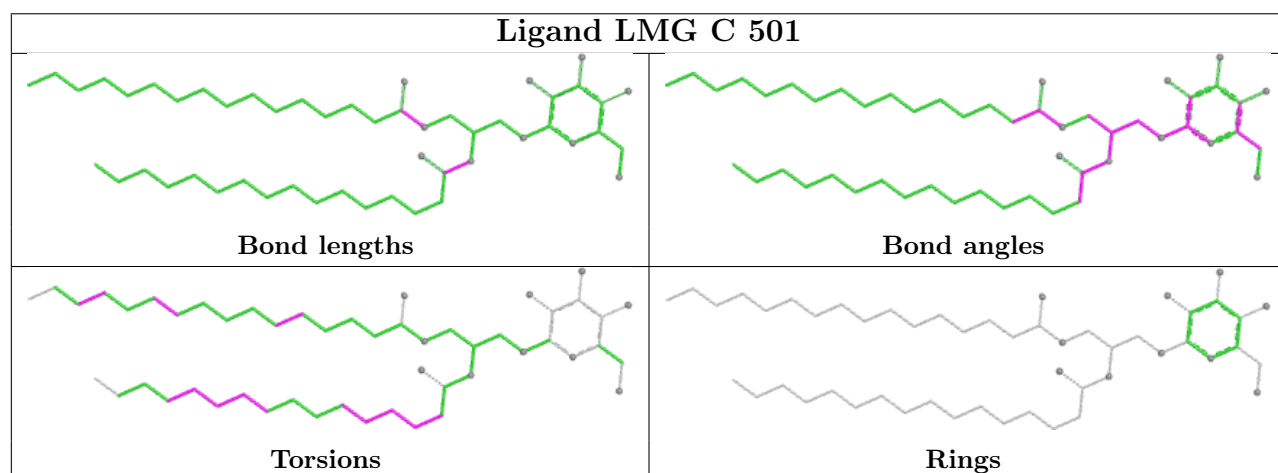
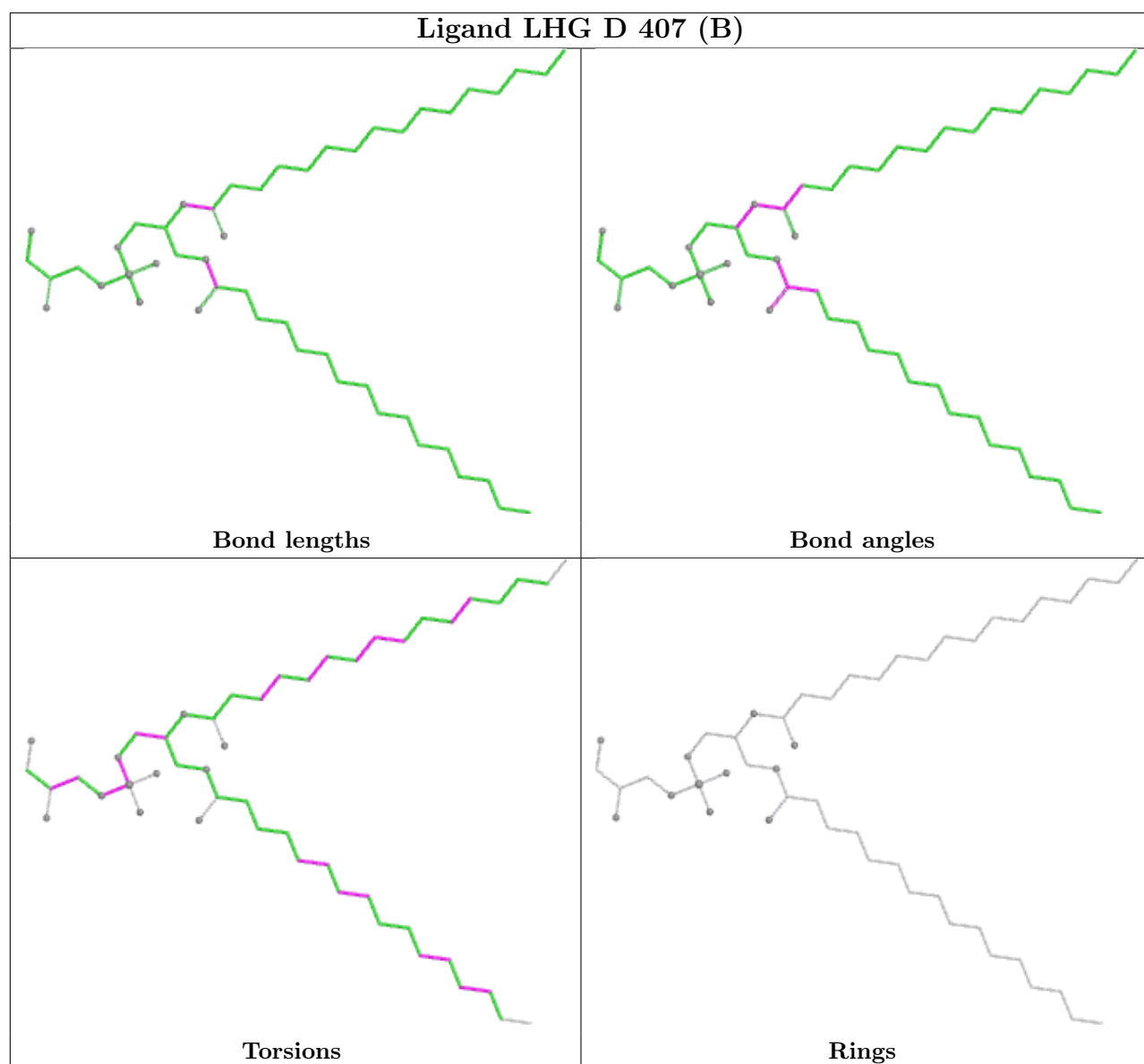


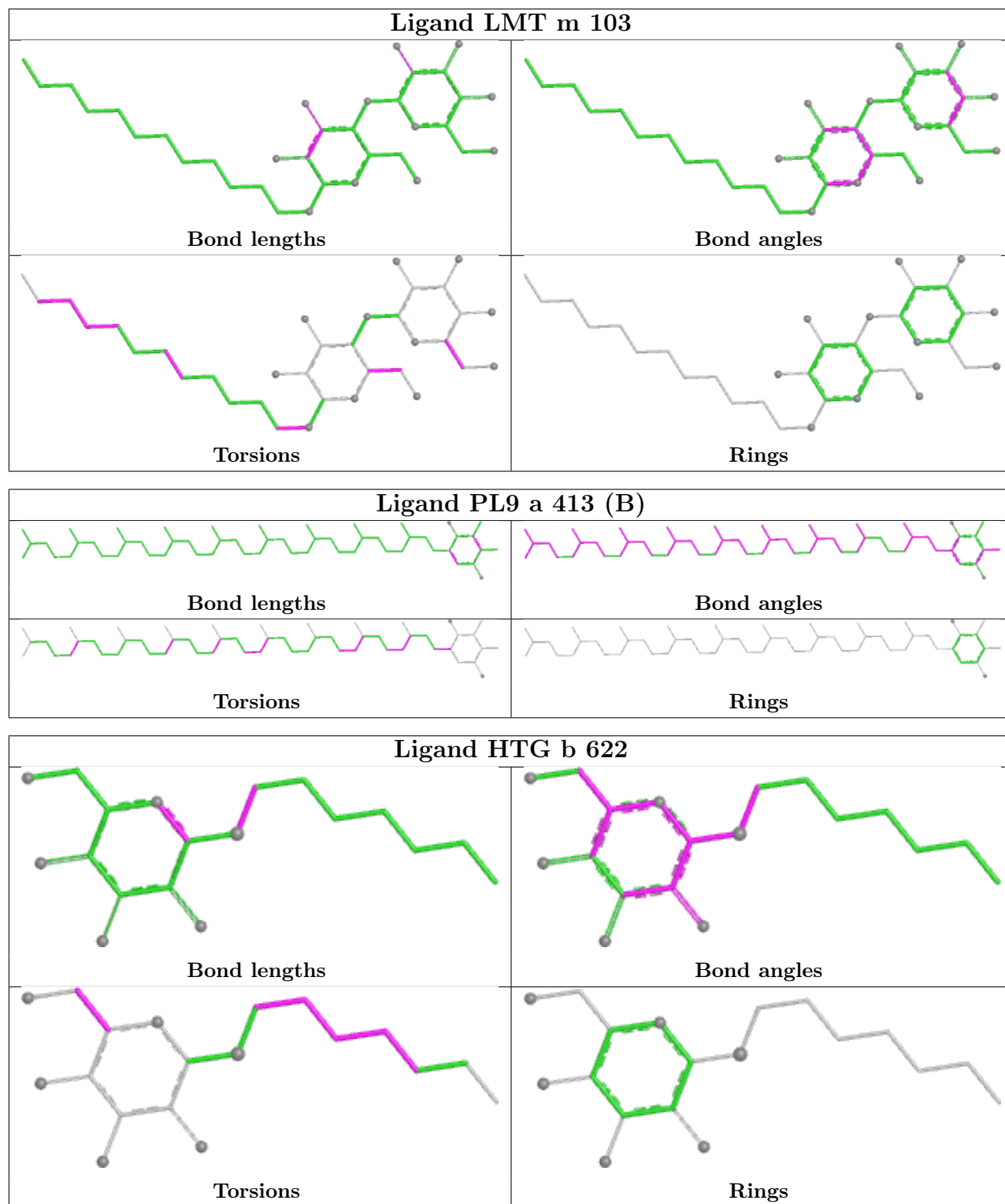


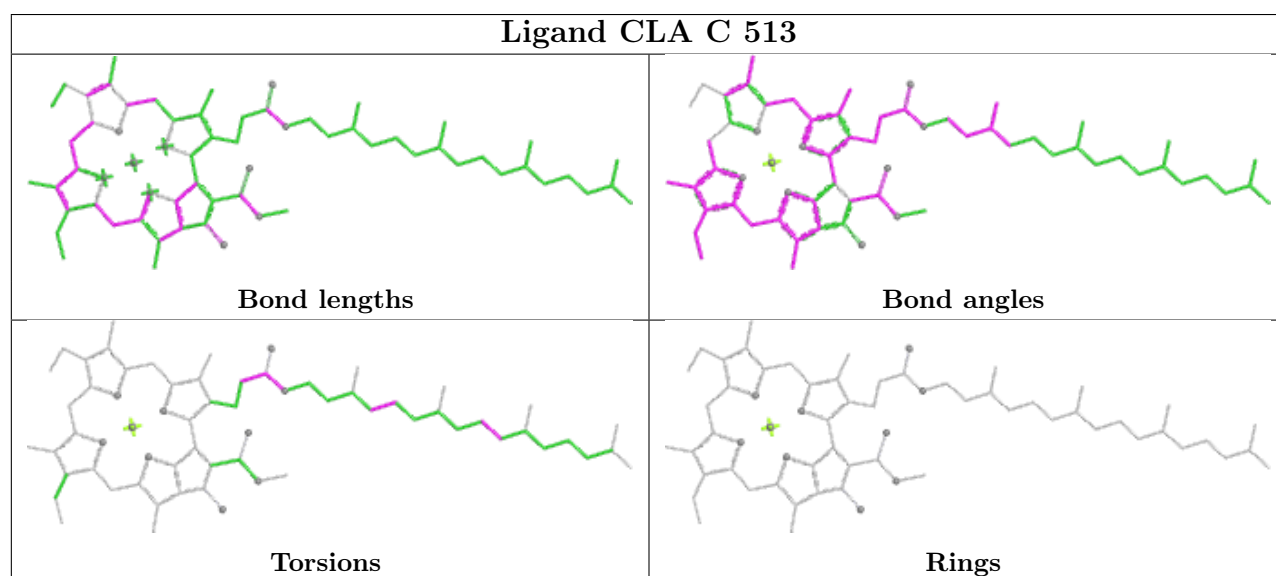
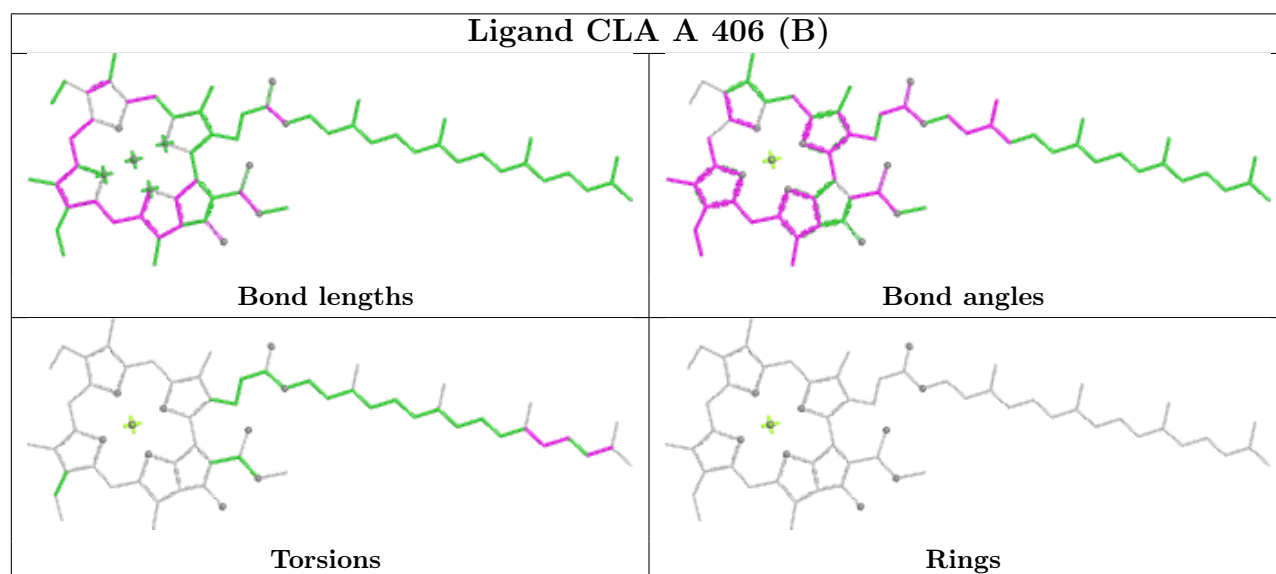
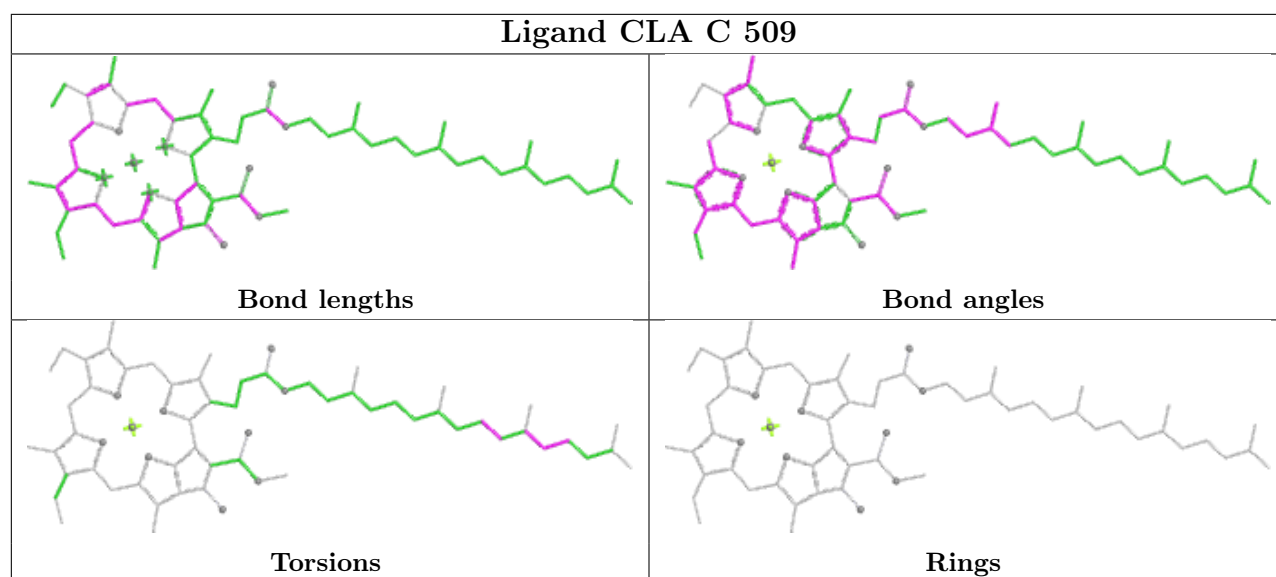


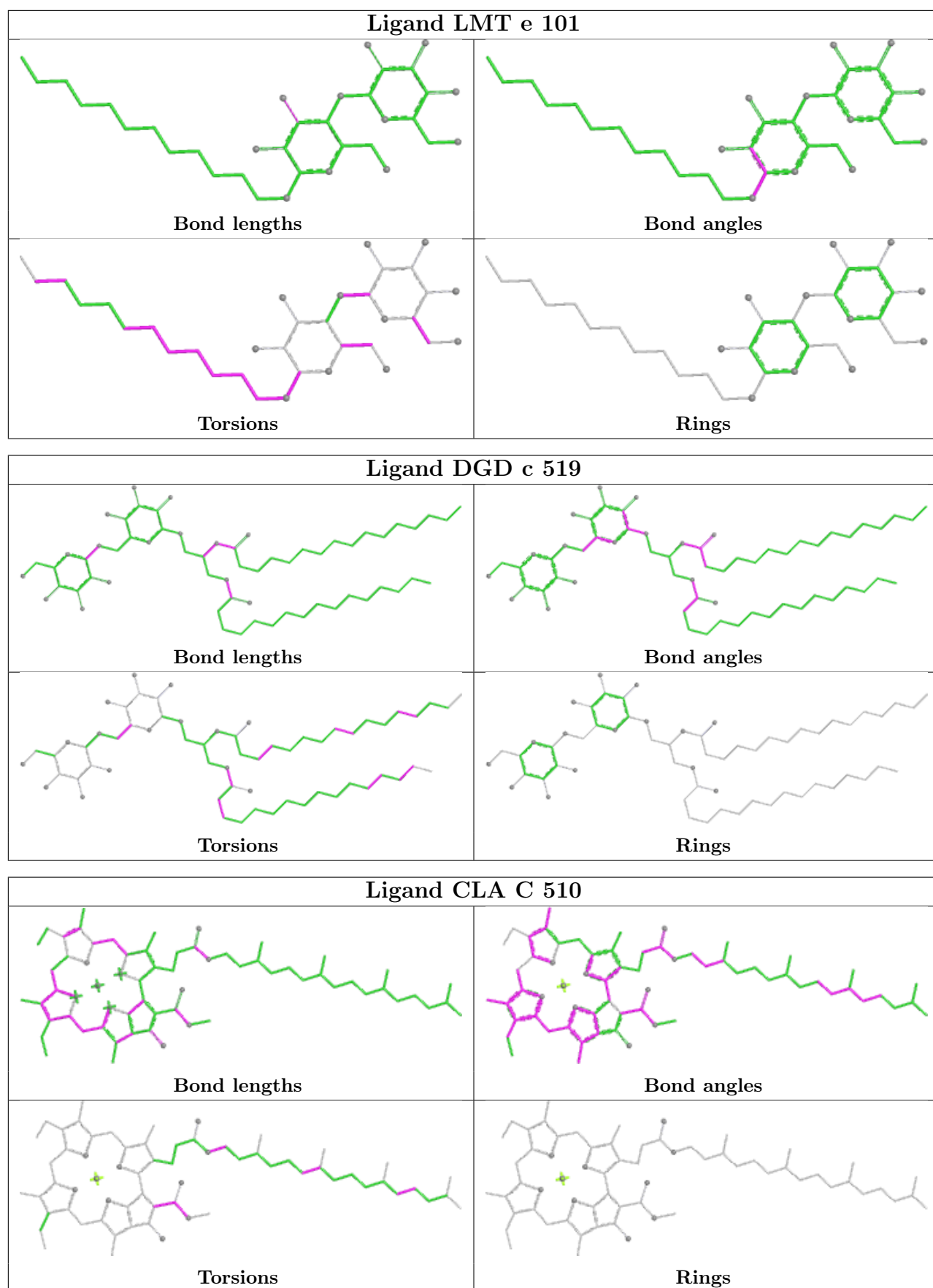


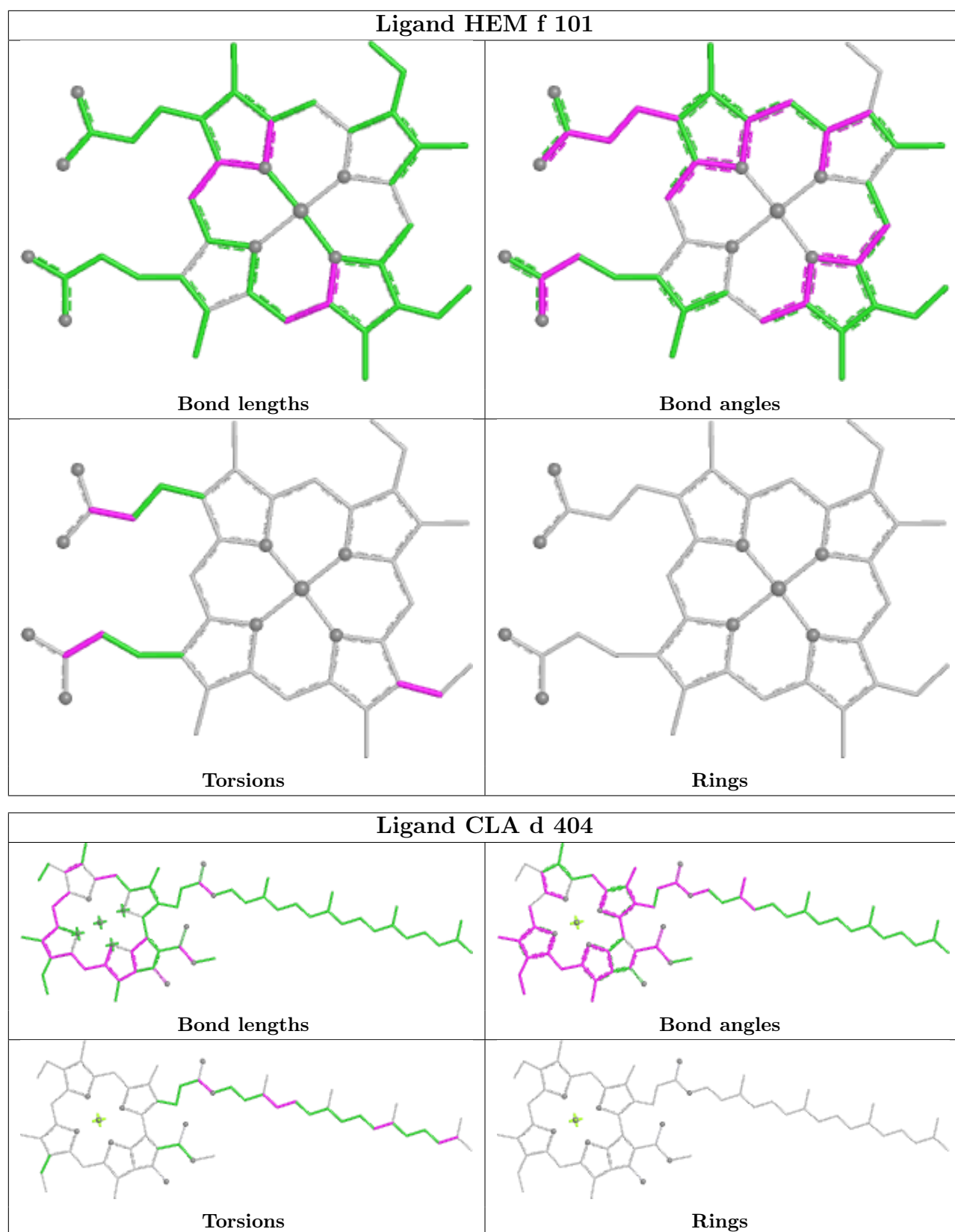


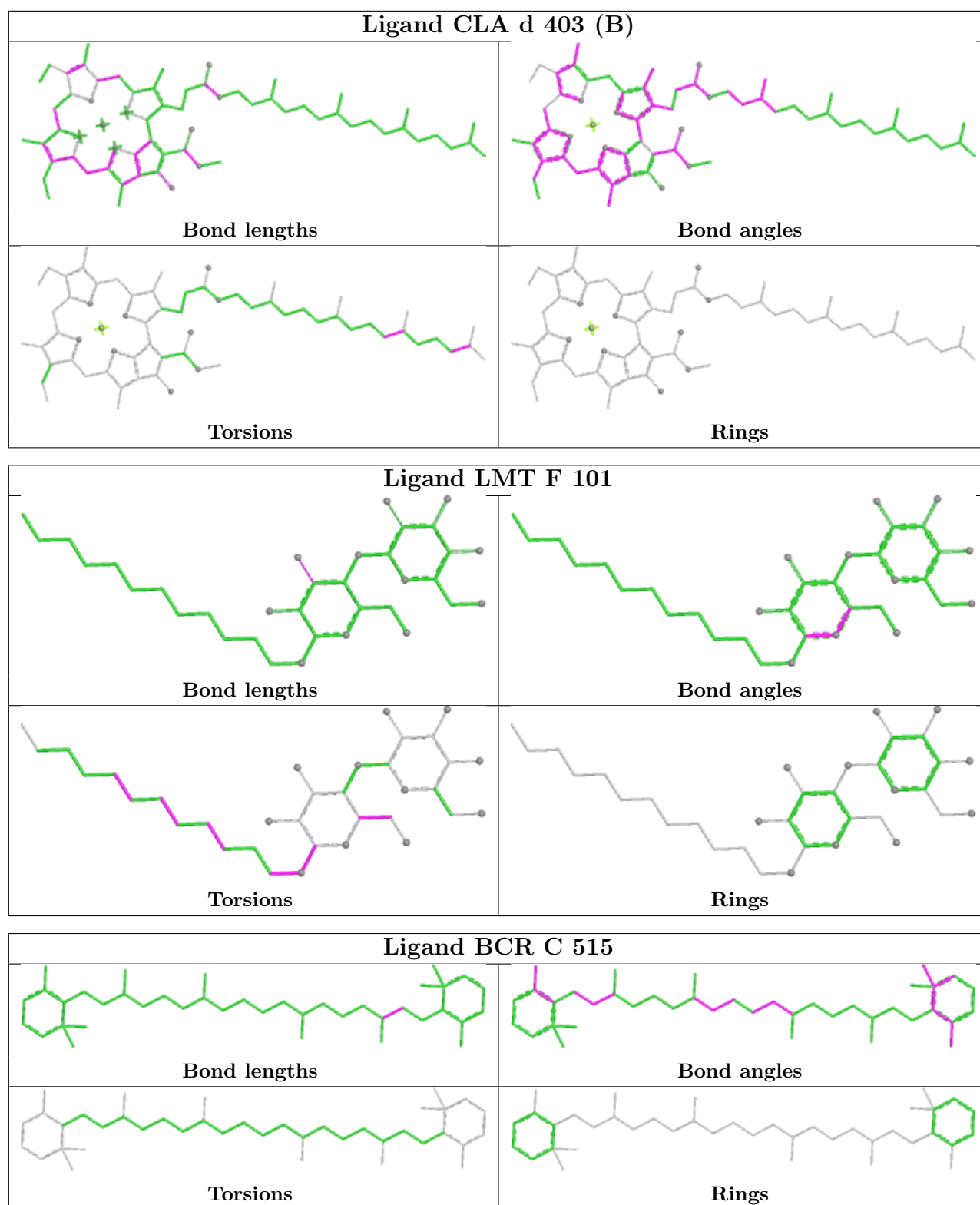


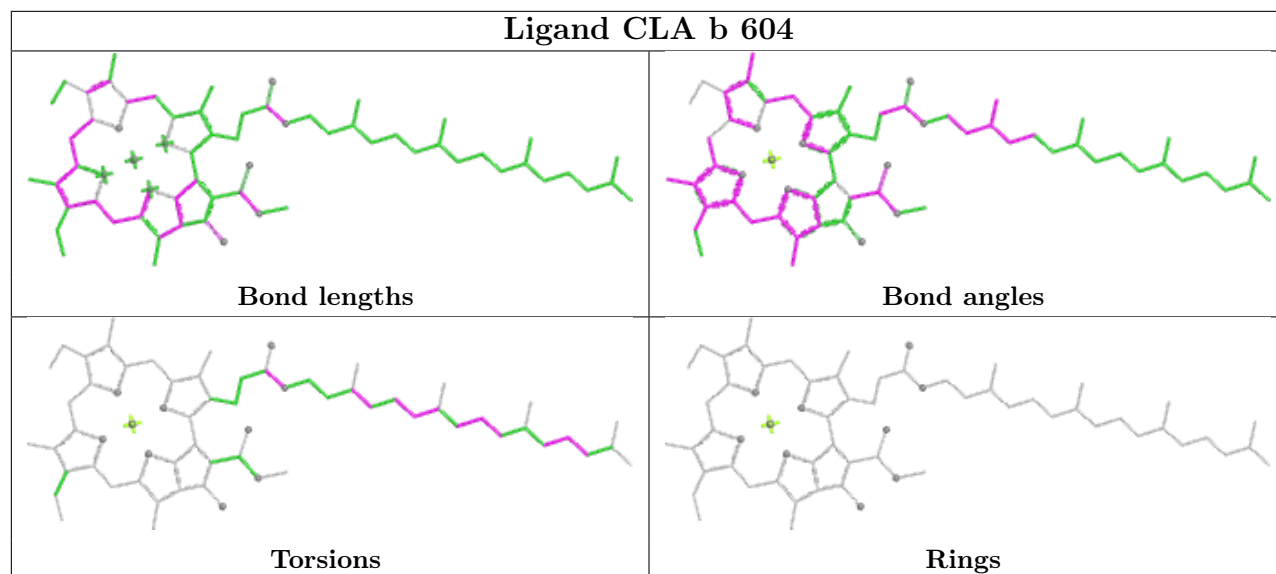












## 5.7 Other polymers [\(i\)](#)

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	334/344 (97%)	-0.79	1 (0%) 90 90	19, 25, 59, 119	222 (66%)
1	a	334/344 (97%)	-0.74	1 (0%) 90 90	20, 28, 64, 128	221 (66%)
2	B	504/505 (99%)	-0.69	0 100 100	21, 52, 82, 116	20 (3%)
2	b	504/505 (99%)	-0.61	0 100 100	23, 57, 98, 150	19 (3%)
3	C	451/455 (99%)	-0.69	0 100 100	21, 59, 82, 134	97 (21%)
3	c	455/455 (100%)	-0.60	1 (0%) 92 92	24, 65, 87, 128	100 (21%)
4	D	342/342 (100%)	-0.83	0 100 100	19, 44, 64, 127	114 (33%)
4	d	341/342 (99%)	-0.82	0 100 100	21, 49, 73, 128	116 (34%)
5	E	81/84 (96%)	-0.47	0 100 100	51, 69, 96, 147	0
5	e	79/84 (94%)	-0.48	1 (1%) 74 75	31, 74, 116, 142	2 (2%)
6	F	34/44 (77%)	-0.65	0 100 100	52, 59, 89, 110	0
6	f	31/44 (70%)	-0.39	1 (3%) 50 52	53, 66, 94, 132	1 (3%)
7	H	64/65 (98%)	-0.45	1 (1%) 70 71	53, 62, 88, 108	0
7	h	64/65 (98%)	-0.48	0 100 100	39, 72, 93, 105	1 (1%)
8	I	37/38 (97%)	-0.29	0 100 100	55, 65, 117, 143	0
8	i	37/38 (97%)	-0.46	0 100 100	53, 64, 111, 130	0
9	J	38/39 (97%)	-0.50	0 100 100	49, 67, 118, 153	0
9	j	39/39 (100%)	-0.41	0 100 100	56, 77, 124, 150	0
10	K	37/37 (100%)	-0.75	0 100 100	57, 66, 85, 105	0
10	k	37/37 (100%)	-0.62	0 100 100	67, 74, 95, 111	0
11	L	36/37 (97%)	-0.81	0 100 100	22, 45, 110, 128	2 (5%)
11	l	36/37 (97%)	-0.70	0 100 100	23, 46, 104, 118	2 (5%)
12	M	32/36 (88%)	-0.81	0 100 100	25, 47, 76, 125	1 (3%)
12	m	33/36 (91%)	-0.75	0 100 100	23, 48, 71, 137	2 (6%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/244 (99%)	-0.64	0 100 100	20, 64, 118, 161	10 (4%)
13	o	243/244 (99%)	-0.58	0 100 100	22, 68, 121, 153	8 (3%)
14	T	29/32 (90%)	-0.75	0 100 100	25, 45, 54, 65	6 (20%)
14	t	29/32 (90%)	-0.75	1 (3%) 48 50	26, 46, 59, 72	5 (17%)
15	U	96/104 (92%)	-0.73	0 100 100	24, 57, 87, 101	4 (4%)
15	u	97/104 (93%)	-0.80	0 100 100	28, 60, 80, 121	4 (4%)
16	V	137/137 (100%)	-0.84	0 100 100	23, 56, 81, 103	6 (4%)
16	v	137/137 (100%)	-0.67	0 100 100	26, 70, 99, 131	6 (4%)
17	X	38/40 (95%)	-0.34	0 100 100	34, 73, 92, 111	1 (2%)
17	x	38/40 (95%)	-0.20	0 100 100	67, 80, 118, 151	0
18	Y	29/30 (96%)	-0.25	0 100 100	67, 81, 117, 120	0
18	y	29/30 (96%)	-0.33	0 100 100	77, 88, 110, 112	0
19	Z	62/62 (100%)	-0.43	0 100 100	67, 81, 130, 150	0
19	z	62/62 (100%)	-0.02	0 100 100	80, 94, 137, 165	0
20	R	34/34 (100%)	0.41	1 (2%) 54 55	87, 110, 132, 143	0
All	All	5283/5384 (98%)	-0.65	8 (0%) 92 92	19, 57, 100, 165	970 (18%)

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	3.7
5	e	79[A]	PHE	3.4
6	f	16[A]	PHE	2.9
3	c	245[A]	ILE	2.1
1	A	11	ALA	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	FME	I	1	10/11	0.95	0.07	60,70,83,88	0
14	FME	T	1	10/11	0.96	0.07	43,53,70,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
14	FME	t	1	10/11	0.96	0.07	41,46,62,73	0
12	FME	m	1	10/11	0.97	0.07	50,61,88,116	0
8	FME	i	1	10/11	0.97	0.07	54,70,80,85	0
12	FME	M	1	10/11	0.98	0.06	43,55,88,98	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
26	GOL	a	417	6/6	0.61	0.17	79,98,105,108	0
32	LMT	F	101	35/35	0.69	0.15	91,127,168,174	0
32	LMT	e	101	35/35	0.69	0.14	100,141,180,182	0
29	UNL	A	414	28/-	0.70	0.14	81,103,122,140	0
29	UNL	a	414	30/-	0.70	0.12	80,106,129,138	0
29	UNL	j	101	10/-	0.71	0.19	73,87,102,104	0
32	LMT	A	419	35/35	0.71	0.12	89,125,143,156	0
29	UNL	K	101[B]	34/-	0.72	0.14	72,97,111,114	34
32	LMT	B	627	35/35	0.72	0.14	62,116,137,153	0
29	UNL	I	101	40/-	0.72	0.15	73,100,150,155	0
29	UNL	K	101[A]	34/-	0.72	0.14	72,97,111,114	34
29	UNL	m	102	10/-	0.73	0.19	61,71,91,93	0
32	LMT	A	417	35/35	0.73	0.12	59,109,132,137	0
25	SQD	f	102	43/54	0.74	0.13	94,125,167,177	0
29	UNL	J	101	10/-	0.74	0.22	60,75,83,91	0
35	HTG	C	522	19/19	0.74	0.12	99,119,131,131	0
32	LMT	a	416	35/35	0.75	0.12	107,126,147,155	0
33	LHG	a	419[A]	42/49	0.76	0.11	85,125,144,152	42
33	LHG	a	419[B]	42/49	0.76	0.11	85,125,144,152	42
29	UNL	l	102	10/-	0.76	0.16	63,77,90,92	0
29	UNL	B	628	40/-	0.78	0.13	71,99,149,159	0
29	UNL	b	626	33/-	0.79	0.13	63,94,149,161	0
29	UNL	c	525[B]	32/-	0.80	0.14	86,104,116,126	32
26	GOL	B	625	6/6	0.80	0.14	68,88,99,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
29	UNL	c	525[A]	32/-	0.80	0.14	86,104,116,126	32
35	HTG	B	621	19/19	0.80	0.14	60,90,112,112	0
32	LMT	b	621	25/35	0.80	0.12	78,103,153,161	0
34	LMG	C	521	51/55	0.81	0.11	56,115,150,170	0
26	GOL	o	303	6/6	0.81	0.15	79,100,105,111	0
26	GOL	o	304	6/6	0.81	0.14	76,87,97,97	0
35	HTG	D	411	16/19	0.81	0.12	88,102,126,149	0
35	HTG	c	522	19/19	0.81	0.10	103,120,141,142	0
26	GOL	d	413	6/6	0.82	0.21	49,63,77,82	0
29	UNL	D	410	40/-	0.82	0.12	62,90,136,141	0
35	HTG	b	623	19/19	0.82	0.12	79,124,158,158	0
26	GOL	O	302	6/6	0.82	0.09	79,87,104,108	0
32	LMT	T	101	35/35	0.83	0.10	61,120,165,176	0
28	PL9	A	413[A]	55/55	0.83	0.14	61,85,102,106	55
28	PL9	A	413[B]	55/55	0.83	0.14	61,85,102,106	55
32	LMT	B	626	35/35	0.83	0.11	66,102,146,152	0
26	GOL	A	410	6/6	0.83	0.13	63,79,84,85	0
26	GOL	O	303	6/6	0.83	0.13	69,83,99,99	0
28	PL9	a	413[A]	55/55	0.84	0.13	72,95,109,116	55
32	LMT	B	629	25/35	0.84	0.12	56,84,135,159	0
29	UNL	d	410	36/-	0.84	0.10	65,96,131,136	0
28	PL9	a	413[B]	55/55	0.84	0.13	72,95,109,117	55
25	SQD	a	411	54/54	0.84	0.10	63,90,135,145	0
34	LMG	Z	101	37/55	0.85	0.13	66,115,142,163	0
29	UNL	B	624	33/-	0.85	0.13	54,104,138,148	0
32	LMT	m	103	35/35	0.85	0.10	54,88,104,115	0
26	GOL	v	202[B]	6/6	0.85	0.11	60,72,79,80	6
35	HTG	b	622	19/19	0.85	0.12	60,90,115,118	0
26	GOL	b	624	6/6	0.85	0.14	84,98,100,109	0
26	GOL	v	202[A]	6/6	0.85	0.11	60,72,80,80	6
35	HTG	d	411	16/19	0.85	0.11	89,124,140,154	0
34	LMG	z	101	39/55	0.86	0.12	72,125,150,157	0
25	SQD	A	411	54/54	0.86	0.10	57,86,128,153	0
34	LMG	c	521	51/55	0.86	0.10	74,126,157,185	0
32	LMT	t	101	26/35	0.86	0.11	64,98,139,140	0
37	CA	F	103	1/1	0.86	0.23	122,122,122,122	0
35	HTG	V	202	11/19	0.87	0.09	78,108,125,127	0
32	LMT	M	101	35/35	0.87	0.10	57,93,120,130	0
32	LMT	b	627	25/35	0.87	0.12	51,88,142,153	0
25	SQD	X	101	43/54	0.88	0.11	72,103,125,141	0
26	GOL	l	103[A]	6/6	0.88	0.15	61,91,98,100	6
26	GOL	l	103[B]	6/6	0.88	0.15	61,91,98,100	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
26	GOL	c	527	6/6	0.88	0.14	89,98,113,115	0
23	CLA	b	601	65/65	0.89	0.10	59,90,123,154	0
29	UNL	D	409	17/-	0.89	0.11	62,72,103,109	0
25	SQD	l	101	54/54	0.89	0.09	59,87,139,148	0
25	SQD	b	620	54/54	0.89	0.09	55,94,121,128	0
33	LHG	E	101[A]	42/49	0.89	0.10	71,96,111,117	42
33	LHG	E	101[B]	42/49	0.89	0.10	71,96,111,117	42
26	GOL	a	410	6/6	0.89	0.12	70,73,91,93	0
35	HTG	o	301	19/19	0.90	0.11	58,83,117,119	0
35	HTG	B	623	19/19	0.90	0.08	64,77,94,103	0
26	GOL	V	203[A]	6/6	0.91	0.11	56,65,67,73	6
26	GOL	V	203[B]	6/6	0.91	0.11	56,65,67,73	6
26	GOL	D	413	6/6	0.91	0.14	45,64,71,91	0
26	GOL	B	622	6/6	0.91	0.13	66,76,84,85	0
26	GOL	a	418	6/6	0.91	0.21	54,74,79,80	0
34	LMG	C	501	51/55	0.91	0.09	64,89,114,133	0
23	CLA	B	601	65/65	0.91	0.09	56,80,112,156	0
37	CA	f	103	1/1	0.91	0.10	117,117,117,117	0
23	CLA	c	514	65/65	0.92	0.09	68,96,126,148	0
34	LMG	C	520	51/55	0.92	0.09	54,81,114,130	0
26	GOL	D	402	6/6	0.92	0.24	47,72,77,80	0
34	LMG	c	501	51/55	0.92	0.08	69,91,107,113	0
34	LMG	c	520	51/55	0.92	0.09	59,90,127,156	0
34	LMG	B	620	51/55	0.92	0.07	49,66,89,112	0
34	LMG	m	101	51/55	0.92	0.08	48,72,97,107	0
25	SQD	A	409[A]	54/54	0.93	0.09	56,78,109,113	54
29	UNL	d	409	17/-	0.93	0.09	67,80,117,121	0
25	SQD	A	409[B]	54/54	0.93	0.09	56,78,109,113	54
23	CLA	c	513	65/65	0.93	0.09	59,80,117,144	0
23	CLA	C	514	65/65	0.93	0.08	63,87,112,119	0
24	BCR	C	515	40/40	0.93	0.08	55,73,87,93	0
24	BCR	D	405	40/40	0.93	0.08	41,56,98,102	0
24	BCR	T	102	40/40	0.93	0.07	43,58,70,78	0
34	LMG	D	412	51/55	0.93	0.08	46,67,120,132	0
24	BCR	d	405	40/40	0.93	0.08	48,64,98,104	0
24	BCR	t	102	40/40	0.93	0.07	40,58,79,85	0
33	LHG	A	418[A]	49/49	0.93	0.08	46,60,79,84	49
36	DGD	C	518[A]	62/66	0.93	0.08	50,63,110,114	62
36	DGD	C	518[B]	62/66	0.93	0.08	50,63,110,114	62
34	LMG	d	412	51/55	0.93	0.08	54,68,116,145	0
33	LHG	A	418[B]	49/49	0.93	0.08	46,60,79,84	49
24	BCR	c	515	40/40	0.94	0.08	66,82,95,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	CLA	C	507	65/65	0.94	0.08	54,70,117,136	0
26	GOL	b	628	6/6	0.94	0.08	75,79,82,86	0
23	CLA	B	614	65/65	0.94	0.07	35,49,100,116	0
33	LHG	D	408[A]	49/49	0.94	0.09	43,58,107,110	49
33	LHG	D	408[B]	49/49	0.94	0.09	43,58,107,110	49
23	CLA	d	404	65/65	0.94	0.09	54,68,124,147	0
26	GOL	C	523[A]	6/6	0.94	0.09	53,56,61,68	6
26	GOL	C	523[B]	6/6	0.94	0.09	54,58,61,68	6
24	BCR	B	619	40/40	0.94	0.08	46,58,90,104	0
33	LHG	d	414[A]	49/49	0.94	0.08	48,65,80,87	49
33	LHG	d	414[B]	49/49	0.94	0.08	48,66,80,87	49
35	HTG	b	625	19/19	0.94	0.07	61,79,95,108	0
23	CLA	C	505	65/65	0.94	0.07	40,56,98,131	0
23	CLA	b	616	65/65	0.94	0.08	50,63,122,134	0
25	SQD	a	409[A]	54/54	0.94	0.09	60,81,112,118	54
25	SQD	a	409[B]	54/54	0.94	0.09	60,80,112,118	54
24	BCR	K	102	40/40	0.94	0.09	54,65,80,91	0
36	DGD	c	517[A]	62/66	0.94	0.08	49,65,100,108	62
36	DGD	c	517[B]	62/66	0.94	0.08	49,65,100,108	62
36	DGD	c	518[A]	62/66	0.94	0.07	53,67,118,128	62
36	DGD	c	518[B]	62/66	0.94	0.07	53,68,118,128	62
36	DGD	c	519	62/66	0.94	0.07	48,63,100,128	0
23	CLA	c	507	65/65	0.94	0.08	47,70,117,134	0
24	BCR	Y	101	40/40	0.94	0.08	54,63,80,89	0
37	CA	o	302	1/1	0.94	0.07	113,113,113,113	0
26	GOL	c	526[B]	6/6	0.95	0.08	64,66,71,74	6
23	CLA	A	407	65/65	0.95	0.08	39,52,127,140	0
24	BCR	A	408	40/40	0.95	0.07	40,51,64,65	0
29	UNL	d	415	18/-	0.95	0.09	66,79,126,127	0
24	BCR	B	618	40/40	0.95	0.06	37,54,69,79	0
23	CLA	a	405[A]	65/65	0.95	0.07	38,52,118,133	65
23	CLA	a	405[B]	65/65	0.95	0.07	38,52,118,133	65
30	BCT	d	401[A]	4/4	0.95	0.07	53,60,61,76	4
30	BCT	d	401[B]	4/4	0.95	0.07	54,60,61,77	4
23	CLA	a	407	65/65	0.95	0.10	42,55,139,160	0
24	BCR	H	101	40/40	0.95	0.08	50,64,84,89	0
23	CLA	B	616	65/65	0.95	0.08	46,59,129,139	0
23	CLA	b	606	65/65	0.95	0.07	42,62,115,119	0
23	CLA	b	614	65/65	0.95	0.07	39,50,98,113	0
28	PL9	D	406[A]	55/55	0.95	0.07	35,47,55,65	55
28	PL9	D	406[B]	55/55	0.95	0.07	35,47,55,64	55
24	BCR	b	617	40/40	0.95	0.06	41,52,64,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	BCR	b	618	40/40	0.95	0.06	42,57,76,84	0
24	BCR	b	619	40/40	0.95	0.07	48,61,90,95	0
23	CLA	B	603	65/65	0.95	0.08	43,53,73,87	0
24	BCR	c	516	40/40	0.95	0.07	57,66,80,82	0
23	CLA	c	505	65/65	0.95	0.07	46,64,108,137	0
24	BCR	h	101	40/40	0.95	0.09	54,69,91,98	0
24	BCR	k	101	40/40	0.95	0.08	56,72,84,86	0
23	CLA	B	606	65/65	0.95	0.08	41,57,108,129	0
24	BCR	y	101	40/40	0.95	0.07	58,72,85,96	0
23	CLA	c	508	65/65	0.95	0.09	49,68,83,90	0
36	DGD	C	519	62/66	0.95	0.07	41,56,101,115	0
29	UNL	X	102	18/-	0.95	0.09	52,68,103,105	0
23	CLA	C	509	65/65	0.95	0.07	44,55,117,141	0
23	CLA	C	513	65/65	0.95	0.08	57,75,108,121	0
26	GOL	c	526[A]	6/6	0.95	0.08	65,66,71,74	6
33	LHG	b	629[A]	49/49	0.95	0.07	45,57,70,81	49
36	DGD	h	102	62/66	0.95	0.07	51,65,80,90	0
33	LHG	b	629[B]	49/49	0.95	0.07	45,57,70,82	49
33	LHG	d	408[A]	49/49	0.95	0.09	49,63,108,129	49
33	LHG	d	408[B]	49/49	0.95	0.09	49,63,108,129	49
23	CLA	c	504	65/65	0.96	0.06	51,71,85,88	0
28	PL9	d	406[A]	55/55	0.96	0.06	37,49,59,65	55
28	PL9	d	406[B]	55/55	0.96	0.06	37,49,59,65	55
23	CLA	C	508	65/65	0.96	0.07	52,64,85,95	0
23	CLA	c	506	65/65	0.96	0.07	47,65,92,105	0
23	CLA	A	406[B]	65/65	0.96	0.06	36,45,110,121	65
23	CLA	C	510	65/65	0.96	0.08	44,59,84,91	0
23	CLA	c	509	65/65	0.96	0.07	47,62,121,152	0
23	CLA	c	512	65/65	0.96	0.07	54,70,85,101	0
23	CLA	B	607	65/65	0.96	0.06	32,46,73,77	0
23	CLA	B	611	65/65	0.96	0.06	32,44,65,72	0
23	CLA	D	404	65/65	0.96	0.07	49,58,120,137	0
23	CLA	B	613	65/65	0.96	0.06	38,46,99,109	0
23	CLA	A	404[A]	65/65	0.96	0.06	35,41,54,66	65
23	CLA	A	404[B]	65/65	0.96	0.06	35,41,56,66	65
23	CLA	C	502	65/65	0.96	0.06	49,60,75,82	0
24	BCR	C	516	40/40	0.96	0.06	49,64,75,83	0
23	CLA	B	602	65/65	0.96	0.07	46,56,75,88	0
23	CLA	b	607	65/65	0.96	0.06	36,46,77,84	0
23	CLA	b	609	65/65	0.96	0.07	51,66,83,88	0
36	DGD	C	517[A]	62/66	0.96	0.06	46,59,101,106	62
36	DGD	C	517[B]	62/66	0.96	0.06	46,59,101,107	62

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	CLA	b	612	65/65	0.96	0.07	38,53,67,76	0
23	CLA	b	613	65/65	0.96	0.06	41,50,85,95	0
24	BCR	a	408	40/40	0.96	0.06	40,54,63,75	0
36	DGD	H	102	62/66	0.96	0.07	44,61,75,90	0
33	LHG	d	407[A]	49/49	0.96	0.07	47,54,69,75	49
33	LHG	d	407[B]	49/49	0.96	0.07	47,54,69,75	49
23	CLA	C	506	65/65	0.96	0.07	50,60,91,105	0
23	CLA	A	406[A]	65/65	0.96	0.06	36,46,110,121	65
31	PHO	A	416[A]	64/64	0.96	0.06	38,48,54,58	64
31	PHO	A	416[B]	64/64	0.96	0.06	38,48,54,57	64
37	CA	C	524	1/1	0.96	0.05	75,75,75,75	0
31	PHO	a	415[A]	64/64	0.96	0.06	45,55,62,66	64
37	CA	O	301	1/1	0.96	0.04	106,106,106,106	0
31	PHO	a	415[B]	64/64	0.96	0.06	45,55,62,67	64
23	CLA	c	502	65/65	0.96	0.07	56,67,81,88	0
23	CLA	A	405[A]	65/65	0.97	0.05	32,42,54,66	65
23	CLA	c	510	65/65	0.97	0.07	41,60,86,100	0
31	PHO	D	401[A]	64/64	0.97	0.04	38,44,51,55	64
31	PHO	D	401[B]	64/64	0.97	0.04	38,44,51,55	64
31	PHO	a	406[A]	64/64	0.97	0.05	40,46,53,60	64
31	PHO	a	406[B]	64/64	0.97	0.05	40,46,53,60	64
23	CLA	c	511	65/65	0.97	0.06	47,61,79,83	0
23	CLA	C	504	65/65	0.97	0.06	49,62,72,83	0
23	CLA	A	405[B]	65/65	0.97	0.05	32,42,54,66	65
23	CLA	B	609	65/65	0.97	0.06	45,59,72,76	0
23	CLA	d	402[A]	65/65	0.97	0.05	36,43,61,73	65
23	CLA	d	402[B]	65/65	0.97	0.05	36,43,61,73	65
23	CLA	d	403[A]	65/65	0.97	0.06	33,45,71,89	65
23	CLA	d	403[B]	65/65	0.97	0.06	33,45,71,89	65
23	CLA	b	602	65/65	0.97	0.07	51,61,81,87	0
23	CLA	b	603	65/65	0.97	0.06	44,57,75,91	0
24	BCR	B	617	40/40	0.97	0.05	39,51,60,67	0
23	CLA	b	604	65/65	0.97	0.06	42,52,94,121	0
23	CLA	b	605	65/65	0.97	0.06	38,50,74,80	0
23	CLA	B	610	65/65	0.97	0.07	41,52,68,84	0
22	CL	a	403[A]	1/1	0.97	0.07	52,52,52,52	1
23	CLA	b	608	65/65	0.97	0.05	37,56,78,98	0
23	CLA	B	612	65/65	0.97	0.06	35,49,60,75	0
23	CLA	b	610	65/65	0.97	0.07	47,59,71,75	0
33	LHG	D	407[A]	49/49	0.97	0.06	45,53,65,73	49
33	LHG	D	407[B]	49/49	0.97	0.06	45,53,65,73	49
23	CLA	b	611	65/65	0.97	0.06	36,48,67,85	0

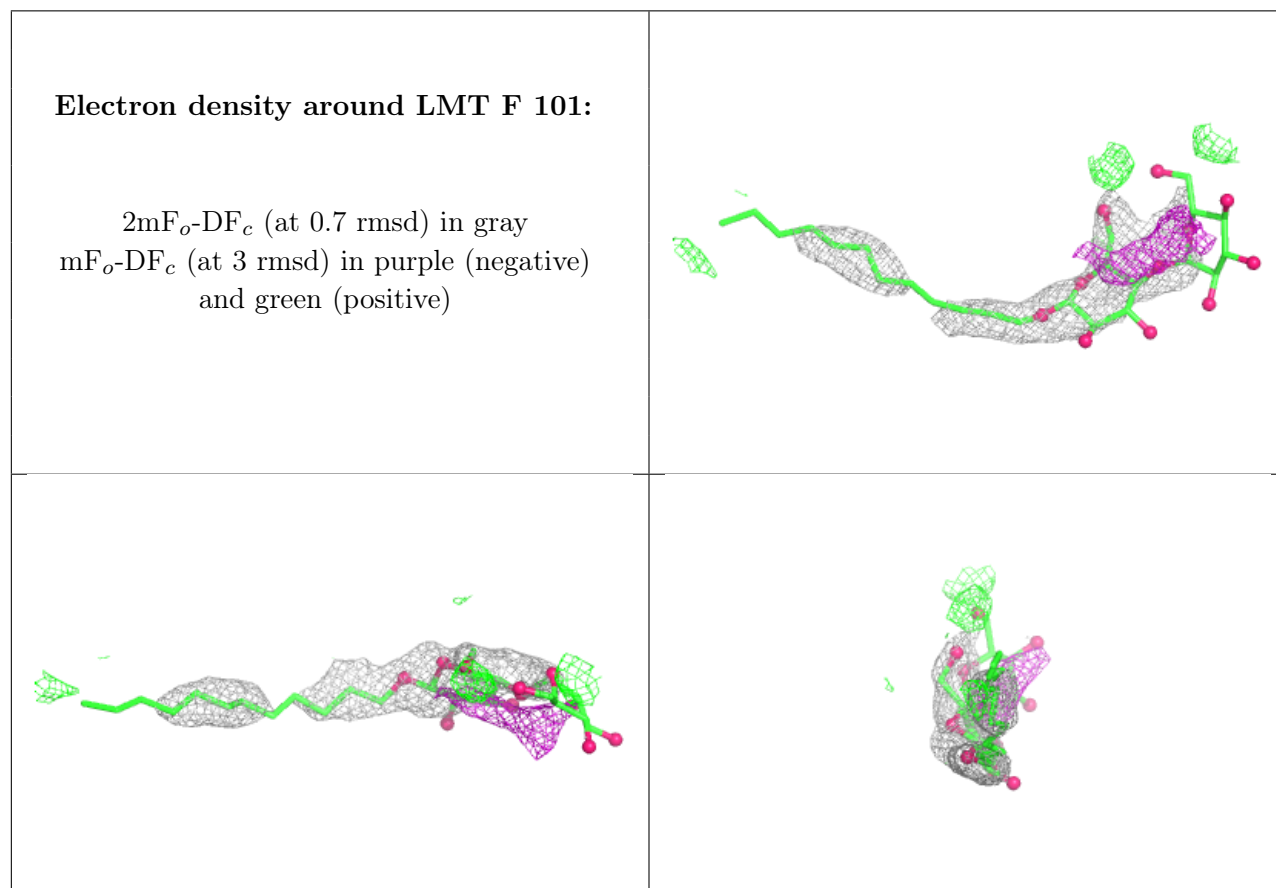
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	CL	a	403[B]	1/1	0.97	0.07	51,51,51,51	1
23	CLA	C	511	65/65	0.97	0.05	44,56,76,87	0
23	CLA	C	512	65/65	0.97	0.07	52,63,82,92	0
33	LHG	L	101[A]	49/49	0.97	0.06	46,54,64,85	49
33	LHG	L	101[B]	49/49	0.97	0.06	46,54,63,85	49
23	CLA	b	615	65/65	0.97	0.06	45,62,85,90	0
23	CLA	B	604	65/65	0.97	0.06	35,47,105,134	0
23	CLA	B	615	65/65	0.97	0.05	42,53,77,94	0
23	CLA	c	503	65/65	0.97	0.06	42,57,87,101	0
23	CLA	D	403[A]	65/65	0.97	0.06	32,42,67,73	65
23	CLA	D	403[B]	65/65	0.97	0.06	32,42,67,73	65
23	CLA	B	605	65/65	0.97	0.06	38,48,63,77	0
37	CA	c	523	1/1	0.97	0.06	78,78,78,78	0
23	CLA	a	404[A]	65/65	0.97	0.06	36,44,61,73	65
23	CLA	a	404[B]	65/65	0.97	0.06	37,44,61,73	65
23	CLA	B	608	65/65	0.98	0.05	35,48,69,73	0
30	BCT	A	415[A]	4/4	0.98	0.05	53,53,57,67	4
30	BCT	A	415[B]	4/4	0.98	0.05	53,53,57,67	4
23	CLA	C	503	65/65	0.98	0.06	38,55,79,86	0
38	HEM	f	101	43/43	0.98	0.07	60,84,110,124	0
40	HEC	V	201	43/43	0.98	0.06	39,52,68,71	0
40	HEC	v	201	43/43	0.98	0.07	50,61,70,75	0
27	OEX	A	412[A]	10/10	0.99	0.03	37,44,51,55	10
27	OEX	A	412[B]	10/10	0.99	0.03	37,44,51,55	10
22	CL	A	402[A]	1/1	0.99	0.07	40,40,40,40	1
37	CA	c	524	1/1	0.99	0.05	81,81,81,81	0
22	CL	A	402[B]	1/1	0.99	0.07	40,40,40,40	1
22	CL	A	403[A]	1/1	0.99	0.05	45,45,45,45	1
38	HEM	F	102	43/43	0.99	0.06	52,68,86,92	0
22	CL	A	403[B]	1/1	0.99	0.05	45,45,45,45	1
39	MG	J	102	1/1	0.99	0.04	57,57,57,57	0
39	MG	j	102	1/1	0.99	0.04	64,64,64,64	0
22	CL	a	402[A]	1/1	0.99	0.07	47,47,47,47	1
22	CL	a	402[B]	1/1	0.99	0.07	47,47,47,47	1
21	FE2	A	401[A]	1/1	1.00	0.01	49,49,49,49	1
21	FE2	A	401[B]	1/1	1.00	0.01	50,50,50,50	1
27	OEX	a	412[A]	10/10	1.00	0.02	47,49,54,54	10
27	OEX	a	412[B]	10/10	1.00	0.02	46,49,53,54	10
21	FE2	a	401[A]	1/1	1.00	0.01	52,52,52,52	1
21	FE2	a	401[B]	1/1	1.00	0.01	52,52,52,52	1

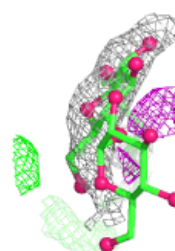
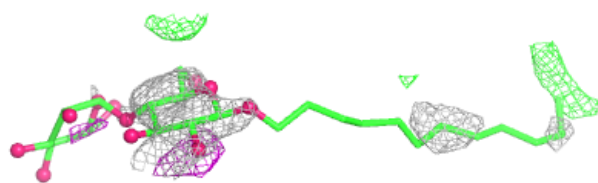
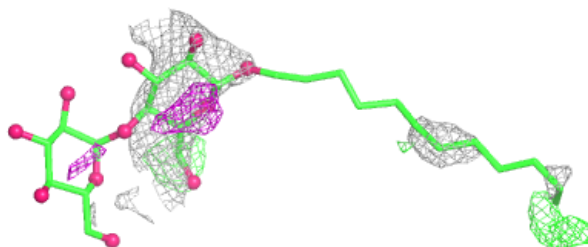
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

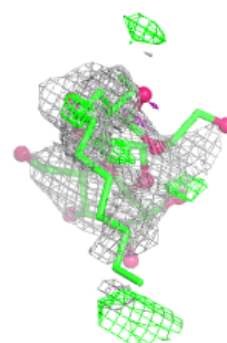
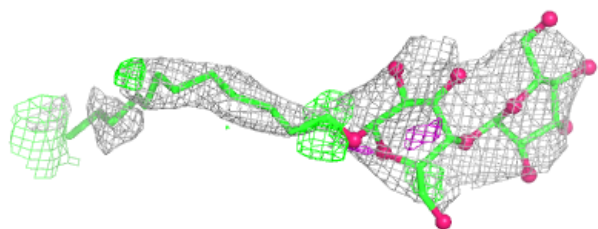
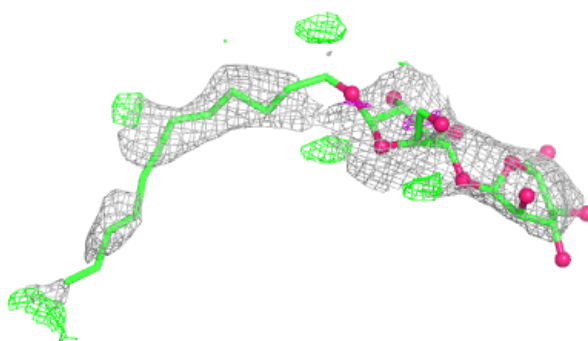


**Electron density around LMT e 101:**

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

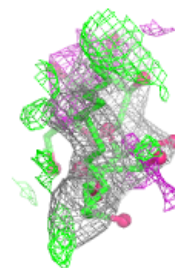
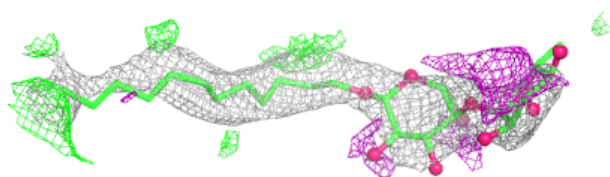
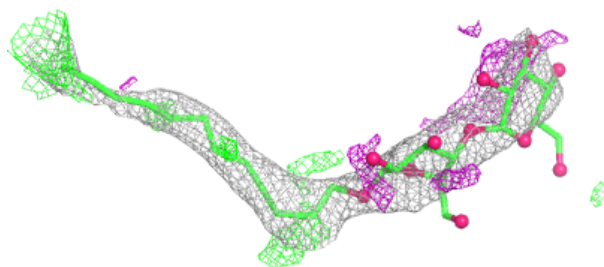
**Electron density around LMT A 419:**

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

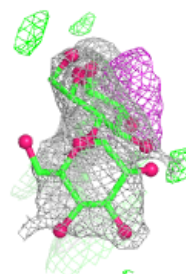
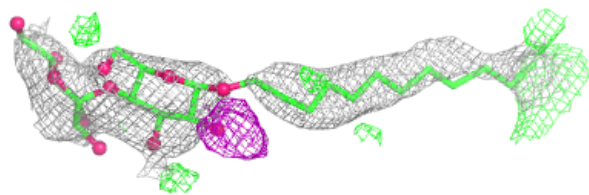
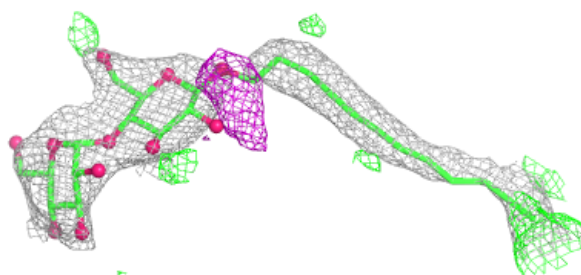


**Electron density around LMT B 627:**

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

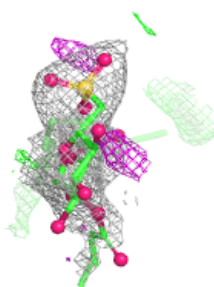
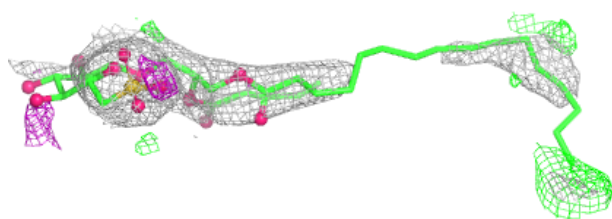
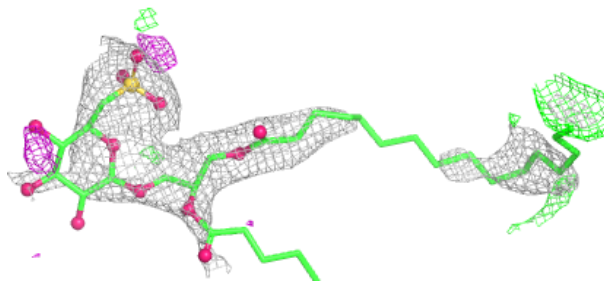
**Electron density around LMT A 417:**

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

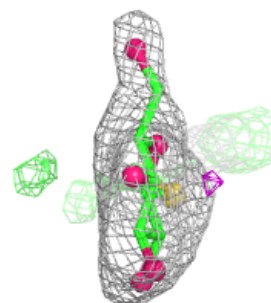
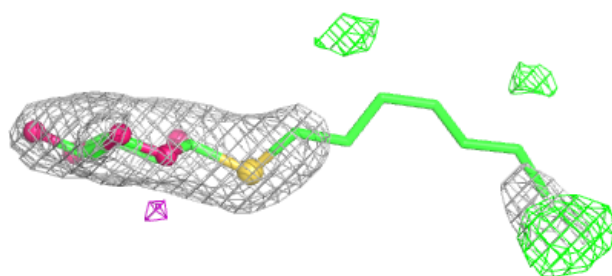
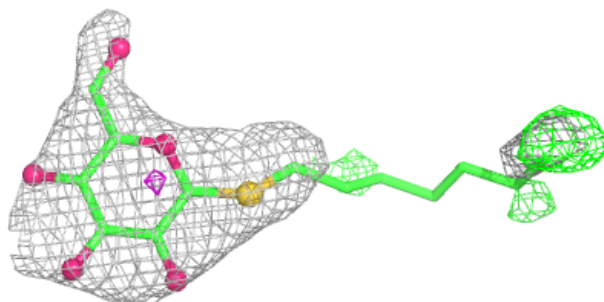


**Electron density around SQD f 102:**

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

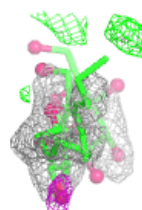
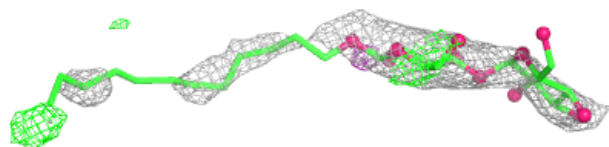
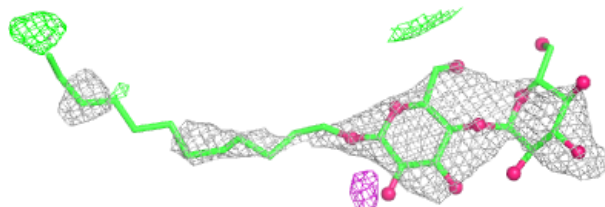
**Electron density around HTG C 522:**

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

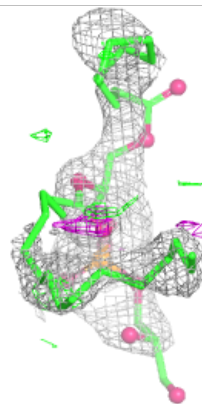
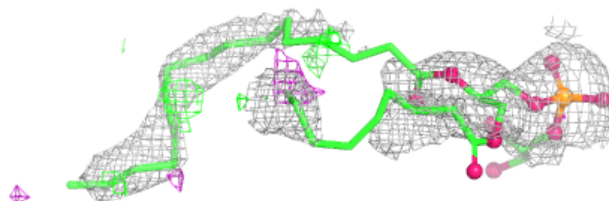
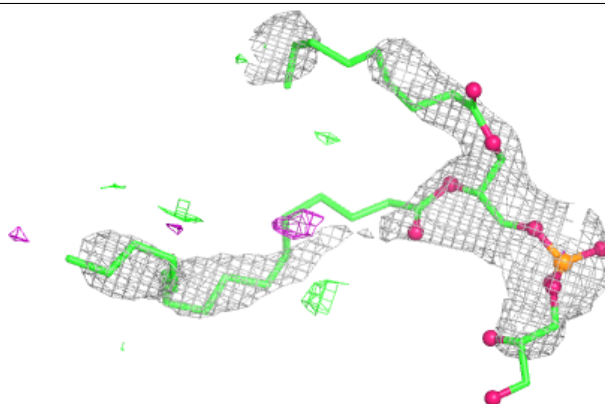


**Electron density around LMT a 416:**

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

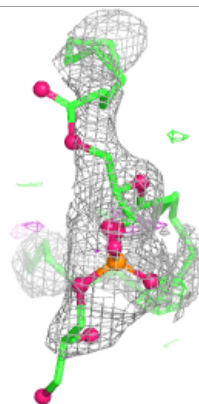
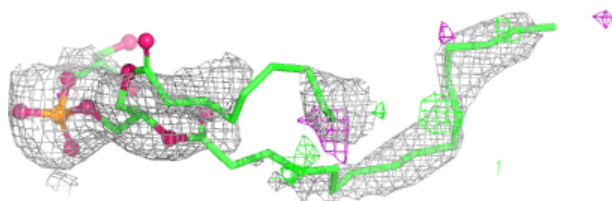
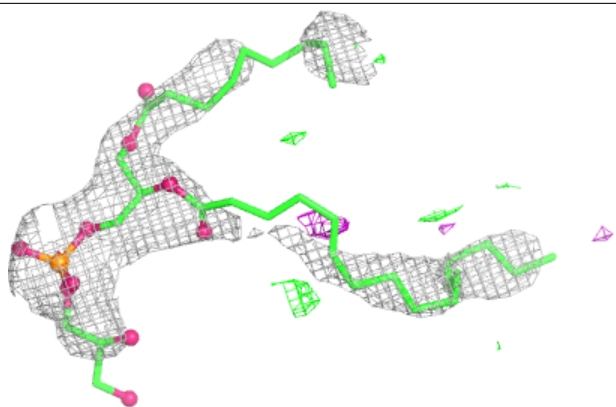
**Electron density around LHG a 419 (A):**

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

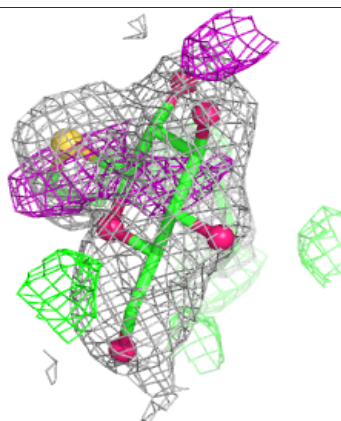
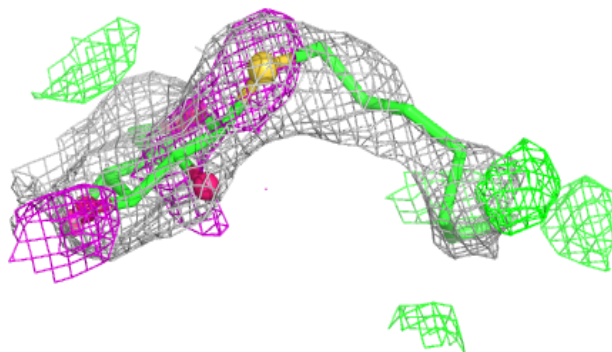
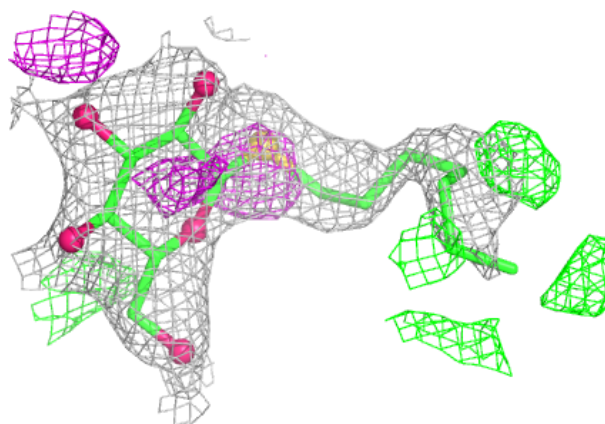


**Electron density around LHG a 419 (B):**

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

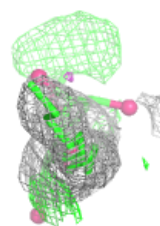
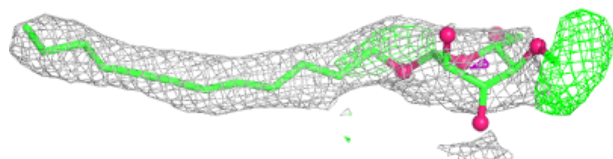
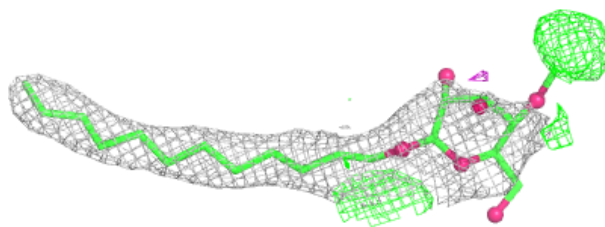
**Electron density around HTG B 621:**

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

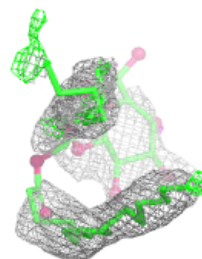
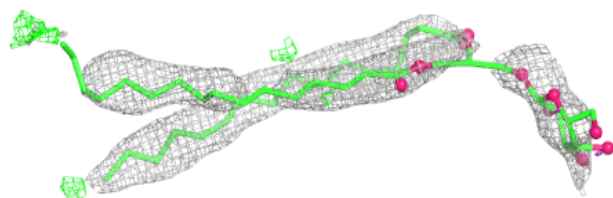
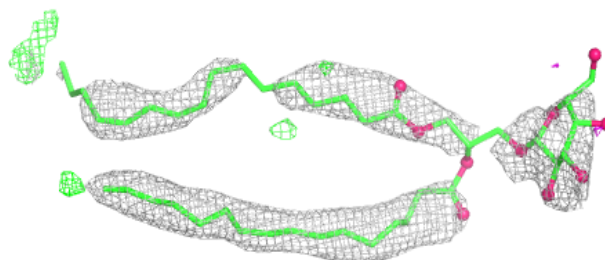


**Electron density around LMT b 621:**

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

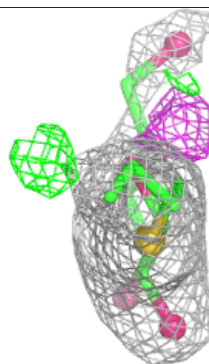
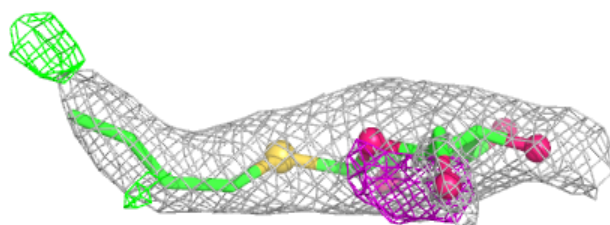
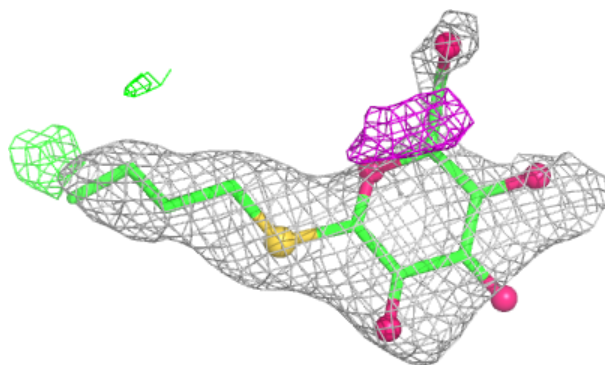
**Electron density around LMG C 521:**

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

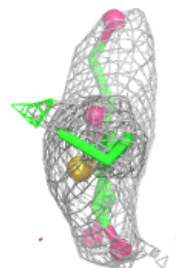
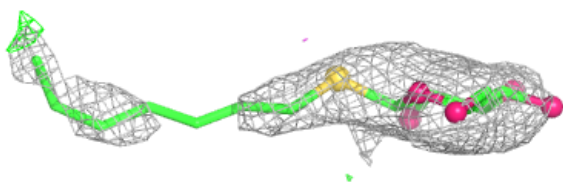
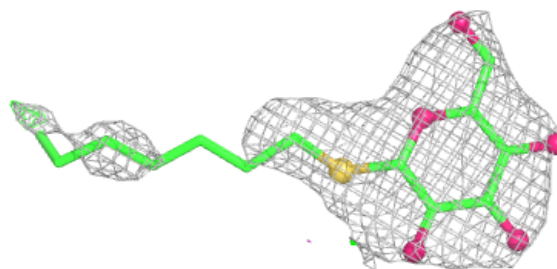


**Electron density around HTG D 411:**

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

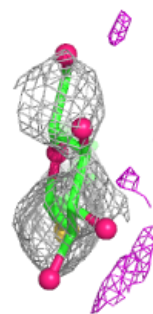
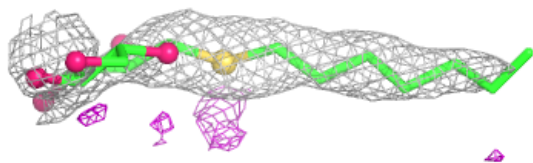
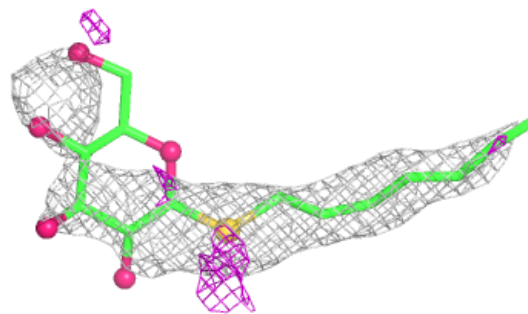
**Electron density around HTG c 522:**

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

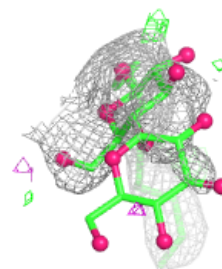
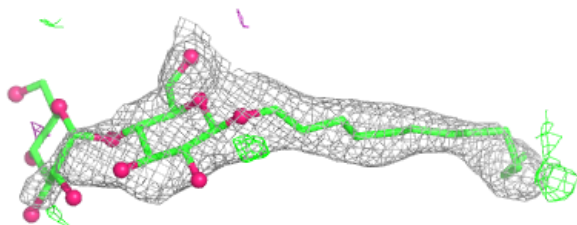
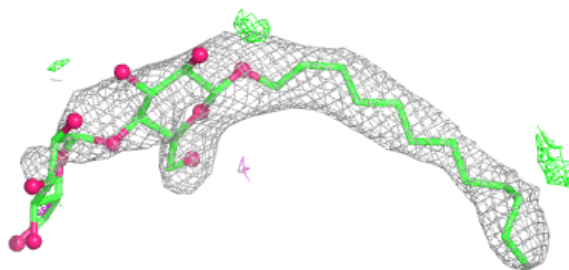


**Electron density around HTG b 623:**

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

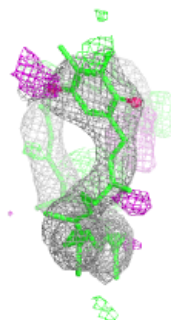
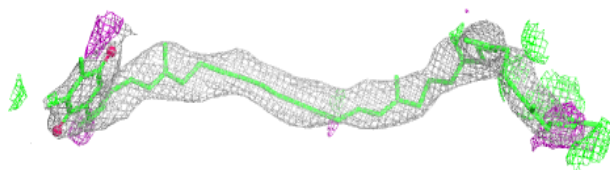
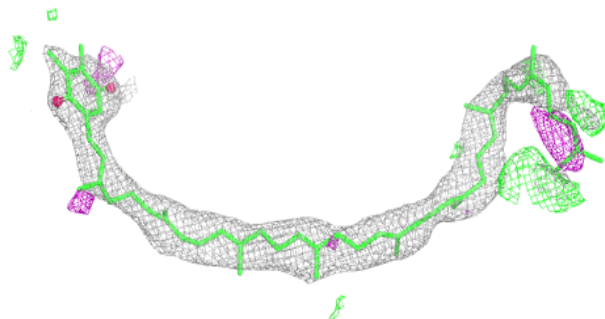
**Electron density around LMT T 101:**

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

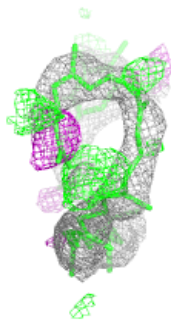
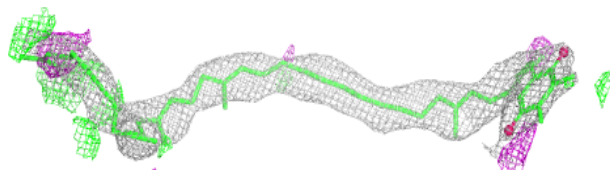
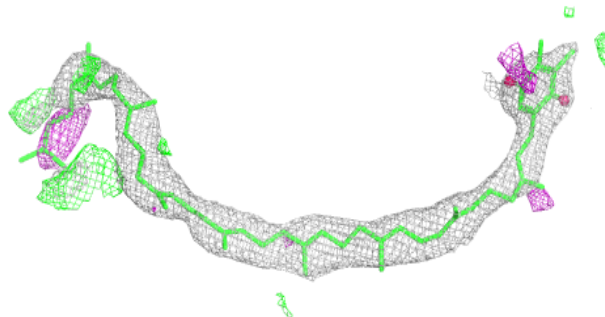


**Electron density around PL9 A 413 (A):**

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

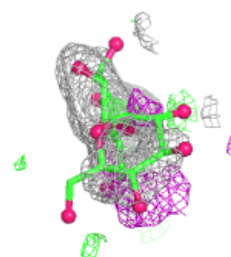
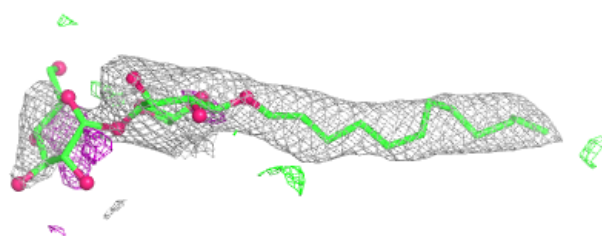
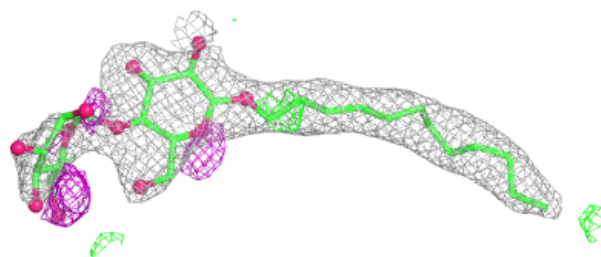
**Electron density around PL9 A 413 (B):**

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

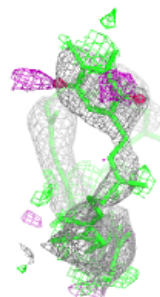
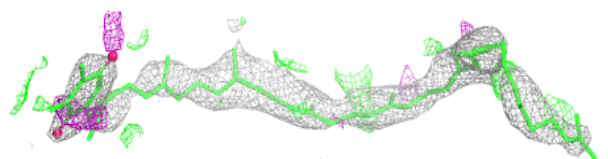
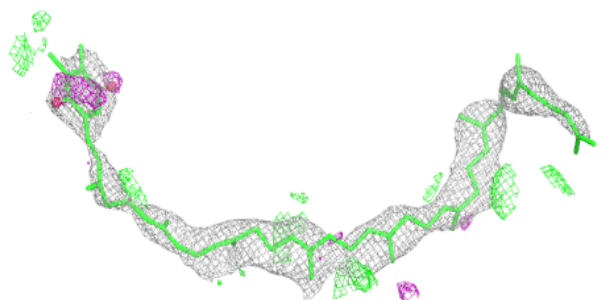


**Electron density around LMT B 626:**

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

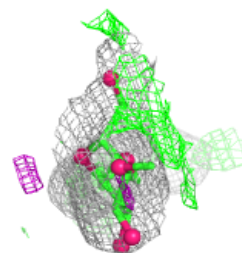
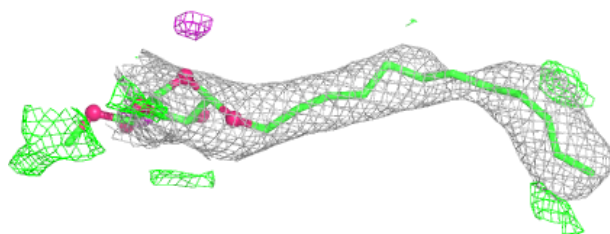
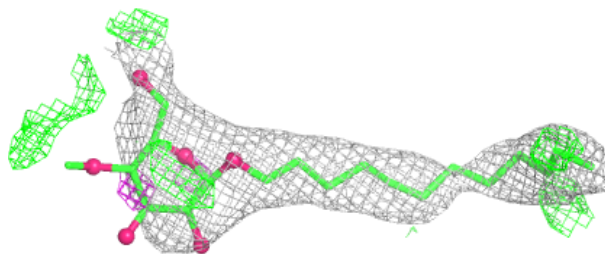
**Electron density around PL9 a 413 (A):**

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

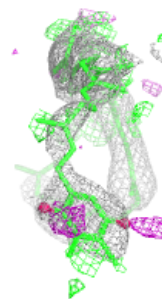
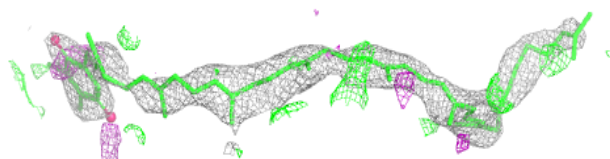
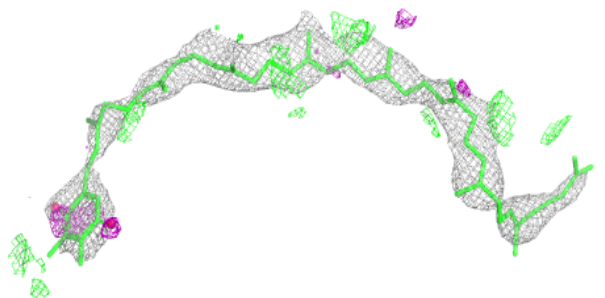


**Electron density around LMT B 629:**

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

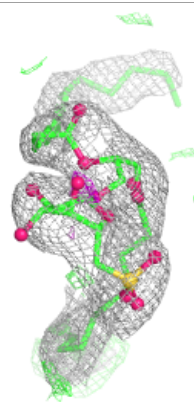
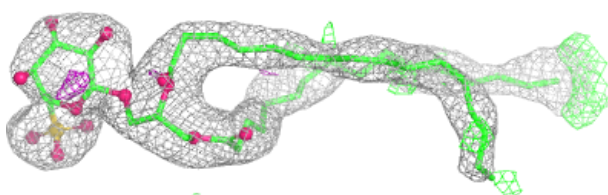
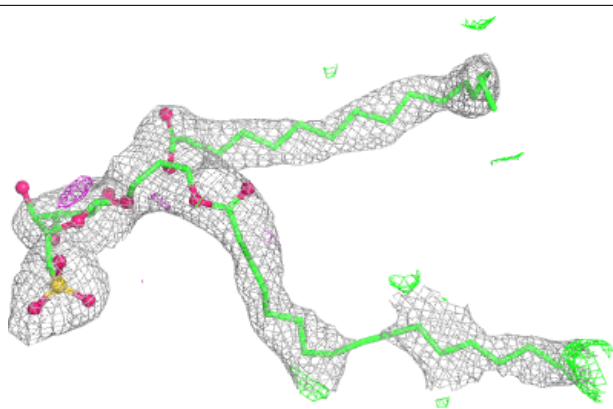
**Electron density around PL9 a 413 (B):**

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

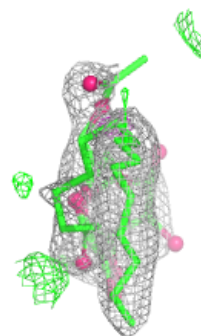
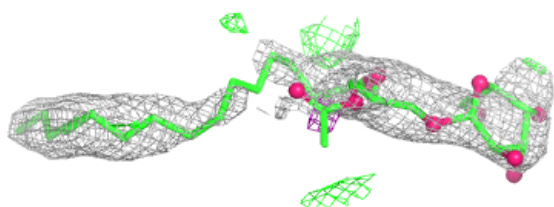
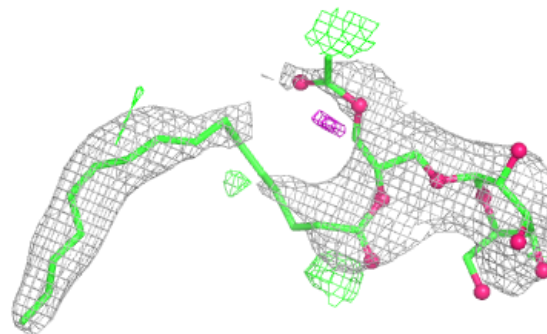


**Electron density around SQD a 411:**

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

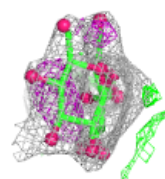
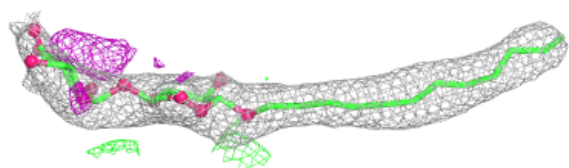
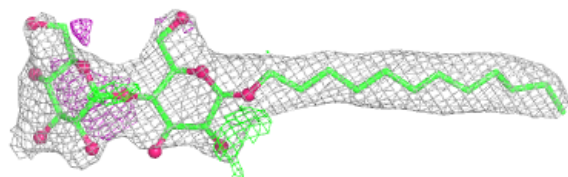
**Electron density around LMG Z 101:**

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

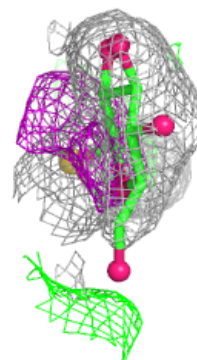
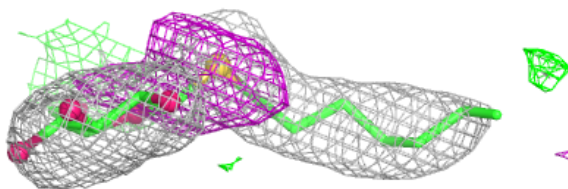
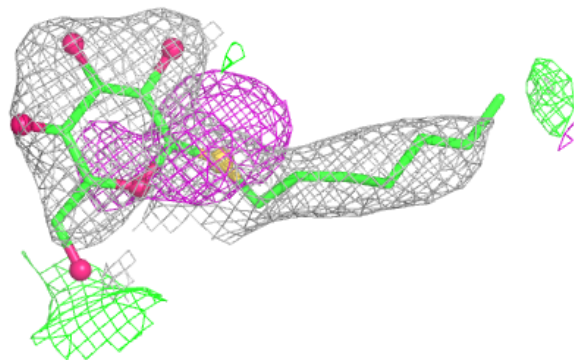


**Electron density around LMT m 103:**

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

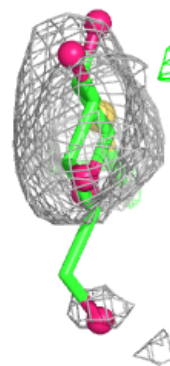
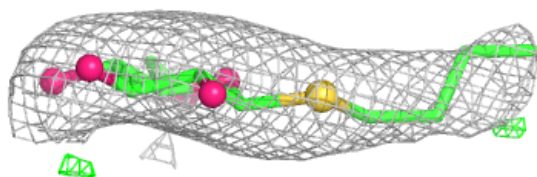
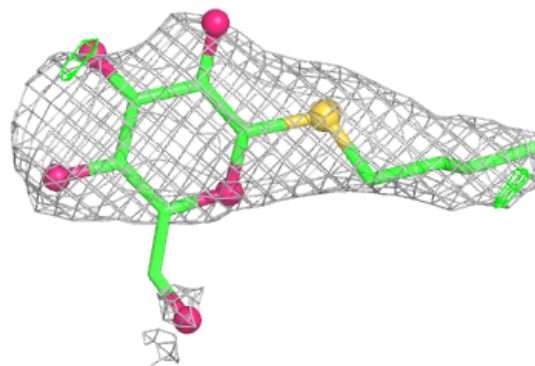
**Electron density around HTG b 622:**

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

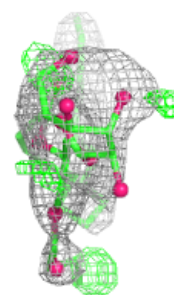
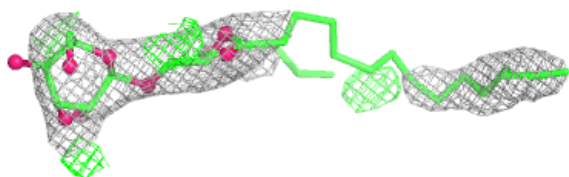
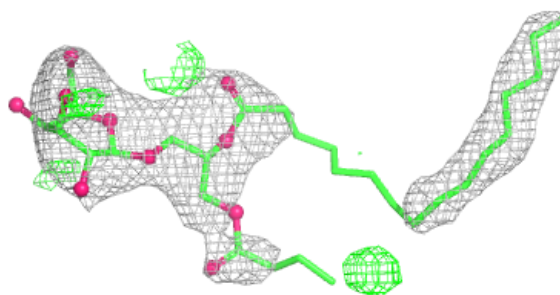


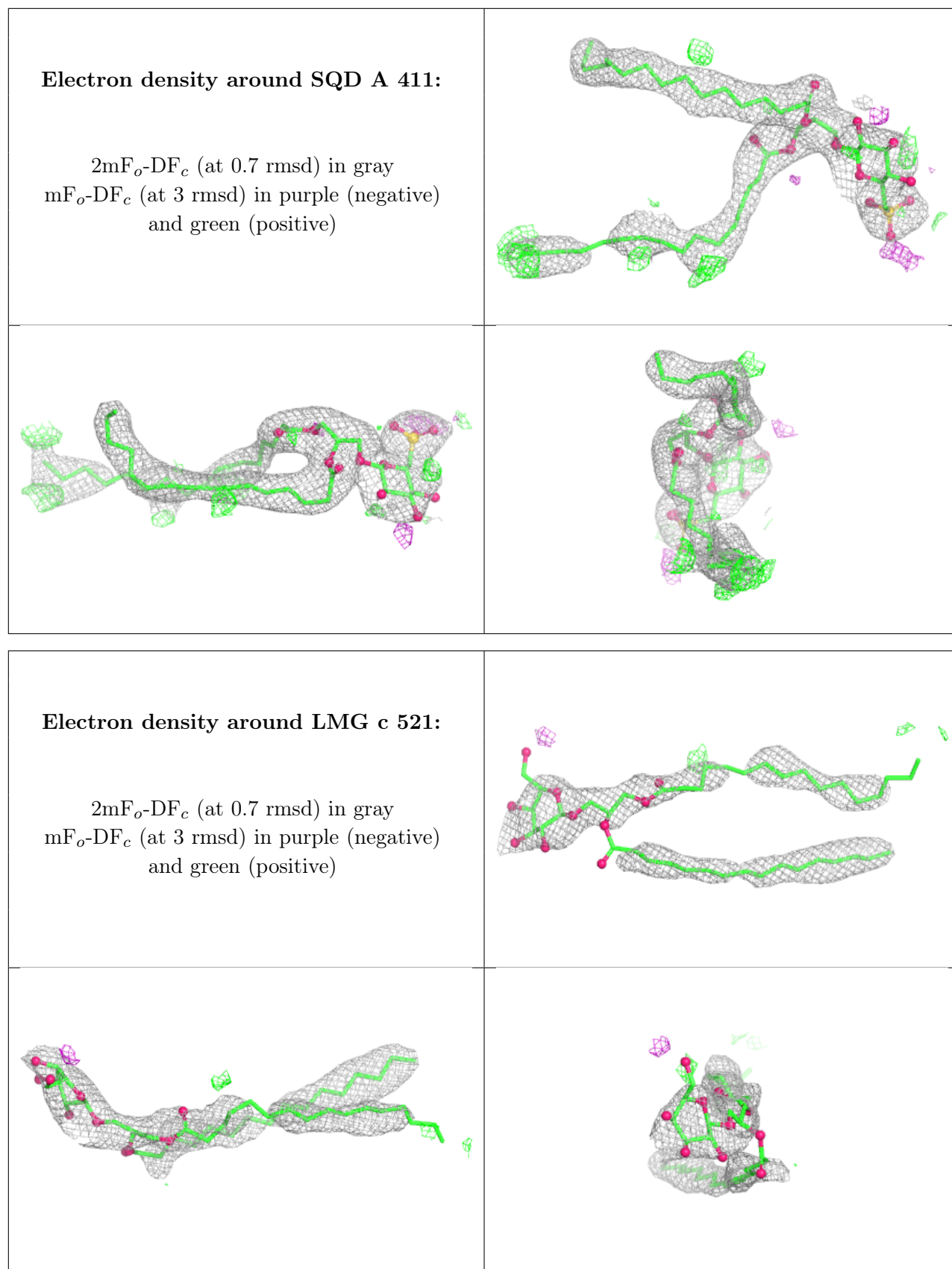
**Electron density around HTG d 411:**

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

**Electron density around LMG z 101:**

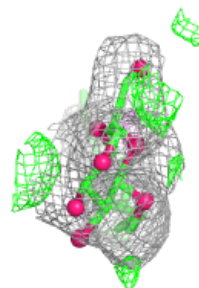
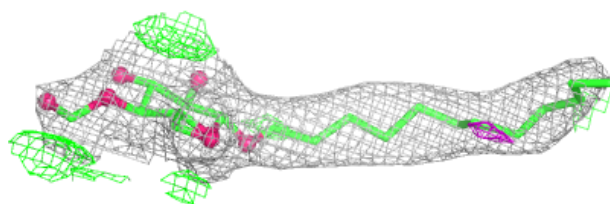
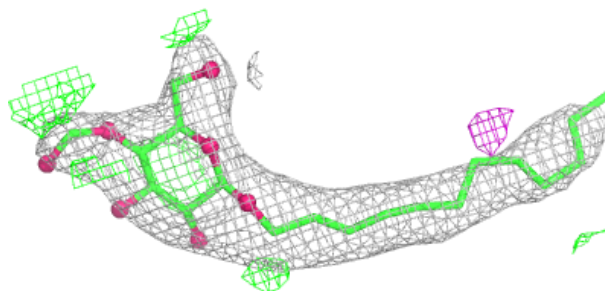
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





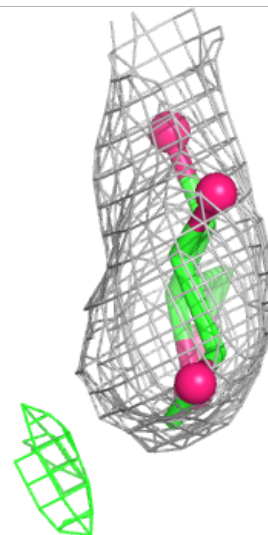
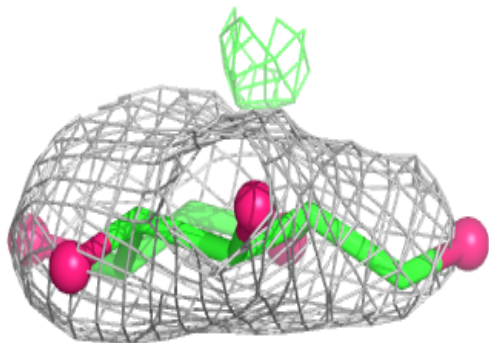
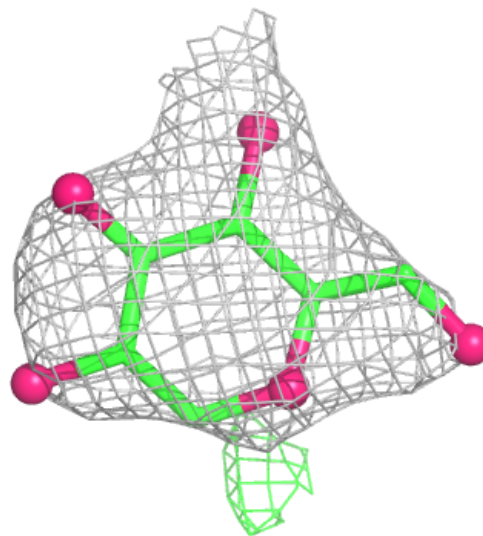
**Electron density around LMT t 101:**

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



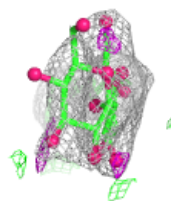
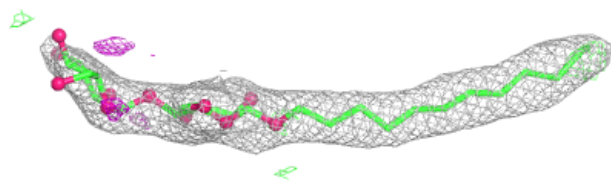
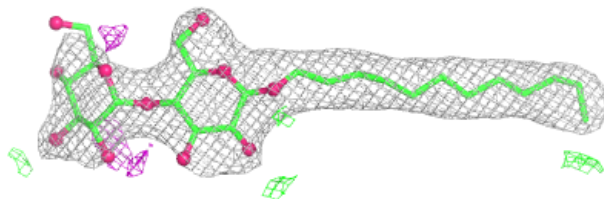
**Electron density around HTG V 202:**

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

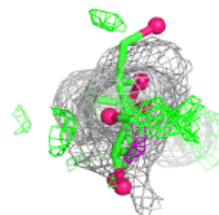
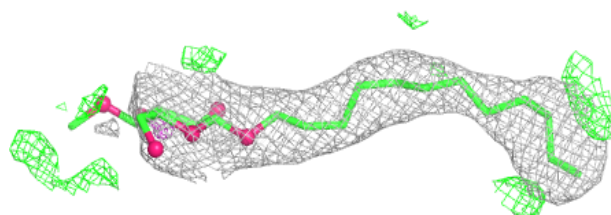
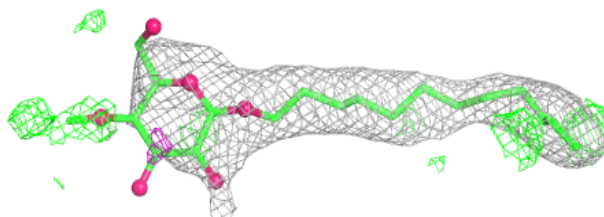


**Electron density around LMT M 101:**

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

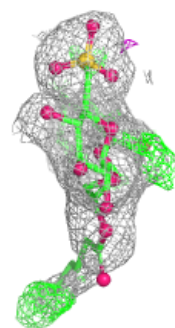
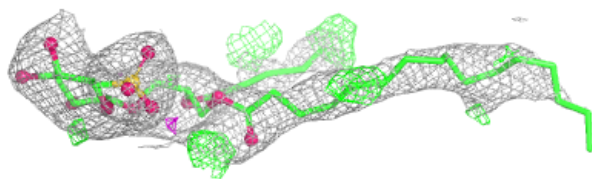
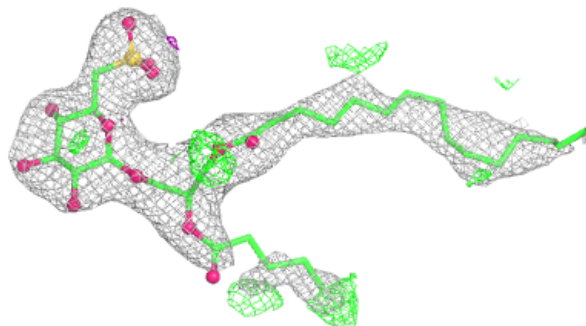
**Electron density around LMT b 627:**

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

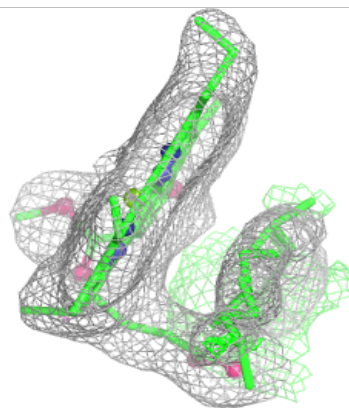
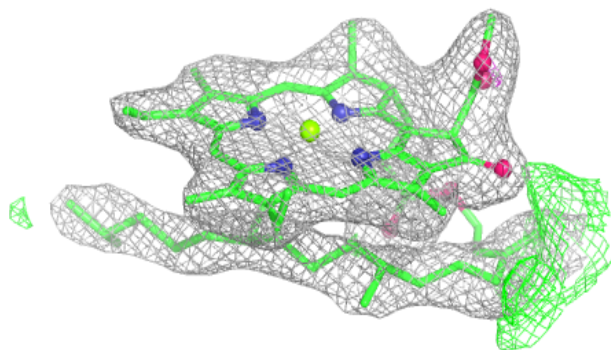
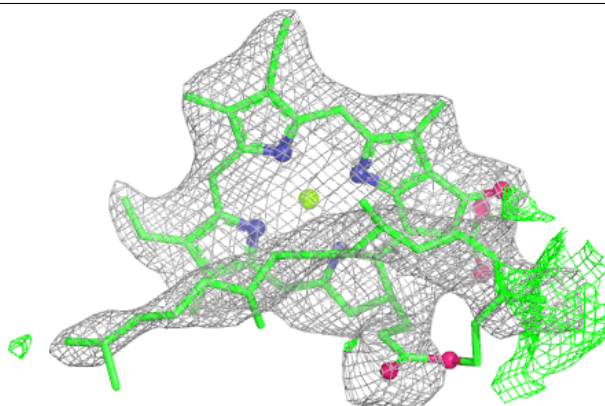


**Electron density around SQD X 101:**

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

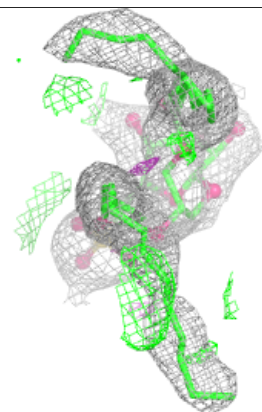
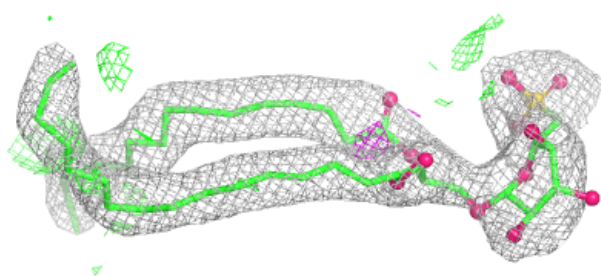
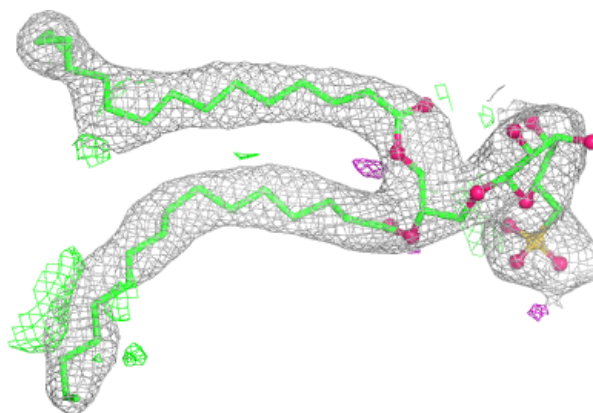
**Electron density around CLA b 601:**

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

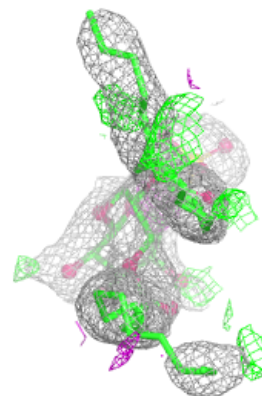
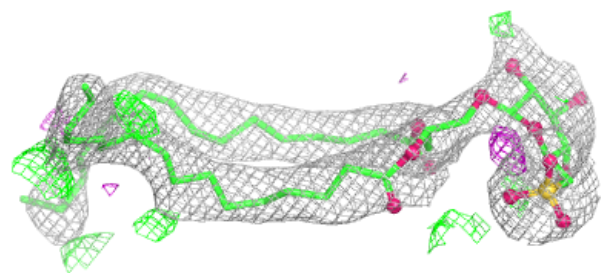
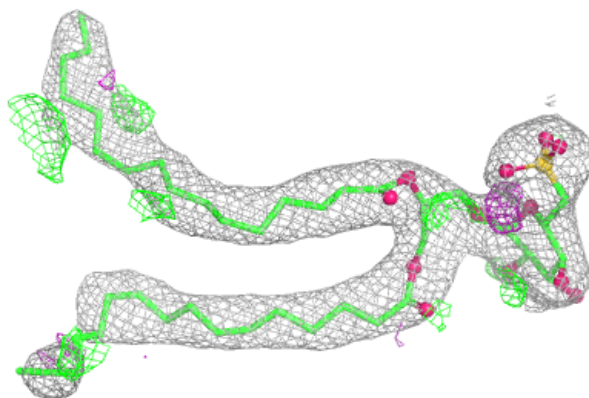


**Electron density around SQD 1 101:**

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

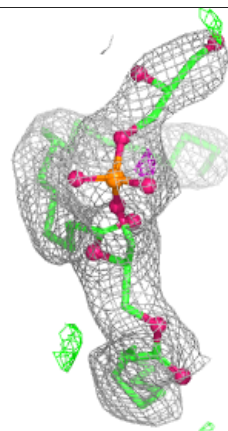
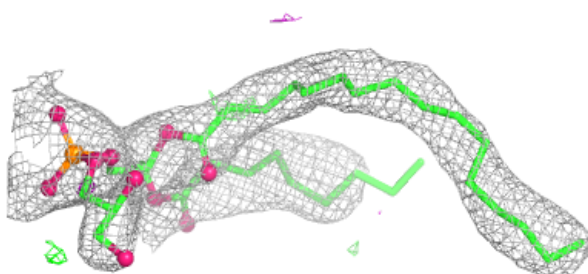
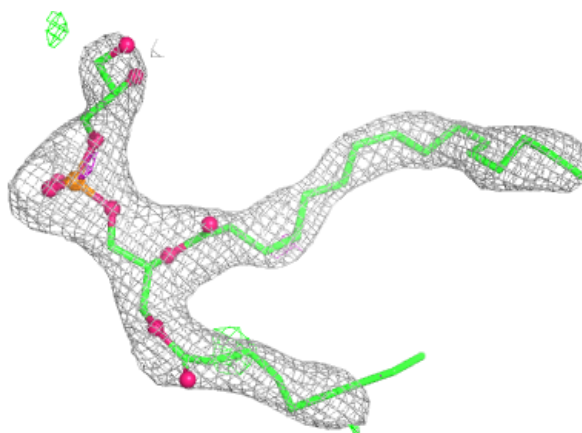
**Electron density around SQD b 620:**

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



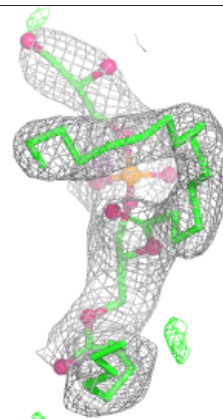
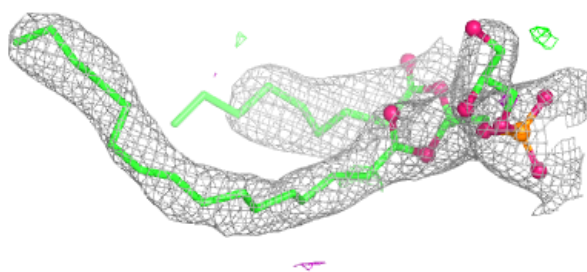
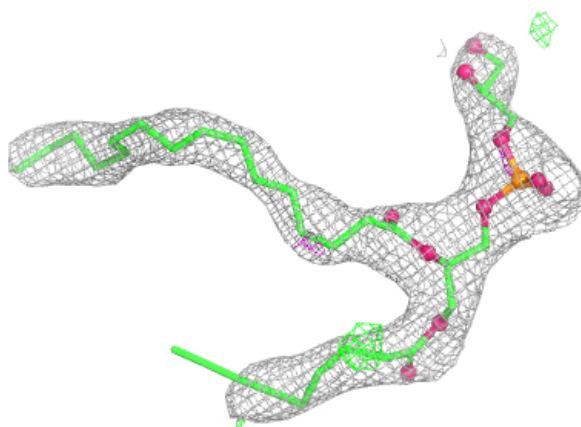
**Electron density around LHG E 101 (A):**

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

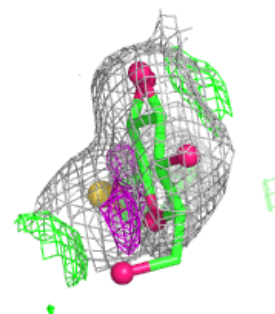
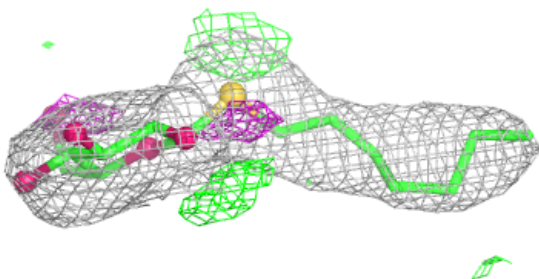
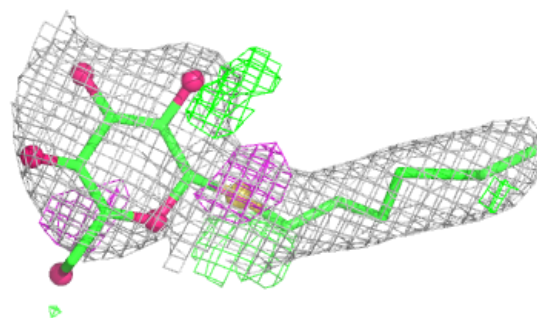


**Electron density around LHG E 101 (B):**

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

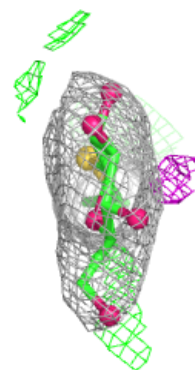
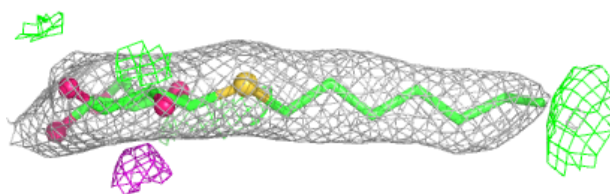
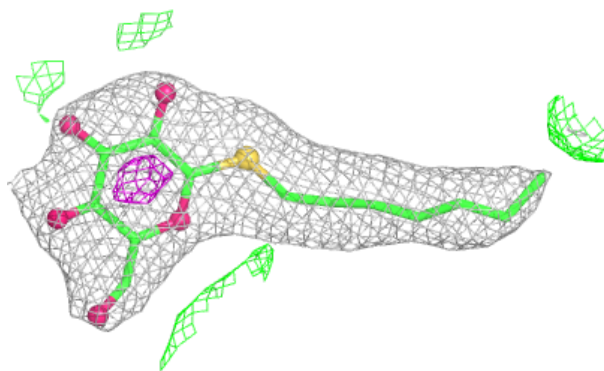
**Electron density around HTG o 301:**

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

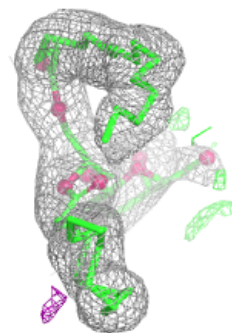
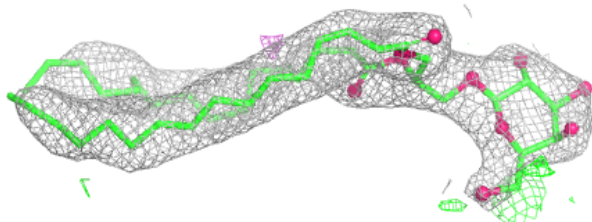
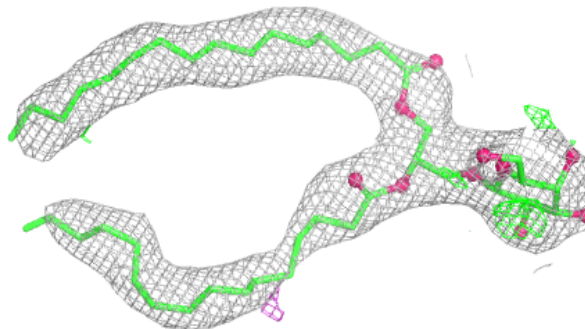


**Electron density around HTG B 623:**

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

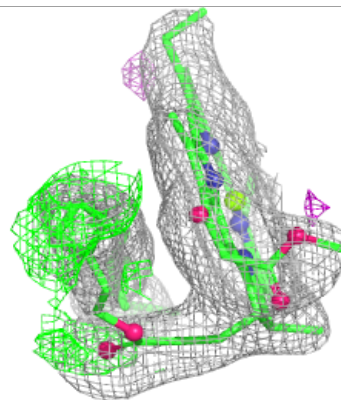
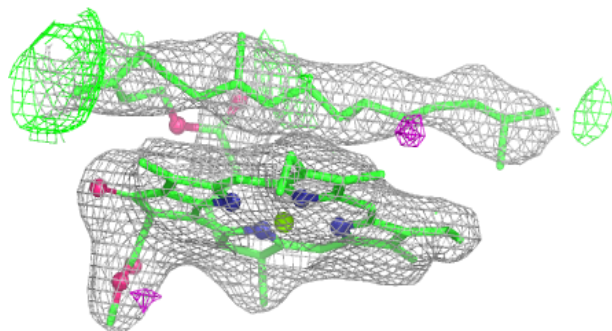
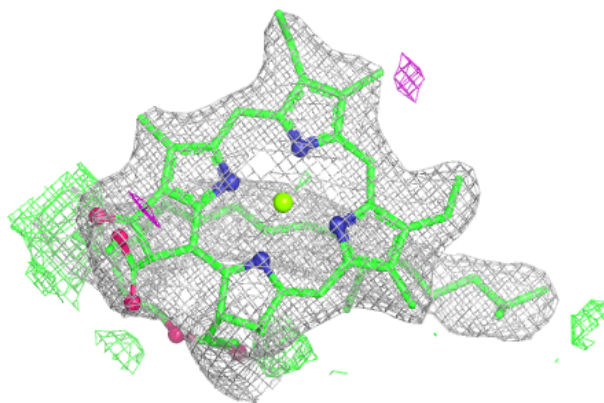
**Electron density around LMG C 501:**

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

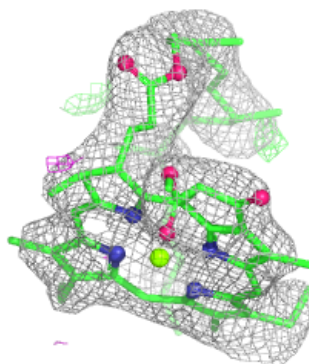
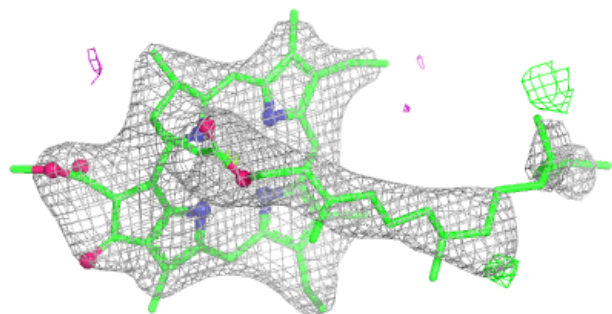
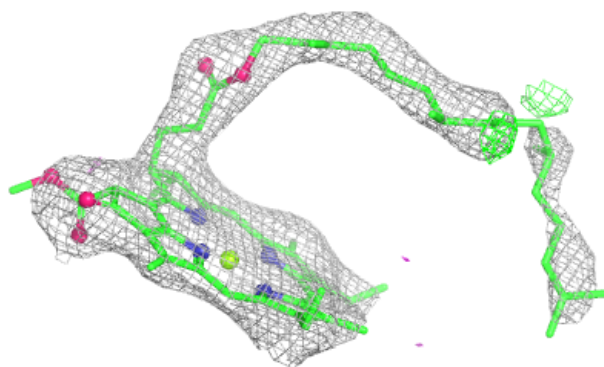


**Electron density around CLA B 601:**

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

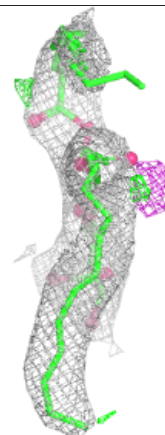
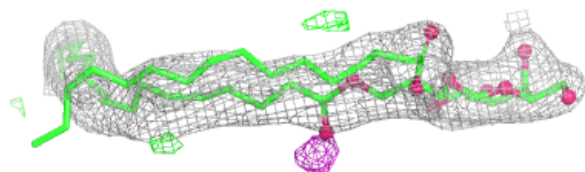
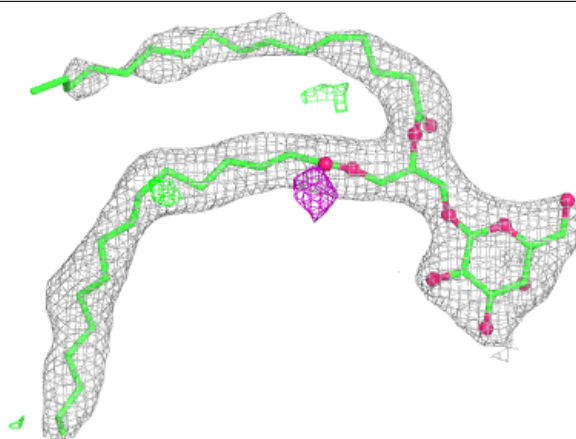
**Electron density around CLA c 514:**

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

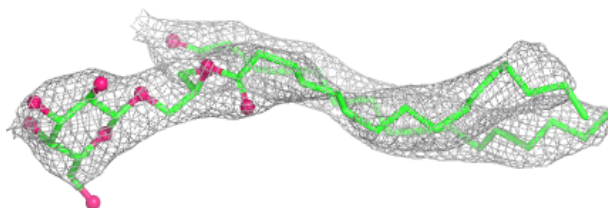
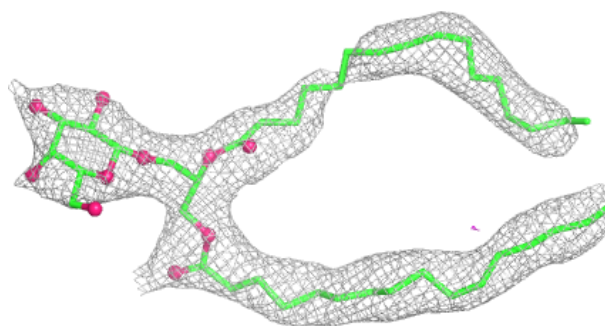


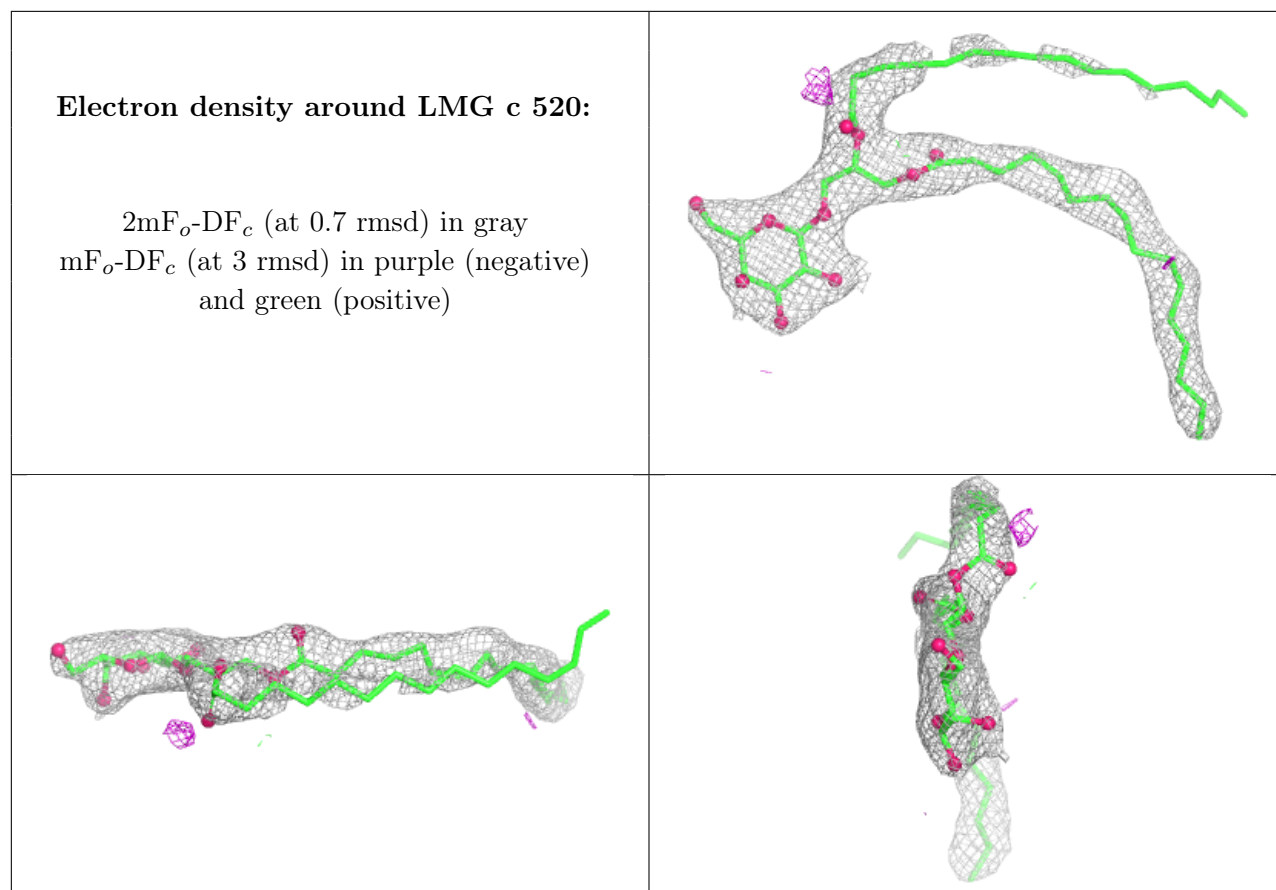
**Electron density around LMG C 520:**

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

**Electron density around LMG c 501:**

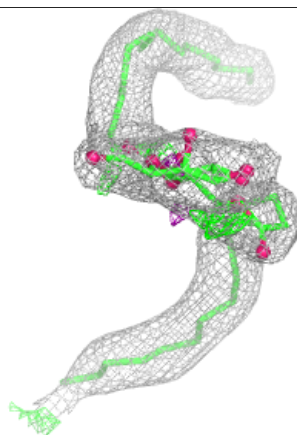
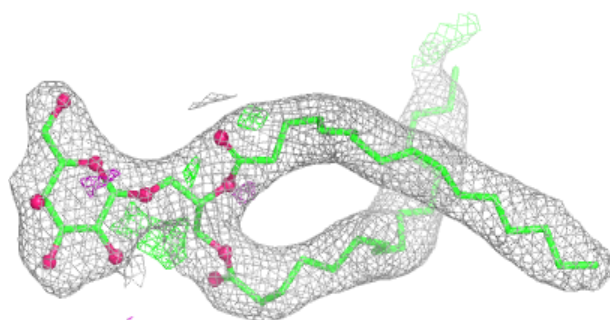
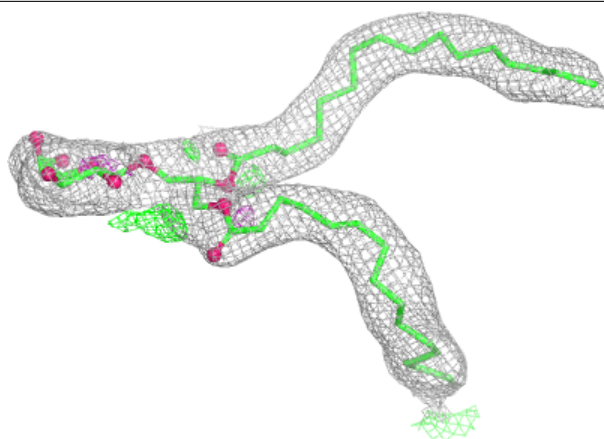
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



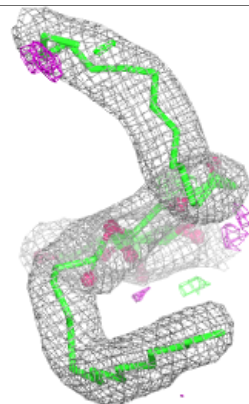
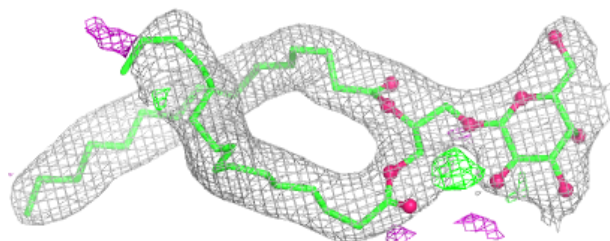
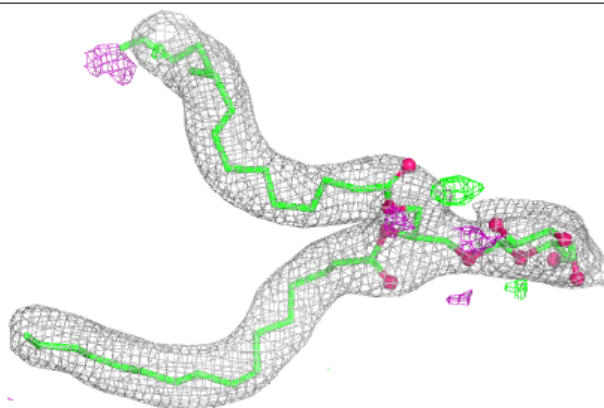


**Electron density around LMG B 620:**

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

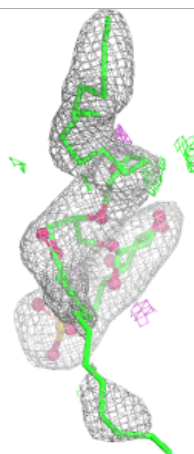
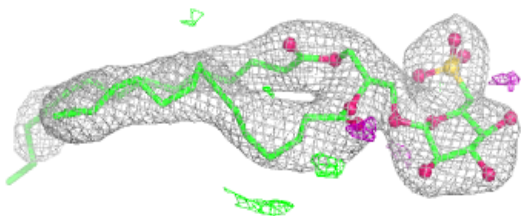
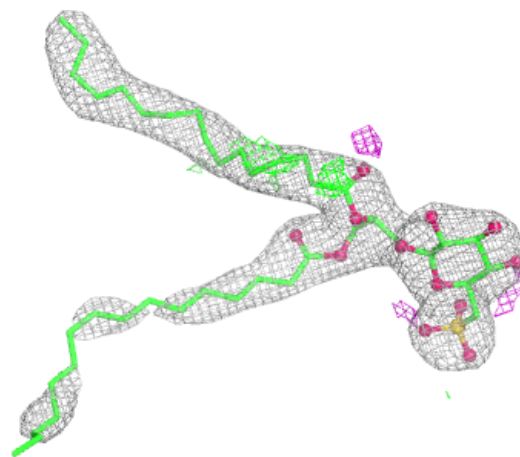
**Electron density around LMG m 101:**

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



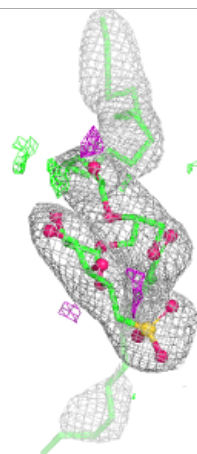
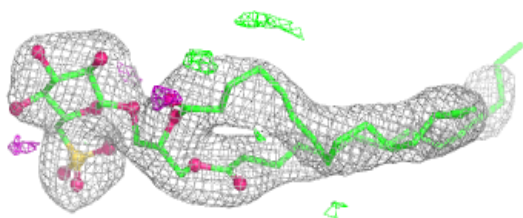
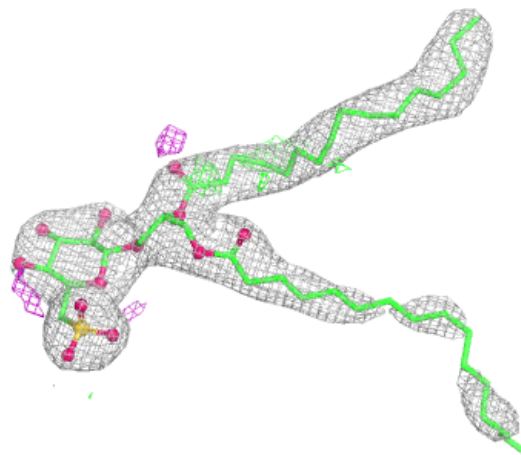
**Electron density around SQD A 409 (A):**

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



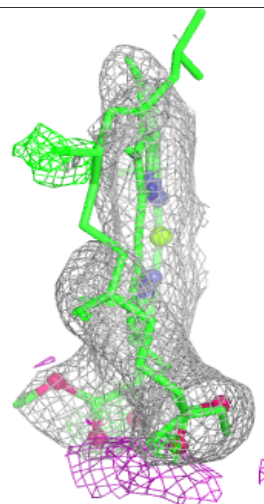
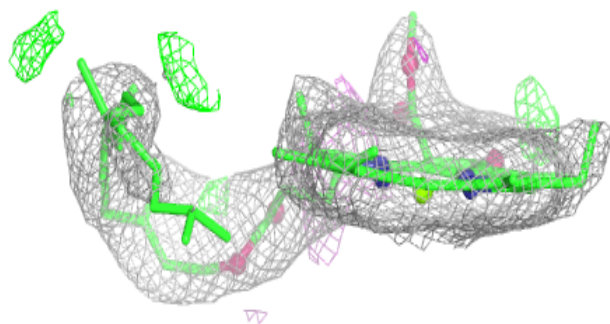
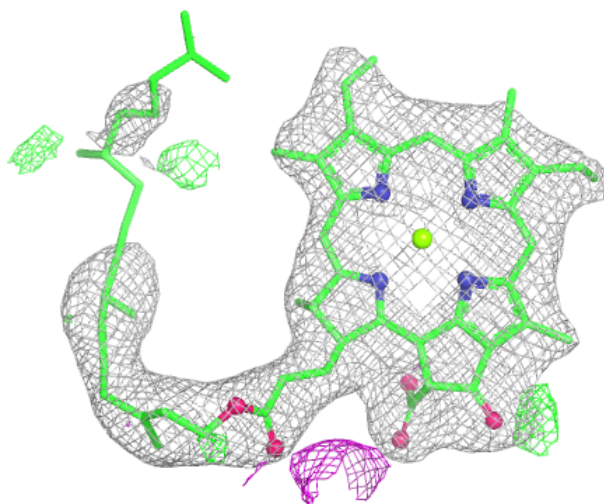
**Electron density around SQD A 409 (B):**

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



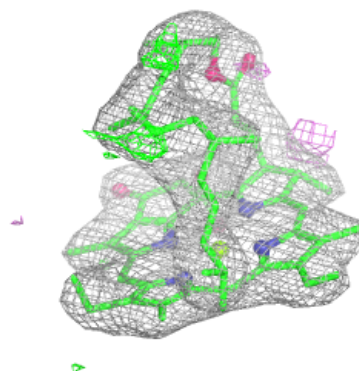
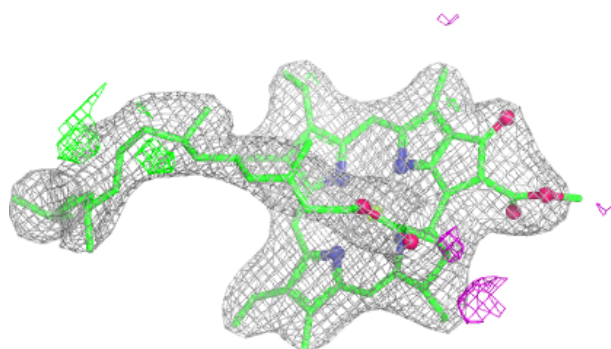
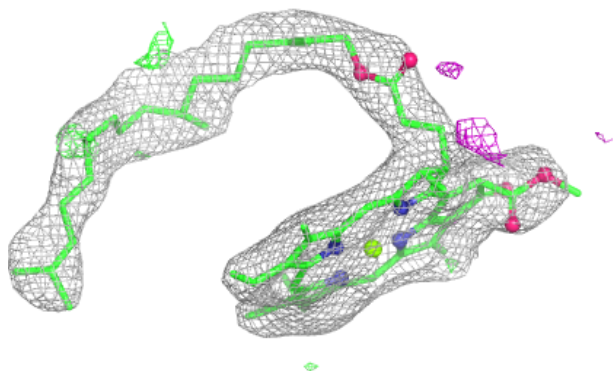
**Electron density around CLA c 513:**

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

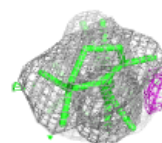
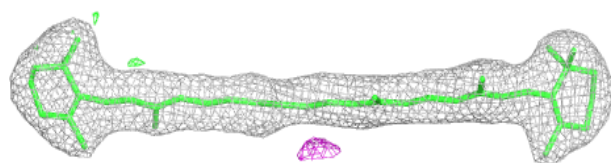
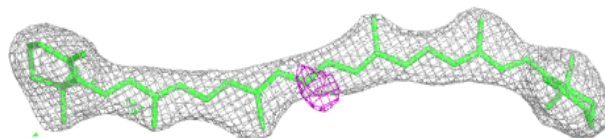


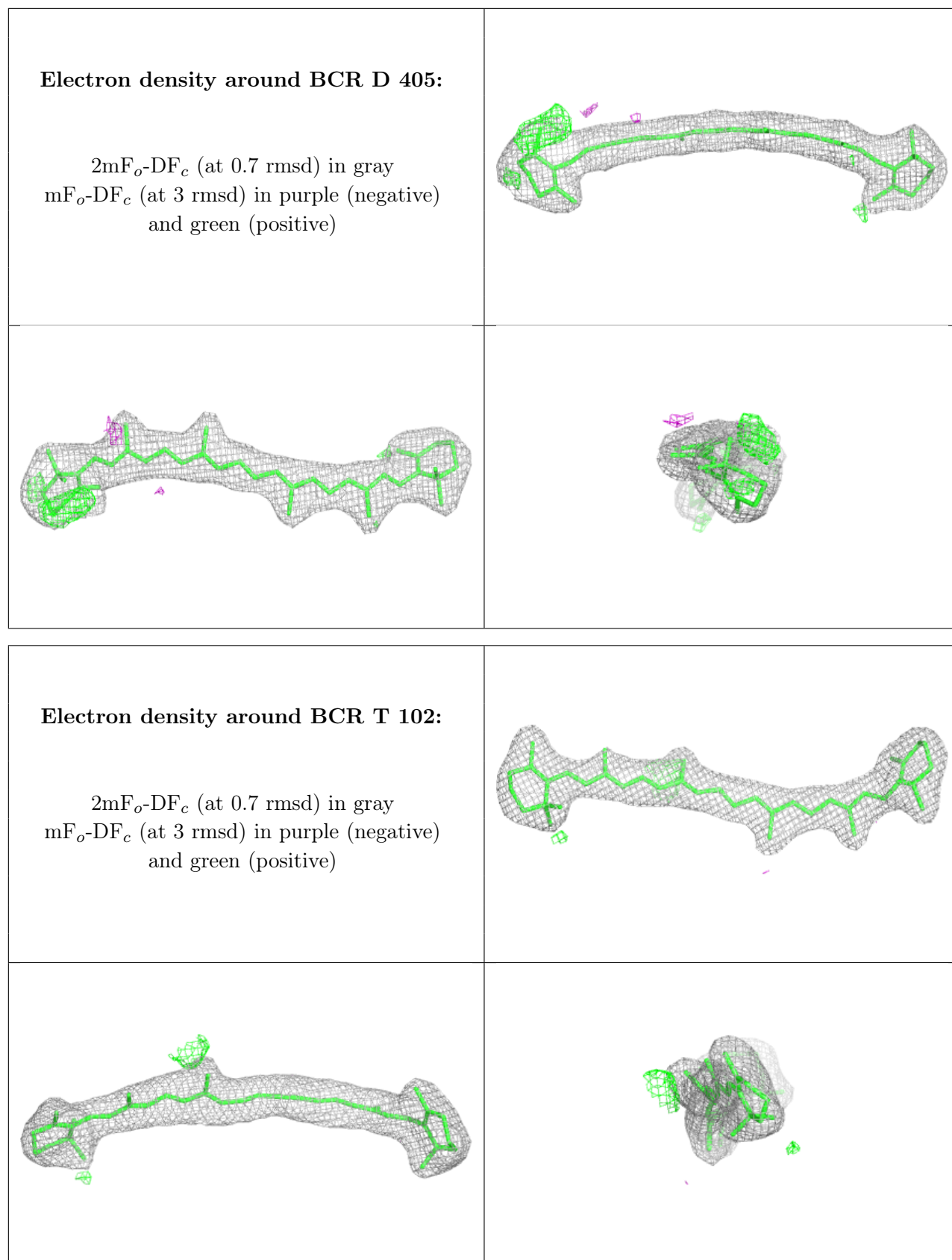
**Electron density around CLA C 514:**

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

**Electron density around BCR C 515:**

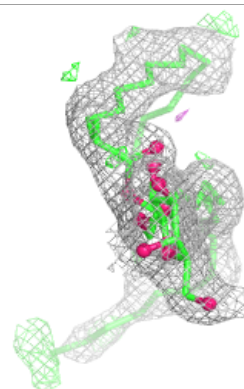
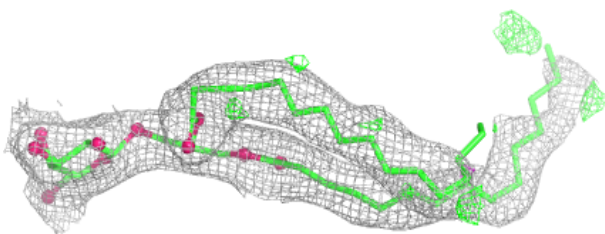
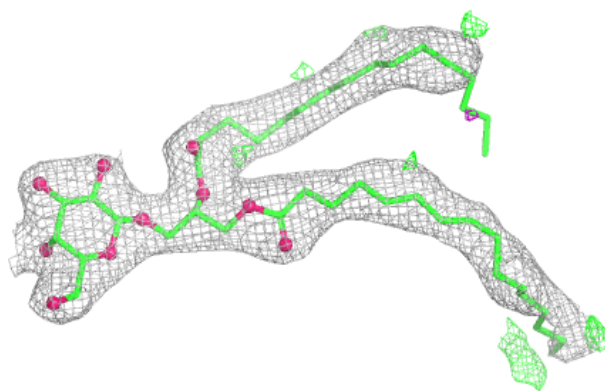
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



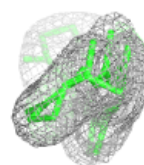
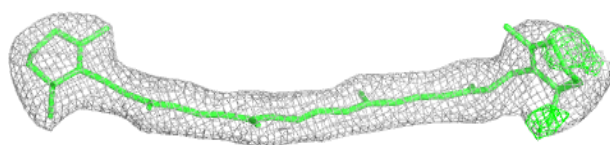
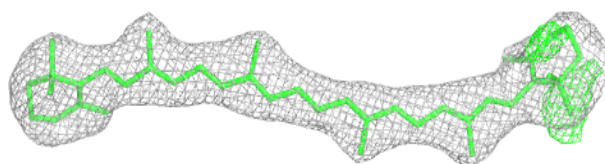


**Electron density around LMG D 412:**

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

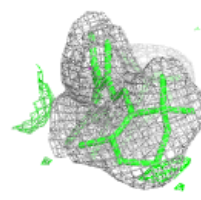
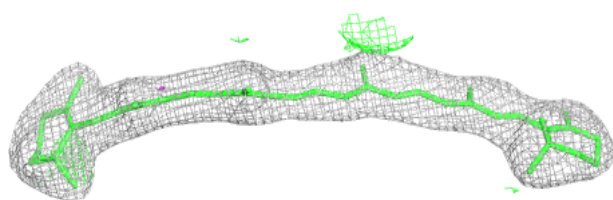
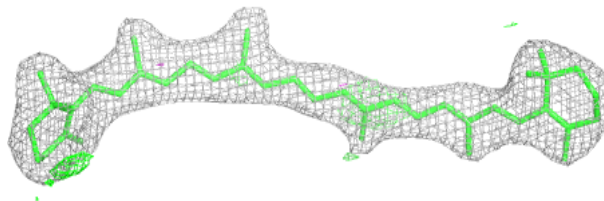
**Electron density around BCR d 405:**

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

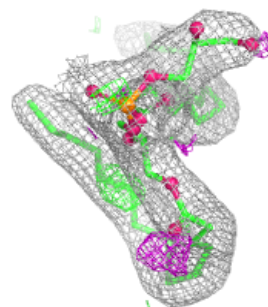
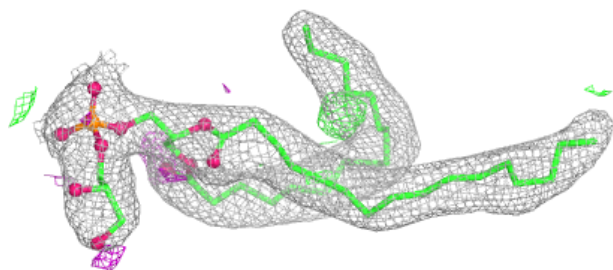
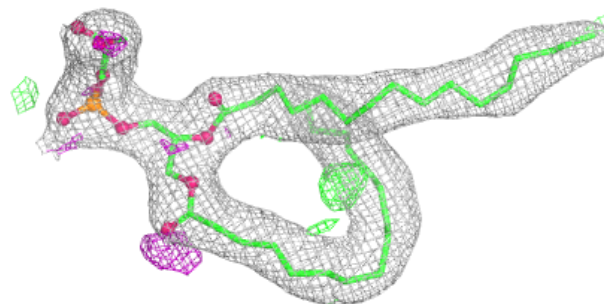


**Electron density around BCR t 102:**

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

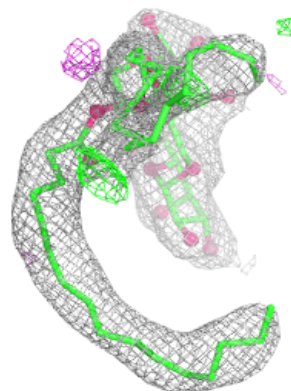
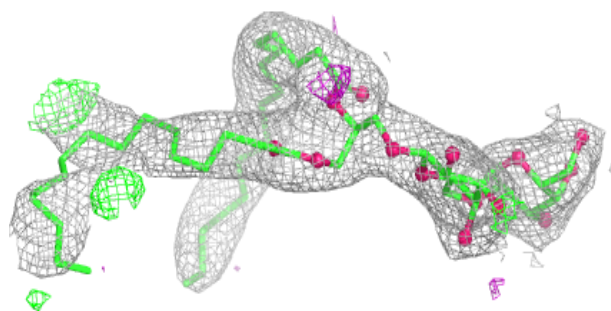
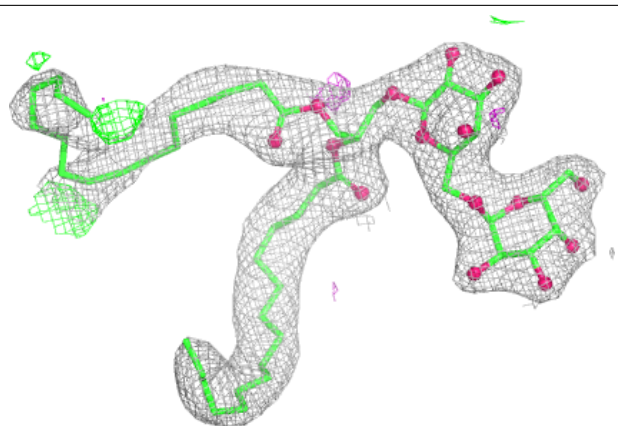
**Electron density around LHG A 418 (A):**

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



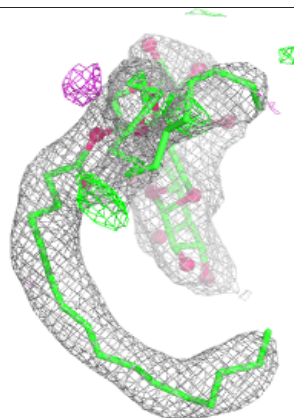
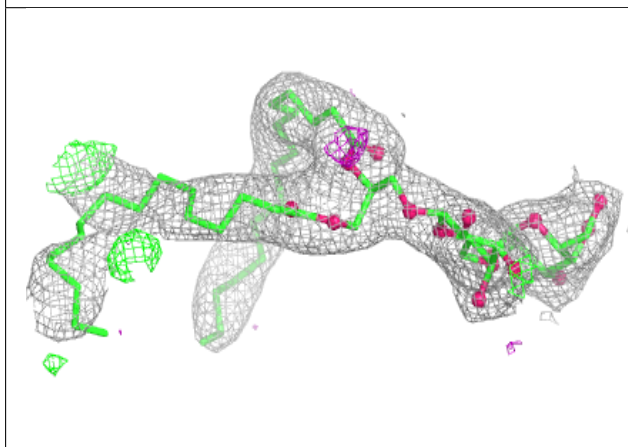
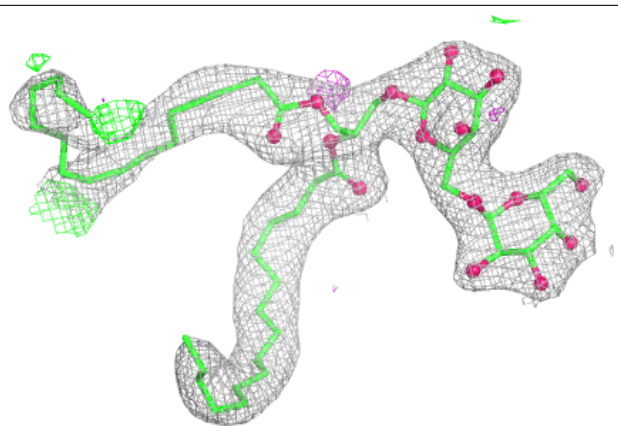
**Electron density around DGD C 518 (A):**

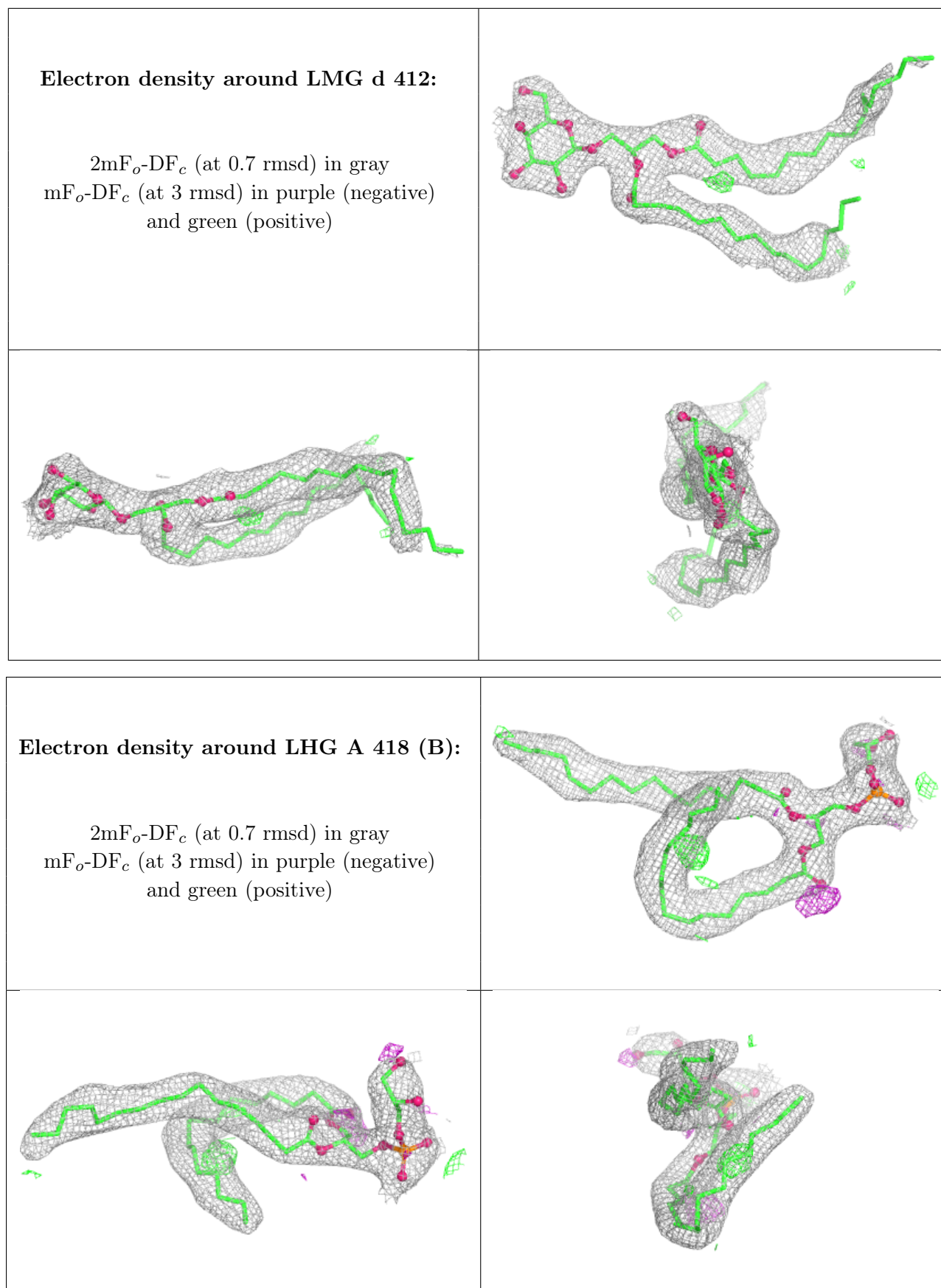
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around DGD C 518 (B):**

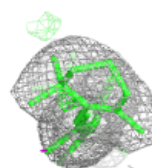
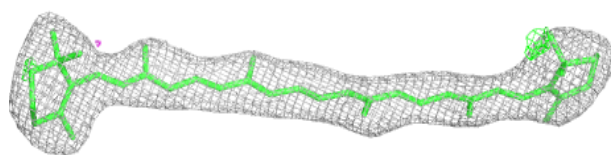
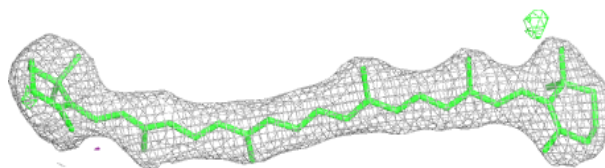
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



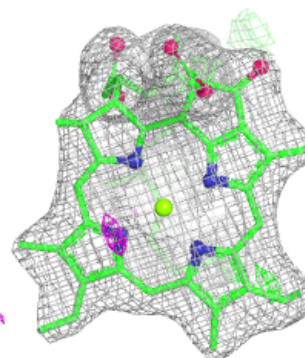
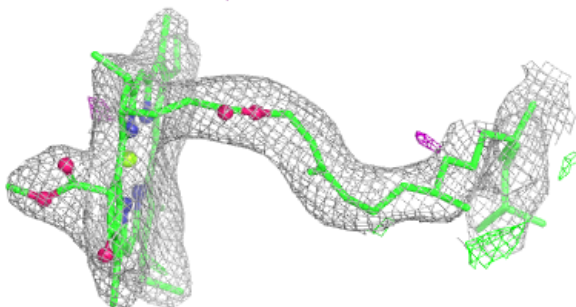
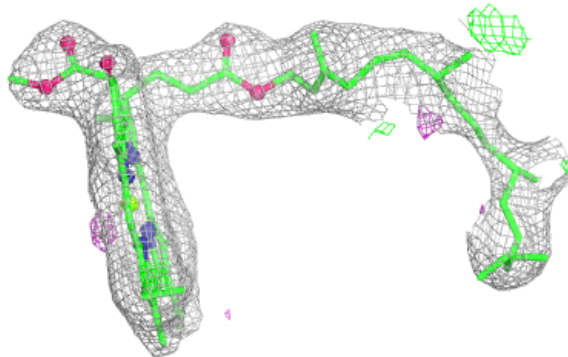


**Electron density around BCR c 515:**

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

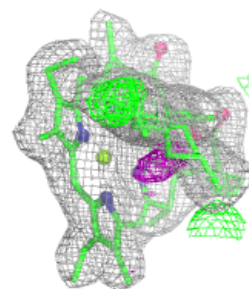
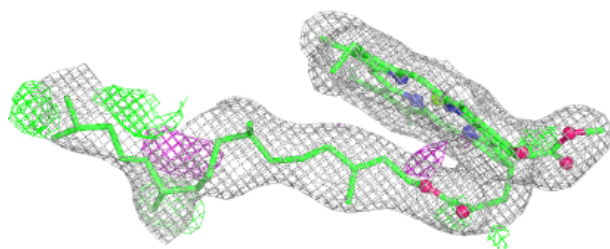
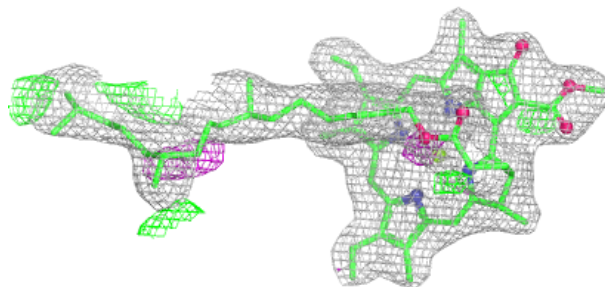
**Electron density around CLA C 507:**

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

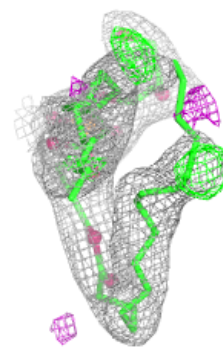
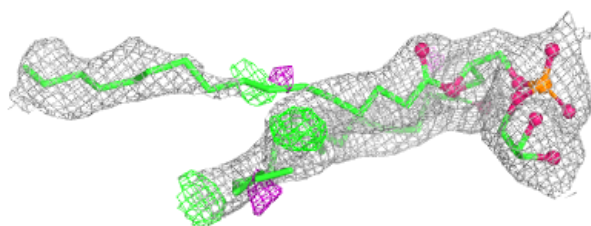
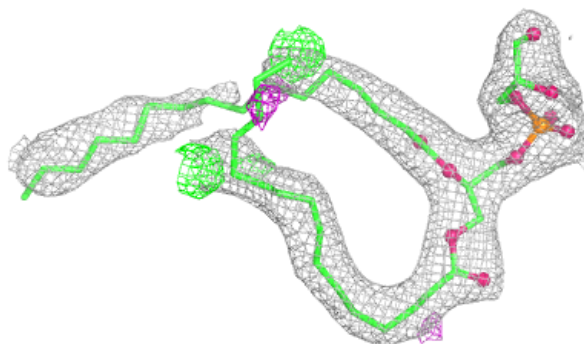


**Electron density around CLA B 614:**

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

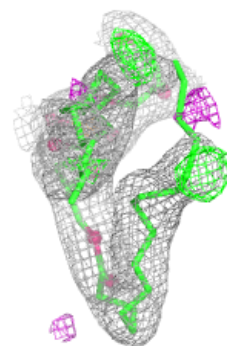
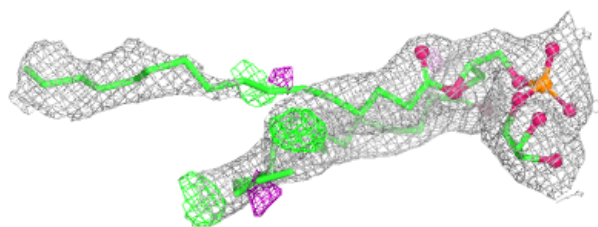
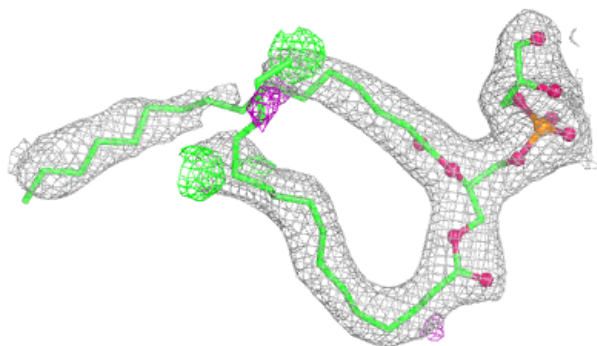
**Electron density around LHG D 408 (A):**

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

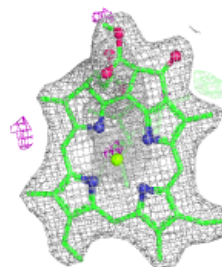
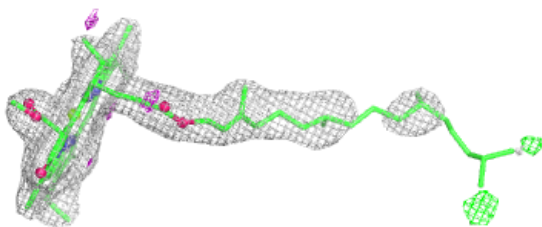
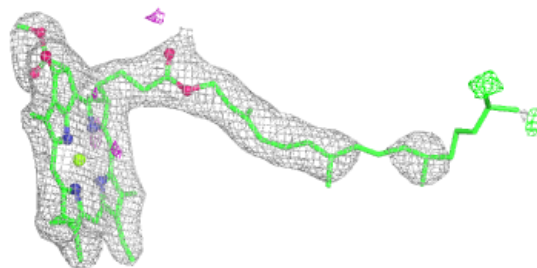


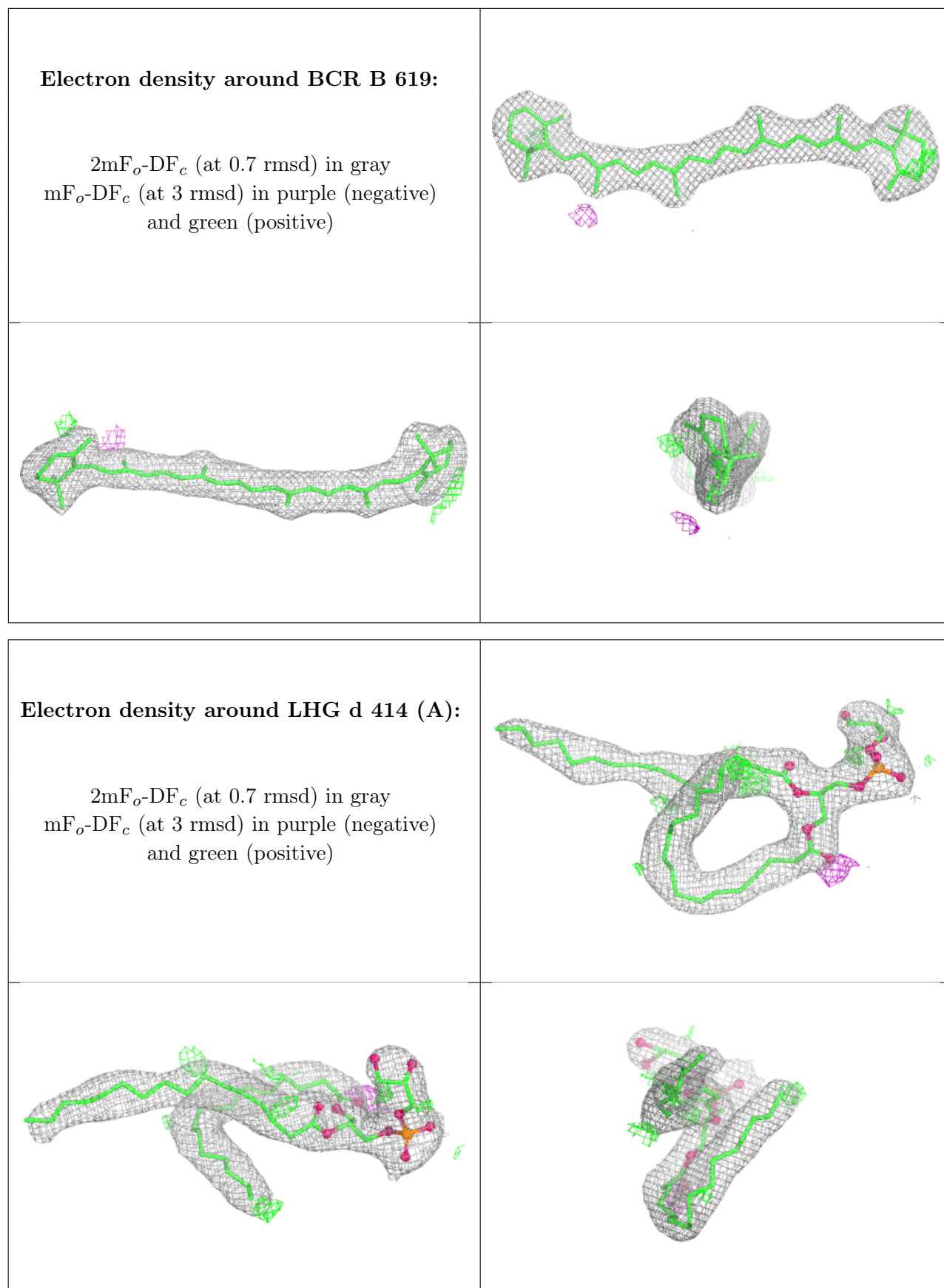
**Electron density around LHG D 408 (B):**

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

**Electron density around CLA d 404:**

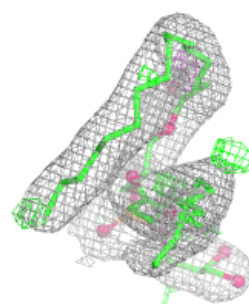
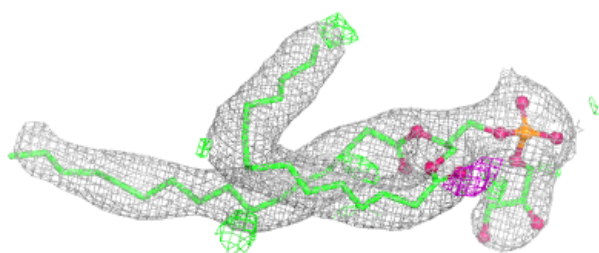
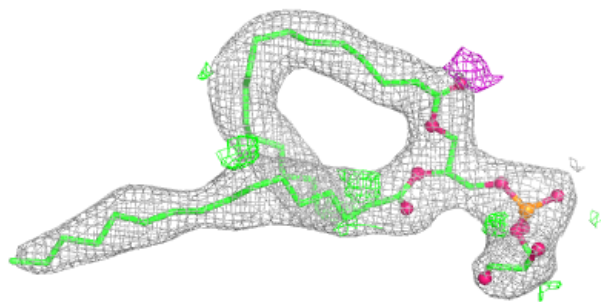
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



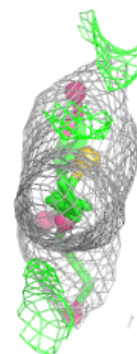
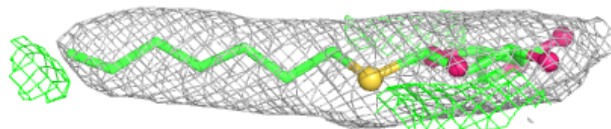
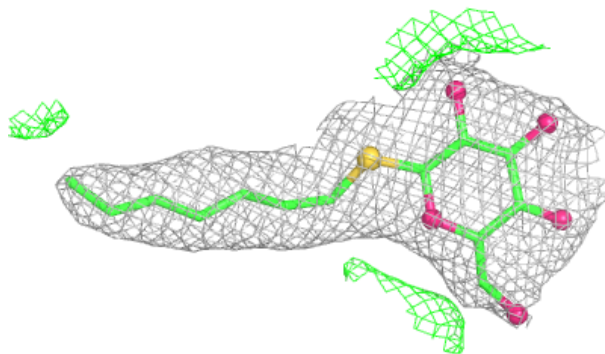


**Electron density around LHG d 414 (B):**

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

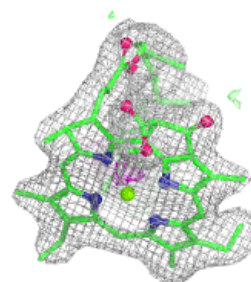
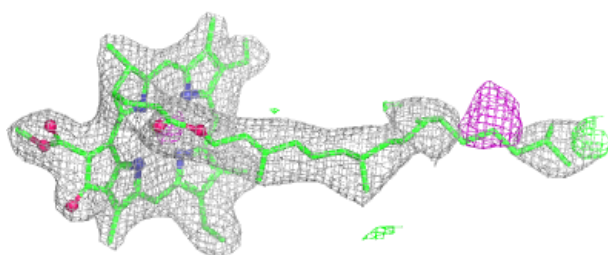
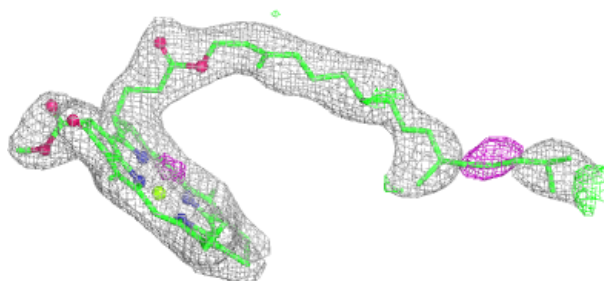
**Electron density around HTG b 625:**

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



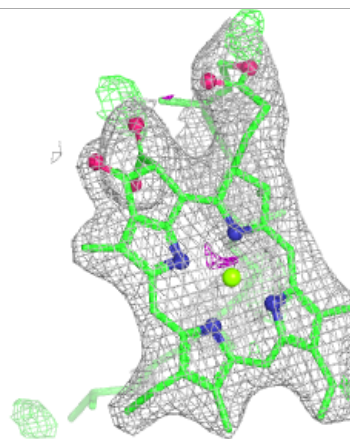
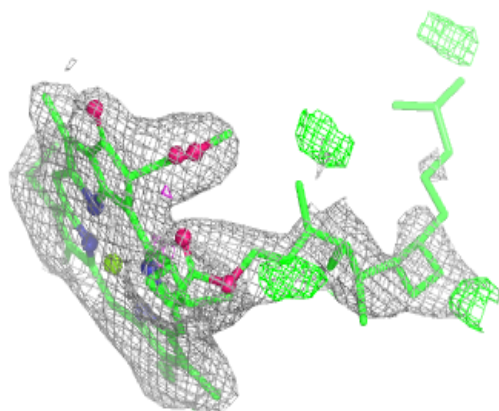
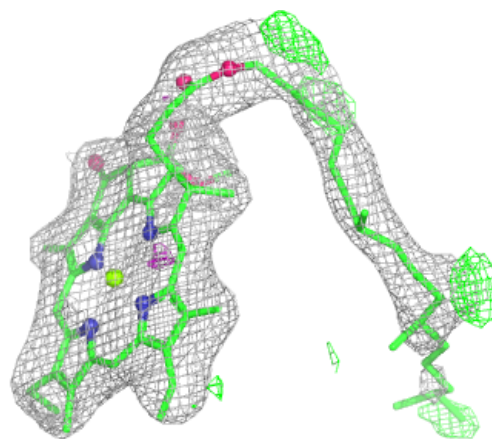
**Electron density around CLA C 505:**

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



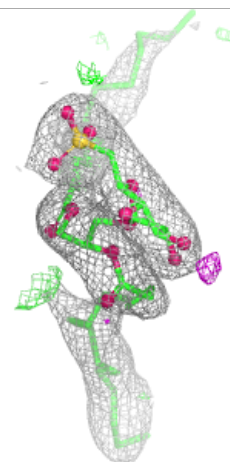
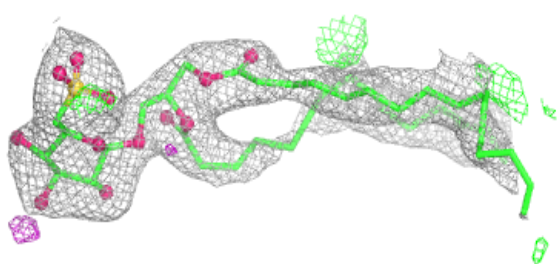
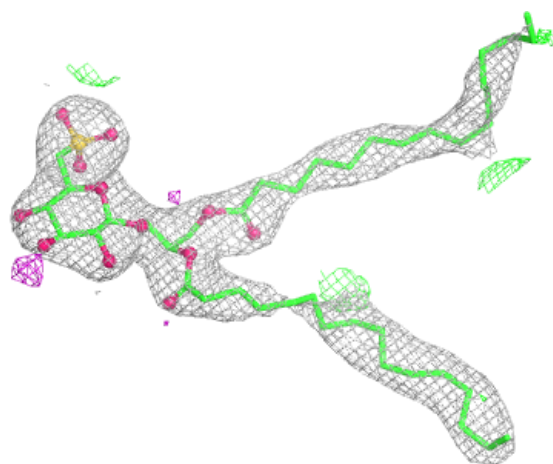
**Electron density around CLA b 616:**

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



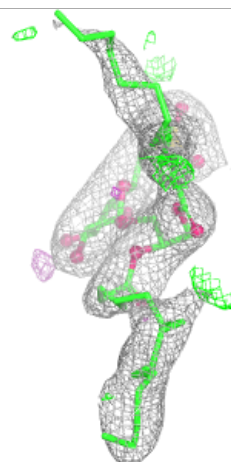
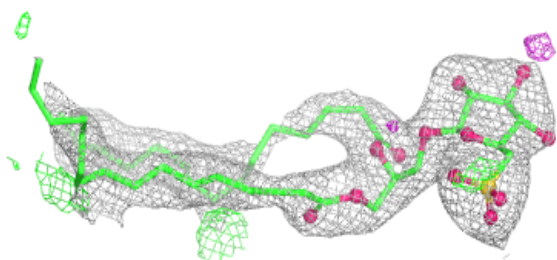
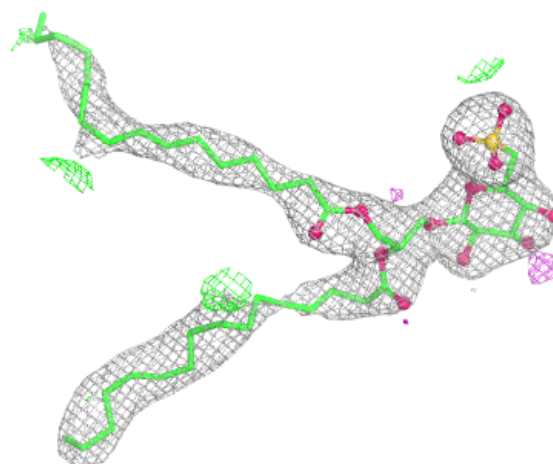
**Electron density around SQD a 409 (A):**

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



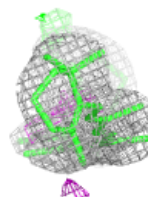
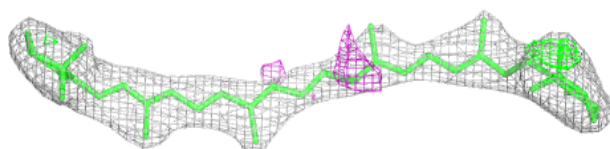
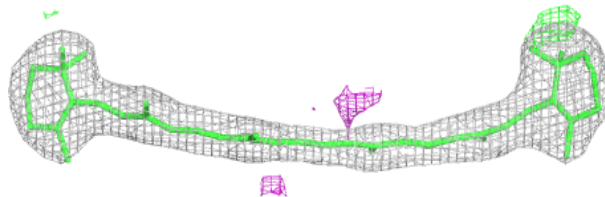
**Electron density around SQD a 409 (B):**

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

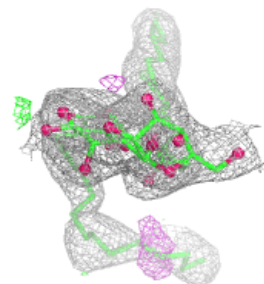
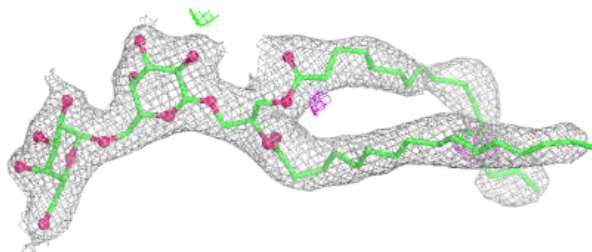
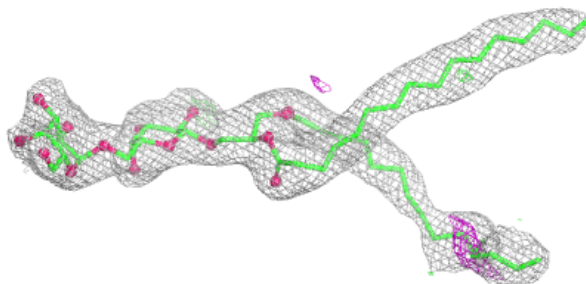


**Electron density around BCR K 102:**

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

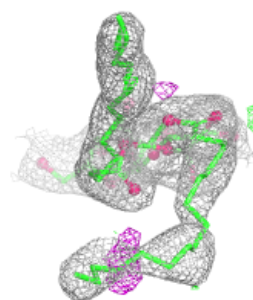
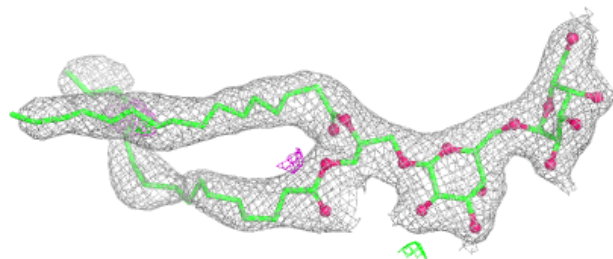
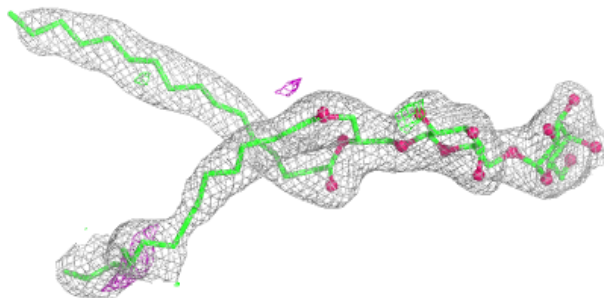
**Electron density around DGD c 517 (A):**

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

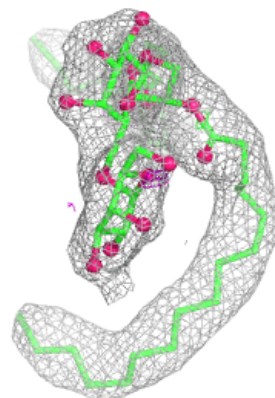
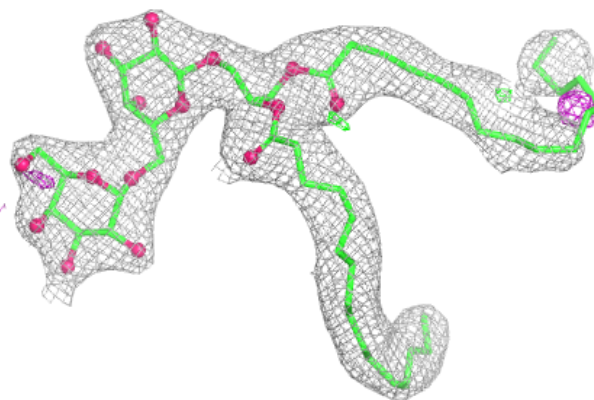


**Electron density around DGD c 517 (B):**

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

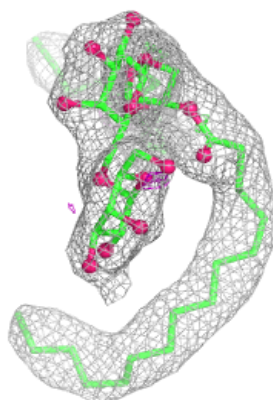
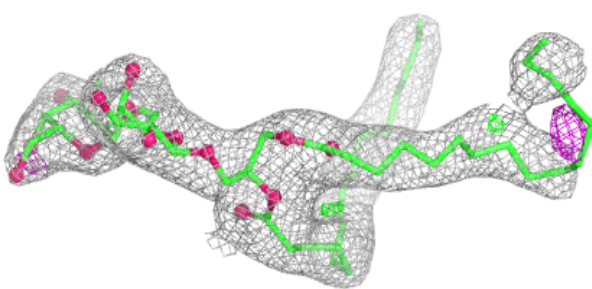
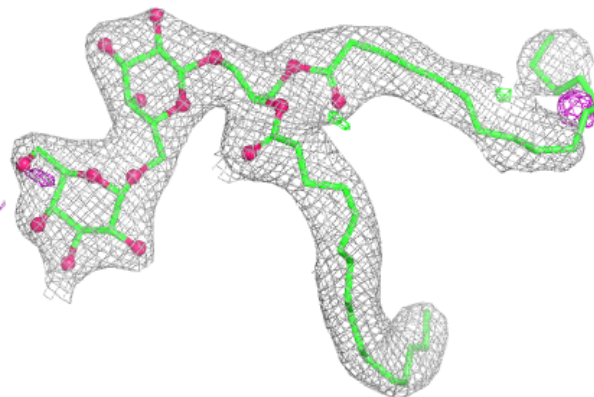
**Electron density around DGD c 518 (A):**

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

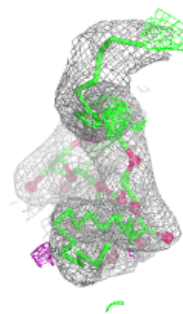
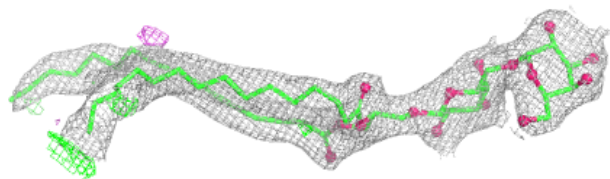
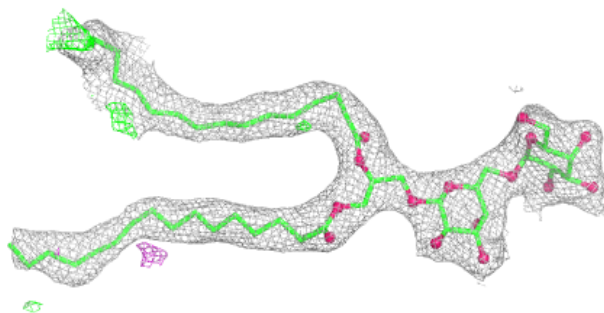


**Electron density around DGD c 518 (B):**

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

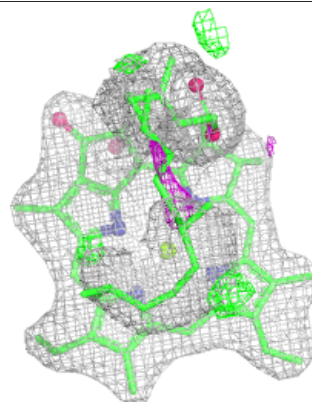
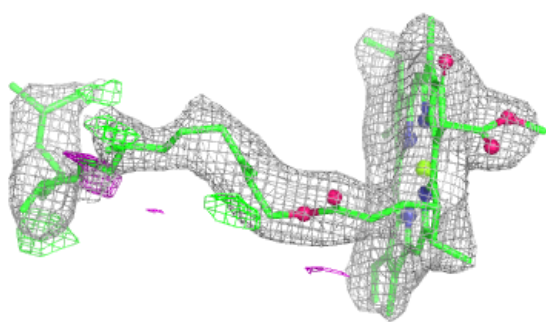
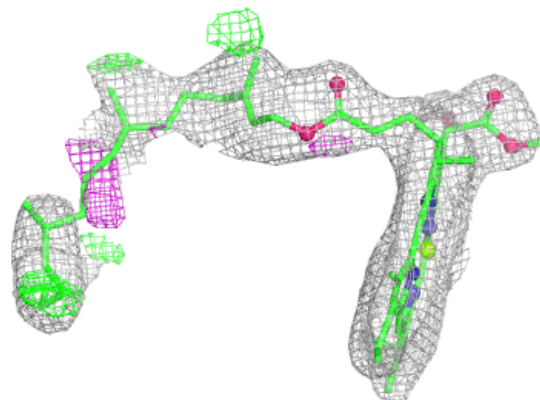
**Electron density around DGD c 519:**

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

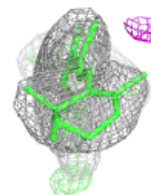
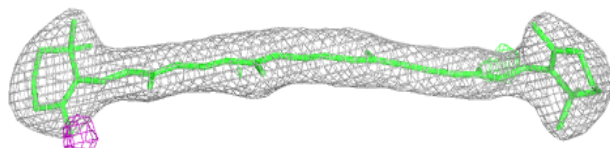
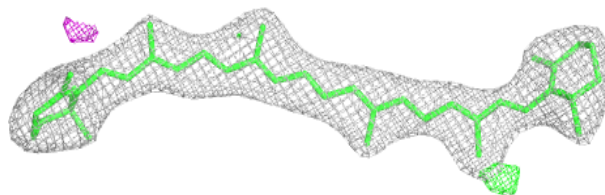


**Electron density around CLA c 507:**

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

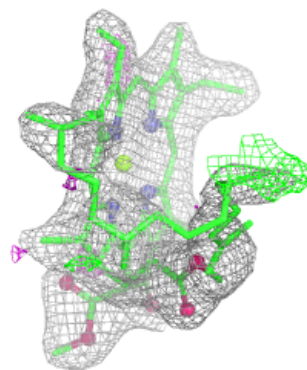
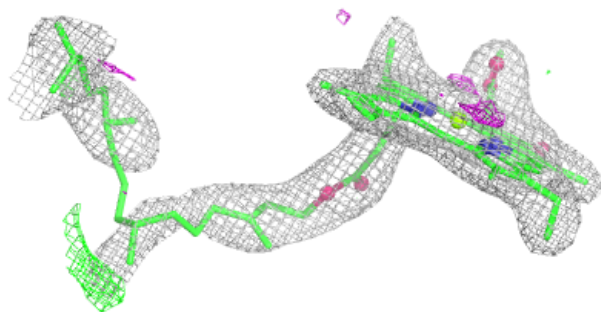
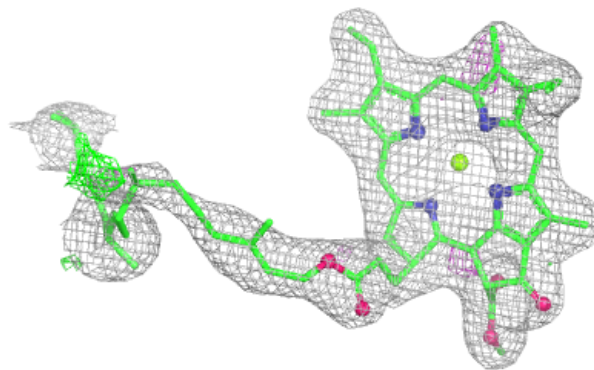
**Electron density around BCR Y 101:**

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

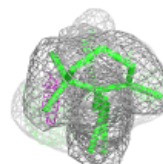
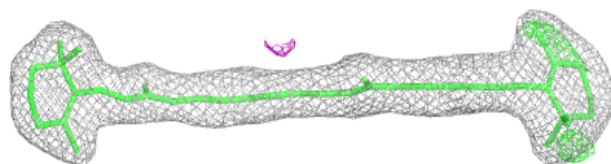
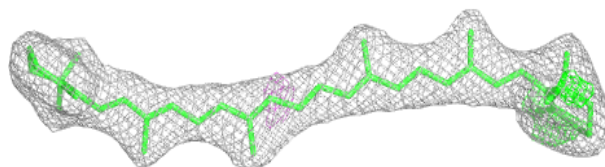


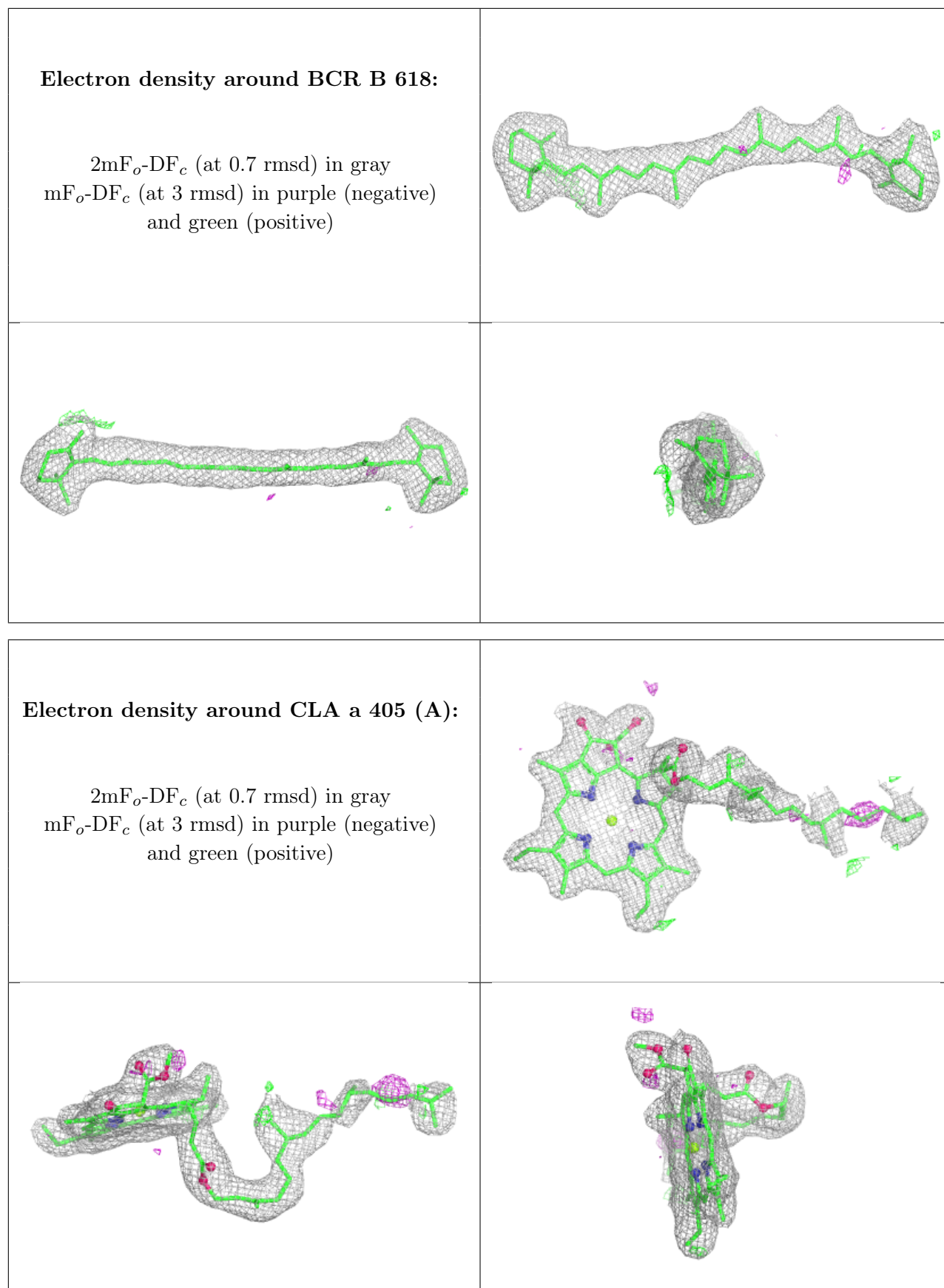
**Electron density around CLA A 407:**

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

**Electron density around BCR A 408:**

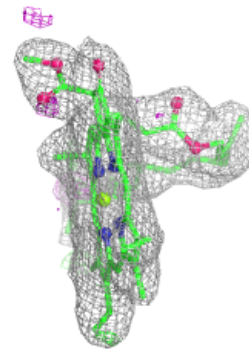
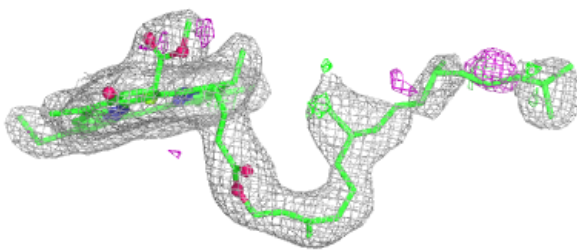
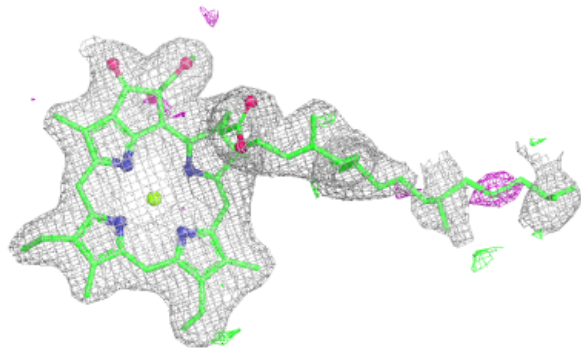
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





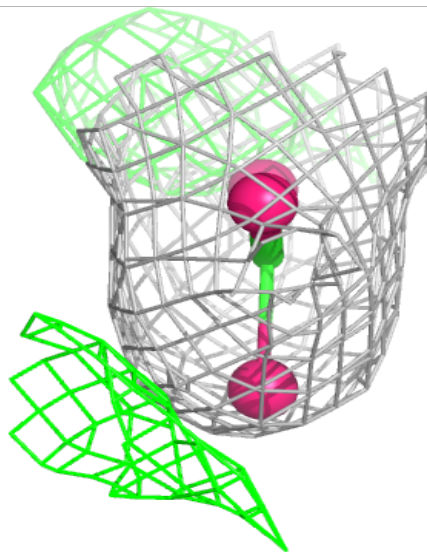
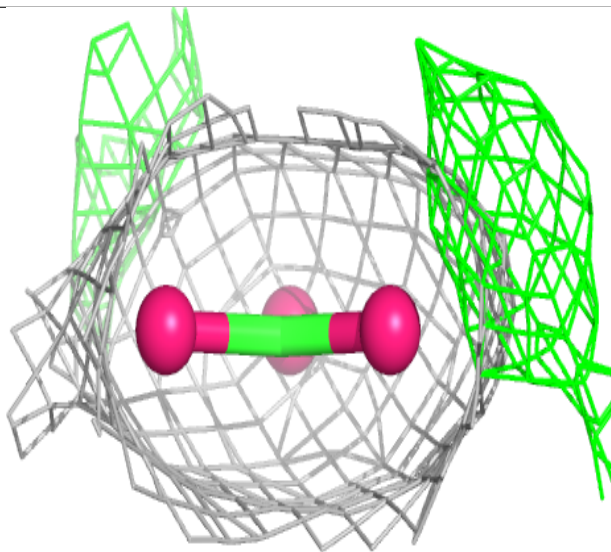
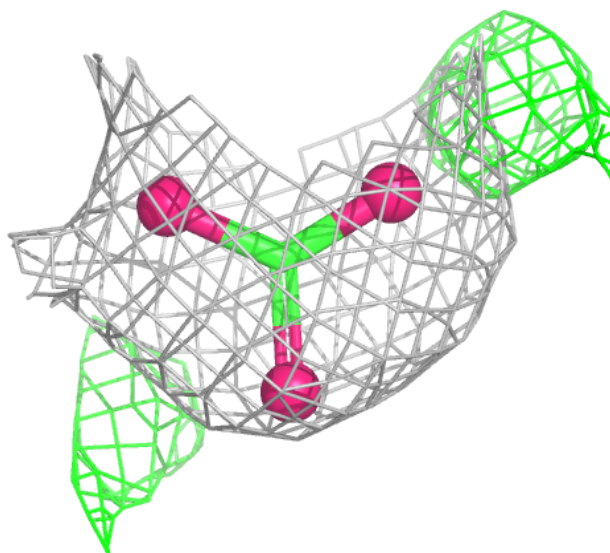
**Electron density around CLA a 405 (B):**

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



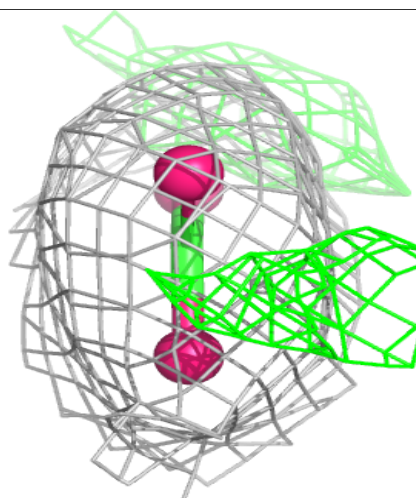
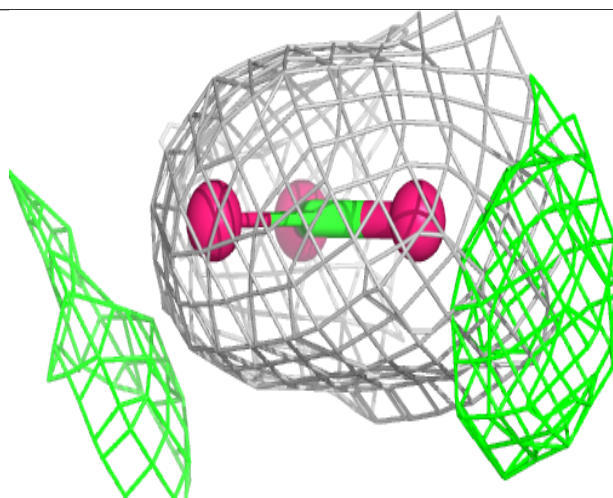
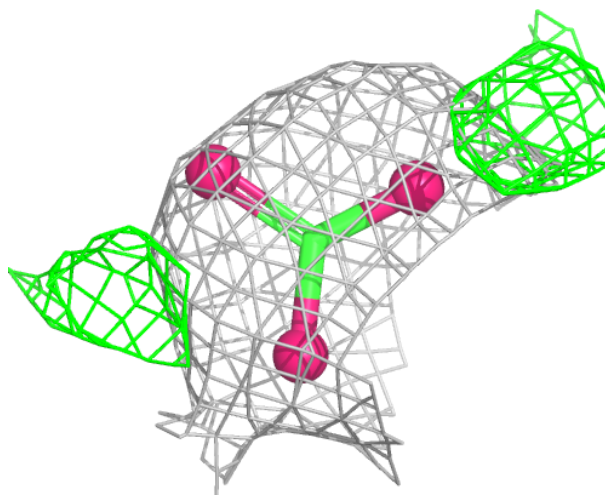
**Electron density around BCT d 401 (A):**

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



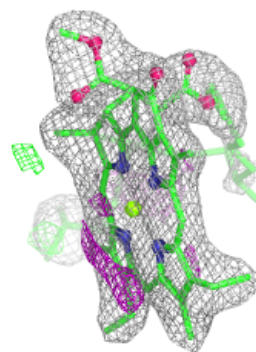
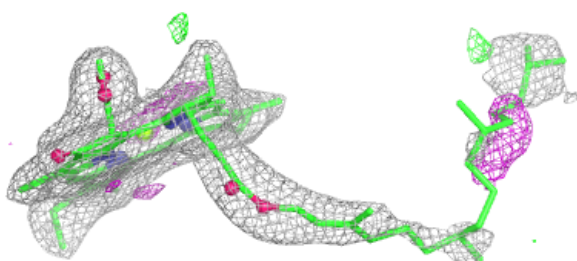
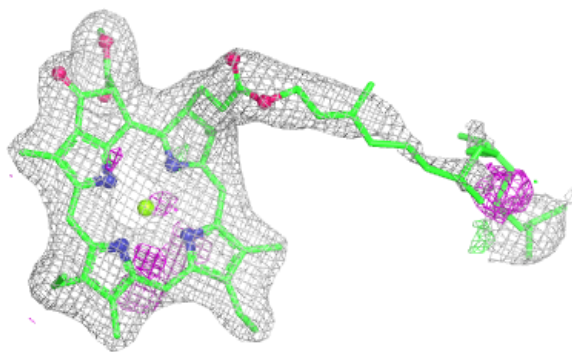
**Electron density around BCT d 401 (B):**

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

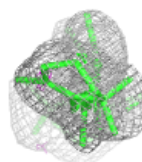
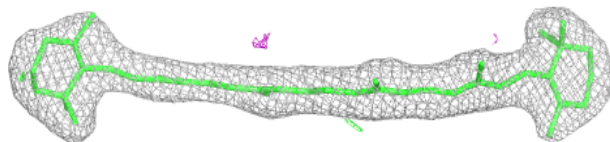
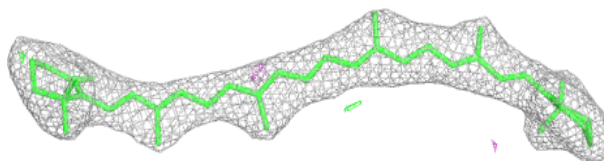


**Electron density around CLA a 407:**

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

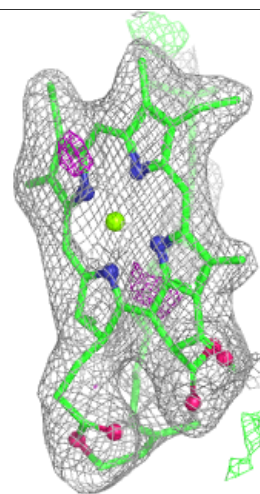
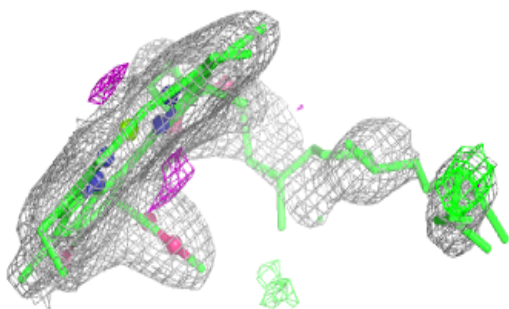
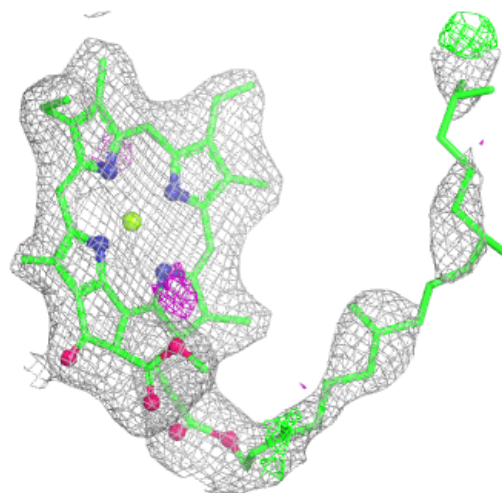
**Electron density around BCR H 101:**

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



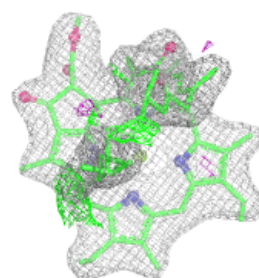
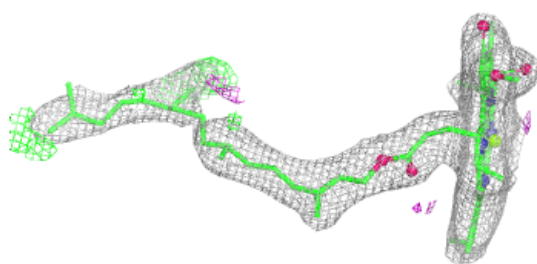
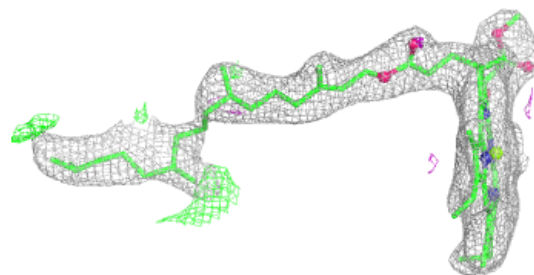
**Electron density around CLA B 616:**

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

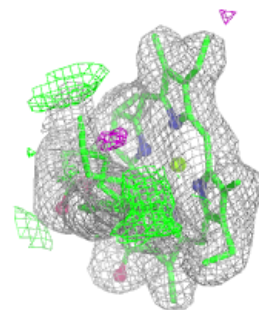
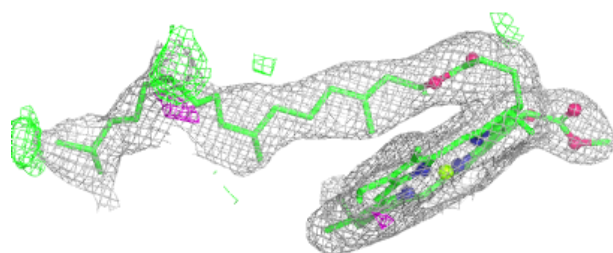
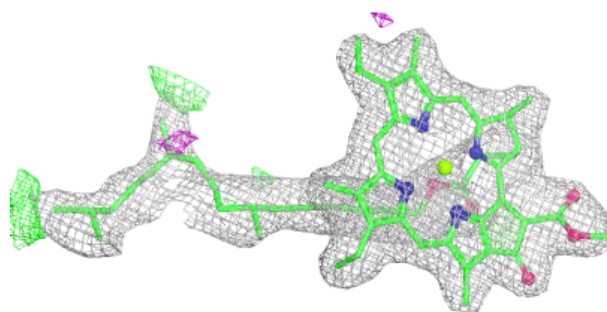


**Electron density around CLA b 606:**

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

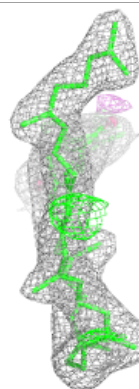
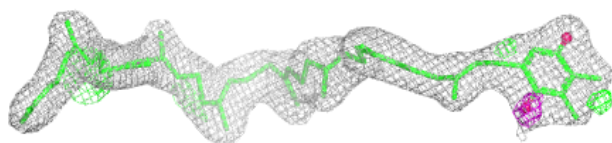
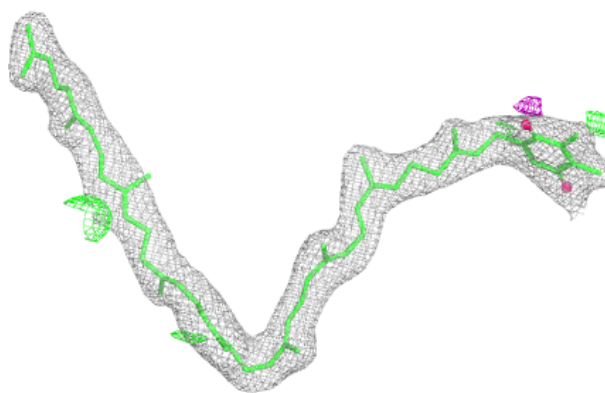
**Electron density around CLA b 614:**

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

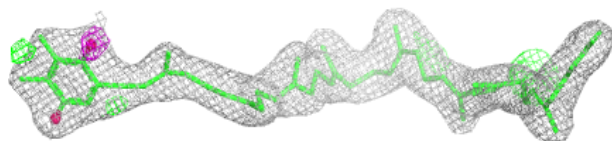
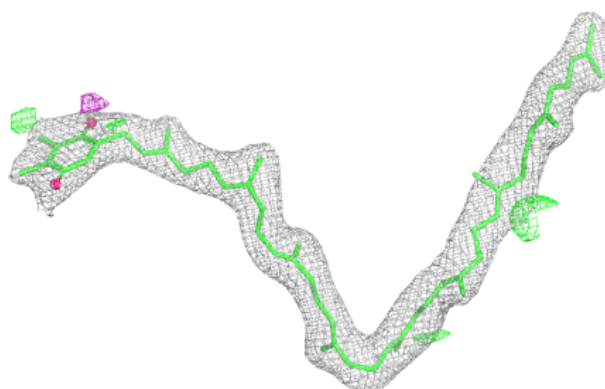


**Electron density around PL9 D 406 (A):**

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

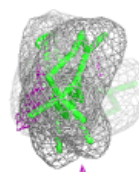
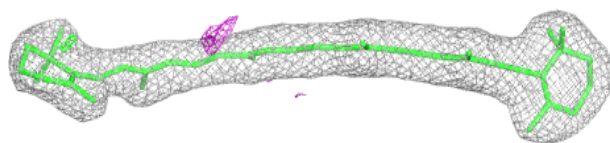
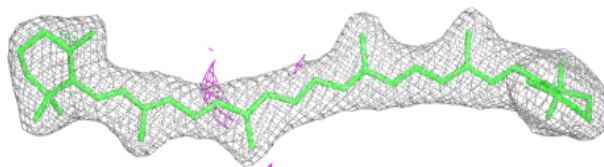
**Electron density around PL9 D 406 (B):**

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

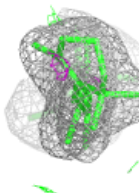
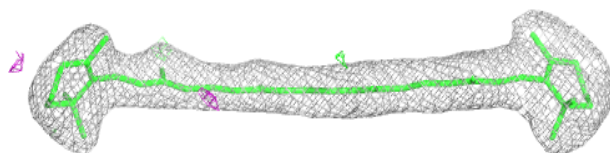
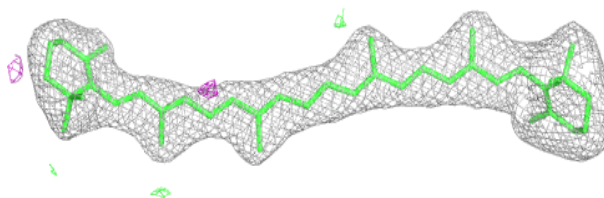


**Electron density around BCR b 617:**

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

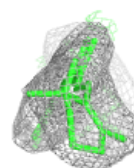
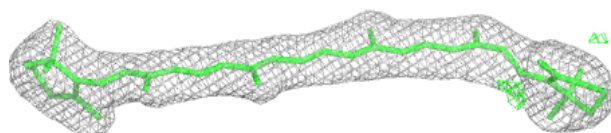
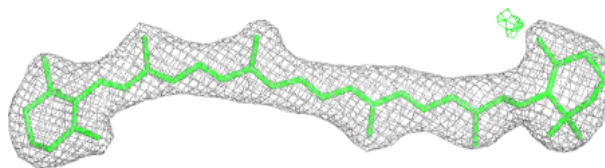
**Electron density around BCR b 618:**

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

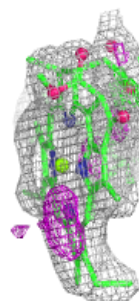
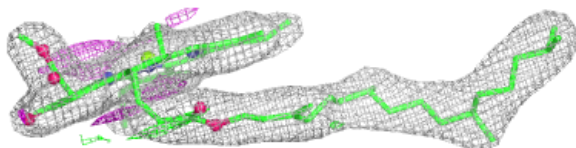
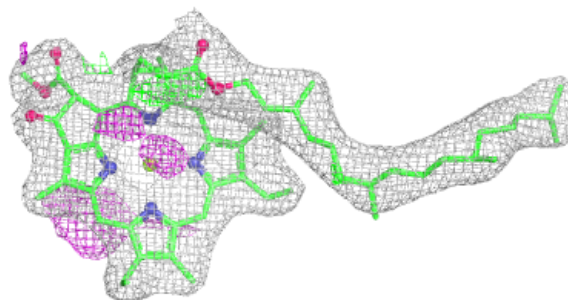


**Electron density around BCR b 619:**

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

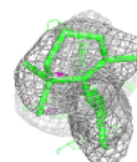
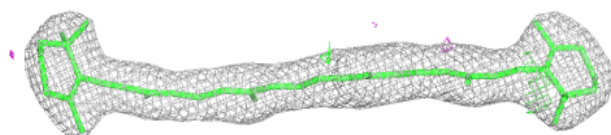
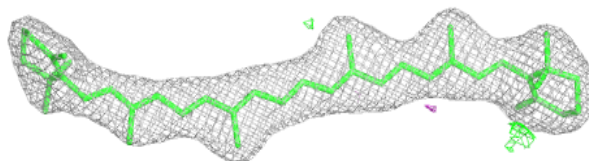
**Electron density around CLA B 603:**

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

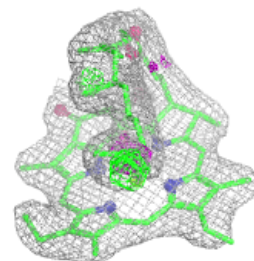
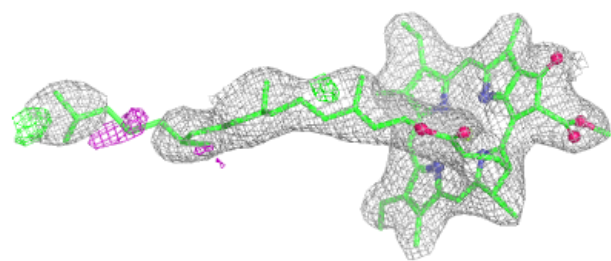
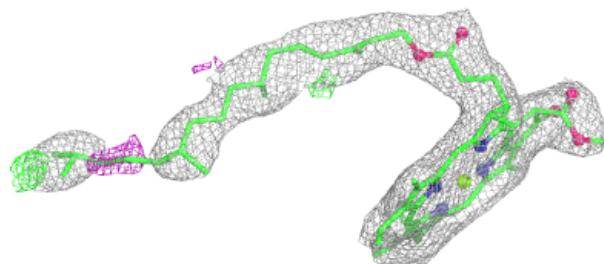


**Electron density around BCR c 516:**

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

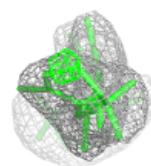
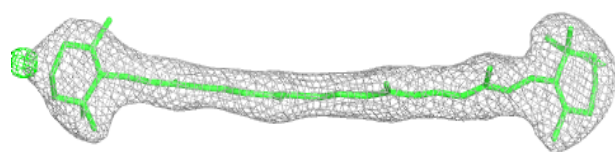
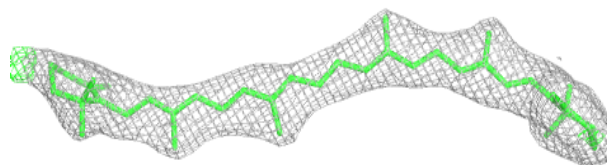
**Electron density around CLA c 505:**

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

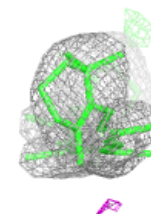
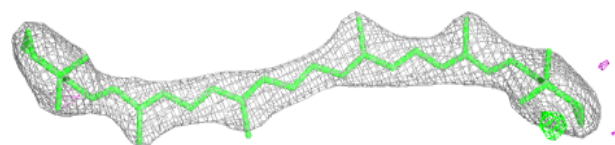
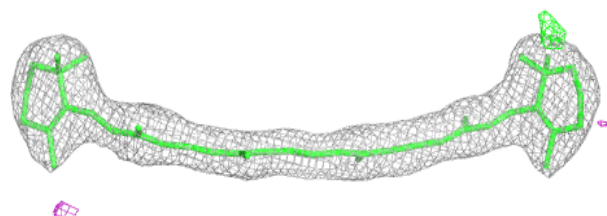


**Electron density around BCR h 101:**

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

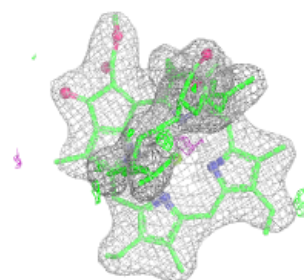
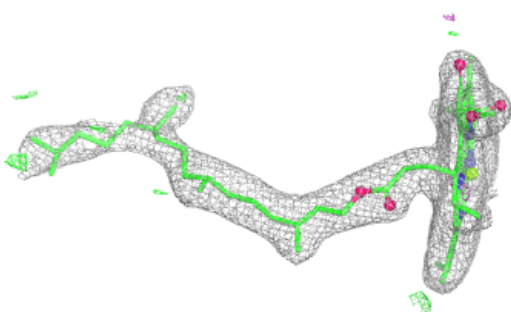
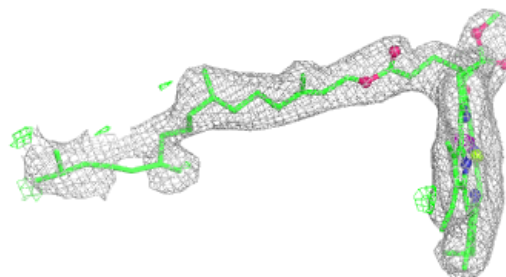
**Electron density around BCR k 101:**

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

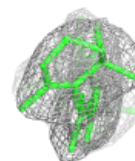
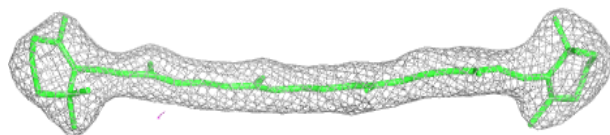
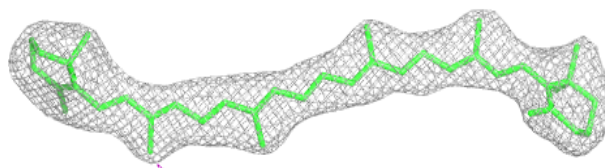


**Electron density around CLA B 606:**

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

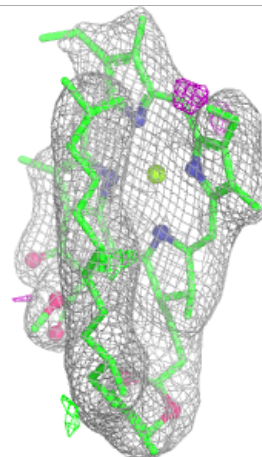
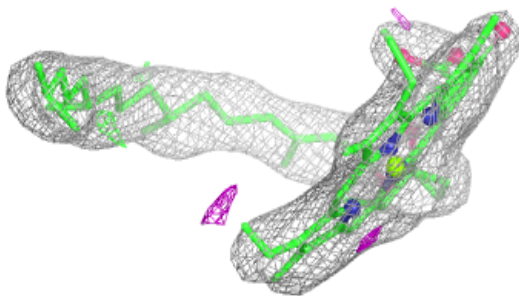
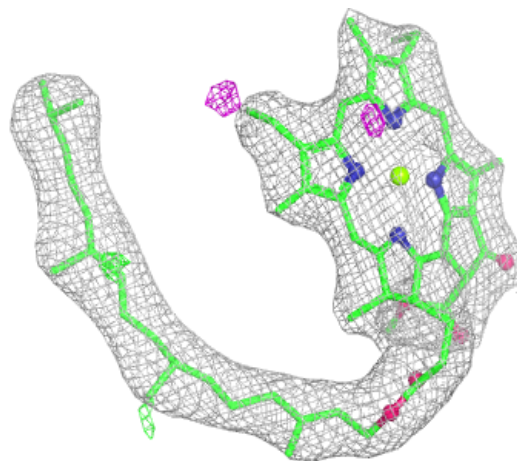
**Electron density around BCR y 101:**

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



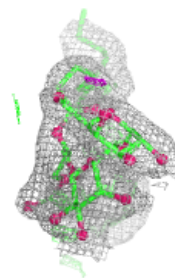
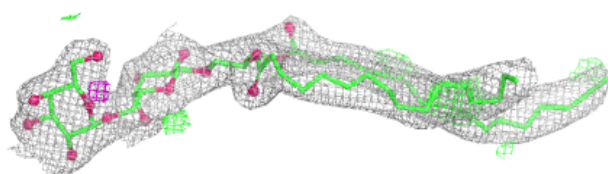
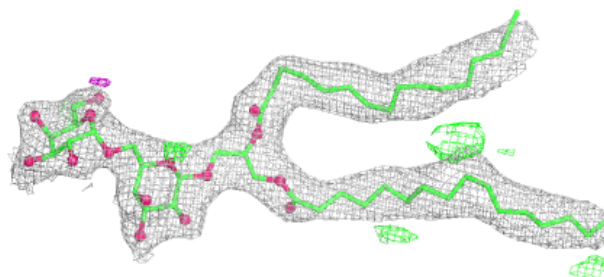
**Electron density around CLA c 508:**

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

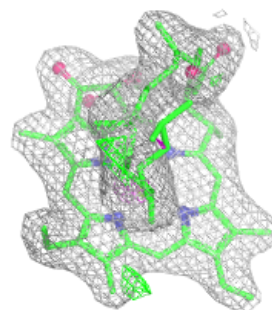
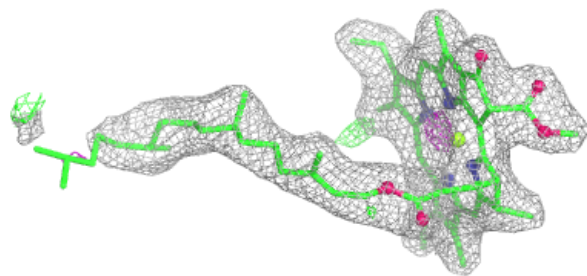
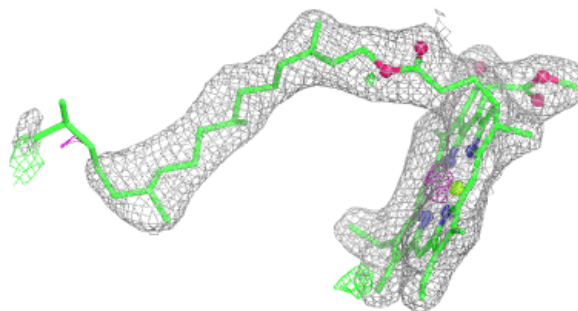


**Electron density around DGD C 519:**

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

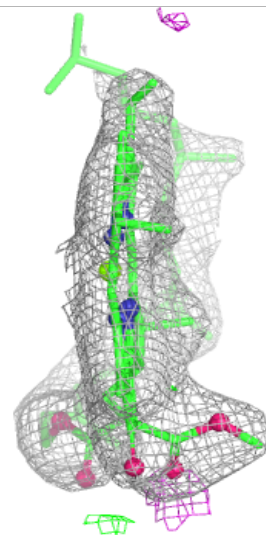
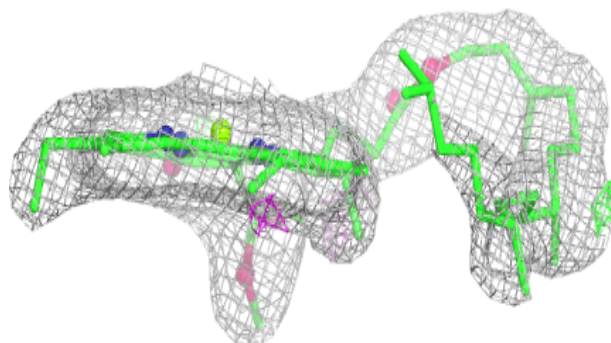
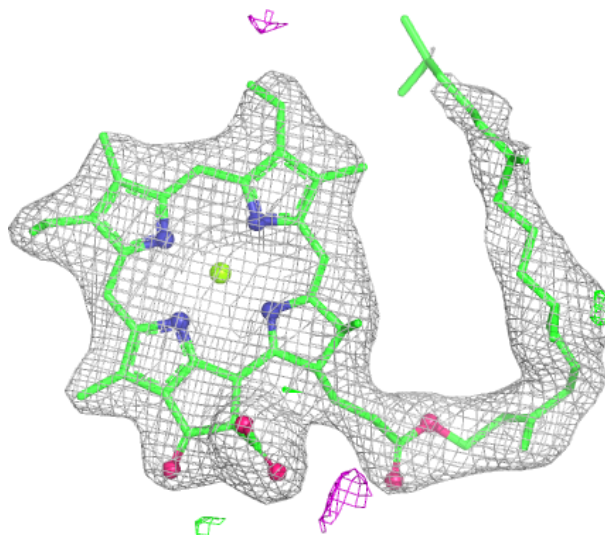
**Electron density around CLA C 509:**

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



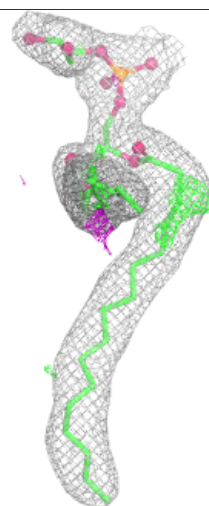
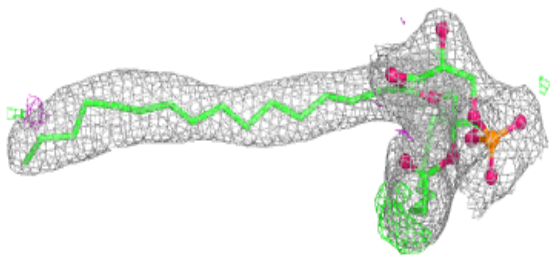
**Electron density around CLA C 513:**

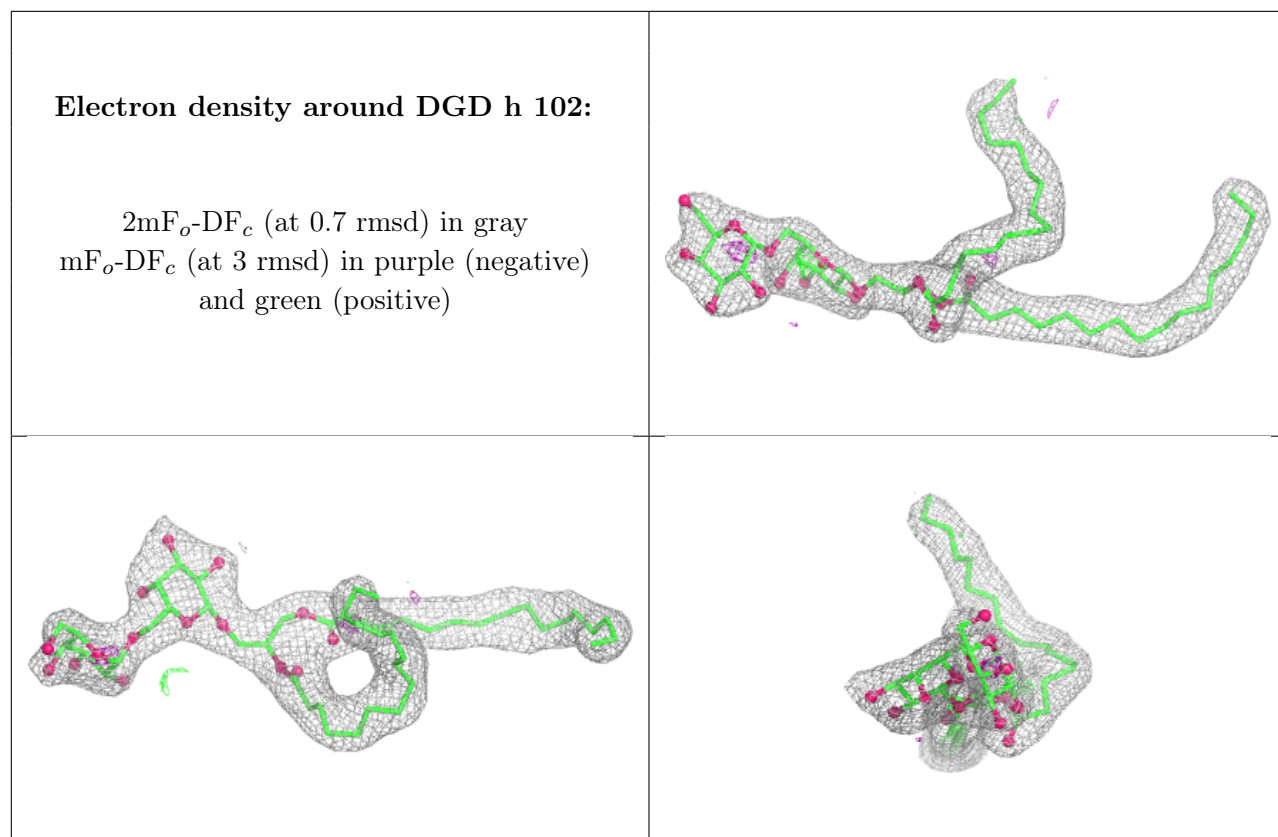
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around LHG b 629 (A):**

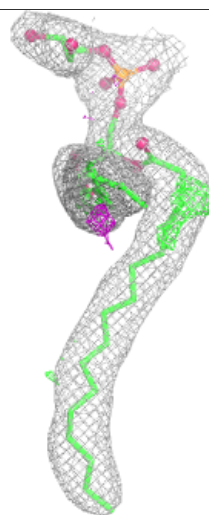
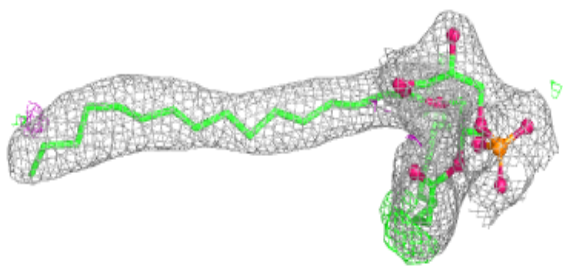
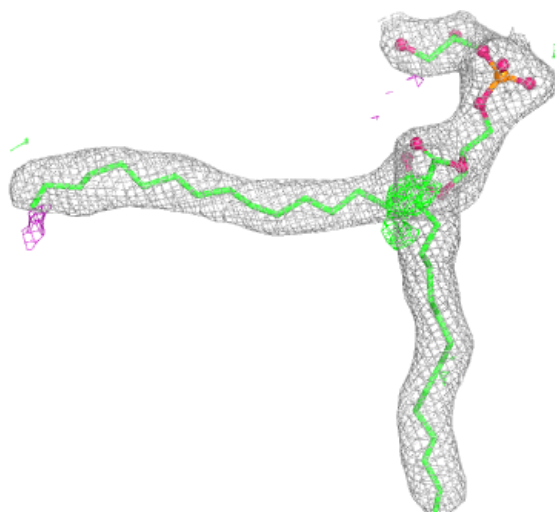
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





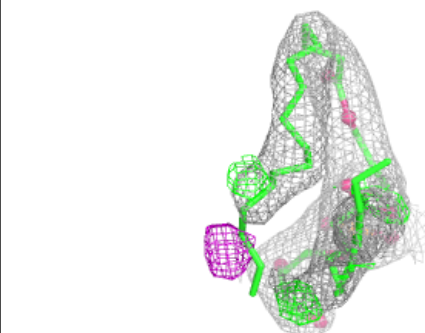
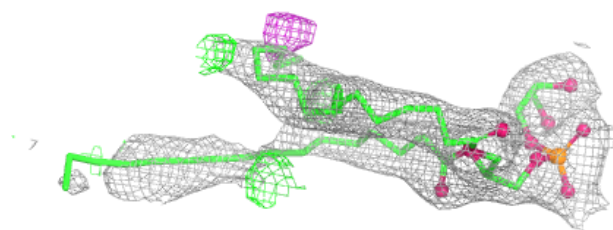
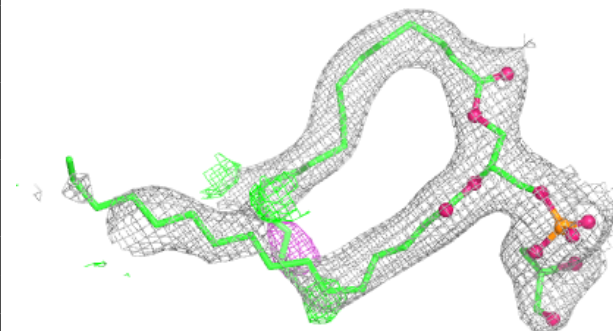
**Electron density around LHG b 629 (B):**

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

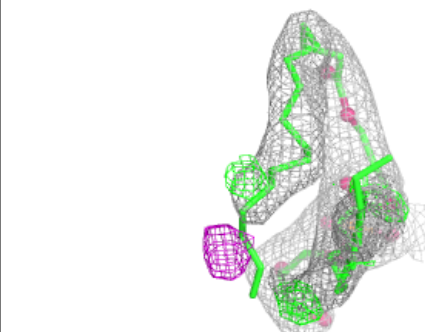
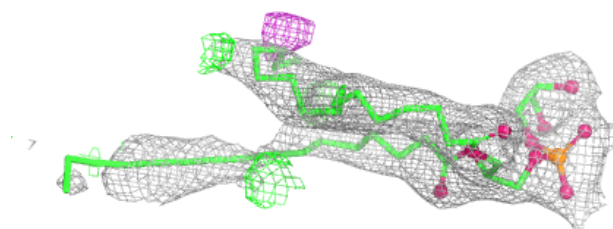
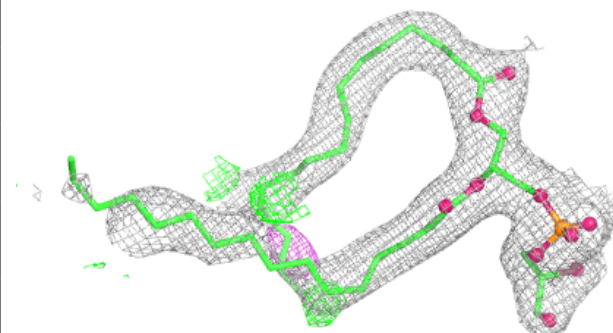


**Electron density around LHG d 408 (A):**

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

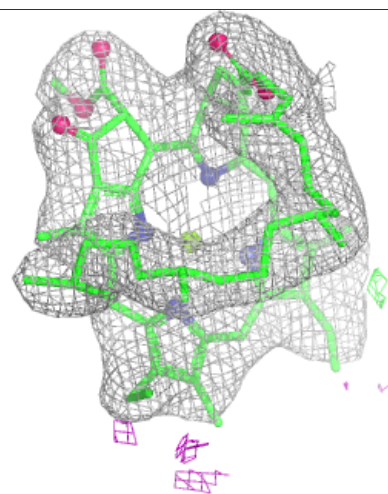
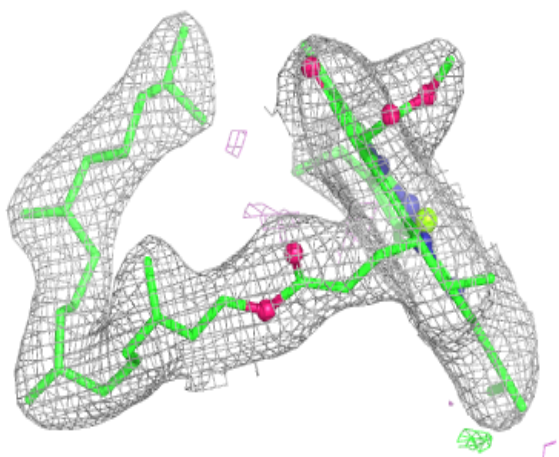
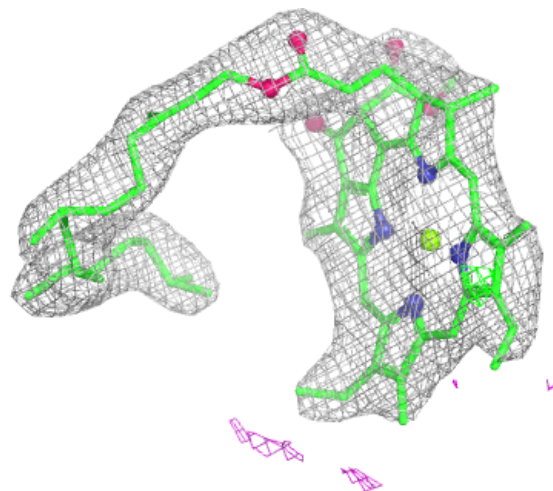
**Electron density around LHG d 408 (B):**

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



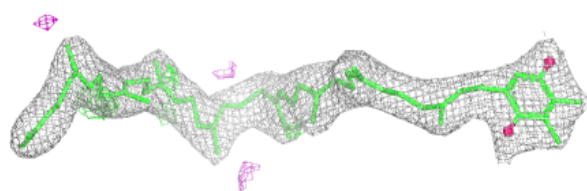
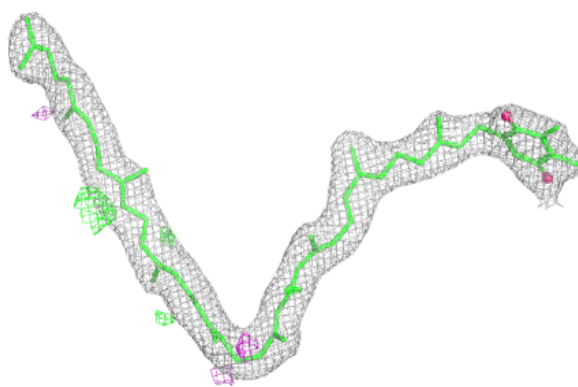
**Electron density around CLA c 504:**

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

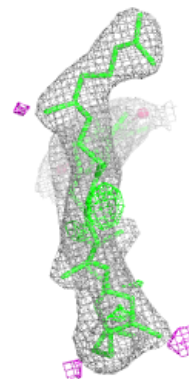
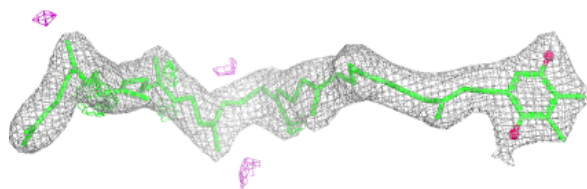
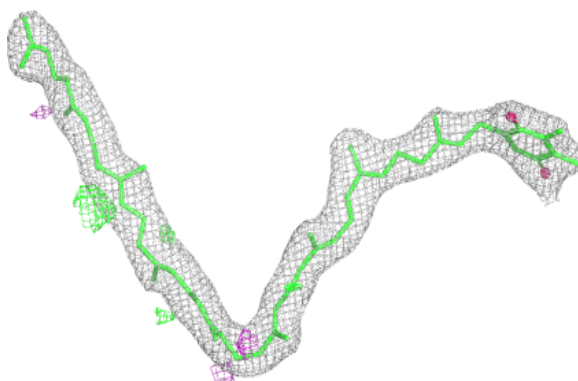


**Electron density around PL9 d 406 (A):**

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

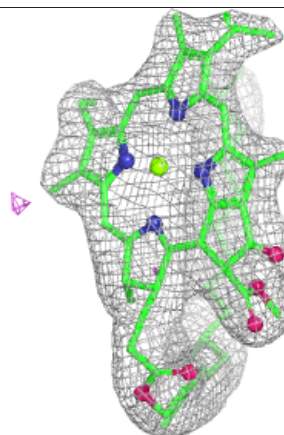
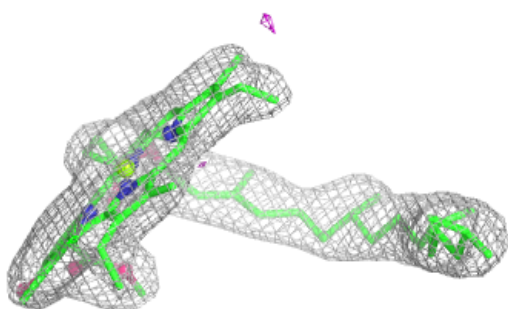
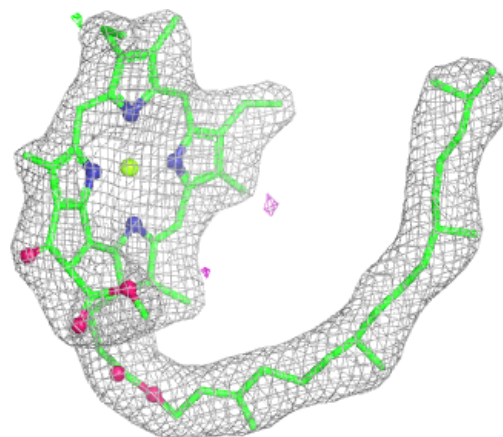
**Electron density around PL9 d 406 (B):**

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



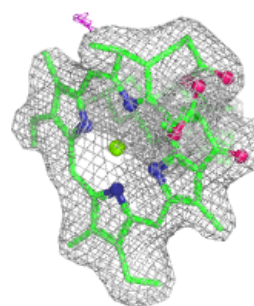
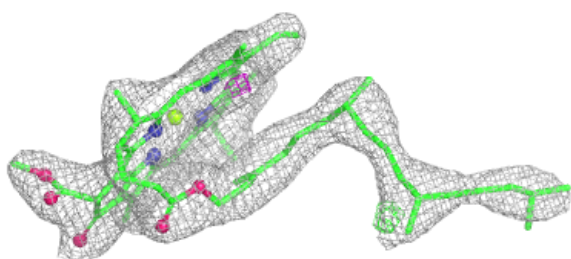
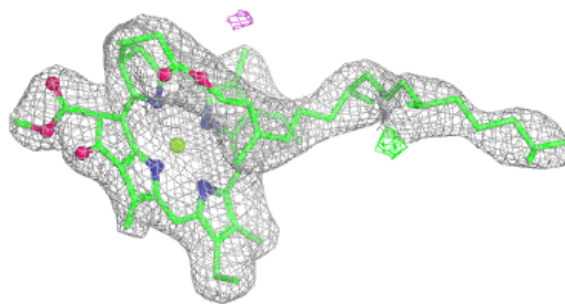
**Electron density around CLA C 508:**

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

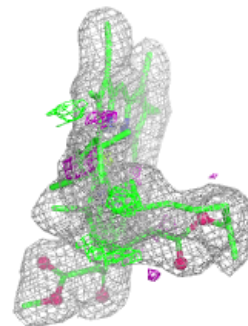
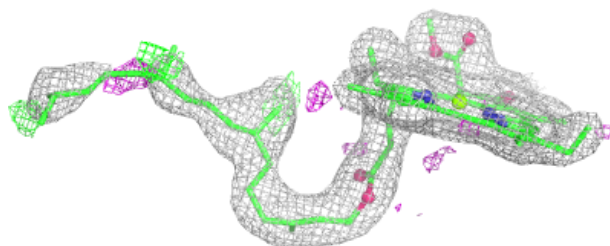
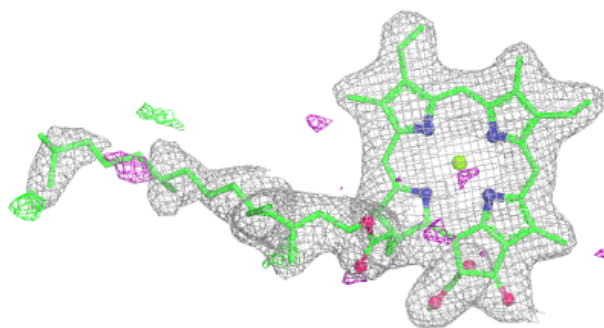


**Electron density around CLA c 506:**

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

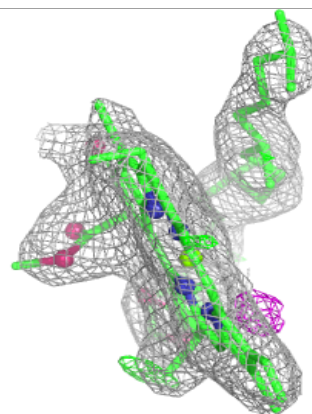
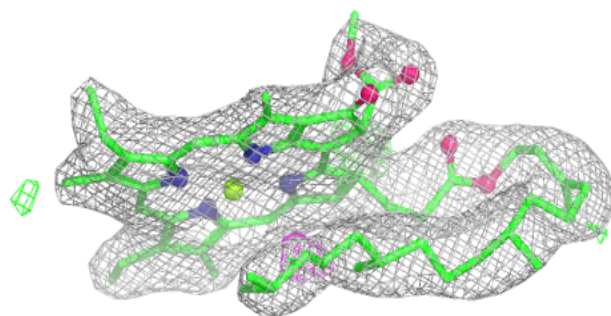
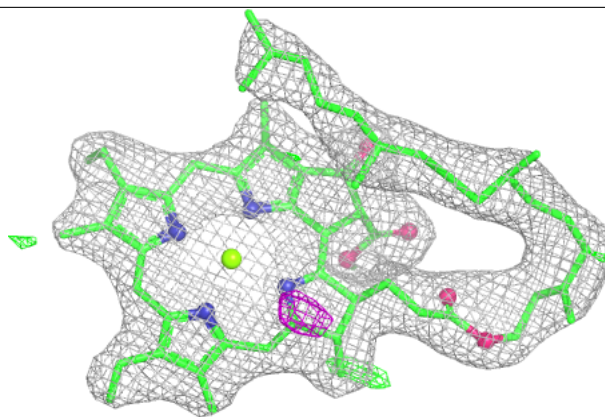
**Electron density around CLA A 406 (B):**

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

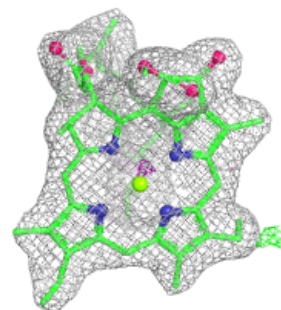
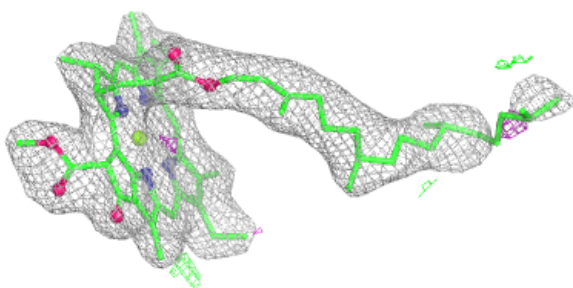
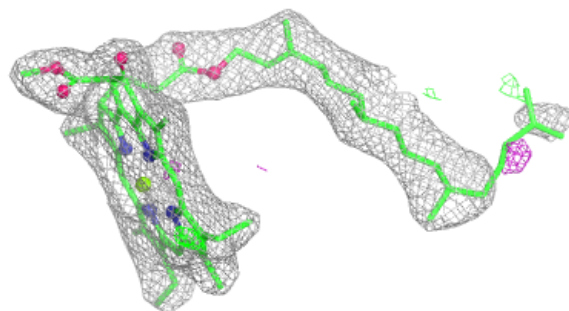


**Electron density around CLA C 510:**

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

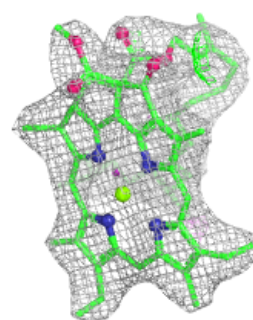
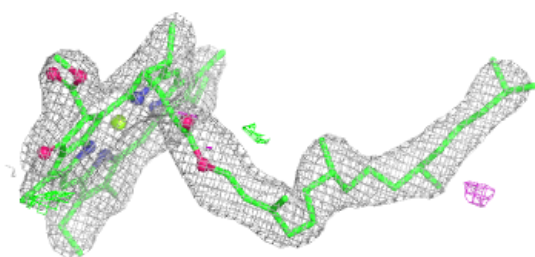
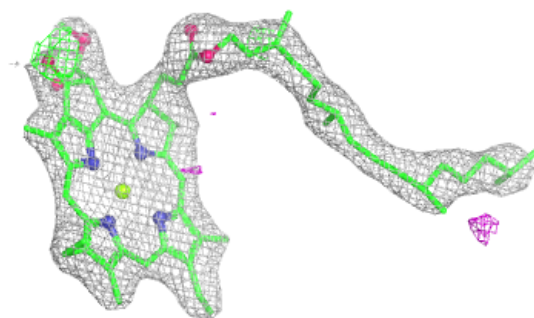
**Electron density around CLA c 509:**

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

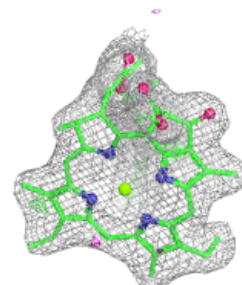
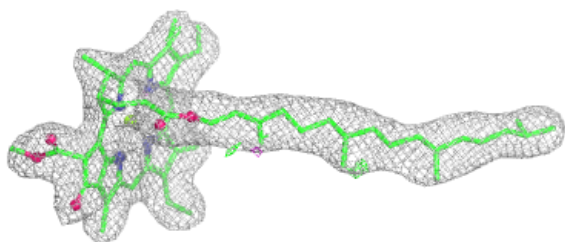
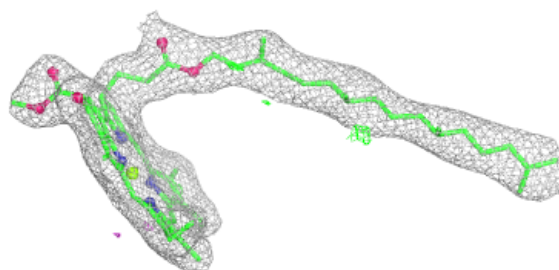


**Electron density around CLA c 512:**

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

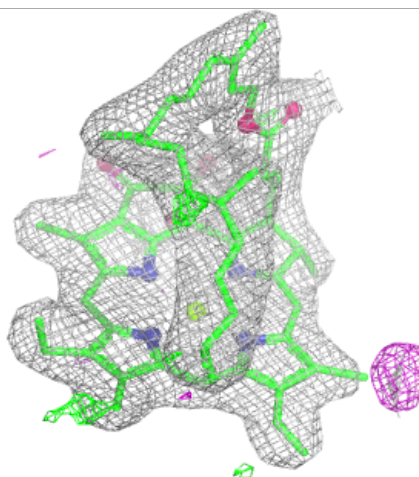
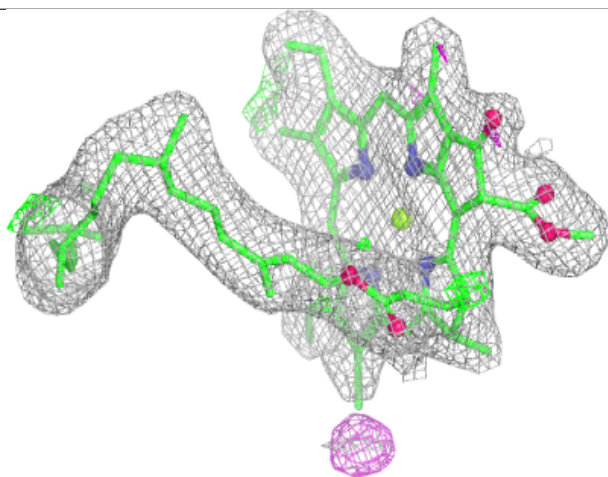
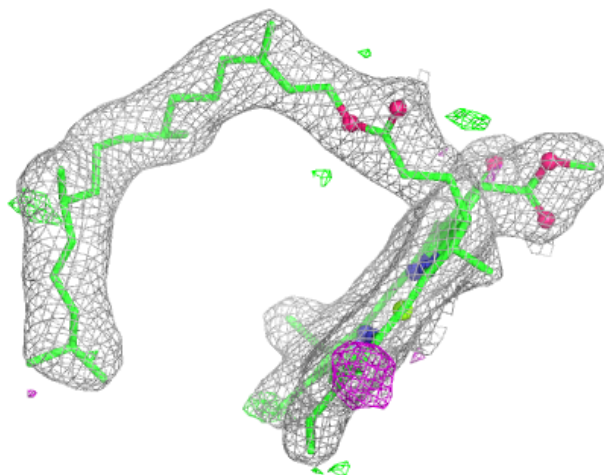
**Electron density around CLA B 607:**

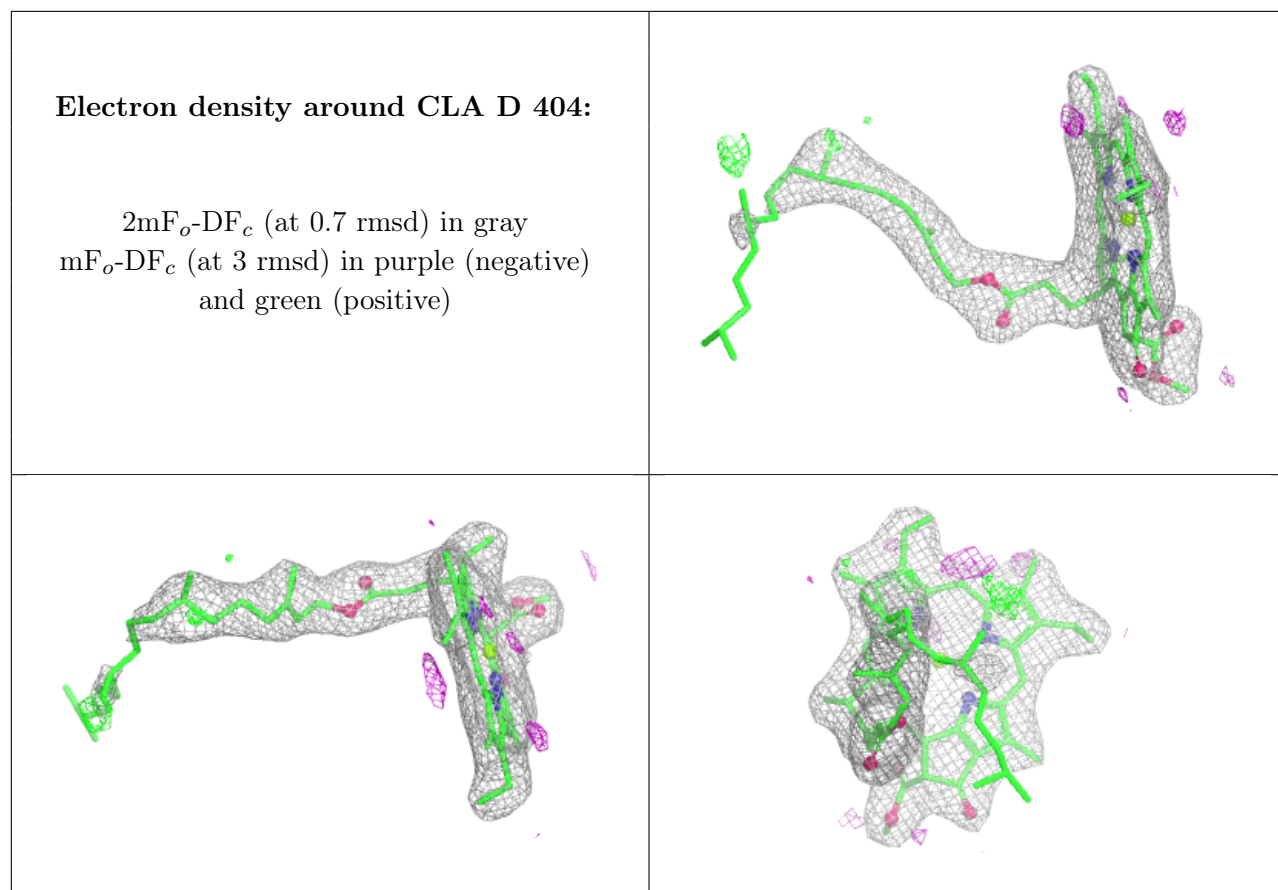
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 611:**

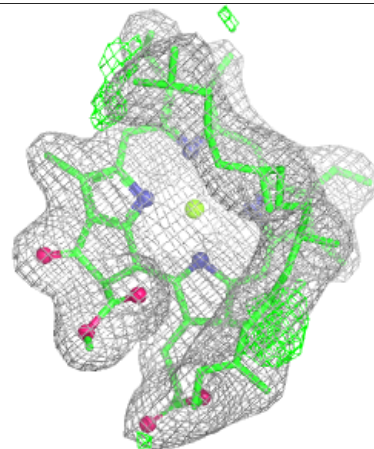
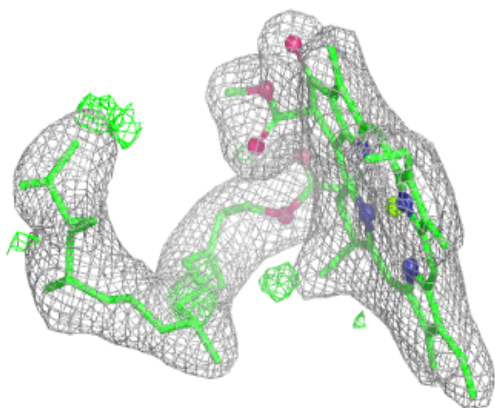
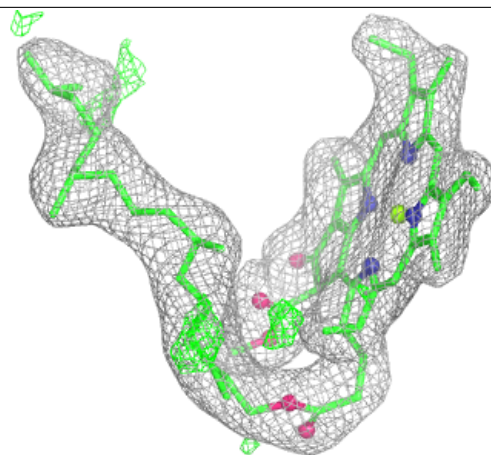
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





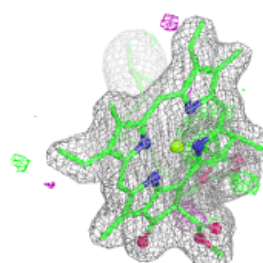
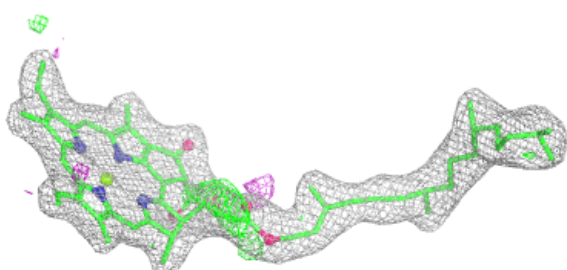
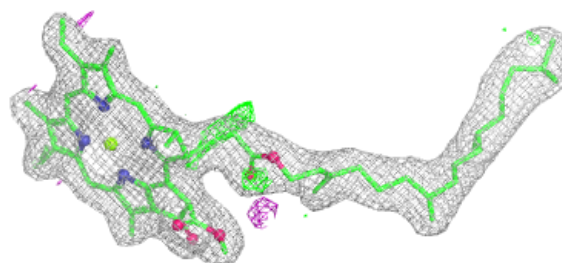
**Electron density around CLA B 613:**

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

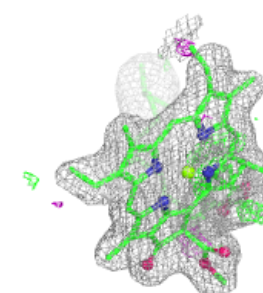
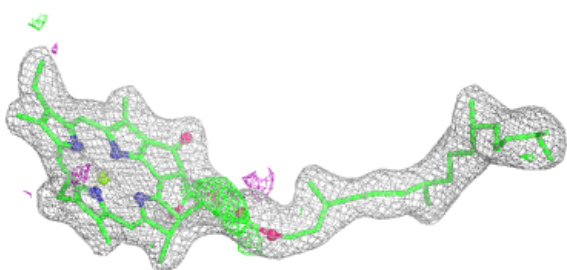
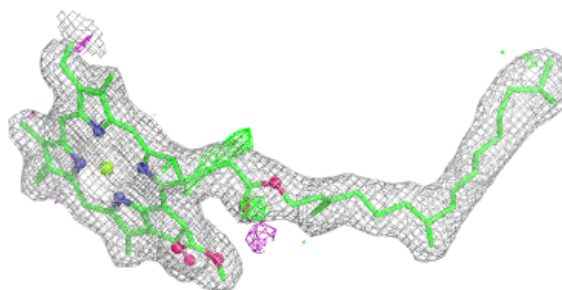


**Electron density around CLA A 404 (A):**

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

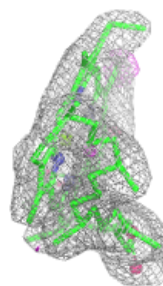
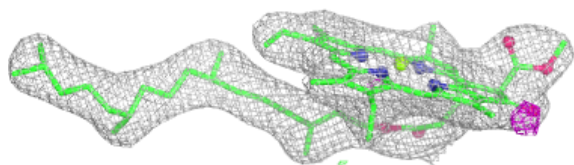
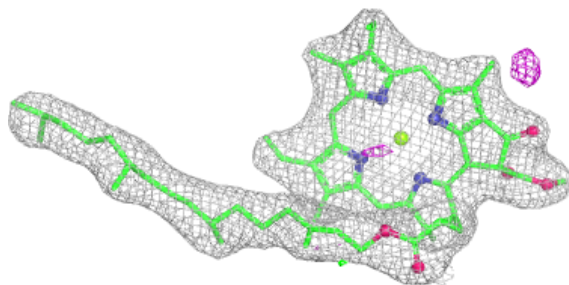
**Electron density around CLA A 404 (B):**

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

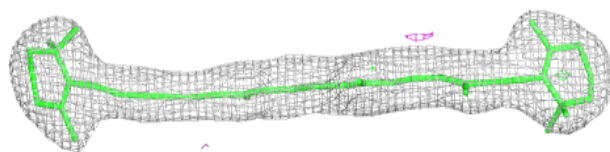
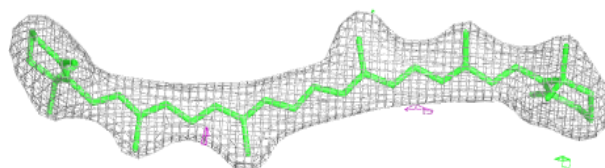


**Electron density around CLA C 502:**

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

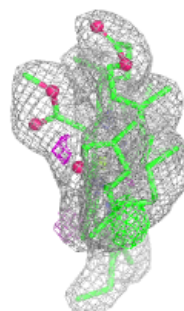
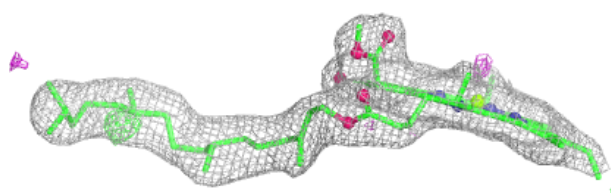
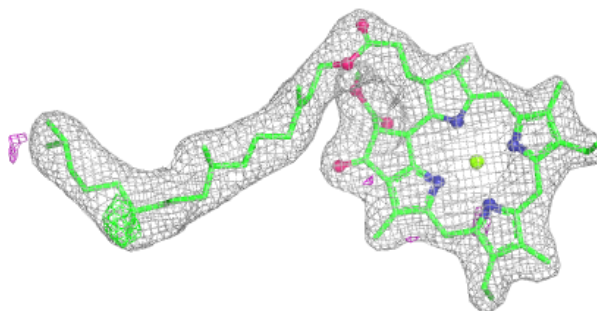
**Electron density around BCR C 516:**

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

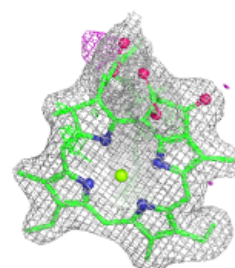
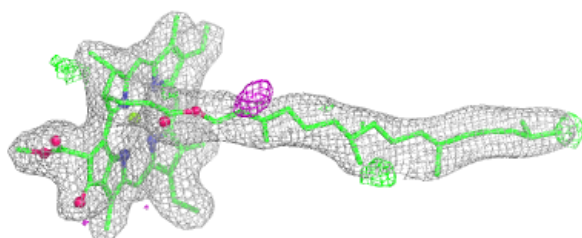
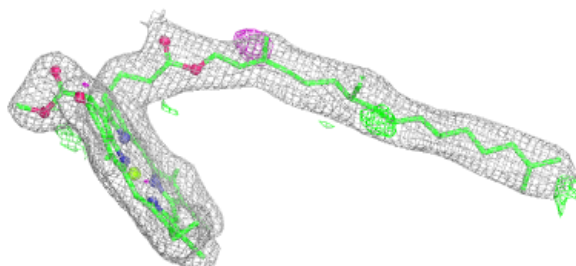


**Electron density around CLA B 602:**

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

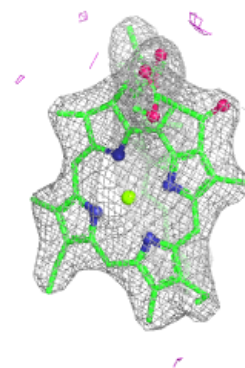
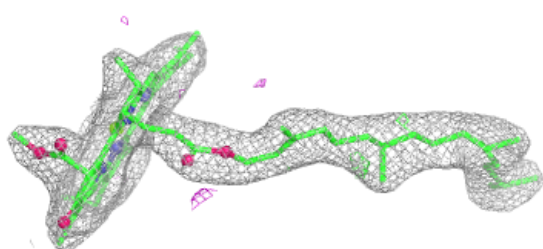
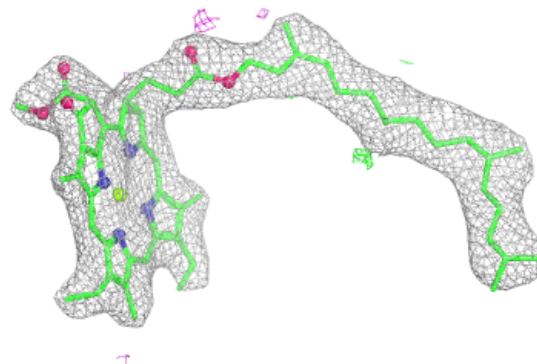
**Electron density around CLA b 607:**

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

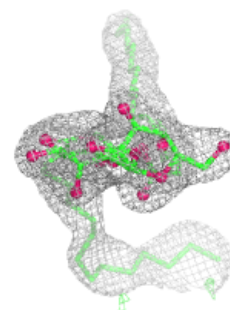
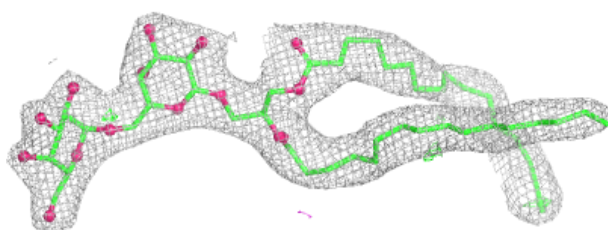
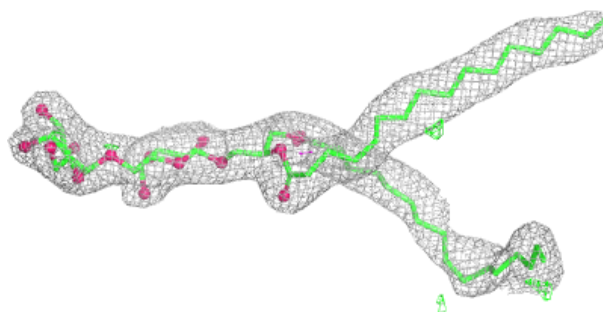


**Electron density around CLA b 609:**

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

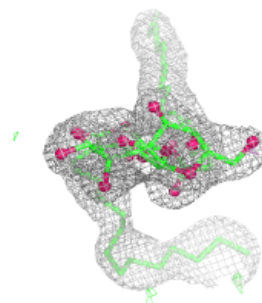
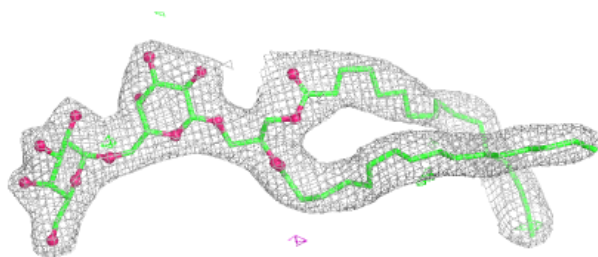
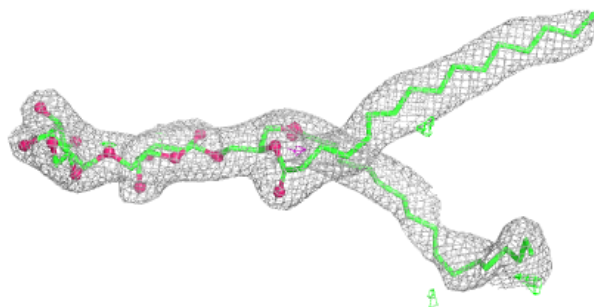
**Electron density around DGD C 517 (A):**

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

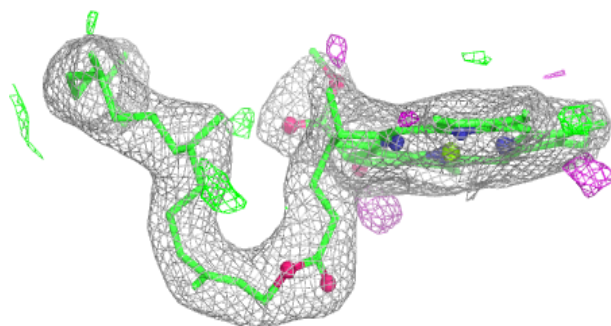
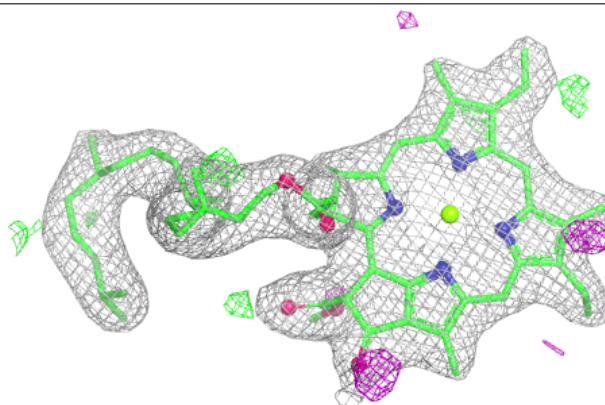


**Electron density around DGD C 517 (B):**

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

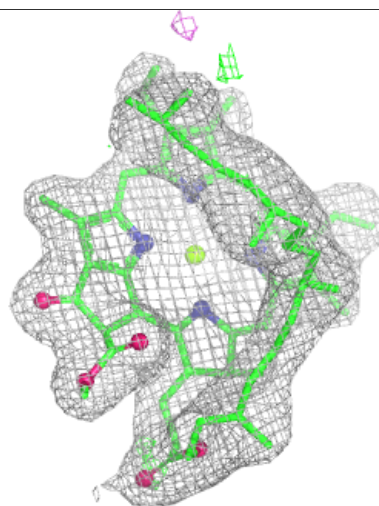
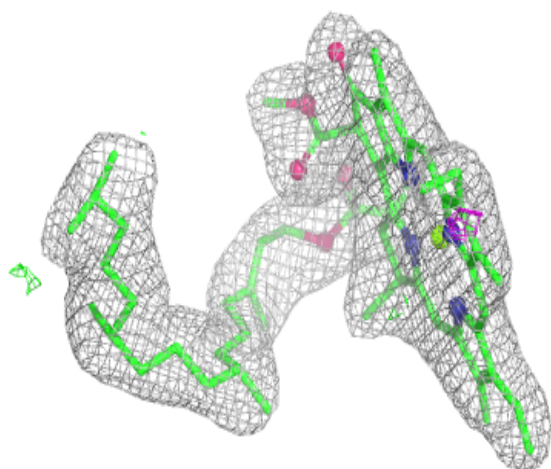
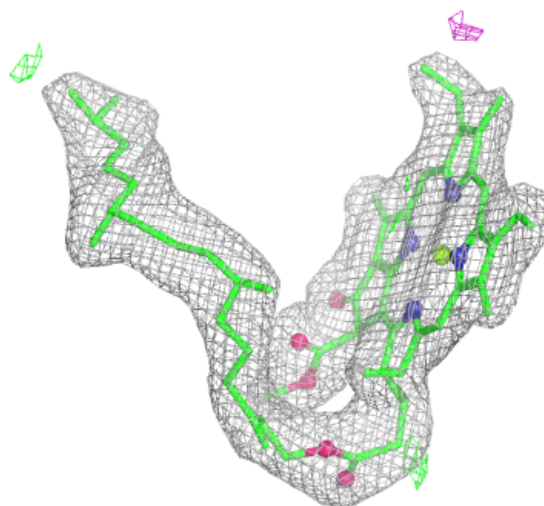
**Electron density around CLA b 612:**

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



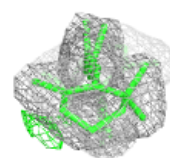
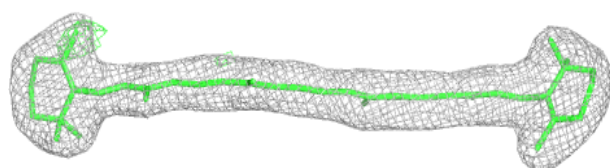
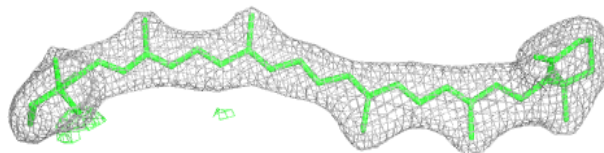
**Electron density around CLA b 613:**

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

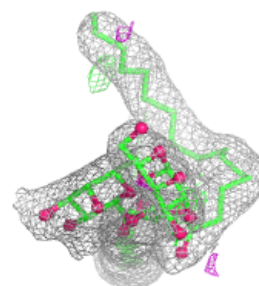
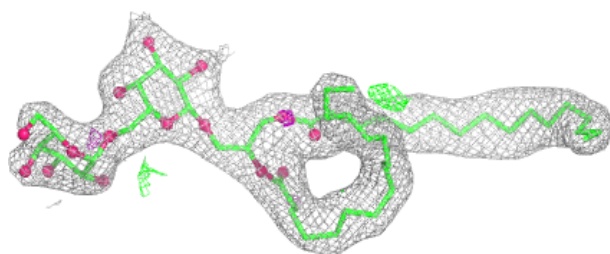
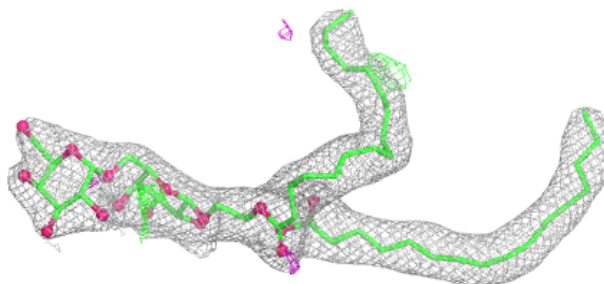


**Electron density around BCR a 408:**

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

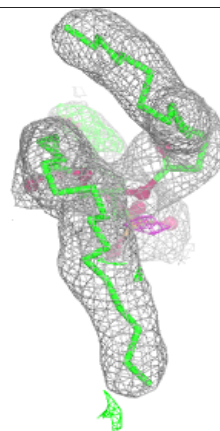
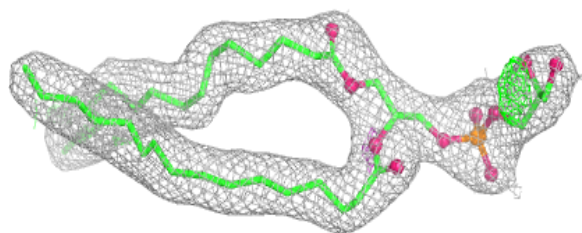
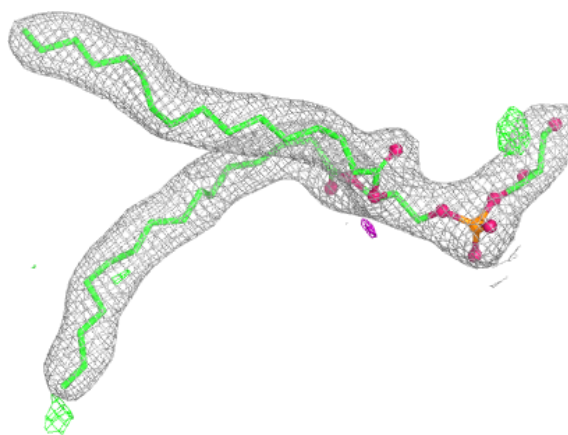
**Electron density around DGD H 102:**

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



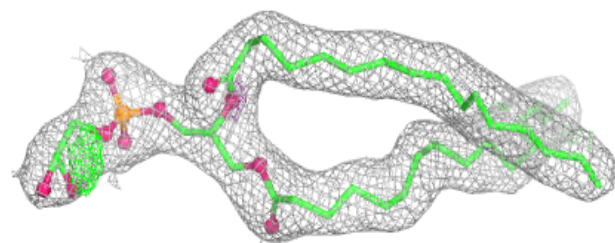
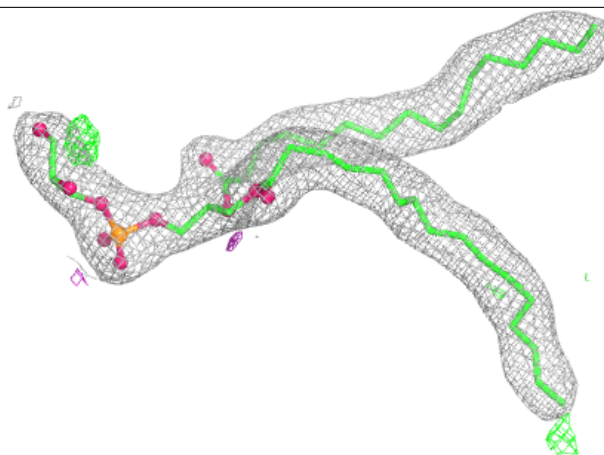
**Electron density around LHG d 407 (A):**

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



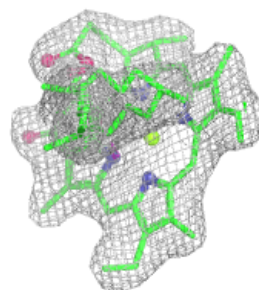
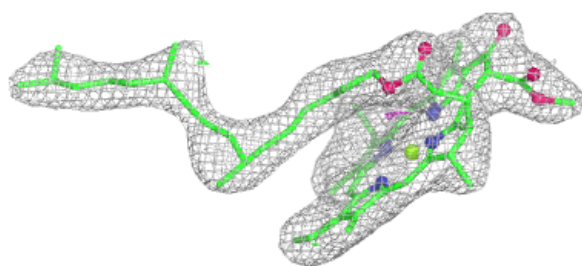
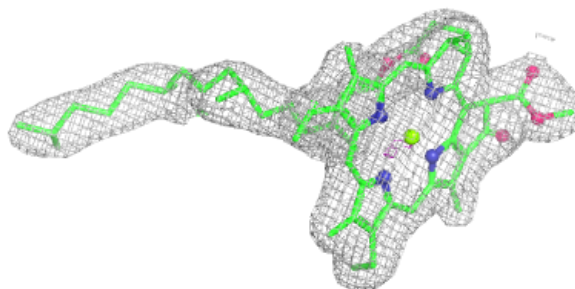
**Electron density around LHG d 407 (B):**

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

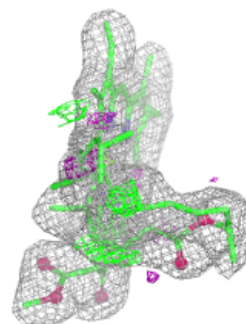
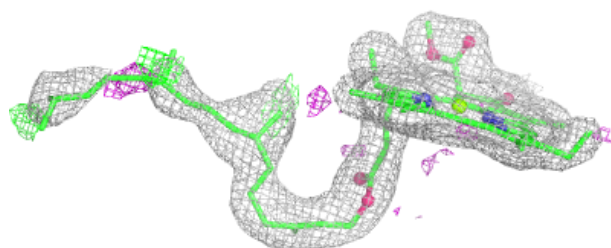
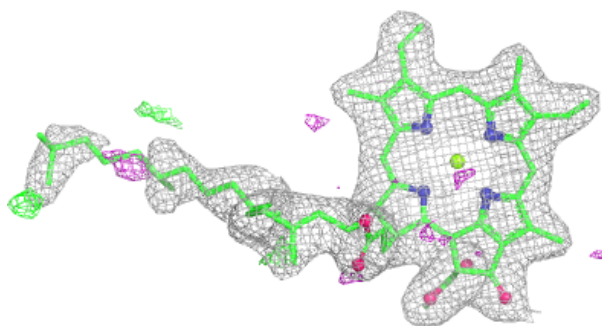


**Electron density around CLA C 506:**

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

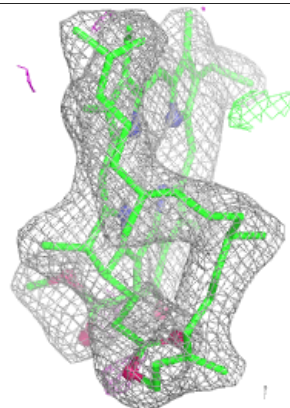
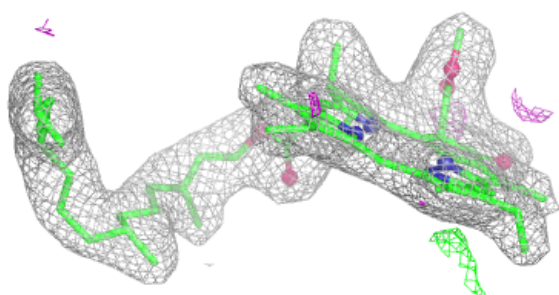
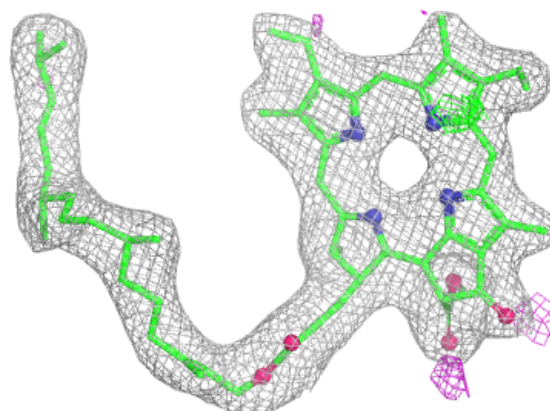
**Electron density around CLA A 406 (A):**

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

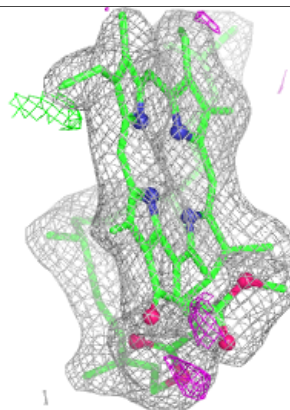
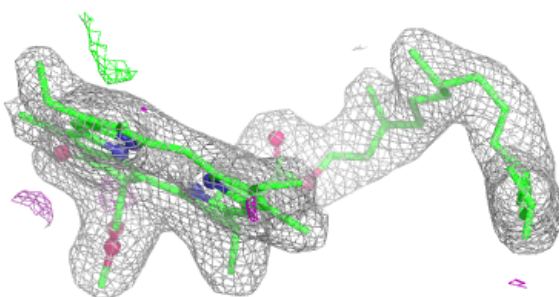
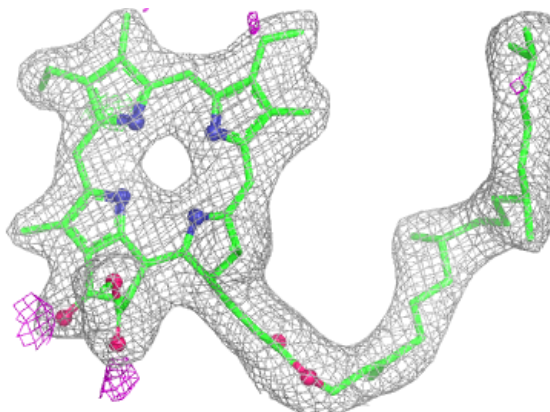


**Electron density around PHO A 416 (A):**

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

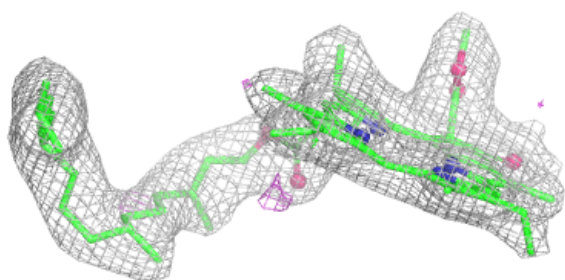
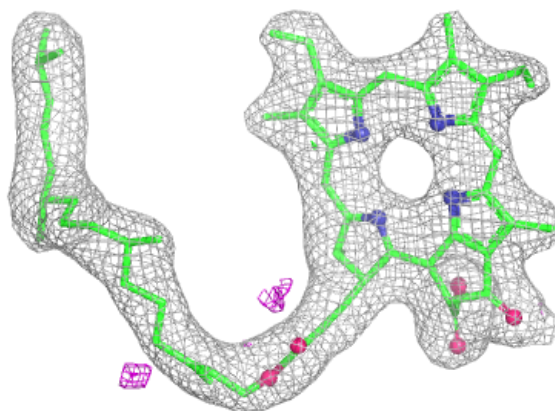
**Electron density around PHO A 416 (B):**

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

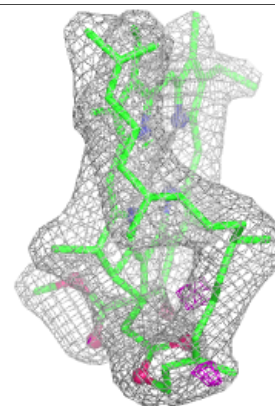
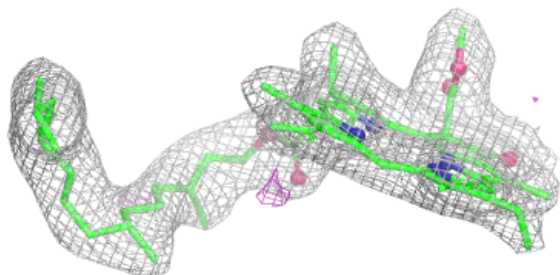
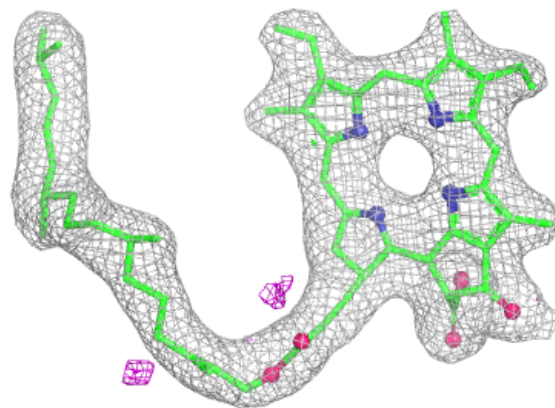


**Electron density around PHO a 415 (A):**

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

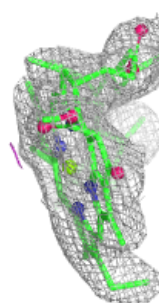
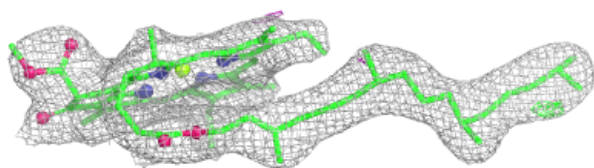
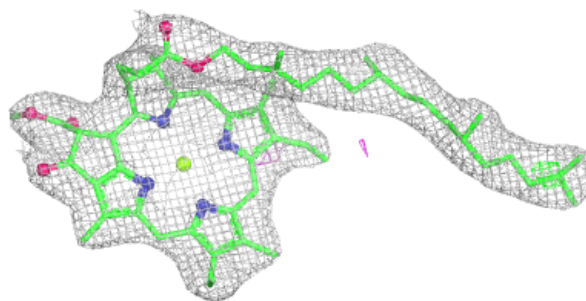
**Electron density around PHO a 415 (B):**

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

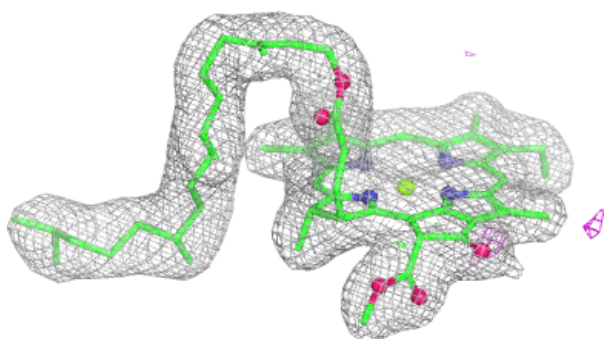
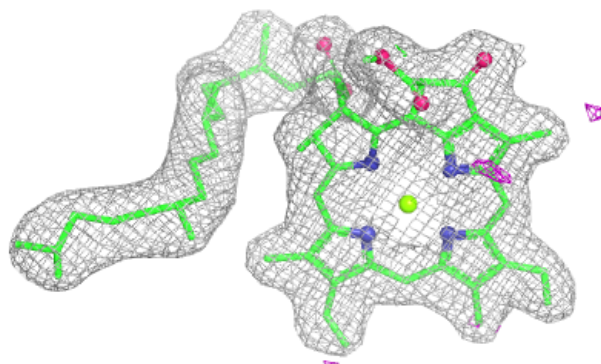


**Electron density around CLA c 502:**

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

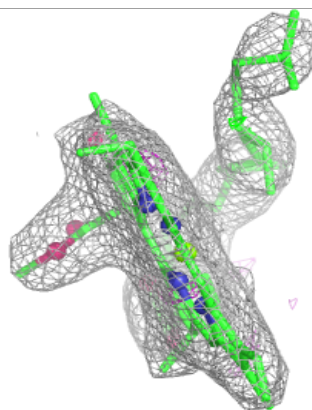
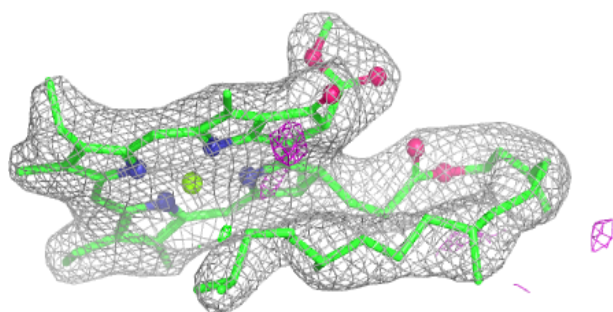
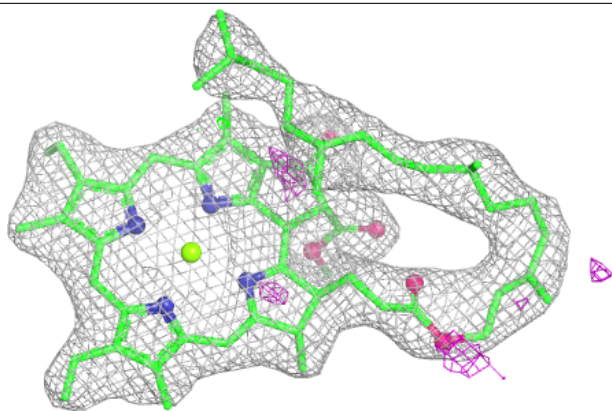
**Electron density around CLA A 405 (A):**

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



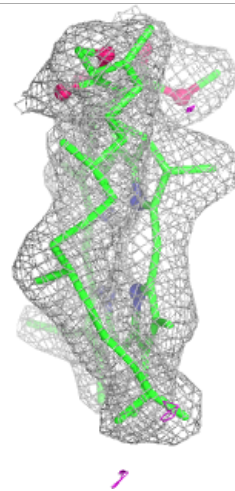
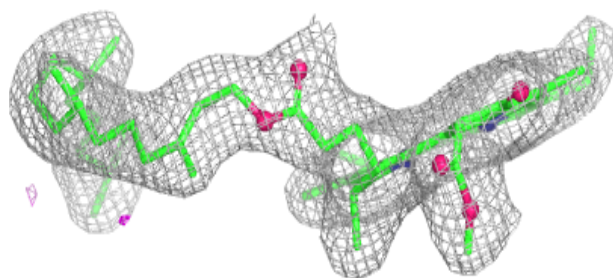
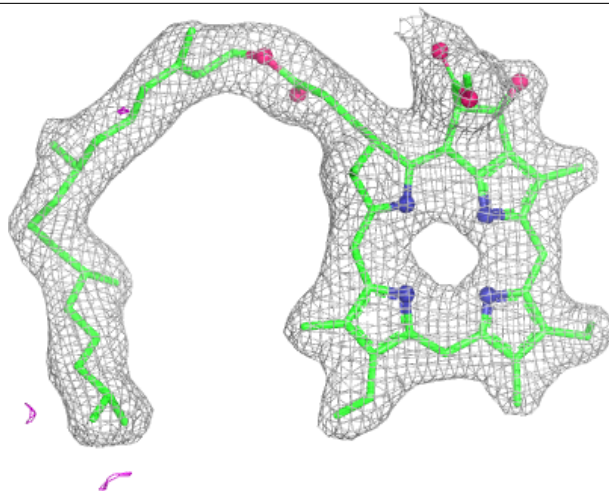
**Electron density around CLA c 510:**

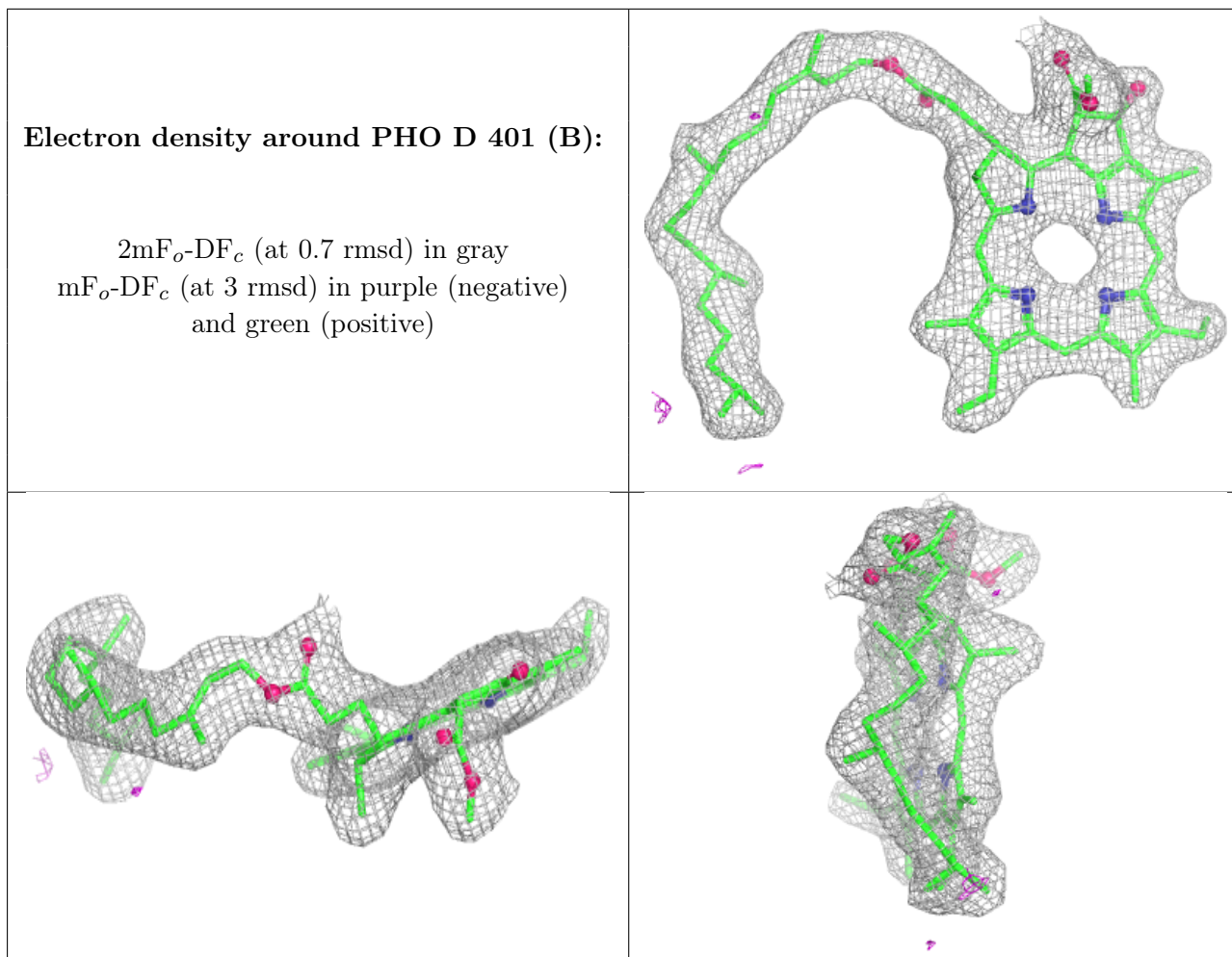
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



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

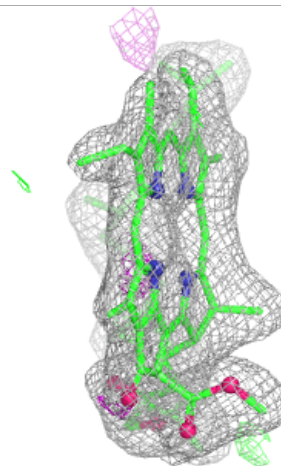
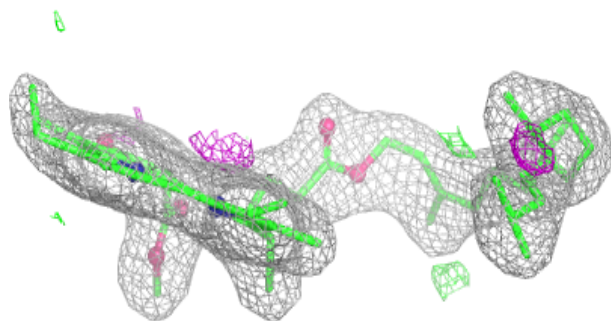
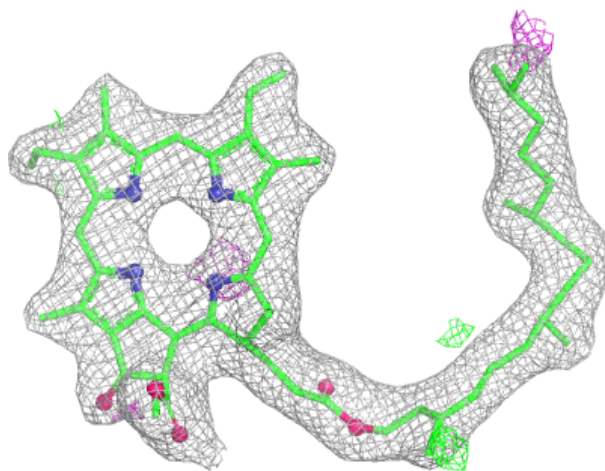
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





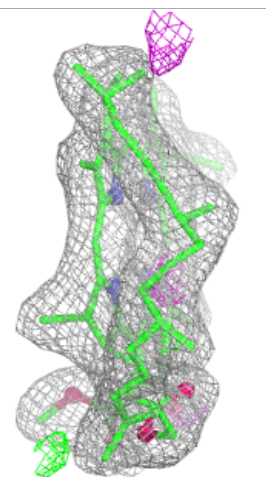
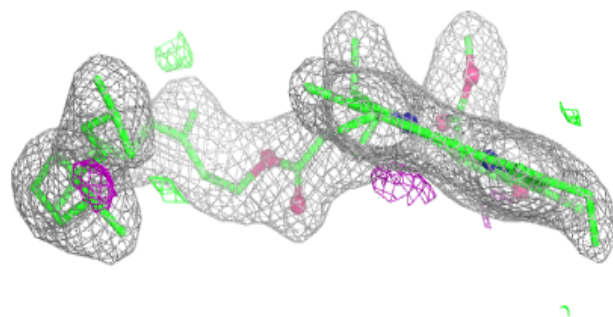
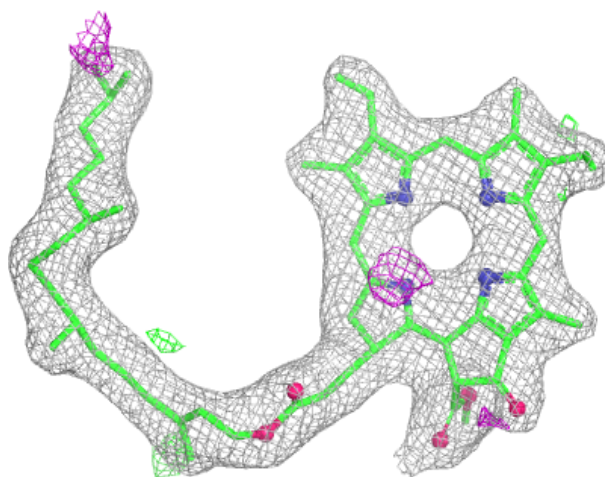
**Electron density around PHO a 406 (A):**

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



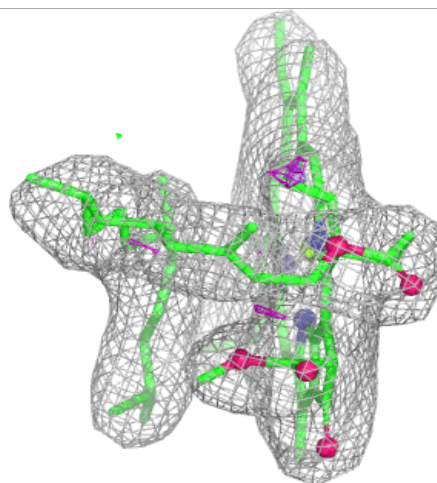
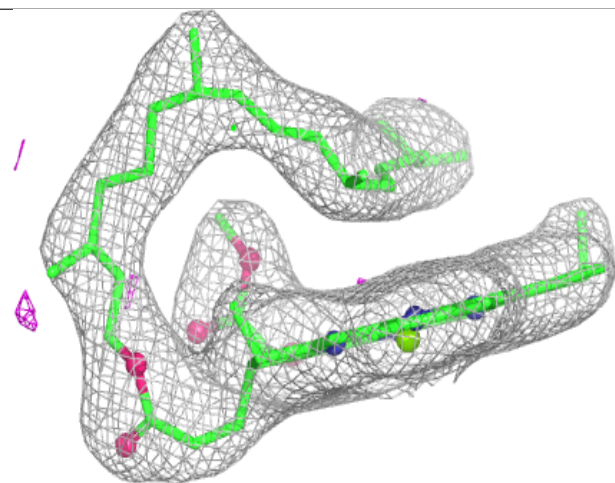
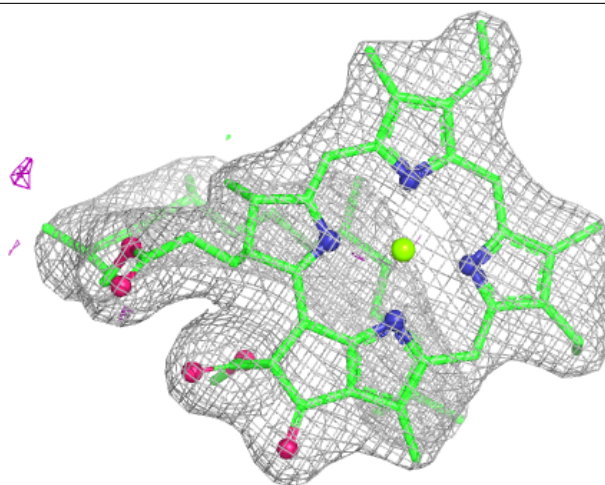
**Electron density around PHO a 406 (B):**

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



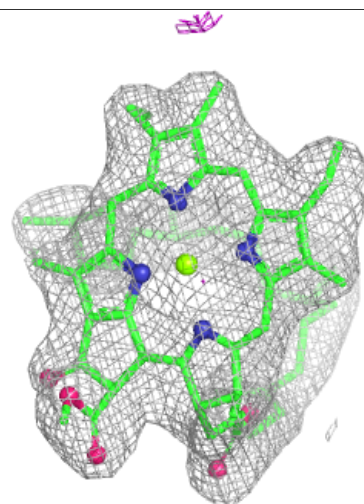
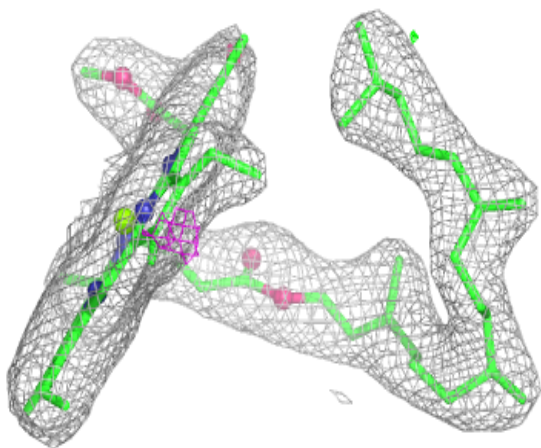
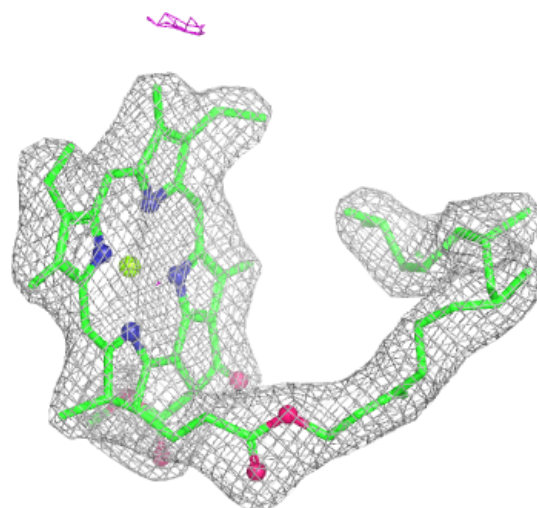
**Electron density around CLA c 511:**

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



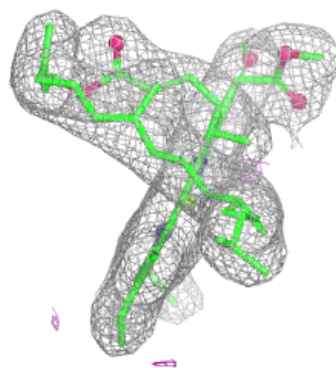
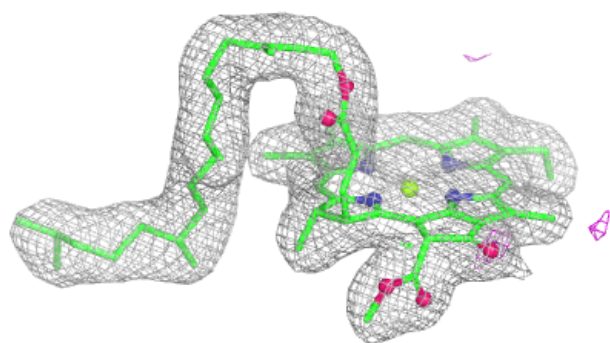
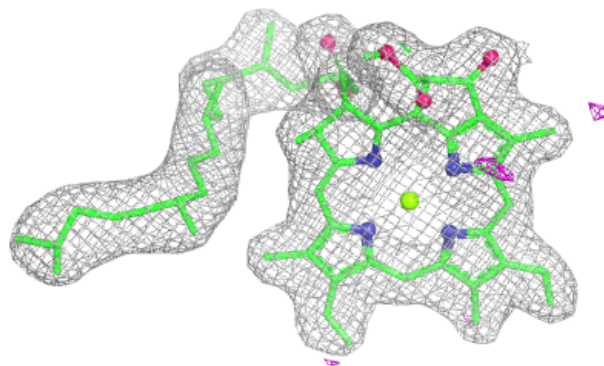
**Electron density around CLA C 504:**

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

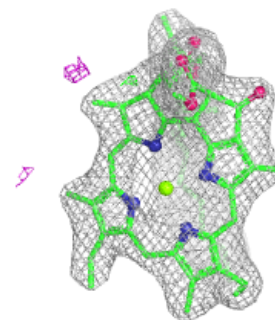
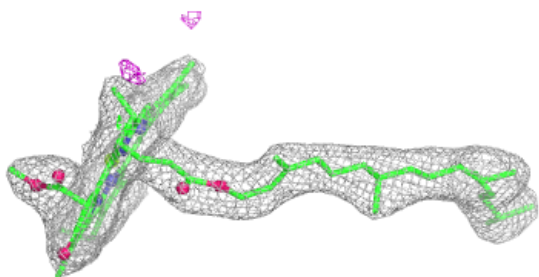
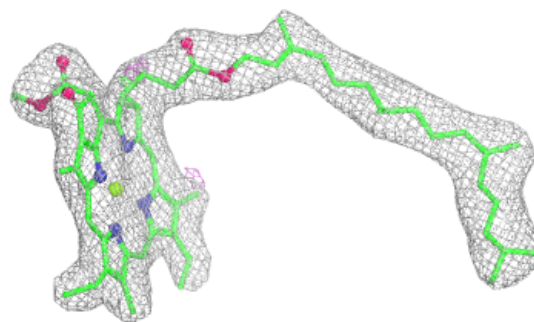


**Electron density around CLA A 405 (B):**

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

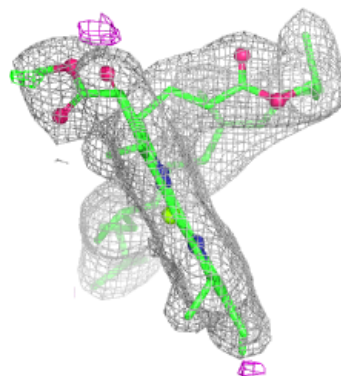
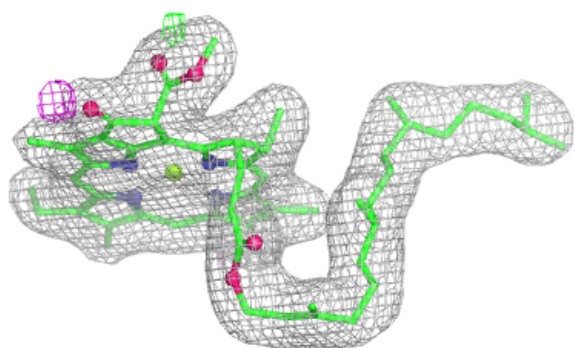
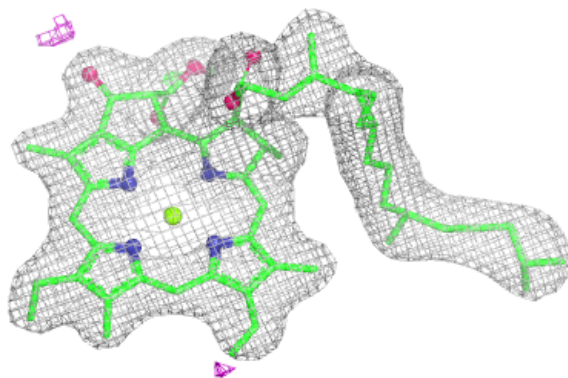
**Electron density around CLA B 609:**

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

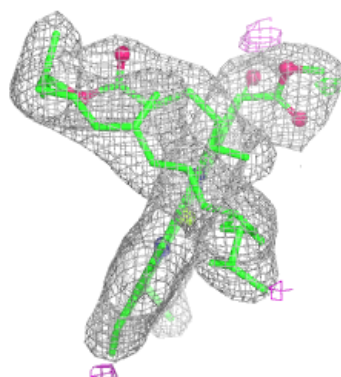
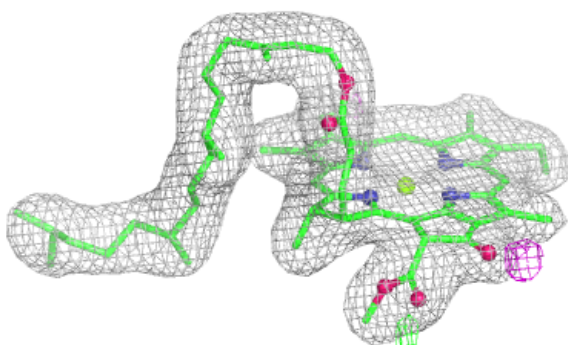
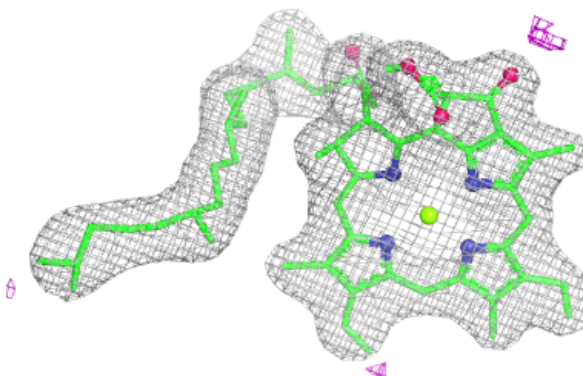


**Electron density around CLA d 402 (A):**

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

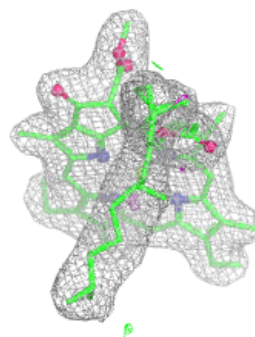
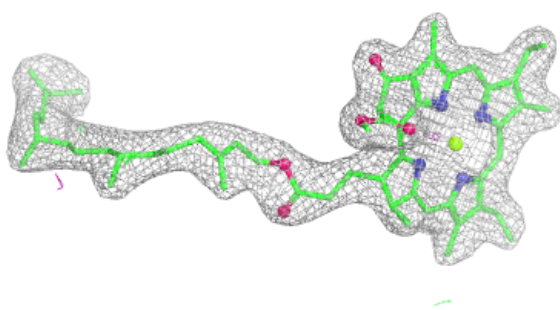
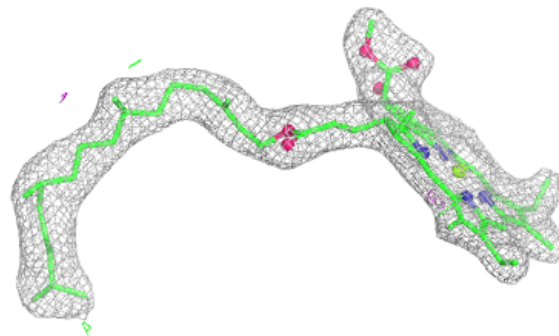
**Electron density around CLA d 402 (B):**

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

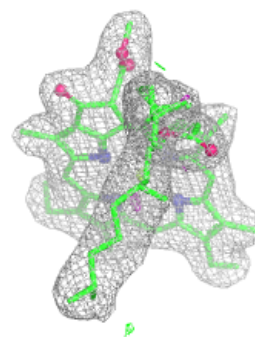
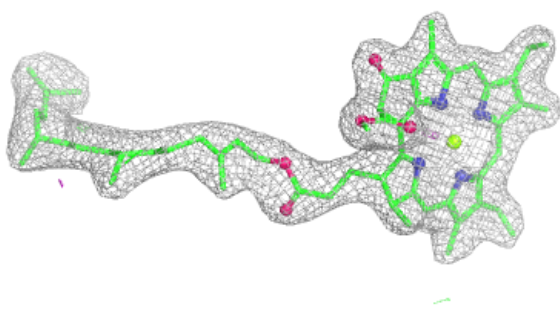
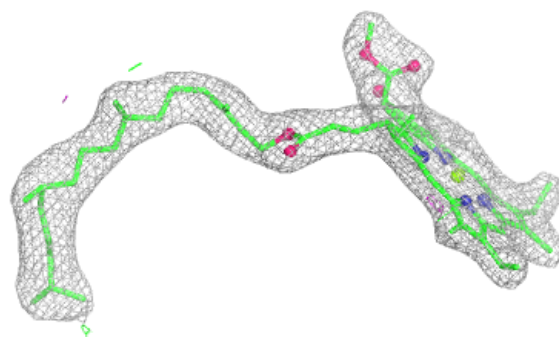


**Electron density around CLA d 403 (A):**

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

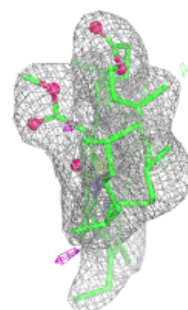
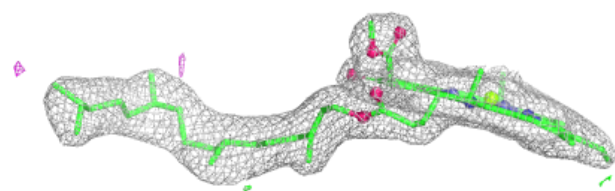
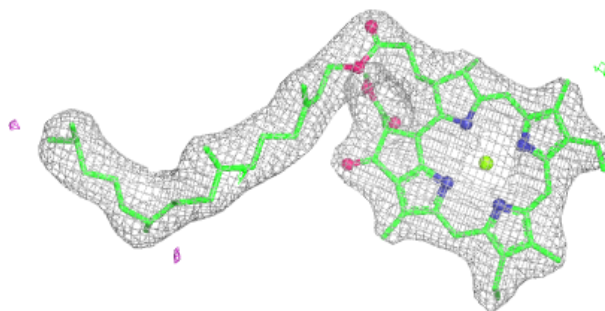
**Electron density around CLA d 403 (B):**

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

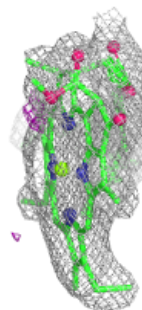
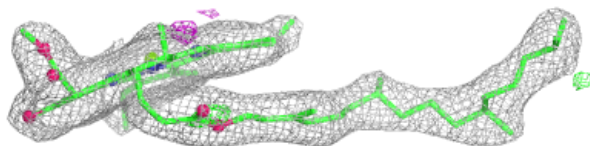
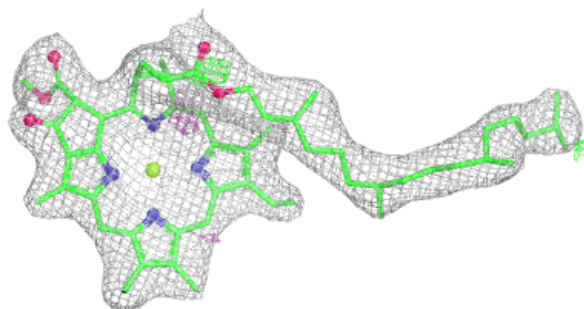


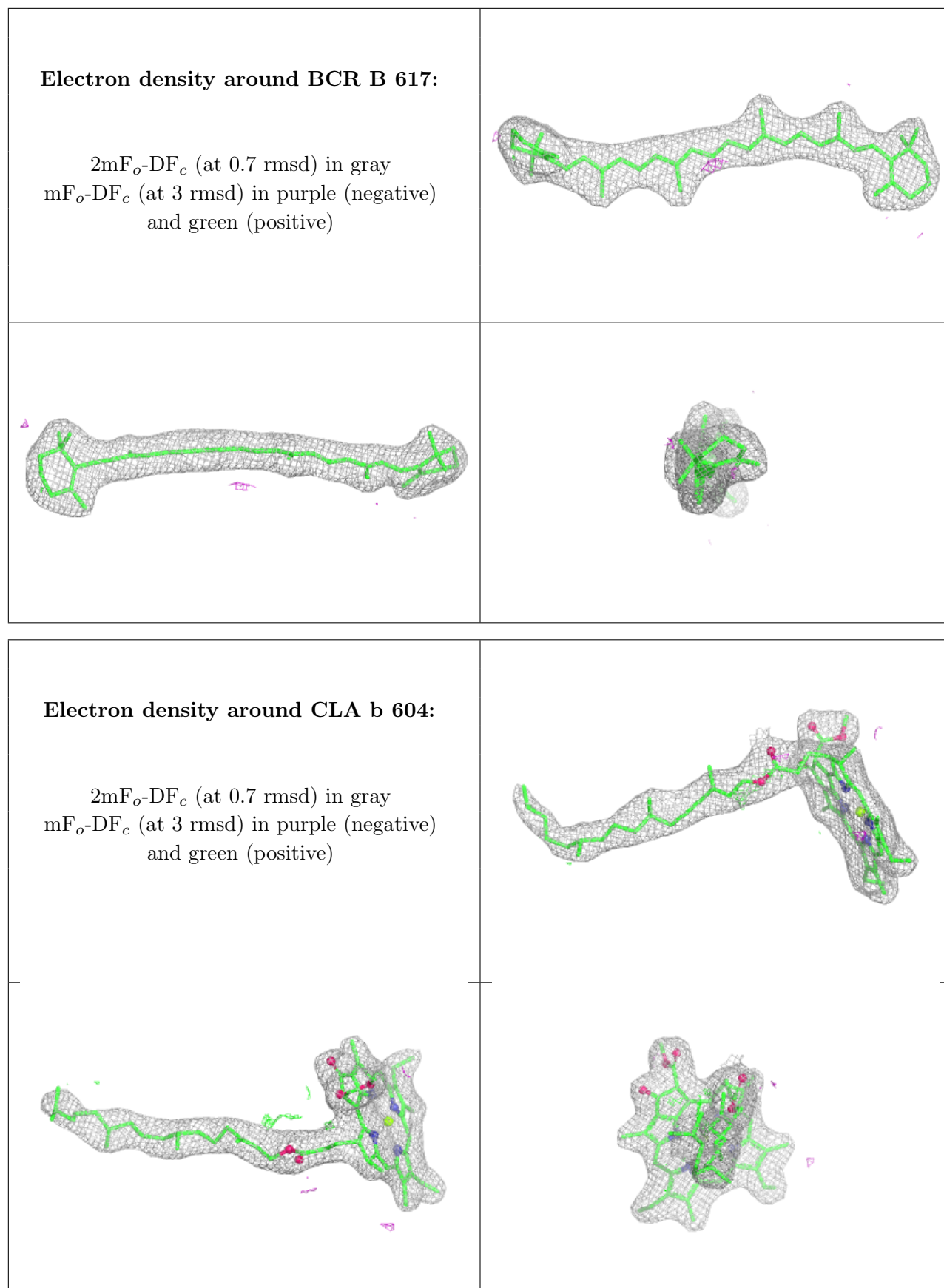
**Electron density around CLA b 602:**

$2mF_o-DF_c$  (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:**

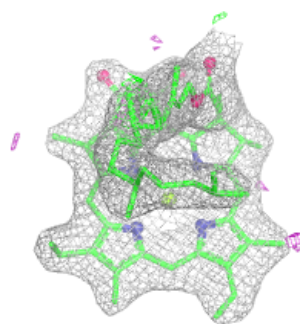
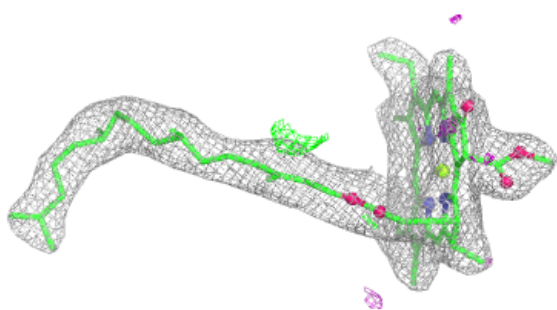
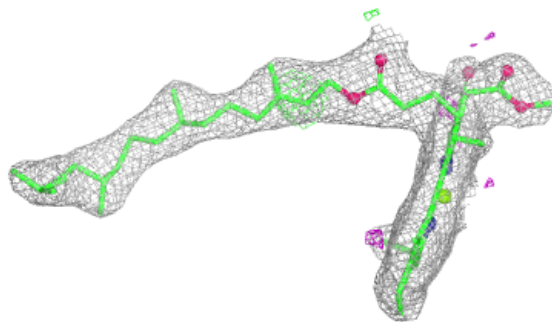
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





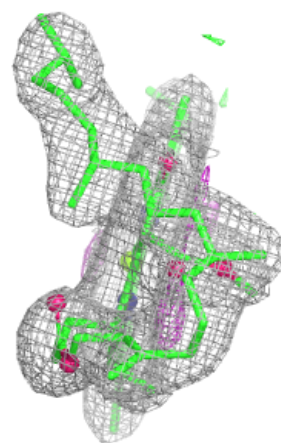
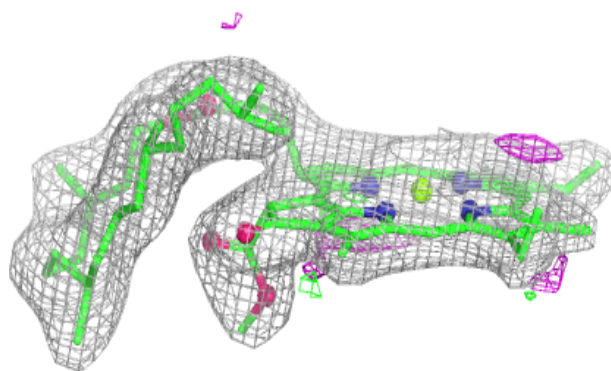
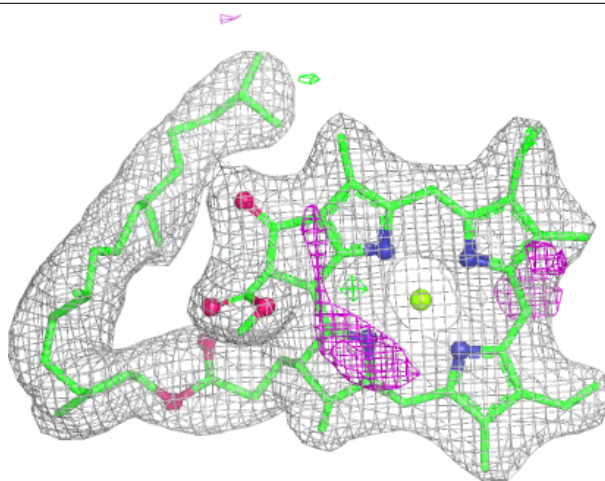
**Electron density around CLA b 605:**

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



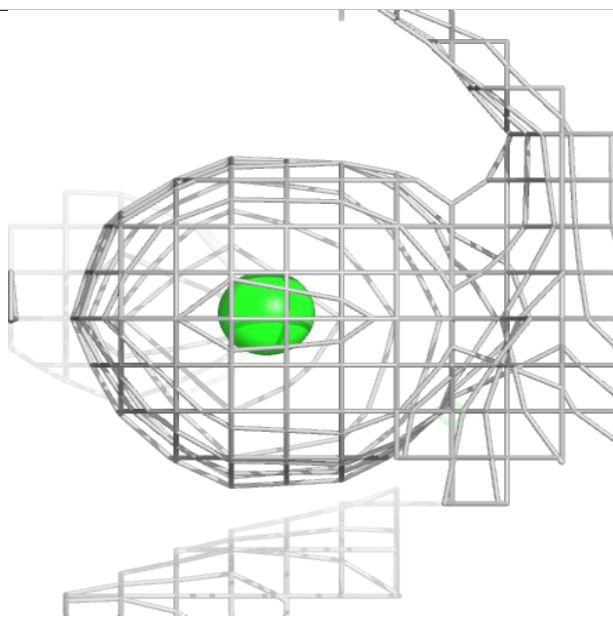
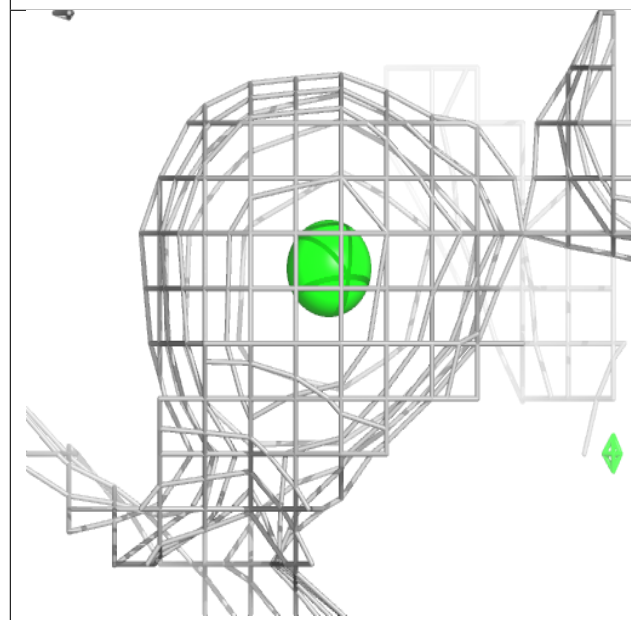
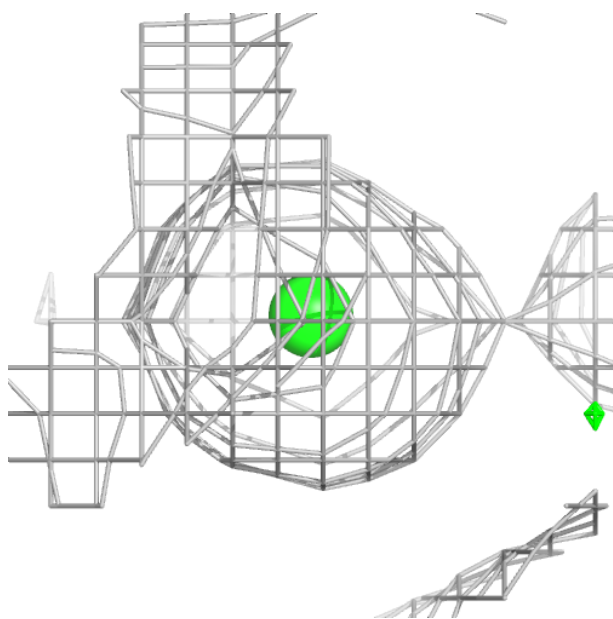
**Electron density around CLA B 610:**

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



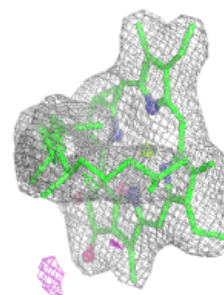
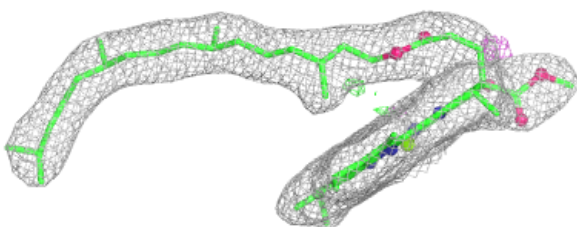
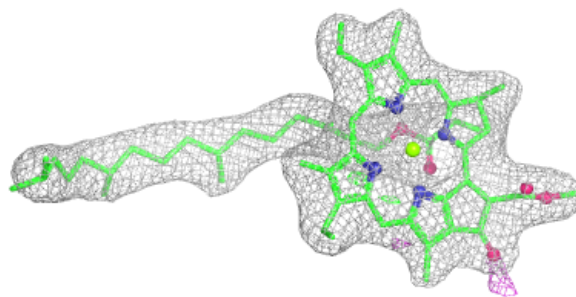
**Electron density around CL a 403 (A):**

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

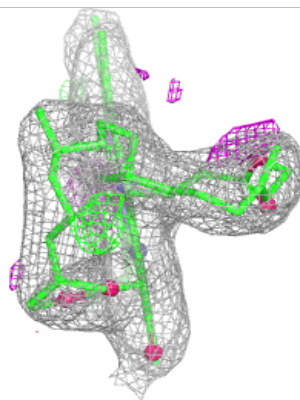
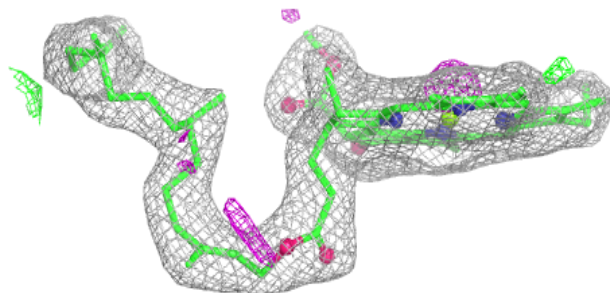
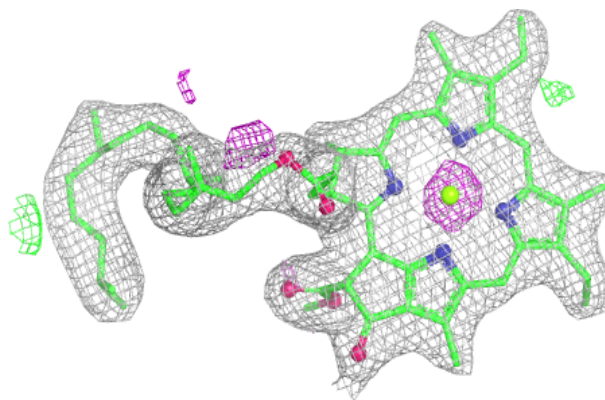


**Electron density around CLA b 608:**

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

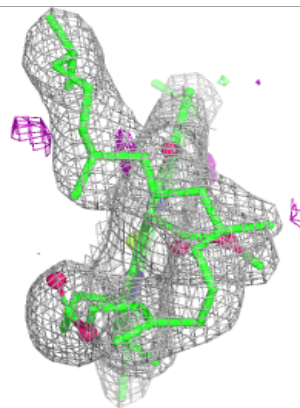
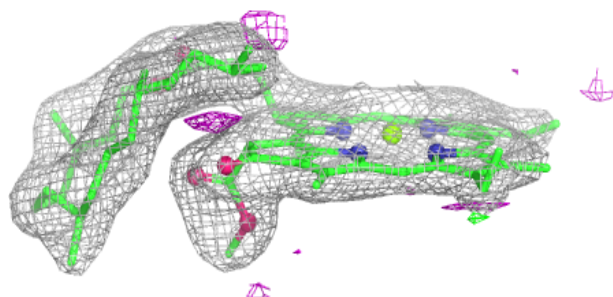
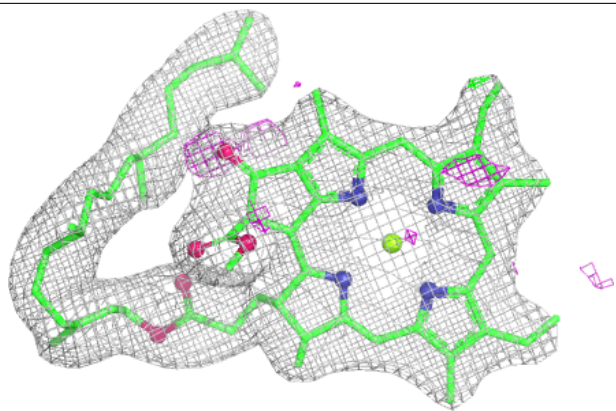
**Electron density around CLA B 612:**

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



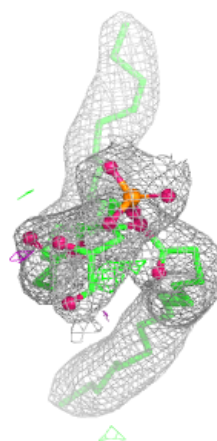
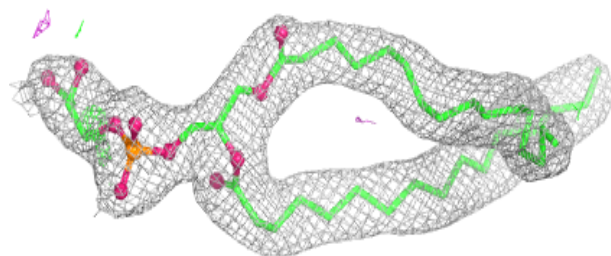
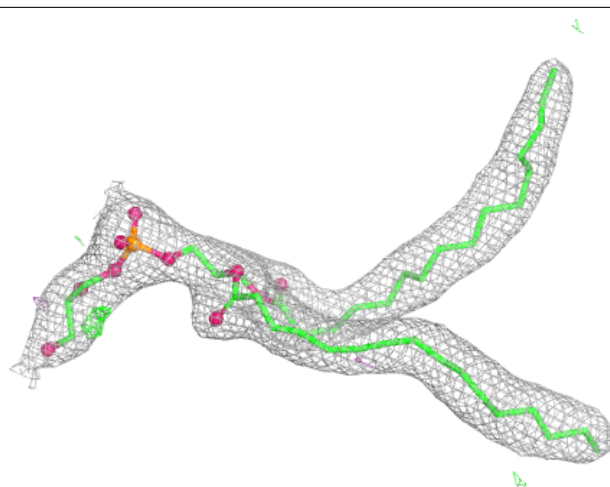
**Electron density around CLA b 610:**

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



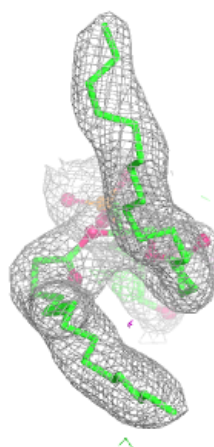
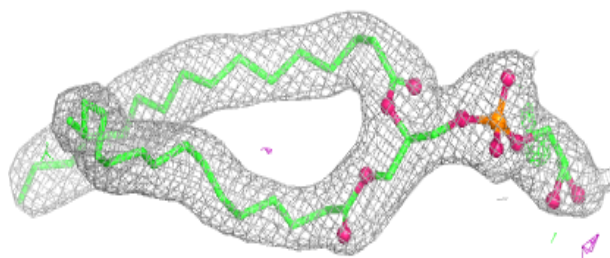
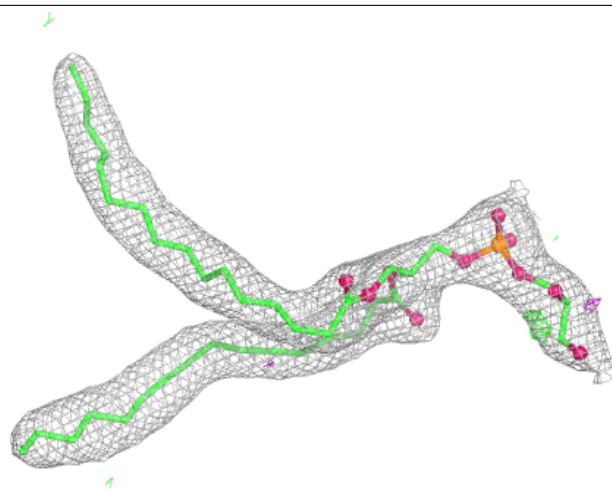
**Electron density around LHG D 407 (A):**

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



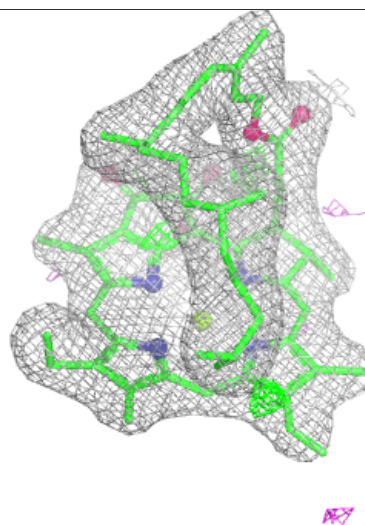
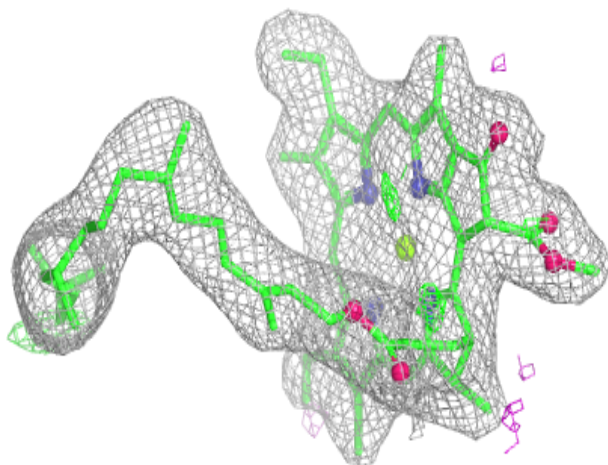
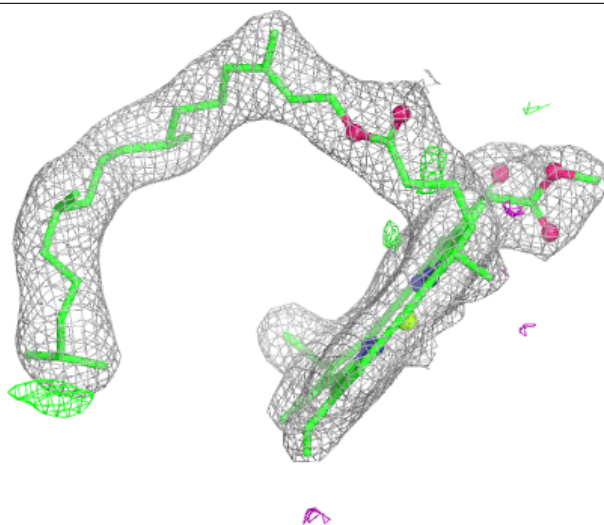
**Electron density around LHG D 407 (B):**

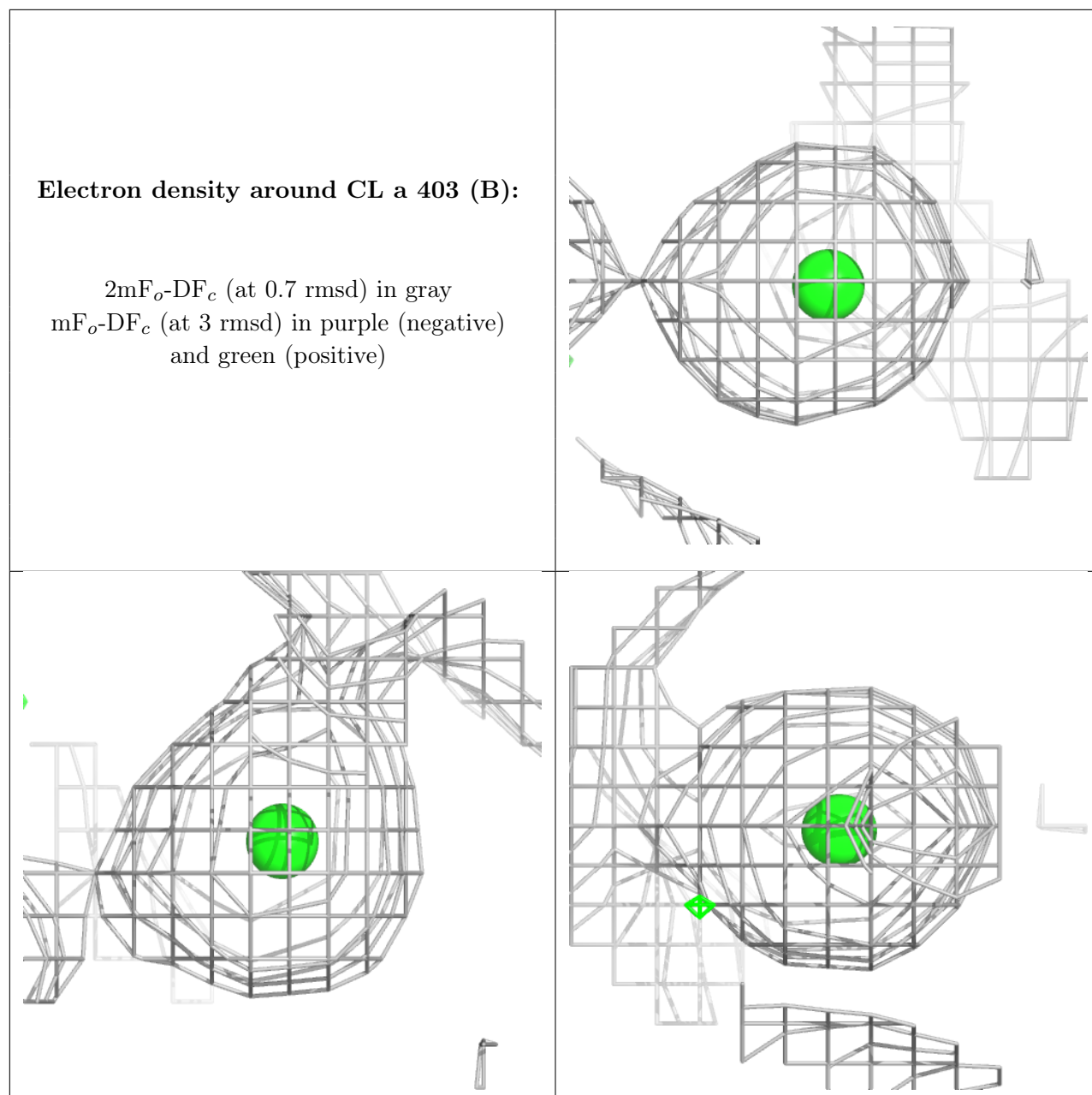
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA b 611:**

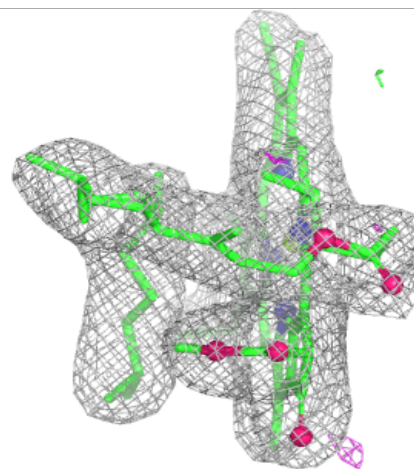
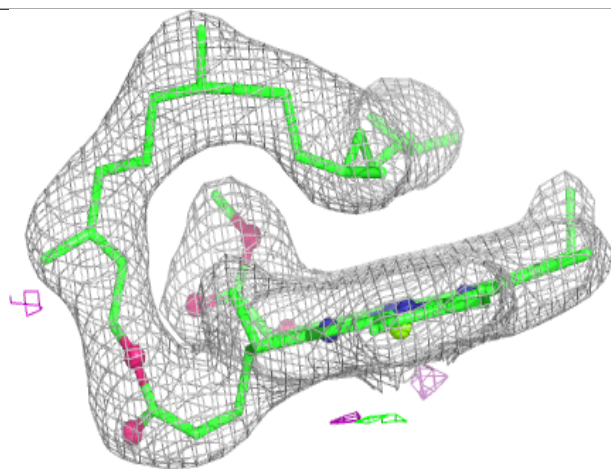
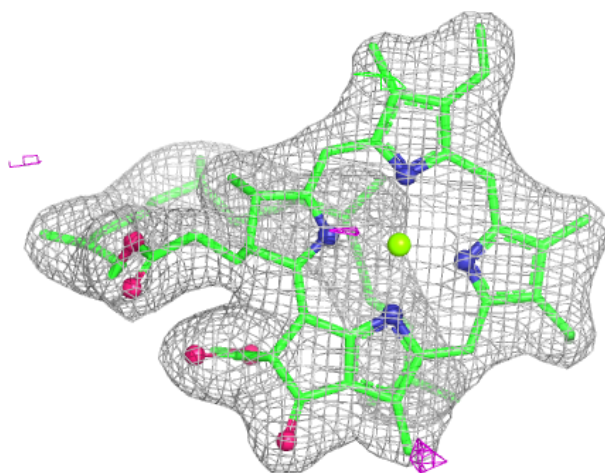
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





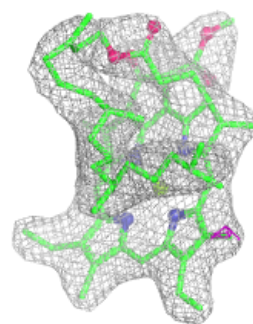
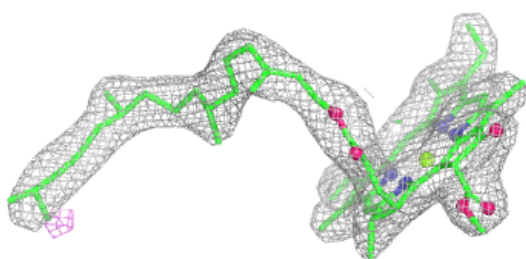
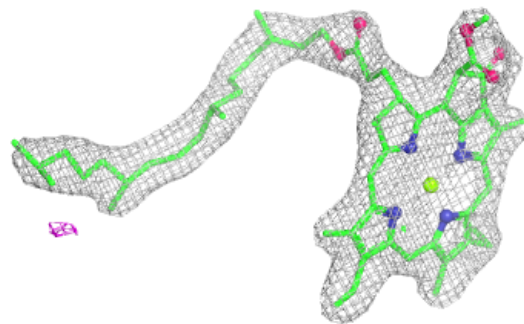
**Electron density around CLA C 511:**

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



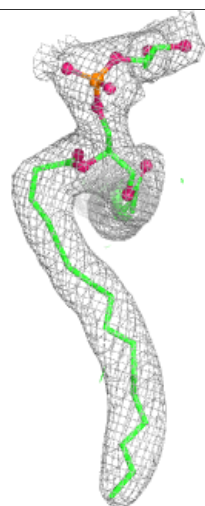
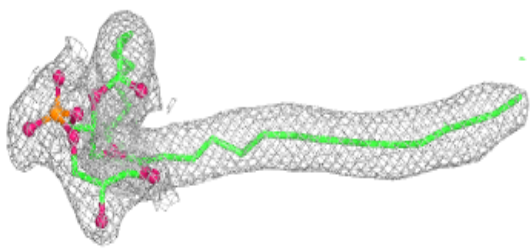
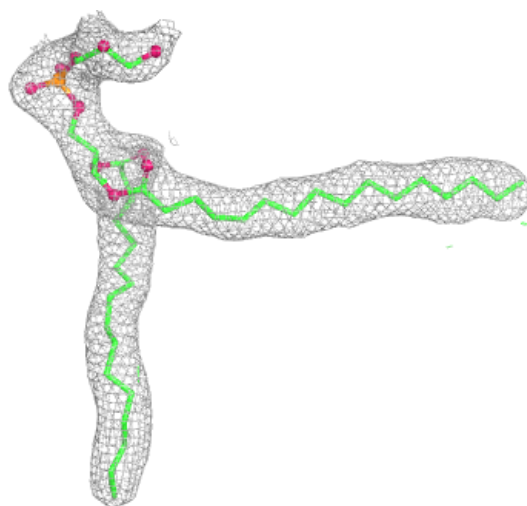
**Electron density around CLA C 512:**

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



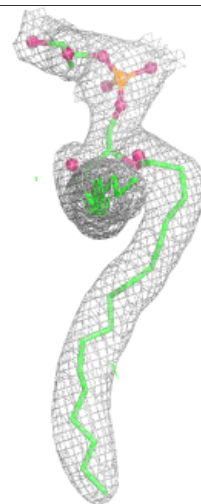
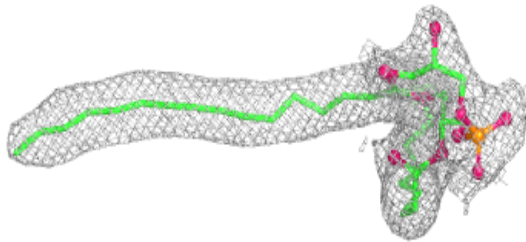
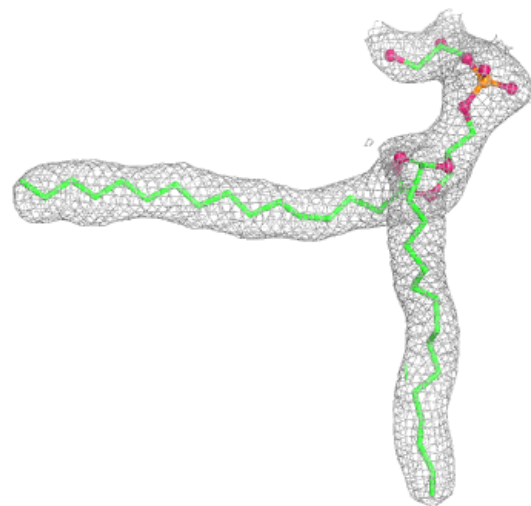
**Electron density around LHG L 101 (A):**

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



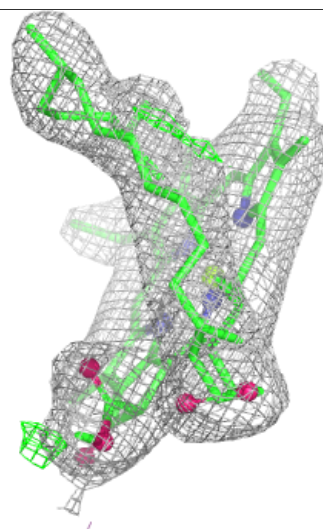
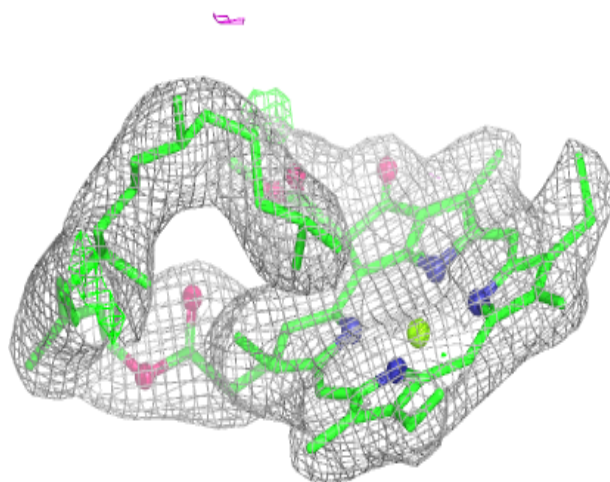
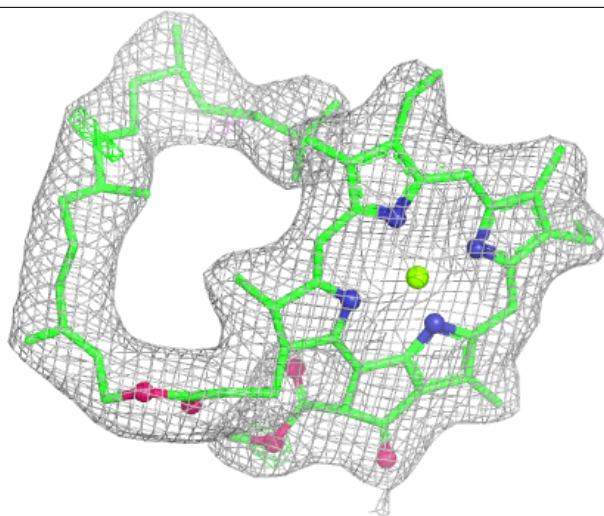
**Electron density around LHG L 101 (B):**

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



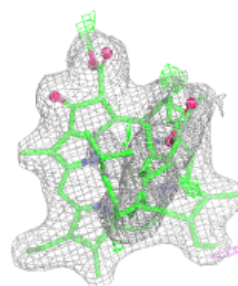
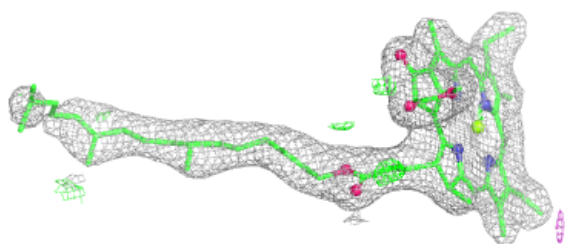
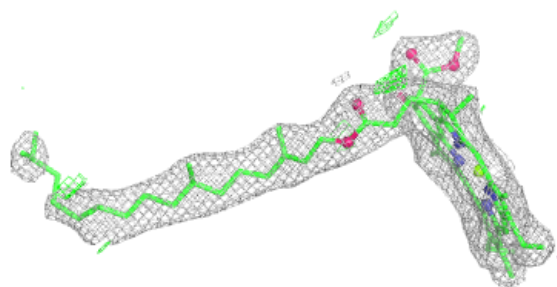
**Electron density around CLA b 615:**

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

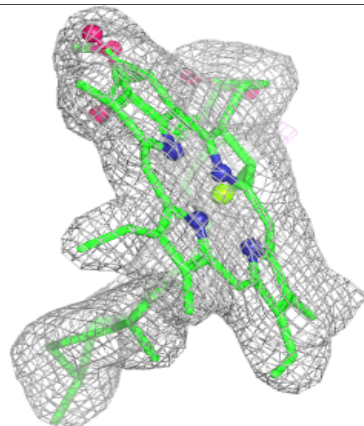
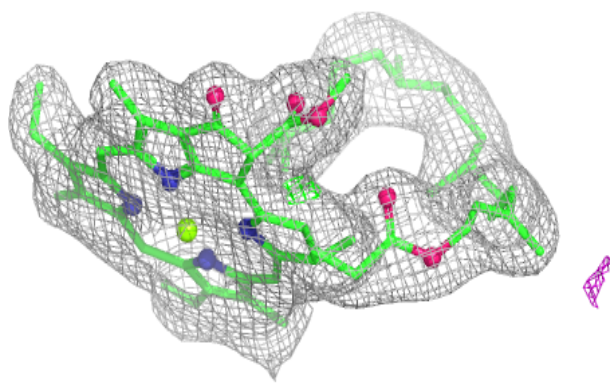
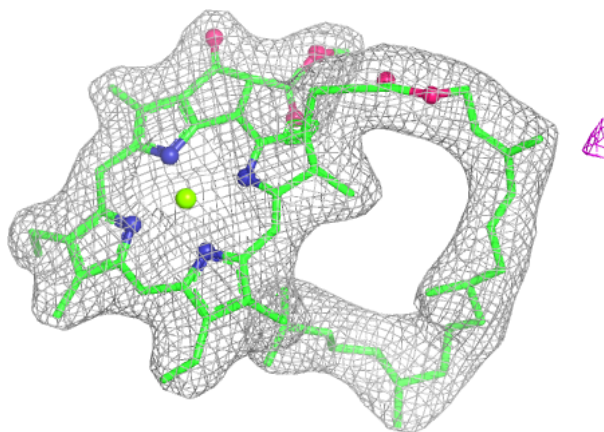


**Electron density around CLA B 604:**

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

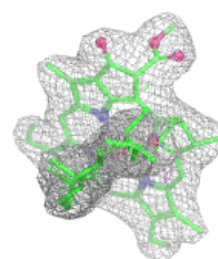
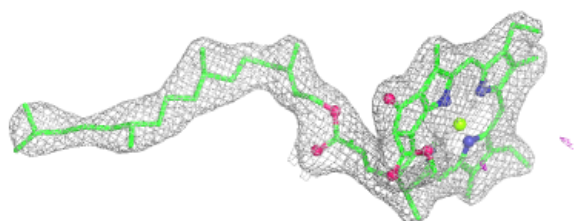
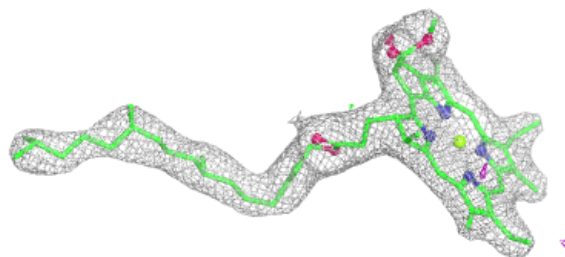
**Electron density around CLA B 615:**

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

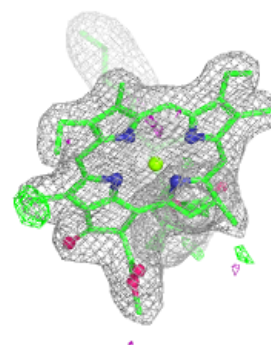
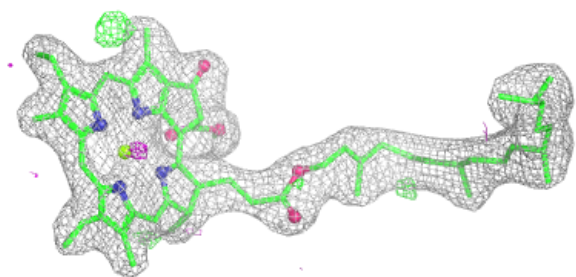
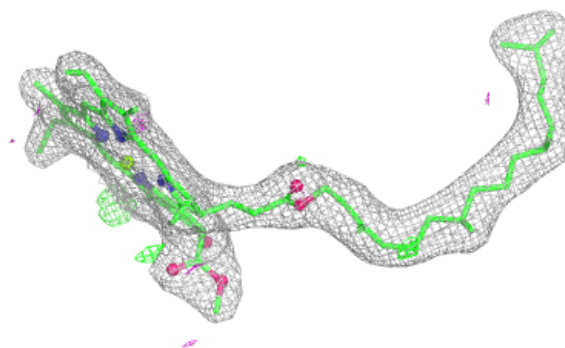


**Electron density around CLA c 503:**

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

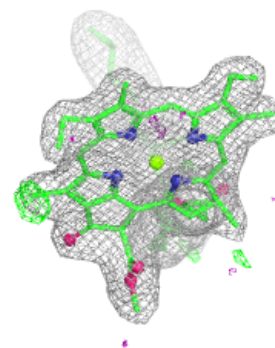
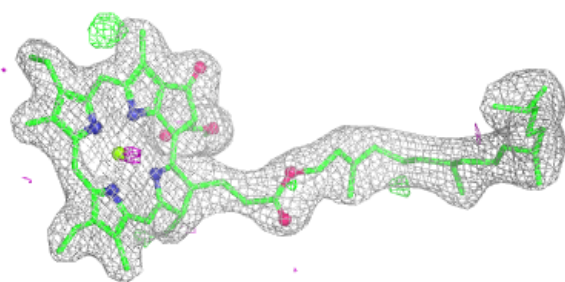
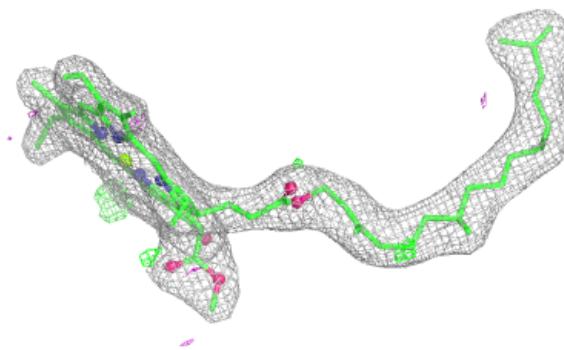
**Electron density around CLA D 403 (A):**

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

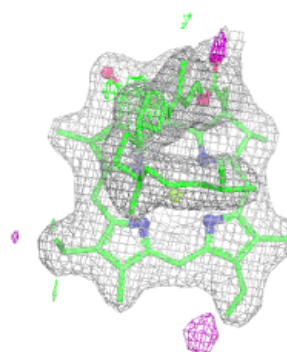
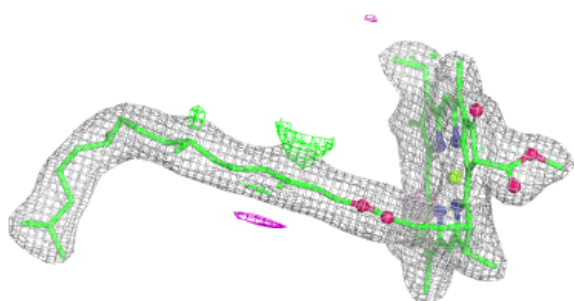
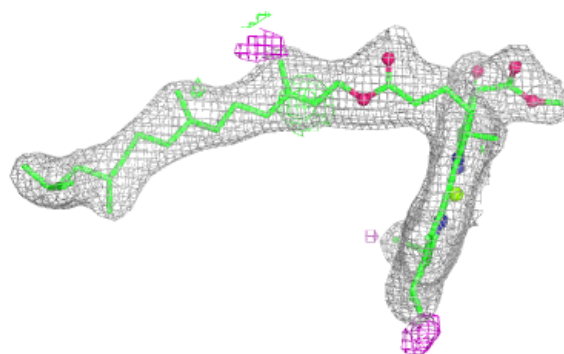


**Electron density around CLA D 403 (B):**

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

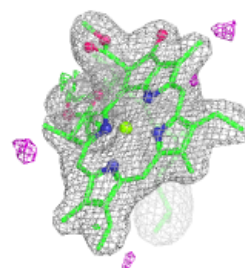
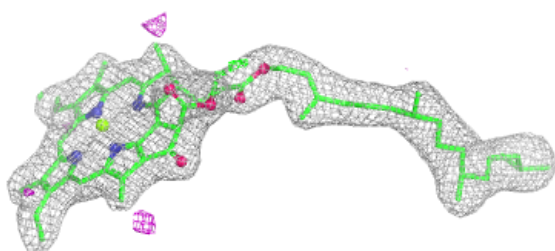
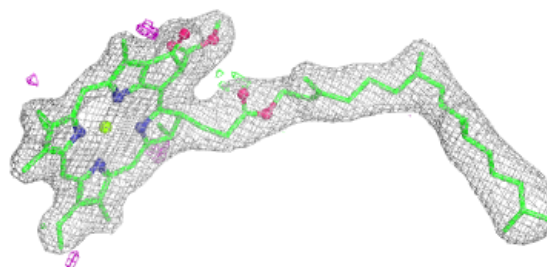
**Electron density around CLA B 605:**

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

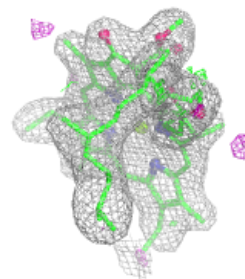
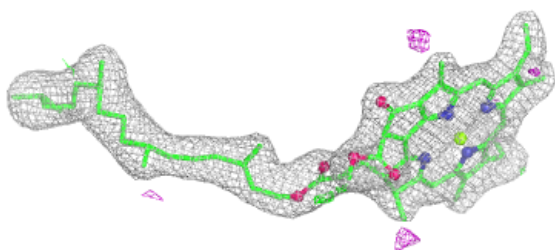
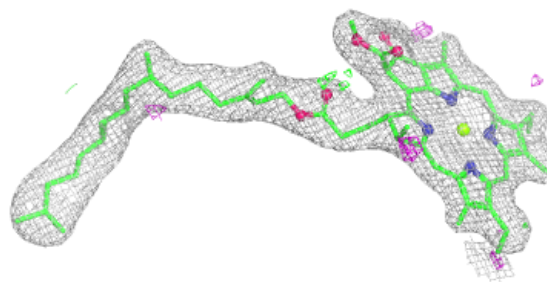


**Electron density around CLA a 404 (A):**

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

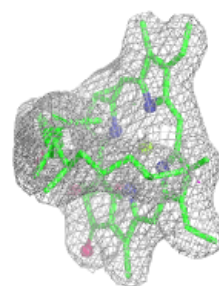
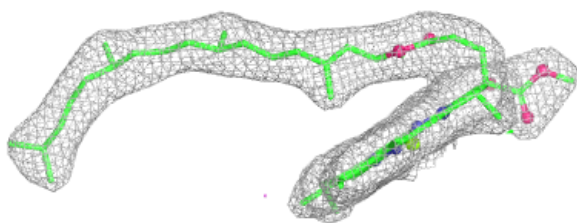
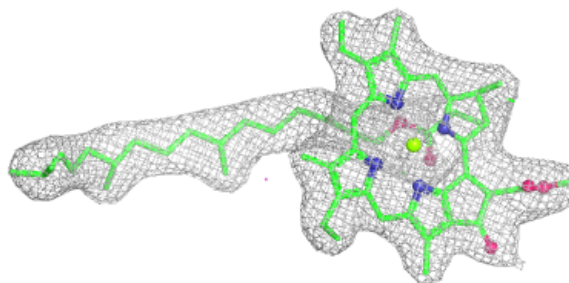
**Electron density around CLA a 404 (B):**

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



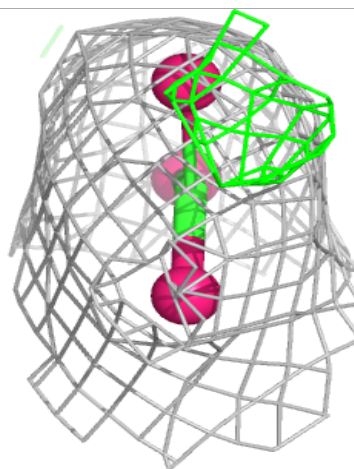
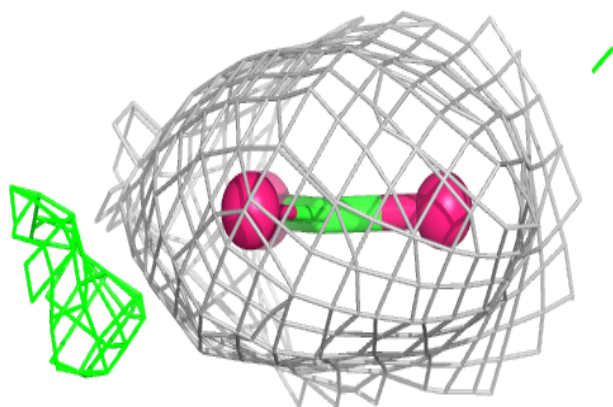
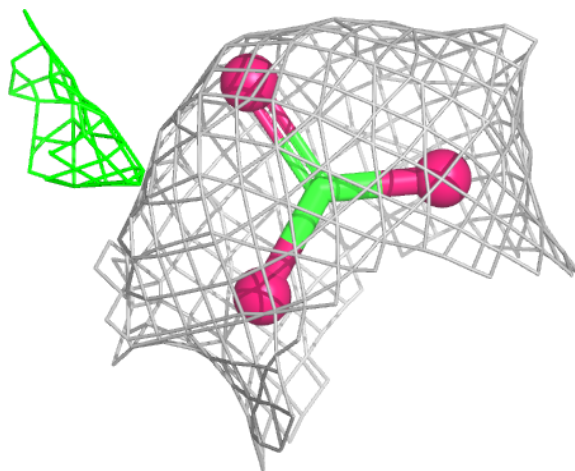
**Electron density around CLA B 608:**

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



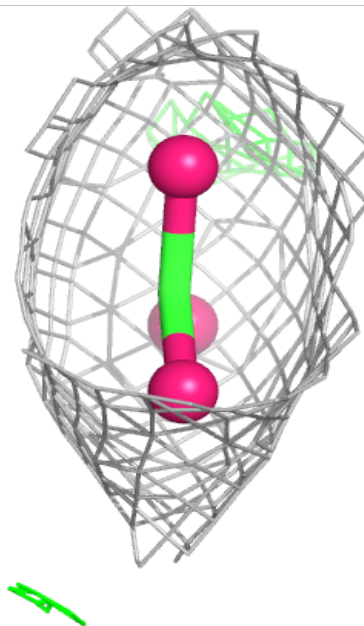
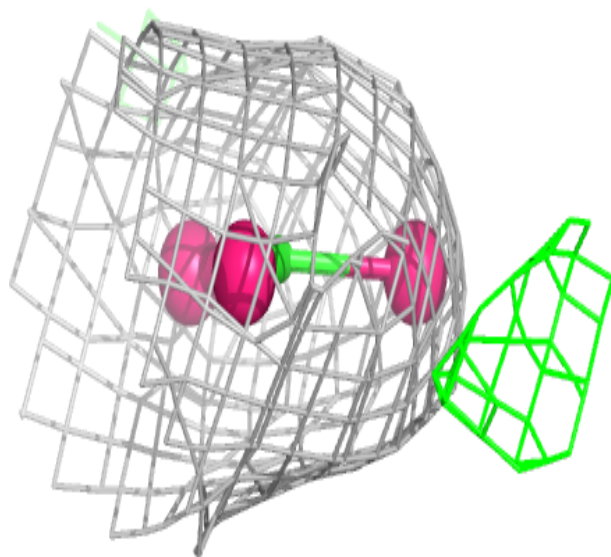
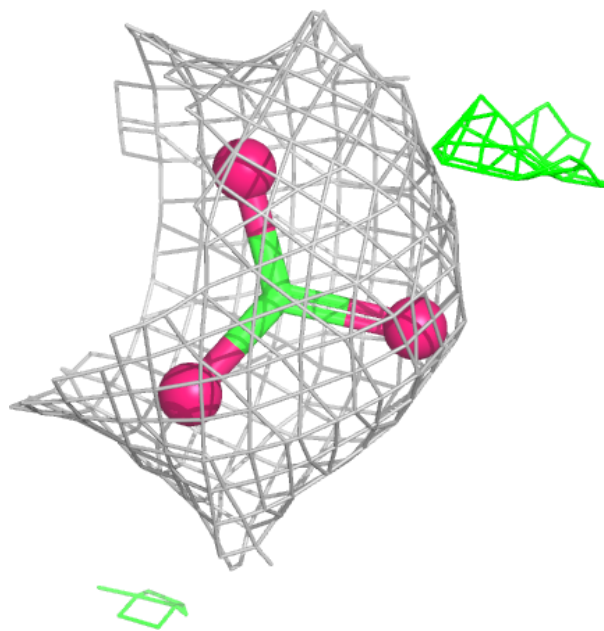
**Electron density around BCT A 415 (A):**

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



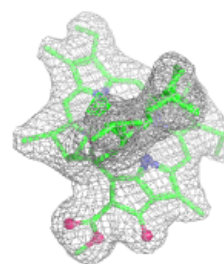
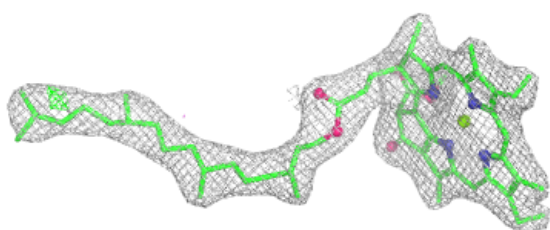
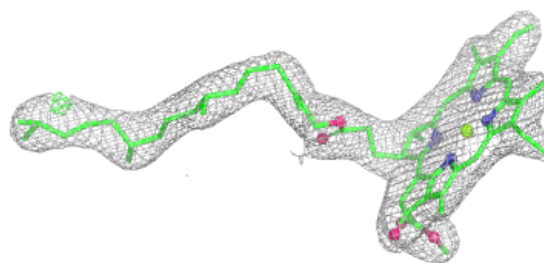
**Electron density around BCT A 415 (B):**

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



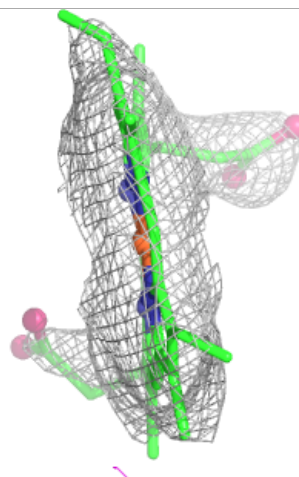
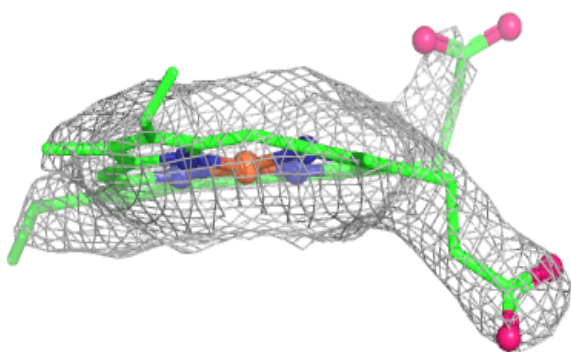
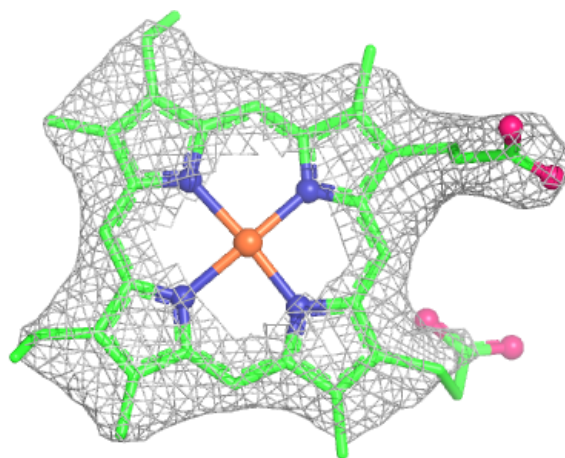
**Electron density around CLA C 503:**

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



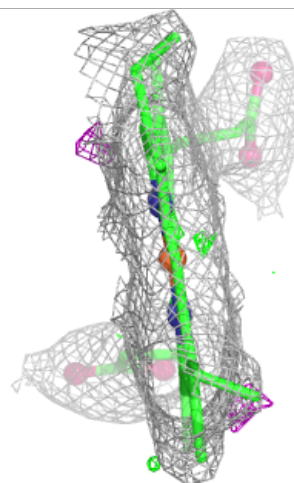
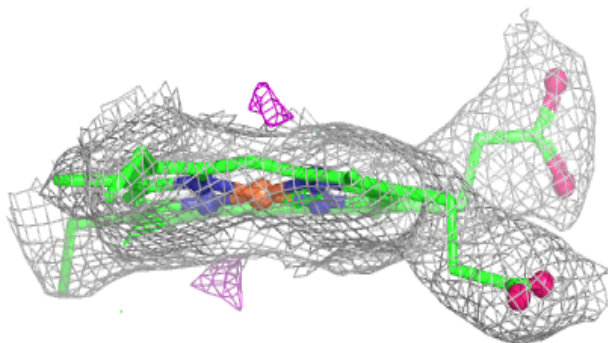
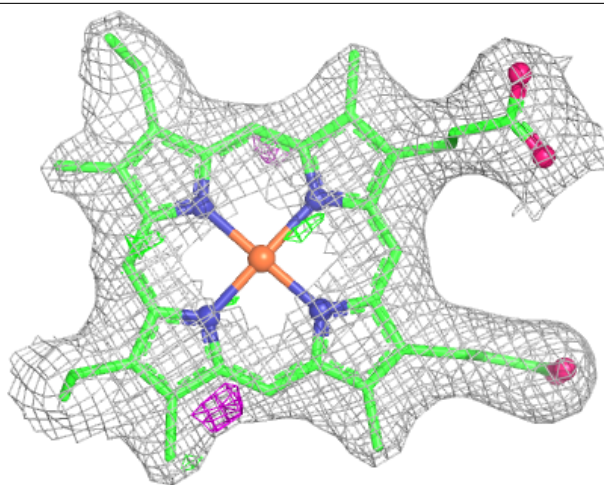
**Electron density around HEM f 101:**

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



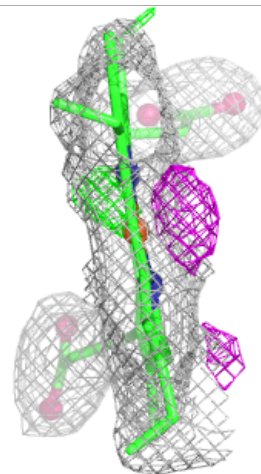
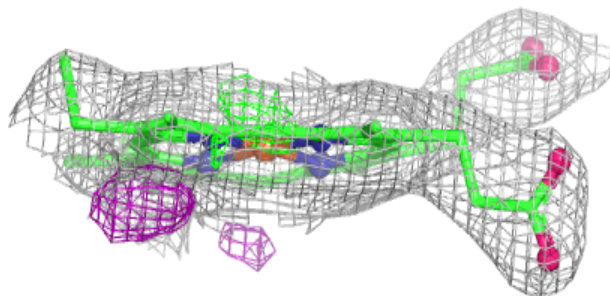
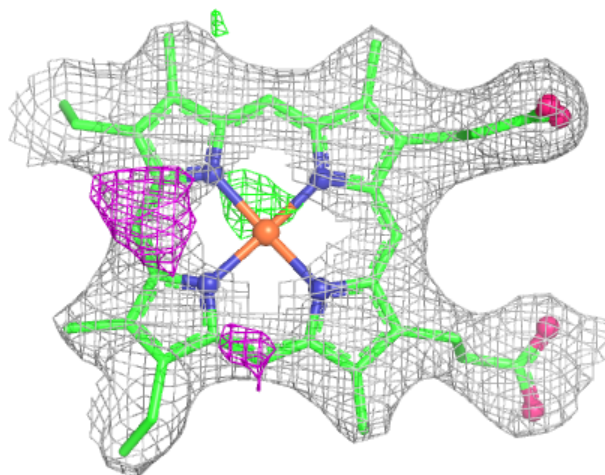
**Electron density around HEC V 201:**

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



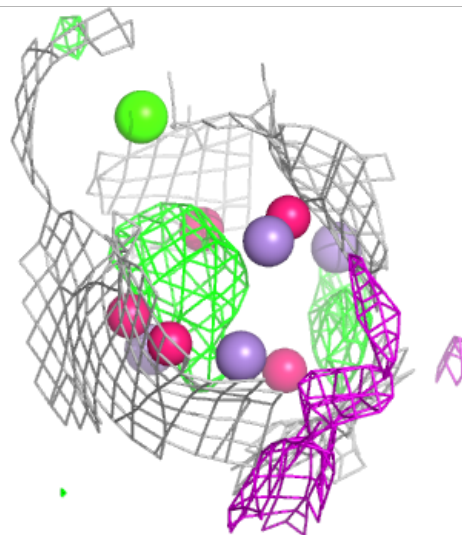
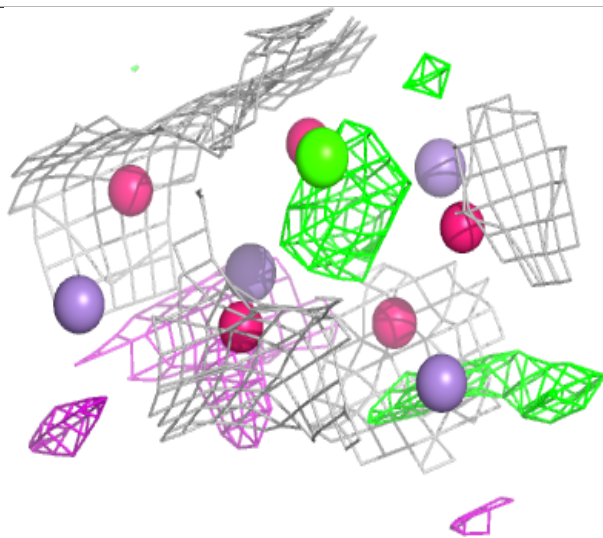
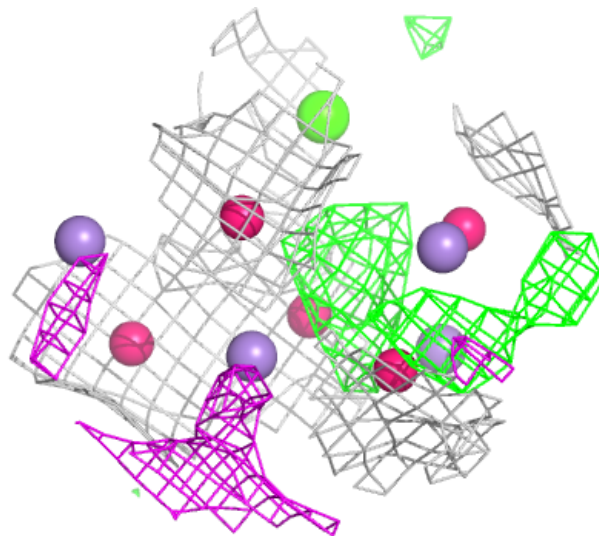
**Electron density around HEC v 201:**

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



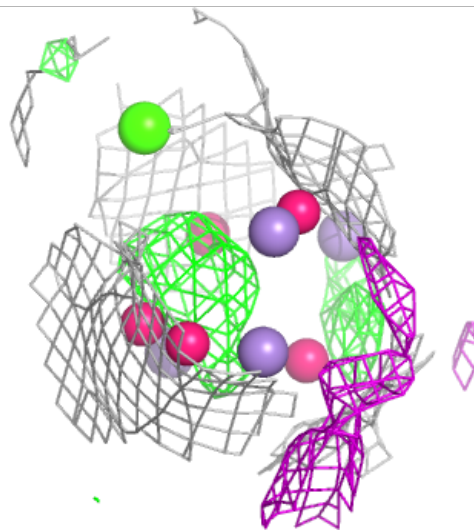
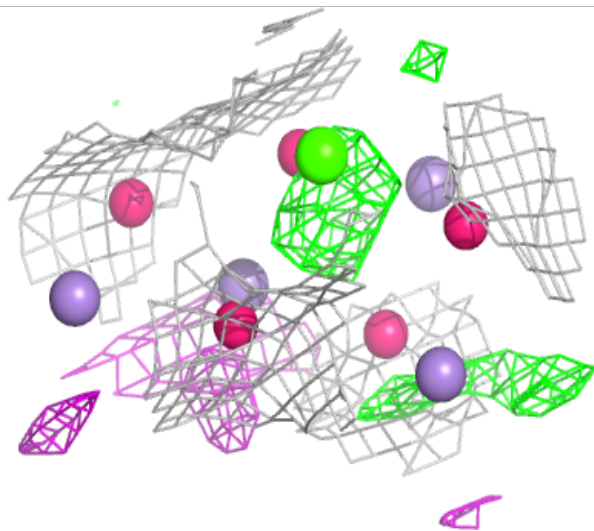
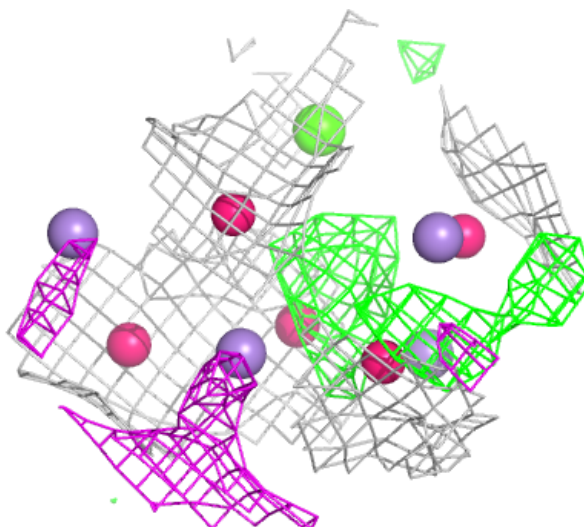
**Electron density around OEX A 412 (A):**

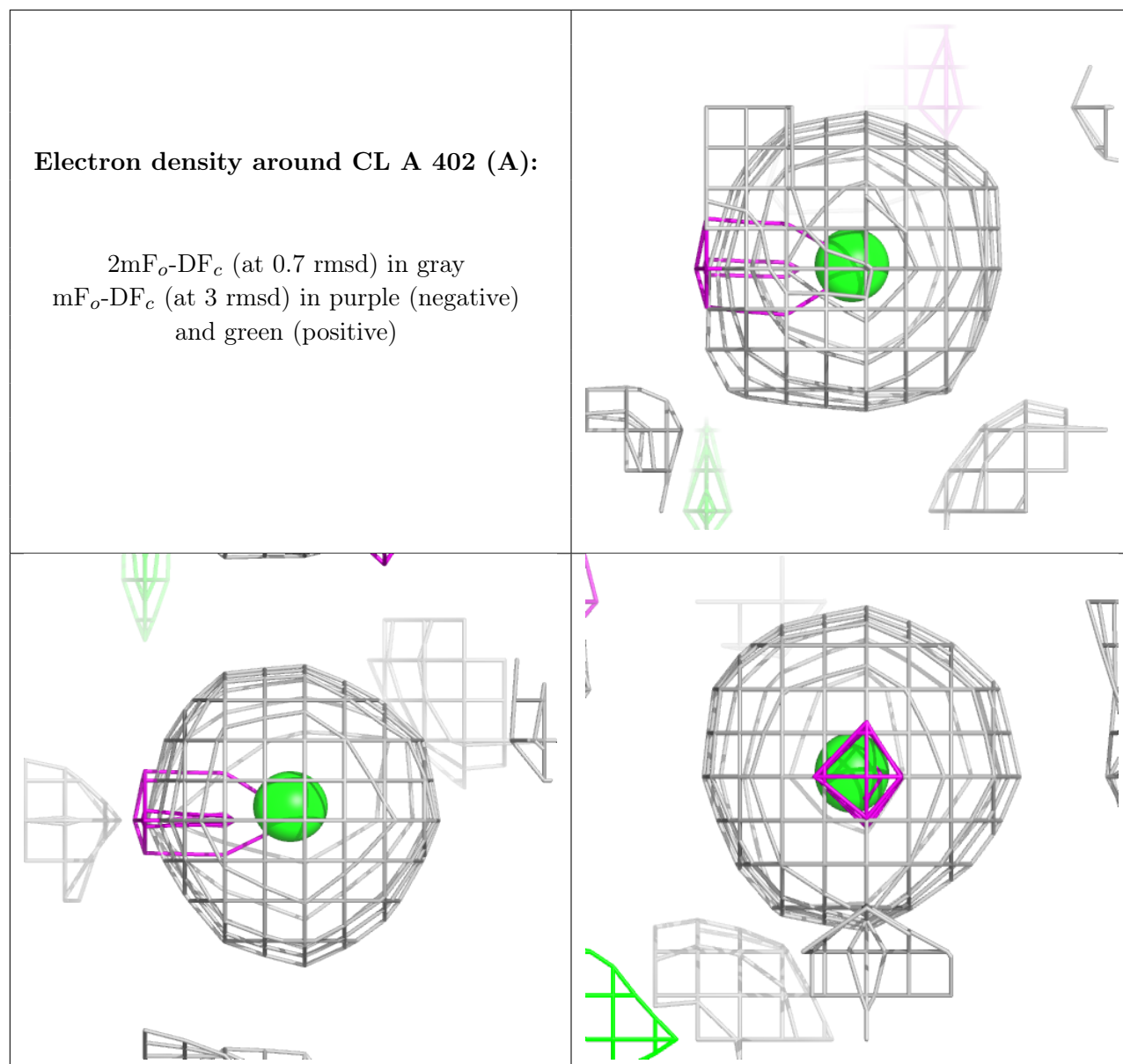
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

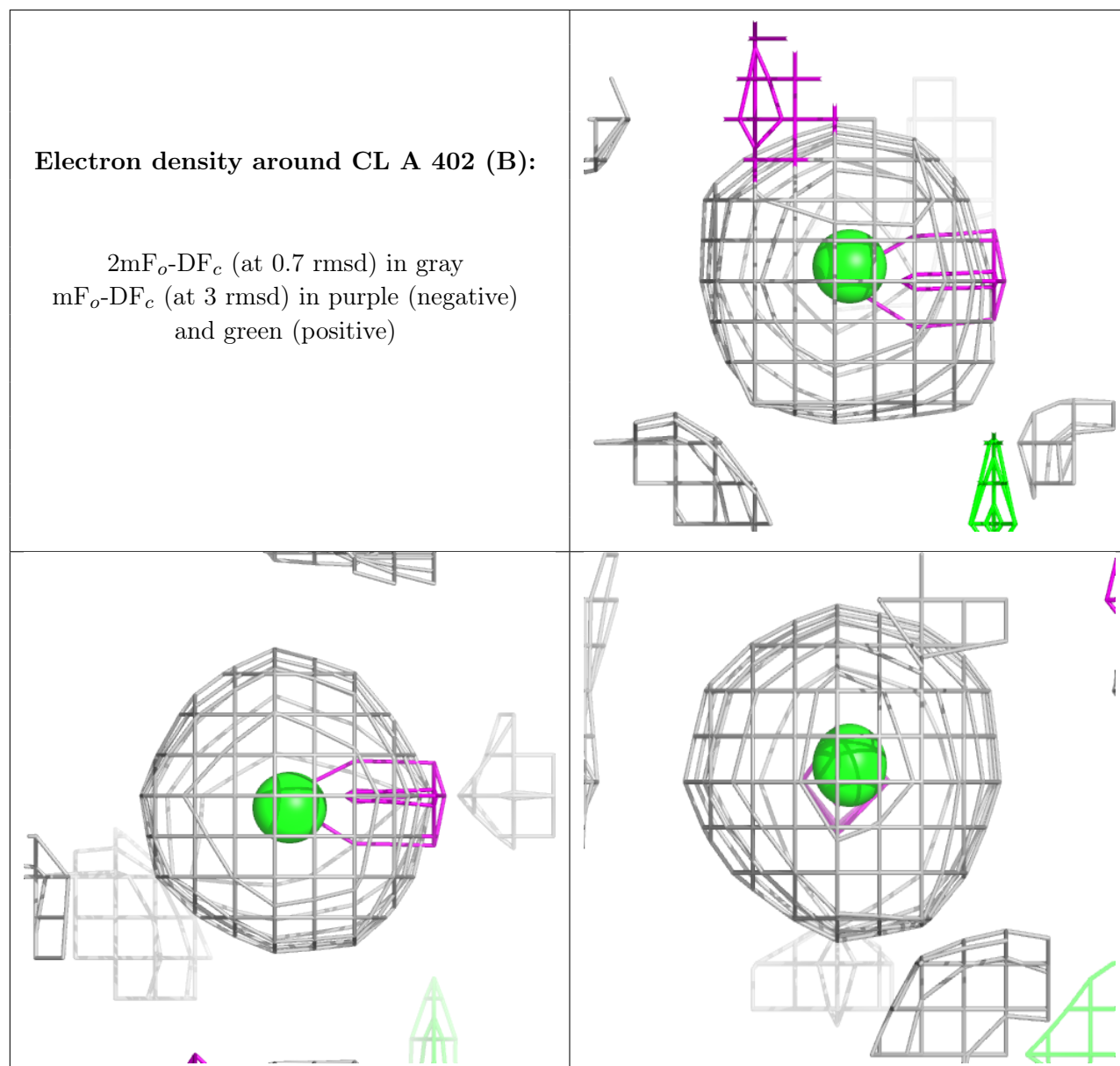


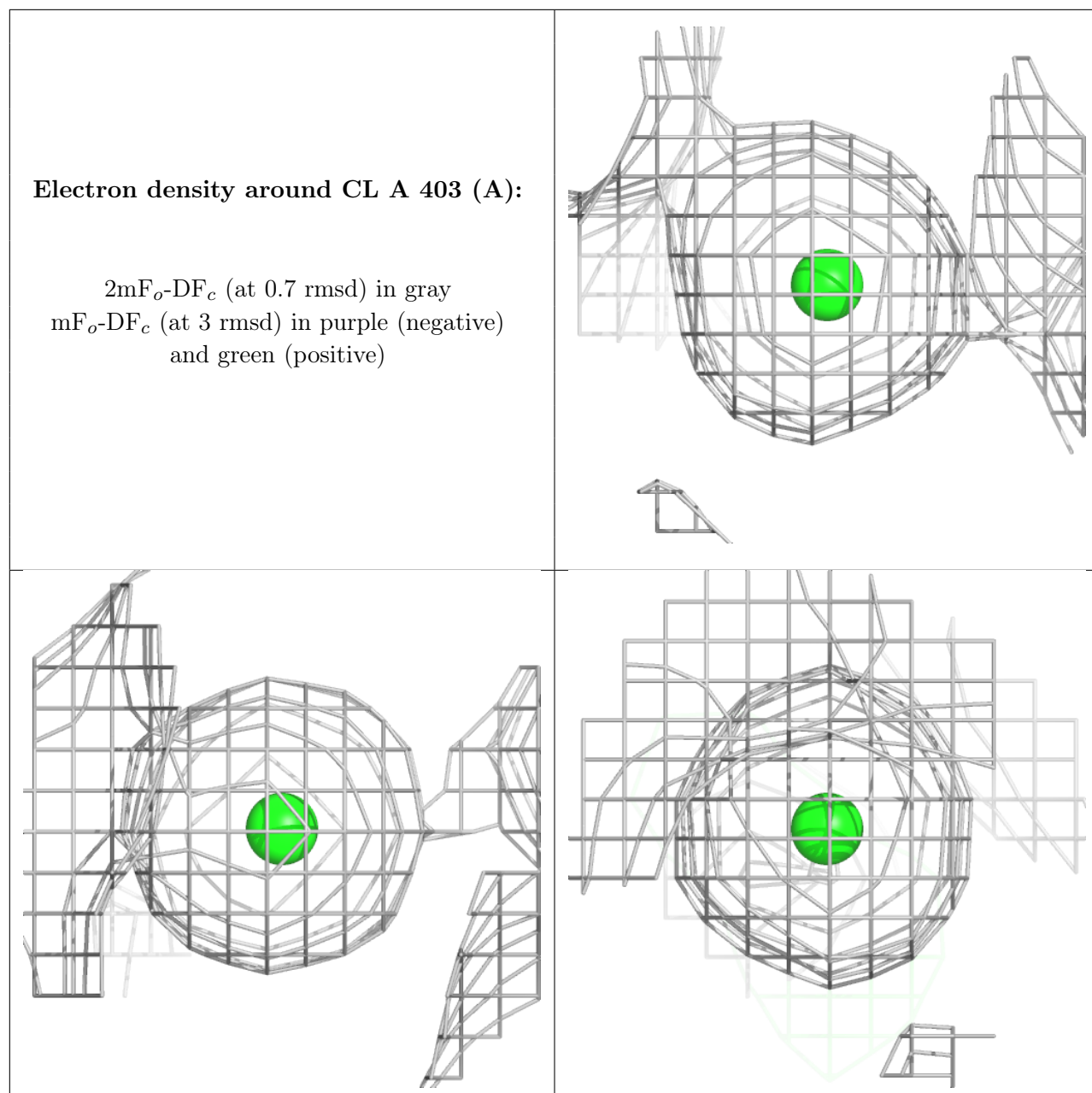
**Electron density around OEX A 412 (B):**

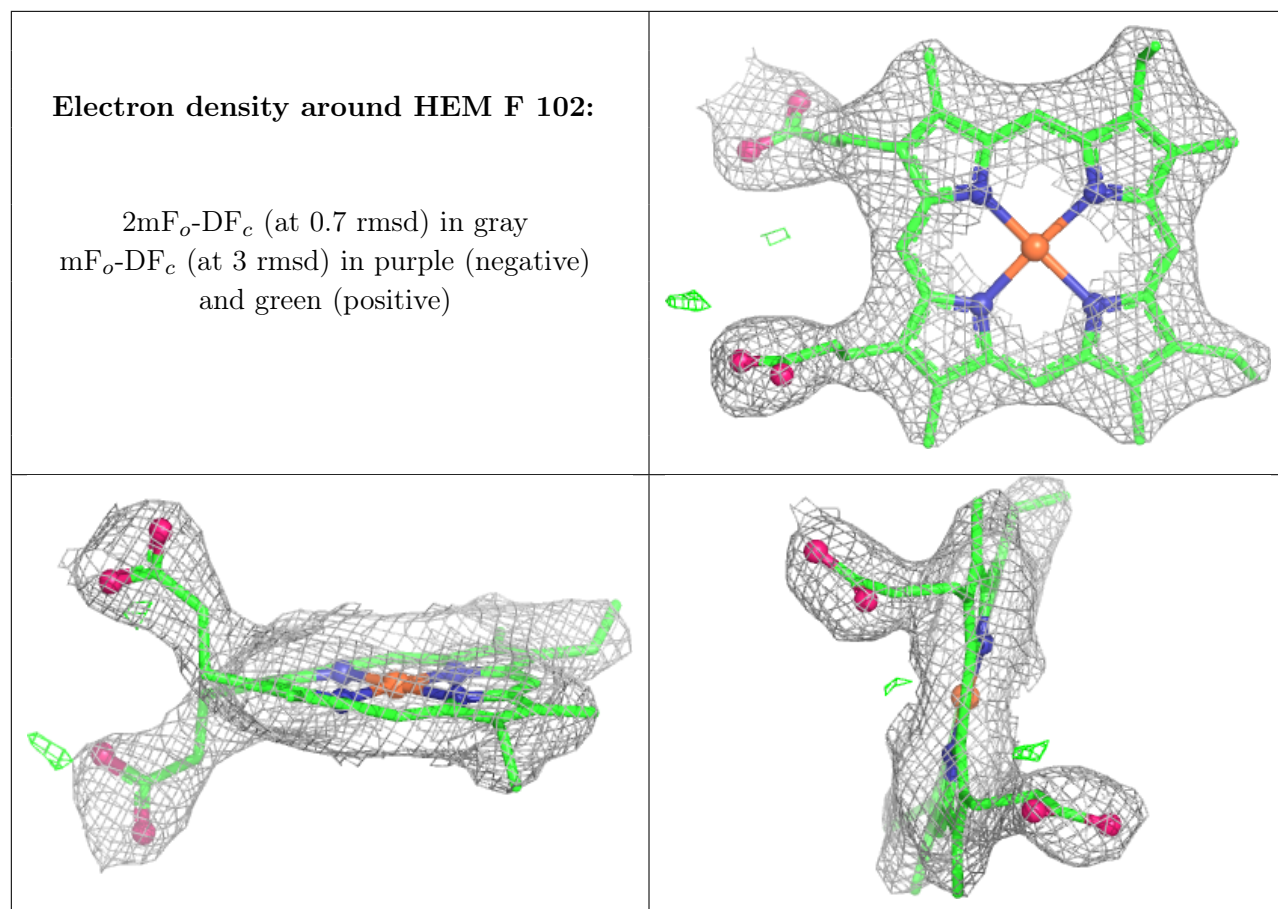
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

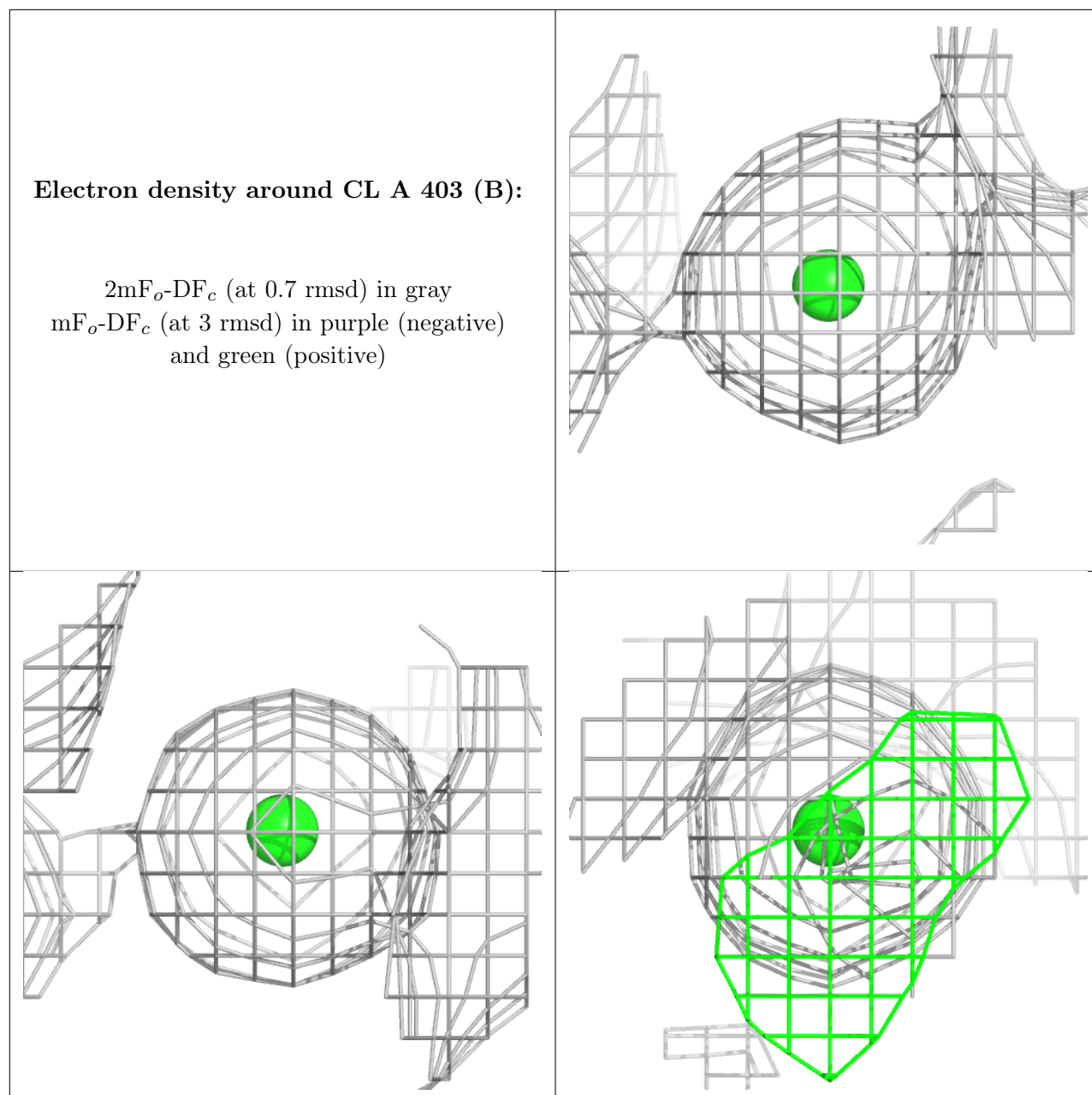






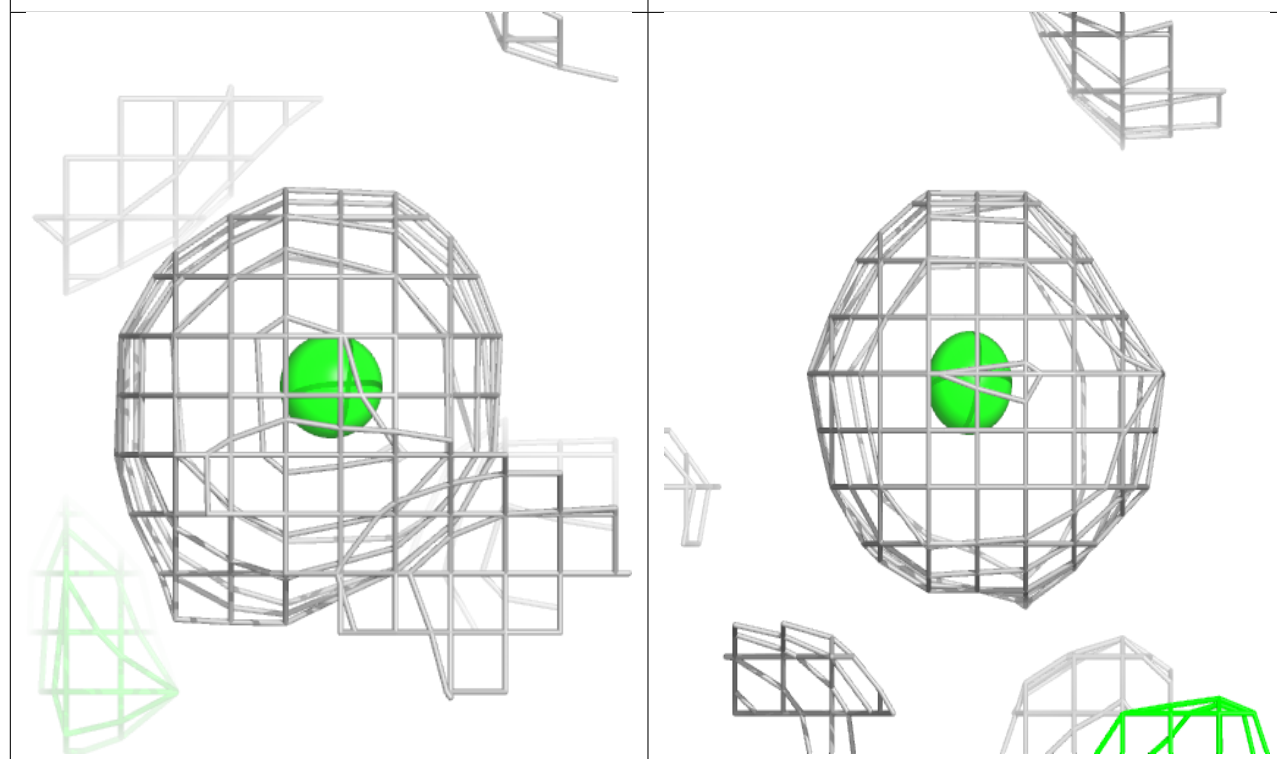
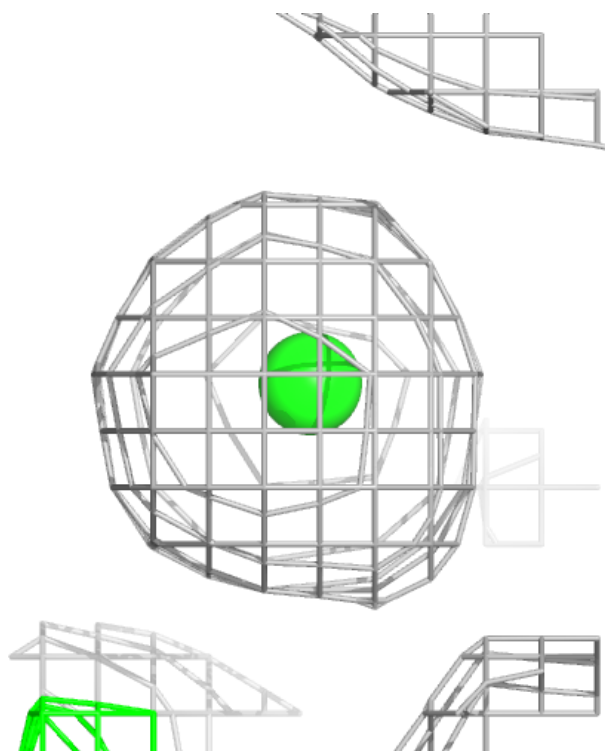






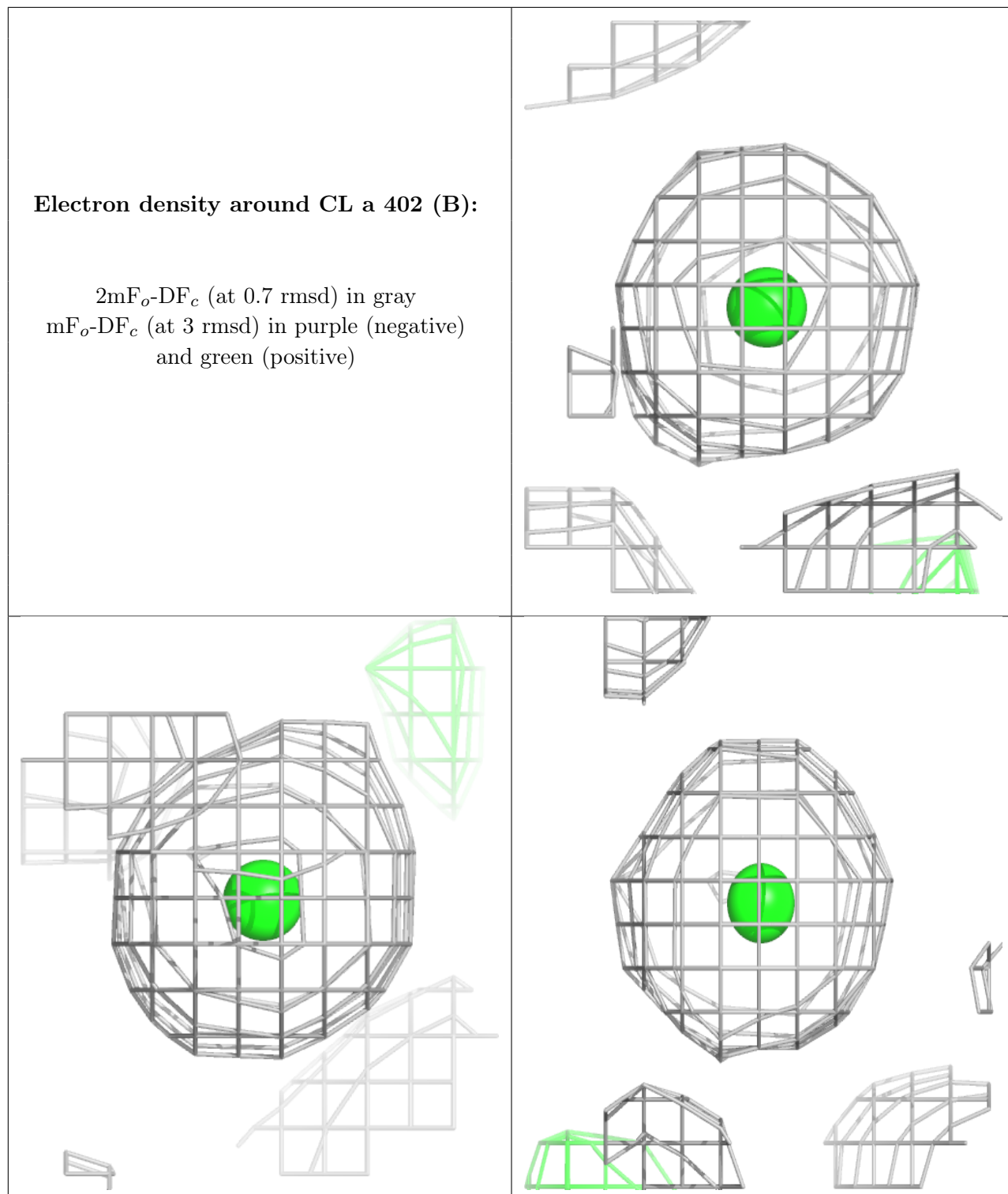
**Electron density around CL a 402 (A):**

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



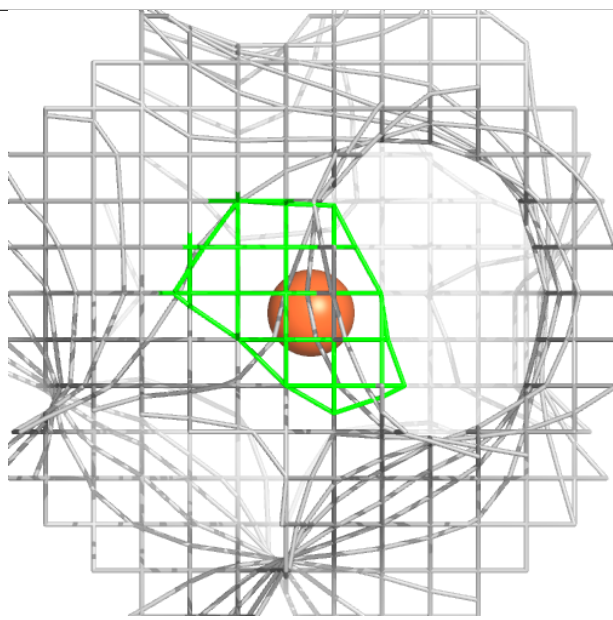
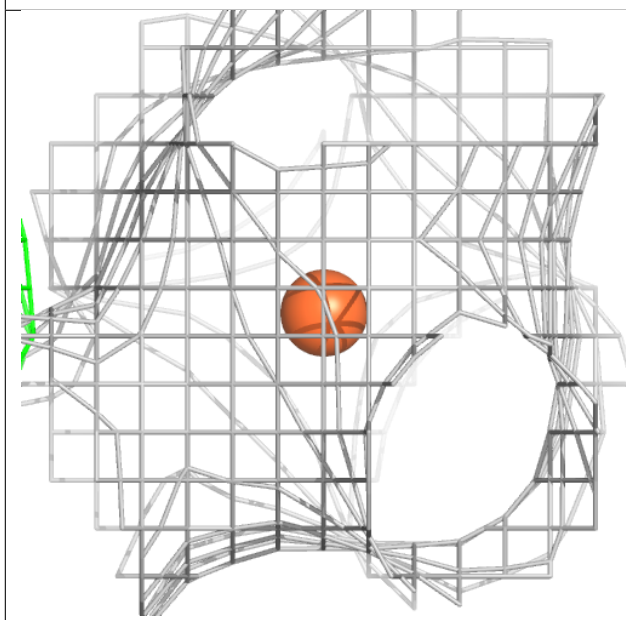
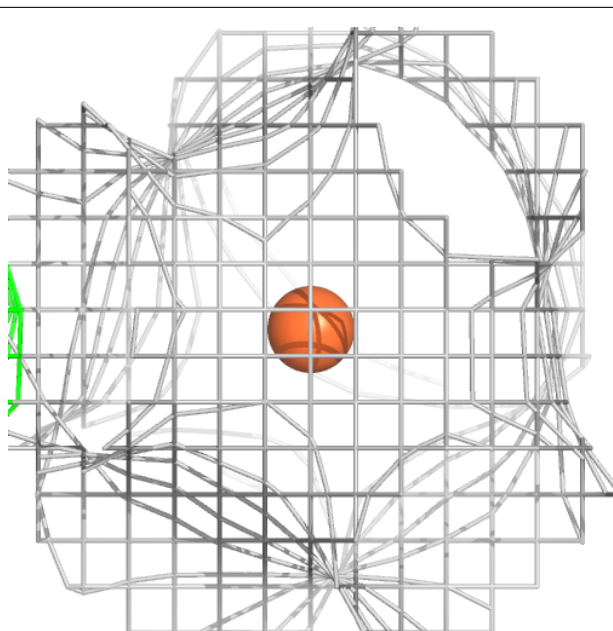
**Electron density around CL a 402 (B):**

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



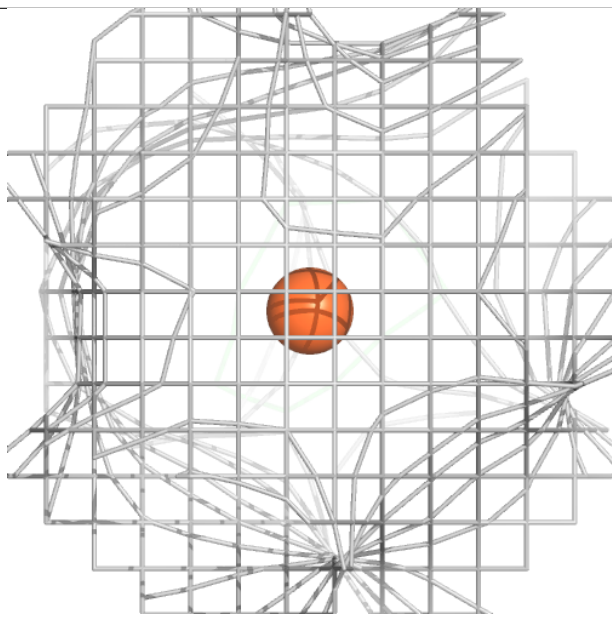
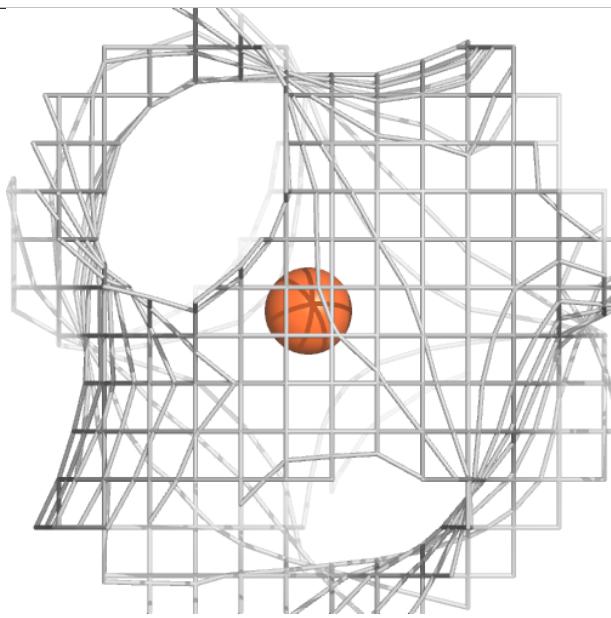
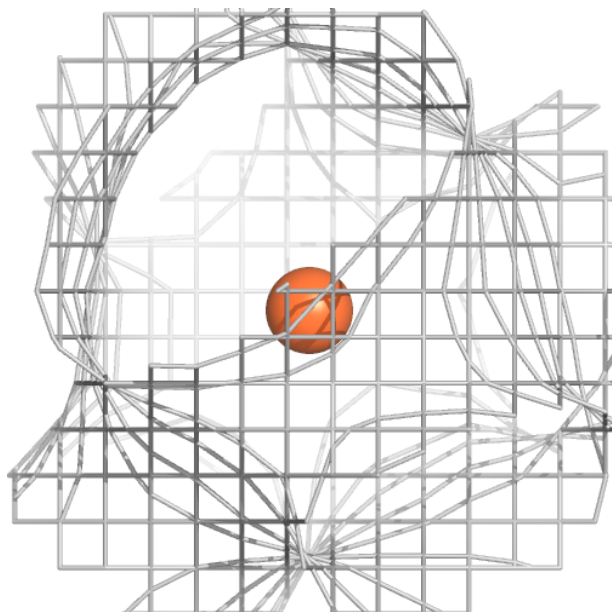
**Electron density around FE2 A 401 (A):**

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



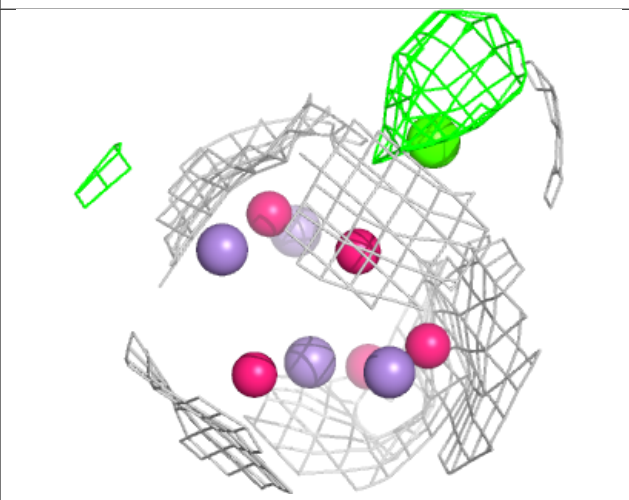
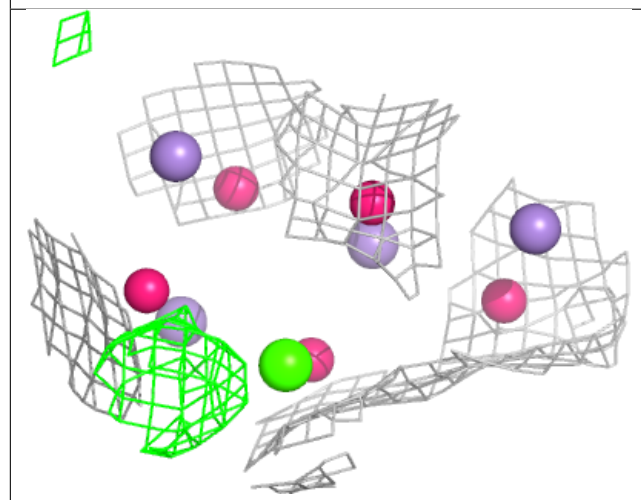
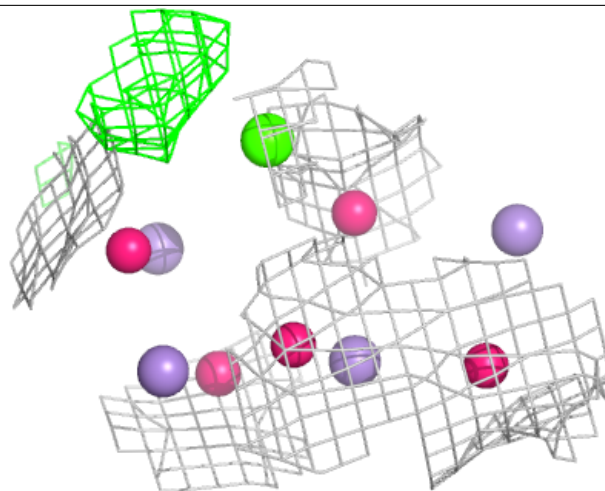
**Electron density around FE2 A 401 (B):**

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



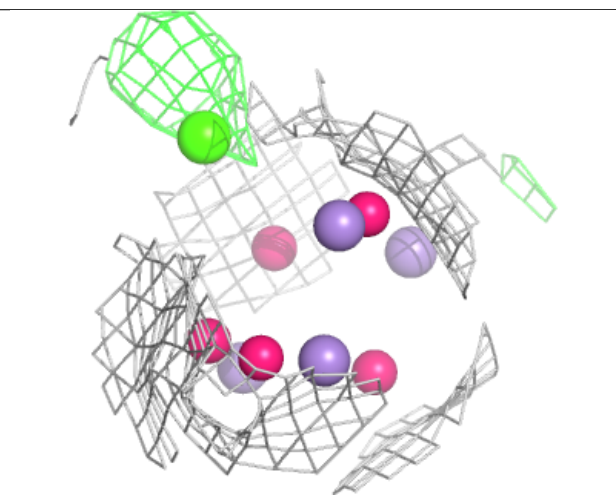
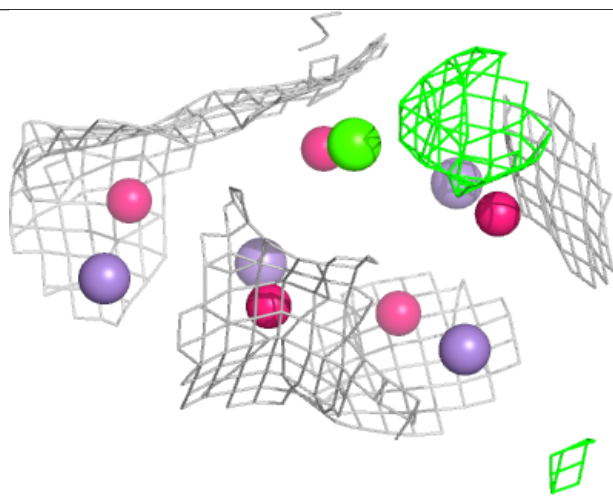
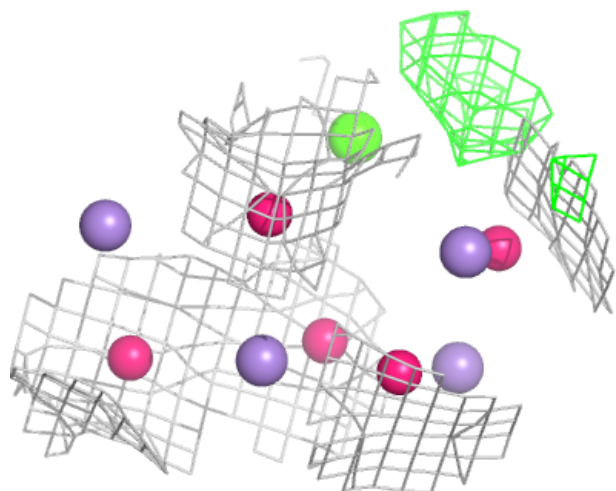
**Electron density around OEX a 412 (A):**

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



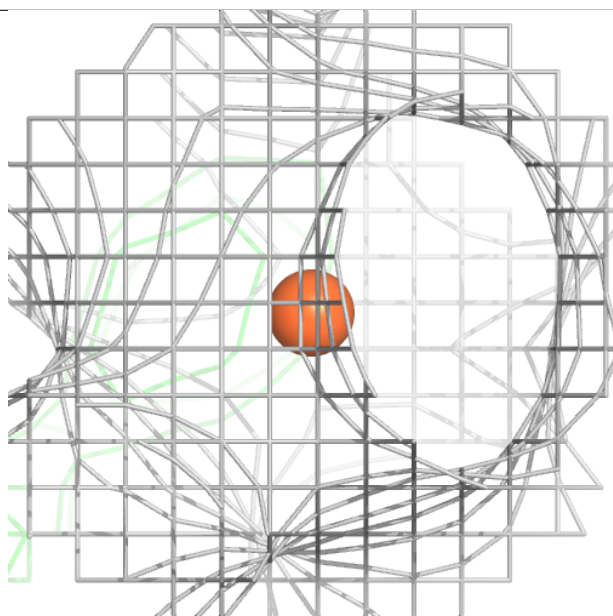
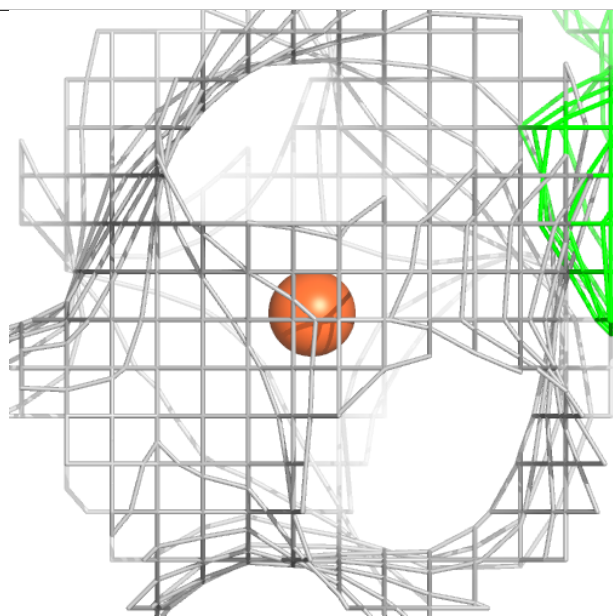
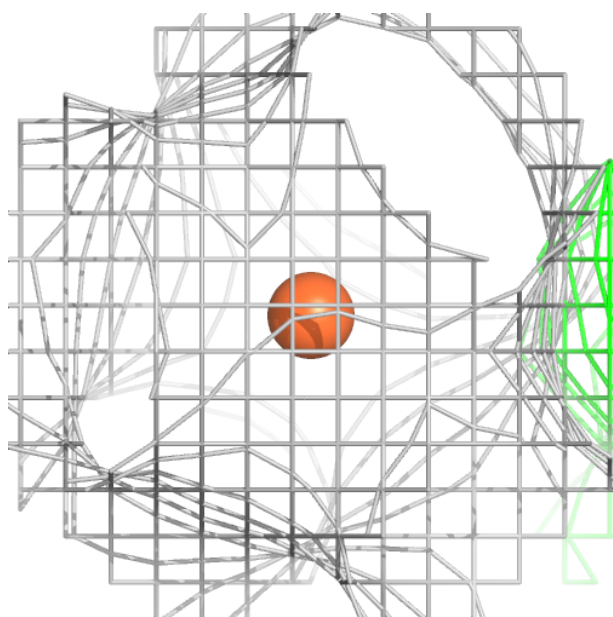
**Electron density around OEX a 412 (B):**

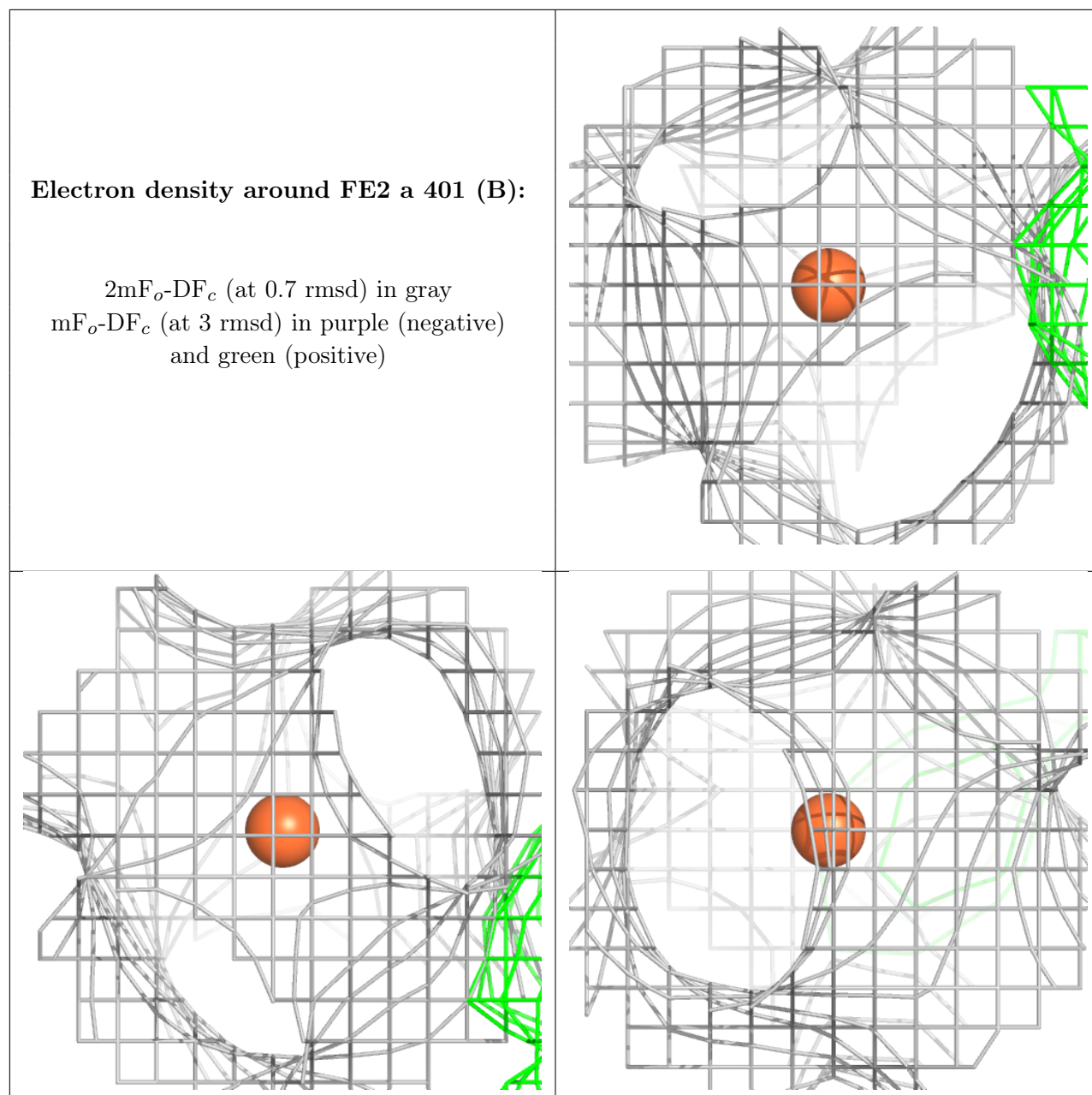
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FE2 a 401 (A):**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.