



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 06:13 AM UTC

PDB ID : 8IRC / pdb_00008irc
Title : XFEL structure of cyanobacterial photosystem II following one flash (1F) with a 5-millisecond delay (Single conformation)
Authors : Li, H.; Suga, M.; Shen, J.R.
Deposited on : 2023-03-17
Resolution : 2.25 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

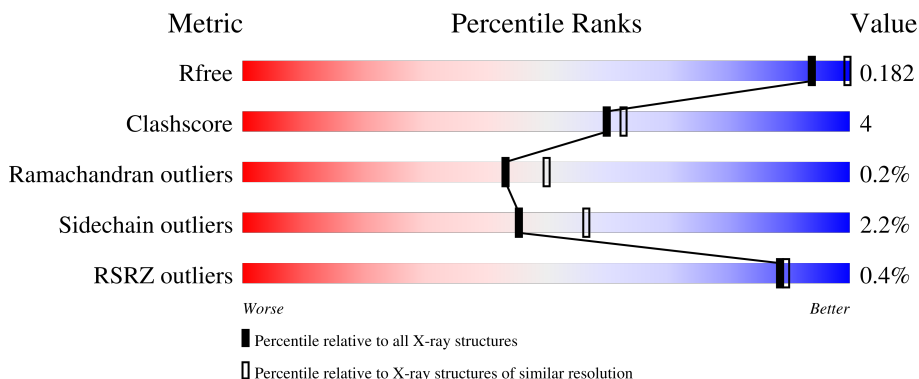
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	344	92%
1	a	344	89% 8%
2	B	505	93% 7%
2	b	505	92% 7%
3	C	455	91% 9%

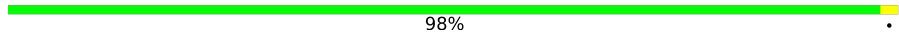
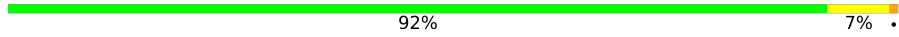







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Mol	Chain	Length	Quality of chain
3	c	455	93% 7% .
4	D	342	91% 9%
4	d	342	94% 6%
5	E	84	80% 17% .
5	e	84	2% 90% . 6%
6	F	44	64% 14% 23%
6	f	44	2% 57% 14% 30%
7	H	65	3% 94% 5% .
7	h	65	2% 86% 12% .
8	I	38	76% 21% .
8	i	38	3% 89% 11%
9	J	39	82% 13% . .
9	j	39	92% 8%
10	K	37	78% 19% .
10	k	37	78% 16% 5%
11	L	37	95% . .
11	l	37	89% 8% .
12	M	36	81% 6% 6% 8%
12	m	36	78% 14% . 6%
13	O	244	88% 12%
13	o	244	91% 8%
14	T	32	84% 9% 6%
14	t	32	81% 12% 6%
15	U	104	84% 9% 8%
15	u	104	87% 6% . 7%

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Mol	Chain	Length	Quality of chain
16	V	137	 98%
16	v	137	 92% 7%
17	X	40	 88% 8% 5%
17	x	40	 88% 8% 5%
18	Y	30	 87% 10% 3%
18	y	30	 70% 27%
19	Z	62	 89% 10%
19	z	62	 79% 19%
20	R	34	 71% 29% 9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	404	X	-	-	-
23	CLA	A	405	X	-	-	-
23	CLA	A	408	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	405	X	-	-	-
23	CLA	D	406	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	406	X	-	-	-
23	CLA	a	409	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	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	c	514	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-
27	GOL	a	801	-	-	X	-

2 Entry composition [i](#)

There are 41 unique types of molecules in this entry. The entry contains 52977 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	2628	1722	432	459	15	0	1	0
1	a	334	2629	1721	432	461	15	0	2	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	4029	2639	674	703	13	0	7	0
2	b	504	4017	2636	669	699	13	0	6	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	3497	2287	588	609	13	0	1	0
3	c	455	3555	2327	595	620	13	0	5	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	1	0
			2732	1808	446	466	12			
4	d	341	Total	C	N	O	S	0	2	0
			2732	1808	447	465	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	S	0	0	0
			662	432	107	123				
5	e	79	Total	C	N	O	S	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	0	0
			296	197	47	52			
11	l	36	Total	C	N	O	0	0	0
			296	197	47	52			

- 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	3	0
			1894	1181	321	388	4			
13	o	243	Total	C	N	O	S	0	0	0
			1865	1165	315	381	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	1	0
			267	186	37	42	2			
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	96	Total	C	N	O	0	1	0
			774	491	129	154			
15	u	97	Total	C	N	O	0	1	0
			781	496	130	155			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	2	0
			1082	685	179	214	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	38	Total	C	N	O	0	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	0
			1	1		
21	a	1	Total	Fe	0	0
			1	1		

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

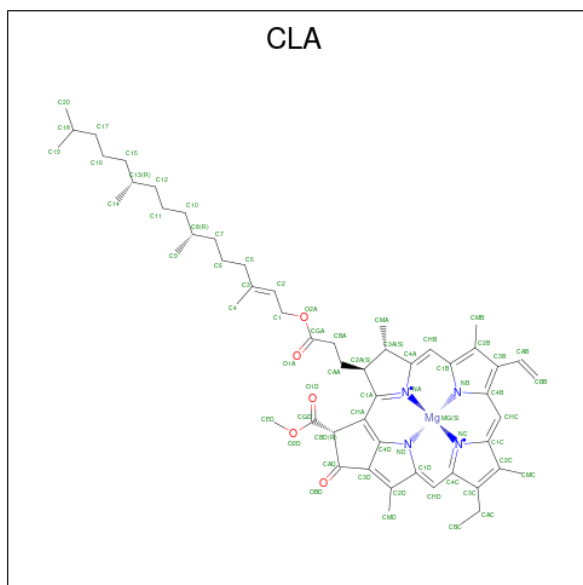
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		

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

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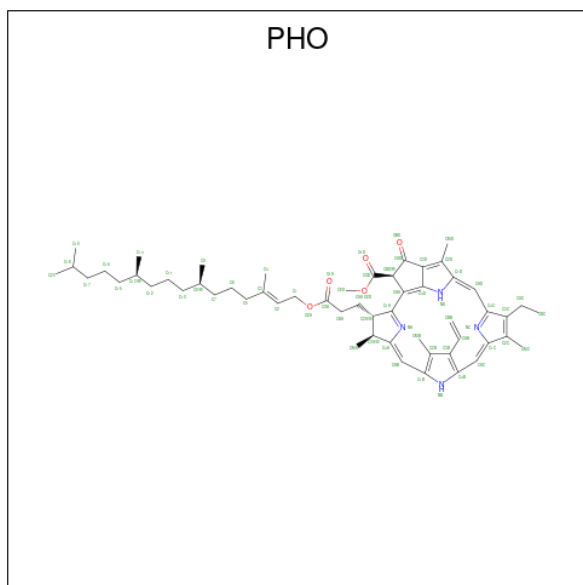
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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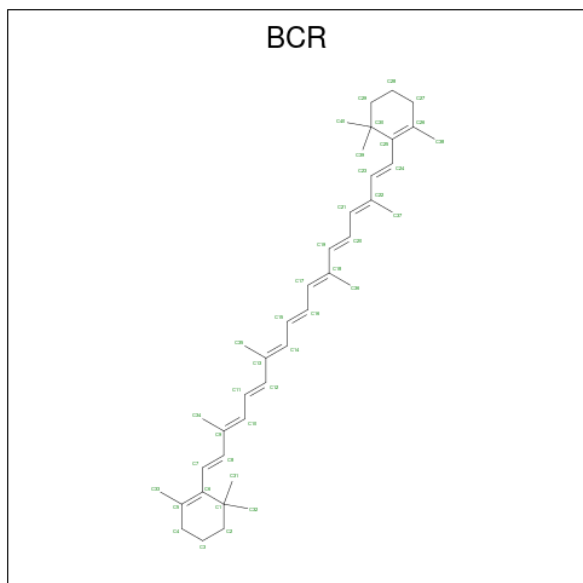
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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



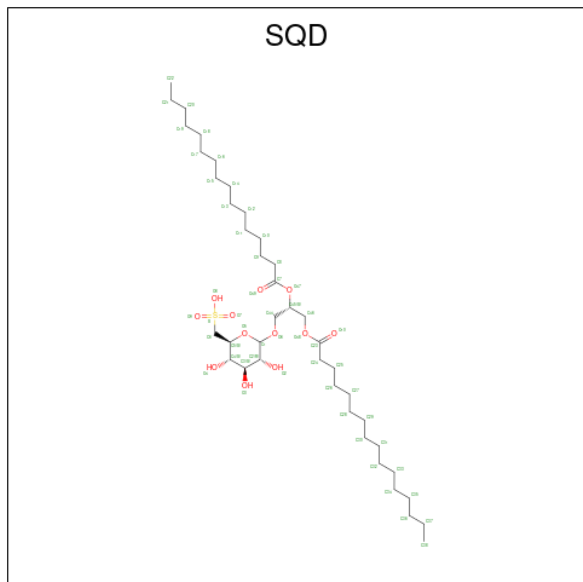
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		

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



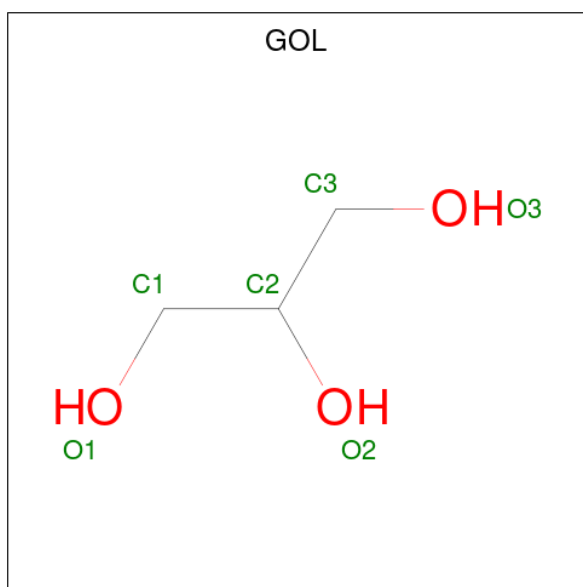
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total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

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



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

- Molecule 27 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



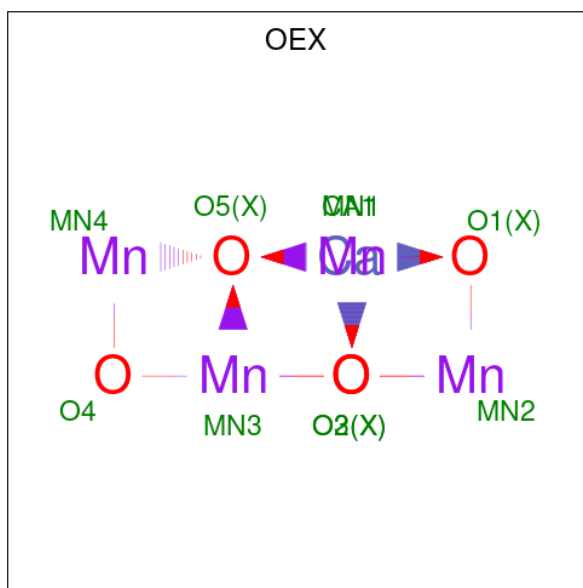
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 6 3 3	0	0
27	A	1	Total C O 6 3 3	0	0
27	B	1	Total C O 6 3 3	0	0
27	B	1	Total C O 6 3 3	0	0
27	C	1	Total C O 6 3 3	0	0
27	D	1	Total C O 6 3 3	0	0
27	O	1	Total C O 6 3 3	0	0
27	O	1	Total C O 6 3 3	0	0
27	V	1	Total C O 6 3 3	0	0
27	a	1	Total C O 6 3 3	0	0
27	a	1	Total C O 6 3 3	0	0
27	a	1	Total C O 6 3 3	0	0
27	b	1	Total C O 6 3 3	0	0
27	b	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	c	1	Total	C	O	0	0
			6	3	3		
27	c	1	Total	C	O	0	0
			6	3	3		
27	d	1	Total	C	O	0	0
			6	3	3		
27	d	1	Total	C	O	0	0
			6	3	3		
27	o	1	Total	C	O	0	0
			6	3	3		
27	o	1	Total	C	O	0	0
			6	3	3		
27	v	1	Total	C	O	0	0
			6	3	3		

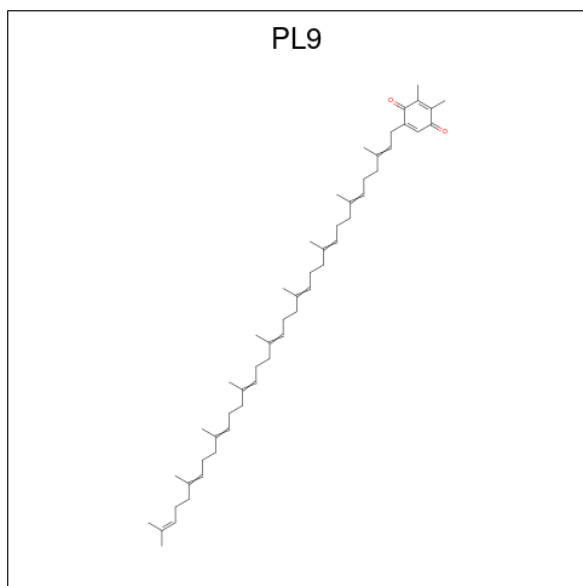
- Molecule 28 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $\text{C}_{53}\text{H}_{80}\text{O}_2$)

(labeled as "Ligand of Interest" by depositor).



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

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

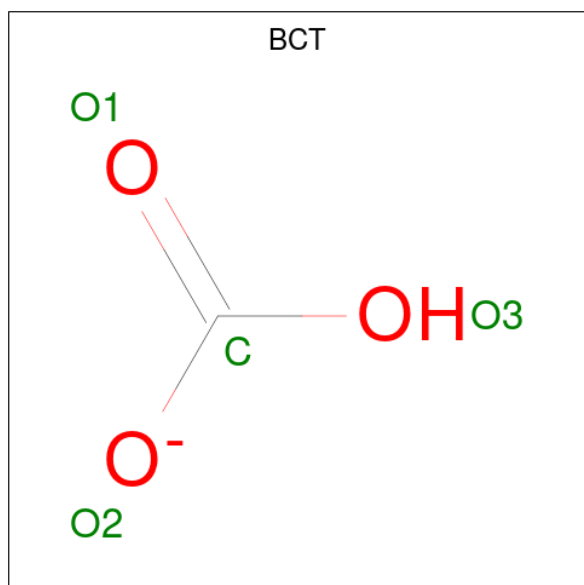
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			28	23	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	I	1	Total	C	O	0	0
			40	35	5		
30	J	1	Total	C		0	0
			10	10			
30	K	1	Total	C	O	0	0
			34	29	5		
30	M	1	Total	C		0	0
			10	10			

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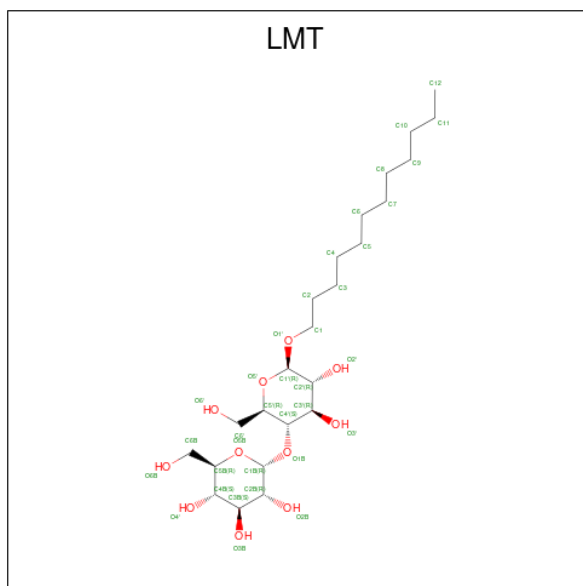
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	X	1	Total	C	O	0	0
			18	16	2		
30	a	1	Total	C	O	0	0
			30	25	5		
30	b	1	Total	C	O	0	0
			33	28	5		
30	c	1	Total	C	O	0	0
			32	27	5		
30	d	2	Total	C	O	0	0
			53	47	6		
30	i	1	Total	C	O	0	0
			40	35	5		
30	j	1	Total	C		0	0
			10	10			
30	m	1	Total	C		0	0
			10	10			
30	x	1	Total	C	O	0	0
			18	16	2		

- Molecule 31 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			4	1	3		
31	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 32 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



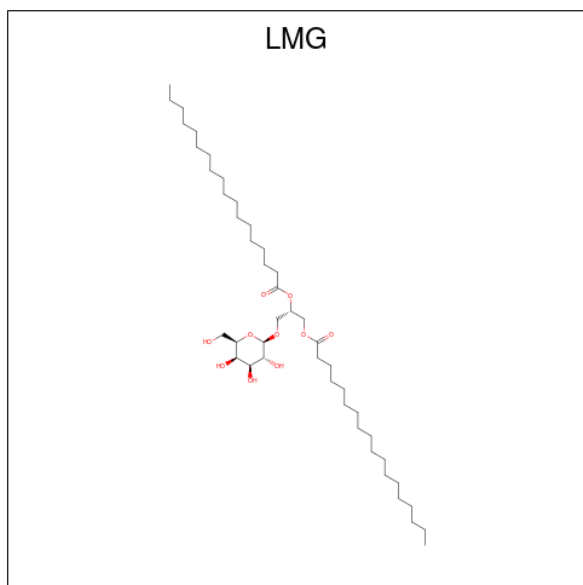
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total C O 35 24 11	0	0
32	D	1	Total C O 35 24 11	0	0
32	E	1	Total C O 35 24 11	0	0
32	I	1	Total C O 35 24 11	0	0
32	M	1	Total C O 35 24 11	0	0
32	M	1	Total C O 35 24 11	0	0
32	a	1	Total C O 35 24 11	0	0
32	a	1	Total C O 35 24 11	0	0
32	b	1	Total C O 25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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
32	t	1	26	19	7	0	0

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



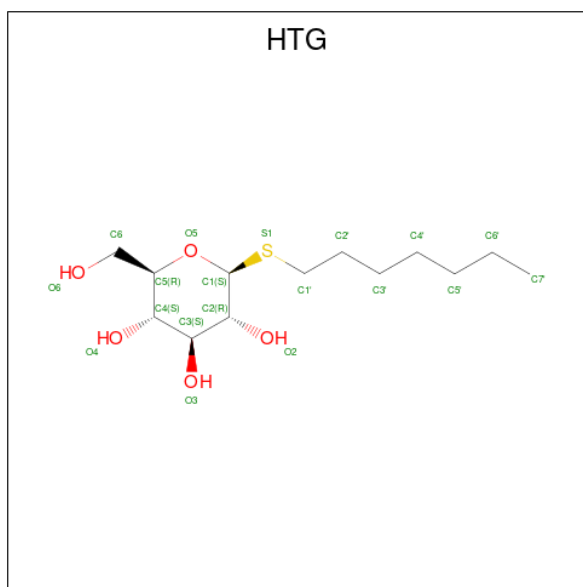
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
33	B	1	51	41	10	0	0
33	C	1	51	41	10	0	0
33	C	1	51	41	10	0	0
33	C	1	51	41	10	0	0
33	D	1	51	41	10	0	0
33	a	1	51	41	10	0	0
33	c	1	51	41	10	0	0
33	c	1	51	41	10	0	0
33	d	1	51	41	10	0	0
33	m	1	51	41	10	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	Z	1	Total	C	O	0	0
			37	27	10		
33	z	1	Total	C	O	0	0
			39	29	10		

- Molecule 34 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C₁₃H₂₆O₅S).



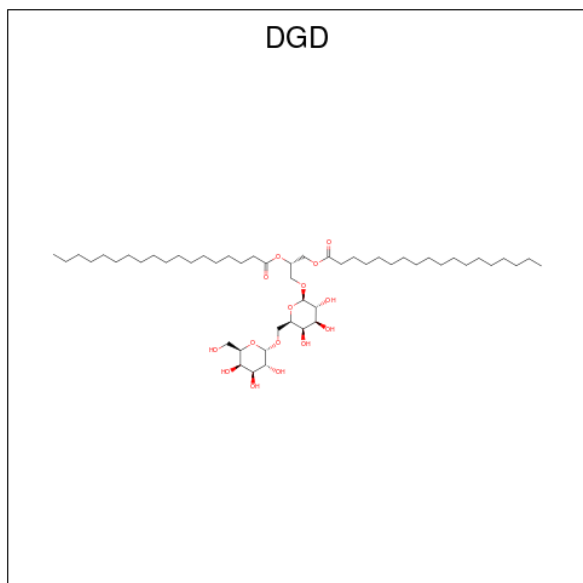
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	C	1	Total	C	O	S	0	0
			19	13	5	1		
34	D	1	Total	C	O	S	0	0
			16	10	5	1		
34	V	1	Total	C	O		0	0
			11	6	5			
34	b	1	Total	C	O	S	0	0
			19	13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

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

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

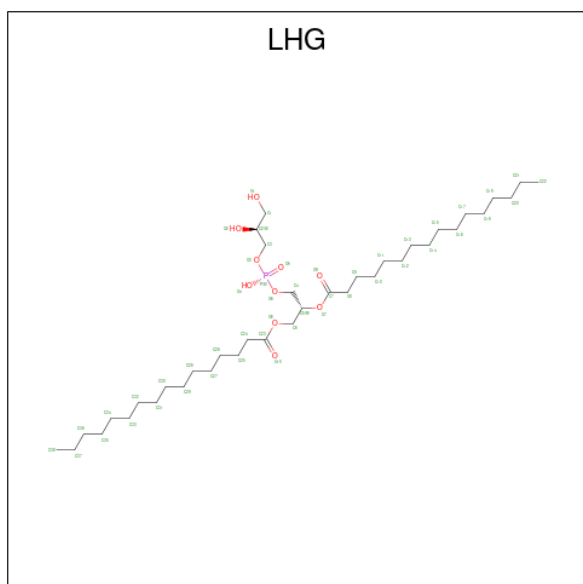


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
35	C	1	62	47	15	0	0
35	C	1	62	47	15	0	0
35	C	1	62	47	15	0	0
35	H	1	62	47	15	0	0
35	c	1	62	47	15	0	0
35	c	1	62	47	15	0	0
35	c	1	62	47	15	0	0
35	h	1	62	47	15	0	0

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

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

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



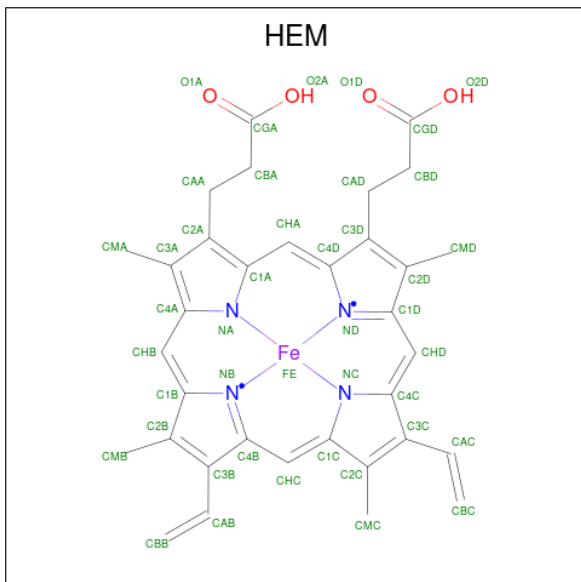
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	D	1	Total C O P 49 38 10 1	0	0
37	D	1	Total C O P 49 38 10 1	0	0
37	D	1	Total C O P 49 38 10 1	0	0
37	E	1	Total C O P 42 31 10 1	0	0
37	L	1	Total C O P 49 38 10 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	d	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0
			49	38	10	1		
37	e	1	Total	C	O	P	0	0
			42	31	10	1		
37	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

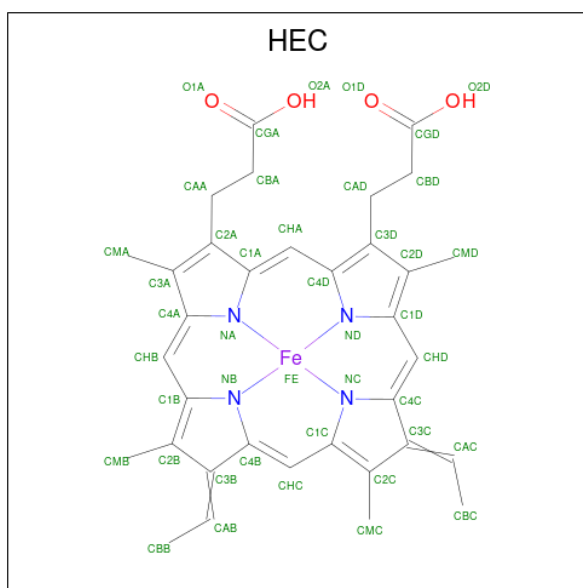


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
38	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
38	e	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

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

- Molecule 40 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	126	Total	O	0	1
			127	127		
41	B	164	Total	O	0	0
			164	164		
41	C	141	Total	O	0	0
			141	141		
41	D	118	Total	O	0	0
			118	118		
41	E	14	Total	O	0	0
			14	14		
41	F	3	Total	O	0	0
			3	3		
41	H	17	Total	O	0	0
			17	17		
41	I	6	Total	O	0	0
			6	6		
41	J	5	Total	O	0	0
			5	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	K	5	Total O 5 5	0	0
41	L	3	Total O 3 3	0	0
41	M	5	Total O 5 5	0	0
41	O	70	Total O 70 70	0	0
41	T	8	Total O 8 8	0	0
41	U	32	Total O 32 32	0	0
41	V	65	Total O 65 65	0	0
41	X	1	Total O 1 1	0	0
41	a	128	Total O 128 128	0	0
41	b	182	Total O 182 182	0	0
41	c	133	Total O 133 133	0	0
41	d	109	Total O 109 109	0	0
41	e	8	Total O 8 8	0	0
41	f	3	Total O 3 3	0	0
41	h	15	Total O 15 15	0	0
41	i	3	Total O 3 3	0	0
41	j	2	Total O 2 2	0	0
41	k	3	Total O 3 3	0	0
41	l	4	Total O 4 4	0	0
41	m	14	Total O 14 14	0	0
41	o	76	Total O 76 76	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	t	6	Total O 6 6	0	0
41	u	47	Total O 47 47	0	0
41	v	41	Total O 41 41	0	0
41	x	2	Total O 2 2	0	0
41	y	1	Total O 1 1	0	0
41	G	264	Total O 264 264	0	1

3 Residue-property plots [i](#)


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

- Molecule 1: Photosystem II protein D1

Chain A:  92%



- Molecule 1: Photosystem II protein D1

Chain a:  89% 8%



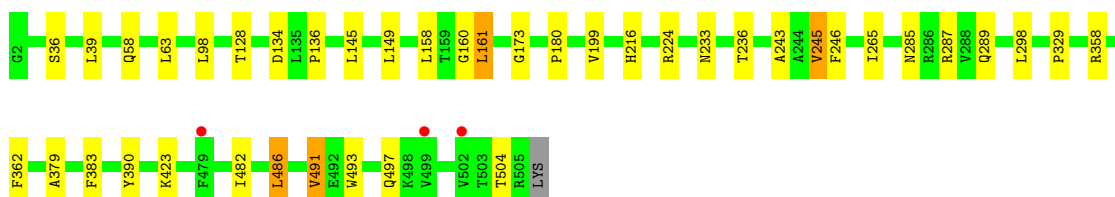
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  93% 7%




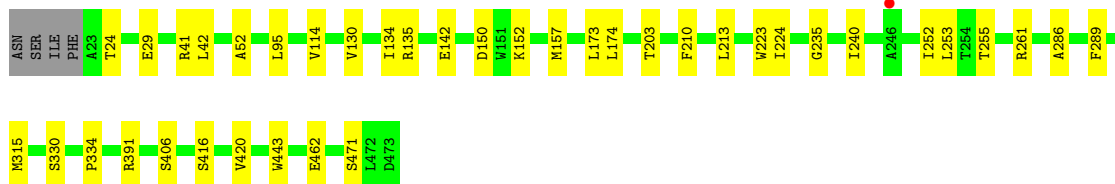
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  92% 7%




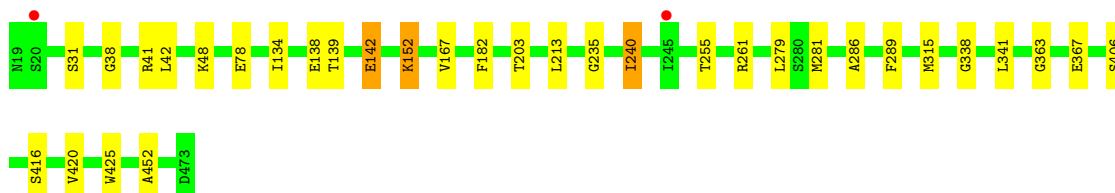
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C:  91% 9%




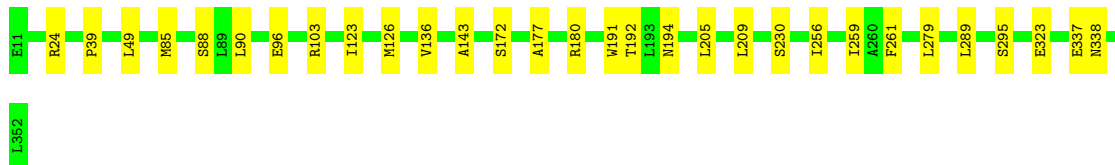
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c:  93% 7%



- Molecule 4: Photosystem II D2 protein

Chain D:  91% 9%




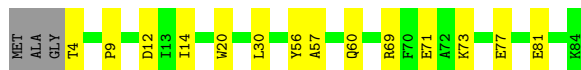
- Molecule 4: Photosystem II D2 protein

Chain d:  94% 6%




- Molecule 5: Cytochrome b559 subunit alpha

Chain E:  80% 17%

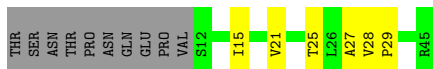


- Molecule 5: Cytochrome b559 subunit alpha

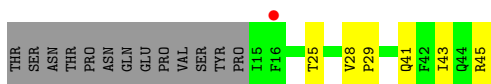
Chain e:  90% 6%



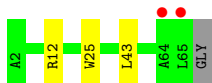
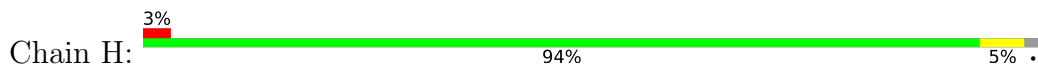
- Molecule 6: Cytochrome b559 subunit beta



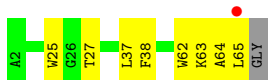
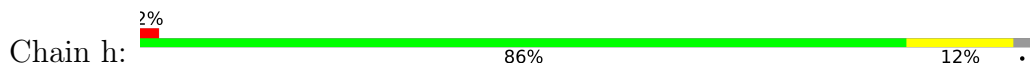
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H



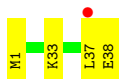
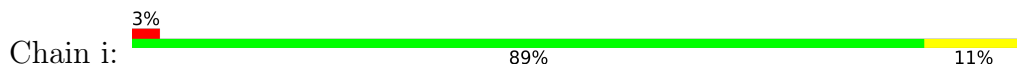
- Molecule 7: Photosystem II reaction center protein H




- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I




- Molecule 9: Photosystem II reaction center protein J

Chain J:  82% 13%




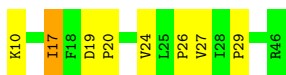
- Molecule 9: Photosystem II reaction center protein J

Chain j:  92% 8%




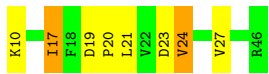
- Molecule 10: Photosystem II reaction center protein K

Chain K:  78% 19%



- Molecule 10: Photosystem II reaction center protein K

Chain k:  78% 16% 5%




- Molecule 11: Photosystem II reaction center protein L

Chain L:  95%




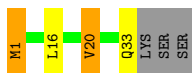
- Molecule 11: Photosystem II reaction center protein L

Chain l:  89% 8%




- Molecule 12: Photosystem II reaction center protein M

Chain M:  81% 6% 6% 8%




- Molecule 12: Photosystem II reaction center protein M

Chain m:  78% 14% 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  88% 12%




- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  91% 8%




- Molecule 14: Photosystem II reaction center protein T

Chain T:  84% 9% 6%




- Molecule 14: Photosystem II reaction center protein T

Chain t:  81% 12% 6%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  84% 9% 8%



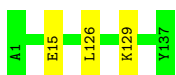
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  87% 6% 7%



- Molecule 16: Cytochrome c-550

Chain V:  98%




- Molecule 16: Cytochrome c-550

Chain v:  92% 7%




- Molecule 17: Photosystem II reaction center protein X

Chain X:  88% 8% 5%




- Molecule 17: Photosystem II reaction center protein X

Chain x:  88% 8% 5%



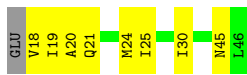
- Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:  87% 10% 3%




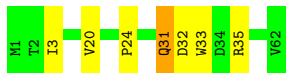
- Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:  70% 27%




- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  89% 10%



- Molecule 19: Photosystem II reaction center protein Z

Chain z:  79% 19%



● Molecule 20: Photosystem II protein Y

Chain R:  9% 71% 29%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	125.77Å 231.76Å 288.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.25 19.99 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.25) 99.8 (19.99-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.26Å)	Xtrriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.145 , 0.180 0.146 , 0.182	Depositor DCC
R_{free} test set	19914 reflections (2.44%)	wwPDB-VP
Wilson B-factor (Å ²)	50.9	Xtrriage
Anisotropy	0.487	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 69.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	52977	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.36	0/2713	0.52	0/3700
1	a	0.33	0/2717	0.49	0/3705
2	B	0.33	0/4169	0.47	0/5679
2	b	0.30	0/4161	0.47	0/5669
3	C	0.29	0/3610	0.44	0/4914
3	c	0.29	0/3675	0.45	0/5002
4	D	0.37	0/2827	0.51	0/3852
4	d	0.34	0/2827	0.48	0/3852
5	E	0.28	0/681	0.47	0/928
5	e	0.25	0/690	0.44	0/939
6	F	0.28	0/284	0.44	0/387
6	f	0.25	0/269	0.38	0/365
7	H	0.29	0/519	0.46	0/708
7	h	0.26	0/530	0.44	0/722
8	I	0.27	0/311	0.45	0/419
8	i	0.30	0/311	0.43	0/419
9	J	0.27	0/278	0.36	0/376
9	j	0.27	0/283	0.40	0/383
10	K	0.29	0/303	0.46	0/416
10	k	0.33	0/303	0.44	0/416
11	L	0.33	0/303	0.46	0/412
11	l	0.35	0/303	0.44	0/412
12	M	0.34	0/261	0.47	0/357
12	m	0.31	0/279	0.44	0/380
13	O	0.30	0/1925	0.48	0/2609
13	o	0.29	0/1896	0.48	0/2571
14	T	0.34	0/266	0.43	0/362
14	t	0.31	0/257	0.42	0/349
15	U	0.32	0/785	0.52	0/1064
15	u	0.32	0/792	0.50	0/1074
16	V	0.32	0/1103	0.46	0/1497

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.27	0/1085	0.44	0/1473
17	X	0.21	0/292	0.33	0/395
17	x	0.20	0/284	0.32	0/384
18	Y	0.21	0/216	0.39	0/289
18	y	0.21	0/216	0.37	0/289
19	Z	0.19	0/490	0.34	0/669
19	z	0.19	0/490	0.36	0/669
20	R	0.21	0/279	0.32	0/383
All	All	0.31	0/42983	0.47	0/58489

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	2628	0	2527	10	0
1	a	2629	0	2526	21	0
2	B	4029	0	3880	24	0
2	b	4017	0	3872	33	0
3	C	3497	0	3419	23	0
3	c	3555	0	3480	23	0
4	D	2732	0	2631	24	0
4	d	2732	0	2632	14	0
5	E	662	0	648	11	0
5	e	670	0	655	2	0
6	F	275	0	282	4	0
6	f	261	0	269	5	0
7	H	506	0	529	3	0
7	h	517	0	541	5	0
8	I	314	0	328	5	0
8	i	314	0	328	2	0
9	J	272	0	279	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	277	0	284	2	0
10	K	293	0	305	4	0
10	k	293	0	305	7	0
11	L	296	0	304	1	0
11	l	296	0	304	3	0
12	M	268	0	285	4	0
12	m	286	0	305	8	0
13	O	1894	0	1860	15	0
13	o	1865	0	1838	8	0
14	T	267	0	267	0	0
14	t	258	0	261	3	0
15	U	774	0	772	4	0
15	u	781	0	781	4	0
16	V	1082	0	1083	1	0
16	v	1064	0	1073	5	0
17	X	289	0	322	2	0
17	x	281	0	312	3	0
18	Y	215	0	246	3	0
18	y	215	0	246	6	0
19	Z	479	0	516	3	0
19	z	479	0	516	3	0
20	R	273	0	305	5	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0
23	A	260	0	288	7	0
23	B	1040	0	1152	24	0
23	C	845	0	936	27	0
23	D	130	0	144	3	0
23	a	260	0	288	10	0
23	b	1040	0	1152	28	0
23	c	845	0	936	25	0
23	d	130	0	144	4	0
24	A	128	0	148	3	0
24	a	128	0	148	1	0
25	A	40	0	56	2	0
25	B	120	0	168	6	0
25	C	80	0	112	2	0
25	D	40	0	56	2	0
25	H	40	0	56	2	0
25	K	40	0	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	T	40	0	56	6	0
25	Y	40	0	56	1	0
25	a	40	0	56	1	0
25	b	120	0	168	10	0
25	c	80	0	112	5	0
25	d	40	0	56	2	0
25	h	40	0	56	3	0
25	k	40	0	56	0	0
25	t	40	0	56	4	0
25	y	40	0	56	1	0
26	A	108	0	156	1	0
26	B	54	0	78	1	0
26	F	43	0	53	1	0
26	a	108	0	155	4	0
26	b	54	0	78	3	0
26	f	43	0	53	0	0
27	A	12	0	16	3	0
27	B	12	0	16	2	0
27	C	6	0	8	0	0
27	D	6	0	7	1	0
27	O	12	0	16	3	0
27	V	6	0	8	0	0
27	a	18	0	24	5	0
27	b	12	0	16	2	0
27	c	12	0	16	0	0
27	d	12	0	16	1	0
27	o	12	0	16	0	0
27	v	6	0	8	1	0
28	A	10	0	0	0	0
28	a	10	0	0	0	0
29	A	55	0	80	10	0
29	D	55	0	80	1	0
29	a	55	0	80	4	0
29	d	55	0	80	0	0
30	A	28	0	0	0	0
30	B	33	0	0	0	0
30	D	57	0	0	0	0
30	I	40	0	0	0	0
30	J	10	0	0	0	0
30	K	34	0	0	0	0
30	M	10	0	0	0	0
30	X	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	a	30	0	0	0	0
30	b	33	0	0	0	0
30	c	32	0	0	0	0
30	d	53	0	0	0	0
30	i	40	0	0	0	0
30	j	10	0	0	0	0
30	m	10	0	0	0	0
30	x	18	0	0	0	0
31	A	4	0	0	0	0
31	a	4	0	0	0	0
32	A	35	0	46	1	0
32	D	35	0	46	1	0
32	E	35	0	46	0	0
32	I	35	0	46	1	0
32	M	70	0	92	2	0
32	a	70	0	92	2	0
32	b	50	0	70	1	0
32	e	35	0	46	1	0
32	m	35	0	46	0	0
32	t	51	0	69	2	0
33	B	51	0	72	1	0
33	C	153	0	216	3	0
33	D	51	0	72	0	0
33	Z	37	0	44	2	0
33	a	51	0	72	0	0
33	c	102	0	144	2	0
33	d	51	0	72	2	0
33	m	51	0	72	0	0
33	z	39	0	48	2	0
34	B	57	0	78	3	0
34	C	19	0	26	0	0
34	D	16	0	17	1	0
34	V	11	0	10	0	0
34	b	57	0	78	2	0
34	c	19	0	26	1	0
34	d	16	0	17	1	0
35	C	186	0	246	3	0
35	H	62	0	82	1	0
35	c	186	0	246	5	0
35	h	62	0	82	0	0
36	C	1	0	0	0	0
36	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	O	1	0	0	0	0
36	c	2	0	0	0	0
36	f	1	0	0	0	0
36	o	1	0	0	0	0
37	D	147	0	222	5	0
37	E	42	0	57	3	0
37	L	49	0	74	0	0
37	d	147	0	222	13	0
37	e	42	0	57	5	0
37	l	49	0	74	0	0
38	E	43	0	30	1	0
38	e	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	127	0	0	0	0
41	B	164	0	0	1	0
41	C	141	0	0	0	0
41	D	118	0	0	0	0
41	E	14	0	0	0	0
41	F	3	0	0	0	0
41	G	264	0	0	4	0
41	H	17	0	0	0	0
41	I	6	0	0	0	0
41	J	5	0	0	2	0
41	K	5	0	0	0	0
41	L	3	0	0	0	0
41	M	5	0	0	0	0
41	O	70	0	0	1	0
41	T	8	0	0	1	0
41	U	32	0	0	0	0
41	V	65	0	0	0	0
41	X	1	0	0	0	0
41	a	128	0	0	1	0
41	b	182	0	0	0	0
41	c	133	0	0	1	0
41	d	109	0	0	0	0
41	e	8	0	0	0	0
41	f	3	0	0	1	0
41	h	15	0	0	0	0
41	i	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	j	2	0	0	0	0
41	k	3	0	0	0	0
41	l	4	0	0	0	0
41	m	14	0	0	0	0
41	o	76	0	0	0	0
41	t	6	0	0	0	0
41	u	47	0	0	0	0
41	v	41	0	0	1	0
41	x	2	0	0	0	0
41	y	1	0	0	0	0
All	All	52977	0	52089	447	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 4.

The worst 5 of 447 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)
27:A:701:GOL:H11	12:M:1:FME:HG2	1.45	0.98
1:a:250:ALA:HA	2:b:491:VAL:HG11	1.51	0.93
23:c:504:CLA:HBB1	23:c:513:CLA:H41	1.57	0.86
23:B:604:CLA:H42	23:B:605:CLA:H2	1.59	0.84
4:D:85:MET:HE2	4:D:90:LEU:HD21	1.64	0.78

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	333/344 (97%)	328 (98%)	4 (1%)	1 (0%)	36 40
1	a	334/344 (97%)	327 (98%)	6 (2%)	1 (0%)	36 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	509/505 (101%)	501 (98%)	8 (2%)	0	100	100
2	b	508/505 (101%)	497 (98%)	11 (2%)	0	100	100
3	C	450/455 (99%)	441 (98%)	8 (2%)	1 (0%)	43	50
3	c	458/455 (101%)	450 (98%)	7 (2%)	1 (0%)	43	50
4	D	341/342 (100%)	328 (96%)	13 (4%)	0	100	100
4	d	341/342 (100%)	332 (97%)	9 (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%)	7	4
8	I	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	4	2
8	i	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
9	J	36/39 (92%)	36 (100%)	0	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	34/37 (92%)	34 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (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	244/244 (100%)	236 (97%)	7 (3%)	1 (0%)	30	31
13	o	241/244 (99%)	236 (98%)	5 (2%)	0	100	100
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
15	u	96/104 (92%)	93 (97%)	3 (3%)	0	100	100
16	V	137/137 (100%)	133 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	131 (97%)	4 (3%)	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%)	25 (93%)	2 (7%)	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	3
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	7	3
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	5252/5384 (98%)	5135 (98%)	108 (2%)	9 (0%)	43	50

5 of 9 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	270/279 (97%)	268 (99%)	2 (1%)	76	82
1	a	271/279 (97%)	270 (100%)	1 (0%)	84	89
2	B	409/403 (102%)	404 (99%)	5 (1%)	63	74
2	b	408/403 (101%)	400 (98%)	8 (2%)	48	59
3	C	353/356 (99%)	345 (98%)	8 (2%)	44	55
3	c	361/356 (101%)	355 (98%)	6 (2%)	53	65
4	D	278/277 (100%)	276 (99%)	2 (1%)	76	82
4	d	278/277 (100%)	275 (99%)	3 (1%)	65	75
5	E	72/73 (99%)	70 (97%)	2 (3%)	38	48
5	e	72/73 (99%)	71 (99%)	1 (1%)	59	70

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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%)	30	37
7	h	55/54 (102%)	54 (98%)	1 (2%)	51	63
8	I	34/34 (100%)	32 (94%)	2 (6%)	18	18
8	i	34/34 (100%)	33 (97%)	1 (3%)	37	47
9	J	26/27 (96%)	24 (92%)	2 (8%)	12	10
9	j	26/27 (96%)	25 (96%)	1 (4%)	29	36
10	K	30/30 (100%)	26 (87%)	4 (13%)	4	2
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	5
11	L	34/35 (97%)	34 (100%)	0	100	100
11	l	34/35 (97%)	34 (100%)	0	100	100
12	M	30/32 (94%)	27 (90%)	3 (10%)	7	5
12	m	32/32 (100%)	30 (94%)	2 (6%)	16	16
13	O	209/207 (101%)	203 (97%)	6 (3%)	37	47
13	o	206/207 (100%)	199 (97%)	7 (3%)	32	40
14	T	27/28 (96%)	24 (89%)	3 (11%)	6	4
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	84/89 (94%)	82 (98%)	2 (2%)	43	54
15	u	85/89 (96%)	83 (98%)	2 (2%)	43	54
16	V	119/117 (102%)	118 (99%)	1 (1%)	73	80
16	v	117/117 (100%)	113 (97%)	4 (3%)	32	40
17	X	32/33 (97%)	31 (97%)	1 (3%)	35	44
17	x	31/33 (94%)	31 (100%)	0	100	100
18	Y	22/23 (96%)	22 (100%)	0	100	100
18	y	22/23 (96%)	19 (86%)	3 (14%)	3	2
19	Z	52/52 (100%)	49 (94%)	3 (6%)	18	19
19	z	52/52 (100%)	44 (85%)	8 (15%)	2	1
20	R	29/29 (100%)	27 (93%)	2 (7%)	14	13
All	All	4358/4403 (99%)	4257 (98%)	101 (2%)	45	55

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	255	THR
12	m	16[B]	LEU
19	z	34	ASP
3	c	315	MET
8	i	33	LYS

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

Mol	Chain	Res	Type
13	o	58	ASN
16	v	86	GLN
15	U	78	ASN
1	a	165	GLN
1	a	296	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	$\# Z > 2$
14	FME	T	1	-	8,9,10	0.69	0	8,9,11	2.09	3 (37%)
8	FME	I	1	-	8,9,10	0.64	0	8,9,11	1.34	2 (25%)
12	FME	m	1	-	8,9,10	0.58	0	8,9,11	1.30	2 (25%)
8	FME	i	1	-	8,9,10	0.69	0	8,9,11	1.15	1 (12%)
14	FME	t	1	-	8,9,10	0.79	0	8,9,11	1.39	1 (12%)
12	FME	M	1	-	8,9,10	0.65	0	8,9,11	1.05	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

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

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	CA-N-CN	3.40	128.05	122.82
14	T	1	FME	CB-CA-N	-2.91	105.22	110.52
14	T	1	FME	C-CA-N	2.74	114.79	109.50
14	t	1	FME	O-C-CA	-2.48	118.39	124.77
8	I	1	FME	O-C-CA	-2.33	118.78	124.77

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	O1-CN-N-CA
12	m	1	FME	O-C-CA-CB
14	t	1	FME	O1-CN-N-CA
14	T	1	FME	CB-CG-SD-CE

There are no ring outliers.

2 monomers are involved in 5 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 225 ligands modelled in this entry, 15 are monoatomic and 18 are unknown - leaving 192 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
23	CLA	c	513	-	69,73,73	2.06	19 (27%)	82,113,113	2.65	34 (41%)
23	CLA	b	613	-	69,73,73	1.98	20 (28%)	82,113,113	2.68	31 (37%)
29	PL9	D	408	-	55,55,55	0.65	1 (1%)	68,69,69	1.61	17 (25%)
23	CLA	C	502	-	69,73,73	1.98	19 (27%)	82,113,113	2.73	33 (40%)
23	CLA	A	406	-	69,73,73	2.01	19 (27%)	82,113,113	2.69	33 (40%)
23	CLA	b	612	-	69,73,73	1.97	19 (27%)	82,113,113	2.68	29 (35%)
27	GOL	b	624	-	5,5,5	1.21	1 (20%)	5,5,5	0.84	0
35	DGD	H	102	-	63,63,67	0.85	3 (4%)	77,77,81	1.03	5 (6%)
25	BCR	C	516	-	41,41,41	1.06	1 (2%)	56,56,56	1.33	7 (12%)
23	CLA	b	611	-	69,73,73	1.91	18 (26%)	82,113,113	2.82	31 (37%)
34	HTG	B	622	-	19,19,19	0.96	1 (5%)	23,24,24	1.60	5 (21%)
23	CLA	c	507	-	69,73,73	2.02	20 (28%)	82,113,113	2.65	30 (36%)
34	HTG	D	414	-	16,16,19	0.96	1 (6%)	20,21,24	1.20	1 (5%)
23	CLA	D	406	-	69,73,73	2.06	19 (27%)	82,113,113	2.65	31 (37%)
23	CLA	C	513	-	69,73,73	2.01	20 (28%)	82,113,113	2.74	35 (42%)
23	CLA	C	510	-	69,73,73	2.05	20 (28%)	82,113,113	2.70	29 (35%)
32	LMT	D	404	-	36,36,36	1.15	3 (8%)	47,47,47	1.32	6 (12%)
32	LMT	E	102	-	36,36,36	1.03	1 (2%)	47,47,47	1.04	3 (6%)
23	CLA	c	514	-	69,73,73	2.09	21 (30%)	82,113,113	2.73	32 (39%)
26	SQD	f	102	-	41,43,54	1.13	2 (4%)	51,54,65	1.55	10 (19%)
31	BCT	A	348	-	3,3,3	0.55	0	2,3,3	1.29	0
23	CLA	b	601	-	69,73,73	2.05	20 (28%)	82,113,113	2.70	31 (37%)
23	CLA	b	603	-	69,73,73	1.94	19 (27%)	82,113,113	2.76	32 (39%)
32	LMT	I	101	-	36,36,36	1.02	2 (5%)	47,47,47	1.17	4 (8%)
27	GOL	O	501	-	5,5,5	0.96	0	5,5,5	1.03	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	GOL	a	801	-	5,5,5	1.19	1 (20%)	5,5,5	1.06	1 (20%)
37	LHG	d	408	-	48,48,48	0.92	2 (4%)	51,54,54	1.02	3 (5%)
40	HEC	v	202	-	46,50,50	1.93	6 (13%)	58,82,82	1.86	6 (10%)
27	GOL	D	701	-	5,5,5	1.38	1 (20%)	5,5,5	0.97	0
25	BCR	B	617	-	41,41,41	1.09	1 (2%)	56,56,56	1.37	10 (17%)
25	BCR	B	618	-	41,41,41	0.97	1 (2%)	56,56,56	1.40	10 (17%)
31	BCT	a	404	-	3,3,3	0.49	0	2,3,3	1.49	0
32	LMT	b	627	-	25,25,36	0.89	0	30,30,47	1.12	3 (10%)
23	CLA	B	604	-	69,73,73	2.02	19 (27%)	82,113,113	2.57	31 (37%)
27	GOL	A	701	-	5,5,5	1.47	2 (40%)	5,5,5	1.11	1 (20%)
23	CLA	C	514	-	69,73,73	2.01	19 (27%)	82,113,113	2.72	31 (37%)
33	LMG	C	501	-	51,51,55	0.93	2 (3%)	59,59,63	1.38	7 (11%)
25	BCR	k	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.44	9 (16%)
25	BCR	B	619	-	41,41,41	1.08	1 (2%)	56,56,56	1.37	9 (16%)
23	CLA	A	408	-	69,73,73	1.95	19 (27%)	82,113,113	2.80	34 (41%)
23	CLA	c	511	-	69,73,73	1.95	20 (28%)	82,113,113	2.71	32 (39%)
33	LMG	C	520	-	51,51,55	0.94	2 (3%)	59,59,63	1.10	4 (6%)
34	HTG	b	622	-	19,19,19	1.09	2 (10%)	23,24,24	1.86	7 (30%)
26	SQD	b	620	-	52,54,54	1.00	3 (5%)	62,65,65	1.58	11 (17%)
23	CLA	C	509	-	69,73,73	2.02	18 (26%)	82,113,113	2.65	30 (36%)
33	LMG	D	415	-	51,51,55	0.82	2 (3%)	59,59,63	1.05	3 (5%)
29	PL9	a	416	-	55,55,55	0.68	2 (3%)	68,69,69	2.03	23 (33%)
33	LMG	Z	101	-	37,37,55	1.01	3 (8%)	45,45,63	1.43	5 (11%)
23	CLA	B	614	-	69,73,73	1.99	19 (27%)	82,113,113	2.87	33 (40%)
23	CLA	B	602	-	69,73,73	2.00	19 (27%)	82,113,113	2.71	32 (39%)
23	CLA	B	610	-	69,73,73	2.01	19 (27%)	82,113,113	2.78	33 (40%)
25	BCR	D	407	-	41,41,41	1.12	1 (2%)	56,56,56	1.82	15 (26%)
23	CLA	B	609	-	69,73,73	2.00	18 (26%)	82,113,113	2.65	31 (37%)
23	CLA	c	504	-	69,73,73	2.04	19 (27%)	82,113,113	2.70	30 (36%)
27	GOL	B	624	-	5,5,5	0.88	0	5,5,5	1.28	1 (20%)
23	CLA	C	512	-	69,73,73	2.02	22 (31%)	82,113,113	2.60	28 (34%)
23	CLA	B	612	-	69,73,73	1.95	19 (27%)	82,113,113	2.67	31 (37%)
27	GOL	C	523	-	5,5,5	1.16	0	5,5,5	0.94	0
25	BCR	C	515	-	41,41,41	1.04	1 (2%)	56,56,56	1.39	5 (8%)
35	DGD	C	519	-	63,63,67	0.88	3 (4%)	77,77,81	1.00	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	b	618	-	41,41,41	1.02	1 (2%)	56,56,56	1.23	6 (10%)
27	GOL	d	801	-	5,5,5	0.98	0	5,5,5	1.05	1 (20%)
23	CLA	C	504	-	69,73,73	1.98	19 (27%)	82,113,113	2.67	30 (36%)
29	PL9	d	405	-	55,55,55	0.72	1 (1%)	68,69,69	1.61	17 (25%)
34	HTG	C	522	-	19,19,19	0.83	1 (5%)	23,24,24	1.32	2 (8%)
26	SQD	a	413	-	52,54,54	1.02	3 (5%)	62,65,65	1.15	6 (9%)
27	GOL	c	743	-	5,5,5	1.24	1 (20%)	5,5,5	0.97	0
27	GOL	o	501	-	5,5,5	1.04	0	5,5,5	1.04	0
24	PHO	A	407	-	58,69,69	2.66	12 (20%)	55,99,99	2.93	14 (25%)
26	SQD	A	412	-	52,54,54	0.97	2 (3%)	62,65,65	1.15	5 (8%)
33	LMG	a	419	-	51,51,55	0.93	2 (3%)	59,59,63	1.20	6 (10%)
34	HTG	B	626	-	19,19,19	0.95	2 (10%)	23,24,24	1.28	4 (17%)
26	SQD	F	101	-	41,43,54	1.15	3 (7%)	51,54,65	2.03	10 (19%)
37	LHG	d	711	-	48,48,48	0.89	3 (6%)	51,54,54	1.13	4 (7%)
32	LMT	e	102	-	36,36,36	0.99	1 (2%)	47,47,47	1.01	1 (2%)
32	LMT	M	103	-	36,36,36	1.04	2 (5%)	47,47,47	1.07	2 (4%)
34	HTG	V	203	-	11,11,19	0.28	0	15,15,24	1.13	1 (6%)
25	BCR	d	404	-	41,41,41	1.14	2 (4%)	56,56,56	1.91	14 (25%)
23	CLA	B	615	-	69,73,73	2.00	20 (28%)	82,113,113	2.68	30 (36%)
34	HTG	b	623	-	19,19,19	0.96	1 (5%)	23,24,24	1.60	2 (8%)
29	PL9	A	414	-	55,55,55	0.71	3 (5%)	68,69,69	2.05	25 (36%)
23	CLA	d	402	-	69,73,73	1.94	19 (27%)	82,113,113	2.64	33 (40%)
33	LMG	m	101	-	51,51,55	0.88	2 (3%)	59,59,63	1.25	5 (8%)
23	CLA	b	610	-	69,73,73	1.98	20 (28%)	82,113,113	2.74	34 (41%)
27	GOL	v	401	-	5,5,5	1.26	0	5,5,5	0.88	0
32	LMT	t	102	-	26,26,36	0.90	1 (3%)	31,31,47	1.33	2 (6%)
35	DGD	c	518	-	63,63,67	0.85	3 (4%)	77,77,81	0.98	4 (5%)
33	LMG	d	412	-	51,51,55	0.89	2 (3%)	59,59,63	1.09	4 (6%)
23	CLA	b	602	-	69,73,73	2.05	19 (27%)	82,113,113	2.81	35 (42%)
23	CLA	C	511	-	69,73,73	2.03	20 (28%)	82,113,113	2.76	33 (40%)
24	PHO	a	353	-	58,69,69	2.79	14 (24%)	55,99,99	3.05	17 (30%)
23	CLA	b	609	-	69,73,73	1.97	18 (26%)	82,113,113	2.67	32 (39%)
27	GOL	V	401	-	5,5,5	1.41	1 (20%)	5,5,5	0.86	0
35	DGD	h	102	-	63,63,67	0.86	3 (4%)	77,77,81	1.10	5 (6%)
25	BCR	K	102	-	41,41,41	1.05	1 (2%)	56,56,56	1.46	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	a	405	-	69,73,73	1.97	19 (27%)	82,113,113	2.75	34 (41%)
35	DGD	c	517	-	63,63,67	0.86	2 (3%)	77,77,81	1.10	8 (10%)
23	CLA	C	507	-	69,73,73	2.00	20 (28%)	82,113,113	2.69	33 (40%)
23	CLA	B	611	-	69,73,73	2.46	21 (30%)	82,113,113	3.59	32 (39%)
23	CLA	a	407	-	69,73,73	1.96	19 (27%)	82,113,113	2.67	32 (39%)
27	GOL	B	901	-	5,5,5	1.11	0	5,5,5	1.03	0
27	GOL	a	701	-	5,5,5	1.09	0	5,5,5	1.09	1 (20%)
33	LMG	z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.10	4 (8%)
37	LHG	D	410	-	48,48,48	0.88	3 (6%)	51,54,54	1.02	3 (5%)
23	CLA	b	615	-	69,73,73	1.97	20 (28%)	82,113,113	2.67	33 (40%)
23	CLA	A	405	-	69,73,73	2.00	18 (26%)	82,113,113	2.70	35 (42%)
35	DGD	C	518	-	63,63,67	0.91	3 (4%)	77,77,81	1.04	5 (6%)
38	HEM	E	103	-	50,50,50	1.55	8 (16%)	67,82,82	1.81	14 (20%)
33	LMG	B	621	-	51,51,55	0.93	2 (3%)	59,59,63	1.26	4 (6%)
40	HEC	V	202	-	46,50,50	1.91	5 (10%)	58,82,82	1.83	8 (13%)
23	CLA	B	603	-	69,73,73	1.98	20 (28%)	82,113,113	2.80	31 (37%)
23	CLA	A	404	-	69,73,73	1.98	19 (27%)	82,113,113	2.74	31 (37%)
34	HTG	b	625	-	19,19,19	0.92	2 (10%)	23,24,24	1.56	3 (13%)
37	LHG	l	101	-	48,48,48	0.84	3 (6%)	51,54,54	1.05	4 (7%)
25	BCR	b	619	-	41,41,41	1.10	1 (2%)	56,56,56	1.39	7 (12%)
34	HTG	B	623	-	19,19,19	0.72	1 (5%)	23,24,24	1.18	1 (4%)
23	CLA	a	406	-	69,73,73	2.01	17 (24%)	82,113,113	2.72	31 (37%)
23	CLA	c	503	-	69,73,73	2.00	18 (26%)	82,113,113	2.66	28 (34%)
25	BCR	T	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.59	13 (23%)
32	LMT	M	101	-	36,36,36	1.11	3 (8%)	47,47,47	1.20	4 (8%)
23	CLA	B	601	-	69,73,73	2.05	19 (27%)	82,113,113	2.74	31 (37%)
25	BCR	h	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.35	9 (16%)
23	CLA	B	606	-	69,73,73	2.00	18 (26%)	82,113,113	2.84	33 (40%)
24	PHO	A	353	-	58,69,69	2.81	14 (24%)	55,99,99	2.93	16 (29%)
32	LMT	A	359	-	36,36,36	0.91	1 (2%)	47,47,47	1.02	1 (2%)
27	GOL	A	411	-	5,5,5	1.10	0	5,5,5	0.78	0
25	BCR	b	617	-	41,41,41	1.06	1 (2%)	56,56,56	1.35	6 (10%)
34	HTG	c	522	-	19,19,19	0.86	1 (5%)	23,24,24	1.44	1 (4%)
27	GOL	c	742	-	5,5,5	1.04	0	5,5,5	1.05	0
23	CLA	C	503	-	69,73,73	2.00	20 (28%)	82,113,113	2.58	29 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	607	-	69,73,73	1.95	19 (27%)	82,113,113	2.66	32 (39%)
23	CLA	c	505	-	69,73,73	2.02	21 (30%)	82,113,113	2.67	33 (40%)
34	HTG	d	411	-	16,16,19	0.91	1 (6%)	20,21,24	1.33	1 (5%)
32	LMT	b	621	-	25,25,36	0.95	1 (4%)	30,30,47	1.18	3 (10%)
25	BCR	H	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.43	10 (17%)
25	BCR	y	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.64	9 (16%)
33	LMG	c	521	-	51,51,55	1.01	2 (3%)	59,59,63	1.37	7 (11%)
35	DGD	c	519	-	63,63,67	0.88	3 (4%)	77,77,81	0.99	4 (5%)
23	CLA	b	606	-	69,73,73	1.99	19 (27%)	82,113,113	2.71	31 (37%)
23	CLA	B	616	-	69,73,73	1.94	19 (27%)	82,113,113	2.74	27 (32%)
25	BCR	Y	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.75	13 (23%)
23	CLA	c	506	-	69,73,73	1.99	19 (27%)	82,113,113	2.68	29 (35%)
37	LHG	D	411	-	48,48,48	0.94	2 (4%)	51,54,54	1.04	4 (7%)
37	LHG	L	101	-	48,48,48	0.89	3 (6%)	51,54,54	1.16	4 (7%)
27	GOL	d	701	-	5,5,5	1.08	0	5,5,5	1.01	0
37	LHG	D	409	-	48,48,48	0.87	2 (4%)	51,54,54	1.29	6 (11%)
23	CLA	b	616	-	69,73,73	1.99	19 (27%)	82,113,113	2.80	30 (36%)
23	CLA	C	505	-	69,73,73	1.96	20 (28%)	82,113,113	2.66	31 (37%)
28	OEX	a	415	-	0,15,15	-	-	-	-	-
23	CLA	c	510	-	69,73,73	2.05	18 (26%)	82,113,113	2.74	32 (39%)
26	SQD	a	411	-	52,54,54	0.89	2 (3%)	62,65,65	1.80	11 (17%)
33	LMG	C	521	-	51,51,55	1.06	3 (5%)	59,59,63	1.33	6 (10%)
23	CLA	b	614	-	69,73,73	1.97	20 (28%)	82,113,113	2.77	29 (35%)
35	DGD	C	517	-	63,63,67	0.84	2 (3%)	77,77,81	1.20	6 (7%)
23	CLA	C	506	-	69,73,73	2.01	18 (26%)	82,113,113	2.68	31 (37%)
23	CLA	d	403	-	69,73,73	2.02	19 (27%)	82,113,113	2.69	31 (37%)
32	LMT	t	101	-	25,25,36	0.88	2 (8%)	30,30,47	1.13	3 (10%)
25	BCR	a	410	-	41,41,41	1.05	1 (2%)	56,56,56	1.31	7 (12%)
32	LMT	m	103	-	36,36,36	1.03	3 (8%)	47,47,47	1.11	3 (6%)
27	GOL	a	412	-	5,5,5	0.93	0	5,5,5	1.18	1 (20%)
32	LMT	a	414	-	36,36,36	0.98	3 (8%)	47,47,47	1.13	3 (6%)
23	CLA	b	605	-	69,73,73	1.95	20 (28%)	82,113,113	2.77	31 (37%)
38	HEM	e	87	-	50,50,50	1.50	6 (12%)	67,82,82	1.64	12 (17%)
28	OEX	A	413	-	0,15,15	-	-	-	-	-
23	CLA	b	608	-	69,73,73	1.97	20 (28%)	82,113,113	2.68	34 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	508	-	69,73,73	2.00	18 (26%)	82,113,113	2.74	31 (37%)
23	CLA	c	512	-	69,73,73	2.04	19 (27%)	82,113,113	2.62	31 (37%)
27	GOL	O	601	-	5,5,5	0.99	0	5,5,5	1.22	1 (20%)
25	BCR	A	409	-	41,41,41	1.01	1 (2%)	56,56,56	1.41	10 (17%)
25	BCR	t	103	-	41,41,41	1.02	1 (2%)	56,56,56	1.50	10 (17%)
37	LHG	E	101	-	41,41,48	1.08	2 (4%)	44,47,54	1.12	3 (6%)
32	LMT	a	420	-	36,36,36	0.99	1 (2%)	47,47,47	1.04	1 (2%)
27	GOL	o	601	-	5,5,5	1.16	1 (20%)	5,5,5	1.10	0
27	GOL	b	901	-	5,5,5	0.44	0	5,5,5	1.58	1 (20%)
33	LMG	c	520	-	51,51,55	0.91	2 (3%)	59,59,63	1.09	5 (8%)
23	CLA	B	613	-	69,73,73	2.03	18 (26%)	82,113,113	2.62	29 (35%)
23	CLA	c	509	-	69,73,73	2.11	20 (28%)	82,113,113	2.61	30 (36%)
23	CLA	C	508	-	69,73,73	1.98	20 (28%)	82,113,113	2.72	32 (39%)
23	CLA	b	604	-	69,73,73	1.99	20 (28%)	82,113,113	2.67	30 (36%)
23	CLA	b	607	-	69,73,73	1.99	19 (27%)	82,113,113	2.73	31 (37%)
25	BCR	c	516	-	41,41,41	1.05	1 (2%)	56,56,56	1.38	10 (17%)
25	BCR	c	515	-	41,41,41	1.00	1 (2%)	56,56,56	1.58	10 (17%)
23	CLA	c	502	-	69,73,73	1.98	21 (30%)	82,113,113	2.69	29 (35%)
37	LHG	d	407	-	48,48,48	0.87	2 (4%)	51,54,54	1.06	4 (7%)
23	CLA	B	605	-	69,73,73	2.01	19 (27%)	82,113,113	2.73	30 (36%)
37	LHG	e	101	-	41,41,48	1.06	2 (4%)	44,47,54	0.93	2 (4%)
23	CLA	B	608	-	69,73,73	1.89	20 (28%)	82,113,113	2.69	33 (40%)
26	SQD	B	620	-	52,54,54	1.02	3 (5%)	62,65,65	1.75	11 (17%)
26	SQD	A	410	-	52,54,54	0.86	2 (3%)	62,65,65	1.85	10 (16%)
23	CLA	D	405	-	69,73,73	1.98	19 (27%)	82,113,113	2.74	34 (41%)
23	CLA	a	409	-	69,73,73	1.98	18 (26%)	82,113,113	2.78	32 (39%)
24	PHO	a	408	-	58,69,69	2.77	13 (22%)	55,99,99	2.94	14 (25%)

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
23	CLA	c	513	-	1/1/15/20	13/39/115/115	-
23	CLA	b	613	-	1/1/15/20	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PL9	D	408	-	-	6/53/73/73	0/1/1/1
23	CLA	C	502	-	1/1/15/20	4/39/115/115	-
23	CLA	b	612	-	1/1/15/20	4/39/115/115	-
23	CLA	A	406	-	-	5/39/115/115	-
27	GOL	b	624	-	-	2/4/4/4	-
35	DGD	H	102	-	-	11/51/91/95	0/2/2/2
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
23	CLA	b	611	-	1/1/15/20	2/39/115/115	-
34	HTG	B	622	-	-	4/10/30/30	0/1/1/1
23	CLA	c	507	-	1/1/15/20	7/39/115/115	-
34	HTG	D	414	-	-	3/7/27/30	0/1/1/1
23	CLA	D	406	-	1/1/15/20	13/39/115/115	-
23	CLA	C	513	-	1/1/15/20	9/39/115/115	-
23	CLA	C	510	-	1/1/15/20	5/39/115/115	-
32	LMT	D	404	-	-	12/21/61/61	0/2/2/2
32	LMT	E	102	-	-	8/21/61/61	0/2/2/2
23	CLA	c	514	-	1/1/15/20	10/39/115/115	-
26	SQD	f	102	-	-	9/38/58/69	0/1/1/1
23	CLA	b	601	-	1/1/15/20	15/39/115/115	-
23	CLA	b	603	-	1/1/15/20	6/39/115/115	-
32	LMT	I	101	-	-	16/21/61/61	0/2/2/2
27	GOL	O	501	-	-	2/4/4/4	-
27	GOL	a	801	-	-	1/4/4/4	-
37	LHG	d	408	-	-	12/53/53/53	-
40	HEC	v	202	-	-	6/14/54/54	-
27	GOL	D	701	-	-	4/4/4/4	-
25	BCR	B	617	-	-	2/29/63/63	0/2/2/2
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
32	LMT	b	627	-	-	10/17/37/61	0/1/1/2
23	CLA	B	604	-	1/1/15/20	1/39/115/115	-
27	GOL	A	701	-	-	0/4/4/4	-
23	CLA	C	514	-	1/1/15/20	7/39/115/115	-
33	LMG	C	501	-	-	14/46/66/70	0/1/1/1
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	A	408	-	1/1/15/20	8/39/115/115	-
23	CLA	c	511	-	1/1/15/20	8/39/115/115	-
33	LMG	C	520	-	-	9/46/66/70	0/1/1/1
34	HTG	b	622	-	-	6/10/30/30	0/1/1/1
26	SQD	b	620	-	-	17/49/69/69	0/1/1/1
23	CLA	C	509	-	1/1/15/20	2/39/115/115	-
33	LMG	D	415	-	-	7/46/66/70	0/1/1/1
29	PL9	a	416	-	-	14/53/73/73	0/1/1/1
33	LMG	Z	101	-	-	9/31/51/70	0/1/1/1
23	CLA	B	614	-	1/1/15/20	11/39/115/115	-
23	CLA	B	602	-	1/1/15/20	9/39/115/115	-
23	CLA	B	610	-	1/1/15/20	7/39/115/115	-
25	BCR	D	407	-	-	4/29/63/63	0/2/2/2
23	CLA	B	609	-	1/1/15/20	1/39/115/115	-
23	CLA	c	504	-	1/1/15/20	2/39/115/115	-
27	GOL	B	624	-	-	4/4/4/4	-
23	CLA	C	512	-	1/1/15/20	4/39/115/115	-
23	CLA	B	612	-	1/1/15/20	5/39/115/115	-
27	GOL	C	523	-	-	0/4/4/4	-
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
35	DGD	C	519	-	-	15/51/91/95	0/2/2/2
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
27	GOL	d	801	-	-	2/4/4/4	-
23	CLA	C	504	-	1/1/15/20	2/39/115/115	-
29	PL9	d	405	-	-	6/53/73/73	0/1/1/1
34	HTG	C	522	-	-	0/10/30/30	0/1/1/1
26	SQD	a	413	-	-	11/49/69/69	0/1/1/1
27	GOL	c	743	-	-	3/4/4/4	-
27	GOL	o	501	-	-	2/4/4/4	-
24	PHO	A	407	-	-	0/37/103/103	0/5/6/6
26	SQD	A	412	-	-	14/49/69/69	0/1/1/1
33	LMG	a	419	-	-	13/46/66/70	0/1/1/1
34	HTG	B	626	-	-	5/10/30/30	0/1/1/1
26	SQD	F	101	-	-	15/38/58/69	0/1/1/1
37	LHG	d	711	-	-	15/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LMT	e	102	-	-	15/21/61/61	0/2/2/2
32	LMT	M	103	-	-	7/21/61/61	0/2/2/2
34	HTG	V	203	-	-	0/2/19/30	0/1/1/1
25	BCR	d	404	-	-	6/29/63/63	0/2/2/2
23	CLA	B	615	-	1/1/15/20	5/39/115/115	-
34	HTG	b	623	-	-	4/10/30/30	0/1/1/1
29	PL9	A	414	-	-	14/53/73/73	0/1/1/1
23	CLA	d	402	-	1/1/15/20	4/39/115/115	-
33	LMG	m	101	-	-	12/46/66/70	0/1/1/1
23	CLA	b	610	-	1/1/15/20	6/39/115/115	-
27	GOL	v	401	-	-	2/4/4/4	-
32	LMT	t	102	-	-	9/17/38/61	0/1/1/2
35	DGD	c	518	-	-	16/51/91/95	0/2/2/2
33	LMG	d	412	-	-	10/46/66/70	0/1/1/1
23	CLA	b	602	-	1/1/15/20	4/39/115/115	-
23	CLA	C	511	-	1/1/15/20	13/39/115/115	-
24	PHO	a	353	-	-	1/37/103/103	0/5/6/6
23	CLA	b	609	-	1/1/15/20	2/39/115/115	-
27	GOL	V	401	-	-	2/4/4/4	-
35	DGD	h	102	-	-	13/51/91/95	0/2/2/2
25	BCR	K	102	-	-	2/29/63/63	0/2/2/2
23	CLA	a	405	-	1/1/15/20	4/39/115/115	-
35	DGD	c	517	-	-	17/51/91/95	0/2/2/2
23	CLA	C	507	-	1/1/15/20	12/39/115/115	-
23	CLA	B	611	-	1/1/15/20	2/39/115/115	-
23	CLA	a	407	-	-	6/39/115/115	-
27	GOL	B	901	-	-	2/4/4/4	-
27	GOL	a	701	-	-	2/4/4/4	-
33	LMG	z	101	-	-	9/34/54/70	0/1/1/1
37	LHG	D	410	-	-	17/53/53/53	-
23	CLA	b	615	-	1/1/15/20	7/39/115/115	-
23	CLA	A	405	-	1/1/15/20	1/39/115/115	-
35	DGD	C	518	-	-	12/51/91/95	0/2/2/2
38	HEM	E	103	-	-	6/14/54/54	-
33	LMG	B	621	-	-	20/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	HEC	V	202	-	-	6/14/54/54	-
23	CLA	B	603	-	1/1/15/20	6/39/115/115	-
23	CLA	A	404	-	1/1/15/20	3/39/115/115	-
34	HTG	b	625	-	-	3/10/30/30	0/1/1/1
37	LHG	l	101	-	-	15/53/53/53	-
25	BCR	b	619	-	-	4/29/63/63	0/2/2/2
34	HTG	B	623	-	-	2/10/30/30	0/1/1/1
23	CLA	a	406	-	1/1/15/20	4/39/115/115	-
23	CLA	c	503	-	1/1/15/20	5/39/115/115	-
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
32	LMT	M	101	-	-	5/21/61/61	0/2/2/2
23	CLA	B	601	-	1/1/15/20	12/39/115/115	-
25	BCR	h	101	-	-	2/29/63/63	0/2/2/2
23	CLA	B	606	-	1/1/15/20	8/39/115/115	-
24	PHO	A	353	-	-	1/37/103/103	0/5/6/6
32	LMT	A	359	-	-	7/21/61/61	0/2/2/2
27	GOL	A	411	-	-	2/4/4/4	-
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
34	HTG	c	522	-	-	1/10/30/30	0/1/1/1
27	GOL	c	742	-	-	0/4/4/4	-
23	CLA	C	503	-	1/1/15/20	11/39/115/115	-
23	CLA	B	607	-	1/1/15/20	3/39/115/115	-
23	CLA	c	505	-	1/1/15/20	5/39/115/115	-
34	HTG	d	411	-	-	1/7/27/30	0/1/1/1
32	LMT	b	621	-	-	8/17/37/61	0/1/1/2
25	BCR	H	101	-	-	1/29/63/63	0/2/2/2
25	BCR	y	101	-	-	3/29/63/63	0/2/2/2
33	LMG	c	521	-	-	10/46/66/70	0/1/1/1
35	DGD	c	519	-	-	11/51/91/95	0/2/2/2
23	CLA	b	606	-	1/1/15/20	11/39/115/115	-
23	CLA	B	616	-	1/1/15/20	6/39/115/115	-
25	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
23	CLA	c	506	-	1/1/15/20	6/39/115/115	-
37	LHG	D	411	-	-	13/53/53/53	-
37	LHG	L	101	-	-	20/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	GOL	d	701	-	-	2/4/4/4	-
37	LHG	D	409	-	-	14/53/53/53	-
23	CLA	b	616	-	1/1/15/20	9/39/115/115	-
23	CLA	C	505	-	1/1/15/20	8/39/115/115	-
23	CLA	c	510	-	1/1/15/20	14/39/115/115	-
26	SQD	a	411	-	-	9/49/69/69	0/1/1/1
33	LMG	C	521	-	-	13/46/66/70	0/1/1/1
23	CLA	b	614	-	1/1/15/20	11/39/115/115	-
35	DGD	C	517	-	-	15/51/91/95	0/2/2/2
23	CLA	C	506	-	1/1/15/20	6/39/115/115	-
23	CLA	d	403	-	1/1/15/20	8/39/115/115	-
32	LMT	t	101	-	-	11/17/37/61	0/1/1/2
25	BCR	a	410	-	-	1/29/63/63	0/2/2/2
32	LMT	m	103	-	-	7/21/61/61	0/2/2/2
27	GOL	a	412	-	-	4/4/4/4	-
32	LMT	a	414	-	-	10/21/61/61	0/2/2/2
23	CLA	b	605	-	1/1/15/20	5/39/115/115	-
38	HEM	e	87	-	-	6/14/54/54	-
23	CLA	c	508	-	1/1/15/20	7/39/115/115	-
23	CLA	c	512	-	1/1/15/20	5/39/115/115	-
23	CLA	b	608	-	-	5/39/115/115	-
27	GOL	O	601	-	-	2/4/4/4	-
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
25	BCR	t	103	-	-	0/29/63/63	0/2/2/2
37	LHG	E	101	-	-	21/46/46/53	-
32	LMT	a	420	-	-	11/21/61/61	0/2/2/2
27	GOL	o	601	-	-	4/4/4/4	-
27	GOL	b	901	-	-	0/4/4/4	-
33	LMG	c	520	-	-	11/46/66/70	0/1/1/1
23	CLA	B	613	-	1/1/15/20	8/39/115/115	-
23	CLA	c	509	-	1/1/15/20	4/39/115/115	-
23	CLA	C	508	-	1/1/15/20	10/39/115/115	-
23	CLA	b	604	-	1/1/15/20	12/39/115/115	-
23	CLA	b	607	-	1/1/15/20	2/39/115/115	-
25	BCR	c	516	-	-	1/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	c	515	-	-	2/29/63/63	0/2/2/2
23	CLA	c	502	-	1/1/15/20	3/39/115/115	-
37	LHG	d	407	-	-	12/53/53/53	-
23	CLA	B	605	-	1/1/15/20	3/39/115/115	-
37	LHG	e	101	-	-	16/46/46/53	-
23	CLA	B	608	-	-	4/39/115/115	-
26	SQD	B	620	-	-	13/49/69/69	0/1/1/1
26	SQD	A	410	-	-	12/49/69/69	0/1/1/1
23	CLA	D	405	-	1/1/15/20	2/39/115/115	-
23	CLA	a	409	-	1/1/15/20	10/39/115/115	-
24	PHO	a	408	-	-	6/37/103/103	0/5/6/6

The worst 5 of 1593 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	408	PHO	C1B-C2B	9.37	1.49	1.39
24	A	407	PHO	C1D-C2D	9.05	1.49	1.39
24	a	353	PHO	C1B-C2B	8.84	1.49	1.39
24	A	353	PHO	C1B-C2B	8.80	1.49	1.39
24	a	353	PHO	C1D-C2D	8.76	1.49	1.39

The worst 5 of 2881 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	C3B-C2B-C1B	-13.30	91.49	107.17
23	B	611	CLA	C1D-ND-C4D	-11.86	97.99	106.31
24	A	407	PHO	C2D-C1D-ND	11.49	117.73	109.43
24	a	353	PHO	C2D-C1D-ND	10.99	117.38	109.43
24	a	408	PHO	C2D-C1D-ND	10.81	117.24	109.43

5 of 66 chirality outliers are listed below:

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

5 of 1263 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	603	CLA	C2-C3-C5-C6
23	B	603	CLA	C4-C3-C5-C6
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	C	508	CLA	C2B-C3B-CAB-CBB

There are no ring outliers.

143 monomers are involved in 261 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	c	513	CLA	4	0
23	b	613	CLA	2	0
29	D	408	PL9	1	0
23	C	502	CLA	5	0
23	A	406	CLA	1	0
23	b	612	CLA	1	0
35	H	102	DGD	1	0
25	C	516	BCR	1	0
34	B	622	HTG	1	0
23	c	507	CLA	2	0
34	D	414	HTG	1	0
23	C	513	CLA	2	0
23	C	510	CLA	1	0
32	D	404	LMT	1	0
23	c	514	CLA	1	0
23	b	601	CLA	1	0
23	b	603	CLA	1	0
32	I	101	LMT	1	0
27	O	501	GOL	1	0
27	a	801	GOL	4	0
37	d	408	LHG	11	0
27	D	701	GOL	1	0
25	B	617	BCR	2	0
25	B	618	BCR	2	0
23	B	604	CLA	1	0
27	A	701	GOL	3	0
23	C	514	CLA	2	0
25	B	619	BCR	2	0
23	A	408	CLA	3	0
23	c	511	CLA	1	0
34	b	622	HTG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	b	620	SQD	3	0
23	C	509	CLA	3	0
29	a	416	PL9	4	0
33	Z	101	LMG	2	0
23	B	614	CLA	3	0
23	B	602	CLA	1	0
25	D	407	BCR	2	0
23	B	609	CLA	2	0
23	c	504	CLA	3	0
27	B	624	GOL	2	0
23	C	512	CLA	3	0
23	B	612	CLA	1	0
25	C	515	BCR	1	0
35	C	519	DGD	1	0
25	b	618	BCR	4	0
27	d	801	GOL	1	0
23	C	504	CLA	3	0
26	a	413	SQD	1	0
24	A	407	PHO	1	0
34	B	626	HTG	1	0
26	F	101	SQD	1	0
32	e	102	LMT	1	0
25	d	404	BCR	2	0
23	B	615	CLA	3	0
29	A	414	PL9	10	0
23	d	402	CLA	1	0
27	v	401	GOL	1	0
32	t	102	LMT	2	0
35	c	518	DGD	3	0
33	d	412	LMG	2	0
23	b	602	CLA	1	0
23	C	511	CLA	3	0
24	a	353	PHO	1	0
23	b	609	CLA	5	0
25	K	102	BCR	1	0
23	a	405	CLA	2	0
35	c	517	DGD	1	0
23	C	507	CLA	3	0
23	a	407	CLA	2	0
27	a	701	GOL	1	0
33	z	101	LMG	2	0
37	D	410	LHG	2	0

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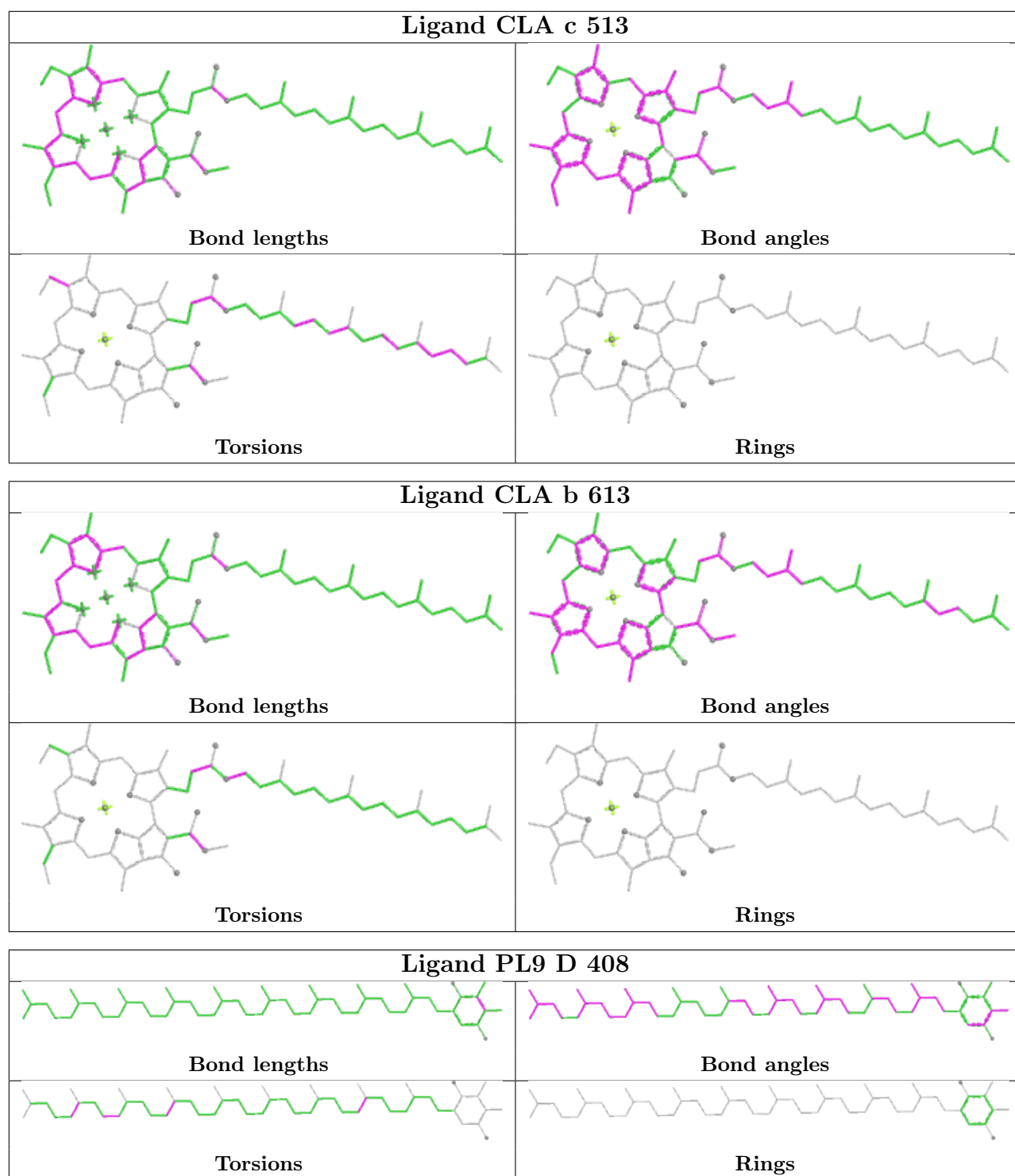
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23	b	615	CLA	2	0
23	A	405	CLA	1	0
35	C	518	DGD	1	0
38	E	103	HEM	1	0
33	B	621	LMG	1	0
23	B	603	CLA	1	0
23	A	404	CLA	2	0
34	b	625	HTG	1	0
25	b	619	BCR	5	0
34	B	623	HTG	1	0
23	a	406	CLA	3	0
23	c	503	CLA	2	0
25	T	101	BCR	6	0
32	M	101	LMT	2	0
23	B	601	CLA	4	0
25	h	101	BCR	3	0
23	B	606	CLA	2	0
24	A	353	PHO	2	0
32	A	359	LMT	1	0
25	b	617	BCR	1	0
34	c	522	HTG	1	0
23	C	503	CLA	2	0
23	c	505	CLA	1	0
34	d	411	HTG	1	0
32	b	621	LMT	1	0
25	H	101	BCR	2	0
25	y	101	BCR	1	0
33	c	521	LMG	1	0
35	c	519	DGD	2	0
23	b	606	CLA	1	0
23	B	616	CLA	3	0
25	Y	101	BCR	1	0
23	c	506	CLA	5	0
37	D	411	LHG	3	0
23	b	616	CLA	1	0
23	C	505	CLA	1	0
23	c	510	CLA	2	0
26	a	411	SQD	3	0
33	C	521	LMG	3	0
23	b	614	CLA	3	0
35	C	517	DGD	1	0
23	C	506	CLA	4	0

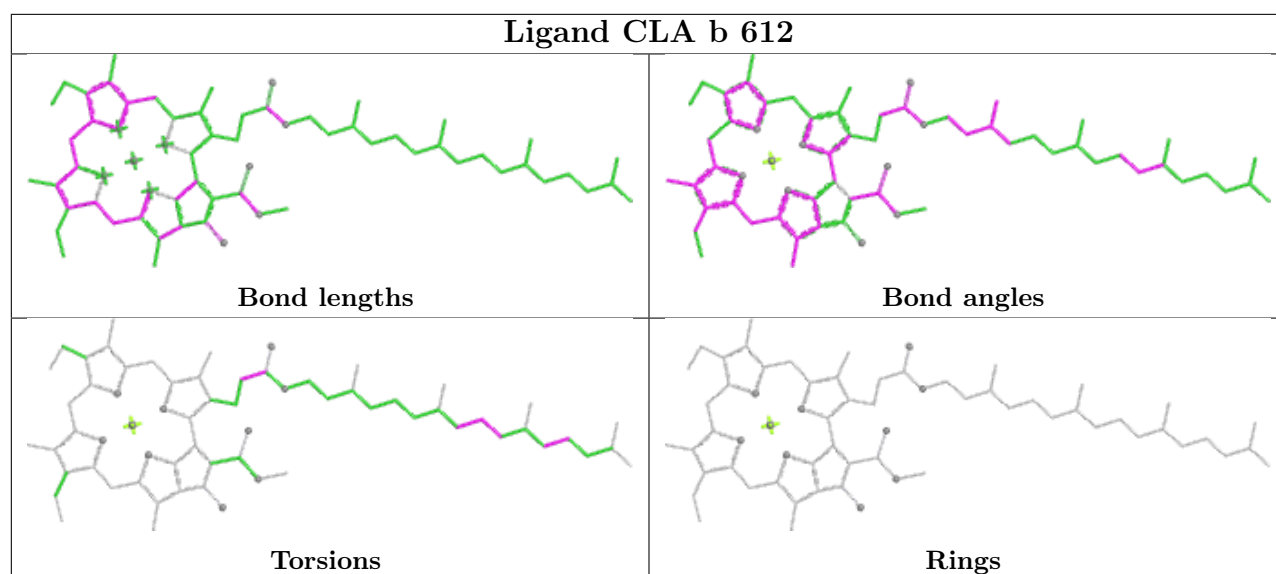
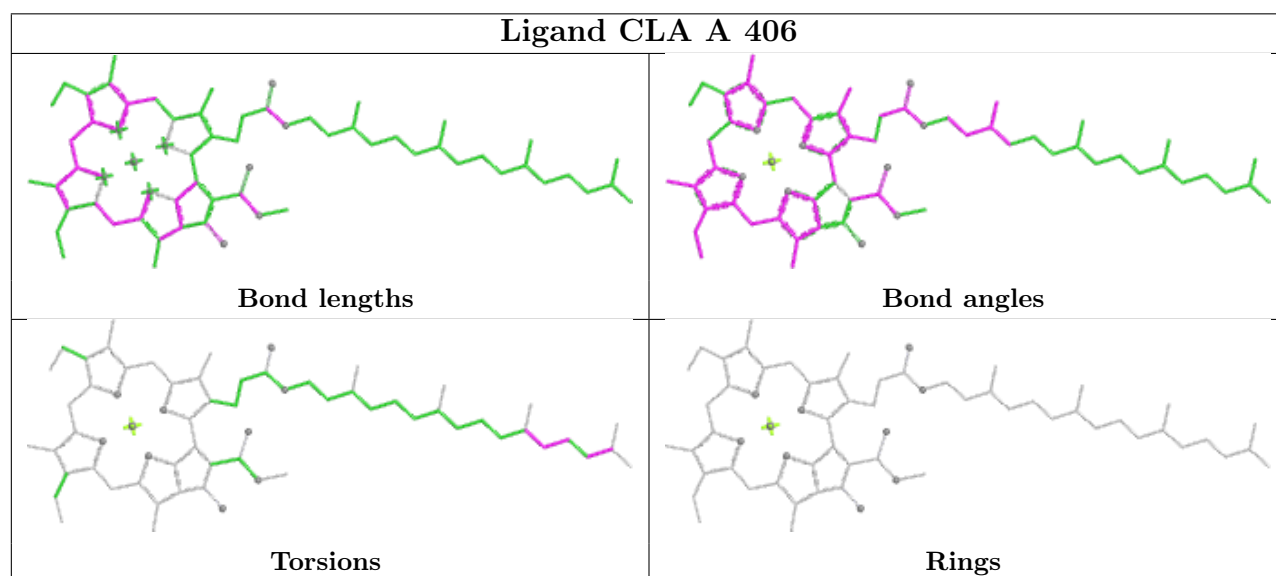
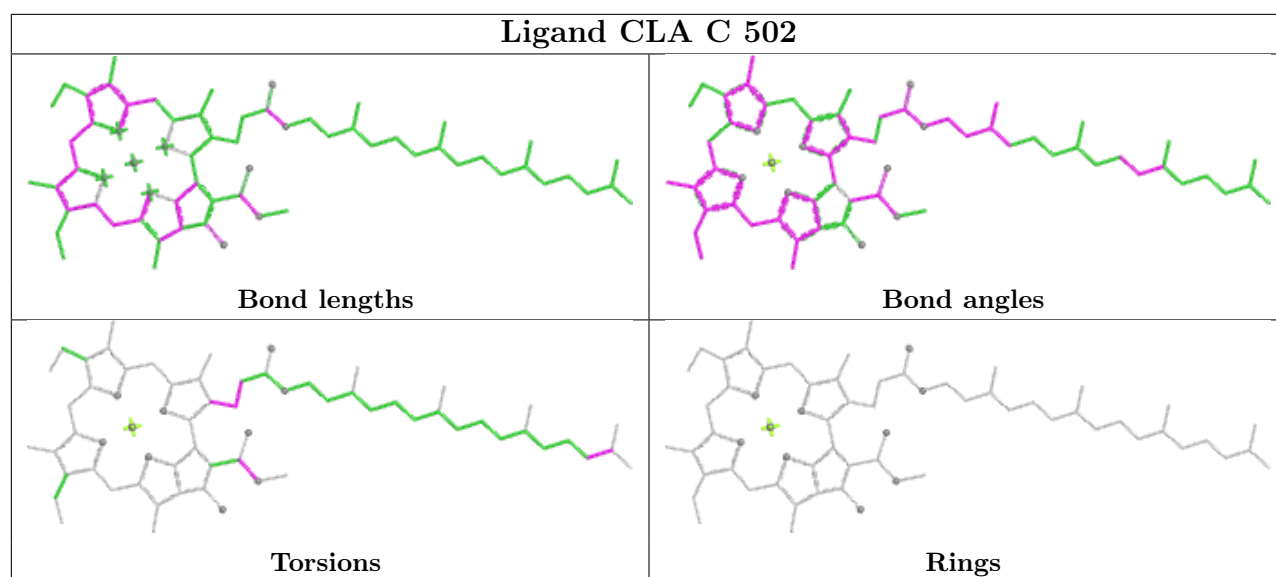
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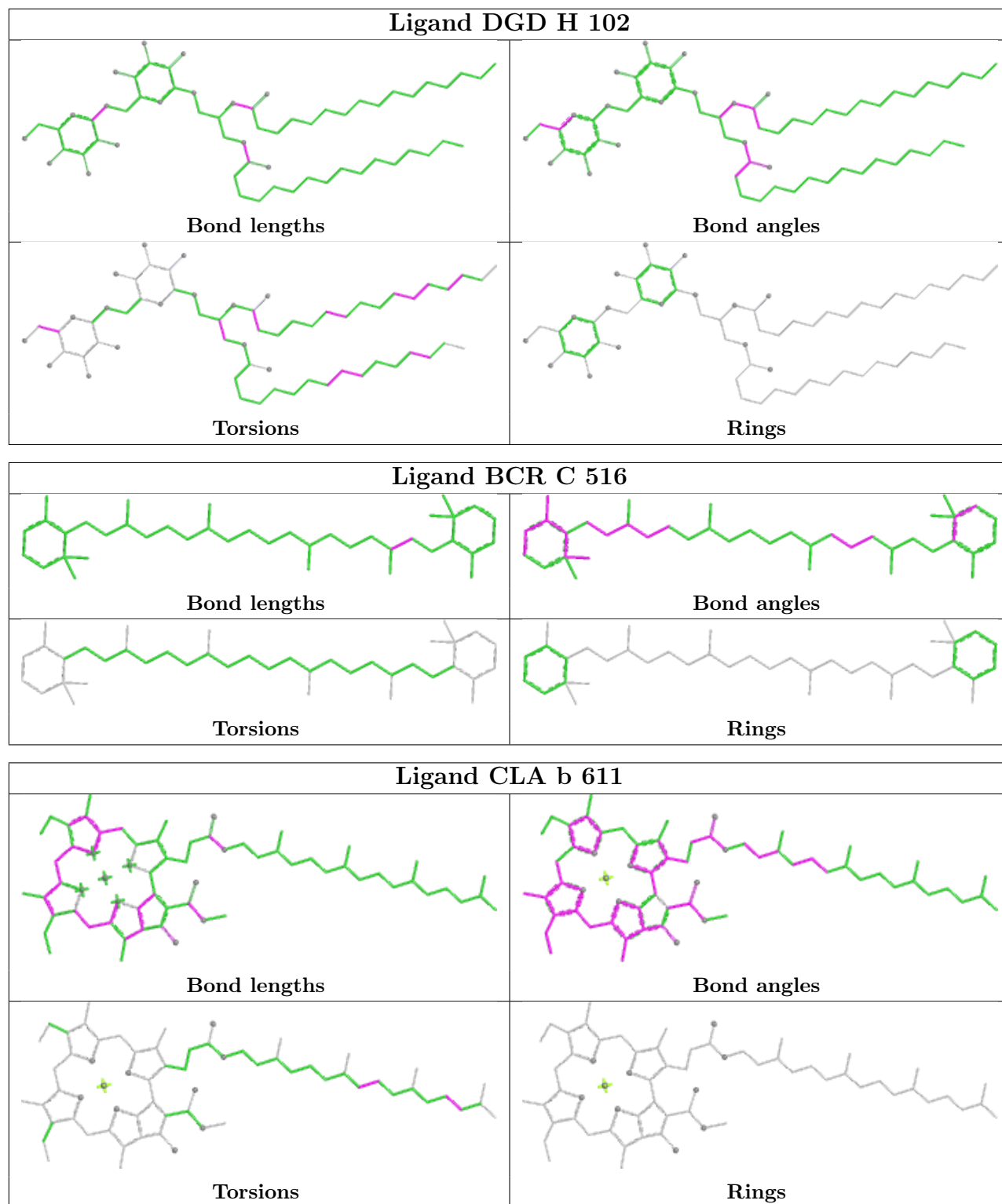
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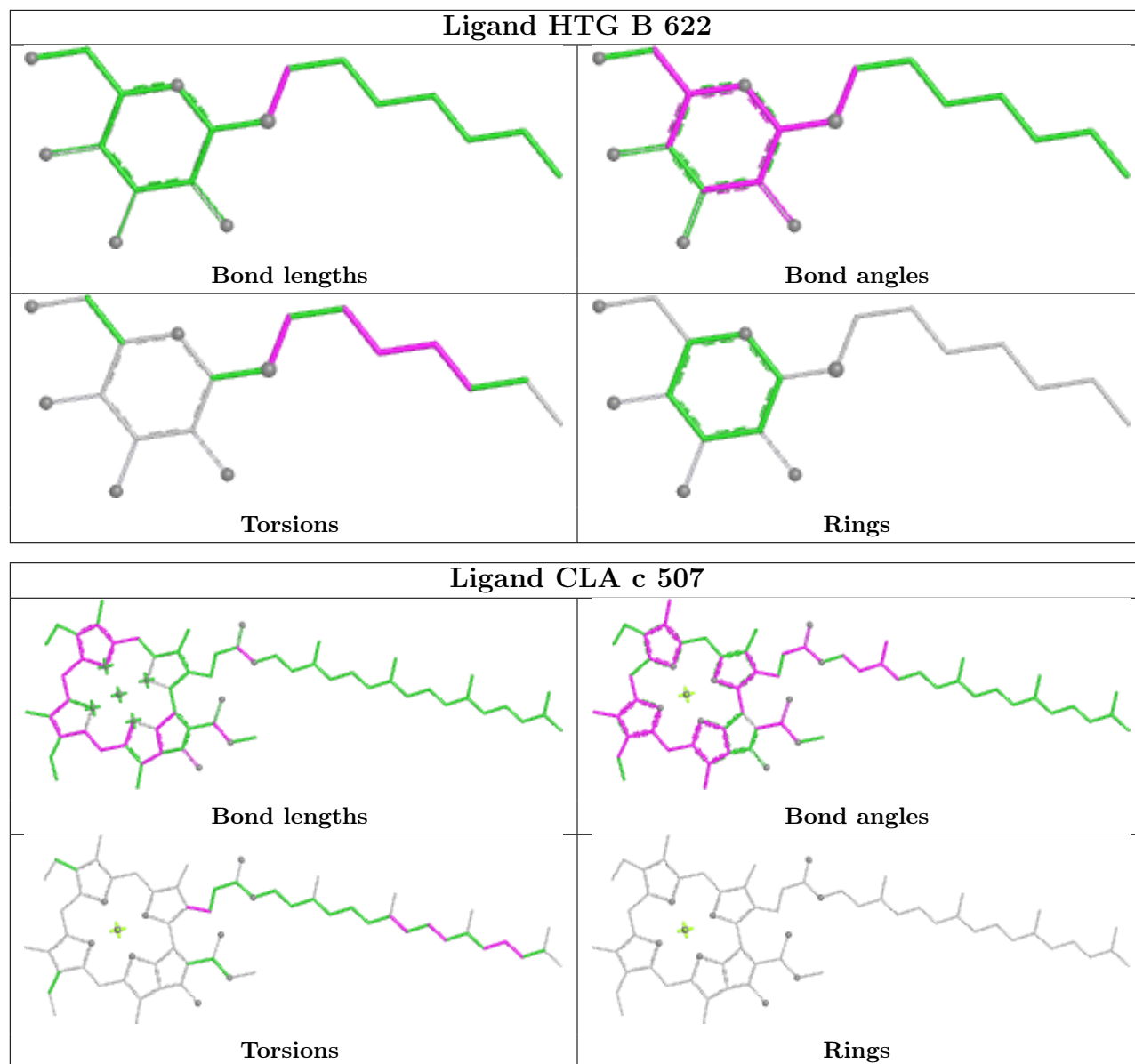
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	d	403	CLA	3	0
32	t	101	LMT	1	0
25	a	410	BCR	1	0
23	b	605	CLA	5	0
23	c	508	CLA	2	0
23	c	512	CLA	5	0
27	O	601	GOL	2	0
25	A	409	BCR	2	0
25	t	103	BCR	4	0
37	E	101	LHG	3	0
32	a	420	LMT	2	0
27	b	901	GOL	2	0
33	c	520	LMG	1	0
23	B	613	CLA	2	0
23	c	509	CLA	2	0
23	C	508	CLA	2	0
23	b	604	CLA	5	0
23	b	607	CLA	1	0
25	c	516	BCR	3	0
25	c	515	BCR	2	0
23	c	502	CLA	2	0
37	d	407	LHG	2	0
23	B	605	CLA	4	0
37	e	101	LHG	5	0
26	B	620	SQD	1	0
26	A	410	SQD	1	0
23	D	405	CLA	3	0
23	a	409	CLA	3	0

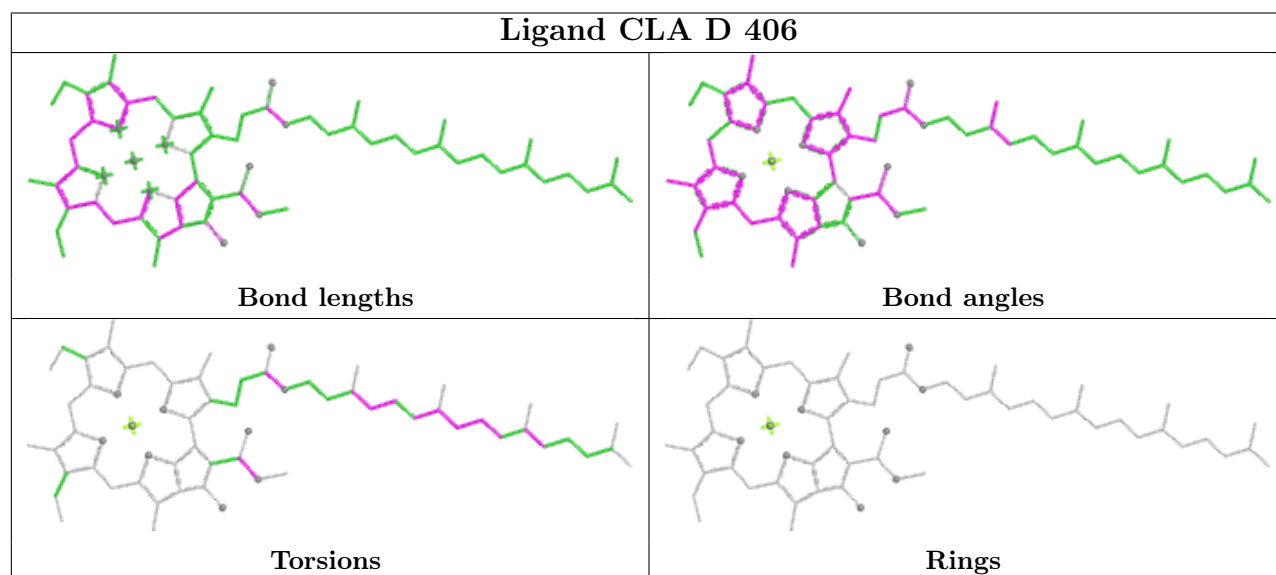
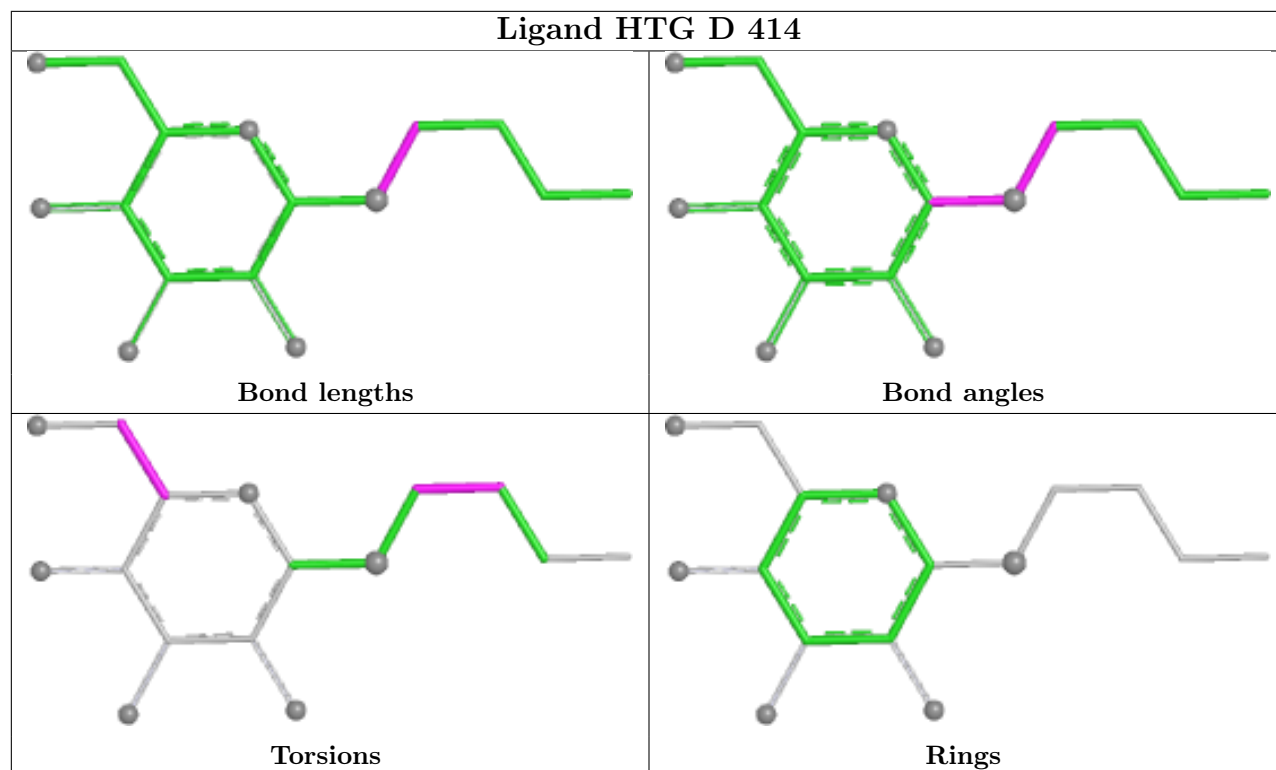
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

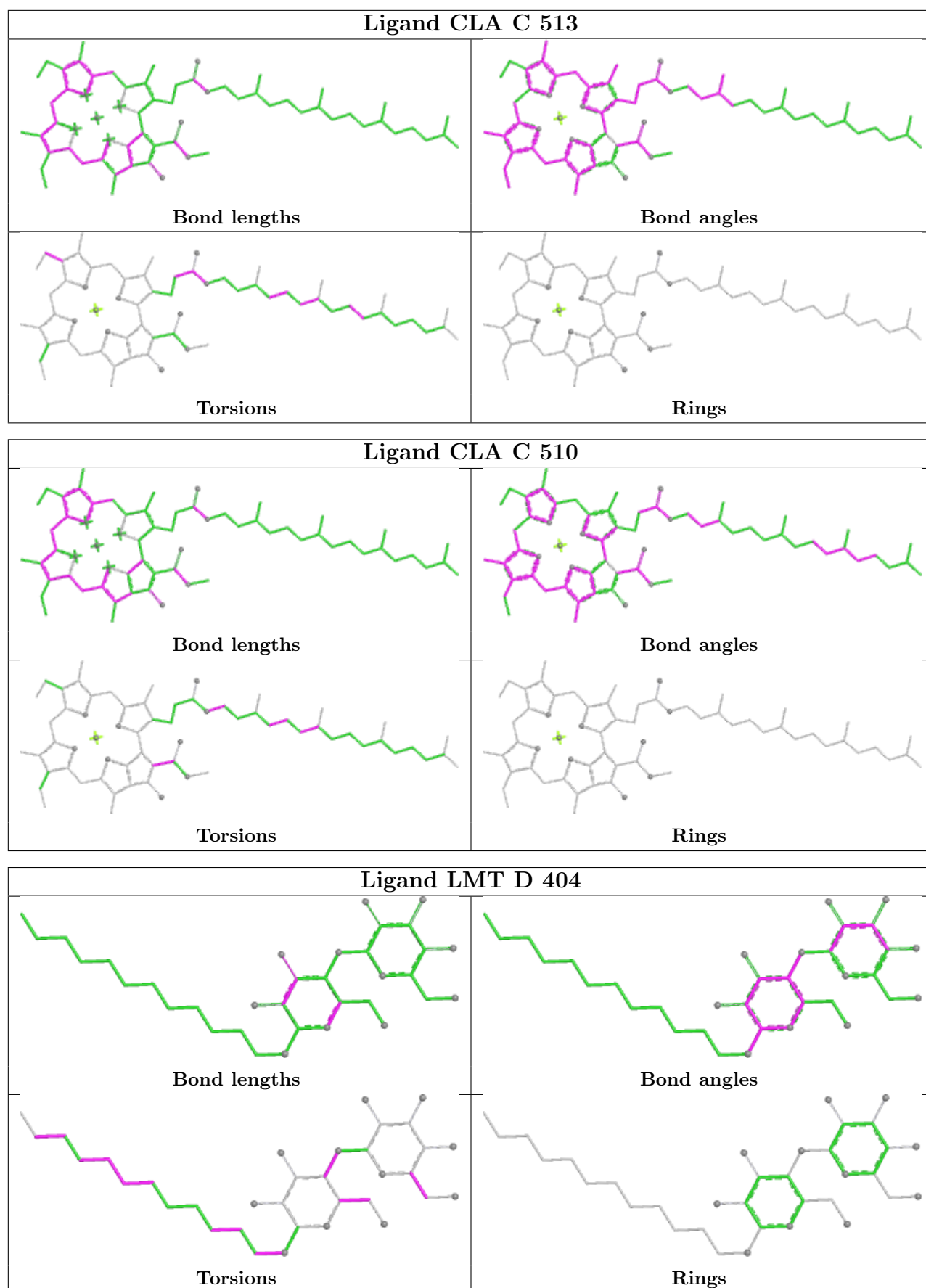


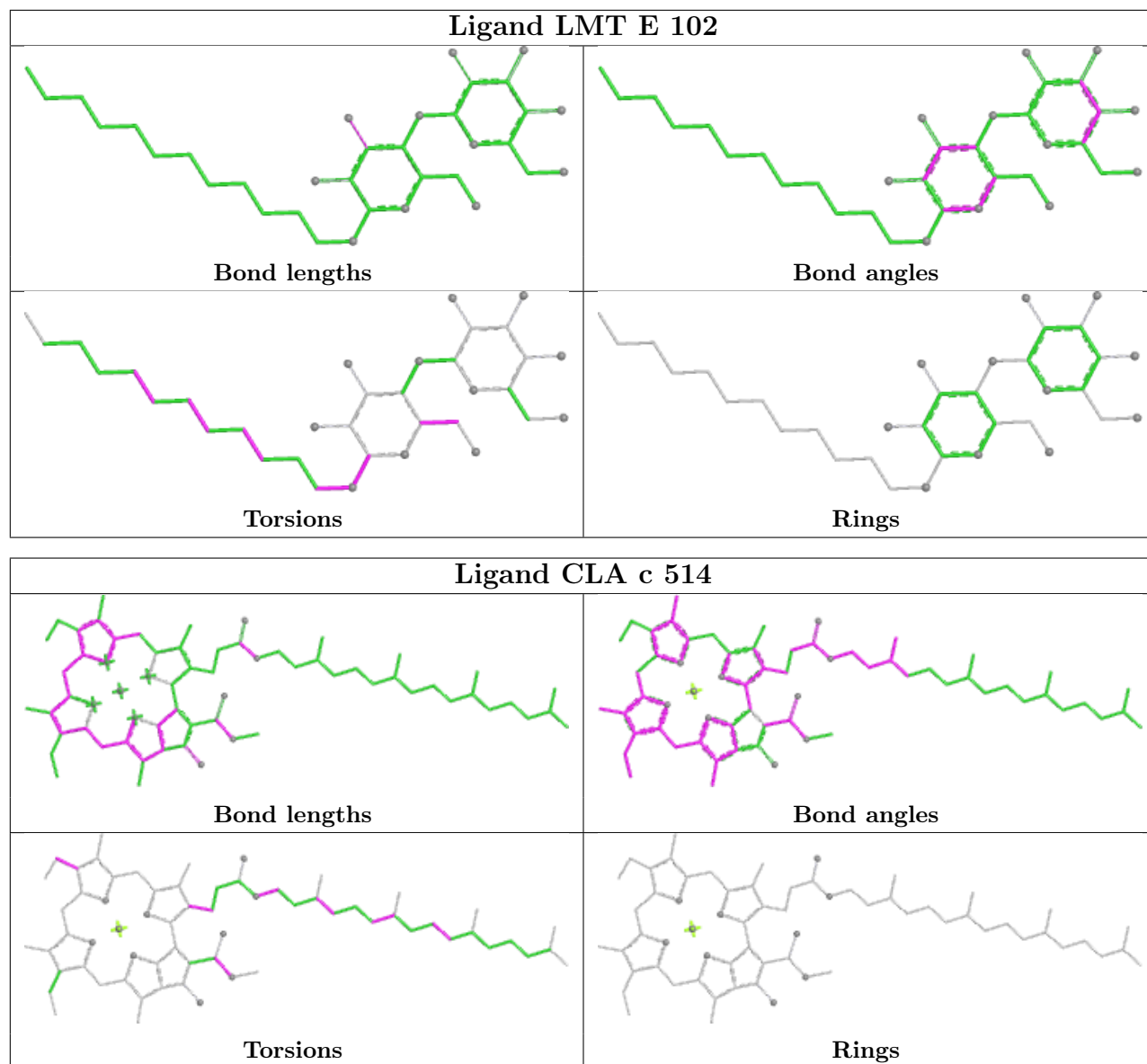


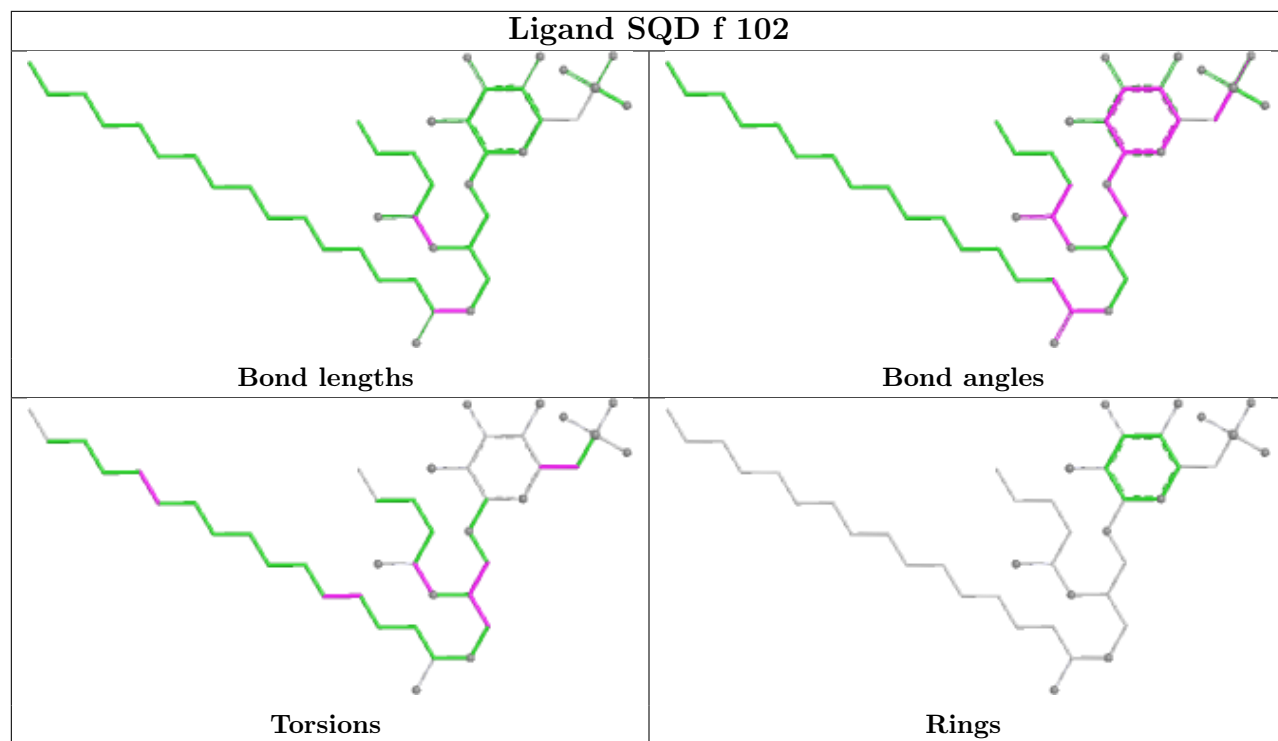


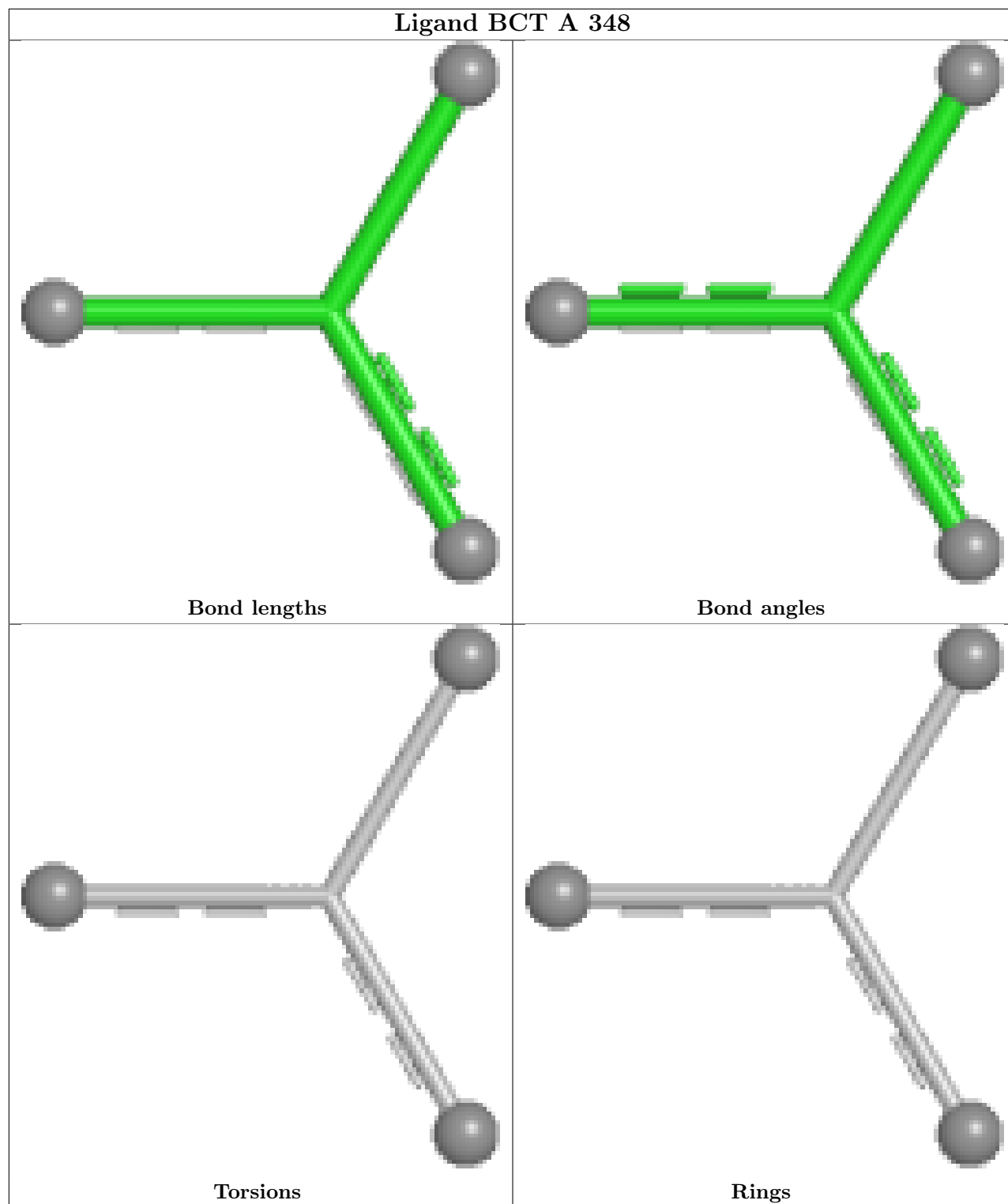


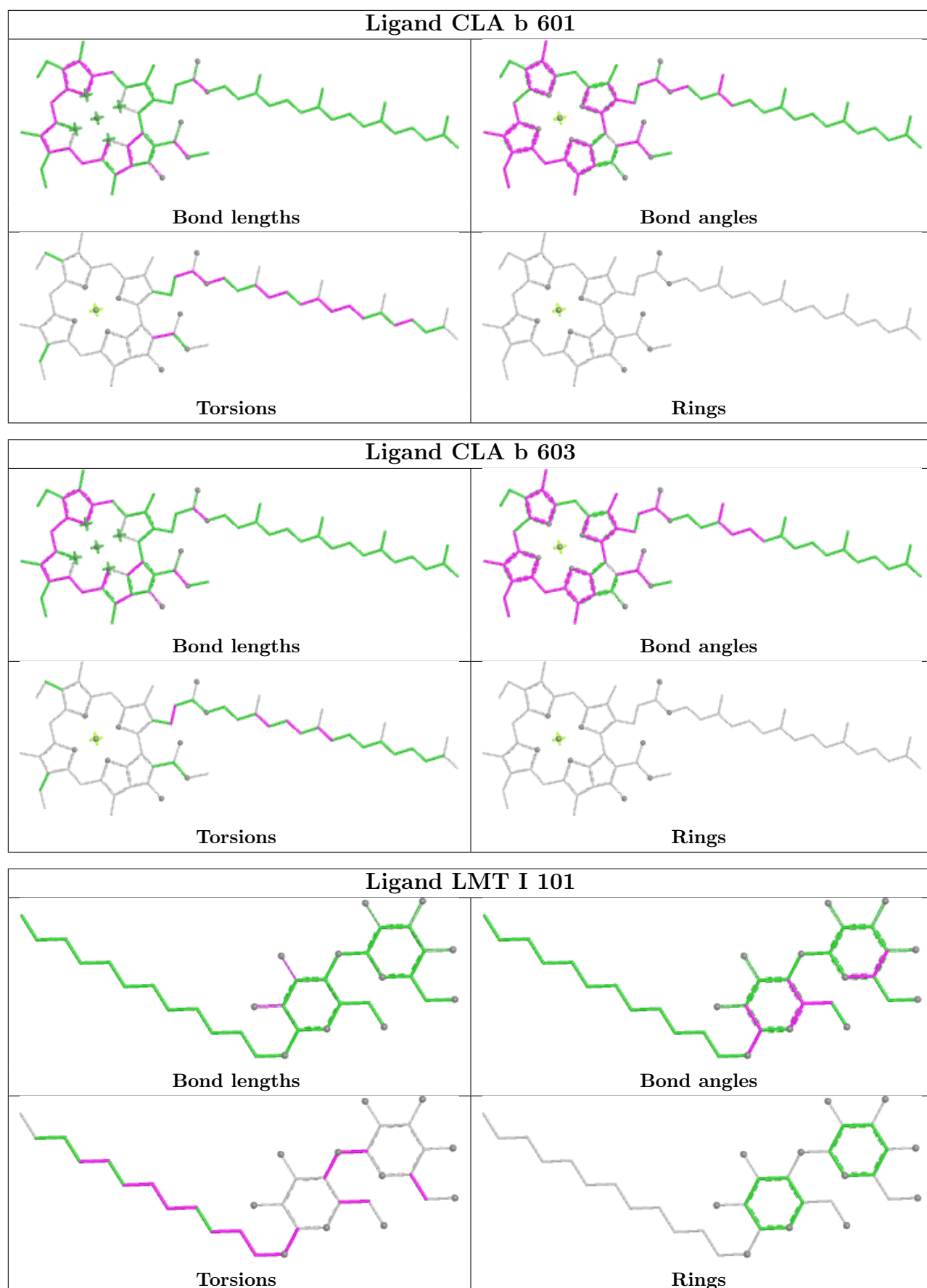


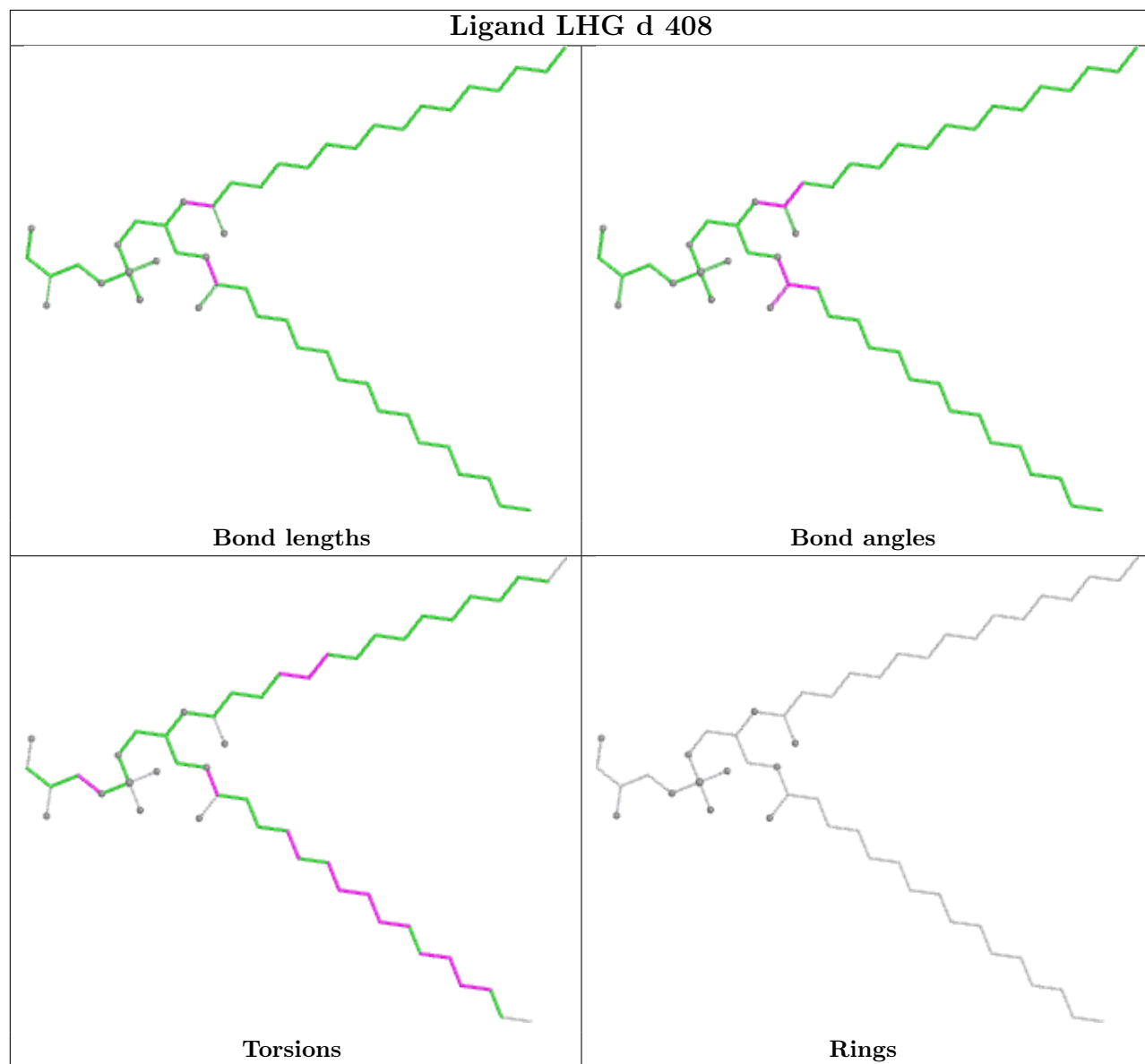


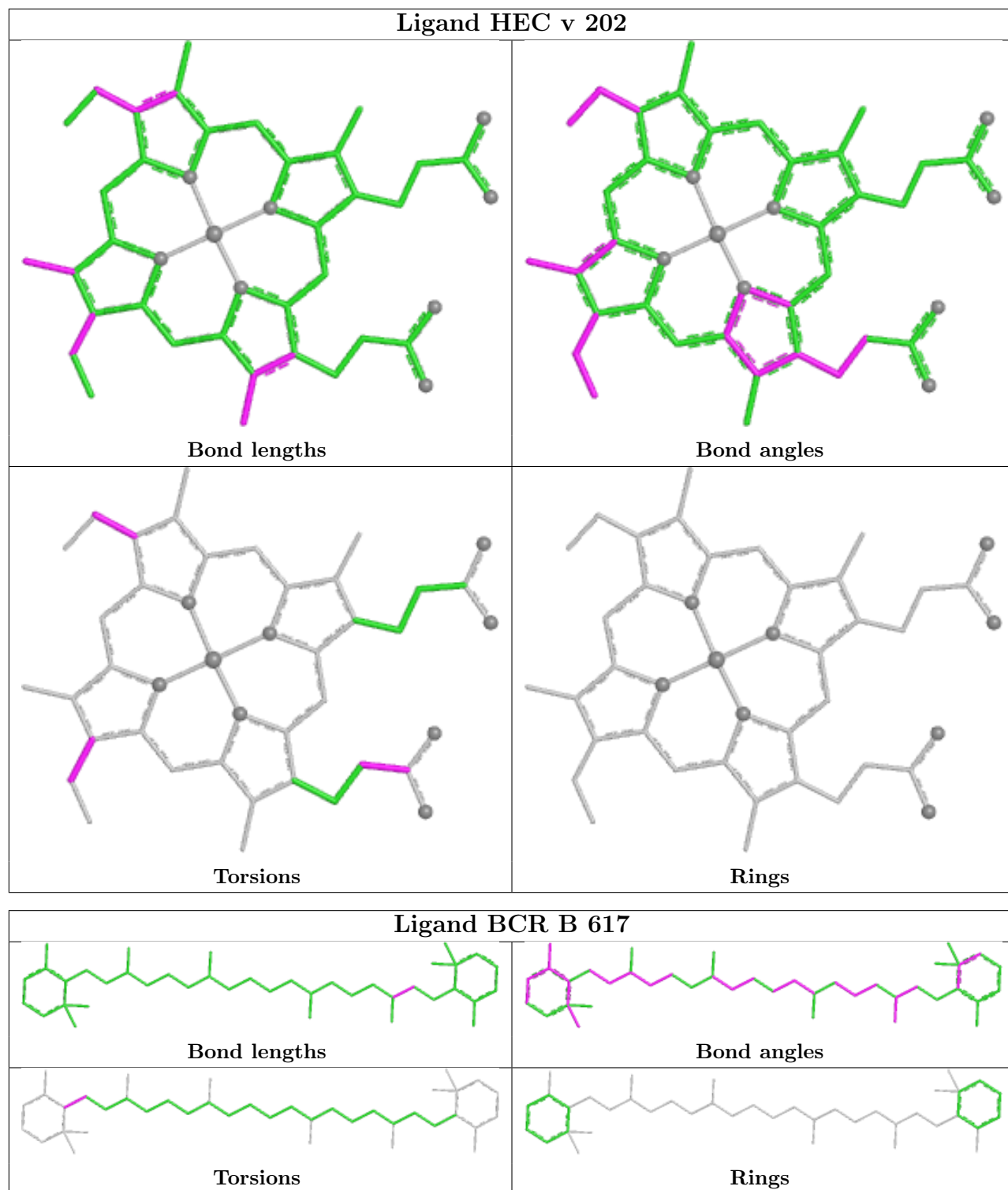


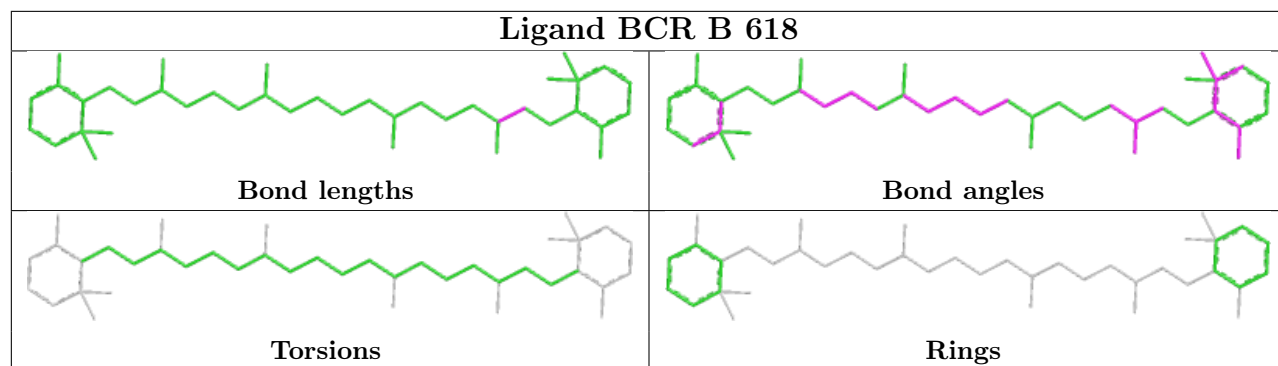


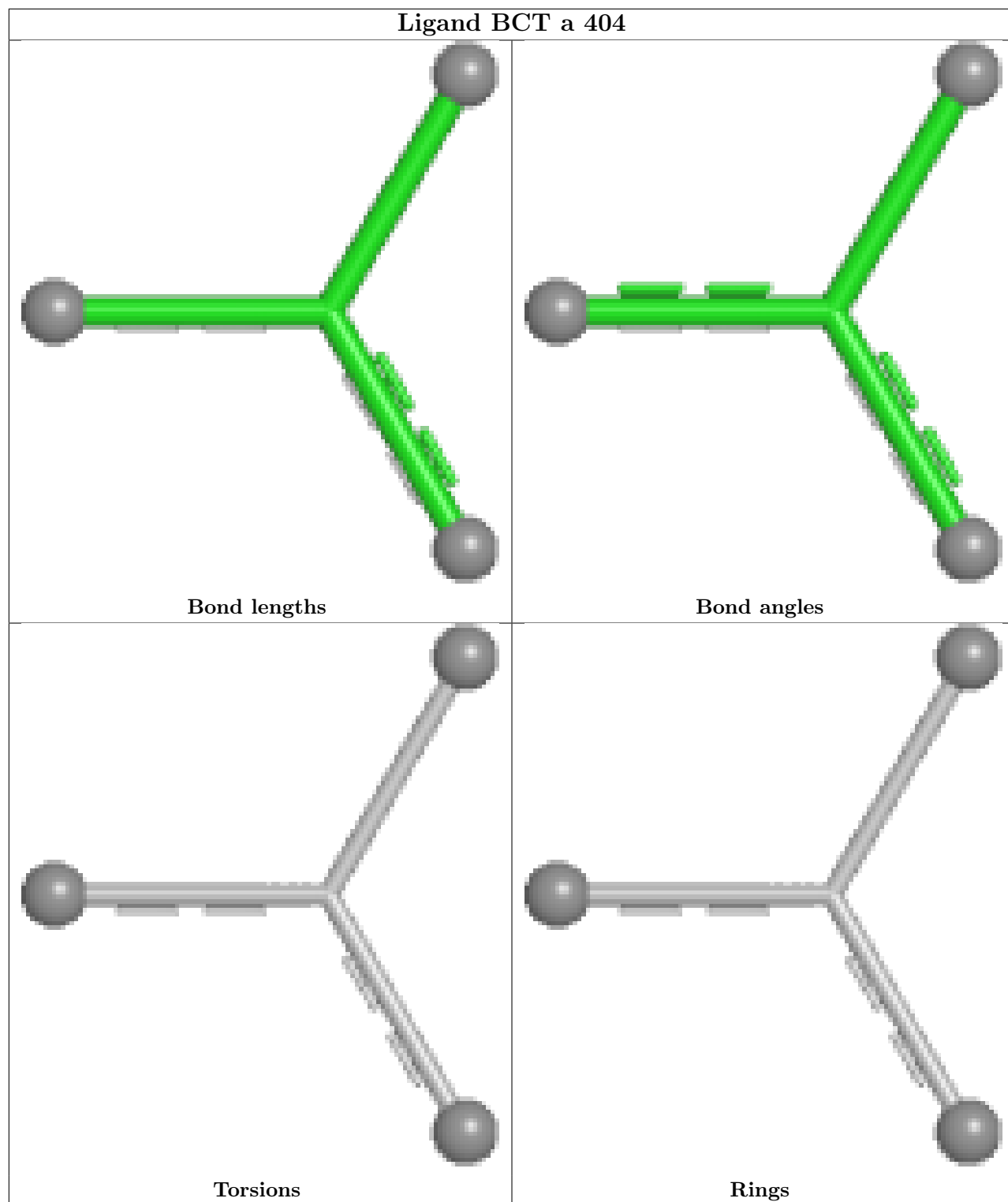


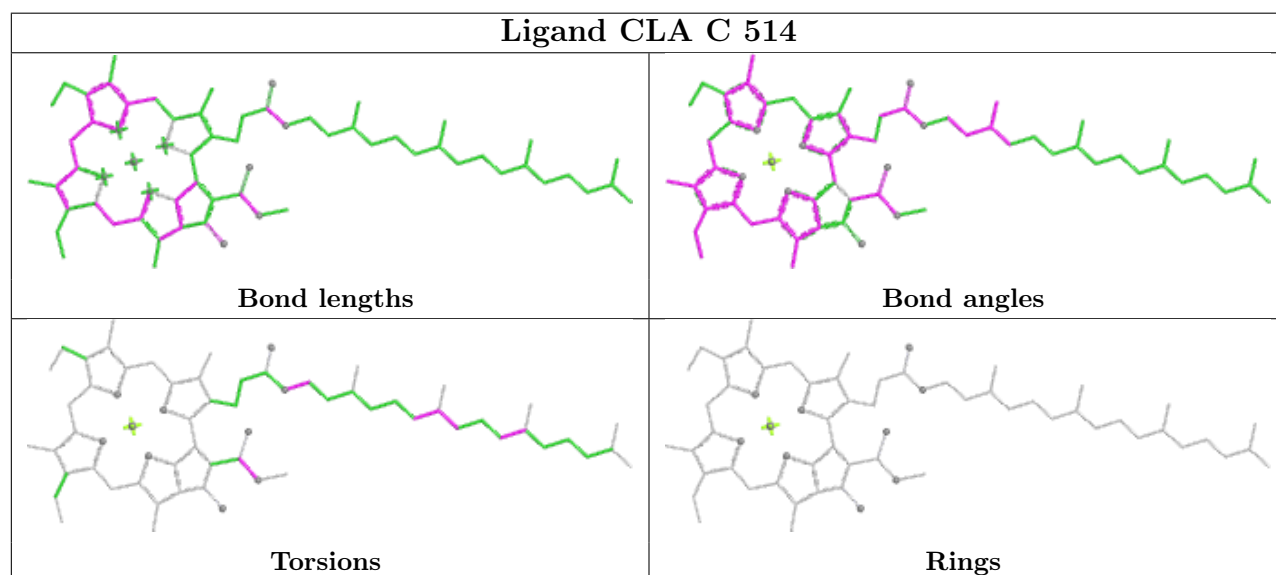
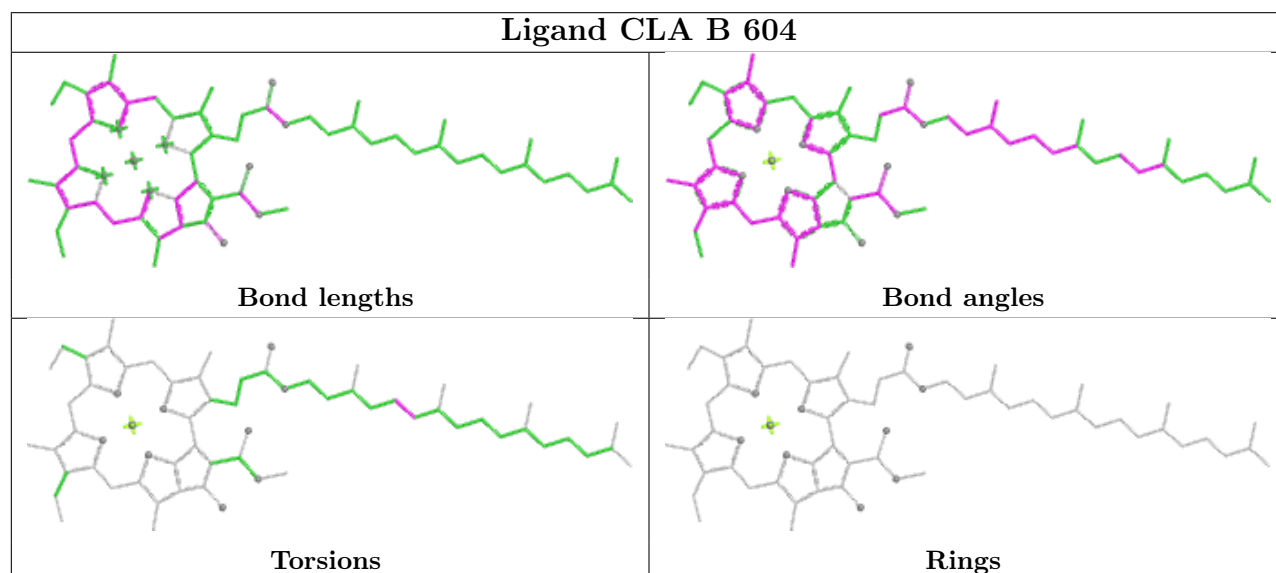
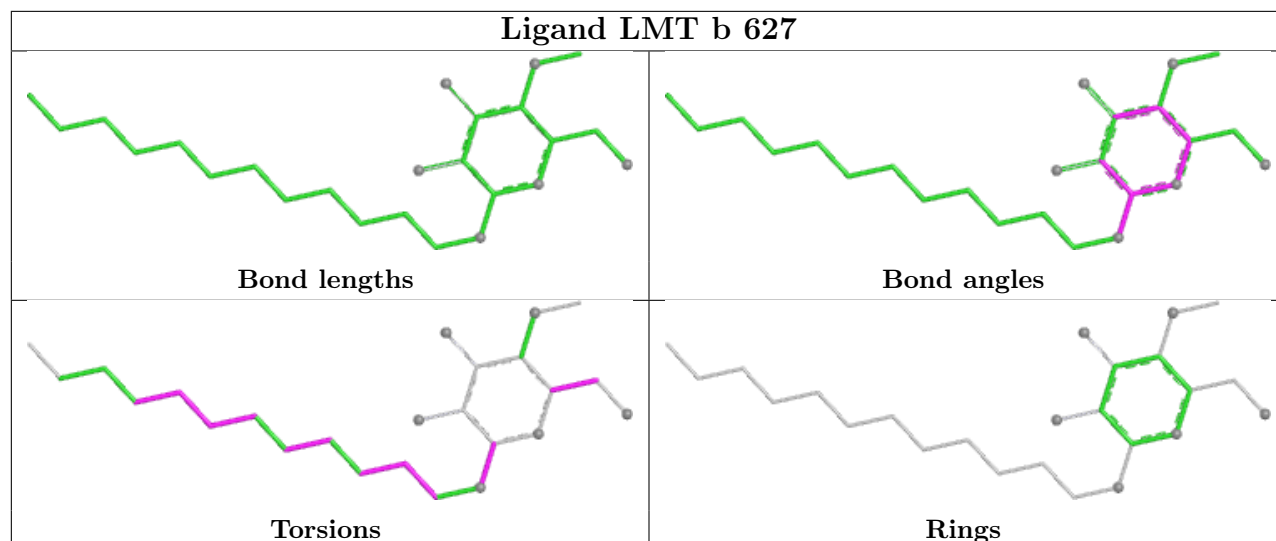


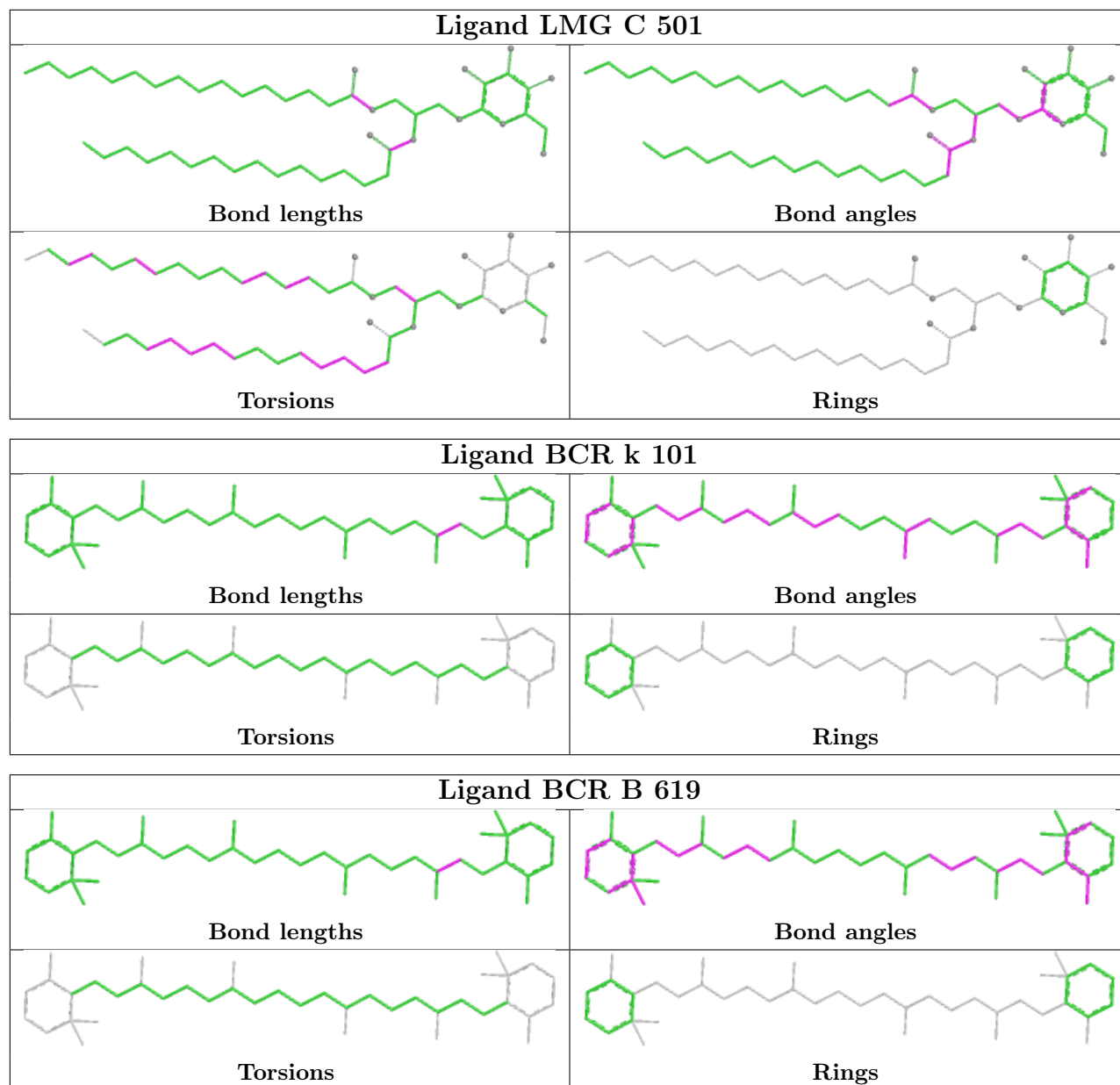


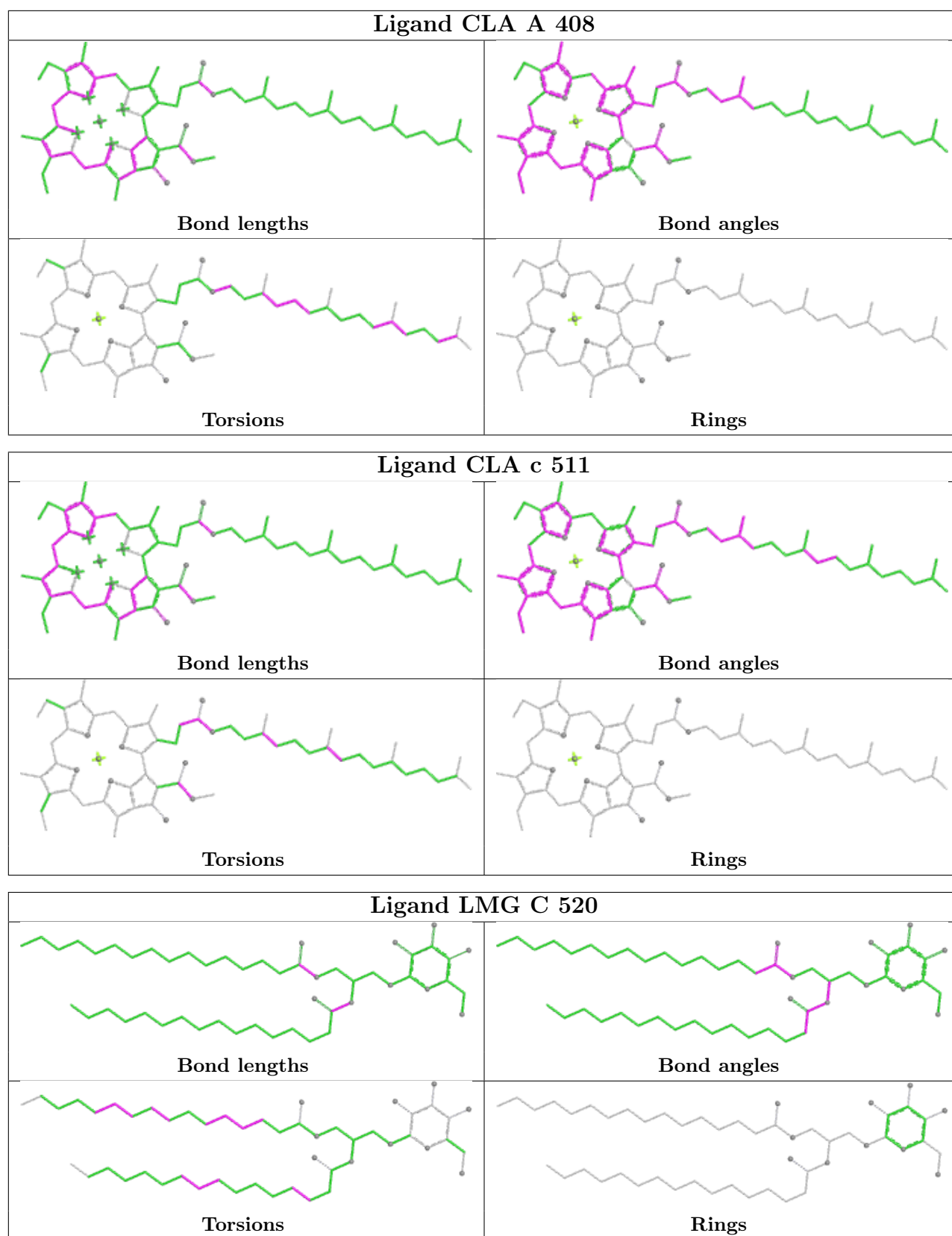


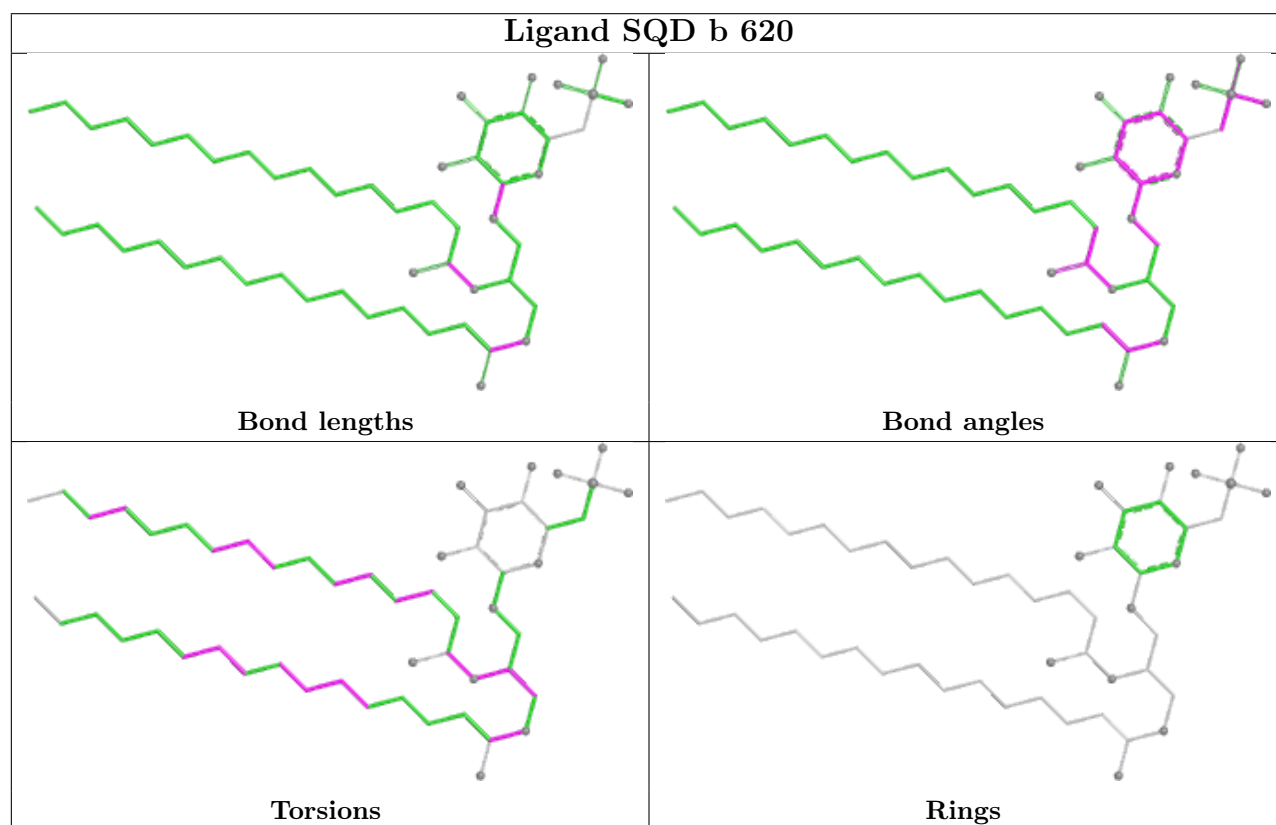
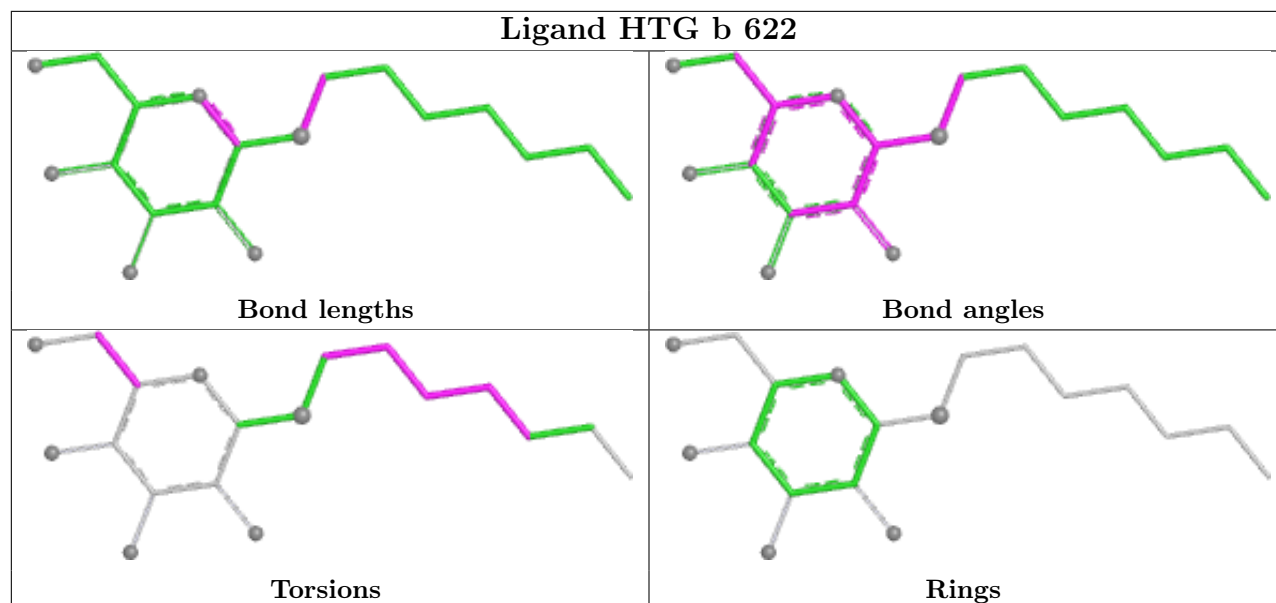


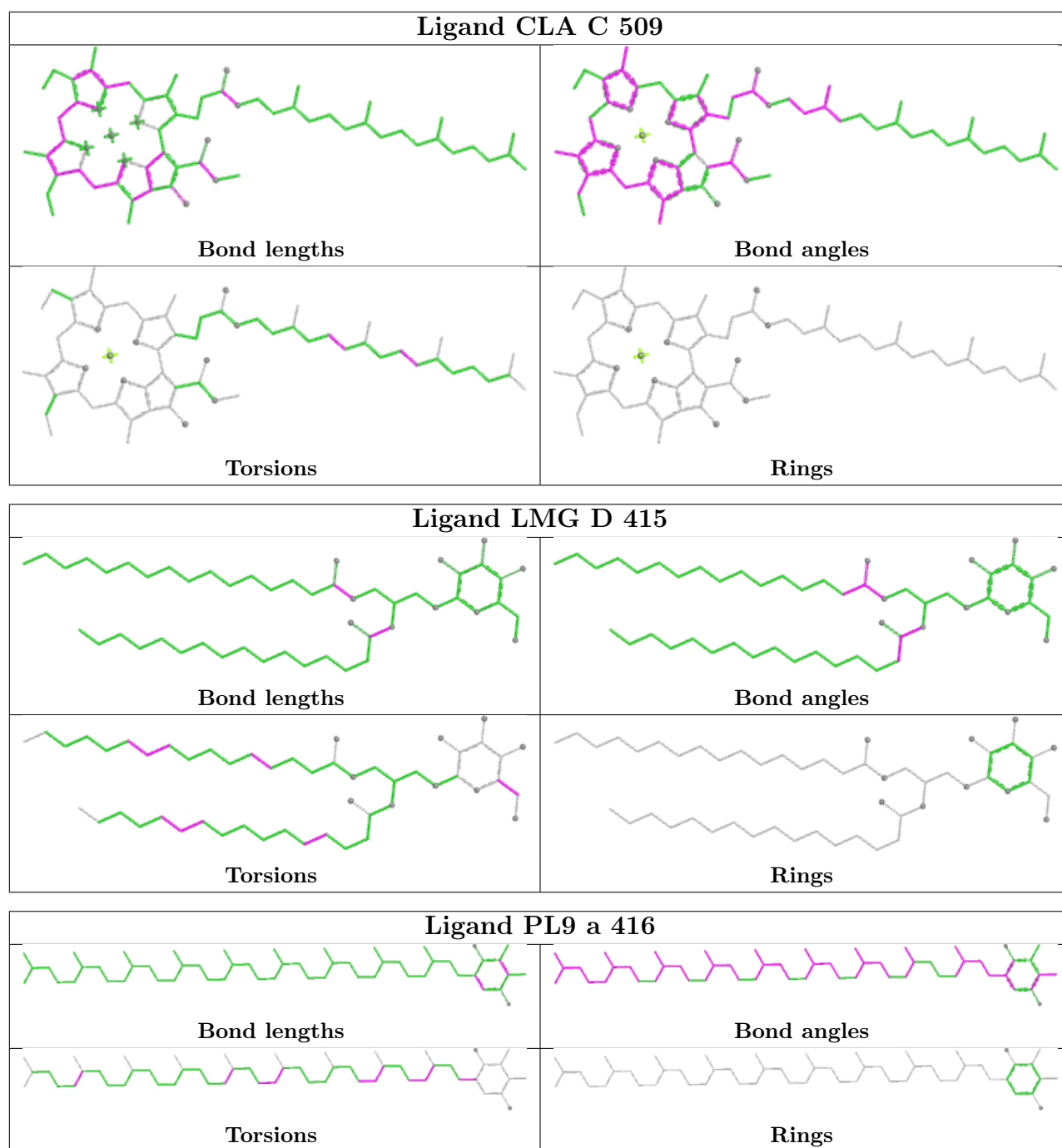


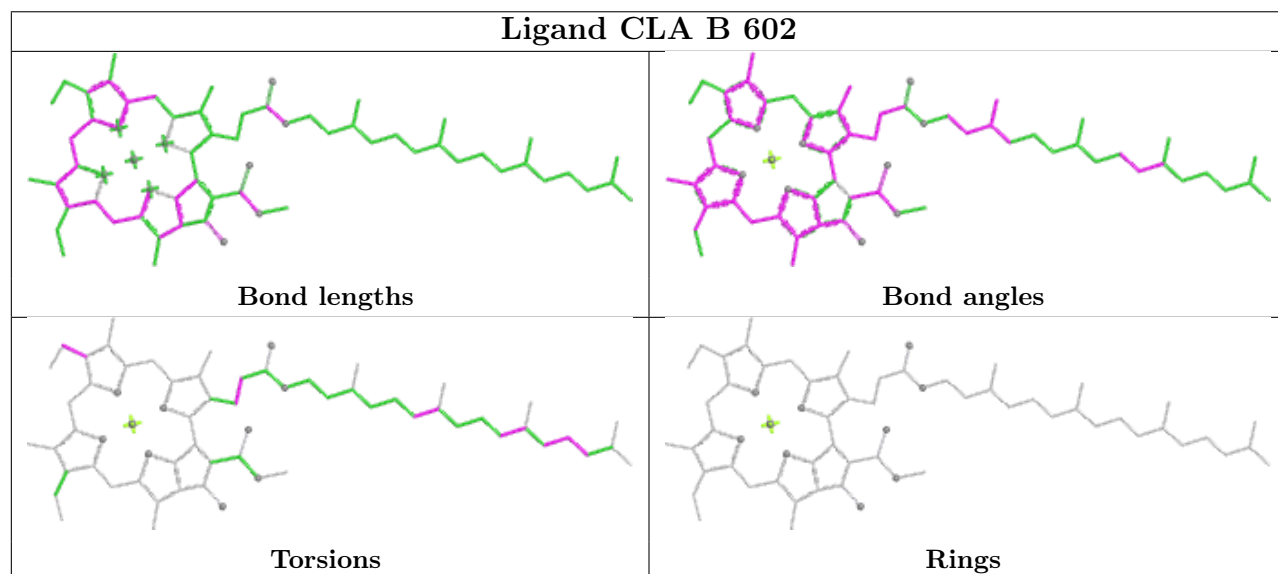
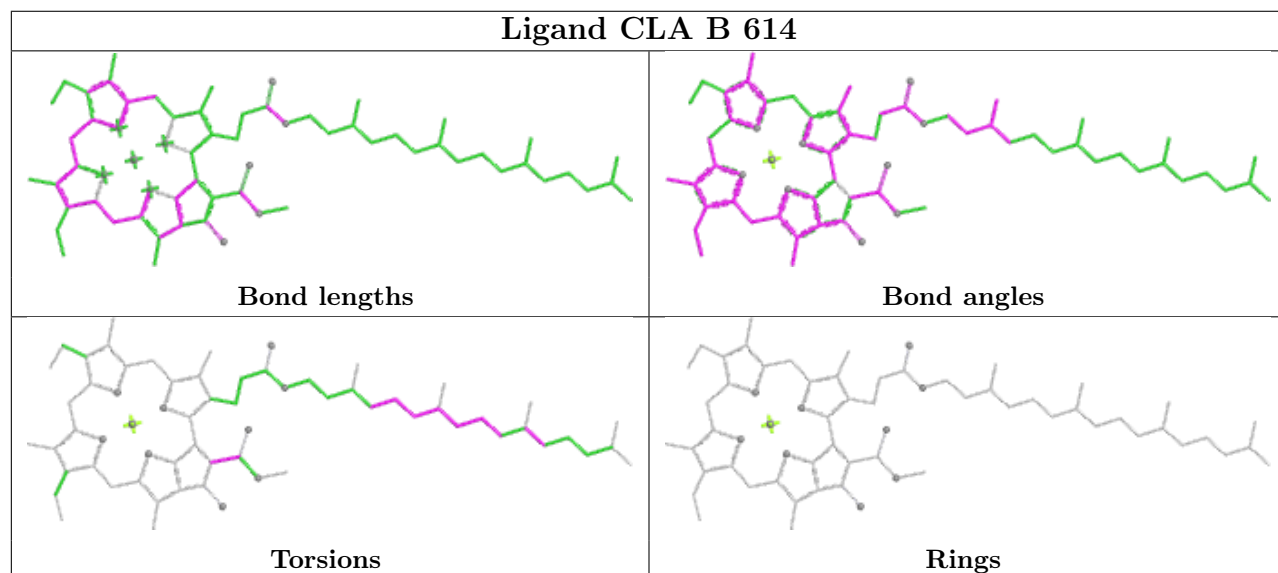
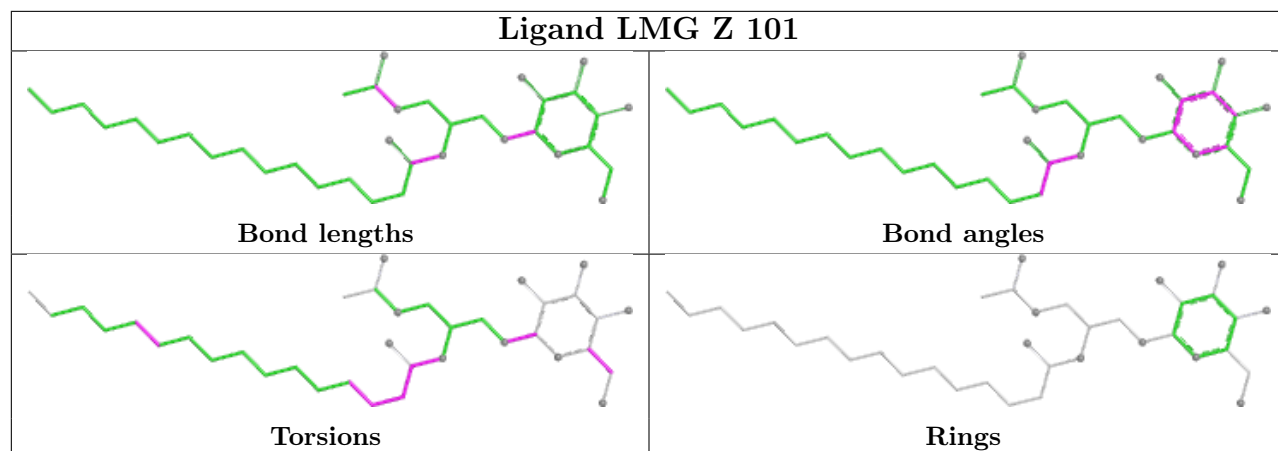


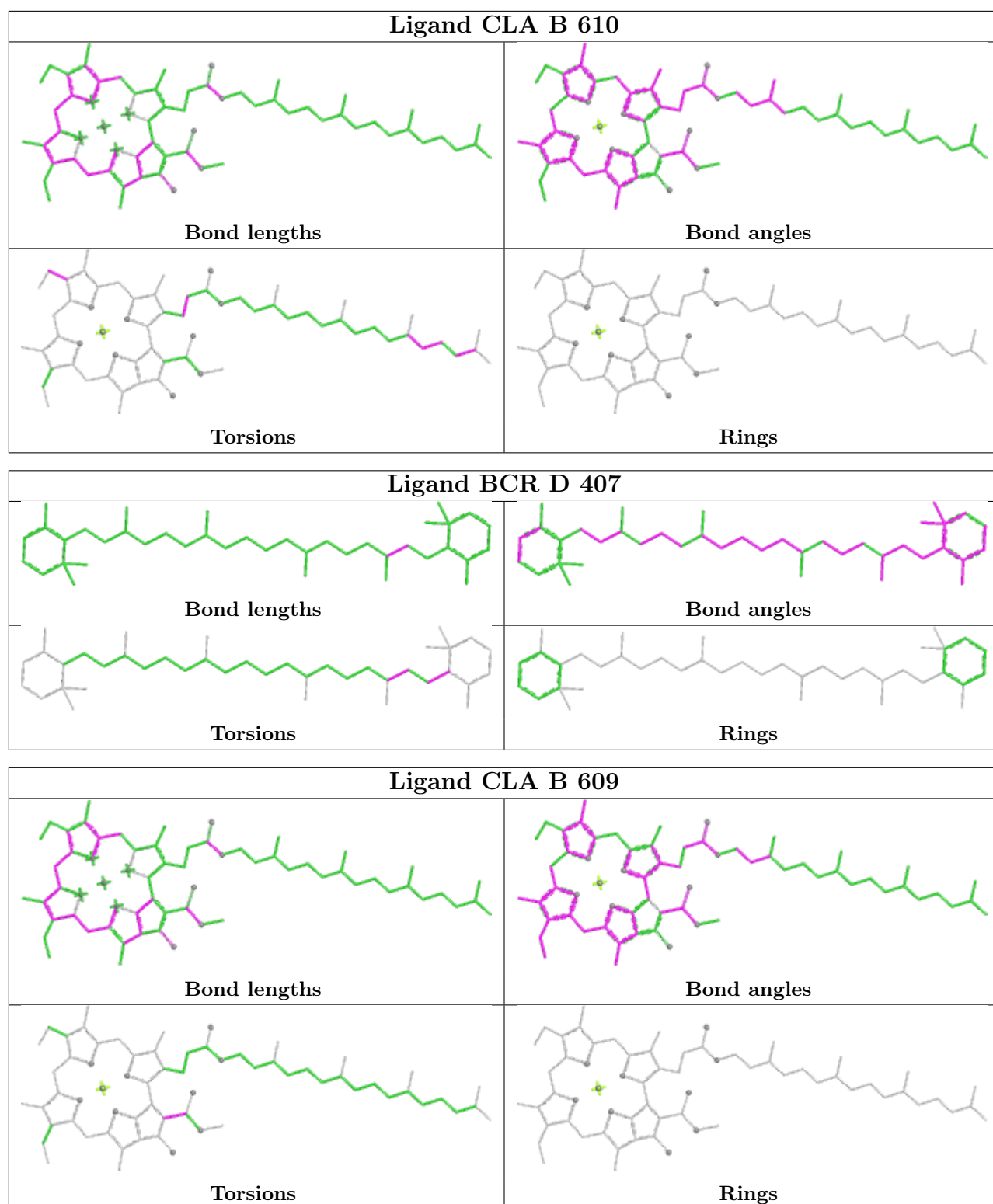


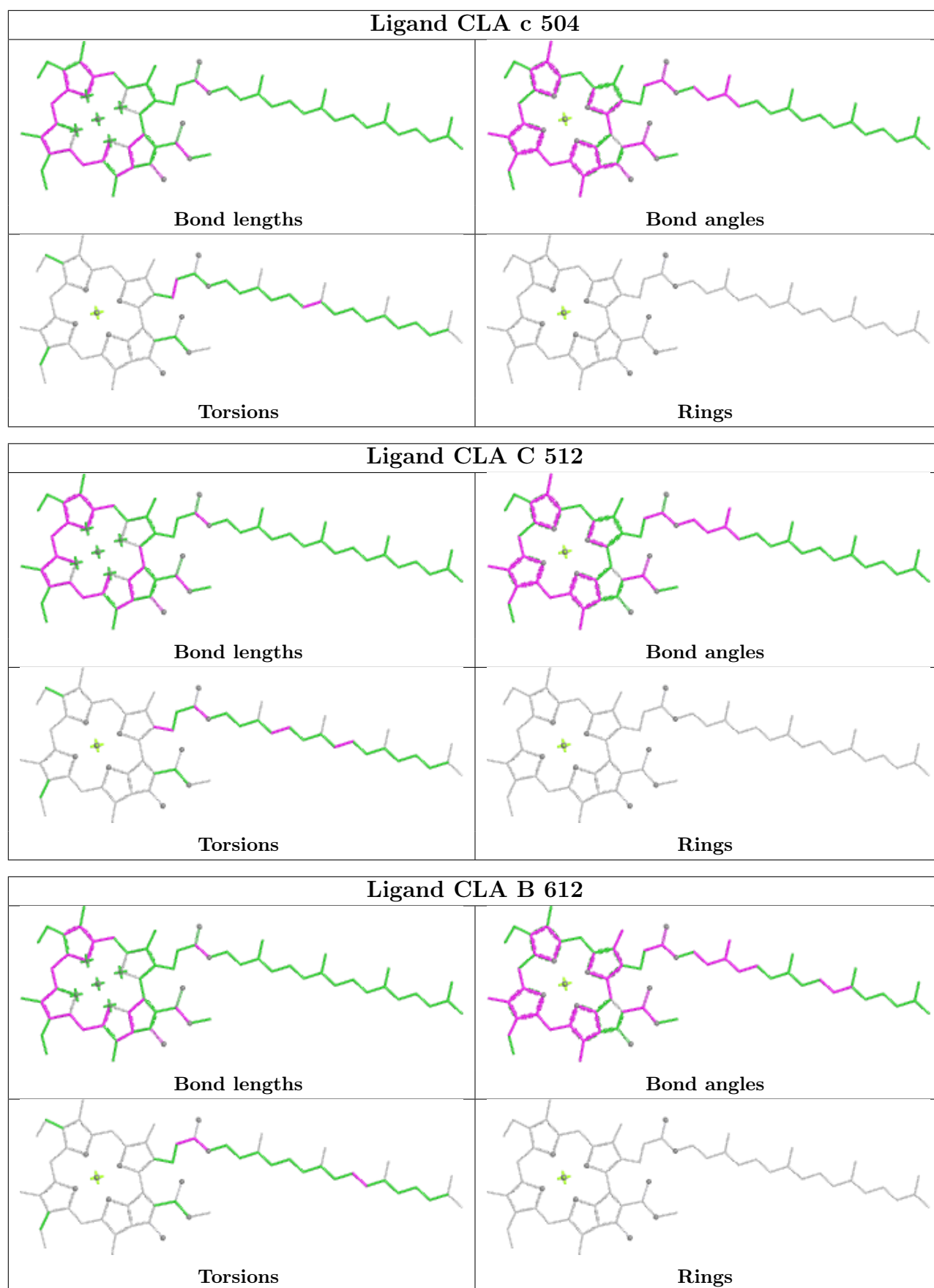


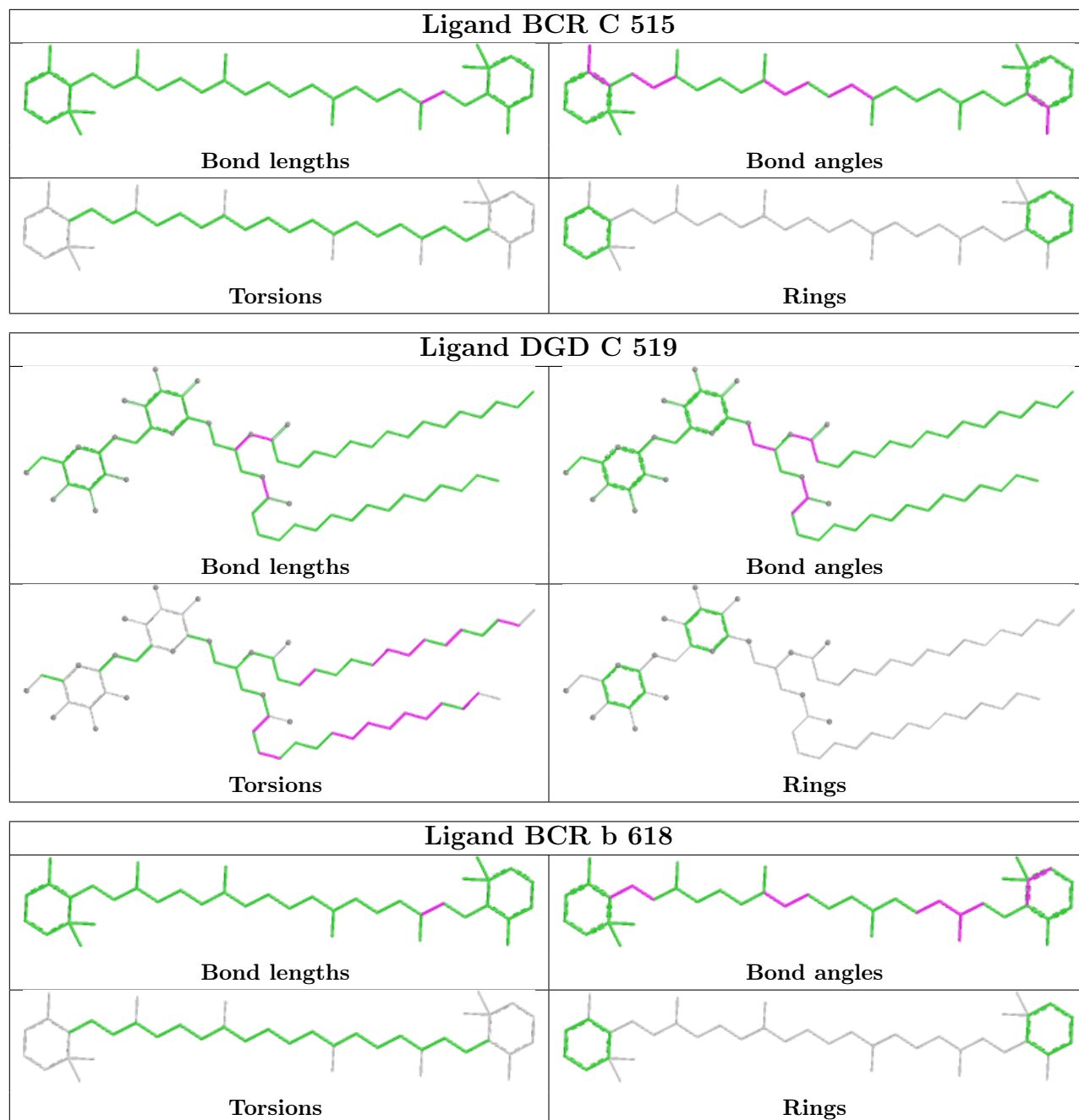


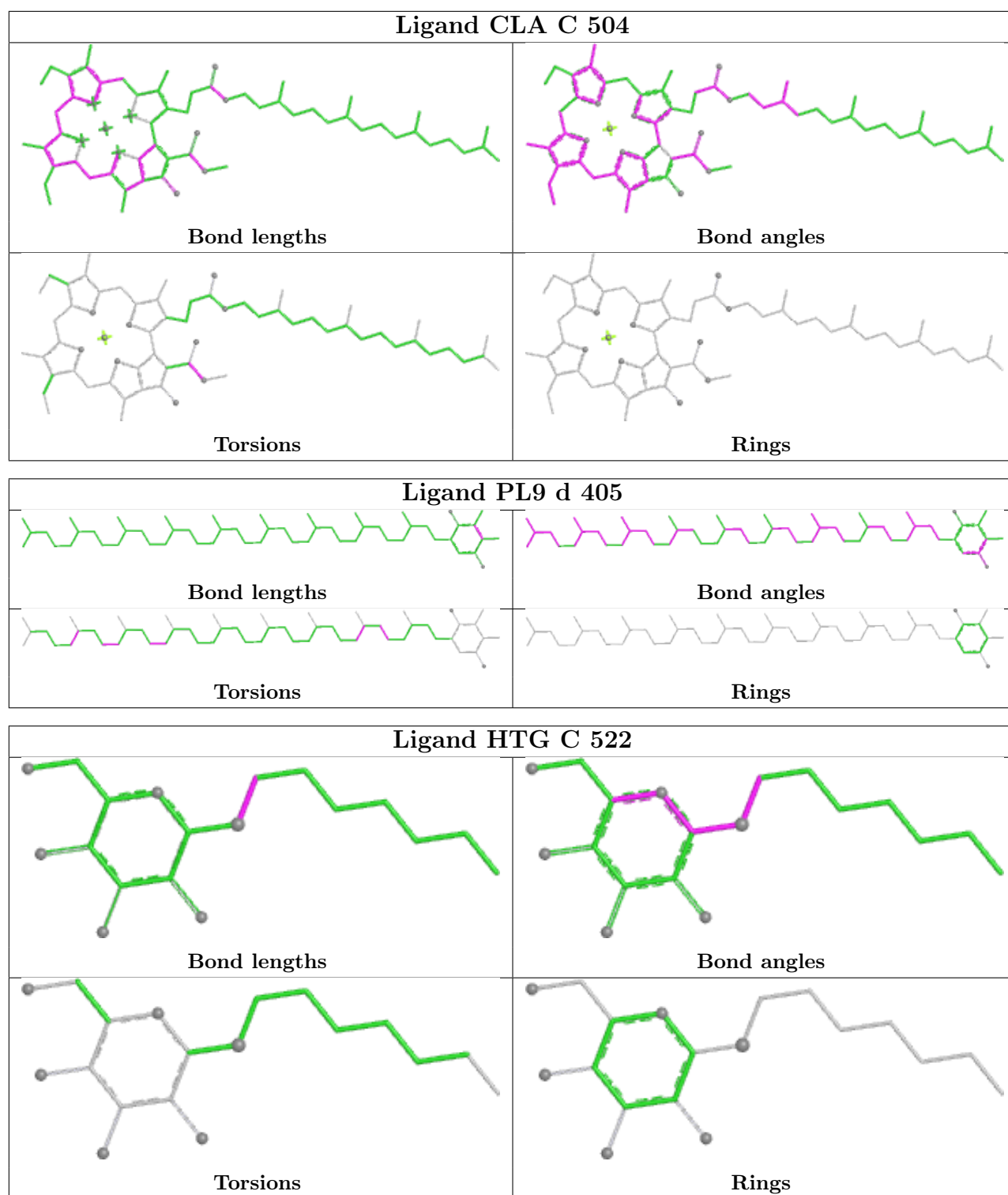


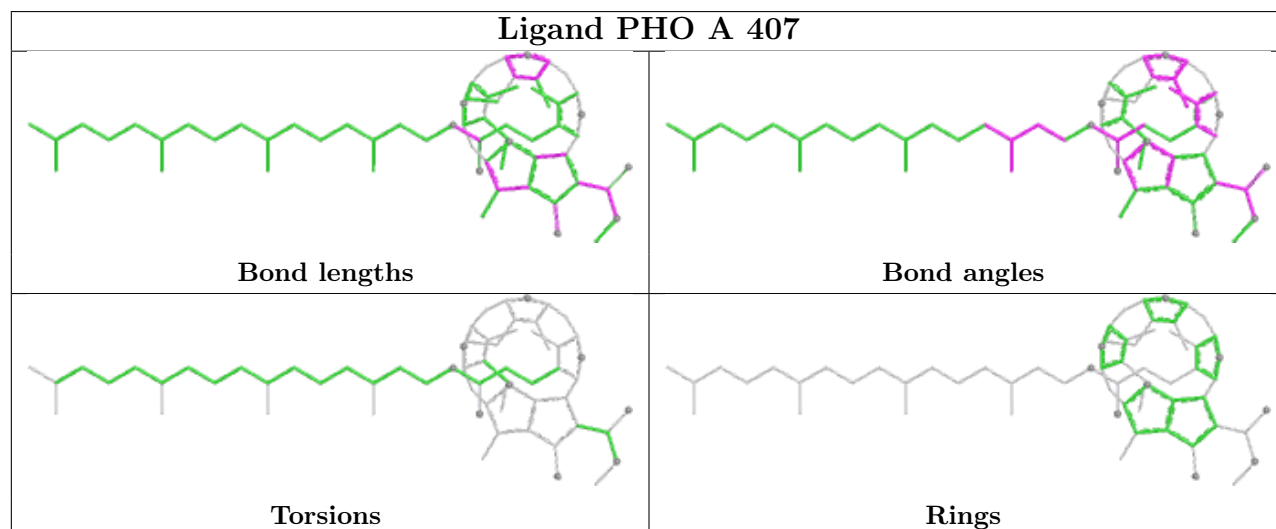
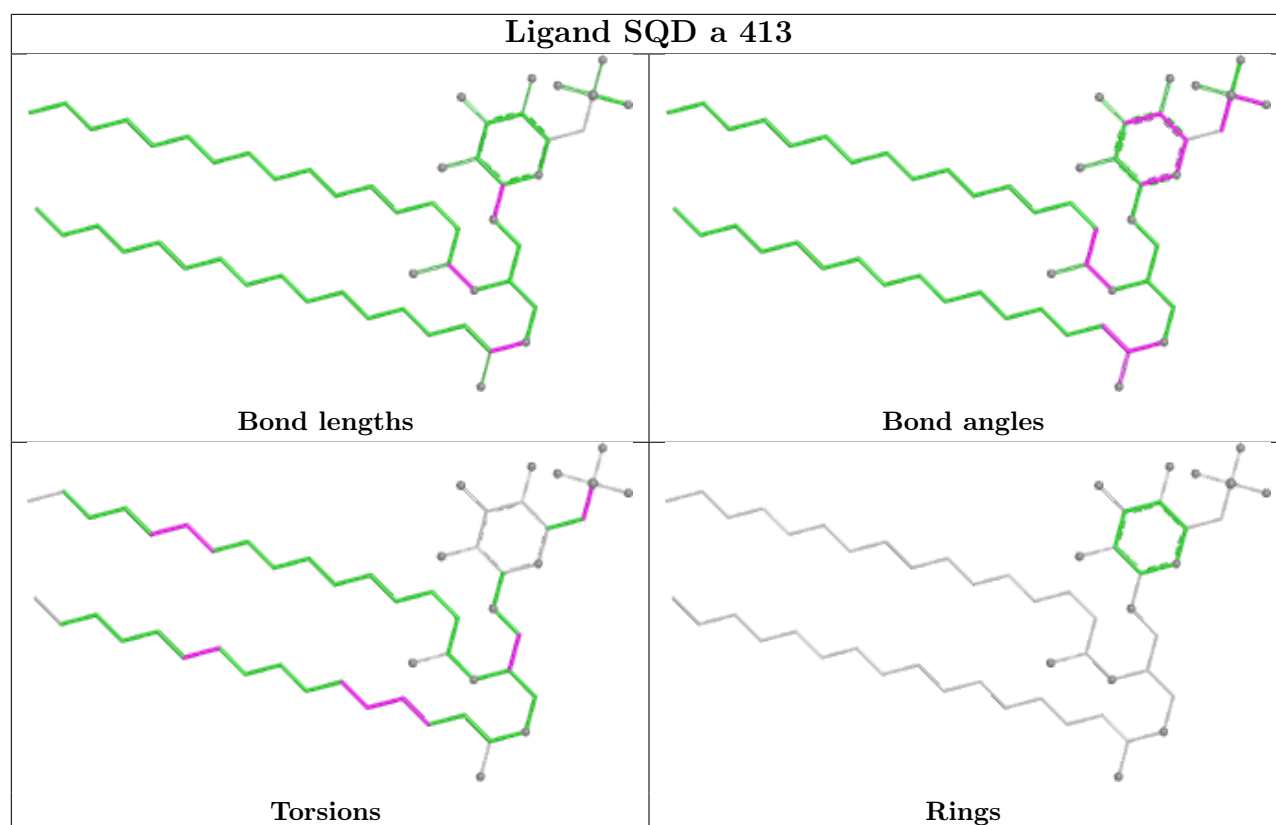


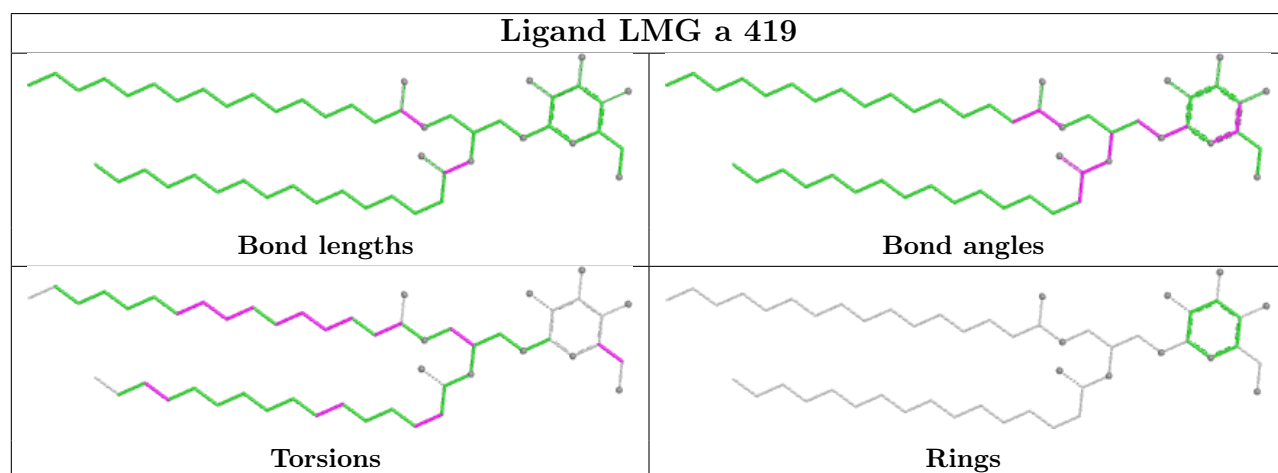
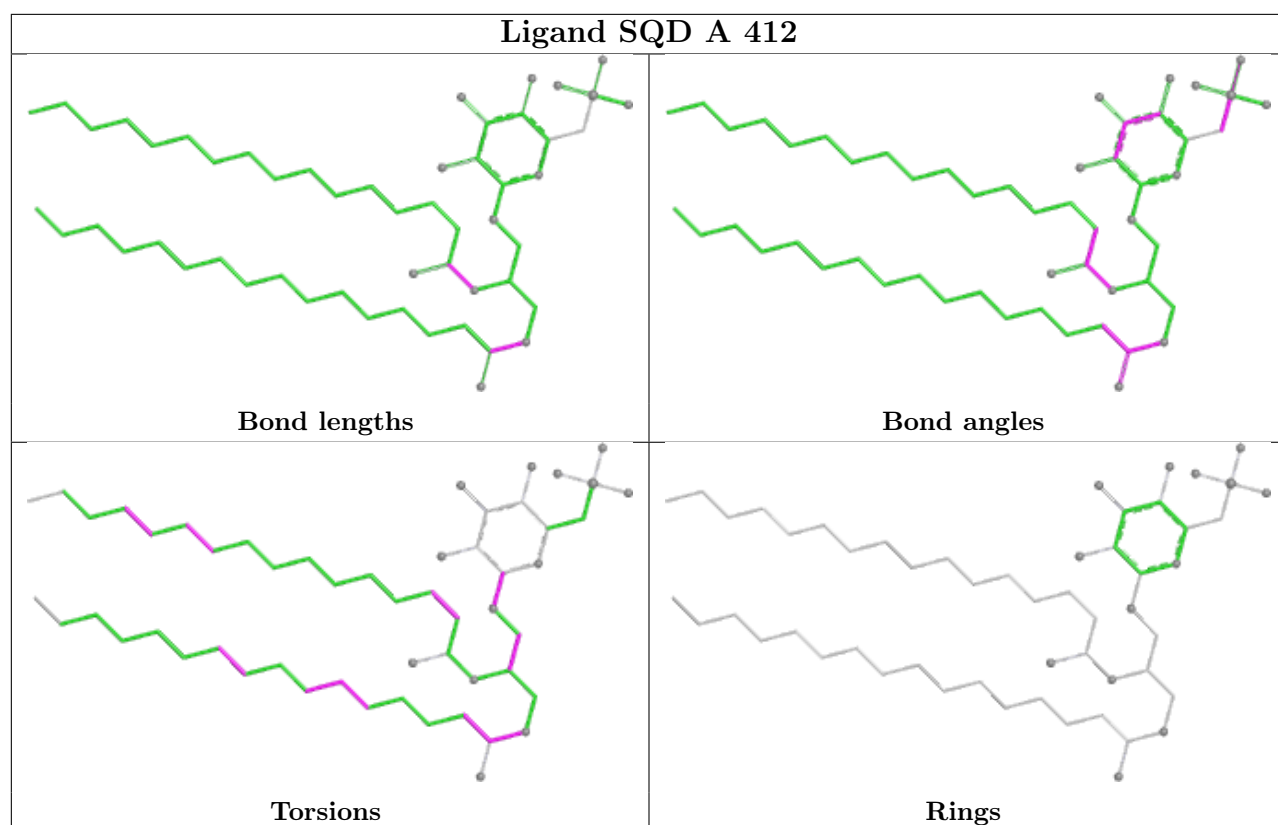


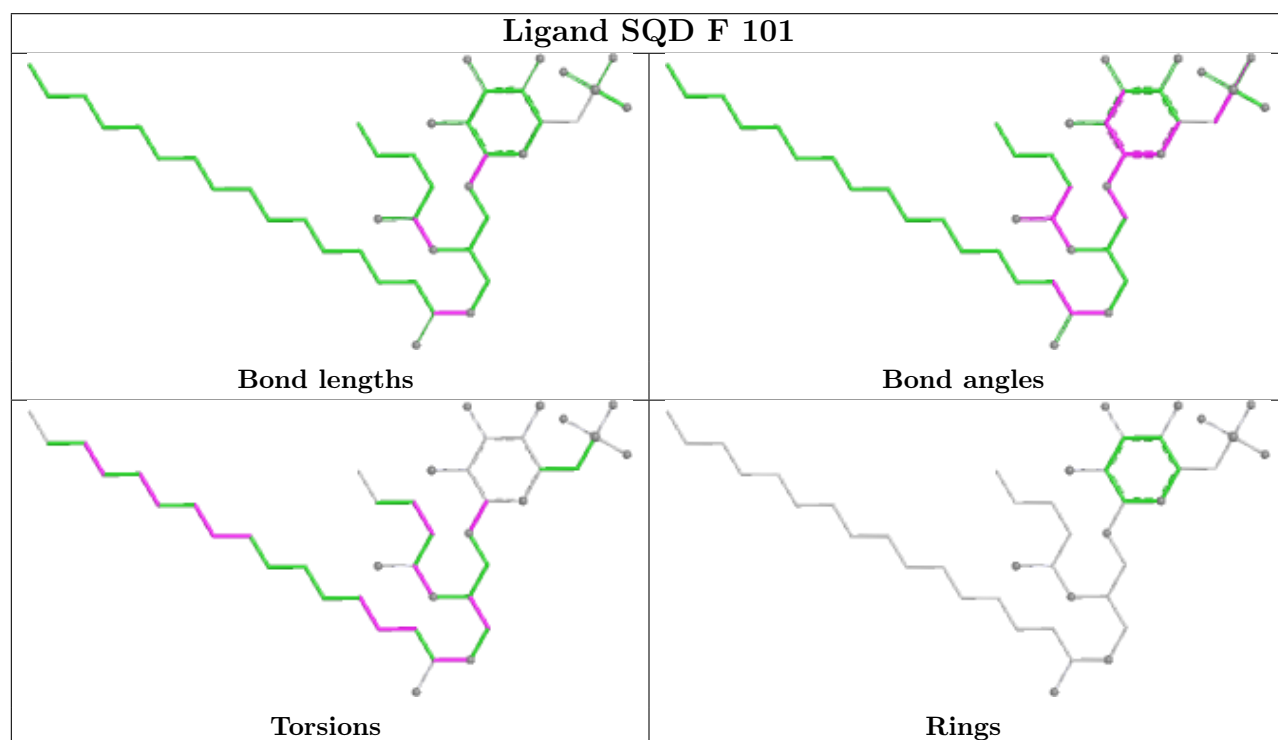
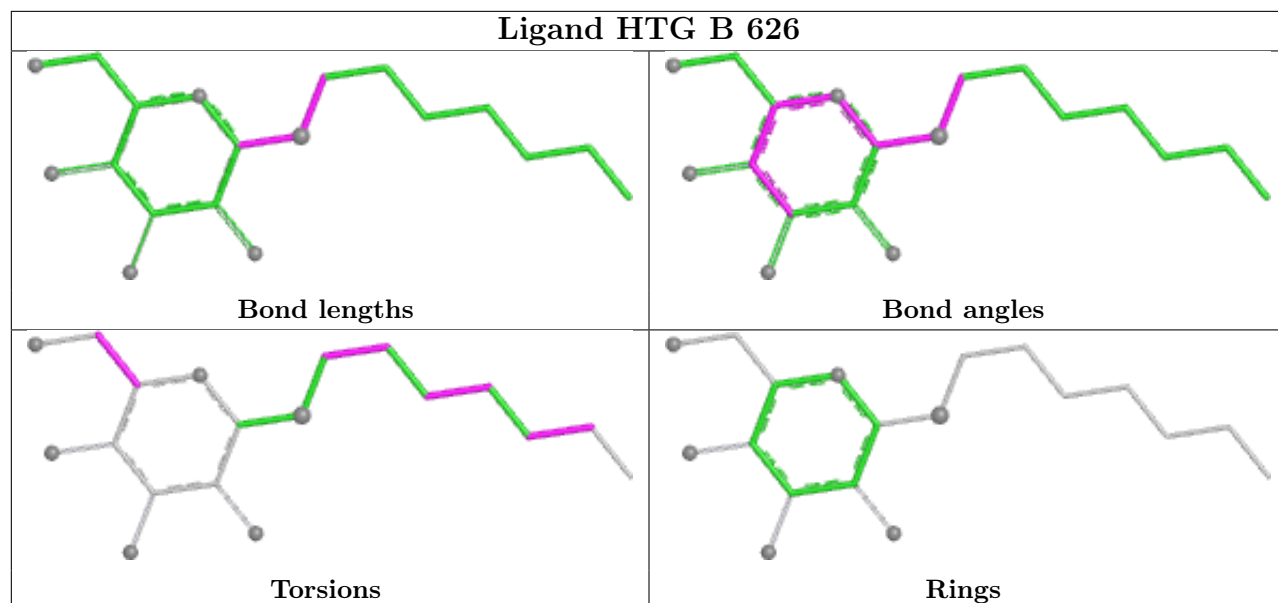


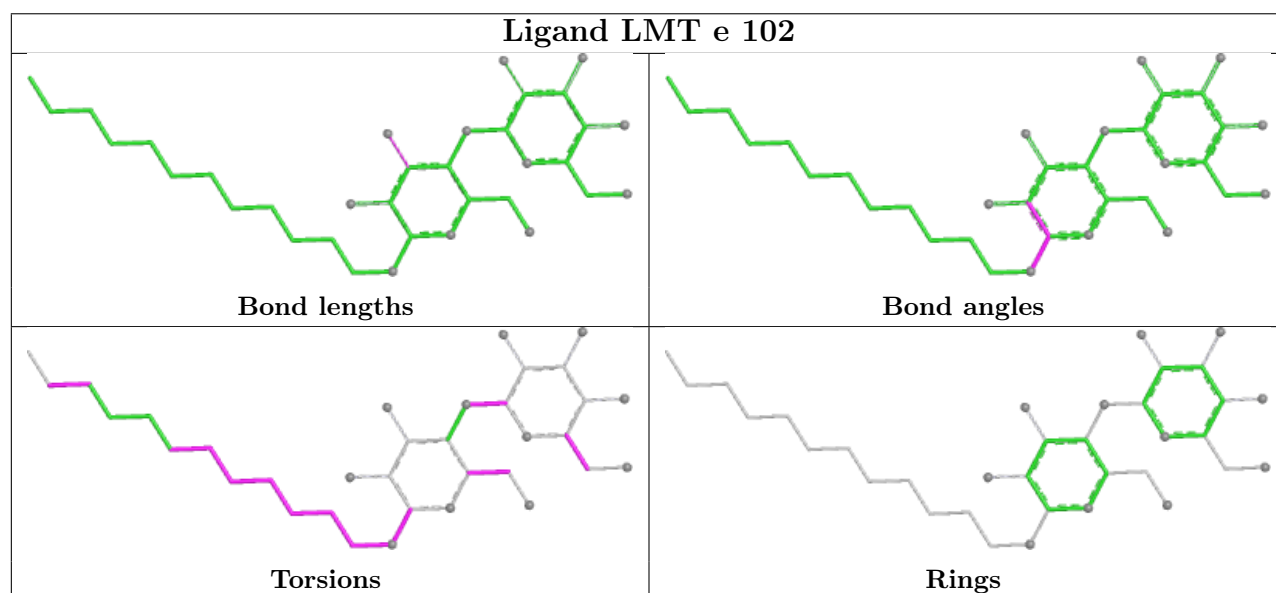
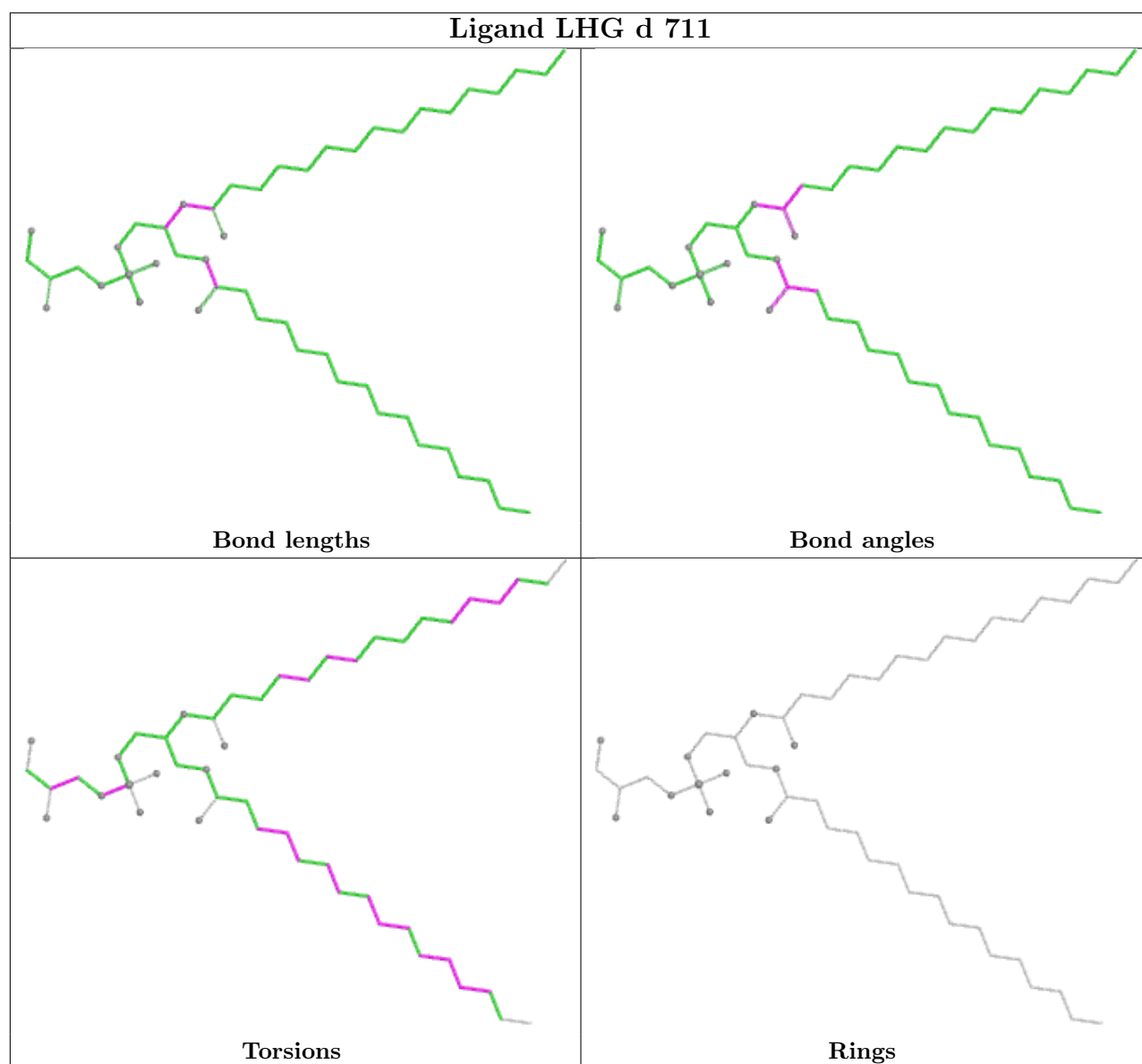


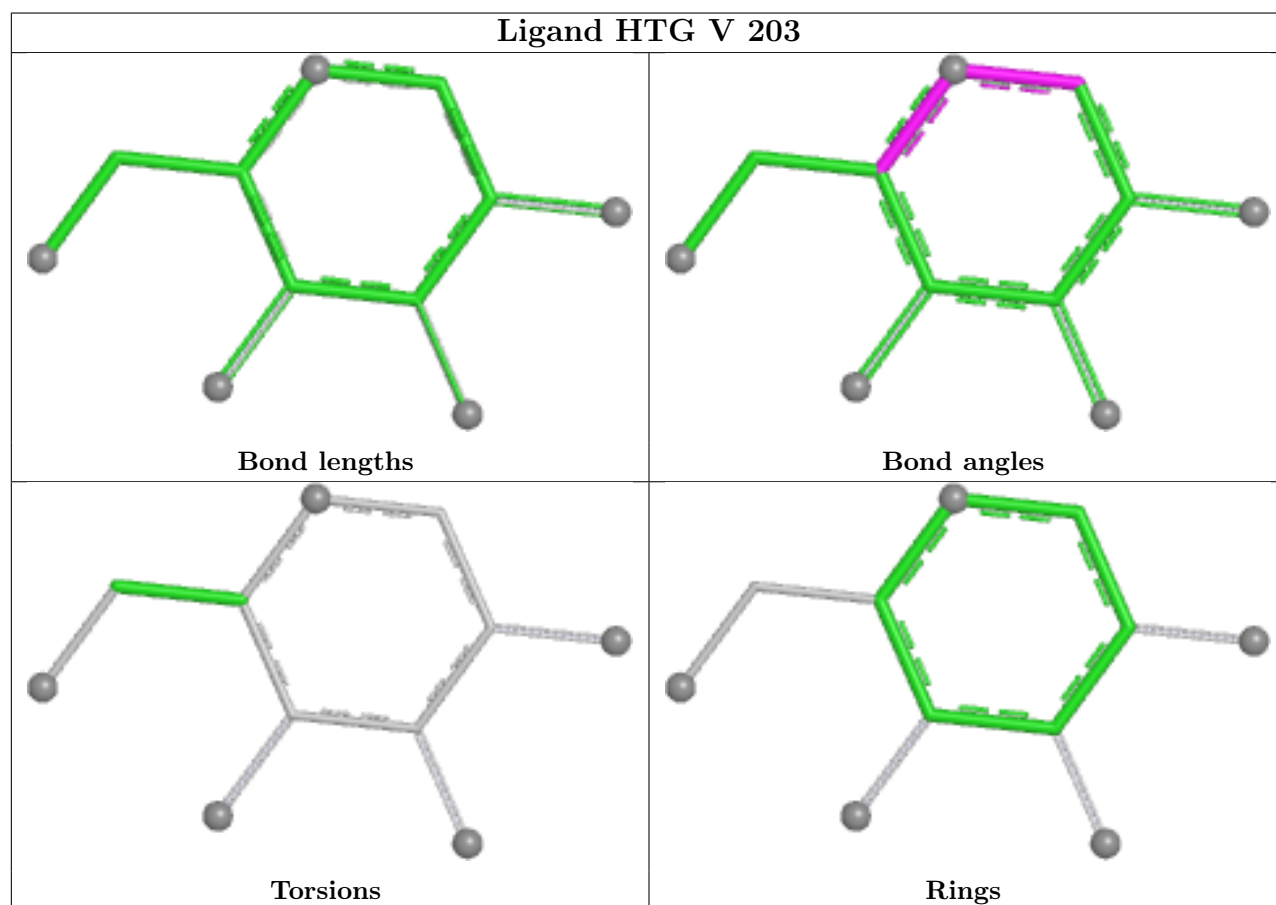
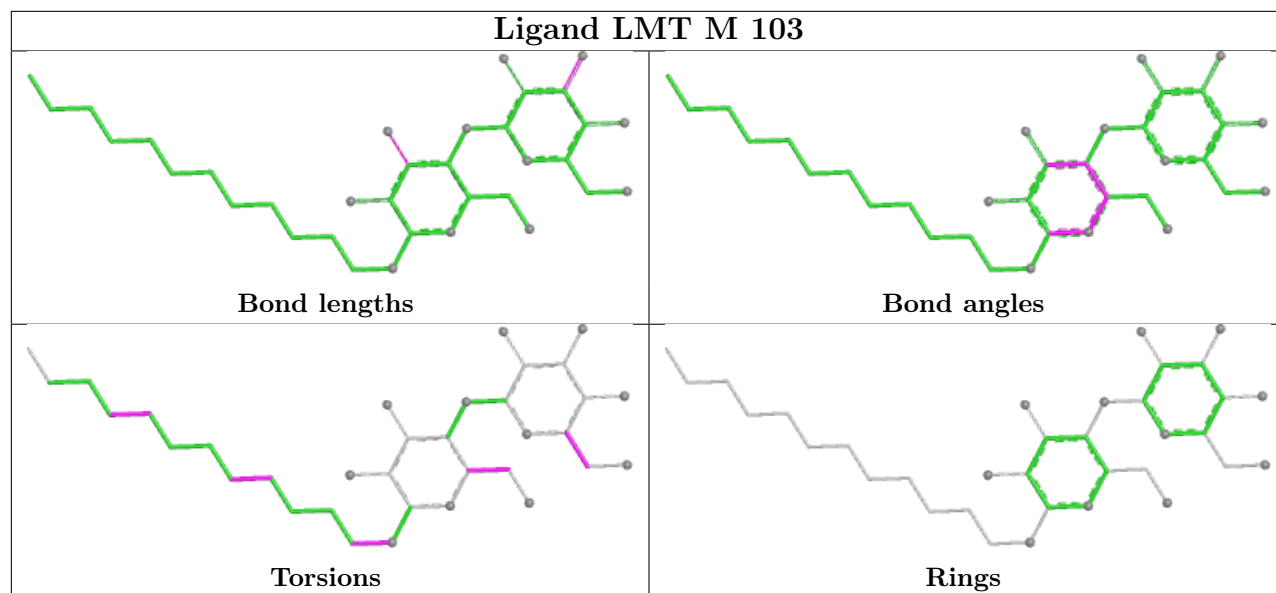


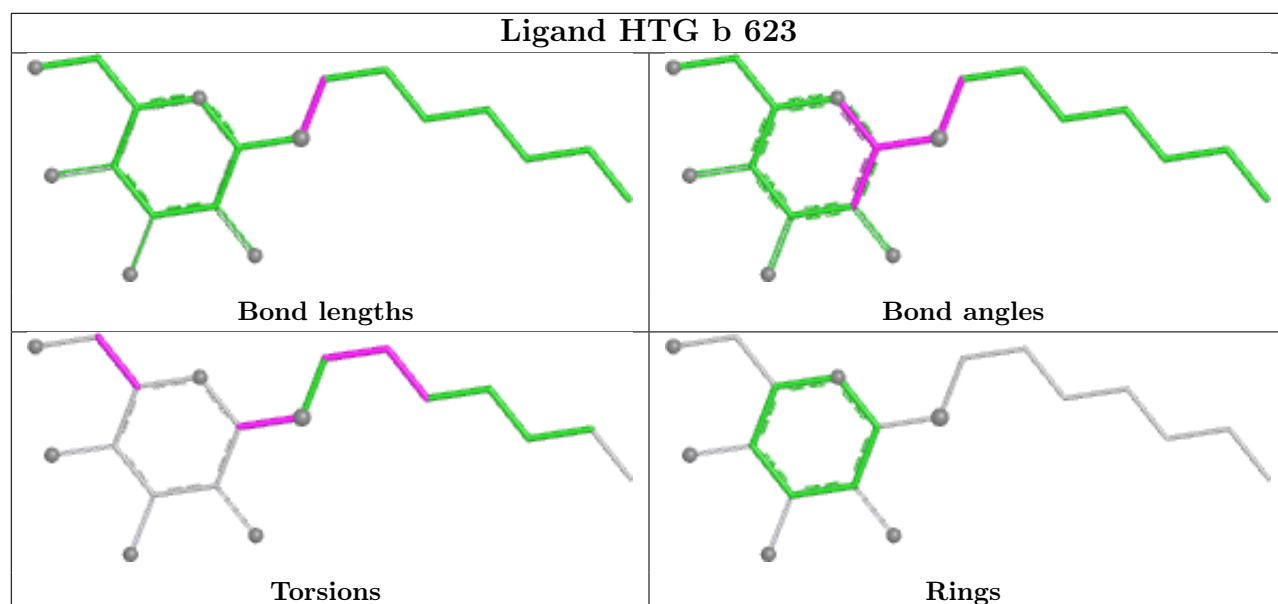
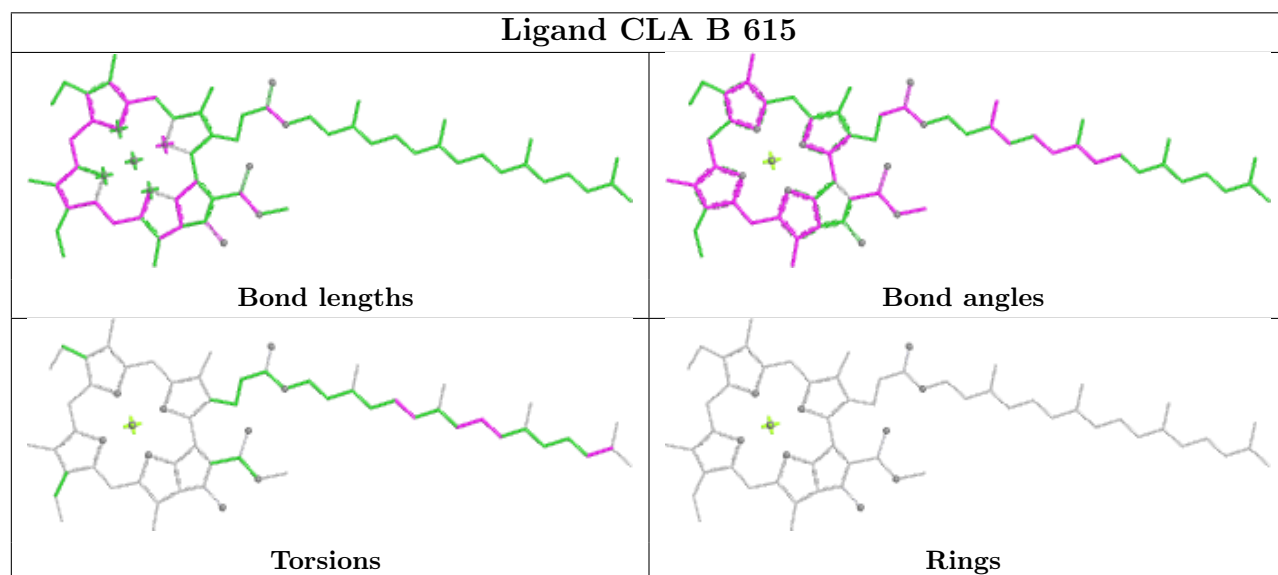
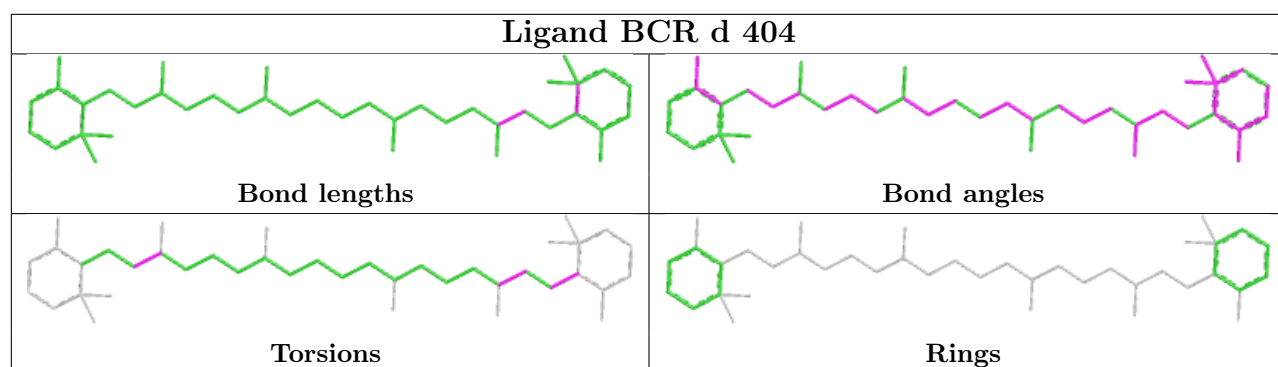


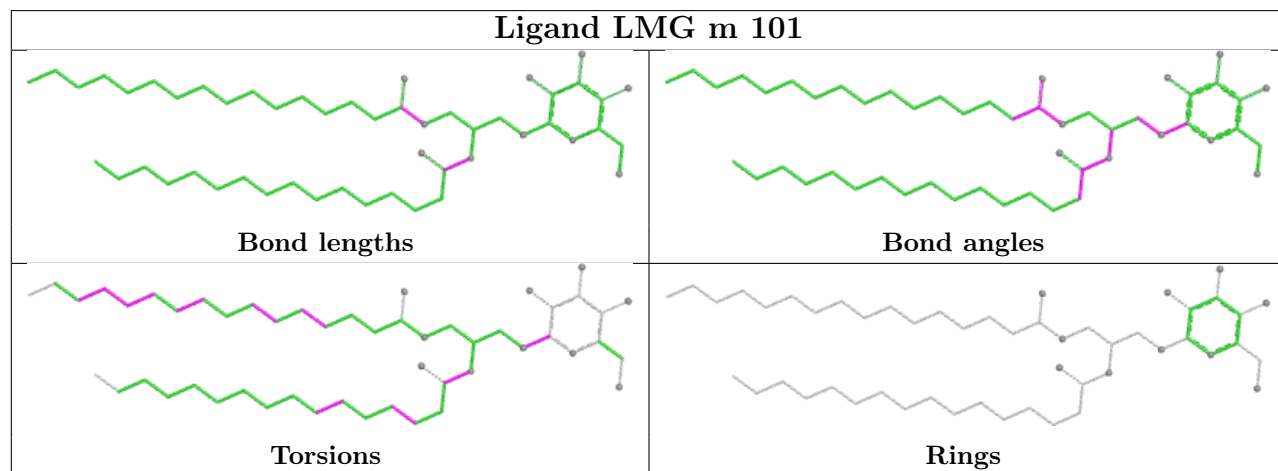
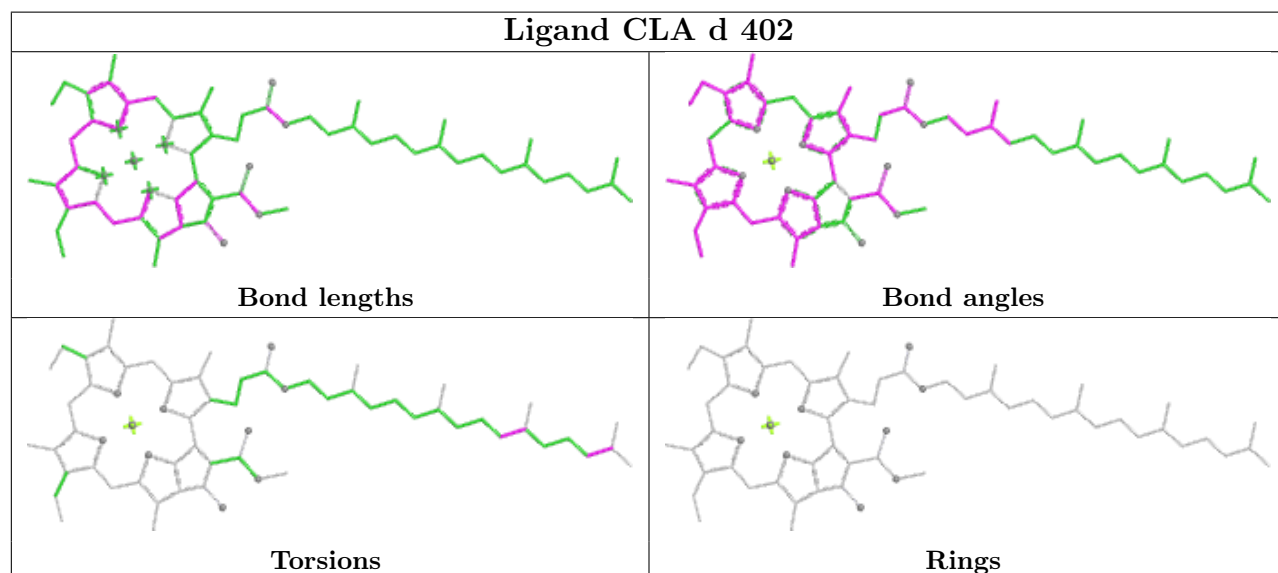
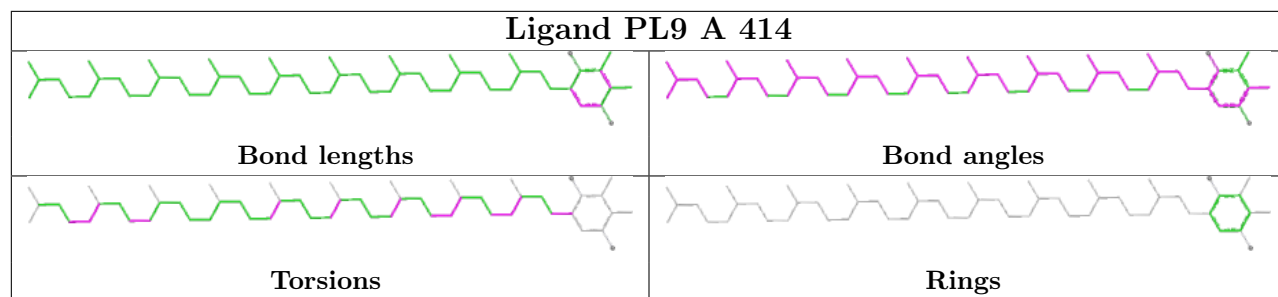


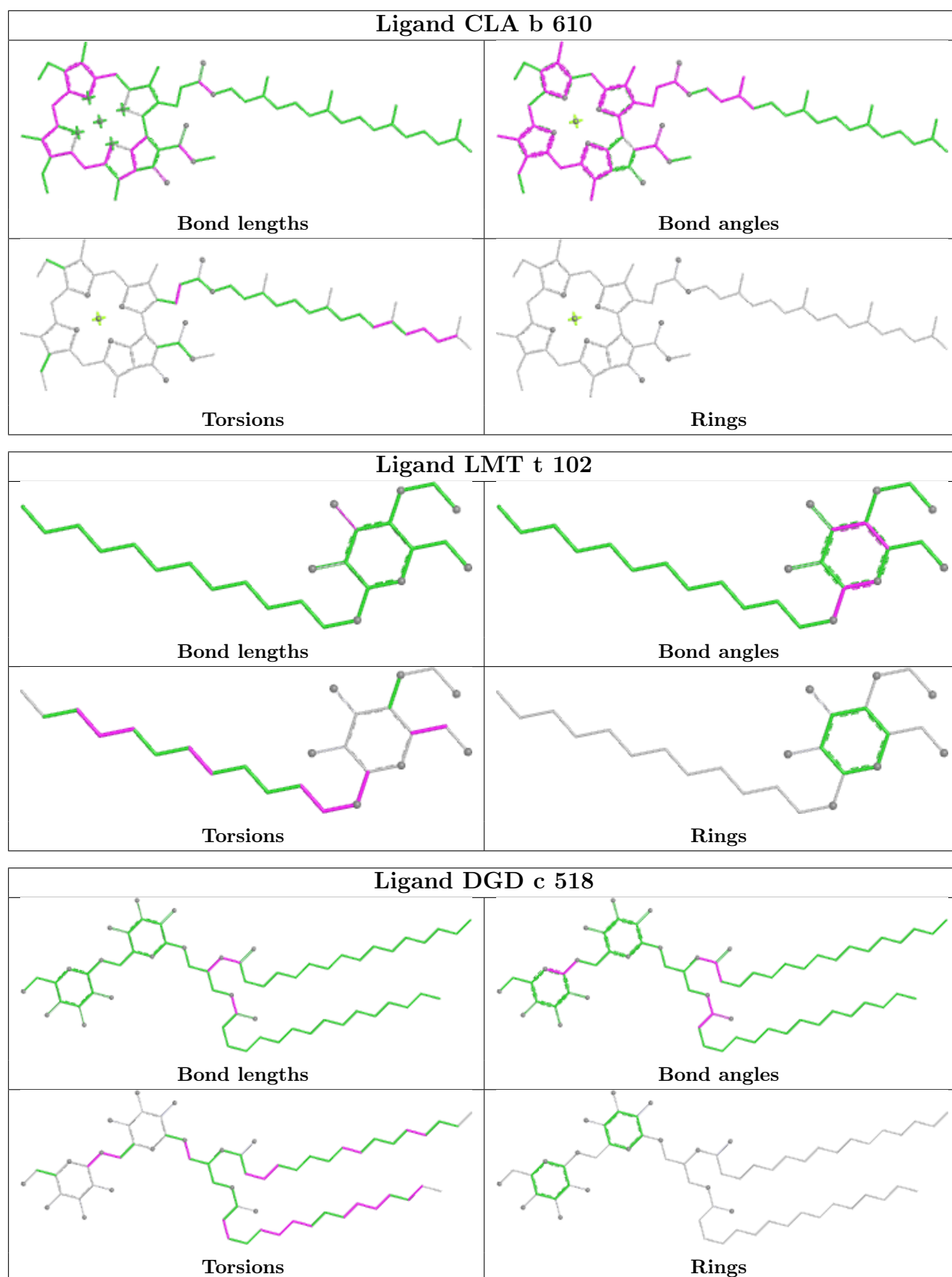


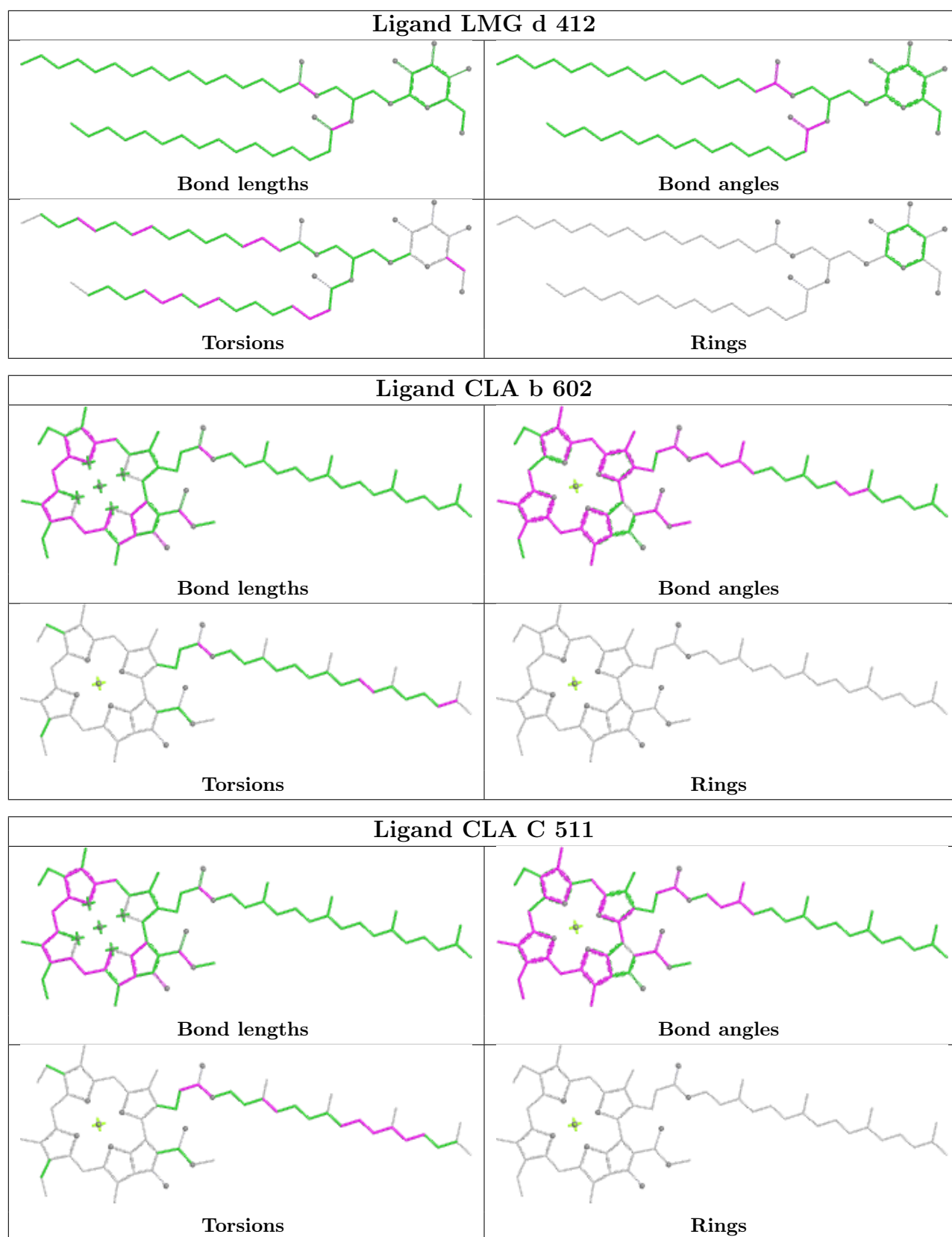


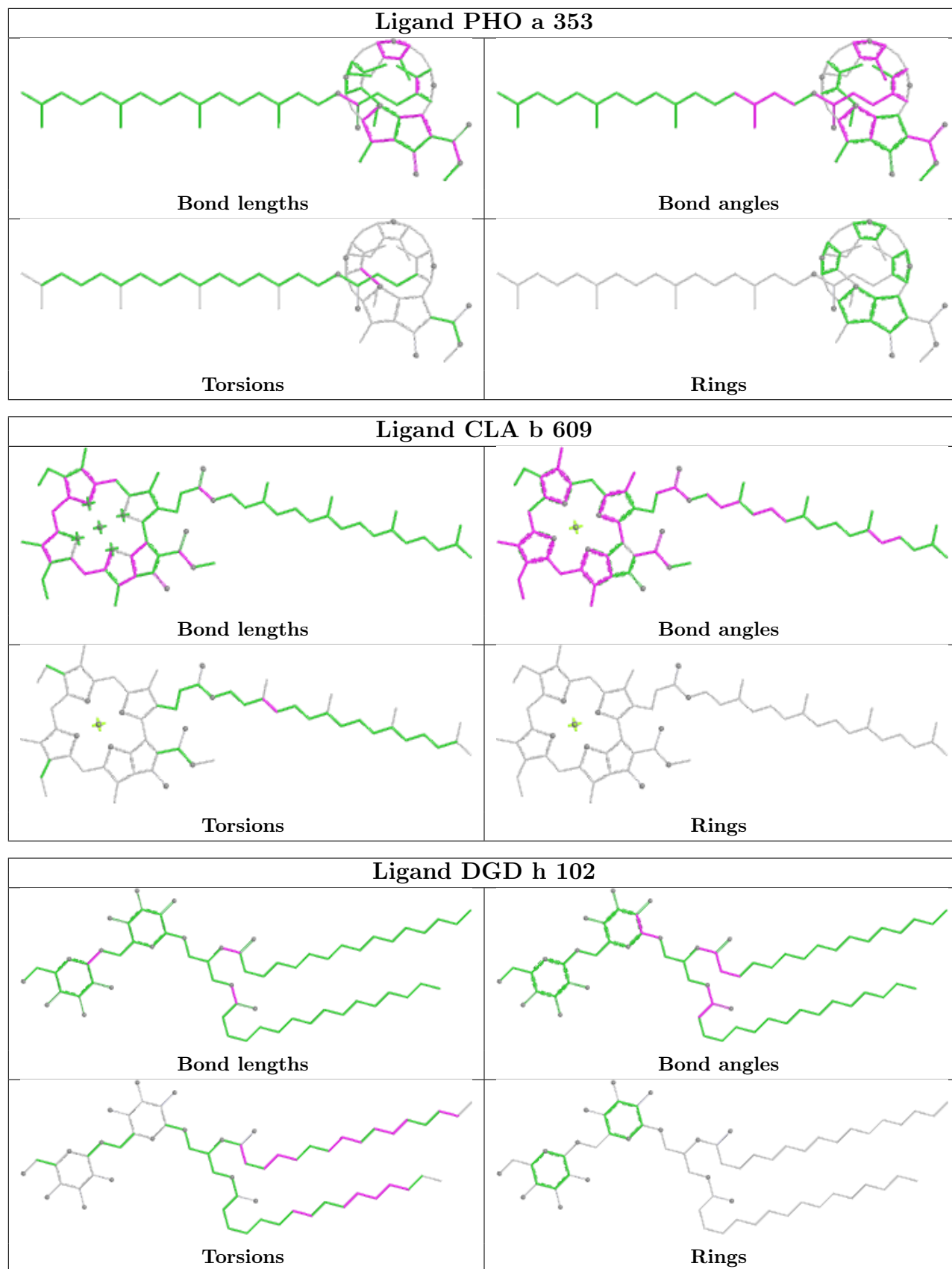


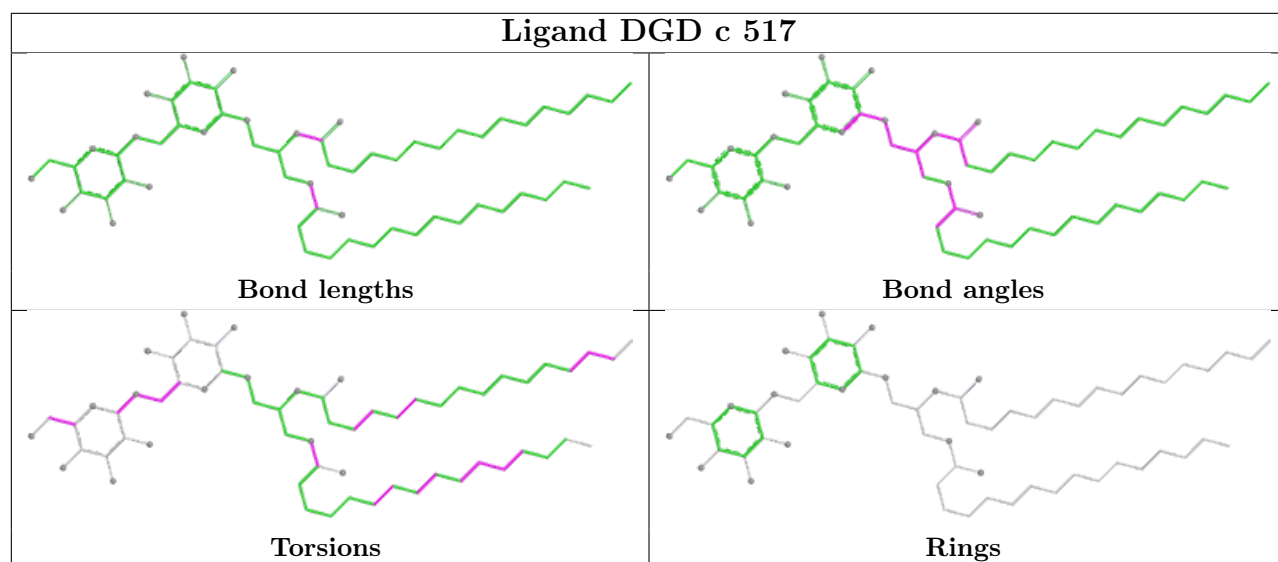
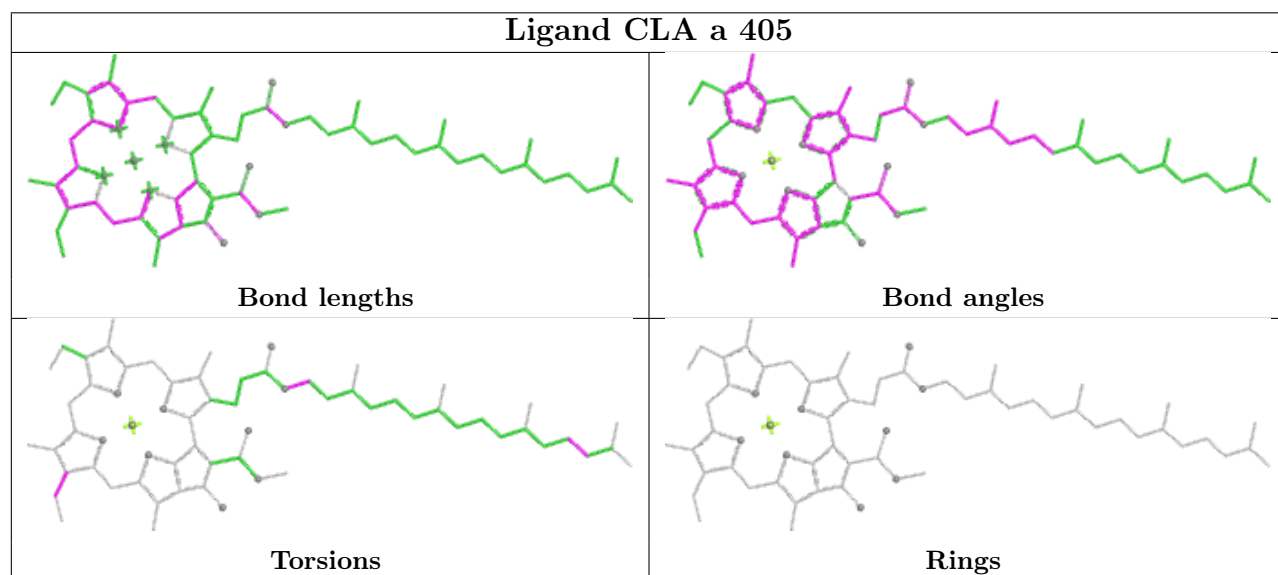
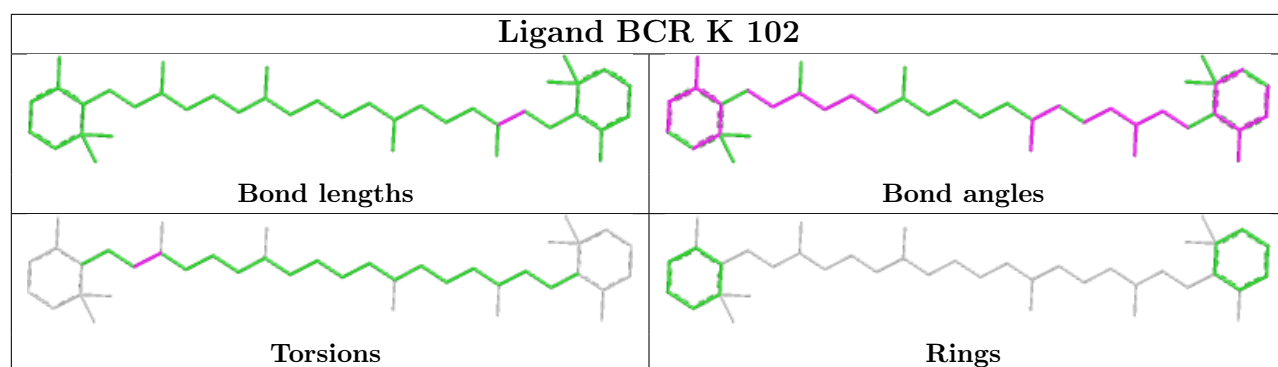


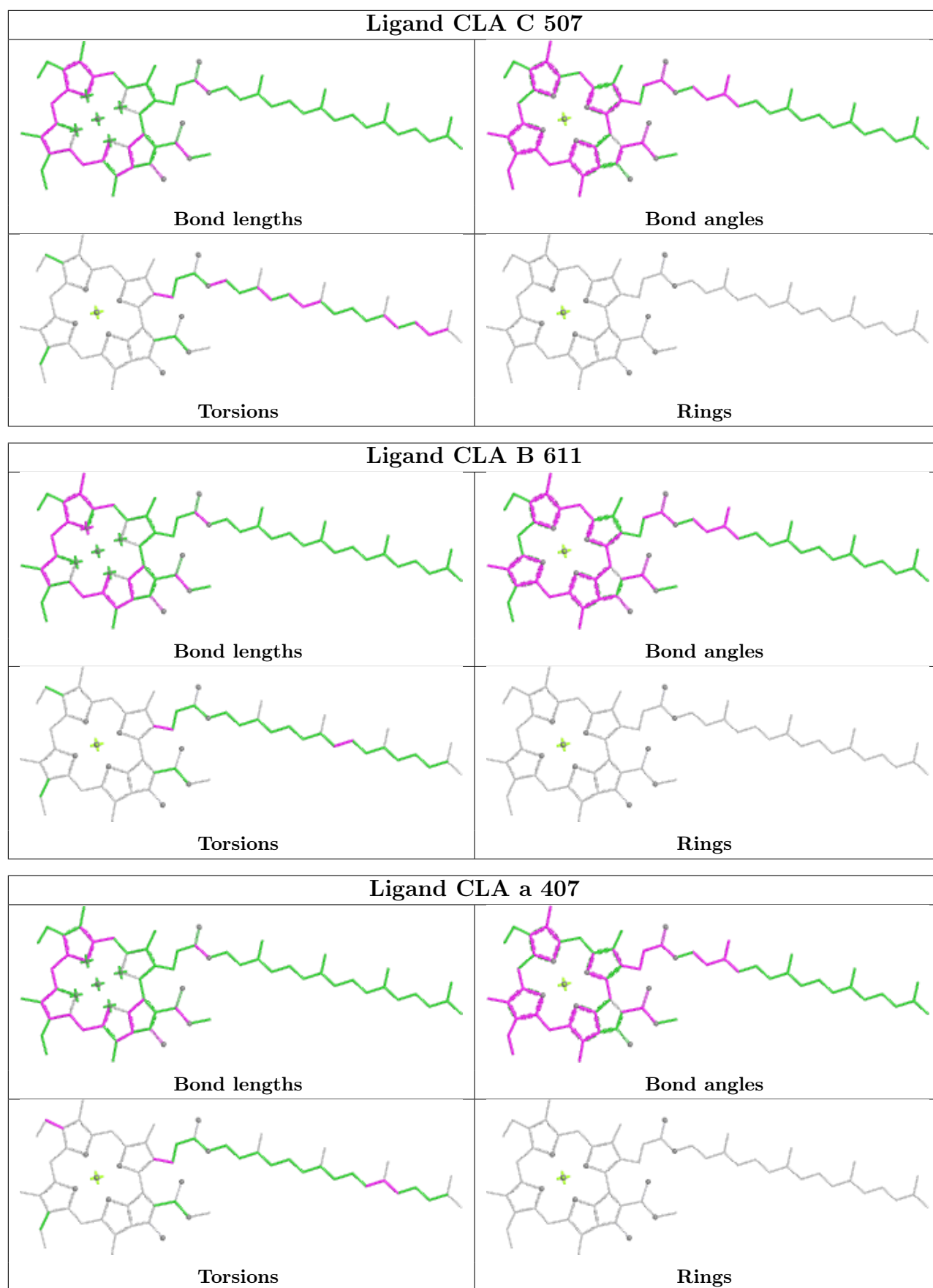


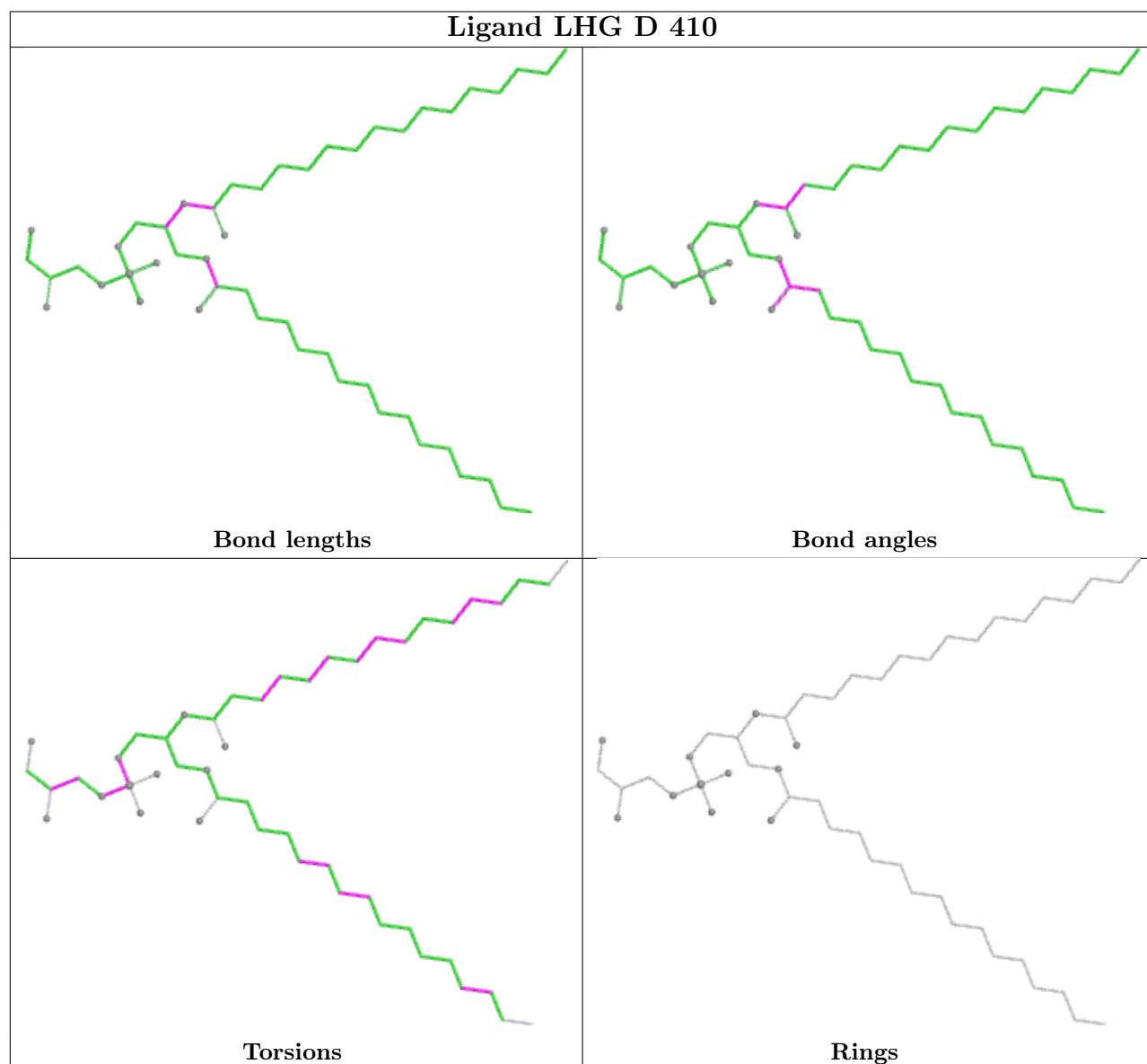
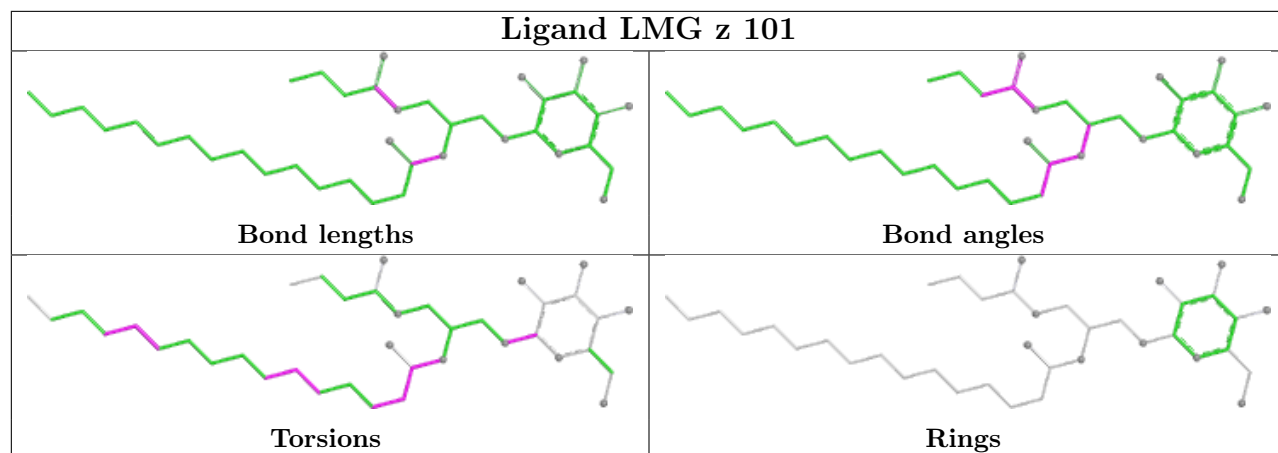


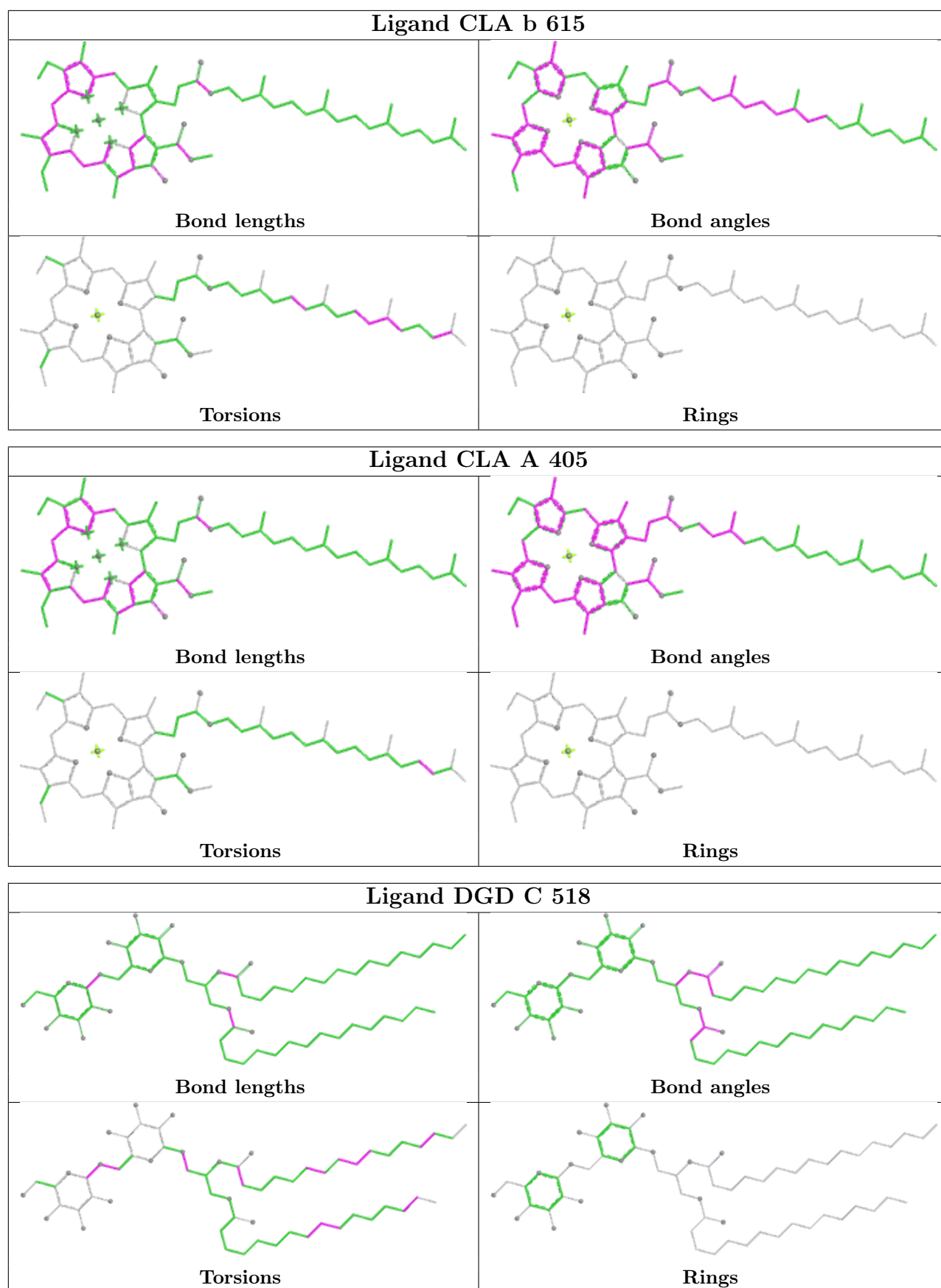


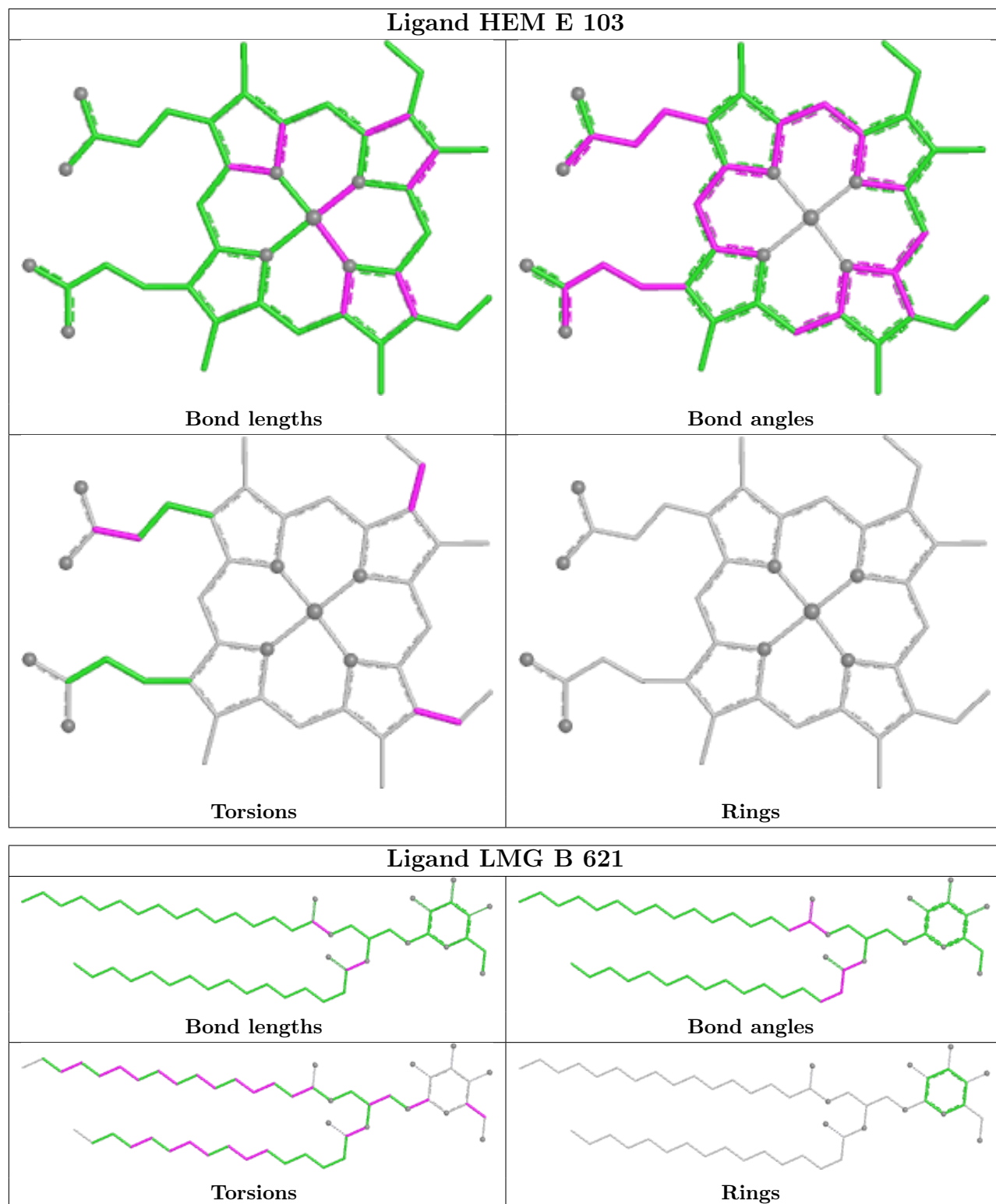


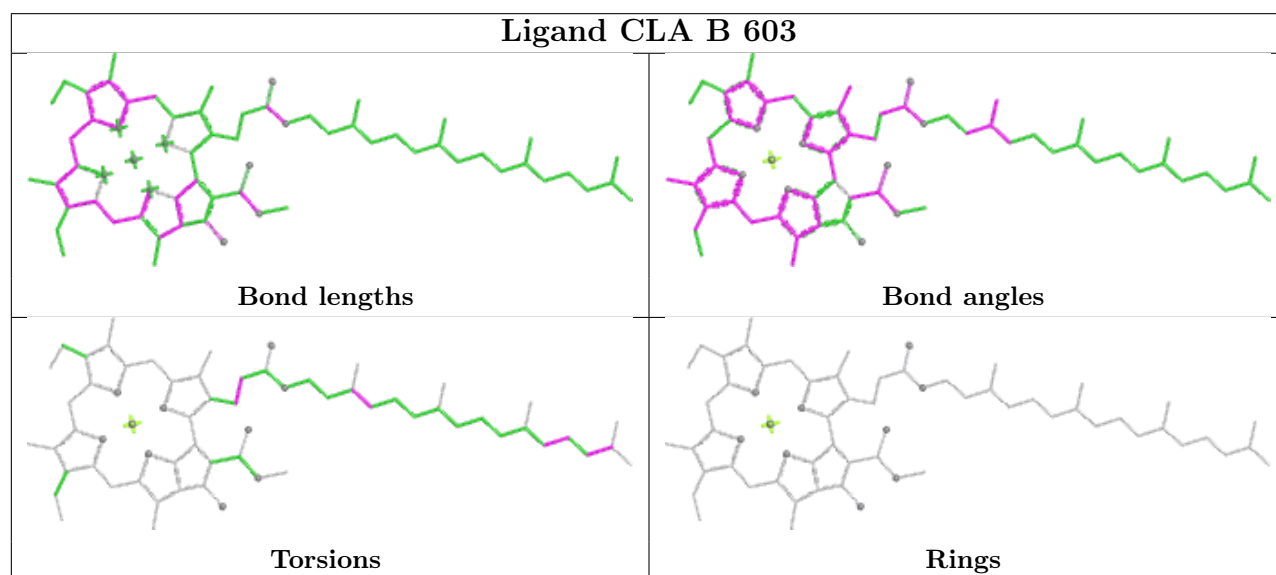
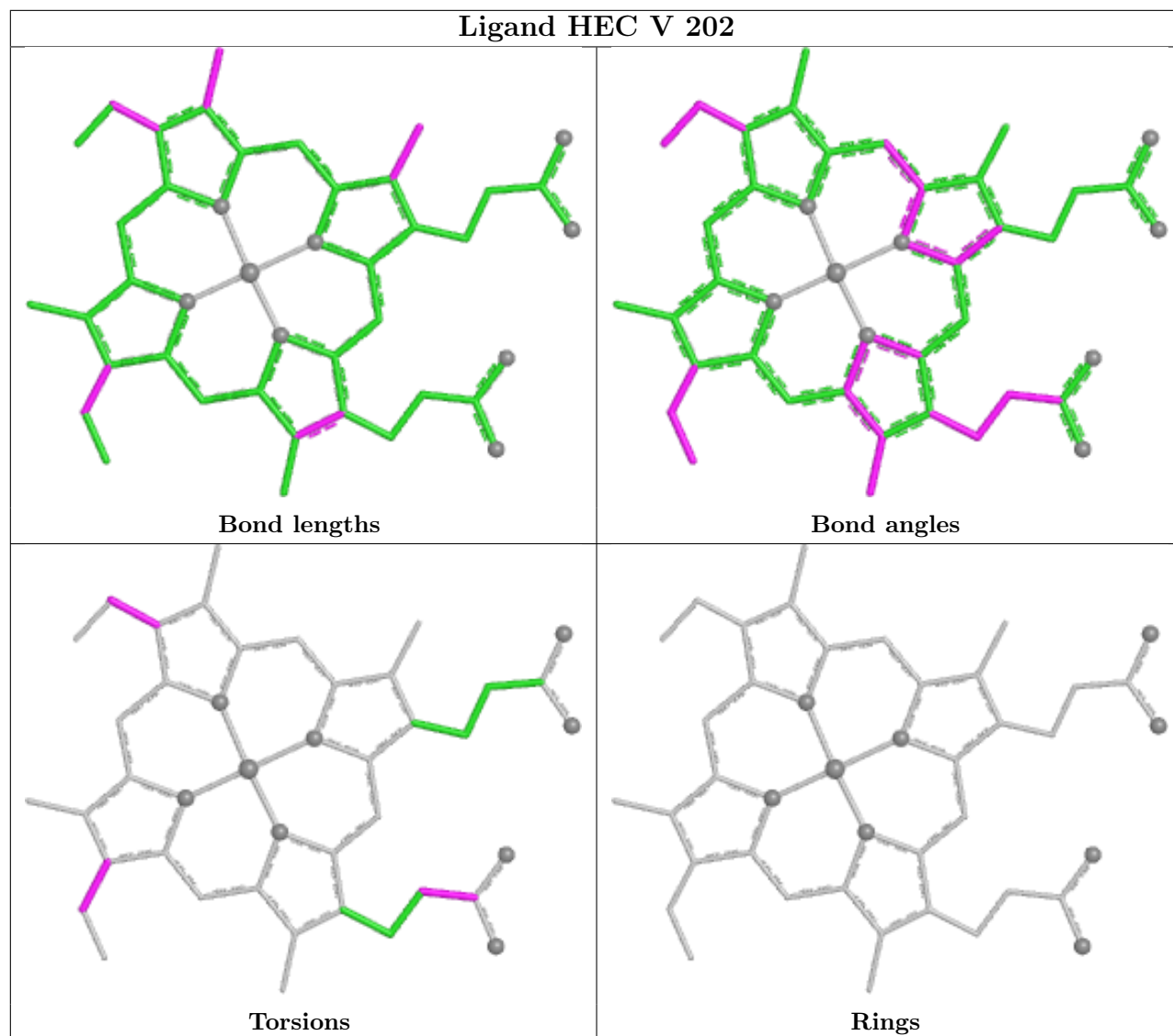


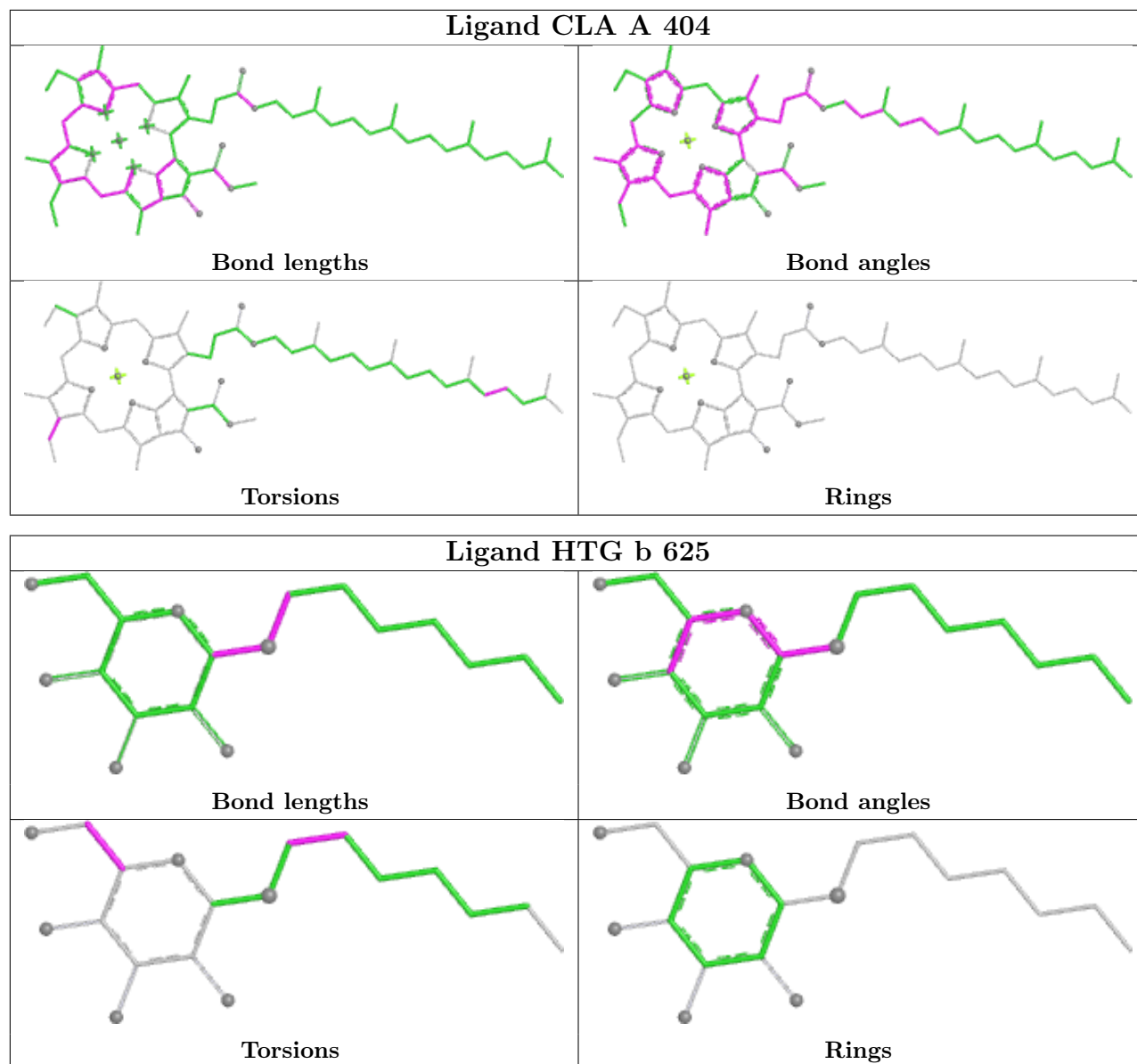


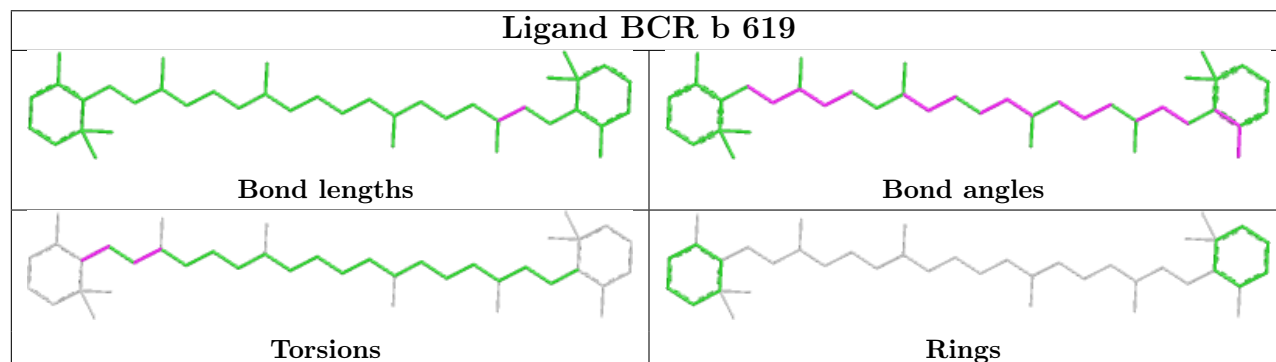
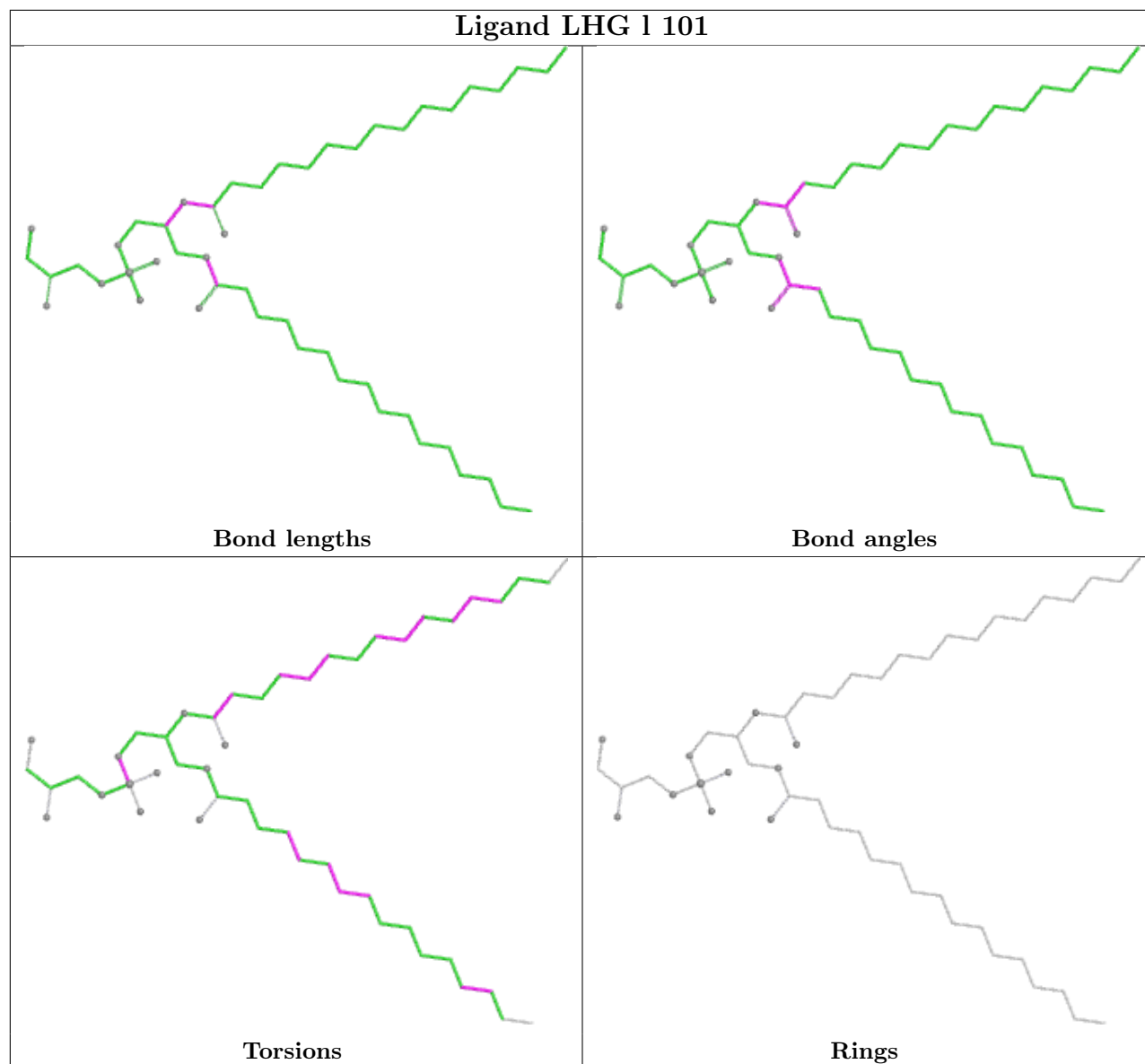


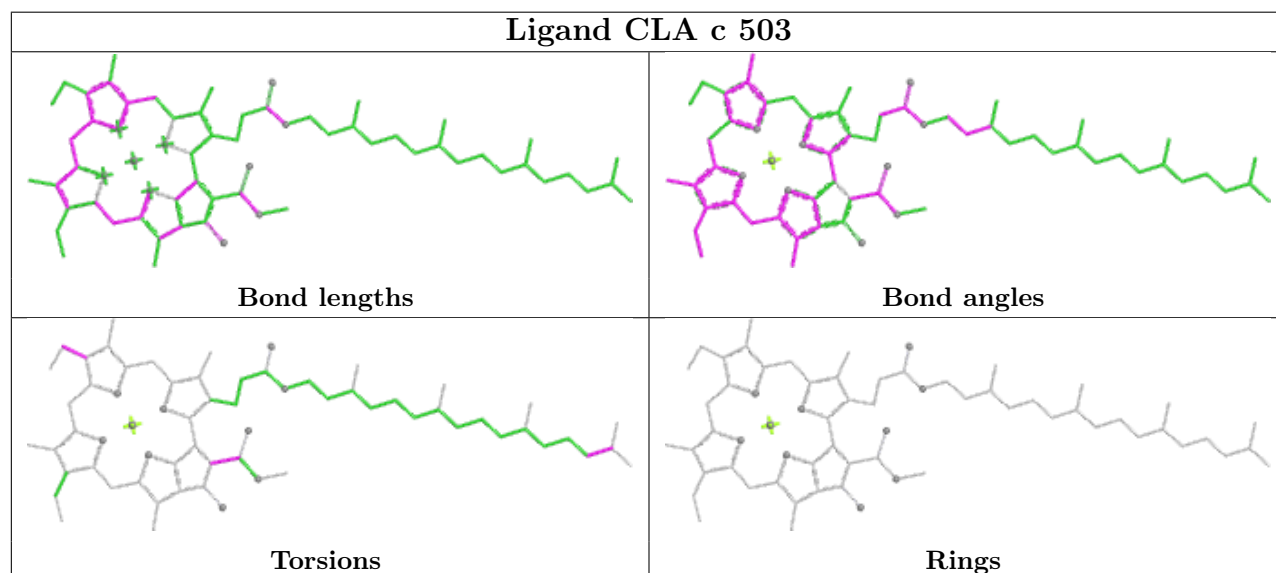
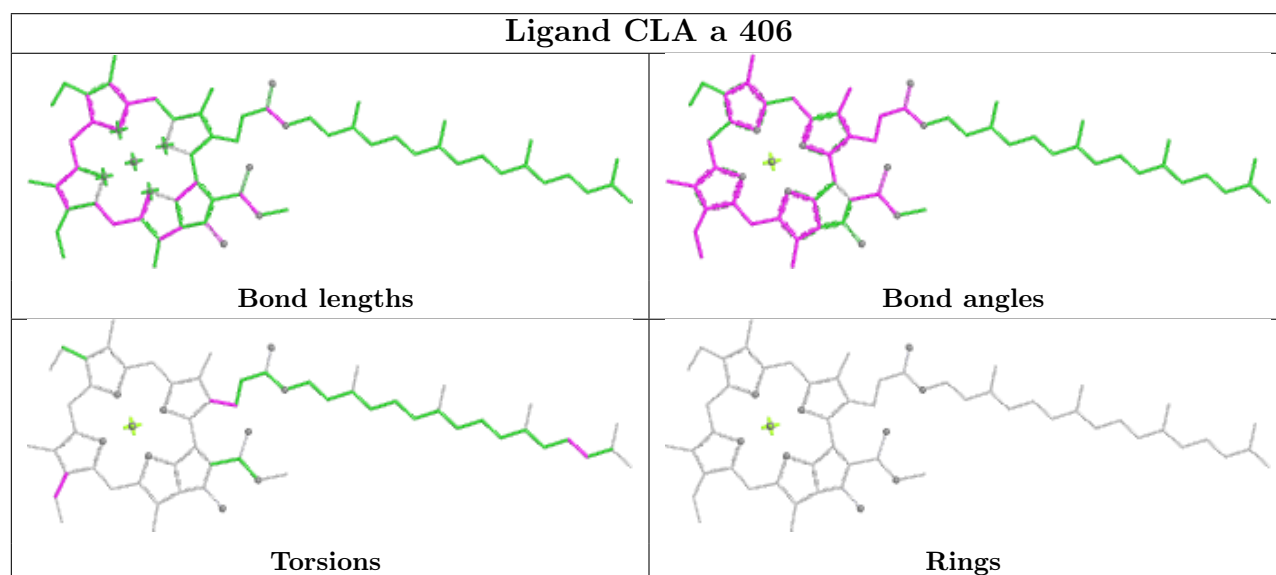
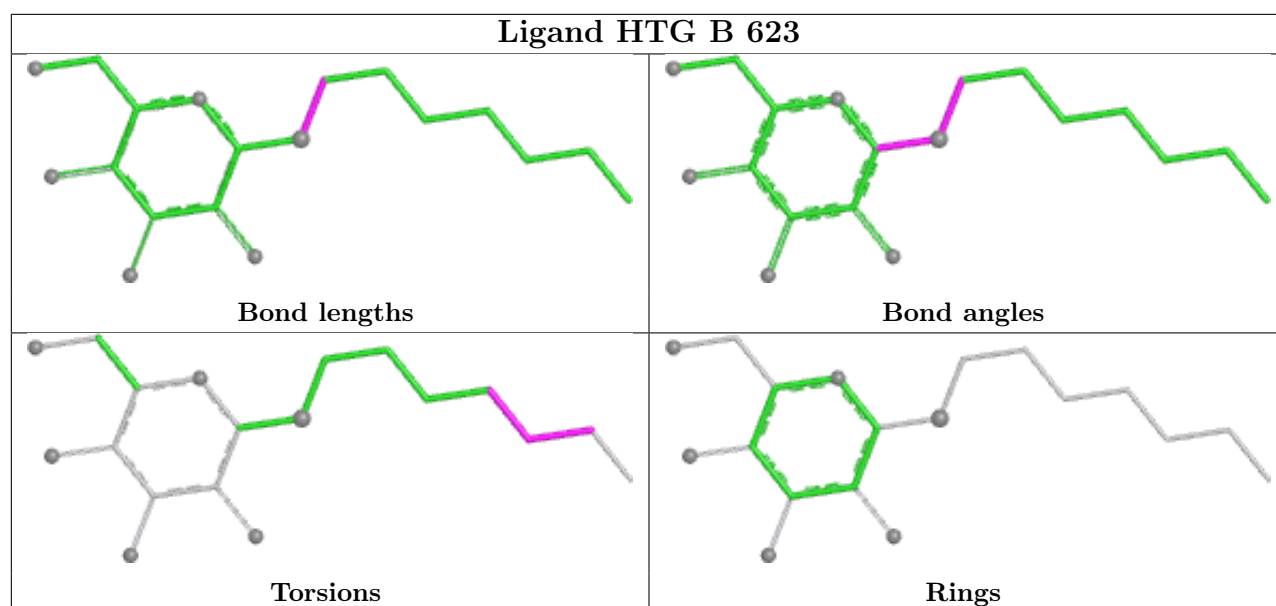


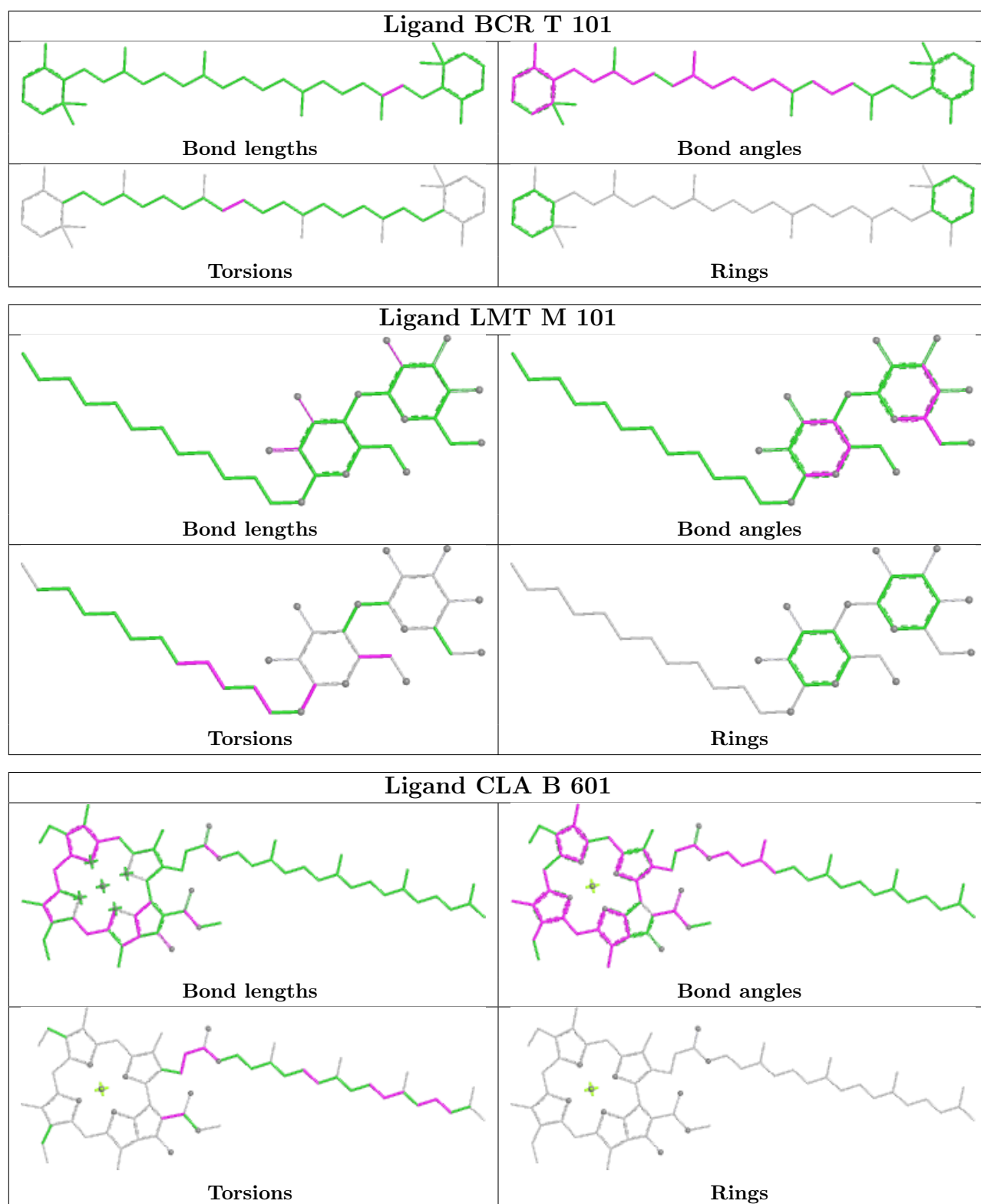


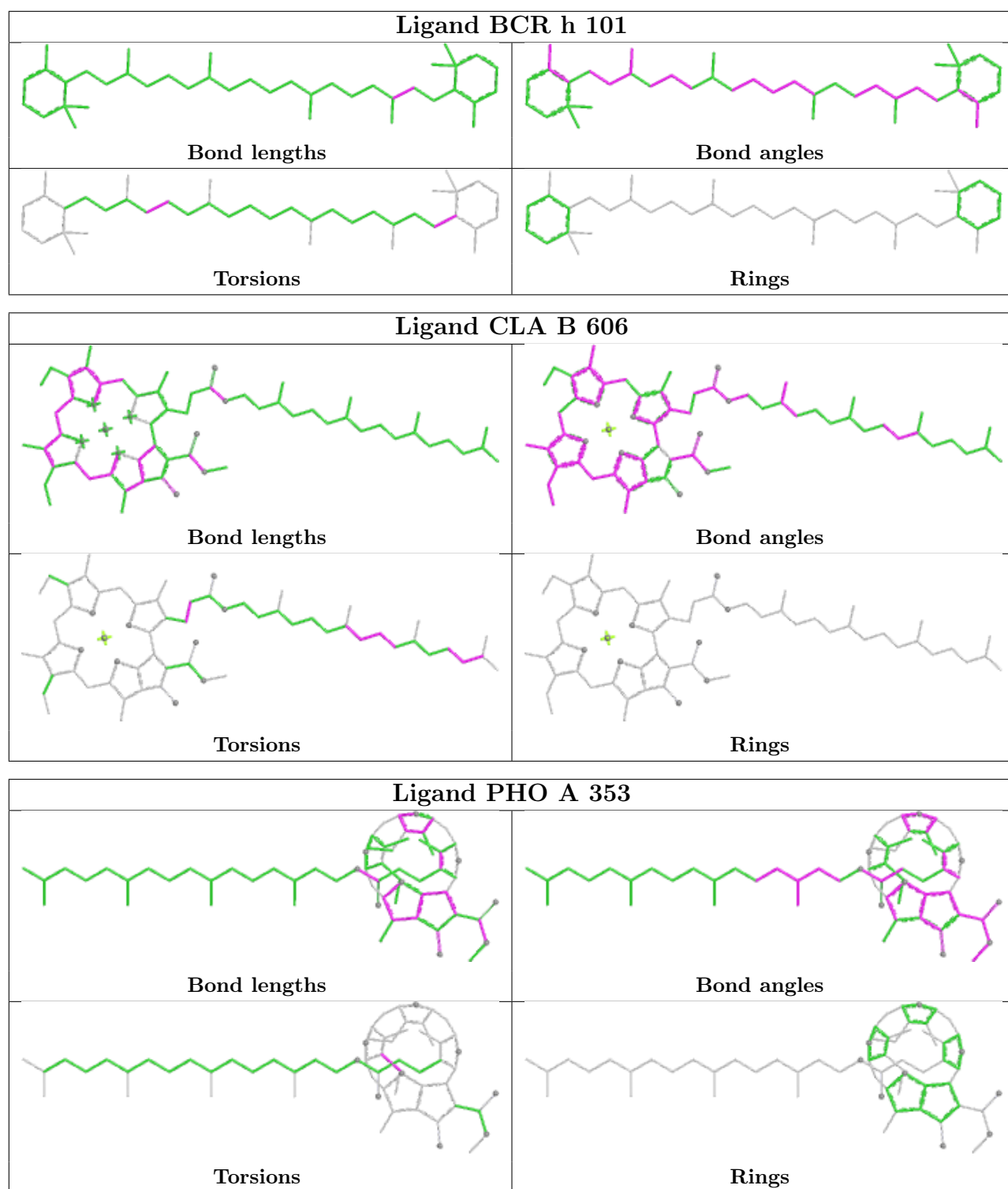


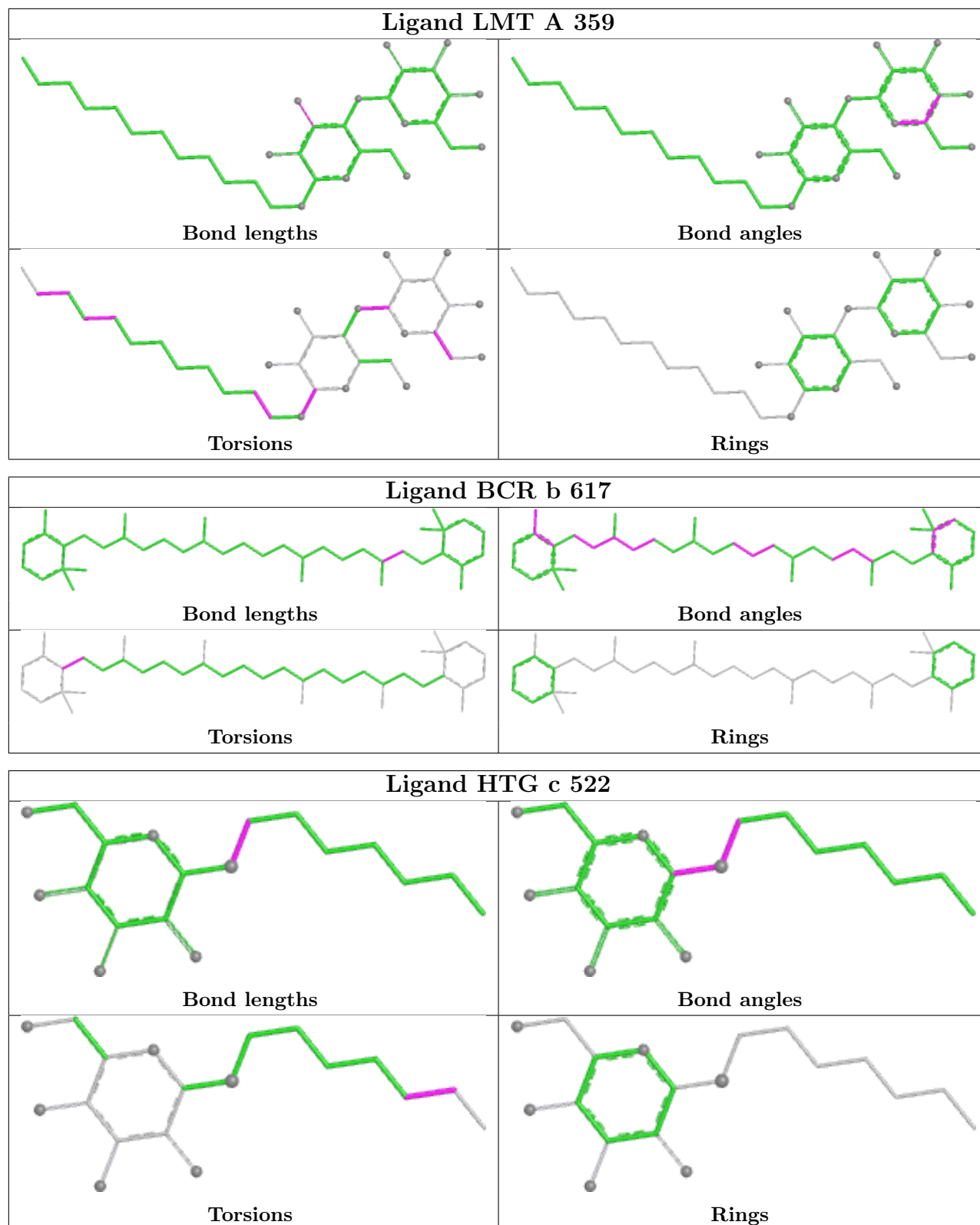


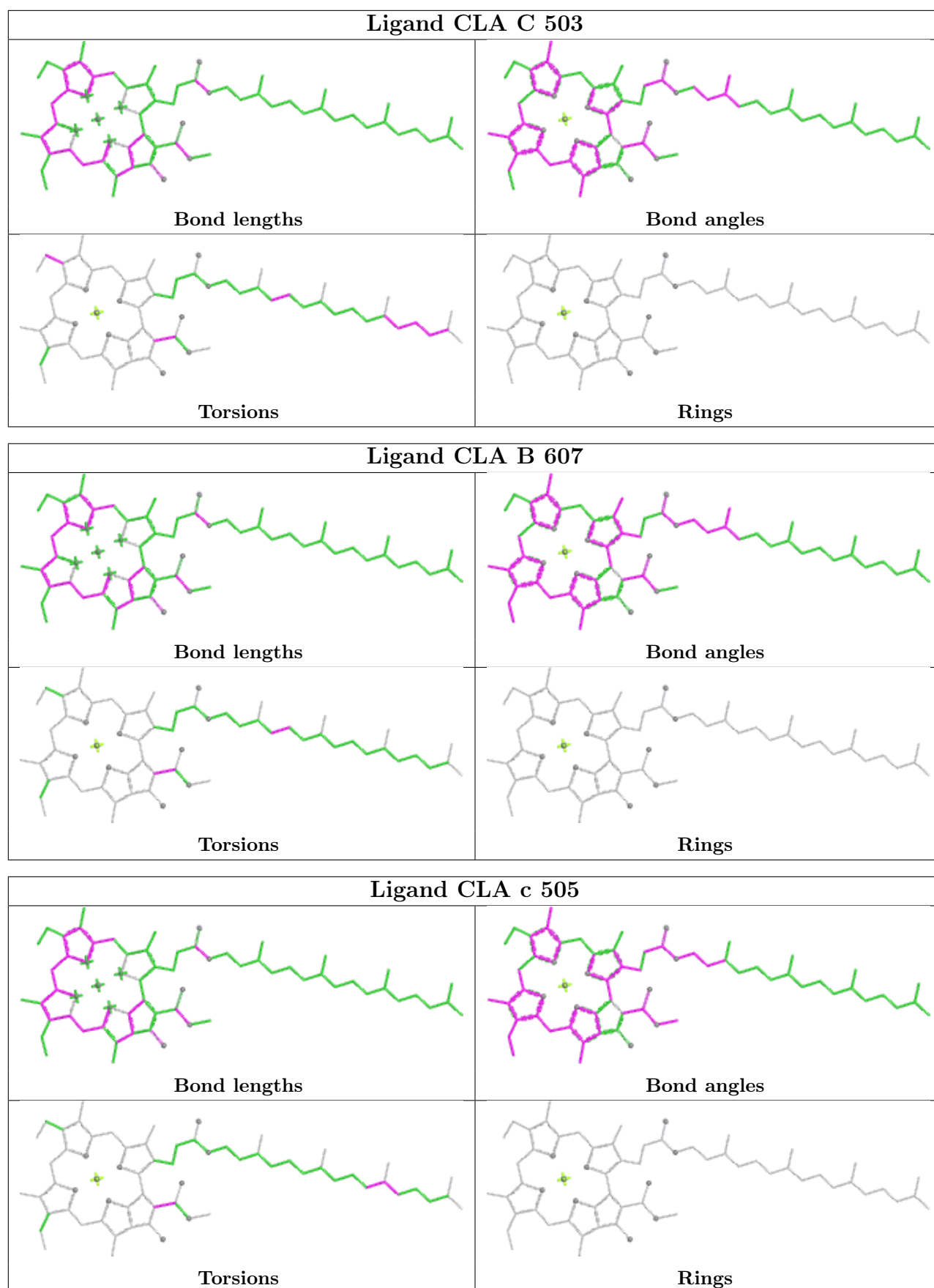


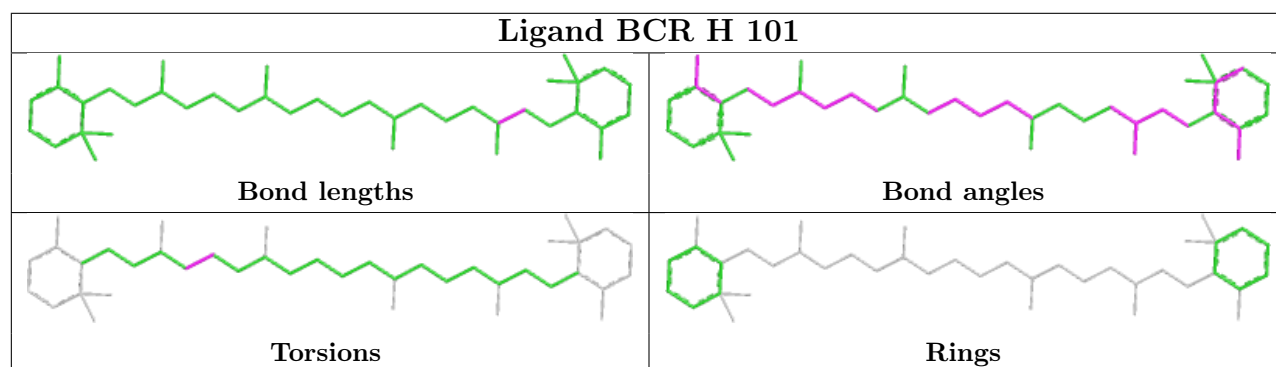
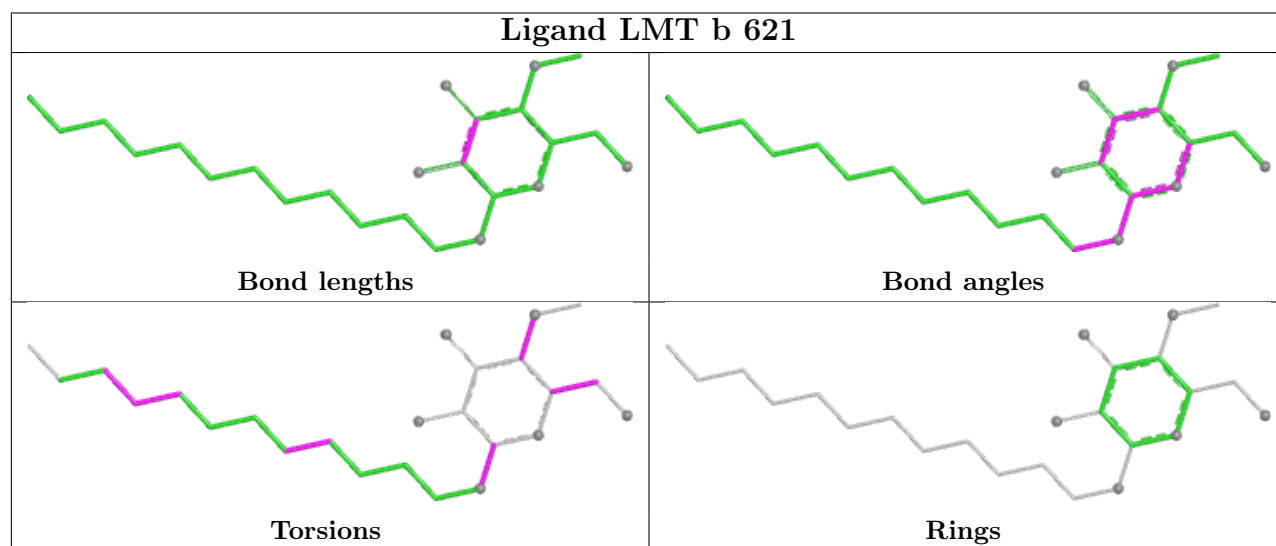
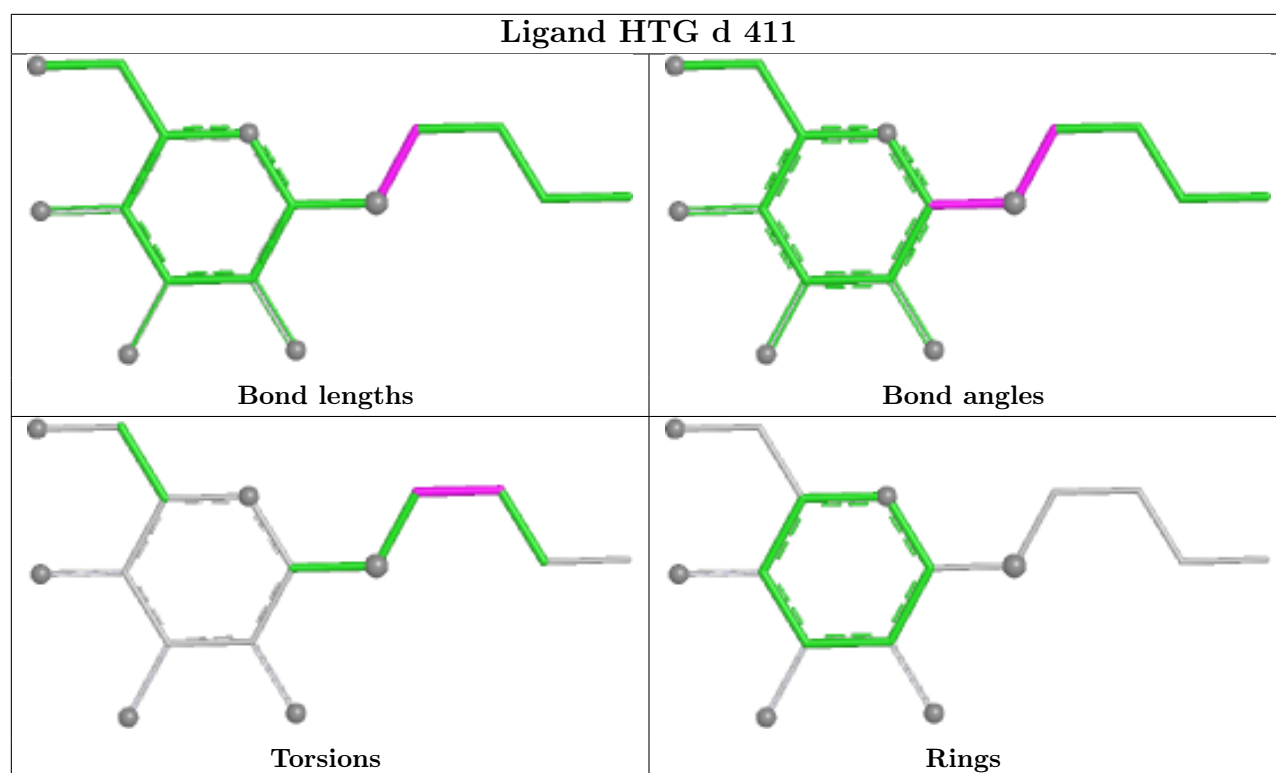


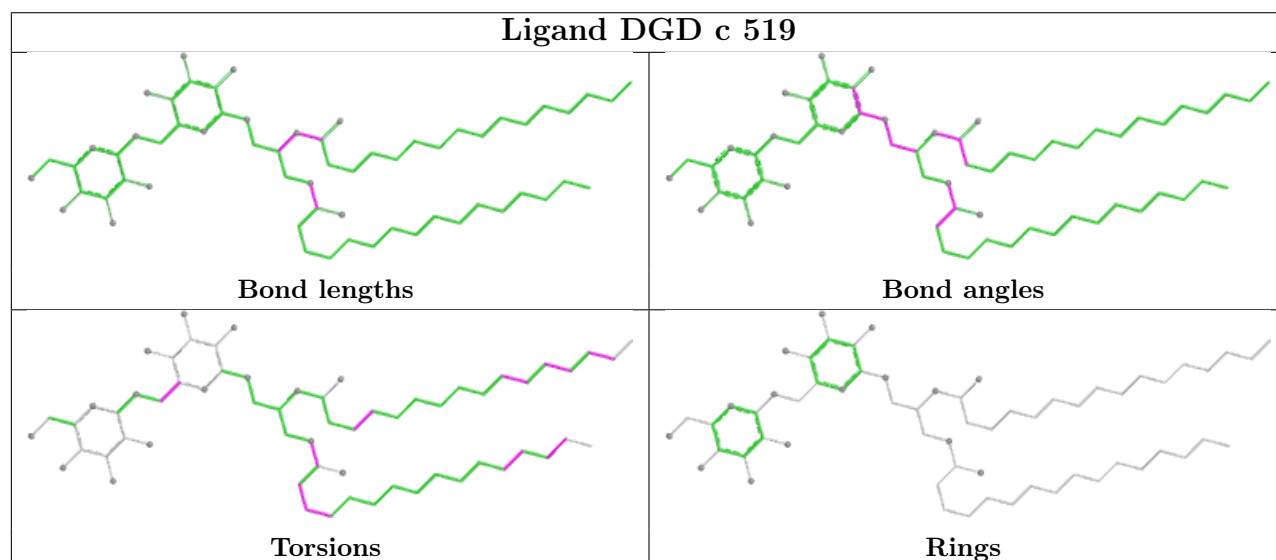
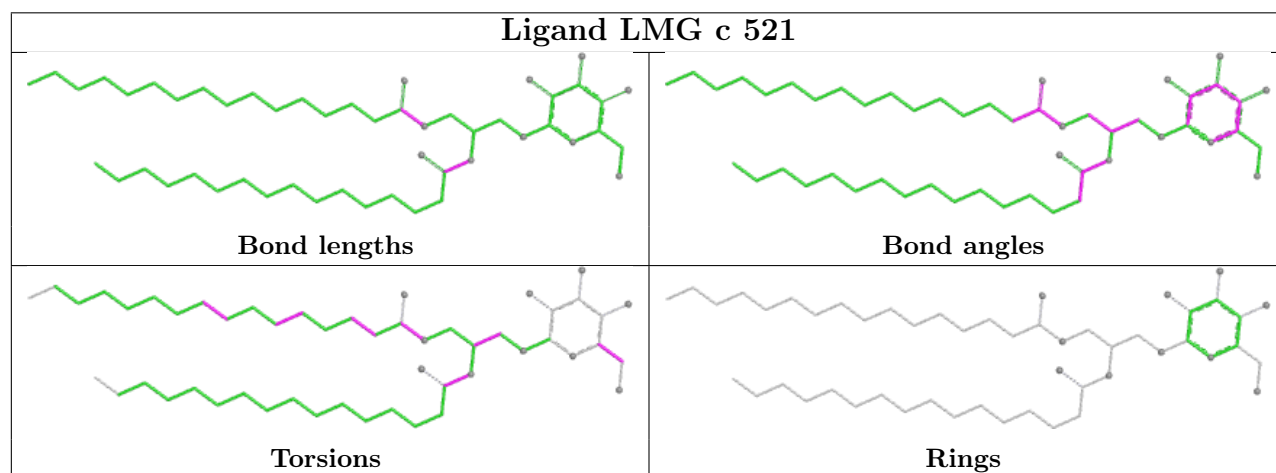
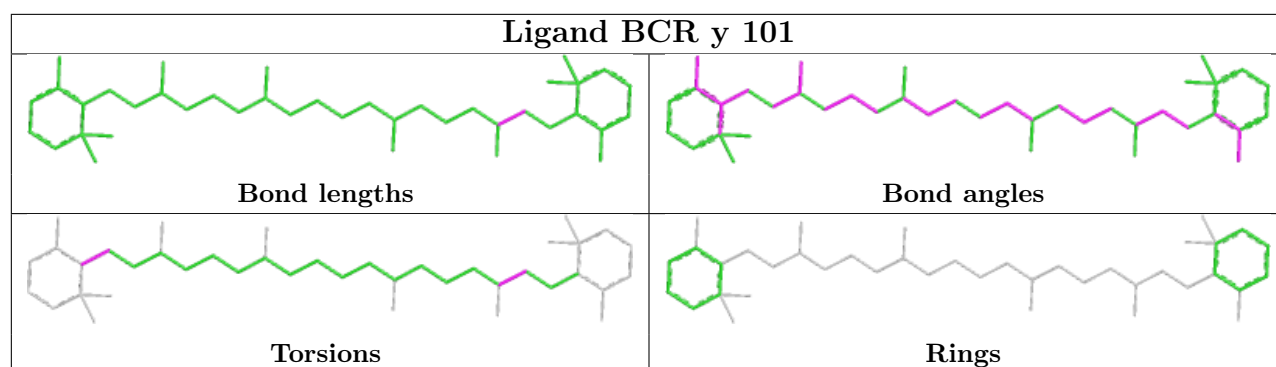


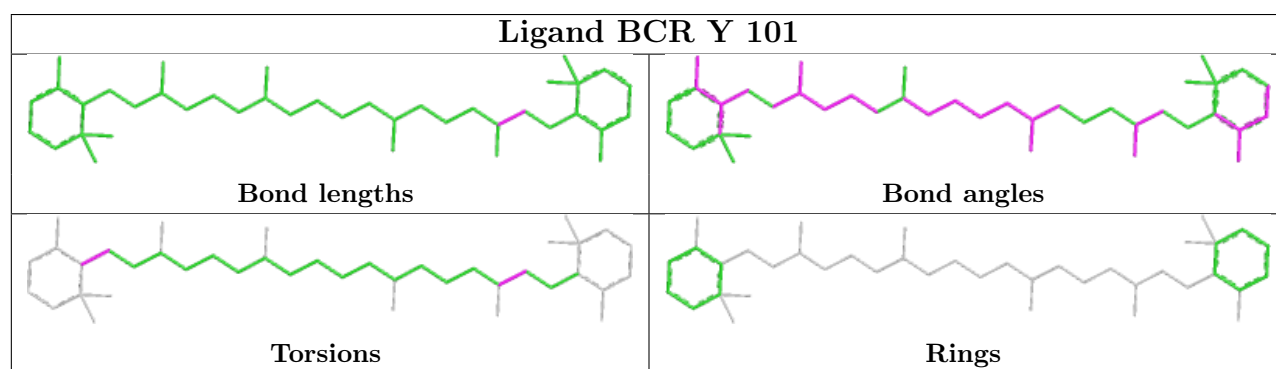
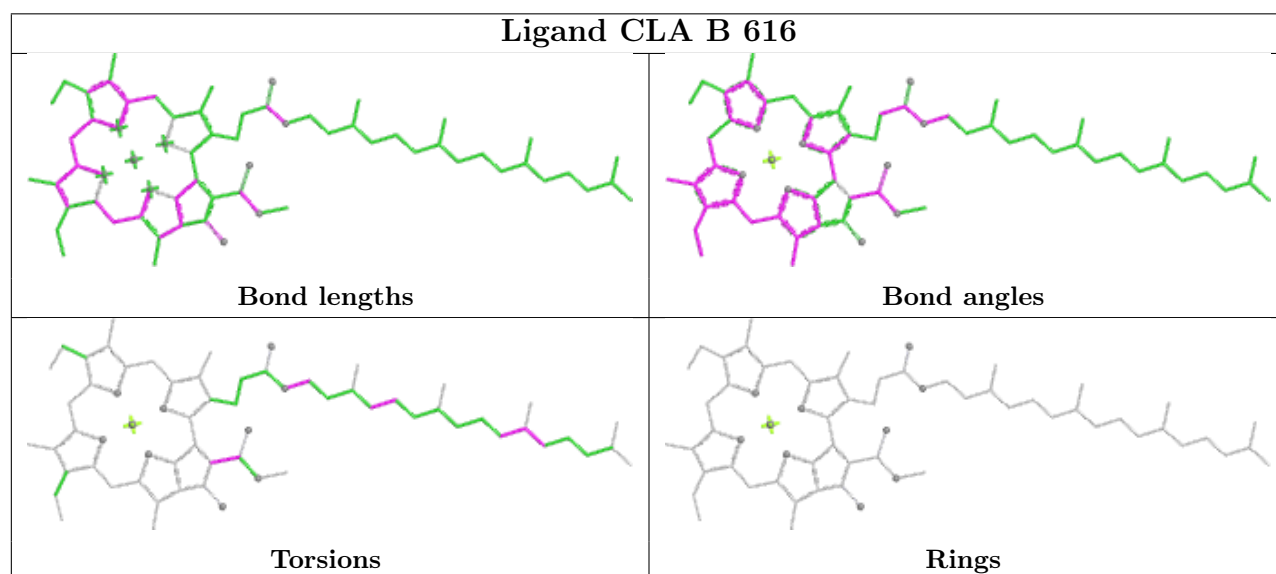
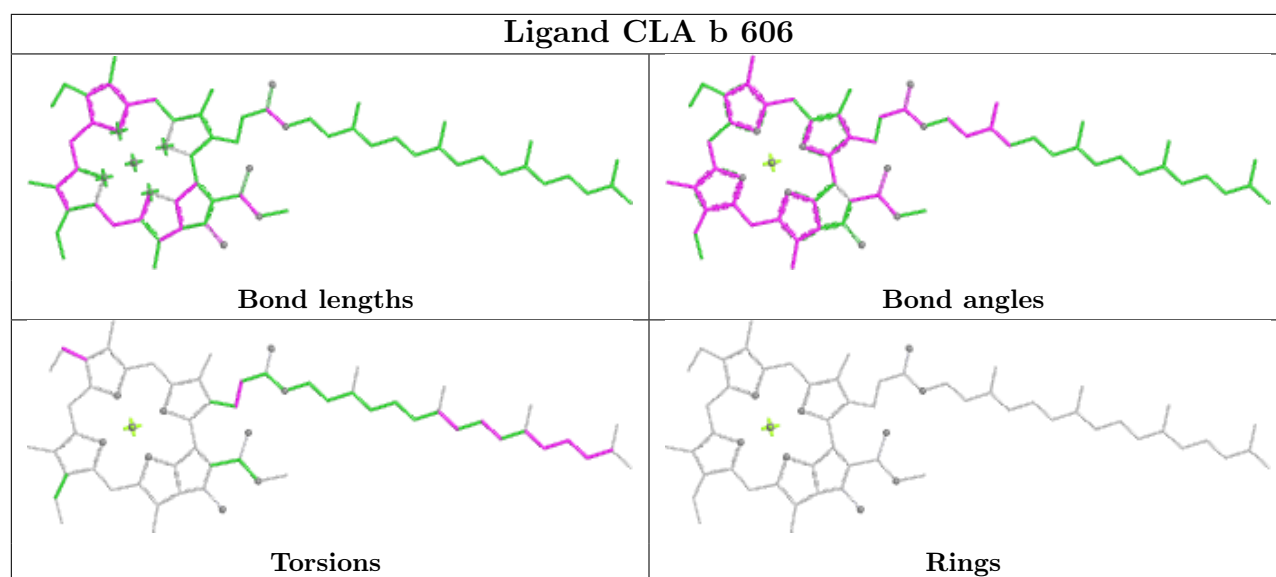


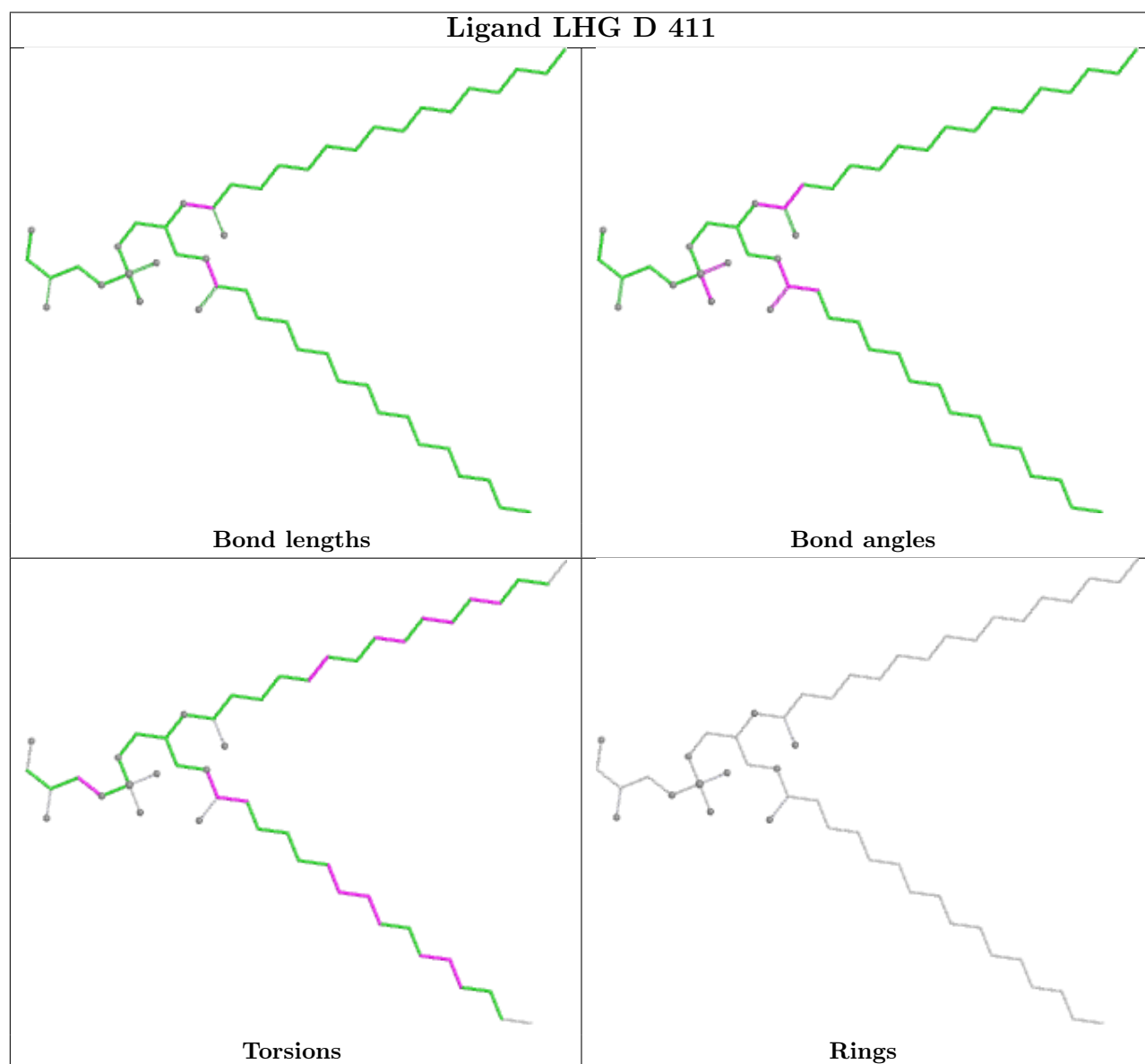
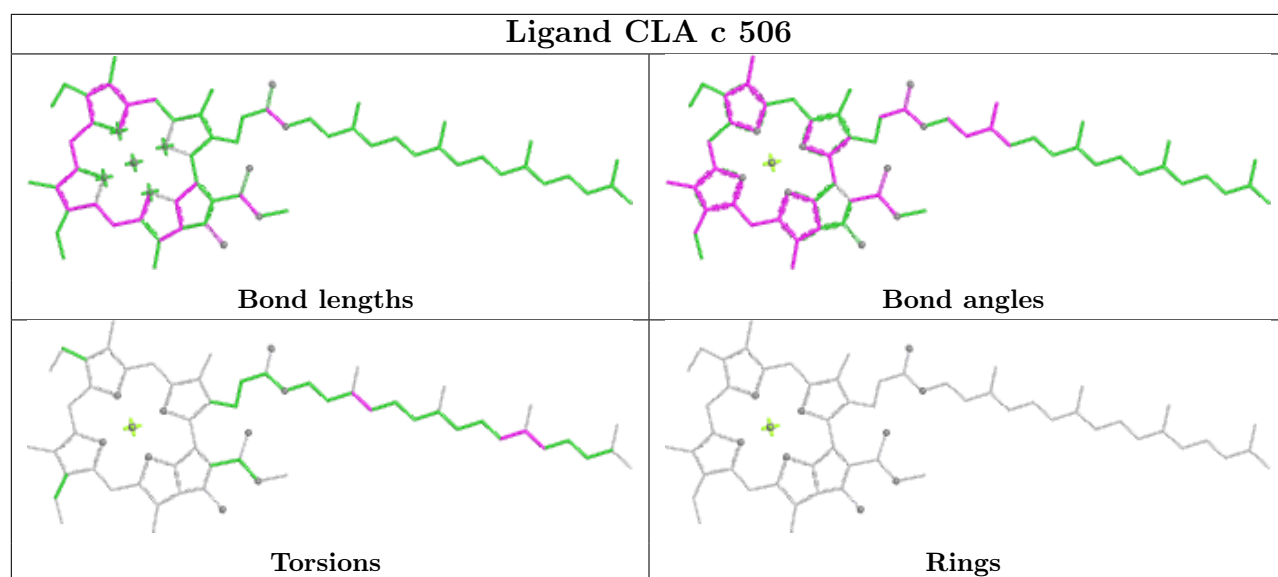


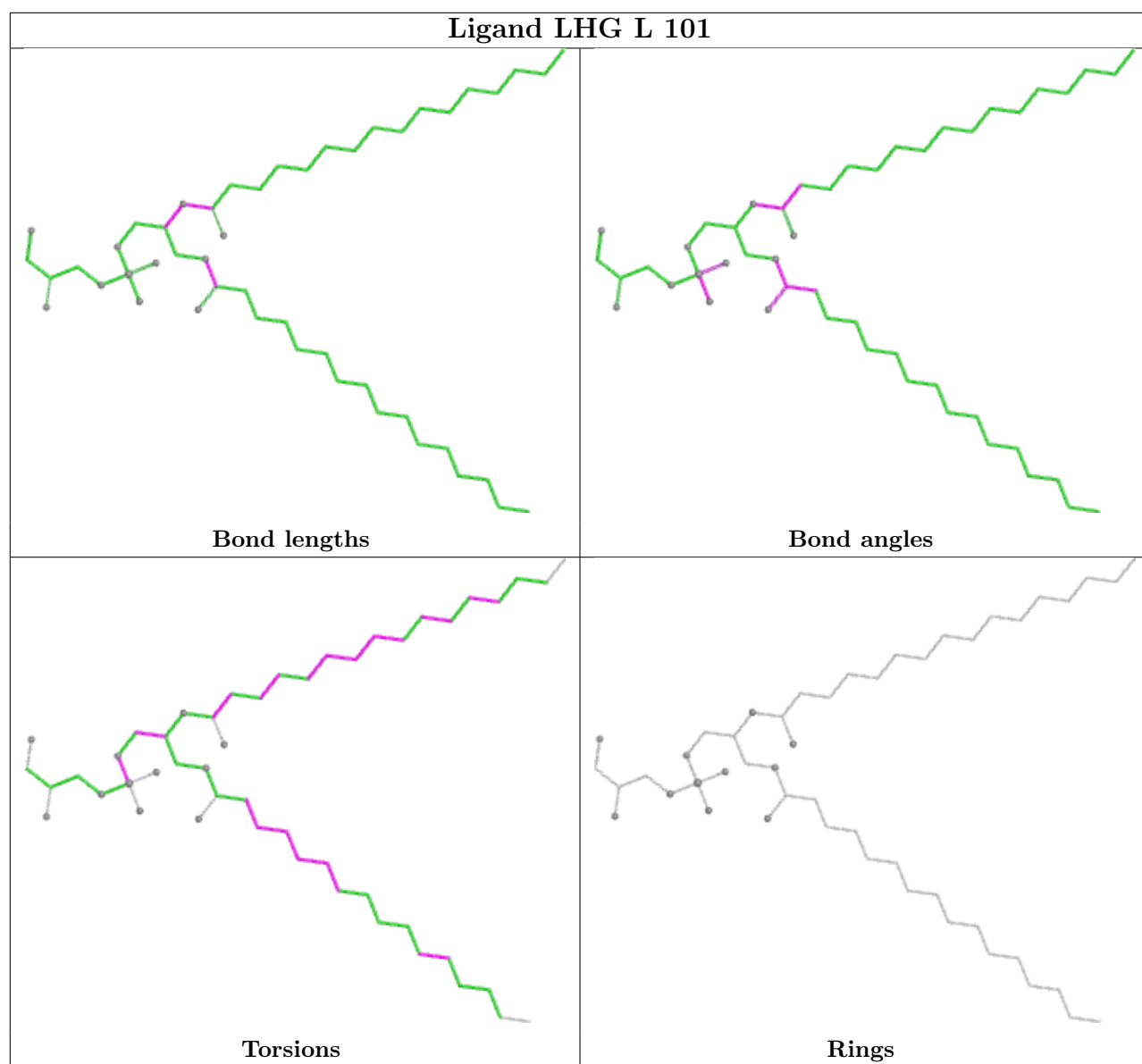


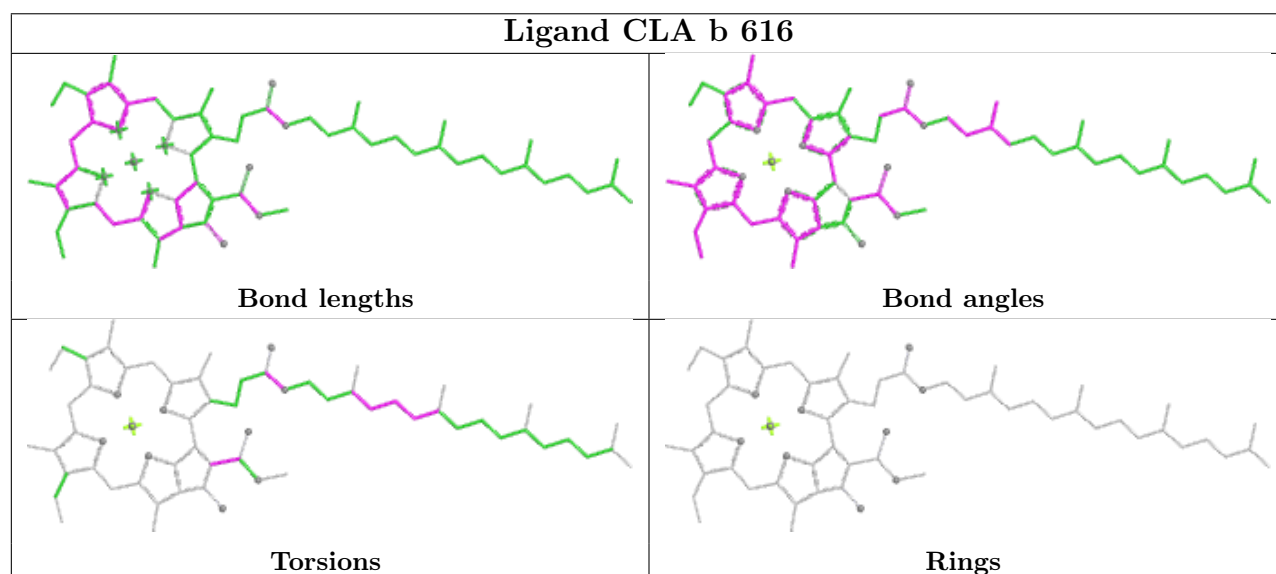
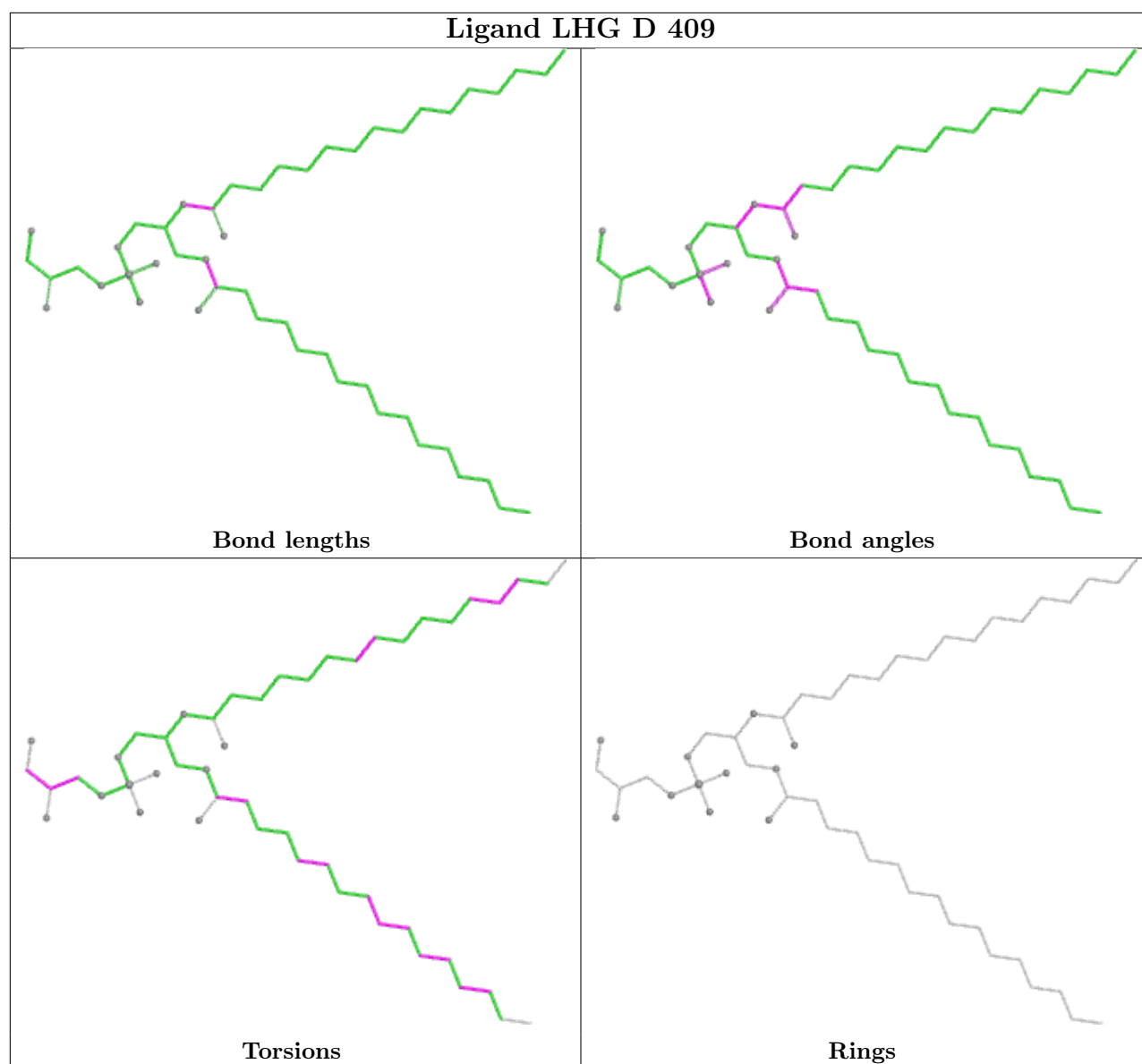


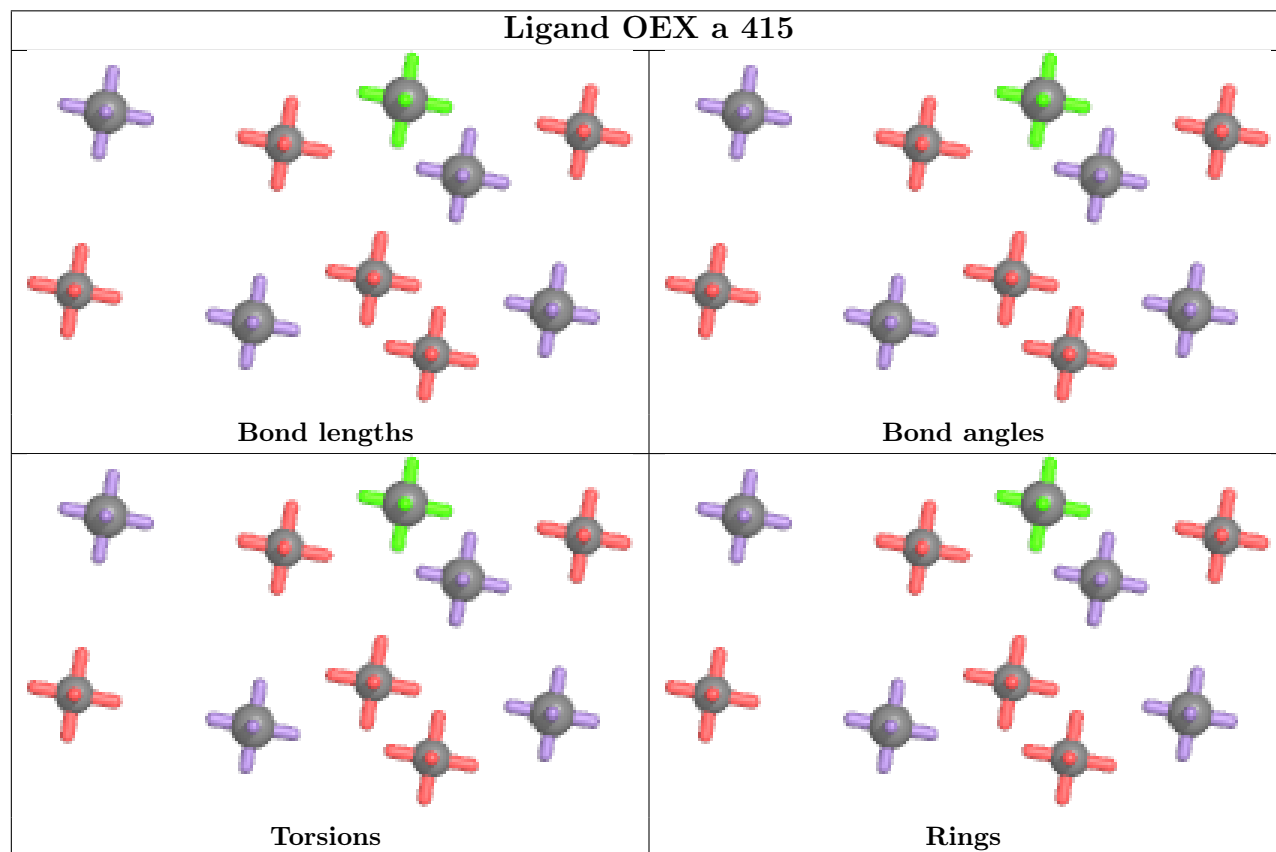
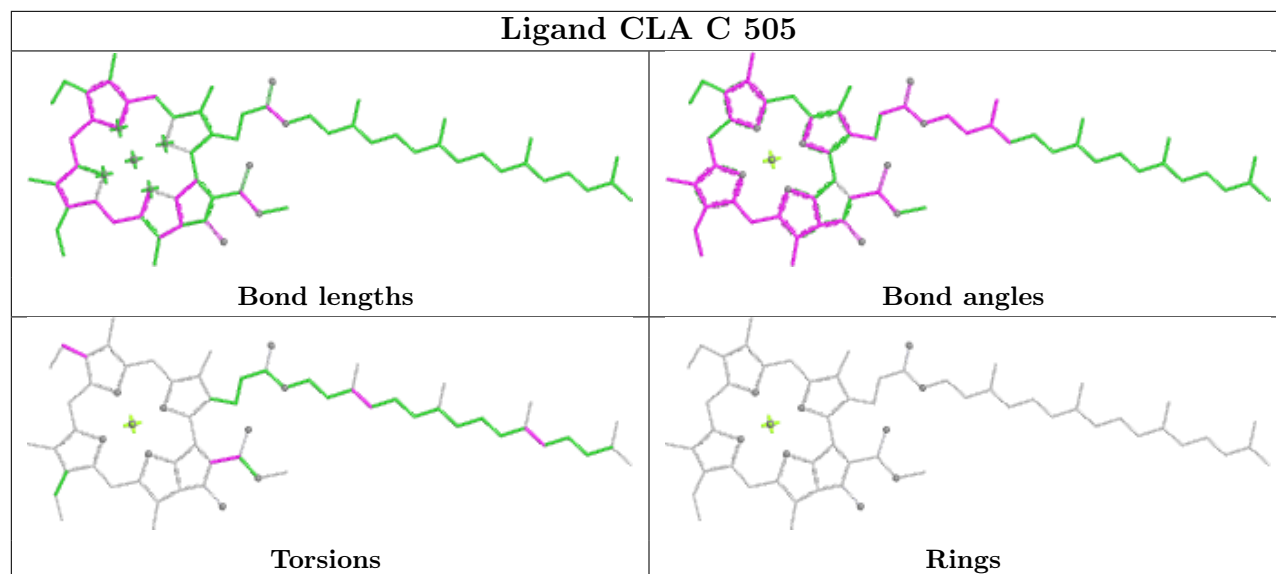


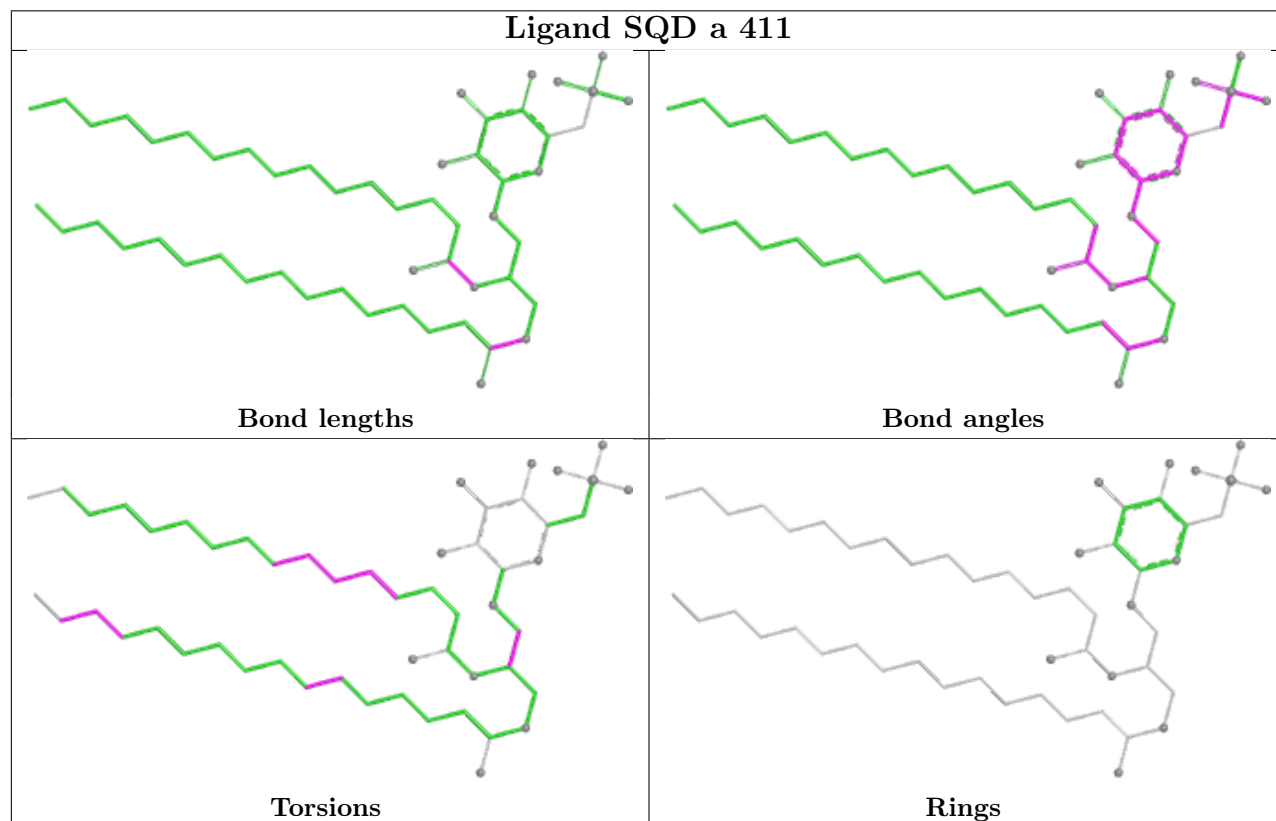
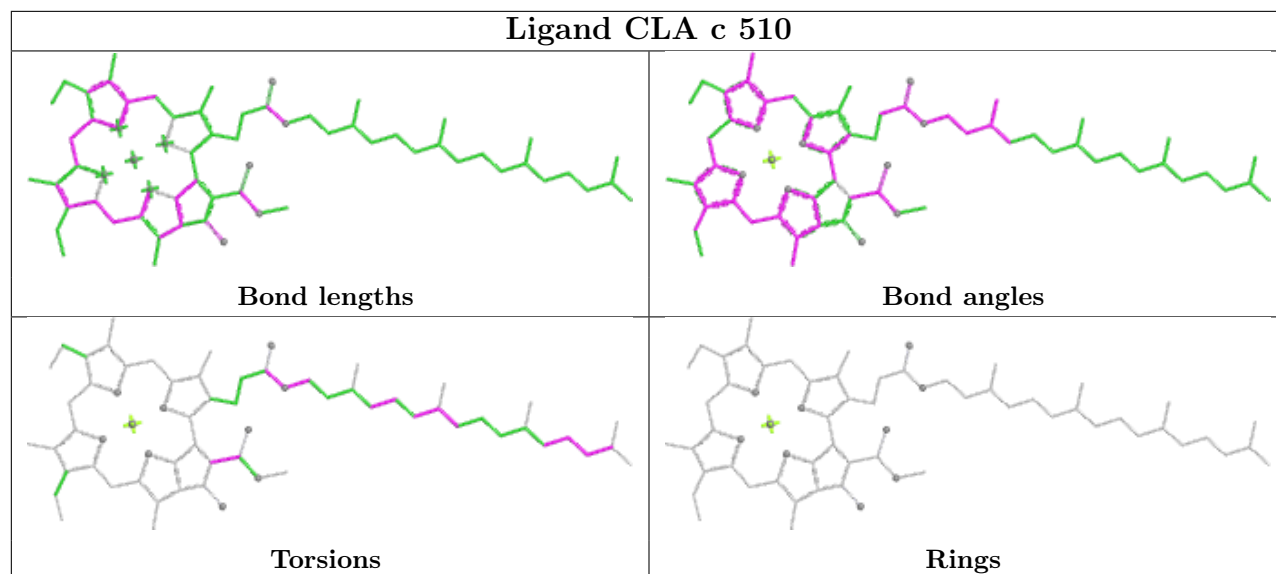


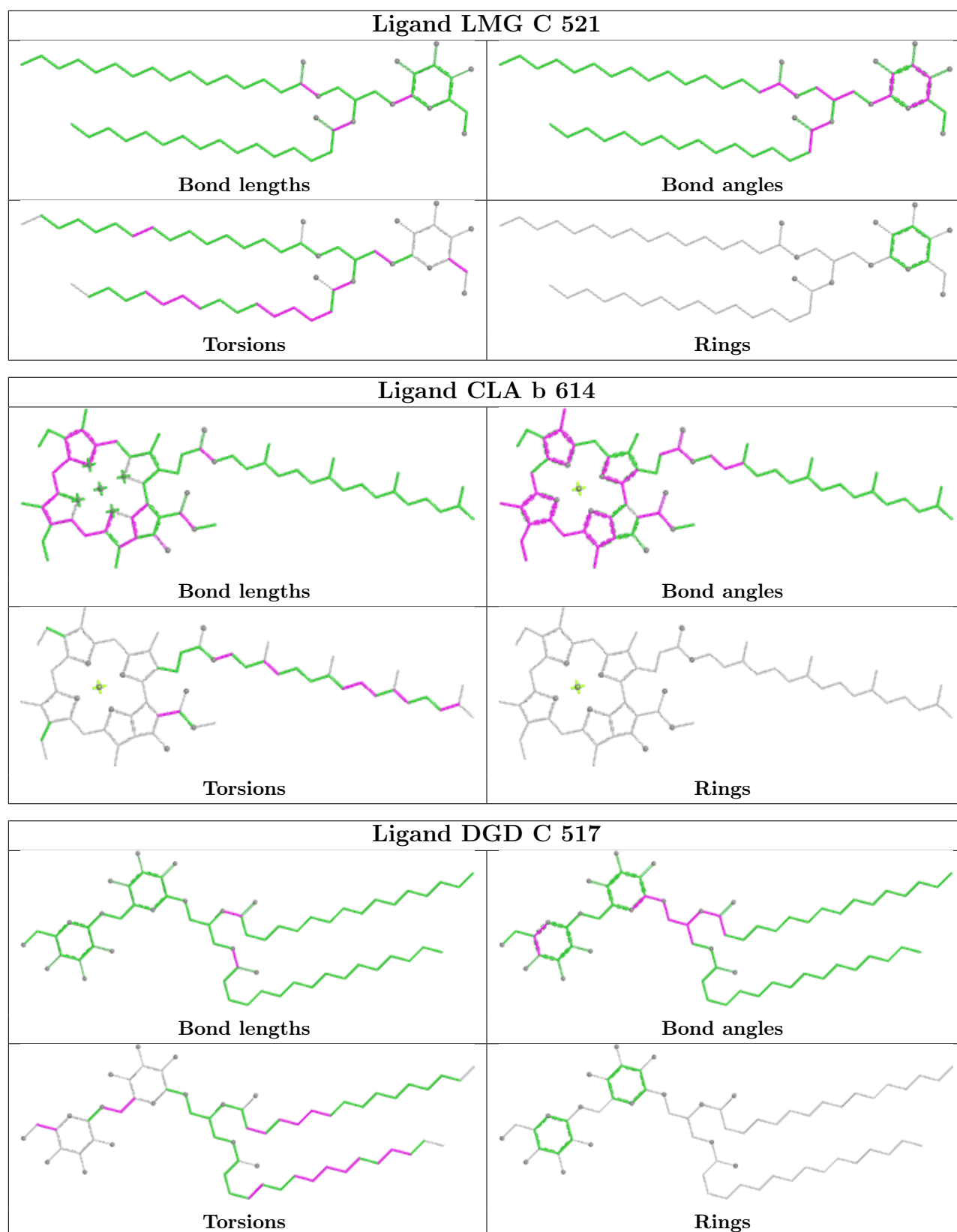


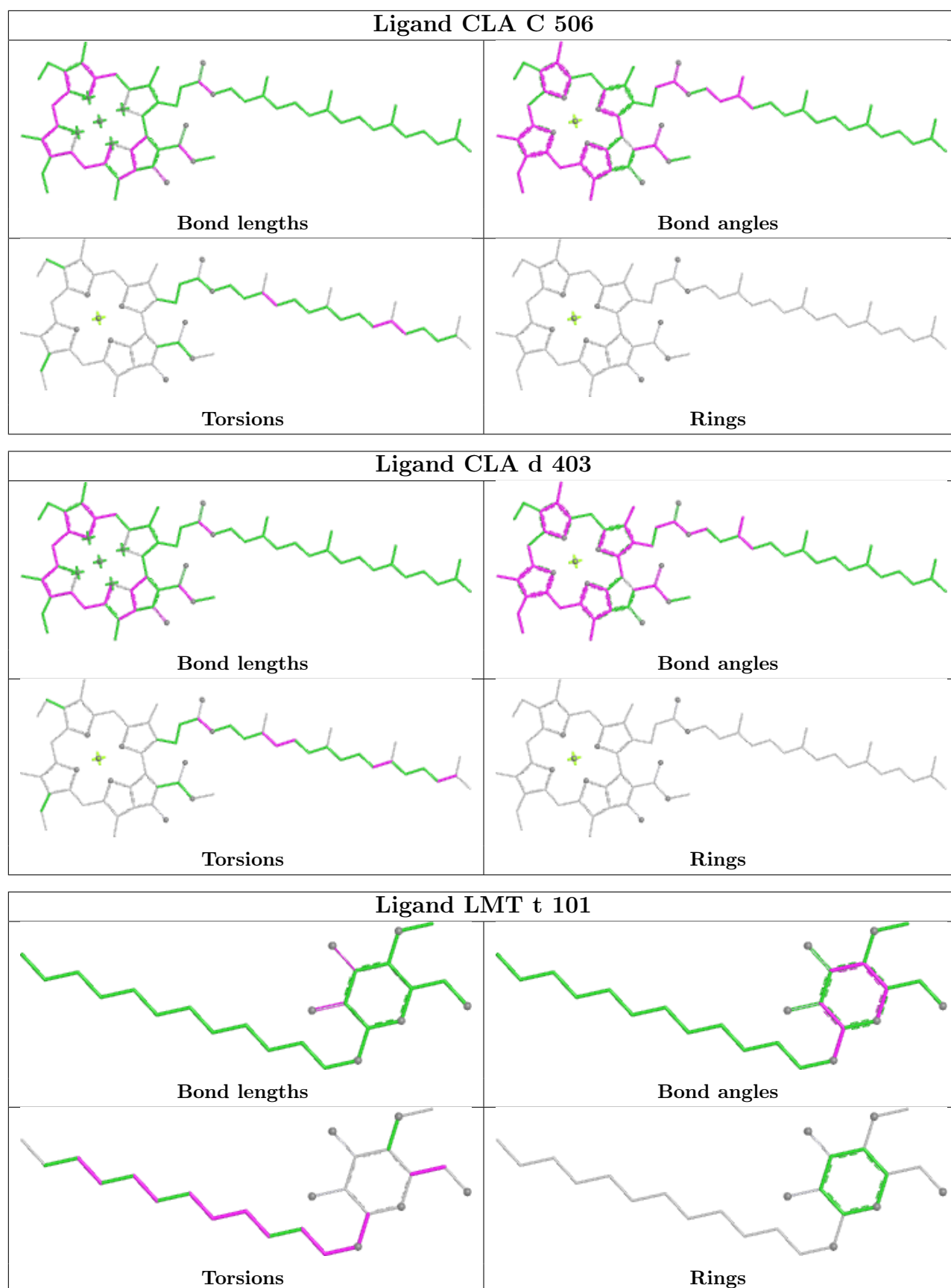


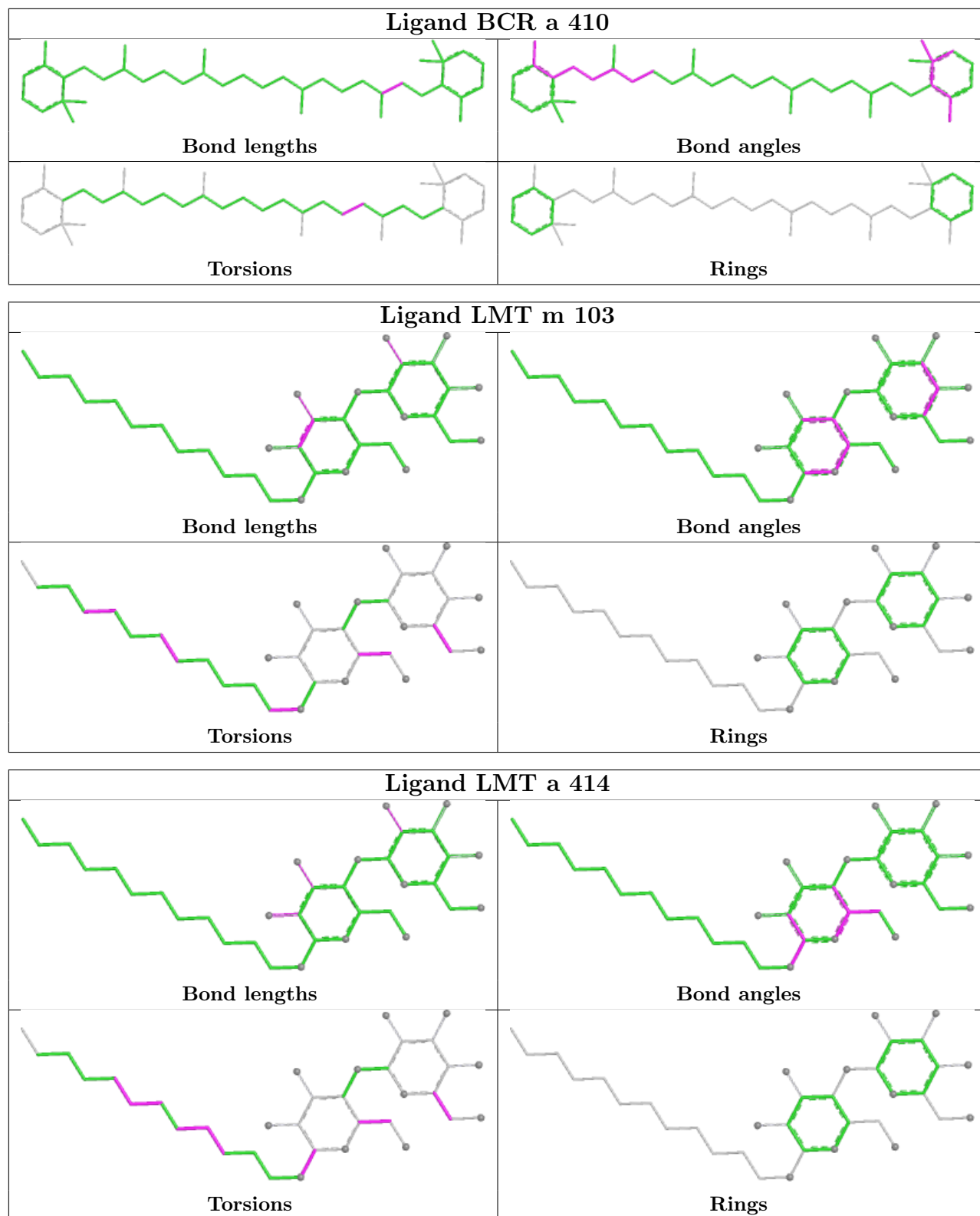


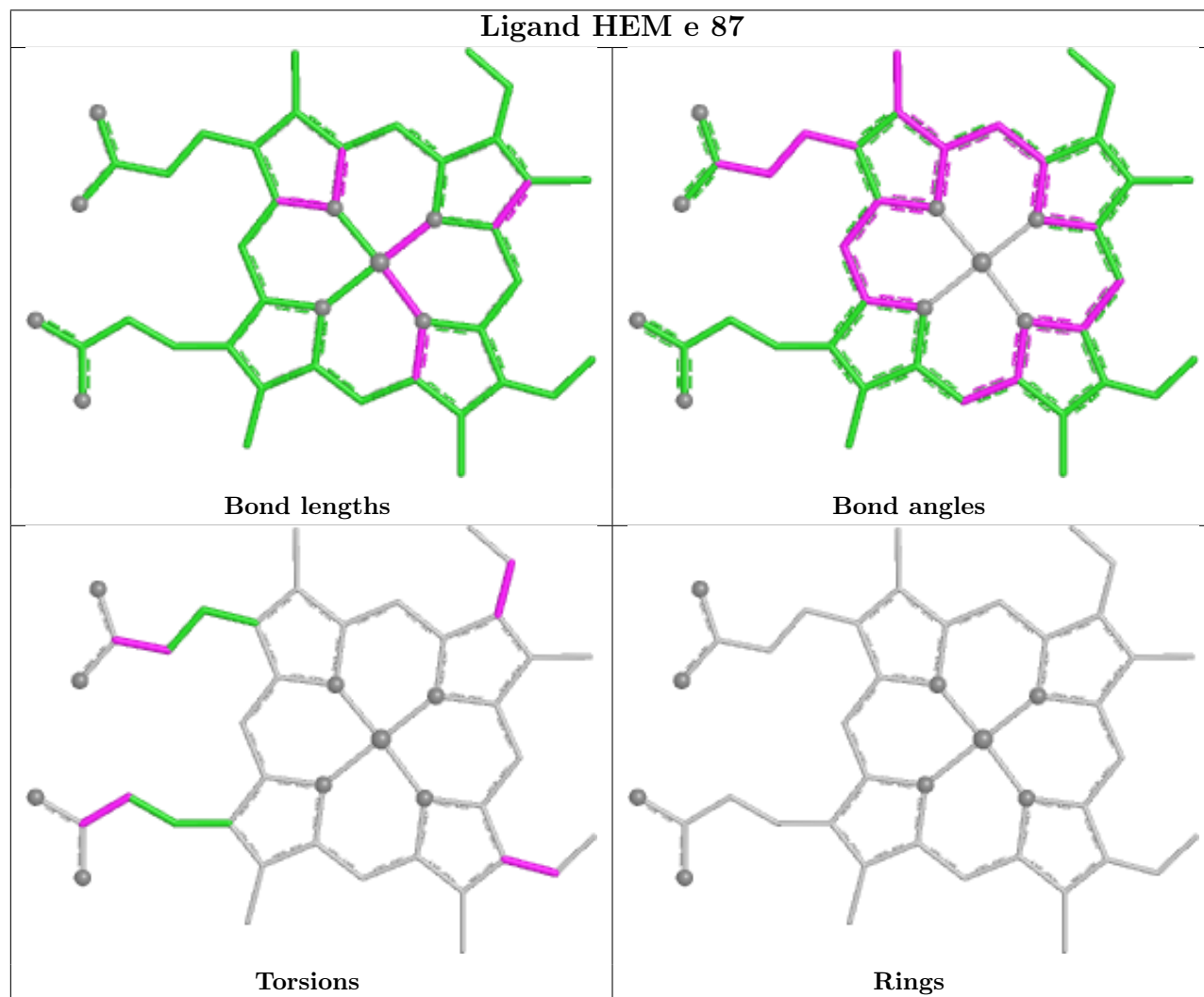
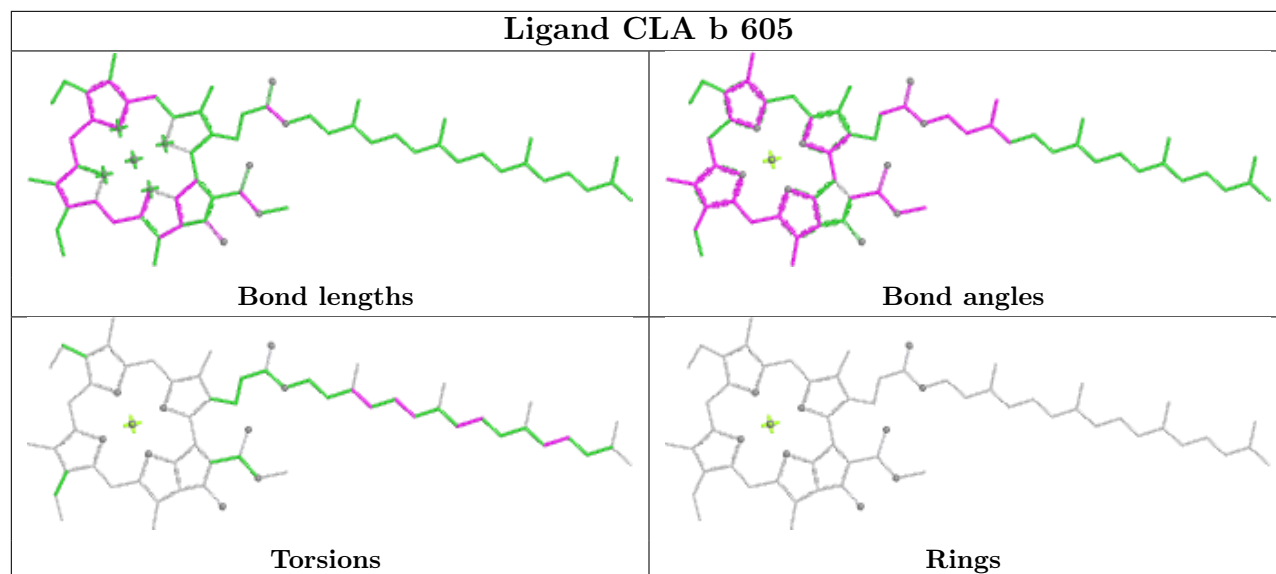


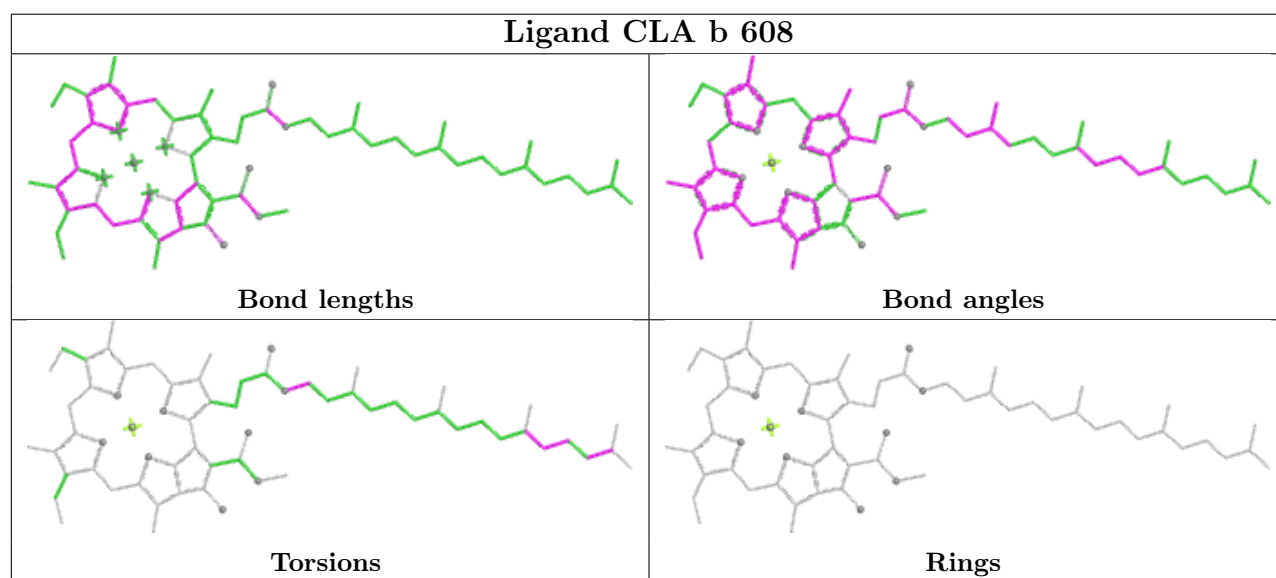
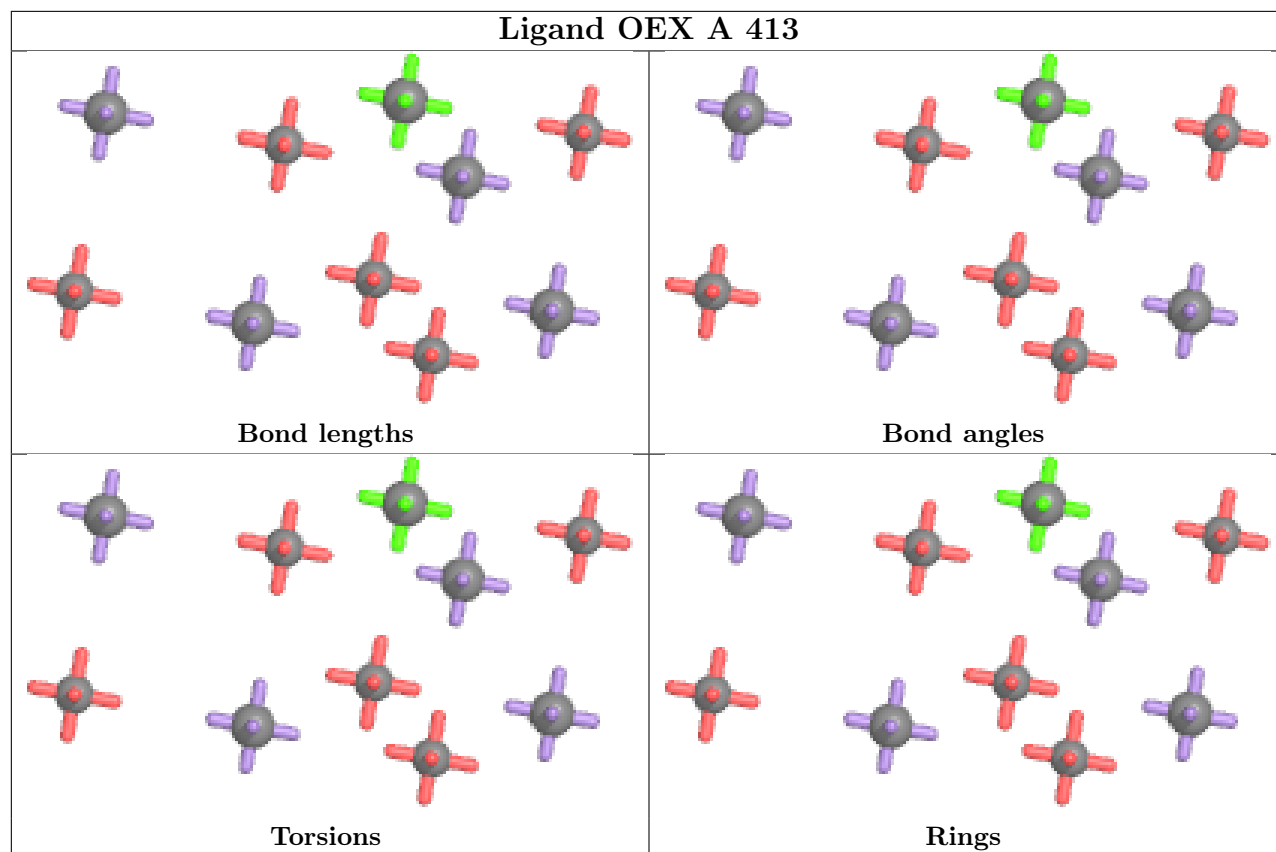


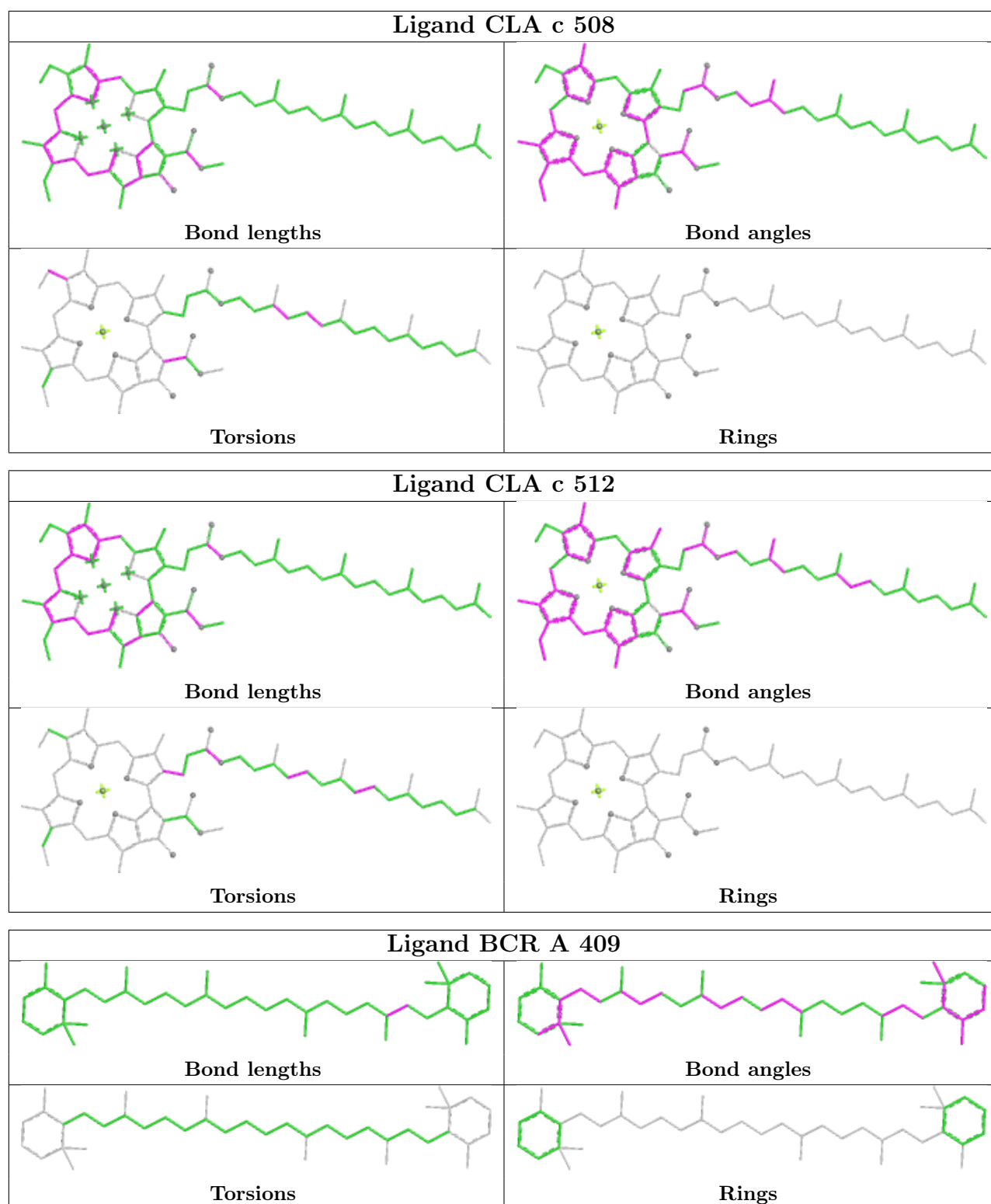


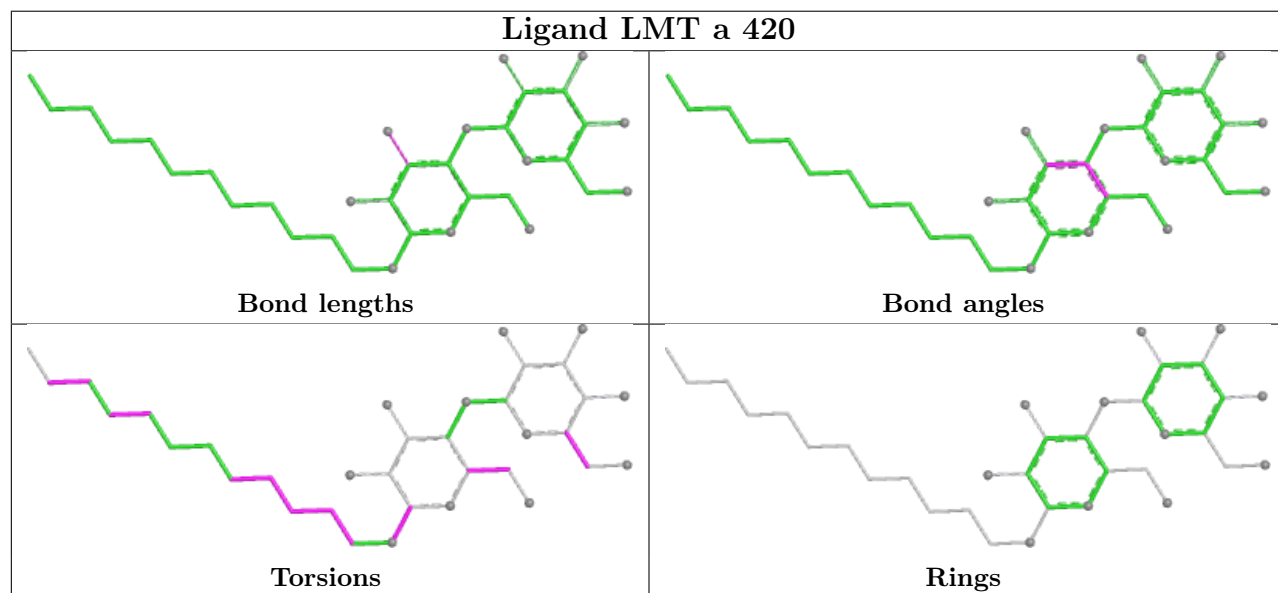
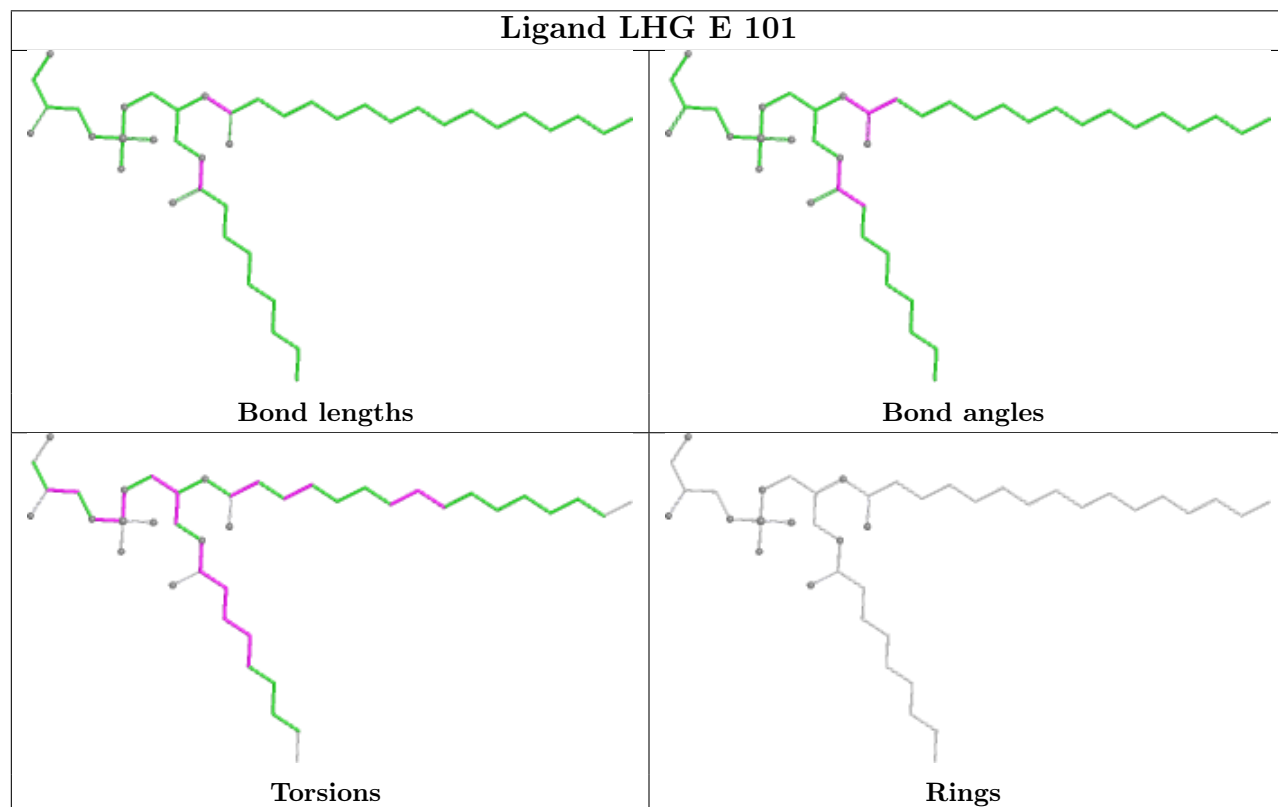
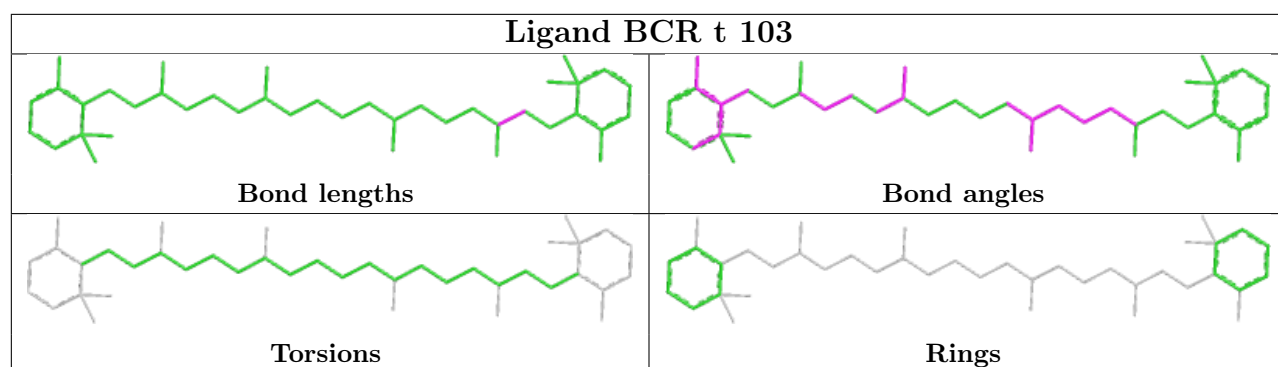


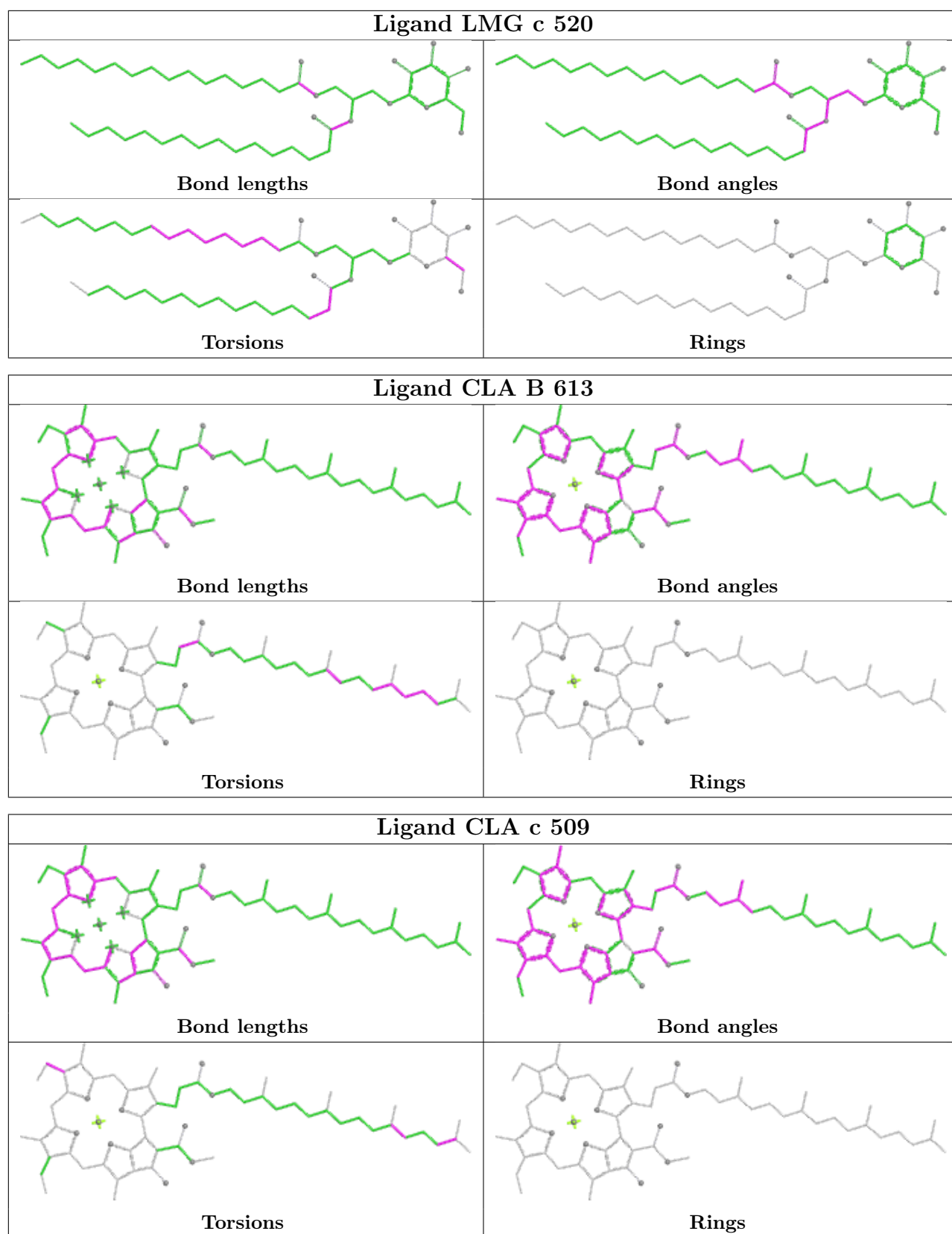


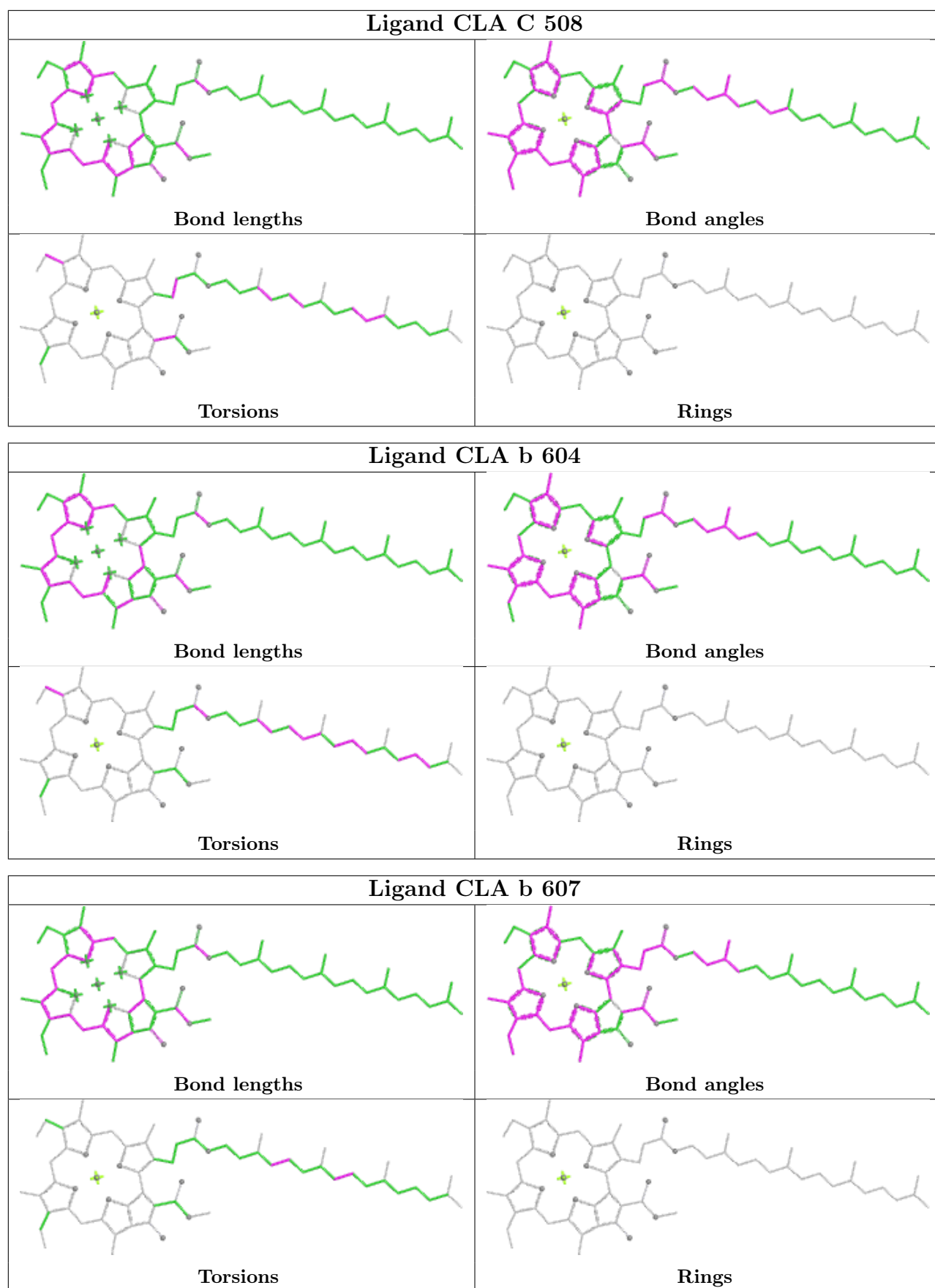


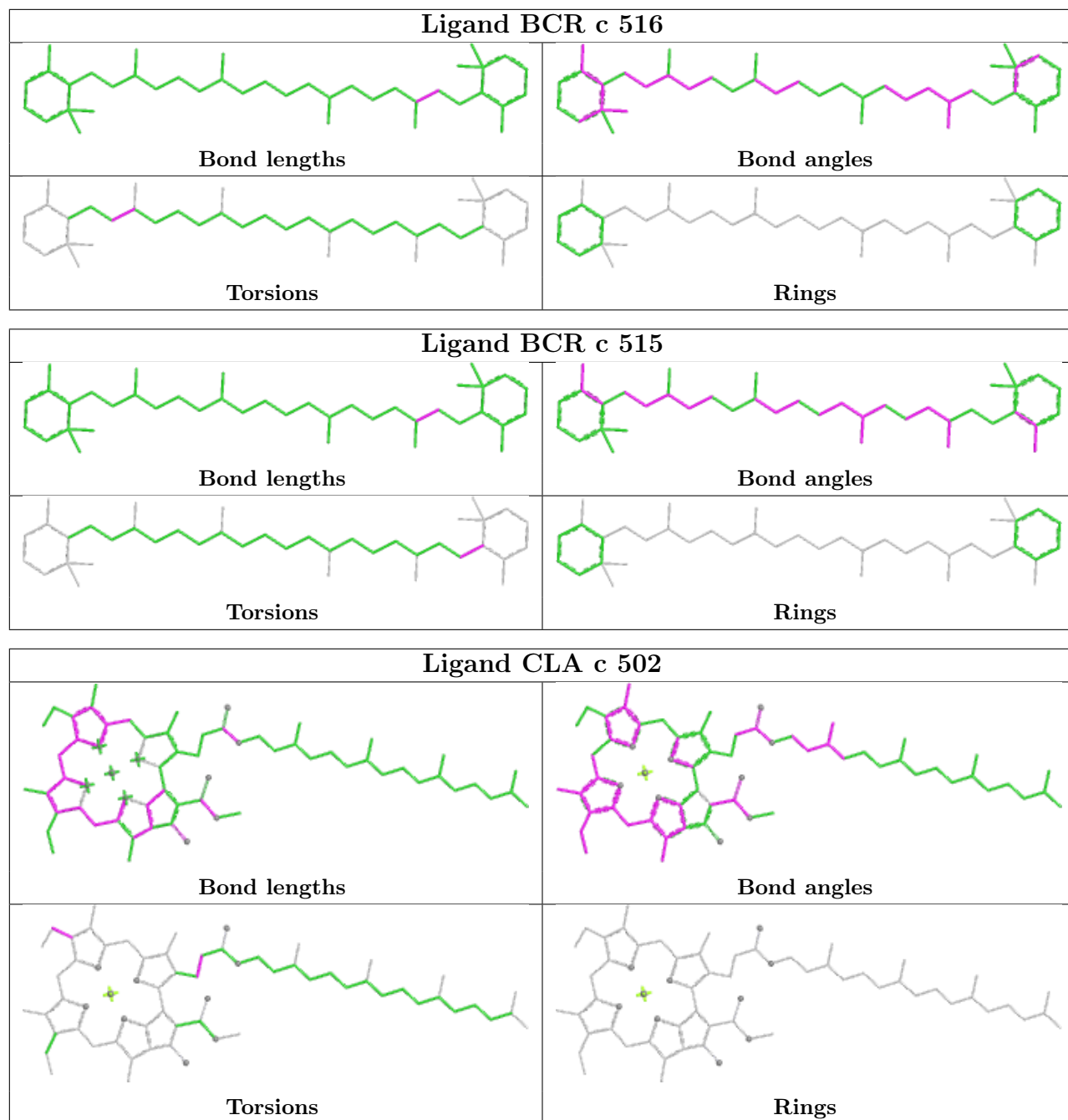


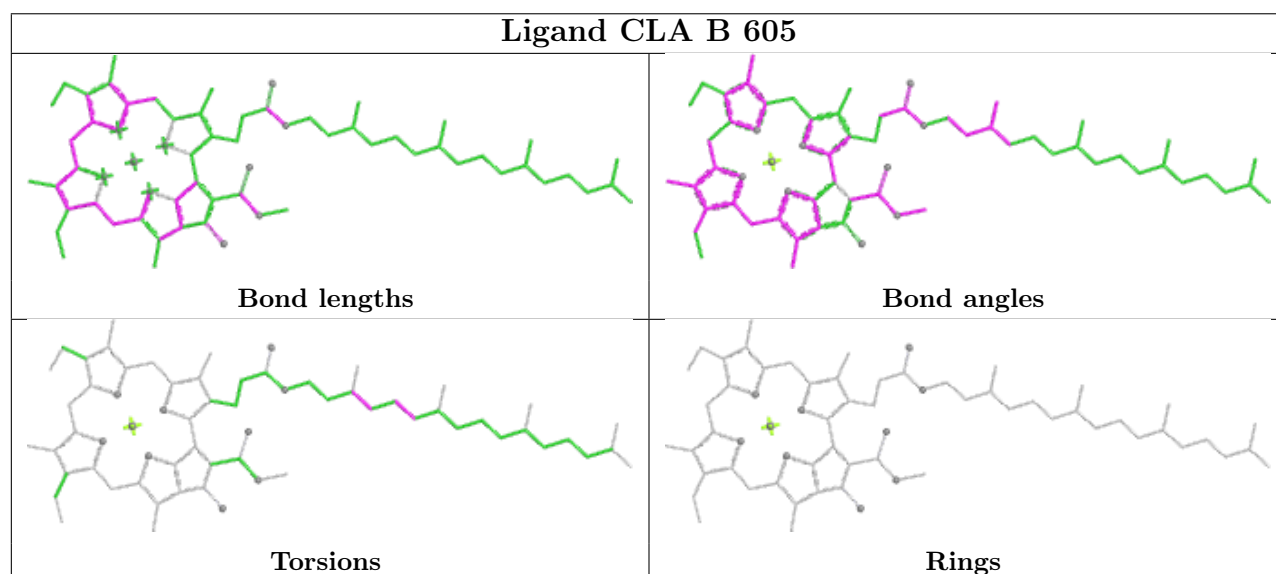
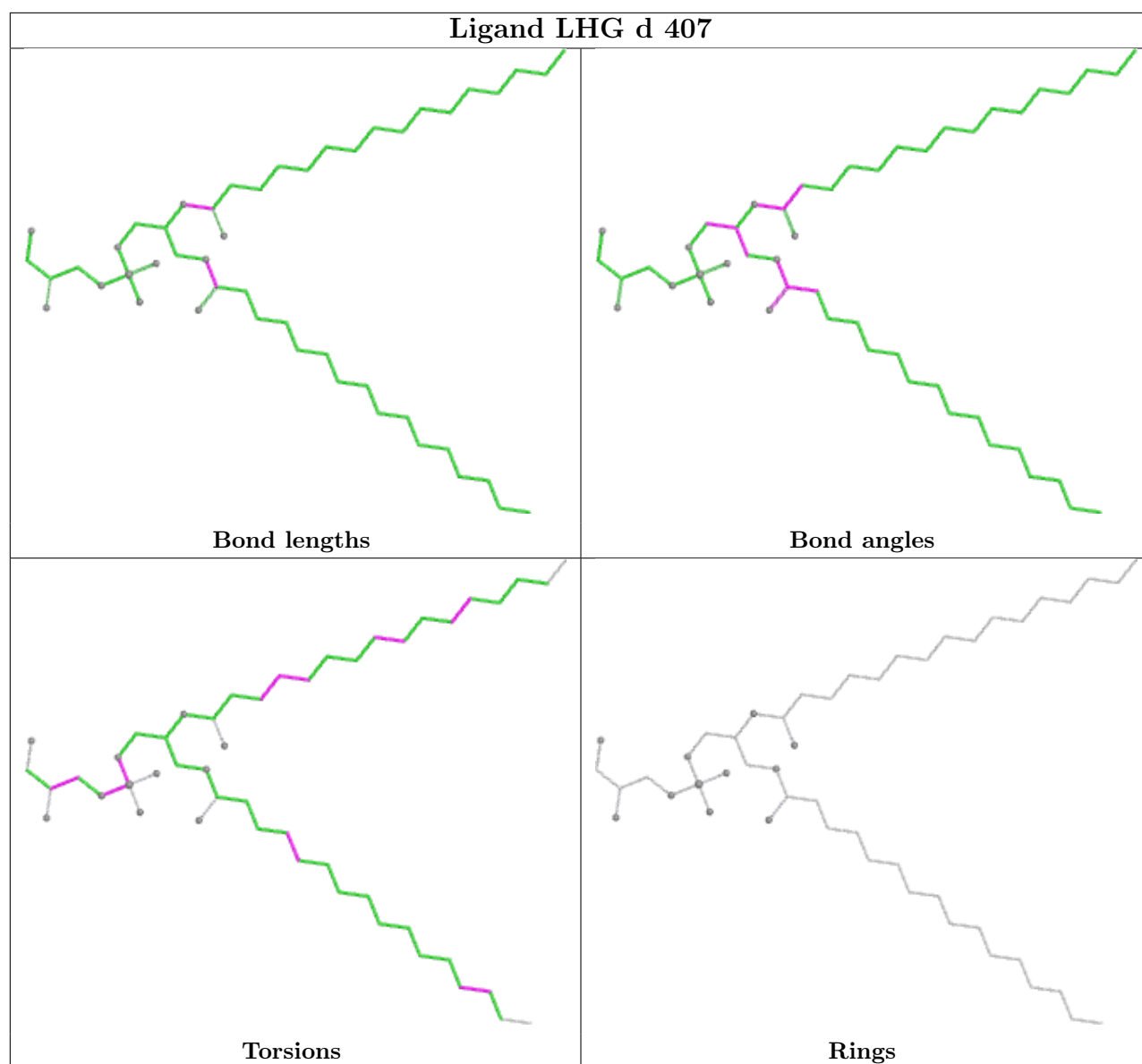


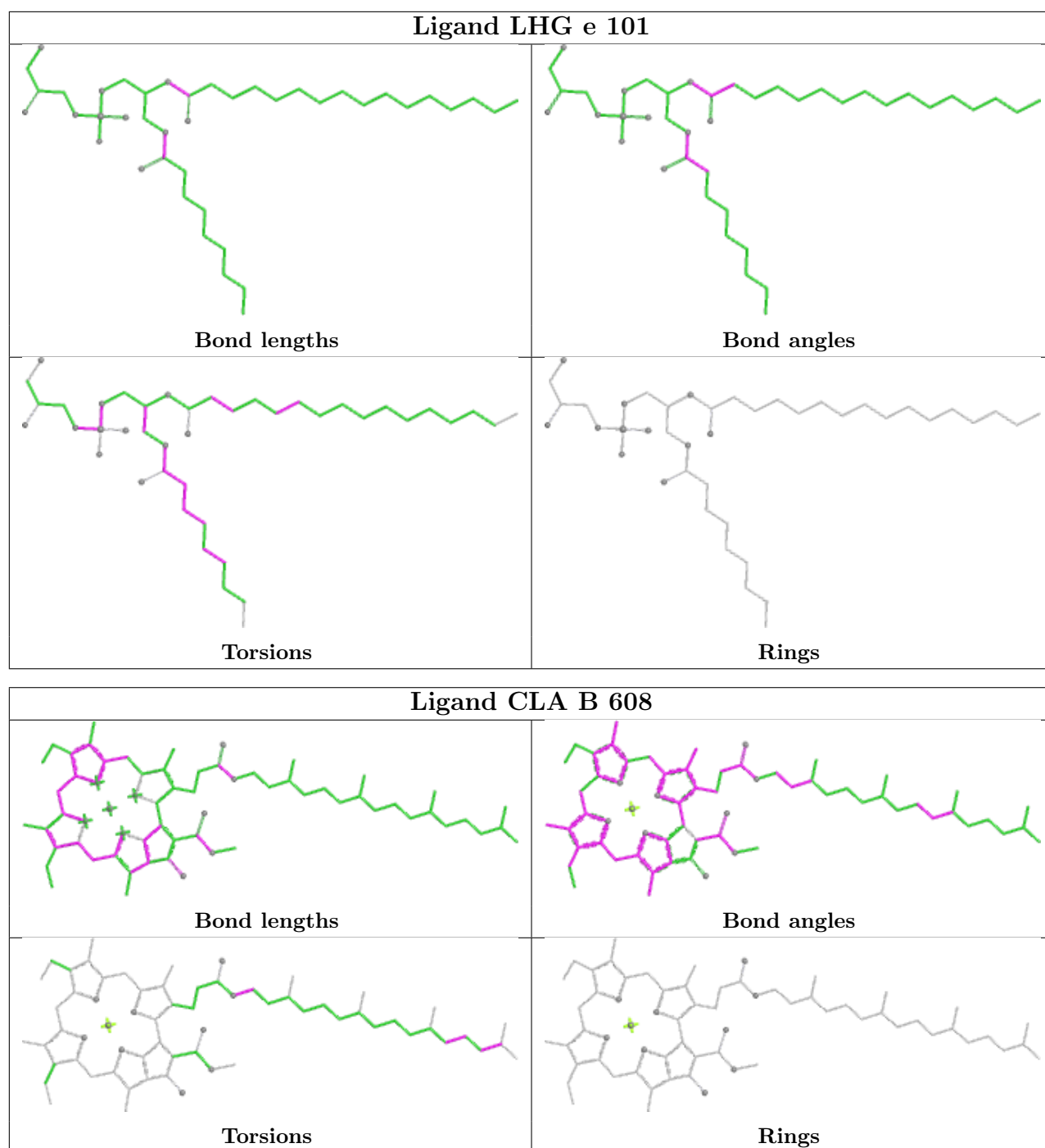


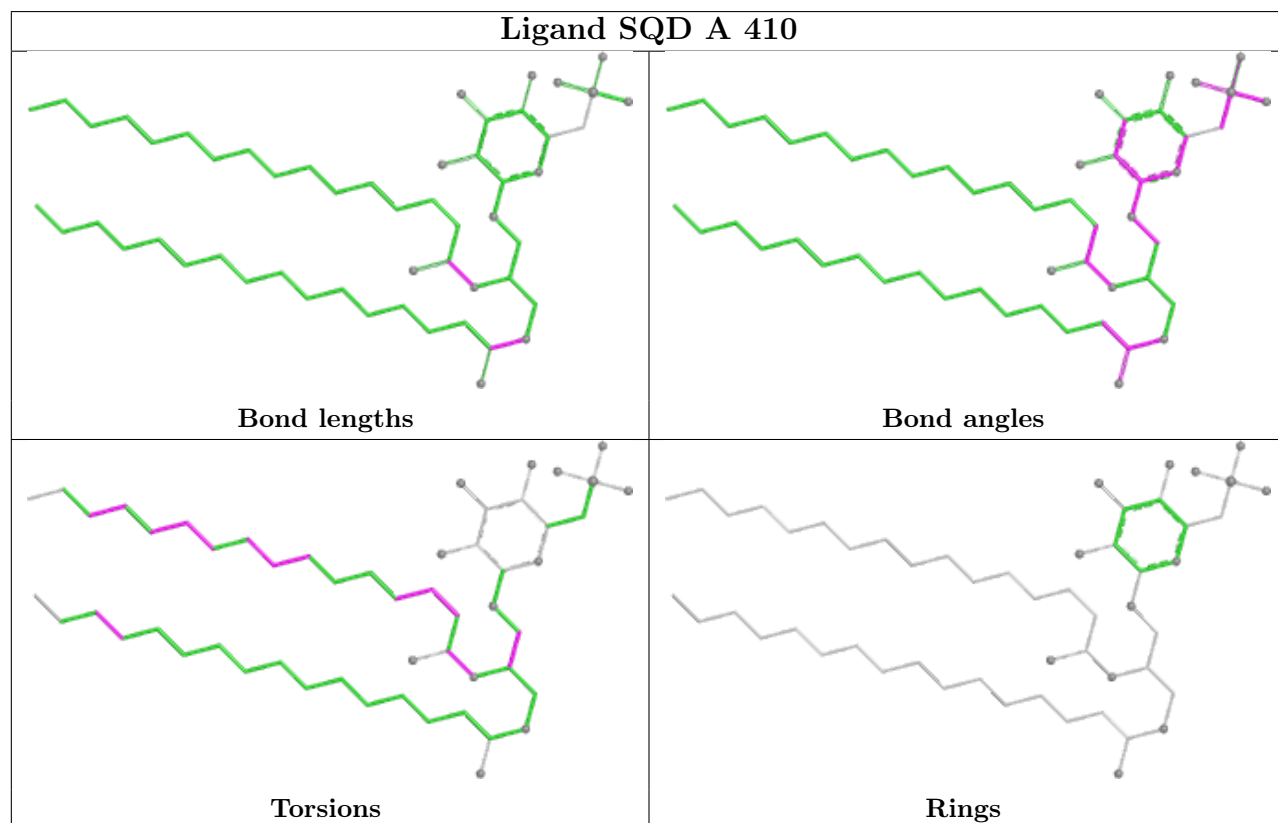
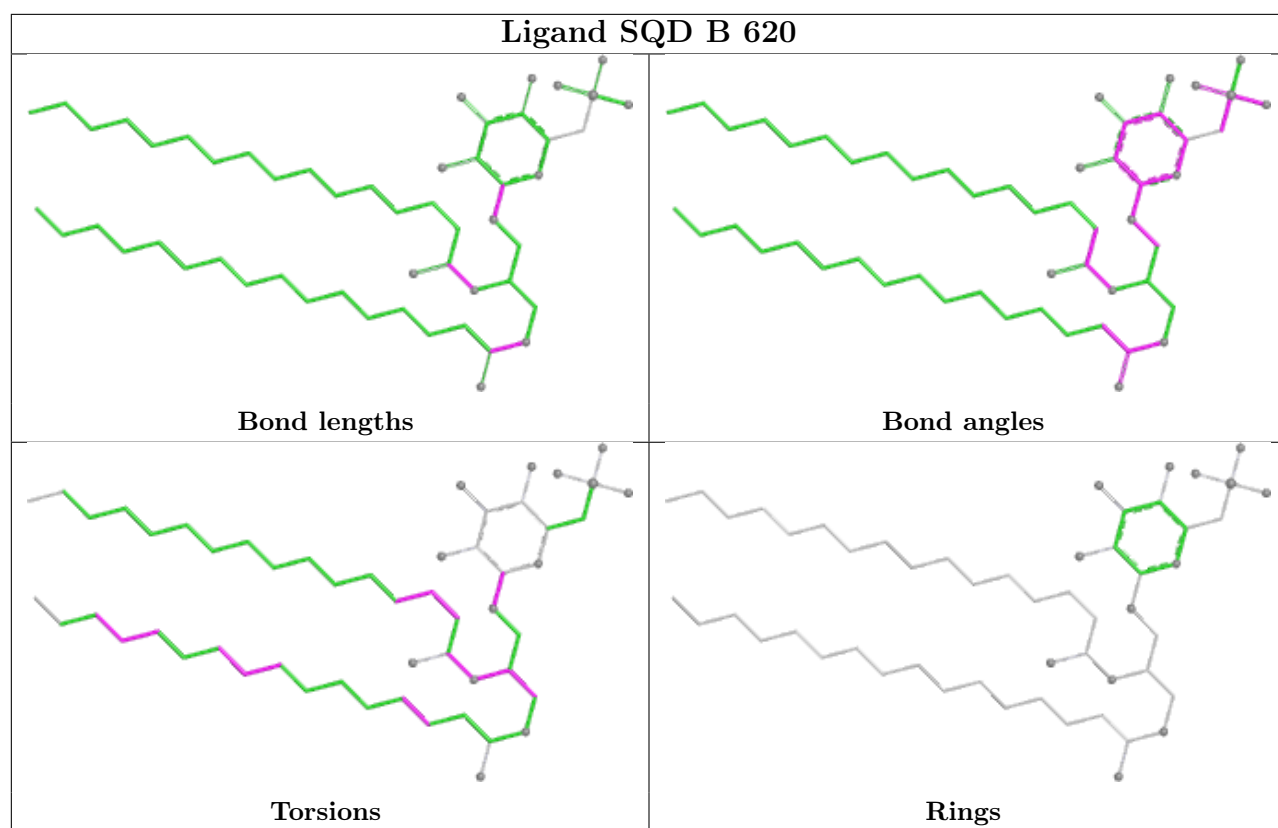


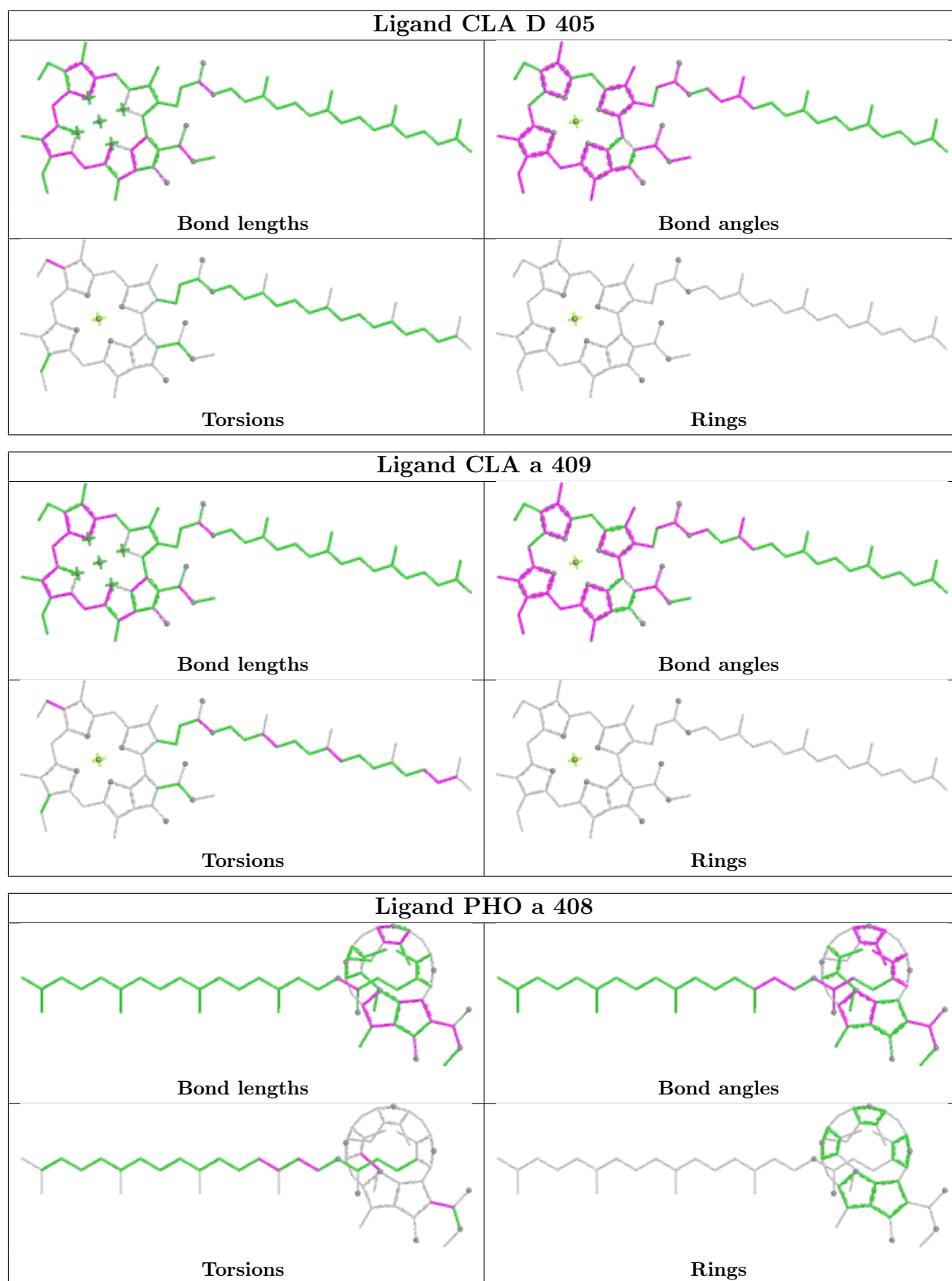












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.66	0 100 100	23, 46, 67, 111	1 (0%)
1	a	334/344 (97%)	-0.64	2 (0%) 85 86	27, 50, 77, 114	2 (0%)
2	B	504/505 (99%)	-0.53	1 (0%) 91 92	23, 53, 79, 105	7 (1%)
2	b	504/505 (99%)	-0.41	3 (0%) 85 86	26, 58, 95, 136	6 (1%)
3	C	451/455 (99%)	-0.53	1 (0%) 91 92	28, 59, 80, 116	1 (0%)
3	c	455/455 (100%)	-0.46	2 (0%) 88 89	30, 64, 86, 118	5 (1%)
4	D	342/342 (100%)	-0.68	0 100 100	20, 48, 66, 117	1 (0%)
4	d	341/342 (99%)	-0.67	0 100 100	22, 53, 78, 114	2 (0%)
5	E	81/84 (96%)	-0.25	0 100 100	53, 68, 89, 140	0
5	e	79/84 (94%)	-0.24	1 (1%) 75 76	32, 74, 107, 128	2 (2%)
6	F	34/44 (77%)	-0.54	0 100 100	52, 61, 86, 106	0
6	f	31/44 (70%)	-0.23	1 (3%) 50 50	53, 69, 89, 125	1 (3%)
7	H	64/65 (98%)	-0.27	2 (3%) 51 51	52, 63, 80, 92	0
7	h	64/65 (98%)	-0.22	1 (1%) 70 71	38, 73, 87, 91	1 (1%)
8	I	37/38 (97%)	-0.05	0 100 100	56, 64, 104, 127	0
8	i	37/38 (97%)	-0.18	1 (2%) 56 57	56, 65, 103, 117	0
9	J	38/39 (97%)	-0.37	0 100 100	50, 68, 108, 135	0
9	j	39/39 (100%)	-0.20	0 100 100	58, 77, 115, 133	0
10	K	37/37 (100%)	-0.63	0 100 100	56, 66, 82, 95	0
10	k	37/37 (100%)	-0.45	0 100 100	65, 73, 91, 101	0
11	L	36/37 (97%)	-0.63	0 100 100	38, 44, 87, 107	0
11	l	36/37 (97%)	-0.62	0 100 100	40, 46, 90, 95	0
12	M	32/36 (88%)	-0.57	0 100 100	24, 46, 68, 107	1 (3%)
12	m	33/36 (91%)	-0.57	0 100 100	23, 47, 68, 123	2 (6%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.47	0 100 100	33, 63, 108, 147	3 (1%)
13	o	243/244 (99%)	-0.37	0 100 100	43, 67, 114, 143	0
14	T	29/32 (90%)	-0.70	0 100 100	28, 47, 72, 93	1 (3%)
14	t	29/32 (90%)	-0.64	0 100 100	43, 49, 75, 100	0
15	U	96/104 (92%)	-0.57	0 100 100	33, 56, 82, 90	1 (1%)
15	u	97/104 (93%)	-0.62	0 100 100	30, 61, 77, 106	1 (1%)
16	V	137/137 (100%)	-0.68	0 100 100	32, 55, 75, 96	2 (1%)
16	v	137/137 (100%)	-0.52	0 100 100	51, 70, 93, 116	0
17	X	38/40 (95%)	-0.13	0 100 100	35, 72, 92, 102	1 (2%)
17	x	38/40 (95%)	0.09	0 100 100	69, 80, 120, 138	0
18	Y	29/30 (96%)	0.03	1 (3%) 48 48	66, 82, 111, 113	0
18	y	29/30 (96%)	-0.10	0 100 100	77, 89, 105, 106	0
19	Z	62/62 (100%)	-0.18	0 100 100	69, 79, 123, 135	0
19	z	62/62 (100%)	0.21	0 100 100	81, 93, 129, 151	0
20	R	34/34 (100%)	0.90	3 (8%) 15 14	89, 106, 127, 134	0
All	All	5283/5384 (98%)	-0.49	19 (0%) 88 89	20, 58, 95, 151	41 (0%)

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	b	479[A]	PHE	4.8
5	e	79[A]	PHE	4.2
7	H	65	LEU	3.6
6	f	16[A]	PHE	3.5
2	B	494	GLY	3.1

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	T	1	10/11	0.94	0.08	42,50,60,69	0
8	FME	I	1	10/11	0.95	0.07	62,71,80,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	t	1	10/11	0.96	0.07	43,48,58,71	0
12	FME	m	1	10/11	0.97	0.07	47,59,81,89	0
8	FME	i	1	10/11	0.97	0.07	60,69,80,82	0
12	FME	M	1	10/11	0.98	0.06	45,57,82,83	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
27	GOL	a	701	6/6	0.58	0.17	67,76,80,87	0
32	LMT	a	414	35/35	0.58	0.16	63,88,104,110	0
30	UNL	a	417	30/-	0.60	0.14	83,97,111,115	0
32	LMT	E	102	35/35	0.60	0.16	91,110,128,136	0
30	UNL	A	415	28/-	0.60	0.15	85,97,103,113	0
32	LMT	e	102	35/35	0.60	0.16	100,117,141,148	0
32	LMT	A	359	35/35	0.62	0.14	62,87,99,103	0
32	LMT	a	420	35/35	0.66	0.14	98,106,117,123	0
32	LMT	I	101	35/35	0.67	0.13	95,106,125,127	0
30	UNL	I	102	40/-	0.67	0.16	73,93,117,117	0
30	UNL	K	101	34/-	0.69	0.14	70,94,106,109	0
30	UNL	J	101	10/-	0.70	0.21	62,76,78,81	0
26	SQD	f	102	43/54	0.71	0.13	95,111,133,137	0
34	HTG	C	522	19/19	0.71	0.13	101,105,118,120	0
27	GOL	o	601	6/6	0.72	0.16	69,76,81,81	0
37	LHG	e	101	42/49	0.72	0.13	77,123,136,141	0
30	UNL	i	101	40/-	0.73	0.13	73,92,119,122	0
30	UNL	m	102	10/-	0.73	0.18	66,69,81,84	0
34	HTG	b	623	19/19	0.74	0.13	82,117,123,124	0
30	UNL	j	101	10/-	0.74	0.17	73,86,89,91	0
30	UNL	M	102	10/-	0.75	0.15	61,69,82,85	0
32	LMT	b	621	25/35	0.75	0.14	78,101,125,128	0
32	LMT	t	102	26/35	0.76	0.13	65,87,107,111	0
30	UNL	c	525	32/-	0.76	0.13	84,98,109,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	UNL	d	410	36/-	0.76	0.12	68,87,107,111	0
30	UNL	D	413	40/-	0.76	0.13	66,84,105,112	0
33	LMG	C	521	51/55	0.77	0.12	62,105,124,128	0
32	LMT	M	103	35/35	0.77	0.12	63,100,125,128	0
32	LMT	t	101	25/35	0.77	0.14	57,76,105,116	0
27	GOL	o	501	6/6	0.77	0.15	78,88,93,93	0
34	HTG	D	414	16/19	0.78	0.12	85,93,108,117	0
34	HTG	B	623	19/19	0.78	0.15	62,74,92,96	0
30	UNL	b	626	33/-	0.78	0.13	68,91,132,133	0
32	LMT	D	404	35/35	0.79	0.12	67,94,113,116	0
27	GOL	O	501	6/6	0.79	0.10	80,89,94,96	0
30	UNL	B	627	33/-	0.79	0.14	56,95,117,120	0
27	GOL	A	411	6/6	0.79	0.13	61,70,75,76	0
32	LMT	b	627	25/35	0.80	0.13	56,78,111,117	0
34	HTG	c	522	19/19	0.80	0.10	106,114,122,125	0
34	HTG	d	411	16/19	0.80	0.12	92,107,116,125	0
34	HTG	V	203	11/19	0.80	0.10	79,95,104,104	0
27	GOL	c	743	6/6	0.81	0.17	84,89,90,93	0
27	GOL	d	701	6/6	0.82	0.21	51,59,69,72	0
34	HTG	b	622	19/19	0.82	0.12	57,74,82,89	0
27	GOL	B	901	6/6	0.82	0.15	62,69,78,92	0
26	SQD	a	413	54/54	0.82	0.10	65,85,111,118	0
29	PL9	A	414	55/55	0.82	0.12	58,81,99,103	0
29	PL9	a	416	55/55	0.82	0.14	71,90,100,107	0
33	LMG	c	521	51/55	0.83	0.11	74,112,132,135	0
27	GOL	b	624	6/6	0.83	0.14	78,85,87,93	0
26	SQD	A	412	54/54	0.84	0.10	63,79,104,118	0
27	GOL	d	801	6/6	0.84	0.16	56,86,90,90	0
36	CA	F	102	1/1	0.84	0.23	114,114,114,114	0
33	LMG	Z	101	37/55	0.84	0.14	71,110,125,133	0
32	LMT	m	103	35/35	0.85	0.11	60,77,86,90	0
27	GOL	O	601	6/6	0.85	0.18	67,71,76,78	0
32	LMT	M	101	35/35	0.85	0.11	58,81,89,94	0
33	LMG	z	101	39/55	0.85	0.12	78,116,128,136	0
34	HTG	B	622	19/19	0.85	0.12	63,76,85,85	0
30	UNL	D	412	17/-	0.86	0.11	57,70,92,98	0
26	SQD	B	620	54/54	0.86	0.10	61,81,106,110	0
23	CLA	b	601	65/65	0.87	0.10	68,87,110,121	0
26	SQD	b	620	54/54	0.87	0.10	58,83,99,104	0
36	CA	f	103	1/1	0.87	0.12	116,116,116,116	0
26	SQD	F	101	43/54	0.87	0.11	71,94,114,123	0
27	GOL	a	412	6/6	0.88	0.12	69,72,83,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	LMG	C	501	51/55	0.88	0.09	66,82,94,99	0
37	LHG	E	101	42/49	0.88	0.10	70,93,106,111	0
27	GOL	D	701	6/6	0.88	0.17	46,57,60,63	0
27	GOL	V	401	6/6	0.89	0.14	54,62,68,69	0
27	GOL	a	801	6/6	0.89	0.24	54,61,68,69	0
33	LMG	a	419	51/55	0.89	0.08	68,85,93,101	0
27	GOL	A	701	6/6	0.89	0.24	48,61,63,69	0
33	LMG	m	101	51/55	0.89	0.09	52,68,81,90	0
30	UNL	d	409	17/-	0.90	0.10	64,75,90,92	0
27	GOL	v	401	6/6	0.90	0.13	62,73,75,76	0
23	CLA	B	601	65/65	0.90	0.09	59,77,99,112	0
33	LMG	c	520	51/55	0.91	0.09	61,86,110,121	0
33	LMG	B	621	51/55	0.91	0.08	53,66,78,88	0
23	CLA	c	514	65/65	0.91	0.10	75,91,113,123	0
33	LMG	d	412	51/55	0.92	0.09	54,69,102,107	0
25	BCR	d	404	40/40	0.92	0.08	50,65,89,95	0
33	LMG	C	520	51/55	0.92	0.09	55,80,98,108	0
34	HTG	b	625	19/19	0.92	0.07	62,72,85,90	0
23	CLA	C	514	65/65	0.92	0.09	68,84,105,108	0
33	LMG	D	415	51/55	0.92	0.09	48,63,100,106	0
27	GOL	C	523	6/6	0.92	0.13	56,58,59,62	0
34	HTG	B	626	19/19	0.92	0.07	64,77,86,89	0
25	BCR	D	407	40/40	0.92	0.09	44,58,89,91	0
25	BCR	T	101	40/40	0.92	0.07	44,57,65,66	0
30	UNL	X	101	18/-	0.93	0.10	59,73,95,100	0
23	CLA	c	513	65/65	0.93	0.09	65,80,111,115	0
27	GOL	c	742	6/6	0.93	0.21	63,64,69,69	0
23	CLA	B	614	65/65	0.93	0.07	37,47,82,91	0
25	BCR	C	515	40/40	0.93	0.09	61,76,85,88	0
23	CLA	C	507	65/65	0.93	0.08	59,69,104,107	0
35	DGD	C	518	62/66	0.93	0.08	48,61,103,107	0
23	CLA	b	616	65/65	0.93	0.09	55,63,116,123	0
23	CLA	c	505	65/65	0.93	0.07	52,61,95,101	0
36	CA	o	301	1/1	0.93	0.06	107,107,107,107	0
37	LHG	D	409	49/49	0.93	0.08	47,59,75,81	0
25	BCR	t	103	40/40	0.93	0.07	46,55,69,73	0
23	CLA	c	507	65/65	0.93	0.09	56,68,100,106	0
23	CLA	B	606	65/65	0.94	0.08	46,56,97,106	0
23	CLA	C	509	65/65	0.94	0.07	50,55,107,116	0
23	CLA	C	513	65/65	0.94	0.09	60,74,100,108	0
26	SQD	a	411	54/54	0.94	0.08	58,77,107,109	0
23	CLA	A	408	65/65	0.94	0.09	42,51,108,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	d	403	65/65	0.94	0.09	56,65,110,122	0
23	CLA	a	409	65/65	0.94	0.10	46,55,108,116	0
23	CLA	B	616	65/65	0.94	0.09	46,57,106,111	0
25	BCR	K	102	40/40	0.94	0.09	59,65,71,72	0
27	GOL	B	624	6/6	0.94	0.12	62,64,69,71	0
23	CLA	b	606	65/65	0.94	0.08	47,61,100,110	0
25	BCR	Y	101	40/40	0.94	0.08	55,63,76,77	0
35	DGD	c	517	62/66	0.94	0.07	48,62,95,101	0
35	DGD	c	518	62/66	0.94	0.07	55,65,110,121	0
35	DGD	c	519	62/66	0.94	0.07	50,64,98,115	0
25	BCR	c	515	40/40	0.94	0.08	77,84,90,91	0
23	CLA	b	614	65/65	0.94	0.07	41,51,84,86	0
25	BCR	h	101	40/40	0.94	0.09	60,70,88,89	0
25	BCR	k	101	40/40	0.94	0.10	63,74,82,85	0
37	LHG	D	411	49/49	0.94	0.09	47,59,99,106	0
23	CLA	C	505	65/65	0.94	0.08	44,55,89,101	0
37	LHG	d	711	49/49	0.94	0.08	49,63,75,77	0
26	SQD	A	410	54/54	0.94	0.08	55,77,101,104	0
25	BCR	B	618	40/40	0.95	0.06	41,51,62,66	0
25	BCR	B	619	40/40	0.95	0.07	49,59,83,89	0
25	BCR	y	101	40/40	0.95	0.07	62,71,80,85	0
29	PL9	d	405	55/55	0.95	0.06	39,49,57,67	0
31	BCT	a	404	4/4	0.95	0.07	53,58,65,74	0
23	CLA	b	604	65/65	0.95	0.07	41,52,88,93	0
23	CLA	a	407	65/65	0.95	0.07	41,52,112,121	0
35	DGD	C	519	62/66	0.95	0.07	43,58,88,95	0
35	DGD	H	102	62/66	0.95	0.08	47,58,67,70	0
25	BCR	H	101	40/40	0.95	0.08	53,66,84,85	0
23	CLA	c	508	65/65	0.95	0.08	58,67,78,80	0
23	CLA	c	509	65/65	0.95	0.07	50,61,118,124	0
35	DGD	h	102	62/66	0.95	0.07	53,63,72,76	0
23	CLA	B	611	65/65	0.95	0.07	37,43,61,67	0
36	CA	O	301	1/1	0.95	0.04	98,98,98,98	0
36	CA	c	523	1/1	0.95	0.06	79,79,79,79	0
27	GOL	b	901	6/6	0.95	0.11	67,70,76,77	0
25	BCR	a	410	40/40	0.95	0.07	44,54,62,63	0
25	BCR	b	618	40/40	0.95	0.06	42,55,72,76	0
25	BCR	b	619	40/40	0.95	0.08	53,62,80,85	0
23	CLA	D	406	65/65	0.95	0.08	49,58,102,105	0
37	LHG	d	408	49/49	0.95	0.08	50,61,105,116	0
23	CLA	c	502	65/65	0.95	0.07	58,68,75,81	0
25	BCR	A	409	40/40	0.95	0.07	40,52,62,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
37	LHG	l	101	49/49	0.95	0.07	48,56,68,82	0
23	CLA	B	603	65/65	0.96	0.07	45,52,68,73	0
23	CLA	c	512	65/65	0.96	0.07	60,67,81,87	0
23	CLA	A	406	65/65	0.96	0.06	36,45,103,112	0
23	CLA	C	502	65/65	0.96	0.06	52,60,68,77	0
23	CLA	b	602	65/65	0.96	0.07	49,61,74,81	0
24	PHO	a	353	64/64	0.96	0.06	45,55,61,66	0
29	PL9	D	408	55/55	0.96	0.06	37,46,55,66	0
23	CLA	b	603	65/65	0.96	0.07	49,56,77,82	0
25	BCR	B	617	40/40	0.96	0.05	42,51,59,61	0
35	DGD	C	517	62/66	0.96	0.06	47,56,94,100	0
23	CLA	B	607	65/65	0.96	0.06	37,45,67,73	0
23	CLA	C	506	65/65	0.96	0.07	52,59,85,91	0
23	CLA	b	607	65/65	0.96	0.06	40,47,70,76	0
25	BCR	C	516	40/40	0.96	0.07	55,65,73,76	0
23	CLA	b	609	65/65	0.96	0.07	55,65,76,82	0
23	CLA	b	611	65/65	0.96	0.06	40,48,66,77	0
23	CLA	b	612	65/65	0.96	0.07	44,53,63,68	0
23	CLA	b	613	65/65	0.96	0.06	41,49,79,86	0
23	CLA	B	609	65/65	0.96	0.07	46,59,67,73	0
23	CLA	b	615	65/65	0.96	0.07	49,60,75,78	0
25	BCR	b	617	40/40	0.96	0.06	46,54,61,64	0
23	CLA	C	508	65/65	0.96	0.07	54,63,76,83	0
23	CLA	B	610	65/65	0.96	0.07	42,53,60,72	0
23	CLA	B	602	65/65	0.96	0.07	49,57,70,80	0
25	BCR	c	516	40/40	0.96	0.06	58,66,76,78	0
37	LHG	d	407	49/49	0.96	0.07	44,54,66,72	0
23	CLA	c	506	65/65	0.96	0.07	52,63,84,87	0
23	CLA	B	612	65/65	0.96	0.06	36,47,56,61	0
30	UNL	x	101	18/-	0.96	0.09	66,77,110,116	0
23	CLA	B	613	65/65	0.96	0.06	37,44,82,88	0
23	CLA	A	405	65/65	0.97	0.05	35,41,52,64	0
23	CLA	b	608	65/65	0.97	0.06	44,56,76,86	0
23	CLA	C	504	65/65	0.97	0.06	51,61,67,75	0
23	CLA	b	610	65/65	0.97	0.07	50,59,66,68	0
24	PHO	A	407	64/64	0.97	0.05	36,44,50,56	0
24	PHO	A	353	64/64	0.97	0.05	38,47,53,57	0
24	PHO	a	408	64/64	0.97	0.05	40,47,51,54	0
23	CLA	D	405	65/65	0.97	0.06	33,42,67,73	0
23	CLA	A	404	65/65	0.97	0.06	36,41,59,64	0
23	CLA	a	405	65/65	0.97	0.06	38,45,61,69	0
23	CLA	a	406	65/65	0.97	0.04	37,43,61,69	0

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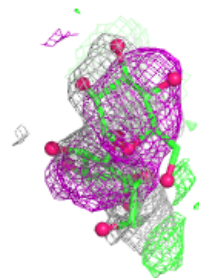
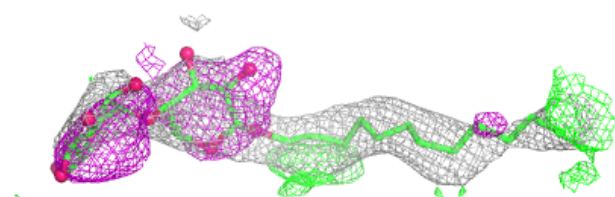
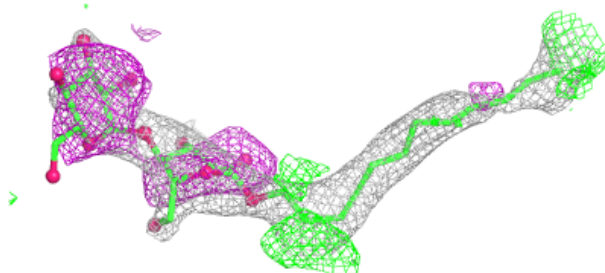
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	B	608	65/65	0.97	0.05	38,48,64,71	0
31	BCT	A	348	4/4	0.97	0.06	53,54,58,67	0
23	CLA	B	604	65/65	0.97	0.06	37,44,95,101	0
23	CLA	B	615	65/65	0.97	0.06	42,52,74,78	0
23	CLA	c	503	65/65	0.97	0.06	46,58,84,98	0
23	CLA	c	504	65/65	0.97	0.06	51,69,78,83	0
37	LHG	D	410	49/49	0.97	0.06	45,52,63,70	0
23	CLA	B	605	65/65	0.97	0.06	40,48,63,69	0
23	CLA	C	510	65/65	0.97	0.07	50,58,76,79	0
37	LHG	L	101	49/49	0.97	0.06	46,52,67,81	0
23	CLA	C	511	65/65	0.97	0.06	49,57,71,75	0
23	CLA	b	605	65/65	0.97	0.07	41,50,68,74	0
23	CLA	C	512	65/65	0.97	0.07	54,63,76,79	0
23	CLA	c	510	65/65	0.97	0.07	50,61,80,82	0
23	CLA	c	511	65/65	0.97	0.06	53,61,72,82	0
38	HEM	e	87	43/43	0.97	0.09	72,84,98,110	0
23	CLA	C	503	65/65	0.98	0.06	48,53,77,83	0
36	CA	C	524	1/1	0.98	0.04	77,77,77,77	0
38	HEM	E	103	43/43	0.98	0.06	57,69,77,88	0
23	CLA	d	402	65/65	0.98	0.05	39,46,72,86	0
40	HEC	V	202	43/43	0.98	0.06	42,50,54,56	0
40	HEC	v	202	43/43	0.98	0.07	54,61,68,70	0
22	CL	a	403	1/1	0.99	0.07	54,54,54,54	0
36	CA	c	524	1/1	0.99	0.05	76,76,76,76	0
22	CL	A	402	1/1	0.99	0.06	40,40,40,40	0
28	OEX	A	413	10/10	0.99	0.03	38,44,47,47	0
39	MG	J	102	1/1	0.99	0.03	57,57,57,57	0
39	MG	j	102	1/1	0.99	0.05	61,61,61,61	0
22	CL	A	403	1/1	0.99	0.03	44,44,44,44	0
22	CL	a	402	1/1	0.99	0.07	47,47,47,47	0
28	OEX	a	415	10/10	1.00	0.02	45,48,51,54	0
21	FE2	A	401	1/1	1.00	0.01	49,49,49,49	0
21	FE2	a	401	1/1	1.00	0.01	52,52,52,52	0

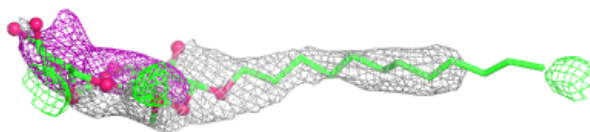
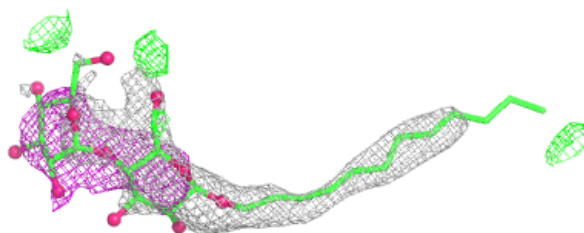
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT a 414:

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

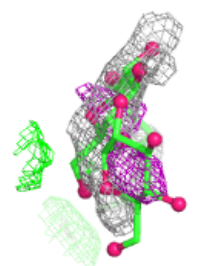
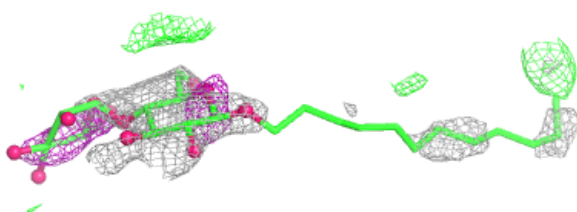
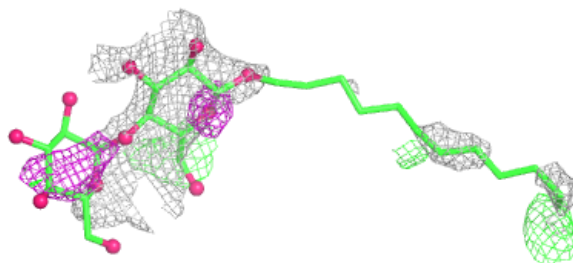
**Electron density around LMT E 102:**

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

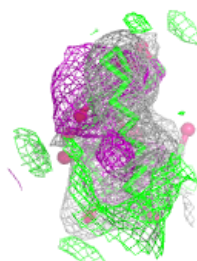
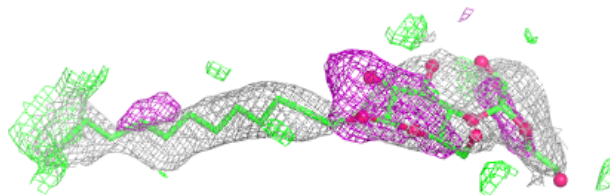
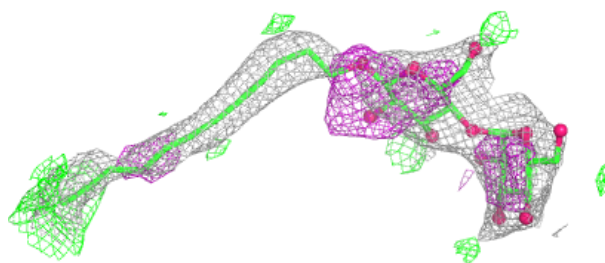


Electron density around LMT e 102:

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

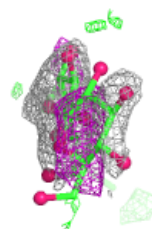
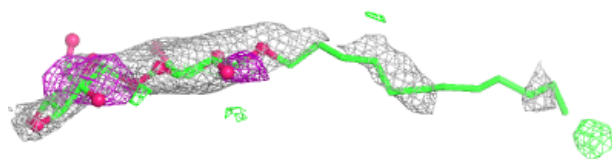
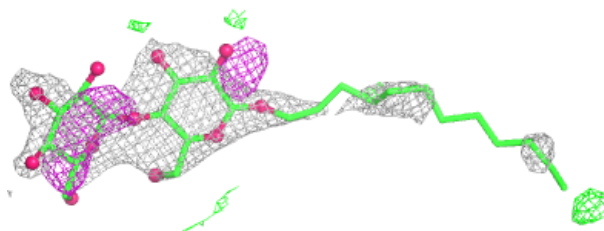
**Electron density around LMT A 359:**

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

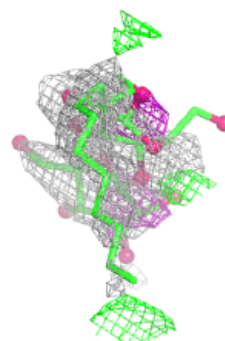
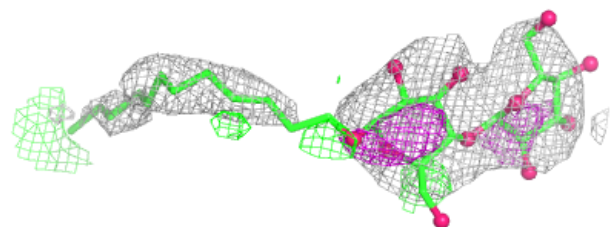
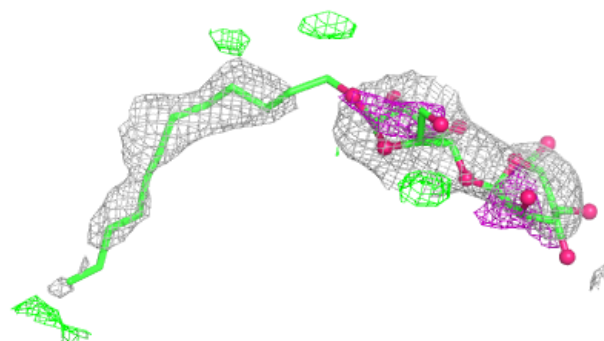


Electron density around LMT a 420:

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

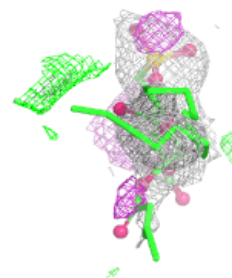
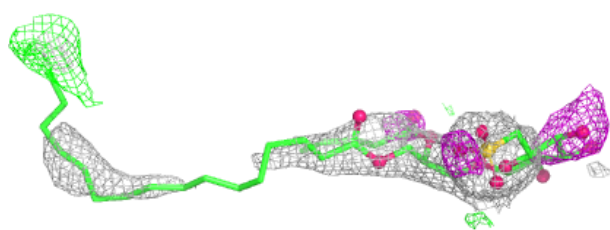
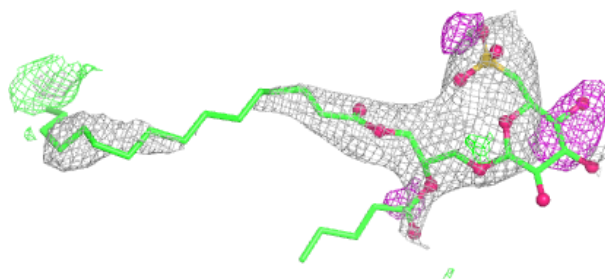
**Electron density around LMT I 101:**

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

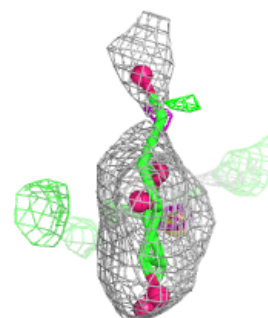
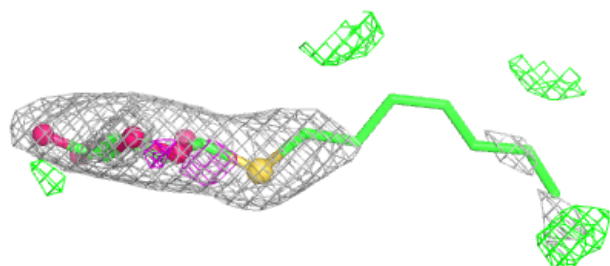
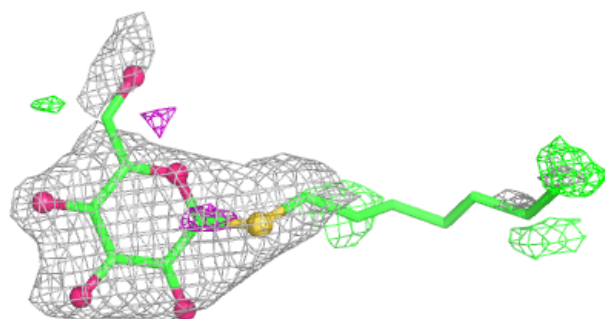


Electron density around SQD f 102:

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

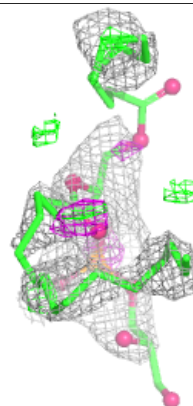
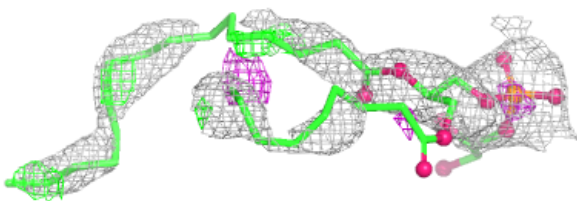
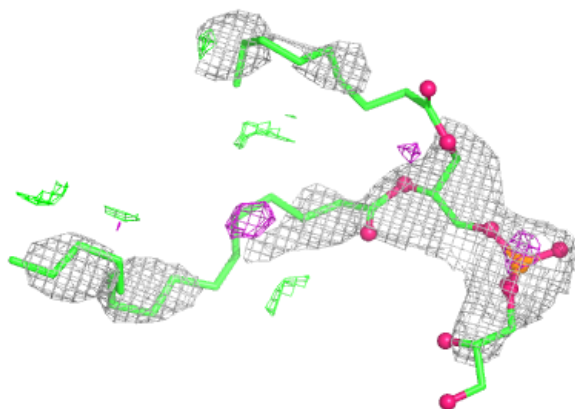
**Electron density around HTG C 522:**

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

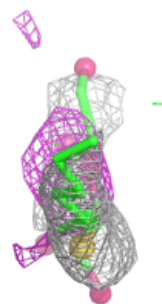
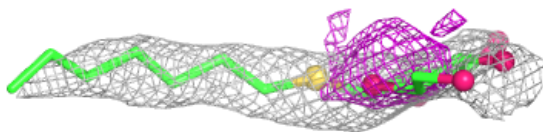
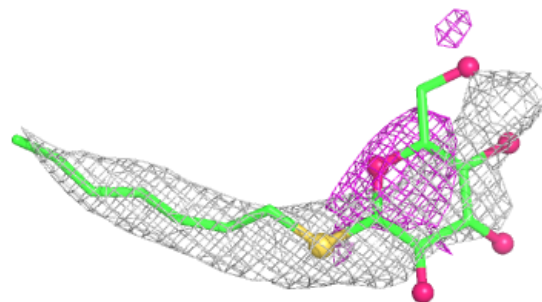


Electron density around LHG e 101:

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

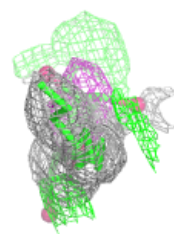
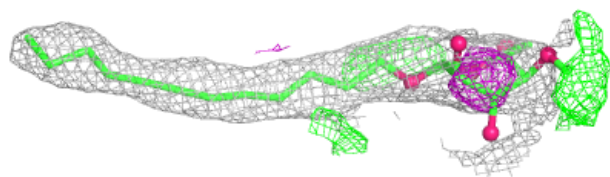
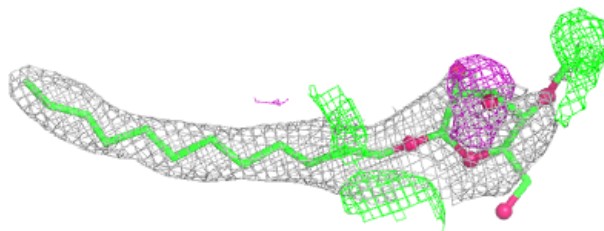
**Electron density around HTG b 623:**

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

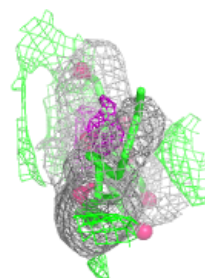
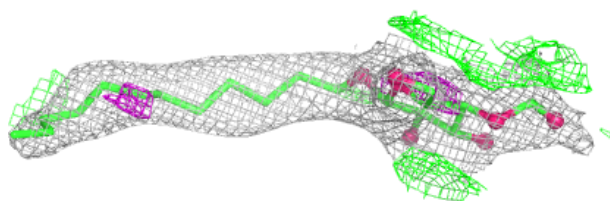
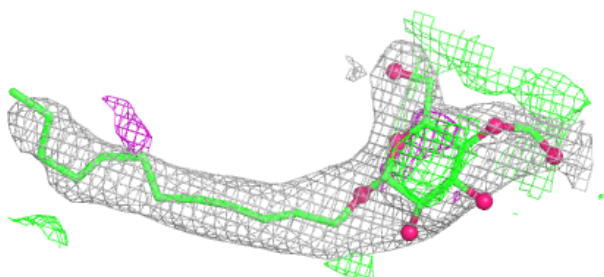


Electron density around LMT b 621:

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

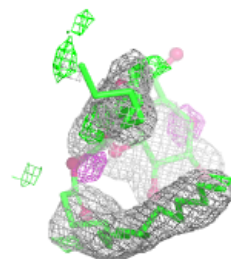
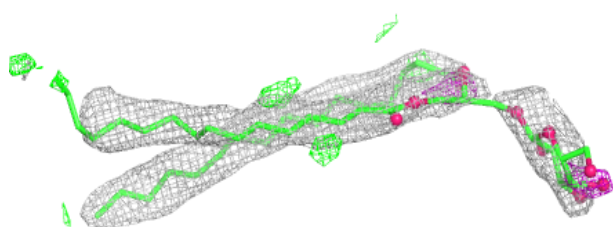
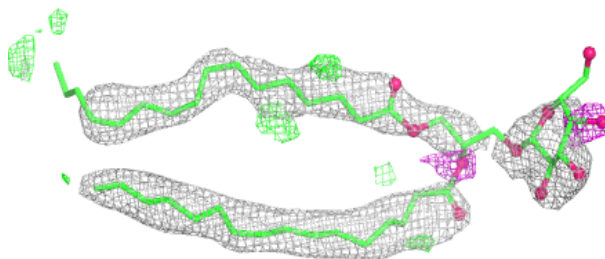
**Electron density around LMT t 102:**

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

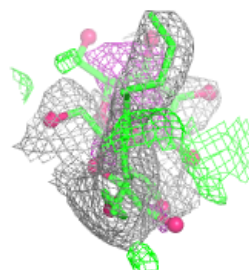
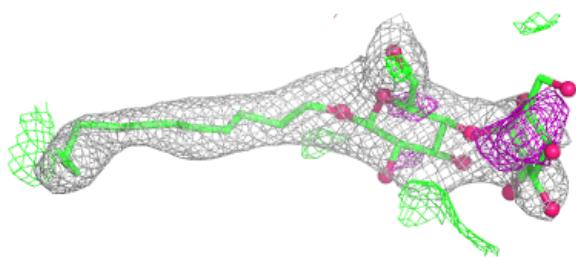
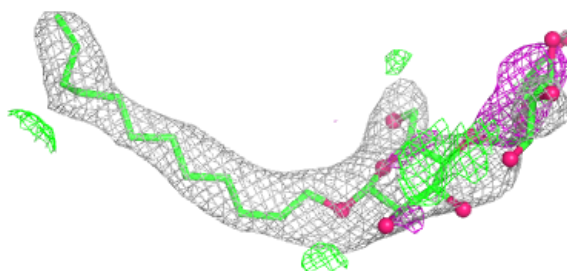


Electron density around LMG C 521:

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

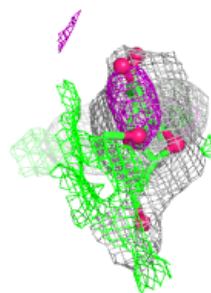
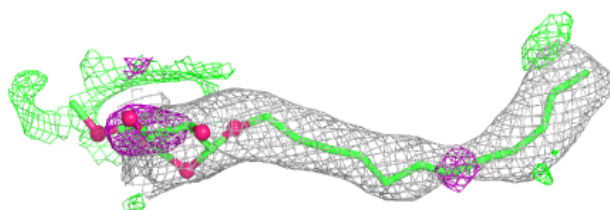
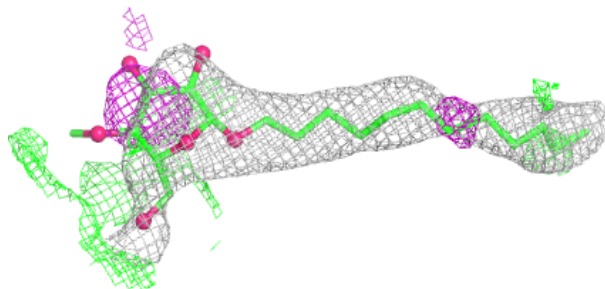
**Electron density around LMT M 103:**

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

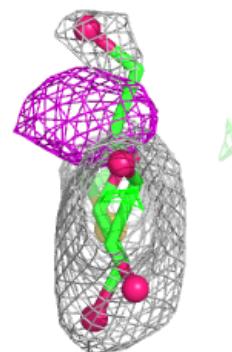
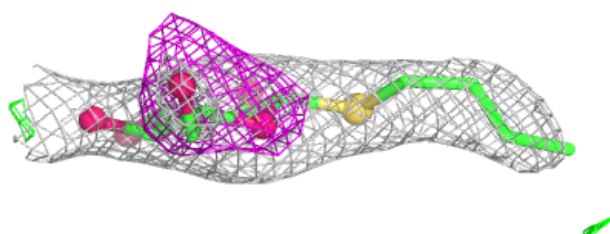
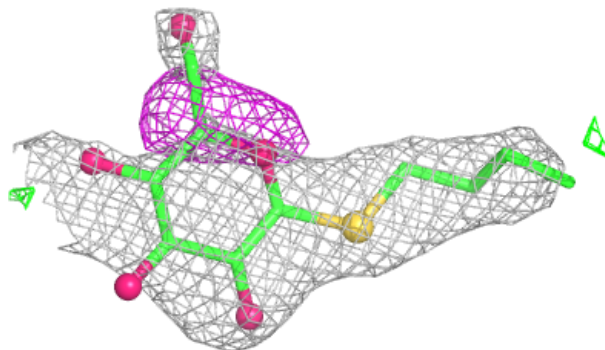


Electron density around LMT t 101:

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

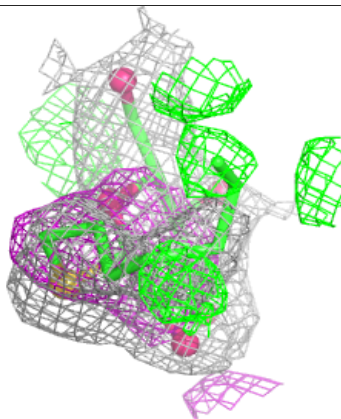
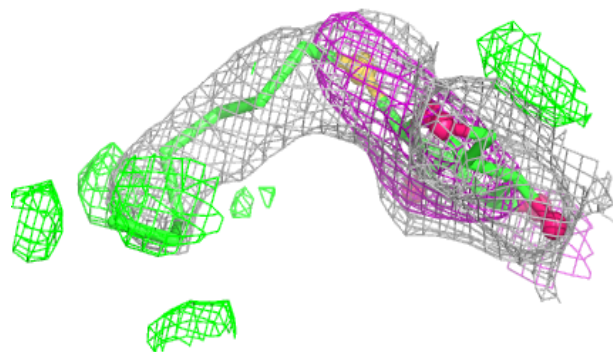
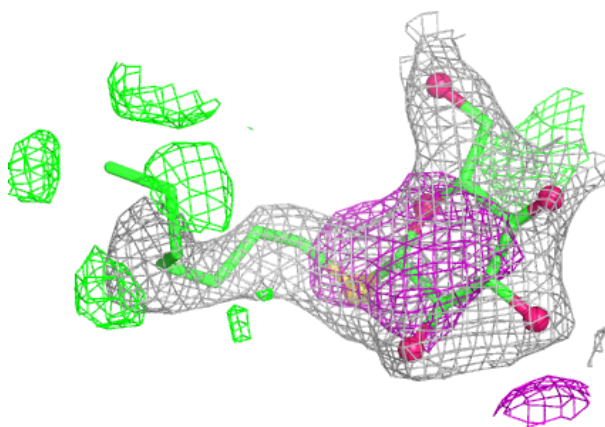
**Electron density around HTG D 414:**

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

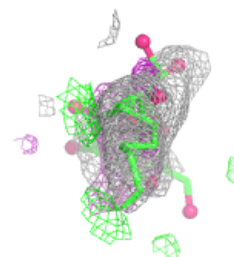
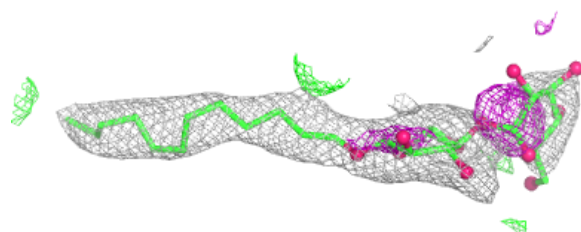
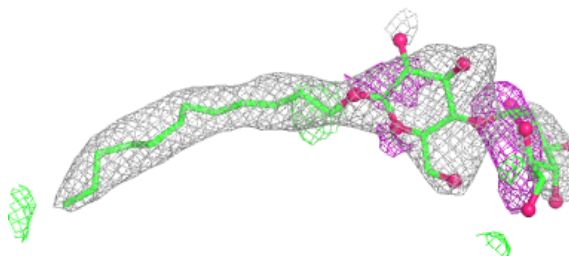


Electron density around HTG B 623:

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

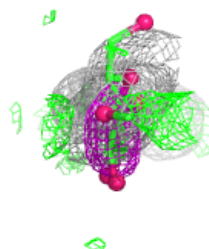
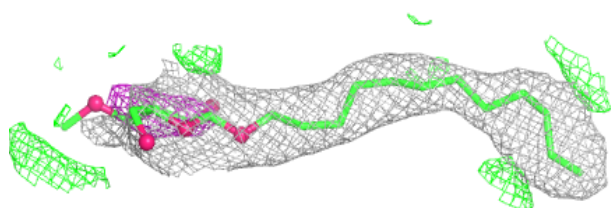
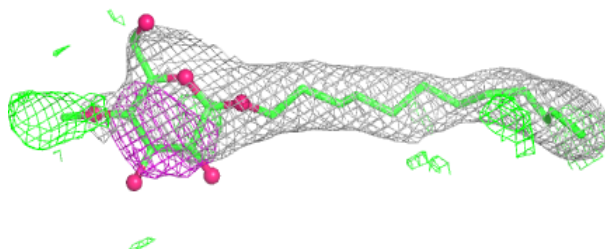
**Electron density around LMT D 404:**

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

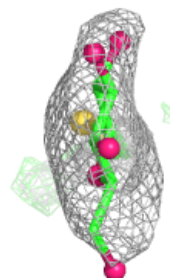
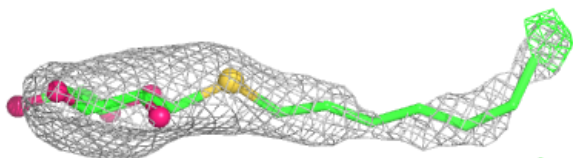
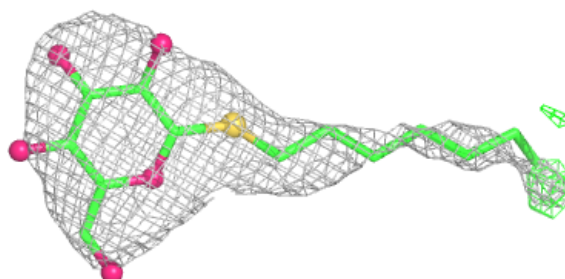


Electron density around LMT b 627:

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

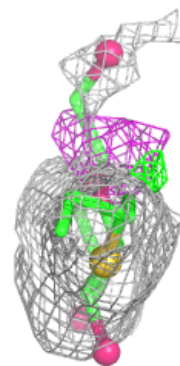
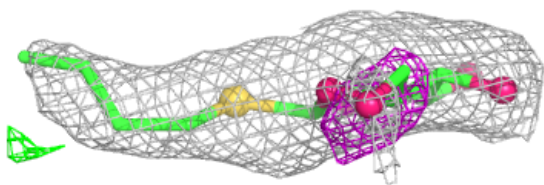
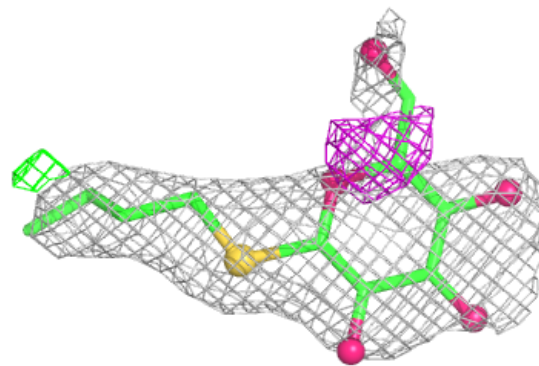
**Electron density around HTG c 522:**

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



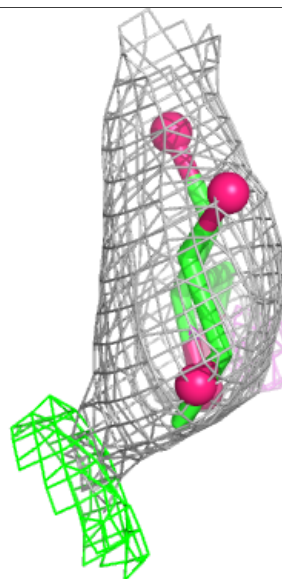
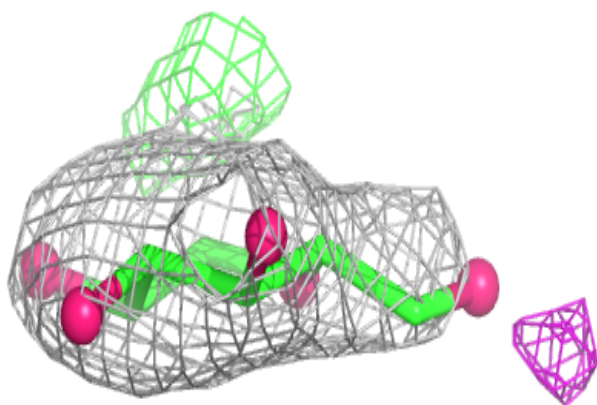
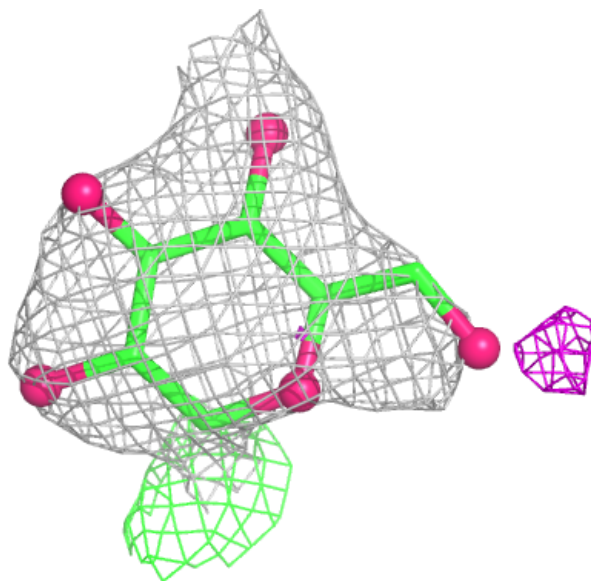
Electron density around HTG d 411:

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



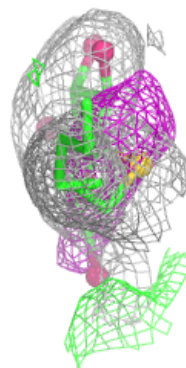
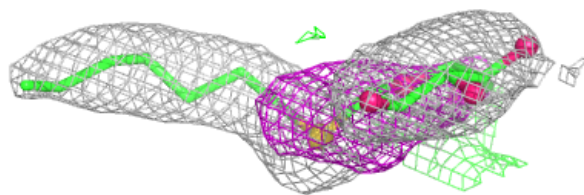
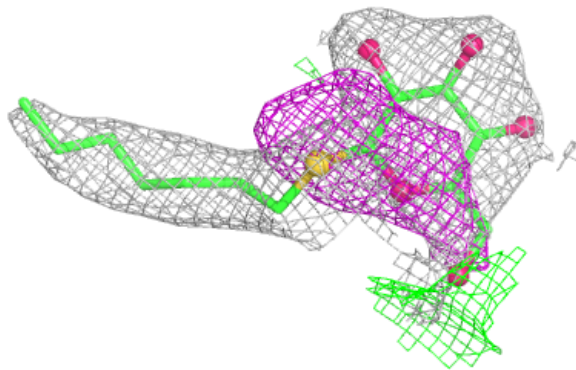
Electron density around HTG V 203:

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

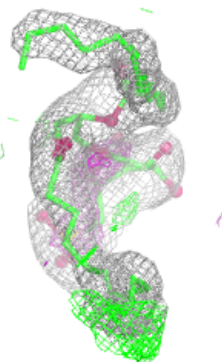
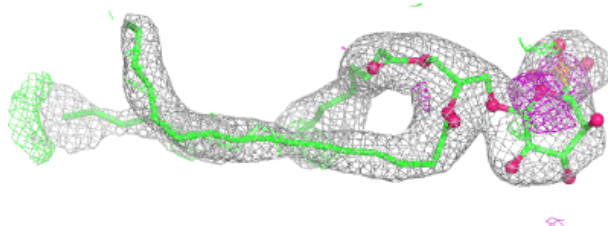
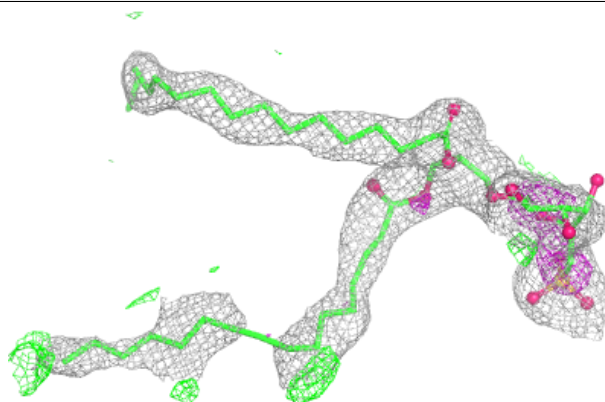


Electron density around HTG b 622:

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

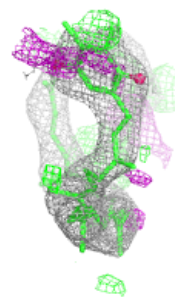
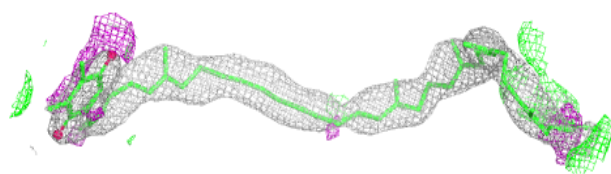
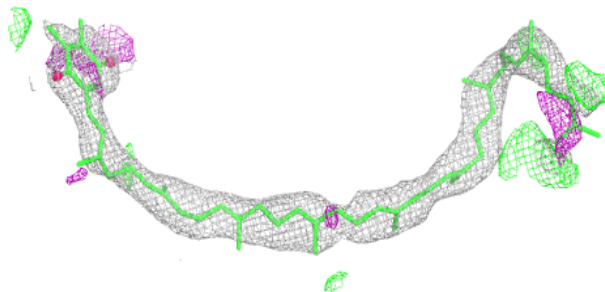
**Electron density around SQD a 413:**

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

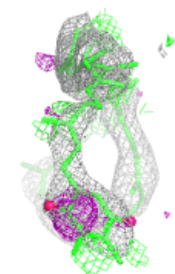
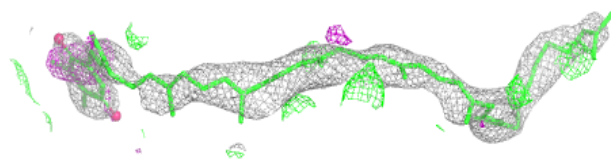
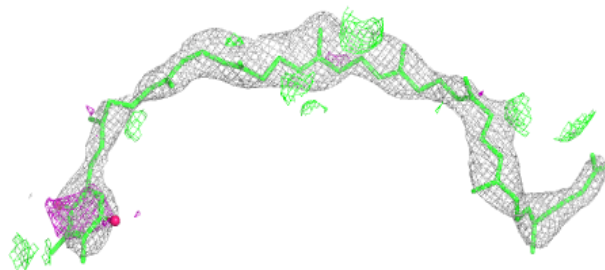


Electron density around PL9 A 414:

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

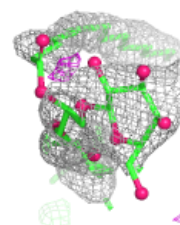
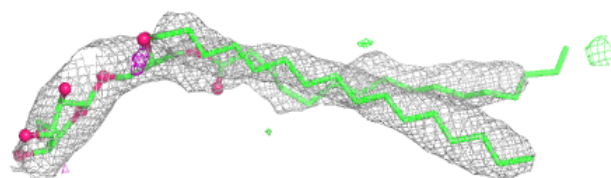
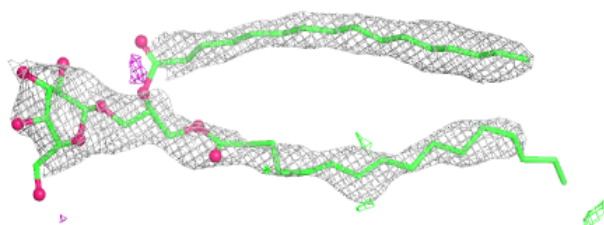
**Electron density around PL9 a 416:**

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

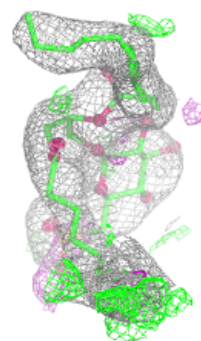
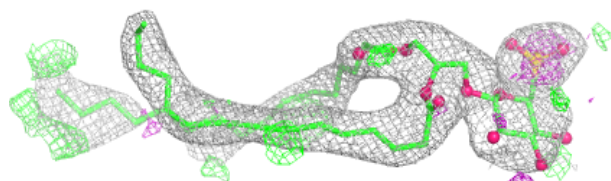
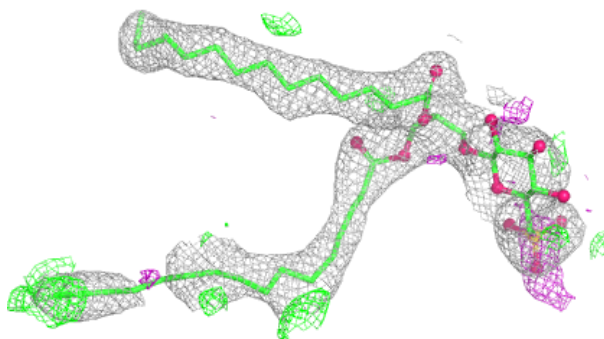


Electron density around LMG c 521:

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

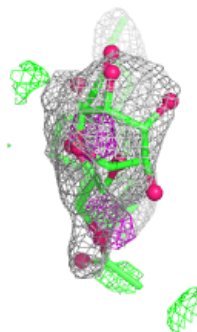
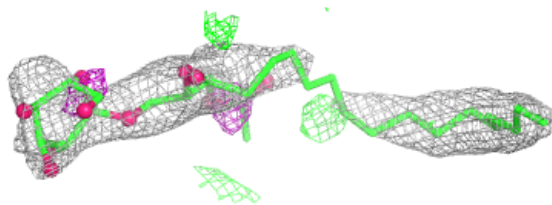
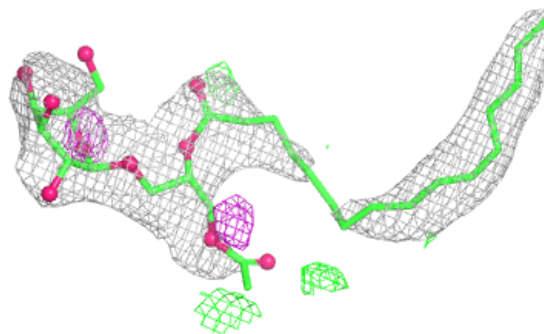
**Electron density around SQD A 412:**

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

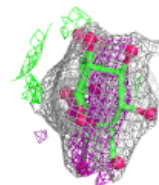
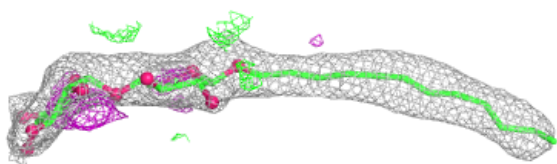
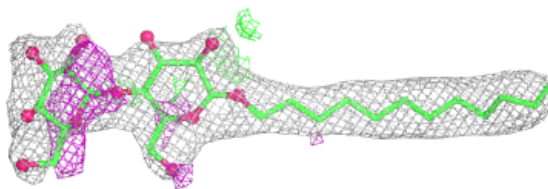


Electron density around LMG Z 101:

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

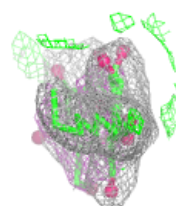
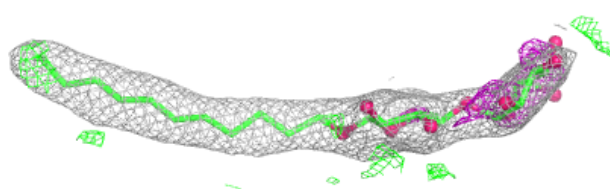
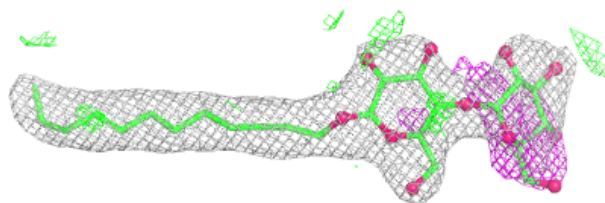
**Electron density around LMT m 103:**

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

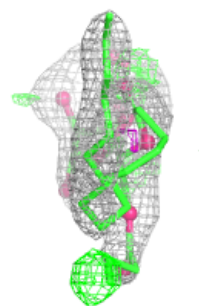
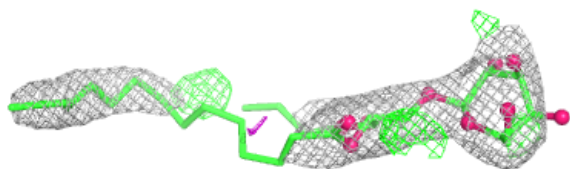
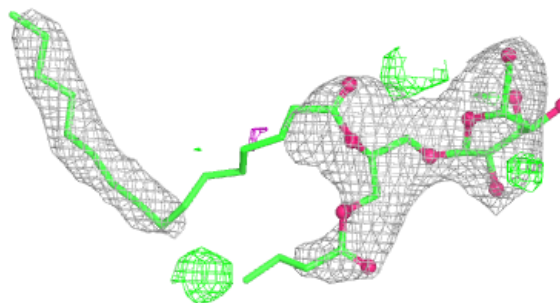


Electron density around LMT M 101:

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

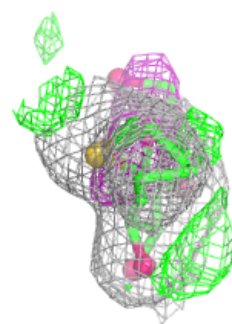
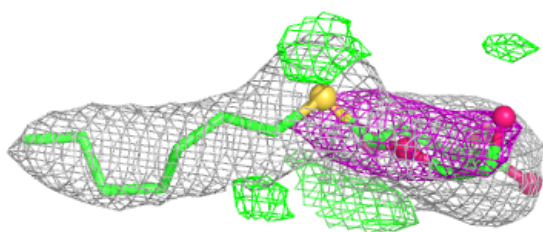
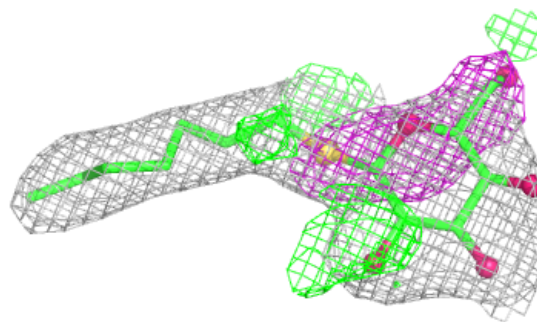
**Electron density around LMG z 101:**

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

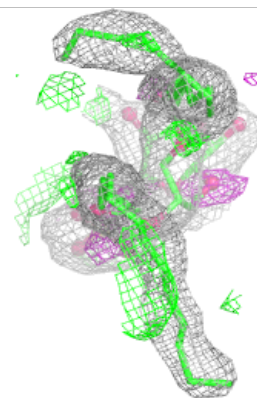
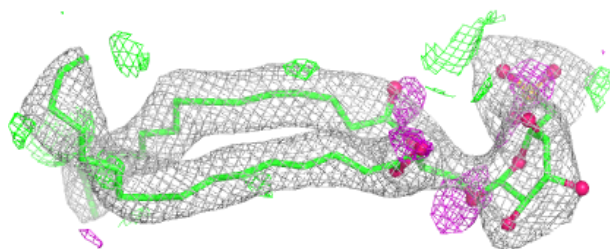
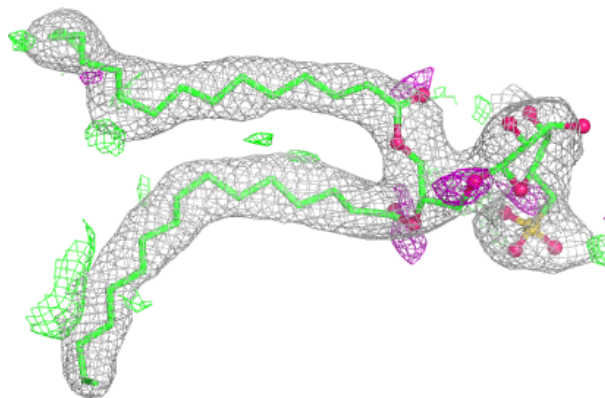


Electron density around HTG B 622:

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

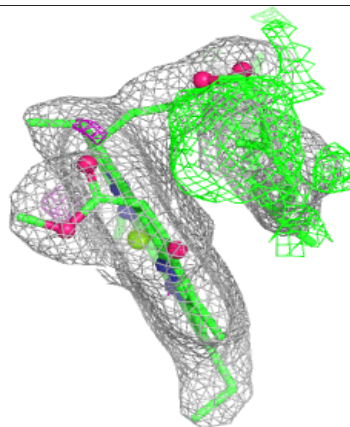
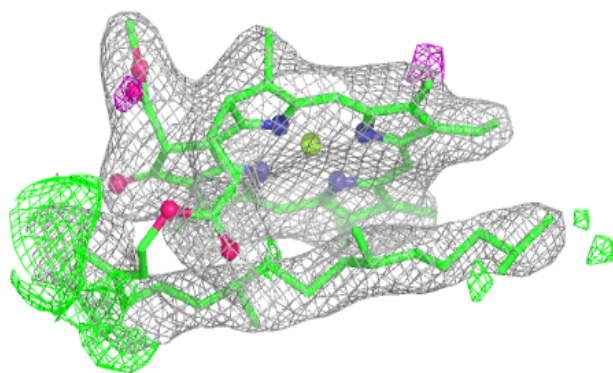
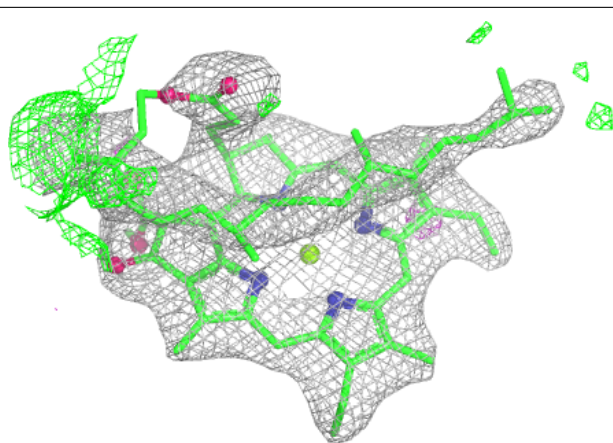
**Electron density around SQD B 620:**

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

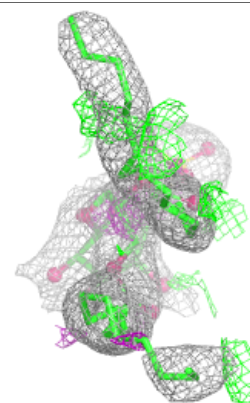
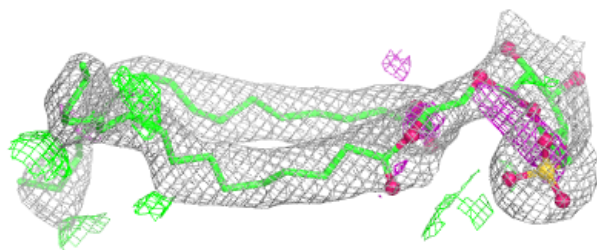
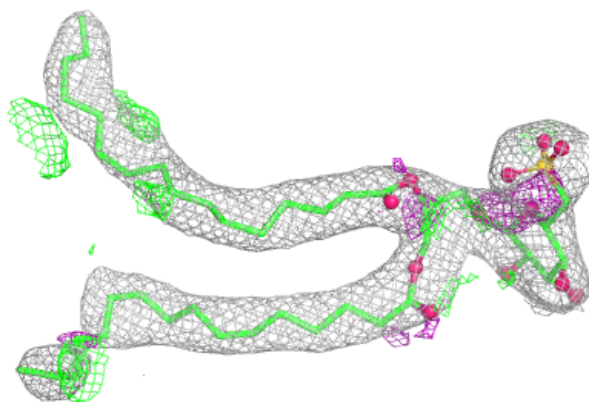


Electron density around CLA b 601:

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

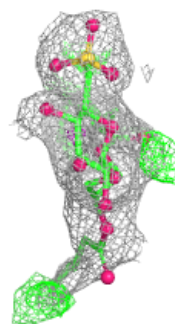
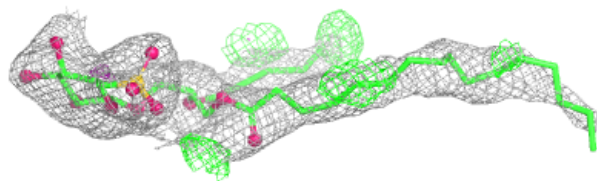
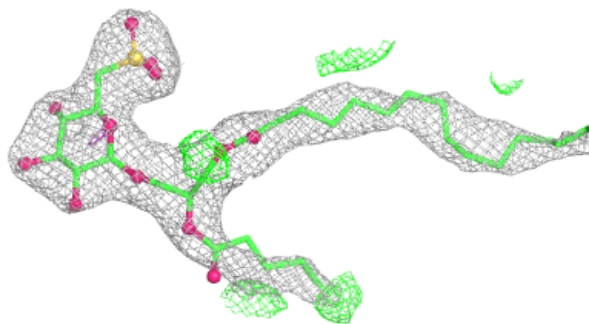
**Electron density around SQD b 620:**

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

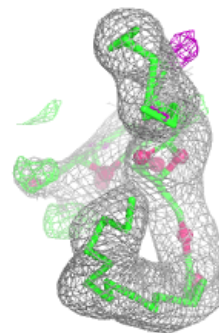
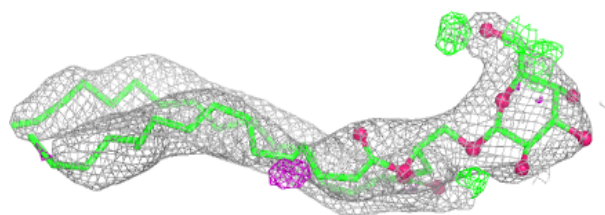
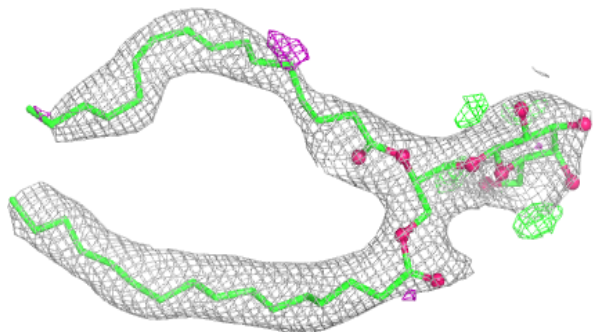


Electron density around SQD F 101:

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

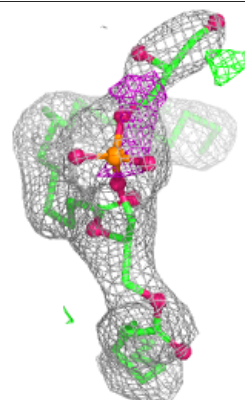
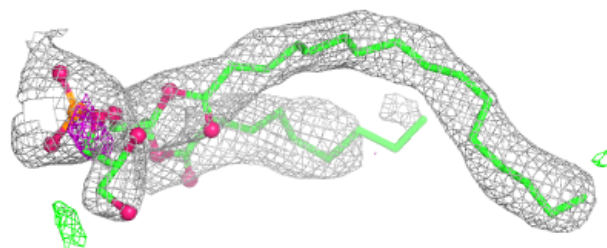
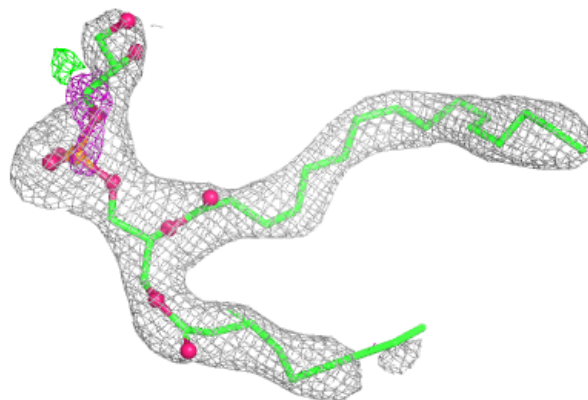
**Electron density around LMG C 501:**

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

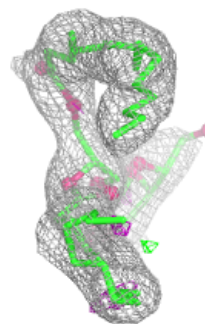
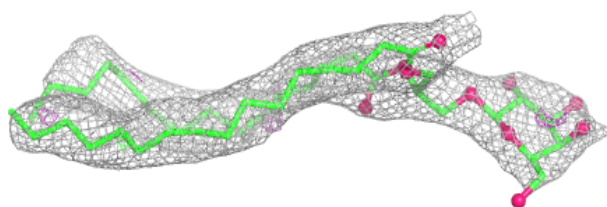
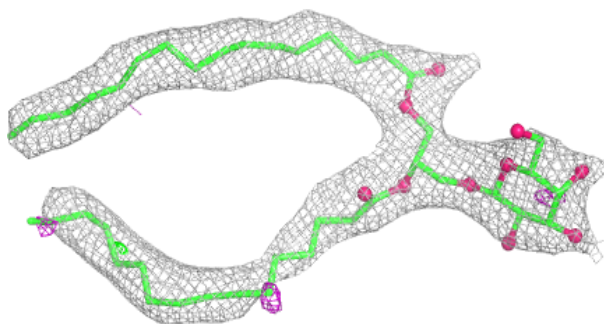


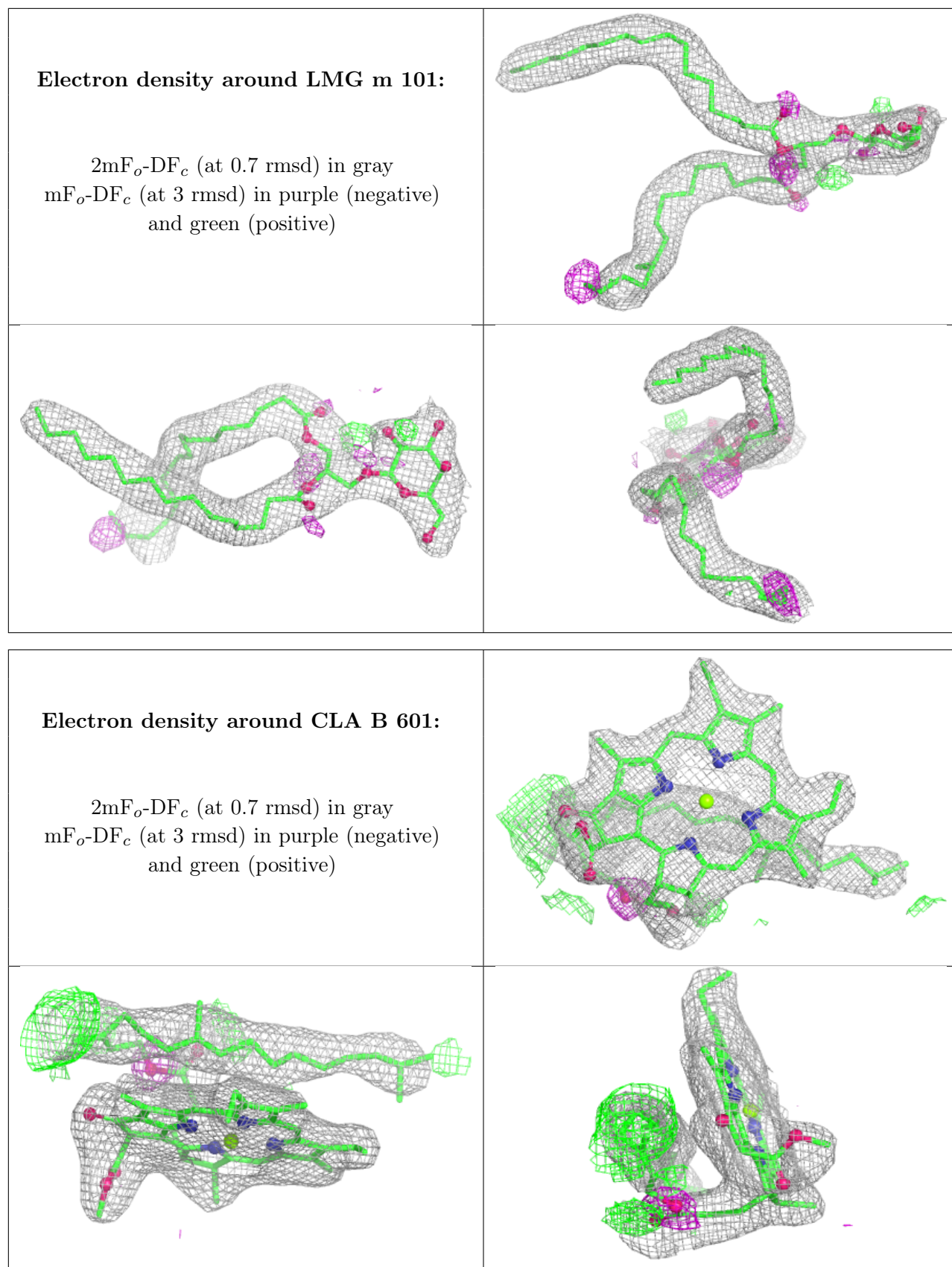
Electron density around LHG E 101:

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

**Electron density around LMG a 419:**

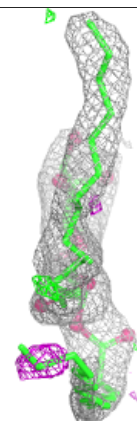
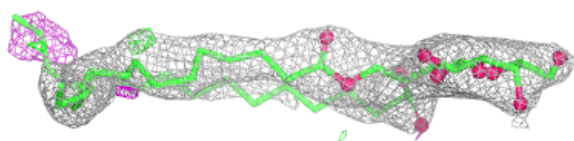
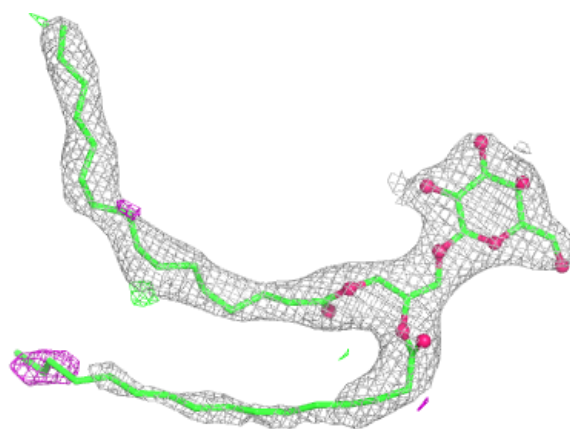
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



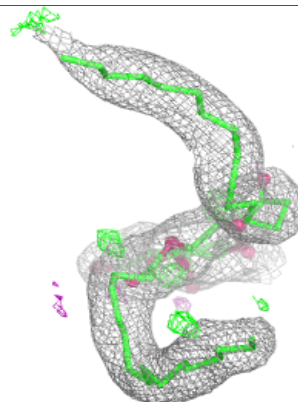
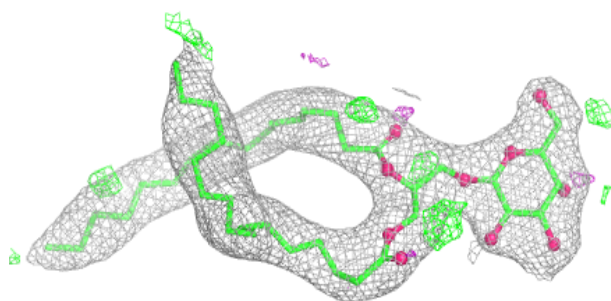
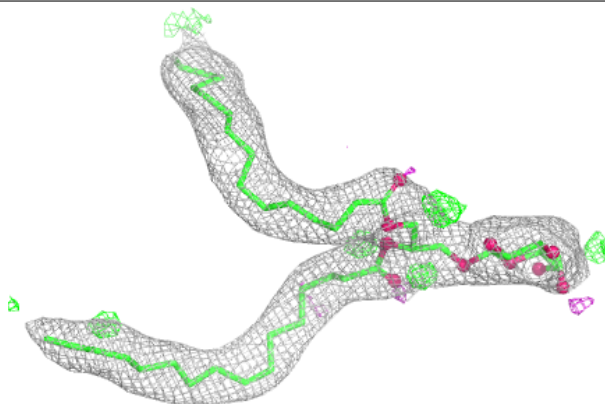


Electron density around LMG c 520:

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

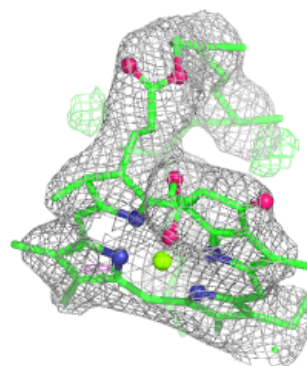
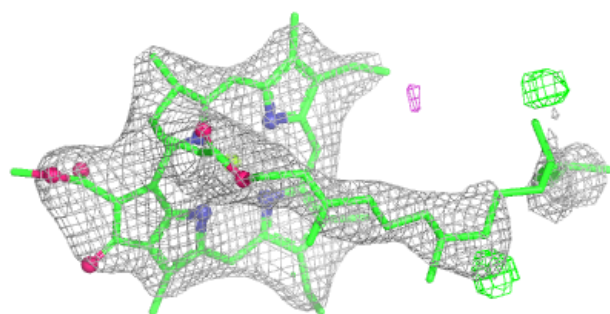
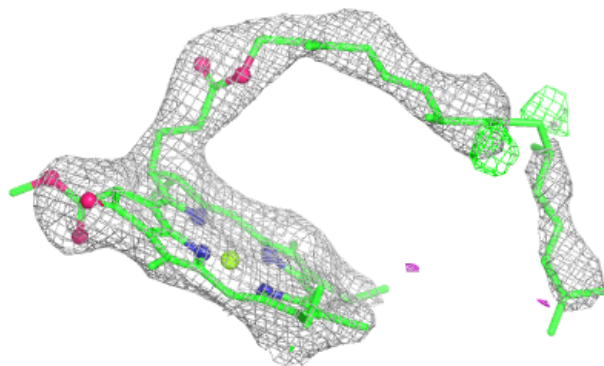
**Electron density around LMG B 621:**

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

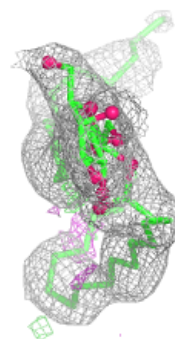
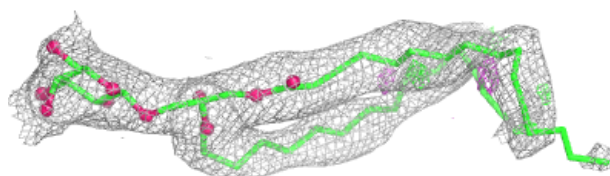
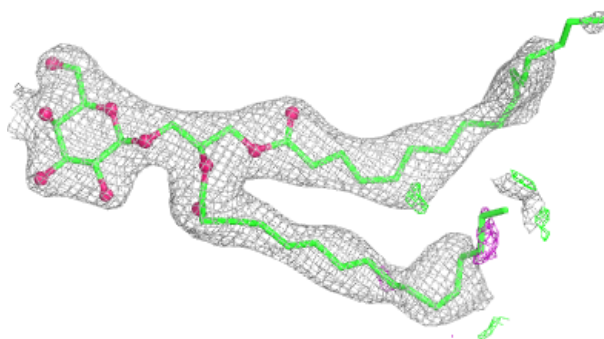


Electron density around CLA c 514:

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

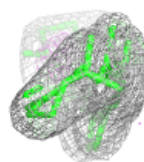
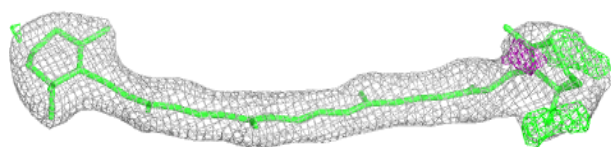
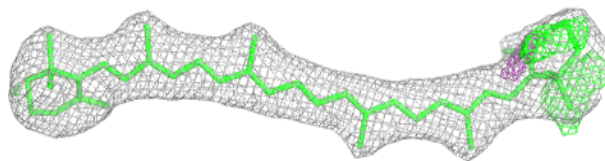
**Electron density around LMG d 412:**

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

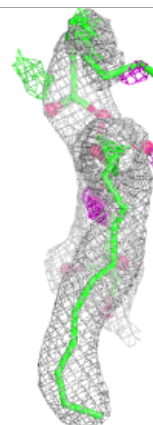
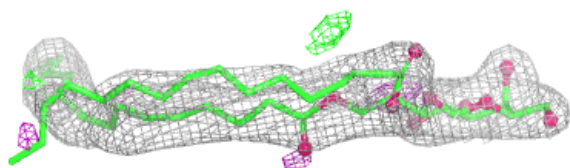
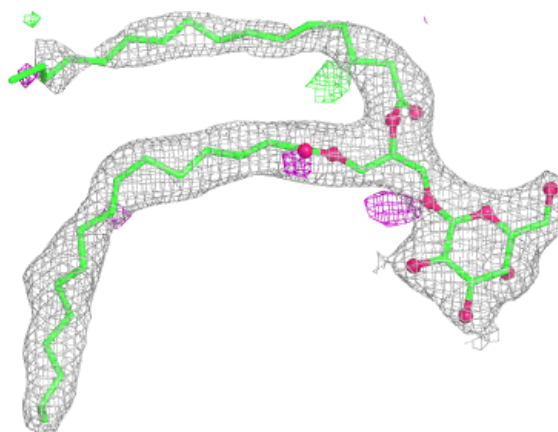


Electron density around BCR d 404:

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

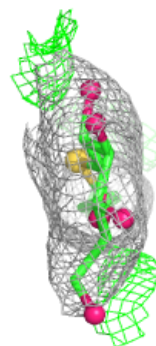
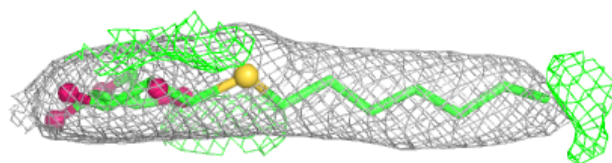
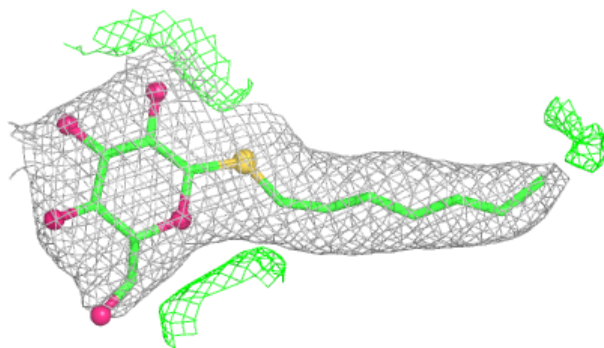
**Electron density around LMG C 520:**

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

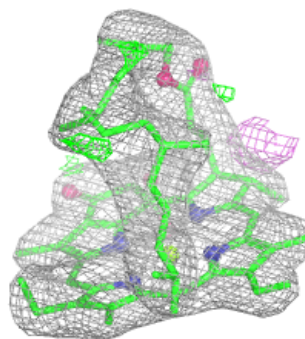
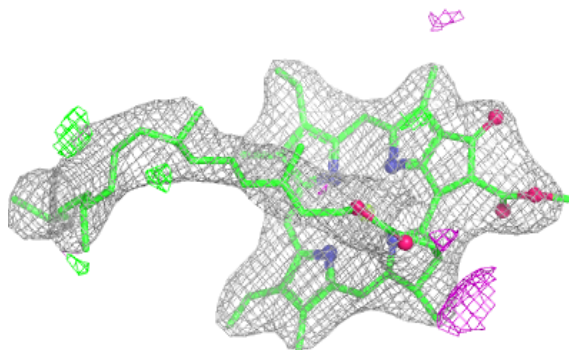
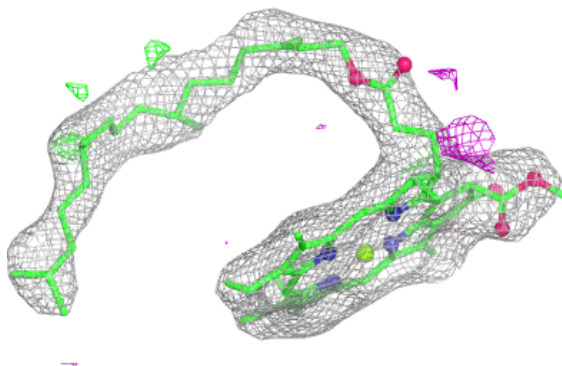


Electron density around HTG b 625:

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

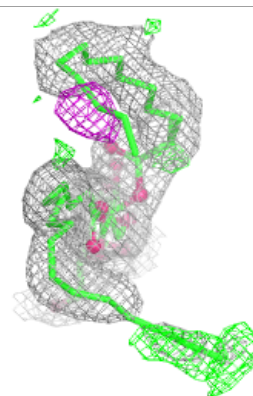
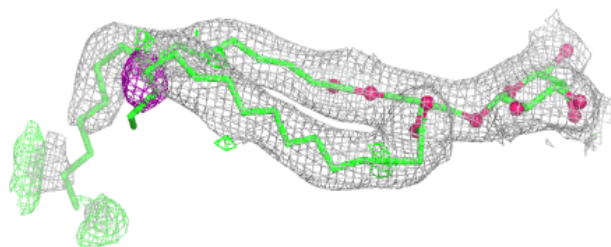
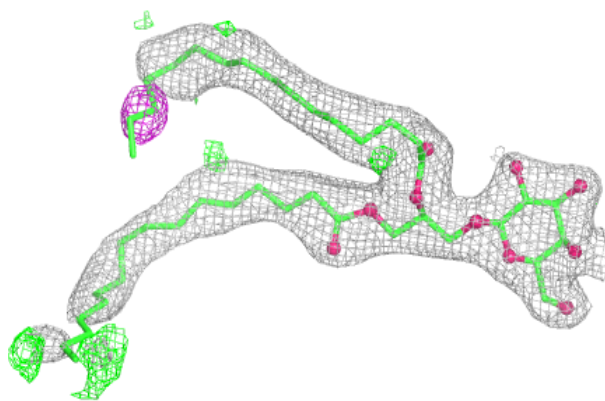
**Electron density around CLA C 514:**

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

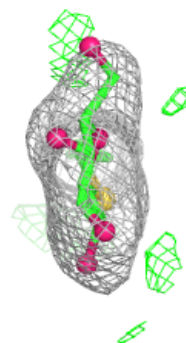
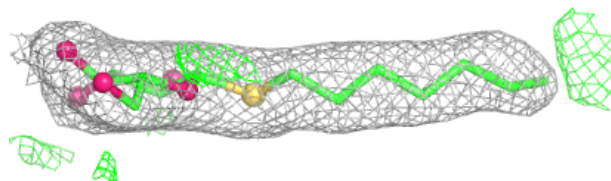
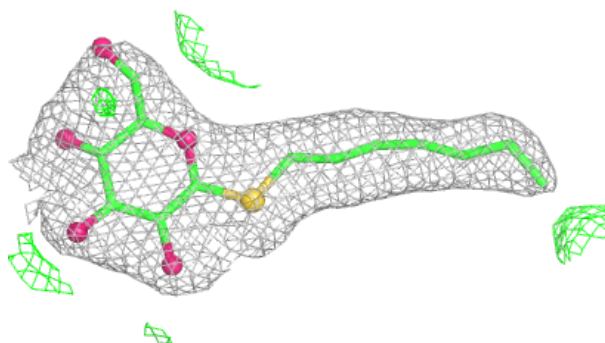


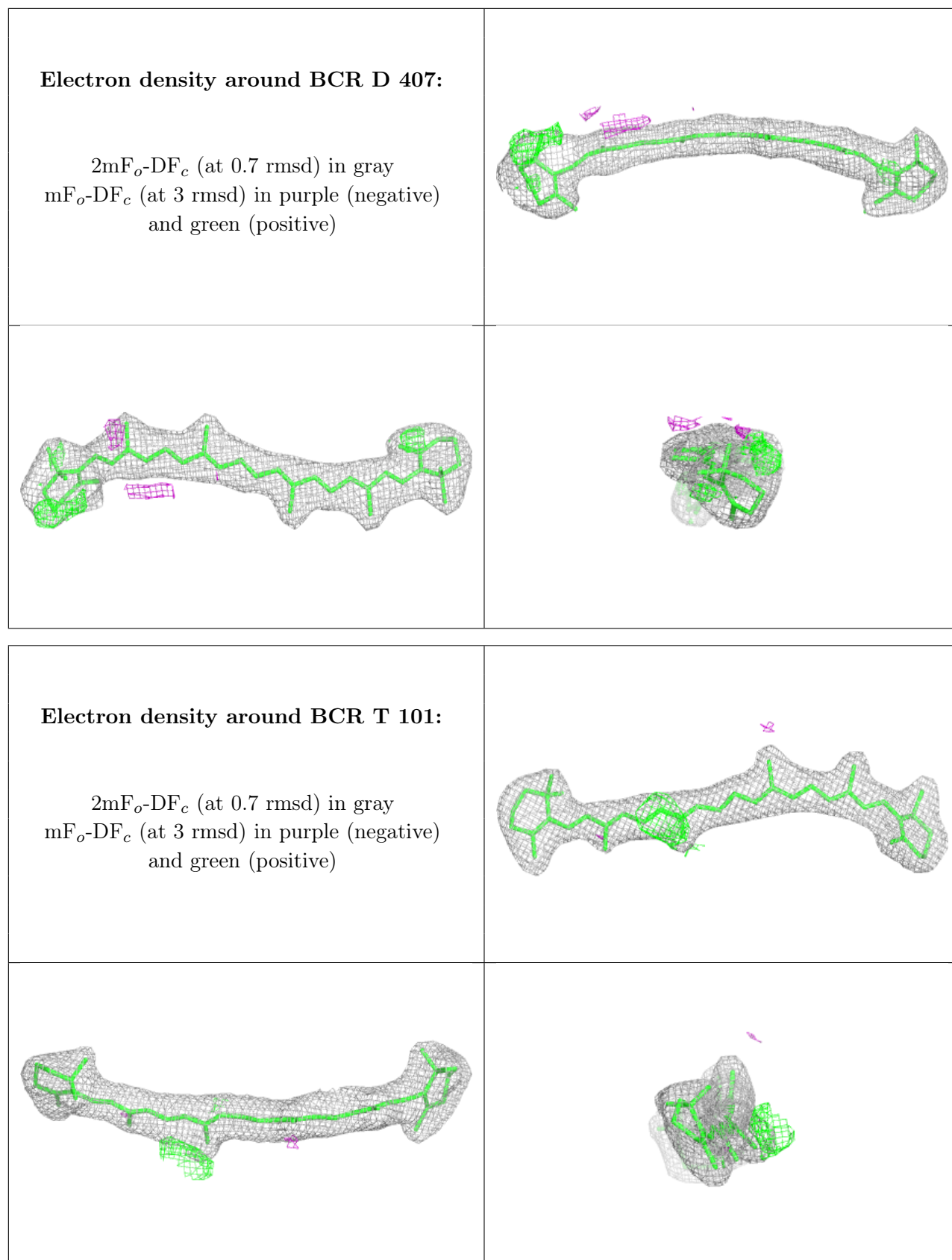
Electron density around LMG D 415:

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

**Electron density around HTG B 626:**

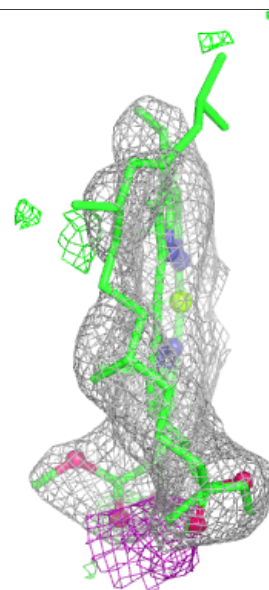
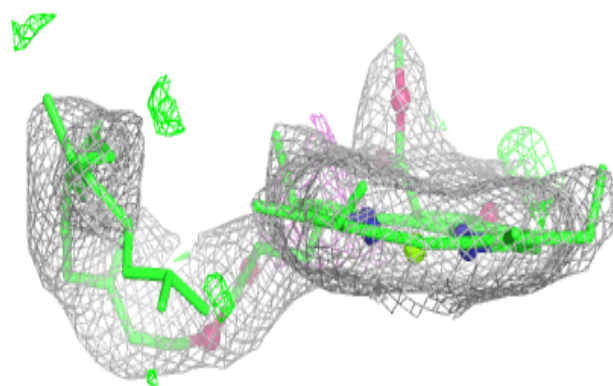
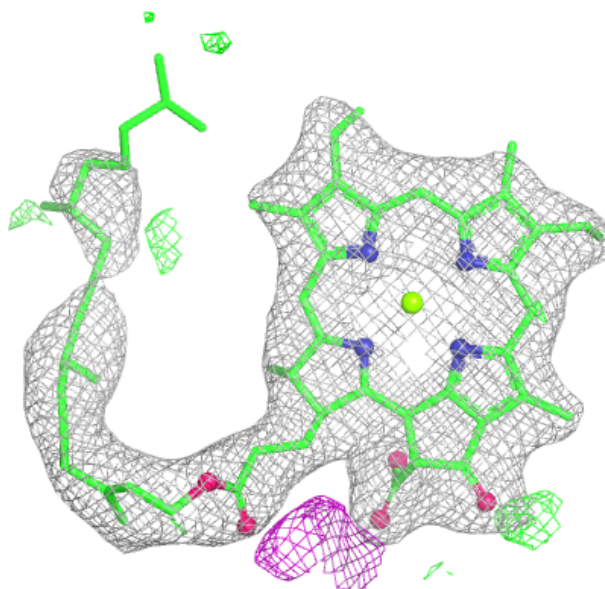
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





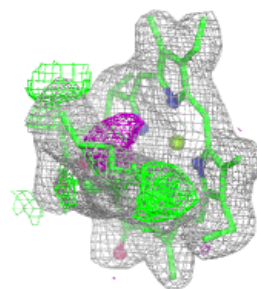
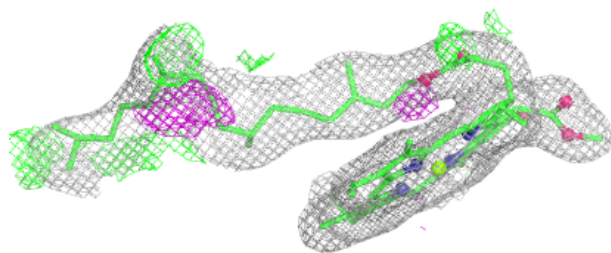
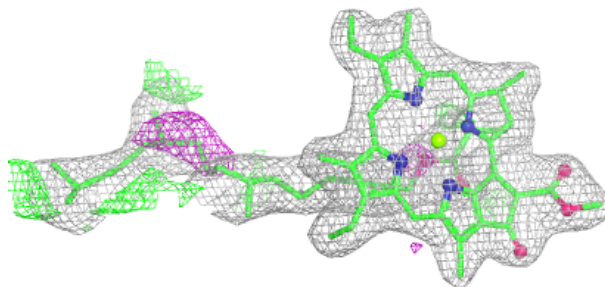
Electron density around CLA c 513:

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

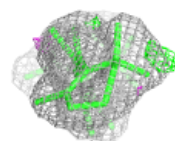
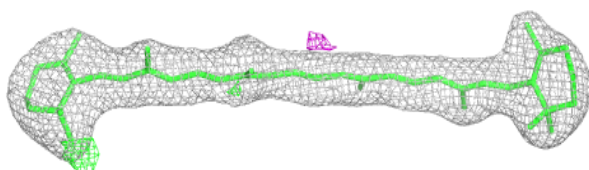
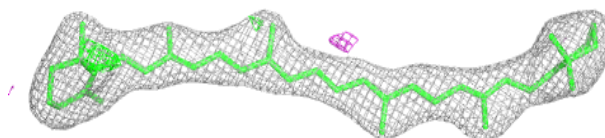


Electron density around CLA B 614:

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

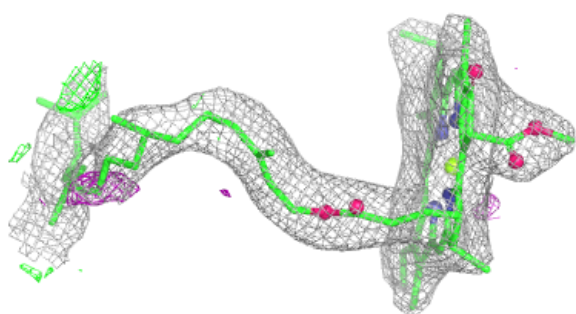
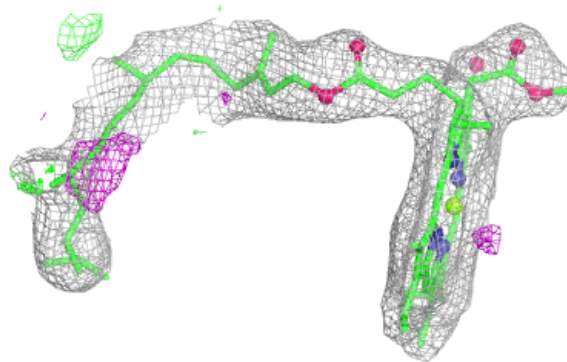
**Electron density around BCR C 515:**

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



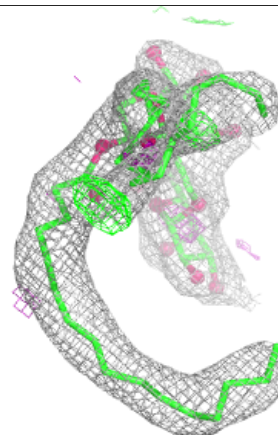
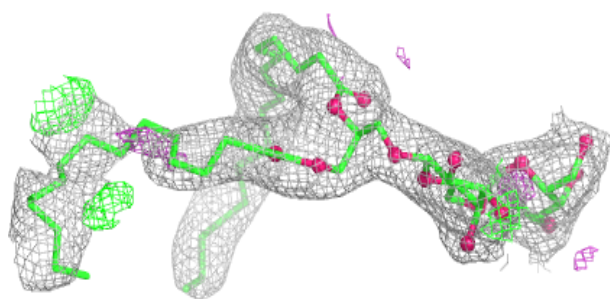
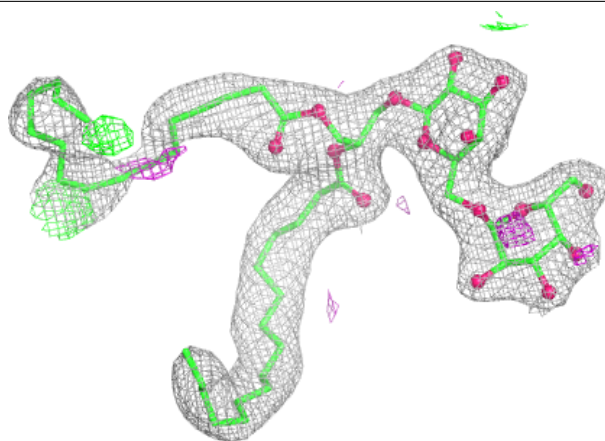
Electron density around CLA C 507:

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



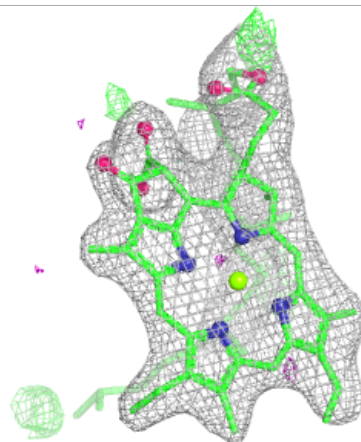
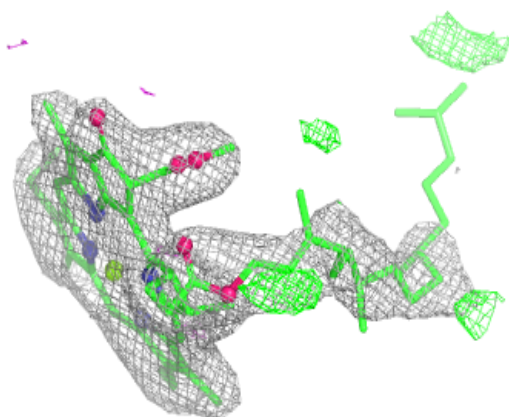
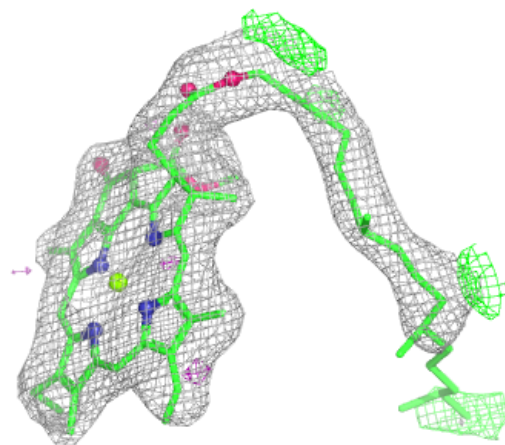
Electron density around DGD C 518:

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



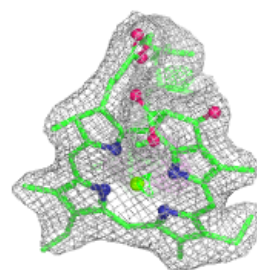
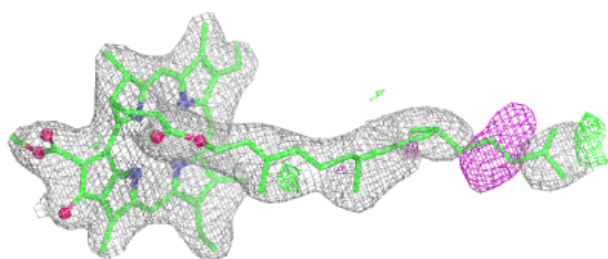
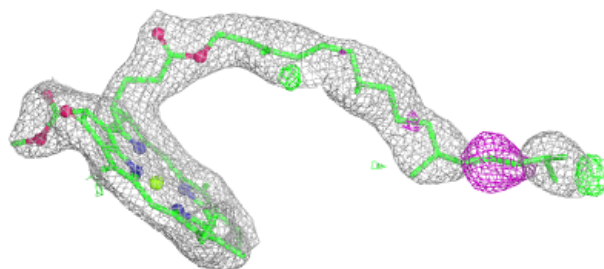
Electron density around CLA b 616:

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

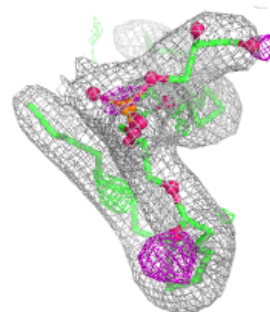
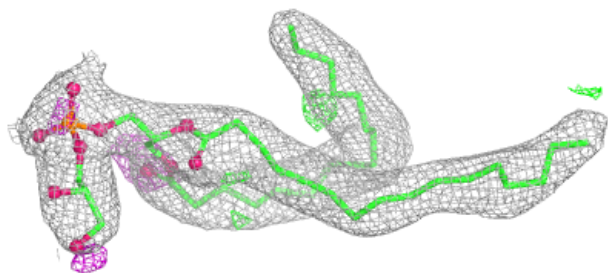
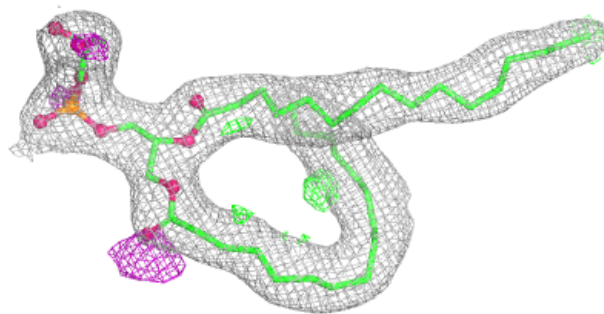


Electron density around CLA c 505:

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

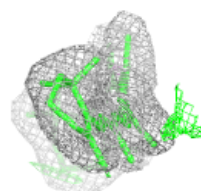
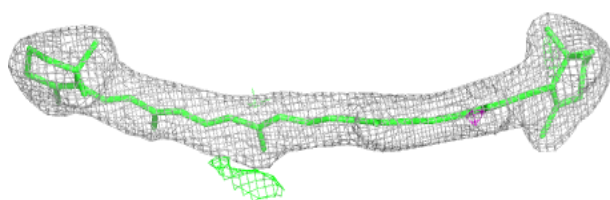
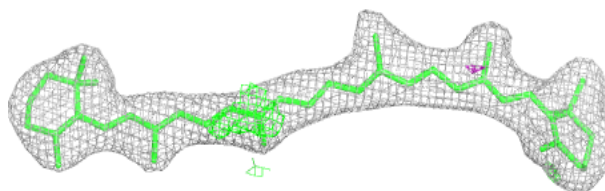
**Electron density around LHG D 409:**

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

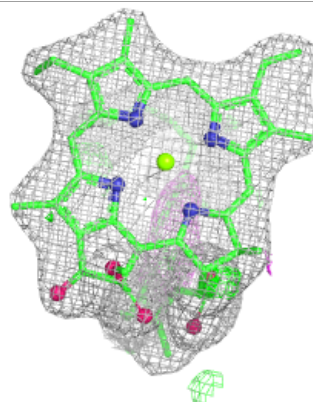
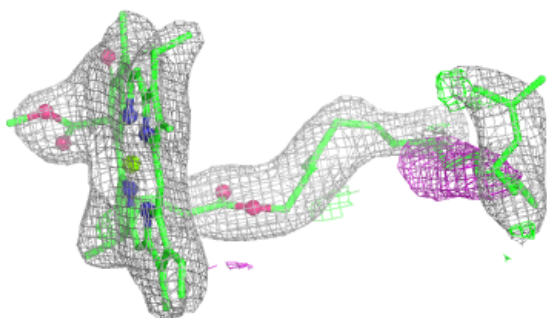
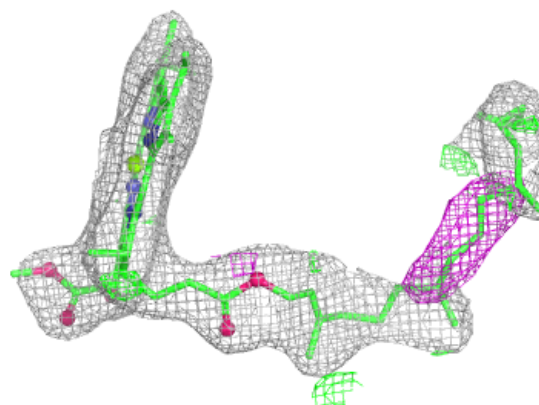


Electron density around BCR t 103:

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

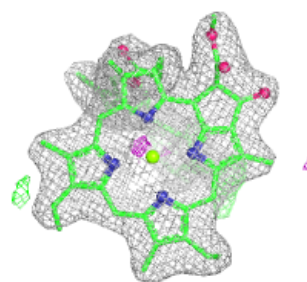
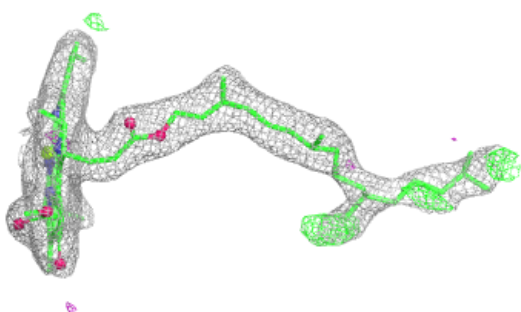
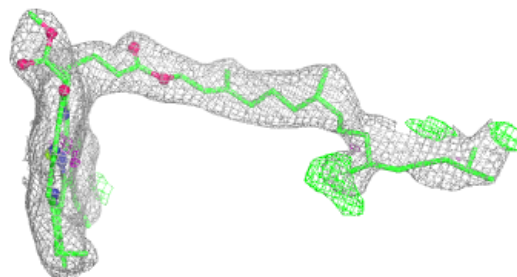
**Electron density around CLA c 507:**

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

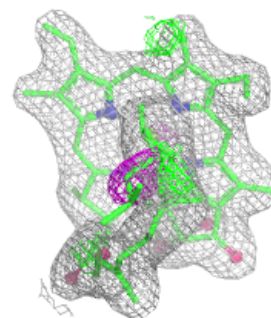
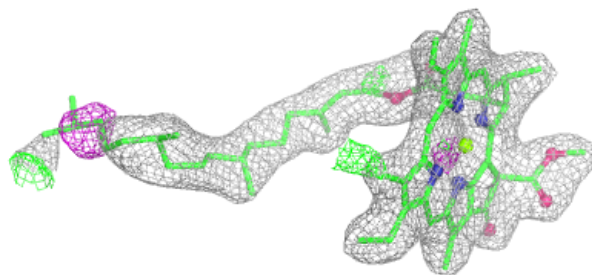
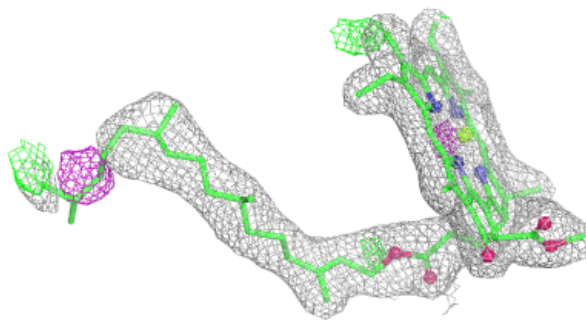


Electron density around CLA B 606:

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

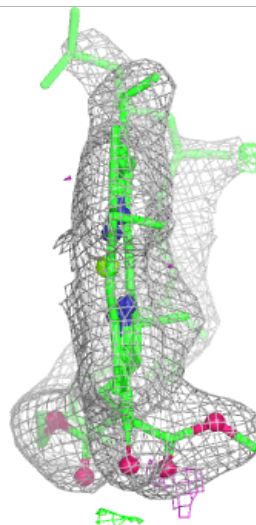
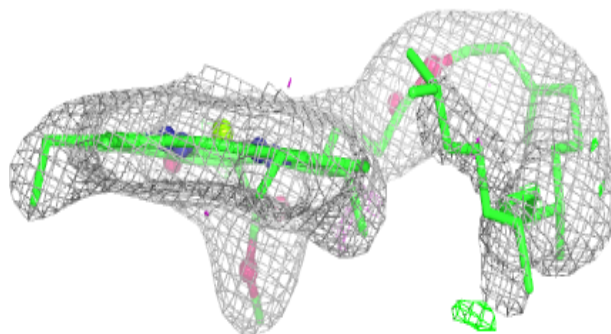
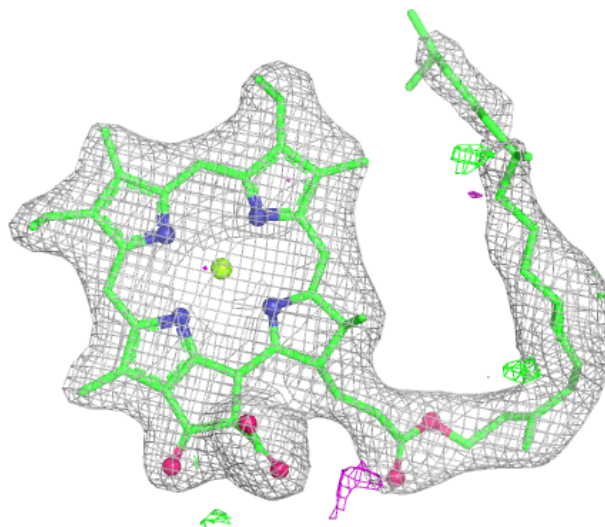
**Electron density around CLA C 509:**

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



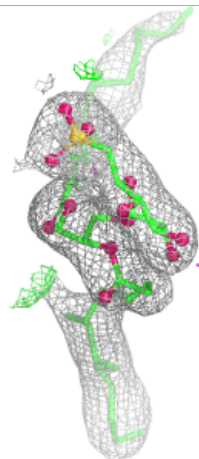
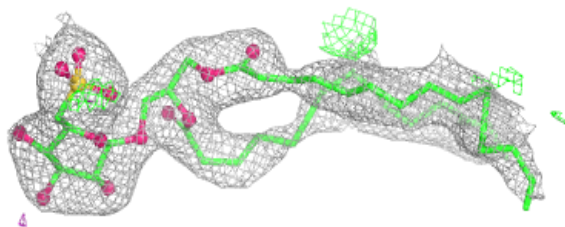
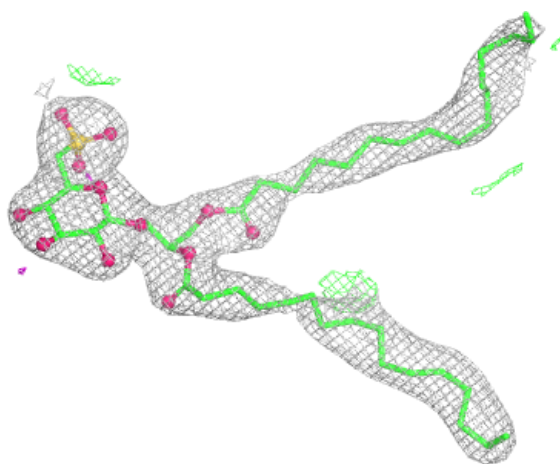
Electron density around CLA C 513:

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



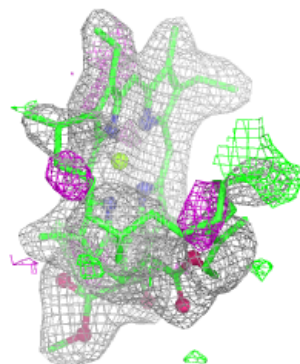
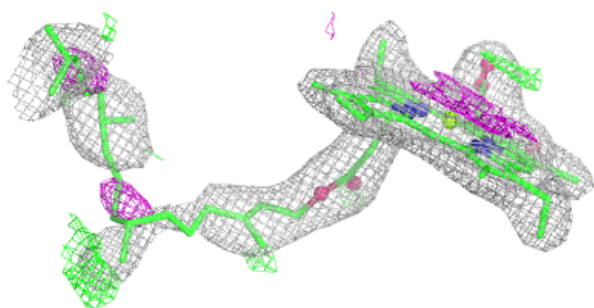
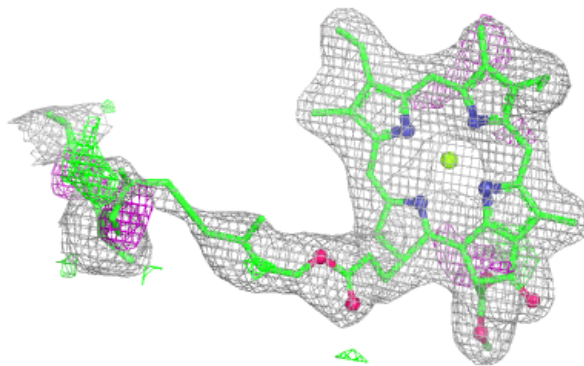
Electron density around SQD a 411:

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

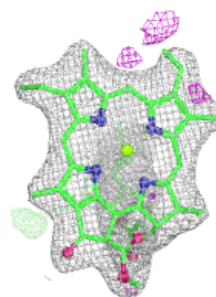
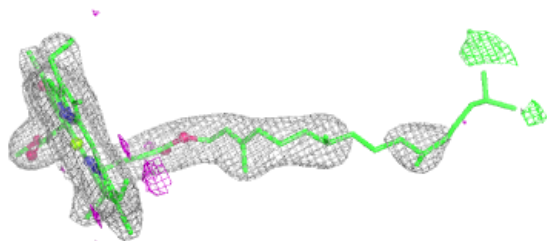
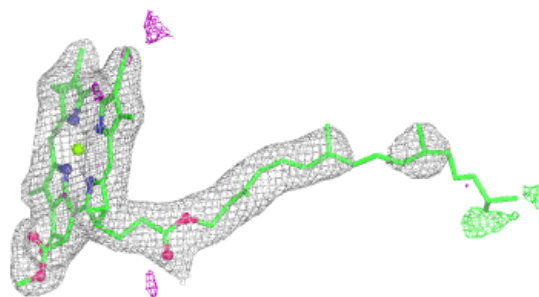


Electron density around CLA A 408:

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

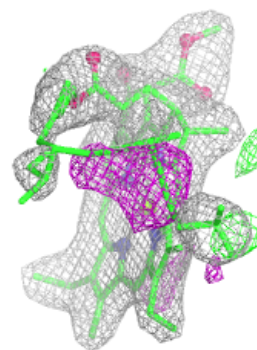
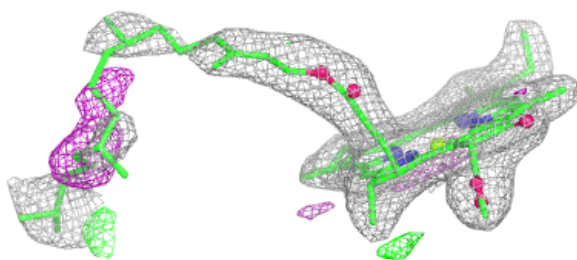
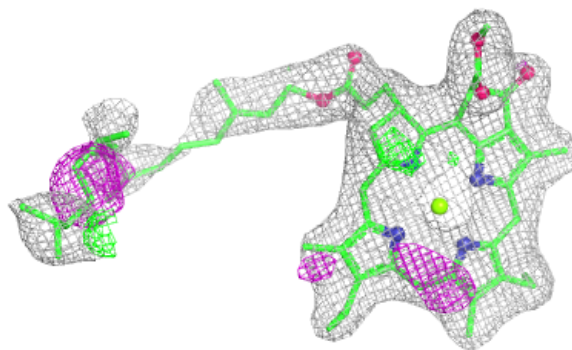
**Electron density around CLA d 403:**

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



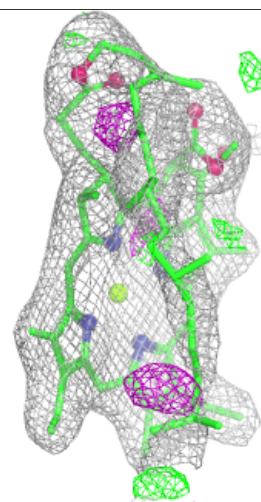
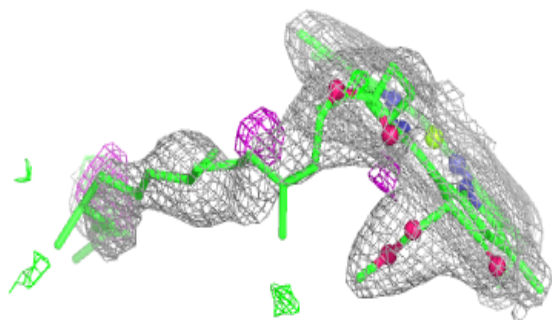
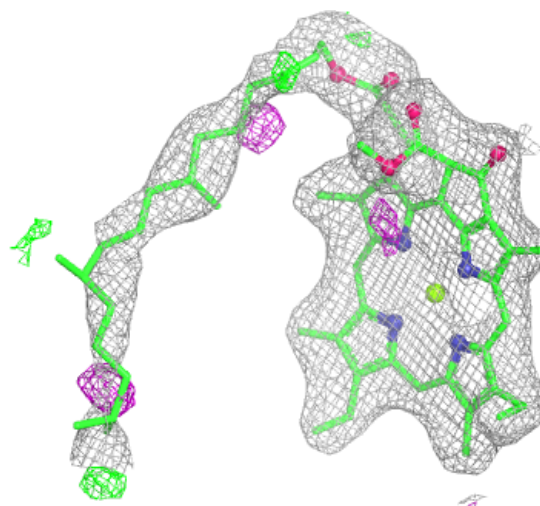
Electron density around CLA a 409:

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



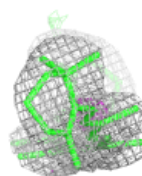
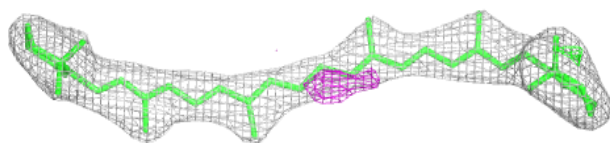
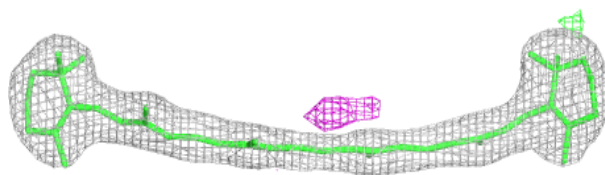
Electron density around CLA B 616:

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

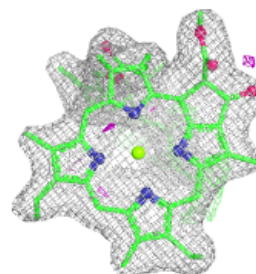
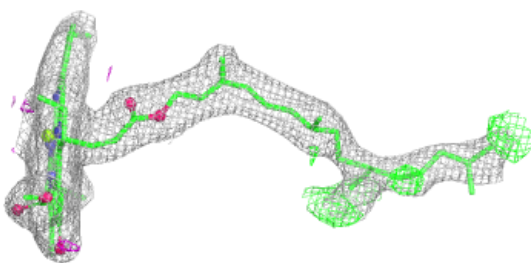
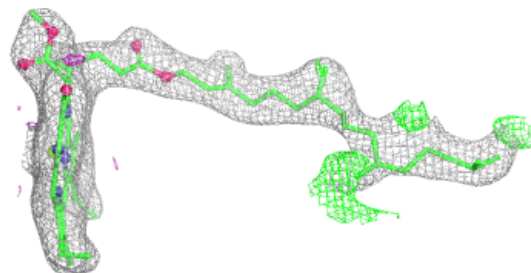


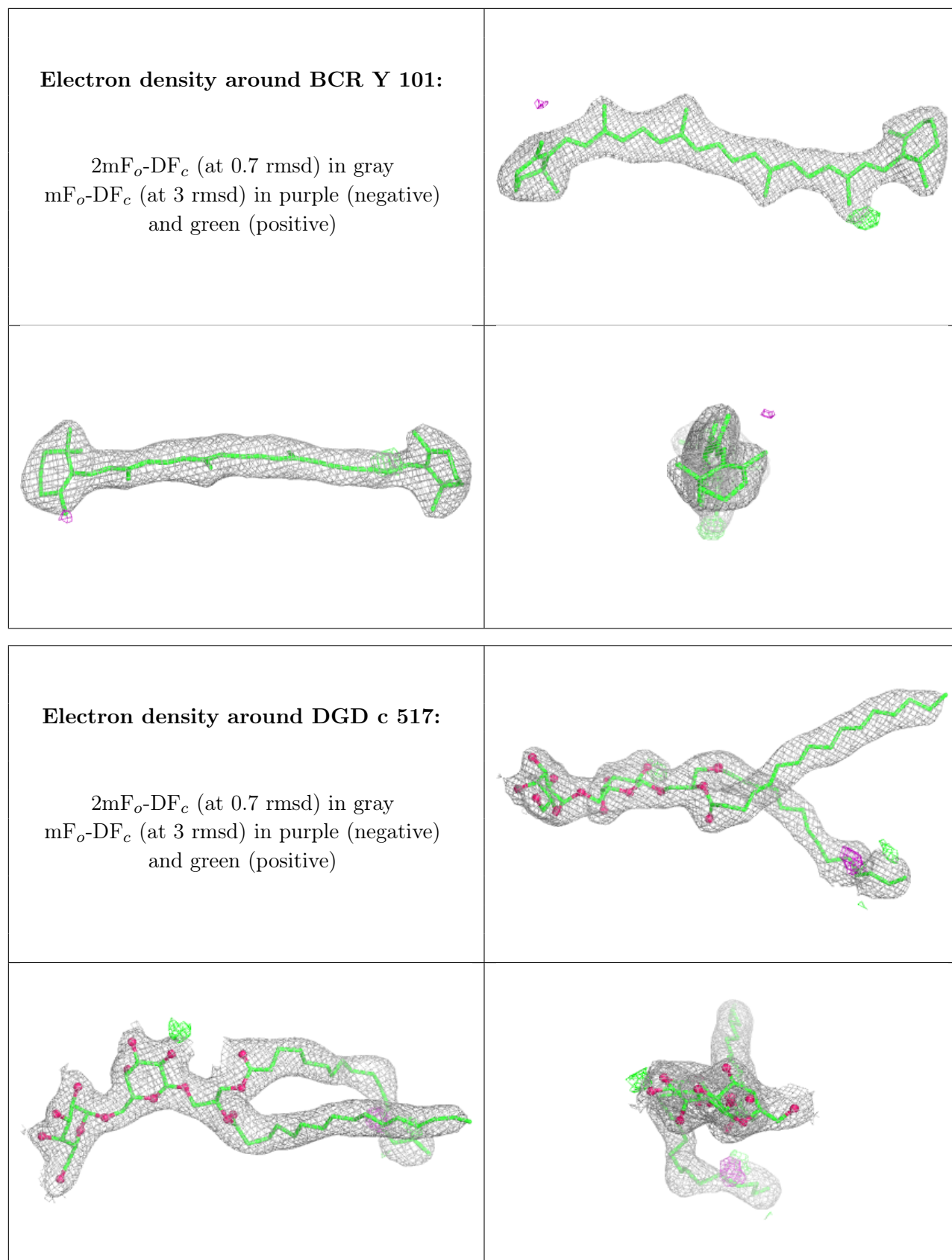
Electron density around BCR K 102:

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

**Electron density around CLA b 606:**

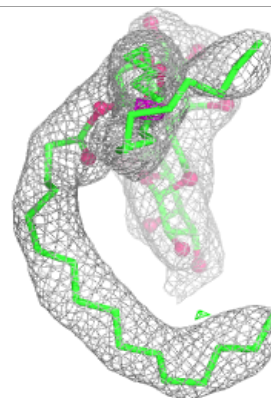
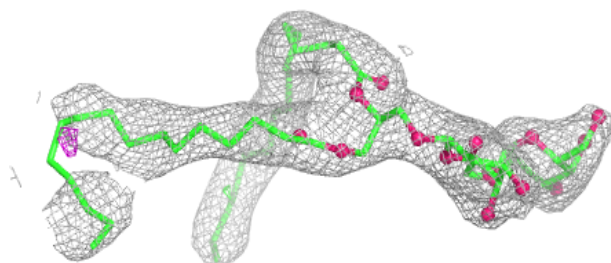
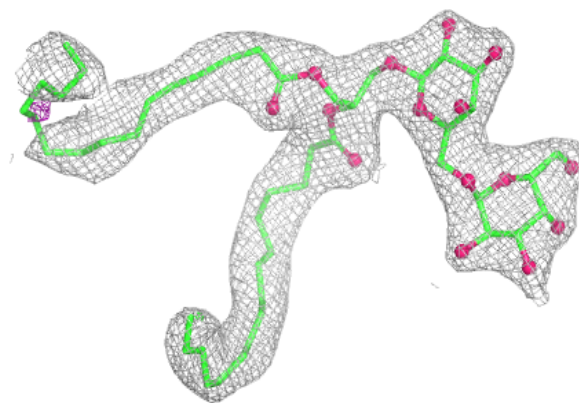
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



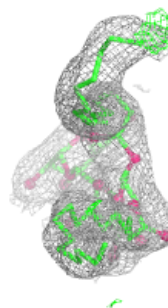
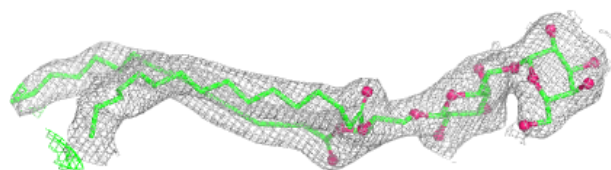
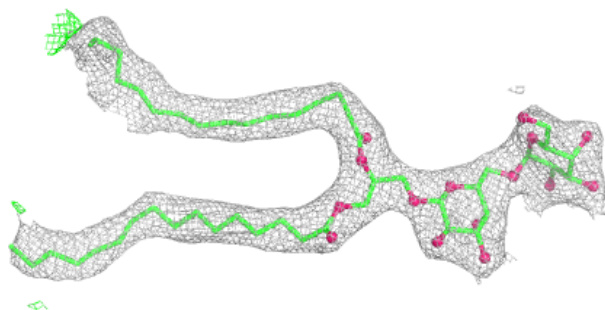


Electron density around DGD c 518:

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

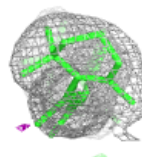
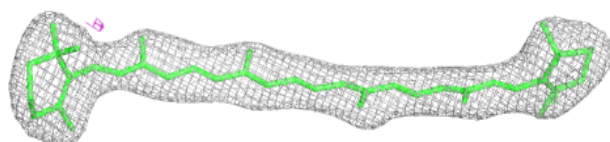
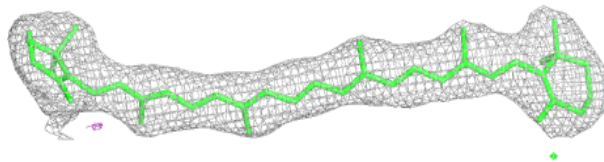
**Electron density around DGD c 519:**

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

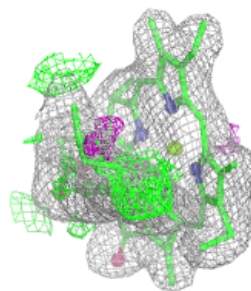
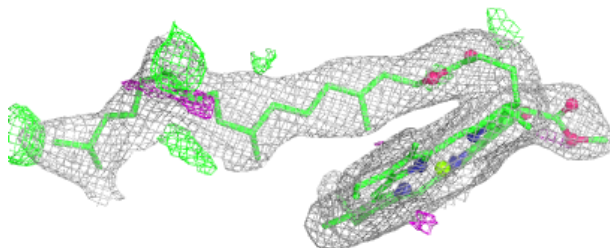
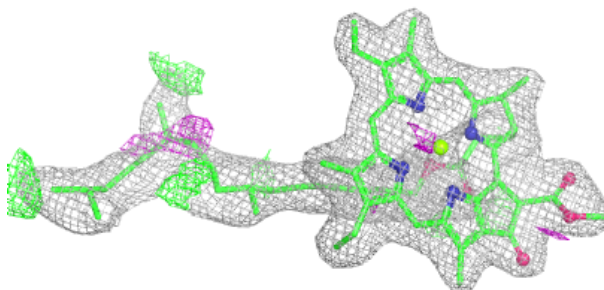


Electron density around BCR c 515:

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

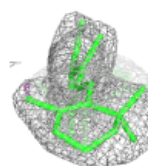
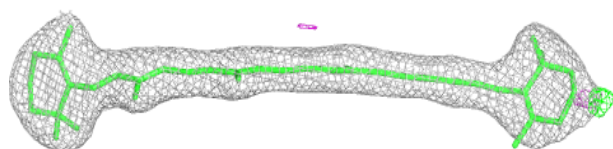
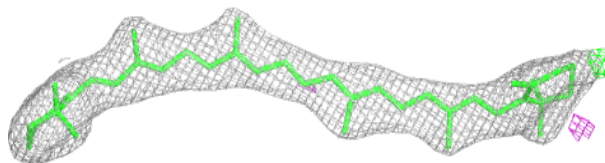
**Electron density around CLA b 614:**

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

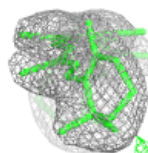
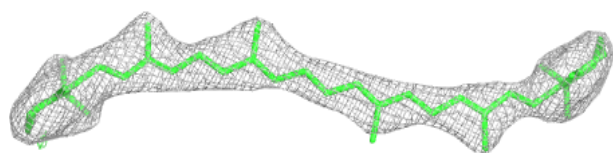
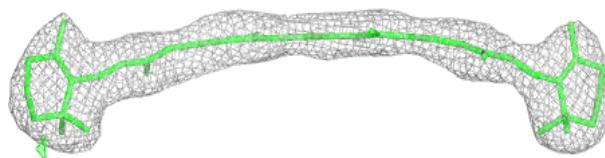


Electron density around BCR h 101:

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

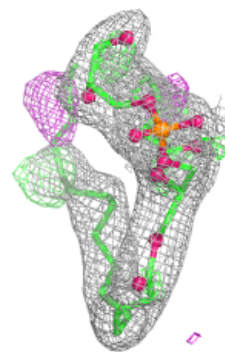
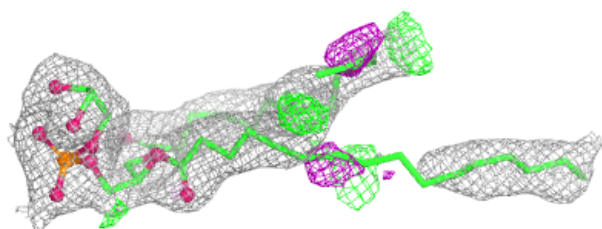
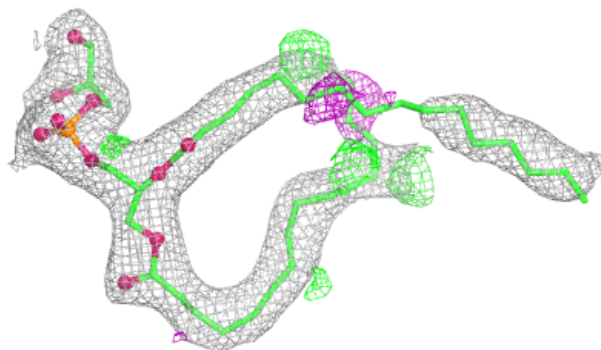
**Electron density around BCR k 101:**

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

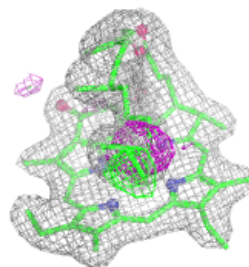
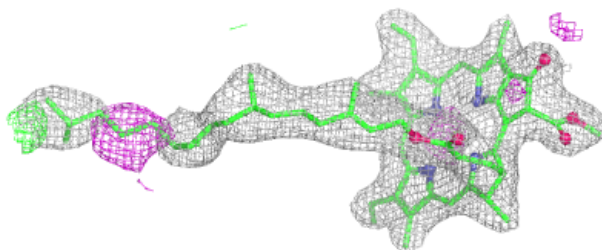
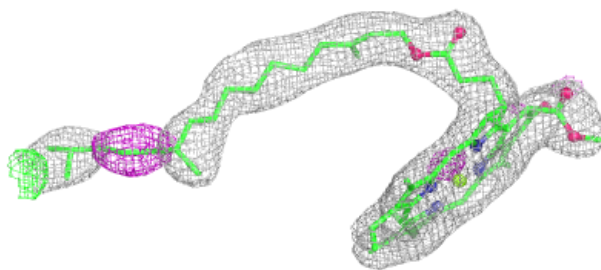


Electron density around LHG D 411:

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

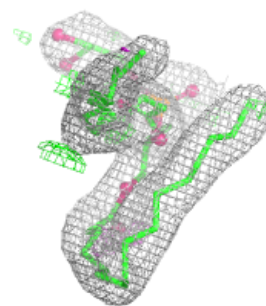
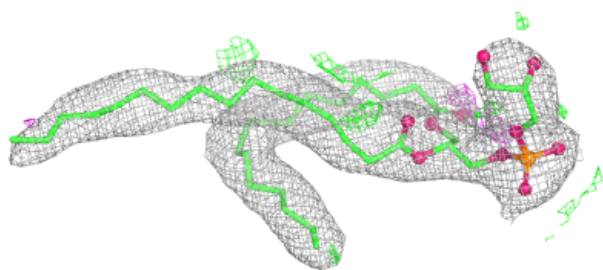
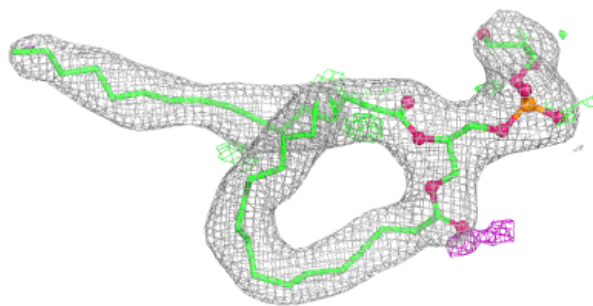
**Electron density around CLA C 505:**

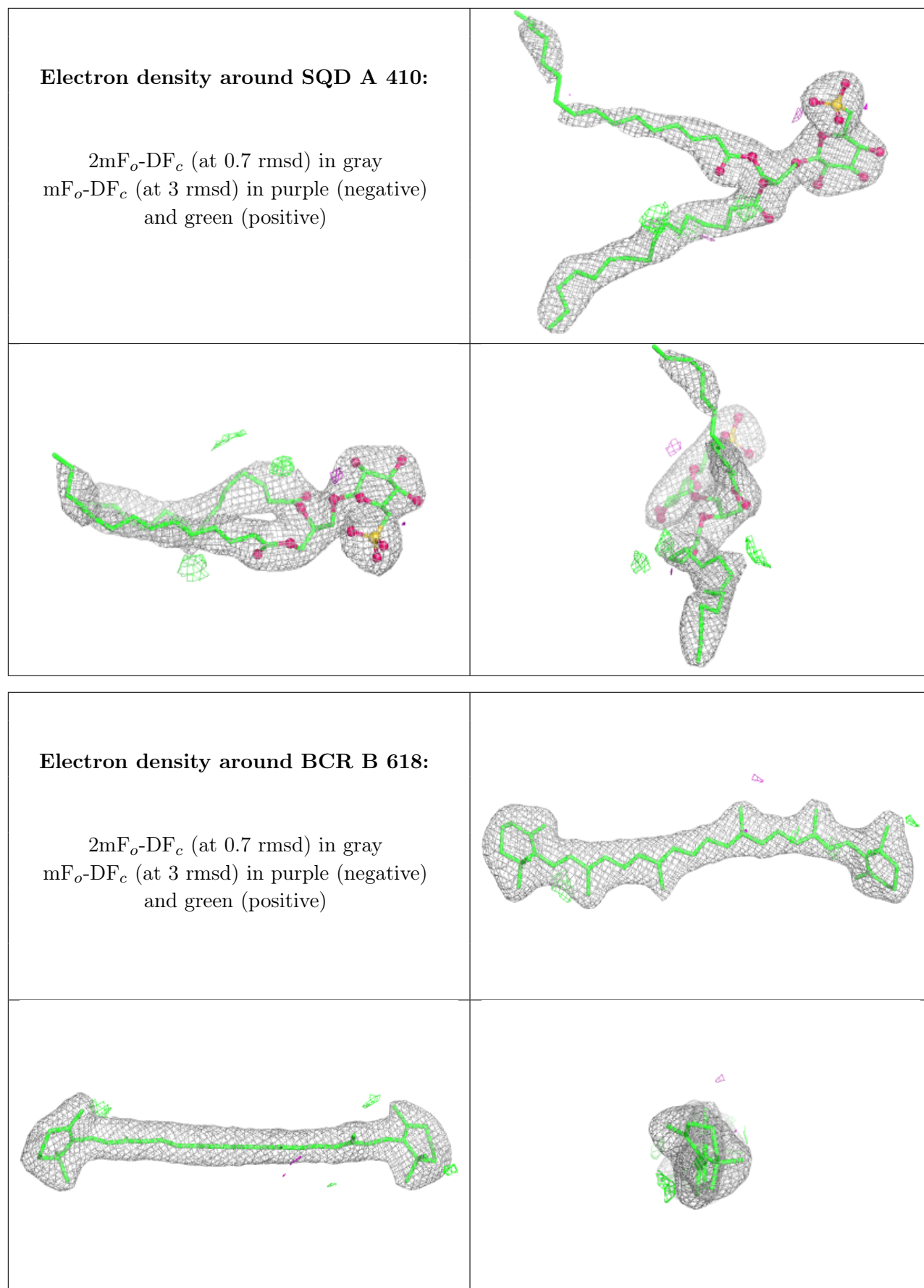
$2mF_o-DF_c$ (at 0.7 rnsd) in gray
 mF_o-DF_c (at 3 rnsd) in purple (negative)
and green (positive)

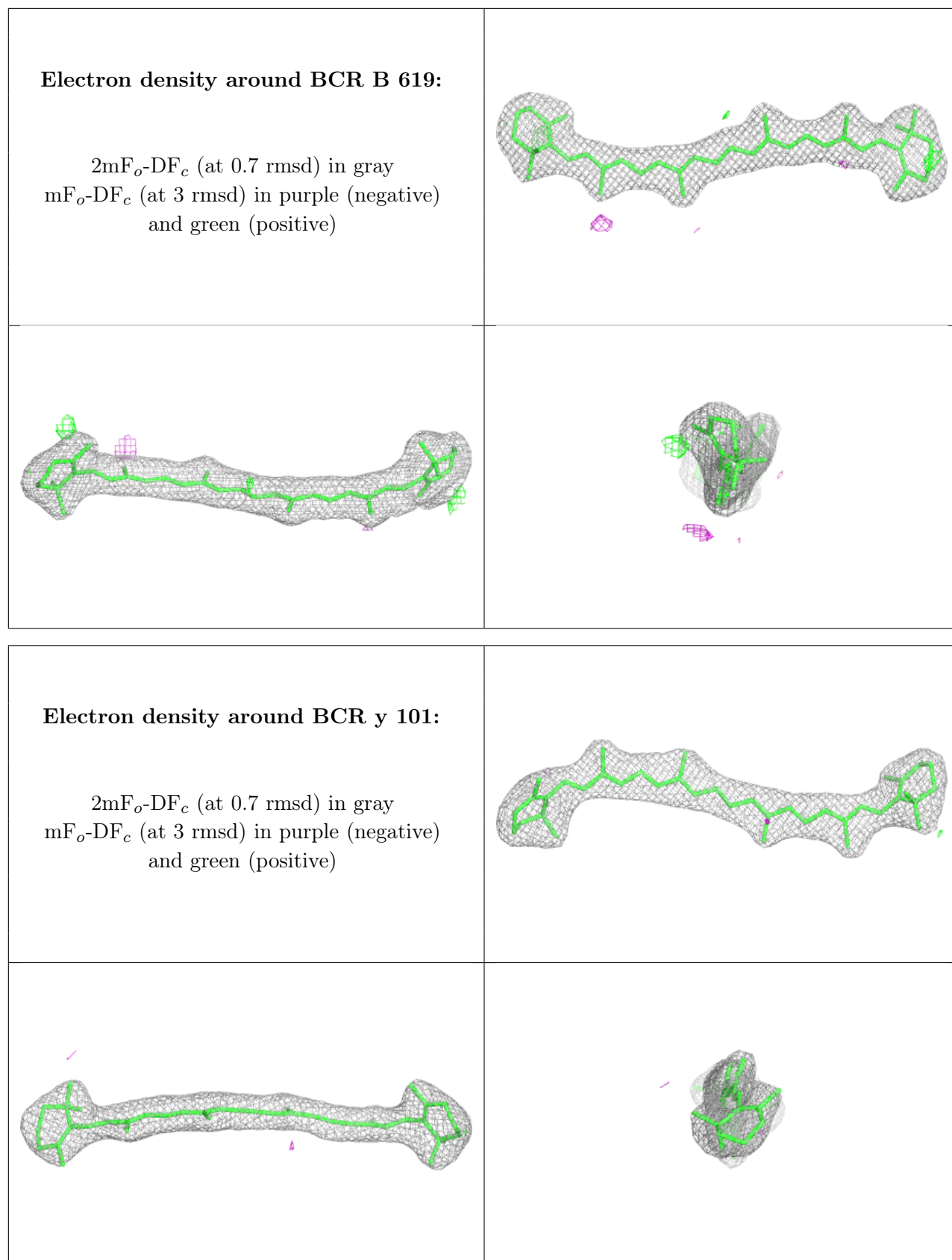


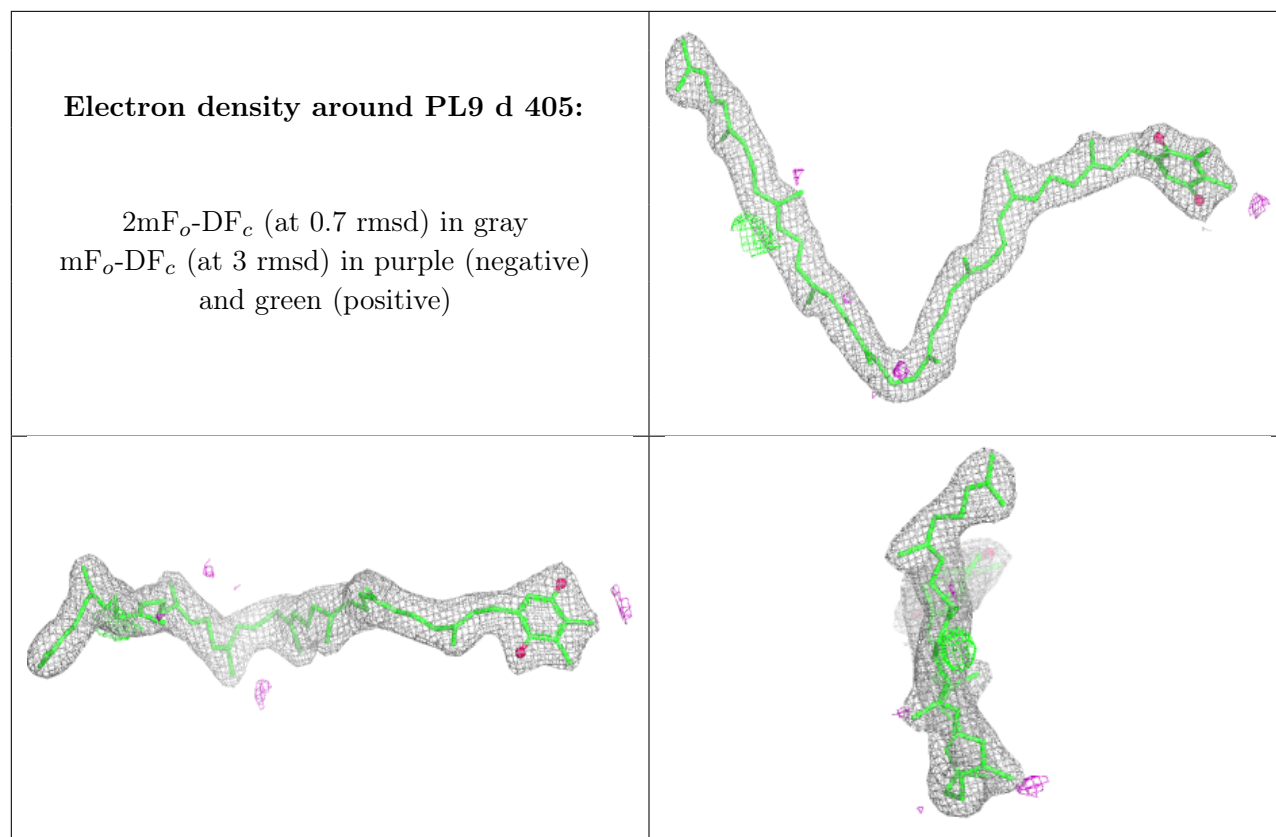
Electron density around LHG d 711:

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



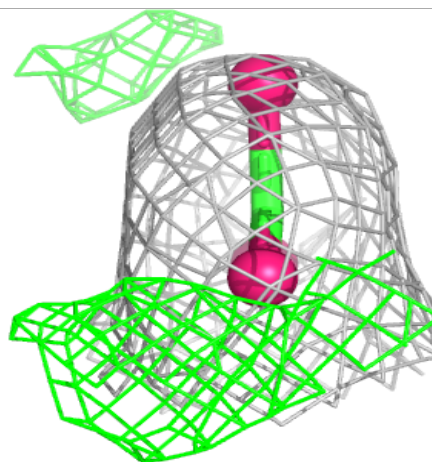
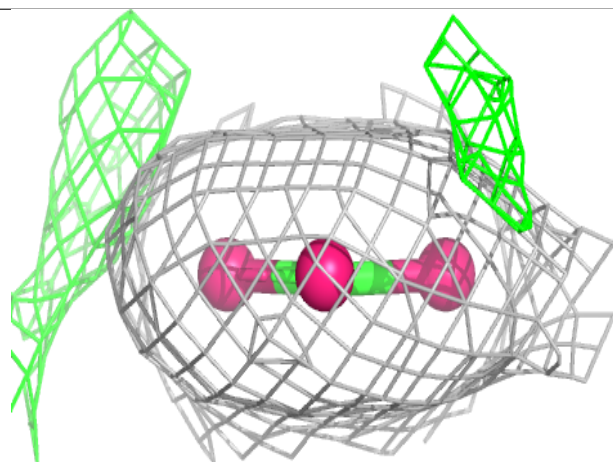
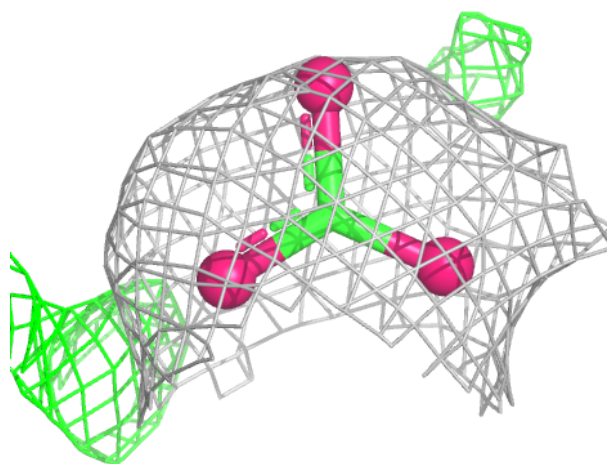






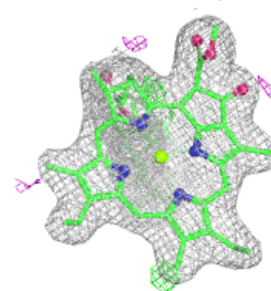
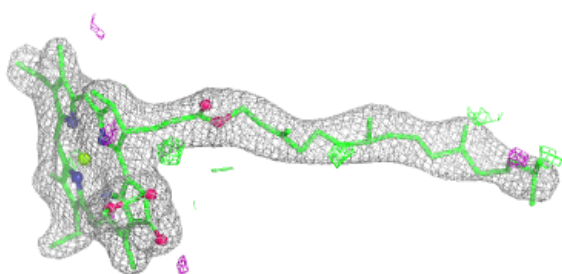
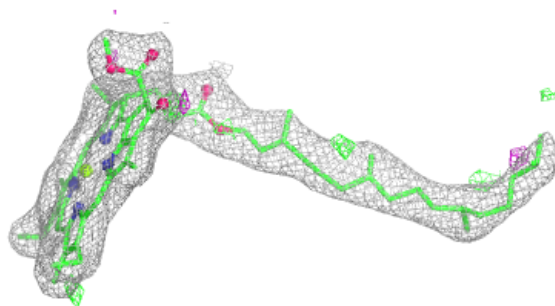
Electron density around BCT a 404:

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

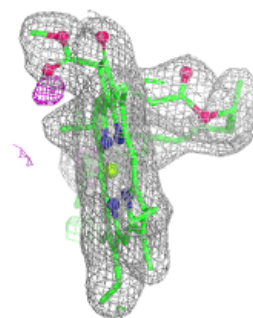
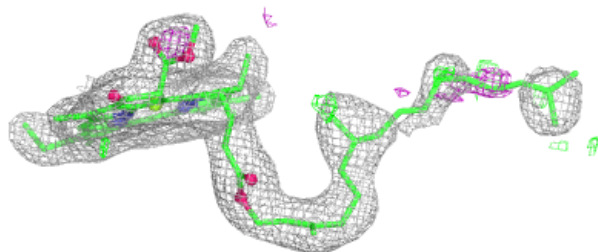
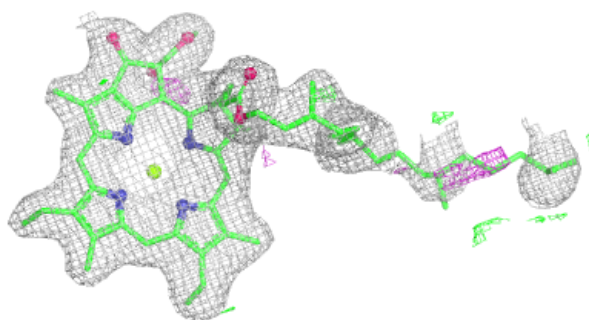


Electron density around CLA b 604:

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

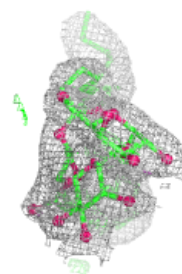
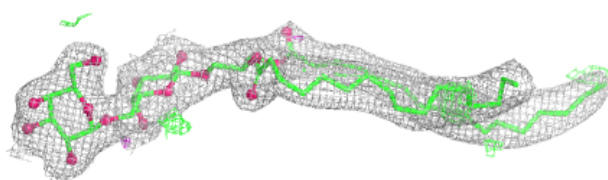
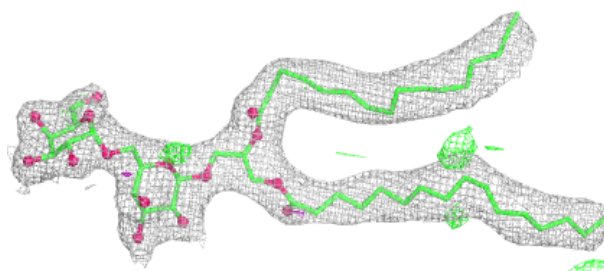
**Electron density around CLA a 407:**

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

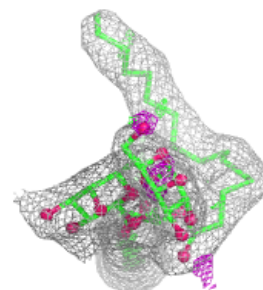
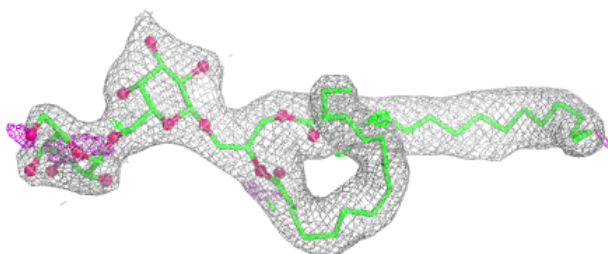
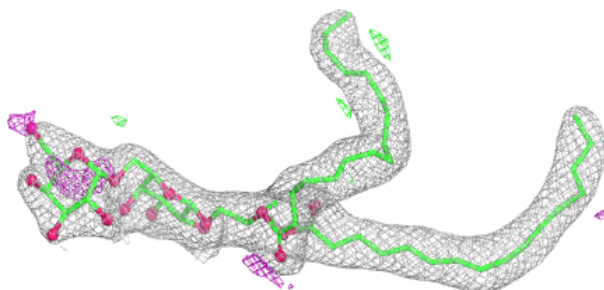


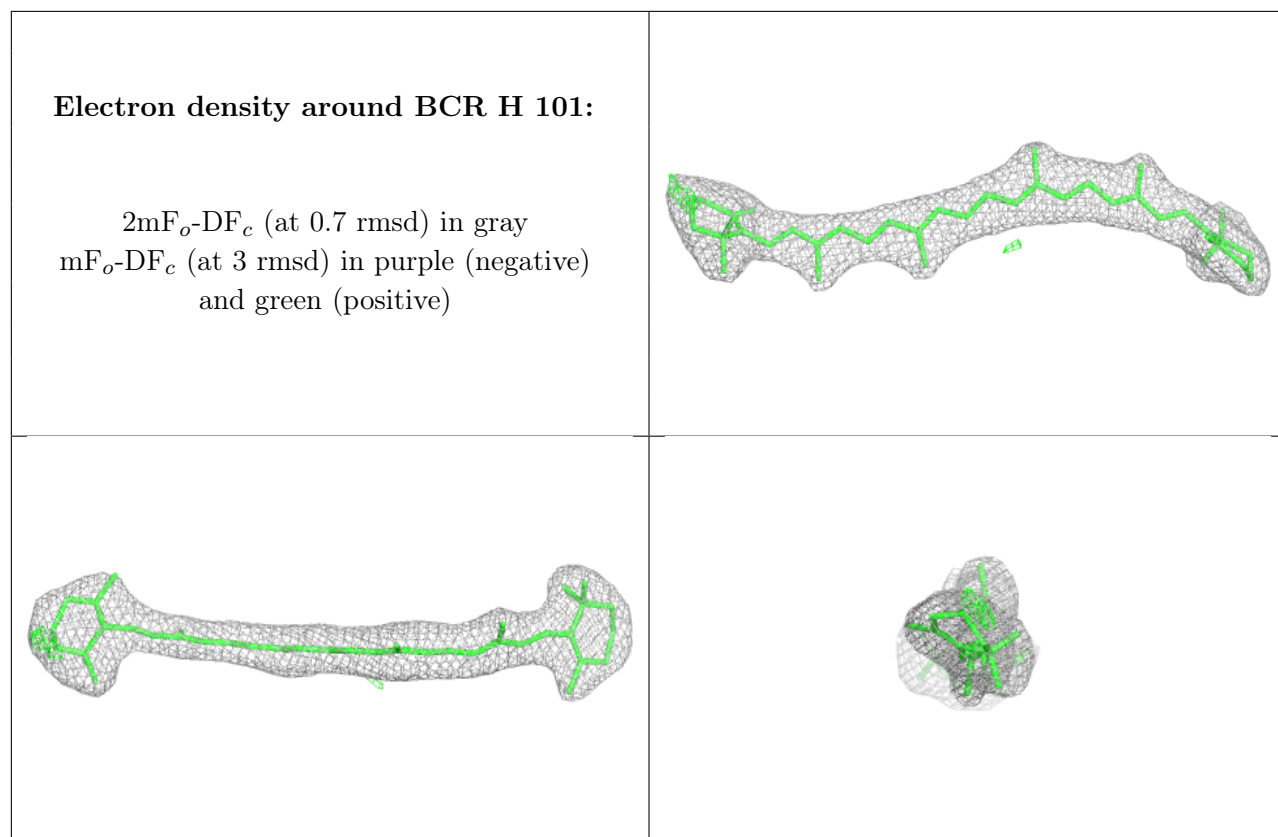
Electron density around DGD C 519:

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

**Electron density around DGD H 102:**

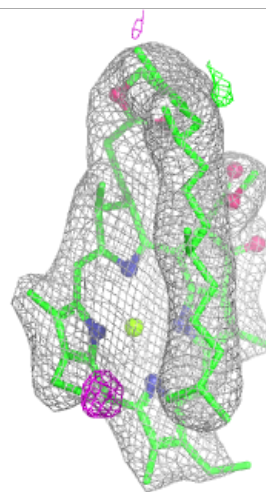
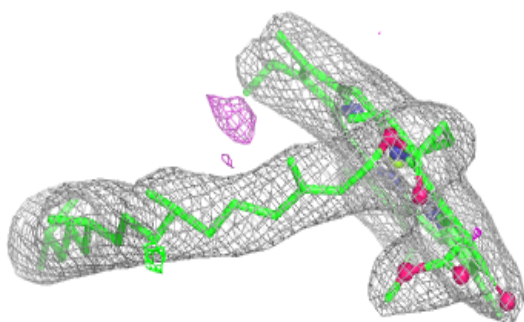
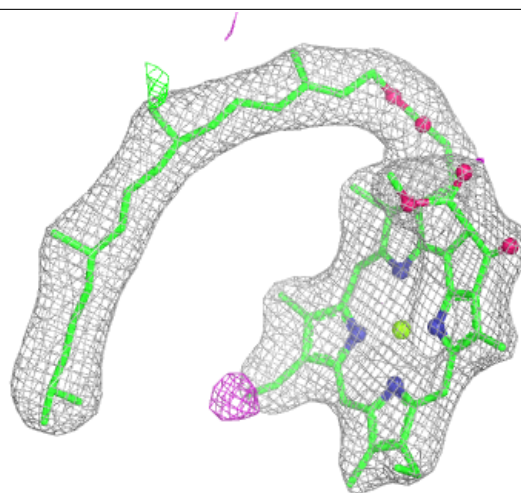
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





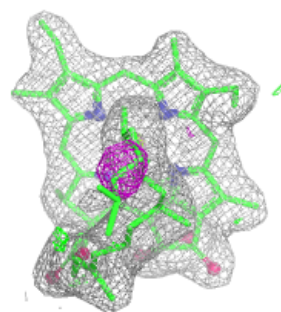
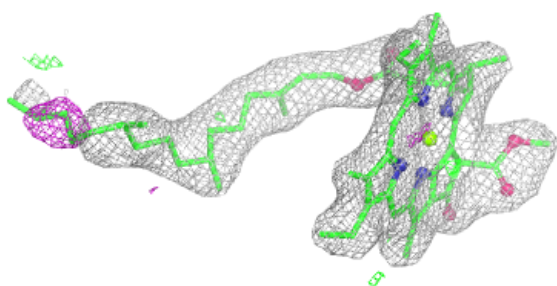
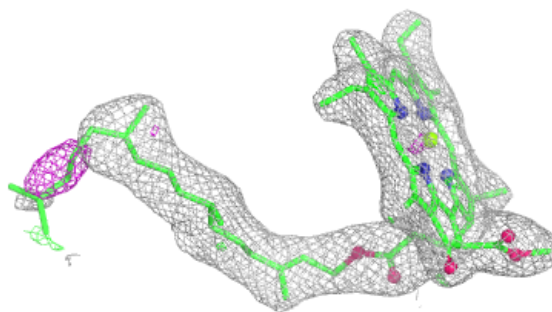
Electron density around CLA c 508:

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

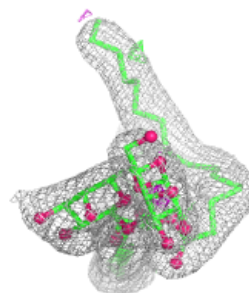
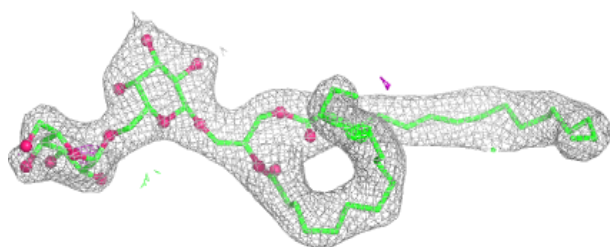
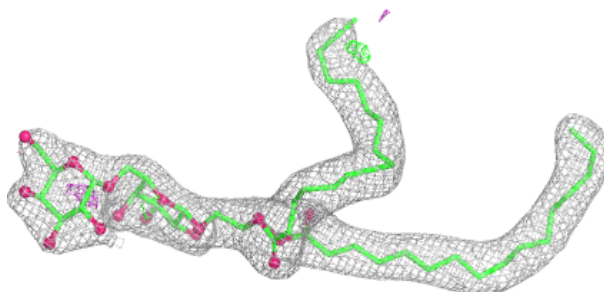


Electron density around CLA c 509:

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

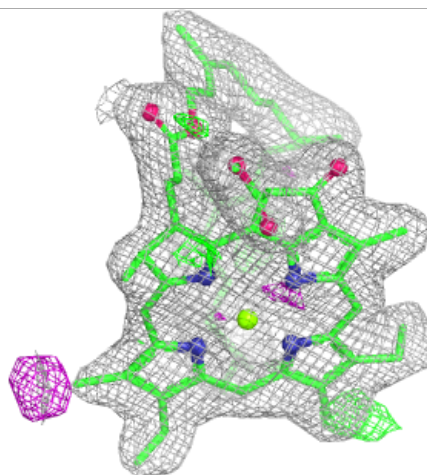
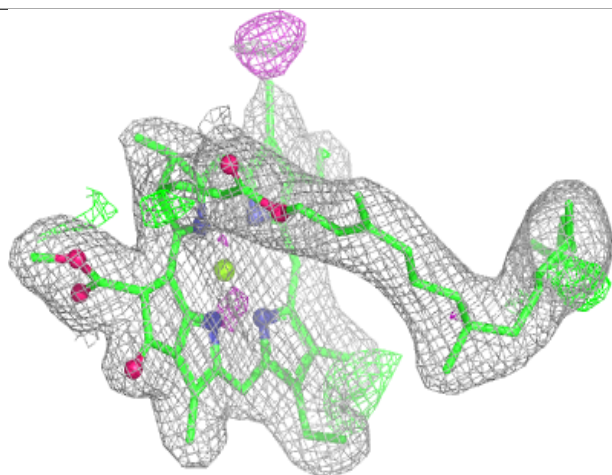
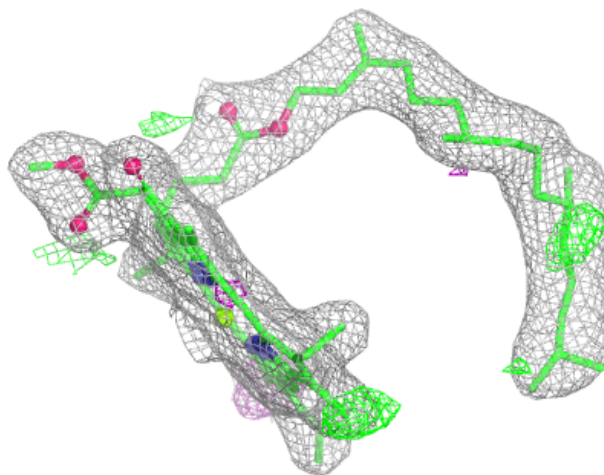
**Electron density around DGD h 102:**

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



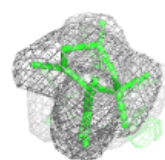
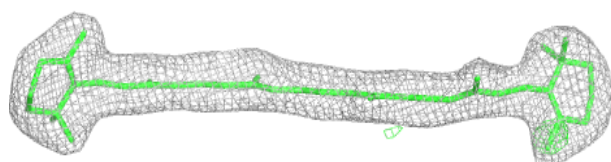
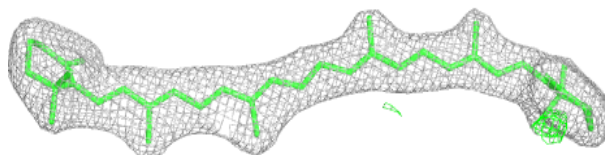
Electron density around CLA B 611:

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

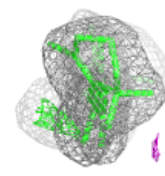
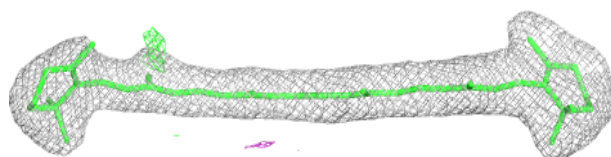
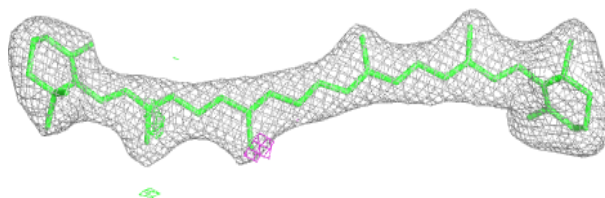


Electron density around BCR a 410:

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

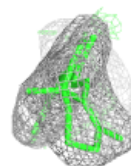
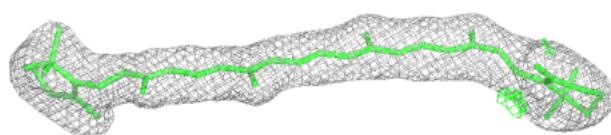
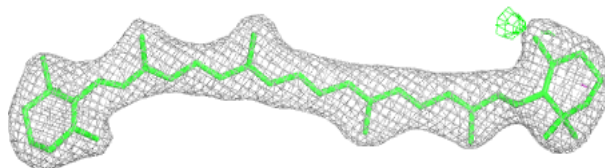
**Electron density around BCR b 618:**

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

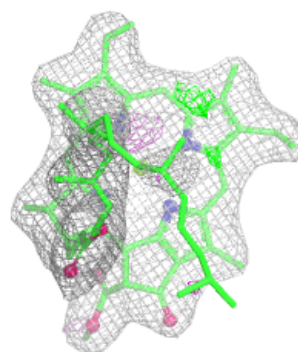
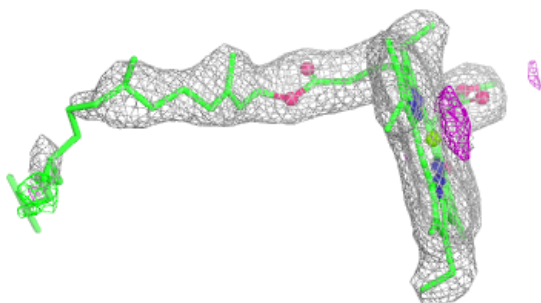
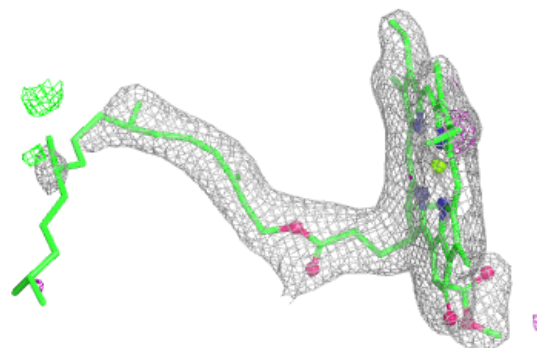


Electron density around BCR b 619:

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

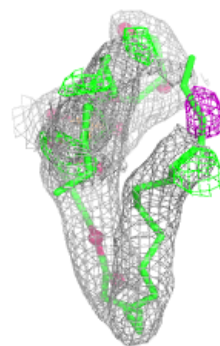
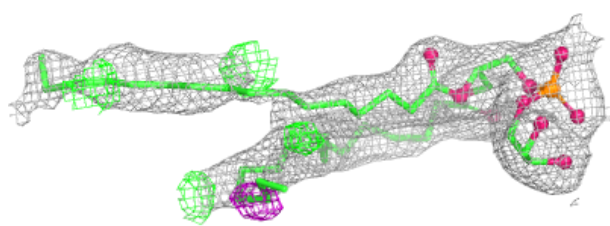
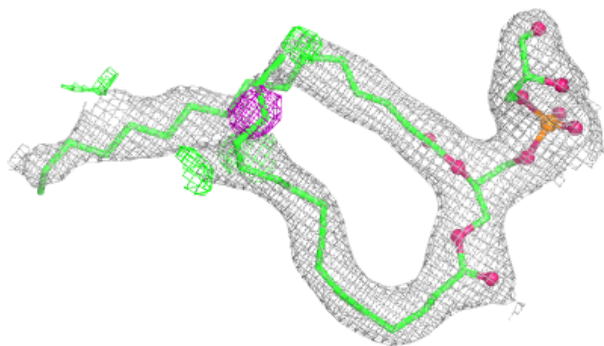
**Electron density around CLA D 406:**

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

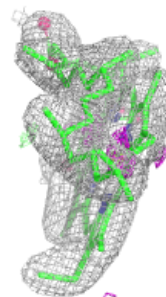
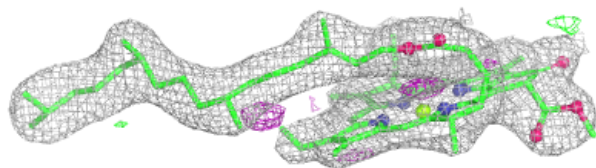
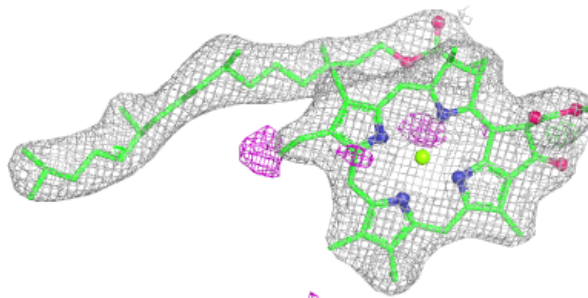


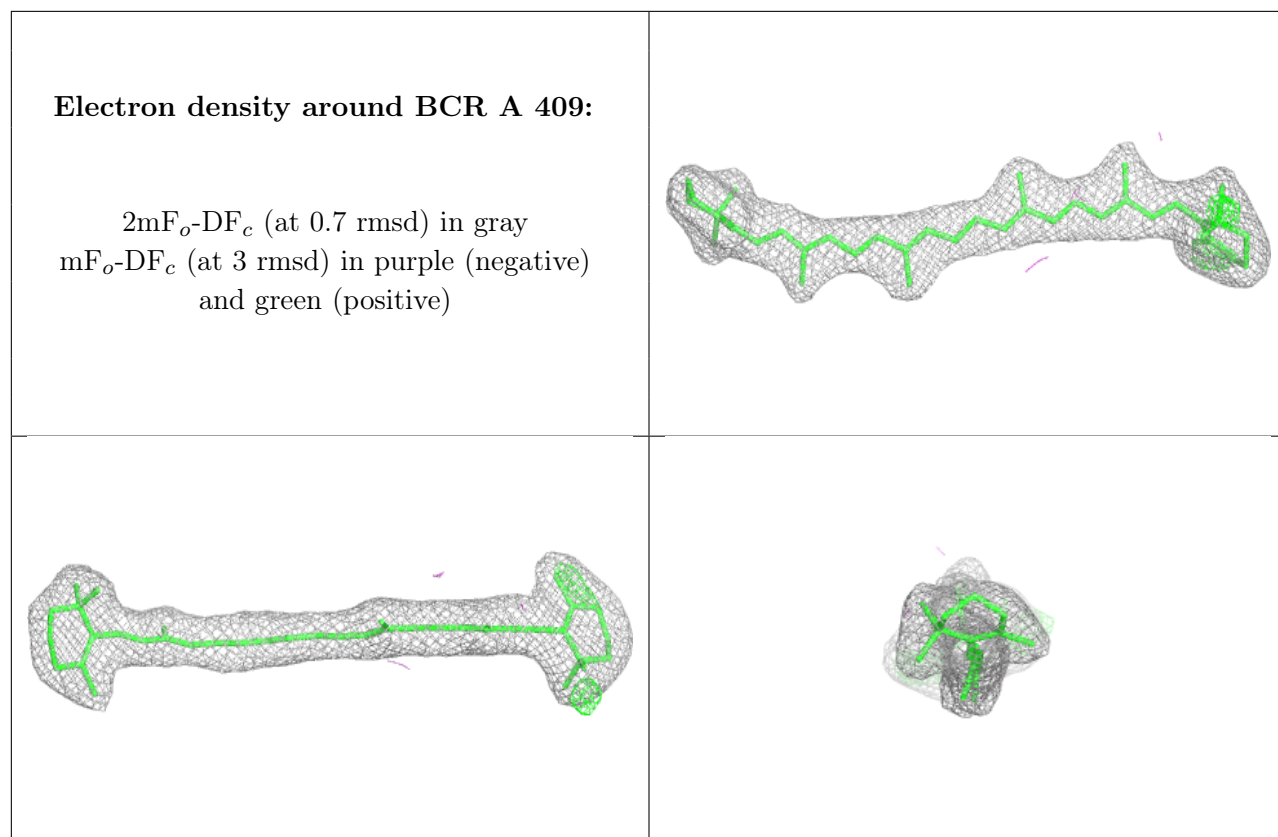
Electron density around LHG d 408:

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

**Electron density around CLA c 502:**

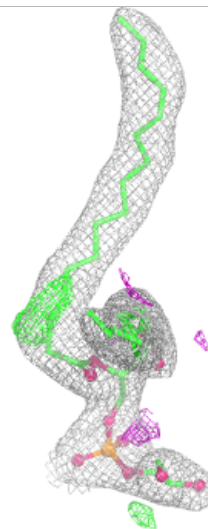
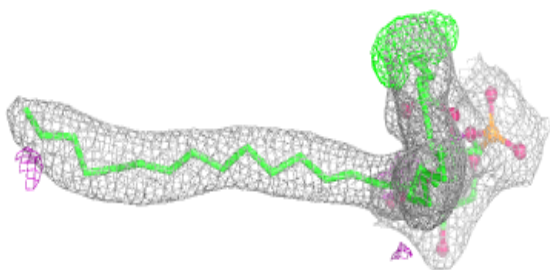
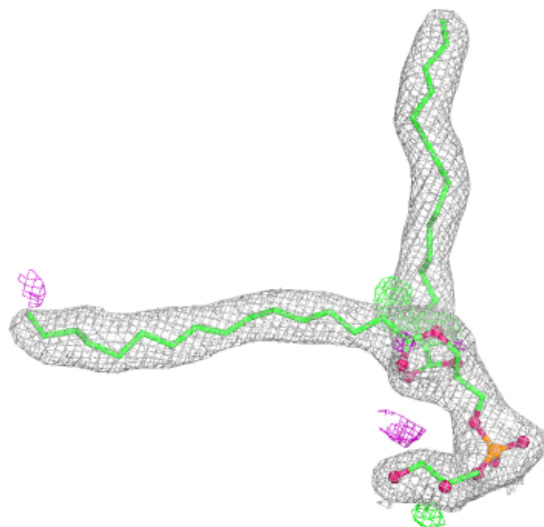
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





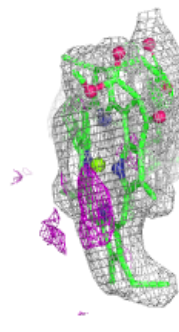
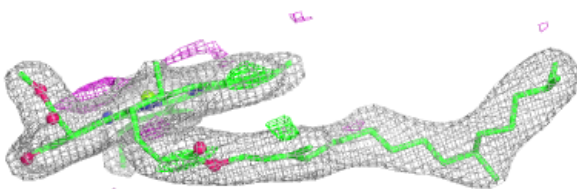
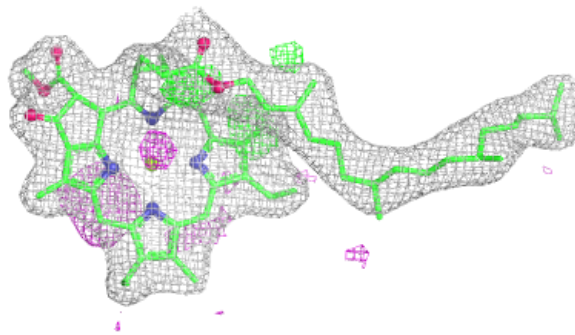
Electron density around LHG 1 101:

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

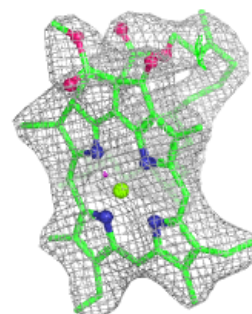
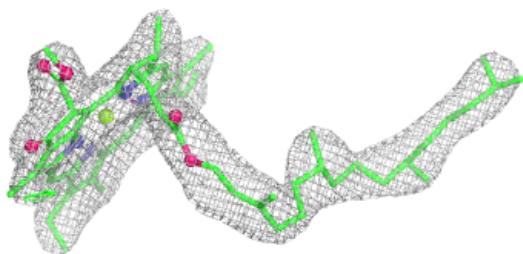
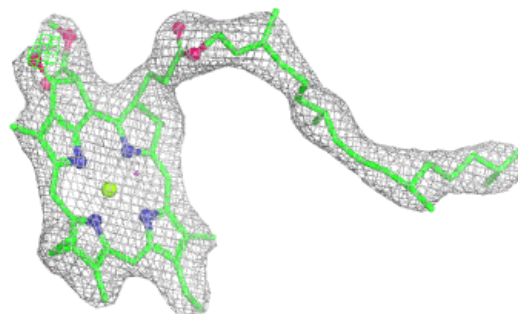


Electron density around CLA B 603:

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

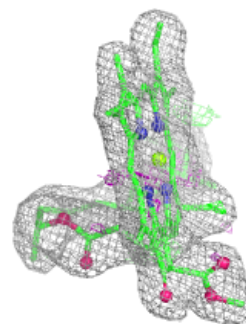
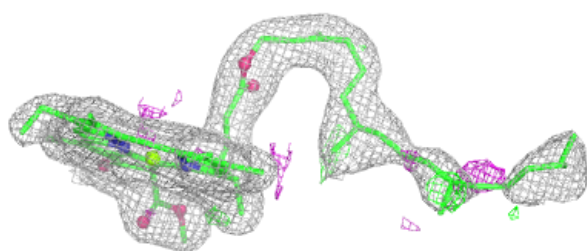
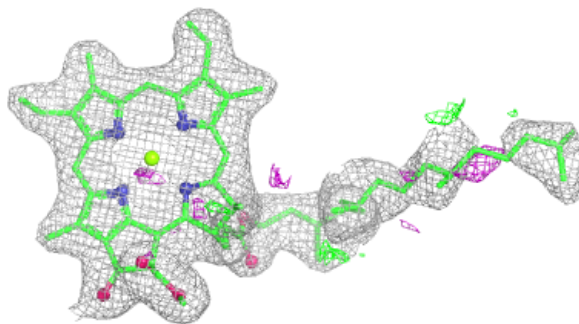
**Electron density around CLA c 512:**

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

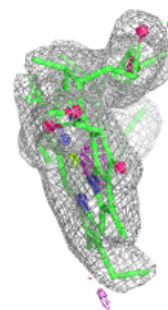
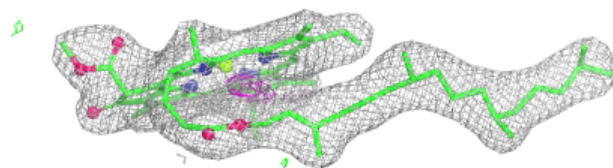
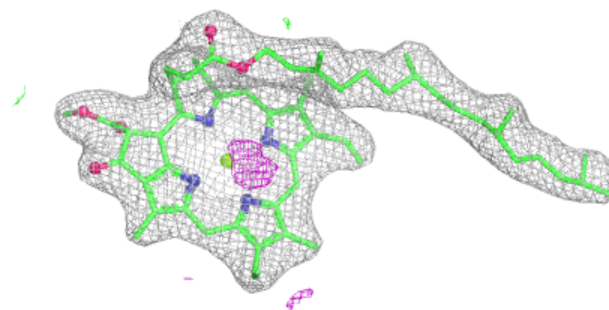


Electron density around CLA A 406:

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

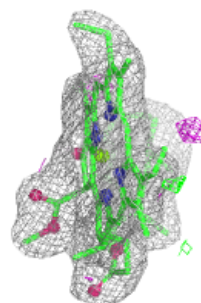
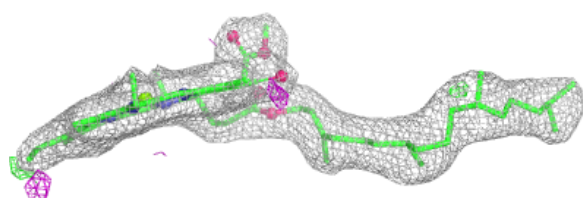
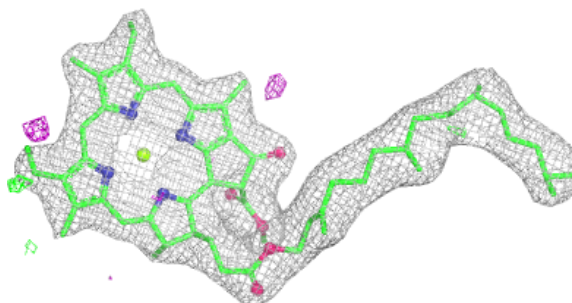
**Electron density around CLA C 502:**

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

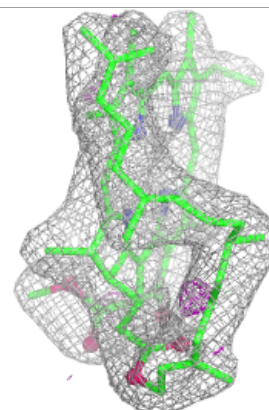
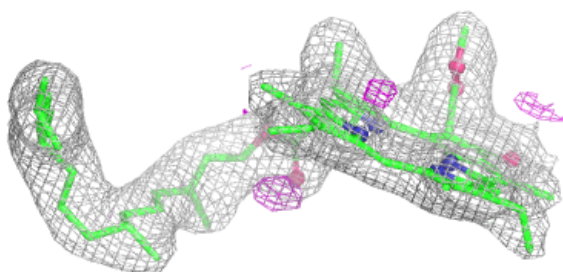
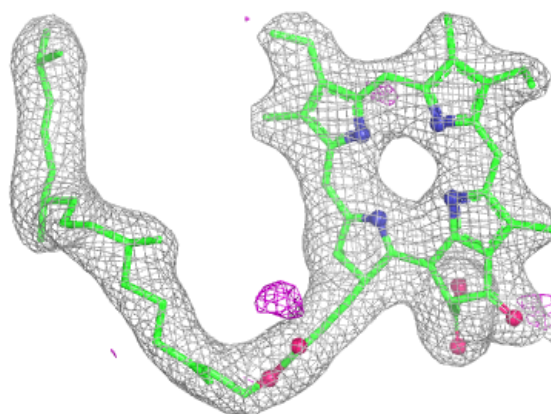


Electron density around CLA b 602:

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

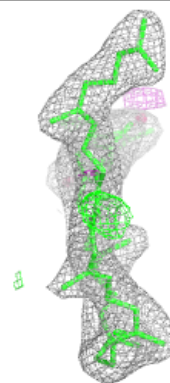
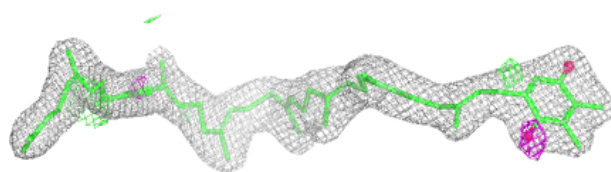
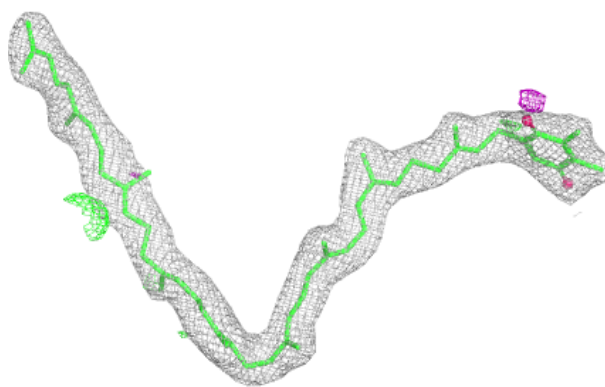
**Electron density around PHO a 353:**

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

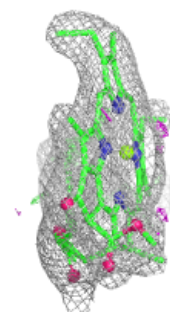
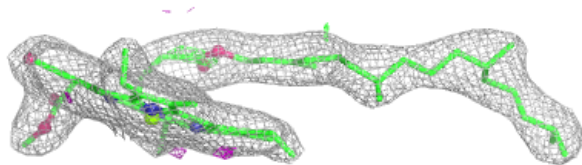
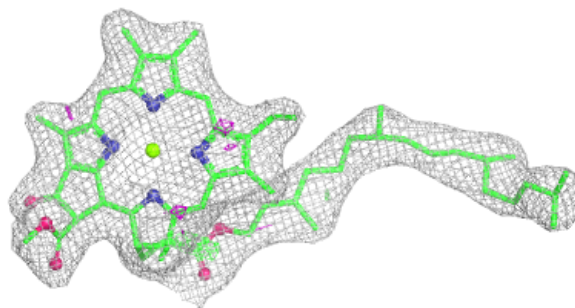


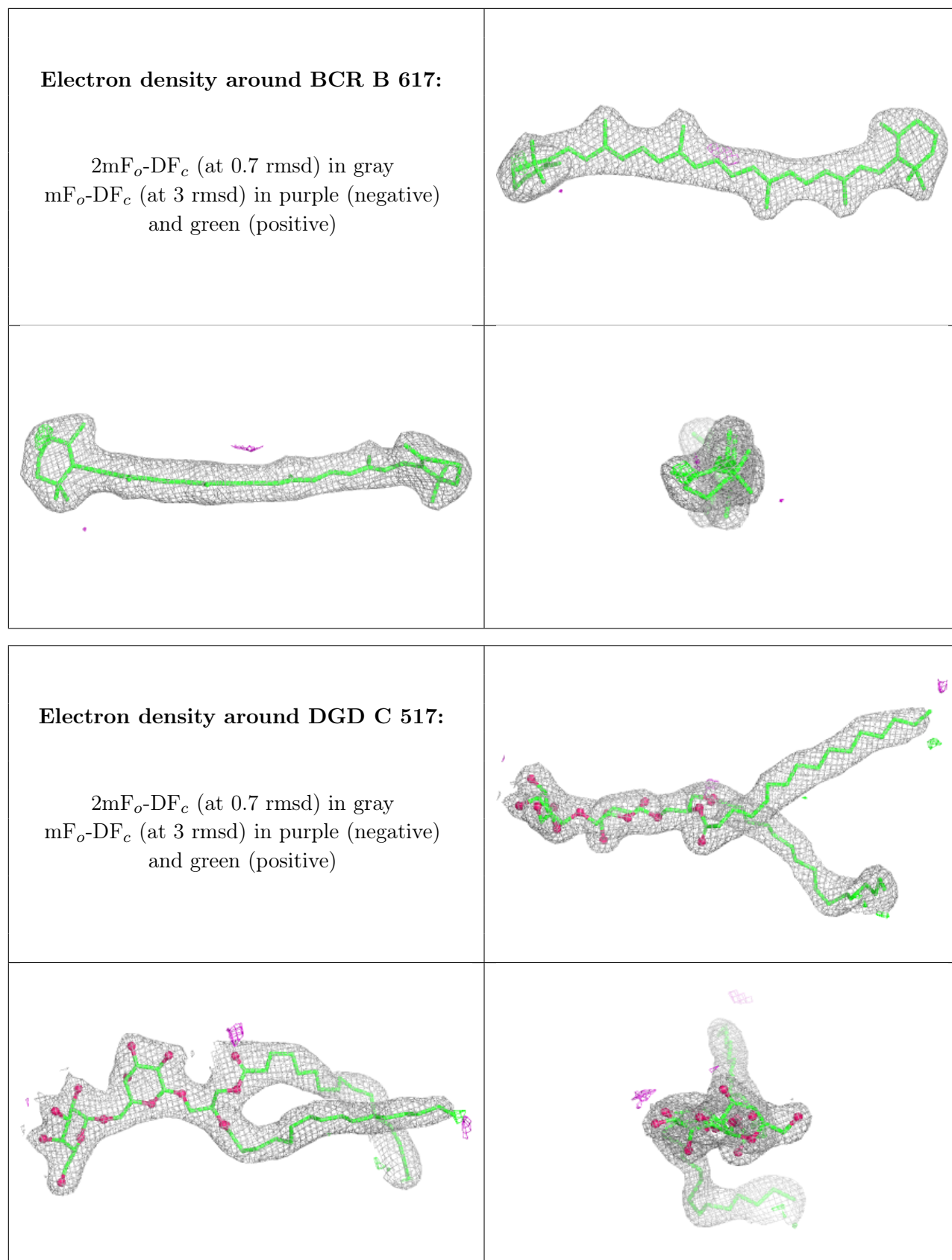
Electron density around PL9 D 408:

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

**Electron density around CLA b 603:**

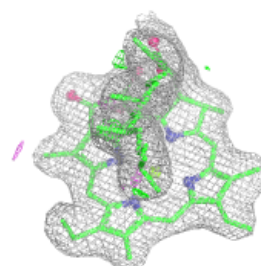
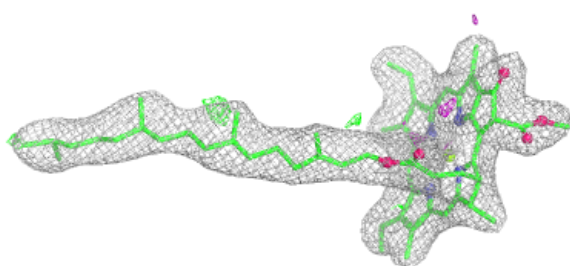
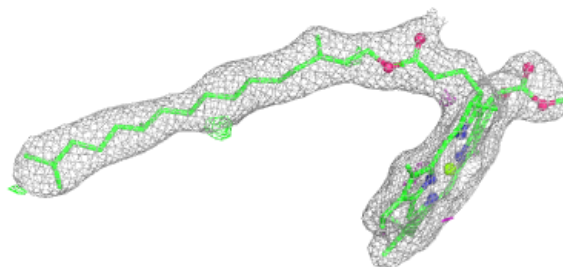
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



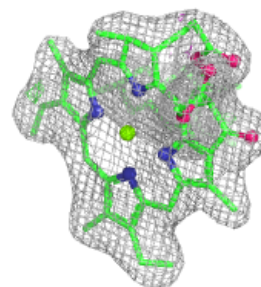
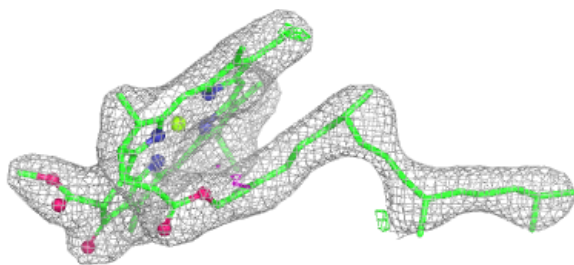
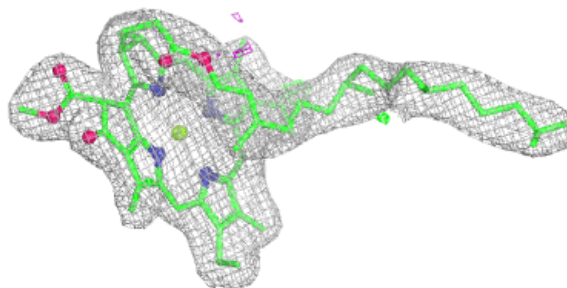


Electron density around CLA B 607:

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

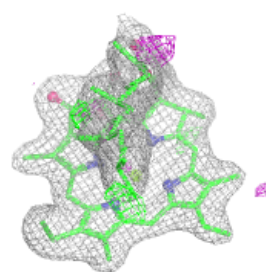
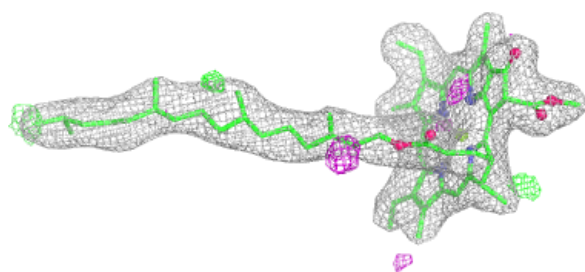
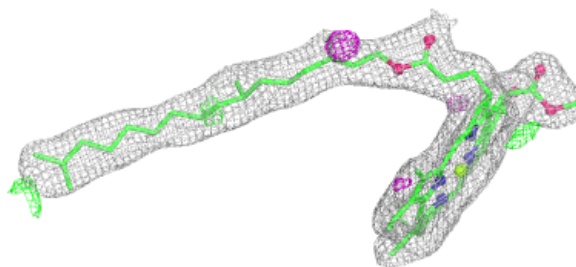
**Electron density around CLA C 506:**

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

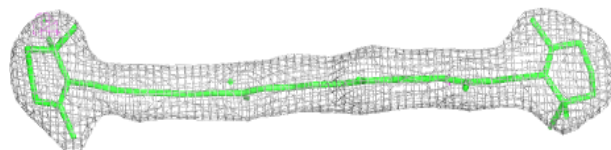
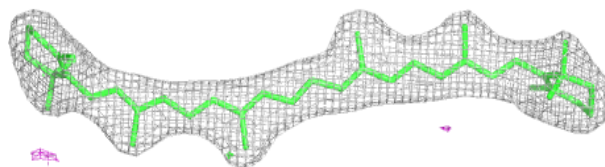


Electron density around CLA b 607:

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

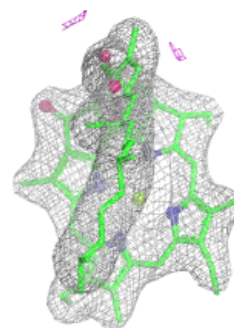
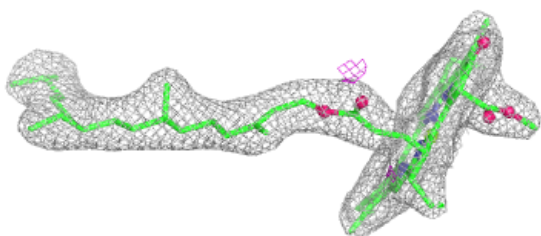
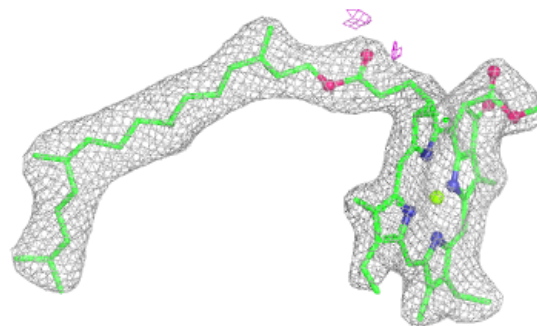
**Electron density around BCR C 516:**

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



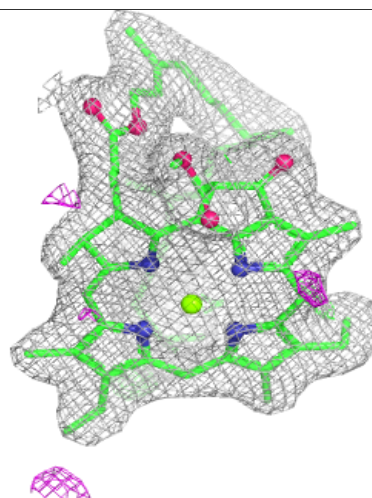
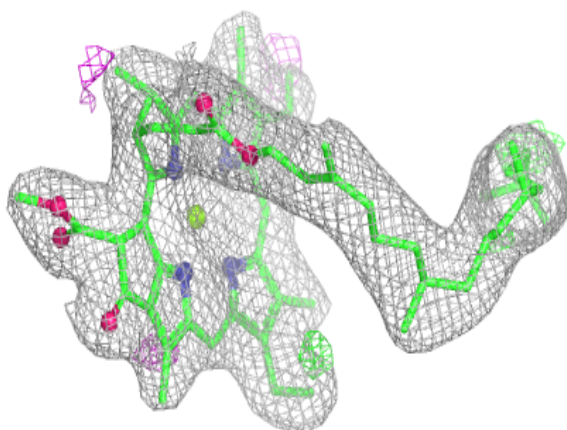
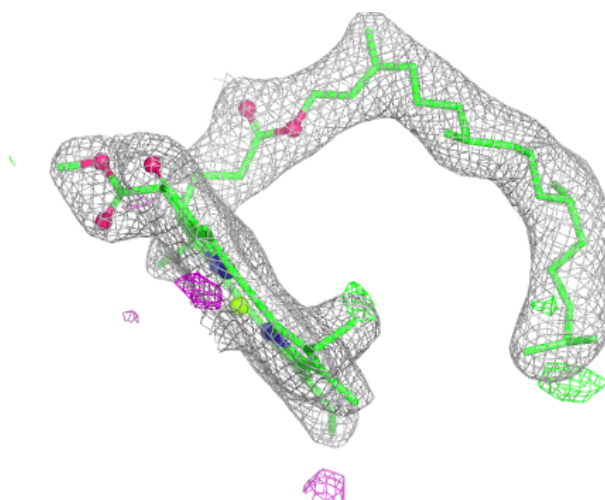
Electron density around CLA b 609:

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



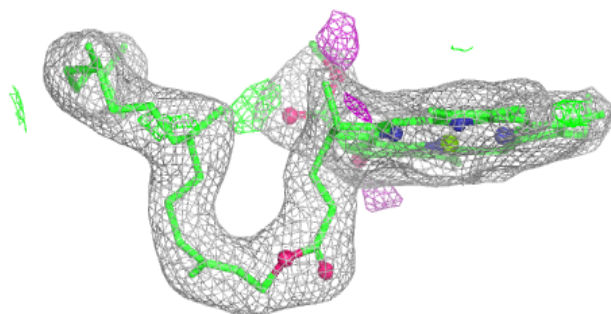
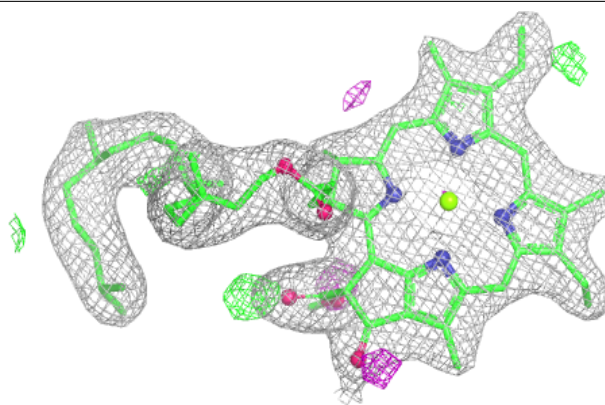
Electron density around CLA b 611:

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



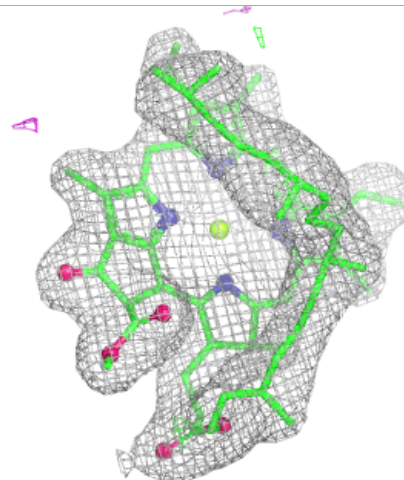
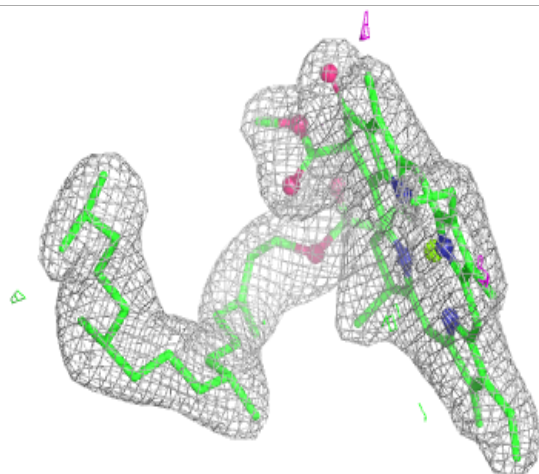
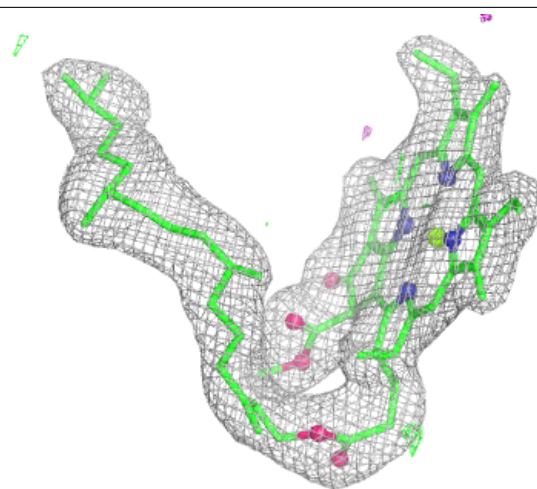
Electron density around CLA b 612:

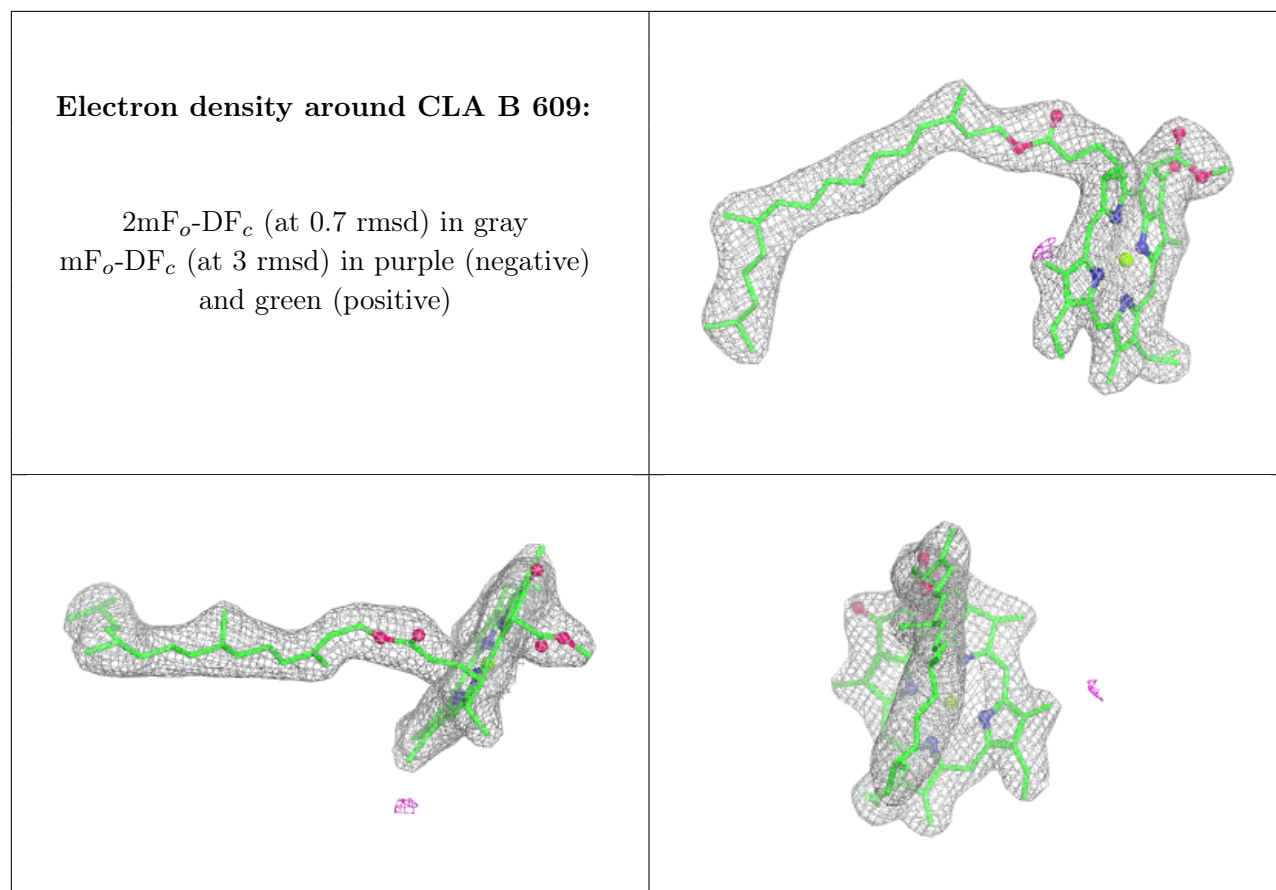
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA b 613:

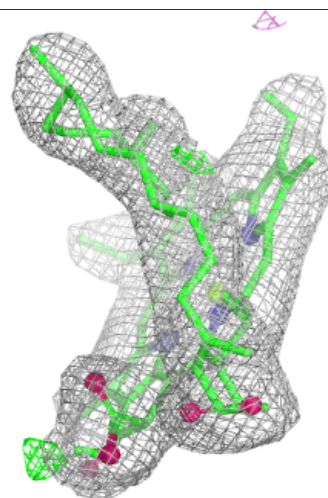
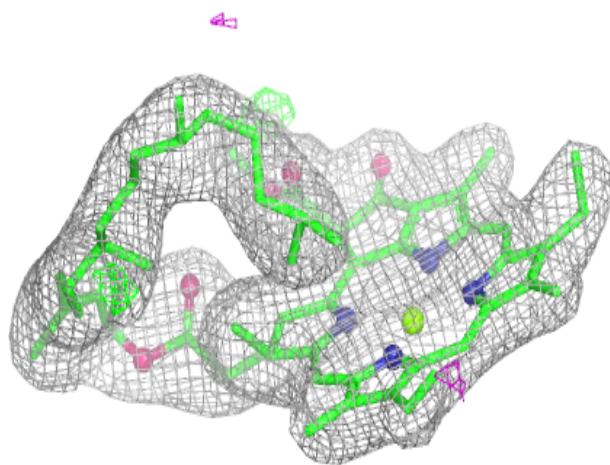
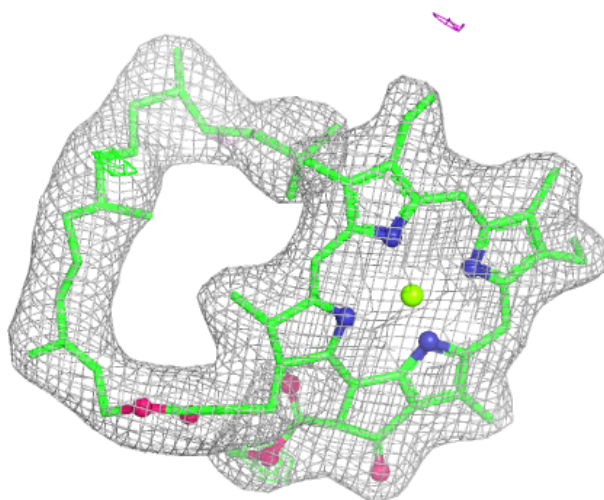
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





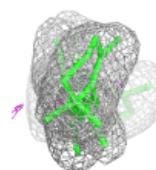
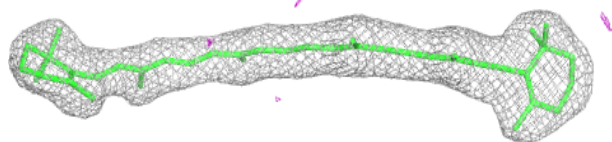
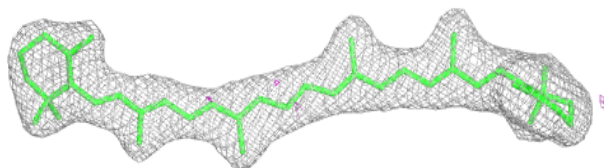
Electron density around CLA b 615:

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

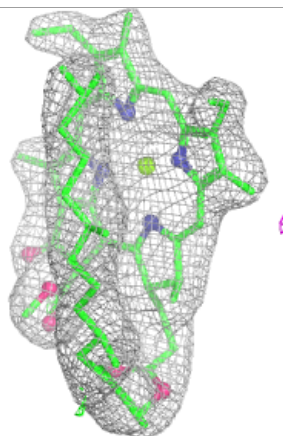
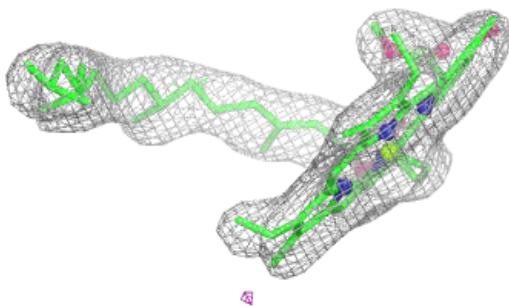
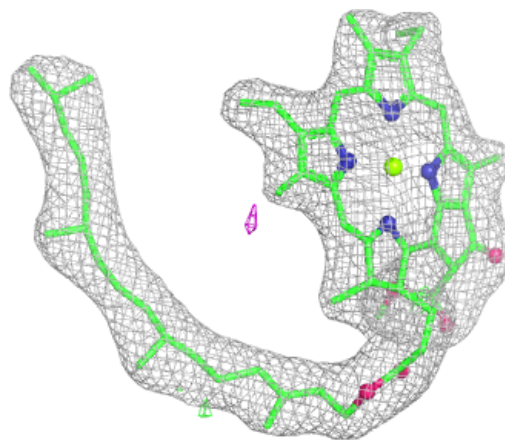


Electron density around BCR b 617:

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

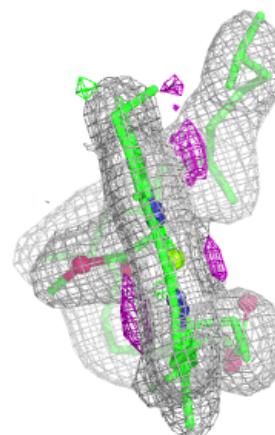
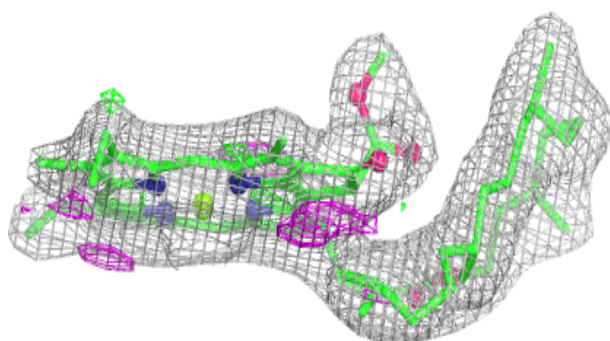
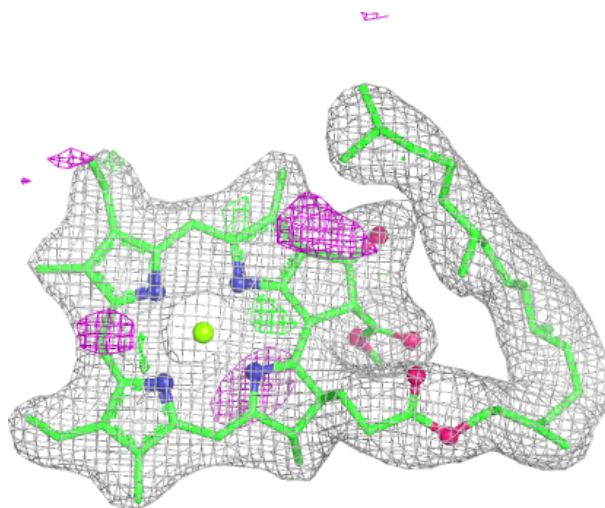
**Electron density around CLA C 508:**

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



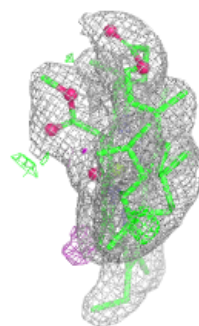
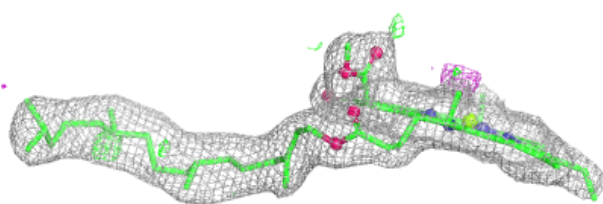
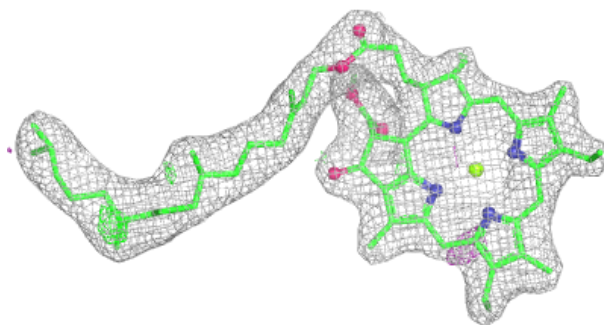
Electron density around CLA B 610:

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

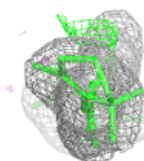
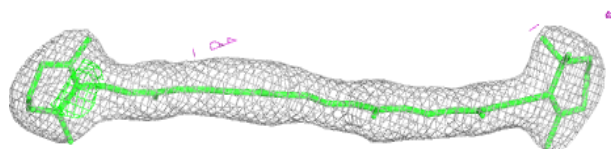
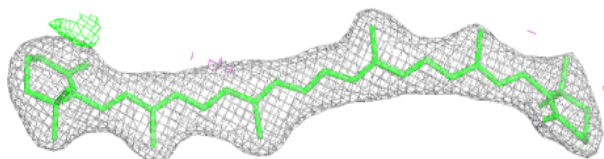


Electron density around CLA B 602:

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

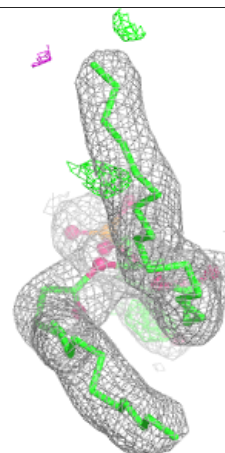
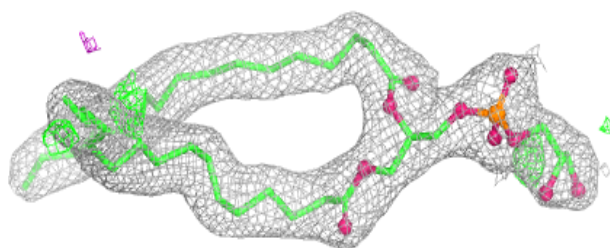
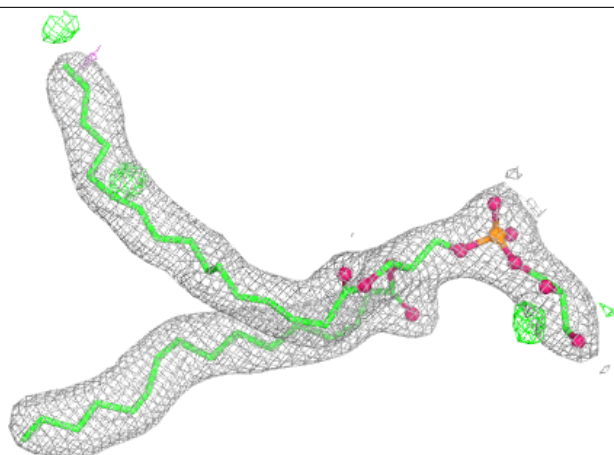
**Electron density around BCR c 516:**

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



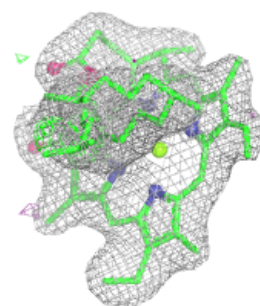
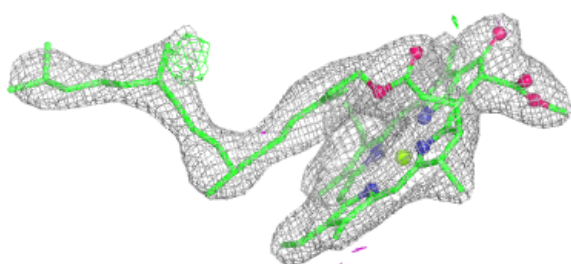
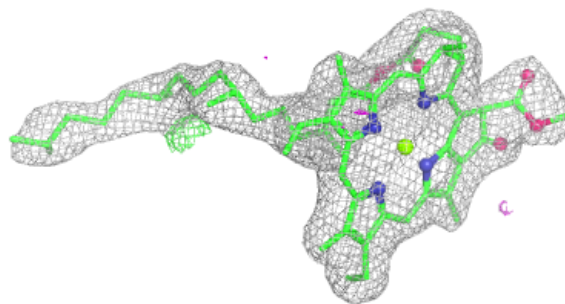
Electron density around LHG d 407:

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

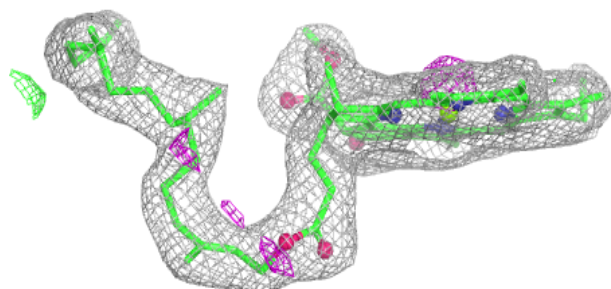
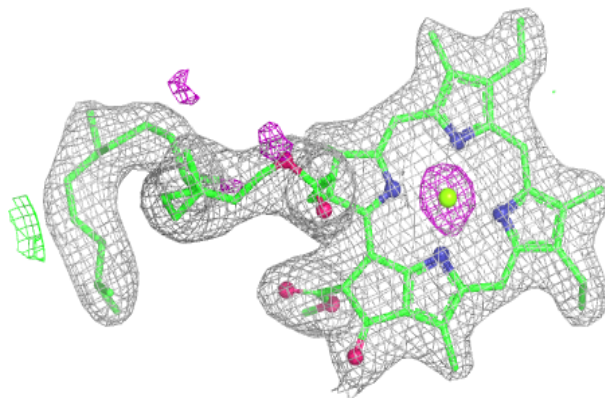


Electron density around CLA c 506:

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

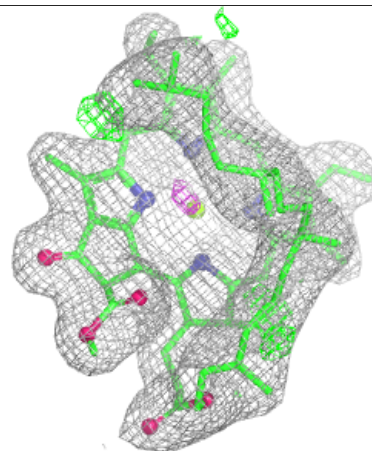
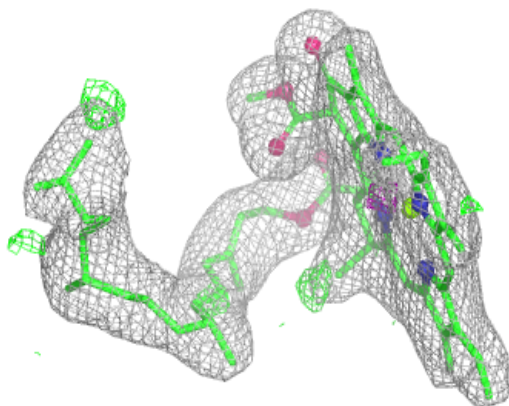
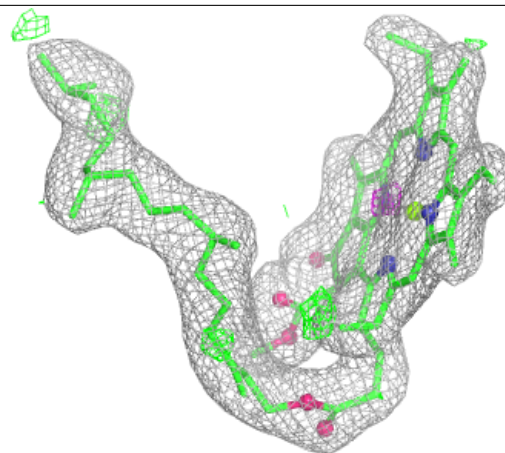
**Electron density around CLA B 612:**

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

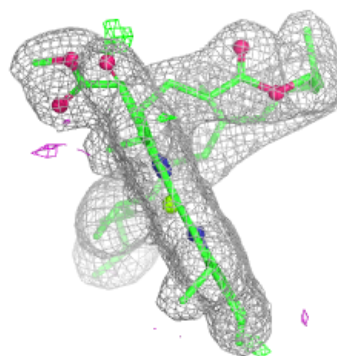
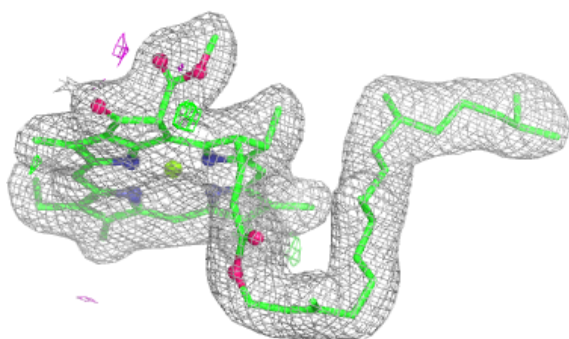
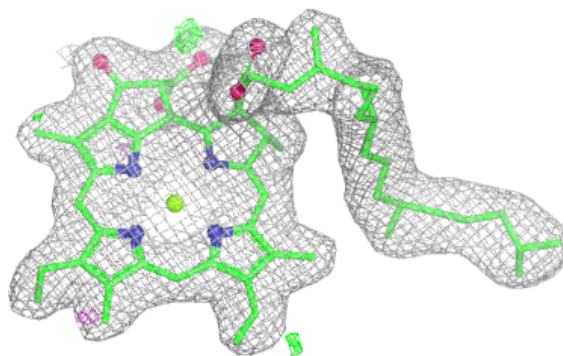


Electron density around CLA B 613:

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

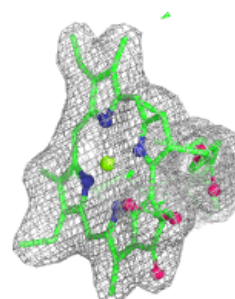
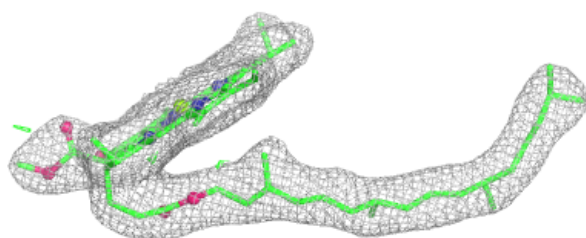
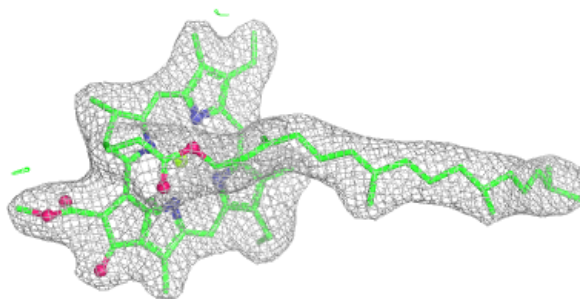
**Electron density around CLA A 405:**

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



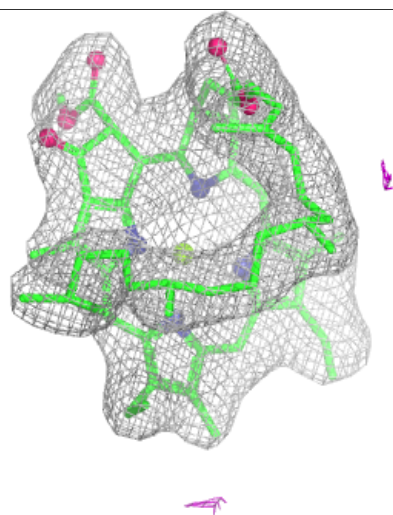
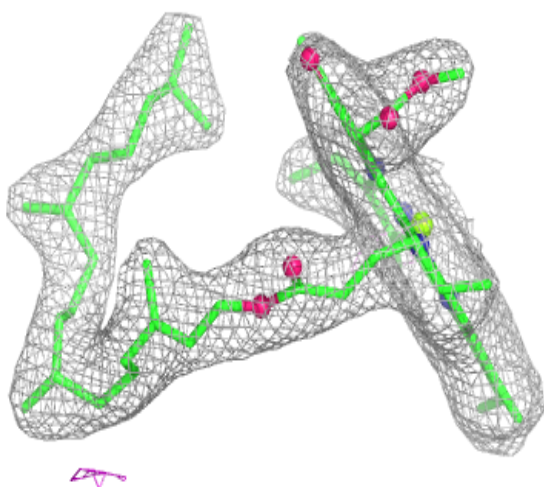
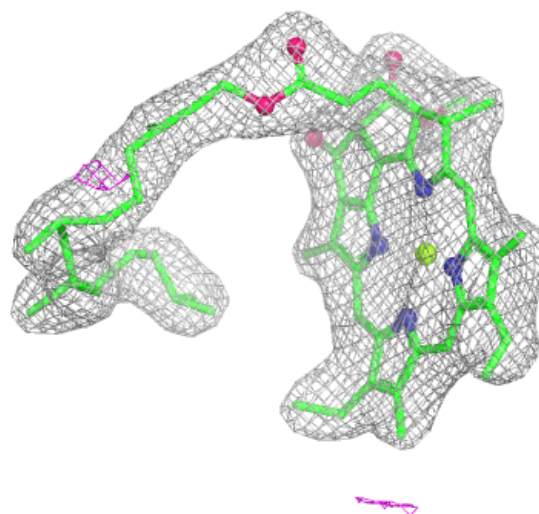
Electron density around CLA b 608:

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



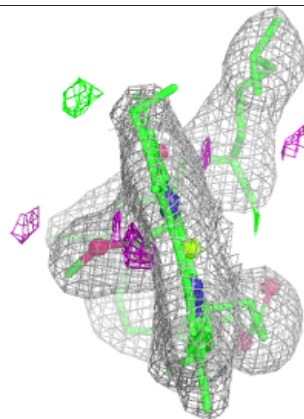
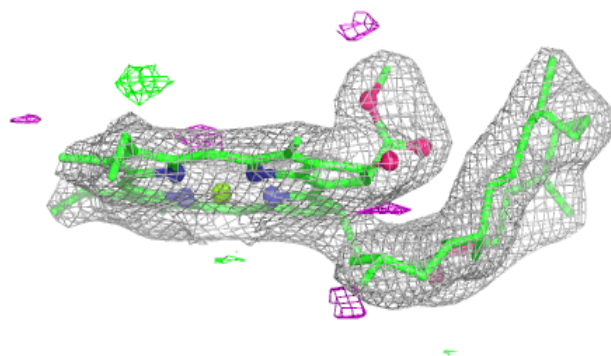
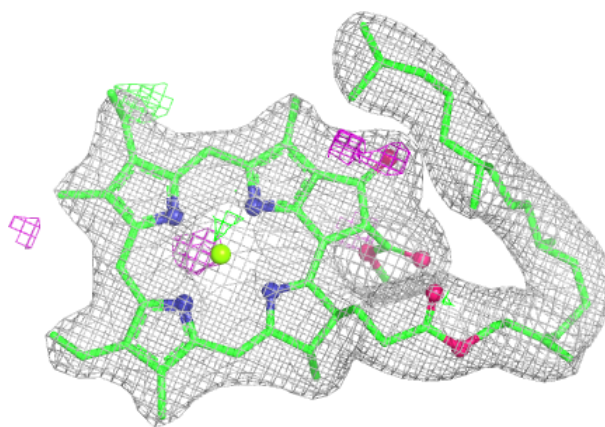
Electron density around CLA C 504:

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



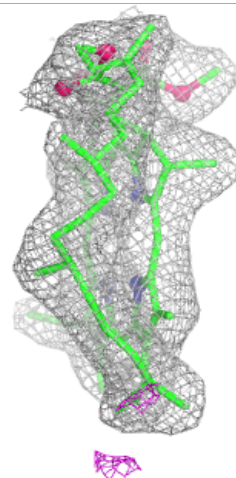
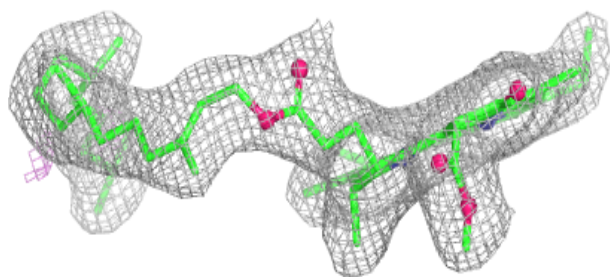
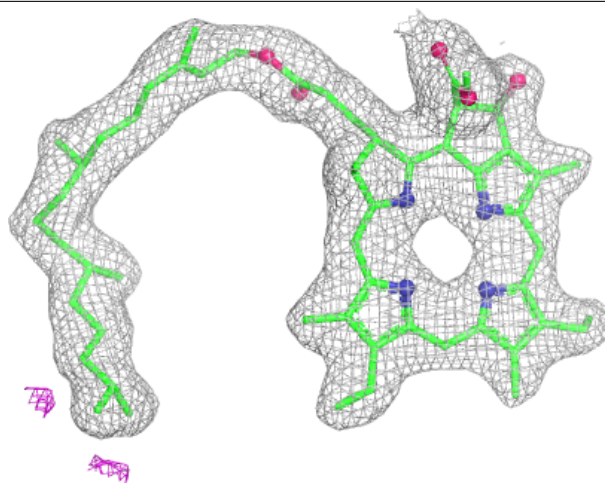
Electron density around CLA b 610:

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



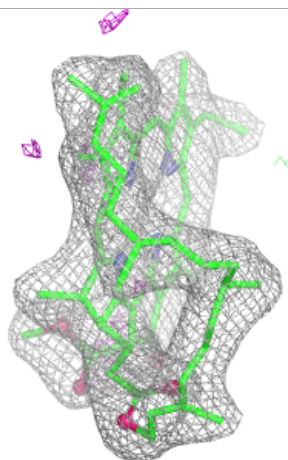
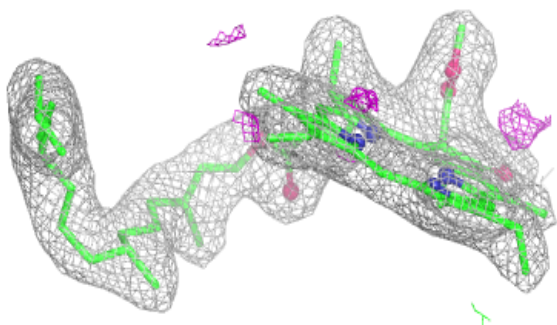
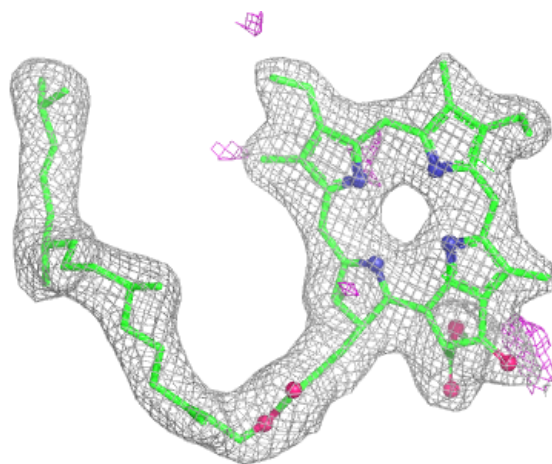
Electron density around PHO A 407:

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



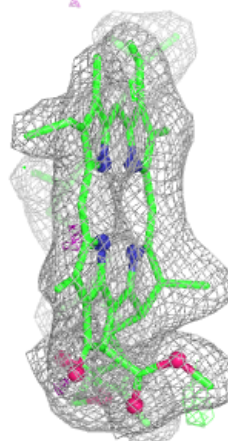
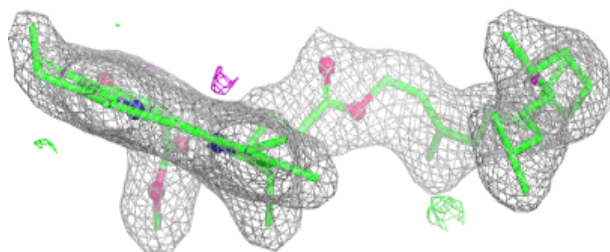
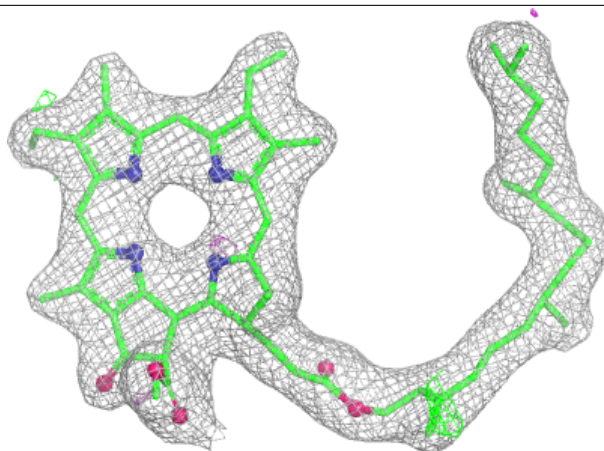
Electron density around PHO A 353:

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



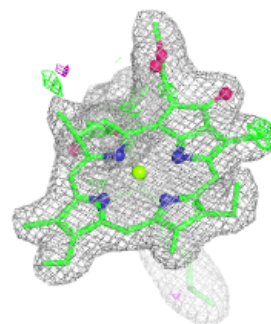
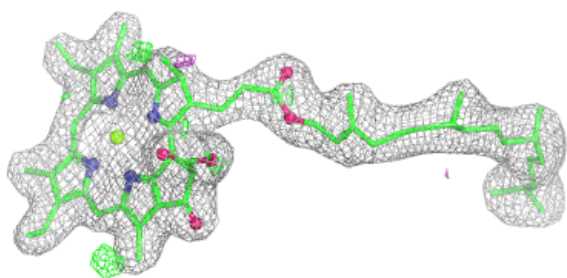
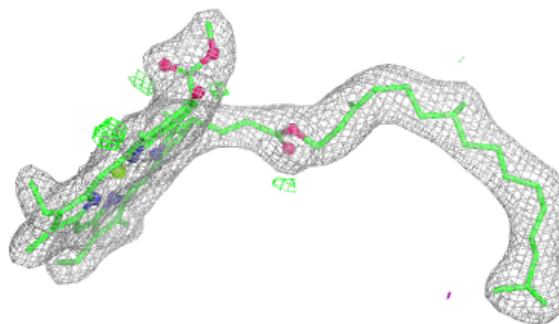
Electron density around PHO a 408:

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

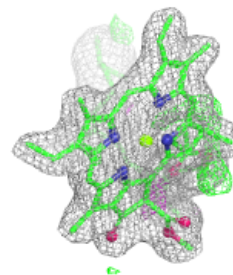
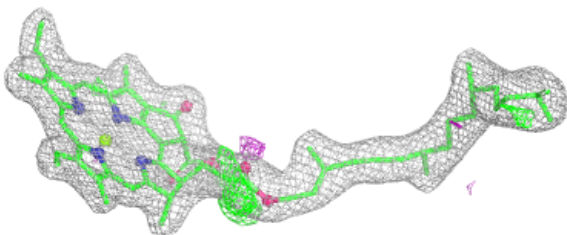
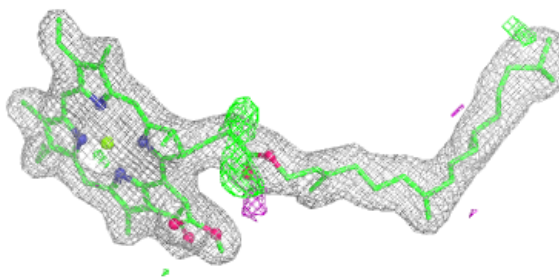


Electron density around CLA D 405:

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

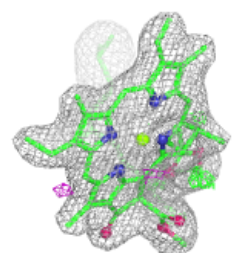
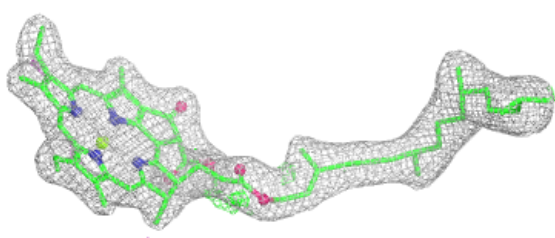
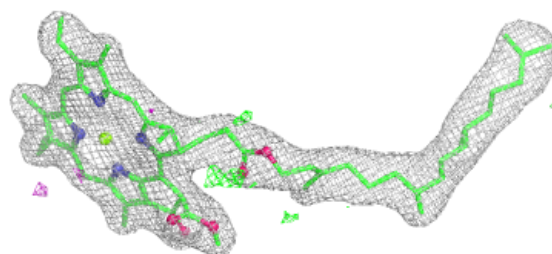
**Electron density around CLA A 404:**

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

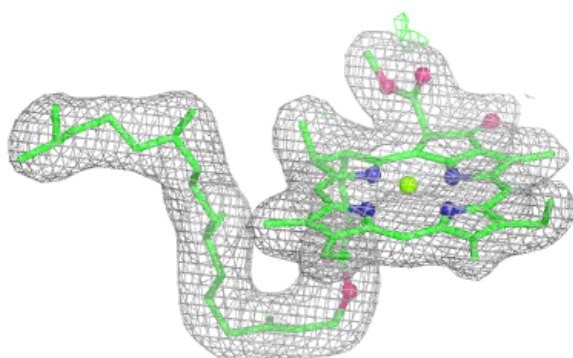
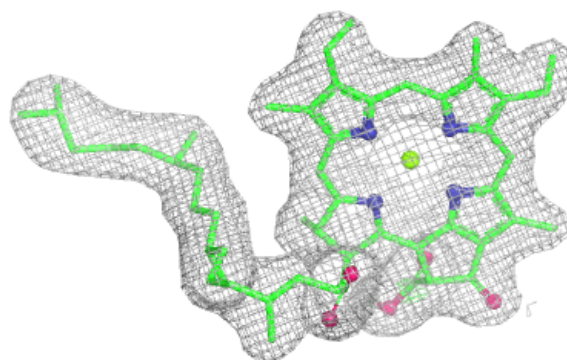


Electron density around CLA a 405:

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

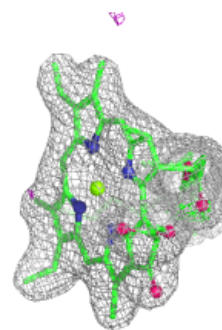
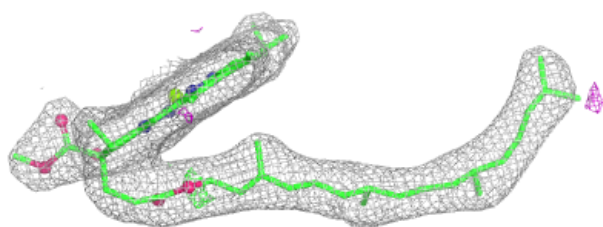
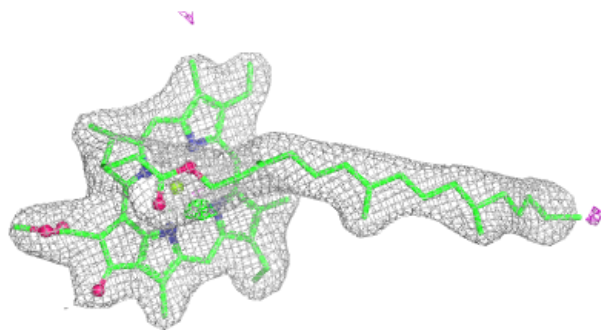
**Electron density around CLA a 406:**

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

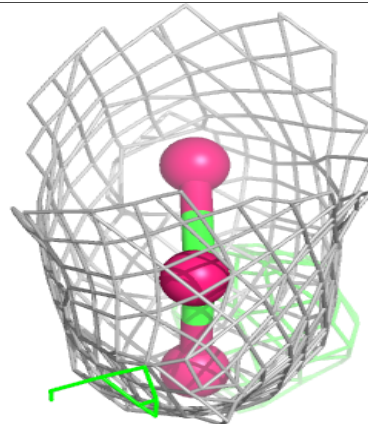
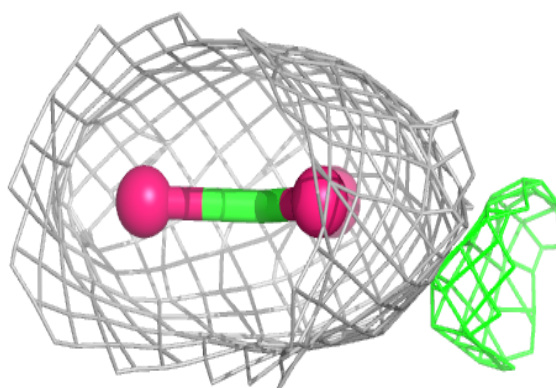
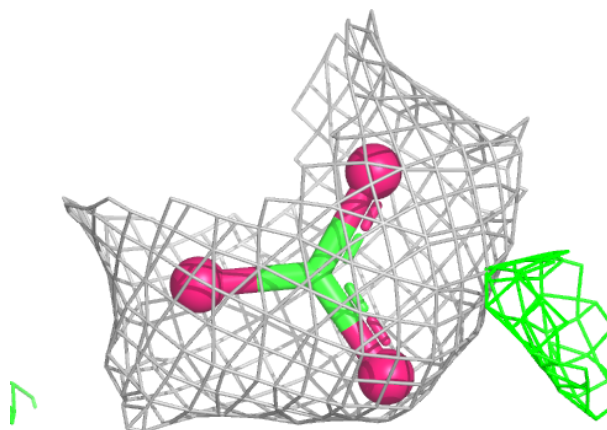


Electron density around CLA B 608:

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

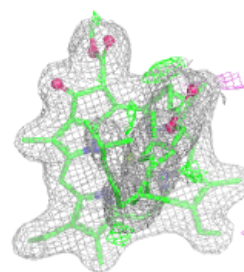
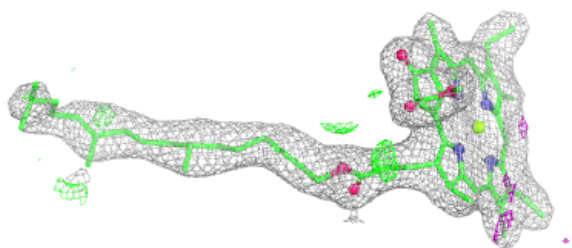
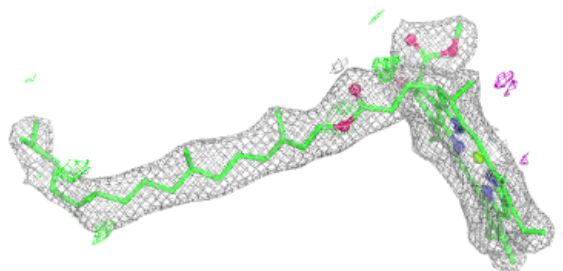
**Electron density around BCT A 348:**

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



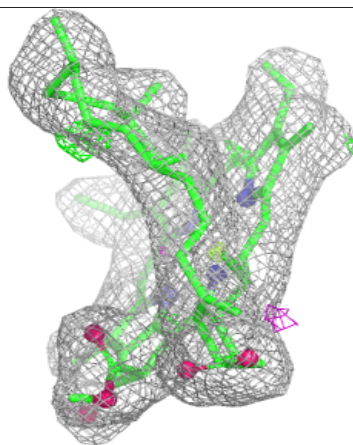
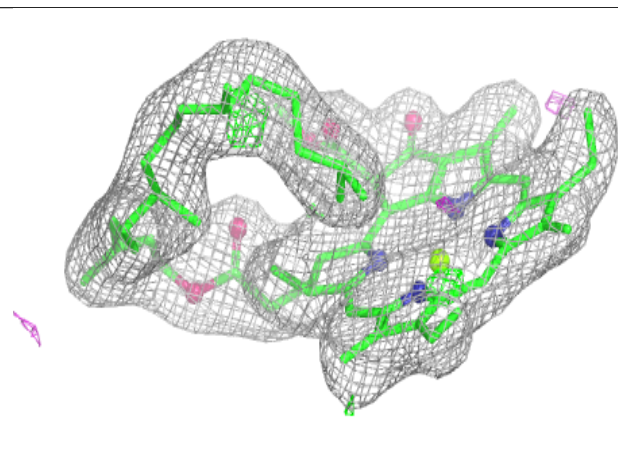
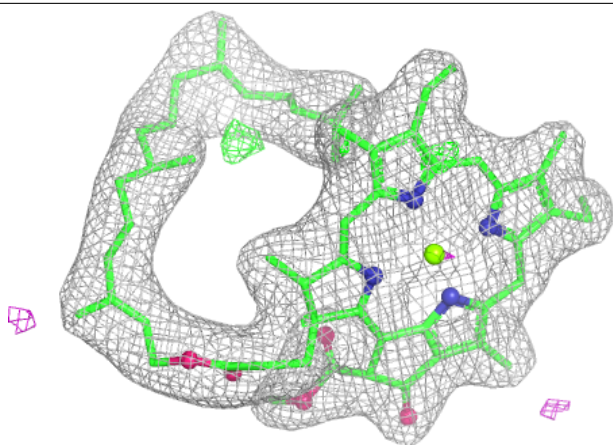
Electron density around CLA B 604:

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



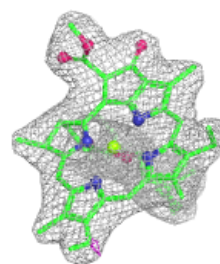
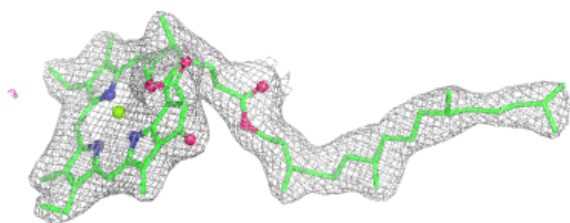
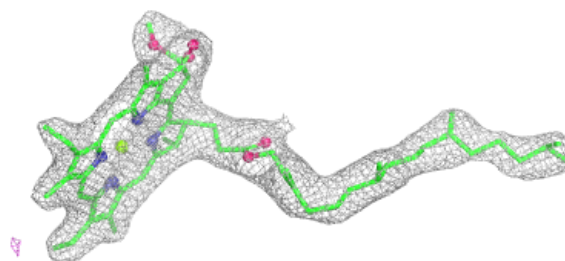
Electron density around CLA B 615:

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



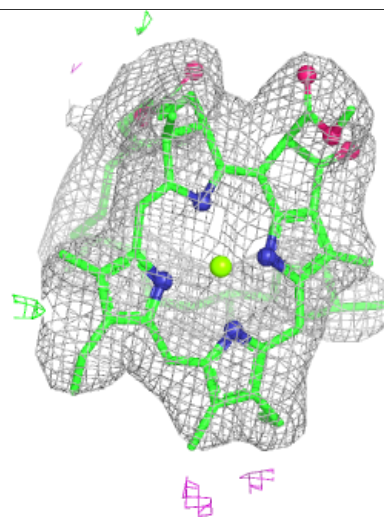
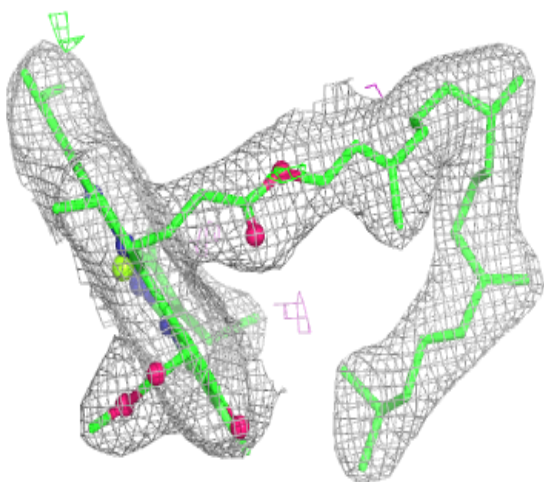
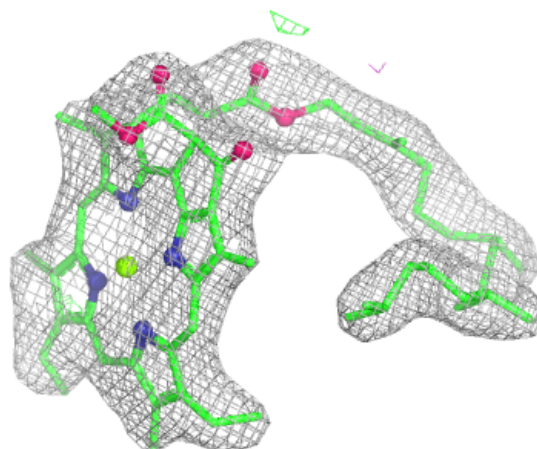
Electron density around CLA c 503:

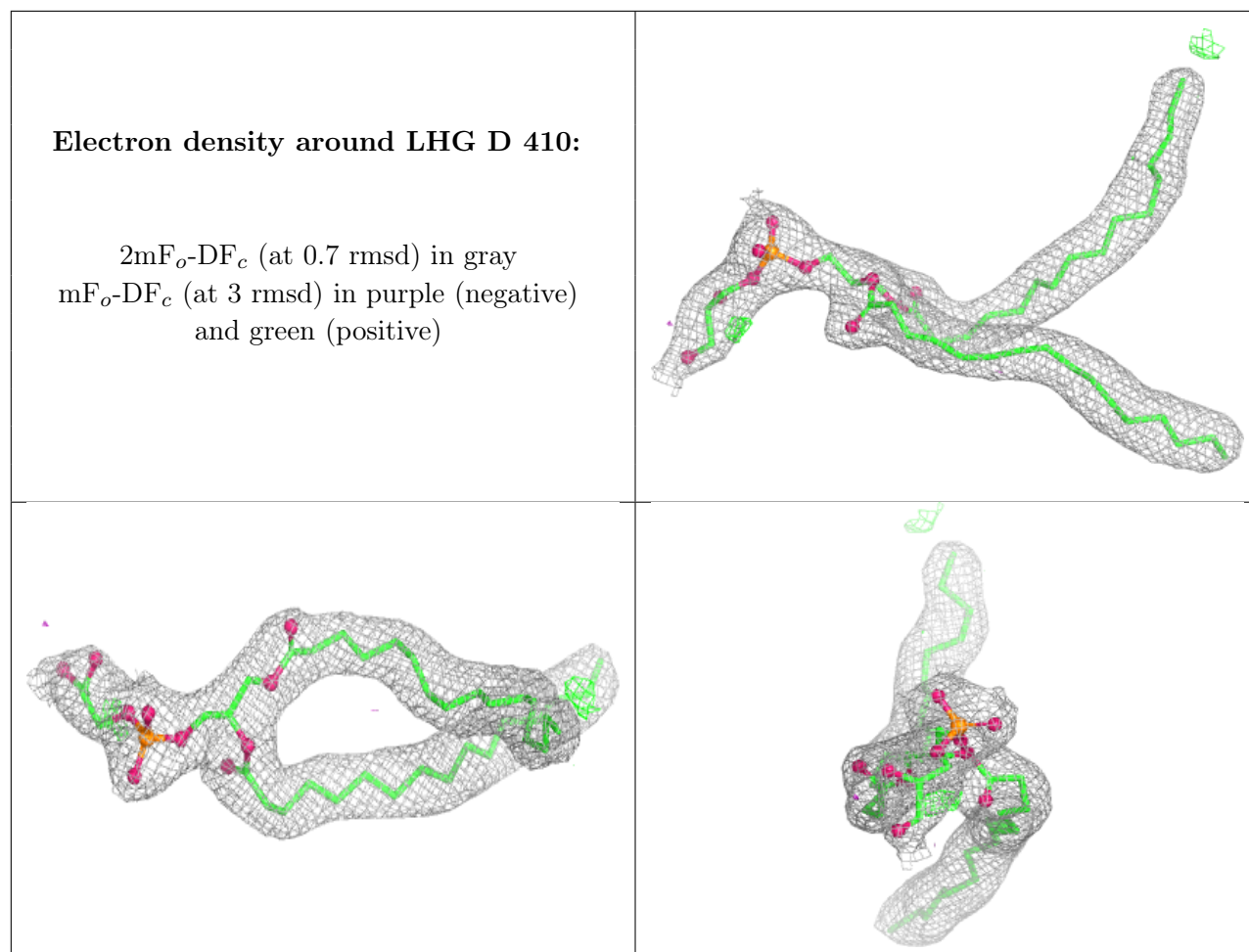
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA c 504:

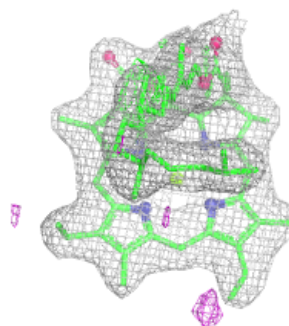
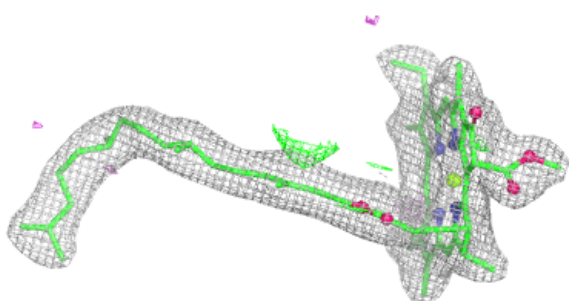
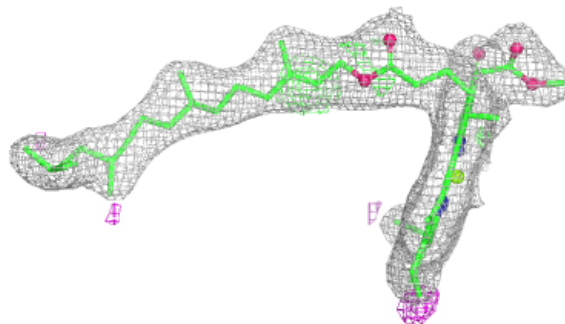
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





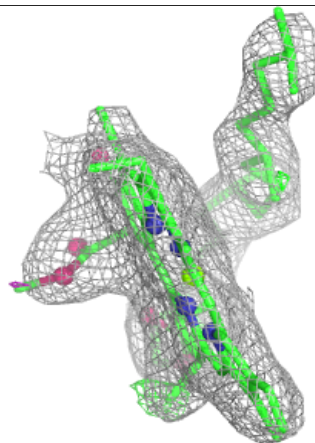
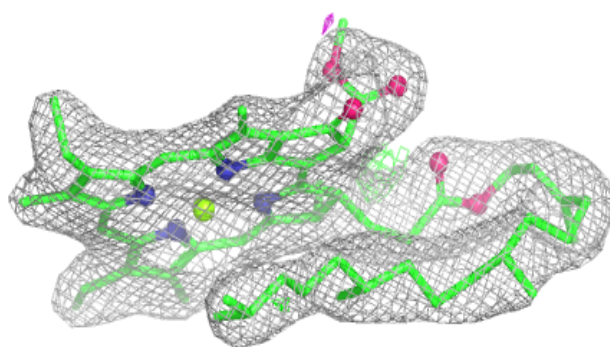
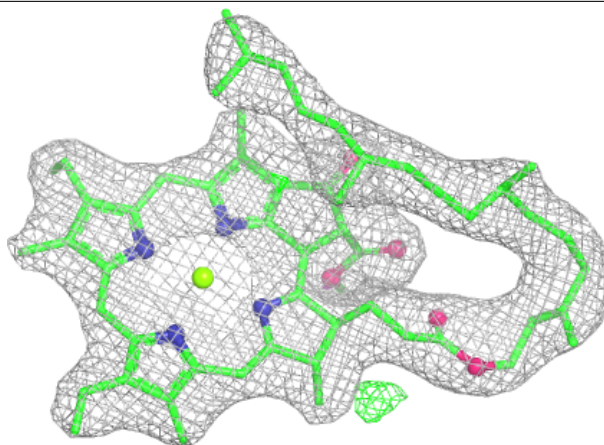
Electron density around CLA B 605:

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



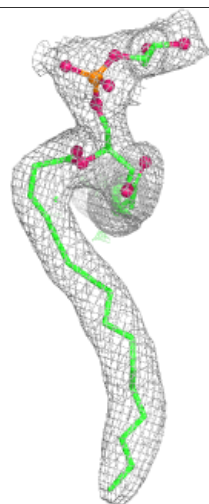
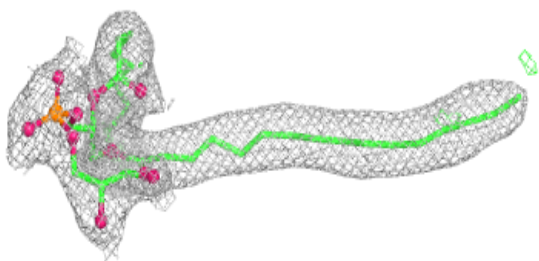
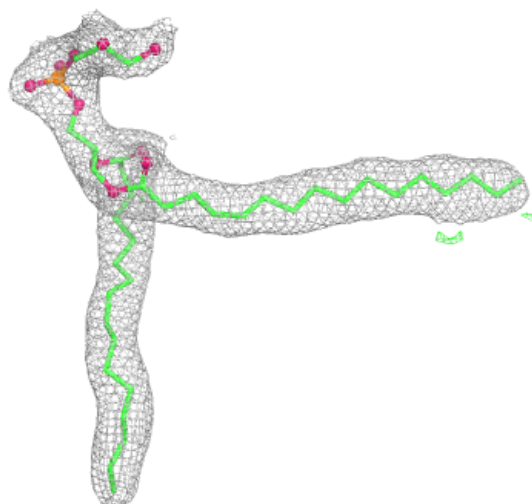
Electron density around CLA C 510:

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



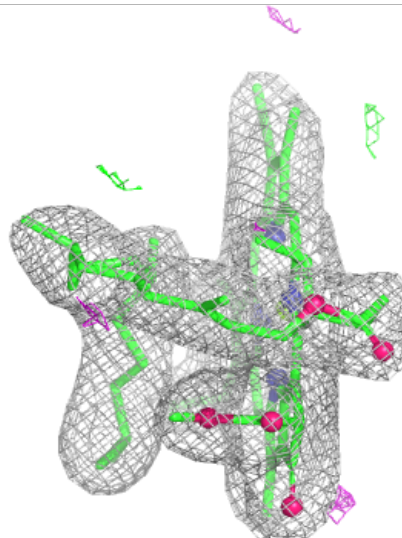
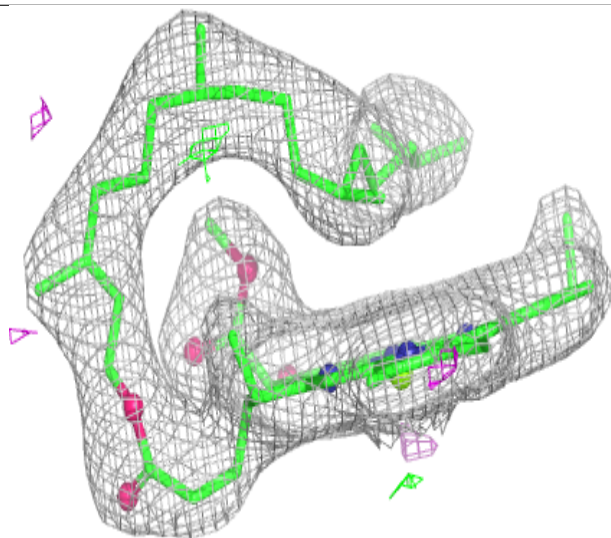
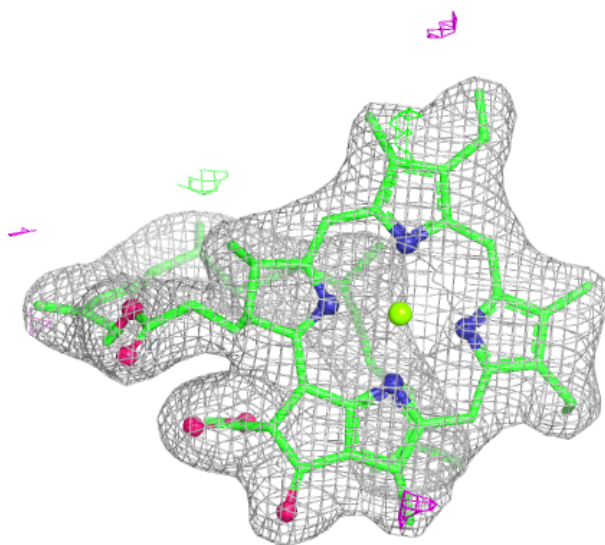
Electron density around LHG L 101:

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



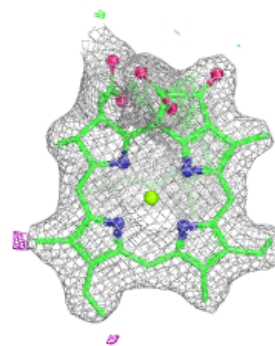
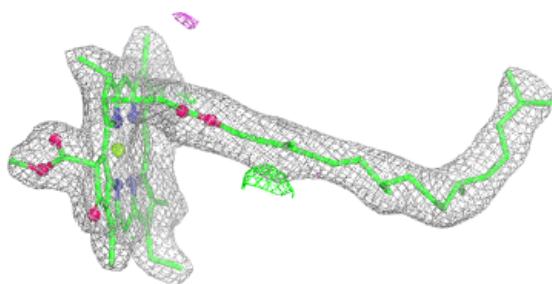
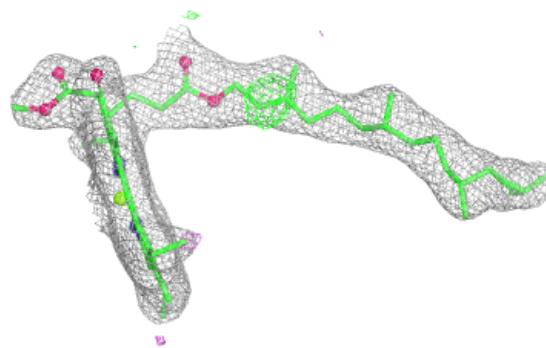
Electron density around CLA C 511:

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

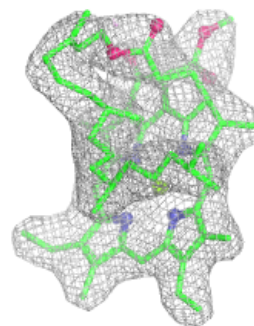
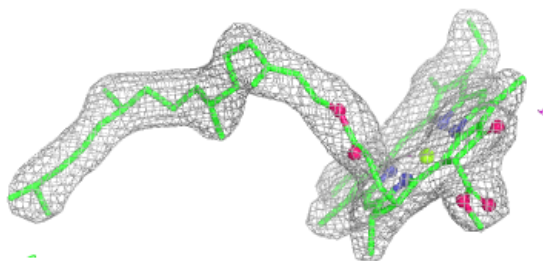
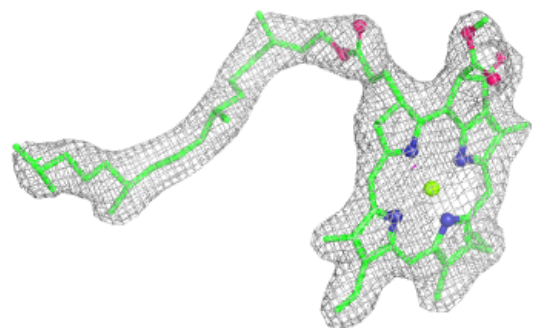


Electron density around CLA b 605:

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

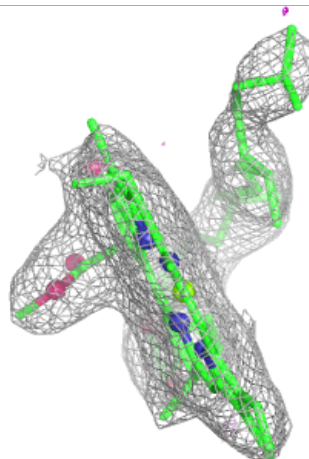
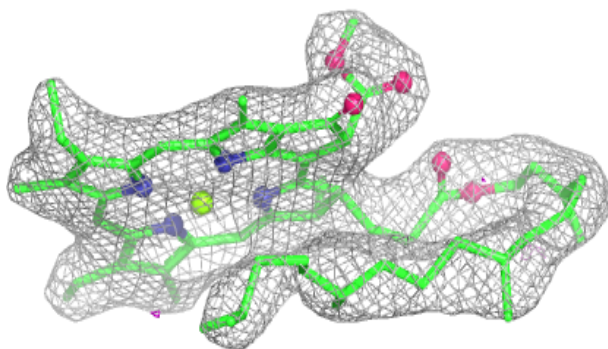
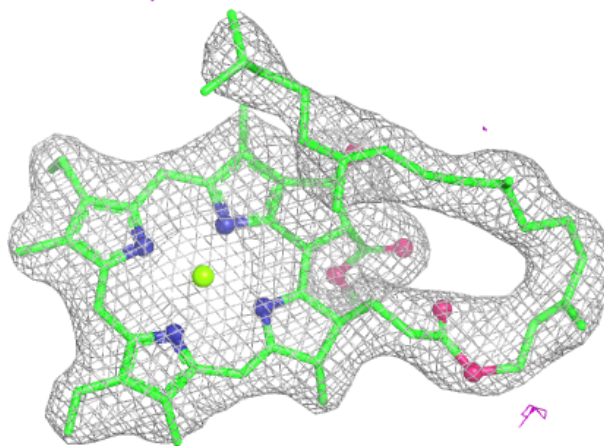
**Electron density around CLA C 512:**

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



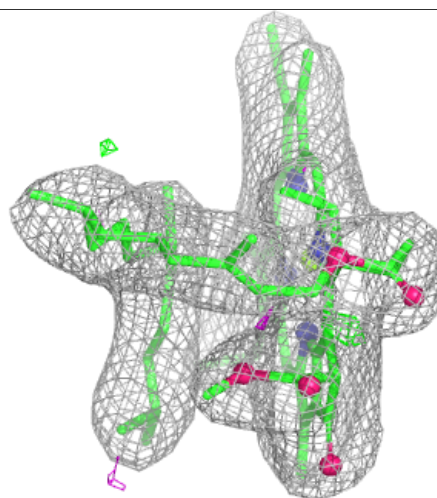
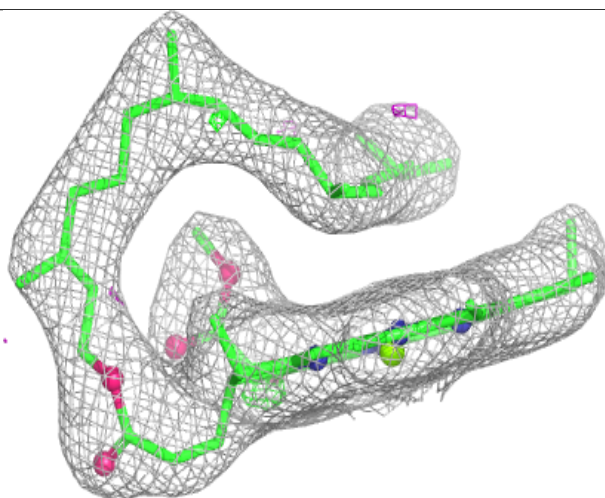
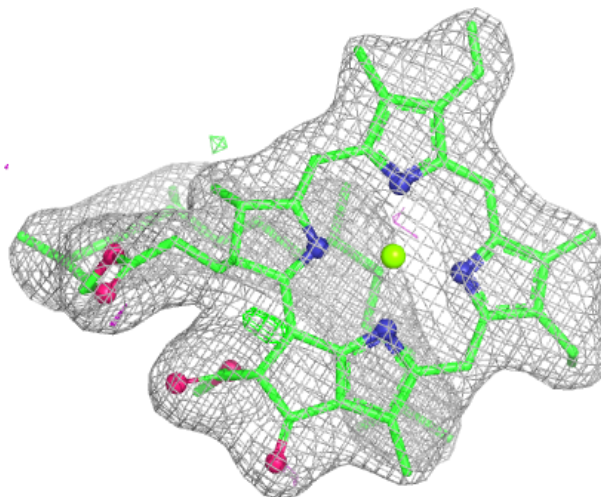
Electron density around CLA c 510:

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



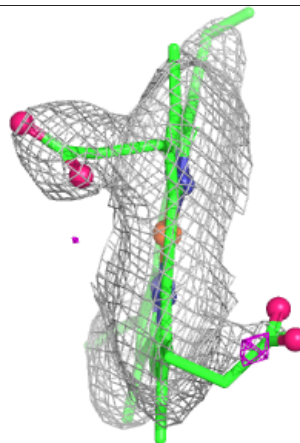
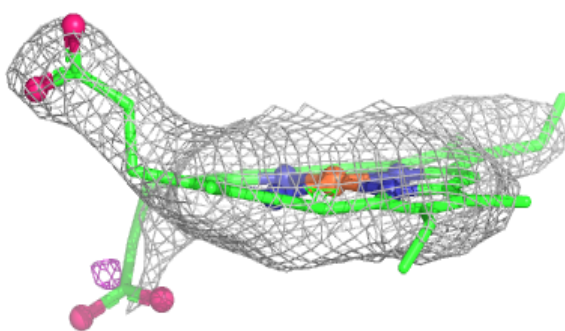
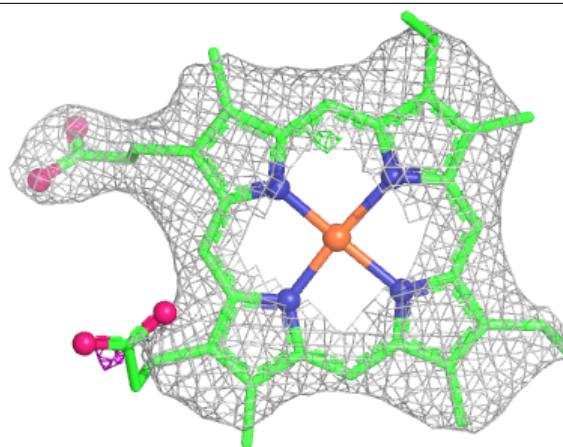
Electron density around CLA c 511:

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



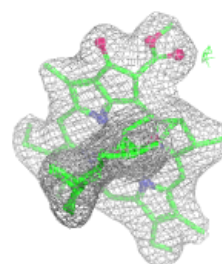
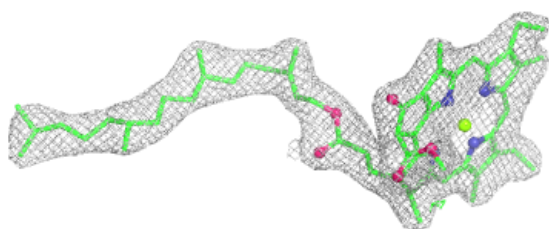
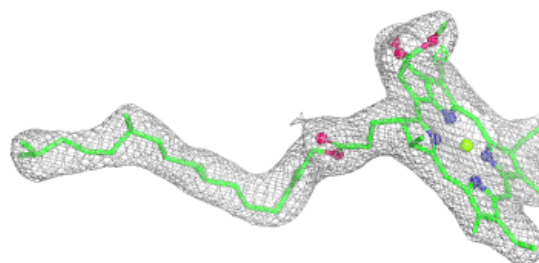
Electron density around HEM e 87:

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



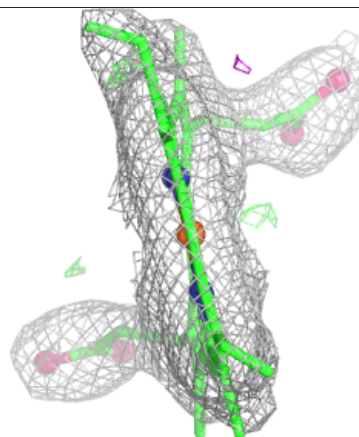
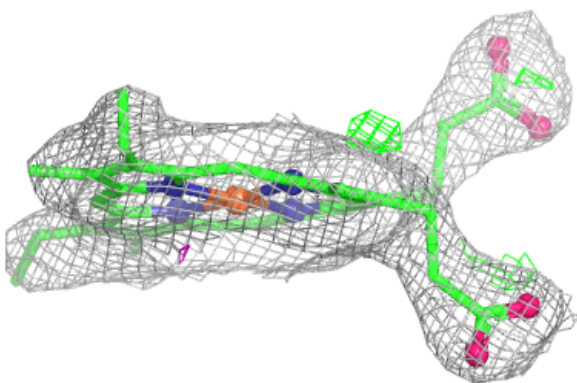
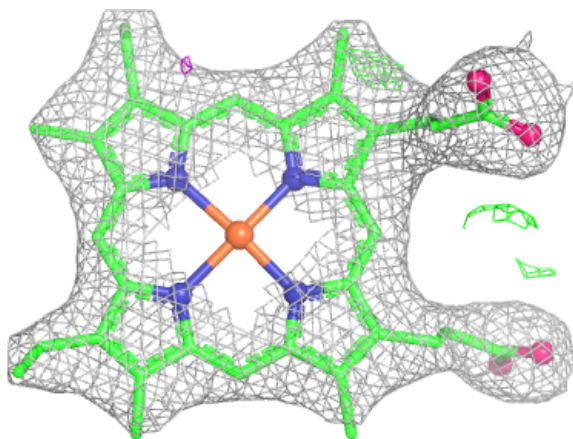
Electron density around CLA C 503:

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



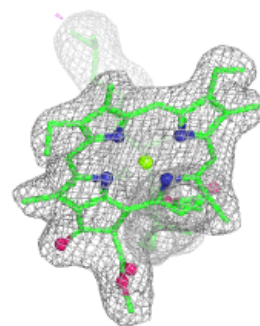
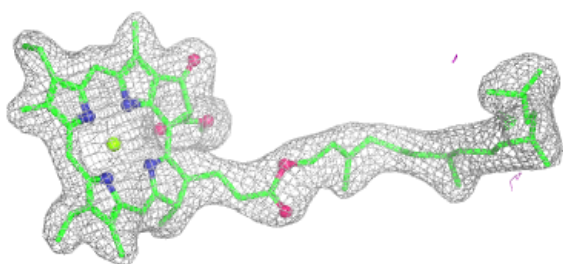
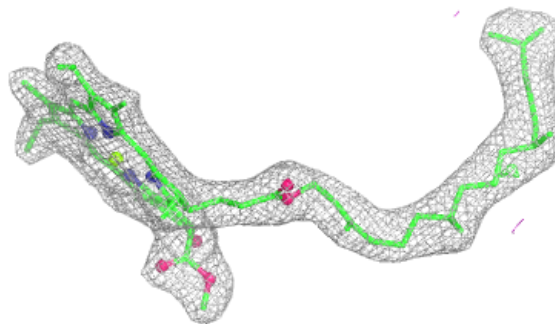
Electron density around HEM E 103:

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



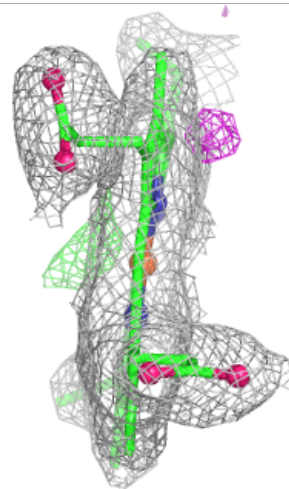
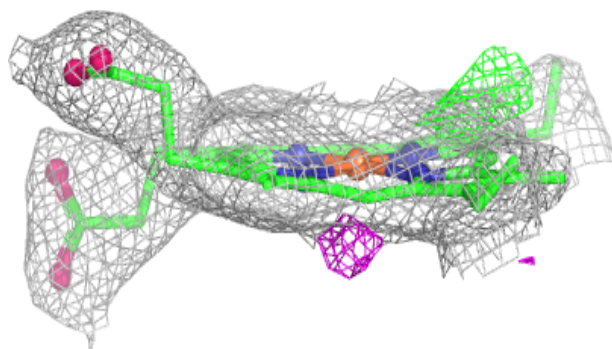
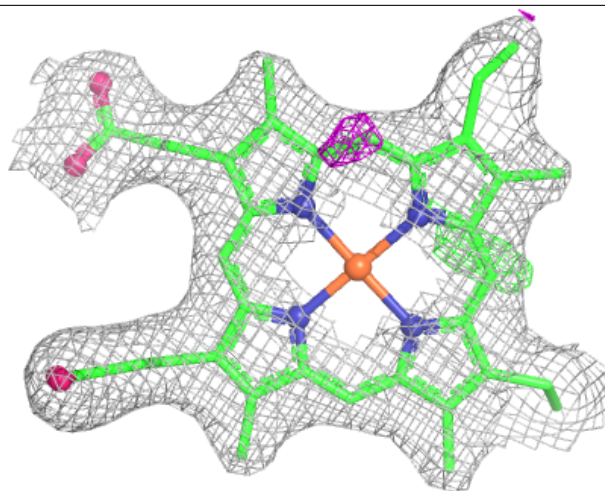
Electron density around CLA d 402:

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



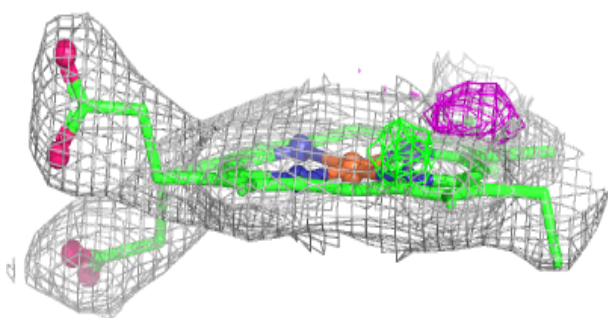
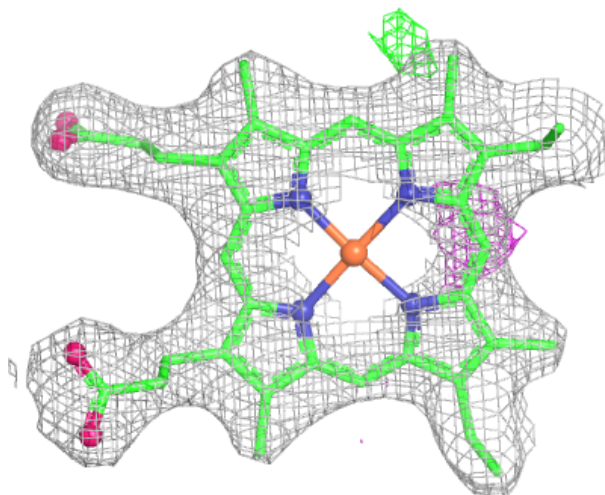
Electron density around HEC V 202:

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



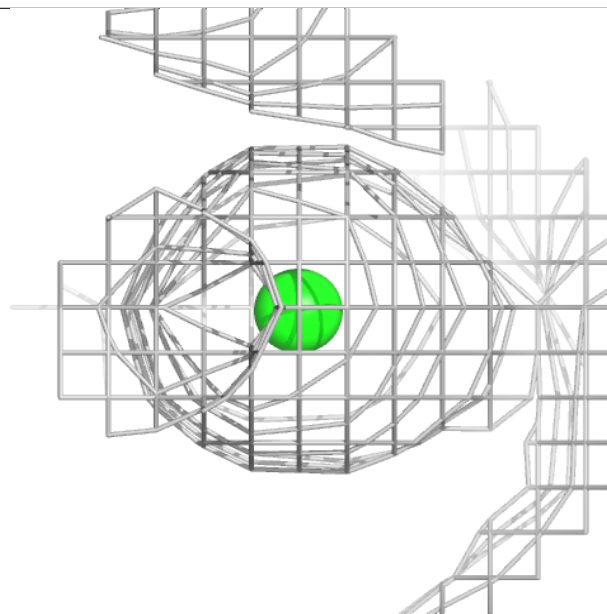
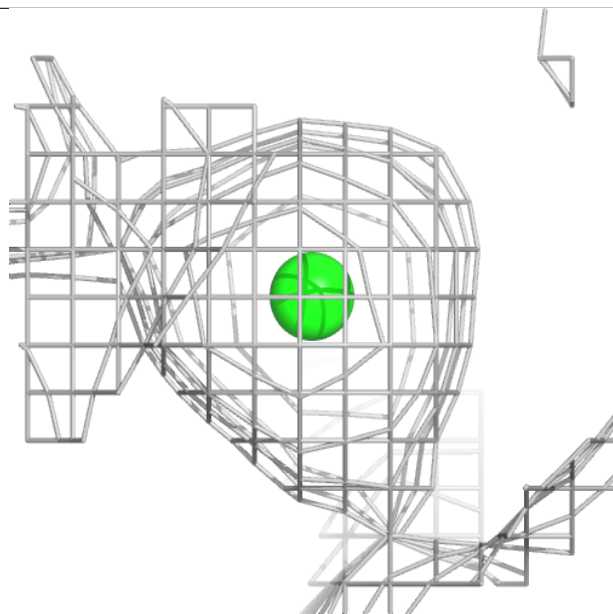
Electron density around HEC v 202:

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



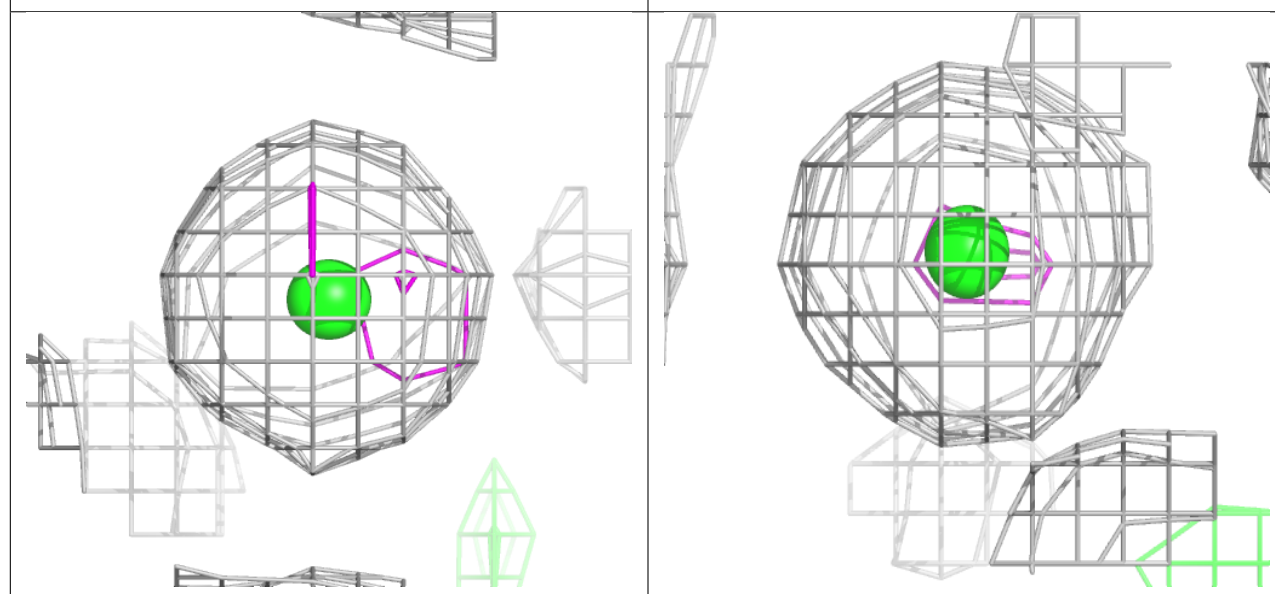
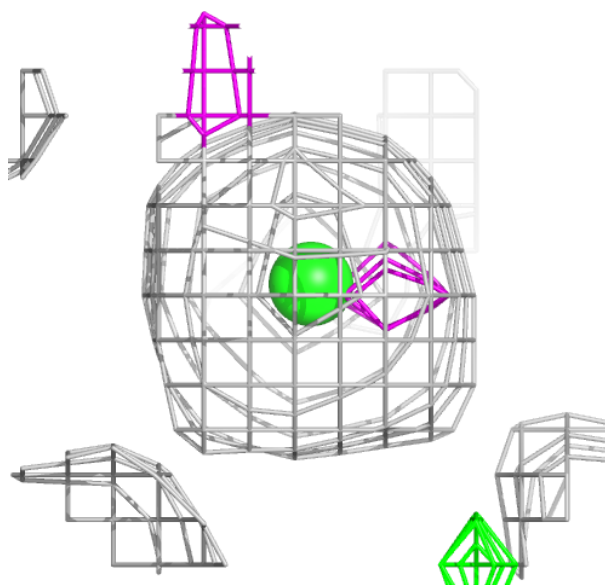
Electron density around CL a 403:

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



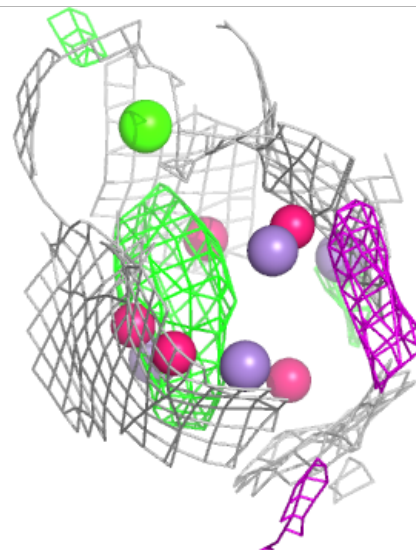
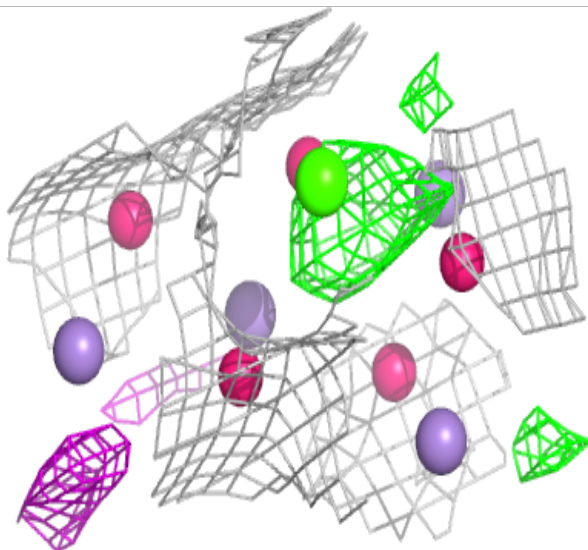
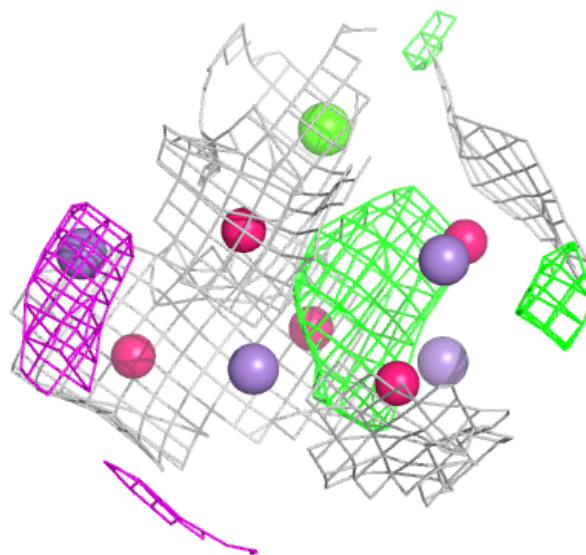
Electron density around CL A 402:

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



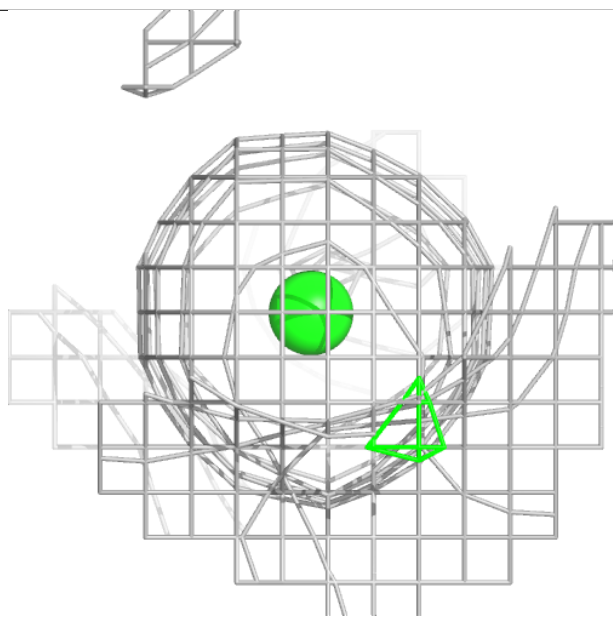
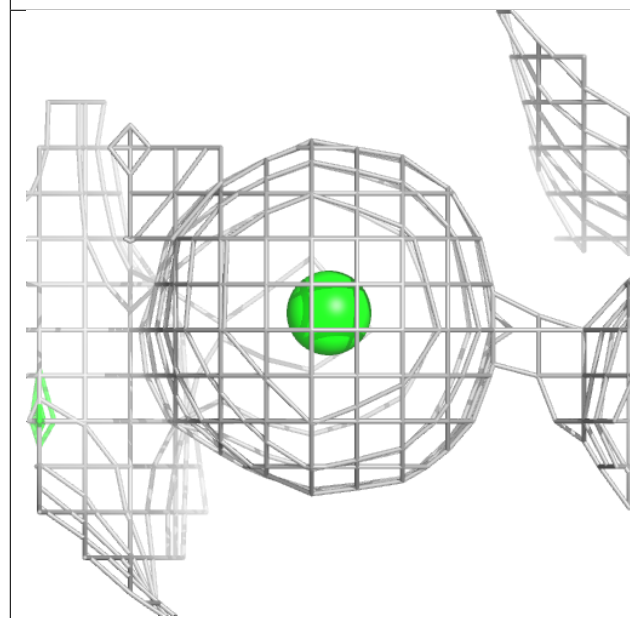
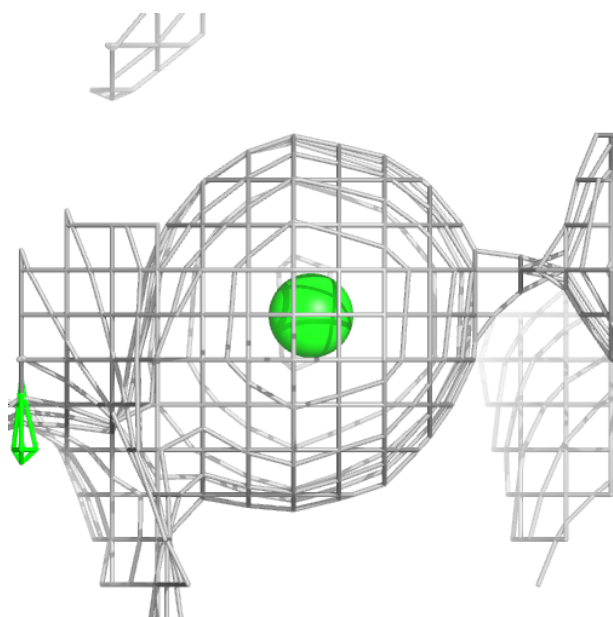
Electron density around OEX A 413:

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



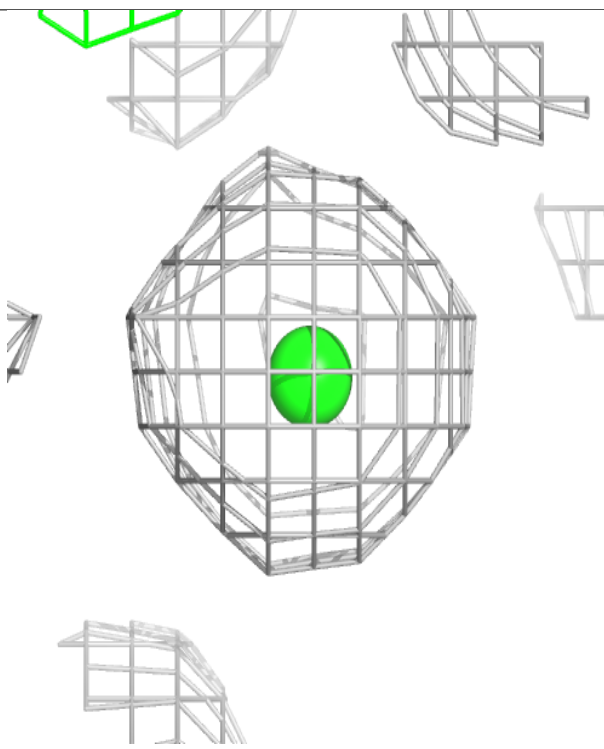
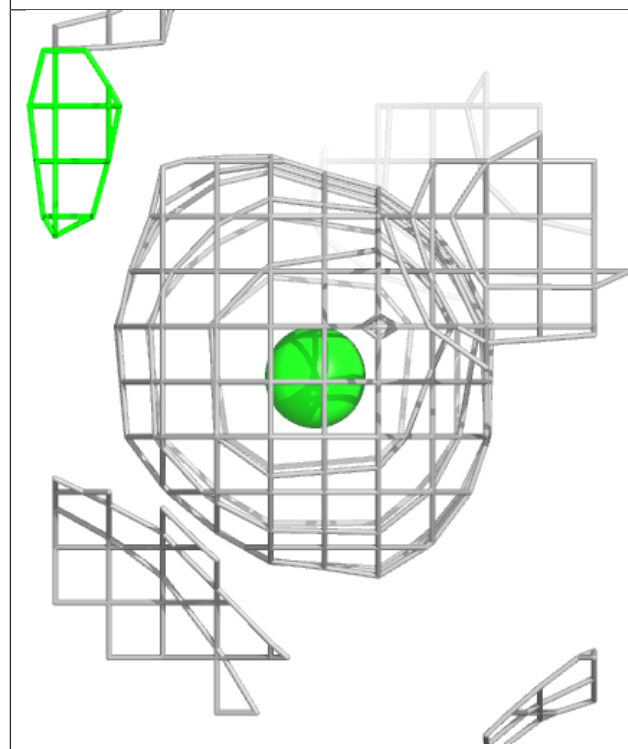
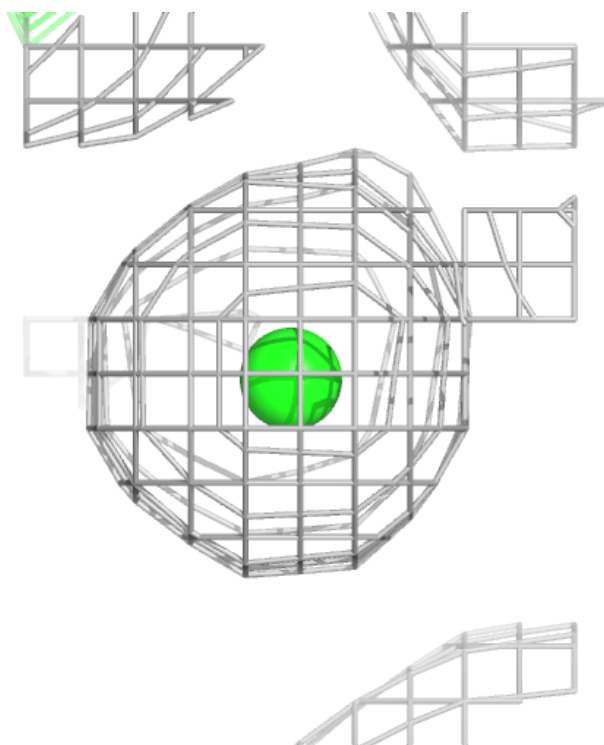
Electron density around CL A 403:

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



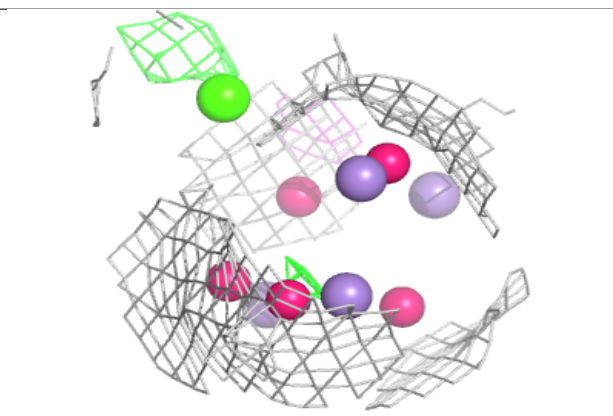
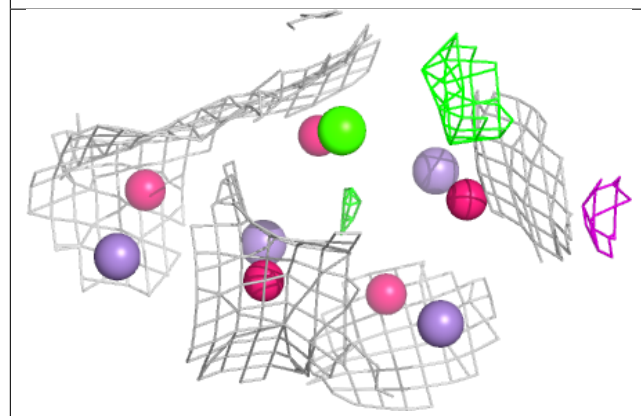
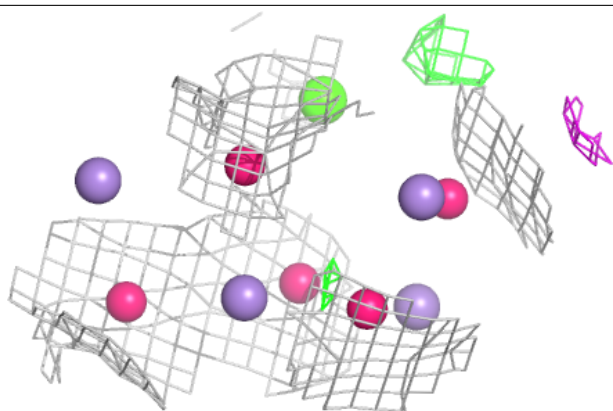
Electron density around CL a 402:

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



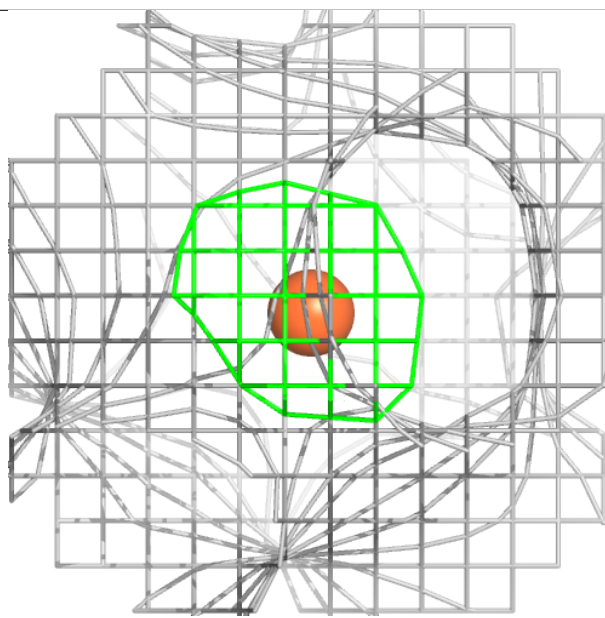
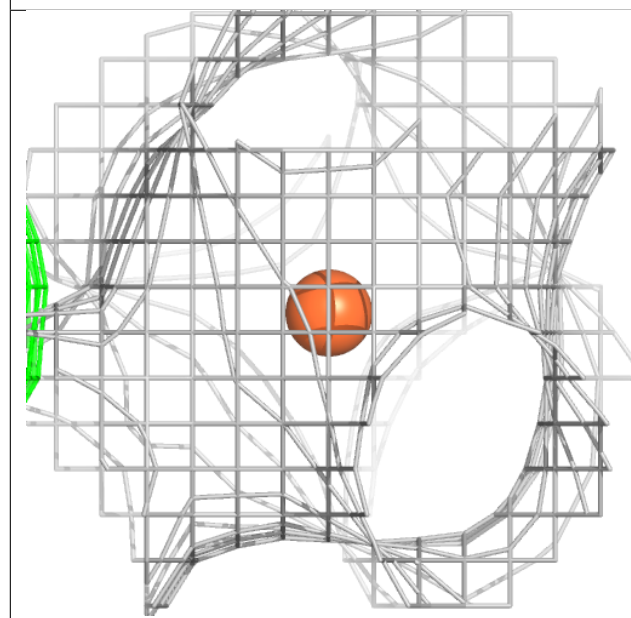
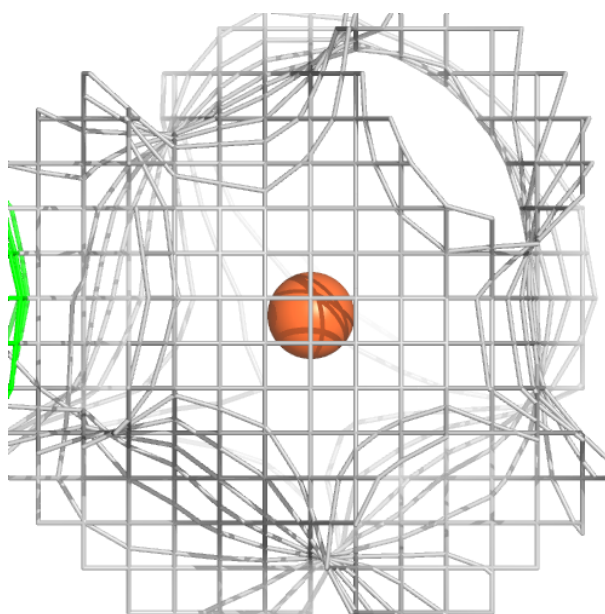
Electron density around OEX a 415:

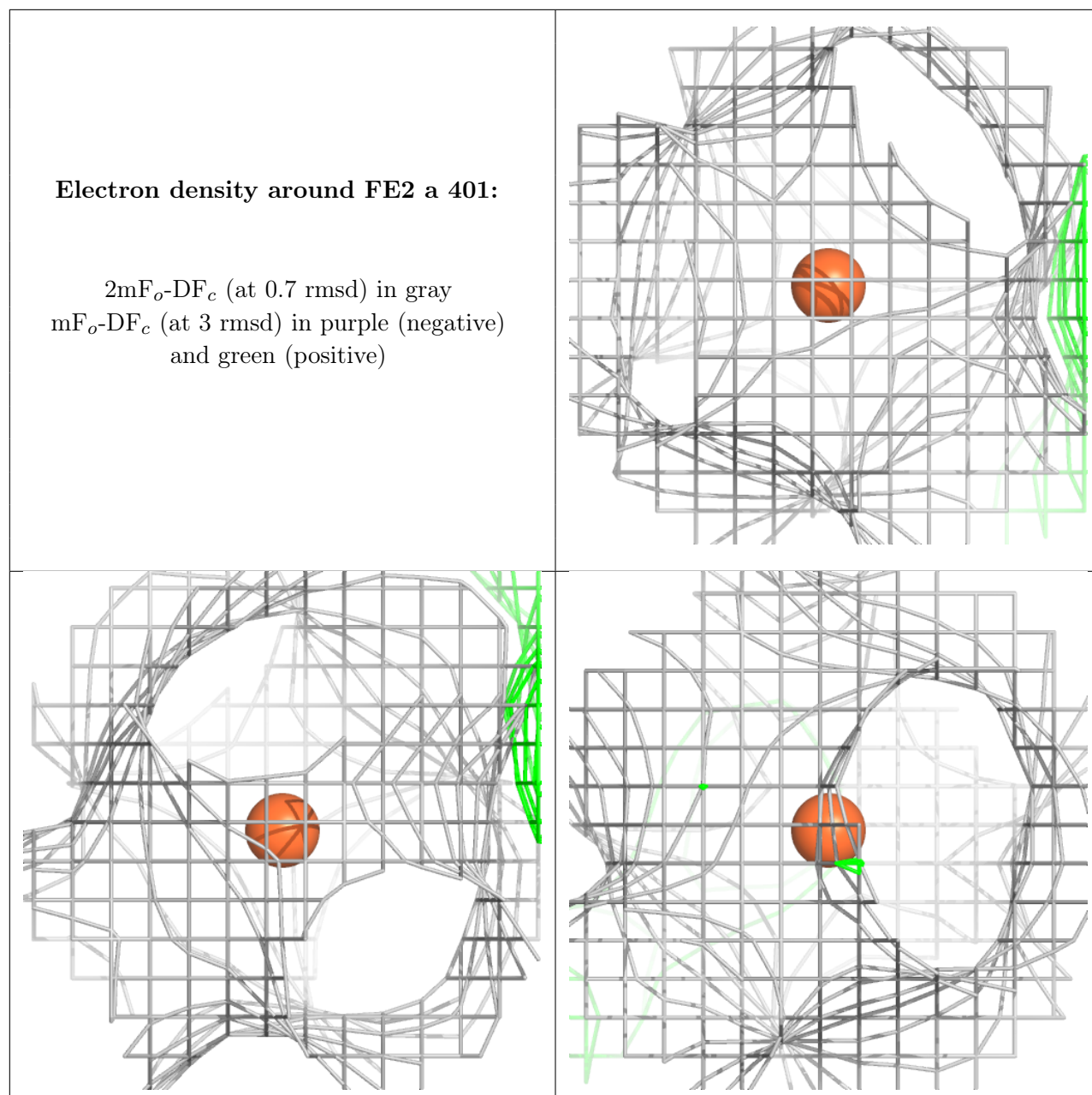
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE2 A 401:

$2mF_o-DF_c$ (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.