



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 12:21 AM UTC

PDB ID : 8IRG / pdb_00008irg
Title : XFEL structure of cyanobacterial photosystem II following two flashes (2F)
with a 30-microsecond delay
Authors : Li, H.; Suga, M.; Shen, J.R.
Deposited on : 2023-03-17
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

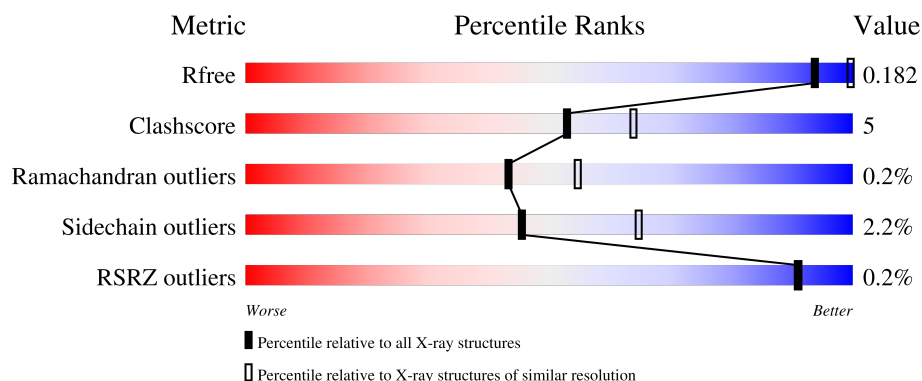
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	88% 9% .
1	a	344	85% 12% .
2	B	505	92% 7%
2	b	505	% 91% 8% .
3	C	455	91% 8% .

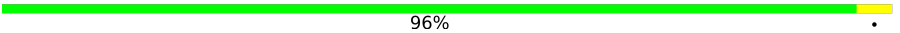
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Mol	Chain	Length	Quality of chain
3	c	455	 89% 10% .
4	D	342	 89% 11%
4	d	342	 91% 9%
5	E	84	 79% 18% .
5	e	84	 79% 15% 6%
6	F	44	 66% 11% 23%
6	f	44	 61% 9% 30%
7	H	65	 92% 6% .
7	h	65	 86% 9% . .
8	I	38	 79% 18% .
8	i	38	 84% 13% .
9	J	39	 82% 13% . .
9	j	39	 92% 8%
10	K	37	 81% 16% .
10	k	37	 76% 19% 5%
11	L	37	 92% 5% .
11	l	37	 92% 5% .
12	M	36	 81% 6% 6% 8%
12	m	36	 81% 11% . 6%
13	O	244	 86% 13%
13	o	244	 92% 7%
14	T	32	 81% 12% 6%
14	t	32	 81% 12% 6%
15	U	104	 85% 8% 8%
15	u	104	 92% . 7%

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Mol	Chain	Length	Quality of chain
16	V	137	 96% .
16	v	137	 91% 9% .
17	X	40	 82% 12% 5%
17	x	40	 88% 8% 5%
18	Y	30	 87% 10% .
18	y	30	 50% 43% . .
19	Z	62	 87% 11% .
19	z	62	 76% 24%
20	R	34	 6% 74% 24% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	404[A]	X	-	-	-
23	CLA	A	404[B]	X	-	-	-
23	CLA	A	405[A]	X	-	-	-
23	CLA	A	405[B]	X	-	-	-
23	CLA	A	407	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	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	C	515	X	-	-	-
23	CLA	D	404[A]	X	-	-	-
23	CLA	D	404[B]	X	-	-	-
23	CLA	D	405	X	-	-	-
23	CLA	a	405[A]	X	-	-	-
23	CLA	a	405[B]	X	-	-	-
23	CLA	a	406[A]	X	-	-	-
23	CLA	b	601	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	513	X	-	-	-
23	CLA	c	514	X	-	-	-
23	CLA	d	401[A]	X	-	-	-
23	CLA	d	401[B]	X	-	-	-
23	CLA	d	402	X	-	-	-
25	GOL	D	403	-	-	X	-
25	GOL	D	414	-	X	-	-
25	GOL	a	419	-	-	X	-

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 62602 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
1	A	334	Total	C	N	O	S	0	222	0
			4338	2836	717	760	25			
1	a	334	Total	C	N	O	S	0	221	0
			4330	2830	716	759	25			

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
2	B	504	Total	C	N	O	S	0	20	0
			4146	2721	692	720	13			
2	b	504	Total	C	N	O	S	0	19	0
			4134	2718	687	716	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	97	0
			4260	2788	713	741	18			
3	c	455	Total	C	N	O	S	0	100	0
			4308	2821	719	750	18			

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O		0	0	0
			662	432	107	123				
5	e	79	Total	C	N	O		0	2	0
			670	439	110	121				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	31	Total	C	N	O	S	0	1	0
			261	179	43	38	1			

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

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

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	36	Total	C	N	O	0	2	0
			311	207	49	55			
11	l	36	Total	C	N	O	0	2	0
			311	207	49	55			

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	10	0
			1958	1221	335	398	4			
13	o	243	Total	C	N	O	S	0	8	0
			1933	1207	330	392	4			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

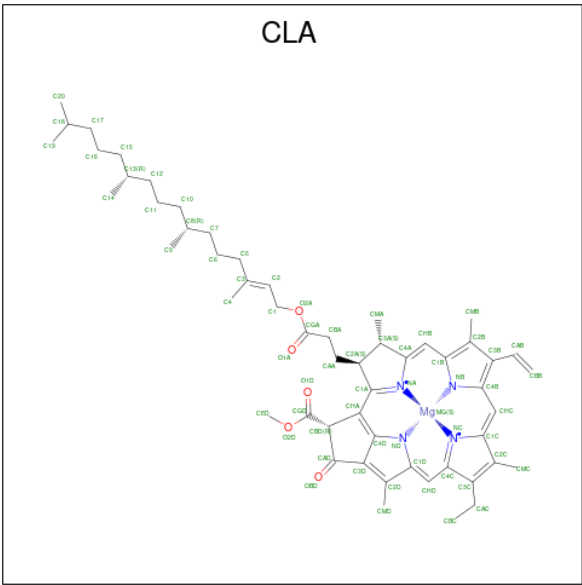
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	2
			4	4		

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

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



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

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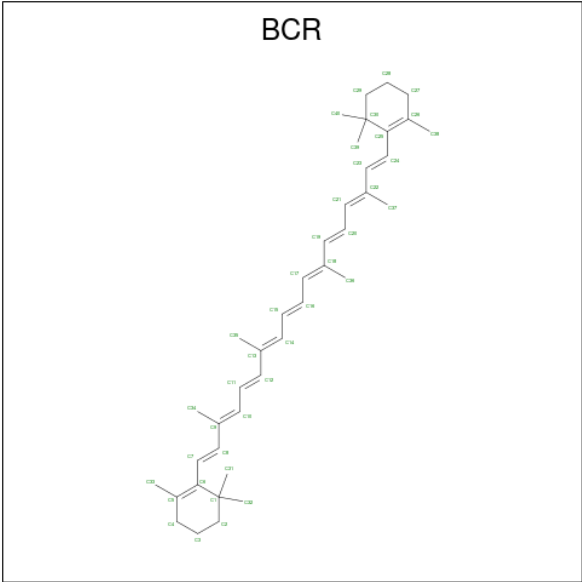
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	a	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	a	1	Total 130	C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

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

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



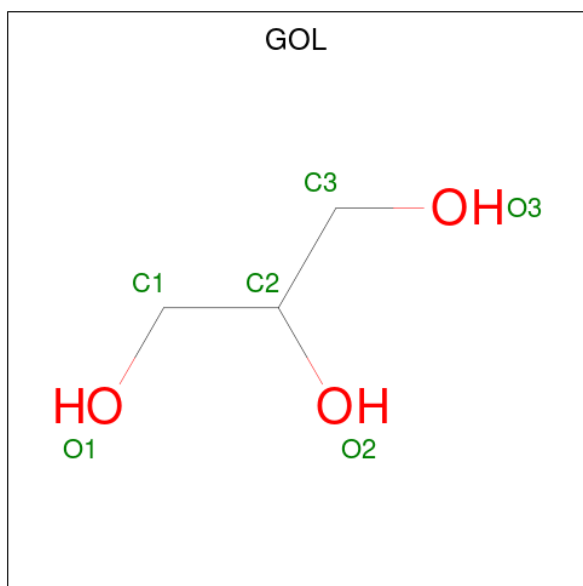
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	T	1	Total C 40 40	0	0
24	Y	1	Total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

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

- Molecule 25 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



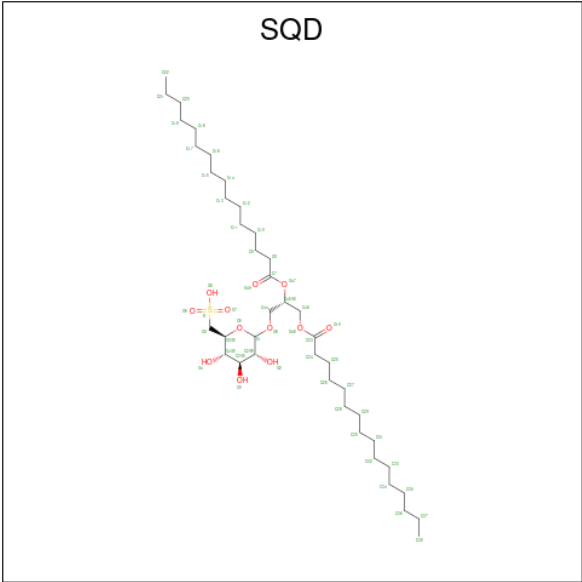
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 6 3 3	0	0
25	B	1	Total C O 6 3 3	0	0
25	B	1	Total C O 6 3 3	0	0

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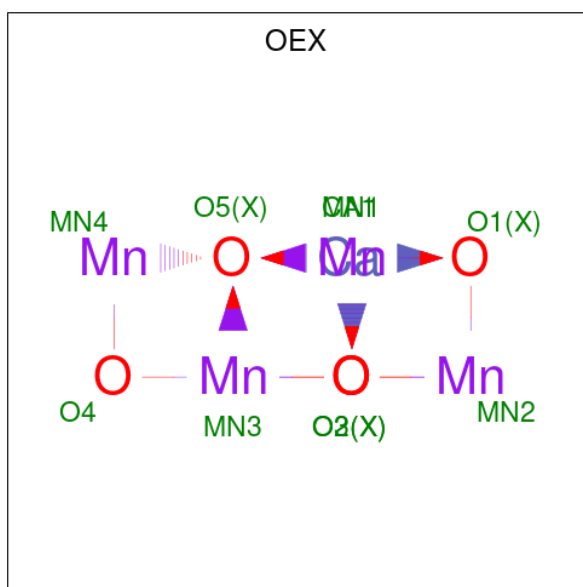
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			6	3	3		
25	C	1	Total	C	O	0	1
			12	6	6		
25	D	1	Total	C	O	0	0
			6	3	3		
25	D	1	Total	C	O	0	0
			6	3	3		
25	O	1	Total	C	O	0	0
			6	3	3		
25	O	1	Total	C	O	0	0
			6	3	3		
25	V	1	Total	C	O	0	1
			12	6	6		
25	a	1	Total	C	O	0	0
			6	3	3		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

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



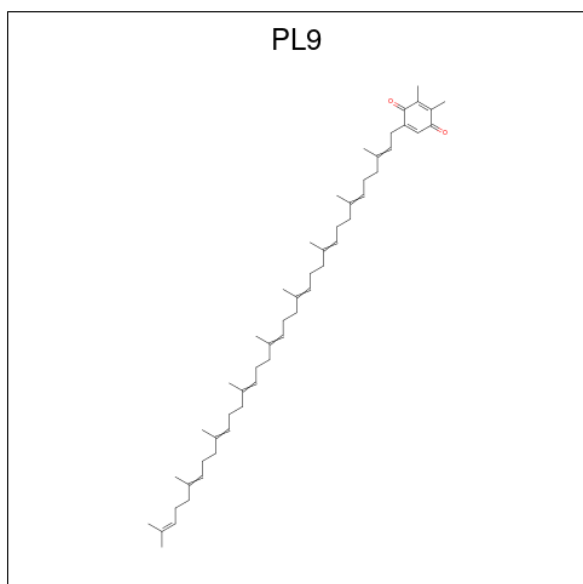
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	B	1	Total	C	O	S	0	0
			54	41	12	1		
26	C	1	Total	C	O	S	0	1
			108	82	24	2		
26	F	1	Total	C	O	S	0	0
			43	30	12	1		
26	a	1	Total	C	O	S	0	1
			108	82	24	2		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	b	1	Total	C	O	S	0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

- Molecule 27 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
27	A	1	Total	Ca	Mn	O	0	1
			20	2	8	10		
27	a	1	Total	Ca	Mn	O	0	1
			20	2	8	10		

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂) (labeled as "Ligand of Interest" by depositor).



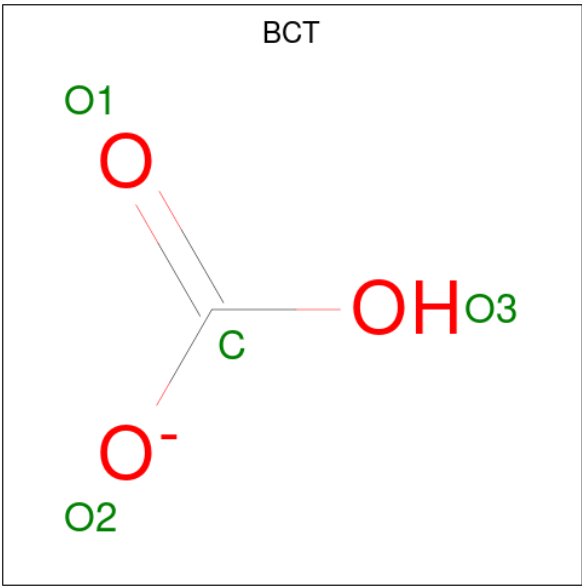
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	1
			110	106	4		
28	D	1	Total	C	O	0	1
			110	106	4		
28	a	1	Total	C	O	0	1
			110	106	4		
28	d	1	Total	C	O	0	1
			110	106	4		

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			28	23	5		
29	B	2	Total	C	O	0	0
			73	63	10		
29	D	2	Total	C	O	0	0
			57	51	6		
29	I	1	Total	C	O	0	0
			40	35	5		
29	J	1	Total	C		0	0
			10	10			
29	K	1	Total	C	O	0	1
			68	58	10		
29	M	1	Total	C		0	0
			10	10			
29	X	1	Total	C	O	0	0
			18	16	2		
29	a	1	Total	C	O	0	0
			30	25	5		
29	b	2	Total	C	O	0	0
			69	59	10		
29	c	1	Total	C	O	0	1
			64	54	10		
29	d	1	Total	C	O	0	0
			17	16	1		
29	j	1	Total	C		0	0
			10	10			
29	m	1	Total	C		0	0
			10	10			
29	x	1	Total	C	O	0	0
			18	16	2		

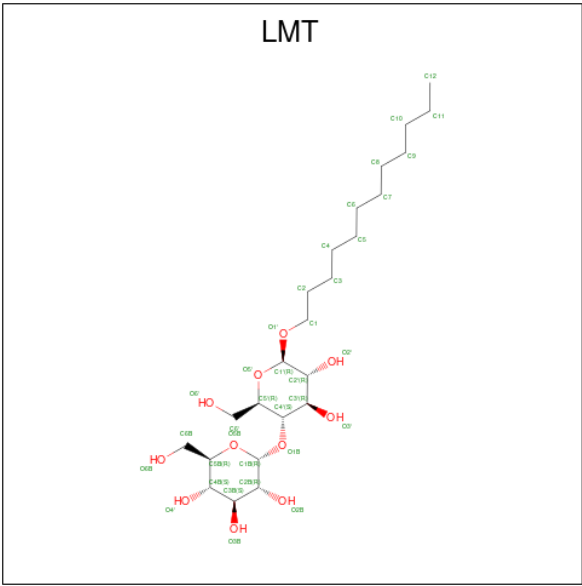
- Molecule 30 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand

of Interest" by depositor).



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

- Molecule 31 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



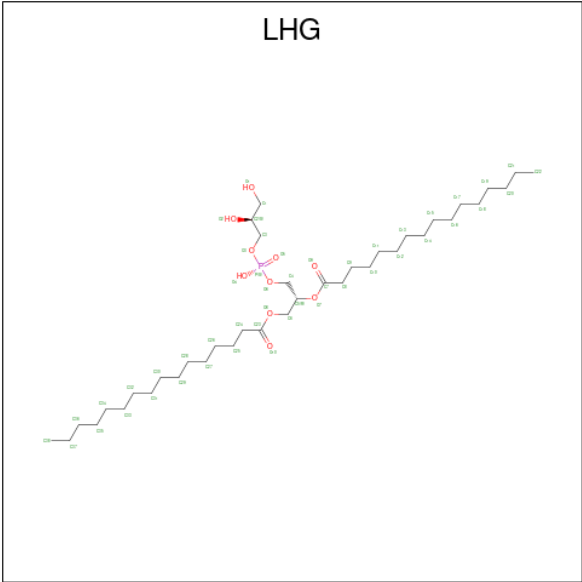
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			35	24	11		

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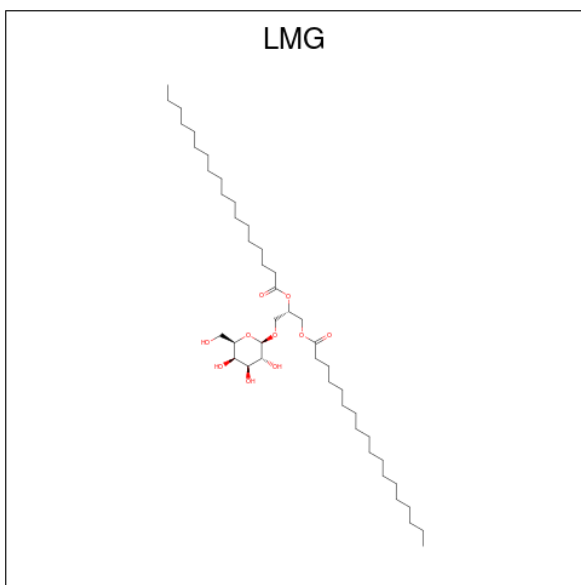
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	F	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total	C	O	0	0
			35	24	11		
31	T	1	Total	C	O	0	0
			35	24	11		
31	b	1	Total	C	O	0	0
			25	19	6		
31	b	1	Total	C	O	0	0
			25	19	6		
31	c	1	Total	C	O	0	0
			35	24	11		
31	e	1	Total	C	O	0	0
			35	24	11		
31	m	1	Total	C	O	0	0
			35	24	11		
31	t	1	Total	C	O	0	0
			25	19	6		
31	t	1	Total	C	O	0	0
			26	19	7		

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



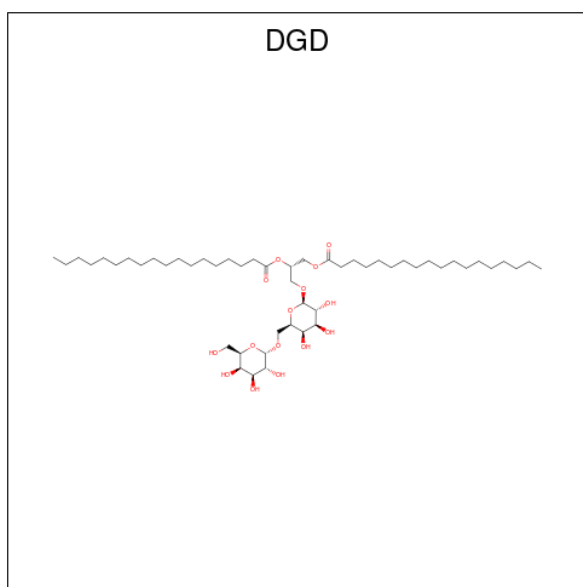
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	A	1	Total	C	O	P	0	1
			98	76	20	2		
32	D	1	Total	C	O	P	0	1
			98	76	20	2		
32	D	1	Total	C	O	P	0	1
			98	76	20	2		
32	E	1	Total	C	O	P	0	1
			84	62	20	2		
32	L	1	Total	C	O	P	0	1
			98	76	20	2		
32	a	1	Total	C	O	P	0	1
			84	62	20	2		
32	d	1	Total	C	O	P	0	1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

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	B	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			37	27	10		
33	D	1	Total	C	O	0	0
			51	41	10		
33	a	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	d	1	Total	C	O	0	0
			51	41	10		
33	m	1	Total	C	O	0	0
			51	41	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
35	C	1	Total	C	O	0	1
			124	94	30		
35	C	1	Total	C	O	0	1
			124	94	30		
35	C	1	Total	C	O	0	0
			62	47	15		
35	H	1	Total	C	O	0	0
			62	47	15		
35	c	1	Total	C	O	0	1
			124	94	30		
35	c	1	Total	C	O	0	1
			124	94	30		
35	c	1	Total	C	O	0	0
			62	47	15		
35	h	1	Total	C	O	0	0
			62	47	15		

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

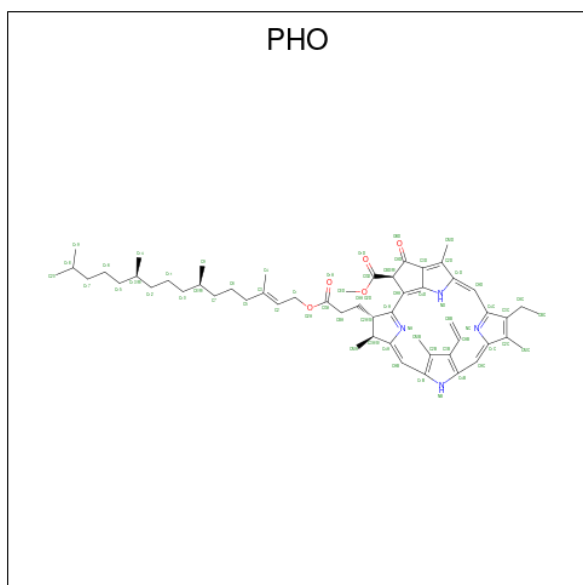
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	C	1	Total	Ca	0	0
			1	1		
36	O	1	Total	Ca	0	0
			1	1		
36	V	1	Total	Ca	0	0
			1	1		
36	c	2	Total	Ca	0	0
			2	2		

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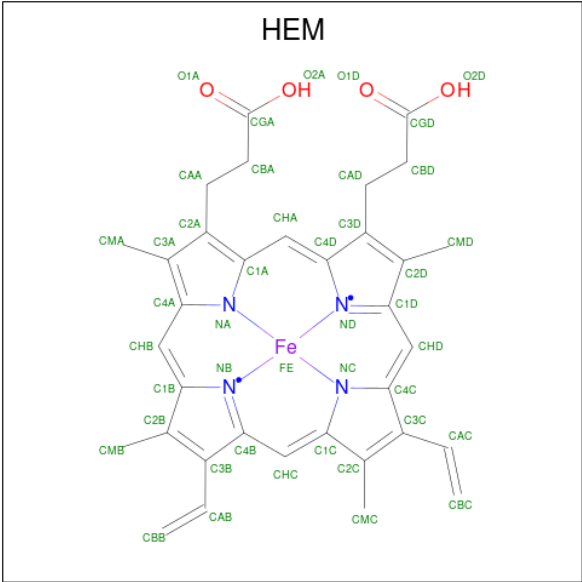
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	f	1	Total Ca 1 1	0	0
36	o	1	Total Ca 1 1	0	0

- Molecule 37 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

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

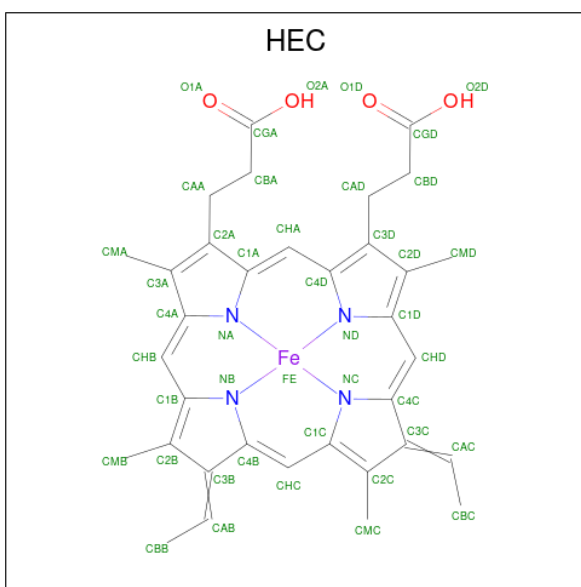


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
38	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
38	f	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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: C₃₄H₃₄FeN₄O₄).



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	A	137	Total O 219 219	0	84
41	B	190	Total O 193 193	0	3
41	C	170	Total O 207 207	0	37
41	D	122	Total O 156 156	0	34
41	E	15	Total O 15 15	0	0
41	F	6	Total O 6 6	0	0
41	H	22	Total O 22 22	0	0
41	I	6	Total O 6 6	0	0
41	J	5	Total O 5 5	0	0
41	K	7	Total O 7 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	L	9	Total O 10 10	0	1
41	M	6	Total O 6 6	0	0
41	O	98	Total O 103 103	0	5
41	T	11	Total O 14 14	0	3
41	U	46	Total O 48 48	0	2
41	V	80	Total O 82 82	0	2
41	X	8	Total O 8 8	0	0
41	a	129	Total O 208 208	0	81
41	b	201	Total O 204 204	0	3
41	c	162	Total O 195 195	0	33
41	d	122	Total O 155 155	0	33
41	e	8	Total O 8 8	0	0
41	f	3	Total O 3 3	0	0
41	h	17	Total O 17 17	0	0
41	i	3	Total O 3 3	0	0
41	j	1	Total O 1 1	0	0
41	k	3	Total O 3 3	0	0
41	l	7	Total O 8 8	0	1
41	m	13	Total O 13 13	0	0
41	o	95	Total O 99 99	0	4
41	t	6	Total O 9 9	0	3

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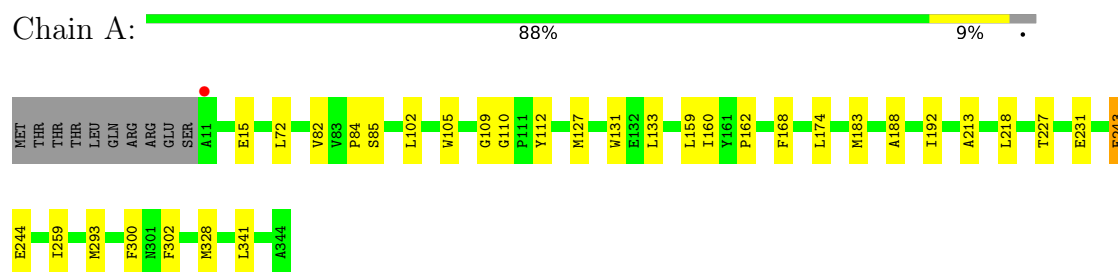
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	u	50	Total 51	O 51	0	1
41	v	57	Total 60	O 60	0	3
41	x	8	Total 8	O 8	0	0
41	y	2	Total 2	O 2	0	0

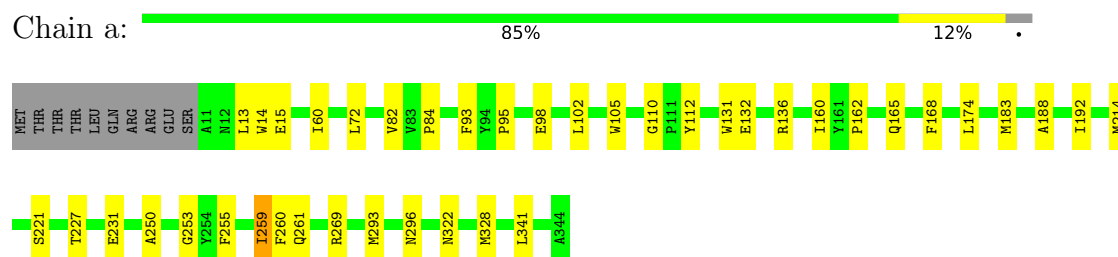
3 Residue-property plots [i](#)

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

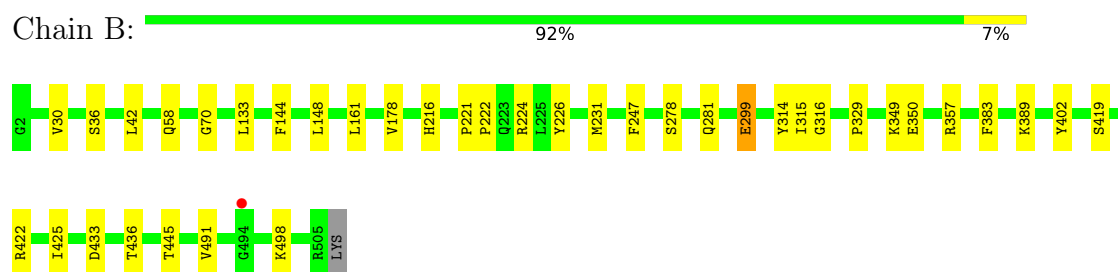
- Molecule 1: Photosystem II protein D1



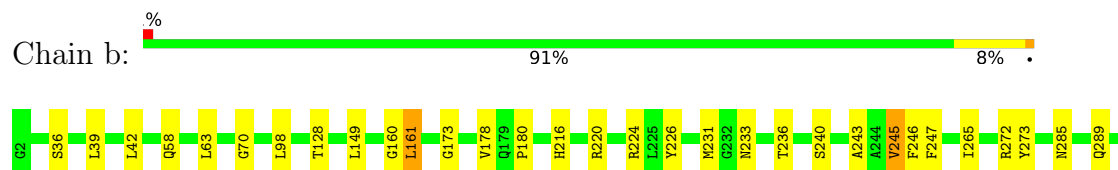
- Molecule 1: Photosystem II protein D1



- Molecule 2: Photosystem II CP47 reaction center protein



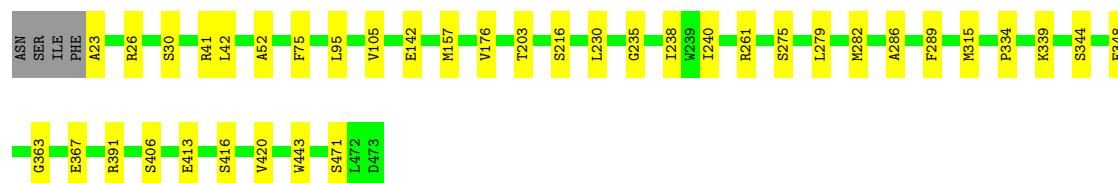
- Molecule 2: Photosystem II CP47 reaction center protein





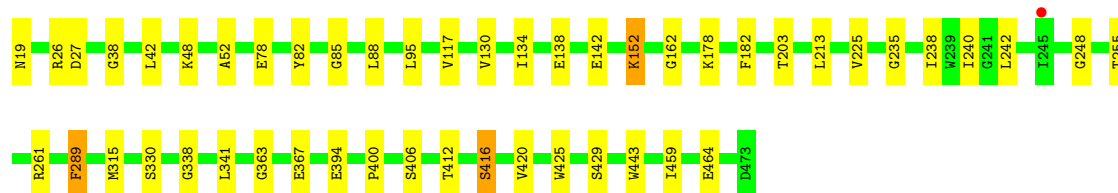
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 91% 8% .



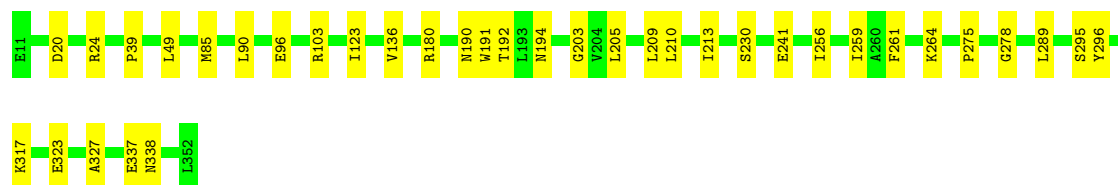
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 89% 10% .



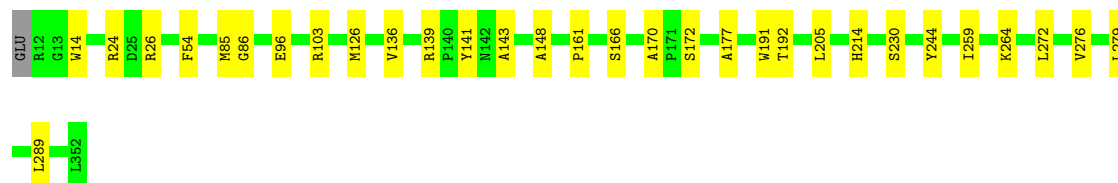
- Molecule 4: Photosystem II D2 protein

Chain D: 89% 11%



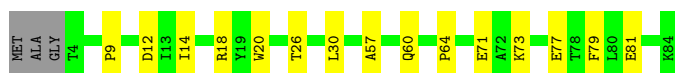
- Molecule 4: Photosystem II D2 protein

Chain d: 91% 9%

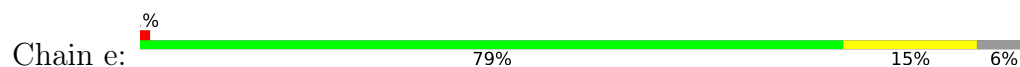


- Molecule 5: Cytochrome b559 subunit alpha

Chain E: 79% 18% .



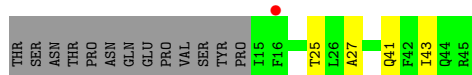
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit beta



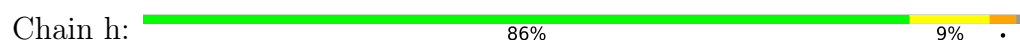
- Molecule 6: Cytochrome b559 subunit beta



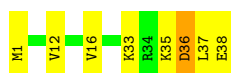
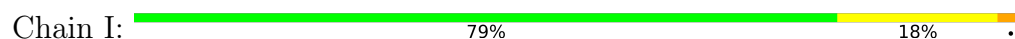
- Molecule 7: Photosystem II reaction center protein H



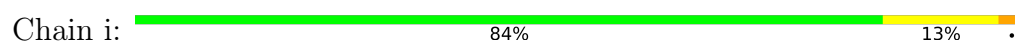
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I





- Molecule 9: Photosystem II reaction center protein J

Chain J: 82% 13% . .



- Molecule 9: Photosystem II reaction center protein J

Chain j: 92% 8%



- Molecule 10: Photosystem II reaction center protein K

Chain K: 81% 16% .



- Molecule 10: Photosystem II reaction center protein K

Chain k: 76% 19% 5%



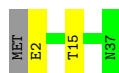
- Molecule 11: Photosystem II reaction center protein L

Chain L: 92% 5% .



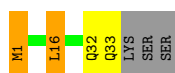
- Molecule 11: Photosystem II reaction center protein L

Chain l: 92% 5% .



- Molecule 12: Photosystem II reaction center protein M

Chain M: 81% 6% 6% 8%



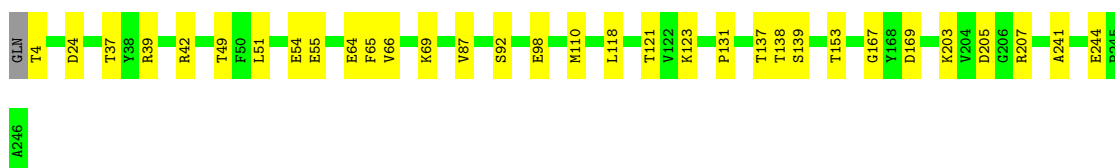
- Molecule 12: Photosystem II reaction center protein M

Chain m: 81% 11% 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 86% 13%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 92% 7%



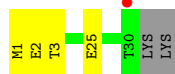
- Molecule 14: Photosystem II reaction center protein T

Chain T: 81% 12% 6%



- Molecule 14: Photosystem II reaction center protein T

Chain t: 3% 81% 12% 6%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 85% 8% 8%

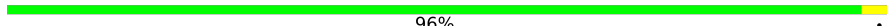


- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  92% • 7%



- Molecule 16: Cytochrome c-550

Chain V:  96% •



- Molecule 16: Cytochrome c-550

Chain v:  91% 9% •



- Molecule 17: Photosystem II reaction center protein X

Chain X:  82% 12% 5%



- Molecule 17: Photosystem II reaction center protein X

Chain x:  88% 8% 5%



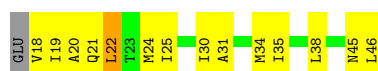
- Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:  87% 10% •



- Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:  50% 43% • •

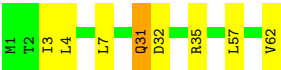


- Molecule 19: Photosystem II reaction center protein Z

Chain Z:

87%

11%

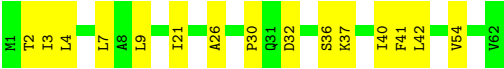


• Molecule 19: Photosystem II reaction center protein Z

Chain z:

76%

24%



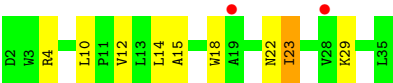
• Molecule 20: Photosystem II protein Y

Chain R:

6%

74%

24%



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 – 2.30 19.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.30) 99.7 (19.99-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.30Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.141 , 0.180 0.142 , 0.182	Depositor DCC
R_{free} test set	28224 reflections (3.46%)	wwPDB-VP
Wilson B-factor (Å ²)	53.0	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 76.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	62602	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage'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

5.1 Standard geometry

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

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	0.27	0/4478	0.43	0/6098
1	a	0.25	0/4470	0.40	0/6087
2	B	0.38	0/4293	0.50	0/5851
2	b	0.34	0/4285	0.49	0/5841
3	C	0.30	0/4404	0.44	0/5997
3	c	0.28	0/4459	0.43	0/6071
4	D	0.34	0/3741	0.47	0/5095
4	d	0.31	0/3749	0.45	0/5106
5	E	0.35	0/681	0.52	0/928
5	e	0.30	0/690	0.48	0/939
6	F	0.35	0/284	0.45	0/387
6	f	0.29	0/269	0.47	0/365
7	H	0.35	0/519	0.53	0/708
7	h	0.31	0/530	0.46	0/722
8	I	0.30	0/311	0.46	0/419
8	i	0.35	0/311	0.45	0/419
9	J	0.32	0/278	0.40	0/376
9	j	0.28	0/283	0.40	0/383
10	K	0.34	0/303	0.48	0/416
10	k	0.33	0/303	0.47	0/416
11	L	0.37	0/318	0.47	0/433
11	l	0.37	0/318	0.45	0/433
12	M	0.38	0/261	0.54	0/357
12	m	0.39	0/279	0.47	0/380
13	O	0.36	0/1991	0.52	0/2698
13	o	0.34	0/1966	0.51	0/2665
14	T	0.34	0/310	0.43	0/419
14	t	0.32	0/301	0.42	0/406
15	U	0.38	0/811	0.54	0/1095
15	u	0.36	0/818	0.54	0/1105
16	V	0.36	0/1142	0.51	0/1545

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.31	0/1139	0.48	0/1542
17	X	0.25	0/292	0.37	0/395
17	x	0.25	0/284	0.37	0/384
18	Y	0.25	0/216	0.47	0/289
18	y	0.24	0/216	0.39	0/289
19	Z	0.23	0/490	0.37	0/669
19	z	0.24	0/490	0.36	0/669
20	R	0.23	0/279	0.35	0/383
All	All	0.32	0/50562	0.46	0/68780

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4338	0	4142	28	0
1	a	4330	0	4132	40	0
2	B	4146	0	3983	25	0
2	b	4134	0	3976	40	0
3	C	4260	0	4123	27	0
3	c	4308	0	4172	36	0
4	D	3620	0	3484	37	0
4	d	3628	0	3490	22	0
5	E	662	0	648	12	0
5	e	670	0	655	9	0
6	F	275	0	282	5	0
6	f	261	0	269	5	0
7	H	506	0	529	3	0
7	h	517	0	541	8	0
8	I	314	0	328	5	0
8	i	314	0	328	3	0
9	J	272	0	279	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	277	0	284	2	0
10	K	293	0	305	4	0
10	k	293	0	305	7	0
11	L	311	0	320	3	0
11	l	311	0	320	2	0
12	M	268	0	285	6	0
12	m	286	0	305	7	0
13	O	1958	0	1920	15	0
13	o	1933	0	1900	9	0
14	T	311	0	318	1	0
14	t	302	0	311	3	0
15	U	800	0	796	5	0
15	u	807	0	805	1	0
16	V	1120	0	1122	3	0
16	v	1117	0	1131	8	0
17	X	289	0	322	4	0
17	x	281	0	312	3	0
18	Y	215	0	246	2	0
18	y	215	0	246	8	0
19	Z	479	0	516	3	0
19	z	479	0	516	5	0
20	R	273	0	305	5	0
21	A	2	0	0	0	0
21	a	2	0	0	0	0
22	A	4	0	0	0	0
22	a	4	0	0	0	0
23	A	455	0	504	14	0
23	B	1040	0	1152	26	0
23	C	845	0	936	37	0
23	D	195	0	216	7	0
23	a	455	0	504	15	0
23	b	1040	0	1152	30	0
23	c	845	0	936	32	0
23	d	195	0	216	7	0
24	A	40	0	56	1	0
24	B	120	0	168	4	0
24	C	80	0	112	0	0
24	D	40	0	56	2	0
24	H	40	0	56	2	0
24	K	40	0	56	1	0
24	T	40	0	56	6	0
24	Y	40	0	56	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	40	0	56	1	0
24	b	120	0	168	10	0
24	c	80	0	112	4	0
24	d	40	0	56	2	0
24	h	40	0	56	5	0
24	k	40	0	56	2	0
24	t	40	0	56	3	0
24	y	40	0	56	2	0
25	A	6	0	8	1	0
25	B	18	0	24	3	0
25	C	12	0	16	1	0
25	D	12	0	14	8	0
25	O	12	0	16	2	0
25	V	12	0	16	1	0
25	a	12	0	16	7	0
25	b	12	0	16	2	0
25	c	24	0	32	1	0
25	d	6	0	8	0	0
25	l	12	0	16	1	0
25	o	6	0	8	0	0
25	v	12	0	16	2	0
26	A	54	0	78	1	0
26	B	54	0	78	3	0
26	C	108	0	155	2	0
26	F	43	0	53	2	0
26	a	162	0	233	9	0
26	b	54	0	78	2	0
26	f	43	0	53	1	0
27	A	20	0	0	0	0
27	a	20	0	0	0	0
28	A	110	0	160	19	0
28	D	110	0	160	1	0
28	a	110	0	160	10	0
28	d	110	0	160	1	0
29	A	28	0	0	0	0
29	B	73	0	0	0	0
29	D	57	0	0	0	0
29	I	40	0	0	0	0
29	J	10	0	0	0	0
29	K	68	0	0	0	0
29	M	10	0	0	0	0
29	X	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	a	30	0	0	0	0
29	b	69	0	0	0	0
29	c	64	0	0	0	0
29	d	17	0	0	0	0
29	j	10	0	0	0	0
29	m	10	0	0	0	0
29	x	18	0	0	0	0
30	A	8	0	0	0	0
30	a	8	0	0	0	0
31	A	70	0	92	3	0
31	B	70	0	92	3	0
31	F	35	0	46	0	0
31	M	35	0	46	0	0
31	T	35	0	45	0	0
31	b	50	0	70	1	0
31	c	35	0	46	2	0
31	e	35	0	46	1	0
31	m	35	0	46	2	0
31	t	51	0	67	2	0
32	A	98	0	148	1	0
32	D	196	0	296	13	0
32	E	84	0	114	6	0
32	L	98	0	148	1	0
32	a	84	0	114	8	0
32	d	294	0	444	24	0
32	l	98	0	148	0	0
33	B	51	0	72	1	0
33	C	190	0	260	4	0
33	D	51	0	72	0	0
33	a	51	0	72	1	0
33	c	102	0	144	2	0
33	d	51	0	72	1	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	310	0	410	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	H	62	0	82	1	0
35	c	310	0	410	12	0
35	h	62	0	82	0	0
36	C	1	0	0	0	0
36	O	1	0	0	0	0
36	V	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	256	0	296	5	0
37	a	256	0	296	4	0
38	F	43	0	30	1	0
38	f	43	0	30	1	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	219	0	0	0	0
41	B	193	0	0	2	0
41	C	207	0	0	3	0
41	D	156	0	0	6	0
41	E	15	0	0	0	0
41	F	6	0	0	0	0
41	H	22	0	0	0	0
41	I	6	0	0	0	0
41	J	5	0	0	2	0
41	K	7	0	0	0	0
41	L	10	0	0	0	0
41	M	6	0	0	0	0
41	O	103	0	0	0	0
41	T	14	0	0	0	0
41	U	48	0	0	0	0
41	V	82	0	0	1	0
41	X	8	0	0	0	0
41	a	208	0	0	2	0
41	b	204	0	0	0	0
41	c	195	0	0	3	0
41	d	155	0	0	1	0
41	e	8	0	0	0	0
41	f	3	0	0	0	0
41	h	17	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	1	0	0	0	0
41	k	3	0	0	0	0
41	l	8	0	0	0	0
41	m	13	0	0	0	0
41	o	99	0	0	0	0
41	t	9	0	0	1	0
41	u	51	0	0	1	0
41	v	60	0	0	0	0
41	x	8	0	0	0	0
41	y	2	0	0	0	0
All	All	62602	0	61441	609	0

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

The worst 5 of 609 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)
25:D:403:GOL:H11	12:M:1:FME:HG2	1.43	0.99
1:a:250[B]:ALA:HA	2:b:491[B]:VAL:HG11	1.50	0.94
1:a:250[A]:ALA:HA	2:b:491[A]:VAL:HG11	1.51	0.93
23:c:504:CLA:HBB1	23:c:513:CLA:H41	1.56	0.88
24:b:619:BCR:H331	24:b:619:BCR:HC8	1.60	0.84

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	553/344 (161%)	548 (99%)	3 (0%)	2 (0%)	30	38
1	a	552/344 (160%)	545 (99%)	5 (1%)	2 (0%)	30	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	522/505 (103%)	515 (99%)	7 (1%)	0	100	100
2	b	521/505 (103%)	509 (98%)	12 (2%)	0	100	100
3	C	546/455 (120%)	540 (99%)	5 (1%)	1 (0%)	43	55
3	c	553/455 (122%)	540 (98%)	12 (2%)	1 (0%)	43	55
4	D	453/342 (132%)	437 (96%)	16 (4%)	0	100	100
4	d	454/342 (133%)	443 (98%)	11 (2%)	0	100	100
5	E	79/84 (94%)	77 (98%)	2 (2%)	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%)	62 (100%)	0	0	100	100
7	h	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
8	I	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	4	2
8	i	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	37 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	34/36 (94%)	34 (100%)	0	0	100	100
13	O	251/244 (103%)	240 (96%)	10 (4%)	1 (0%)	30	38
13	o	249/244 (102%)	243 (98%)	6 (2%)	0	100	100
14	T	33/32 (103%)	33 (100%)	0	0	100	100
14	t	32/32 (100%)	32 (100%)	0	0	100	100
15	U	97/104 (93%)	92 (95%)	5 (5%)	0	100	100
15	u	98/104 (94%)	95 (97%)	3 (3%)	0	100	100
16	V	140/137 (102%)	137 (98%)	3 (2%)	0	100	100
16	v	140/137 (102%)	133 (95%)	7 (5%)	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%)	24 (89%)	3 (11%)	0	100	100
18	y	27/30 (90%)	27 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	7
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	7	7
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	6171/5384 (115%)	6035 (98%)	126 (2%)	10 (0%)	43	55

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
8	I	36	ASP
3	c	416	SER
19	Z	31	GLN
13	O	138	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	444/279 (159%)	440 (99%)	4 (1%)	70	84
1	a	443/279 (159%)	442 (100%)	1 (0%)	87	94
2	B	421/403 (104%)	416 (99%)	5 (1%)	63	79
2	b	420/403 (104%)	410 (98%)	10 (2%)	43	62
3	C	430/356 (121%)	424 (99%)	6 (1%)	59	76
3	c	436/356 (122%)	428 (98%)	8 (2%)	51	70
4	D	368/277 (133%)	365 (99%)	3 (1%)	73	86
4	d	369/277 (133%)	362 (98%)	7 (2%)	50	69
5	E	72/73 (99%)	71 (99%)	1 (1%)	59	76
5	e	72/73 (99%)	70 (97%)	2 (3%)	38	56

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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%)	51 (94%)	3 (6%)	19	28
7	h	55/54 (102%)	53 (96%)	2 (4%)	31	47
8	I	34/34 (100%)	33 (97%)	1 (3%)	37	55
8	i	34/34 (100%)	33 (97%)	1 (3%)	37	55
9	J	26/27 (96%)	25 (96%)	1 (4%)	29	44
9	j	26/27 (96%)	25 (96%)	1 (4%)	29	44
10	K	30/30 (100%)	27 (90%)	3 (10%)	7	9
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	9
11	L	36/35 (103%)	36 (100%)	0	100	100
11	l	36/35 (103%)	35 (97%)	1 (3%)	38	56
12	M	30/32 (94%)	28 (93%)	2 (7%)	15	21
12	m	32/32 (100%)	30 (94%)	2 (6%)	16	23
13	O	216/207 (104%)	207 (96%)	9 (4%)	26	40
13	o	213/207 (103%)	206 (97%)	7 (3%)	33	50
14	T	32/28 (114%)	28 (88%)	4 (12%)	4	5
14	t	31/28 (111%)	31 (100%)	0	100	100
15	U	86/89 (97%)	84 (98%)	2 (2%)	44	63
15	u	87/89 (98%)	85 (98%)	2 (2%)	44	63
16	V	123/117 (105%)	123 (100%)	0	100	100
16	v	123/117 (105%)	119 (97%)	4 (3%)	33	50
17	X	32/33 (97%)	32 (100%)	0	100	100
17	x	31/33 (94%)	31 (100%)	0	100	100
18	Y	22/23 (96%)	22 (100%)	0	100	100
18	y	22/23 (96%)	17 (77%)	5 (23%)	1	1
19	Z	52/52 (100%)	49 (94%)	3 (6%)	18	26
19	z	52/52 (100%)	46 (88%)	6 (12%)	5	6
20	R	29/29 (100%)	26 (90%)	3 (10%)	7	8
All	All	5103/4403 (116%)	4991 (98%)	112 (2%)	45	65

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	152	LYS
19	z	21	ILE
5	e	71	GLU
19	z	7	LEU
18	y	45	ASN

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

Mol	Chain	Res	Type
15	u	78	ASN
19	Z	31	GLN
2	b	14	ASN
2	b	331	ASN
3	c	19	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	i	1	8	8,9,10	0.70	0	8,9,11	1.26	1 (12%)
12	FME	m	1	12	8,9,10	0.51	0	8,9,11	1.35	2 (25%)
14	FME	T	1	14	8,9,10	0.62	0	8,9,11	1.50	1 (12%)
8	FME	I	1	8	8,9,10	0.69	0	8,9,11	1.05	1 (12%)
14	FME	t	1	14	8,9,10	0.82	0	8,9,11	1.37	1 (12%)
12	FME	M	1	12	8,9,10	0.74	0	8,9,11	1.31	2 (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
8	FME	i	1	8	-	0/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
14	FME	T	1	14	-	3/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
14	FME	t	1	14	-	0/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	O-C-CA	-2.81	117.54	124.77
12	m	1	FME	O-C-CA	-2.40	118.59	124.77
12	m	1	FME	O1-CN-N	-2.26	119.49	125.32
14	T	1	FME	CB-CA-N	-2.25	106.42	110.52
8	i	1	FME	O-C-CA	-2.21	119.08	124.77

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	O1-CN-N-CA
14	T	1	FME	C-CA-CB-CG
14	T	1	FME	N-CA-CB-CG
14	T	1	FME	O1-CN-N-CA
8	I	1	FME	CB-CA-N-CN

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	m	1	FME	4	0
12	M	1	FME	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 274 ligands modelled in this entry, 21 are monoatomic and 20 are unknown - leaving 233 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	a	407[B]	41	69,73,73	2.02	19 (27%)	82,113,113	2.73	32 (39%)
25	GOL	l	801[A]	-	5,5,5	0.98	0	5,5,5	1.05	1 (20%)
40	HEC	V	202	16	46,50,50	1.87	5 (10%)	58,82,82	1.81	7 (12%)
23	CLA	c	510	-	69,73,73	2.01	19 (27%)	82,113,113	2.81	32 (39%)
25	GOL	O	302	-	5,5,5	1.04	0	5,5,5	0.94	0
23	CLA	b	604	-	69,73,73	1.96	20 (28%)	82,113,113	2.63	30 (36%)
30	BCT	A	414[B]	21	3,3,3	0.51	0	2,3,3	0.87	0
31	LMT	t	101	-	25,25,36	0.88	1 (4%)	30,30,47	1.21	3 (10%)
32	LHG	D	409[B]	-	48,48,48	0.94	2 (4%)	51,54,54	1.03	3 (5%)
35	DGD	c	518[A]	-	63,63,67	0.85	3 (4%)	77,77,81	0.98	4 (5%)
26	SQD	C	501[A]	-	52,54,54	0.86	2 (3%)	62,65,65	1.85	10 (16%)
24	BCR	c	515	-	41,41,41	1.03	1 (2%)	56,56,56	1.58	12 (21%)
32	LHG	d	405[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.06	4 (7%)
23	CLA	C	505	-	69,73,73	1.93	19 (27%)	82,113,113	2.67	30 (36%)
28	PL9	A	412[A]	-	55,55,55	0.71	3 (5%)	68,69,69	2.05	25 (36%)
23	CLA	C	506	41	69,73,73	1.90	19 (27%)	82,113,113	2.66	31 (37%)
23	CLA	C	508	-	69,73,73	2.00	21 (30%)	82,113,113	2.71	33 (40%)
25	GOL	V	204[B]	-	5,5,5	1.00	0	5,5,5	1.09	0
37	PHO	D	401[B]	-	58,69,69	2.72	15 (25%)	55,99,99	3.00	16 (29%)
23	CLA	B	602	-	69,73,73	2.06	20 (28%)	82,113,113	2.72	33 (40%)
25	GOL	B	629	-	5,5,5	0.90	0	5,5,5	1.12	0
23	CLA	C	511	-	69,73,73	2.03	20 (28%)	82,113,113	2.68	30 (36%)
26	SQD	F	103	-	41,43,54	1.17	3 (7%)	51,54,65	2.03	14 (27%)
23	CLA	a	405[B]	-	69,73,73	2.02	19 (27%)	82,113,113	2.74	36 (43%)
37	PHO	a	416[A]	-	58,69,69	2.79	14 (24%)	55,99,99	3.05	17 (30%)
23	CLA	b	616	-	69,73,73	1.96	19 (27%)	82,113,113	2.81	32 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	608	-	69,73,73	1.90	21 (30%)	82,113,113	2.70	35 (42%)
23	CLA	B	606	-	69,73,73	1.97	20 (28%)	82,113,113	2.77	33 (40%)
23	CLA	b	608	-	69,73,73	2.00	21 (30%)	82,113,113	2.67	31 (37%)
23	CLA	B	613	-	69,73,73	2.00	19 (27%)	82,113,113	2.63	31 (37%)
23	CLA	c	502	-	69,73,73	2.00	21 (30%)	82,113,113	2.61	29 (35%)
23	CLA	D	404[A]	-	69,73,73	1.98	19 (27%)	82,113,113	2.74	34 (41%)
24	BCR	d	403	-	41,41,41	1.10	2 (4%)	56,56,56	1.95	15 (26%)
28	PL9	d	404[B]	-	55,55,55	0.65	1 (1%)	68,69,69	1.69	18 (26%)
26	SQD	a	411[A]	-	52,54,54	0.89	2 (3%)	62,65,65	1.80	11 (17%)
23	CLA	c	512	3	69,73,73	2.05	20 (28%)	82,113,113	2.70	32 (39%)
23	CLA	c	508	41	69,73,73	1.97	17 (24%)	82,113,113	2.75	32 (39%)
25	GOL	c	526[B]	-	5,5,5	0.98	0	5,5,5	1.03	0
23	CLA	a	406[A]	41	69,73,73	2.01	17 (24%)	82,113,113	2.72	31 (37%)
32	LHG	E	101[A]	-	41,41,48	1.08	2 (4%)	44,47,54	1.12	3 (6%)
27	OEX	A	411[B]	41,1,3	0,15,15	-	-	-	-	-
25	GOL	b	628	-	5,5,5	0.55	0	5,5,5	1.43	1 (20%)
35	DGD	C	518[B]	-	63,63,67	0.84	2 (3%)	77,77,81	1.10	7 (9%)
31	LMT	t	102	-	26,26,36	0.93	2 (7%)	31,31,47	1.24	2 (6%)
31	LMT	T	101	-	36,36,36	1.05	1 (2%)	47,47,47	1.12	3 (6%)
23	CLA	B	612	-	69,73,73	1.96	19 (27%)	82,113,113	2.70	33 (40%)
23	CLA	b	612	-	69,73,73	2.03	20 (28%)	82,113,113	2.66	32 (39%)
25	GOL	c	527	-	5,5,5	1.28	1 (20%)	5,5,5	0.98	0
35	DGD	C	520	-	63,63,67	0.88	3 (4%)	77,77,81	1.02	5 (6%)
23	CLA	A	404[B]	-	69,73,73	2.04	19 (27%)	82,113,113	2.75	33 (40%)
33	LMG	C	521	-	51,51,55	0.97	2 (3%)	59,59,63	1.18	4 (6%)
28	PL9	D	407[B]	-	55,55,55	0.62	2 (3%)	68,69,69	1.69	17 (25%)
23	CLA	B	609	-	69,73,73	2.02	17 (24%)	82,113,113	2.68	31 (37%)
23	CLA	A	407	-	69,73,73	1.94	20 (28%)	82,113,113	2.80	36 (43%)
25	GOL	B	624	-	5,5,5	0.80	0	5,5,5	1.17	1 (20%)
25	GOL	D	403	-	5,5,5	1.57	2 (40%)	5,5,5	0.89	0
38	HEM	F	102	5,6	50,50,50	1.53	8 (16%)	67,82,82	1.80	15 (22%)
24	BCR	A	408	-	41,41,41	1.08	2 (4%)	56,56,56	1.47	8 (14%)
24	BCR	T	102	-	41,41,41	1.02	1 (2%)	56,56,56	1.57	11 (19%)
25	GOL	o	302	-	5,5,5	1.32	1 (20%)	5,5,5	1.13	0
23	CLA	B	603	-	69,73,73	1.96	18 (26%)	82,113,113	2.83	31 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LHG	d	411[A]	-	48,48,48	0.89	3 (6%)	51,54,54	1.13	4 (7%)
24	BCR	k	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.59	11 (19%)
34	HTG	b	623	-	19,19,19	0.98	1 (5%)	23,24,24	1.76	4 (17%)
28	PL9	a	414[A]	-	55,55,55	0.68	2 (3%)	68,69,69	2.03	23 (33%)
24	BCR	b	619	-	41,41,41	1.06	1 (2%)	56,56,56	1.40	10 (17%)
23	CLA	b	611	-	69,73,73	1.93	20 (28%)	82,113,113	2.78	30 (36%)
25	GOL	B	627	-	5,5,5	1.04	0	5,5,5	1.03	0
30	BCT	a	404[A]	21	3,3,3	0.49	0	2,3,3	1.49	0
35	DGD	H	102	-	63,63,67	0.82	3 (4%)	77,77,81	1.11	9 (11%)
23	CLA	C	509	41	69,73,73	1.96	18 (26%)	82,113,113	2.79	31 (37%)
23	CLA	b	614	-	69,73,73	2.01	20 (28%)	82,113,113	2.78	32 (39%)
33	LMG	m	101	-	51,51,55	0.86	2 (3%)	59,59,63	1.41	8 (13%)
32	LHG	L	101[A]	-	48,48,48	0.89	3 (6%)	51,54,54	1.16	4 (7%)
24	BCR	t	103	-	41,41,41	1.07	1 (2%)	56,56,56	1.58	12 (21%)
23	CLA	b	613	-	69,73,73	1.94	18 (26%)	82,113,113	2.70	31 (37%)
26	SQD	f	102	-	41,43,54	1.15	2 (4%)	51,54,65	1.55	12 (23%)
23	CLA	a	407[A]	41	69,73,73	1.96	19 (27%)	82,113,113	2.67	32 (39%)
33	LMG	c	520	-	51,51,55	0.93	2 (3%)	59,59,63	1.17	6 (10%)
23	CLA	C	503	-	69,73,73	1.99	19 (27%)	82,113,113	2.70	31 (37%)
31	LMT	F	101	-	36,36,36	1.02	1 (2%)	47,47,47	1.05	3 (6%)
23	CLA	A	405[A]	41	69,73,73	2.00	18 (26%)	82,113,113	2.70	35 (42%)
30	BCT	A	414[A]	21	3,3,3	0.55	0	2,3,3	1.29	0
37	PHO	a	408[B]	-	58,69,69	2.75	14 (24%)	55,99,99	2.86	16 (29%)
32	LHG	A	416[B]	-	48,48,48	0.87	2 (4%)	51,54,54	1.20	5 (9%)
25	GOL	a	419	-	5,5,5	1.47	1 (20%)	5,5,5	1.08	1 (20%)
32	LHG	a	420[B]	-	41,41,48	1.04	2 (4%)	44,47,54	0.94	2 (4%)
32	LHG	l	802[B]	-	48,48,48	0.88	2 (4%)	51,54,54	1.05	4 (7%)
38	HEM	f	101	5,6	50,50,50	1.51	6 (12%)	67,82,82	1.68	12 (17%)
33	LMG	C	526	-	37,37,55	1.01	2 (5%)	45,45,63	1.48	8 (17%)
34	HTG	b	622	-	19,19,19	1.16	3 (15%)	23,24,24	2.15	8 (34%)
23	CLA	b	610	41	69,73,73	1.99	19 (27%)	82,113,113	2.80	32 (39%)
23	CLA	A	406[B]	41	69,73,73	2.08	20 (28%)	82,113,113	2.73	33 (40%)
25	GOL	V	204[A]	-	5,5,5	1.41	1 (20%)	5,5,5	0.86	0
33	LMG	C	502	-	51,51,55	0.91	2 (3%)	59,59,63	1.58	10 (16%)
23	CLA	d	402	-	69,73,73	2.01	20 (28%)	82,113,113	2.67	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	PHO	D	401[A]	-	58,69,69	2.66	12 (20%)	55,99,99	2.93	14 (25%)
23	CLA	b	609	-	69,73,73	2.01	18 (26%)	82,113,113	2.72	32 (39%)
23	CLA	c	504	-	69,73,73	2.08	20 (28%)	82,113,113	2.78	30 (36%)
23	CLA	a	405[A]	-	69,73,73	1.97	19 (27%)	82,113,113	2.75	34 (41%)
26	SQD	B	620	-	52,54,54	1.02	3 (5%)	62,65,65	1.70	11 (17%)
34	HTG	C	523	-	19,19,19	0.82	1 (5%)	23,24,24	1.24	2 (8%)
23	CLA	b	602	-	69,73,73	2.05	20 (28%)	82,113,113	2.89	33 (40%)
34	HTG	V	203	-	11,11,19	0.35	0	15,15,24	1.32	1 (6%)
35	DGD	C	519[A]	-	63,63,67	0.91	3 (4%)	77,77,81	1.04	5 (6%)
25	GOL	l	801[B]	-	5,5,5	0.93	0	5,5,5	1.08	0
32	LHG	d	406[B]	-	48,48,48	0.91	2 (4%)	51,54,54	1.02	4 (7%)
23	CLA	B	611	-	69,73,73	2.49	20 (28%)	82,113,113	3.53	31 (37%)
23	CLA	C	514	-	69,73,73	2.01	19 (27%)	82,113,113	2.66	32 (39%)
24	BCR	y	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.76	12 (21%)
32	LHG	D	408[A]	-	48,48,48	0.88	3 (6%)	51,54,54	1.02	3 (5%)
34	HTG	D	412	-	16,16,19	0.94	1 (6%)	20,21,24	1.29	1 (5%)
35	DGD	c	518[B]	-	63,63,67	0.88	2 (3%)	77,77,81	0.96	5 (6%)
25	GOL	v	202[A]	-	5,5,5	1.26	0	5,5,5	0.88	0
26	SQD	A	410	-	52,54,54	1.01	2 (3%)	62,65,65	1.19	4 (6%)
26	SQD	C	501[B]	-	52,54,54	0.88	2 (3%)	62,65,65	1.61	11 (17%)
31	LMT	A	415	-	36,36,36	0.86	0	47,47,47	1.11	2 (4%)
32	LHG	d	405[B]	-	48,48,48	0.91	3 (6%)	51,54,54	1.06	4 (7%)
25	GOL	O	303	-	5,5,5	0.88	0	5,5,5	1.16	1 (20%)
23	CLA	C	512	-	69,73,73	2.00	20 (28%)	82,113,113	2.81	34 (41%)
25	GOL	D	414	-	5,5,5	1.90	2 (40%)	5,5,5	0.60	0
25	GOL	c	526[A]	-	5,5,5	1.04	0	5,5,5	1.05	0
28	PL9	A	412[B]	-	55,55,55	0.65	2 (3%)	68,69,69	2.04	25 (36%)
35	DGD	c	519	-	63,63,67	0.87	4 (6%)	77,77,81	1.12	6 (7%)
23	CLA	B	604	-	69,73,73	2.04	21 (30%)	82,113,113	2.62	31 (37%)
24	BCR	D	406	-	41,41,41	1.09	1 (2%)	56,56,56	1.83	18 (32%)
27	OEX	A	411[A]	41,1,3	0,15,15	-	-	-	-	-
35	DGD	C	518[A]	-	63,63,67	0.84	2 (3%)	77,77,81	1.20	6 (7%)
33	LMG	z	101	-	39,39,55	1.11	2 (5%)	47,47,63	1.12	5 (10%)
40	HEC	v	201	16	46,50,50	1.94	6 (13%)	58,82,82	1.75	5 (8%)
31	LMT	B	630	-	36,36,36	0.98	2 (5%)	47,47,47	1.20	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LMT	b	621	-	25,25,36	0.94	1 (4%)	30,30,47	1.16	2 (6%)
23	CLA	d	401[B]	-	69,73,73	1.98	19 (27%)	82,113,113	2.71	31 (37%)
25	GOL	c	528	-	5,5,5	1.23	1 (20%)	5,5,5	0.92	0
24	BCR	H	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.46	11 (19%)
28	PL9	D	407[A]	-	55,55,55	0.65	1 (1%)	68,69,69	1.61	17 (25%)
26	SQD	b	620	-	52,54,54	1.01	2 (3%)	62,65,65	1.67	11 (17%)
25	GOL	C	524[B]	-	5,5,5	1.27	0	5,5,5	0.88	0
24	BCR	c	516	-	41,41,41	1.06	1 (2%)	56,56,56	1.45	12 (21%)
31	LMT	c	501	-	36,36,36	0.97	2 (5%)	47,47,47	1.03	1 (2%)
24	BCR	B	619	-	41,41,41	1.13	2 (4%)	56,56,56	1.31	7 (12%)
24	BCR	C	516	-	41,41,41	1.05	1 (2%)	56,56,56	1.50	7 (12%)
23	CLA	B	615	-	69,73,73	2.02	18 (26%)	82,113,113	2.73	32 (39%)
31	LMT	M	101	-	36,36,36	1.08	3 (8%)	47,47,47	1.26	5 (10%)
34	HTG	b	625	-	19,19,19	0.94	2 (10%)	23,24,24	1.44	3 (13%)
23	CLA	c	513	-	69,73,73	2.05	20 (28%)	82,113,113	2.66	32 (39%)
23	CLA	a	406[B]	41	69,73,73	2.02	19 (27%)	82,113,113	2.67	32 (39%)
32	LHG	D	409[A]	-	48,48,48	0.94	2 (4%)	51,54,54	1.04	4 (7%)
24	BCR	C	517	-	41,41,41	1.07	2 (4%)	56,56,56	1.50	11 (19%)
23	CLA	C	513	3	69,73,73	2.01	20 (28%)	82,113,113	2.53	28 (34%)
23	CLA	C	507	-	69,73,73	1.99	19 (27%)	82,113,113	2.72	30 (36%)
37	PHO	D	402[B]	-	58,69,69	2.84	14 (24%)	55,99,99	2.92	16 (29%)
24	BCR	B	617	-	41,41,41	1.06	2 (4%)	56,56,56	1.35	8 (14%)
23	CLA	c	509	-	69,73,73	2.08	20 (28%)	82,113,113	2.63	31 (37%)
35	DGD	c	517[B]	-	63,63,67	0.87	2 (3%)	77,77,81	1.03	5 (6%)
35	DGD	h	102	-	63,63,67	0.87	3 (4%)	77,77,81	1.12	5 (6%)
23	CLA	C	510	-	69,73,73	2.04	19 (27%)	82,113,113	2.70	30 (36%)
27	OEX	a	413[B]	41,1,3	0,15,15	-	-	-	-	-
31	LMT	e	101	-	36,36,36	0.98	1 (2%)	47,47,47	1.04	1 (2%)
23	CLA	C	504	-	69,73,73	2.01	19 (27%)	82,113,113	2.54	29 (35%)
23	CLA	A	406[A]	41	69,73,73	2.01	19 (27%)	82,113,113	2.69	33 (40%)
23	CLA	b	603	-	69,73,73	1.96	20 (28%)	82,113,113	2.74	32 (39%)
24	BCR	h	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.46	11 (19%)
28	PL9	a	414[B]	-	55,55,55	0.65	2 (3%)	68,69,69	1.95	22 (32%)
23	CLA	b	606	-	69,73,73	1.96	19 (27%)	82,113,113	2.81	33 (40%)
31	LMT	B	628	-	36,36,36	1.13	3 (8%)	47,47,47	1.34	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LMG	B	621	-	51,51,55	0.89	2 (3%)	59,59,63	1.32	5 (8%)
23	CLA	c	511	-	69,73,73	1.99	20 (28%)	82,113,113	2.75	35 (42%)
23	CLA	b	601	41	69,73,73	2.04	18 (26%)	82,113,113	2.72	29 (35%)
23	CLA	B	605	-	69,73,73	2.01	18 (26%)	82,113,113	2.82	29 (35%)
23	CLA	b	605	-	69,73,73	1.93	19 (27%)	82,113,113	2.97	30 (36%)
23	CLA	b	607	41	69,73,73	1.95	20 (28%)	82,113,113	2.62	28 (34%)
24	BCR	K	102	-	41,41,41	1.03	1 (2%)	56,56,56	1.45	11 (19%)
28	PL9	d	404[A]	-	55,55,55	0.72	1 (1%)	68,69,69	1.61	17 (25%)
32	LHG	L	101[B]	-	48,48,48	0.91	3 (6%)	51,54,54	1.06	5 (9%)
33	LMG	D	413	39	51,51,55	0.83	2 (3%)	59,59,63	1.07	4 (6%)
24	BCR	Y	101	-	41,41,41	0.99	1 (2%)	56,56,56	1.82	15 (26%)
23	CLA	c	507	-	69,73,73	2.02	19 (27%)	82,113,113	2.61	31 (37%)
23	CLA	c	505	41	69,73,73	2.02	20 (28%)	82,113,113	2.62	32 (39%)
23	CLA	b	615	-	69,73,73	1.99	17 (24%)	82,113,113	2.66	35 (42%)
24	BCR	b	617	-	41,41,41	1.07	2 (4%)	56,56,56	1.36	6 (10%)
32	LHG	d	406[A]	-	48,48,48	0.92	2 (4%)	51,54,54	1.02	3 (5%)
23	CLA	c	503	-	69,73,73	1.95	19 (27%)	82,113,113	2.62	28 (34%)
24	BCR	a	410	-	41,41,41	1.04	2 (4%)	56,56,56	1.36	9 (16%)
23	CLA	A	405[B]	41	69,73,73	1.97	21 (30%)	82,113,113	2.71	34 (41%)
23	CLA	c	506	-	69,73,73	2.01	18 (26%)	82,113,113	2.64	28 (34%)
34	HTG	c	522	-	19,19,19	0.85	1 (5%)	23,24,24	1.39	3 (13%)
23	CLA	B	601	41	69,73,73	2.07	21 (30%)	82,113,113	2.70	31 (37%)
23	CLA	A	404[A]	-	69,73,73	1.98	19 (27%)	82,113,113	2.74	31 (37%)
33	LMG	a	417	-	51,51,55	0.93	2 (3%)	59,59,63	1.19	6 (10%)
23	CLA	B	607	41	69,73,73	1.91	21 (30%)	82,113,113	2.69	33 (40%)
25	GOL	d	410	-	5,5,5	1.09	0	5,5,5	1.02	0
37	PHO	a	416[B]	-	58,69,69	2.80	14 (24%)	55,99,99	3.03	16 (29%)
34	HTG	B	623	-	19,19,19	0.73	1 (5%)	23,24,24	1.39	2 (8%)
23	CLA	B	610	41	69,73,73	2.01	19 (27%)	82,113,113	2.84	32 (39%)
23	CLA	D	404[B]	-	69,73,73	1.98	19 (27%)	82,113,113	2.80	30 (36%)
23	CLA	d	401[A]	-	69,73,73	1.94	19 (27%)	82,113,113	2.64	33 (40%)
34	HTG	d	408	-	16,16,19	0.88	1 (6%)	20,21,24	1.39	2 (10%)
25	GOL	a	418	-	5,5,5	1.40	2 (40%)	5,5,5	0.97	0
31	LMT	b	627	-	25,25,36	0.88	1 (4%)	30,30,47	1.13	2 (6%)
25	GOL	C	524[A]	-	5,5,5	1.16	0	5,5,5	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	616	-	69,73,73	1.97	19 (27%)	82,113,113	2.75	31 (37%)
26	SQD	a	411[B]	-	52,54,54	0.92	2 (3%)	62,65,65	1.53	10 (16%)
35	DGD	C	519[B]	-	63,63,67	0.88	3 (4%)	77,77,81	1.04	6 (7%)
23	CLA	B	614	-	69,73,73	2.01	20 (28%)	82,113,113	2.87	32 (39%)
32	LHG	E	101[B]	-	41,41,48	1.05	2 (4%)	44,47,54	1.13	4 (9%)
32	LHG	D	408[B]	-	48,48,48	0.92	2 (4%)	51,54,54	1.03	5 (9%)
33	LMG	C	522	-	51,51,55	1.08	3 (5%)	59,59,63	1.35	6 (10%)
25	GOL	v	202[B]	-	5,5,5	1.07	0	5,5,5	0.98	0
26	SQD	a	412	-	52,54,54	1.04	2 (3%)	62,65,65	1.15	7 (11%)
25	GOL	A	409	-	5,5,5	1.17	0	5,5,5	0.83	0
37	PHO	a	408[A]	-	58,69,69	2.77	13 (22%)	55,99,99	2.94	14 (25%)
33	LMG	c	521	-	51,51,55	1.02	2 (3%)	59,59,63	1.33	6 (10%)
32	LHG	A	416[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.29	6 (11%)
23	CLA	c	514	-	69,73,73	2.08	21 (30%)	82,113,113	2.71	32 (39%)
31	LMT	A	417	-	36,36,36	1.01	2 (5%)	47,47,47	1.15	4 (8%)
32	LHG	a	420[A]	-	41,41,48	1.06	2 (4%)	44,47,54	0.93	2 (4%)
32	LHG	l	802[A]	-	48,48,48	0.84	3 (6%)	51,54,54	1.05	4 (7%)
34	HTG	B	625	-	19,19,19	1.04	2 (10%)	23,24,24	1.19	4 (17%)
34	HTG	B	622	-	19,19,19	1.11	2 (10%)	23,24,24	1.58	6 (26%)
23	CLA	a	409	-	69,73,73	1.97	19 (27%)	82,113,113	2.82	31 (37%)
37	PHO	D	402[A]	-	58,69,69	2.81	14 (24%)	55,99,99	2.93	16 (29%)
23	CLA	C	515	-	69,73,73	2.01	19 (27%)	82,113,113	2.74	31 (37%)
31	LMT	m	103	-	36,36,36	1.04	2 (5%)	47,47,47	1.17	4 (8%)
32	LHG	d	411[B]	-	48,48,48	0.92	2 (4%)	51,54,54	1.07	4 (7%)
35	DGD	c	517[A]	-	63,63,67	0.86	2 (3%)	77,77,81	1.10	8 (10%)
25	GOL	b	624	-	5,5,5	1.24	1 (20%)	5,5,5	0.86	0
33	LMG	d	409	39	51,51,55	0.92	2 (3%)	59,59,63	1.12	5 (8%)
24	BCR	B	618	-	41,41,41	1.02	2 (4%)	56,56,56	1.33	5 (8%)
24	BCR	b	618	-	41,41,41	1.06	1 (2%)	56,56,56	1.26	9 (16%)
30	BCT	a	404[B]	21	3,3,3	0.51	0	2,3,3	0.90	0
27	OEX	a	413[A]	41,1,3	0,15,15	-	-	-	-	-
23	CLA	D	405	-	69,73,73	2.12	18 (26%)	82,113,113	2.64	31 (37%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	a	407[B]	41	-	5/39/115/115	-
25	GOL	l	801[A]	-	-	2/4/4/4	-
40	HEC	V	202	16	-	6/14/54/54	-
23	CLA	c	510	-	1/1/15/20	15/39/115/115	-
25	GOL	O	302	-	-	2/4/4/4	-
23	CLA	b	604	-	1/1/15/20	11/39/115/115	-
31	LMT	t	101	-	-	11/17/37/61	0/1/1/2
32	LHG	D	409[B]	-	-	12/53/53/53	-
35	DGD	c	518[A]	-	-	16/51/91/95	0/2/2/2
26	SQD	C	501[A]	-	-	12/49/69/69	0/1/1/1
24	BCR	c	515	-	-	0/29/63/63	0/2/2/2
32	LHG	d	405[A]	-	-	12/53/53/53	-
23	CLA	C	505	-	-	4/39/115/115	-
28	PL9	A	412[A]	-	-	14/53/73/73	0/1/1/1
23	CLA	C	506	41	1/1/15/20	7/39/115/115	-
23	CLA	C	508	-	1/1/15/20	11/39/115/115	-
25	GOL	V	204[B]	-	-	2/4/4/4	-
37	PHO	D	401[B]	-	-	4/37/103/103	0/5/6/6
23	CLA	B	602	-	1/1/15/20	12/39/115/115	-
25	GOL	B	629	-	-	4/4/4/4	-
23	CLA	C	511	-	1/1/15/20	4/39/115/115	-
26	SQD	F	103	-	-	13/38/58/69	0/1/1/1
23	CLA	a	405[B]	-	1/1/15/20	9/39/115/115	-
37	PHO	a	416[A]	-	-	1/37/103/103	0/5/6/6
23	CLA	b	616	-	1/1/15/20	9/39/115/115	-
23	CLA	B	608	-	-	3/39/115/115	-
23	CLA	B	606	-	1/1/15/20	4/39/115/115	-
23	CLA	b	608	-	-	6/39/115/115	-
23	CLA	B	613	-	1/1/15/20	7/39/115/115	-
23	CLA	c	502	-	1/1/15/20	7/39/115/115	-
23	CLA	D	404[A]	-	1/1/15/20	2/39/115/115	-
24	BCR	d	403	-	-	4/29/63/63	0/2/2/2
28	PL9	d	404[B]	-	-	8/53/73/73	0/1/1/1
26	SQD	a	411[A]	-	-	9/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	512	3	1/1/15/20	6/39/115/115	-
23	CLA	c	508	41	1/1/15/20	8/39/115/115	-
25	GOL	c	526[B]	-	-	0/4/4/4	-
23	CLA	a	406[A]	41	1/1/15/20	4/39/115/115	-
32	LHG	E	101[A]	-	-	21/46/46/53	-
25	GOL	b	628	-	-	0/4/4/4	-
35	DGD	C	518[B]	-	-	15/51/91/95	0/2/2/2
31	LMT	t	102	-	-	9/17/38/61	0/1/1/2
31	LMT	T	101	-	-	9/21/61/61	0/2/2/2
23	CLA	B	612	-	1/1/15/20	3/39/115/115	-
23	CLA	b	612	-	1/1/15/20	5/39/115/115	-
25	GOL	c	527	-	-	3/4/4/4	-
35	DGD	C	520	-	-	23/51/91/95	0/2/2/2
23	CLA	A	404[B]	-	1/1/15/20	5/39/115/115	-
33	LMG	C	521	-	-	10/46/66/70	0/1/1/1
28	PL9	D	407[B]	-	-	7/53/73/73	0/1/1/1
23	CLA	B	609	-	1/1/15/20	2/39/115/115	-
23	CLA	A	407	-	1/1/15/20	8/39/115/115	-
25	GOL	B	624	-	-	2/4/4/4	-
25	GOL	D	403	-	-	2/4/4/4	-
38	HEM	F	102	5,6	-	6/14/54/54	-
24	BCR	A	408	-	-	0/29/63/63	0/2/2/2
24	BCR	T	102	-	-	1/29/63/63	0/2/2/2
25	GOL	o	302	-	-	2/4/4/4	-
23	CLA	B	603	-	1/1/15/20	2/39/115/115	-
32	LHG	d	411[A]	-	-	15/53/53/53	-
24	BCR	k	101	-	-	0/29/63/63	0/2/2/2
34	HTG	b	623	-	-	3/10/30/30	0/1/1/1
28	PL9	a	414[A]	-	-	14/53/73/73	0/1/1/1
24	BCR	b	619	-	-	4/29/63/63	0/2/2/2
23	CLA	b	611	-	1/1/15/20	2/39/115/115	-
25	GOL	B	627	-	-	4/4/4/4	-
35	DGD	H	102	-	-	10/51/91/95	0/2/2/2
23	CLA	C	509	41	1/1/15/20	11/39/115/115	-
23	CLA	b	614	-	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	m	101	-	-	14/46/66/70	0/1/1/1
32	LHG	L	101[A]	-	-	20/53/53/53	-
24	BCR	t	103	-	-	1/29/63/63	0/2/2/2
23	CLA	b	613	-	1/1/15/20	3/39/115/115	-
26	SQD	f	102	-	-	15/38/58/69	0/1/1/1
23	CLA	a	407[A]	41	-	6/39/115/115	-
33	LMG	c	520	-	-	11/46/66/70	0/1/1/1
23	CLA	C	503	-	1/1/15/20	4/39/115/115	-
31	LMT	F	101	-	-	8/21/61/61	0/2/2/2
23	CLA	A	405[A]	41	1/1/15/20	1/39/115/115	-
37	PHO	a	408[B]	-	-	4/37/103/103	0/5/6/6
32	LHG	A	416[B]	-	-	11/53/53/53	-
25	GOL	a	419	-	-	0/4/4/4	-
32	LHG	a	420[B]	-	-	15/46/46/53	-
32	LHG	l	802[B]	-	-	15/53/53/53	-
38	HEM	f	101	5,6	-	8/14/54/54	-
33	LMG	C	526	-	-	10/31/51/70	0/1/1/1
34	HTG	b	622	-	-	5/10/30/30	0/1/1/1
23	CLA	b	610	41	1/1/15/20	6/39/115/115	-
23	CLA	A	406[B]	41	-	4/39/115/115	-
25	GOL	V	204[A]	-	-	2/4/4/4	-
33	LMG	C	502	-	-	16/46/66/70	0/1/1/1
23	CLA	d	402	-	1/1/15/20	8/39/115/115	-
37	PHO	D	401[A]	-	-	0/37/103/103	0/5/6/6
23	CLA	b	609	-	1/1/15/20	1/39/115/115	-
23	CLA	c	504	-	1/1/15/20	3/39/115/115	-
23	CLA	a	405[A]	-	1/1/15/20	4/39/115/115	-
26	SQD	B	620	-	-	16/49/69/69	0/1/1/1
34	HTG	C	523	-	-	0/10/30/30	0/1/1/1
23	CLA	b	602	-	1/1/15/20	5/39/115/115	-
34	HTG	V	203	-	-	0/2/19/30	0/1/1/1
35	DGD	C	519[A]	-	-	12/51/91/95	0/2/2/2
25	GOL	l	801[B]	-	-	0/4/4/4	-
32	LHG	d	406[B]	-	-	13/53/53/53	-
23	CLA	B	611	-	1/1/15/20	3/39/115/115	-
23	CLA	C	514	-	1/1/15/20	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	y	101	-	-	5/29/63/63	0/2/2/2
32	LHG	D	408[A]	-	-	17/53/53/53	-
34	HTG	D	412	-	-	3/7/27/30	0/1/1/1
35	DGD	c	518[B]	-	-	14/51/91/95	0/2/2/2
25	GOL	v	202[A]	-	-	2/4/4/4	-
26	SQD	A	410	-	-	14/49/69/69	0/1/1/1
26	SQD	C	501[B]	-	-	9/49/69/69	0/1/1/1
31	LMT	A	415	-	-	8/21/61/61	0/2/2/2
32	LHG	d	405[B]	-	-	13/53/53/53	-
25	GOL	O	303	-	-	2/4/4/4	-
23	CLA	C	512	-	1/1/15/20	13/39/115/115	-
25	GOL	D	414	-	-	4/4/4/4	-
25	GOL	c	526[A]	-	-	0/4/4/4	-
28	PL9	A	412[B]	-	-	14/53/73/73	0/1/1/1
35	DGD	c	519	-	-	10/51/91/95	0/2/2/2
23	CLA	B	604	-	1/1/15/20	4/39/115/115	-
24	BCR	D	406	-	-	4/29/63/63	0/2/2/2
35	DGD	C	518[A]	-	-	15/51/91/95	0/2/2/2
33	LMG	z	101	-	-	10/34/54/70	0/1/1/1
40	HEC	v	201	16	-	6/14/54/54	-
31	LMT	B	630	-	-	11/21/61/61	0/2/2/2
31	LMT	b	621	-	-	9/17/37/61	0/1/1/2
23	CLA	d	401[B]	-	1/1/15/20	4/39/115/115	-
25	GOL	c	528	-	-	2/4/4/4	-
24	BCR	H	101	-	-	2/29/63/63	0/2/2/2
28	PL9	D	407[A]	-	-	6/53/73/73	0/1/1/1
26	SQD	b	620	-	-	18/49/69/69	0/1/1/1
25	GOL	C	524[B]	-	-	0/4/4/4	-
24	BCR	c	516	-	-	2/29/63/63	0/2/2/2
31	LMT	c	501	-	-	10/21/61/61	0/2/2/2
24	BCR	B	619	-	-	0/29/63/63	0/2/2/2
24	BCR	C	516	-	-	1/29/63/63	0/2/2/2
23	CLA	B	615	-	1/1/15/20	6/39/115/115	-
31	LMT	M	101	-	-	5/21/61/61	0/2/2/2
34	HTG	b	625	-	-	4/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	513	-	1/1/15/20	13/39/115/115	-
23	CLA	a	406[B]	41	-	4/39/115/115	-
32	LHG	D	409[A]	-	-	13/53/53/53	-
24	BCR	C	517	-	-	0/29/63/63	0/2/2/2
23	CLA	C	513	3	1/1/15/20	4/39/115/115	-
23	CLA	C	507	-	1/1/15/20	4/39/115/115	-
37	PHO	D	402[B]	-	-	1/37/103/103	0/5/6/6
24	BCR	B	617	-	-	2/29/63/63	0/2/2/2
23	CLA	c	509	-	1/1/15/20	3/39/115/115	-
35	DGD	c	517[B]	-	-	18/51/91/95	0/2/2/2
35	DGD	h	102	-	-	13/51/91/95	0/2/2/2
23	CLA	C	510	-	1/1/15/20	6/39/115/115	-
31	LMT	e	101	-	-	12/21/61/61	0/2/2/2
23	CLA	C	504	-	1/1/15/20	9/39/115/115	-
23	CLA	A	406[A]	41	-	5/39/115/115	-
23	CLA	b	603	-	1/1/15/20	6/39/115/115	-
24	BCR	h	101	-	-	2/29/63/63	0/2/2/2
28	PL9	a	414[B]	-	-	17/53/73/73	0/1/1/1
23	CLA	b	606	-	1/1/15/20	12/39/115/115	-
31	LMT	B	628	-	-	12/21/61/61	0/2/2/2
33	LMG	B	621	-	-	21/46/66/70	0/1/1/1
23	CLA	c	511	-	1/1/15/20	11/39/115/115	-
23	CLA	b	601	41	1/1/15/20	18/39/115/115	-
23	CLA	B	605	-	1/1/15/20	5/39/115/115	-
23	CLA	b	605	-	1/1/15/20	6/39/115/115	-
23	CLA	b	607	41	1/1/15/20	3/39/115/115	-
24	BCR	K	102	-	-	2/29/63/63	0/2/2/2
28	PL9	d	404[A]	-	-	6/53/73/73	0/1/1/1
32	LHG	L	101[B]	-	-	18/53/53/53	-
33	LMG	D	413	39	-	10/46/66/70	0/1/1/1
24	BCR	Y	101	-	-	3/29/63/63	0/2/2/2
23	CLA	c	507	-	1/1/15/20	7/39/115/115	-
23	CLA	c	505	41	1/1/15/20	11/39/115/115	-
23	CLA	b	615	-	1/1/15/20	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	b	617	-	-	2/29/63/63	0/2/2/2
32	LHG	d	406[A]	-	-	12/53/53/53	-
23	CLA	c	503	-	1/1/15/20	2/39/115/115	-
24	BCR	a	410	-	-	3/29/63/63	0/2/2/2
23	CLA	A	405[B]	41	1/1/15/20	4/39/115/115	-
23	CLA	c	506	-	1/1/15/20	6/39/115/115	-
34	HTG	c	522	-	-	1/10/30/30	0/1/1/1
23	CLA	B	601	41	1/1/15/20	12/39/115/115	-
23	CLA	A	404[A]	-	1/1/15/20	3/39/115/115	-
33	LMG	a	417	-	-	14/46/66/70	0/1/1/1
23	CLA	B	607	41	1/1/15/20	3/39/115/115	-
25	GOL	d	410	-	-	1/4/4/4	-
37	PHO	a	416[B]	-	-	2/37/103/103	0/5/6/6
34	HTG	B	623	-	-	3/10/30/30	0/1/1/1
23	CLA	B	610	41	1/1/15/20	9/39/115/115	-
23	CLA	D	404[B]	-	1/1/15/20	3/39/115/115	-
23	CLA	d	401[A]	-	1/1/15/20	4/39/115/115	-
34	HTG	d	408	-	-	1/7/27/30	0/1/1/1
25	GOL	a	418	-	-	2/4/4/4	-
31	LMT	b	627	-	-	11/17/37/61	0/1/1/2
25	GOL	C	524[A]	-	-	0/4/4/4	-
23	CLA	B	616	-	1/1/15/20	8/39/115/115	-
26	SQD	a	411[B]	-	-	9/49/69/69	0/1/1/1
35	DGD	C	519[B]	-	-	10/51/91/95	0/2/2/2
23	CLA	B	614	-	1/1/15/20	12/39/115/115	-
32	LHG	E	101[B]	-	-	20/46/46/53	-
32	LHG	D	408[B]	-	-	19/53/53/53	-
33	LMG	C	522	-	-	14/46/66/70	0/1/1/1
25	GOL	v	202[B]	-	-	2/4/4/4	-
26	SQD	a	412	-	-	14/49/69/69	0/1/1/1
25	GOL	A	409	-	-	2/4/4/4	-
37	PHO	a	408[A]	-	-	6/37/103/103	0/5/6/6
33	LMG	c	521	-	-	9/46/66/70	0/1/1/1
32	LHG	A	416[A]	-	-	14/53/53/53	-
23	CLA	c	514	-	1/1/15/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	A	417	-	-	16/21/61/61	0/2/2/2
32	LHG	a	420[A]	-	-	16/46/46/53	-
32	LHG	l	802[A]	-	-	15/53/53/53	-
34	HTG	B	625	-	-	3/10/30/30	0/1/1/1
34	HTG	B	622	-	-	4/10/30/30	0/1/1/1
23	CLA	a	409	-	-	9/39/115/115	-
37	PHO	D	402[A]	-	-	1/37/103/103	0/5/6/6
23	CLA	C	515	-	1/1/15/20	6/39/115/115	-
31	LMT	m	103	-	-	6/21/61/61	0/2/2/2
32	LHG	d	411[B]	-	-	14/53/53/53	-
35	DGD	c	517[A]	-	-	17/51/91/95	0/2/2/2
25	GOL	b	624	-	-	2/4/4/4	-
33	LMG	d	409	39	-	8/46/66/70	0/1/1/1
24	BCR	B	618	-	-	0/29/63/63	0/2/2/2
24	BCR	b	618	-	-	0/29/63/63	0/2/2/2
23	CLA	D	405	-	1/1/15/20	13/39/115/115	-

The worst 5 of 1859 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	a	408[A]	PHO	C1B-C2B	9.37	1.49	1.39
37	a	416[B]	PHO	C1B-C2B	9.27	1.49	1.39
37	D	401[B]	PHO	C1D-C2D	9.25	1.49	1.39
37	D	402[B]	PHO	C1B-C2B	9.11	1.49	1.39
37	D	401[A]	PHO	C1D-C2D	9.05	1.49	1.39

The worst 5 of 3430 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	C3B-C2B-C1B	-13.46	91.30	107.17
37	D	401[A]	PHO	C2D-C1D-ND	11.49	117.73	109.43
23	B	611	CLA	C1D-ND-C4D	-11.26	98.41	106.31
23	a	409	CLA	C1D-ND-C4D	-11.25	98.42	106.31
37	a	416[A]	PHO	C2D-C1D-ND	10.99	117.38	109.43

5 of 69 chirality outliers are listed below:

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

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Mol	Chain	Res	Type	Atom
23	A	404[B]	CLA	ND
23	A	405[A]	CLA	ND
23	A	405[B]	CLA	ND
23	A	407	CLA	ND

5 of 1636 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	404[B]	CLA	C2B-C3B-CAB-CBB
23	A	404[B]	CLA	C4B-C3B-CAB-CBB
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	C	509	CLA	C2B-C3B-CAB-CBB

There are no ring outliers.

183 monomers are involved in 358 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	a	407[B]	CLA	2	0
25	l	801[A]	GOL	1	0
23	c	510	CLA	1	0
25	O	302	GOL	1	0
23	b	604	CLA	1	0
31	t	101	LMT	1	0
32	D	409[B]	LHG	4	0
35	c	518[A]	DGD	3	0
26	C	501[A]	SQD	1	0
24	c	515	BCR	3	0
32	d	405[A]	LHG	2	0
23	C	505	CLA	4	0
28	A	412[A]	PL9	11	0
23	C	506	CLA	1	0
23	C	508	CLA	4	0
25	V	204[B]	GOL	1	0
37	D	401[B]	PHO	1	0
23	B	602	CLA	3	0
25	B	629	GOL	1	0
23	C	511	CLA	3	0
26	F	103	SQD	2	0
23	a	405[B]	CLA	3	0
37	a	416[A]	PHO	1	0
23	b	616	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	606	CLA	2	0
23	B	613	CLA	3	0
23	c	502	CLA	4	0
23	D	404[A]	CLA	3	0
24	d	403	BCR	2	0
28	d	404[B]	PL9	1	0
26	a	411[A]	SQD	4	0
23	c	512	CLA	5	0
23	c	508	CLA	2	0
25	c	526[B]	GOL	1	0
23	a	406[A]	CLA	3	0
32	E	101[A]	LHG	3	0
25	b	628	GOL	2	0
35	C	518[B]	DGD	4	0
31	t	102	LMT	2	0
23	B	612	CLA	3	0
23	b	612	CLA	2	0
35	C	520	DGD	2	0
23	A	404[B]	CLA	2	0
23	B	609	CLA	2	0
23	A	407	CLA	3	0
25	B	624	GOL	1	0
25	D	403	GOL	5	0
38	F	102	HEM	1	0
24	A	408	BCR	1	0
24	T	102	BCR	6	0
23	B	603	CLA	1	0
24	k	101	BCR	2	0
28	a	414[A]	PL9	5	0
24	b	619	BCR	5	0
25	B	627	GOL	1	0
35	H	102	DGD	1	0
23	C	509	CLA	2	0
23	b	614	CLA	2	0
24	t	103	BCR	3	0
23	b	613	CLA	1	0
26	f	102	SQD	1	0
23	a	407[A]	CLA	1	0
33	c	520	LMG	1	0
23	C	503	CLA	4	0
23	A	405[A]	CLA	1	0
37	a	408[B]	PHO	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	a	419	GOL	5	0
32	a	420[B]	LHG	3	0
38	f	101	HEM	1	0
33	C	526	LMG	1	0
34	b	622	HTG	1	0
23	A	406[B]	CLA	3	0
33	C	502	LMG	2	0
23	d	402	CLA	2	0
37	D	401[A]	PHO	1	0
23	b	609	CLA	5	0
23	c	504	CLA	4	0
23	a	405[A]	CLA	2	0
26	B	620	SQD	3	0
23	b	602	CLA	1	0
35	C	519[A]	DGD	1	0
32	d	406[B]	LHG	7	0
23	C	514	CLA	2	0
24	y	101	BCR	2	0
32	D	408[A]	LHG	2	0
34	D	412	HTG	1	0
35	c	518[B]	DGD	4	0
25	v	202[A]	GOL	1	0
26	A	410	SQD	1	0
26	C	501[B]	SQD	1	0
31	A	415	LMT	1	0
32	d	405[B]	LHG	1	0
25	O	303	GOL	1	0
23	C	512	CLA	5	0
25	D	414	GOL	3	0
28	A	412[B]	PL9	8	0
35	c	519	DGD	4	0
23	B	604	CLA	2	0
24	D	406	BCR	2	0
35	C	518[A]	DGD	1	0
33	z	101	LMG	2	0
31	B	630	LMT	2	0
31	b	621	LMT	1	0
23	d	401[B]	CLA	4	0
24	H	101	BCR	2	0
28	D	407[A]	PL9	1	0
26	b	620	SQD	2	0
25	C	524[B]	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	c	516	BCR	1	0
31	c	501	LMT	2	0
24	B	619	BCR	1	0
23	B	615	CLA	2	0
34	b	625	HTG	1	0
23	c	513	CLA	2	0
23	a	406[B]	CLA	2	0
32	D	409[A]	LHG	5	0
23	C	513	CLA	4	0
23	C	507	CLA	6	0
37	D	402[B]	PHO	2	0
23	c	509	CLA	6	0
35	c	517[B]	DGD	2	0
23	C	510	CLA	4	0
31	e	101	LMT	1	0
23	C	504	CLA	3	0
23	A	406[A]	CLA	1	0
23	b	603	CLA	1	0
24	h	101	BCR	5	0
28	a	414[B]	PL9	5	0
23	b	606	CLA	3	0
31	B	628	LMT	1	0
33	B	621	LMG	1	0
23	b	601	CLA	3	0
23	B	605	CLA	4	0
23	b	605	CLA	3	0
23	b	607	CLA	2	0
24	K	102	BCR	1	0
32	L	101[B]	LHG	1	0
24	Y	101	BCR	3	0
23	c	507	CLA	3	0
23	c	505	CLA	4	0
23	b	615	CLA	2	0
24	b	617	BCR	2	0
32	d	406[A]	LHG	11	0
23	c	503	CLA	2	0
24	a	410	BCR	1	0
23	A	405[B]	CLA	3	0
23	c	506	CLA	6	0
34	c	522	HTG	1	0
23	B	601	CLA	3	0
23	A	404[A]	CLA	2	0

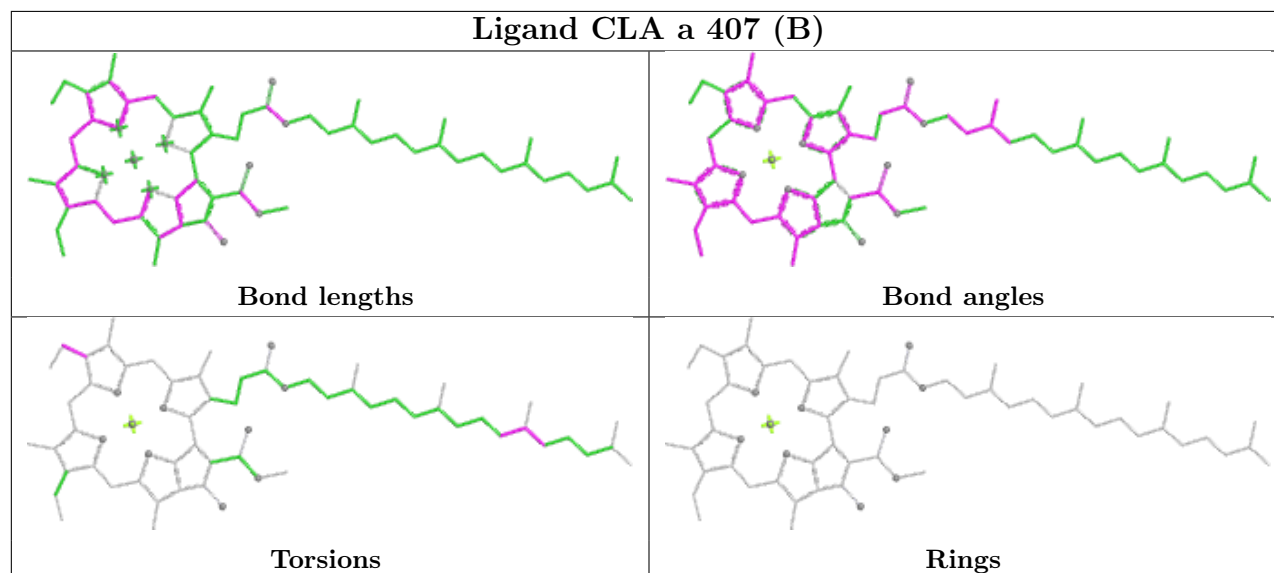
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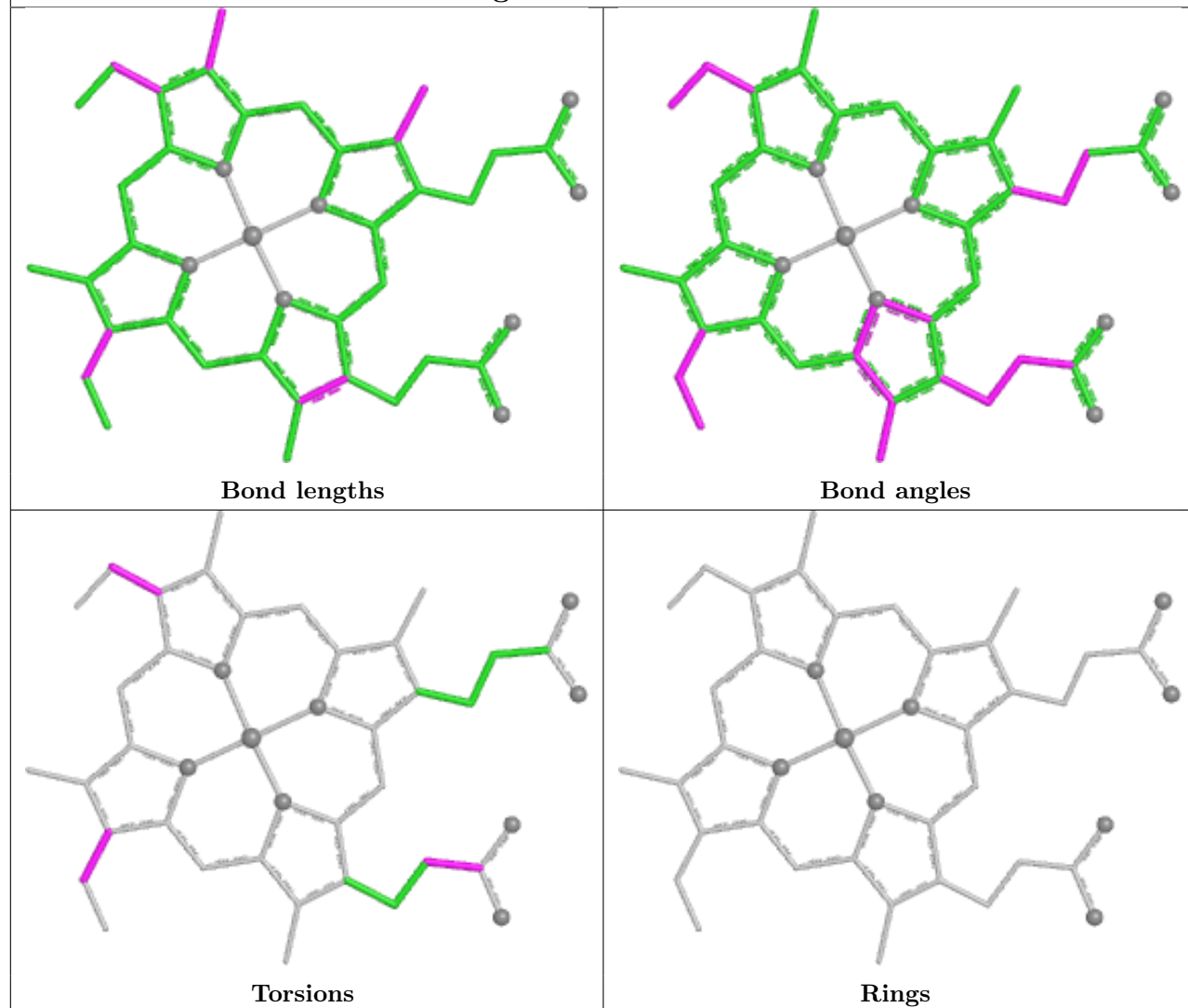
Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	a	417	LMG	1	0
23	B	607	CLA	1	0
37	a	416[B]	PHO	1	0
23	D	404[B]	CLA	4	0
23	d	401[A]	CLA	1	0
34	d	408	HTG	1	0
25	a	418	GOL	2	0
23	B	616	CLA	4	0
26	a	411[B]	SQD	4	0
35	C	519[B]	DGD	1	0
23	B	614	CLA	1	0
32	E	101[B]	LHG	3	0
32	D	408[B]	LHG	2	0
33	C	522	LMG	1	0
25	v	202[B]	GOL	1	0
26	a	412	SQD	1	0
25	A	409	GOL	1	0
33	c	521	LMG	1	0
32	A	416[A]	LHG	1	0
23	c	514	CLA	1	0
31	A	417	LMT	2	0
32	a	420[A]	LHG	5	0
34	B	625	HTG	1	0
34	B	622	HTG	2	0
23	a	409	CLA	2	0
37	D	402[A]	PHO	1	0
23	C	515	CLA	2	0
31	m	103	LMT	2	0
32	d	411[B]	LHG	3	0
35	c	517[A]	DGD	1	0
33	d	409	LMG	1	0
24	B	618	BCR	3	0
24	b	618	BCR	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

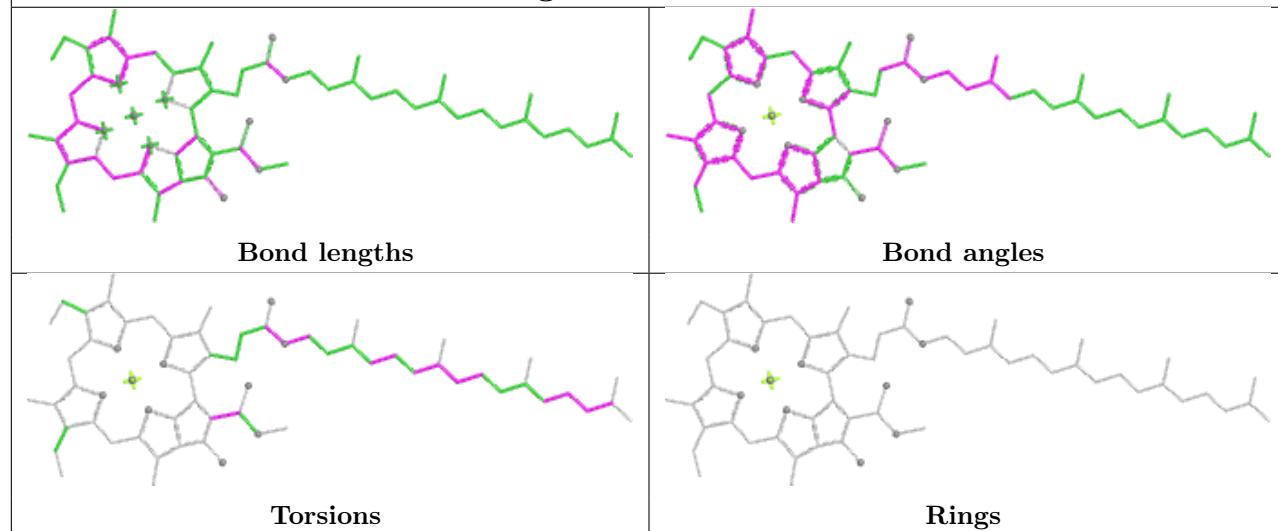
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

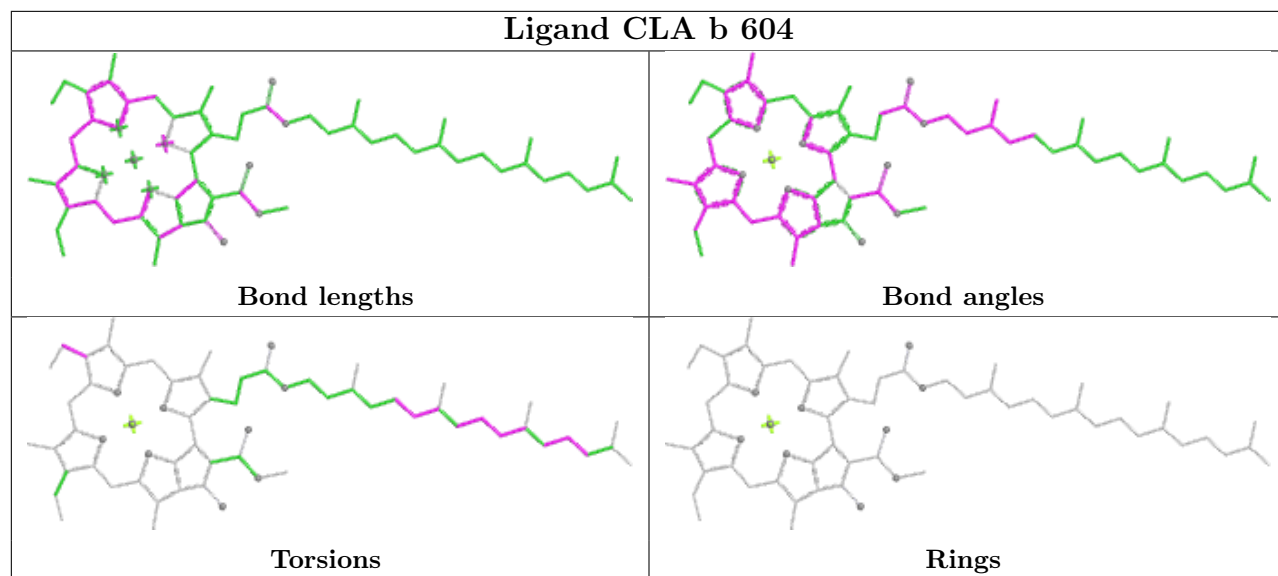


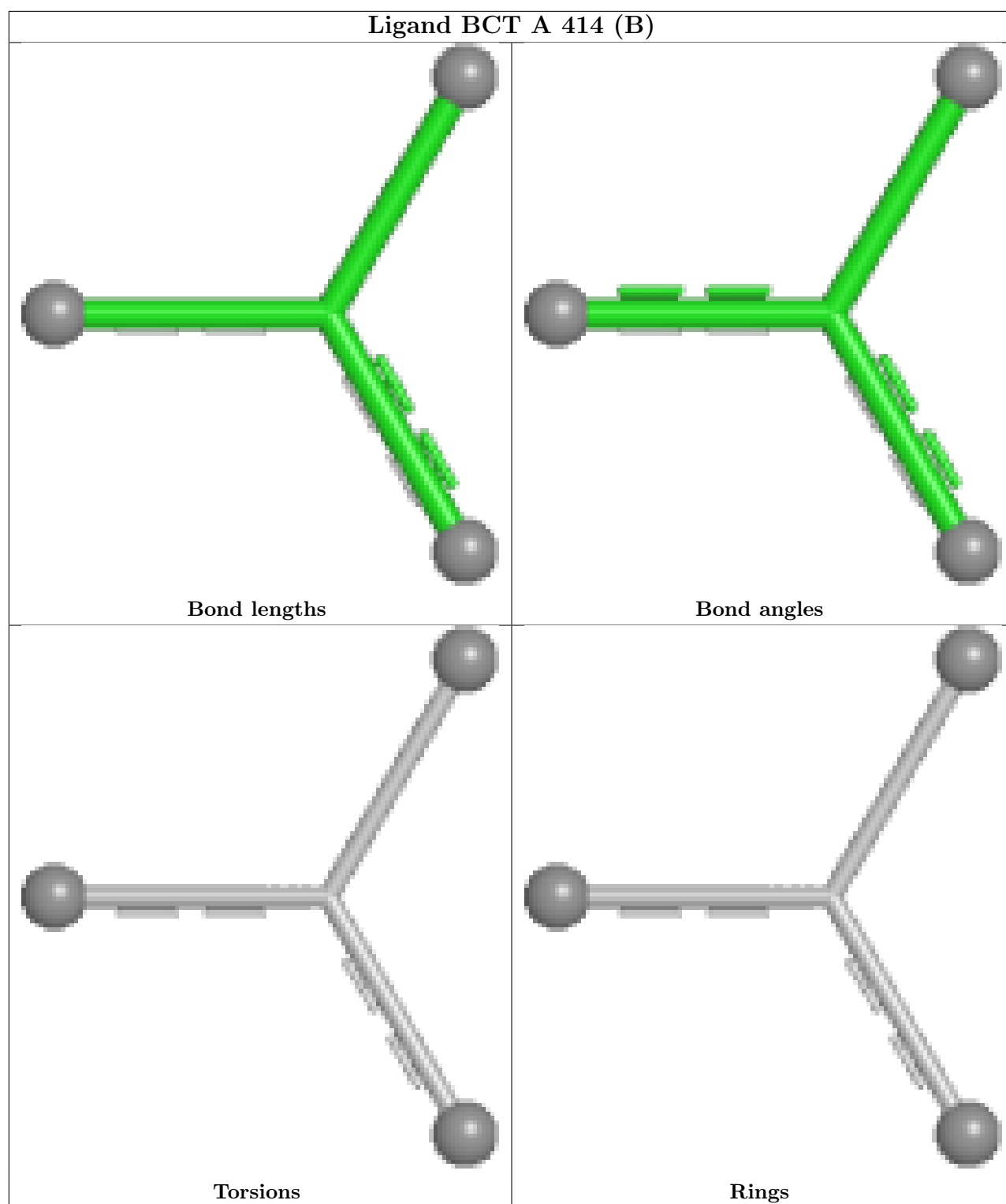
Ligand HEC V 202

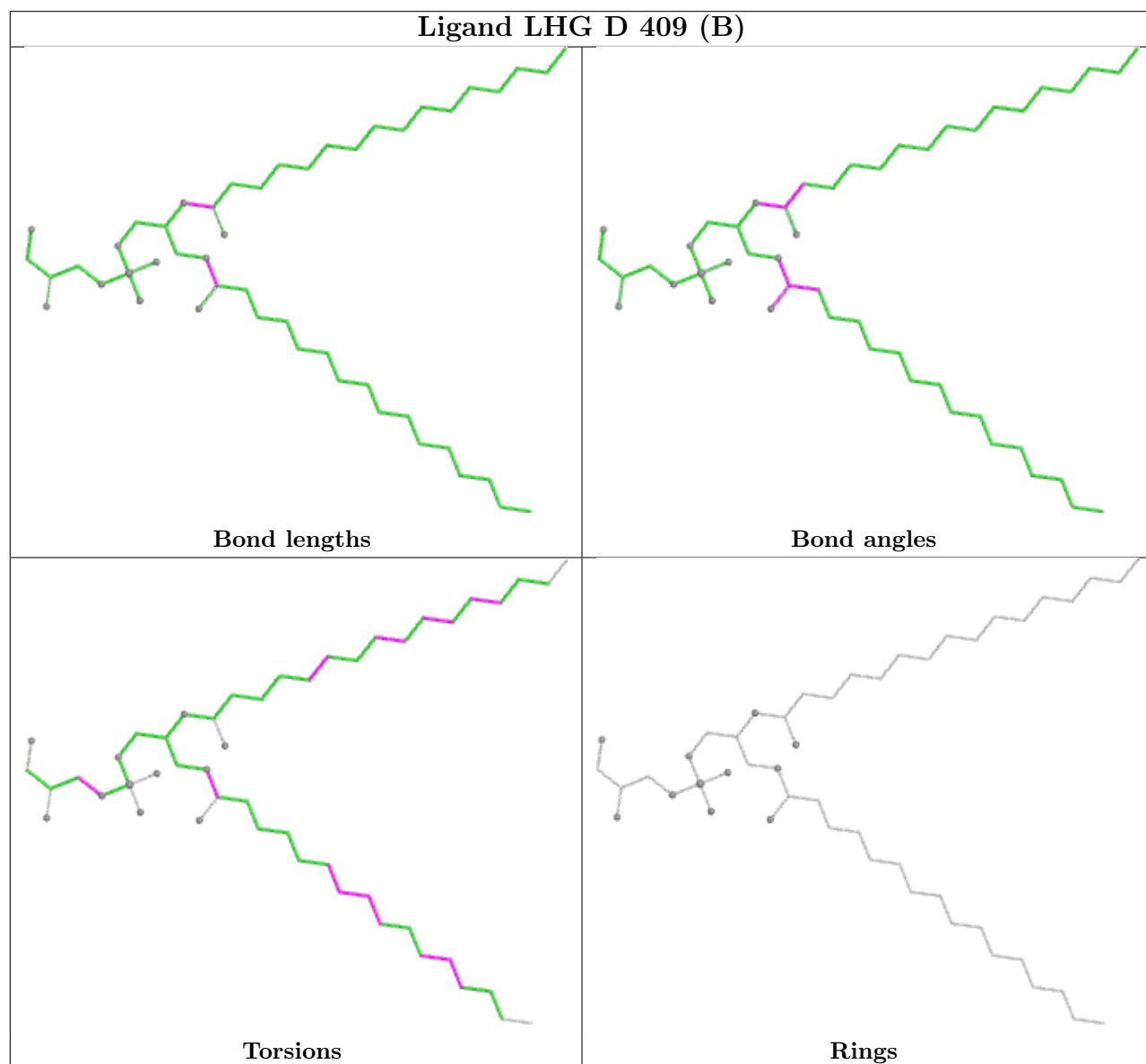
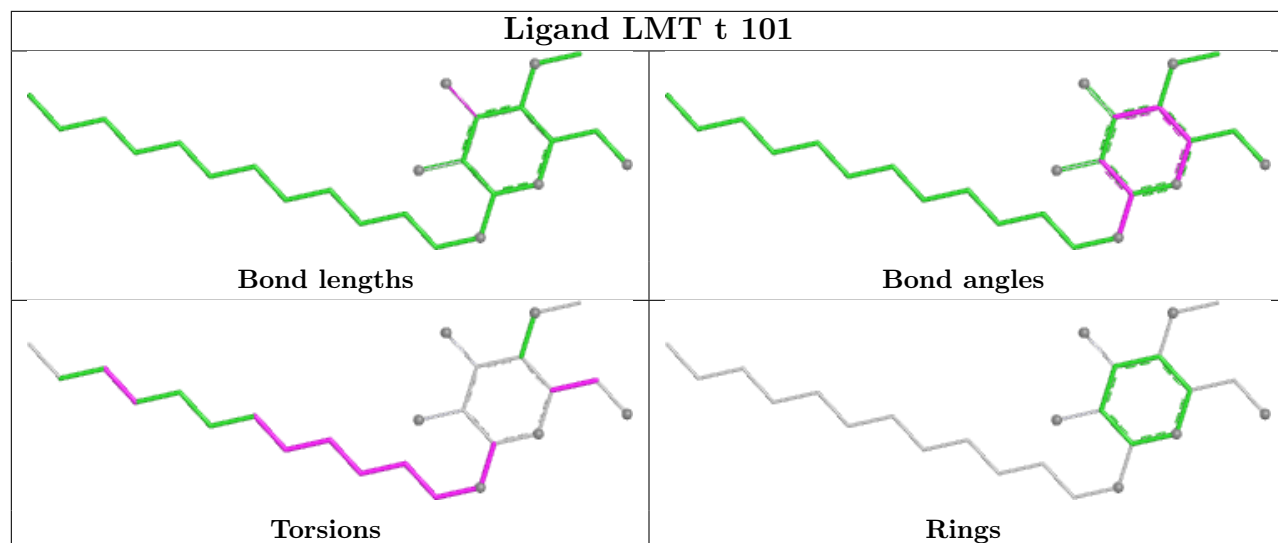


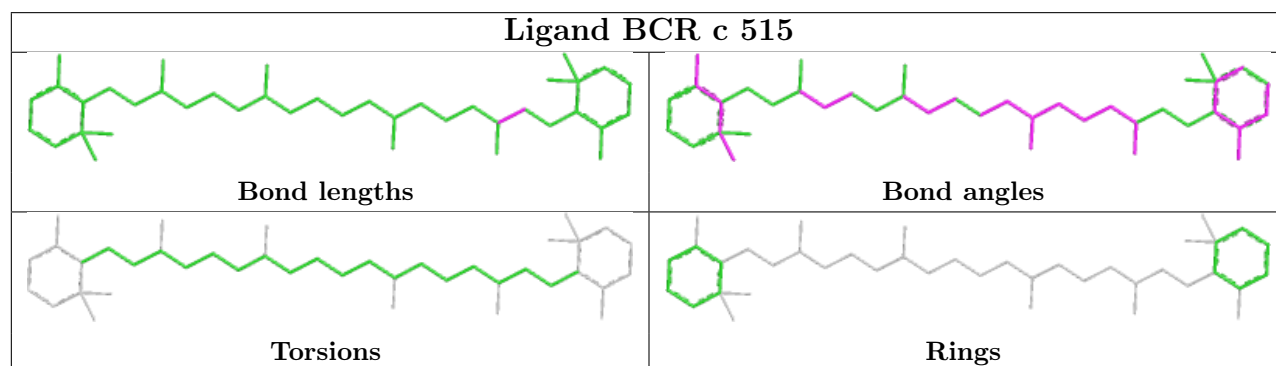
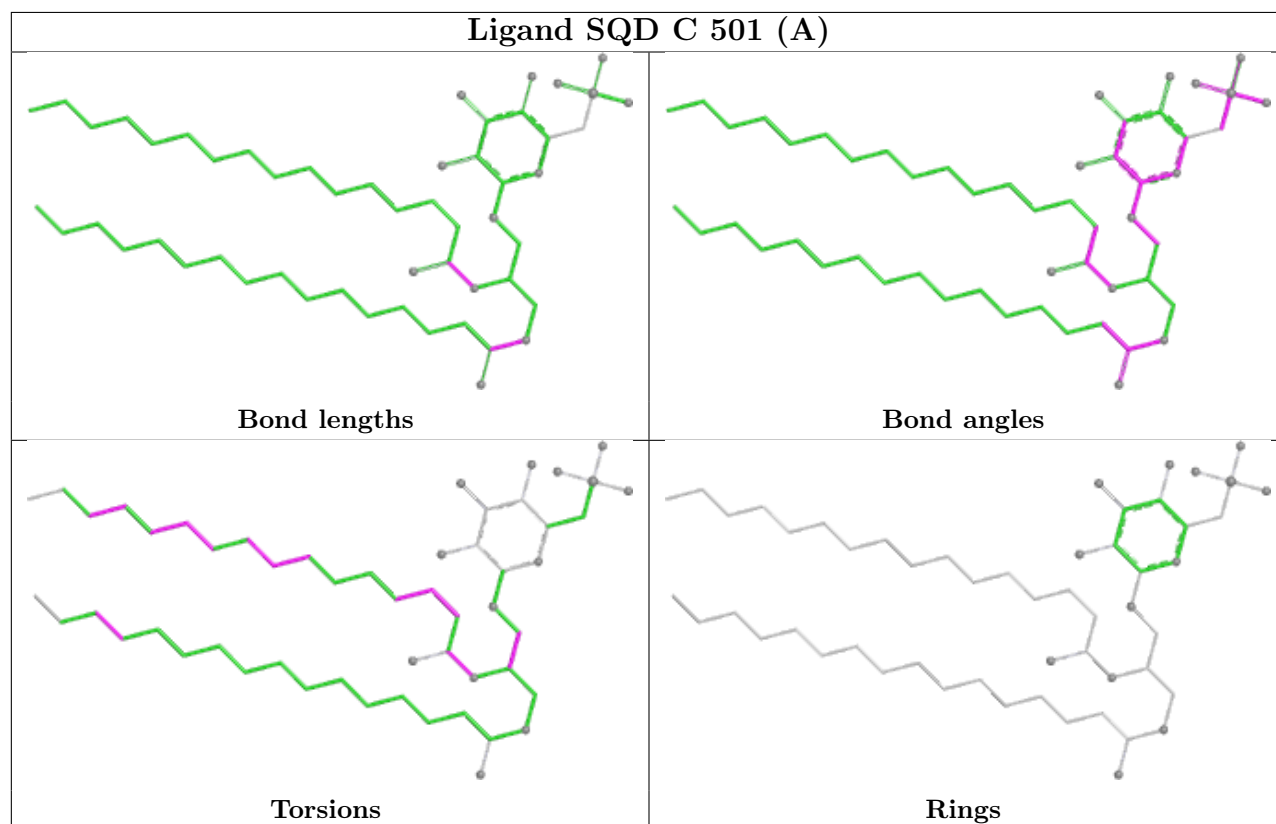
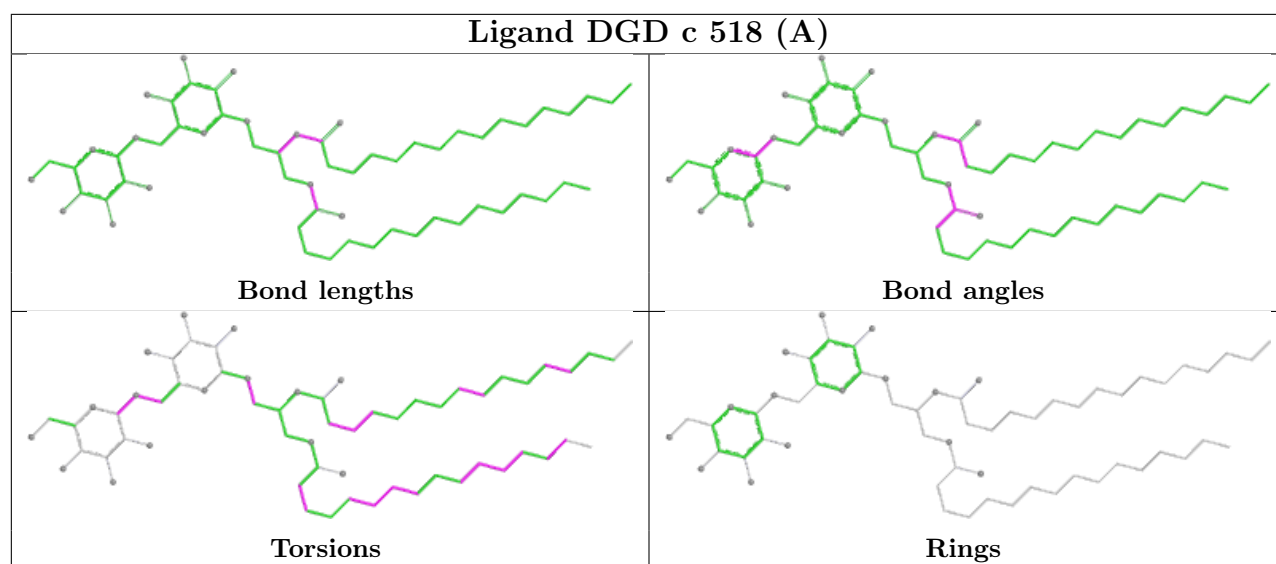
Ligand CLA c 510

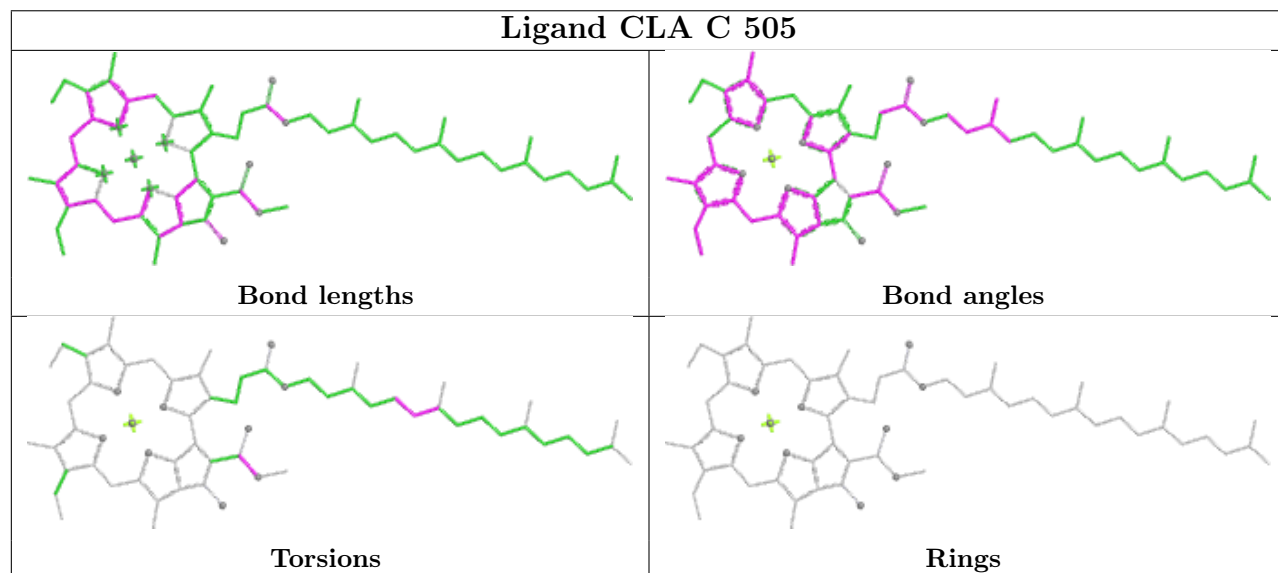
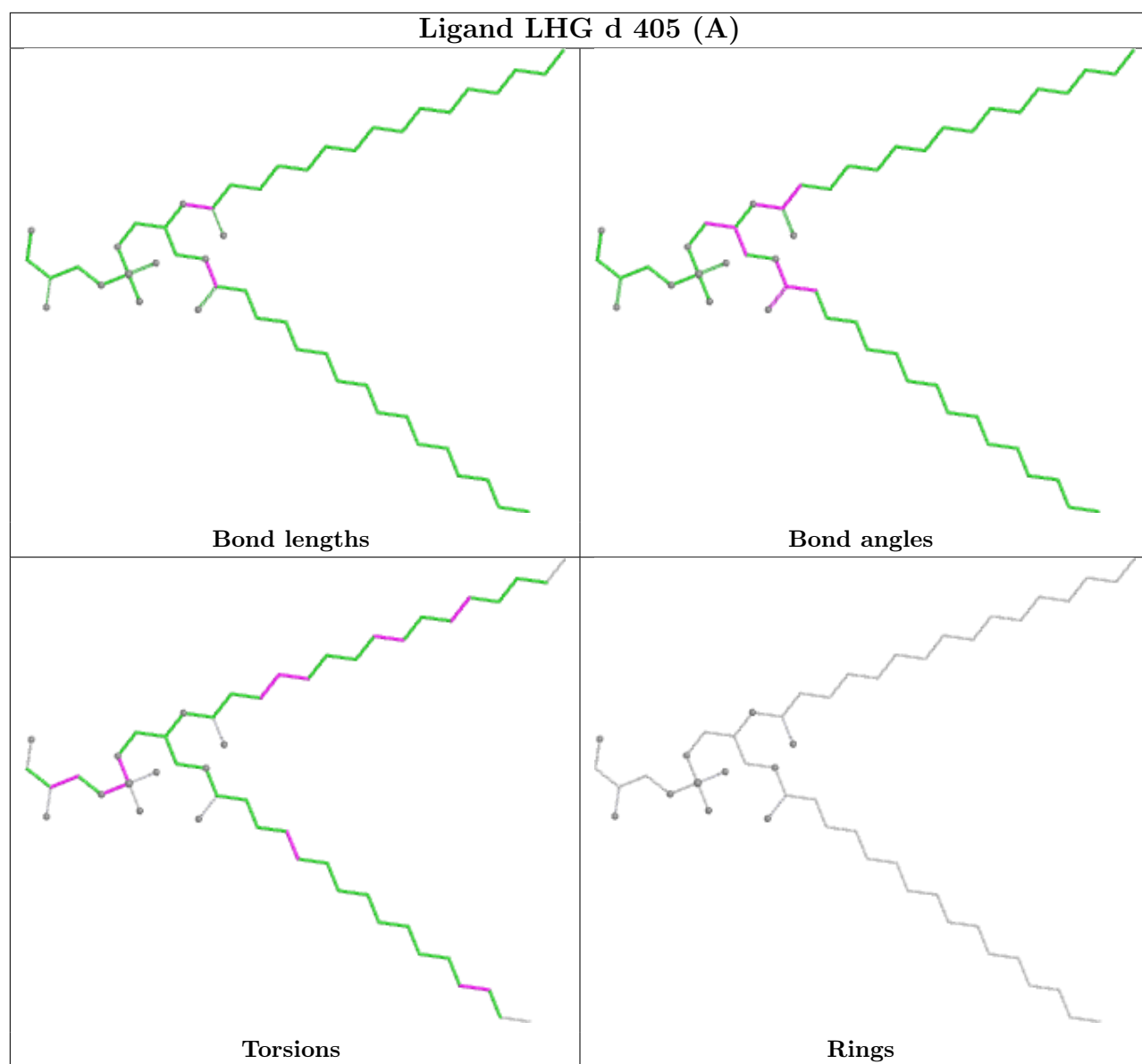


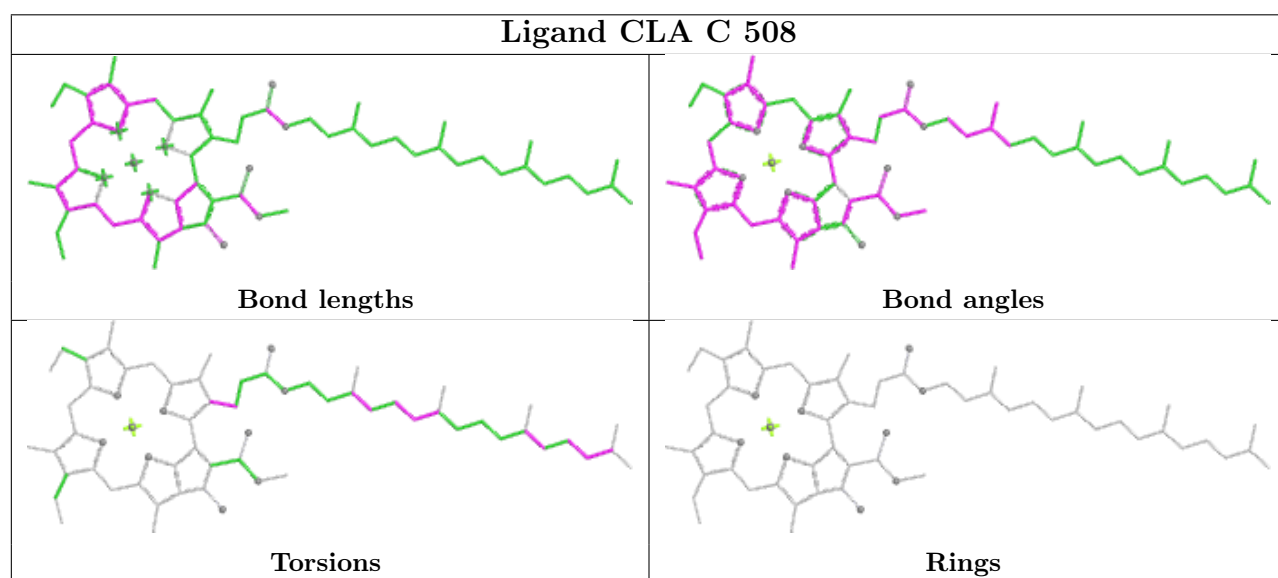
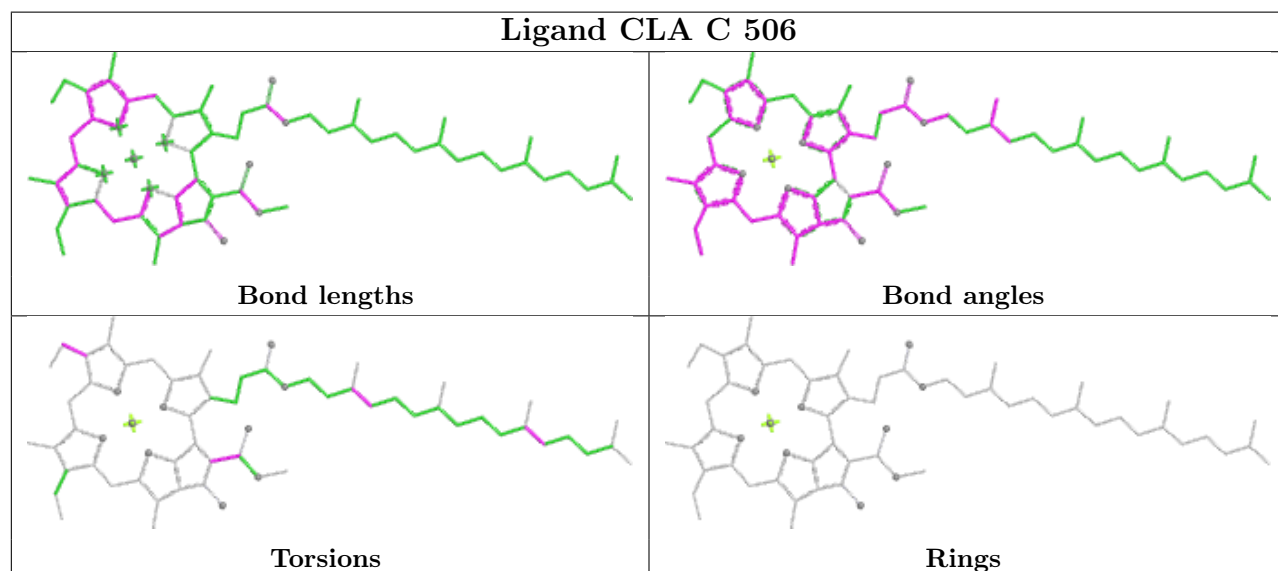
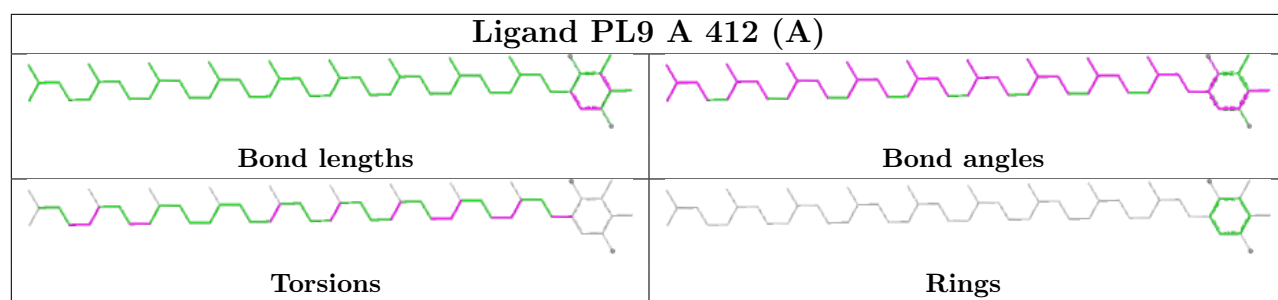


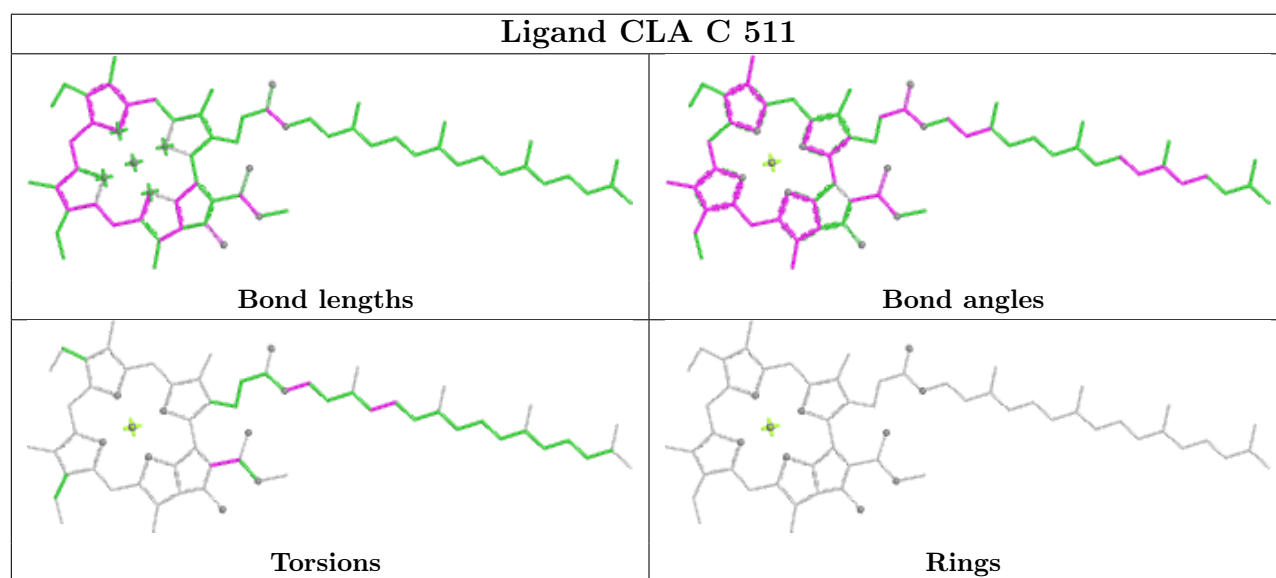
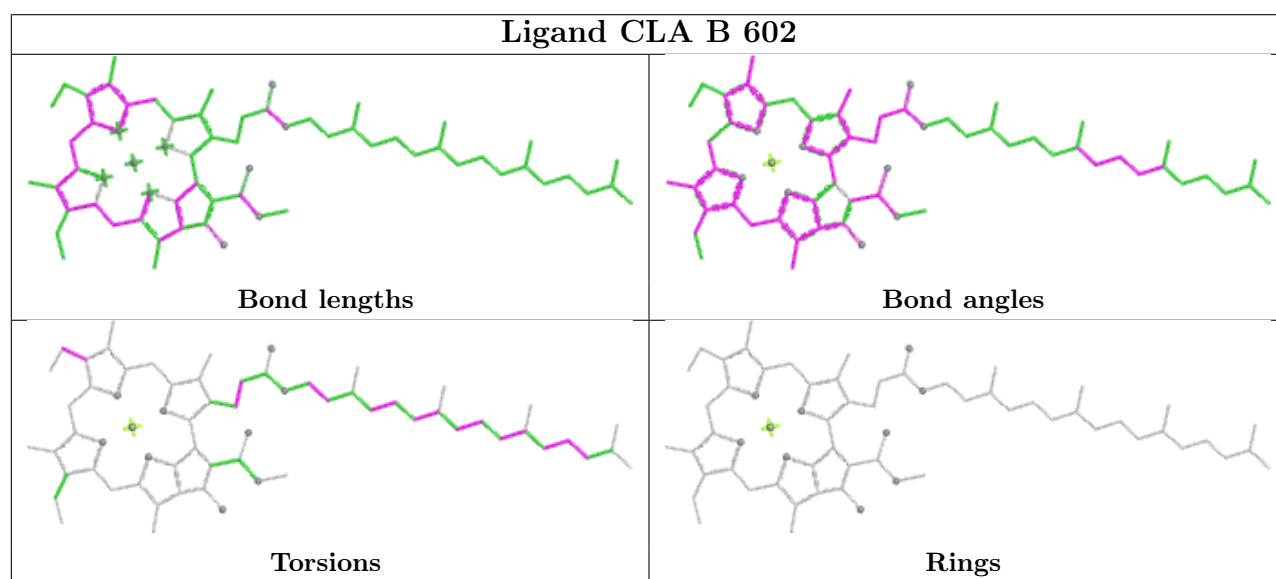
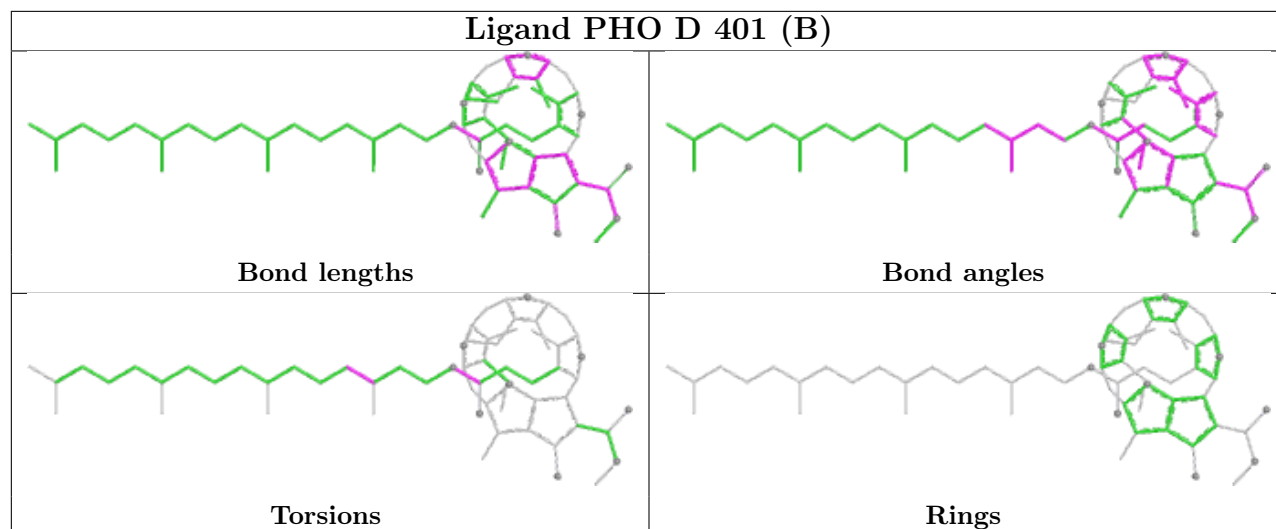


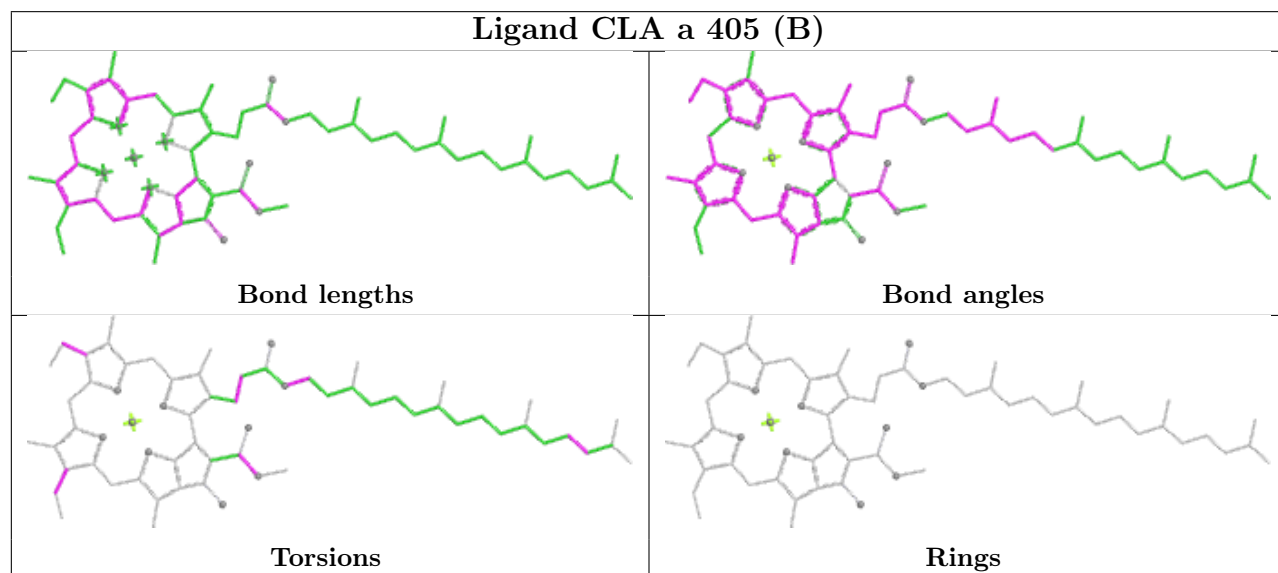
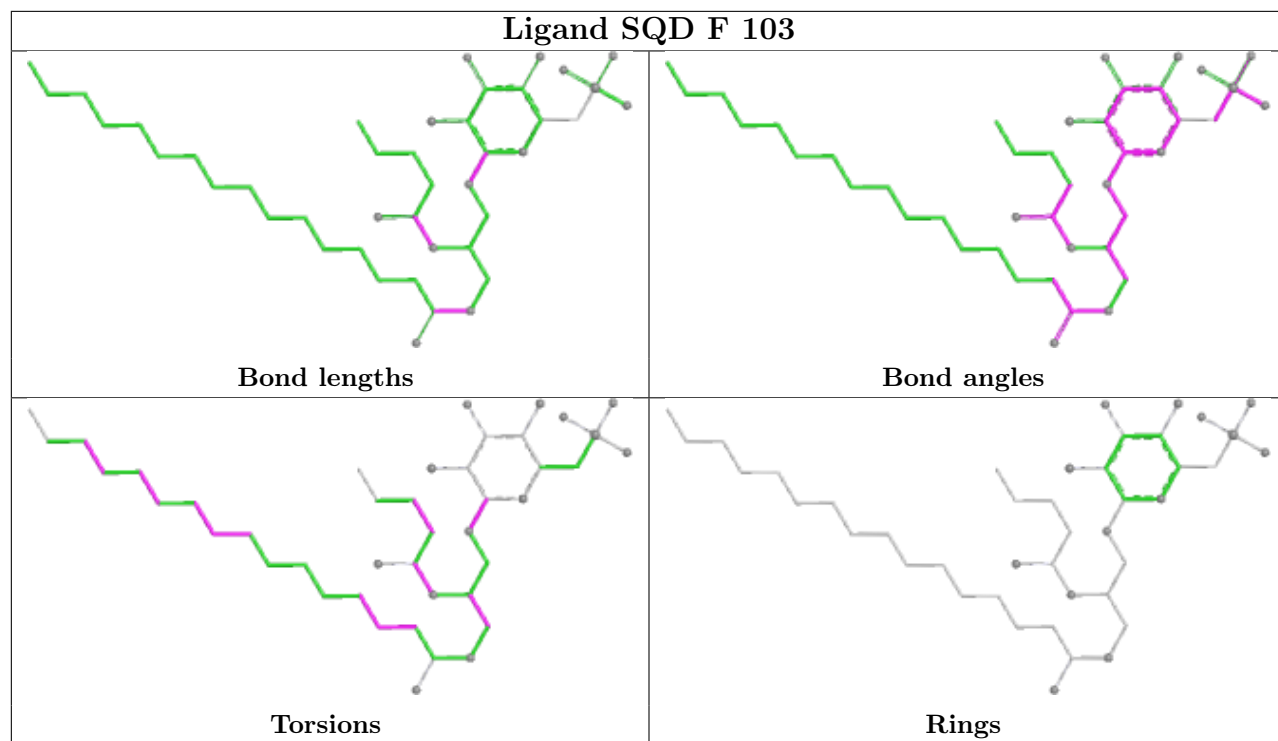


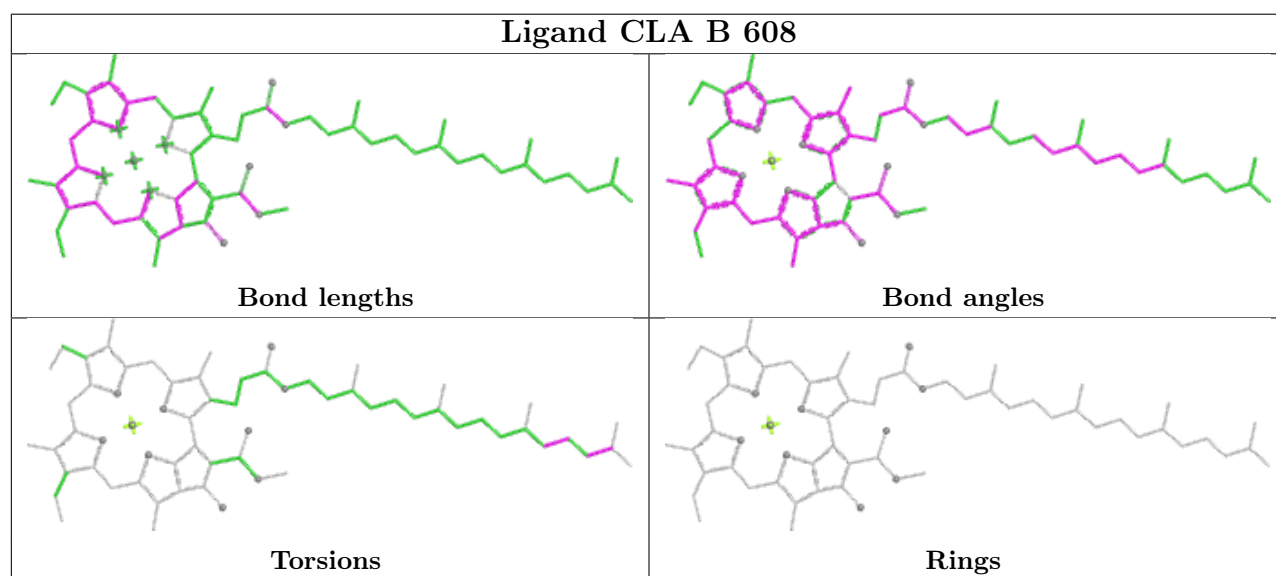
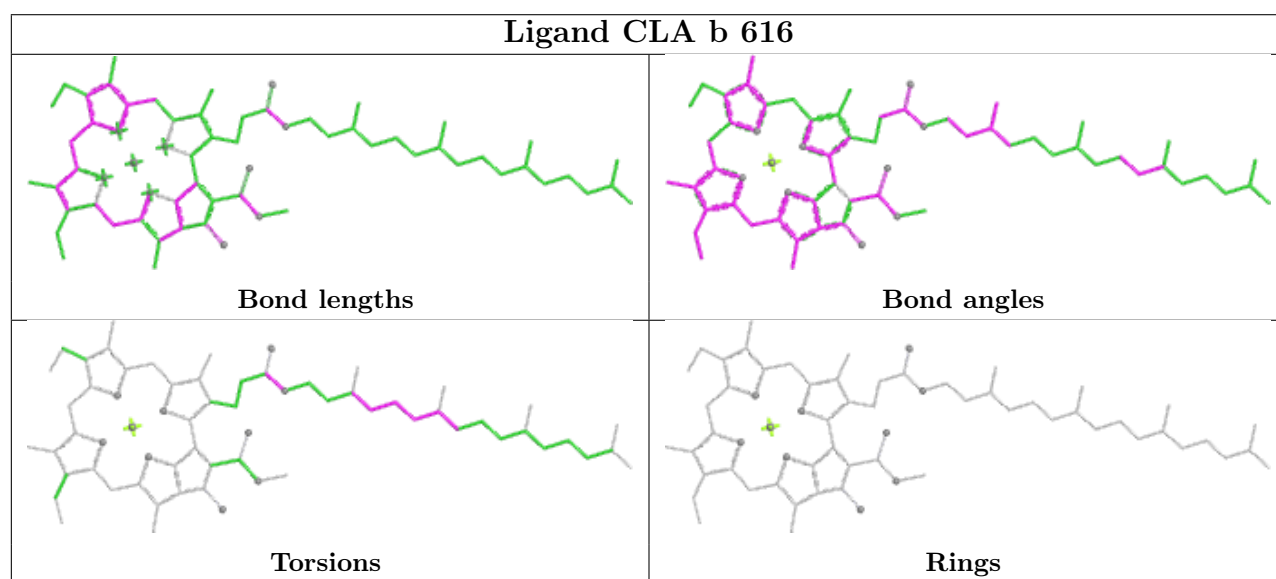
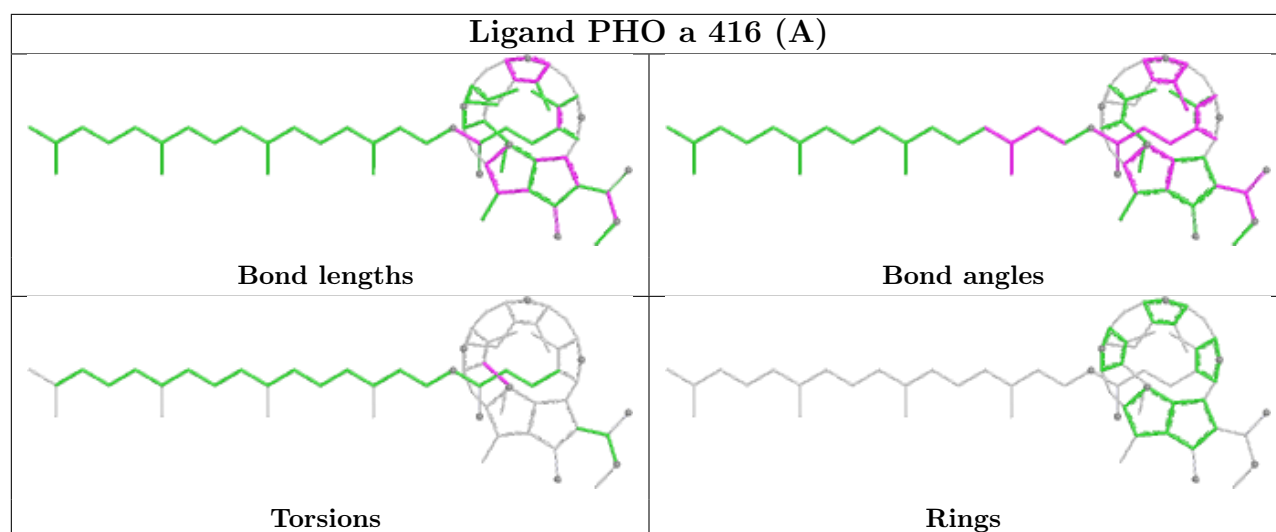


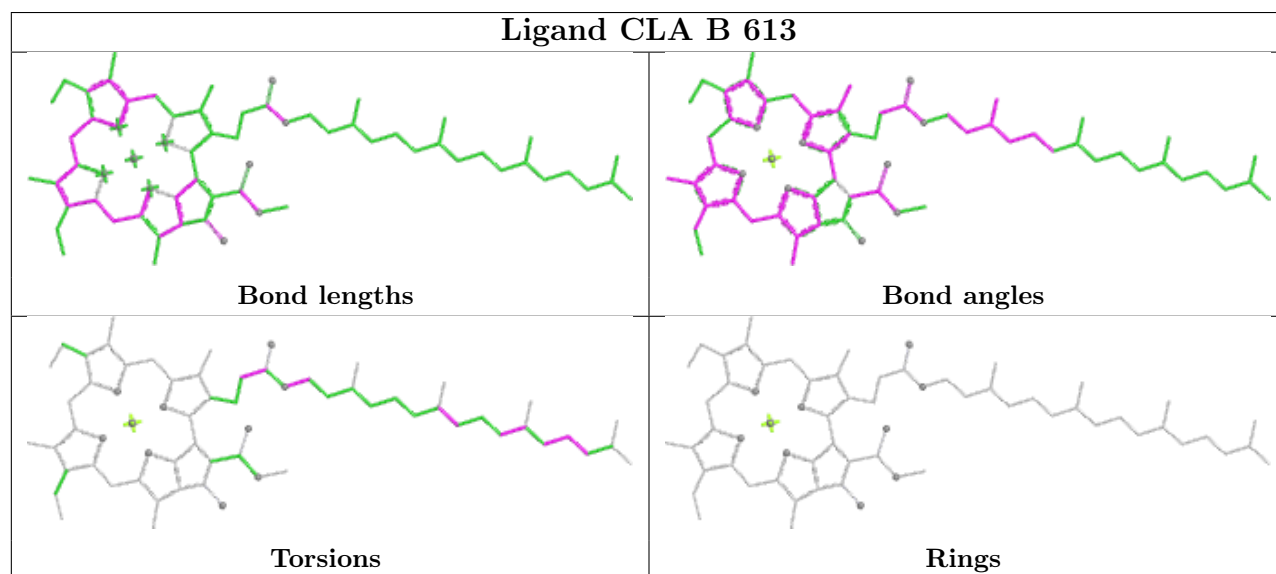
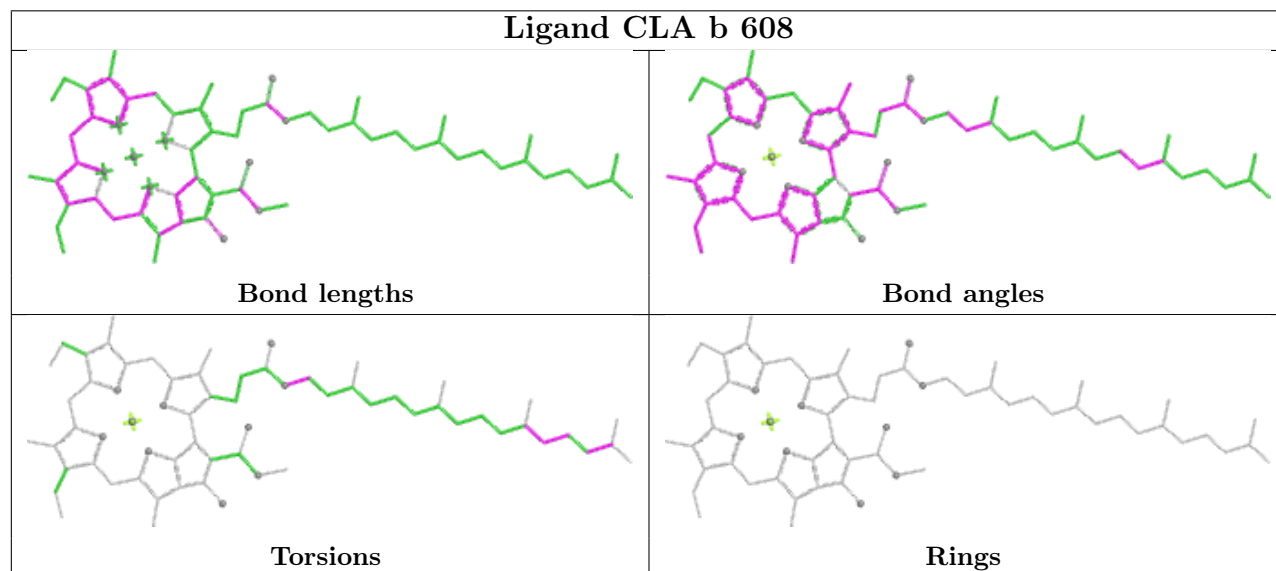
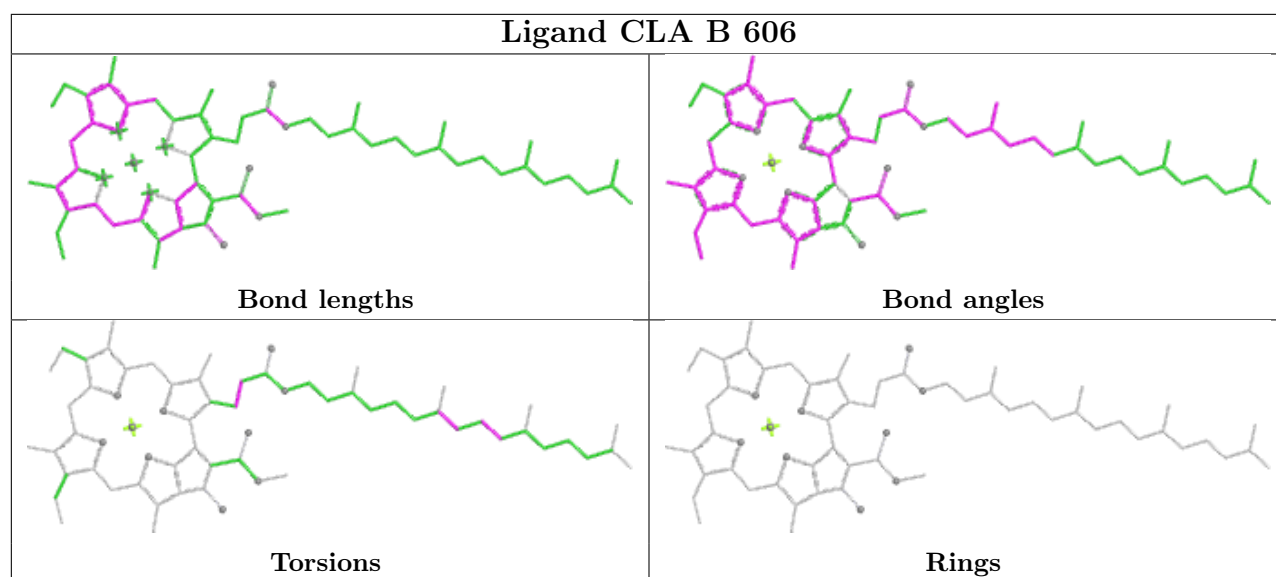


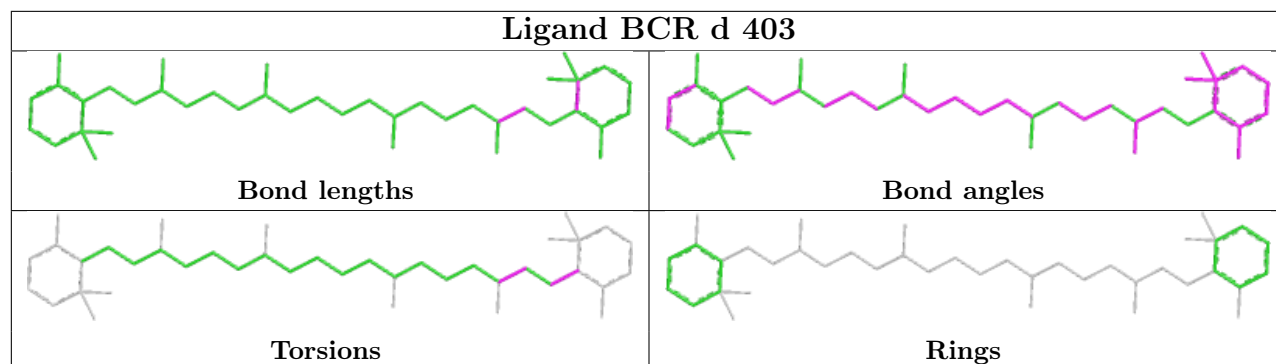
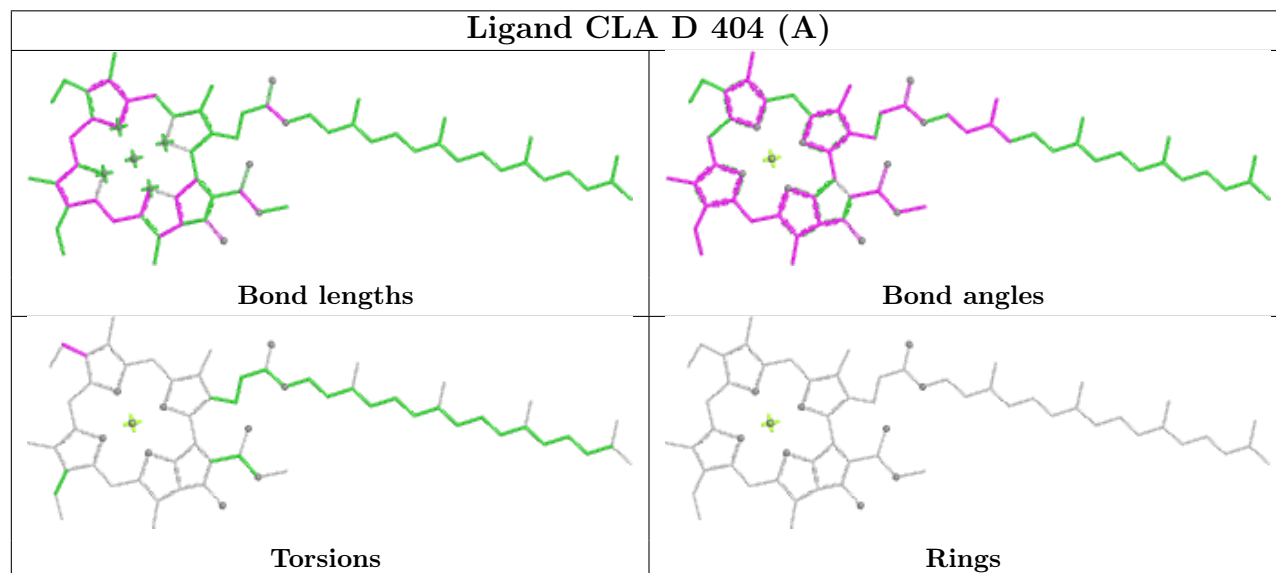
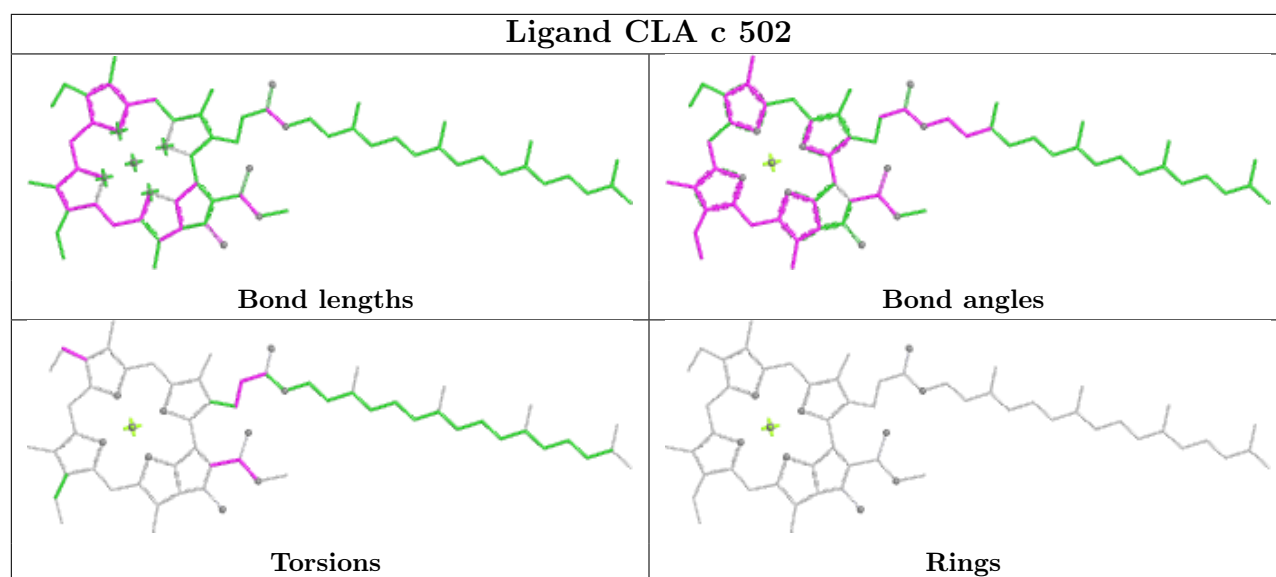


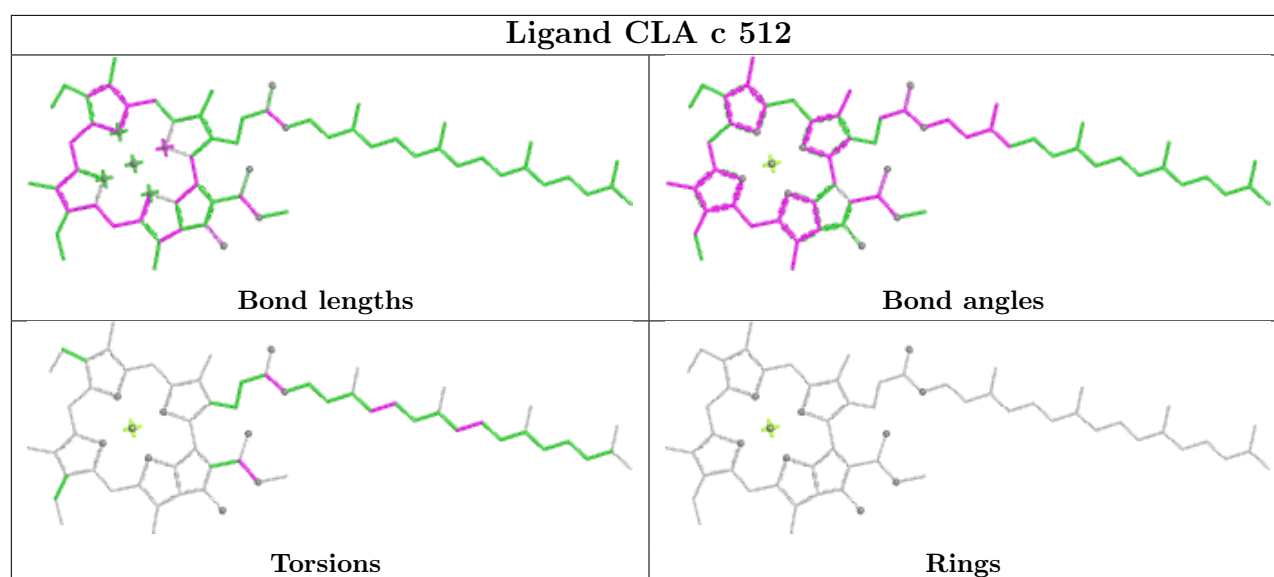
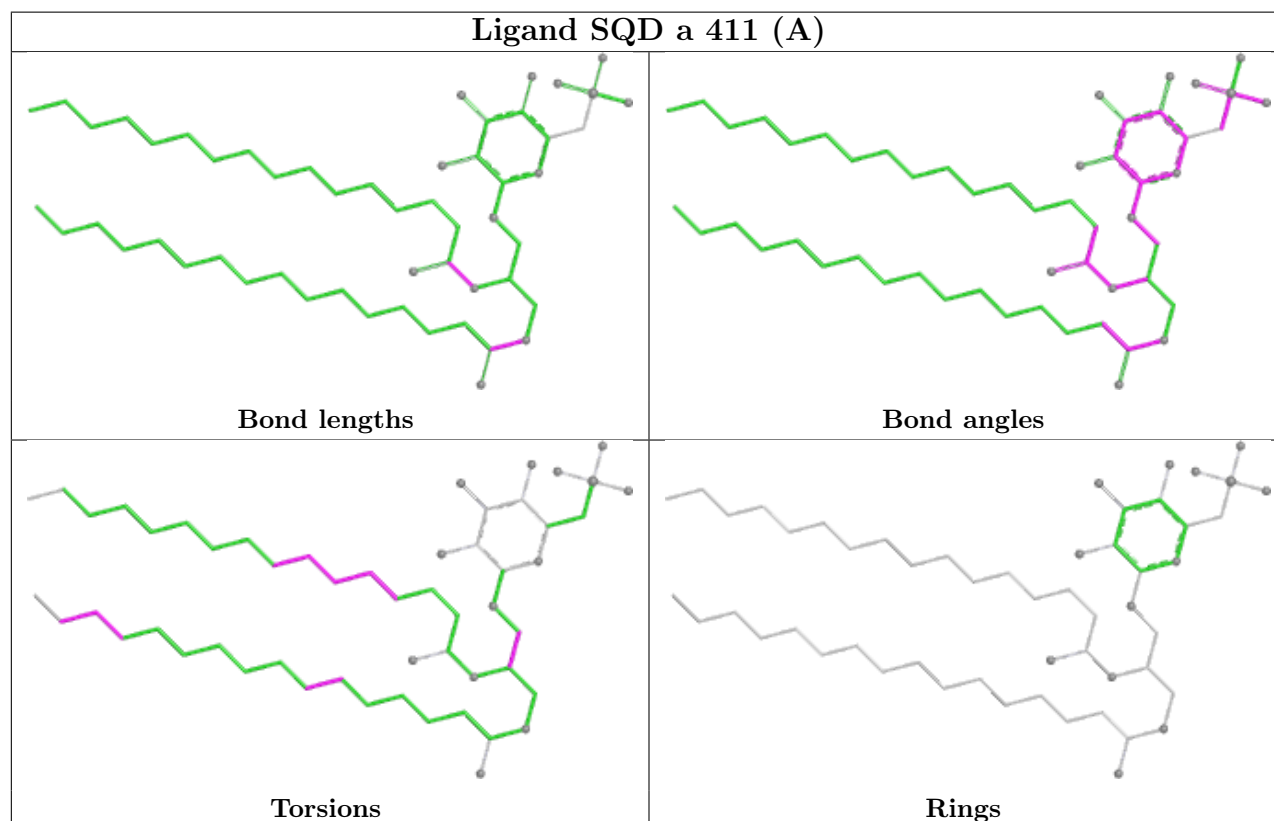
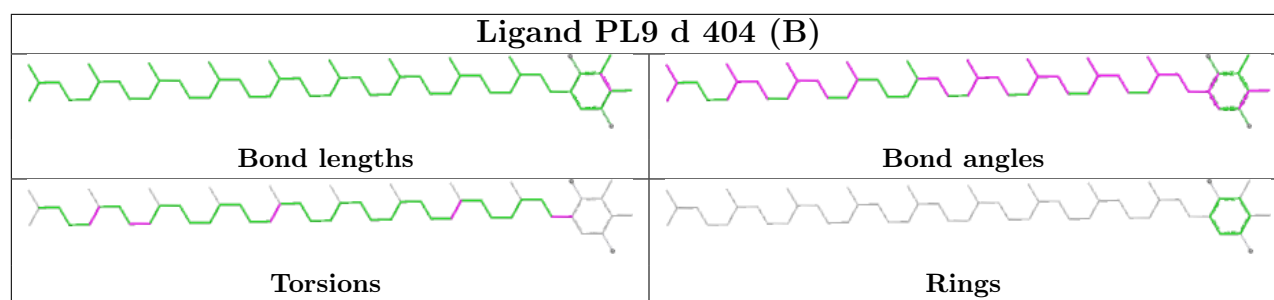




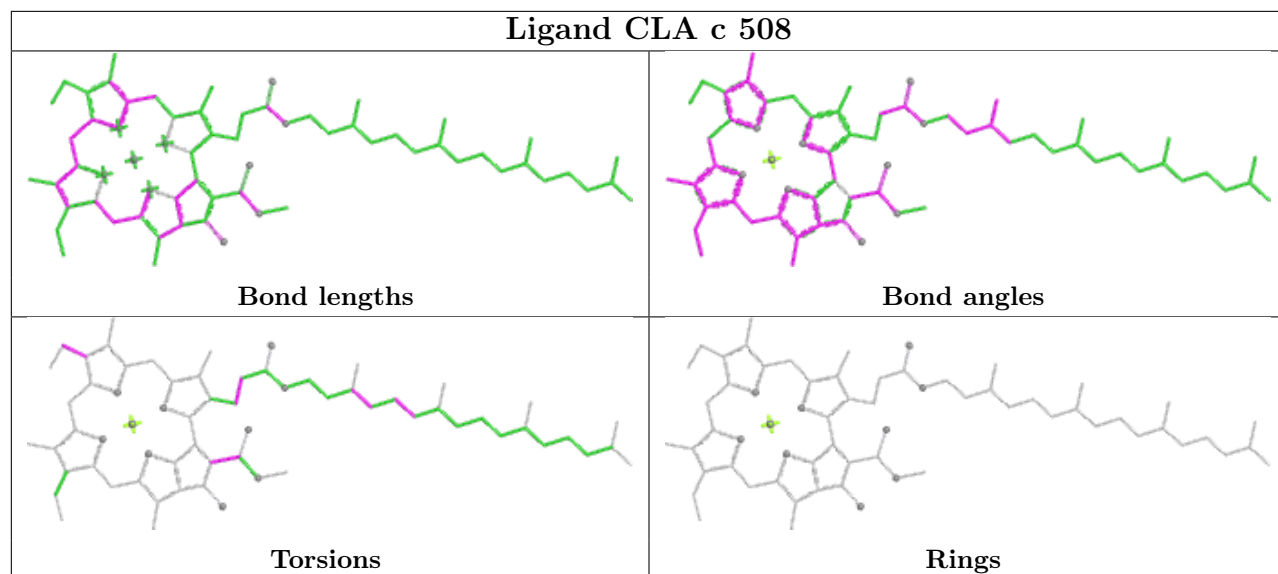




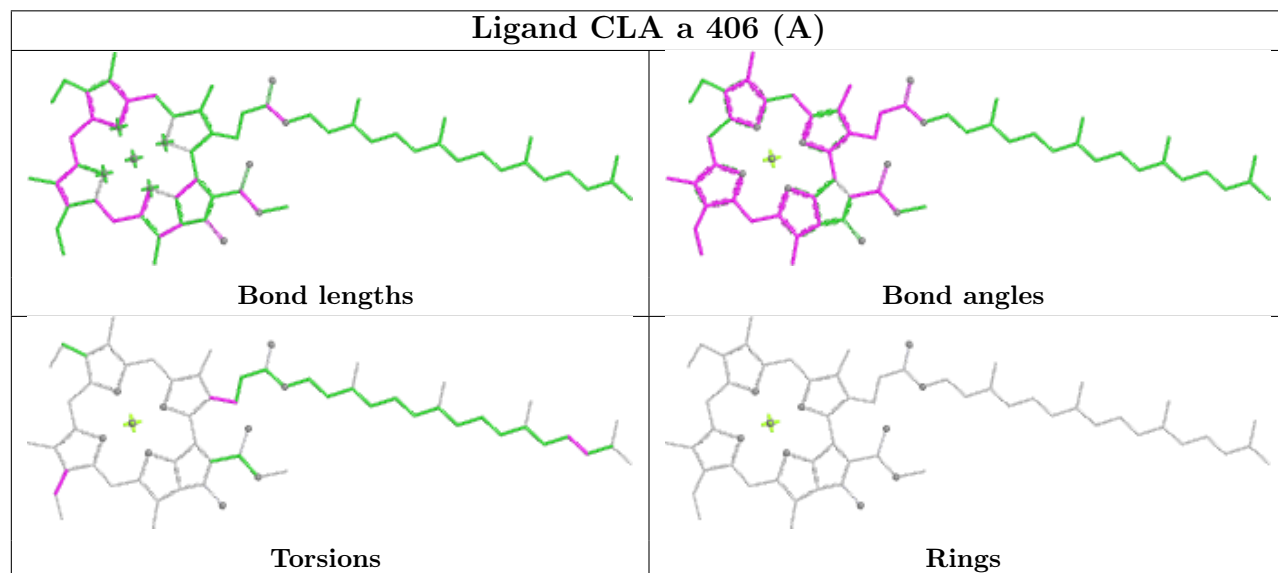


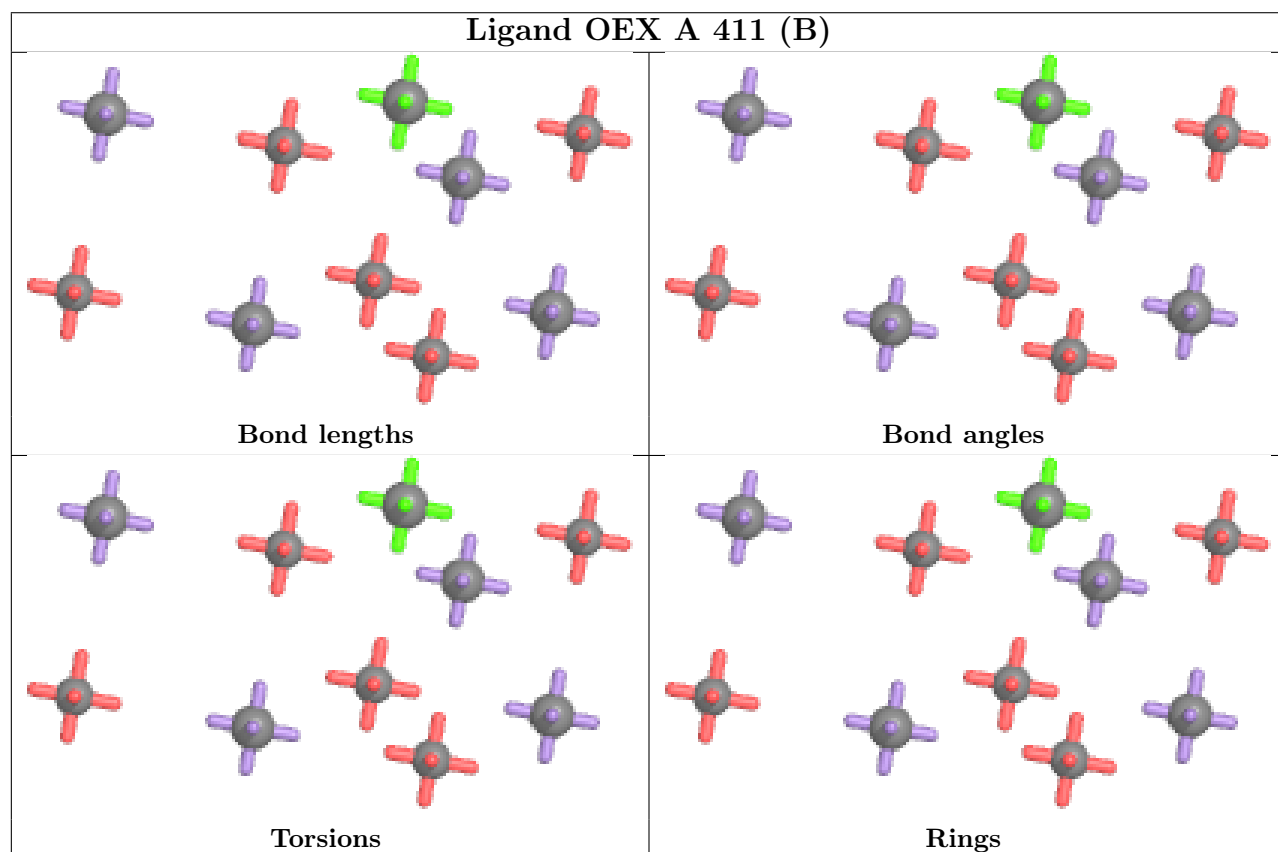
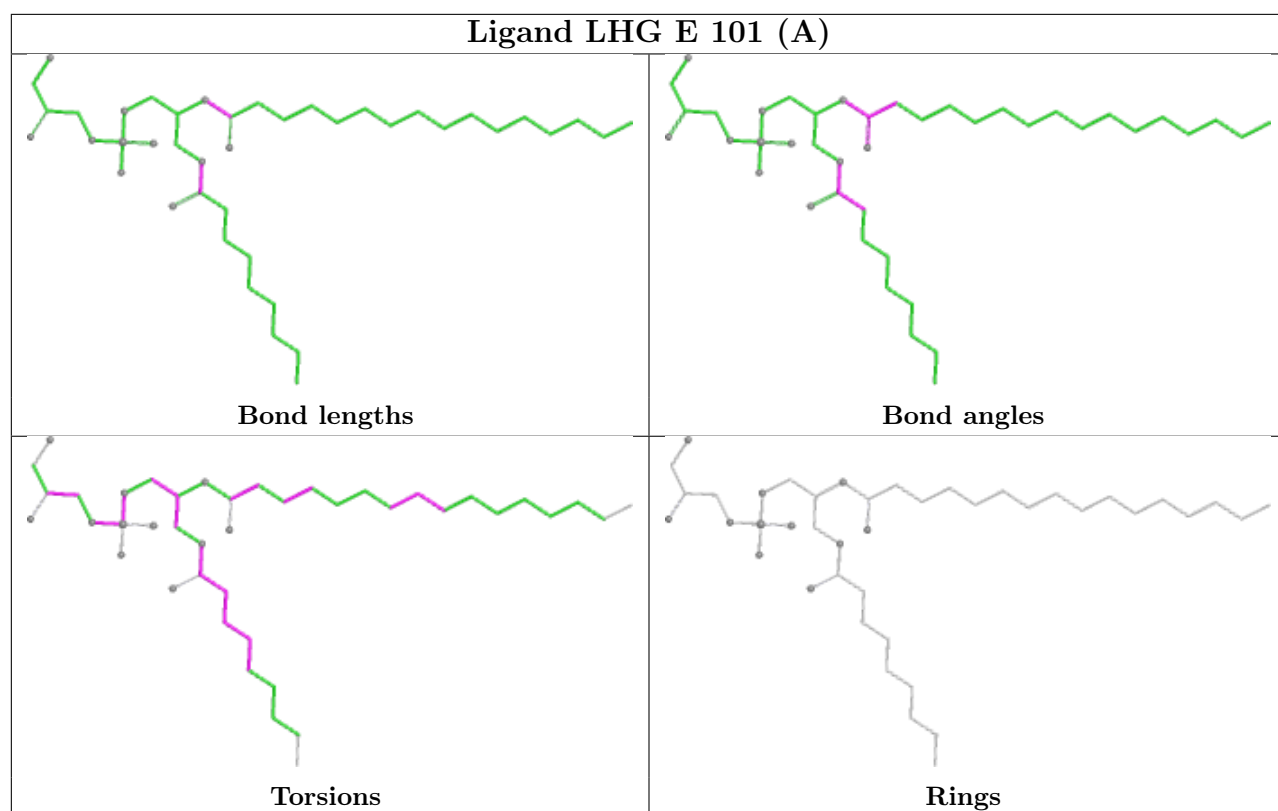


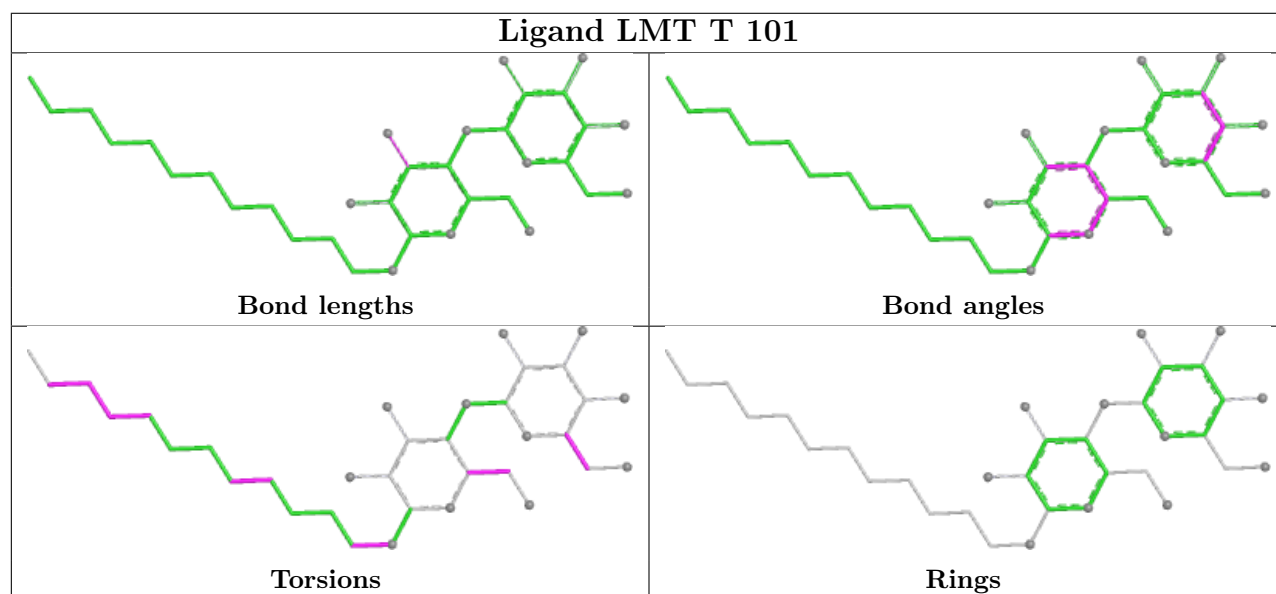
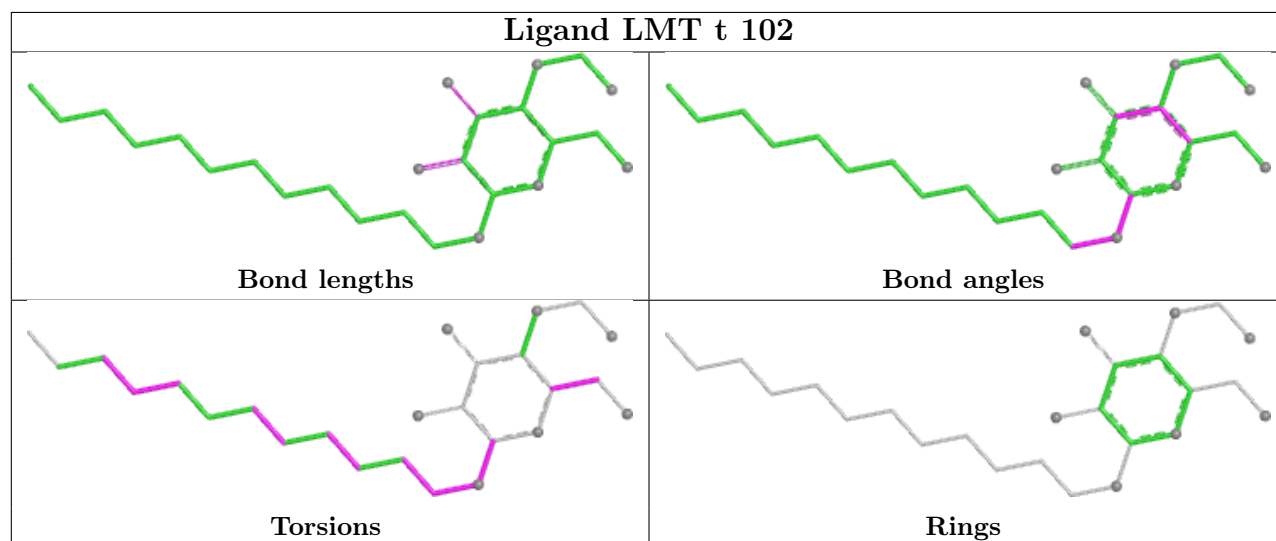
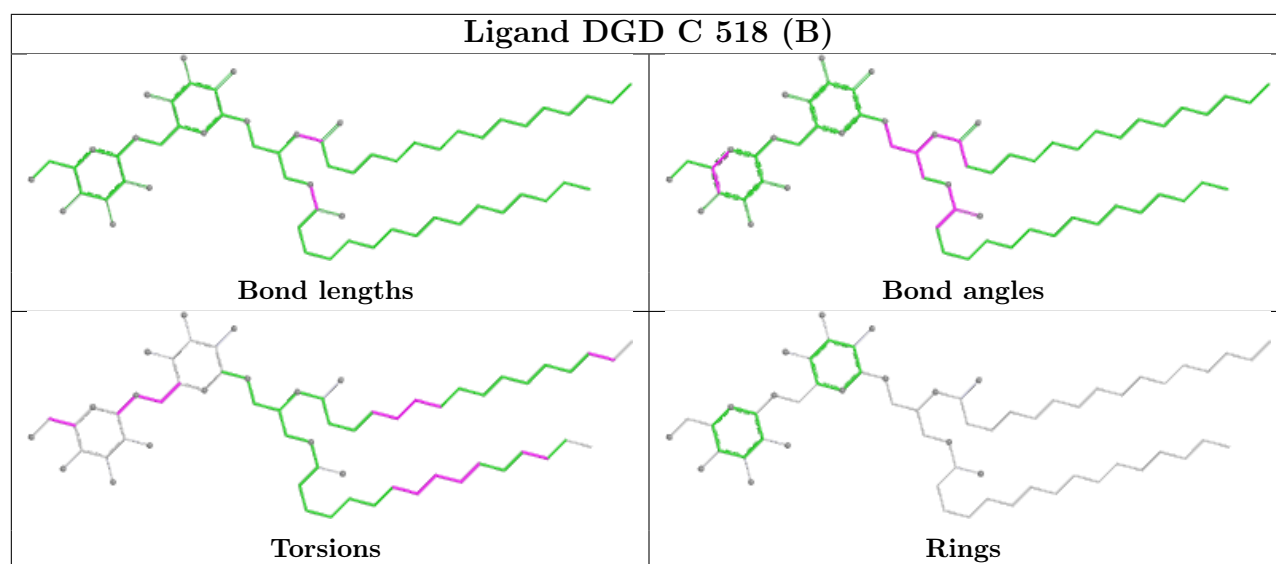
Ligand CLA c 508

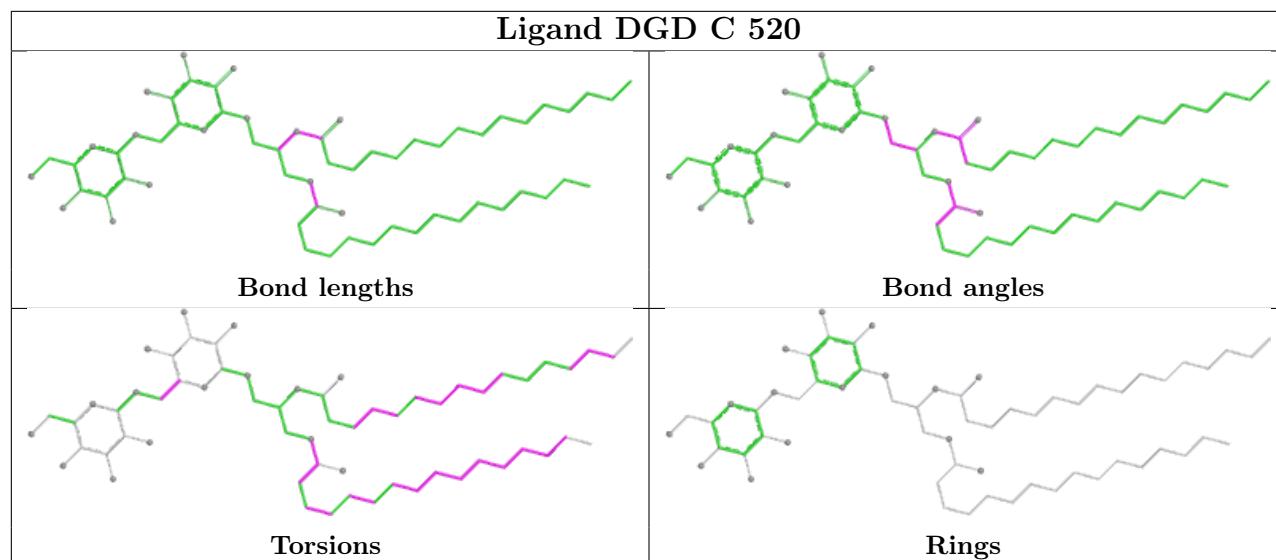
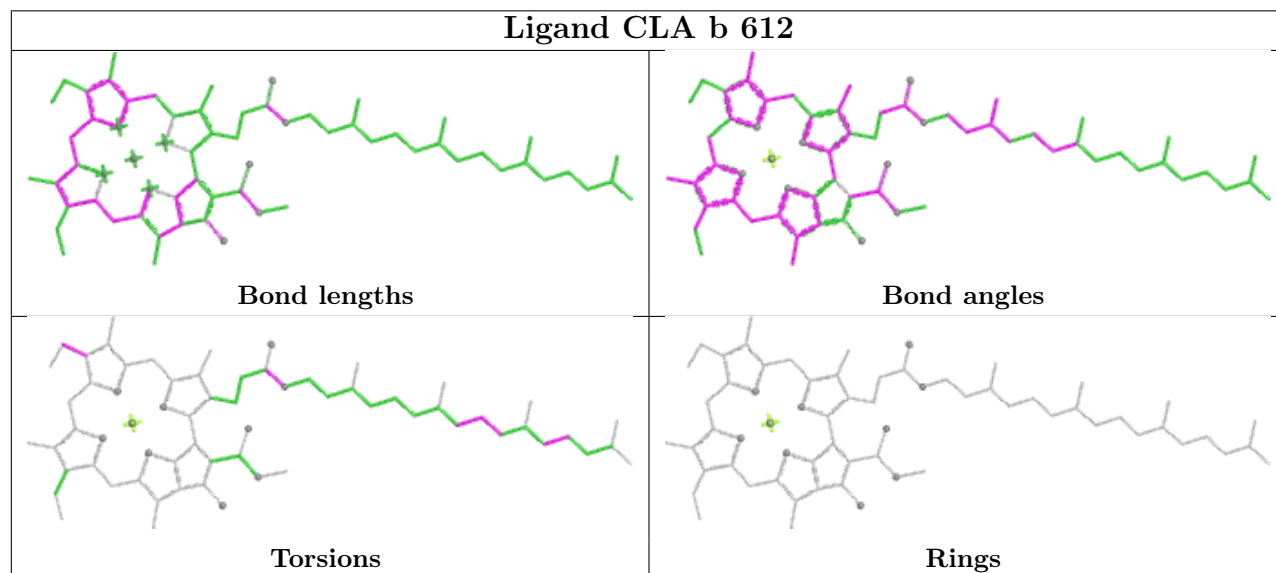
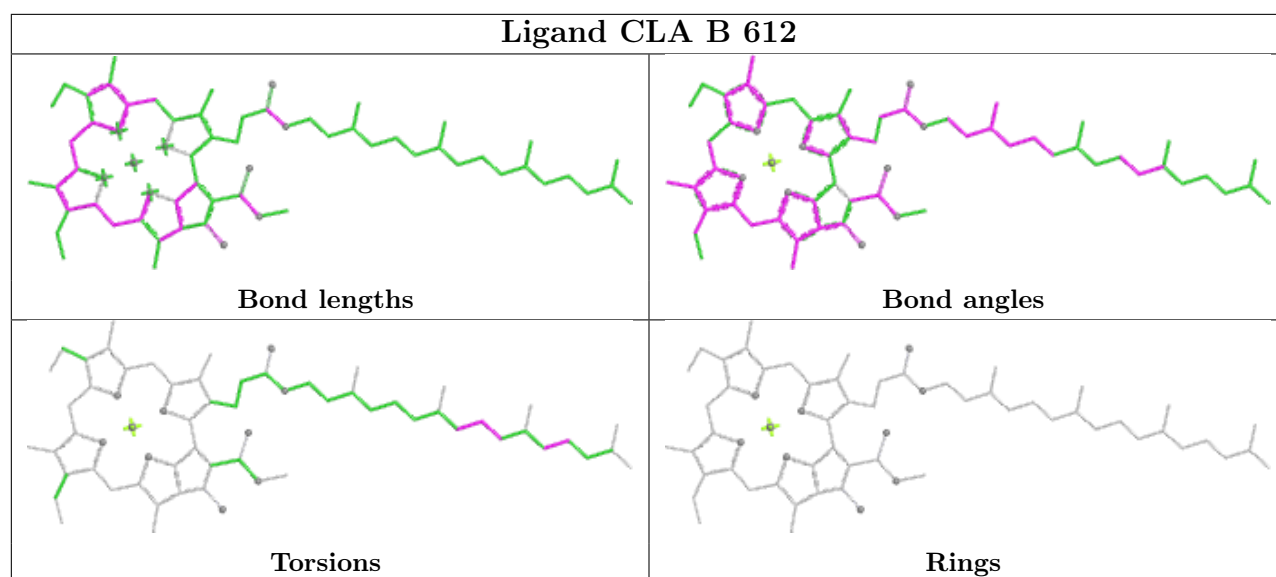


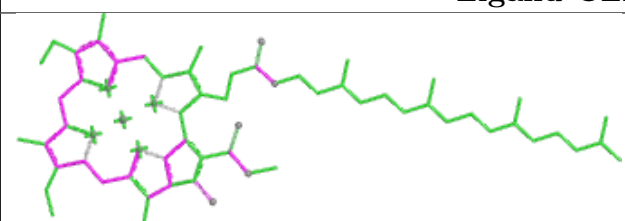
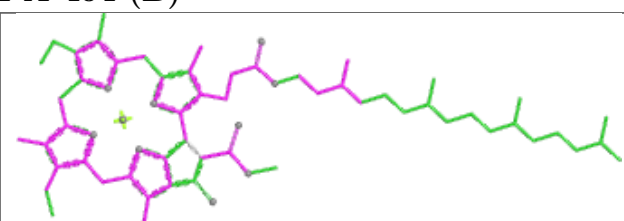
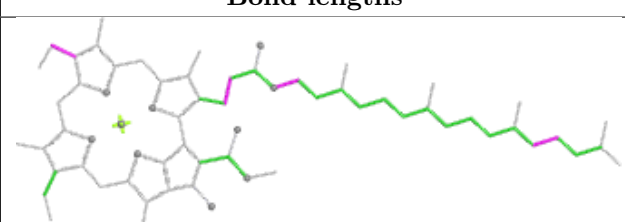
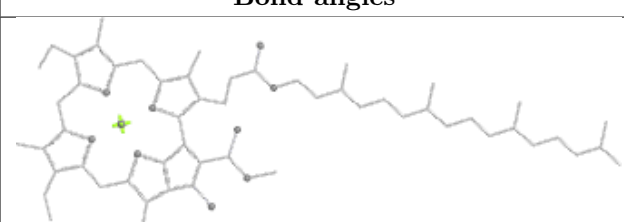
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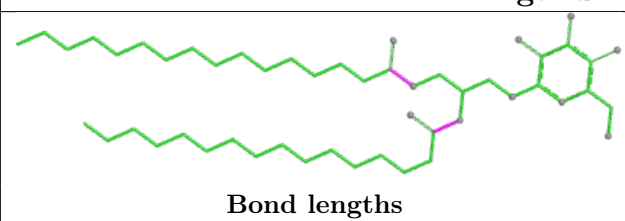
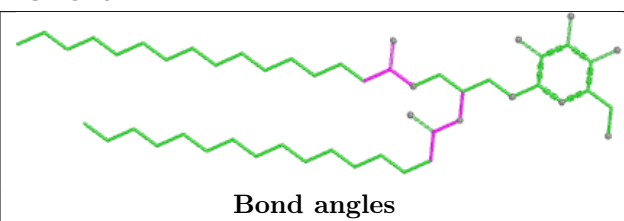
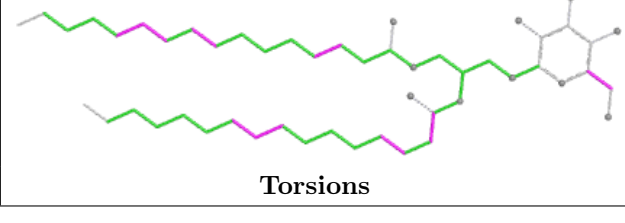
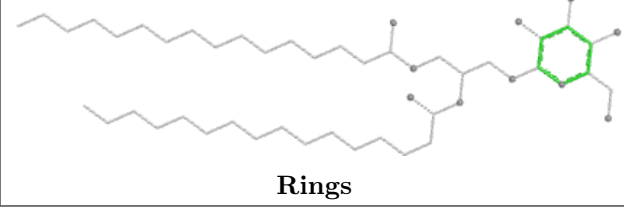


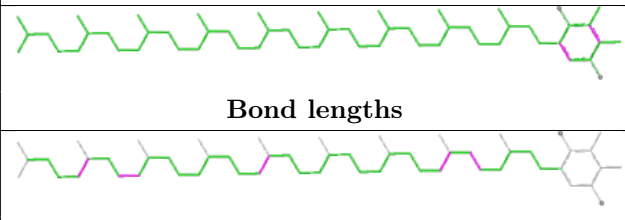
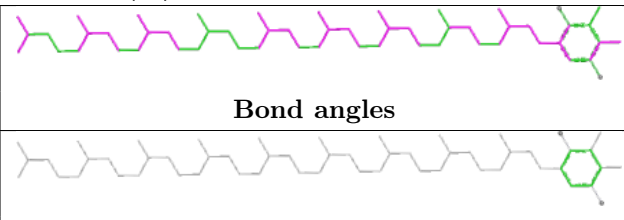


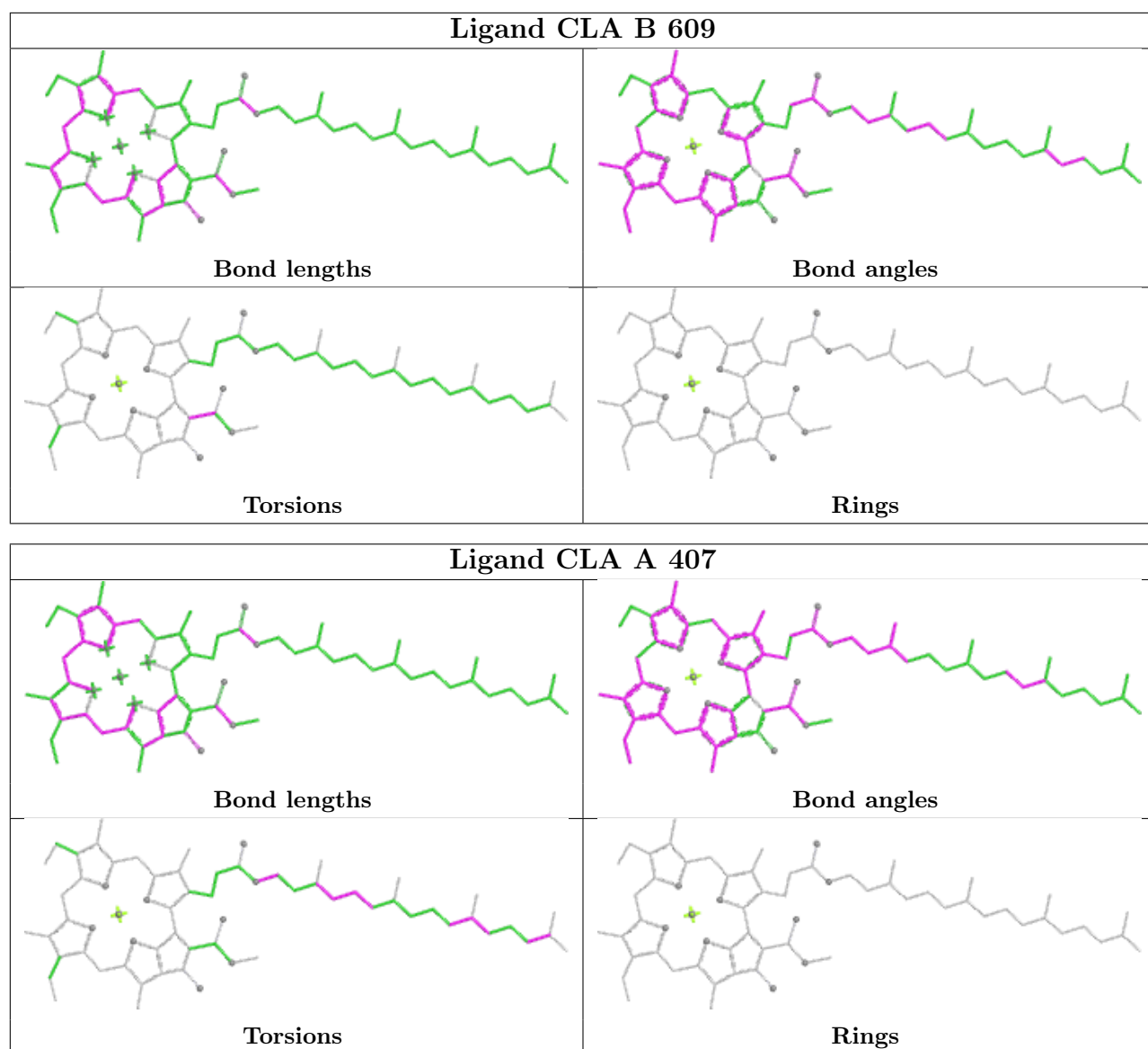


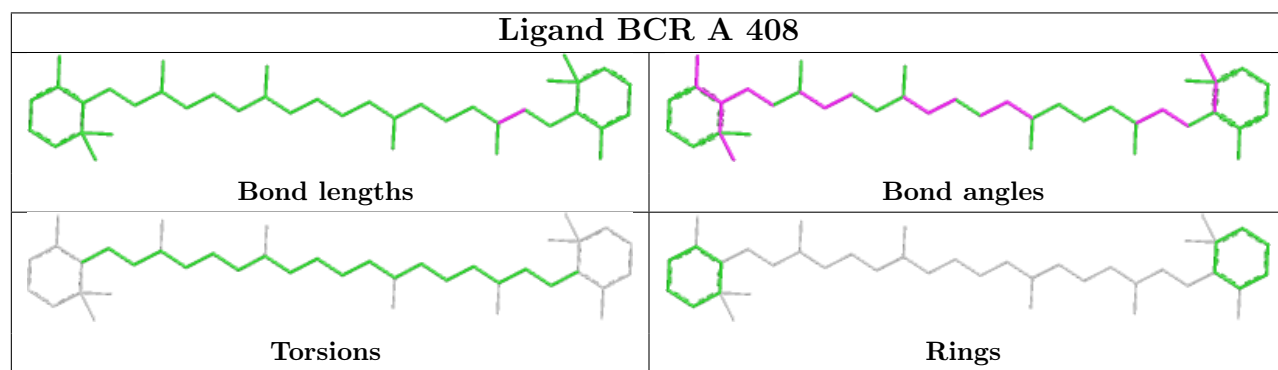
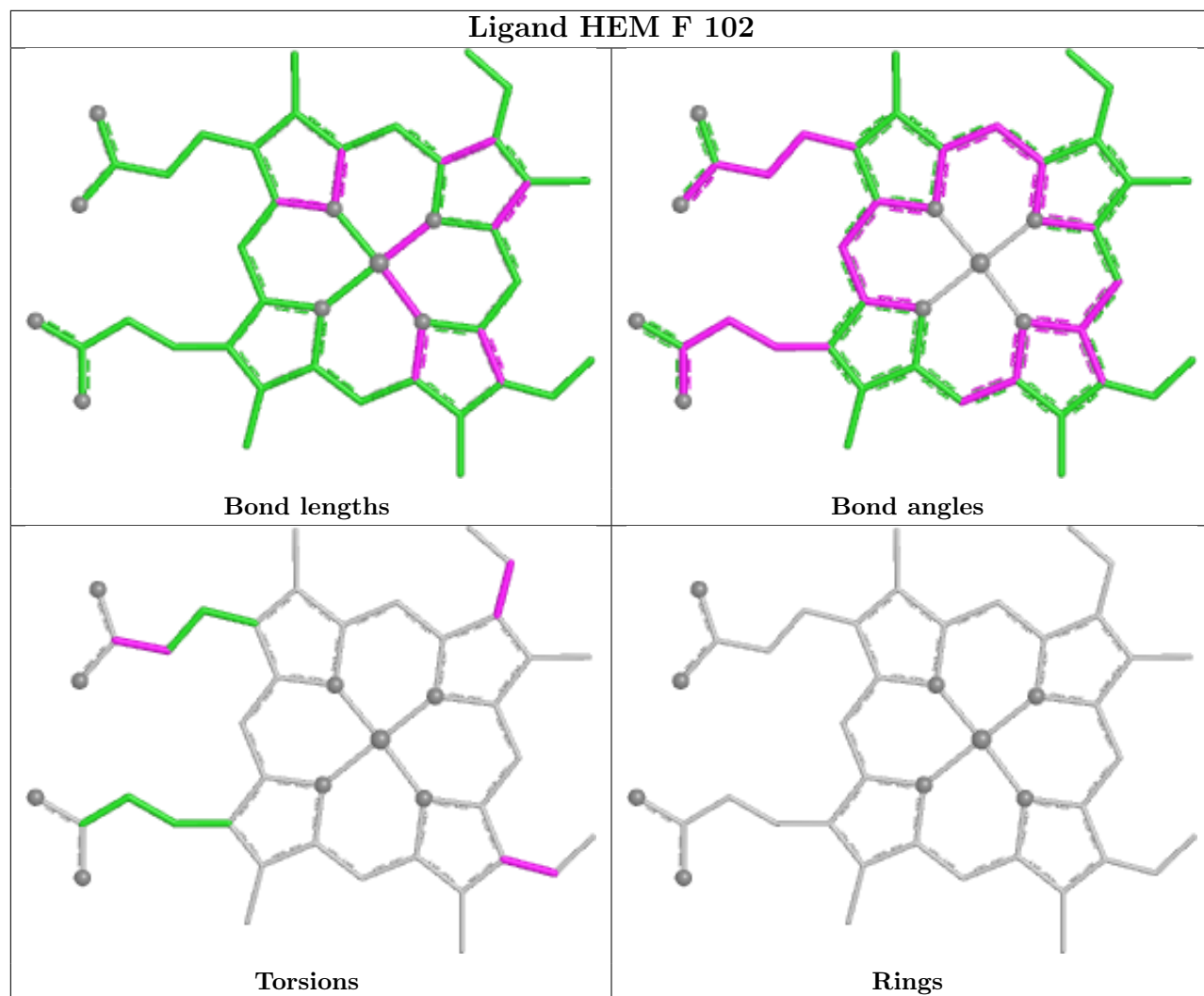


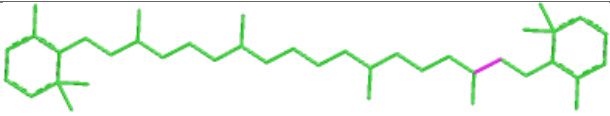
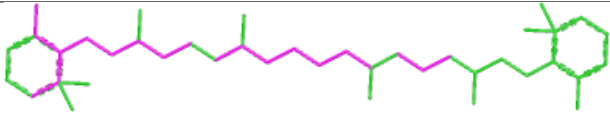
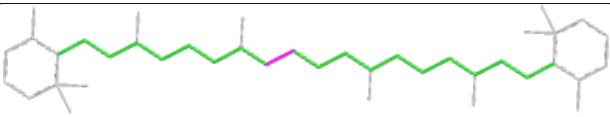
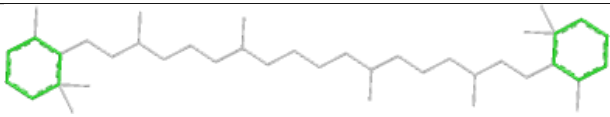
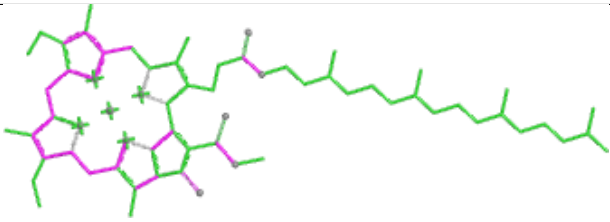
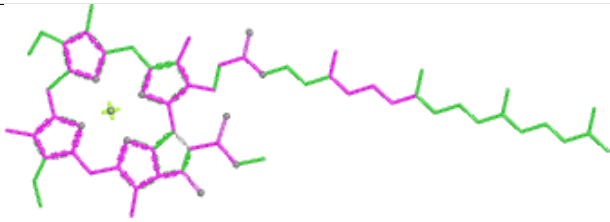
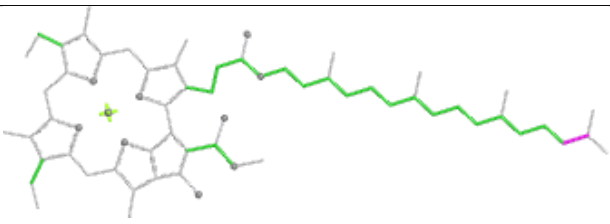
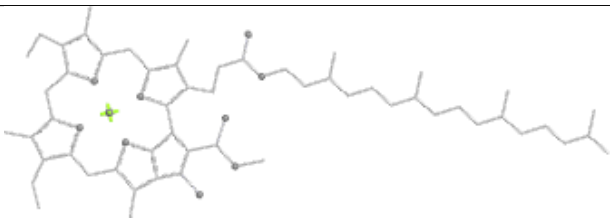
Ligand CLA A 404 (B)	
	
Bond lengths	Bond angles
	
Torsions	Rings

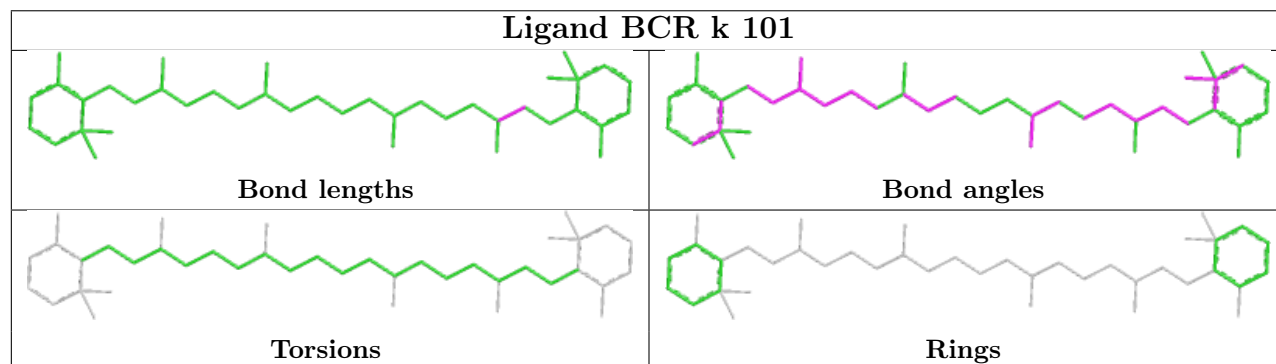
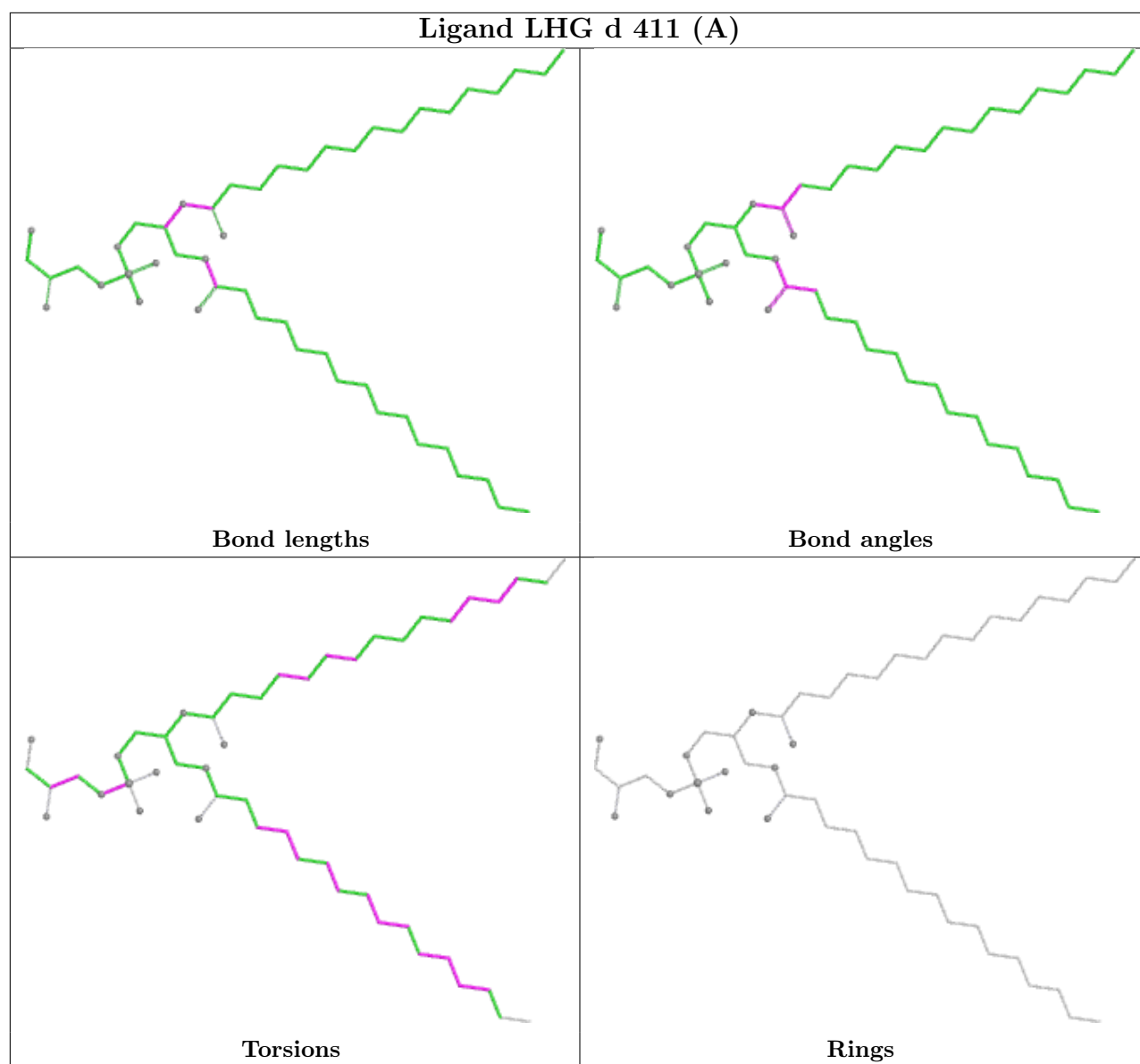
Ligand LMG C 521	
	
Bond lengths	Bond angles
	
Torsions	Rings

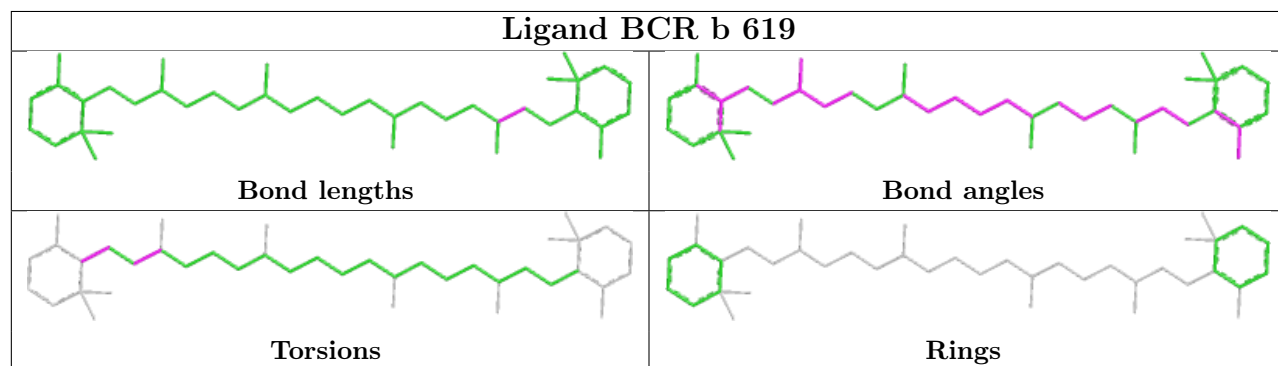
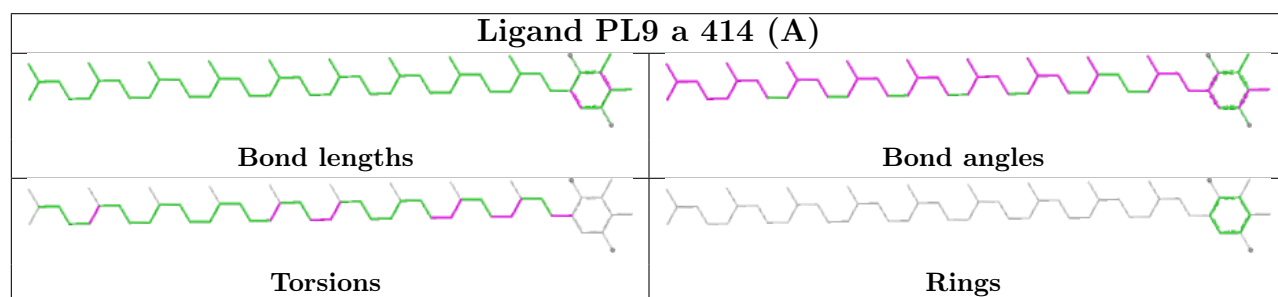
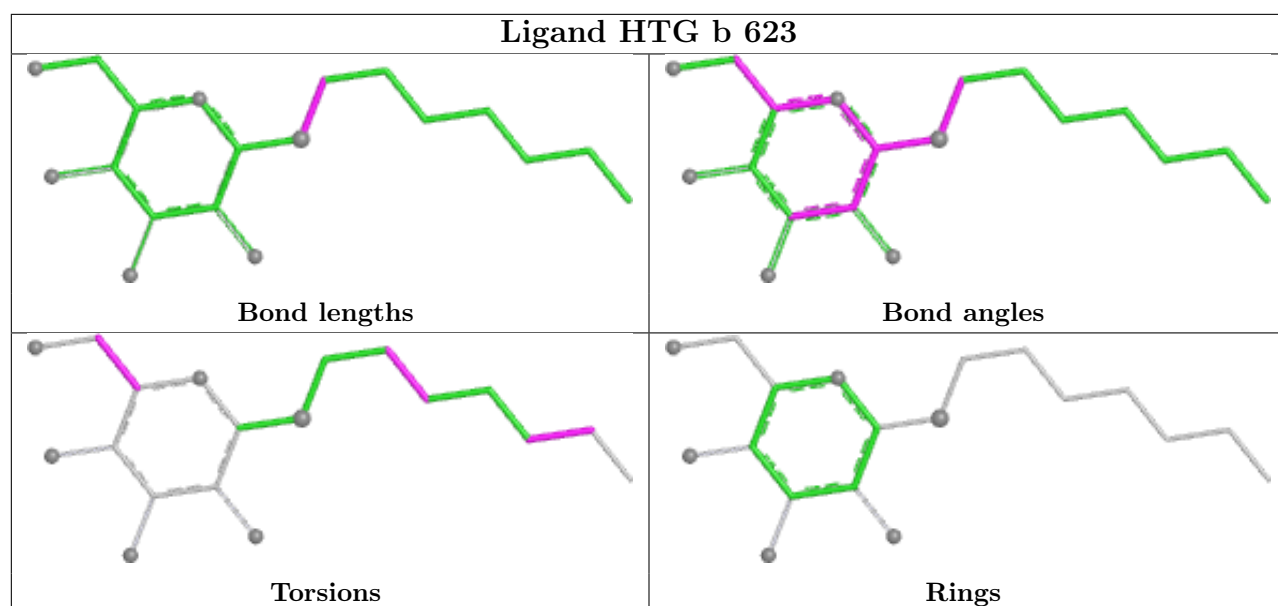
Ligand PL9 D 407 (B)	
	
Bond lengths	Bond angles
	
Torsions	Rings

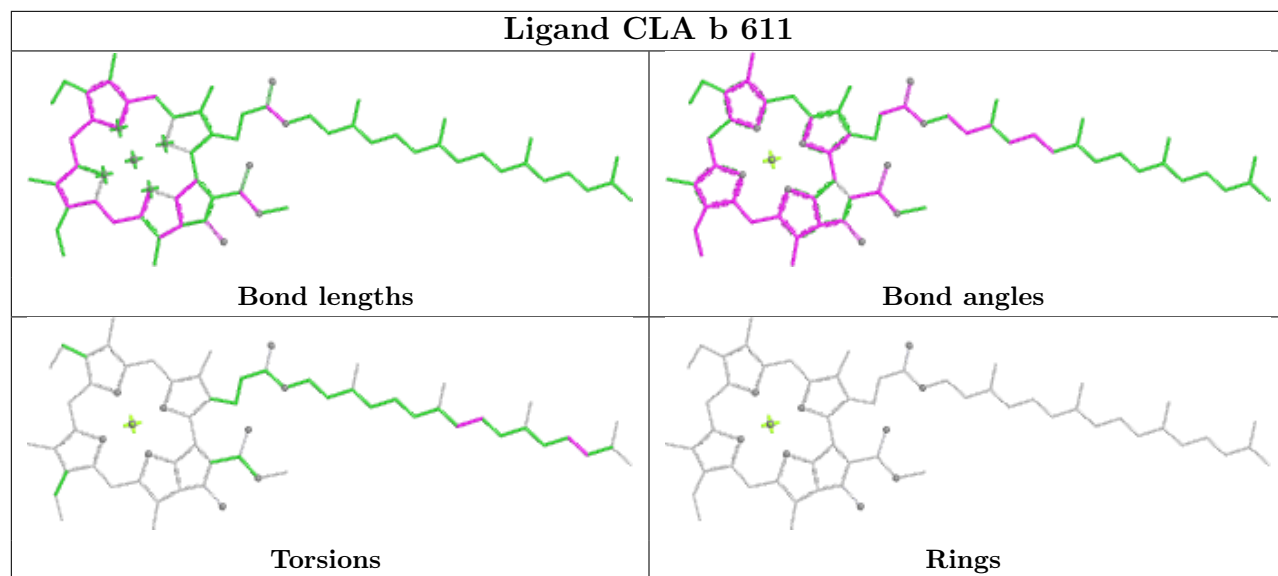


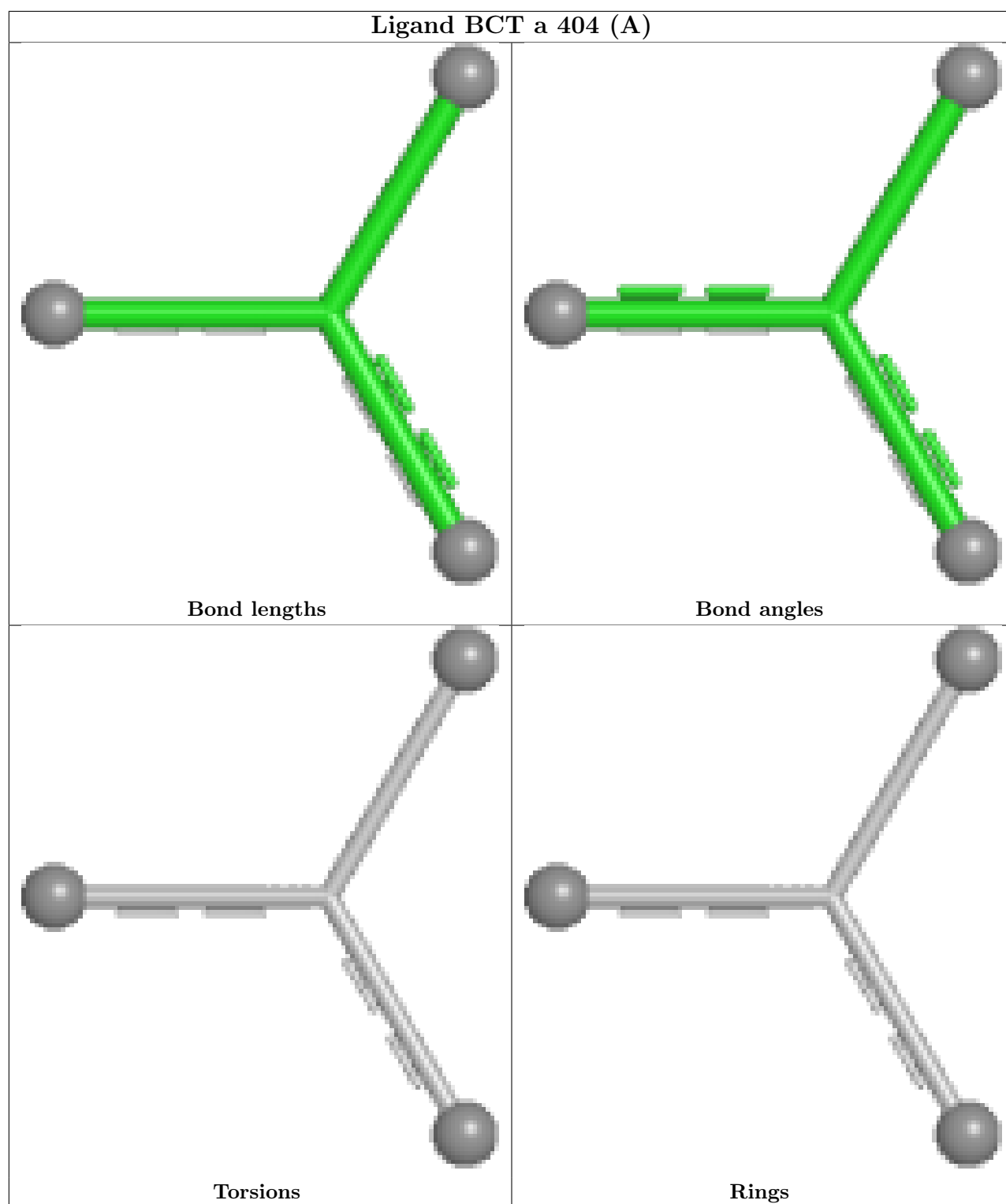


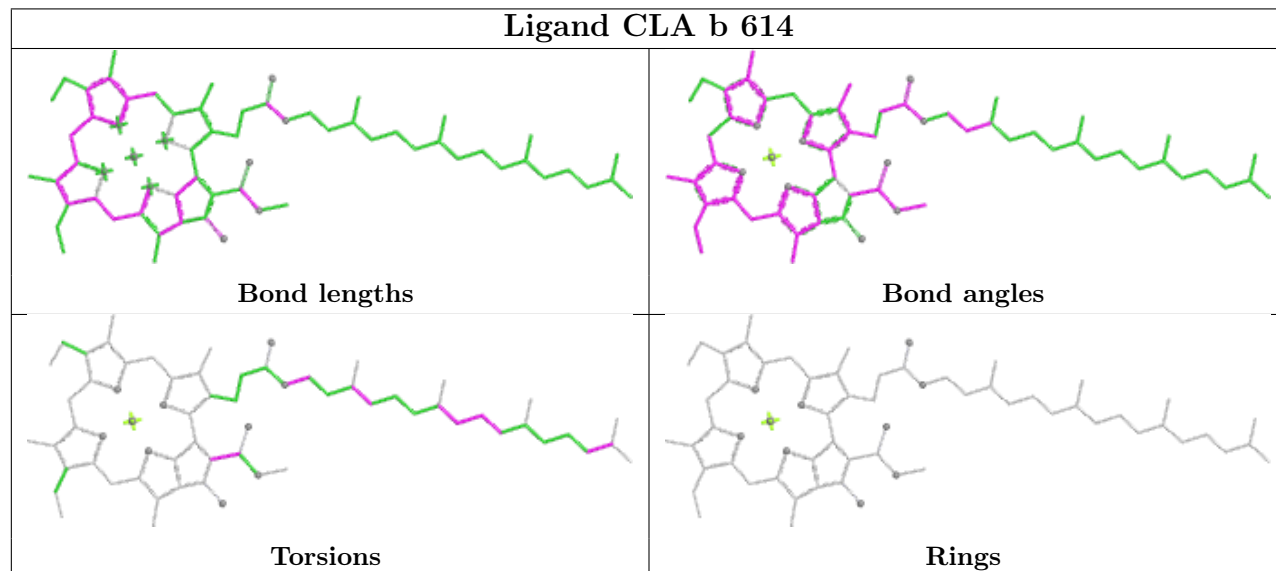
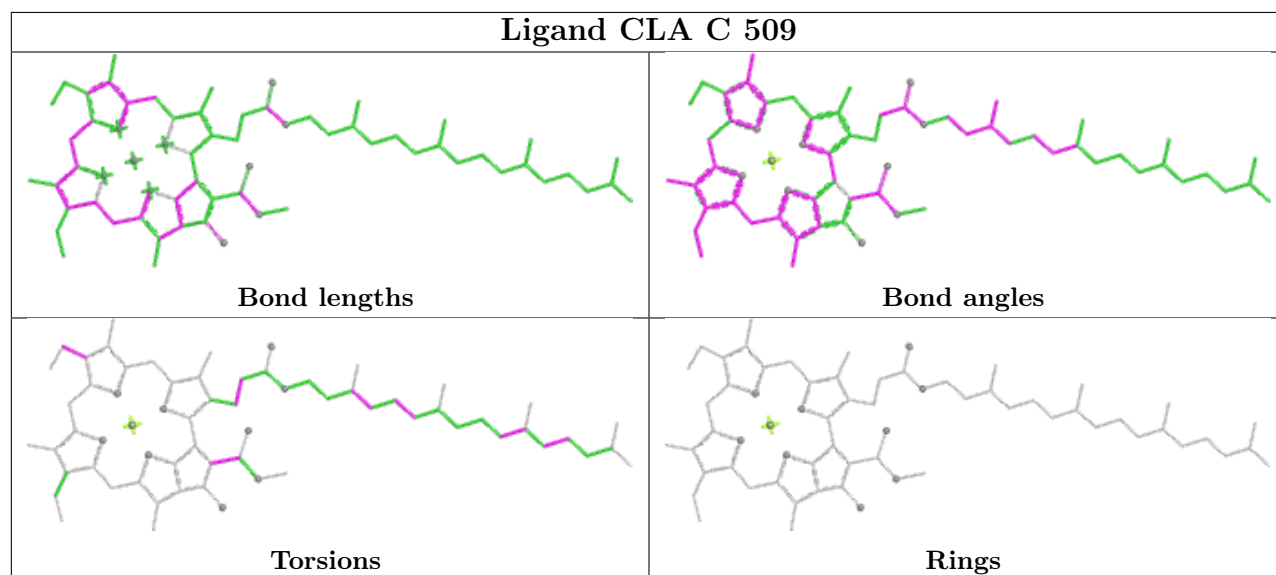
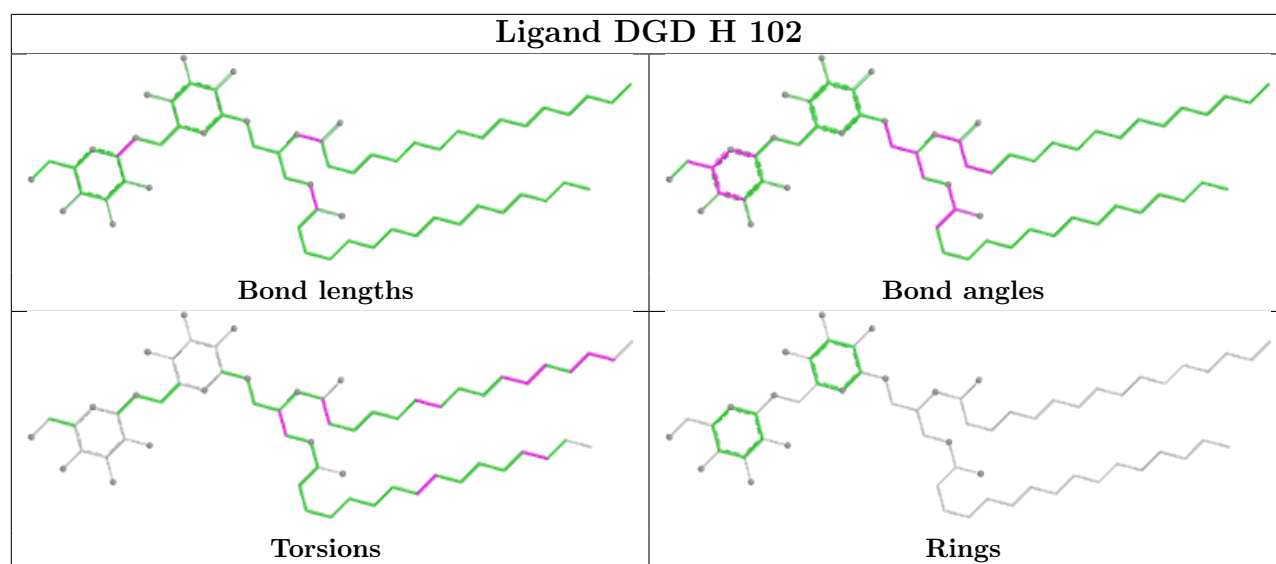
Ligand BCR T 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

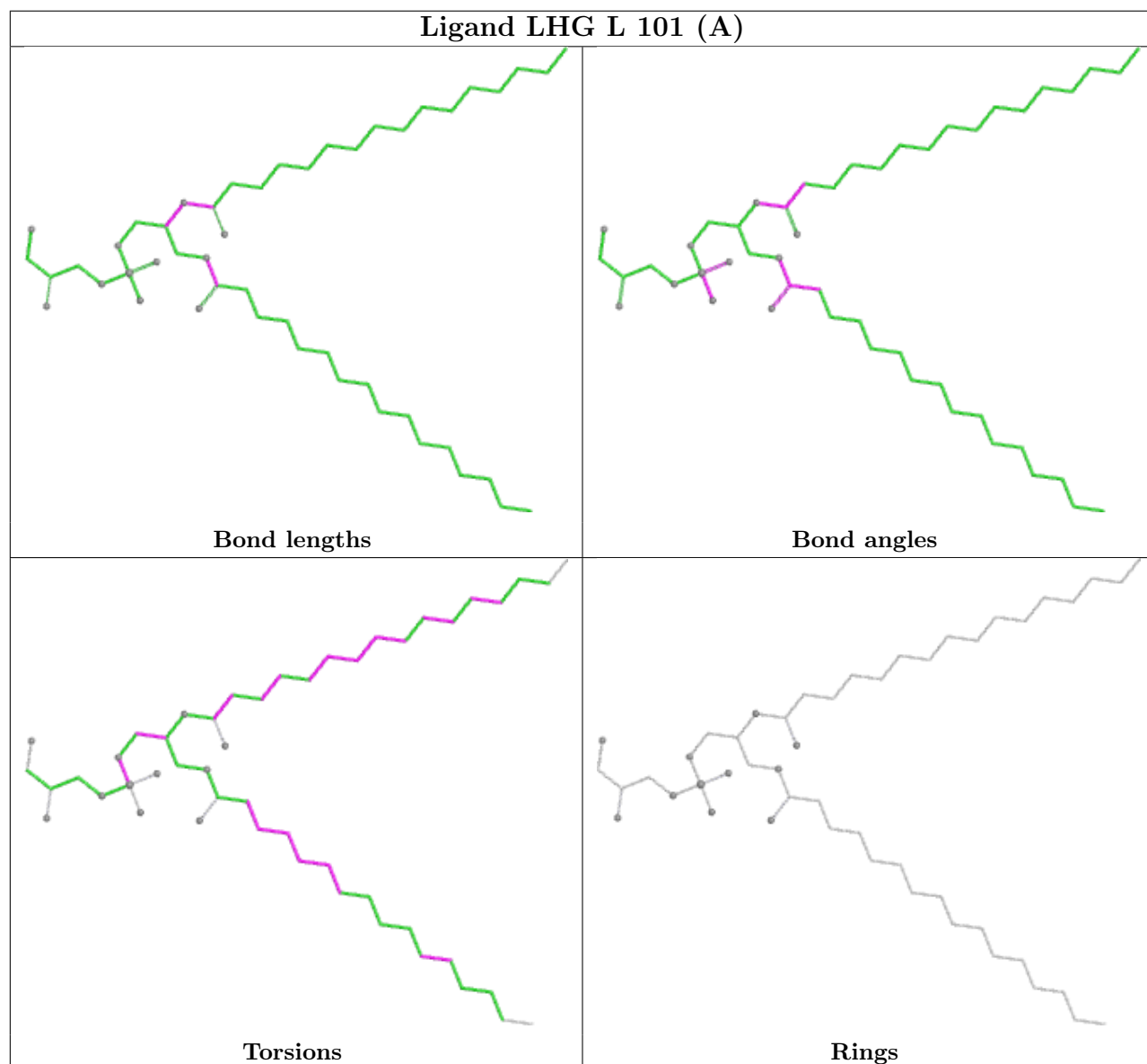
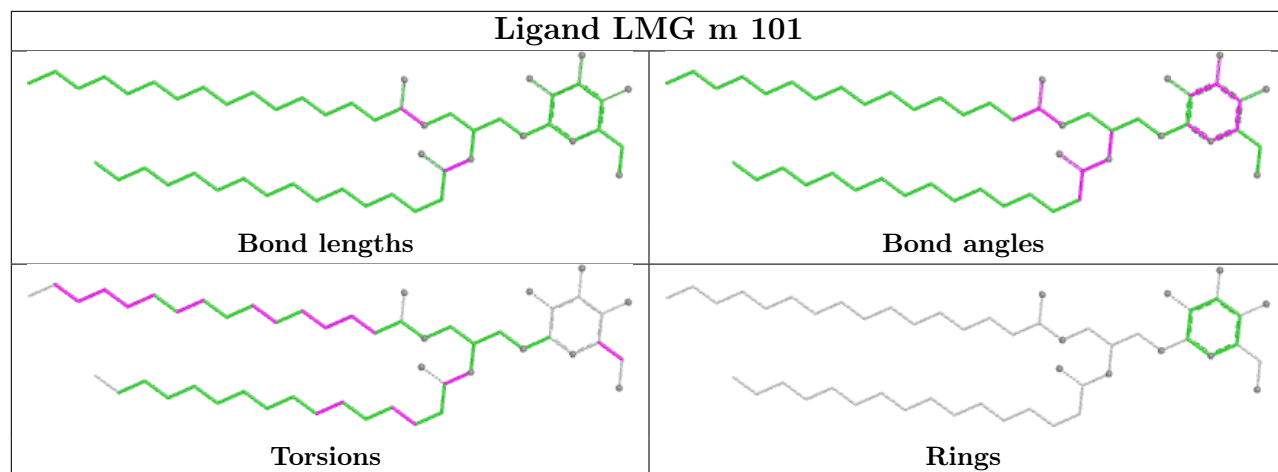


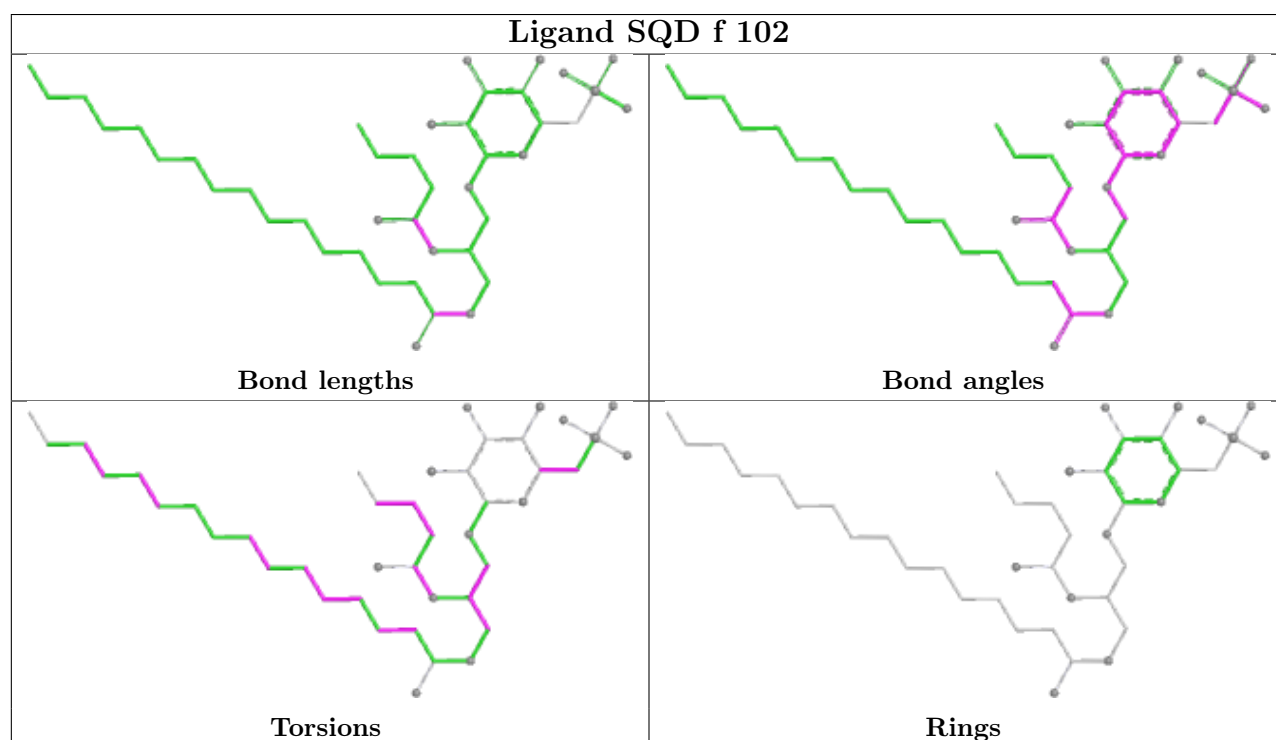
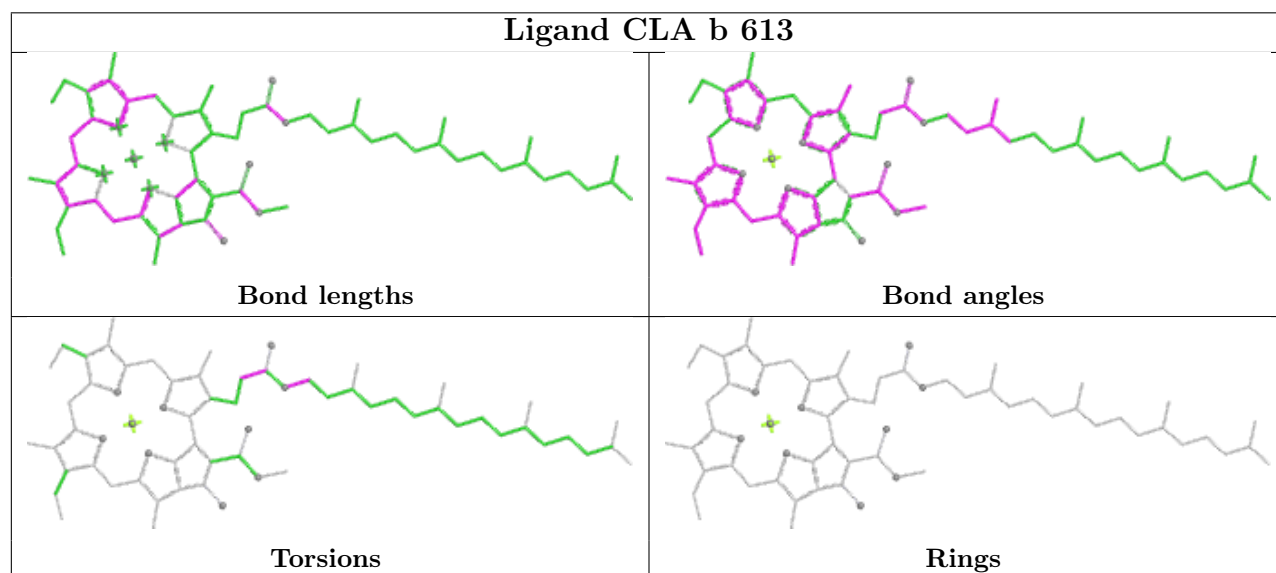
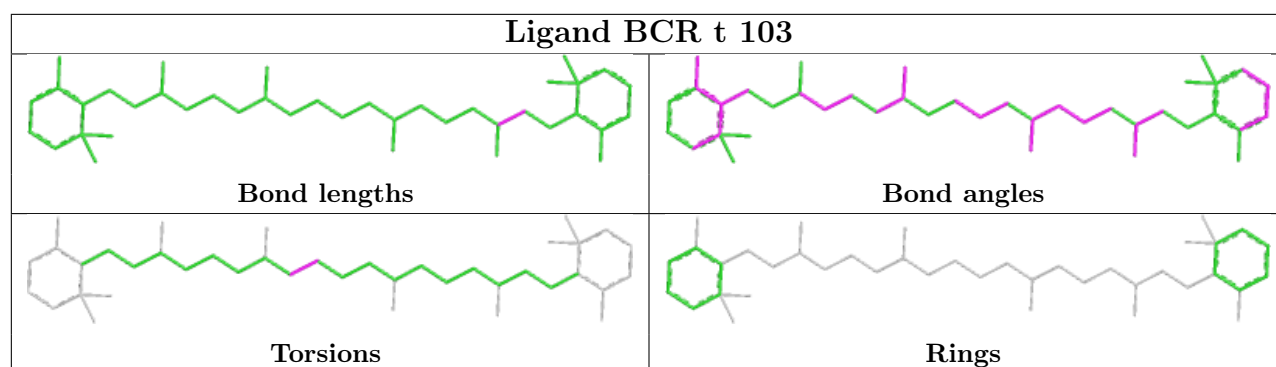


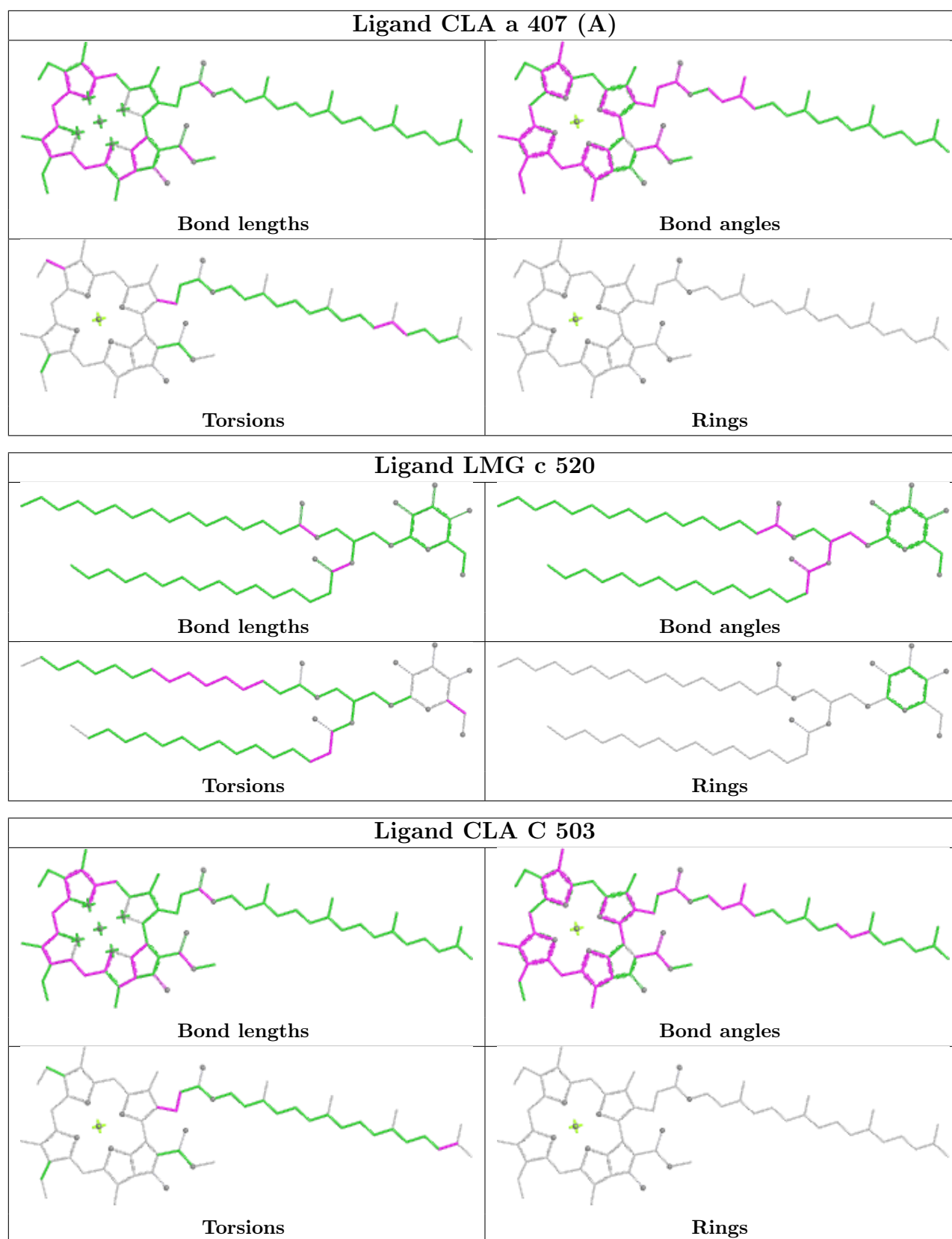


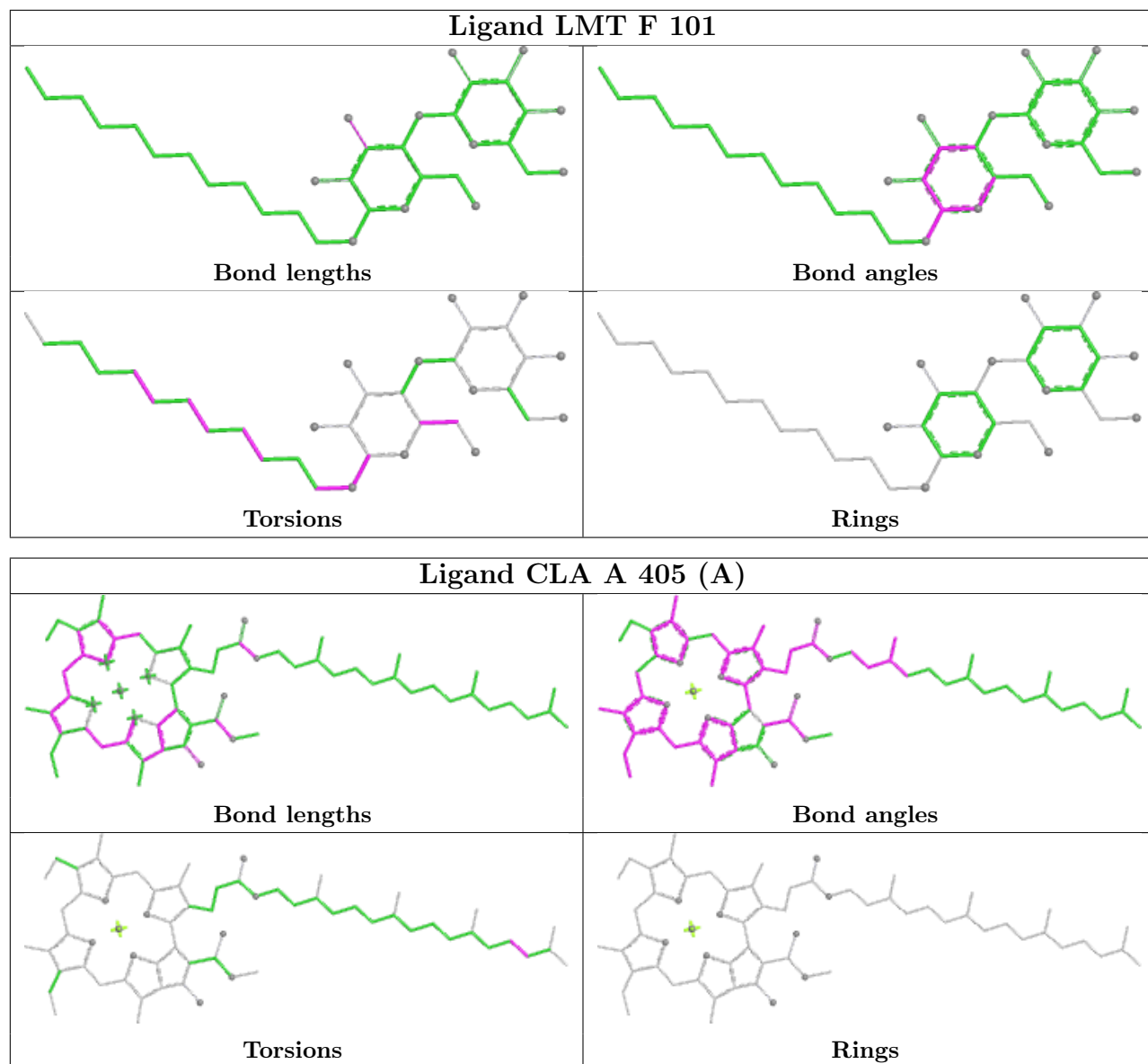


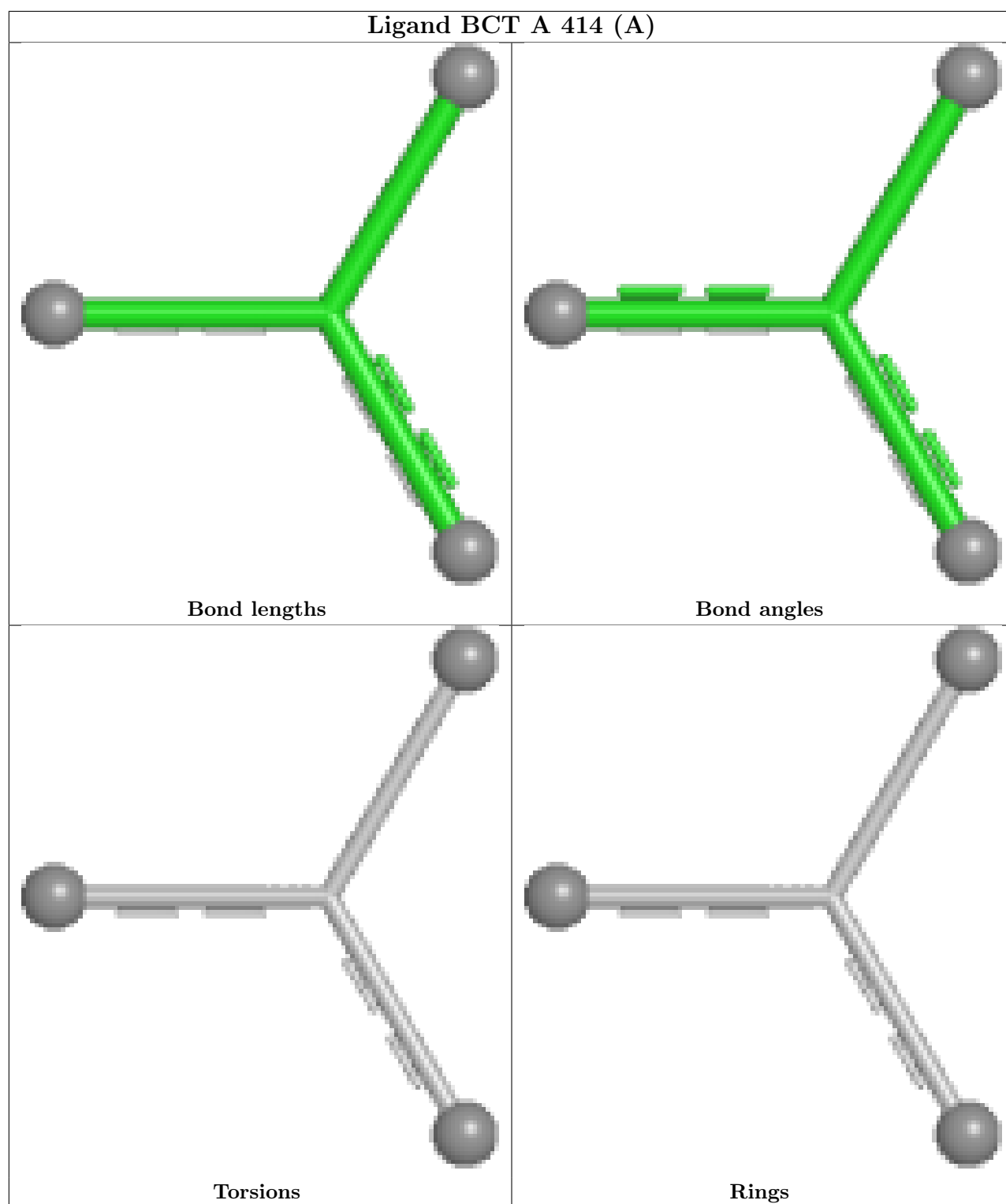


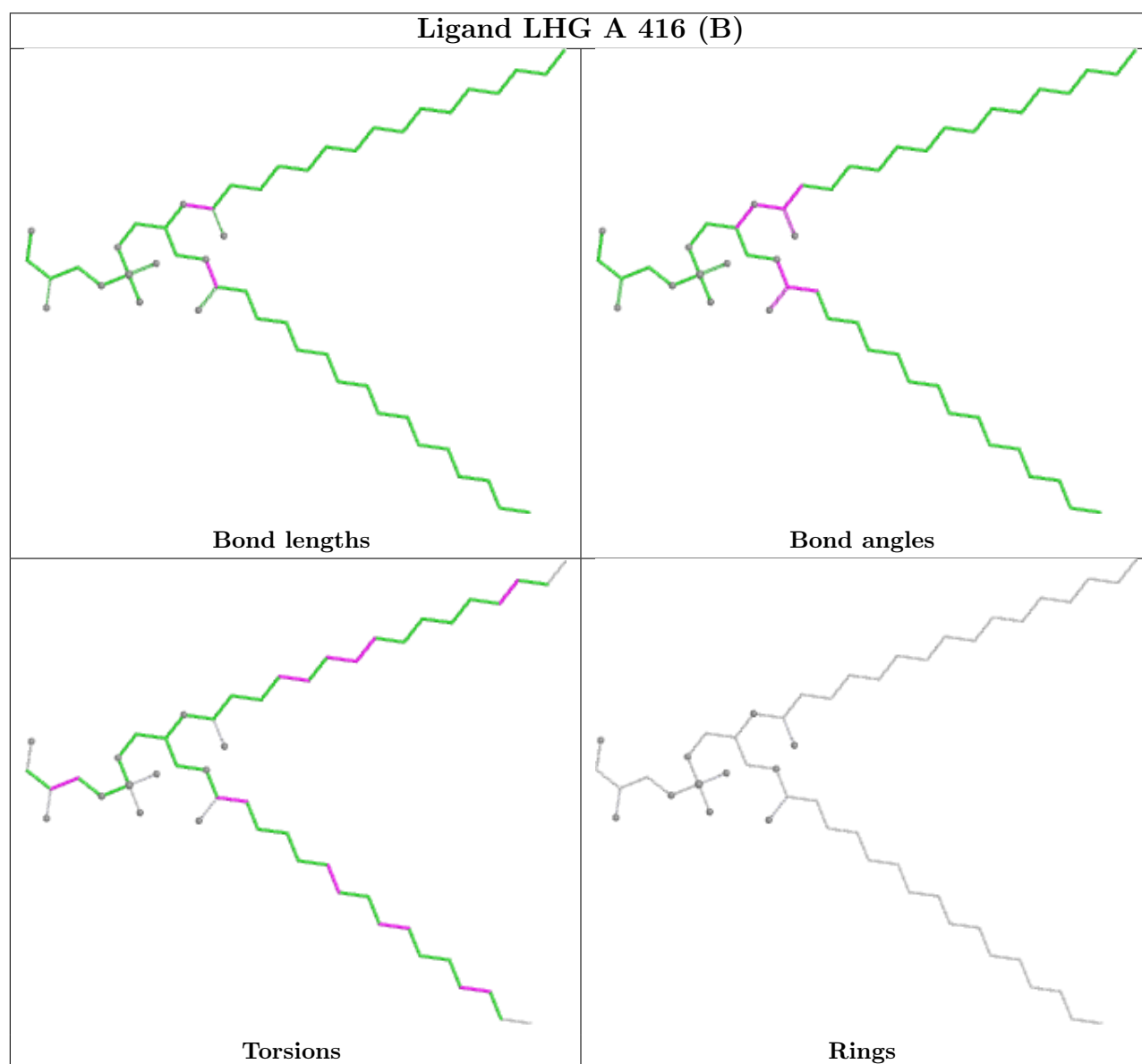
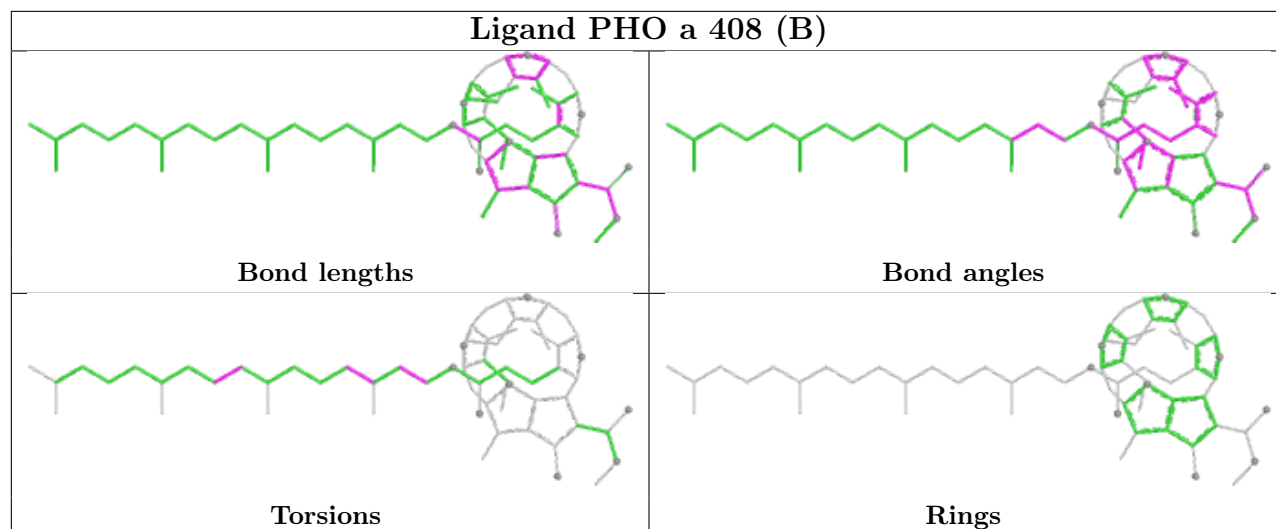


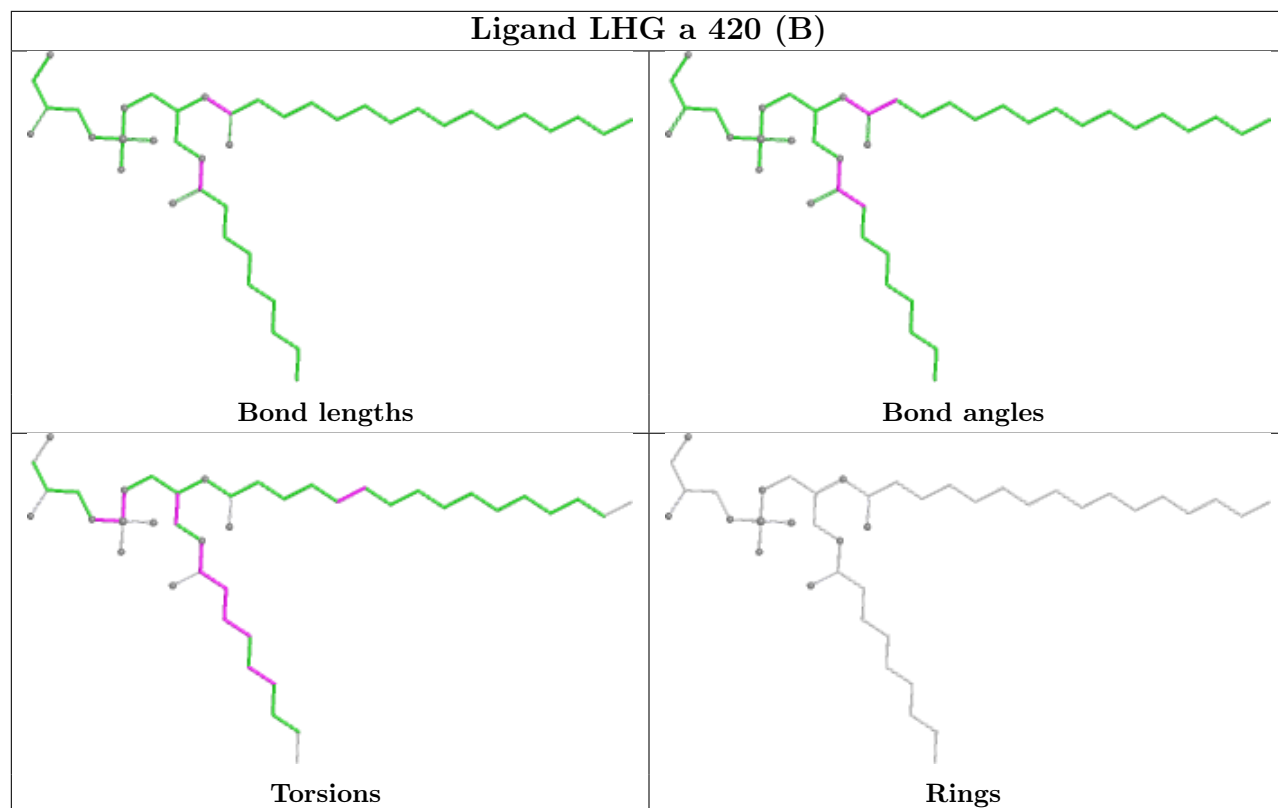


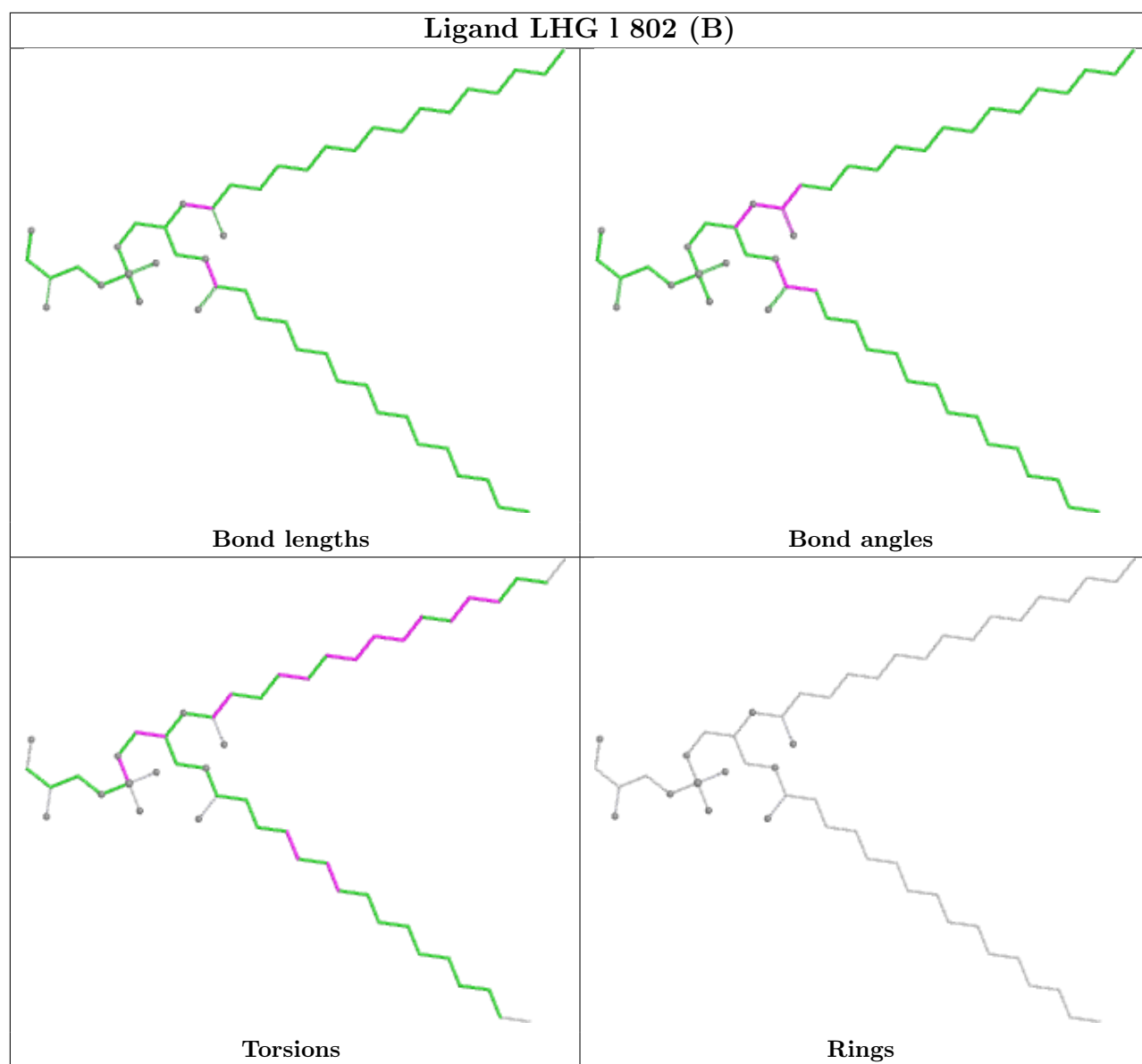




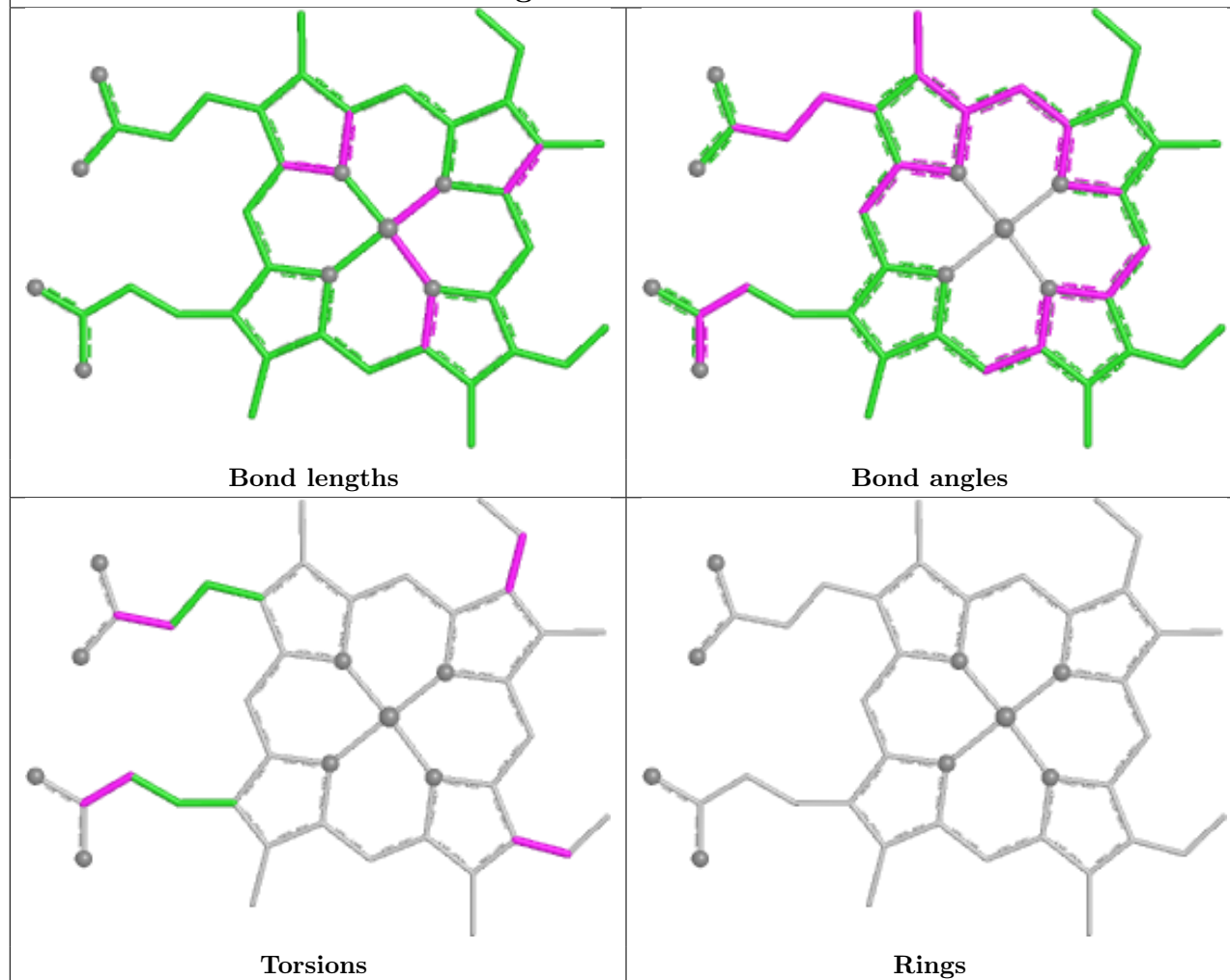




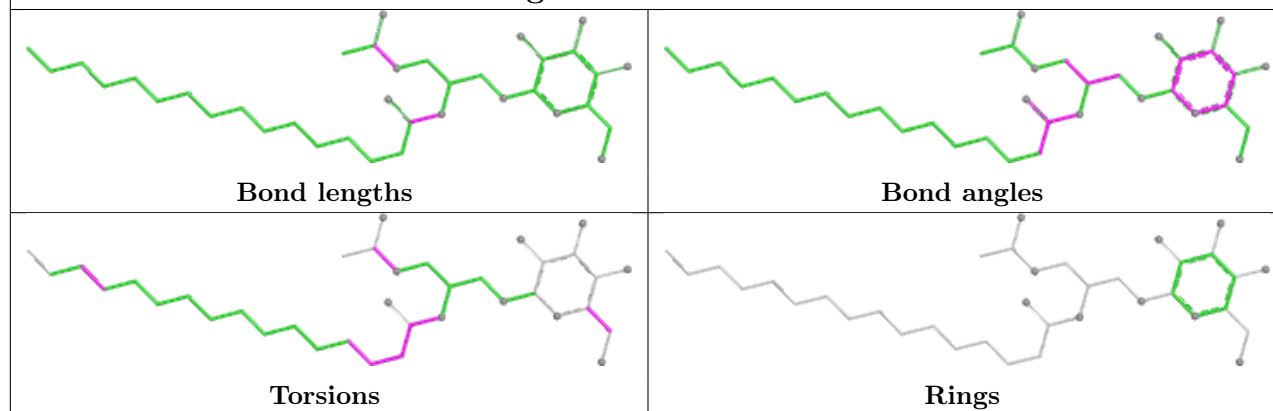


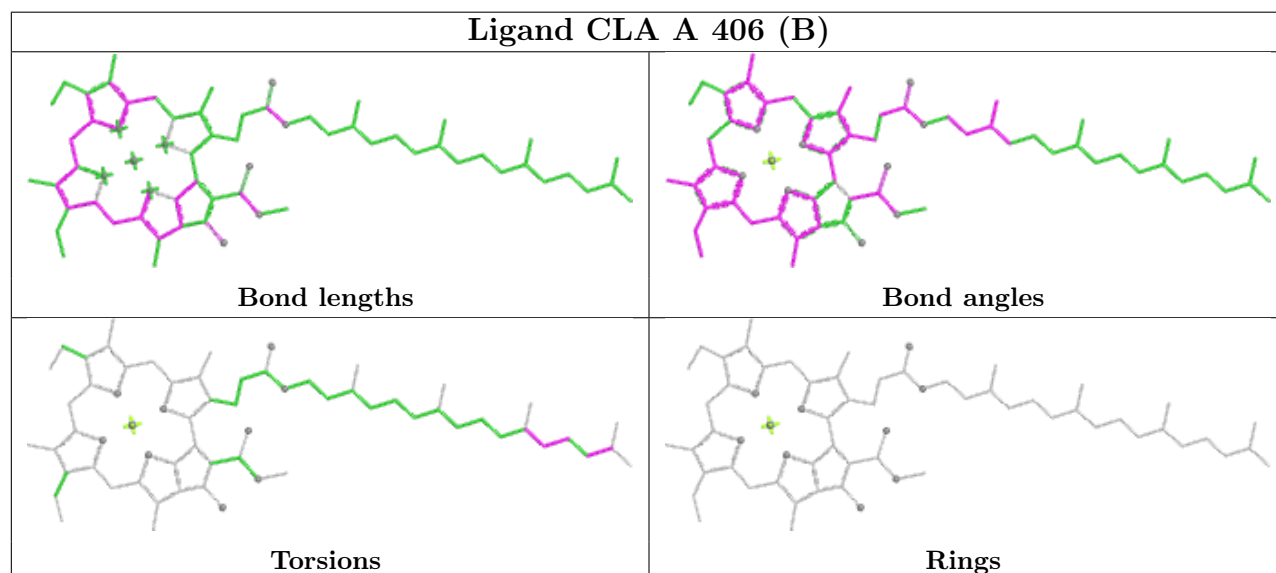
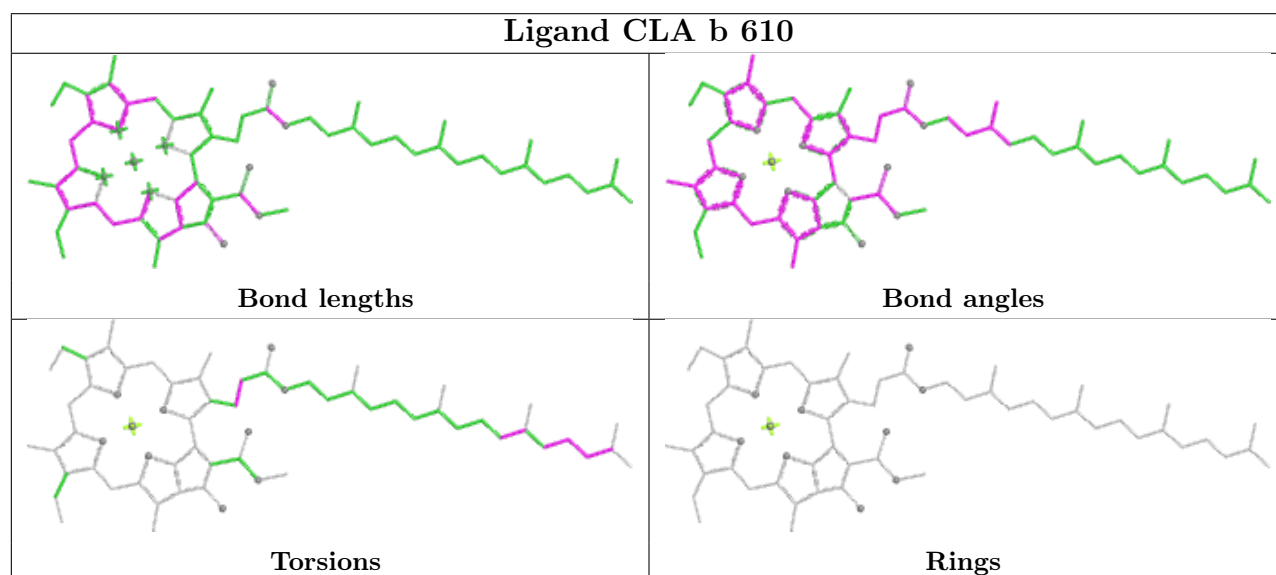
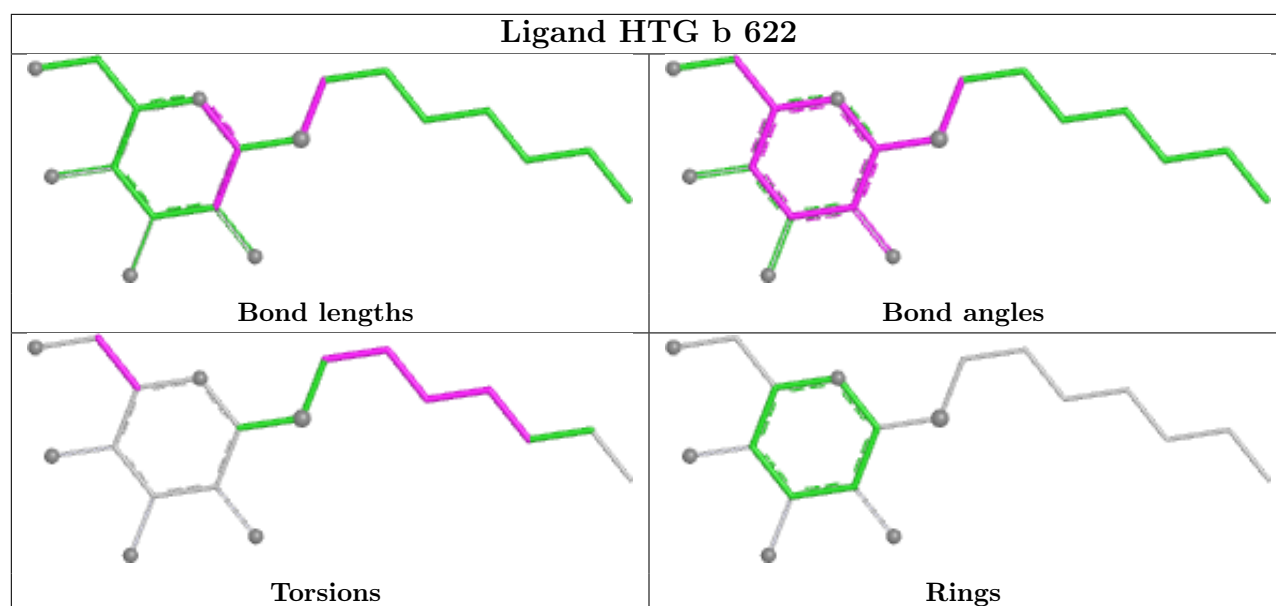


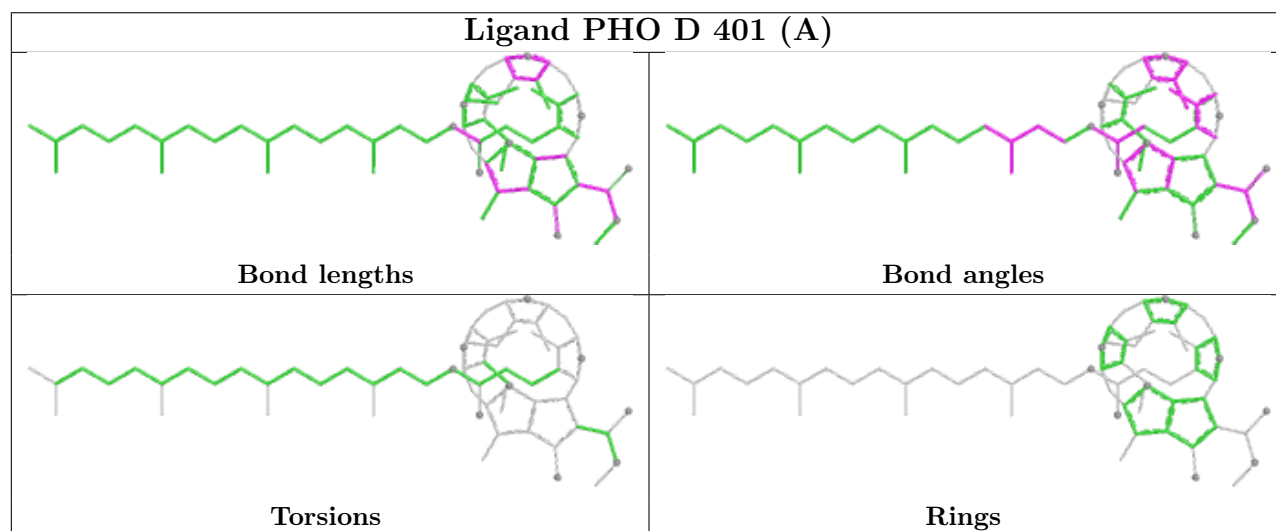
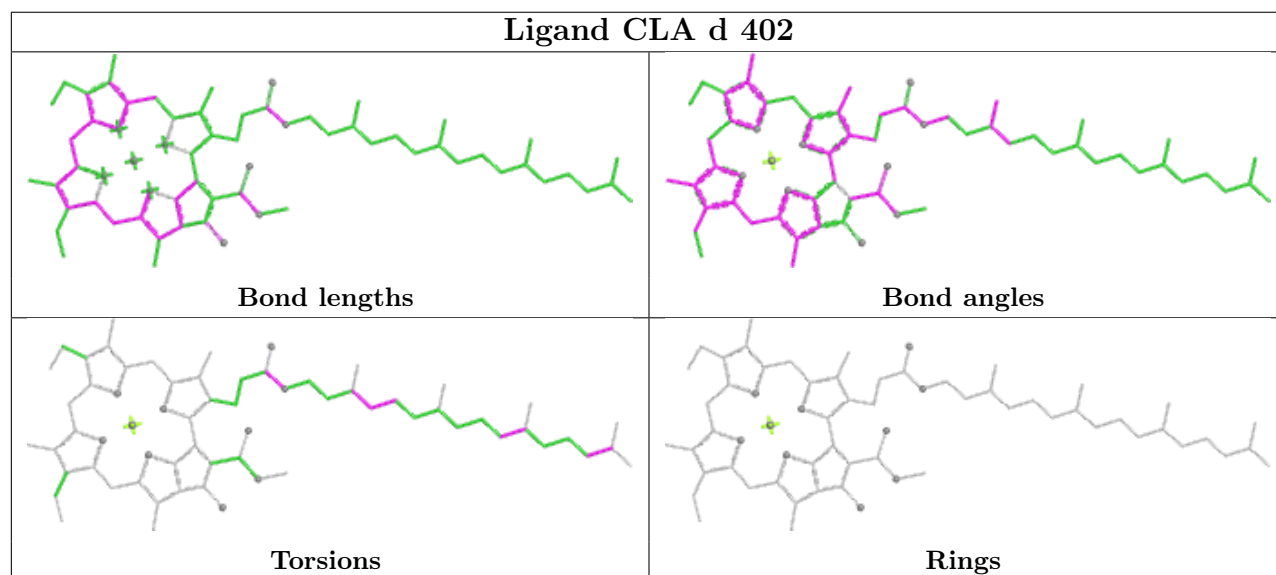
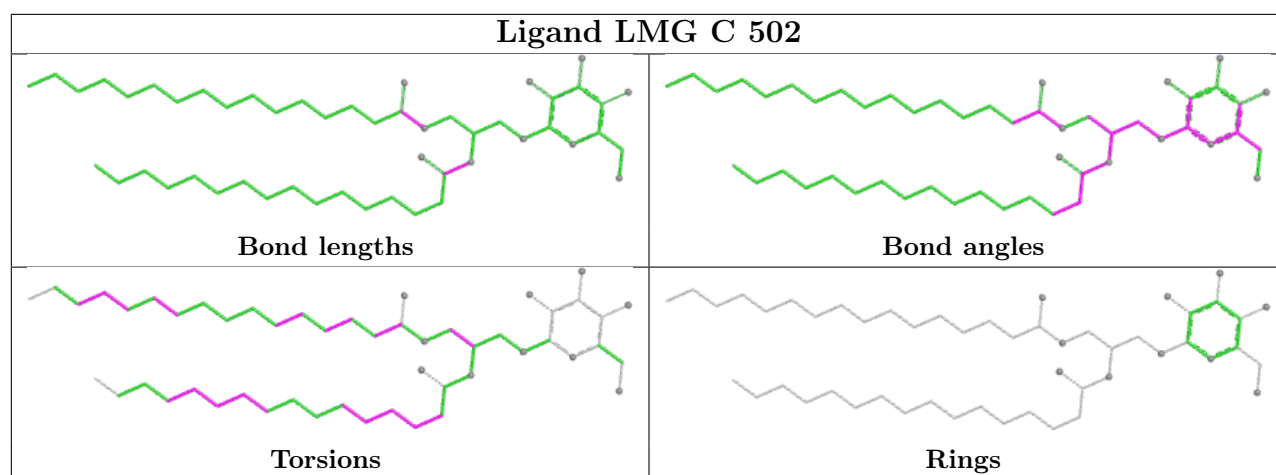
Ligand HEM f 101

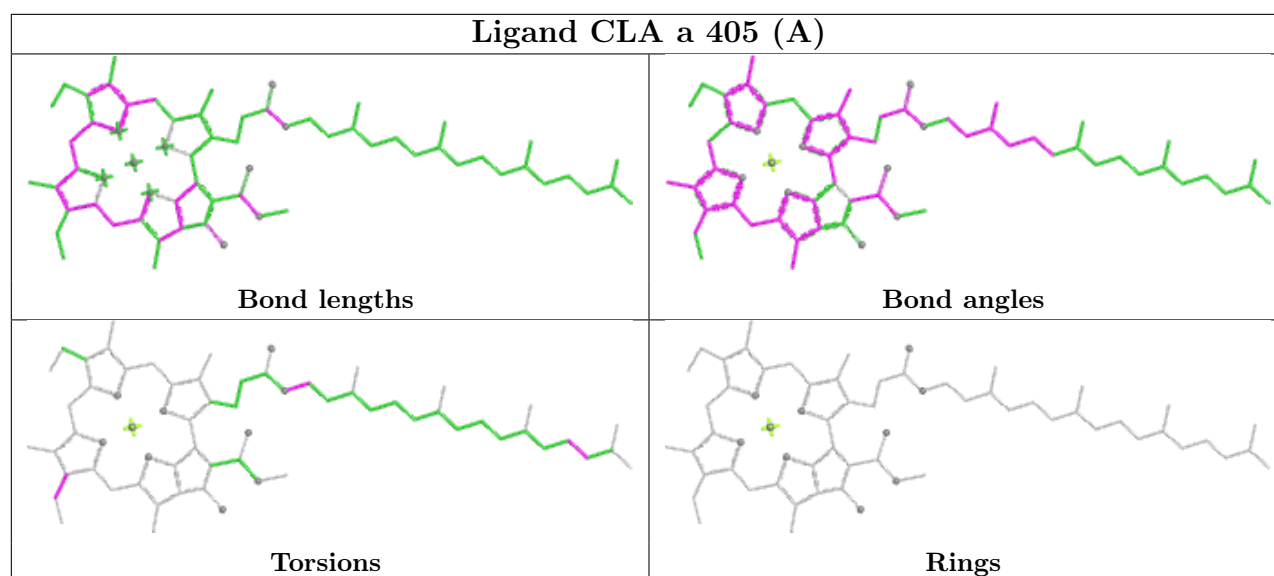
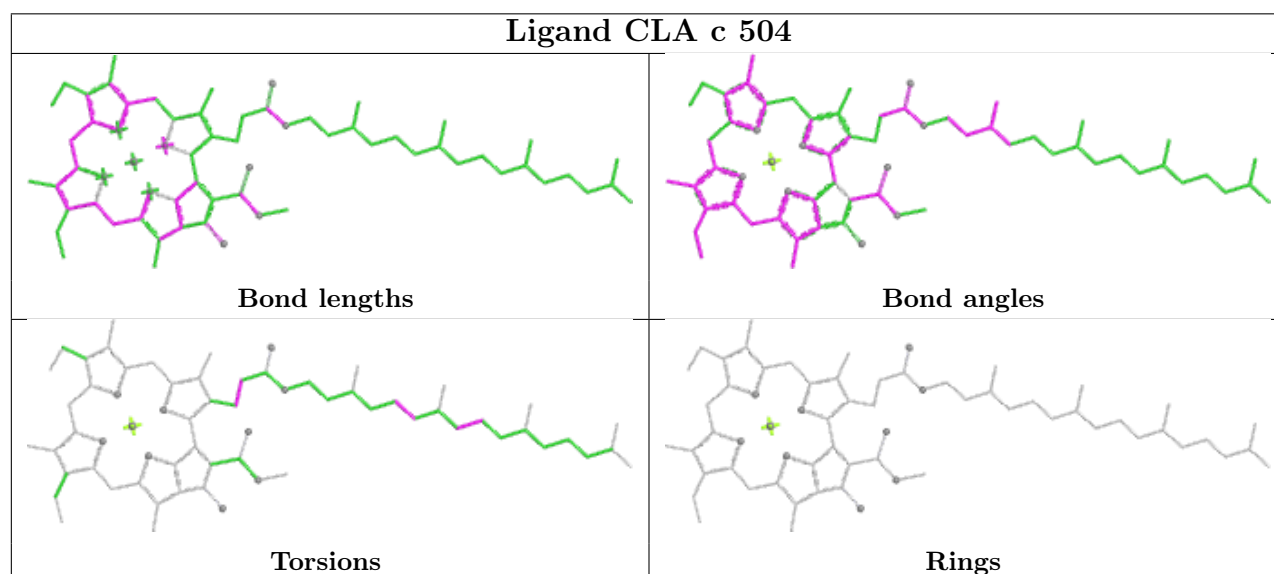
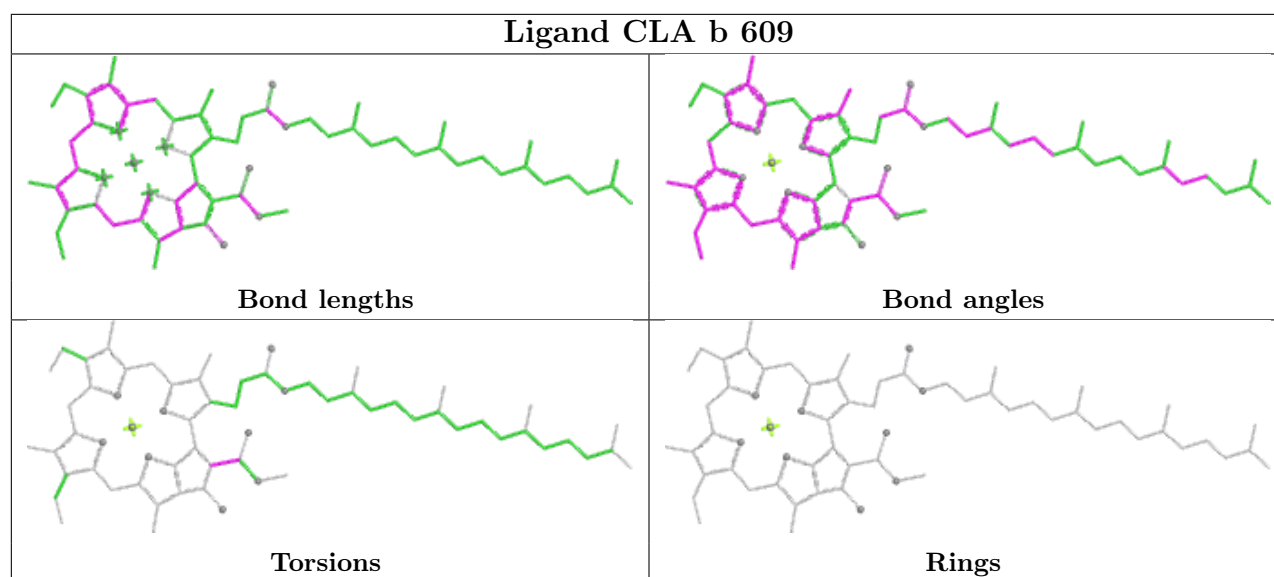


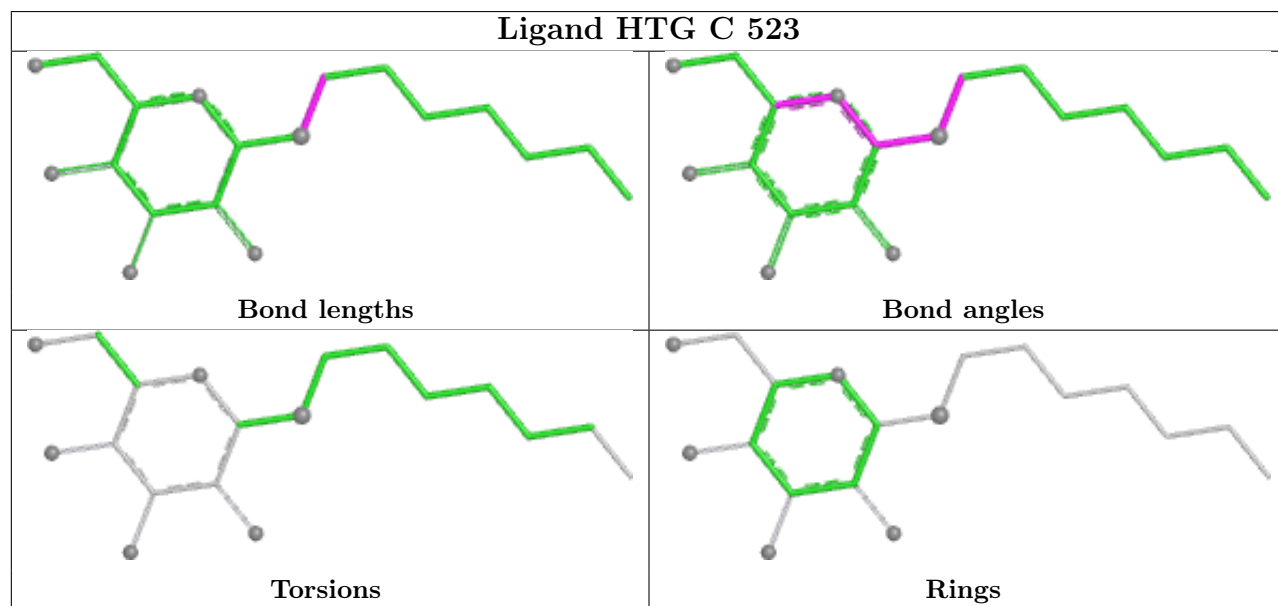
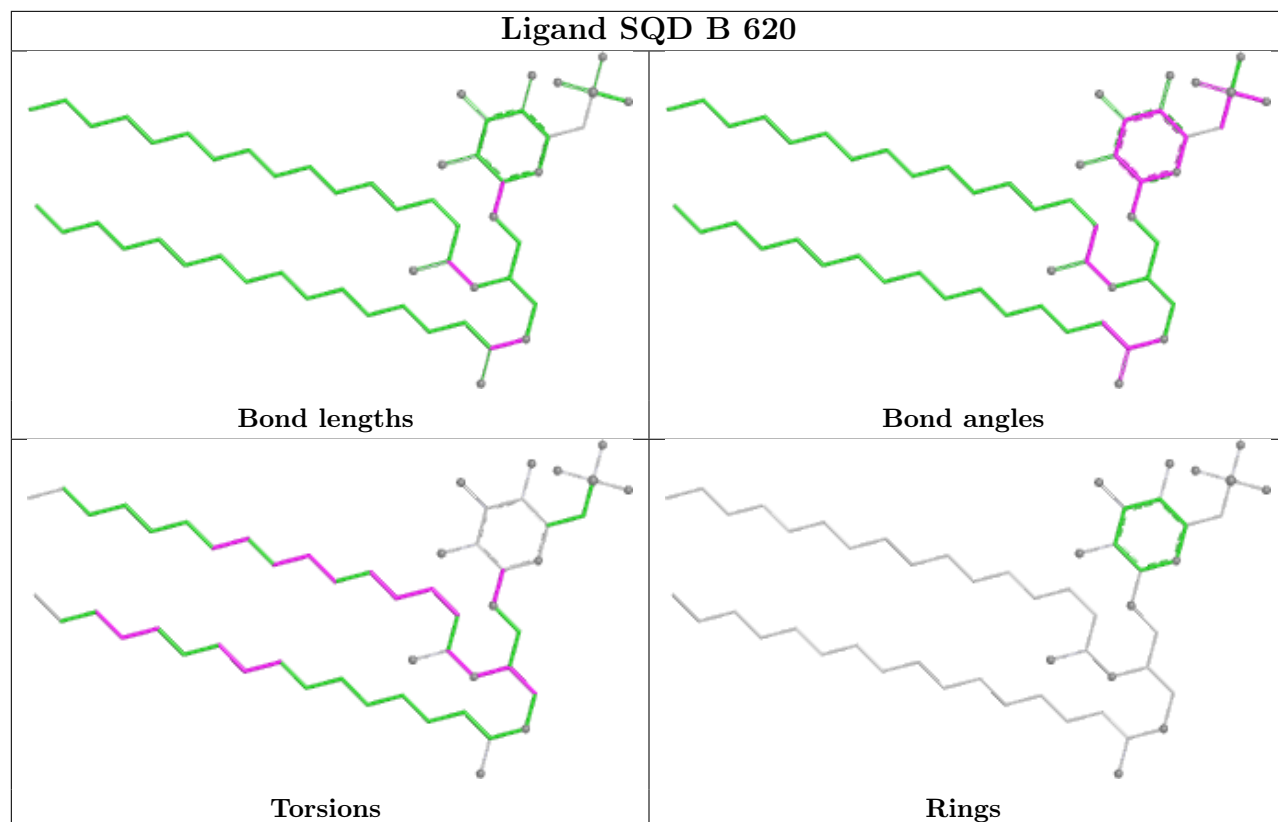
Ligand LMG C 526



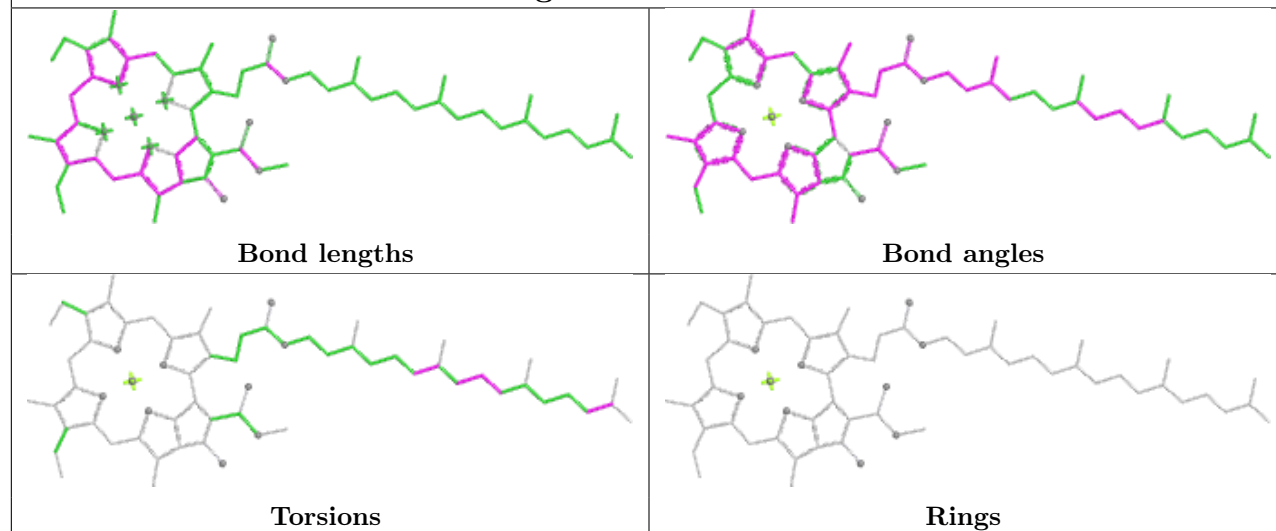




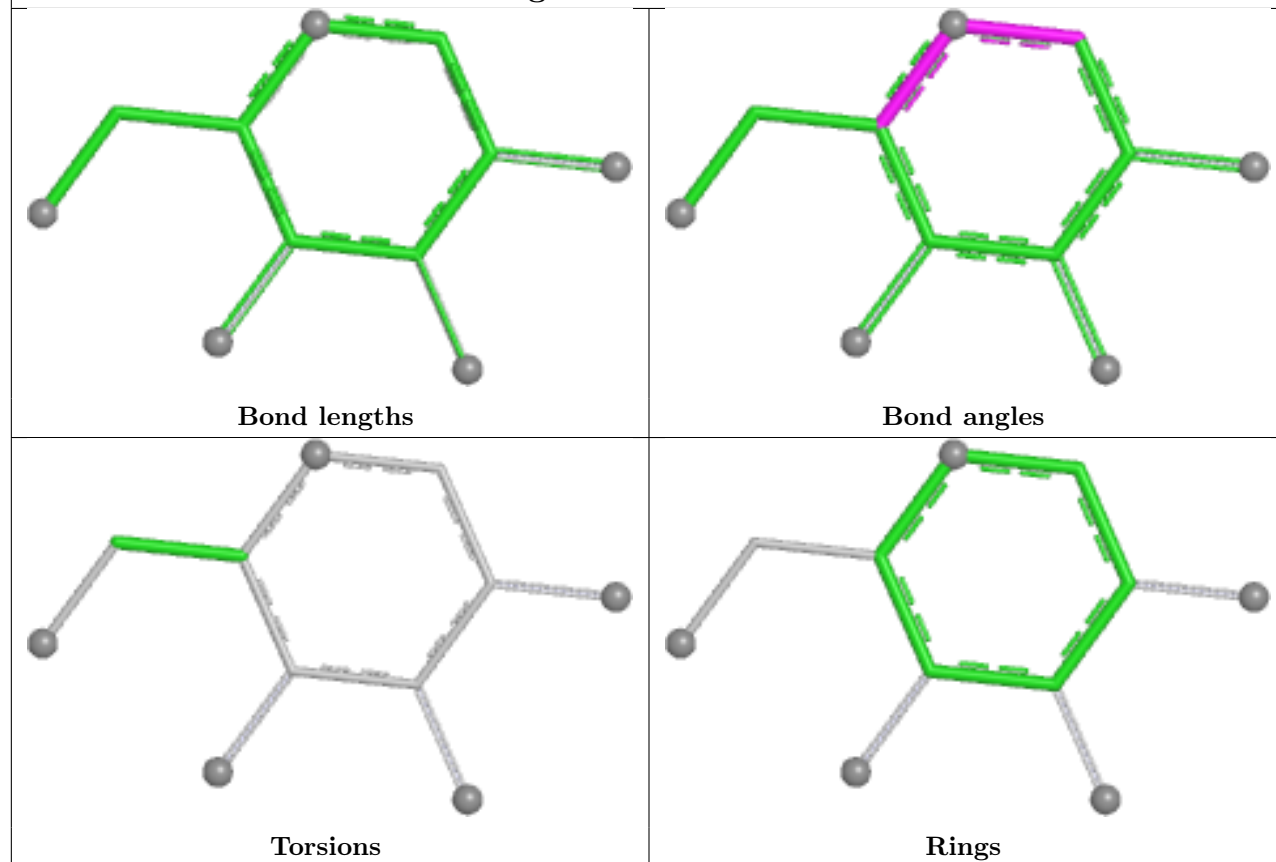


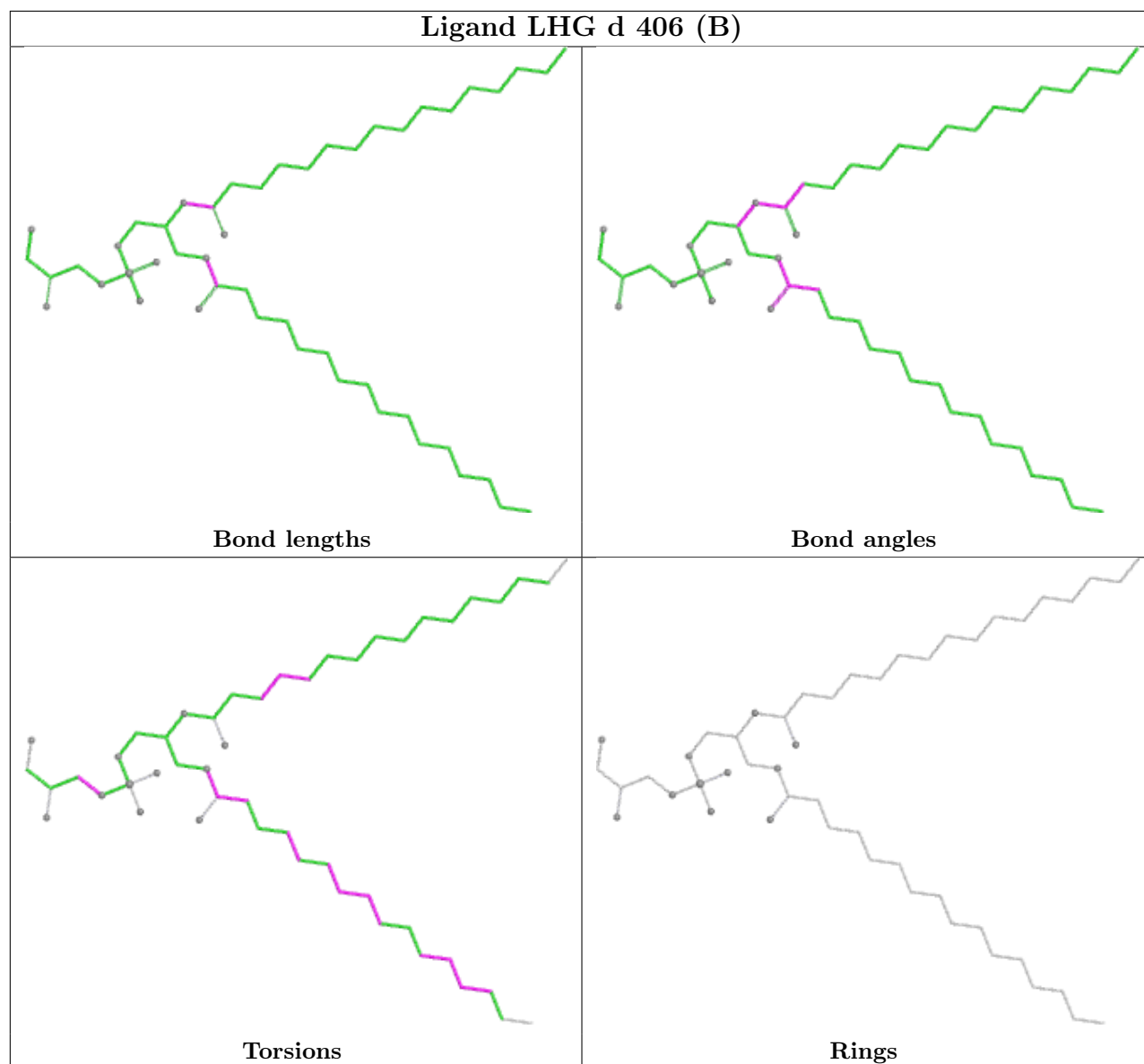
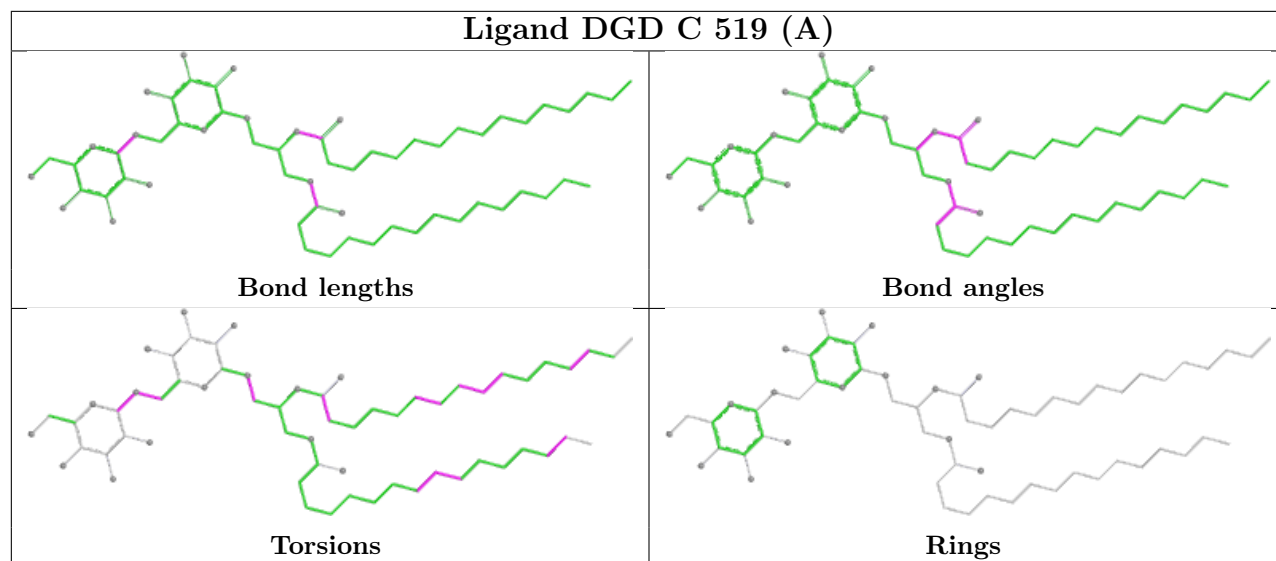


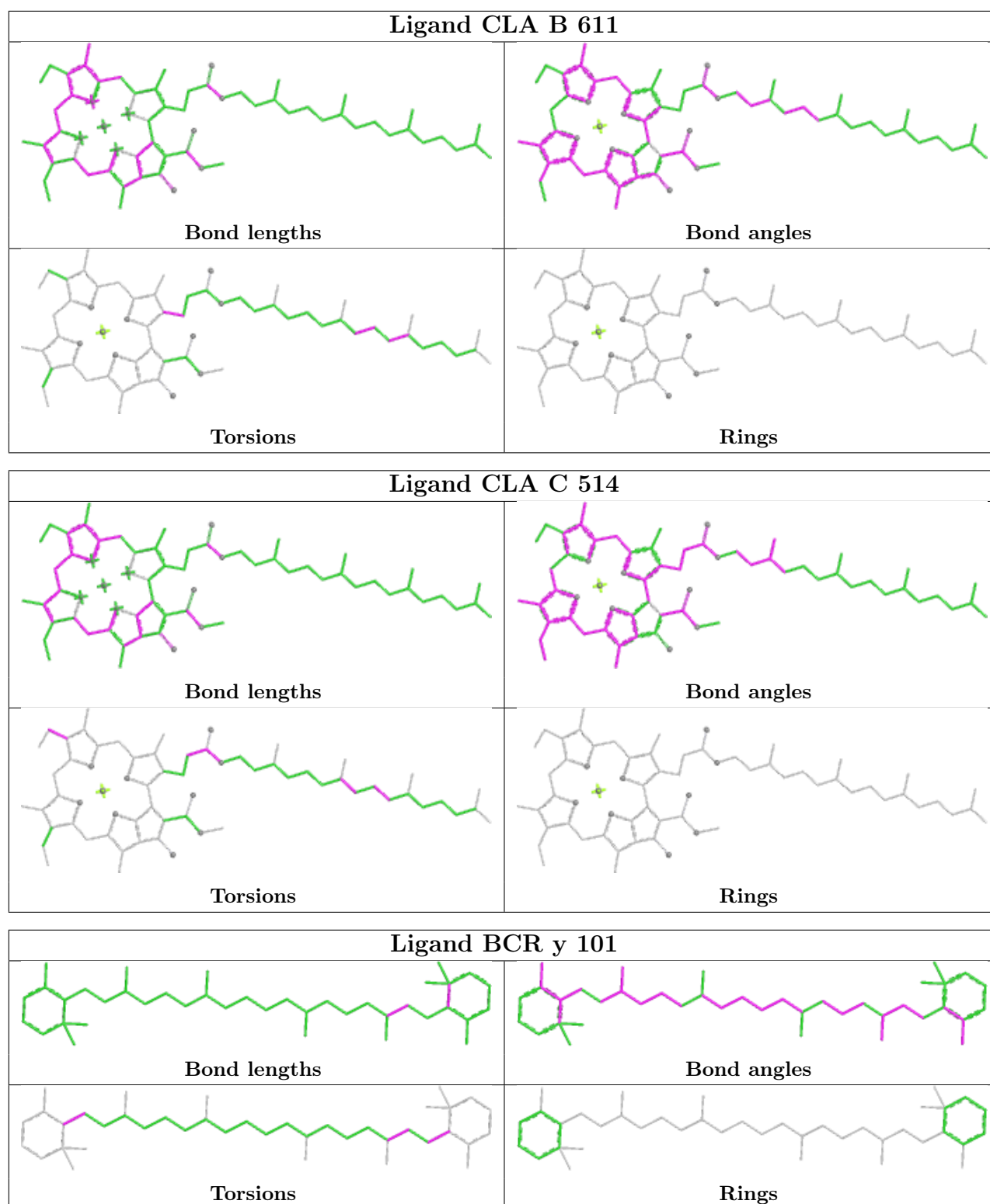
Ligand CLA b 602

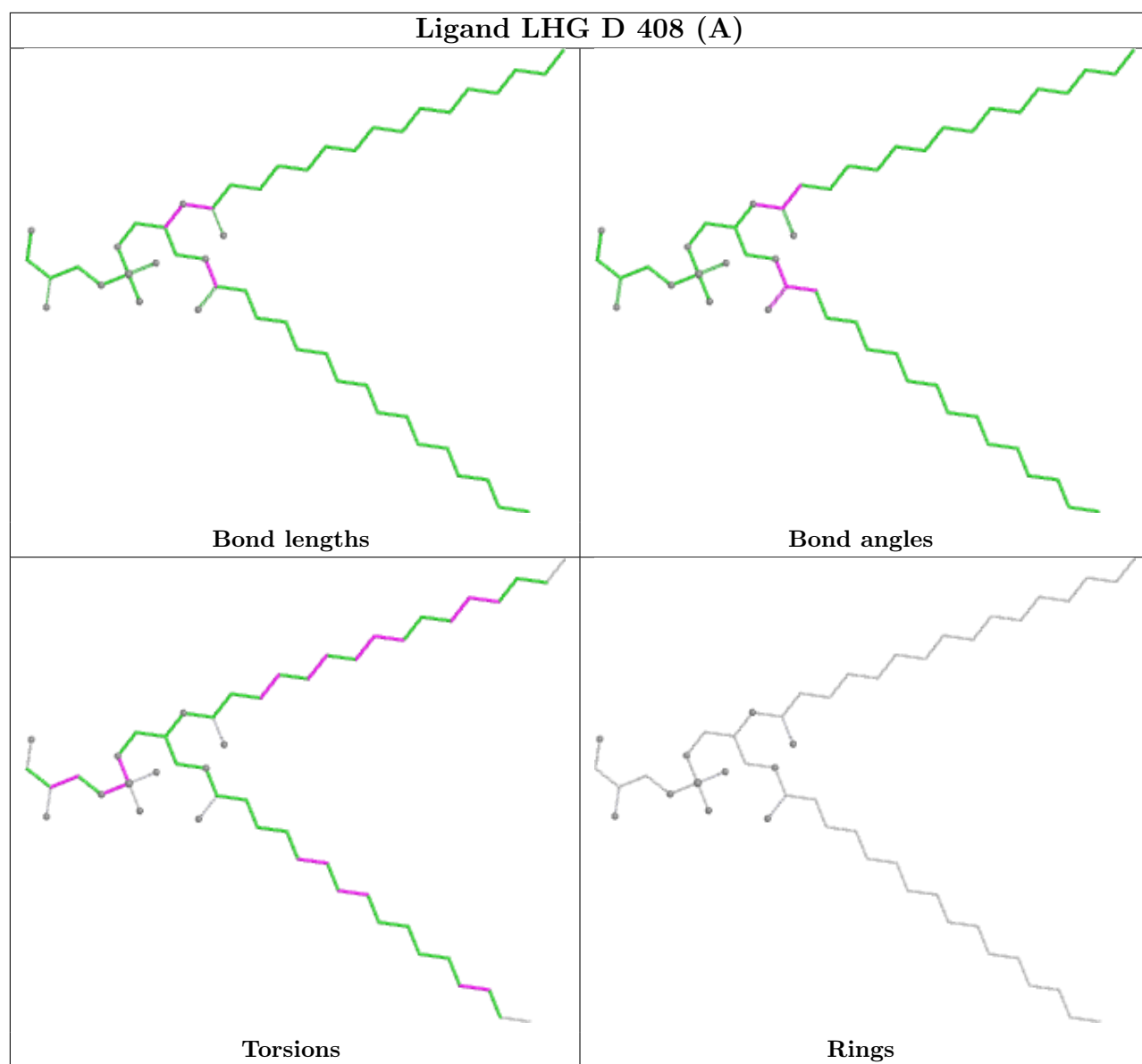


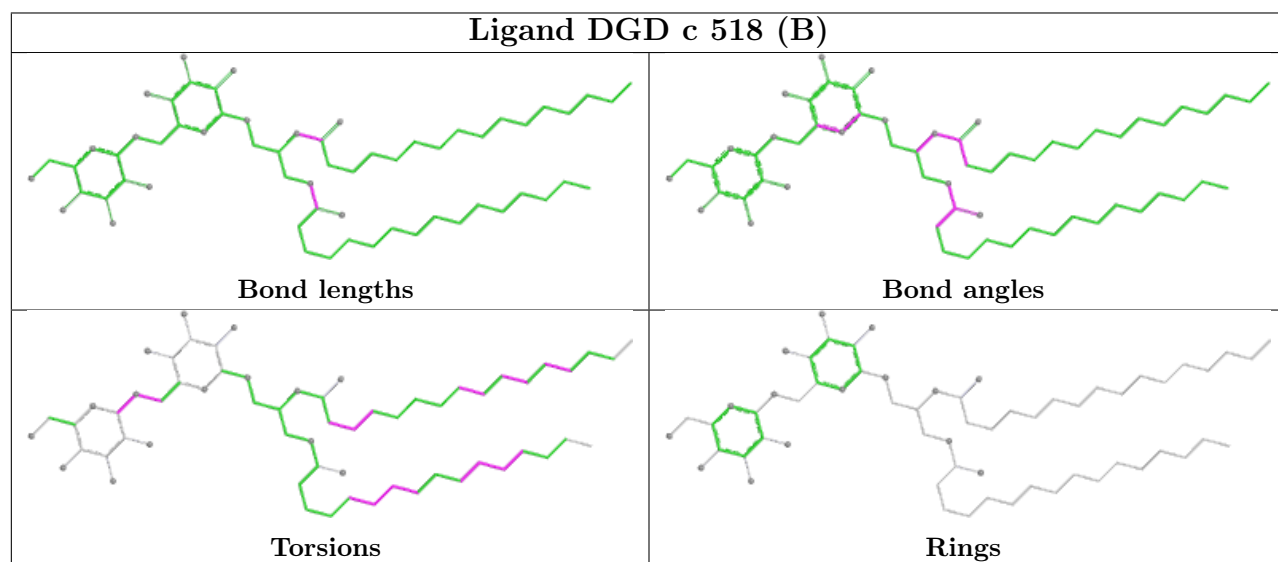
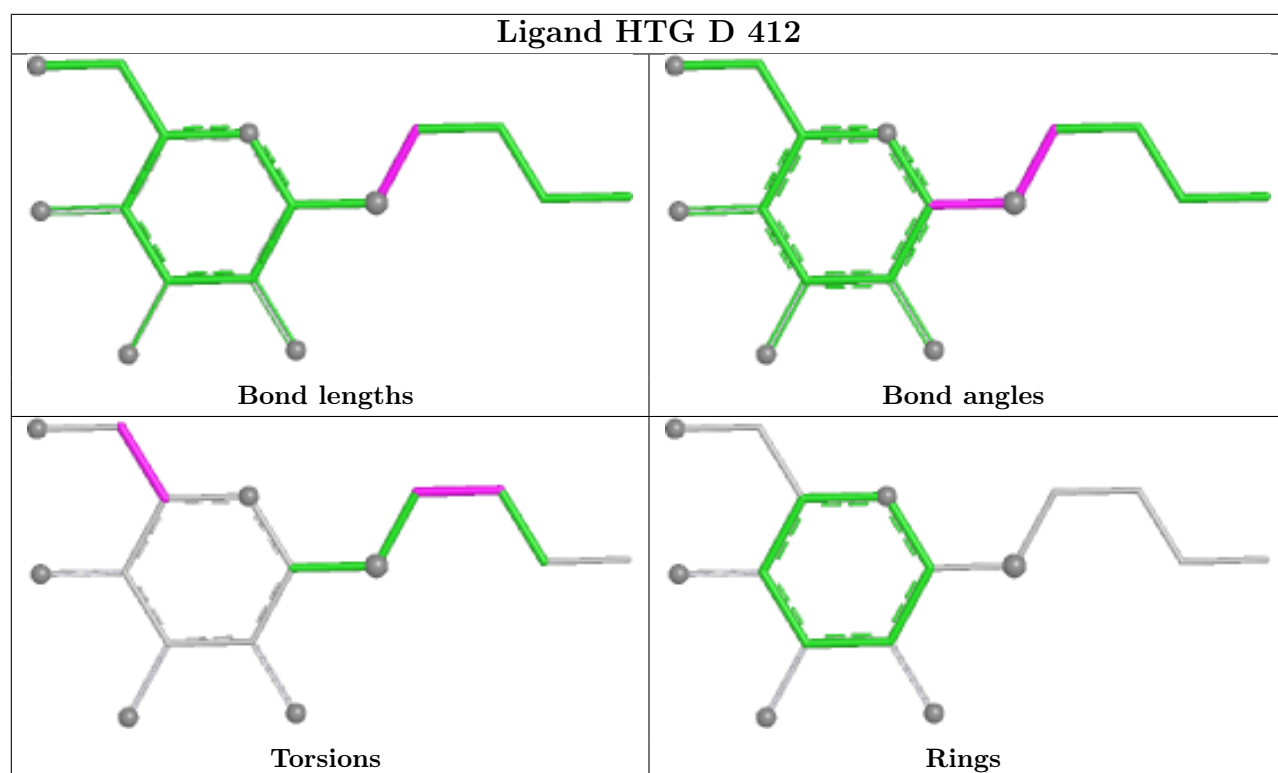
Ligand HTG V 203

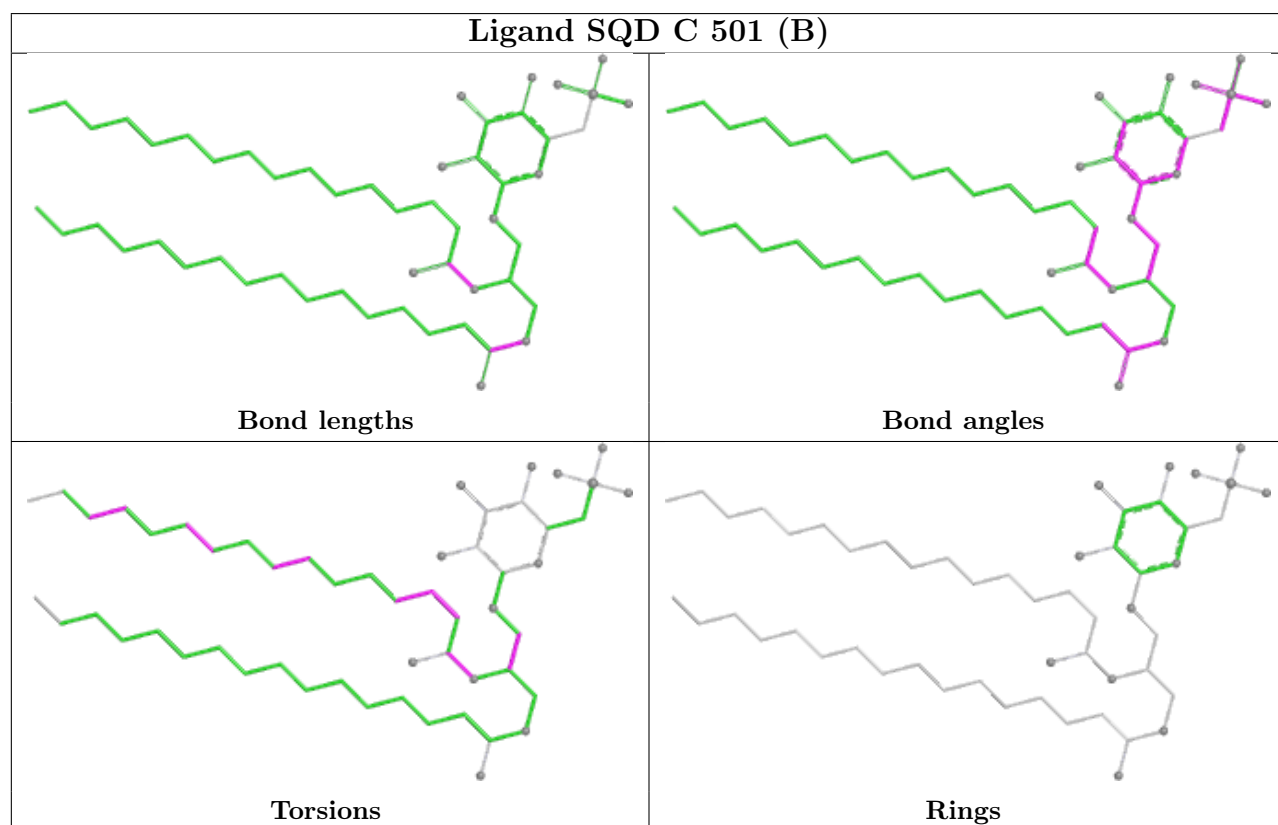
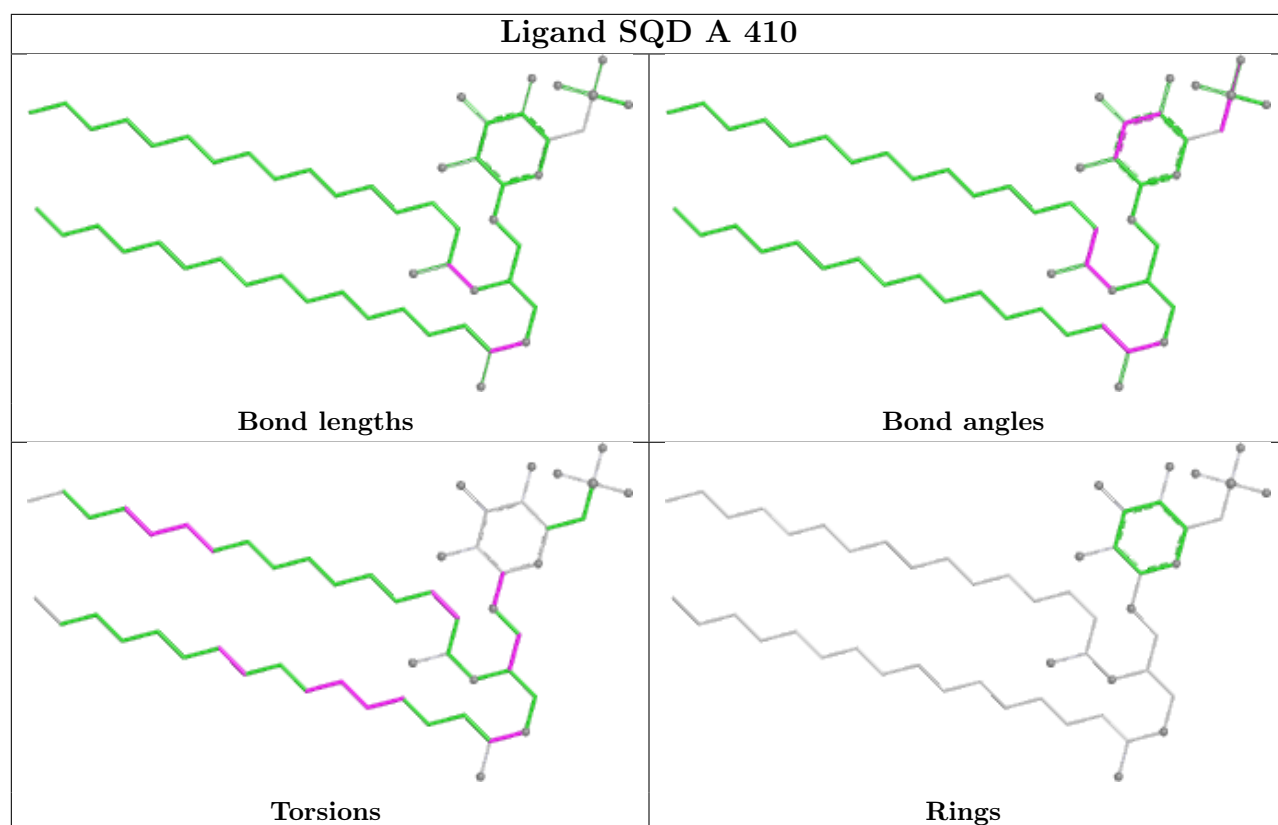


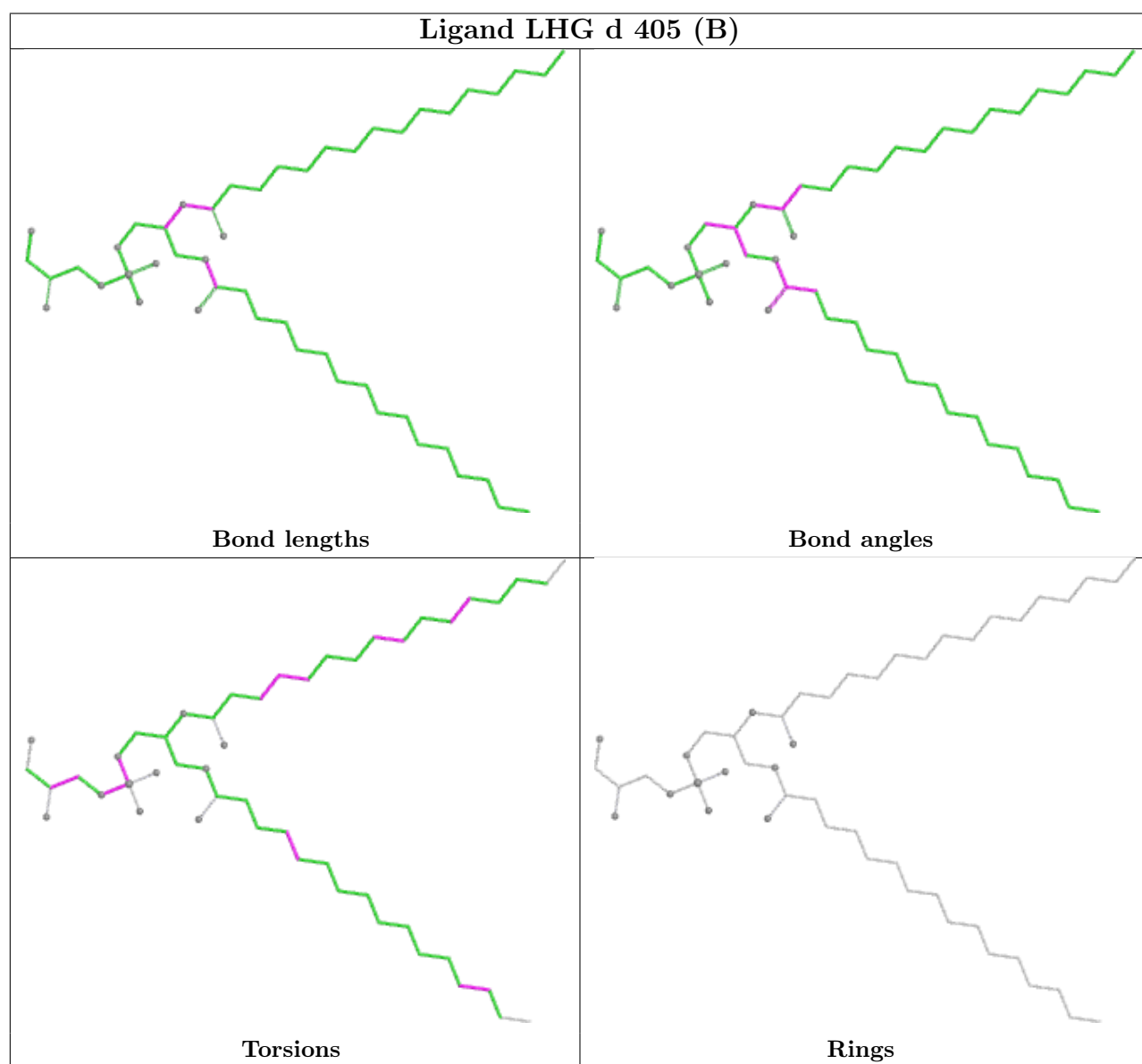
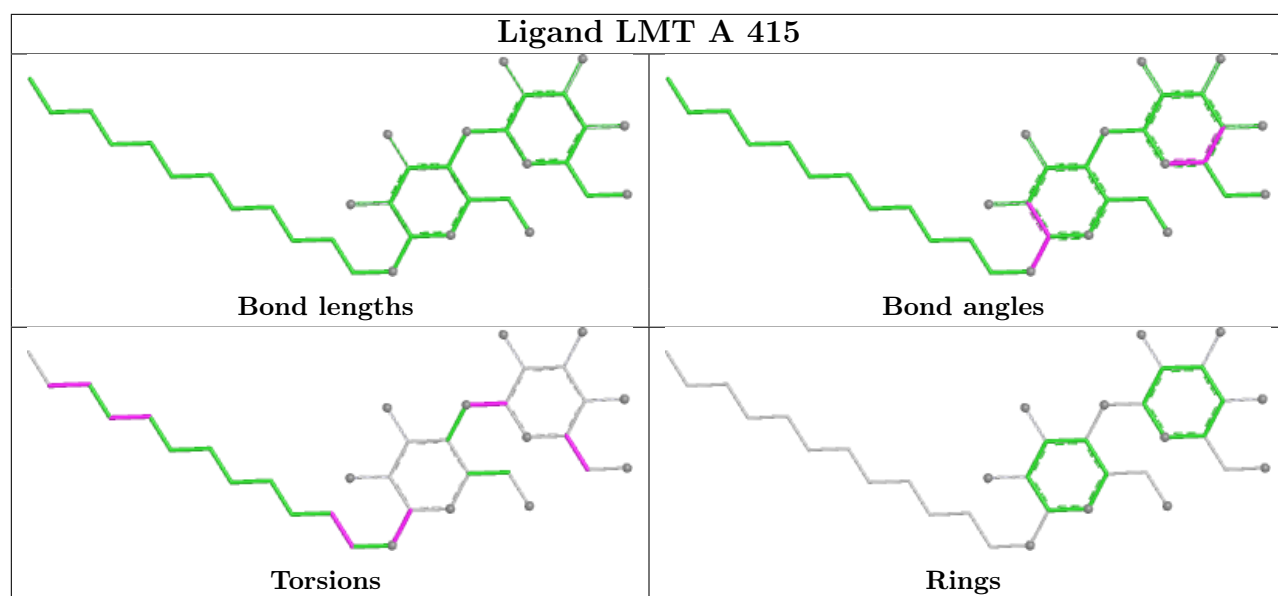


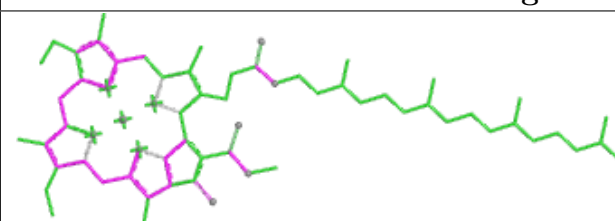
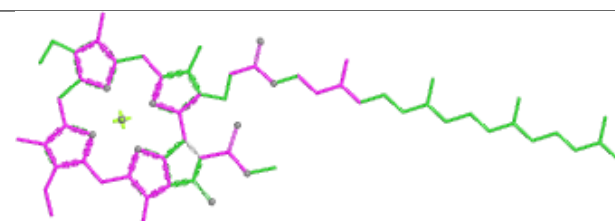
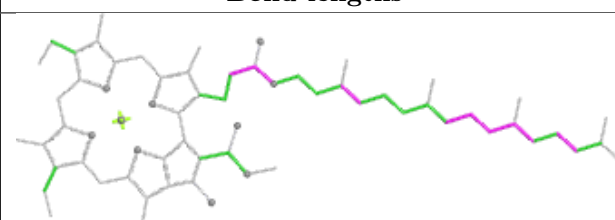
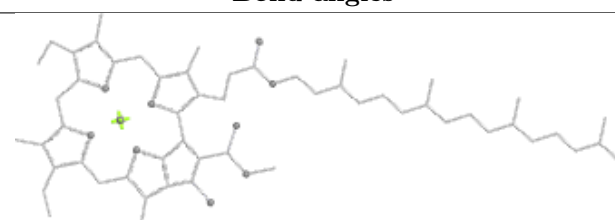


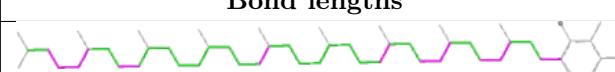
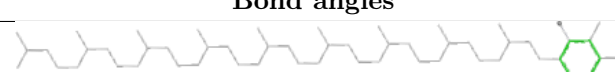


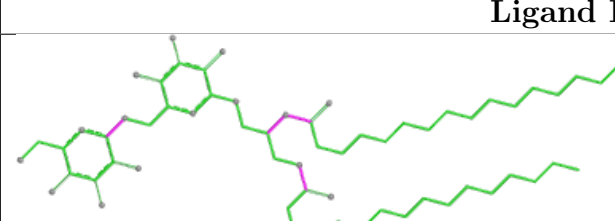
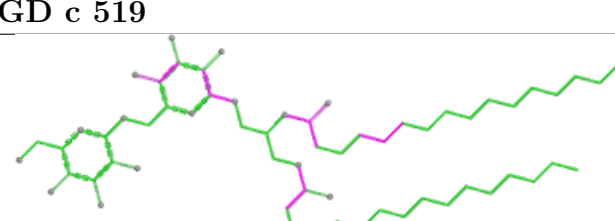
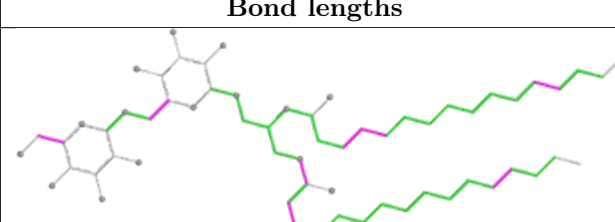
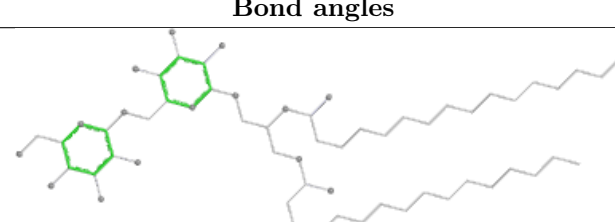


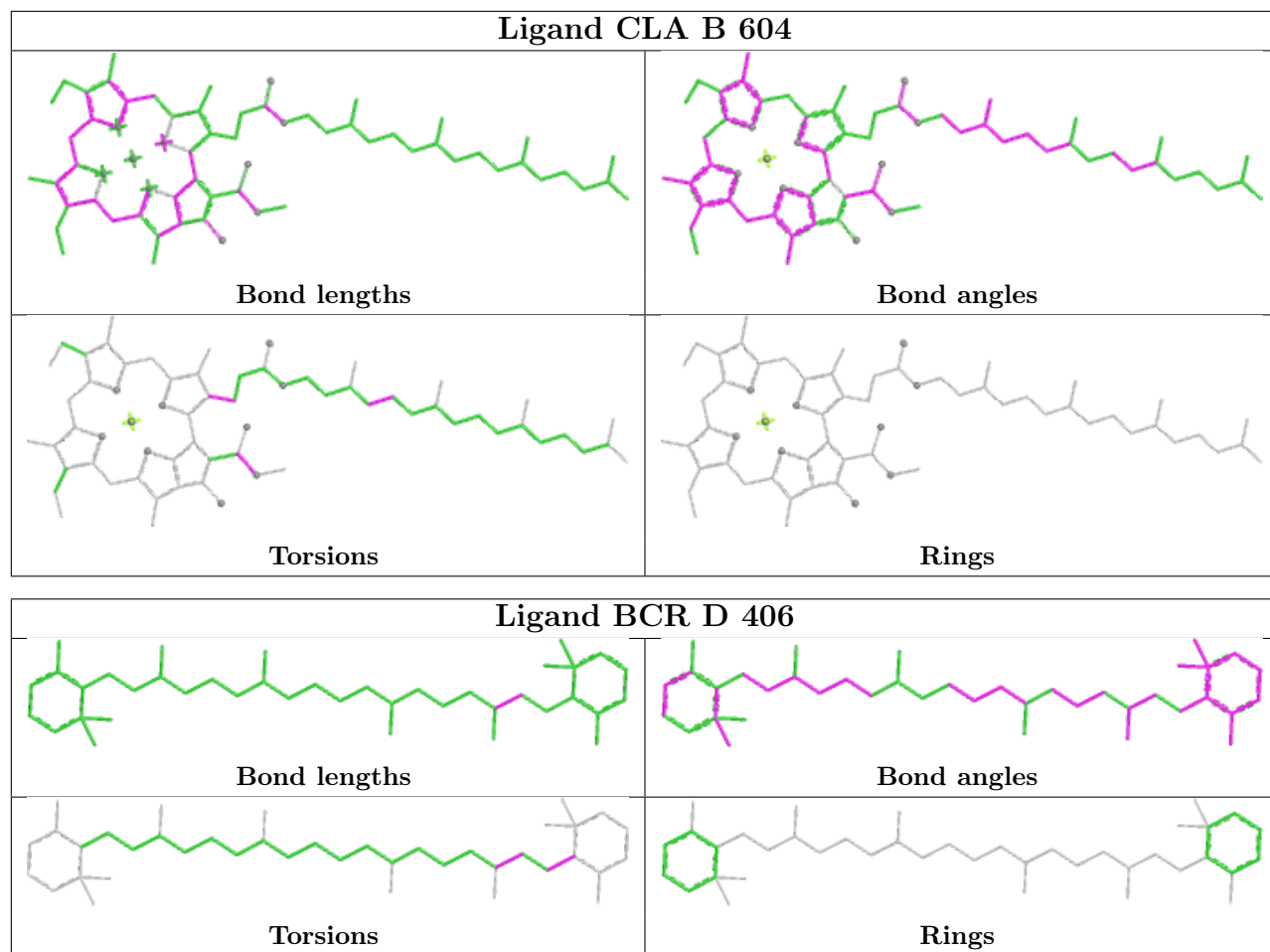


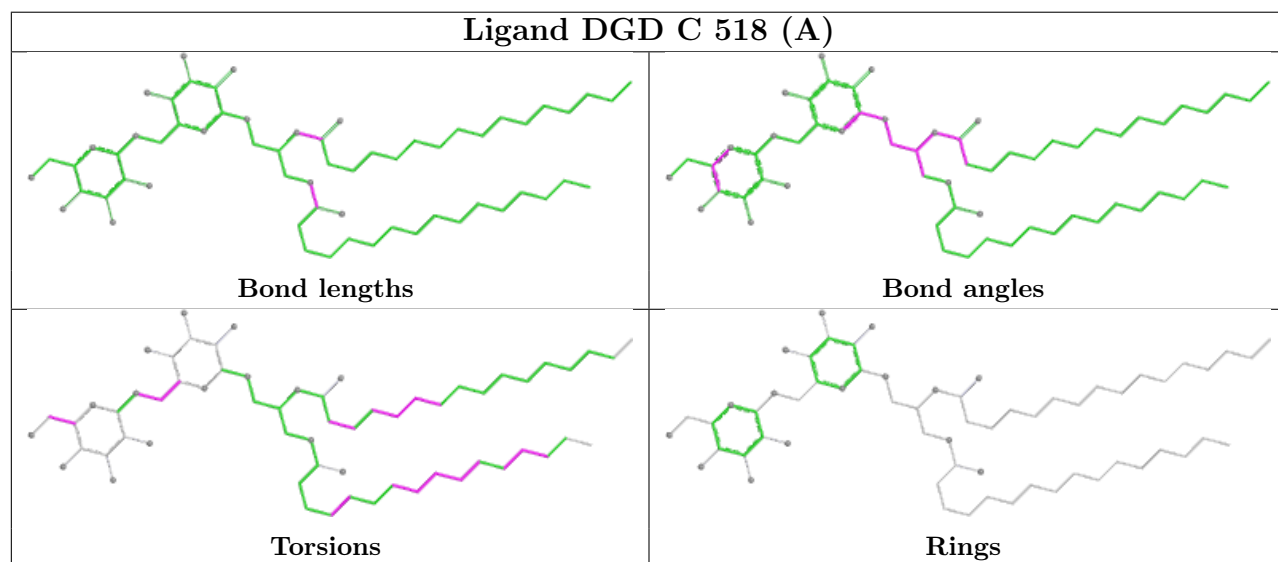
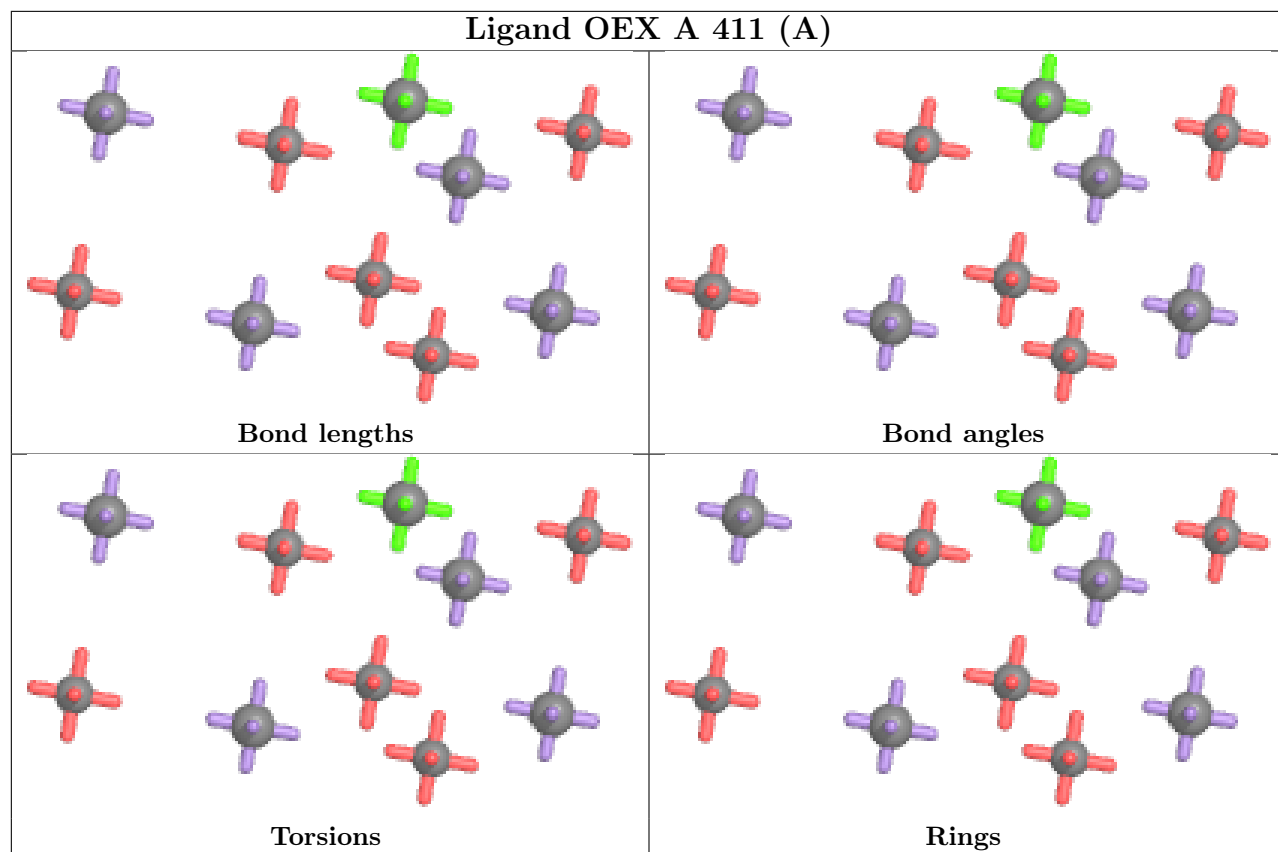


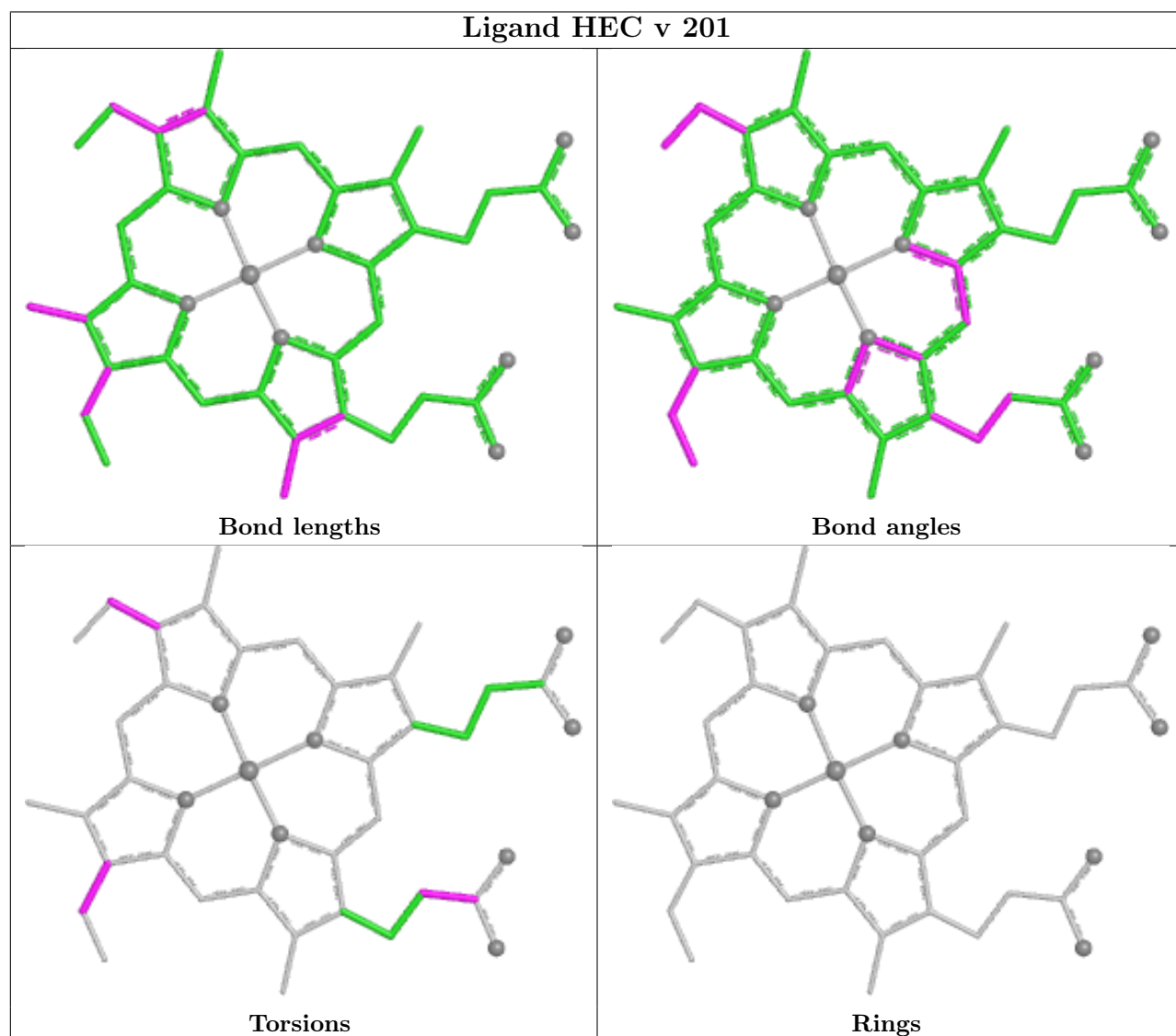
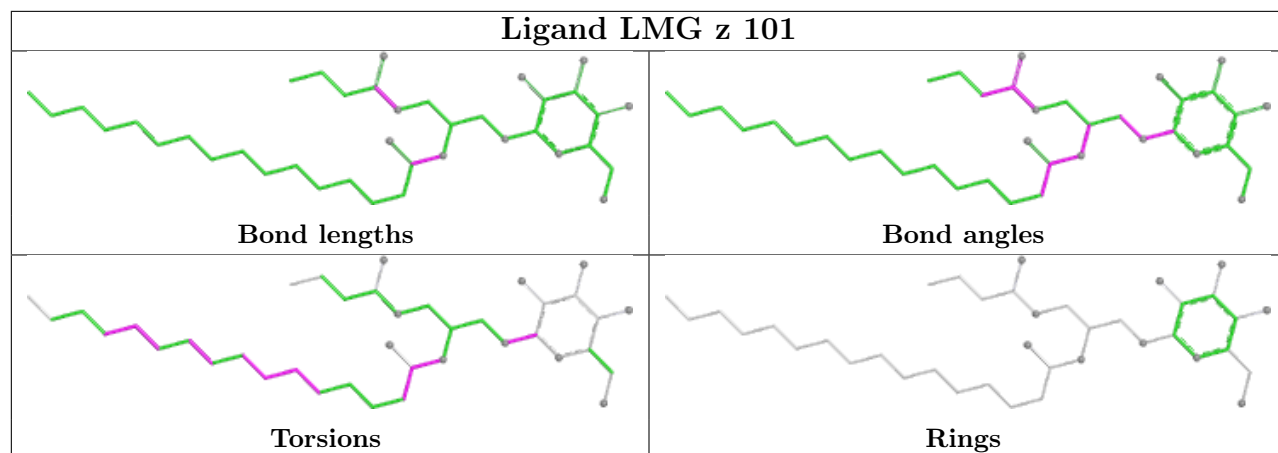
Ligand CLA C 512	
	
Bond lengths	Bond angles
	
Torsions	Rings

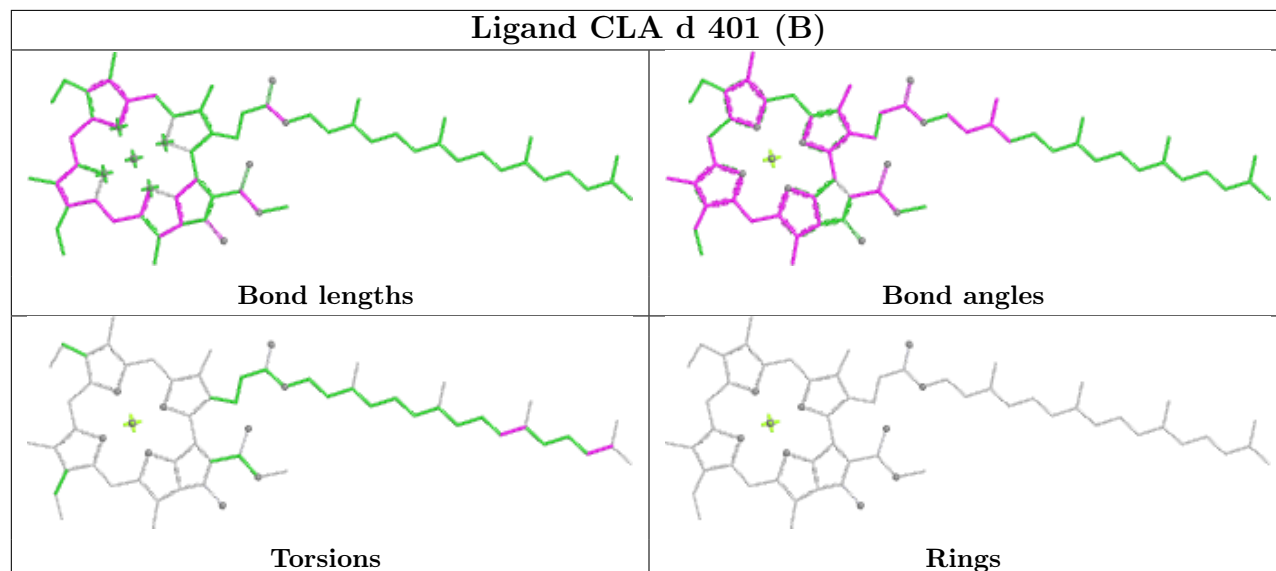
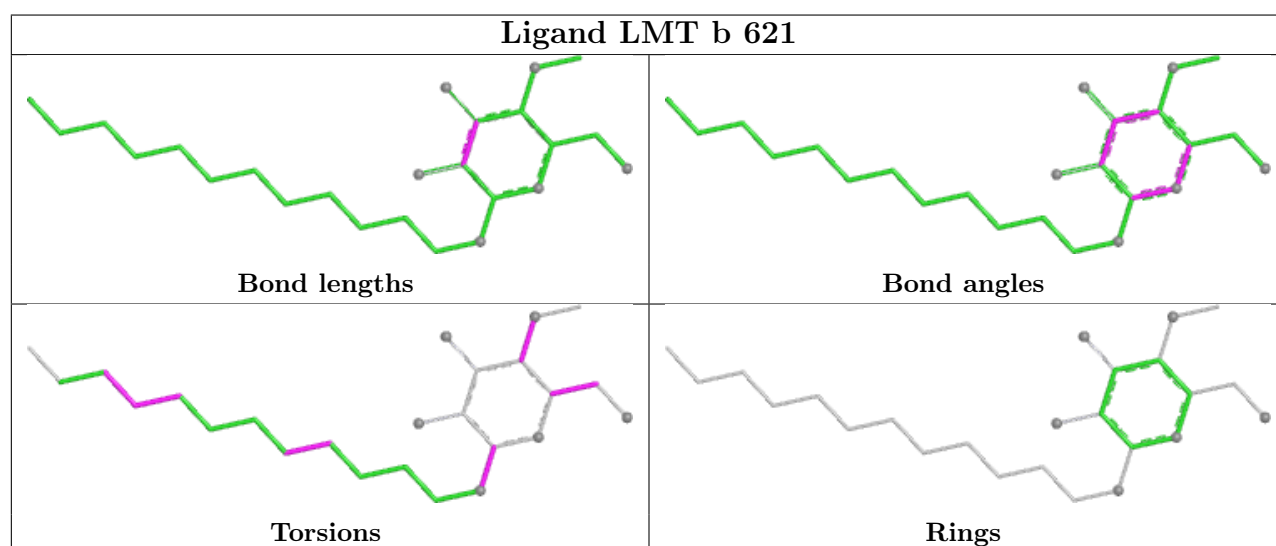
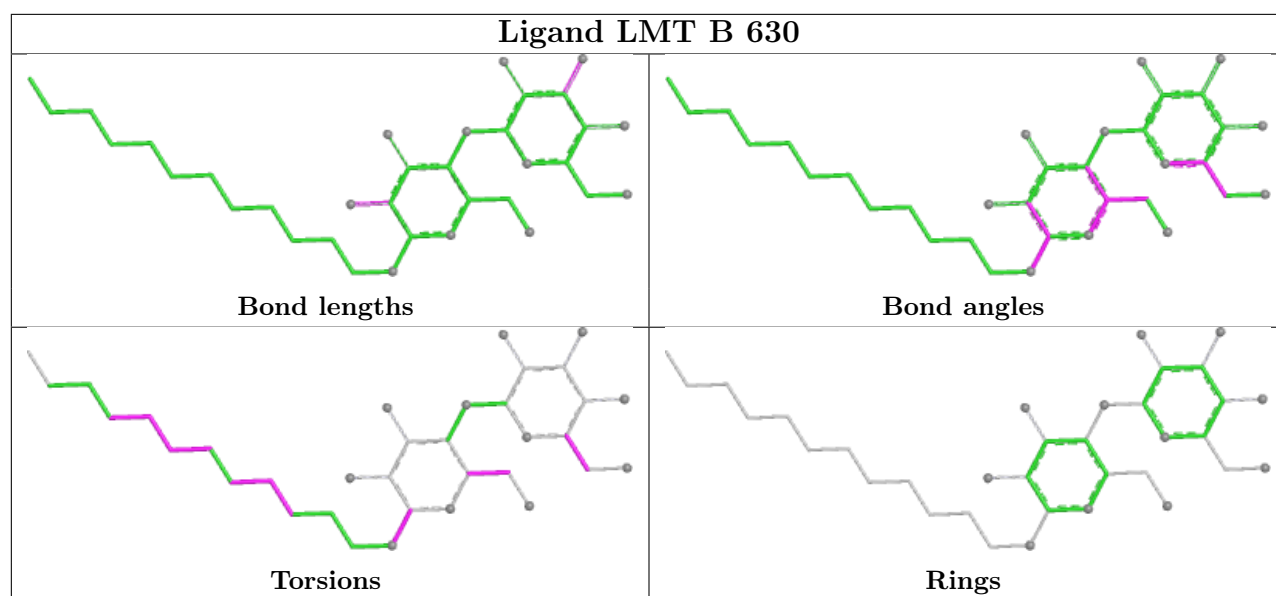
Ligand PL9 A 412 (B)	
	
Bond lengths	Bond angles
	
Torsions	Rings

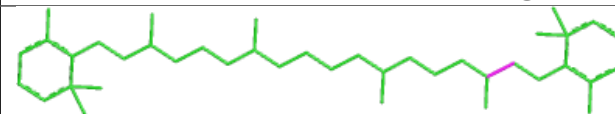
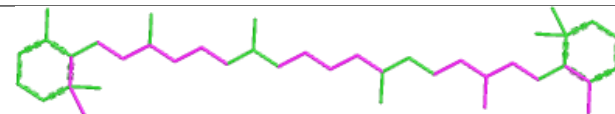
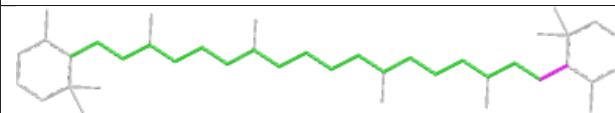
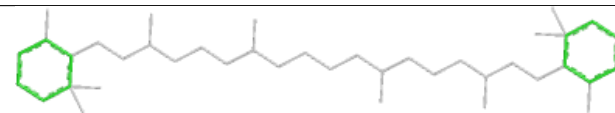
Ligand DGD c 519	
	
Bond lengths	Bond angles
	
Torsions	Rings

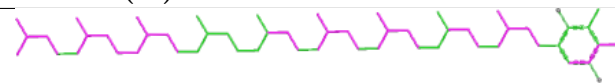


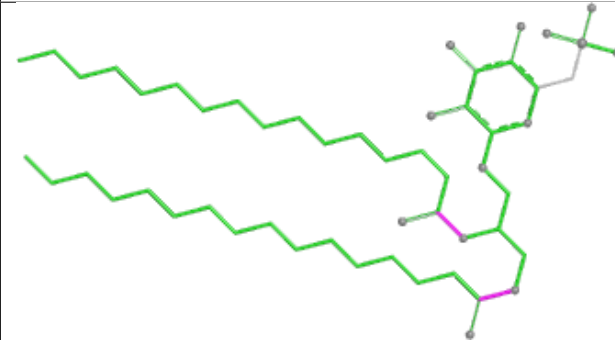
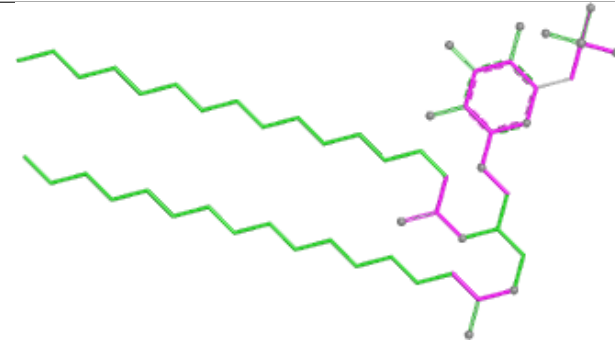
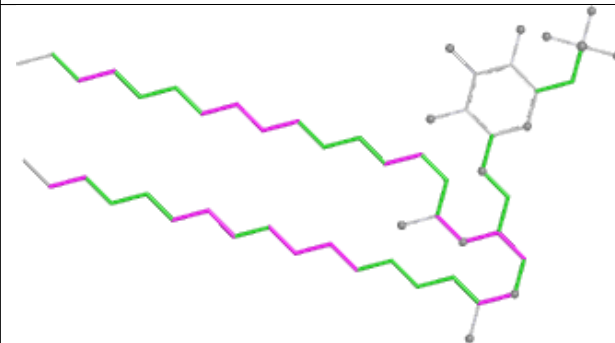
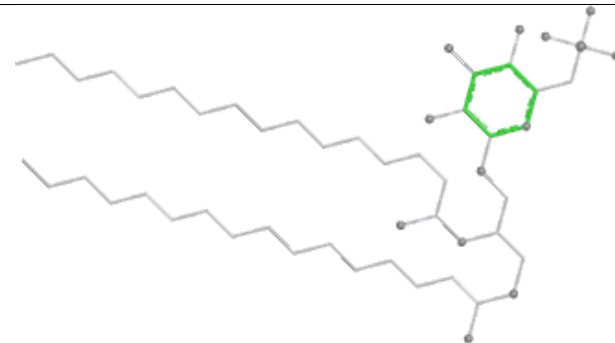


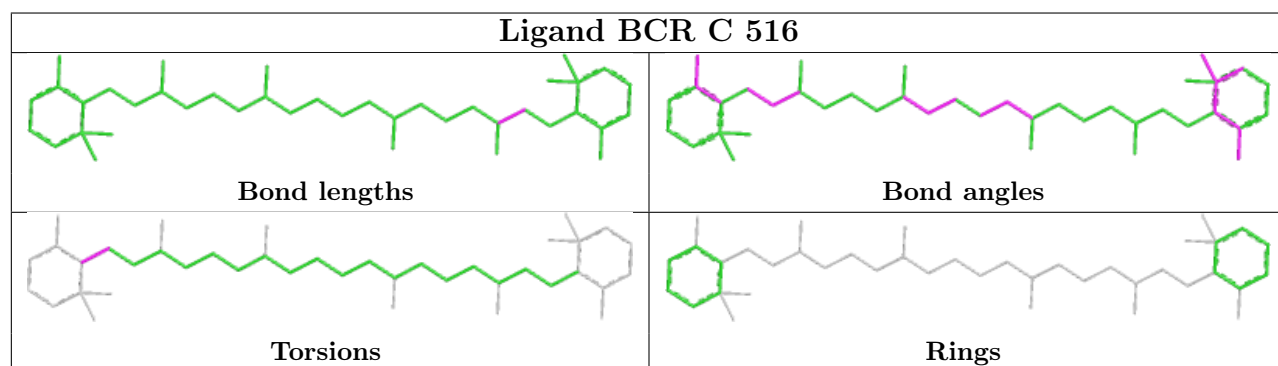
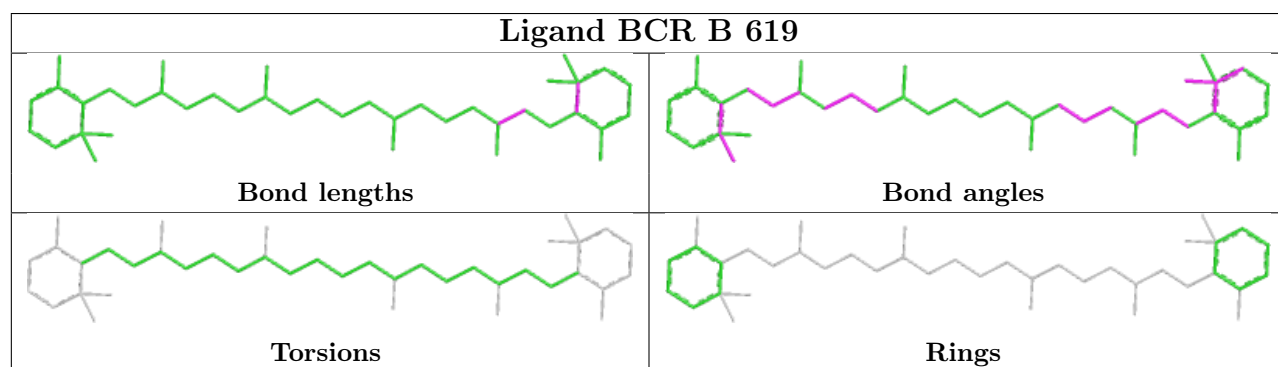
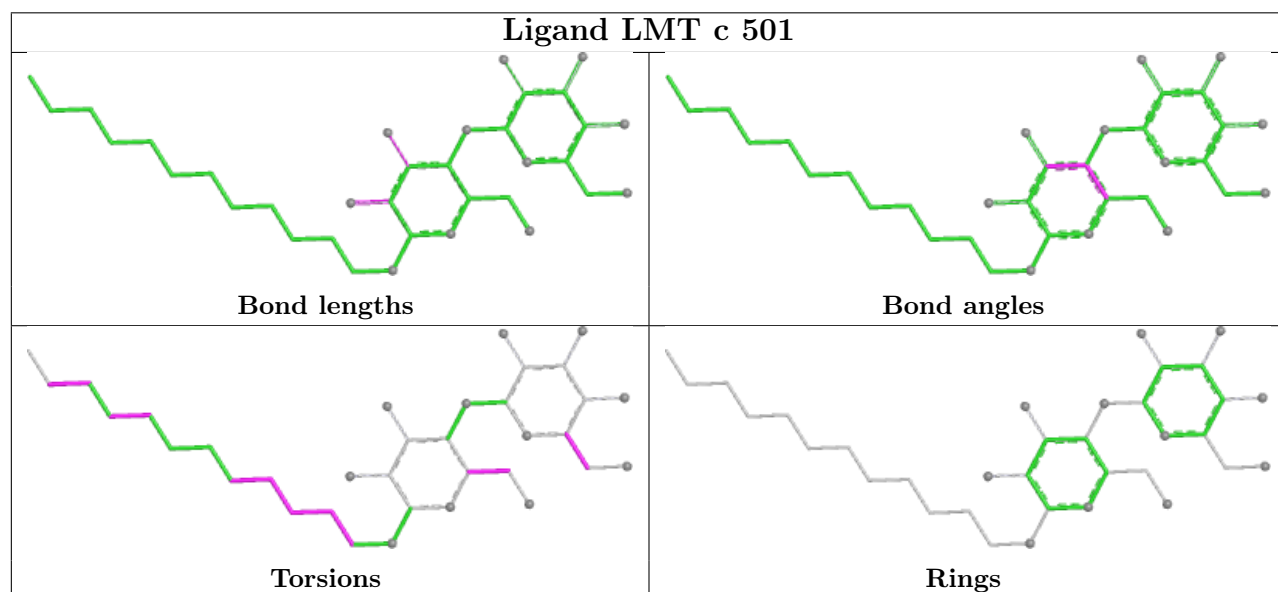
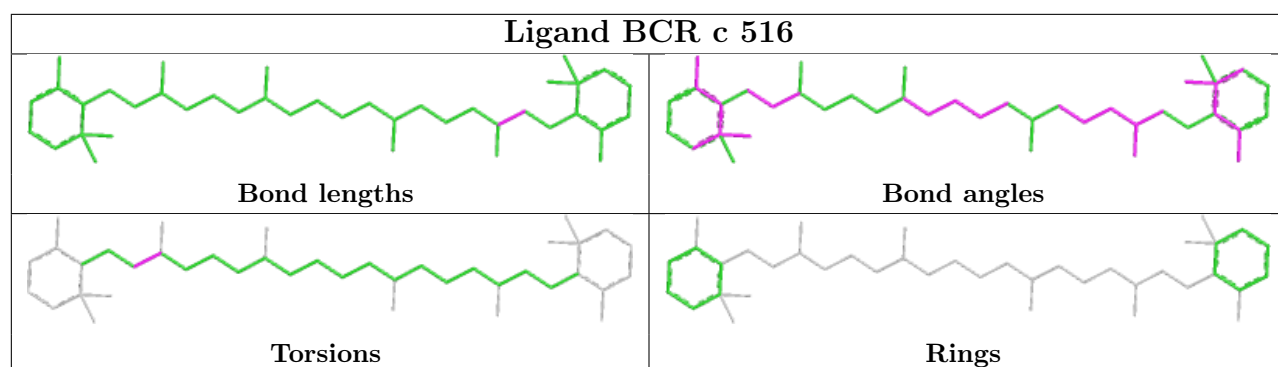


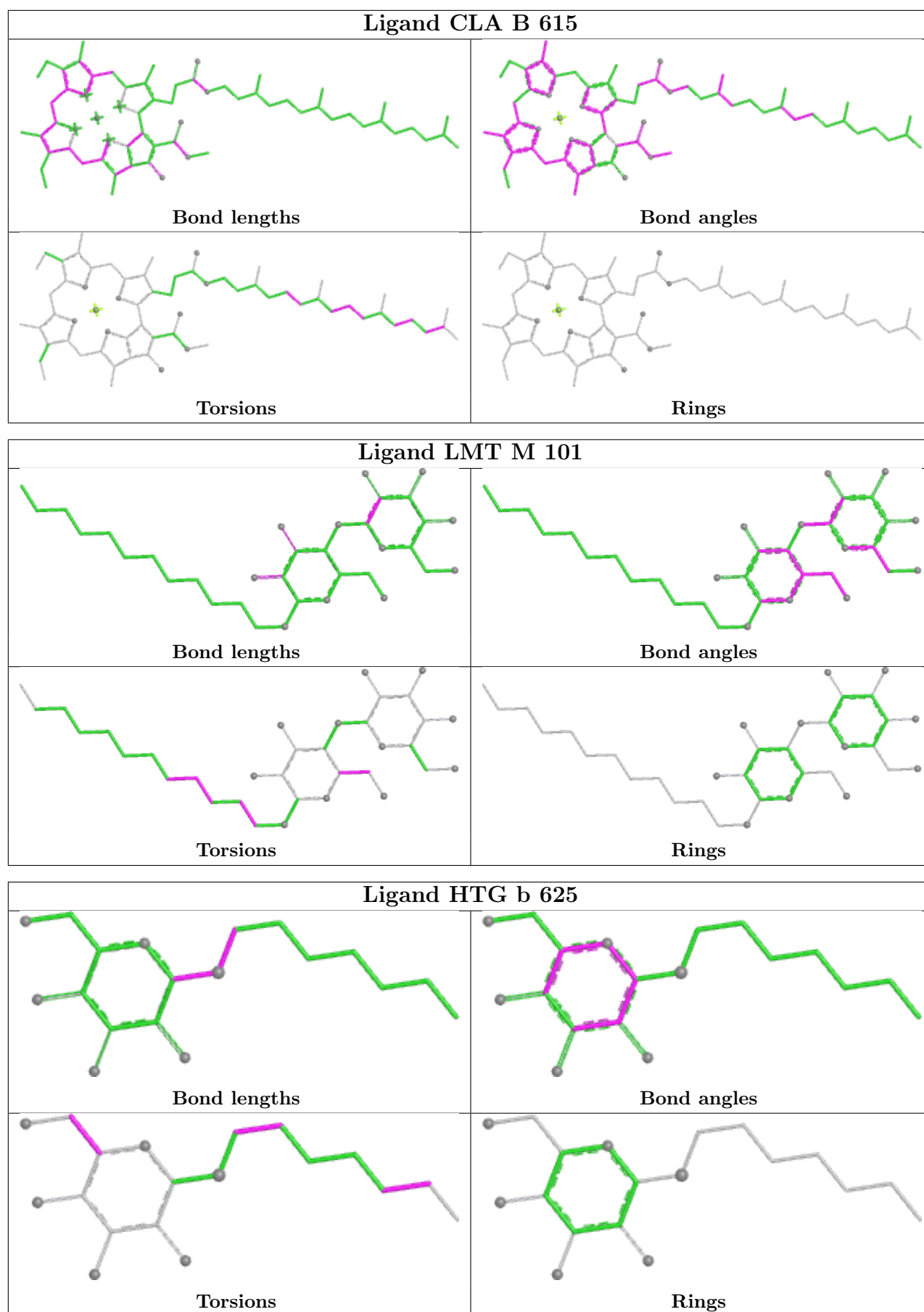


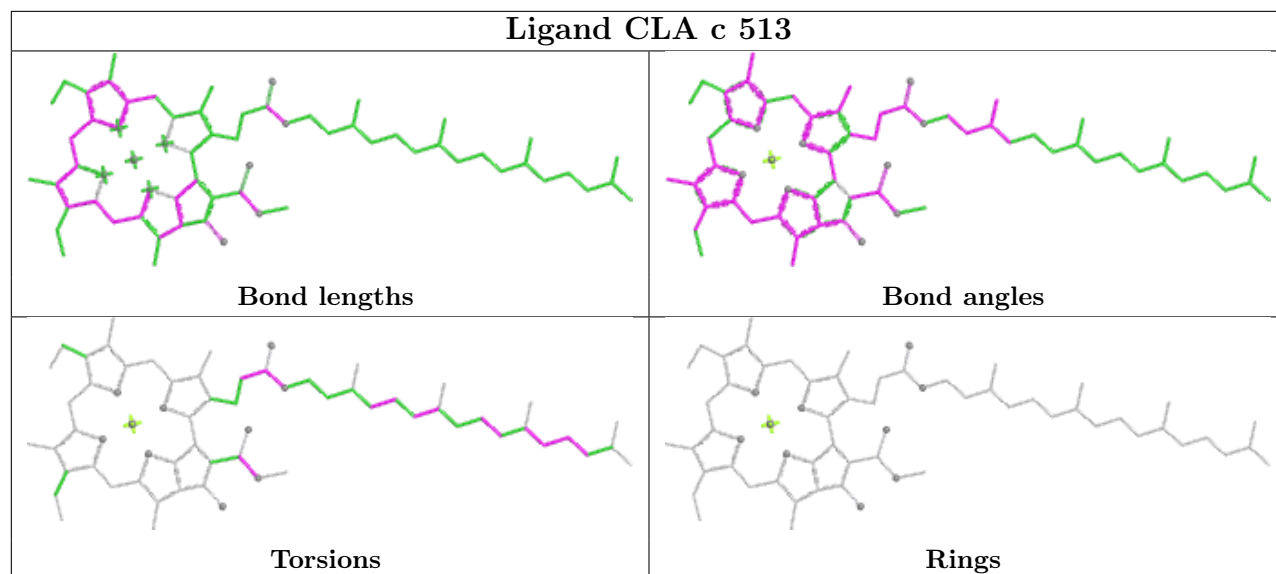
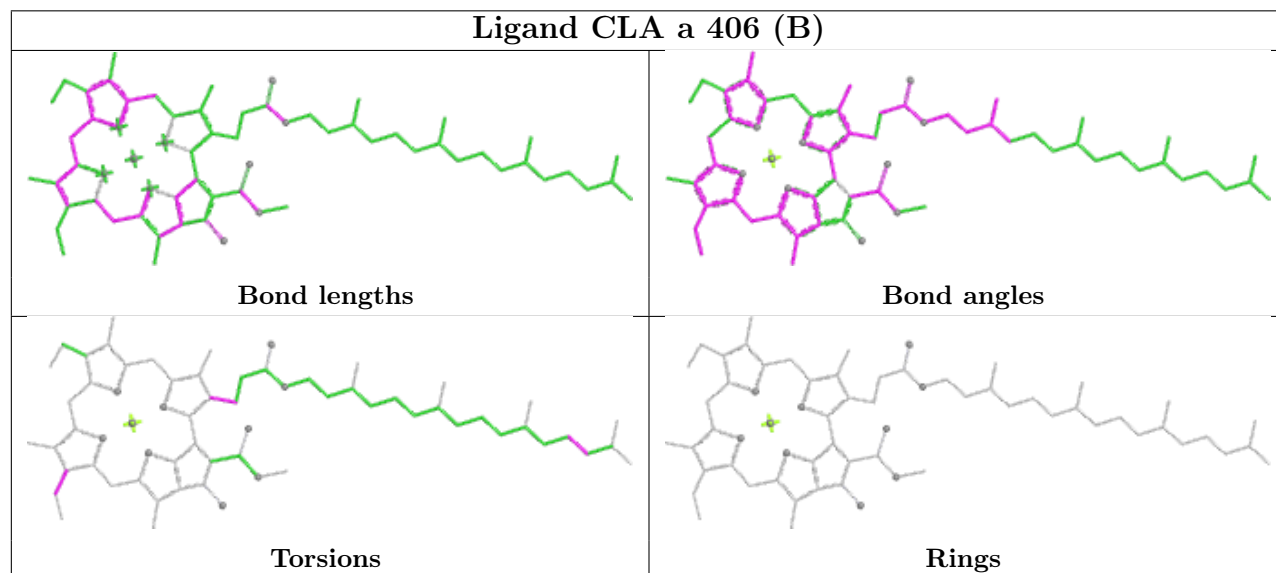
Ligand BCR H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 D 407 (A)	
	
Bond lengths	Bond angles
	
Torsions	Rings

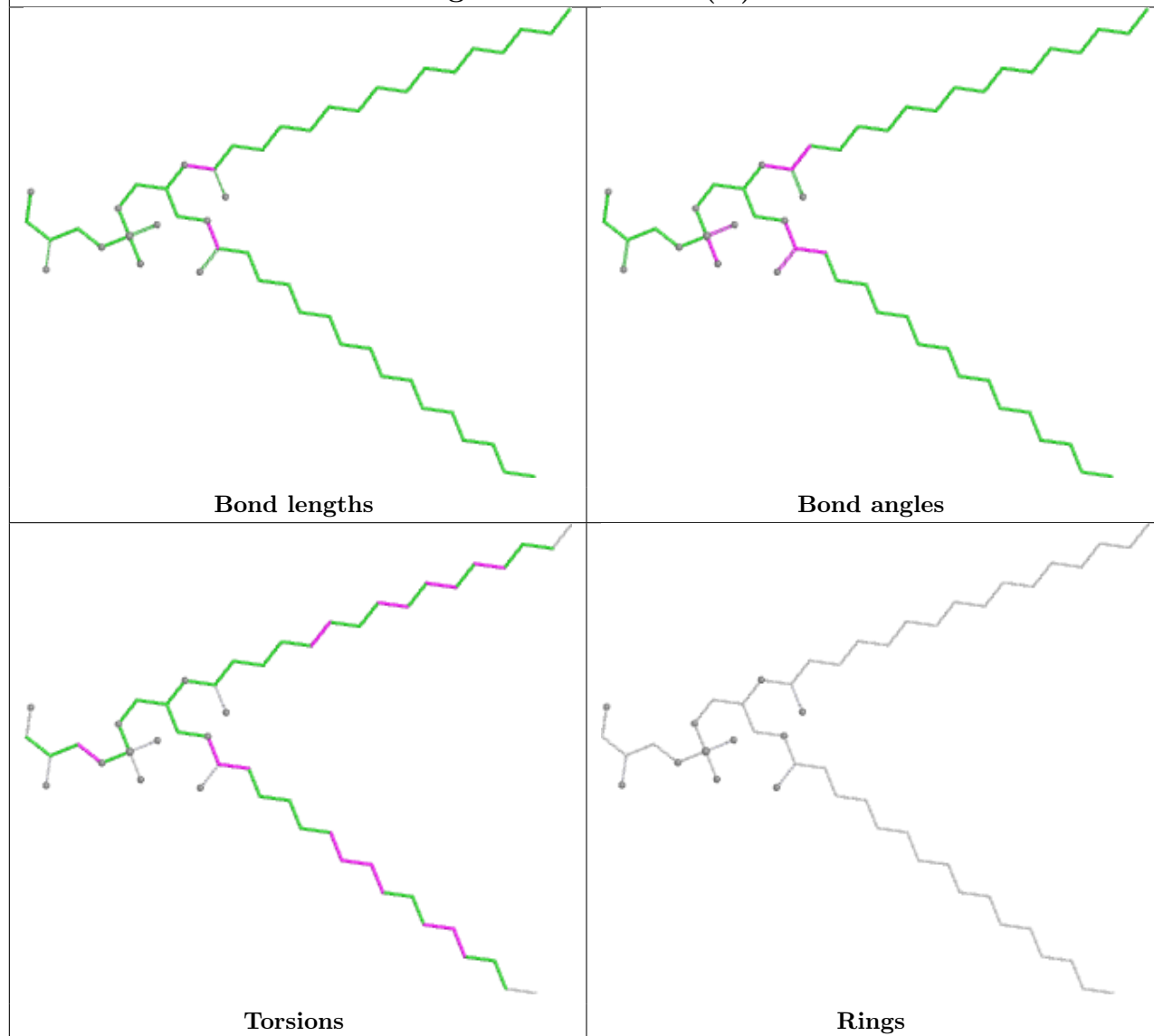
Ligand SQD b 620	
	
Bond lengths	Bond angles
	
Torsions	Rings



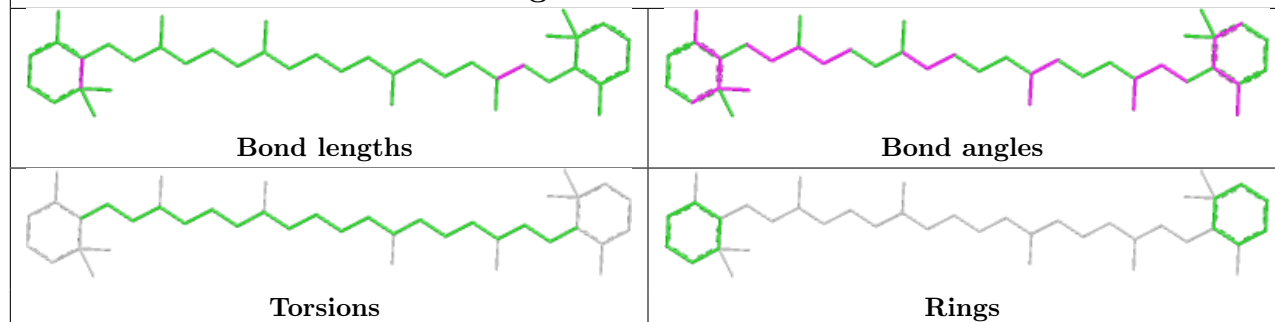


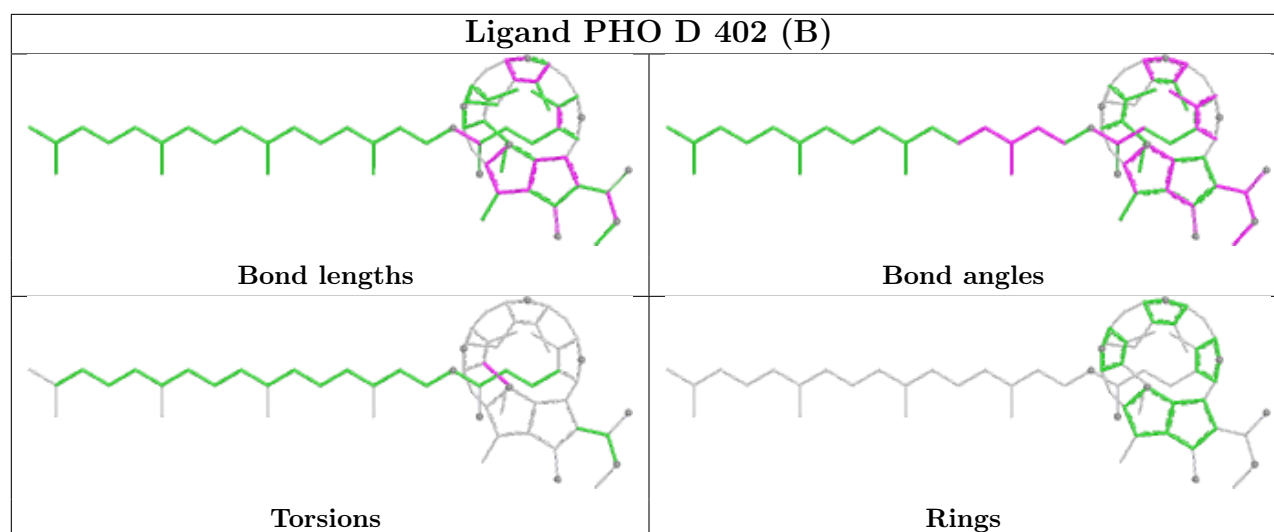
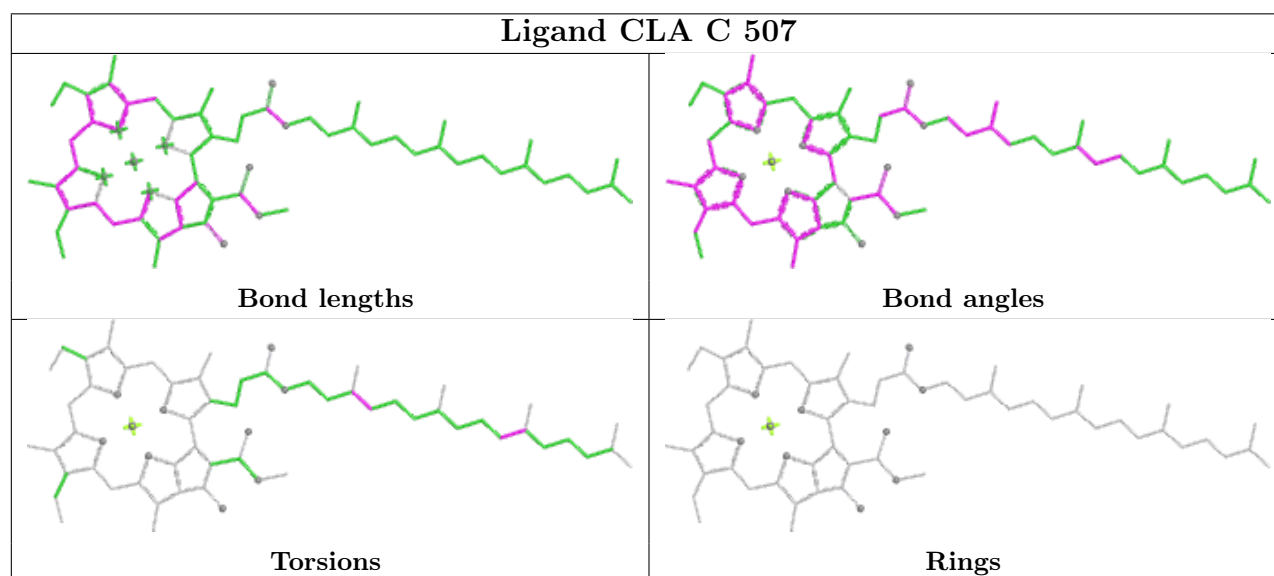
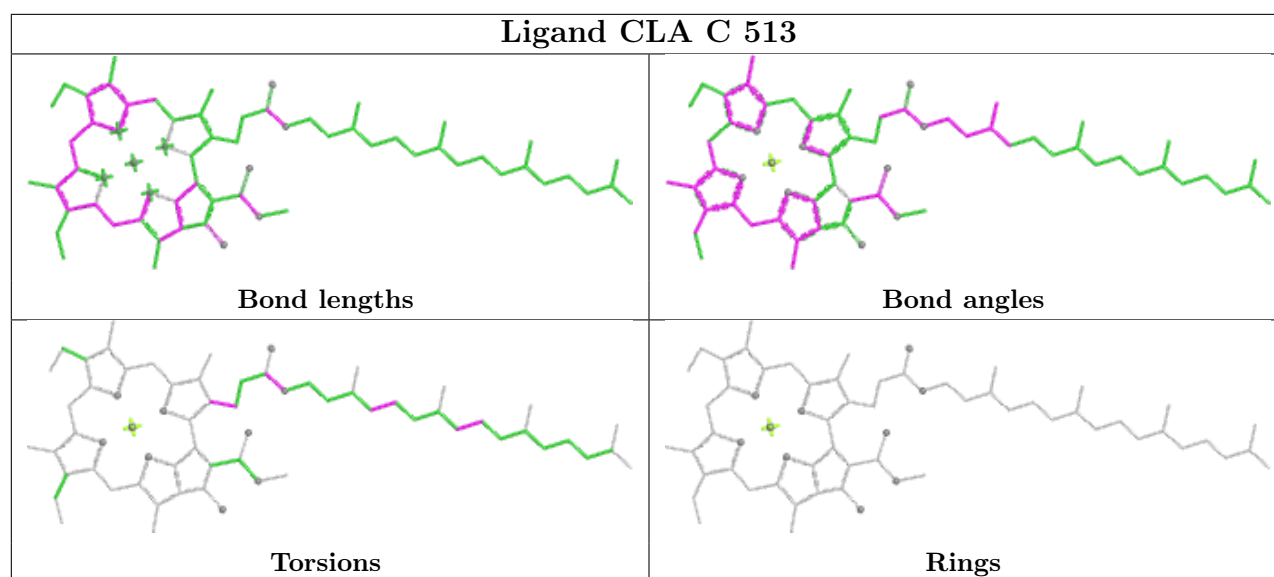
Ligand CLA c 513**Ligand CLA a 406 (B)**

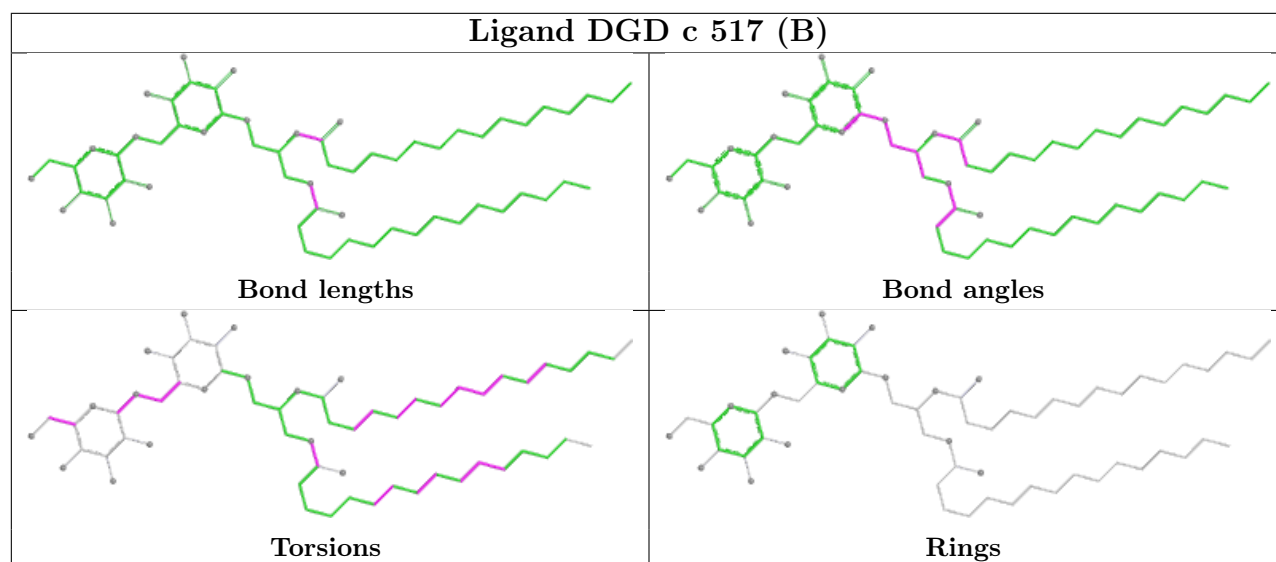
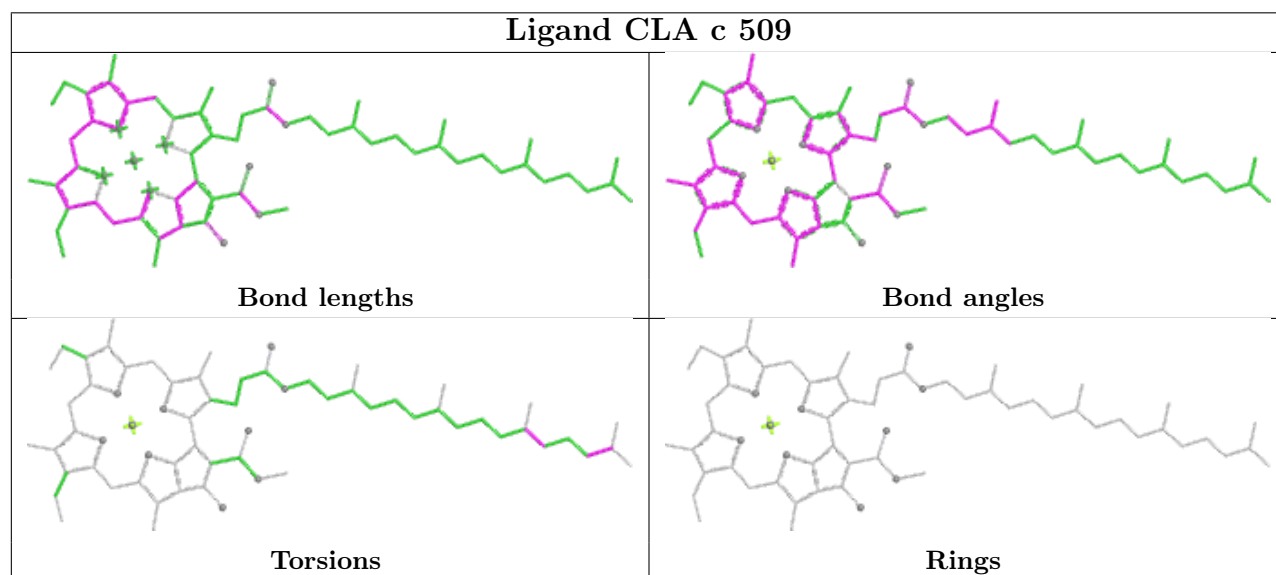
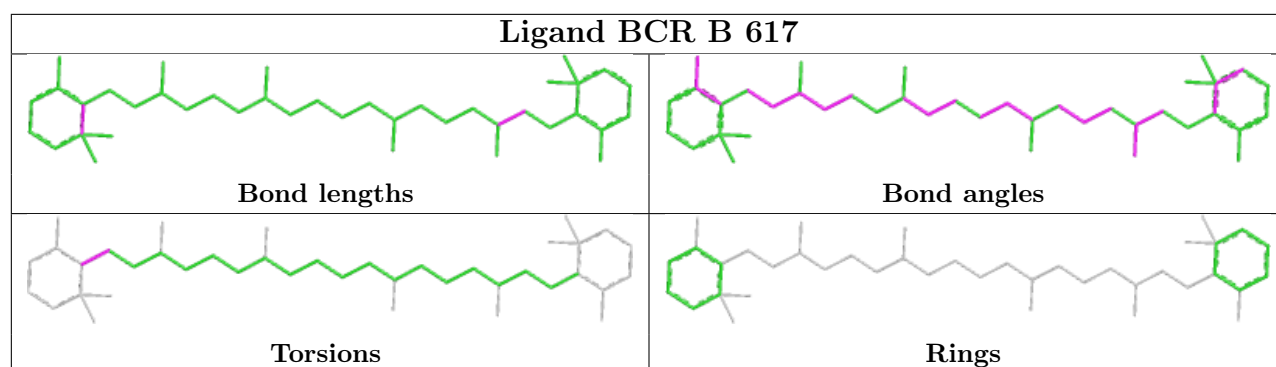
Ligand LHG D 409 (A)

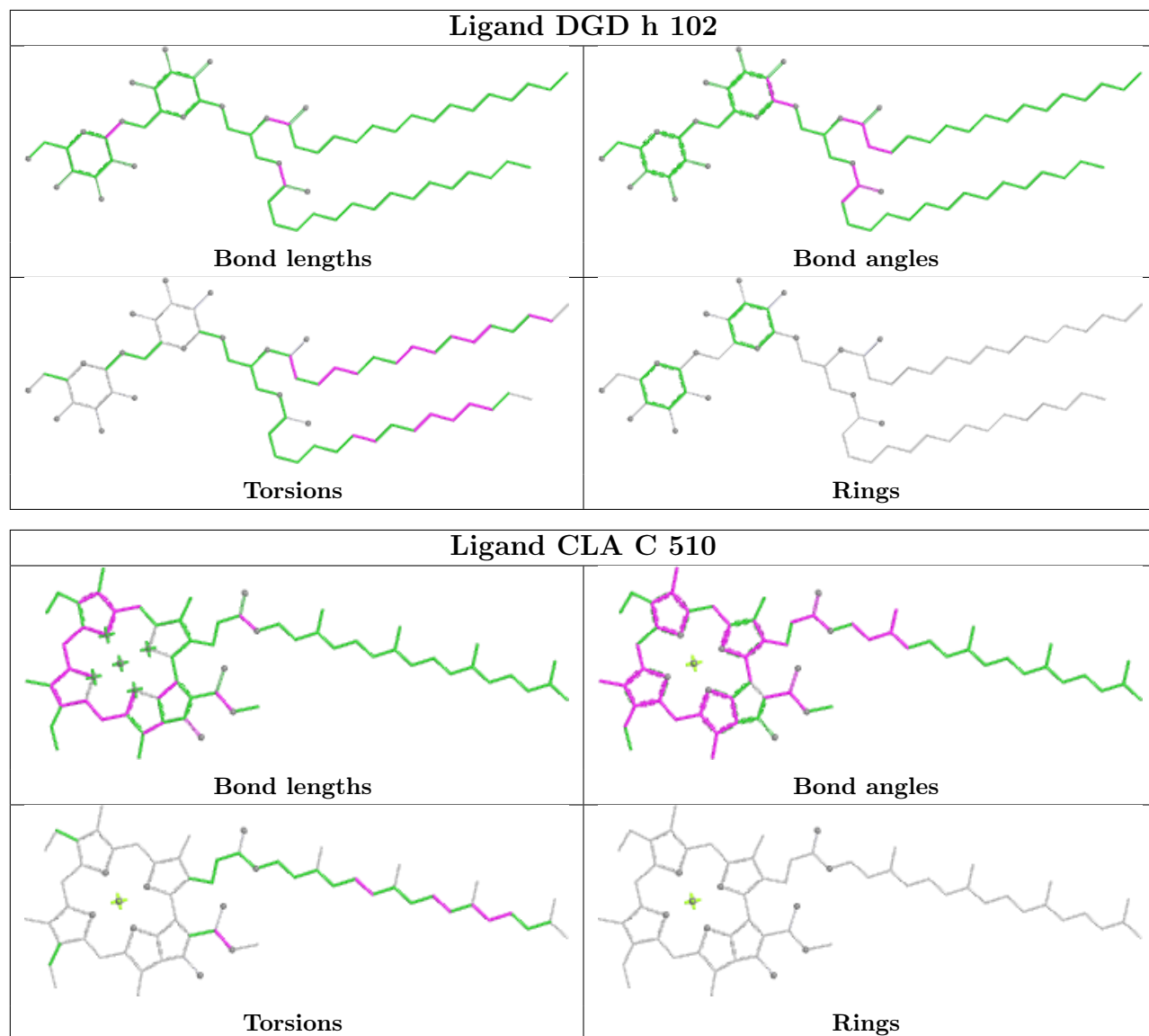


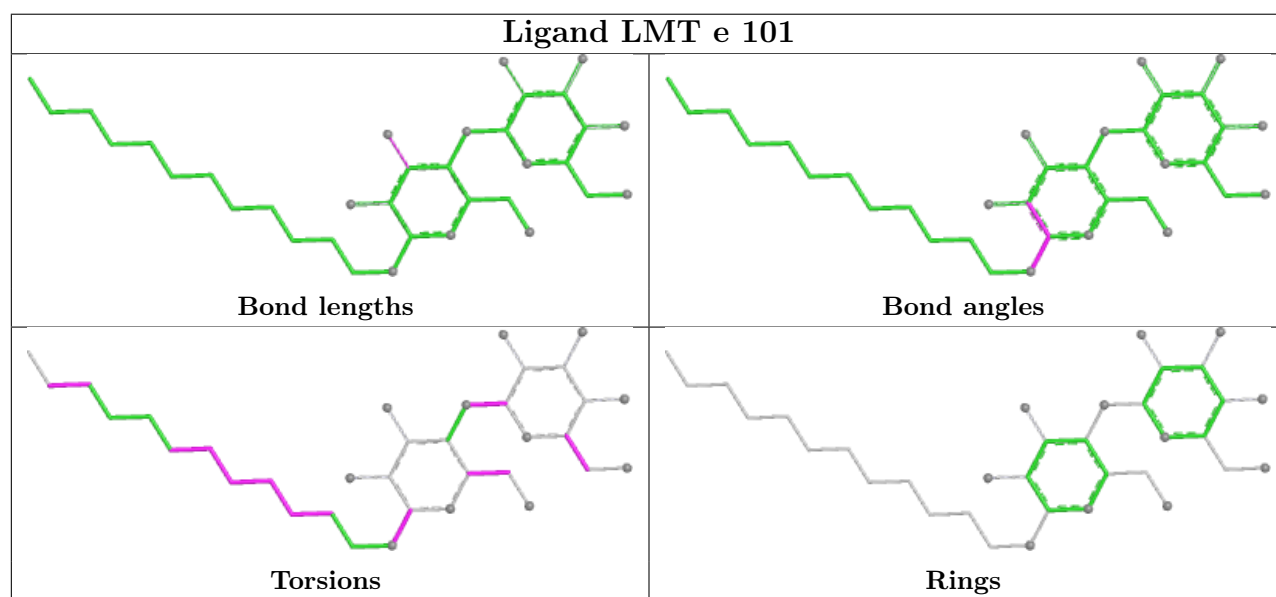
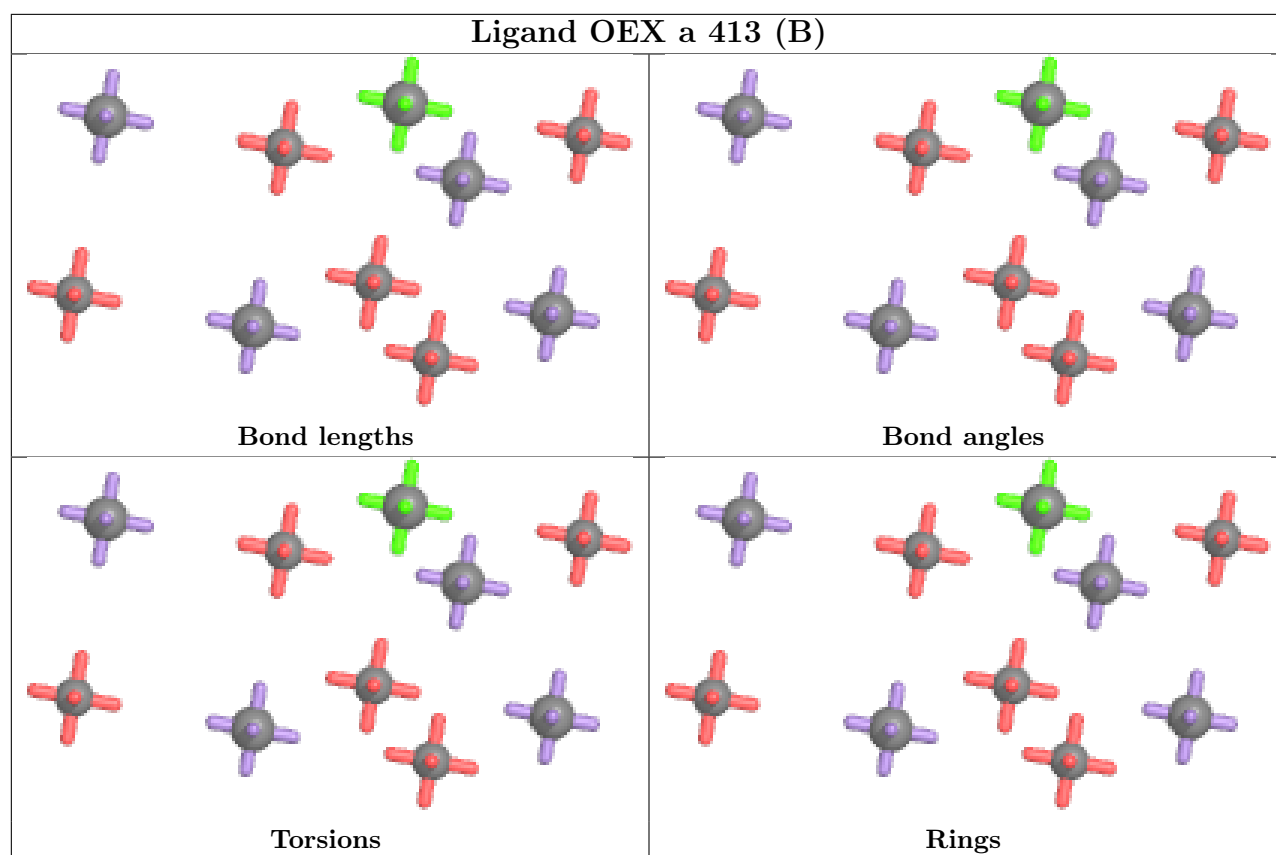
Ligand BCR C 517

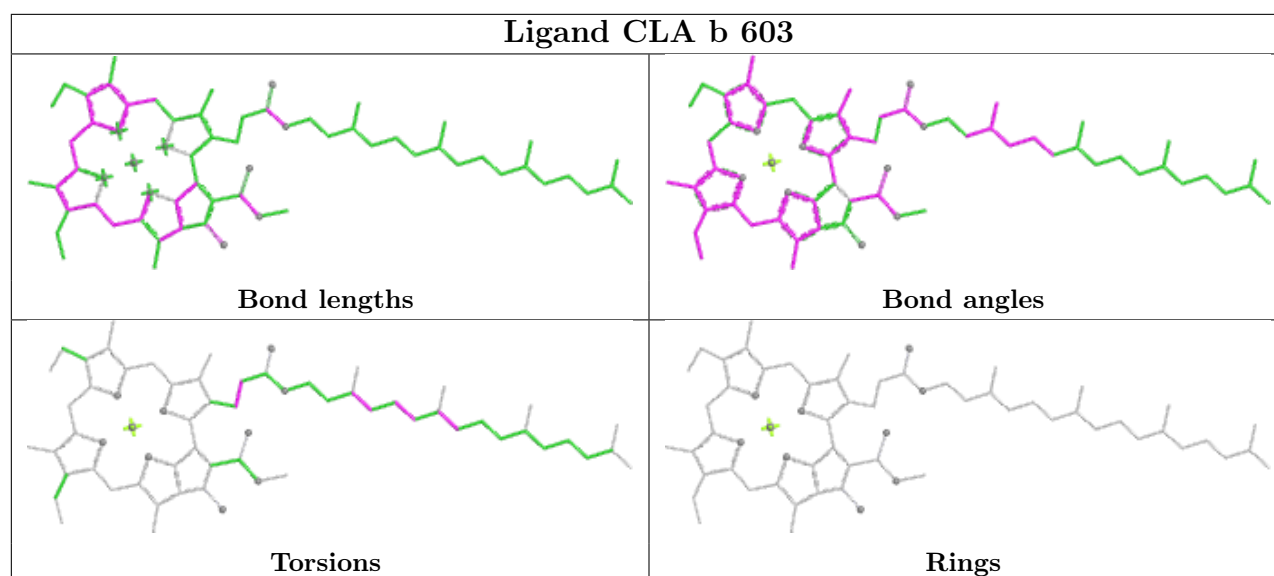
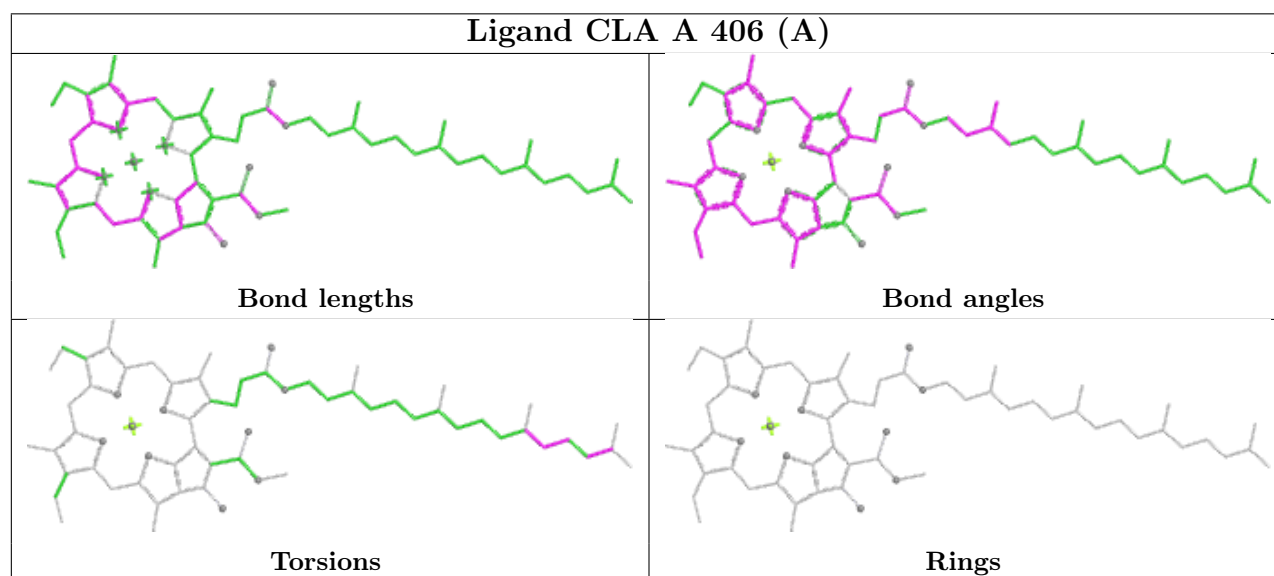
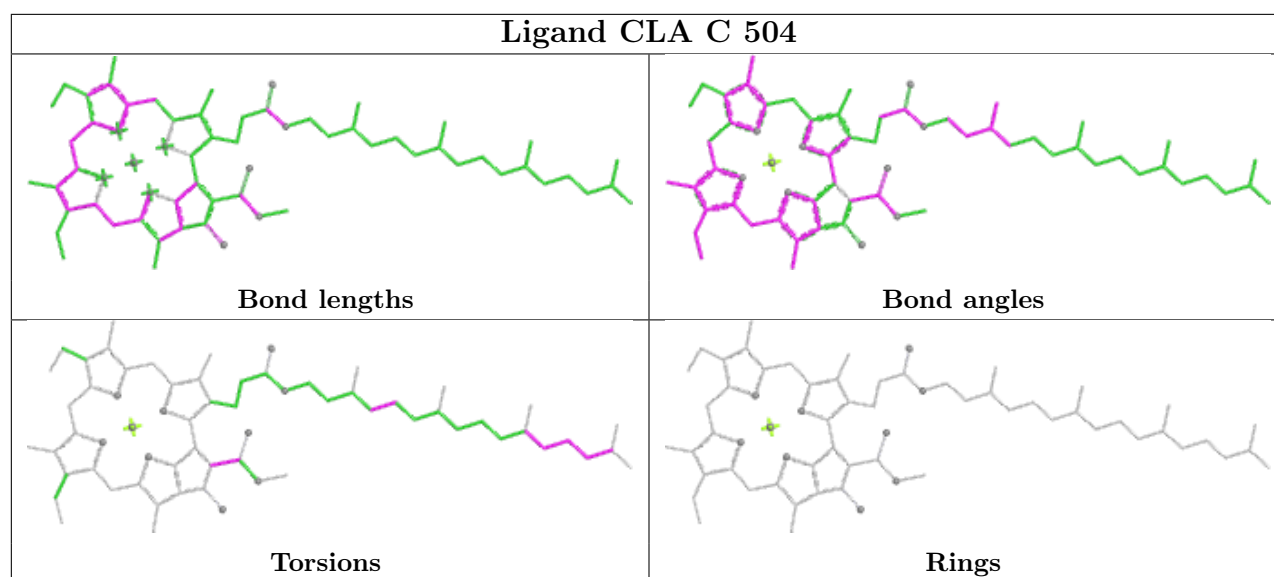


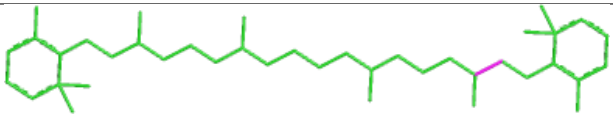
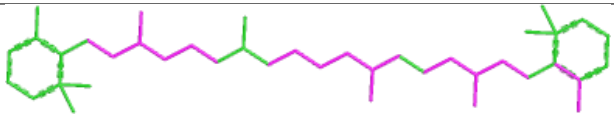
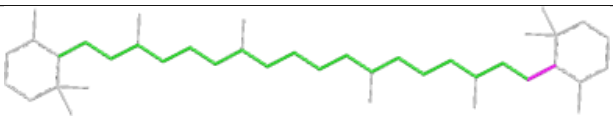
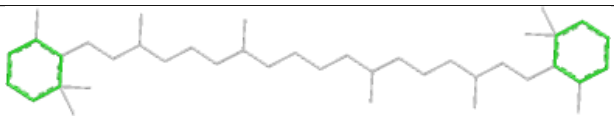
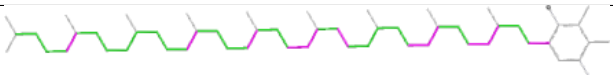
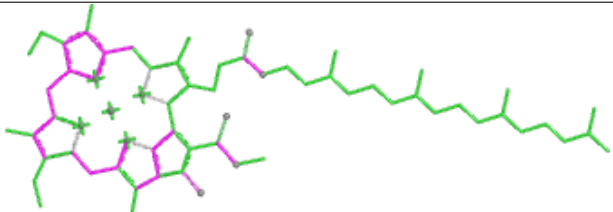
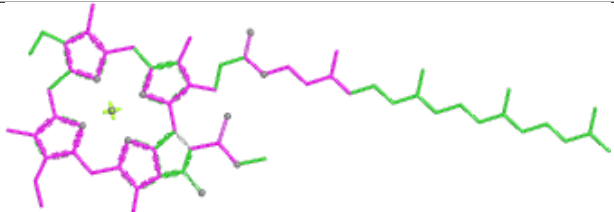
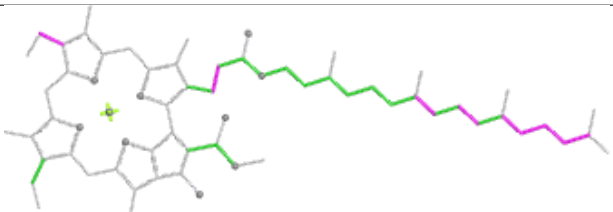
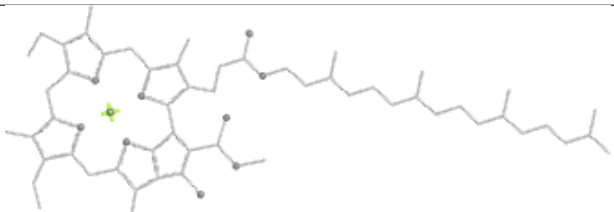


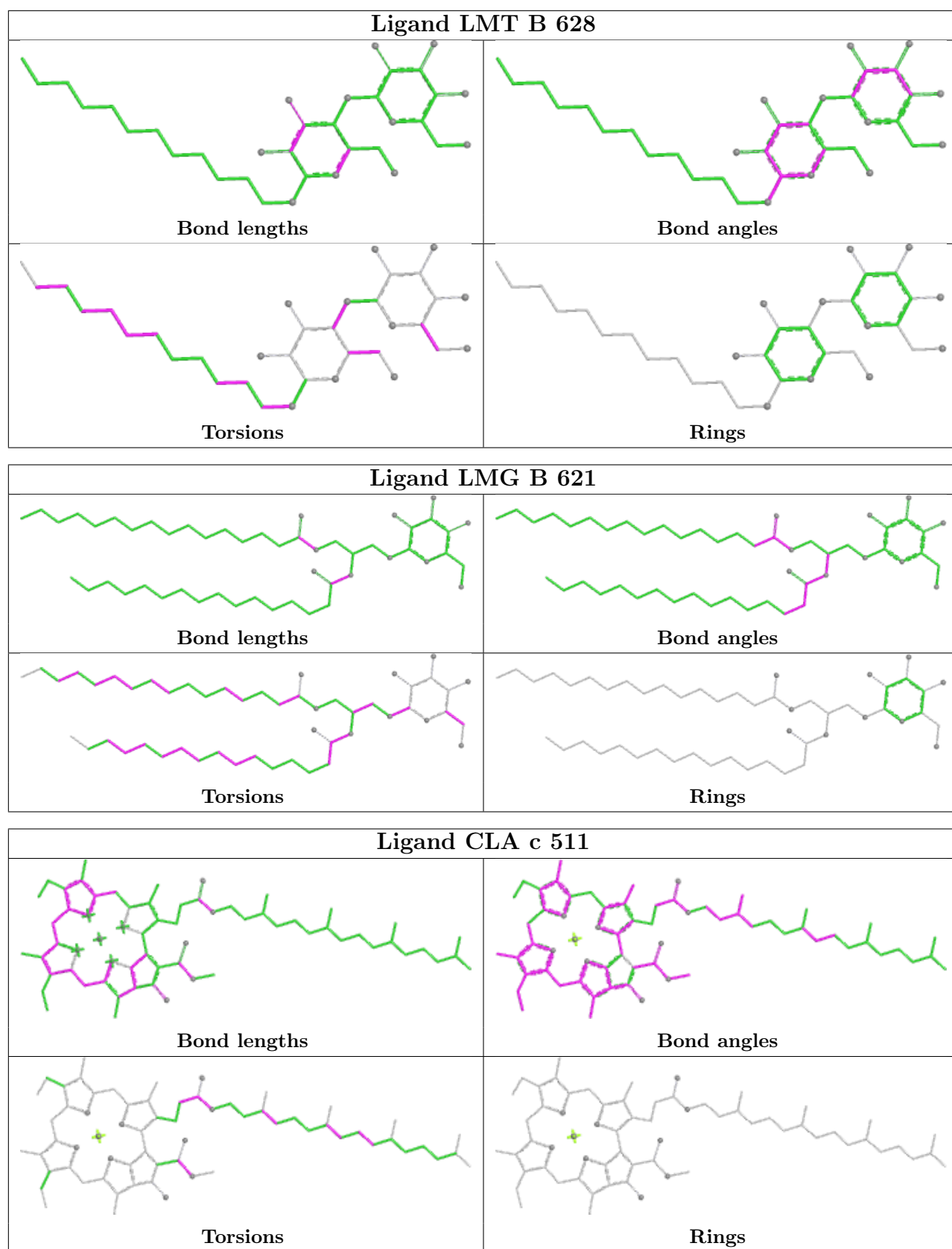


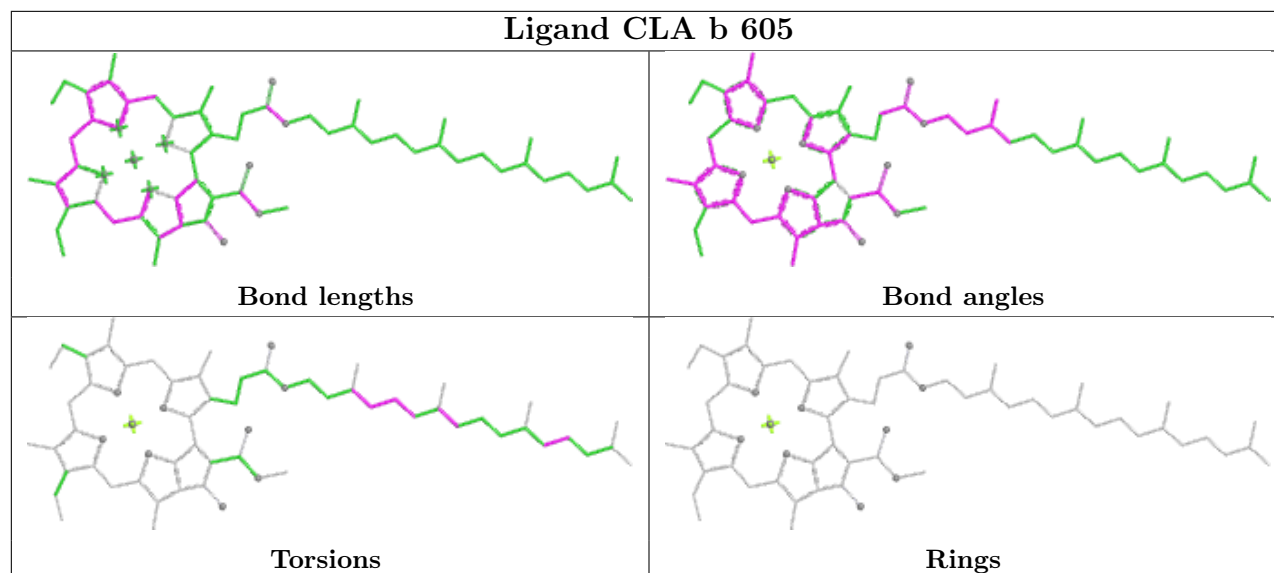
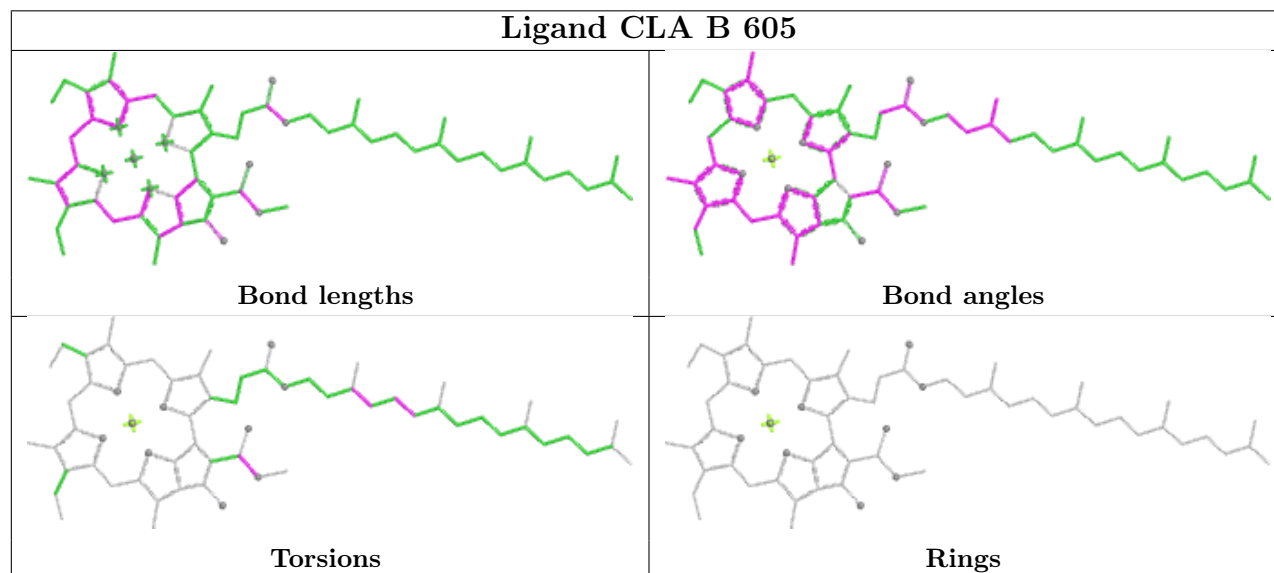
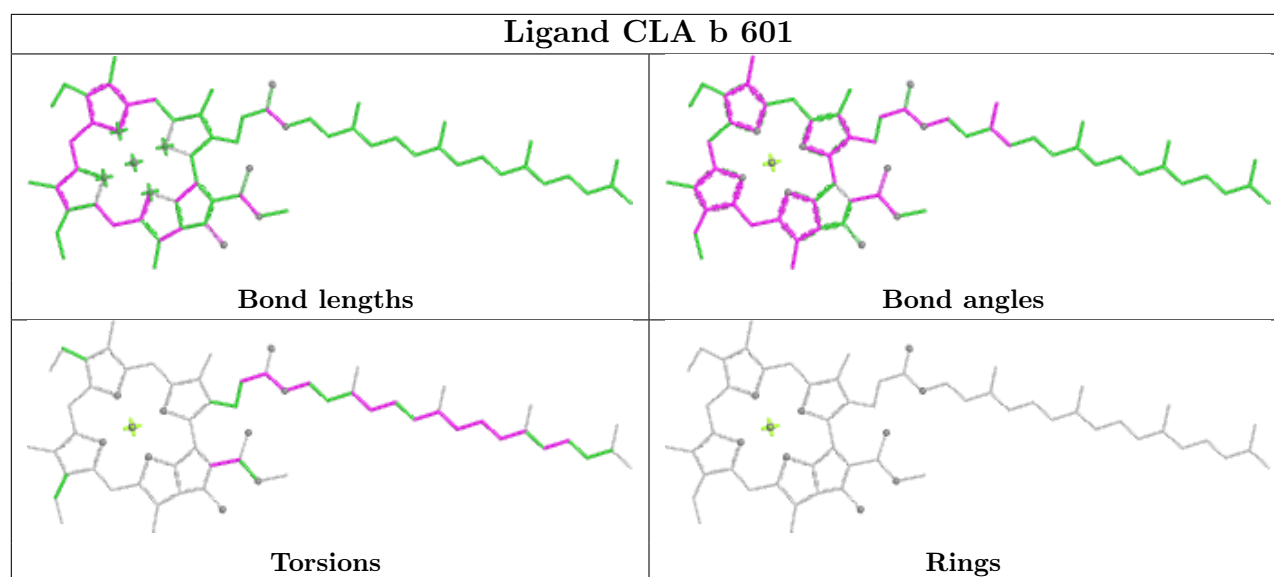


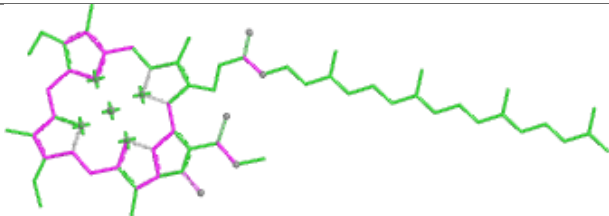
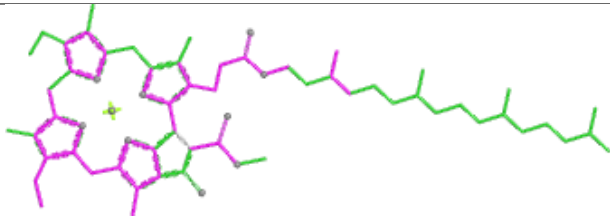
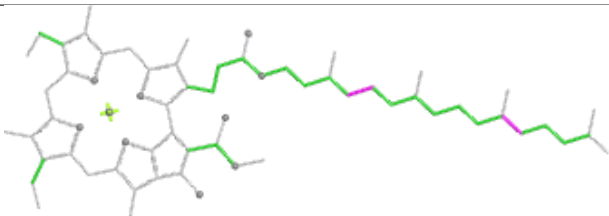
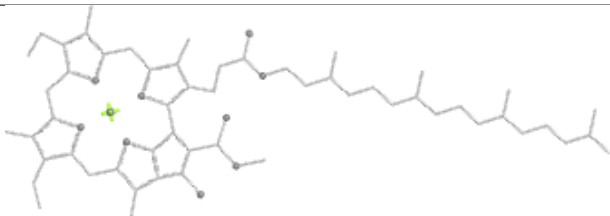


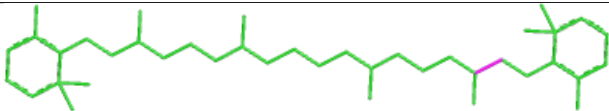
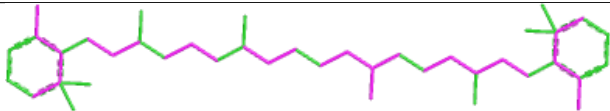
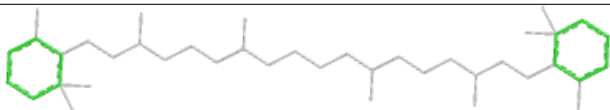


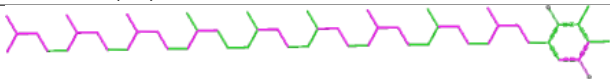
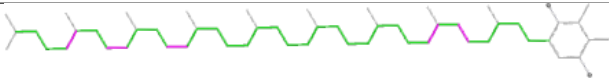
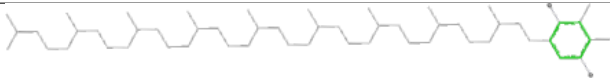
Ligand BCR h 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 a 414 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA b 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

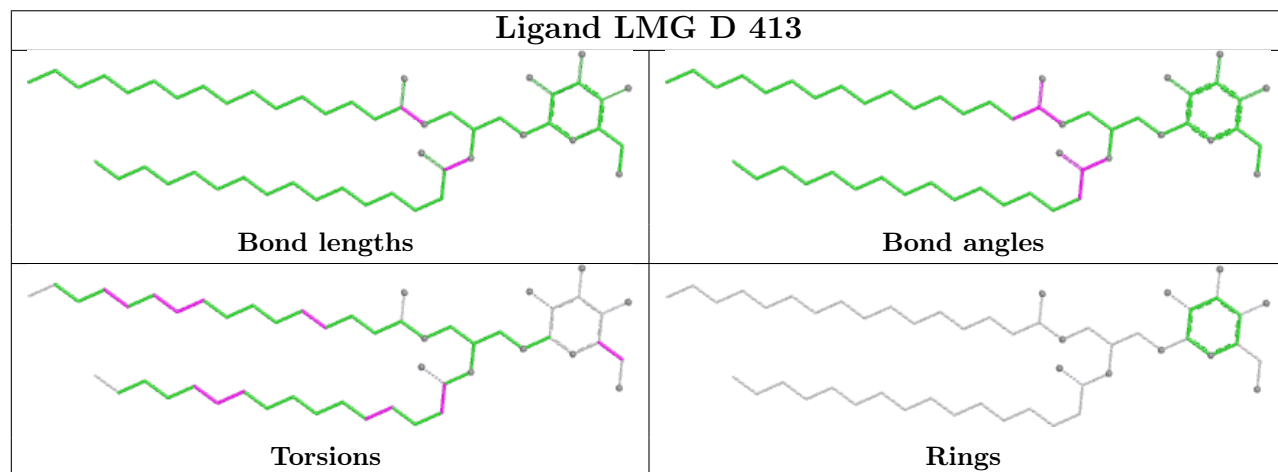
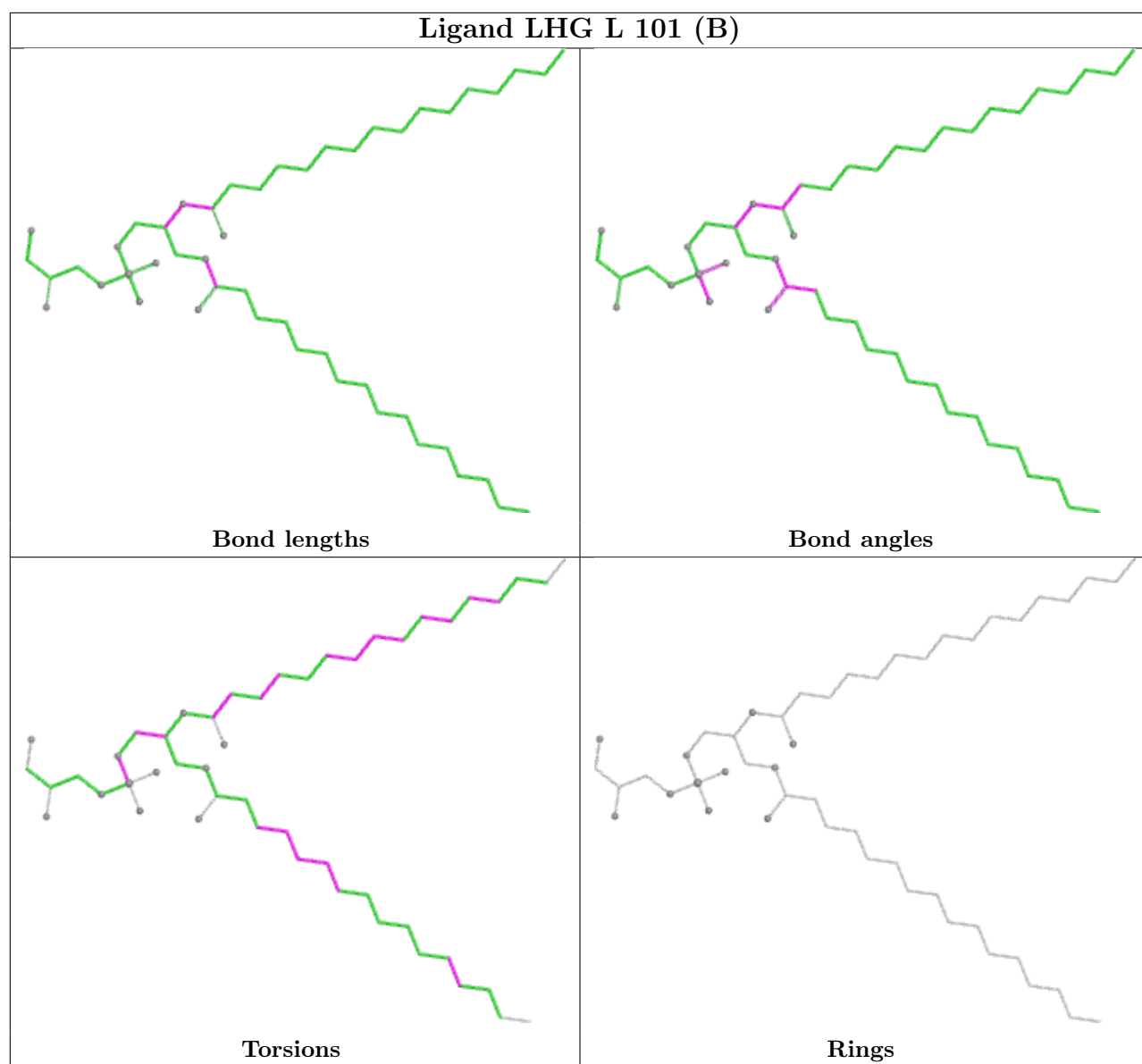


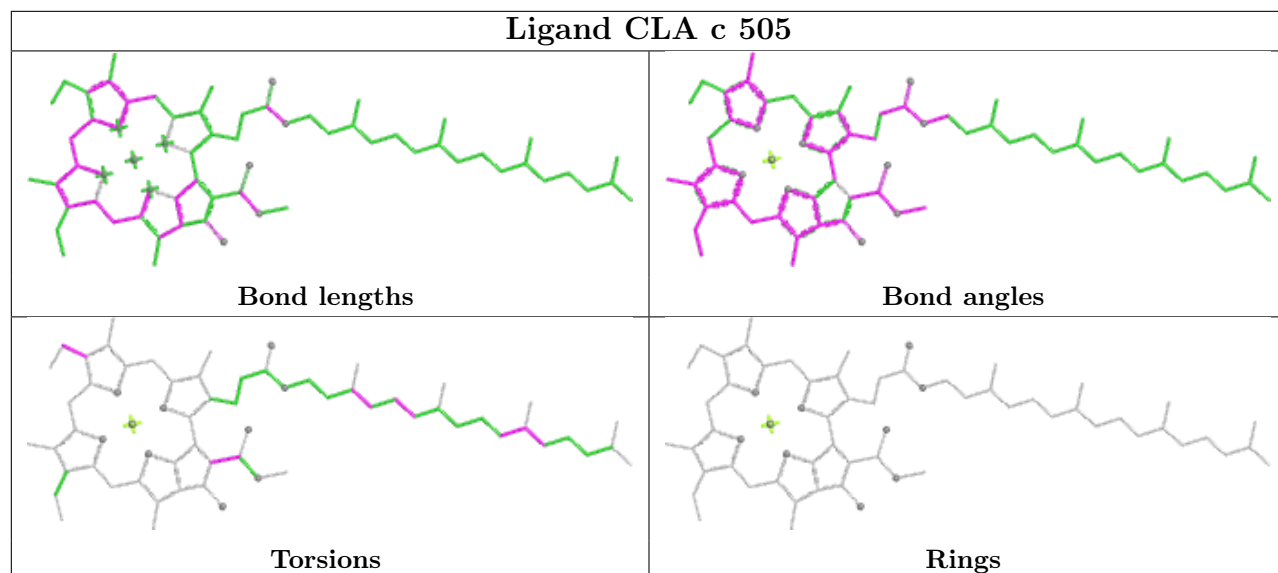
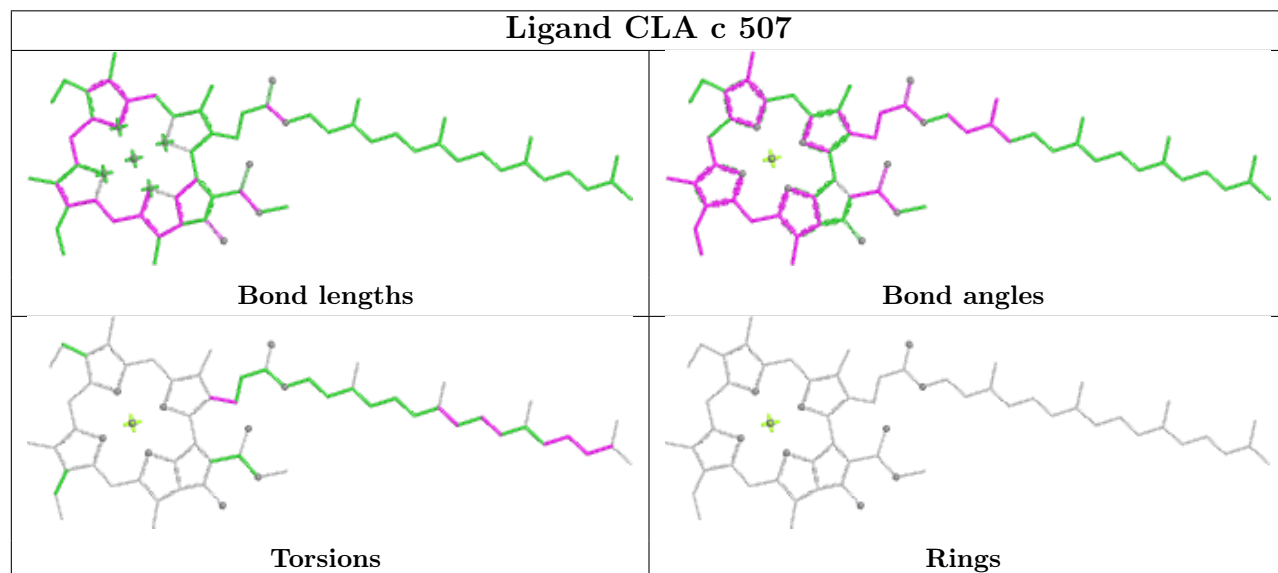
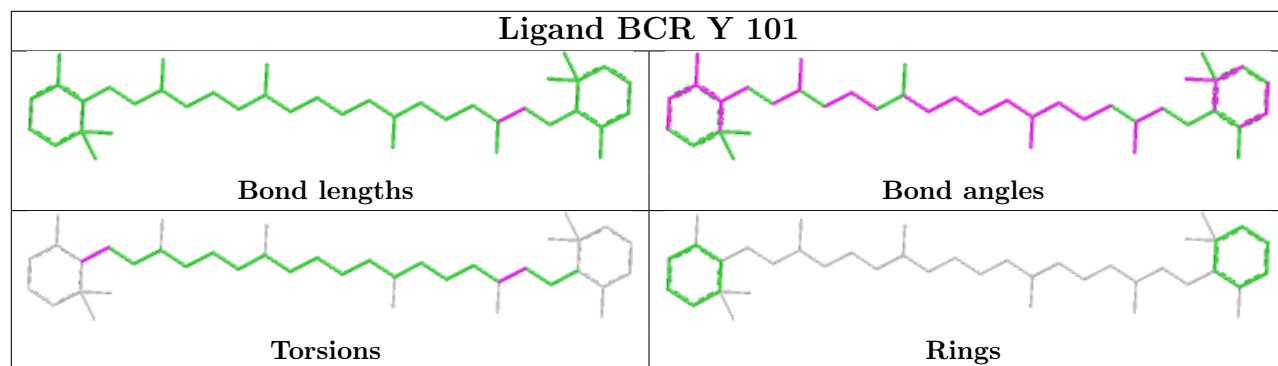


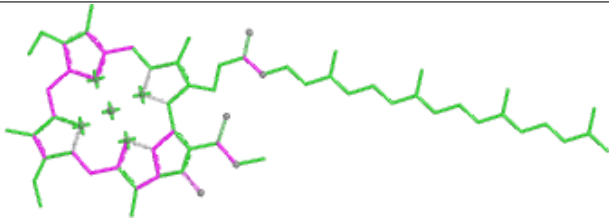
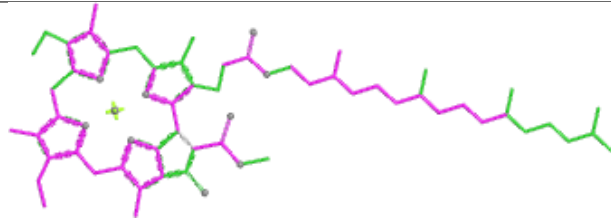
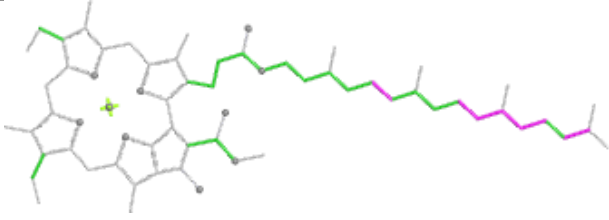
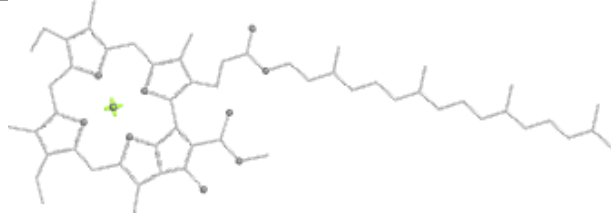
Ligand CLA b 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

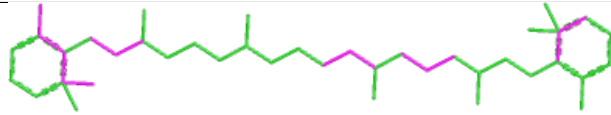
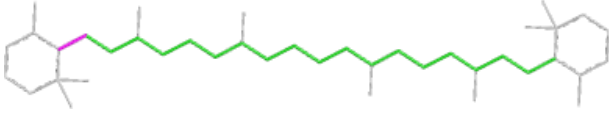
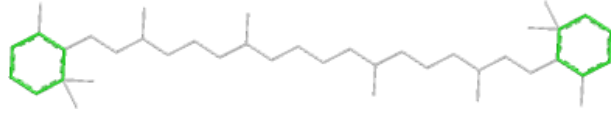
Ligand BCR K 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

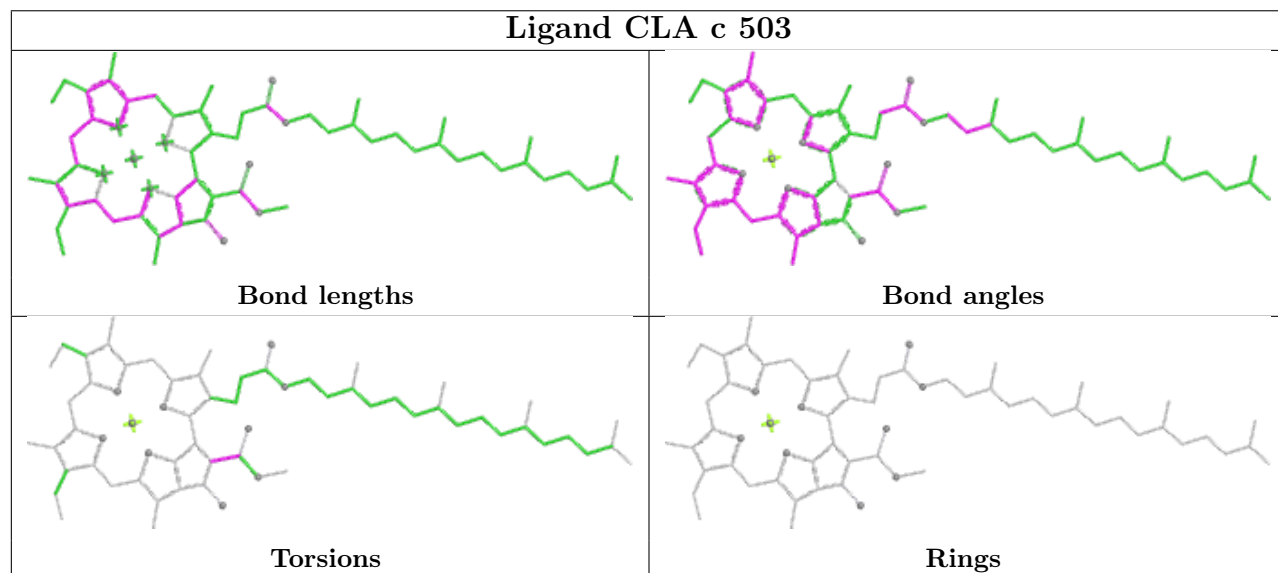
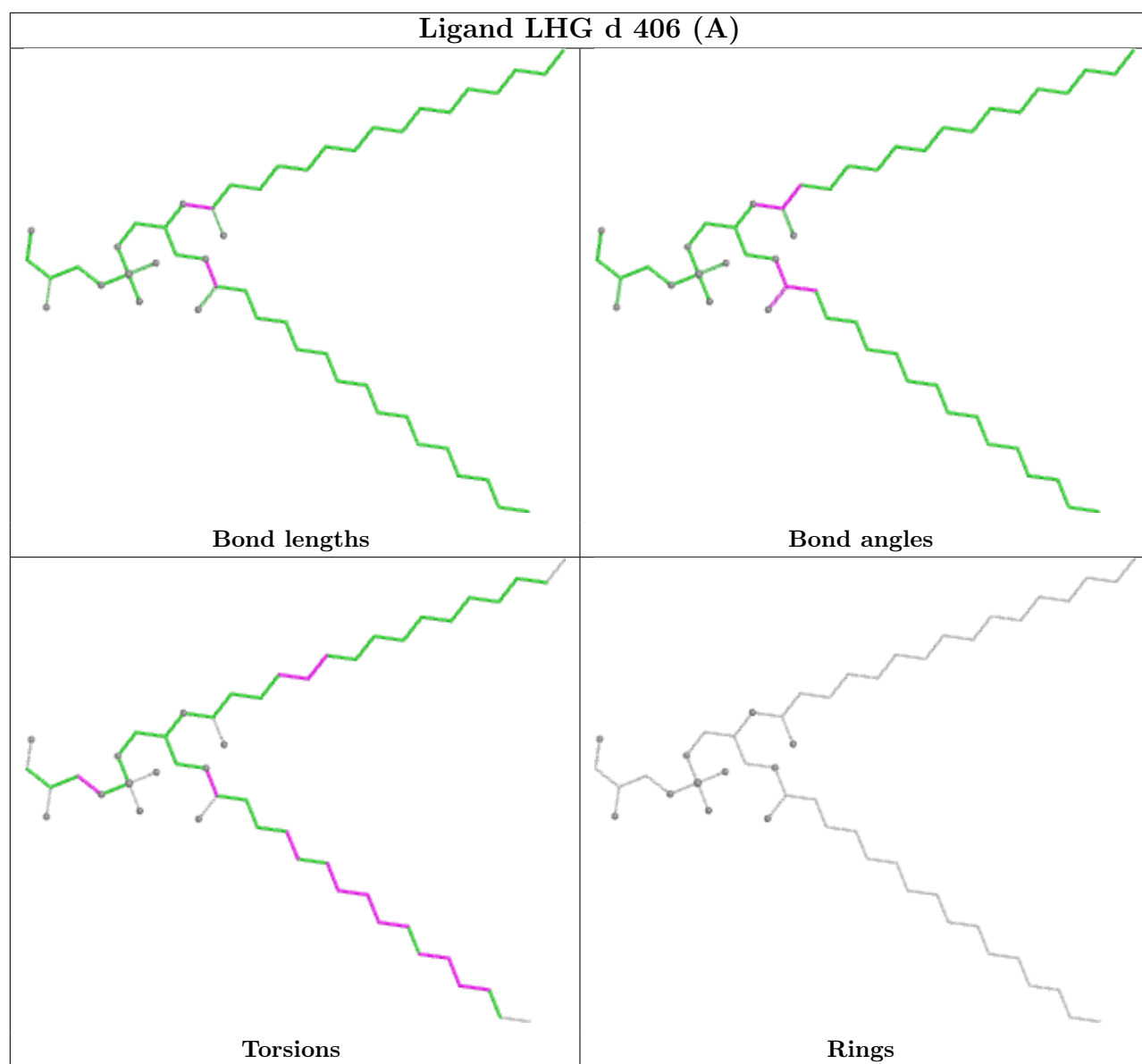
Ligand PL9 d 404 (A)	
	
Bond lengths	Bond angles
	
Torsions	Rings

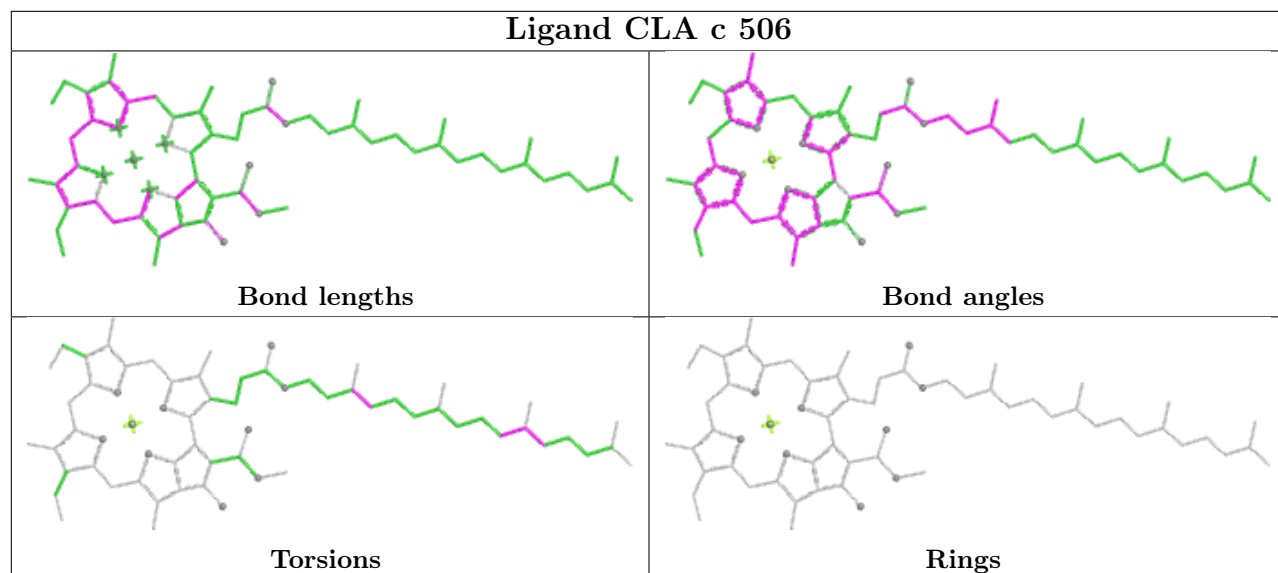
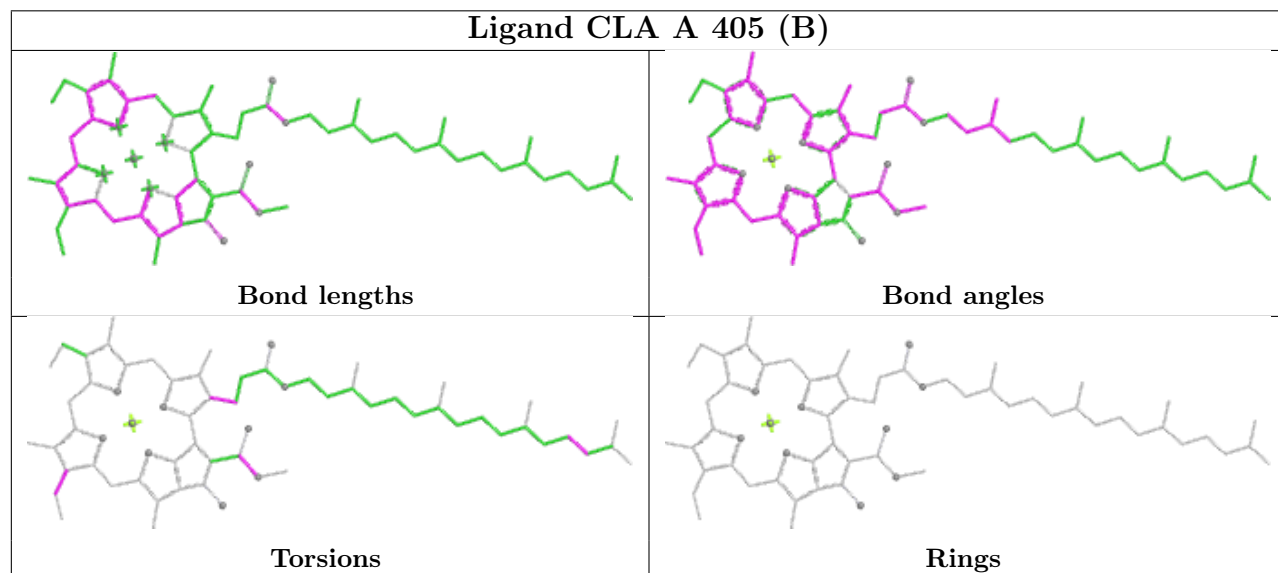
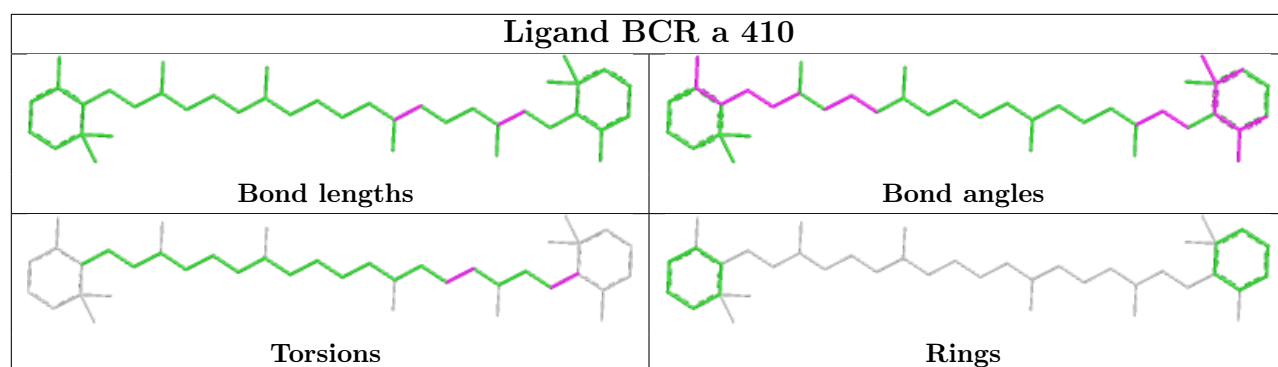


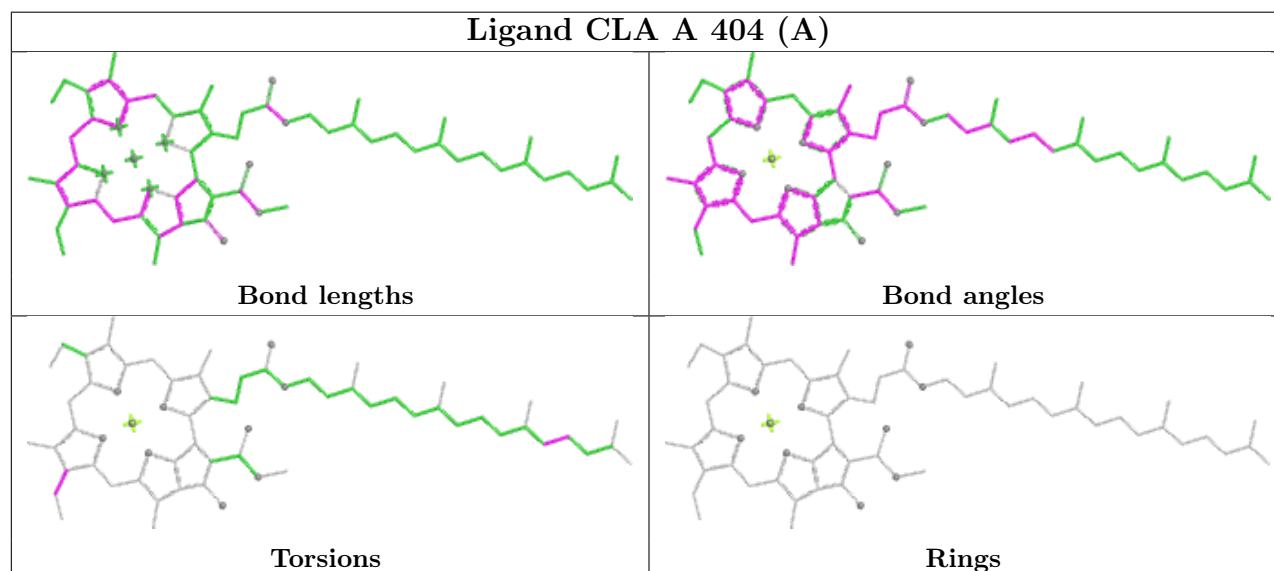
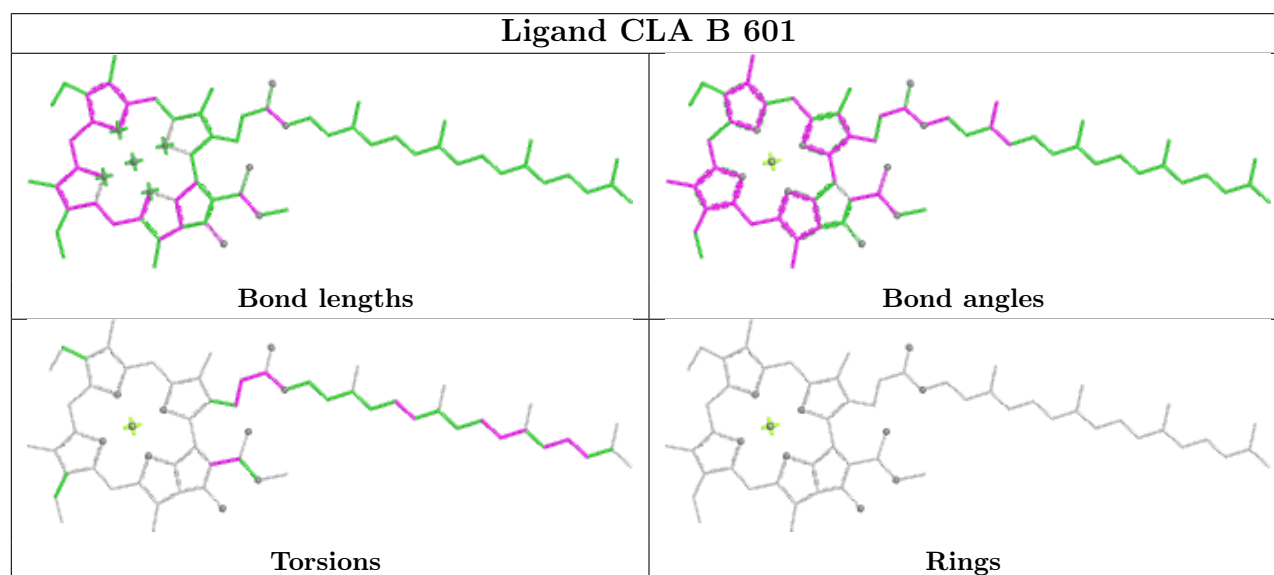
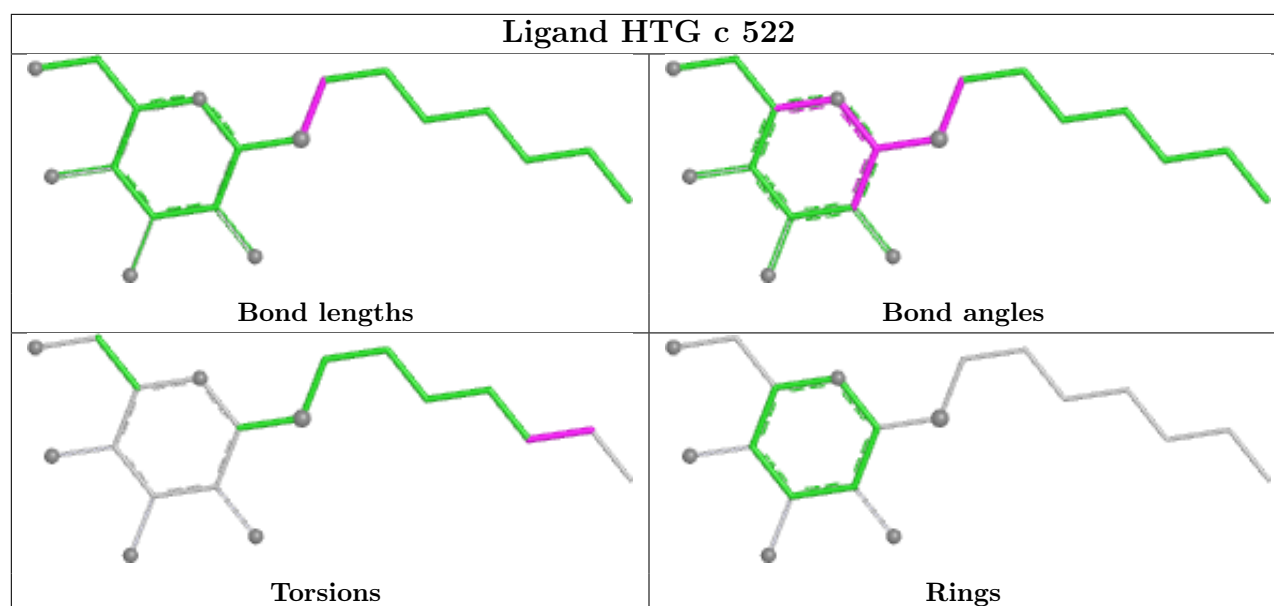


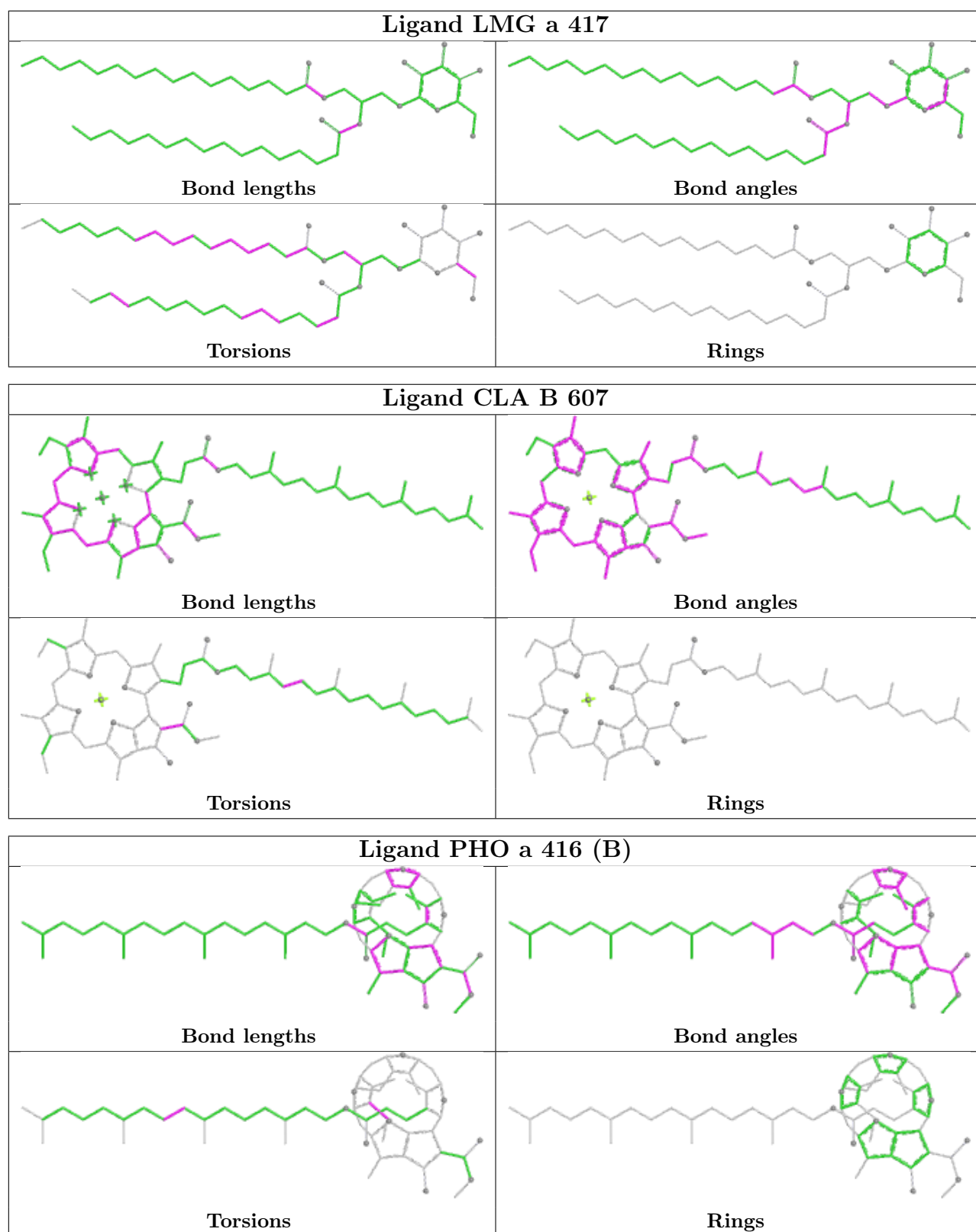
Ligand CLA b 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

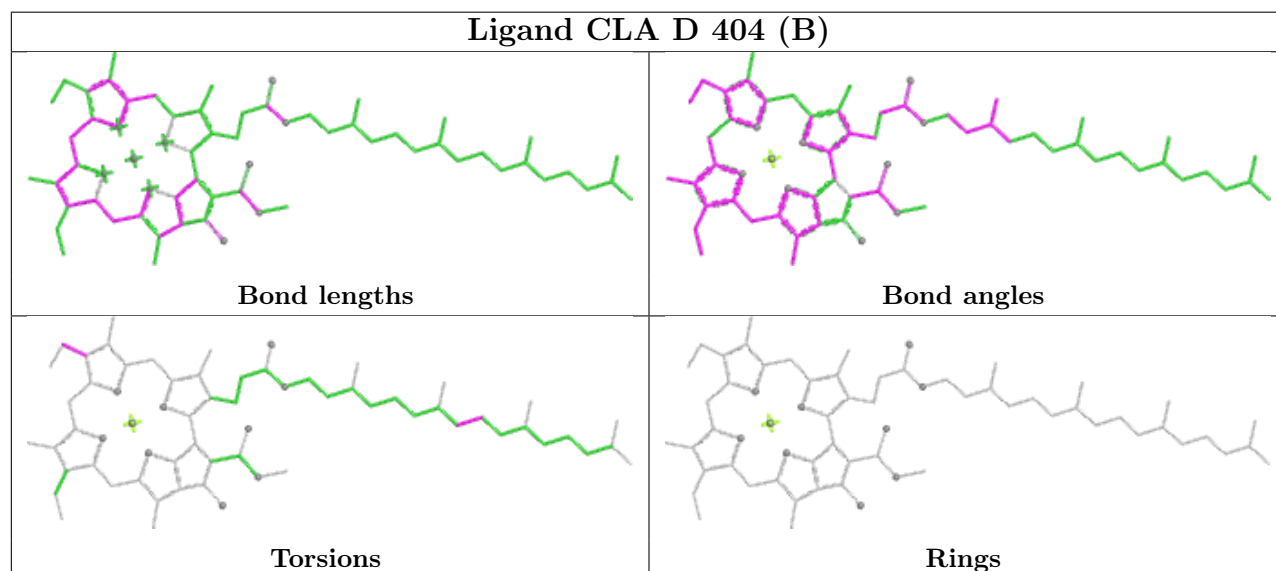
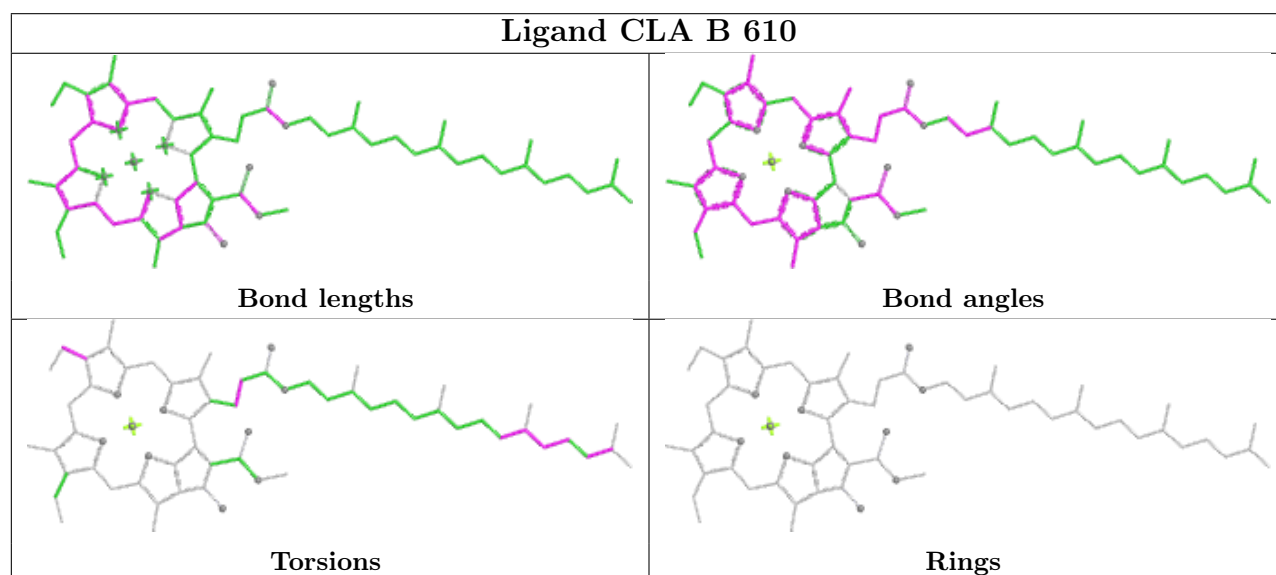
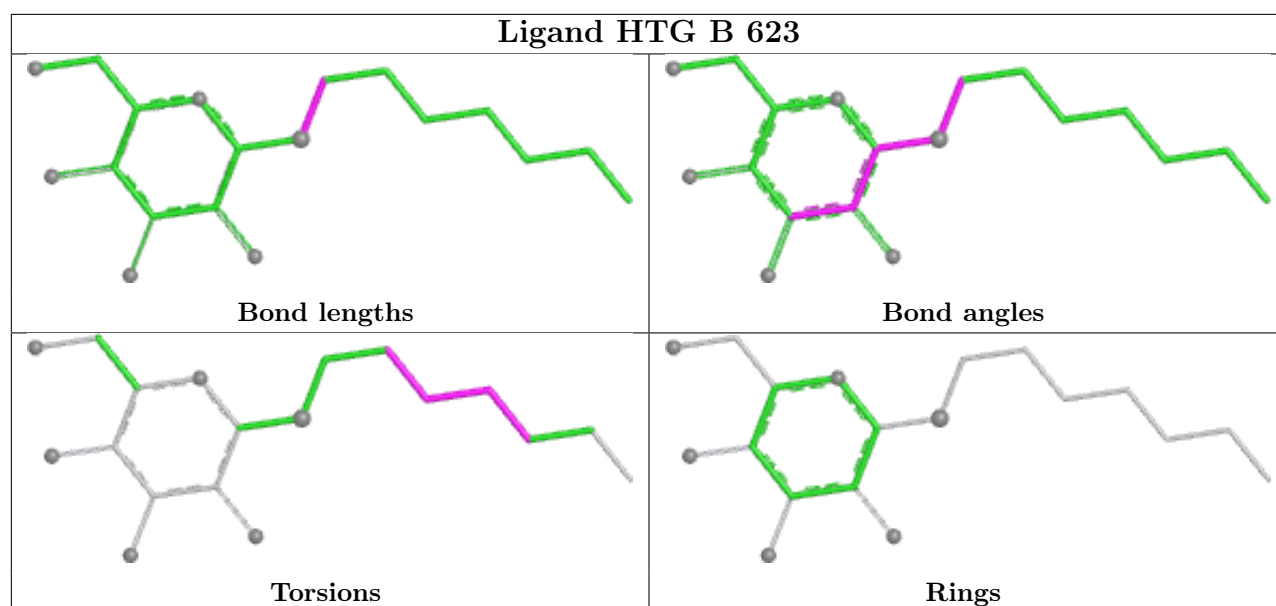
Ligand BCR b 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

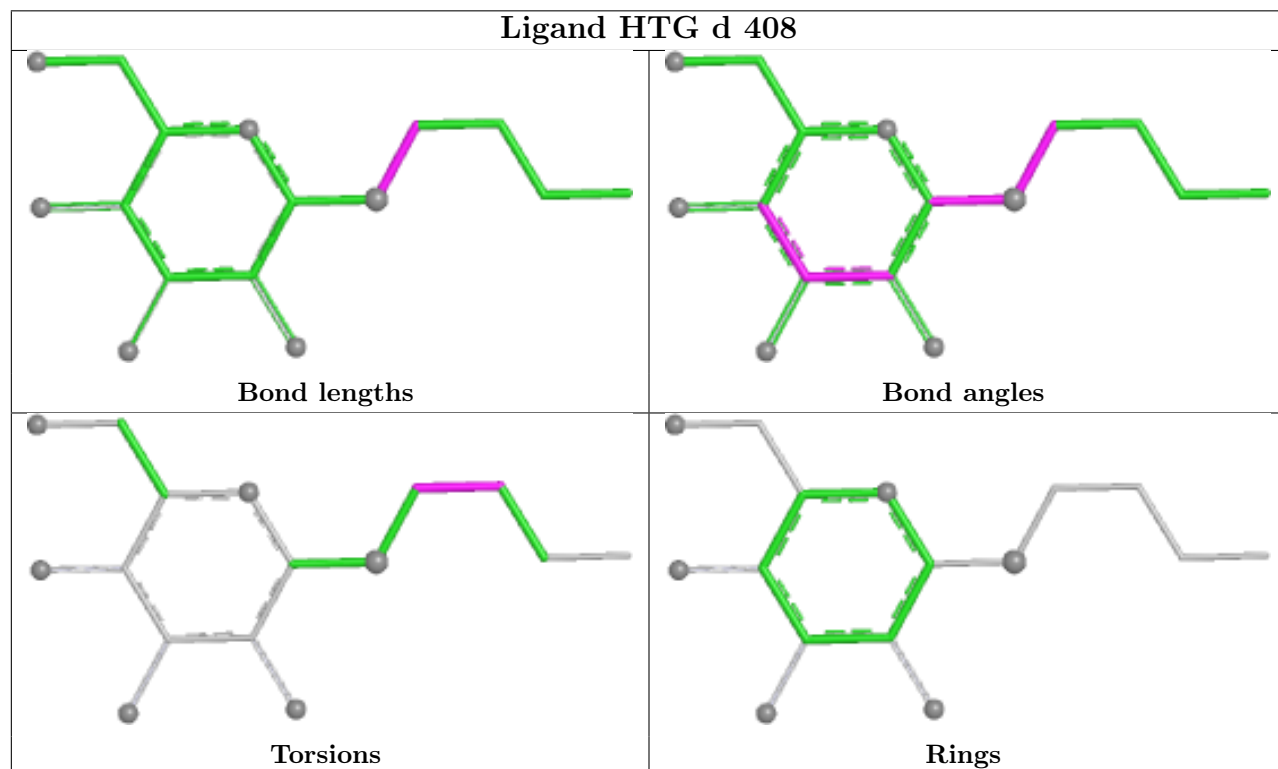
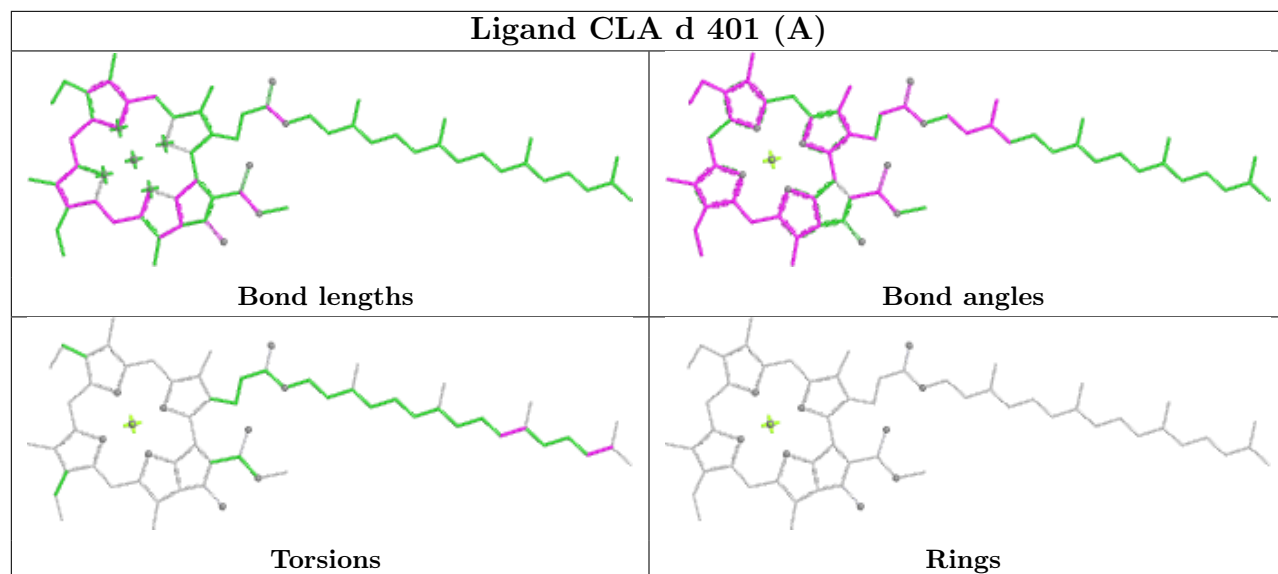


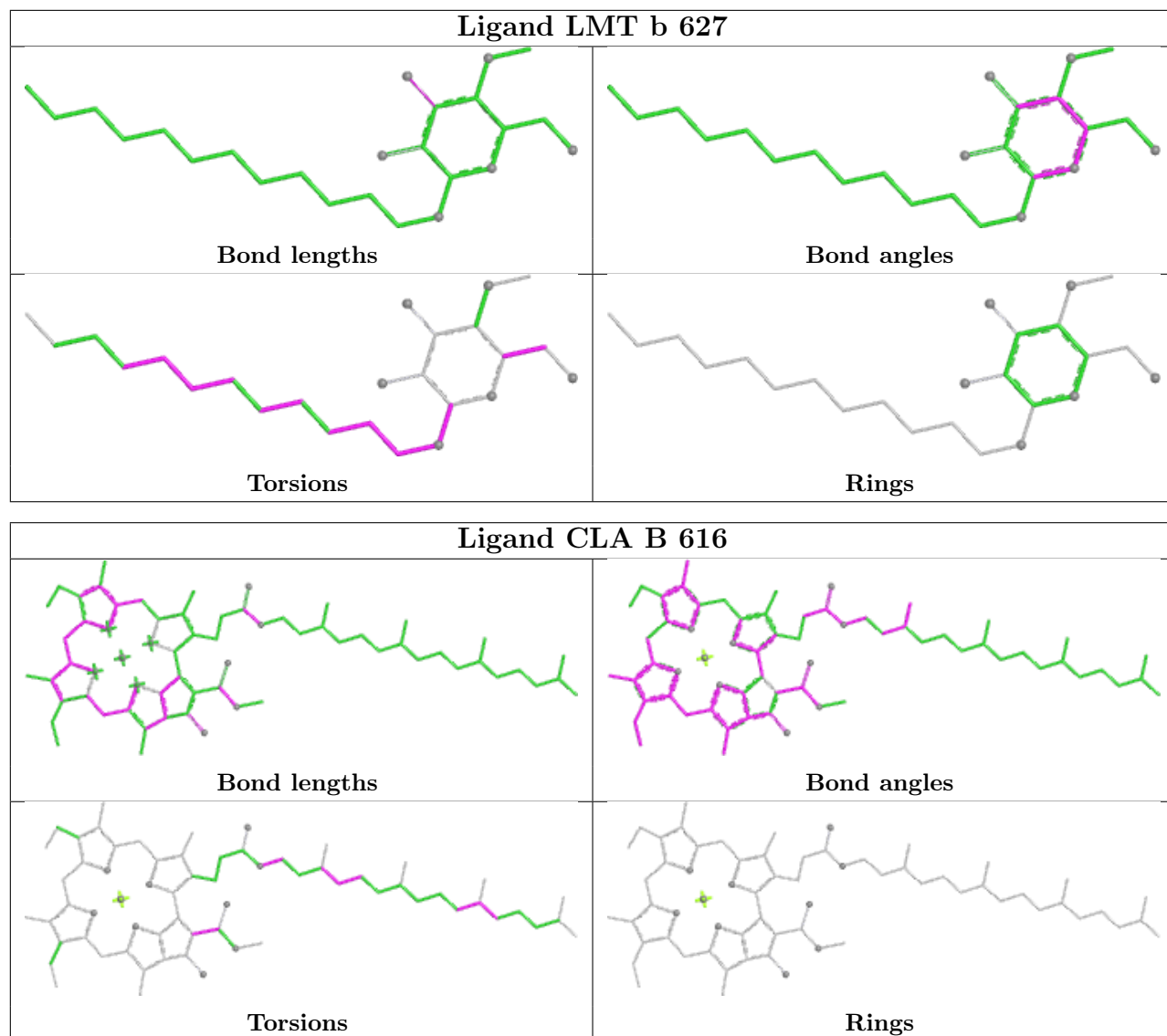


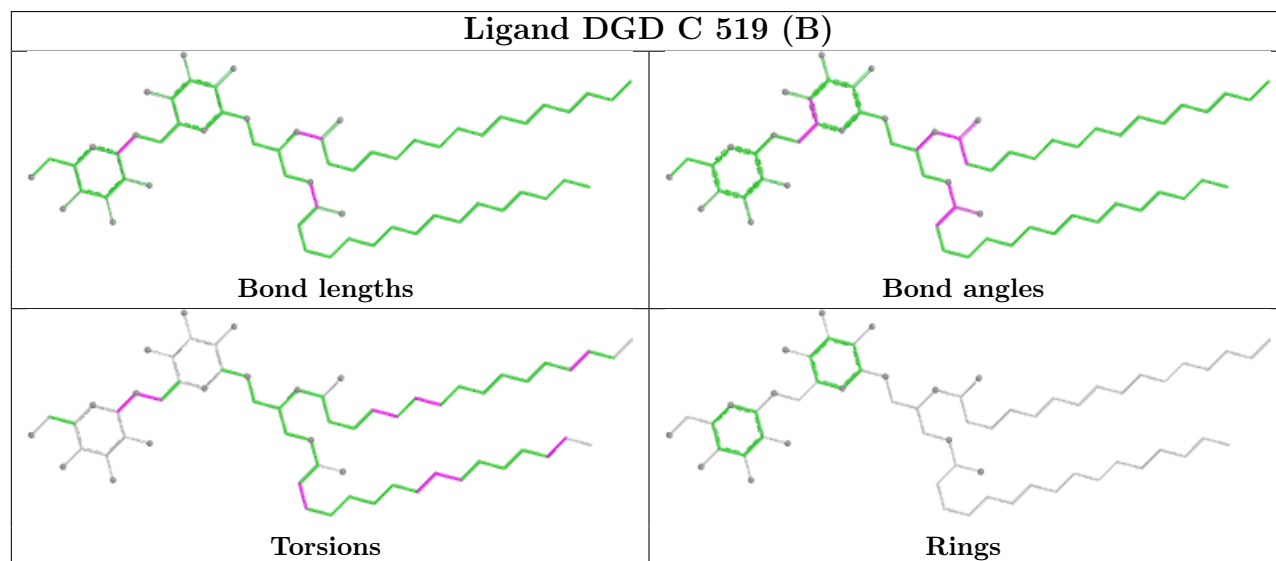
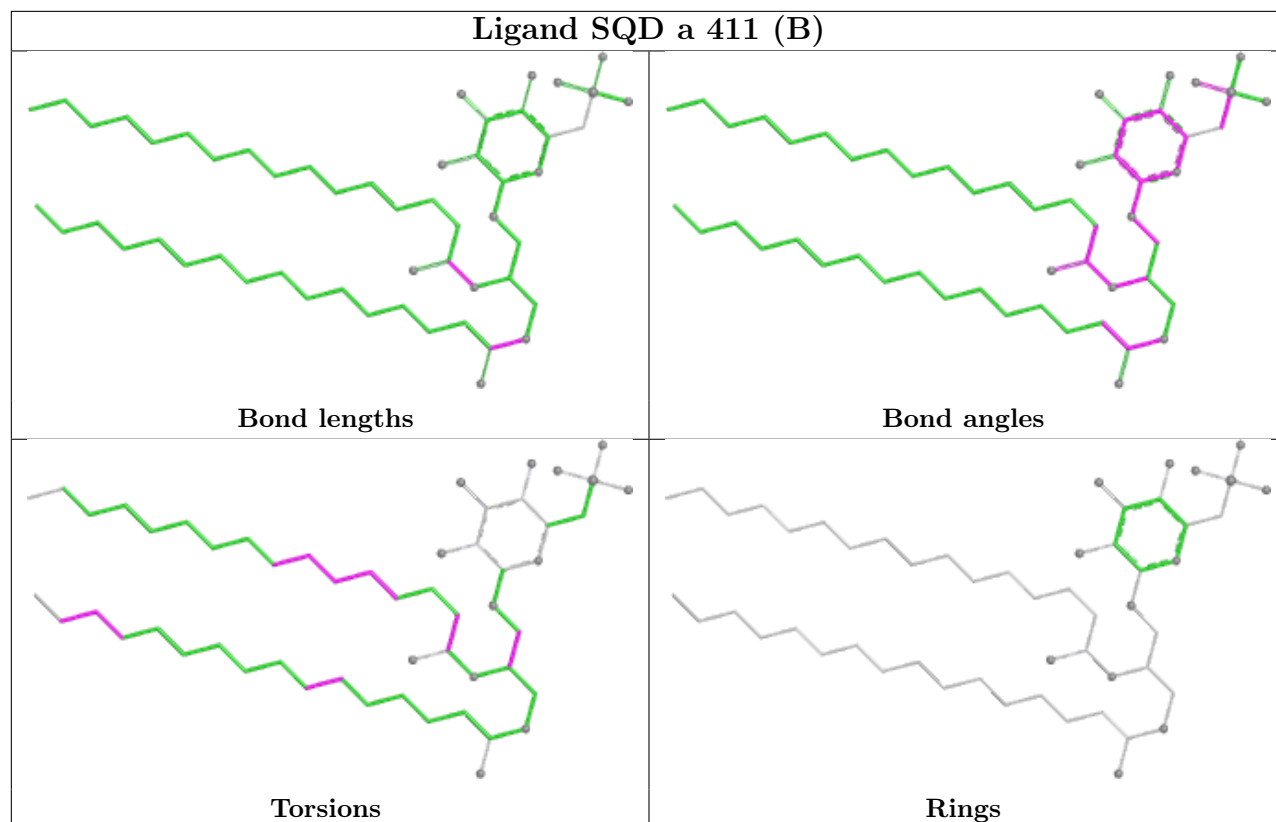


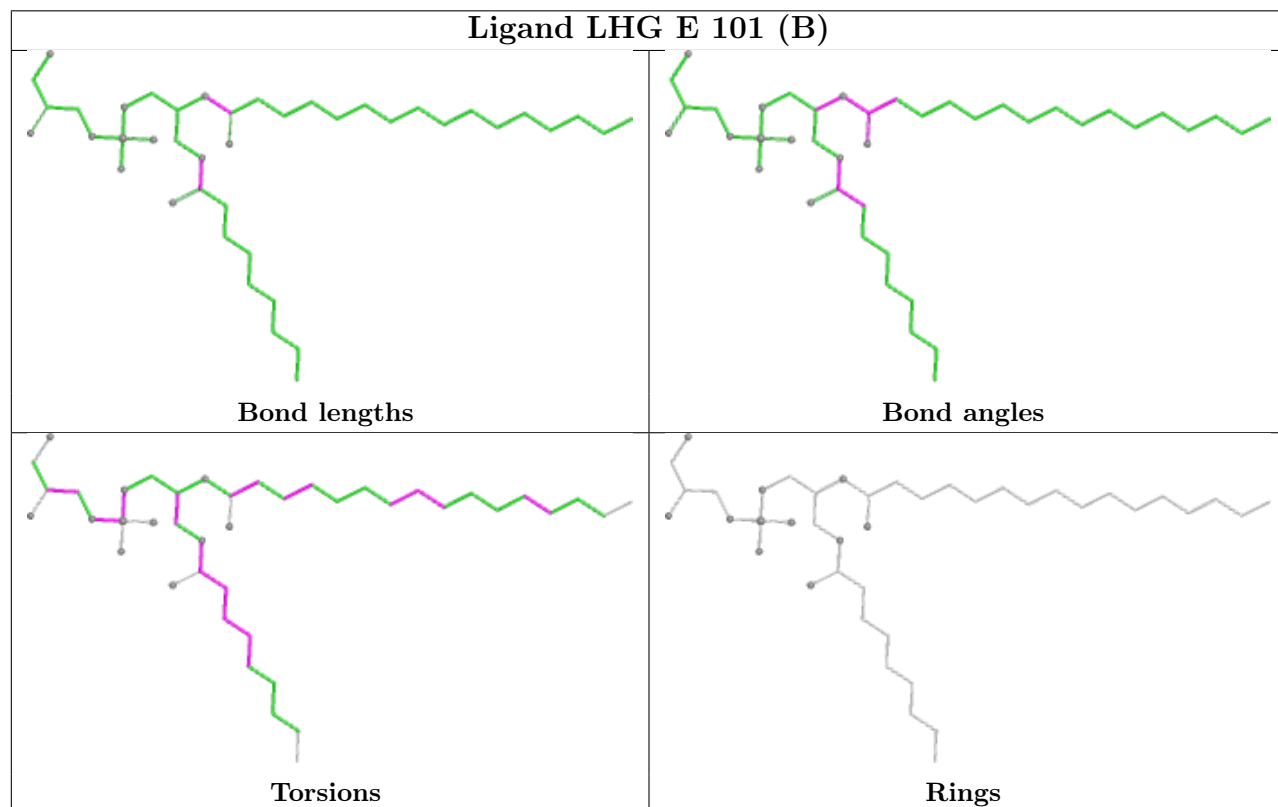
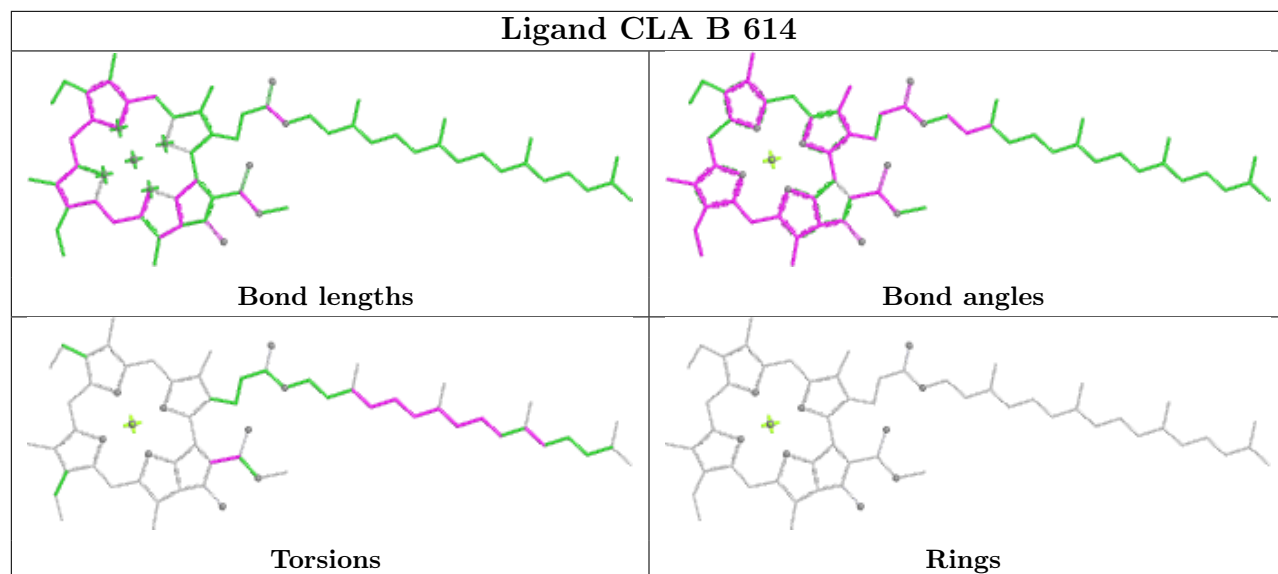


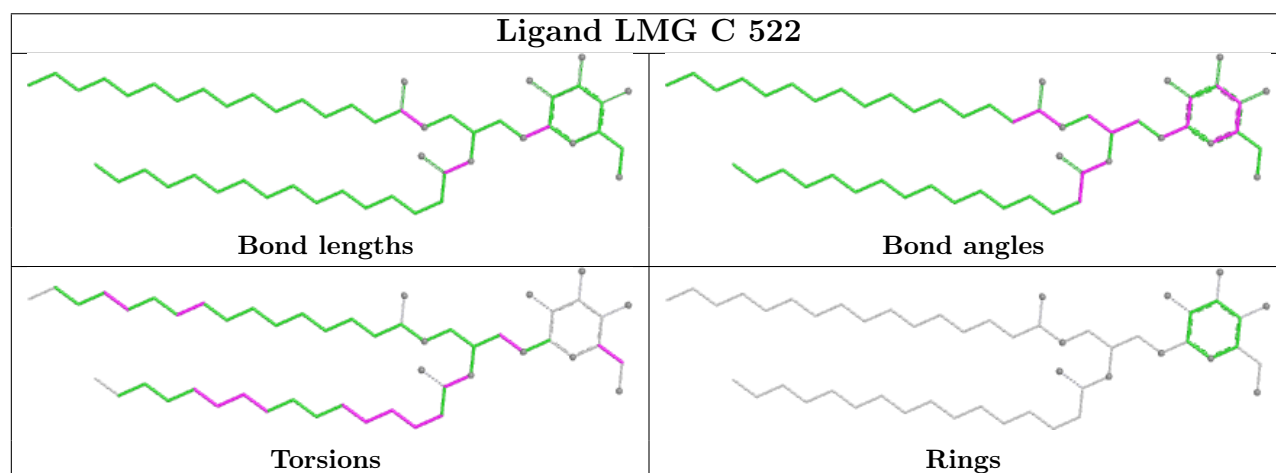
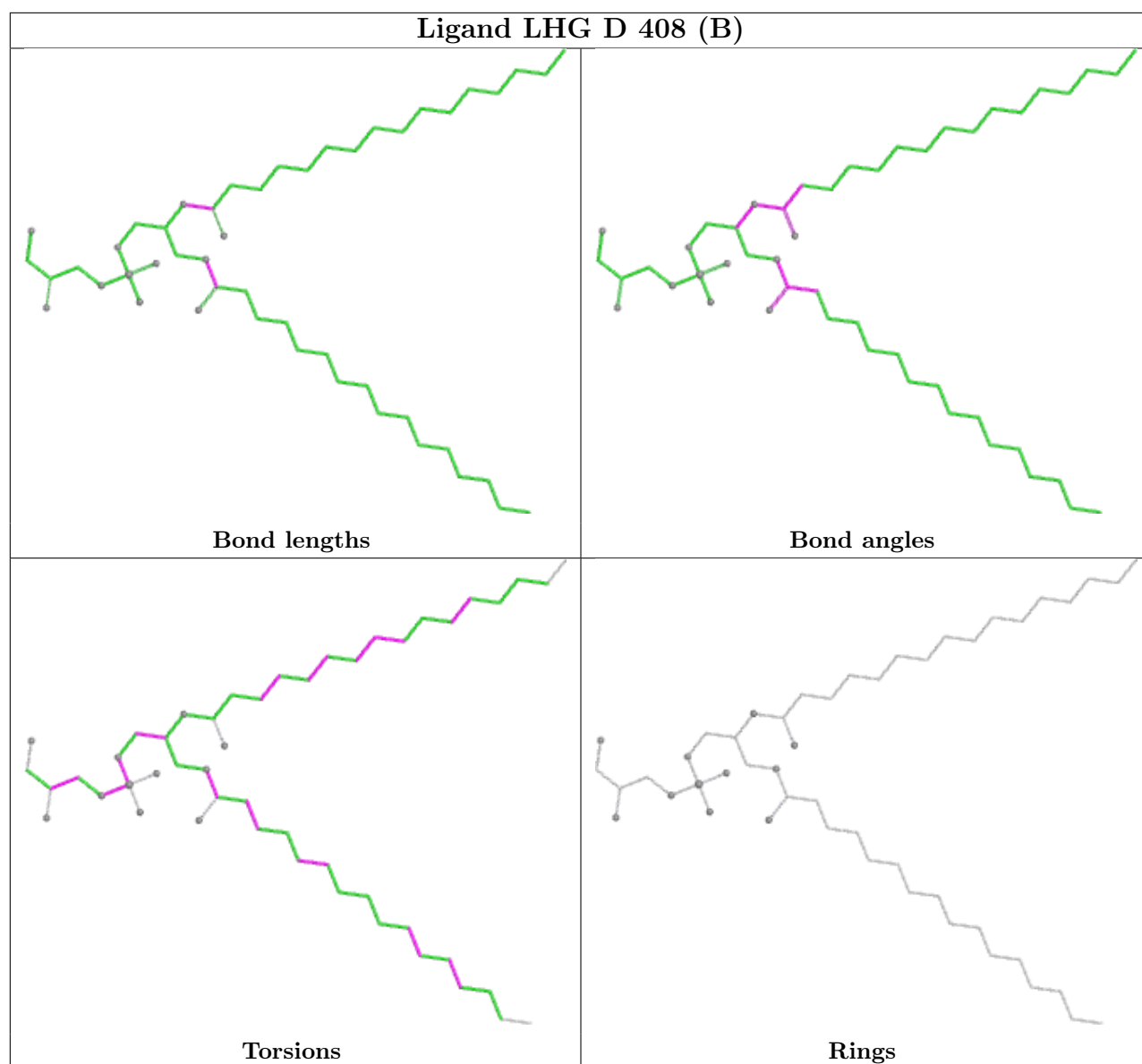


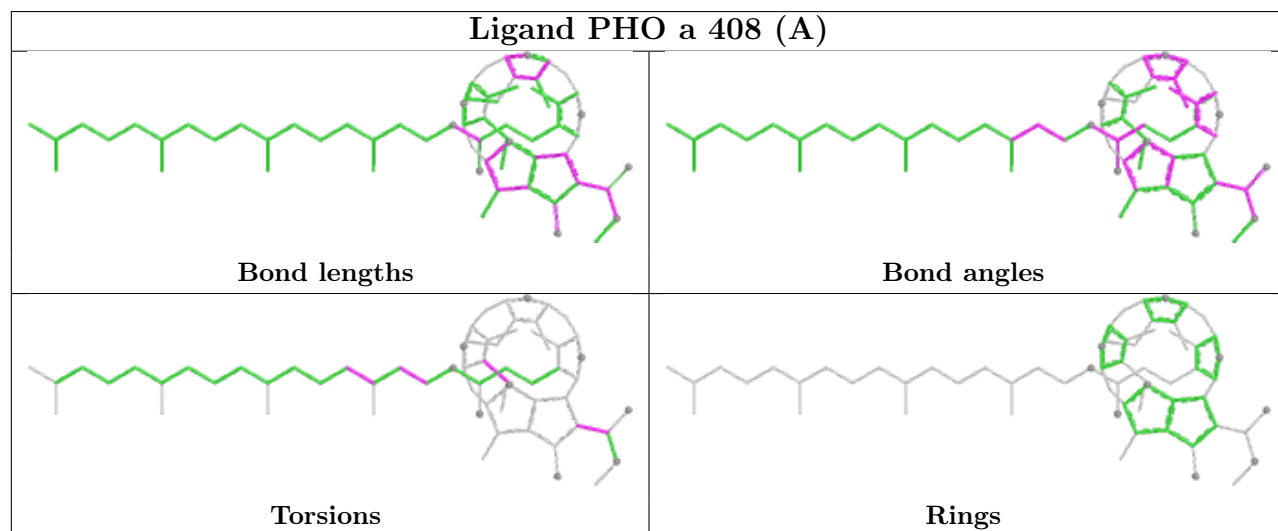
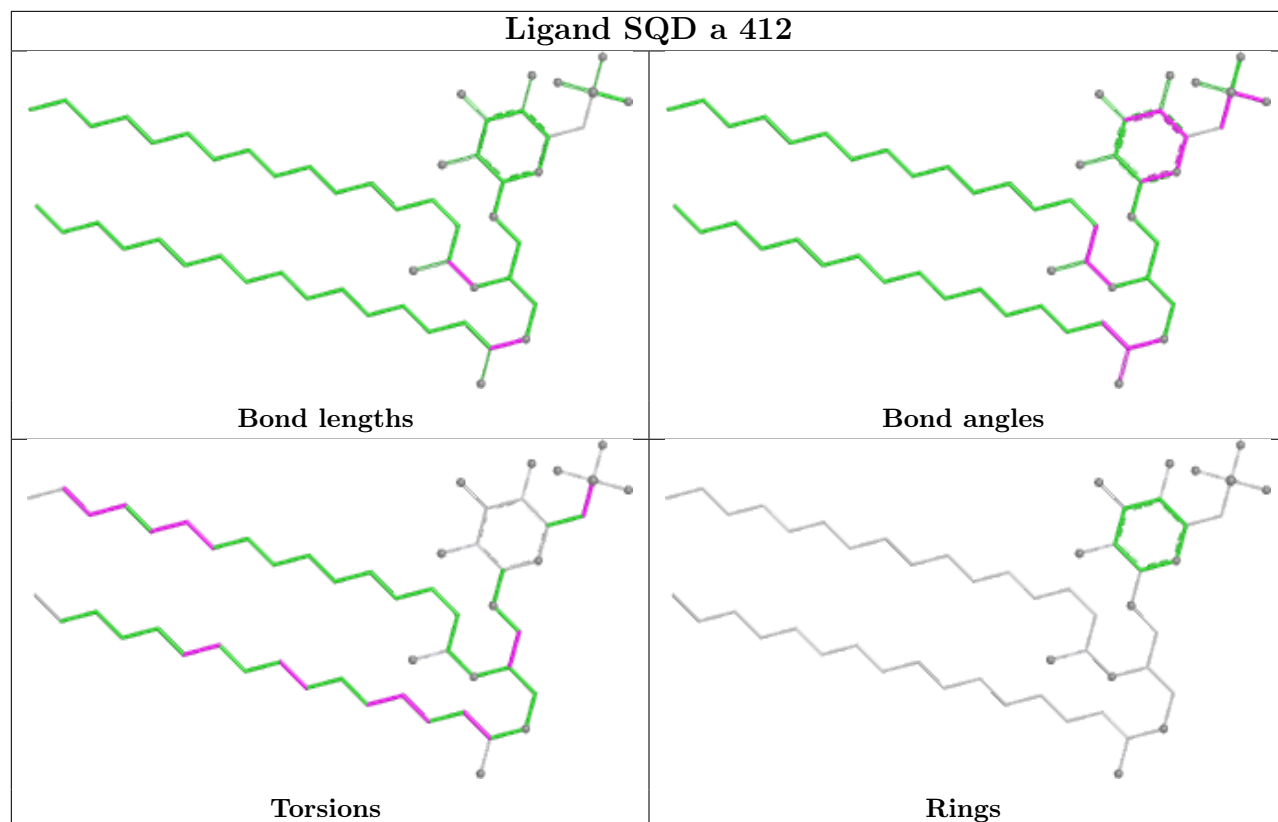


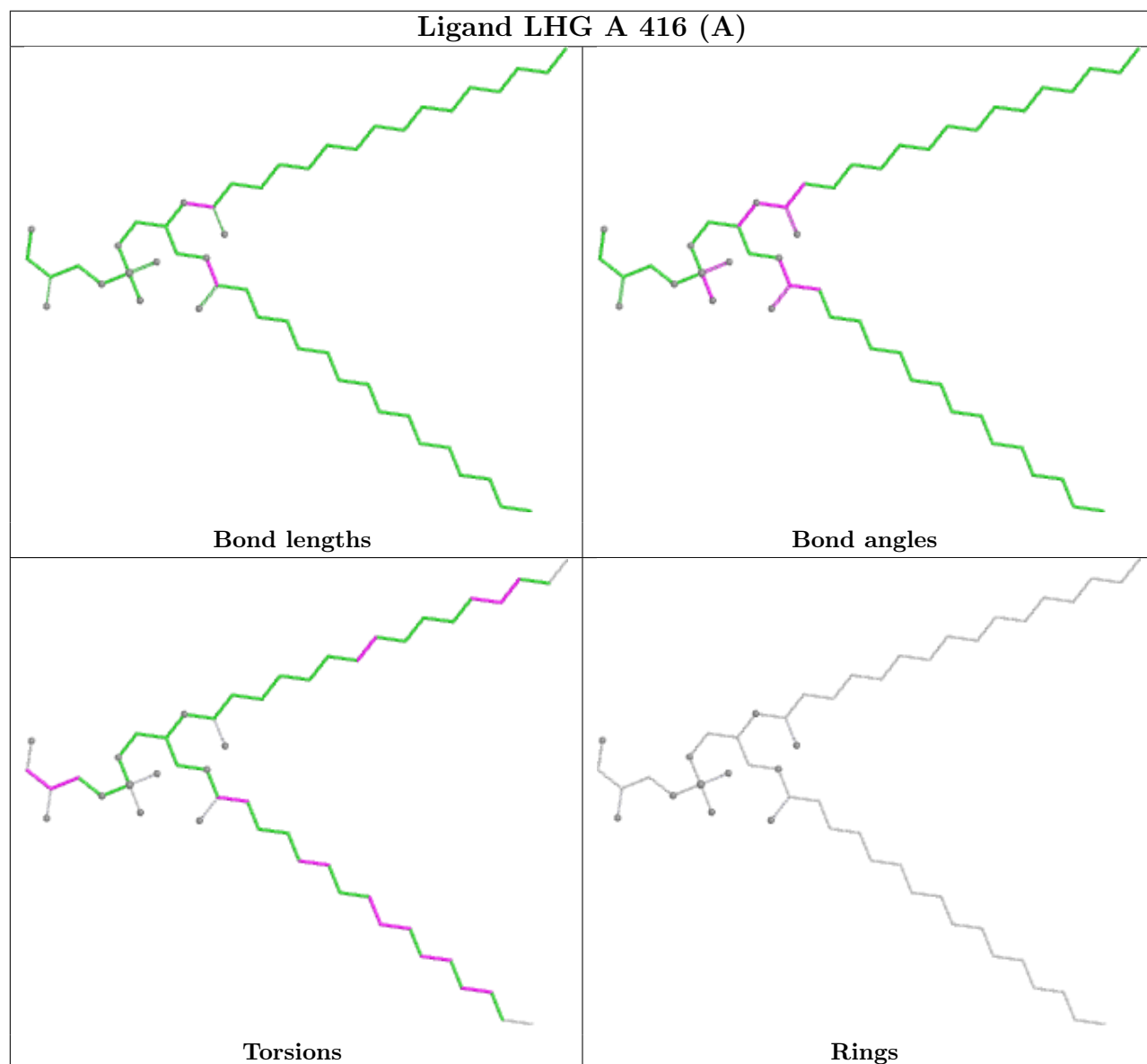
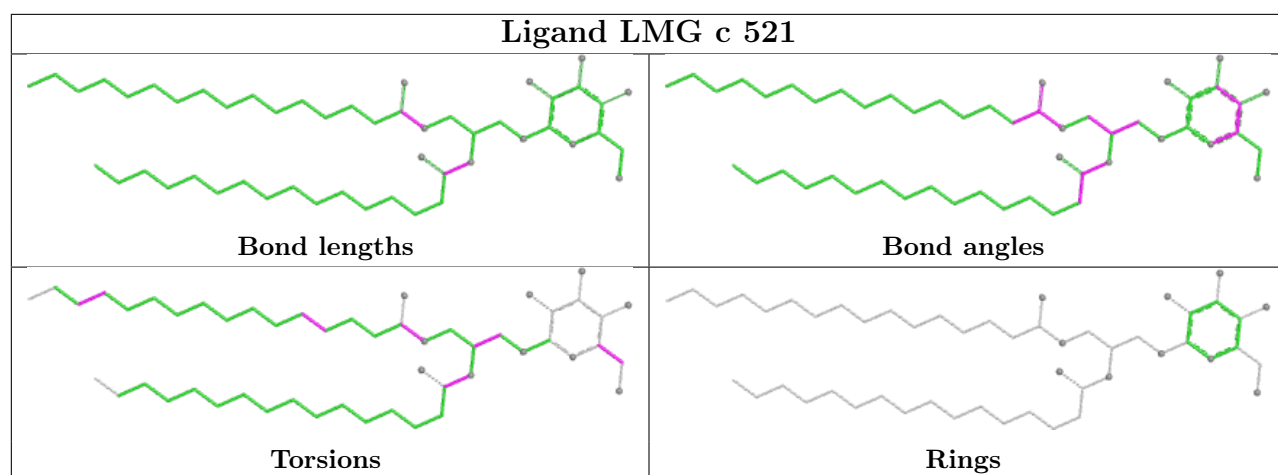


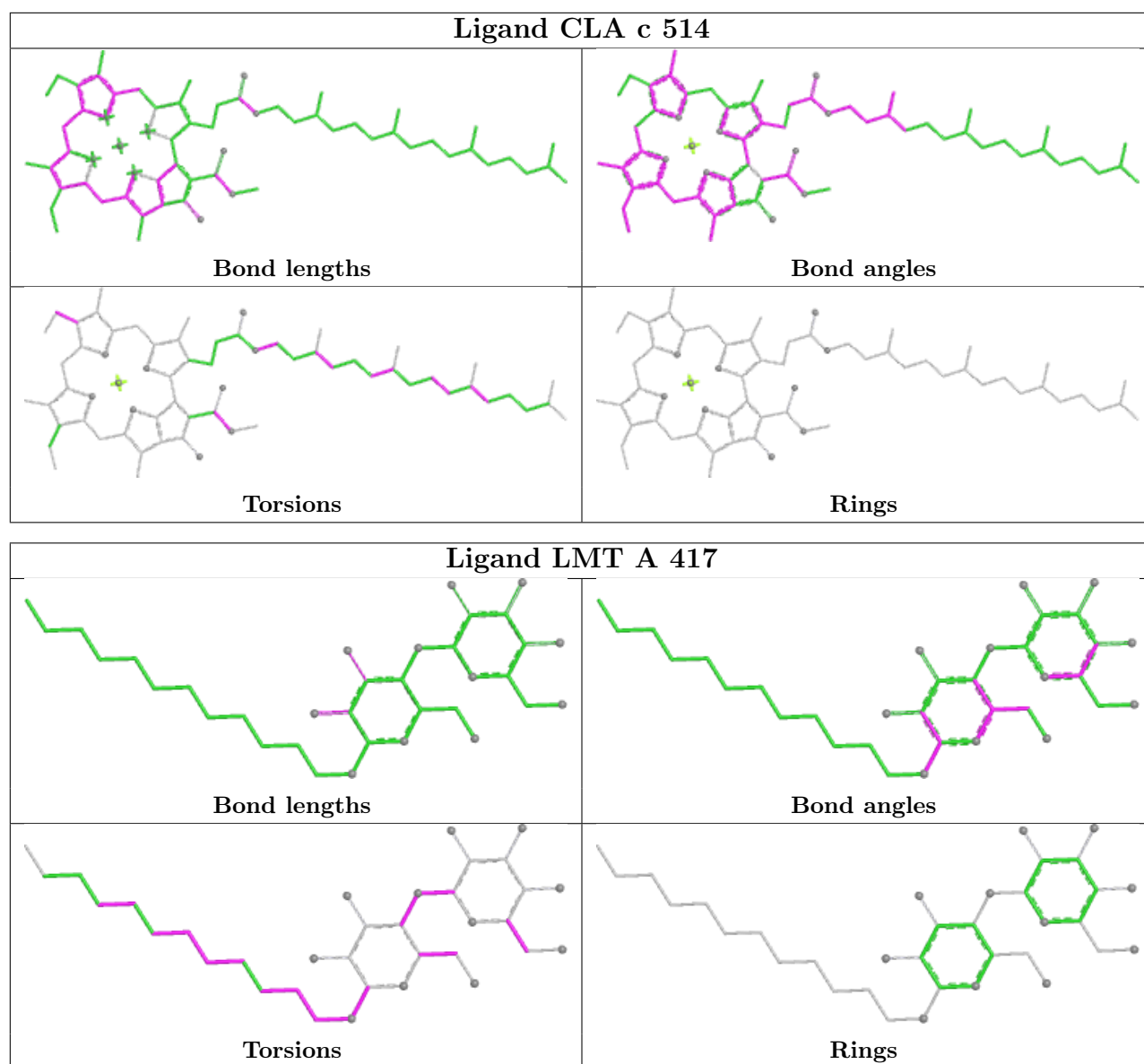


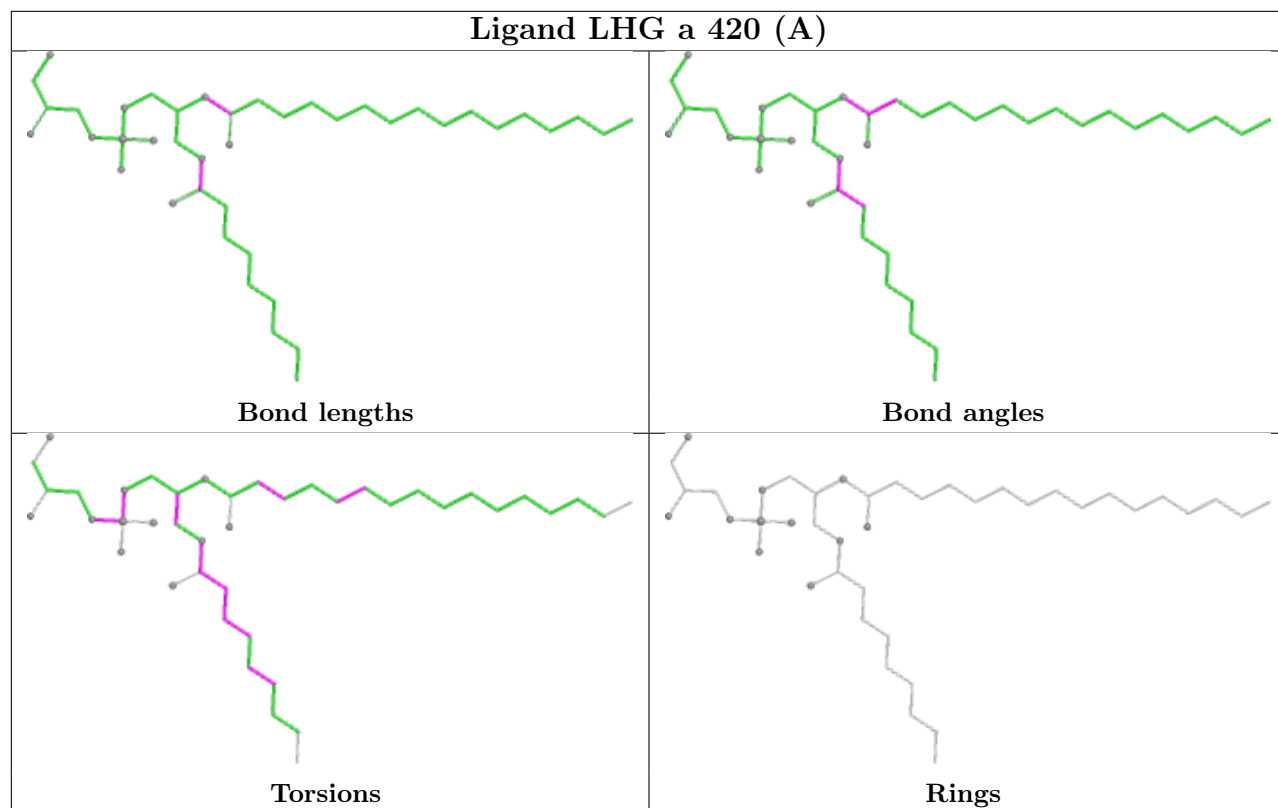




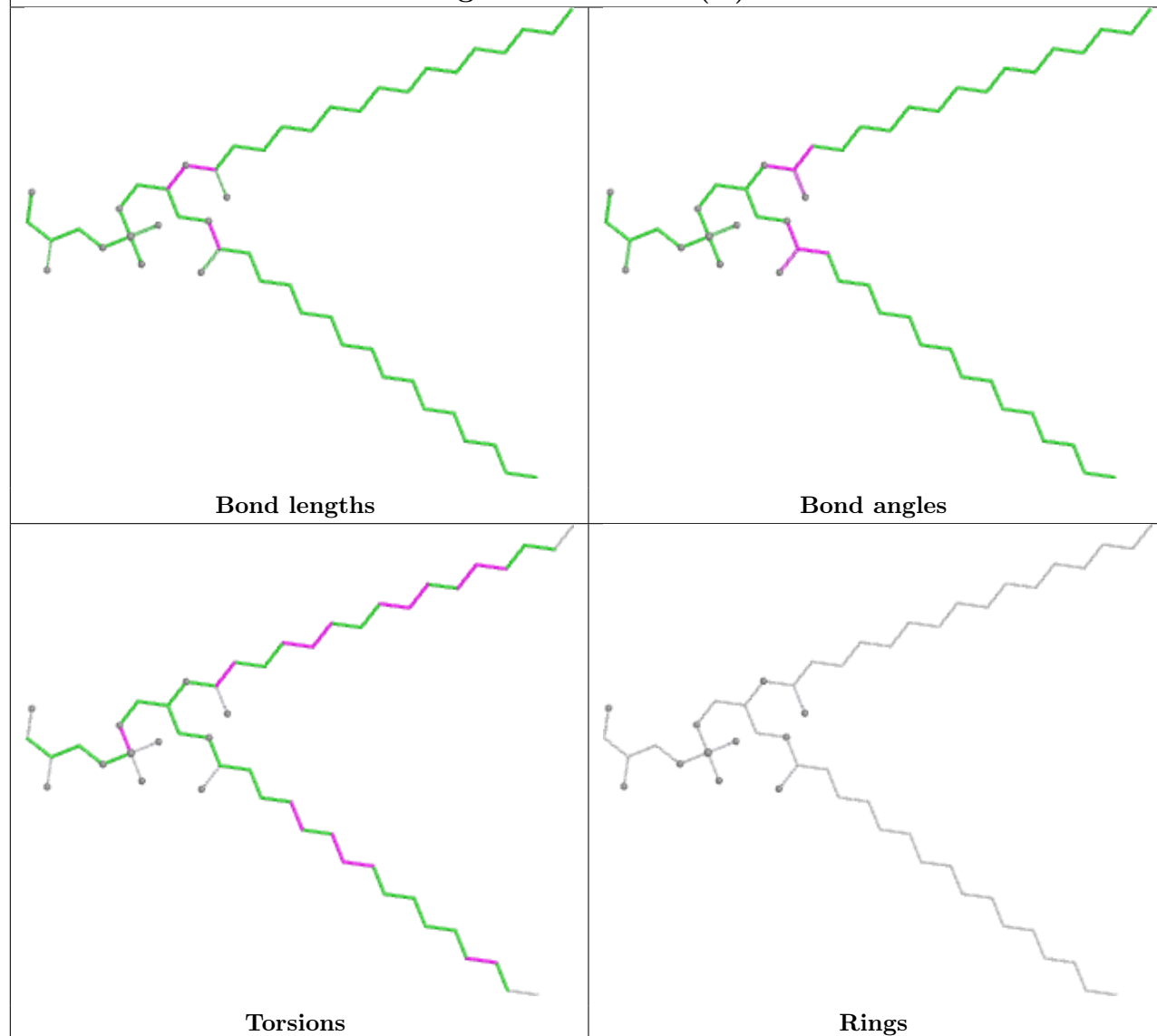




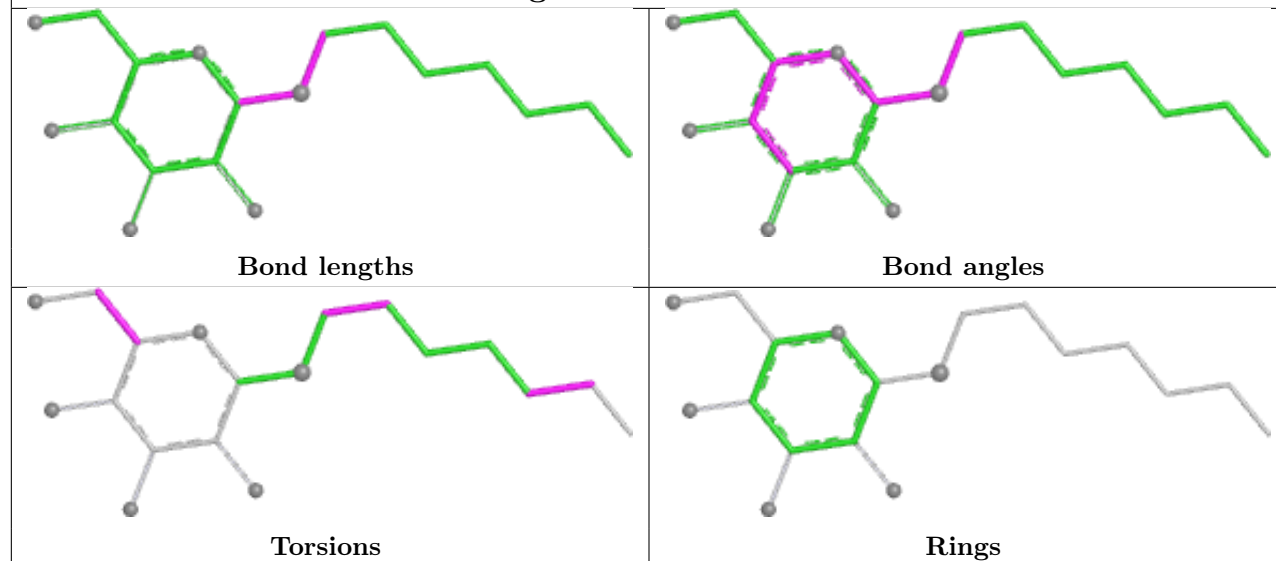


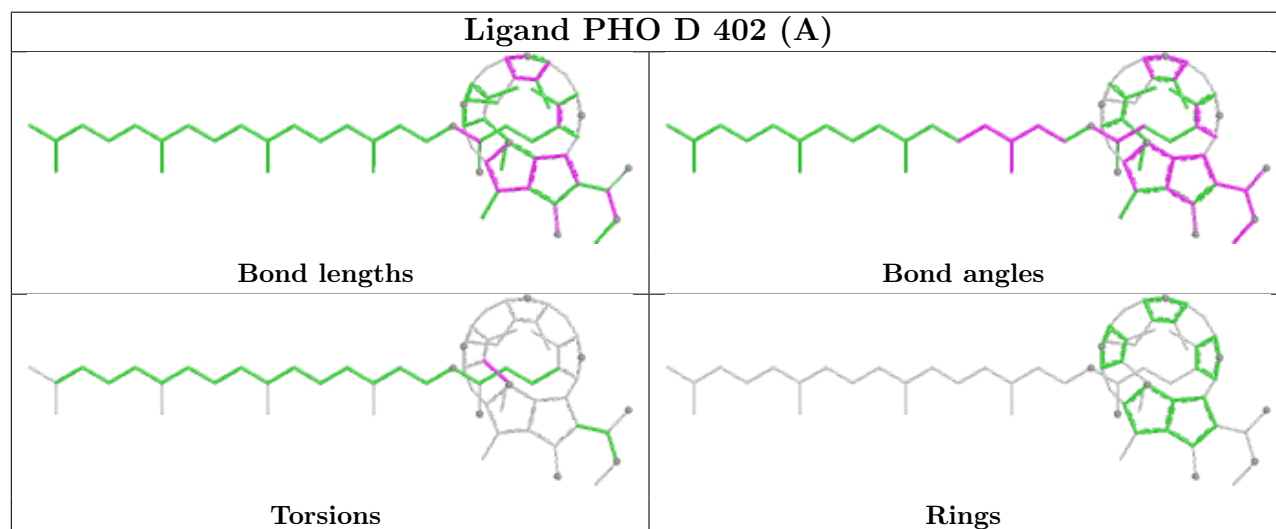
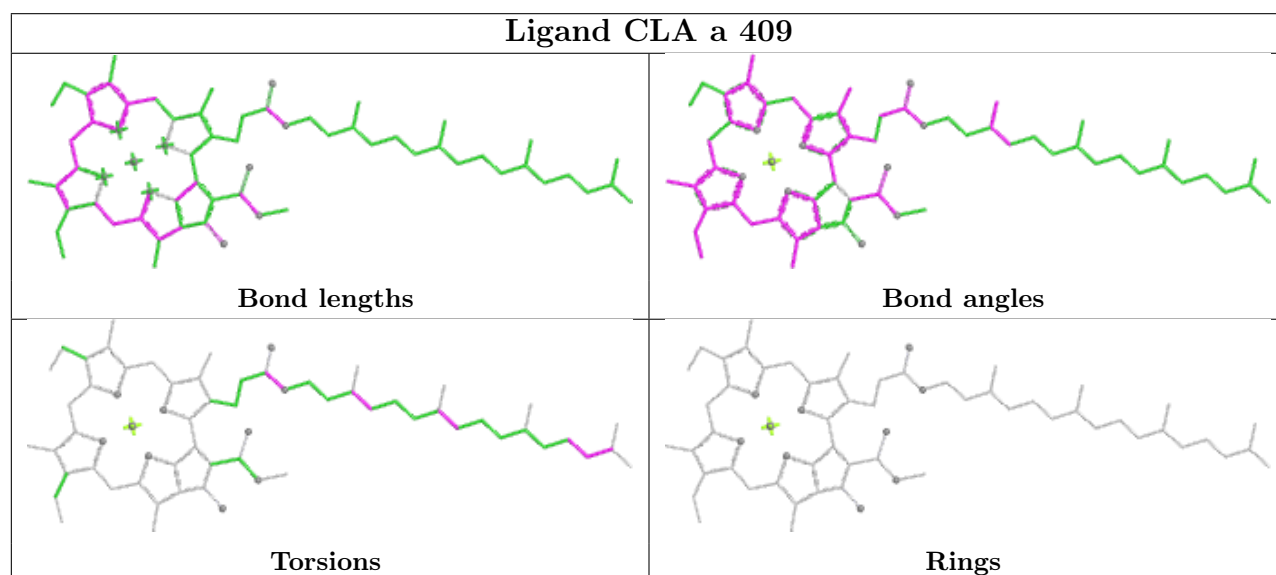
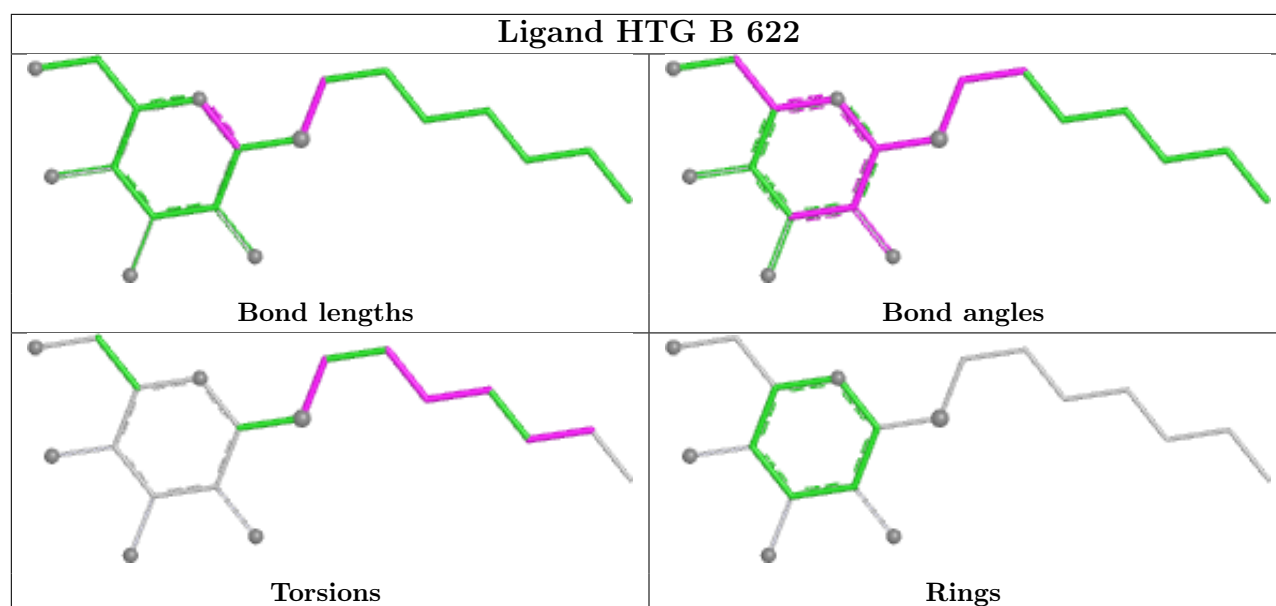


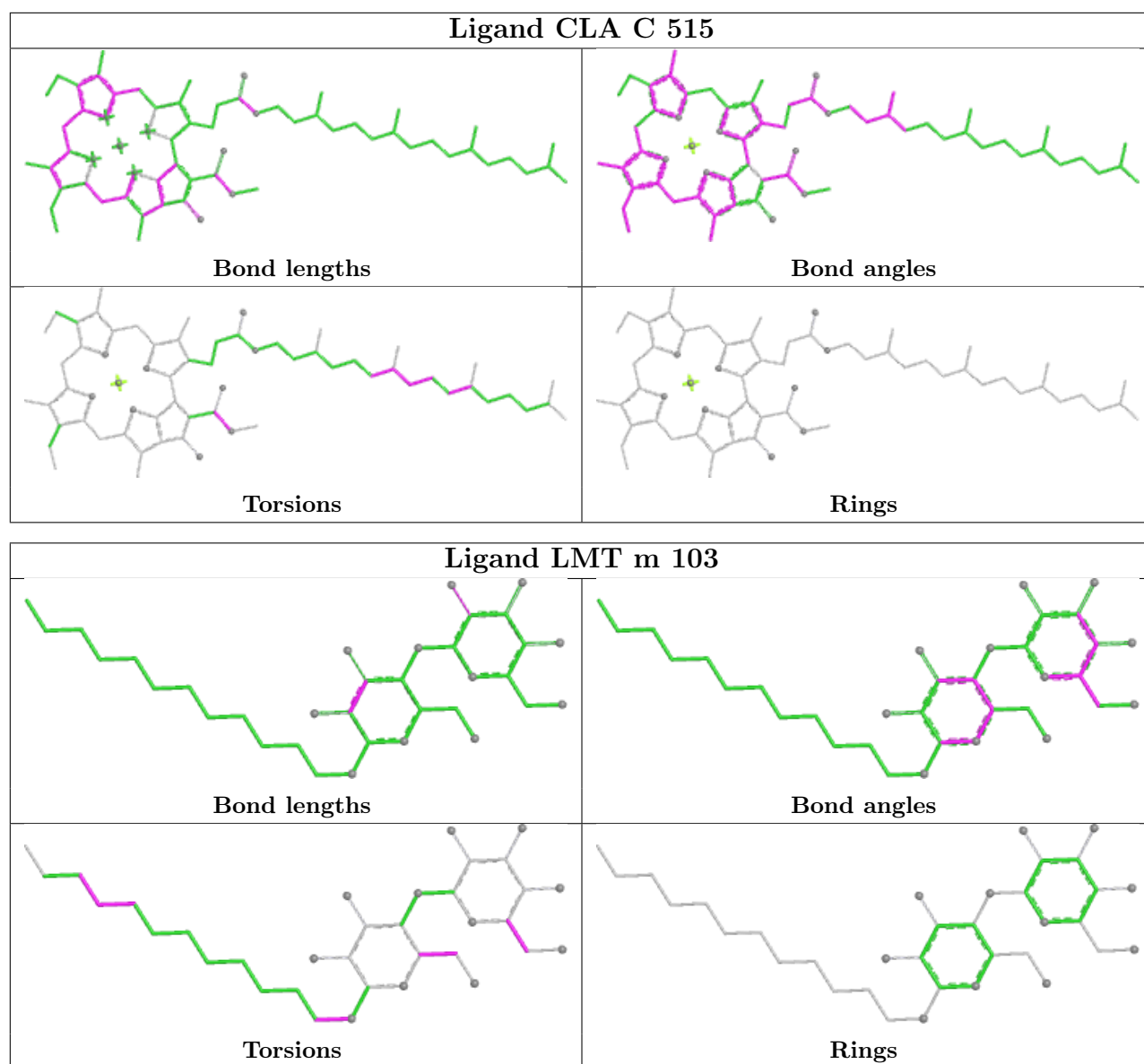
Ligand LHG 1 802 (A)



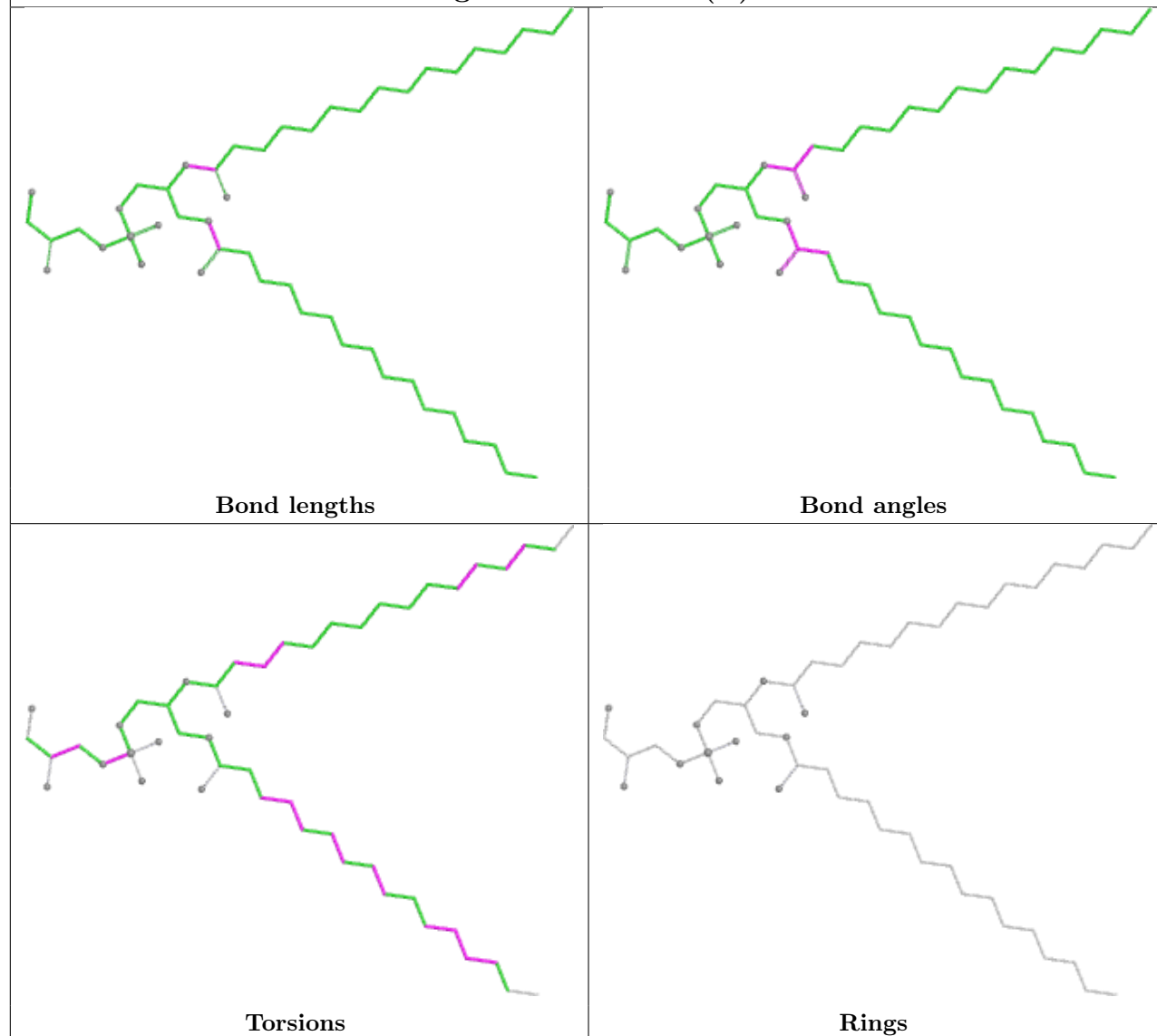
Ligand HTG B 625



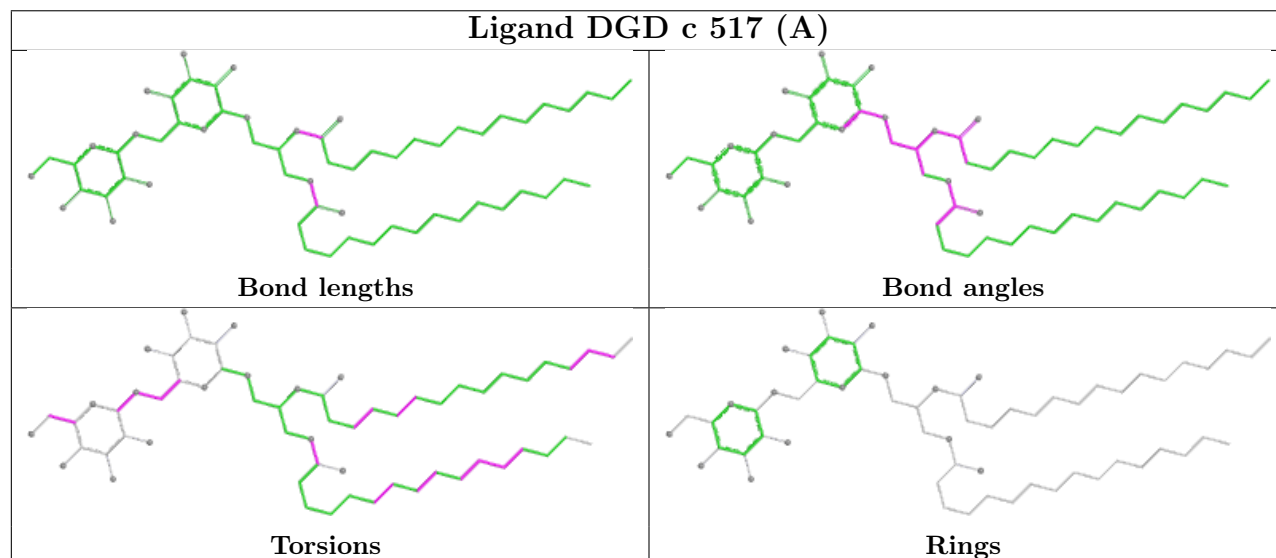


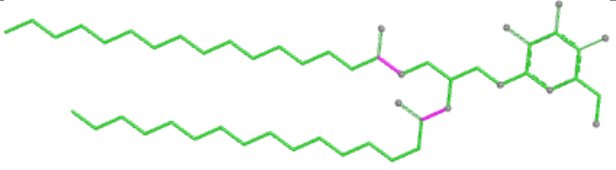
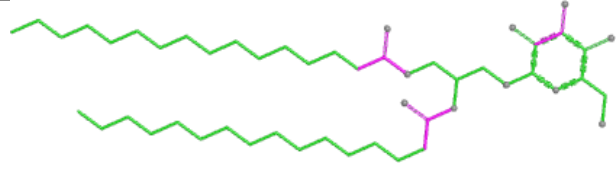
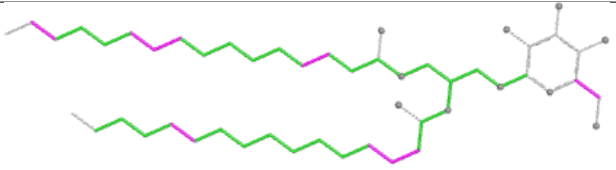
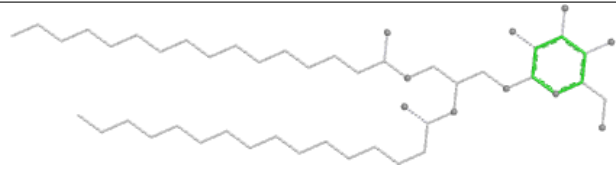


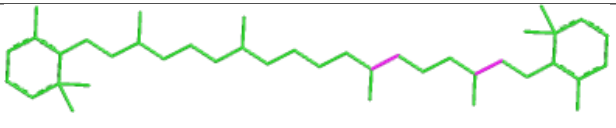
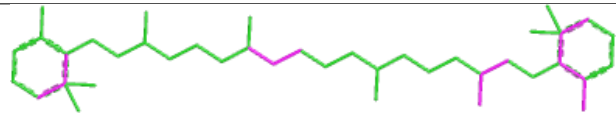
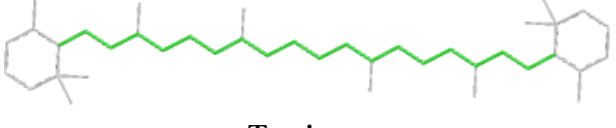
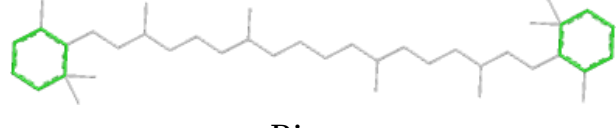
Ligand LHG d 411 (B)

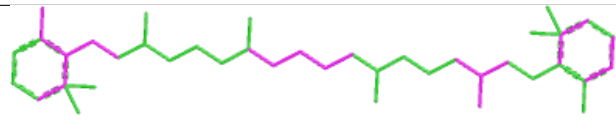
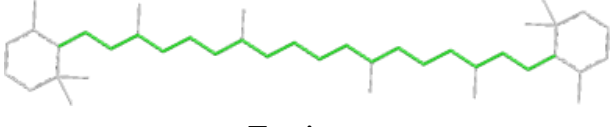
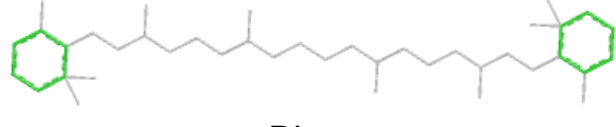


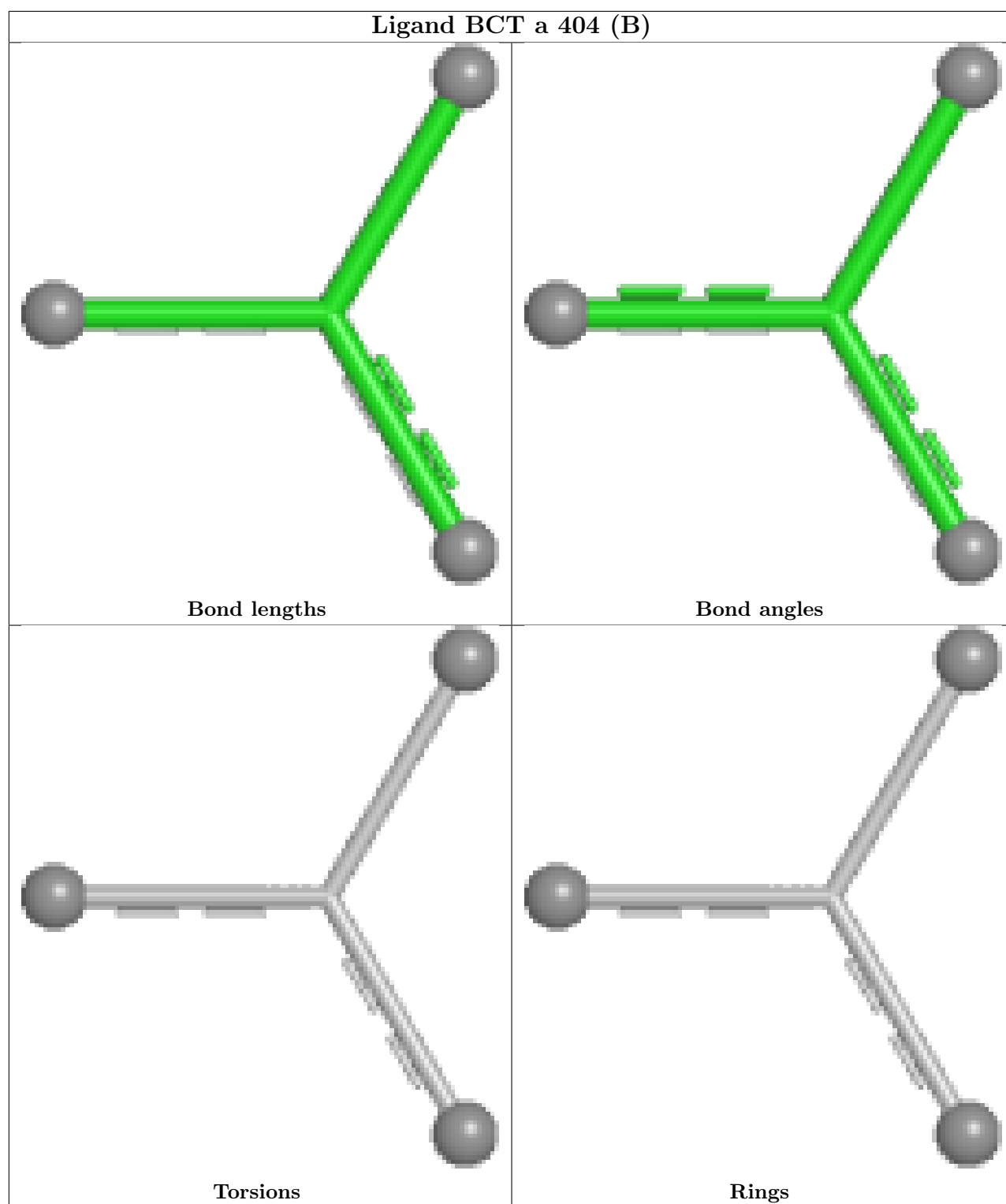
Ligand DGD c 517 (A)

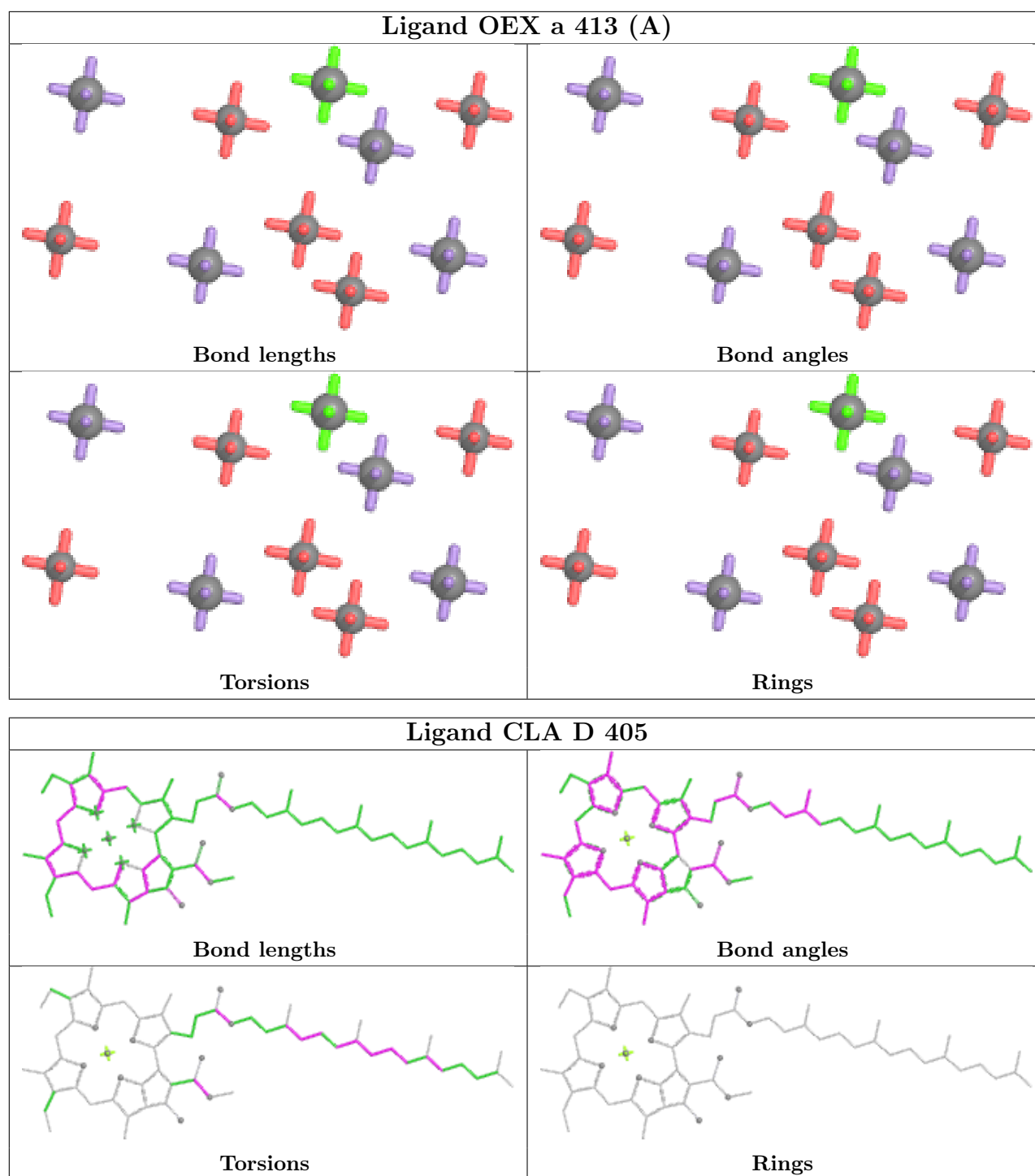


Ligand LMG d 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR b 618	
	
Bond lengths	Bond angles
	
Torsions	Rings





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%)	-0.69	1 (0%) 90 90	20, 26, 61, 122	222 (66%)
1	a	334/344 (97%)	-0.63	0 100 100	21, 29, 65, 126	221 (66%)
2	B	504/505 (99%)	-0.61	1 (0%) 91 91	23, 54, 84, 113	20 (3%)
2	b	504/505 (99%)	-0.48	3 (0%) 85 86	24, 58, 95, 154	19 (3%)
3	C	451/455 (99%)	-0.56	0 100 100	22, 61, 84, 136	97 (21%)
3	c	455/455 (100%)	-0.47	1 (0%) 91 91	25, 67, 88, 125	100 (21%)
4	D	342/342 (100%)	-0.72	0 100 100	20, 46, 66, 129	114 (33%)
4	d	341/342 (99%)	-0.71	0 100 100	22, 51, 76, 130	116 (34%)
5	E	81/84 (96%)	-0.39	0 100 100	53, 71, 98, 147	0
5	e	79/84 (94%)	-0.32	1 (1%) 75 76	33, 76, 116, 143	2 (2%)
6	F	34/44 (77%)	-0.57	0 100 100	55, 61, 89, 113	0
6	f	31/44 (70%)	-0.35	1 (3%) 50 52	55, 69, 94, 138	1 (3%)
7	H	64/65 (98%)	-0.35	1 (1%) 70 72	54, 65, 89, 105	0
7	h	64/65 (98%)	-0.36	0 100 100	40, 73, 96, 101	1 (1%)
8	I	37/38 (97%)	-0.26	0 100 100	58, 66, 123, 146	0
8	i	37/38 (97%)	-0.29	0 100 100	56, 66, 115, 134	0
9	J	38/39 (97%)	-0.47	0 100 100	49, 70, 119, 153	0
9	j	39/39 (100%)	-0.30	0 100 100	58, 78, 129, 151	0
10	K	37/37 (100%)	-0.63	0 100 100	54, 68, 88, 110	0
10	k	37/37 (100%)	-0.52	0 100 100	65, 75, 98, 112	0
11	L	36/37 (97%)	-0.70	0 100 100	23, 46, 112, 127	2 (5%)
11	l	36/37 (97%)	-0.67	0 100 100	23, 47, 105, 115	2 (5%)
12	M	32/36 (88%)	-0.67	0 100 100	27, 50, 75, 131	1 (3%)
12	m	33/36 (91%)	-0.63	0 100 100	25, 49, 71, 140	2 (6%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.52	0 100 100	21, 66, 119, 161	10 (4%)
13	o	243/244 (99%)	-0.45	0 100 100	23, 68, 125, 155	8 (3%)
14	T	29/32 (90%)	-0.63	0 100 100	27, 47, 56, 66	6 (20%)
14	t	29/32 (90%)	-0.71	1 (3%) 48 50	27, 47, 61, 72	5 (17%)
15	U	96/104 (92%)	-0.63	0 100 100	25, 58, 93, 100	4 (4%)
15	u	97/104 (93%)	-0.68	0 100 100	28, 62, 81, 120	4 (4%)
16	V	137/137 (100%)	-0.75	0 100 100	24, 58, 81, 109	6 (4%)
16	v	137/137 (100%)	-0.55	0 100 100	27, 72, 102, 128	6 (4%)
17	X	38/40 (95%)	-0.20	0 100 100	37, 74, 97, 114	1 (2%)
17	x	38/40 (95%)	-0.04	0 100 100	69, 82, 131, 154	0
18	Y	29/30 (96%)	-0.08	0 100 100	68, 85, 113, 123	0
18	y	29/30 (96%)	-0.24	0 100 100	78, 91, 109, 115	0
19	Z	62/62 (100%)	-0.30	0 100 100	68, 83, 130, 153	0
19	z	62/62 (100%)	0.10	0 100 100	80, 95, 144, 168	0
20	R	34/34 (100%)	0.59	2 (5%) 28 30	85, 111, 136, 142	0
All	All	5283/5384 (98%)	-0.54	12 (0%) 91 91	20, 59, 101, 168	970 (18%)

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	3.4
5	e	79[A]	PHE	3.4
6	f	16[A]	PHE	3.2
20	R	19	ALA	2.5
1	A	11	ALA	2.5

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	FME	I	1	10/11	0.95	0.07	67,71,79,85	0
14	FME	T	1	10/11	0.95	0.07	43,53,62,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	FME	i	1	10/11	0.97	0.07	54,75,84,86	0
12	FME	m	1	10/11	0.97	0.07	48,63,87,111	0
14	FME	t	1	10/11	0.97	0.06	44,48,61,77	0
12	FME	M	1	10/11	0.98	0.06	46,62,94,98	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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($\text{\AA}^2$)	Q<0.9
25	GOL	a	418	6/6	0.59	0.17	74,98,100,102	0
29	UNL	A	413	28/-	0.67	0.15	80,110,132,143	0
31	LMT	A	417	35/35	0.68	0.13	97,127,153,163	0
31	LMT	F	101	35/35	0.68	0.15	88,126,165,171	0
31	LMT	e	101	35/35	0.68	0.15	98,140,176,179	0
31	LMT	B	630	35/35	0.69	0.15	65,111,140,146	0
29	UNL	J	101	10/-	0.70	0.22	69,80,87,101	0
29	UNL	K	101[A]	34/-	0.71	0.14	76,104,114,118	34
29	UNL	K	101[B]	34/-	0.71	0.14	75,104,114,118	34
29	UNL	a	415	30/-	0.71	0.12	85,113,133,140	0
31	LMT	A	415	35/35	0.71	0.13	61,109,130,134	0
29	UNL	m	102	10/-	0.72	0.20	68,75,102,103	0
34	HTG	C	523	19/19	0.73	0.13	100,124,139,139	0
31	LMT	c	501	35/35	0.74	0.13	103,128,147,150	0
29	UNL	I	101	40/-	0.74	0.15	73,102,150,162	0
34	HTG	B	623	19/19	0.74	0.16	61,95,108,117	0
26	SQD	f	102	43/54	0.74	0.13	101,124,167,183	0
25	GOL	o	302	6/6	0.75	0.16	82,89,96,104	0
25	GOL	O	302	6/6	0.76	0.12	81,90,105,109	0
34	HTG	D	412	16/19	0.76	0.12	93,103,134,149	0
29	UNL	j	101	10/-	0.77	0.15	73,90,97,98	0
32	LHG	a	420[A]	42/49	0.78	0.12	88,131,146,154	42
32	LHG	a	420[B]	42/49	0.78	0.12	87,131,146,154	42
29	UNL	c	525[B]	32/-	0.78	0.14	86,106,118,127	32

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	GOL	B	627	6/6	0.78	0.14	75,86,96,114	0
29	UNL	c	525[A]	32/-	0.78	0.14	86,106,118,127	32
34	HTG	c	522	19/19	0.78	0.10	109,124,142,145	0
33	LMG	C	522	51/55	0.79	0.11	61,115,156,161	0
29	UNL	M	102	10/-	0.80	0.15	63,77,98,100	0
29	UNL	B	631	40/-	0.80	0.13	74,103,154,159	0
29	UNL	b	626	33/-	0.80	0.13	67,98,162,171	0
29	UNL	D	411	40/-	0.80	0.13	63,88,138,150	0
29	UNL	b	629	36/-	0.81	0.11	68,96,134,143	0
25	GOL	c	528	6/6	0.81	0.16	82,104,109,121	0
36	CA	V	201	1/1	0.81	0.24	129,129,129,129	0
31	LMT	T	101	35/35	0.82	0.10	65,121,165,169	0
31	LMT	b	621	25/35	0.82	0.11	77,114,158,164	0
25	GOL	A	409	6/6	0.82	0.13	60,77,80,83	0
25	GOL	b	624	6/6	0.82	0.15	93,96,104,113	0
28	PL9	a	414[B]	55/55	0.83	0.14	75,97,111,114	55
25	GOL	d	410	6/6	0.83	0.23	51,69,79,86	0
28	PL9	A	412[A]	55/55	0.83	0.13	60,88,103,106	55
31	LMT	B	628	35/35	0.83	0.11	63,102,135,149	0
34	HTG	b	622	19/19	0.83	0.13	63,85,118,119	0
28	PL9	A	412[B]	55/55	0.83	0.13	60,88,103,106	55
28	PL9	a	414[A]	55/55	0.83	0.14	75,97,111,114	55
29	UNL	B	626	33/-	0.84	0.14	60,106,142,146	0
25	GOL	O	303	6/6	0.84	0.13	76,91,93,95	0
34	HTG	V	203	11/19	0.84	0.09	81,111,125,126	0
26	SQD	a	412	54/54	0.84	0.10	66,93,140,149	0
34	HTG	b	623	19/19	0.84	0.10	85,129,154,161	0
33	LMG	c	521	51/55	0.84	0.10	78,131,161,183	0
31	LMT	t	102	26/35	0.84	0.11	67,101,137,148	0
31	LMT	t	101	25/35	0.85	0.12	54,81,132,154	0
26	SQD	A	410	54/54	0.85	0.10	66,89,130,150	0
25	GOL	c	527	6/6	0.85	0.16	96,97,106,110	0
33	LMG	z	101	39/55	0.85	0.12	74,126,151,164	0
31	LMT	b	627	25/35	0.86	0.11	58,93,140,154	0
34	HTG	B	622	19/19	0.86	0.12	69,85,110,123	0
33	LMG	C	526	37/55	0.87	0.12	70,124,146,160	0
34	HTG	d	408	16/19	0.87	0.10	89,116,139,152	0
31	LMT	m	103	35/35	0.87	0.10	62,92,105,108	0
25	GOL	l	801[A]	6/6	0.88	0.17	67,93,96,98	6
25	GOL	l	801[B]	6/6	0.88	0.17	68,93,96,98	6
25	GOL	V	204[B]	6/6	0.88	0.13	59,70,77,78	6
31	LMT	M	101	35/35	0.88	0.10	59,96,115,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	GOL	v	202[A]	6/6	0.88	0.11	70,80,83,86	6
25	GOL	v	202[B]	6/6	0.88	0.11	70,80,83,86	6
25	GOL	V	204[A]	6/6	0.88	0.13	62,72,77,78	6
32	LHG	E	101[A]	42/49	0.89	0.11	74,100,113,119	42
32	LHG	E	101[B]	42/49	0.89	0.11	74,100,113,119	42
26	SQD	b	620	54/54	0.89	0.09	61,94,119,129	0
26	SQD	B	620	54/54	0.89	0.09	59,92,137,145	0
26	SQD	F	103	43/54	0.89	0.11	77,107,129,137	0
25	GOL	B	629	6/6	0.89	0.11	71,78,90,91	0
25	GOL	a	419	6/6	0.90	0.25	54,76,81,87	0
23	CLA	b	601	65/65	0.90	0.10	63,89,128,157	0
33	LMG	a	417	51/55	0.90	0.09	71,93,110,118	0
33	LMG	c	520	51/55	0.91	0.09	65,89,136,153	0
23	CLA	c	514	65/65	0.91	0.09	69,94,127,149	0
33	LMG	C	502	51/55	0.91	0.09	64,87,110,124	0
29	UNL	D	410	17/-	0.91	0.10	59,78,106,113	0
23	CLA	B	601	65/65	0.91	0.09	59,81,115,150	0
34	HTG	B	625	19/19	0.91	0.08	65,81,97,104	0
25	GOL	D	414	6/6	0.91	0.16	43,62,69,85	0
36	CA	f	103	1/1	0.91	0.13	120,120,120,120	0
36	CA	o	301	1/1	0.91	0.06	116,116,116,116	0
33	LMG	B	621	51/55	0.92	0.07	49,68,87,107	0
25	GOL	c	526[B]	6/6	0.92	0.09	68,70,75,77	6
33	LMG	C	521	51/55	0.92	0.09	55,85,119,129	0
33	LMG	m	101	51/55	0.92	0.09	51,73,100,110	0
25	GOL	D	403	6/6	0.92	0.28	50,72,82,83	0
25	GOL	c	526[A]	6/6	0.92	0.09	68,70,75,77	6
33	LMG	D	413	51/55	0.93	0.08	47,67,125,131	0
29	UNL	d	407	17/-	0.93	0.09	67,79,113,114	0
26	SQD	C	501[A]	54/54	0.93	0.09	57,79,116,121	54
26	SQD	C	501[B]	54/54	0.93	0.09	57,80,116,121	54
33	LMG	d	409	51/55	0.93	0.08	53,76,118,148	0
23	CLA	c	513	65/65	0.93	0.09	61,84,127,139	0
23	CLA	C	515	65/65	0.93	0.08	64,87,116,123	0
32	LHG	A	416[A]	49/49	0.93	0.09	48,61,83,86	49
32	LHG	A	416[B]	49/49	0.93	0.09	48,61,83,86	49
24	BCR	T	102	40/40	0.93	0.07	48,59,70,75	0
23	CLA	B	614	65/65	0.94	0.08	39,52,102,126	0
24	BCR	Y	101	40/40	0.94	0.08	54,67,83,93	0
24	BCR	c	515	40/40	0.94	0.08	70,83,97,99	0
24	BCR	d	403	40/40	0.94	0.08	54,67,98,107	0
24	BCR	t	103	40/40	0.94	0.06	43,59,74,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	BCR	y	101	40/40	0.94	0.07	60,72,86,98	0
23	CLA	a	409	65/65	0.94	0.10	43,59,139,154	0
23	CLA	C	506	65/65	0.94	0.08	44,58,101,133	0
23	CLA	b	614	65/65	0.94	0.07	43,54,101,107	0
25	GOL	C	524[A]	6/6	0.94	0.09	59,62,66,70	6
25	GOL	C	524[B]	6/6	0.94	0.09	61,61,68,70	6
23	CLA	c	505	65/65	0.94	0.07	52,62,111,132	0
23	CLA	c	507	65/65	0.94	0.08	55,70,119,137	0
23	CLA	C	508	65/65	0.94	0.08	54,72,122,143	0
23	CLA	C	514	65/65	0.94	0.08	62,77,112,128	0
24	BCR	C	516	40/40	0.94	0.08	62,77,88,93	0
26	SQD	a	411[A]	54/54	0.94	0.09	61,81,115,120	54
32	LHG	D	409[A]	49/49	0.94	0.09	51,60,109,116	49
32	LHG	D	409[B]	49/49	0.94	0.09	51,61,109,116	49
26	SQD	a	411[B]	54/54	0.94	0.09	61,81,115,120	54
34	HTG	b	625	19/19	0.94	0.07	63,82,95,106	0
24	BCR	D	406	40/40	0.94	0.08	45,59,102,109	0
24	BCR	H	101	40/40	0.94	0.08	52,69,86,91	0
35	DGD	C	519[A]	62/66	0.94	0.08	48,66,110,113	62
35	DGD	C	519[B]	62/66	0.94	0.08	48,65,110,113	62
35	DGD	c	517[A]	62/66	0.94	0.08	51,66,102,113	62
35	DGD	c	517[B]	62/66	0.94	0.08	51,66,102,113	62
35	DGD	c	518[A]	62/66	0.94	0.08	53,70,120,136	62
35	DGD	c	518[B]	62/66	0.94	0.08	53,70,120,136	62
24	BCR	K	102	40/40	0.94	0.09	57,65,75,81	0
32	LHG	d	411[A]	49/49	0.94	0.08	51,66,80,89	49
32	LHG	d	411[B]	49/49	0.94	0.08	51,66,80,89	49
24	BCR	A	408	40/40	0.95	0.07	40,53,65,68	0
24	BCR	B	619	40/40	0.95	0.07	50,61,96,102	0
23	CLA	b	606	65/65	0.95	0.07	47,62,122,131	0
28	PL9	D	407[A]	55/55	0.95	0.06	36,49,57,68	55
28	PL9	D	407[B]	55/55	0.95	0.06	36,49,57,68	55
23	CLA	D	405	65/65	0.95	0.08	49,60,123,131	0
23	CLA	b	616	65/65	0.95	0.08	52,65,133,147	0
23	CLA	a	407[A]	65/65	0.95	0.07	41,52,121,129	65
32	LHG	d	406[A]	49/49	0.95	0.09	54,64,115,127	49
32	LHG	d	406[B]	49/49	0.95	0.09	54,64,115,127	49
23	CLA	a	407[B]	65/65	0.95	0.07	41,52,121,129	65
23	CLA	c	508	65/65	0.95	0.09	53,70,87,94	0
24	BCR	b	619	40/40	0.95	0.07	51,64,86,91	0
23	CLA	c	509	65/65	0.95	0.07	45,64,127,142	0
24	BCR	c	516	40/40	0.95	0.07	55,68,84,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	DGD	C	520	62/66	0.95	0.07	44,58,92,112	0
35	DGD	H	102	62/66	0.95	0.08	46,61,74,83	0
23	CLA	A	407	65/65	0.95	0.08	40,54,129,145	0
24	BCR	h	101	40/40	0.95	0.09	58,72,98,100	0
24	BCR	k	101	40/40	0.95	0.09	60,74,90,92	0
25	GOL	b	628	6/6	0.95	0.08	80,82,87,90	0
35	DGD	c	519	62/66	0.95	0.07	51,65,109,131	0
35	DGD	h	102	62/66	0.95	0.08	51,65,79,84	0
29	UNL	X	101	18/-	0.95	0.10	64,76,108,112	0
23	CLA	C	510	65/65	0.95	0.07	44,57,120,146	0
23	CLA	d	402	65/65	0.95	0.09	55,68,126,147	0
23	CLA	B	611	65/65	0.96	0.06	33,45,65,86	0
23	CLA	A	406[A]	65/65	0.96	0.06	38,47,111,118	65
24	BCR	B	617	40/40	0.96	0.05	42,52,64,65	0
29	UNL	x	101	18/-	0.96	0.10	68,81,119,137	0
24	BCR	B	618	40/40	0.96	0.05	37,57,69,76	0
23	CLA	B	616	65/65	0.96	0.08	45,61,131,138	0
23	CLA	b	602	65/65	0.96	0.07	52,63,84,91	0
24	BCR	C	517	40/40	0.96	0.07	52,67,79,90	0
23	CLA	C	503	65/65	0.96	0.07	50,62,76,89	0
23	CLA	b	607	65/65	0.96	0.06	39,48,84,93	0
23	CLA	b	612	65/65	0.96	0.07	47,56,66,78	0
23	CLA	A	406[B]	65/65	0.96	0.06	38,47,111,119	65
28	PL9	d	404[A]	55/55	0.96	0.06	39,51,61,68	55
28	PL9	d	404[B]	55/55	0.96	0.06	39,50,61,68	55
23	CLA	A	404[A]	65/65	0.96	0.06	38,42,60,67	65
24	BCR	a	410	40/40	0.96	0.06	46,54,66,68	0
24	BCR	b	617	40/40	0.96	0.06	44,54,66,67	0
24	BCR	b	618	40/40	0.96	0.06	43,59,78,89	0
23	CLA	c	502	65/65	0.96	0.07	54,69,80,87	0
23	CLA	c	504	65/65	0.96	0.07	55,71,85,90	0
32	LHG	D	408[A]	49/49	0.96	0.07	46,54,66,76	49
32	LHG	D	408[B]	49/49	0.96	0.07	46,55,66,77	49
23	CLA	C	509	65/65	0.96	0.07	52,66,83,93	0
35	DGD	C	518[A]	62/66	0.96	0.07	47,60,102,111	62
35	DGD	C	518[B]	62/66	0.96	0.07	47,60,102,111	62
23	CLA	c	506	65/65	0.96	0.06	51,65,94,103	0
23	CLA	A	404[B]	65/65	0.96	0.06	38,43,63,67	65
23	CLA	B	602	65/65	0.96	0.07	50,59,73,91	0
23	CLA	B	603	65/65	0.96	0.07	44,54,75,85	0
23	CLA	c	511	65/65	0.96	0.06	49,65,80,90	0
32	LHG	d	405[A]	49/49	0.96	0.07	48,55,70,76	49

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	LHG	d	405[B]	49/49	0.96	0.07	47,56,70,77	49
23	CLA	c	512	65/65	0.96	0.07	59,70,86,96	0
25	GOL	B	624	6/6	0.96	0.11	67,78,81,82	0
23	CLA	B	606	65/65	0.96	0.07	43,58,110,134	0
36	CA	O	301	1/1	0.96	0.04	105,105,105,105	0
23	CLA	B	609	65/65	0.96	0.07	46,61,72,83	0
32	LHG	l	802[A]	49/49	0.96	0.07	48,58,72,91	49
32	LHG	l	802[B]	49/49	0.96	0.07	48,57,72,91	49
37	PHO	D	402[A]	64/64	0.96	0.06	41,50,55,59	64
37	PHO	D	402[B]	64/64	0.96	0.06	40,50,55,60	64
37	PHO	a	416[A]	64/64	0.96	0.07	47,57,62,67	64
37	PHO	a	416[B]	64/64	0.96	0.07	47,57,62,66	64
23	CLA	a	406[B]	65/65	0.97	0.05	37,44,64,72	65
23	CLA	A	405[A]	65/65	0.97	0.05	35,43,53,64	65
23	CLA	d	401[A]	65/65	0.97	0.06	40,47,73,94	65
23	CLA	d	401[B]	65/65	0.97	0.06	40,47,73,94	65
23	CLA	B	607	65/65	0.97	0.06	33,48,76,83	0
23	CLA	C	505	65/65	0.97	0.06	48,65,73,84	0
23	CLA	A	405[B]	65/65	0.97	0.05	35,43,53,64	65
23	CLA	C	507	65/65	0.97	0.06	49,63,99,114	0
23	CLA	b	603	65/65	0.97	0.06	45,60,85,98	0
23	CLA	b	604	65/65	0.97	0.06	42,54,100,119	0
23	CLA	b	605	65/65	0.97	0.07	37,52,74,80	0
23	CLA	B	610	65/65	0.97	0.07	40,56,71,84	0
23	CLA	B	604	65/65	0.97	0.06	36,47,108,129	0
23	CLA	b	609	65/65	0.97	0.07	53,68,83,102	0
23	CLA	b	610	65/65	0.97	0.07	48,59,73,78	0
23	CLA	b	611	65/65	0.97	0.06	37,48,71,88	0
23	CLA	B	612	65/65	0.97	0.06	35,50,63,71	0
32	LHG	L	101[A]	49/49	0.97	0.06	47,55,68,87	49
32	LHG	L	101[B]	49/49	0.97	0.06	47,56,68,87	49
23	CLA	b	613	65/65	0.97	0.06	42,52,90,108	0
23	CLA	C	511	65/65	0.97	0.07	50,59,84,91	0
23	CLA	b	615	65/65	0.97	0.07	48,64,87,90	0
23	CLA	C	512	65/65	0.97	0.06	48,59,78,84	0
23	CLA	C	513	65/65	0.97	0.07	51,65,81,83	0
23	CLA	c	503	65/65	0.97	0.06	46,60,90,109	0
23	CLA	B	613	65/65	0.97	0.06	38,47,90,106	0
23	CLA	B	605	65/65	0.97	0.05	40,50,67,84	0
23	CLA	D	404[A]	65/65	0.97	0.06	36,44,67,75	65
36	CA	C	525	1/1	0.97	0.06	79,79,79,79	0
23	CLA	D	404[B]	65/65	0.97	0.06	36,44,67,76	65

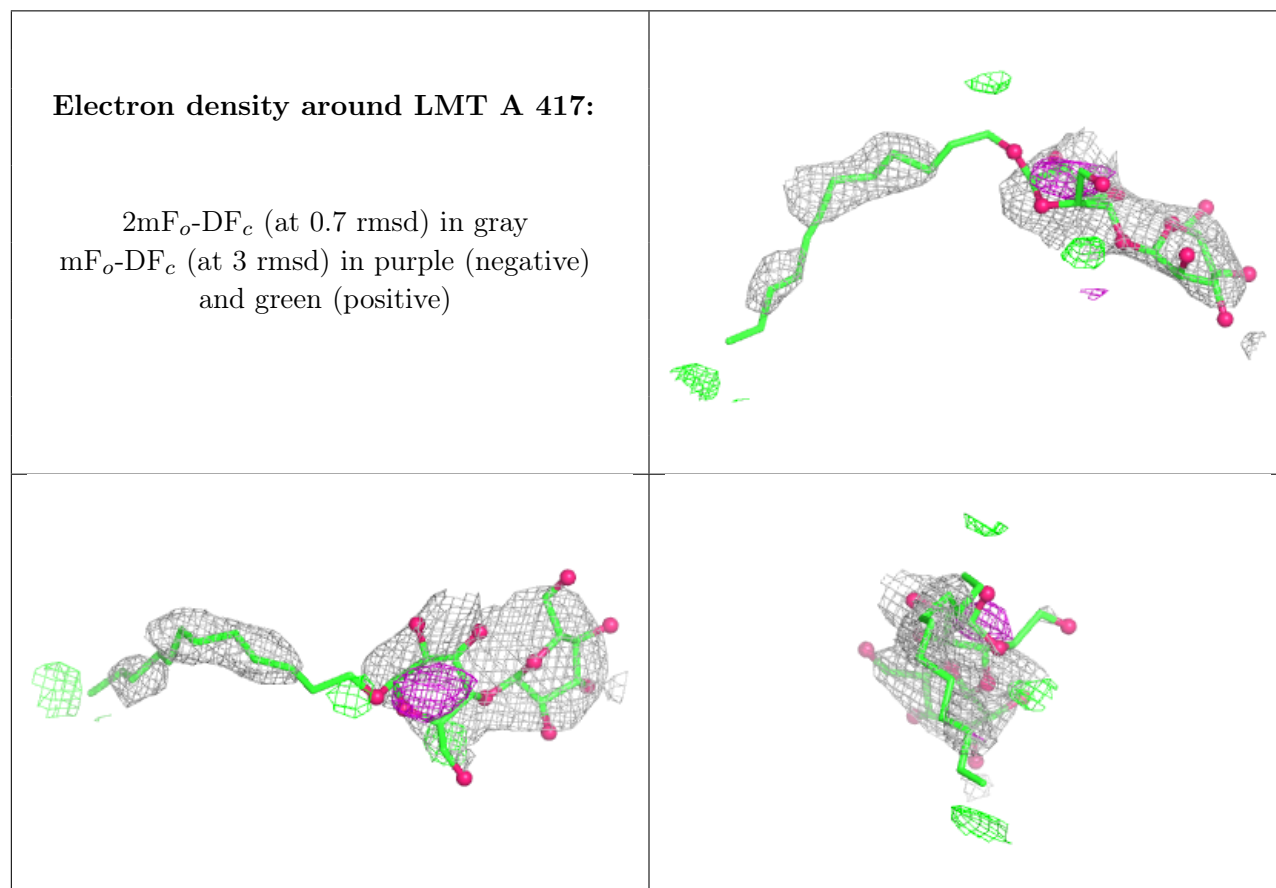
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	BCT	a	404[A]	4/4	0.97	0.05	57,59,65,72	4
36	CA	c	523	1/1	0.97	0.05	78,78,78,78	0
30	BCT	a	404[B]	4/4	0.97	0.05	56,59,65,72	4
23	CLA	B	615	65/65	0.97	0.06	43,55,75,89	0
37	PHO	D	401[A]	64/64	0.97	0.04	39,46,52,56	64
37	PHO	D	401[B]	64/64	0.97	0.04	39,46,52,56	64
23	CLA	a	405[A]	65/65	0.97	0.06	36,46,63,76	65
23	CLA	c	510	65/65	0.97	0.07	45,62,86,94	0
37	PHO	a	408[A]	64/64	0.97	0.05	42,48,53,57	64
37	PHO	a	408[B]	64/64	0.97	0.05	42,48,53,57	64
23	CLA	a	405[B]	65/65	0.97	0.06	39,46,63,76	65
23	CLA	a	406[A]	65/65	0.97	0.05	37,43,63,72	65
23	CLA	B	608	65/65	0.98	0.05	41,52,70,84	0
22	CL	a	403[A]	1/1	0.98	0.09	53,53,53,53	1
22	CL	a	403[B]	1/1	0.98	0.09	53,53,53,53	1
30	BCT	A	414[A]	4/4	0.98	0.06	54,55,61,67	4
30	BCT	A	414[B]	4/4	0.98	0.06	54,55,61,67	4
22	CL	a	402[A]	1/1	0.98	0.05	49,49,49,49	1
23	CLA	b	608	65/65	0.98	0.05	44,57,80,96	0
22	CL	a	402[B]	1/1	0.98	0.05	49,49,49,49	1
23	CLA	C	504	65/65	0.98	0.06	43,55,83,93	0
38	HEM	f	101	43/43	0.98	0.08	69,88,123,141	0
40	HEC	v	201	43/43	0.98	0.06	54,64,74,80	0
22	CL	A	403[B]	1/1	0.99	0.04	47,47,47,47	1
27	OEX	A	411[A]	10/10	0.99	0.03	39,46,50,51	10
27	OEX	A	411[B]	10/10	0.99	0.03	40,46,50,52	10
22	CL	A	402[A]	1/1	0.99	0.06	43,43,43,43	1
38	HEM	F	102	43/43	0.99	0.06	57,72,84,91	0
22	CL	A	402[B]	1/1	0.99	0.06	42,42,42,42	1
39	MG	J	102	1/1	0.99	0.03	60,60,60,60	0
39	MG	j	102	1/1	0.99	0.03	67,67,67,67	0
40	HEC	V	202	43/43	0.99	0.06	37,51,58,60	0
22	CL	A	403[A]	1/1	0.99	0.04	48,48,48,48	1
27	OEX	a	413[B]	10/10	1.00	0.02	46,50,55,56	10
21	FE2	a	401[A]	1/1	1.00	0.01	53,53,53,53	1
21	FE2	a	401[B]	1/1	1.00	0.01	53,53,53,53	1
21	FE2	A	401[A]	1/1	1.00	0.01	51,51,51,51	1
36	CA	c	524	1/1	1.00	0.04	80,80,80,80	0
21	FE2	A	401[B]	1/1	1.00	0.01	51,51,51,51	1
27	OEX	a	413[A]	10/10	1.00	0.02	46,50,55,56	10

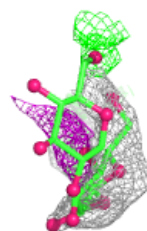
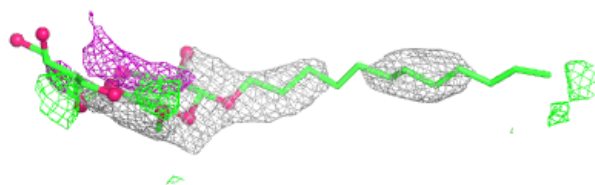
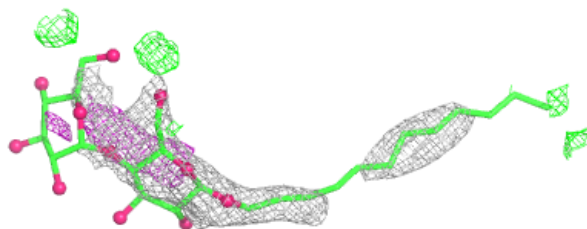
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

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

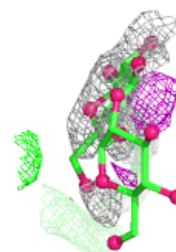
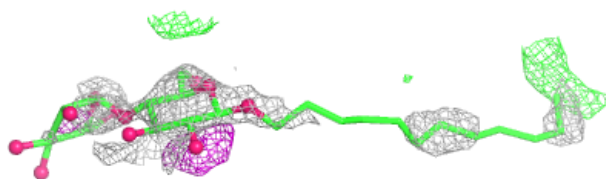
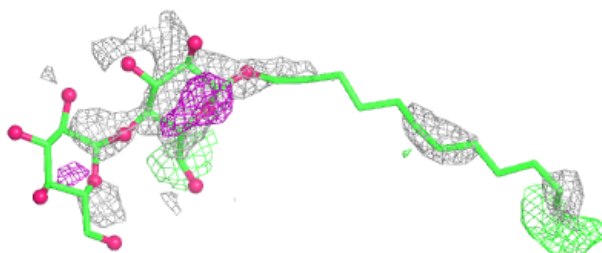


Electron density around LMT F 101:

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

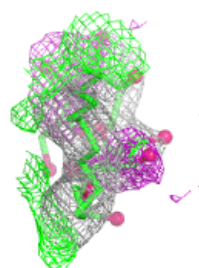
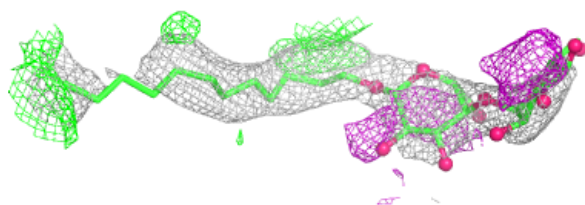
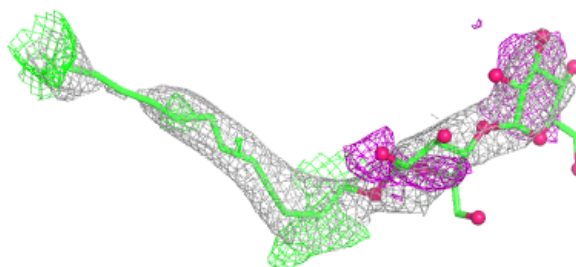
**Electron density around LMT e 101:**

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

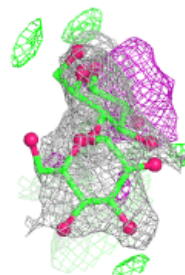
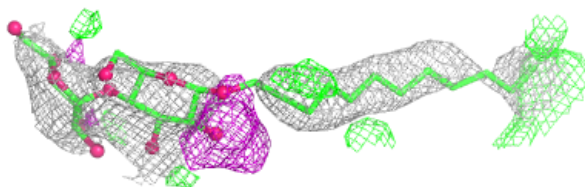
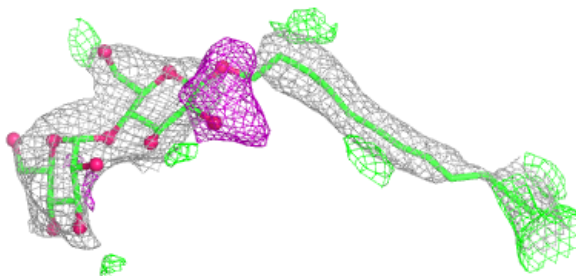


Electron density around LMT B 630:

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

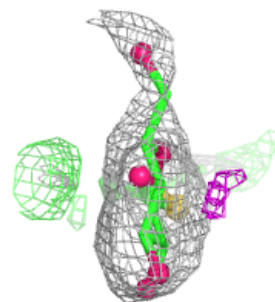
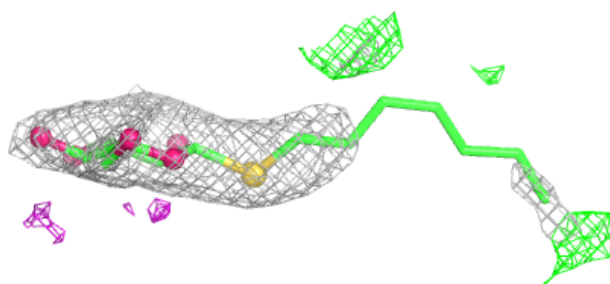
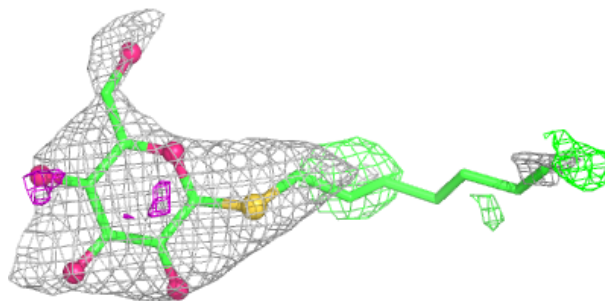
**Electron density around LMT A 415:**

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

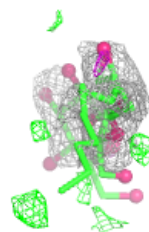
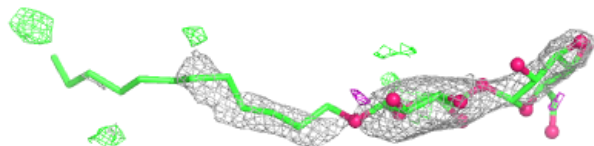
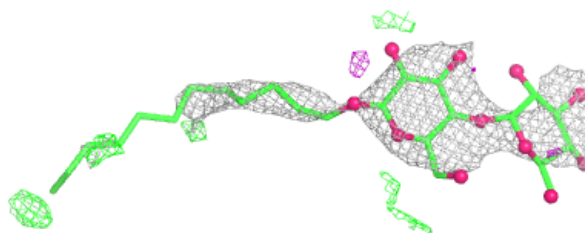


Electron density around HTG C 523:

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

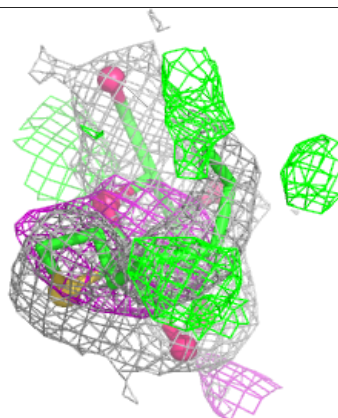
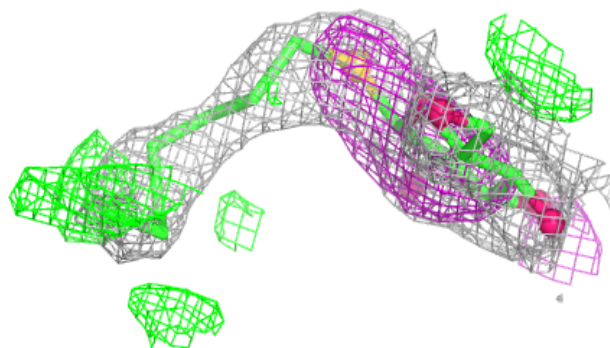
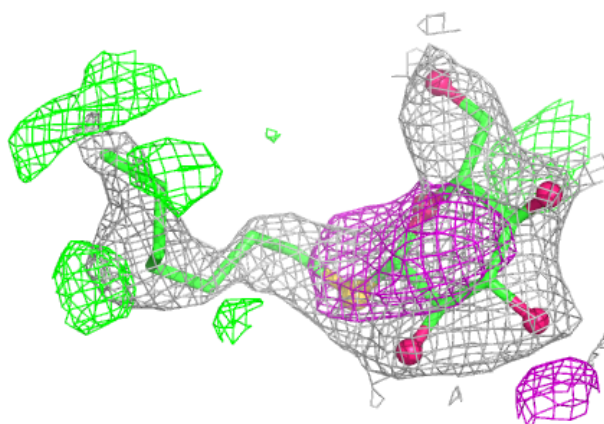
**Electron density around LMT c 501:**

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

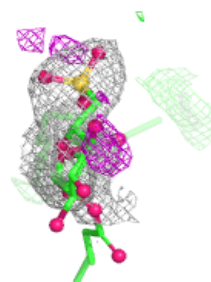
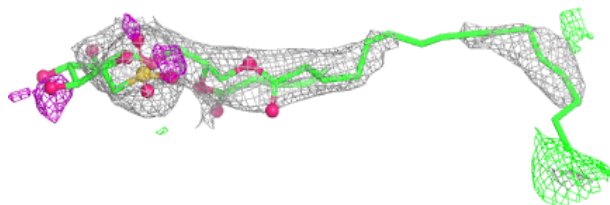
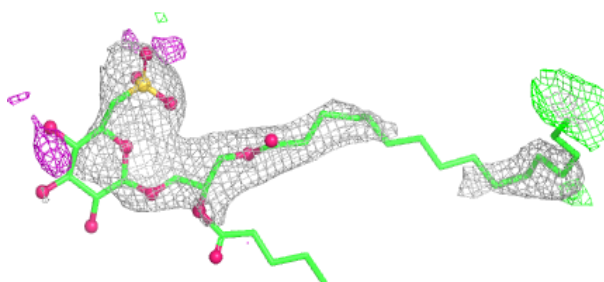


Electron density around HTG B 623:

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

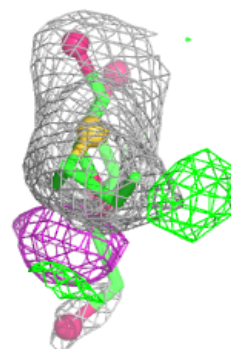
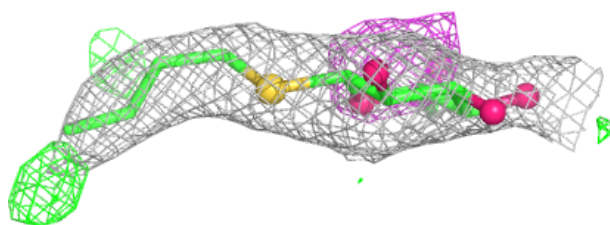
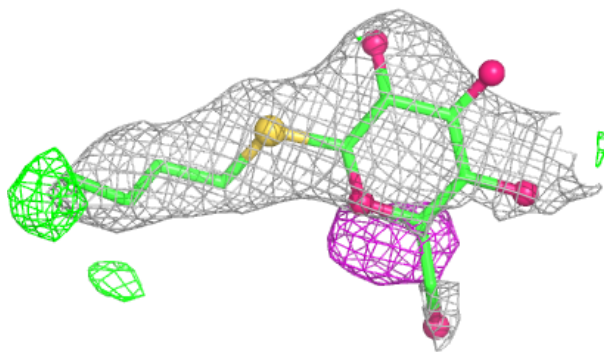
**Electron density around SQD f 102:**

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

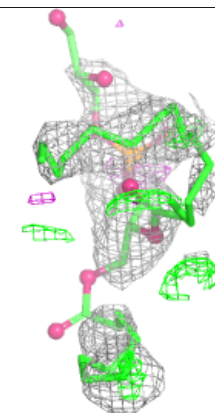
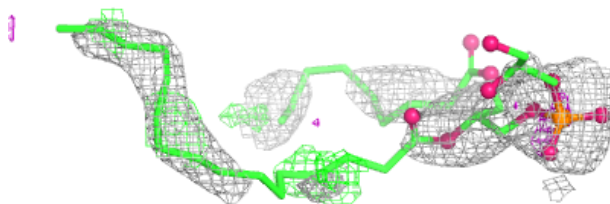
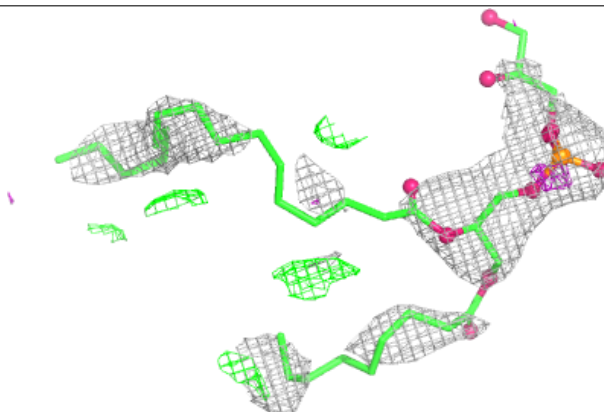


Electron density around HTG D 412:

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

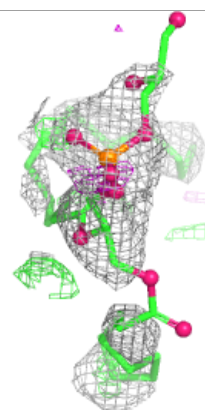
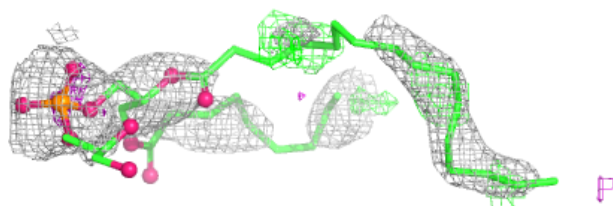
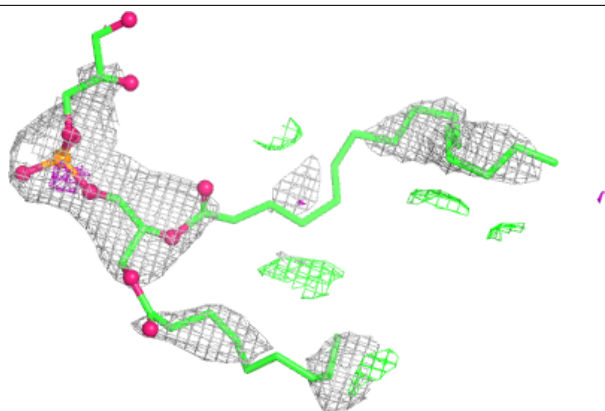
**Electron density around LHG a 420 (A):**

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

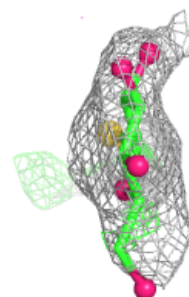
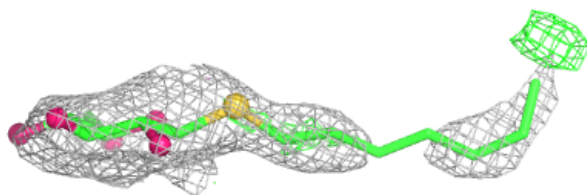


Electron density around LHG a 420 (B):

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

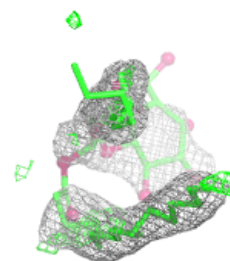
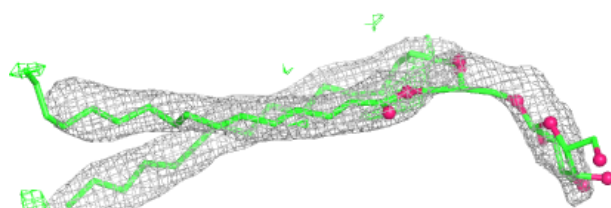
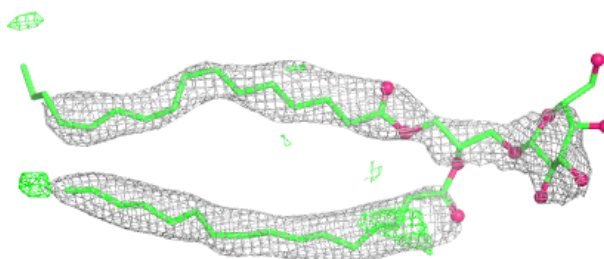
**Electron density around HTG c 522:**

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

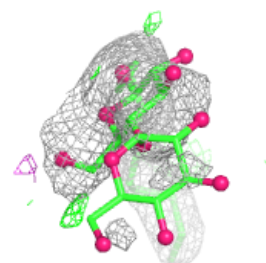
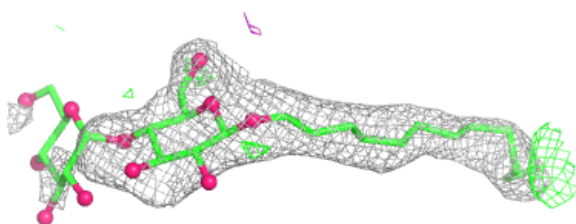
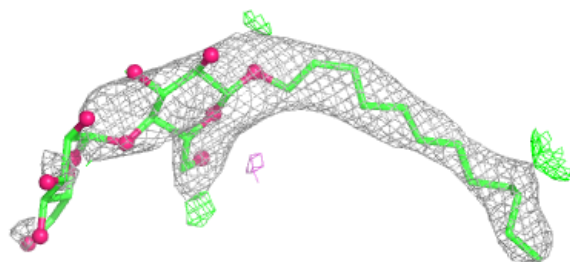


Electron density around LMG C 522:

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

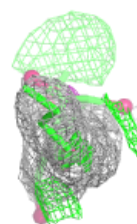
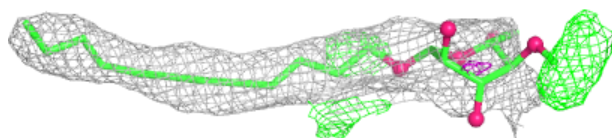
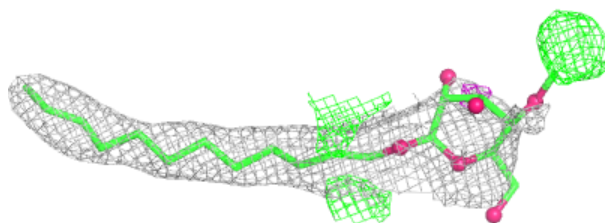
**Electron density around LMT T 101:**

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

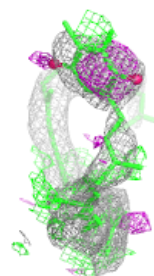
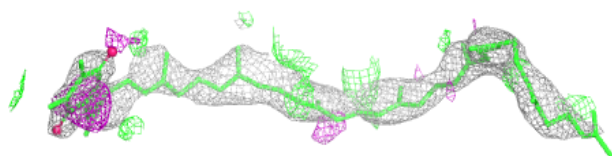
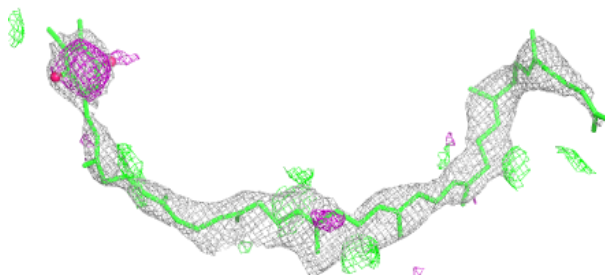


Electron density around LMT b 621:

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

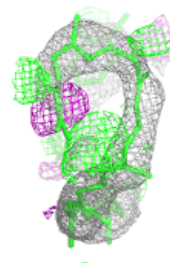
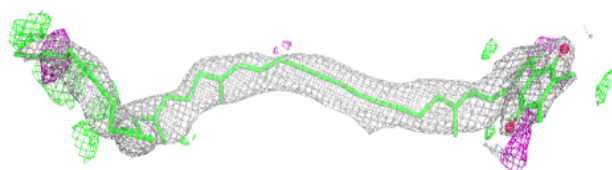
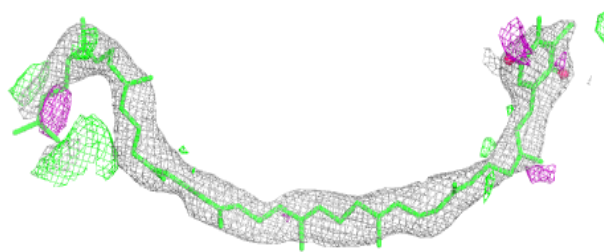
**Electron density around PL9 a 414 (B):**

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

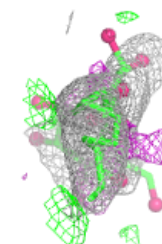
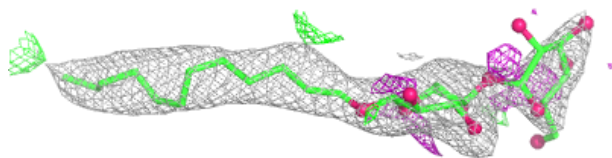
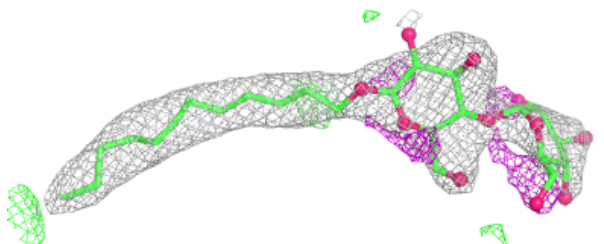


Electron density around PL9 A 412 (A):

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

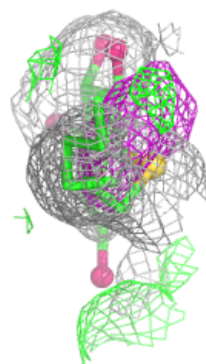
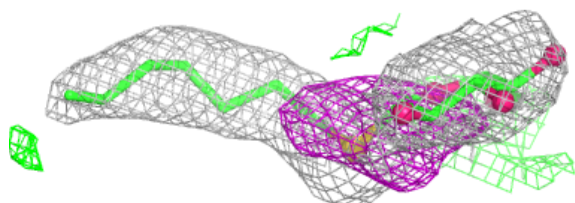
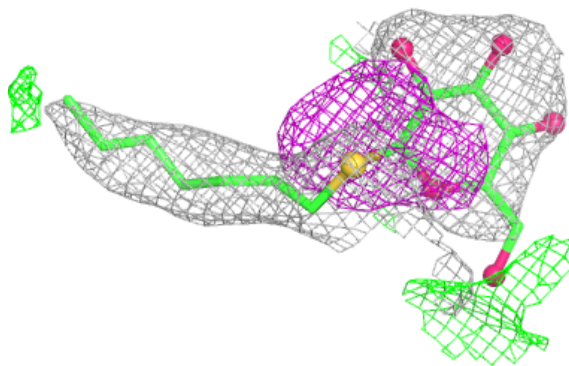
**Electron density around LMT B 628:**

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

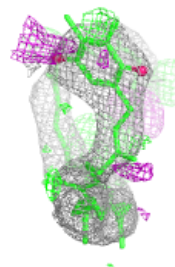
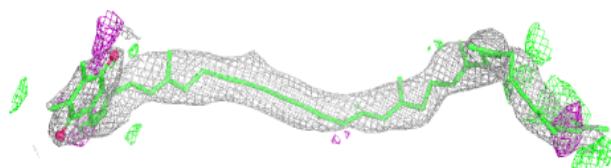
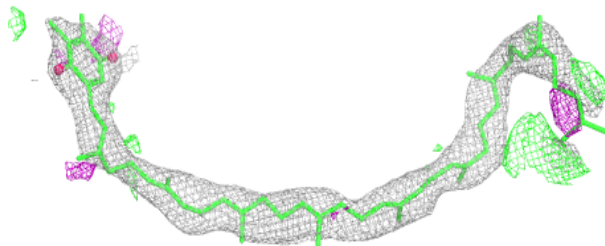


Electron density around HTG b 622:

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

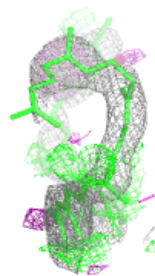
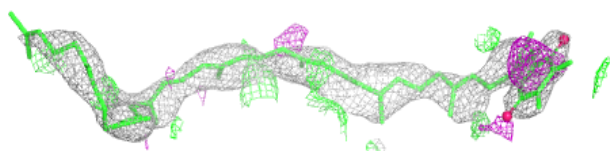
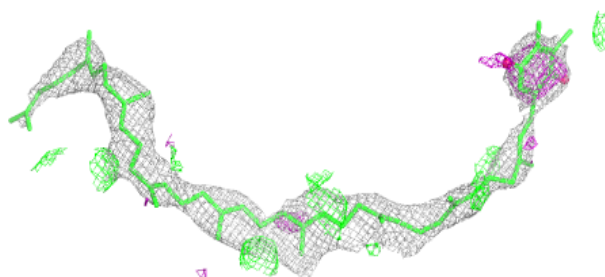
**Electron density around PL9 A 412 (B):**

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



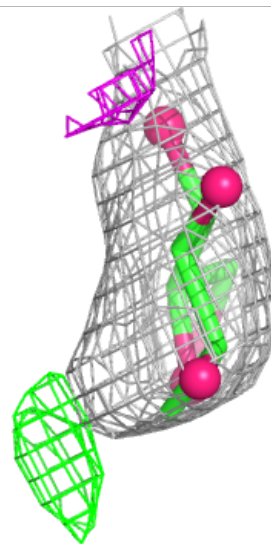
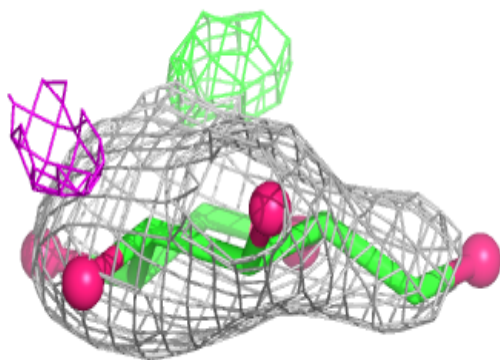
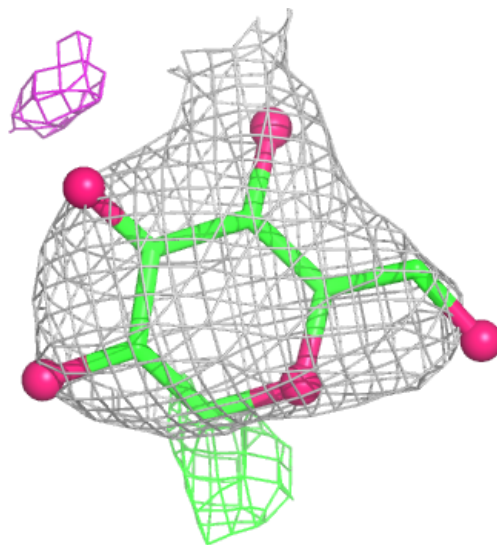
Electron density around PL9 a 414 (A):

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



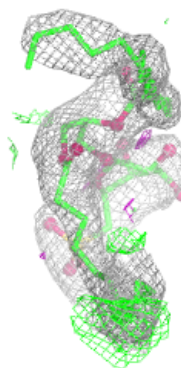
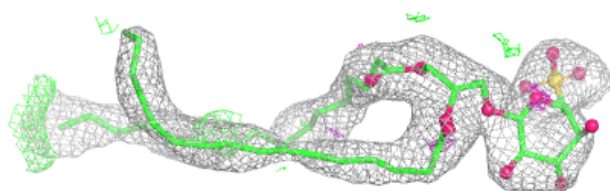
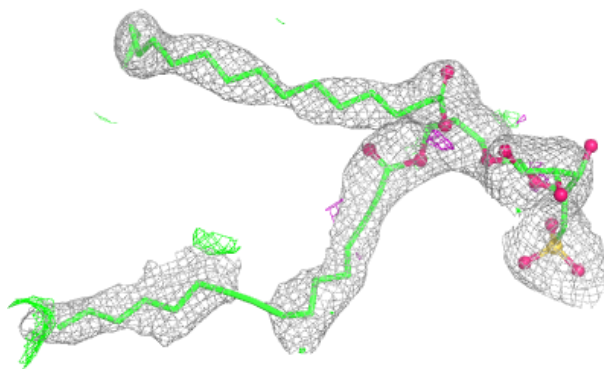
Electron density around HTG V 203:

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

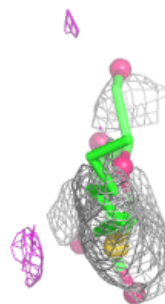
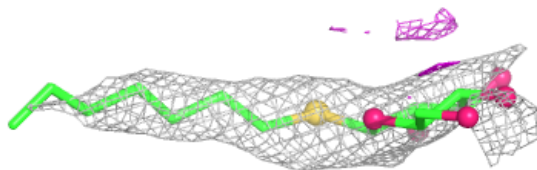
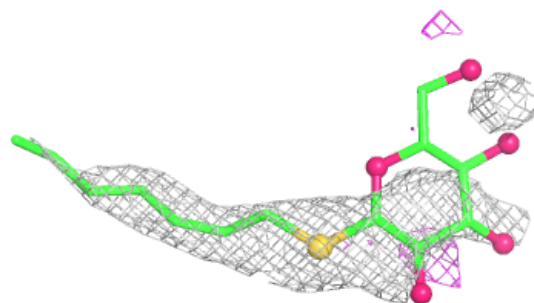


Electron density around SQD a 412:

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

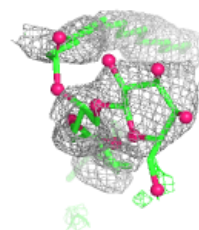
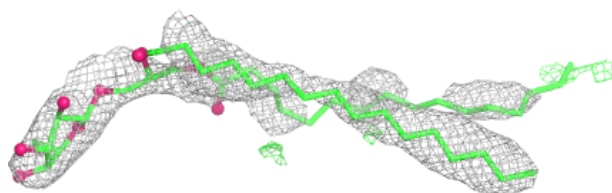
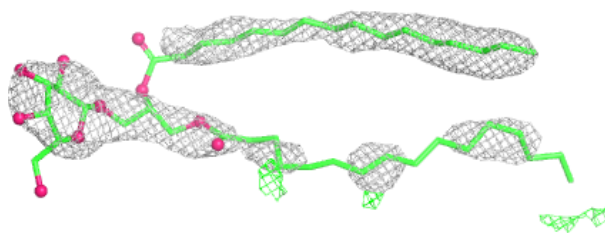
**Electron density around HTG b 623:**

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

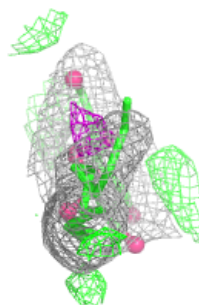
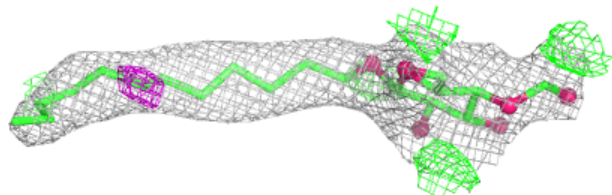
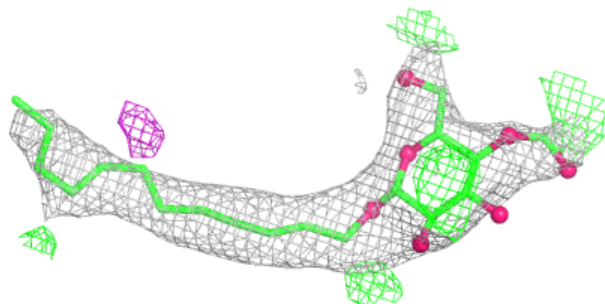


Electron density around LMG c 521:

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

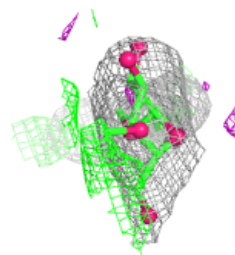
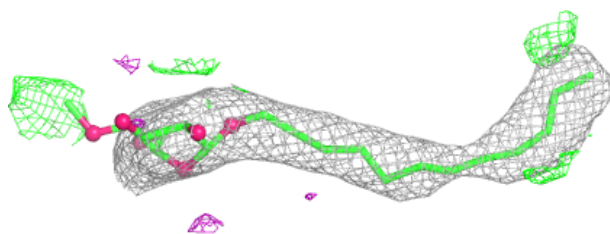
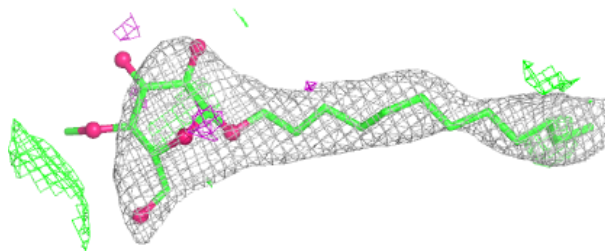
**Electron density around LMT t 102:**

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

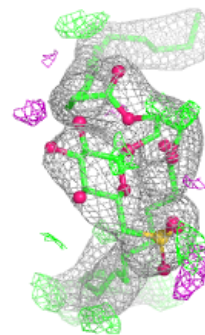
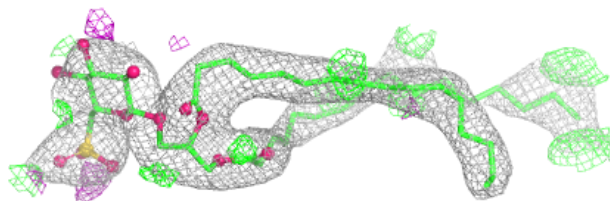
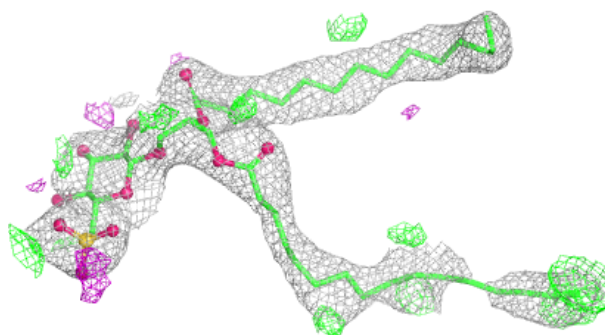


Electron density around LMT t 101:

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

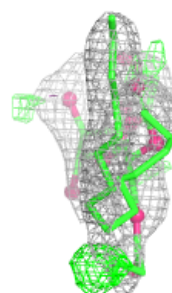
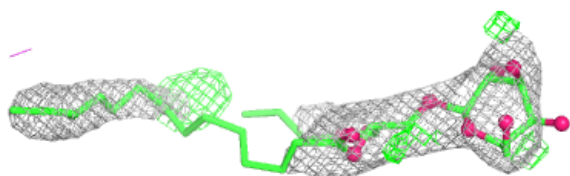
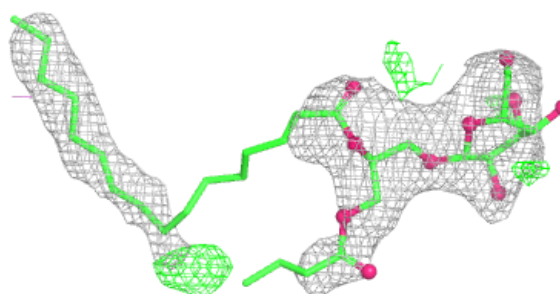
**Electron density around SQD A 410:**

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

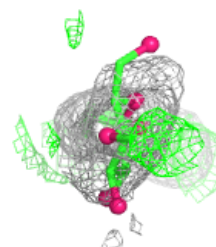
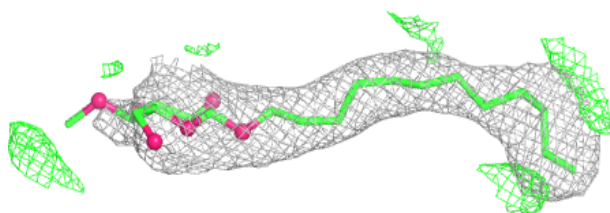
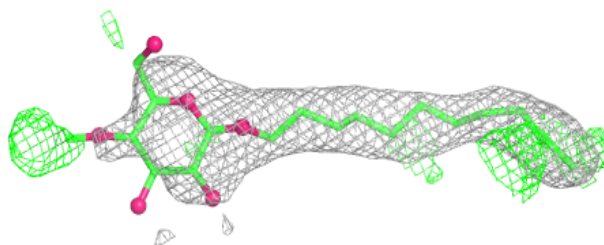


Electron density around LMG z 101:

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

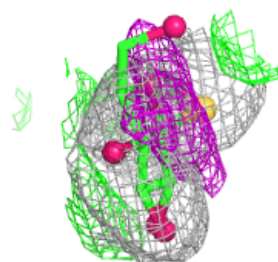
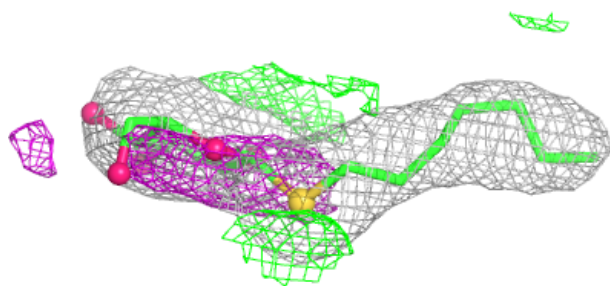
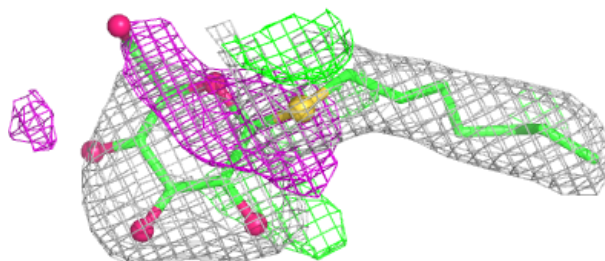
**Electron density around LMT b 627:**

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

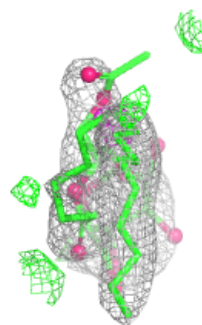
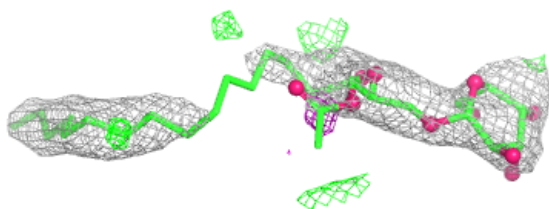
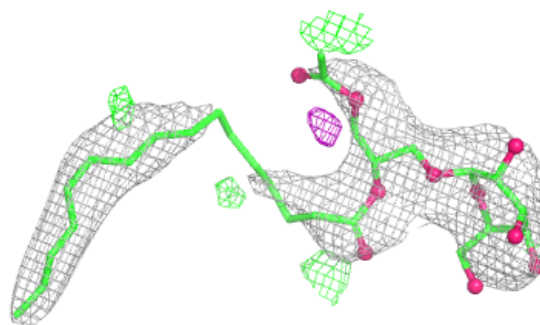


Electron density around HTG B 622:

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

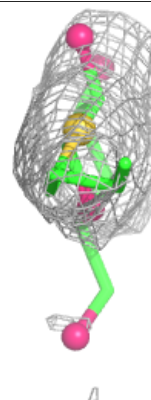
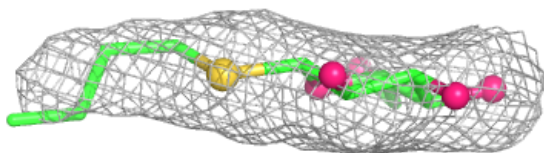
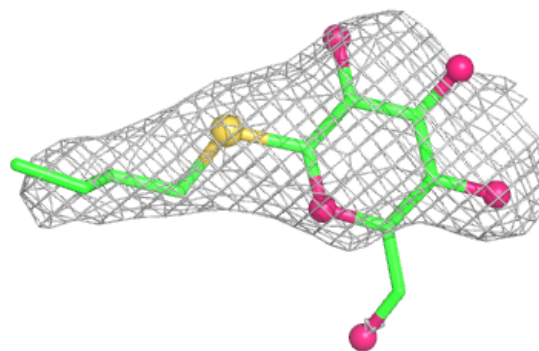
**Electron density around LMG C 526:**

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

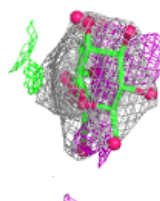
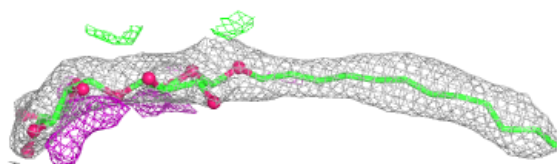
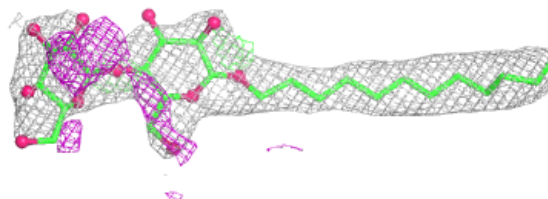


Electron density around HTG d 408:

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

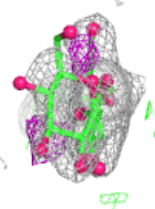
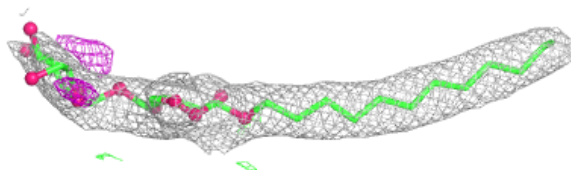
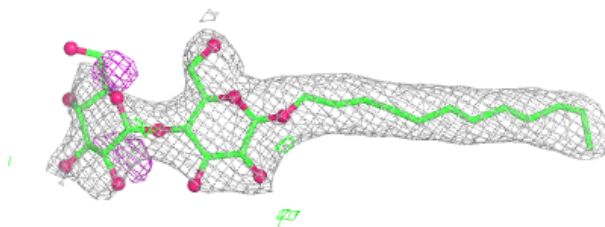
**Electron density around LMT m 103:**

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

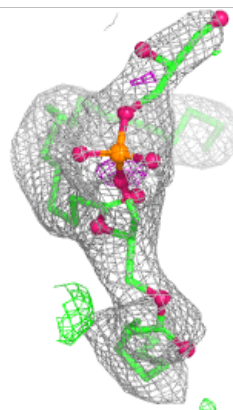
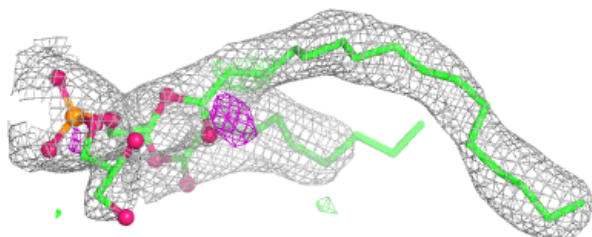
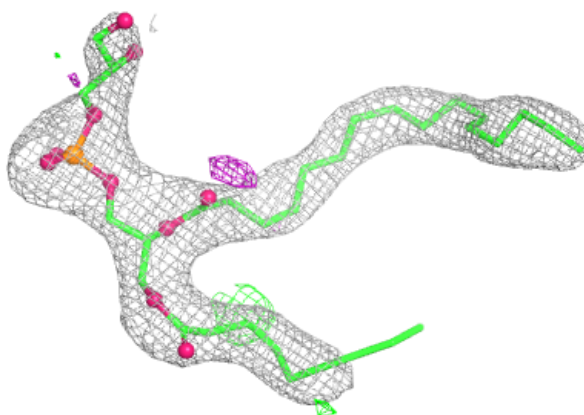


Electron density around LMT M 101:

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

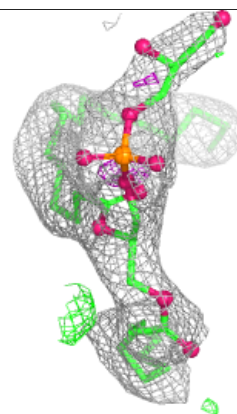
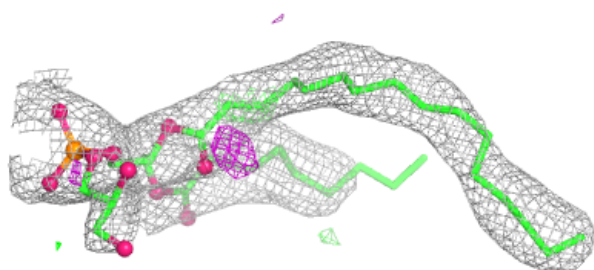
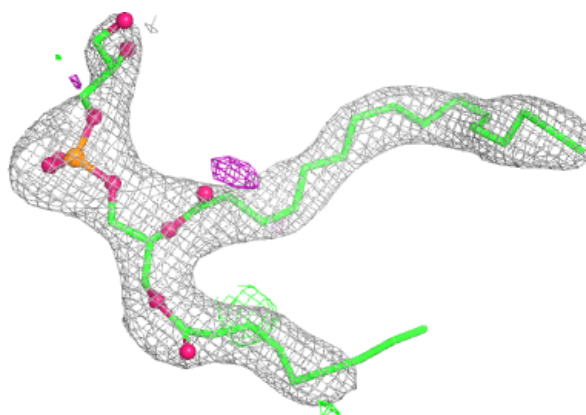
**Electron density around LHG E 101 (A):**

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

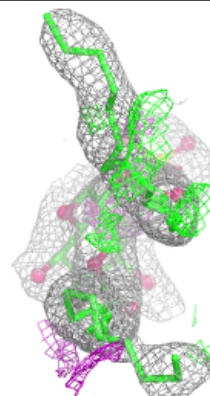
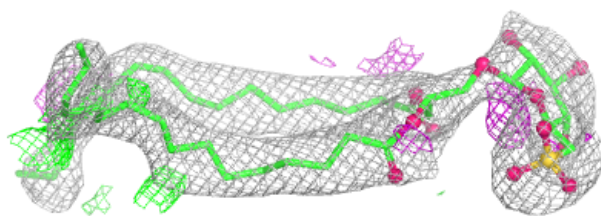
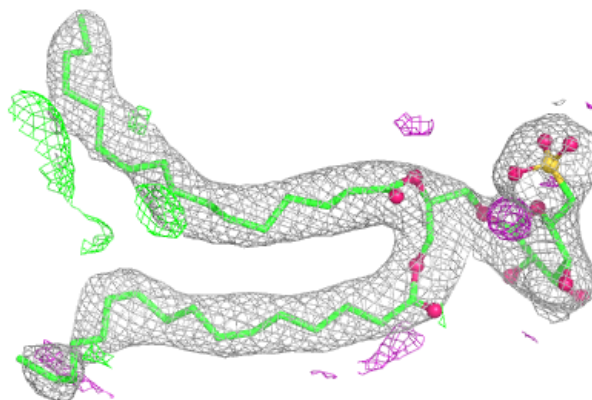


Electron density around LHG E 101 (B):

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

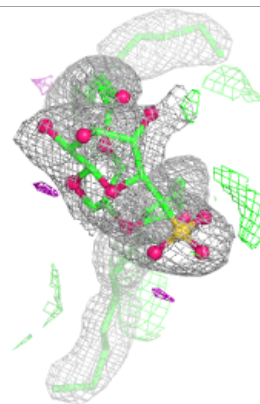
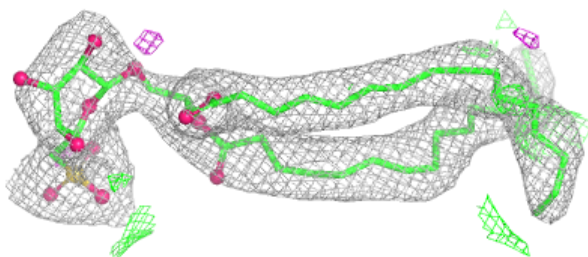
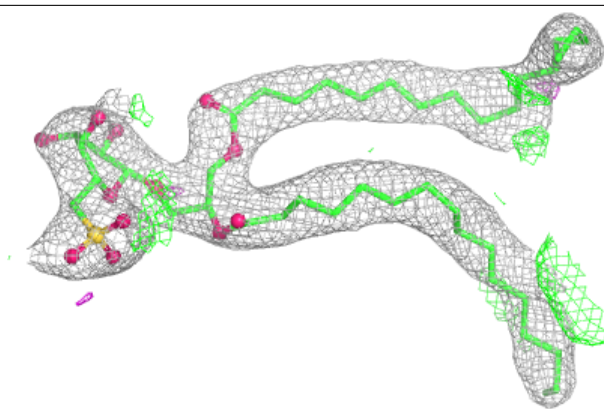
**Electron density around SQD b 620:**

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

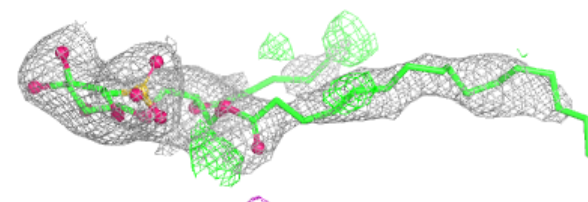
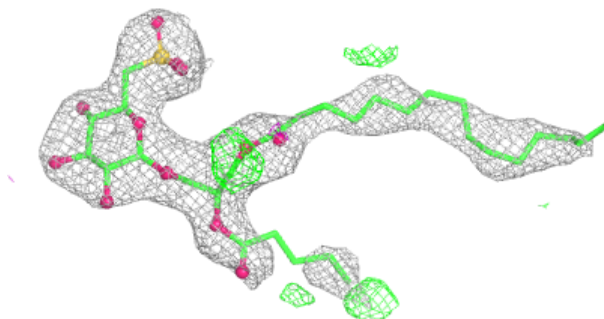


Electron density around SQD B 620:

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

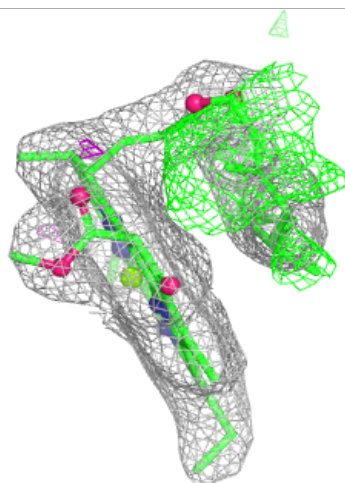
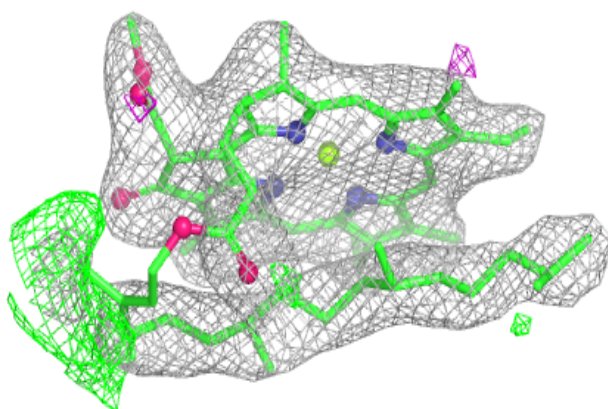
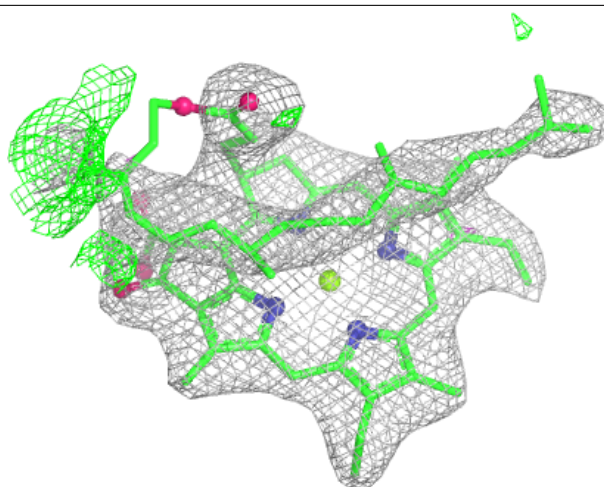
**Electron density around SQD F 103:**

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



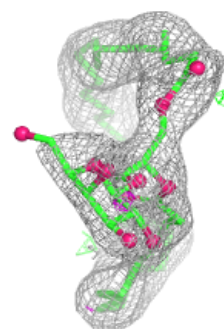
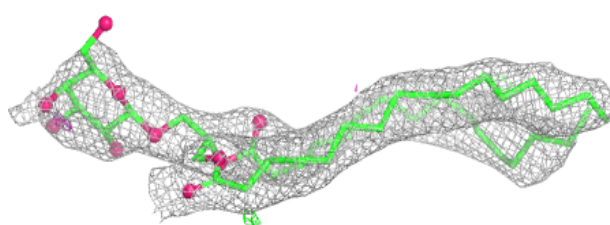
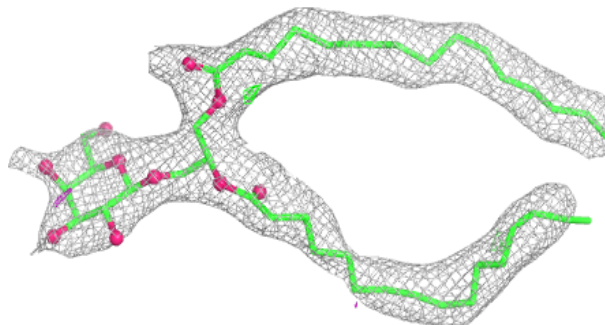
Electron density around CLA b 601:

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

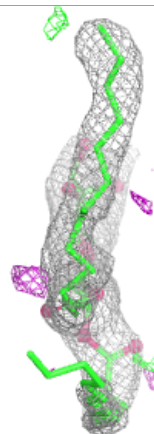
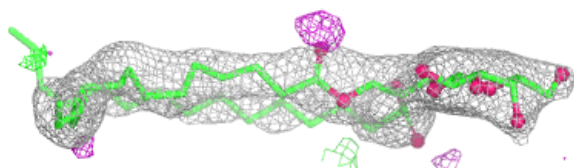
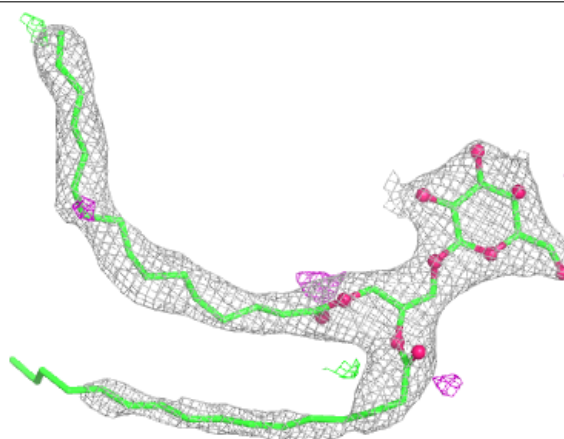


Electron density around LMG a 417:

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

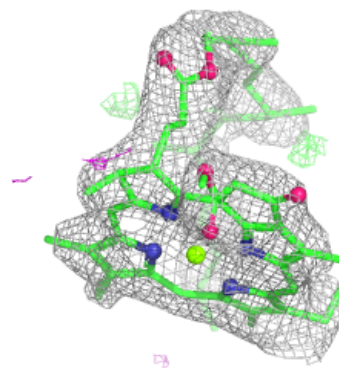
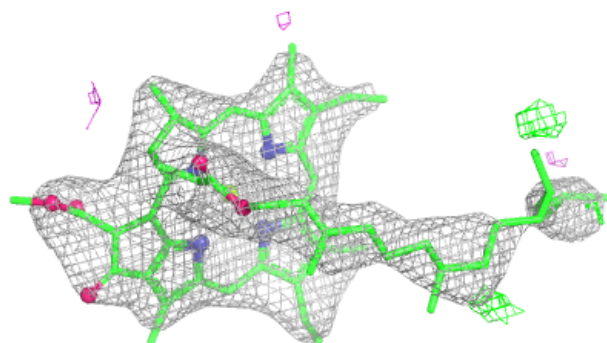
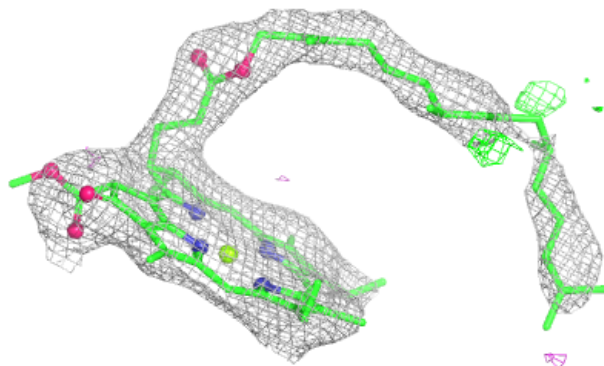
**Electron density around LMG c 520:**

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

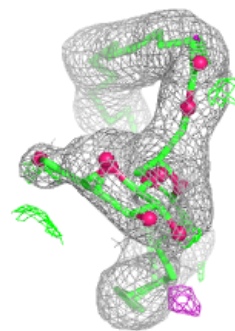
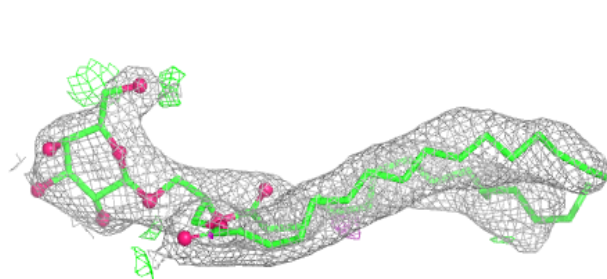
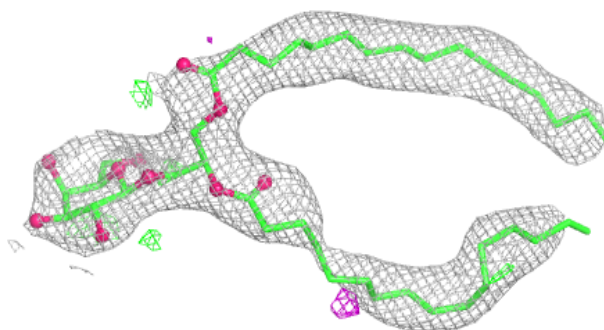


Electron density around CLA c 514:

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

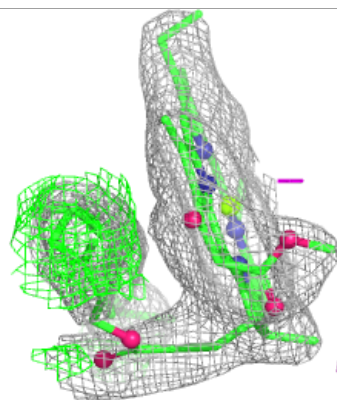
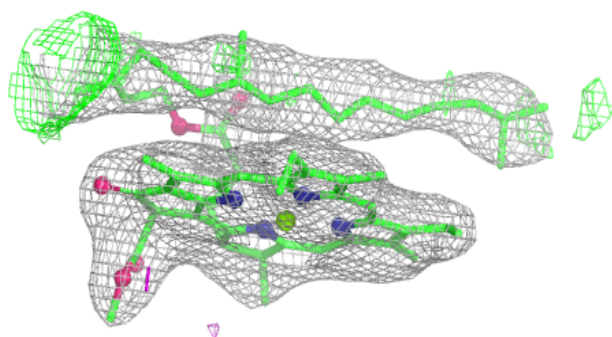
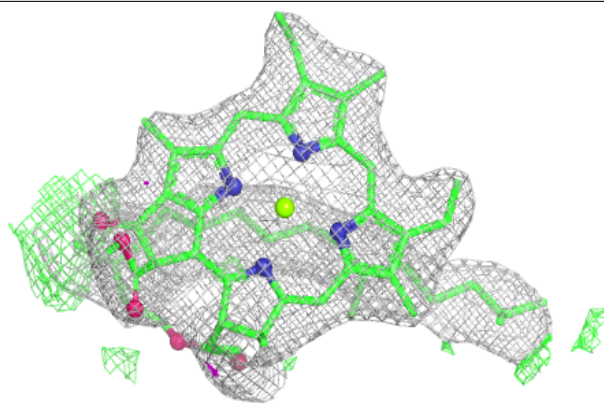
**Electron density around LMG C 502:**

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

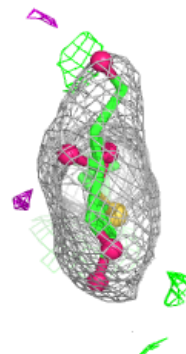
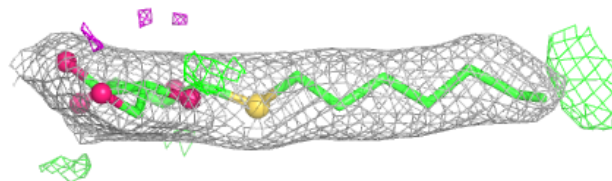
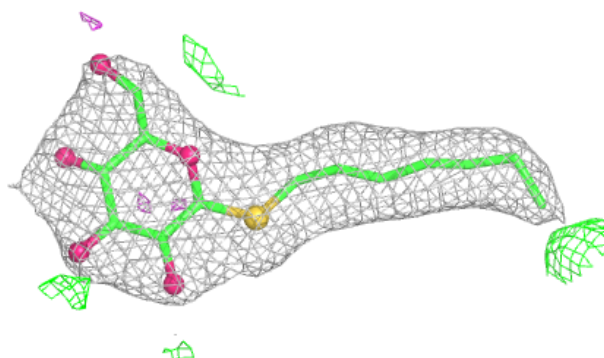


Electron density around CLA B 601:

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

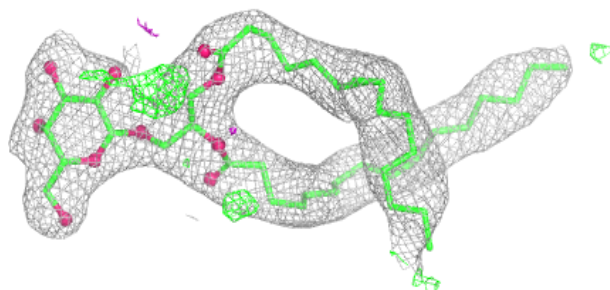
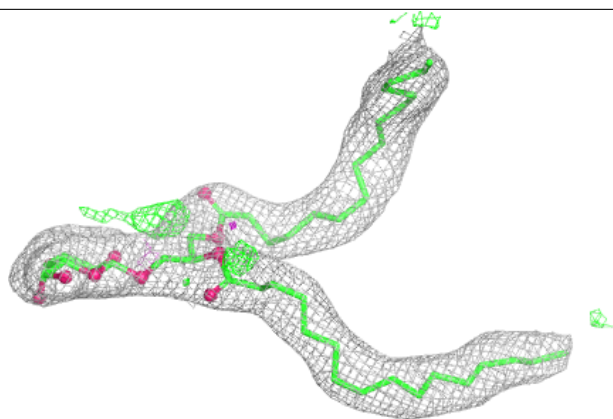
**Electron density around HTG B 625:**

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

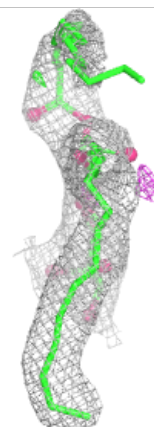
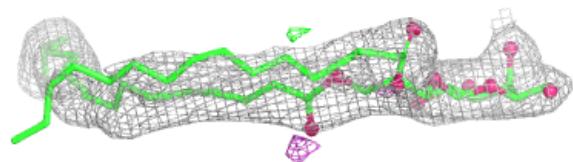
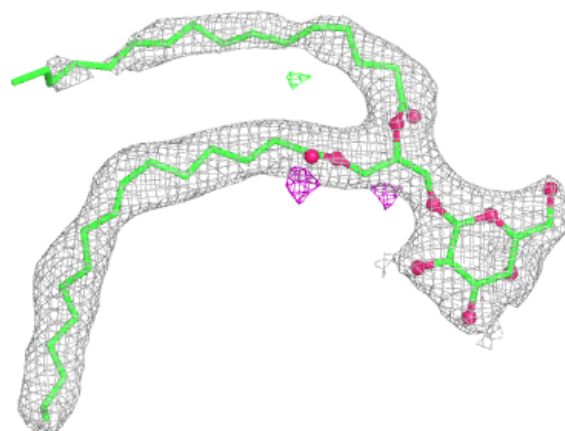


Electron density around LMG B 621:

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

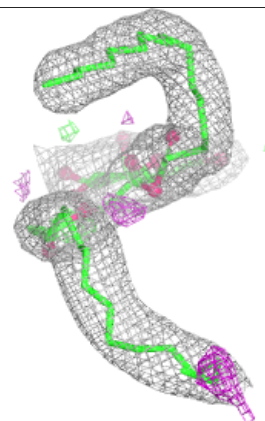
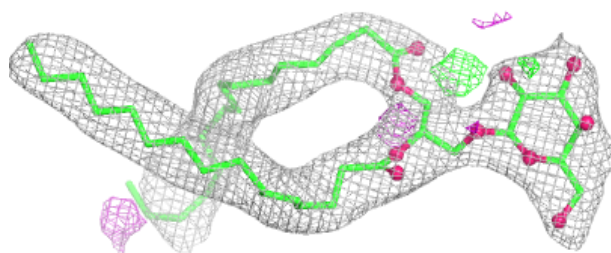
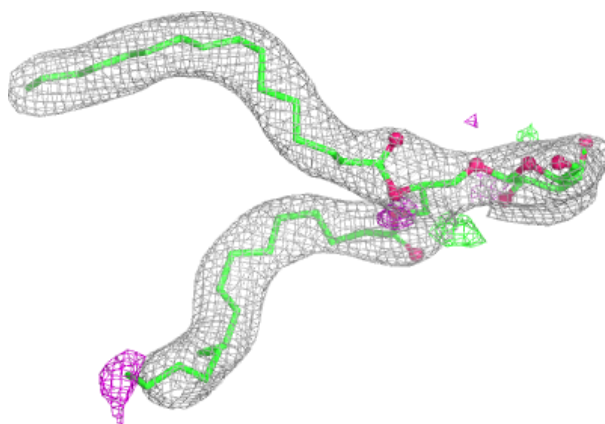
**Electron density around LMG C 521:**

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

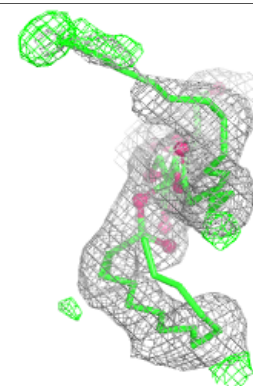
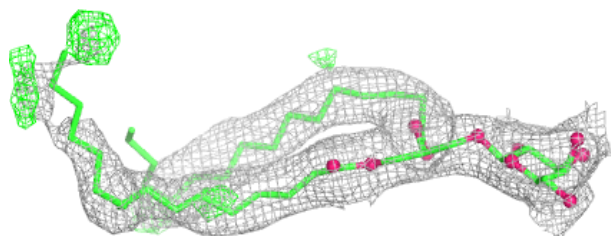
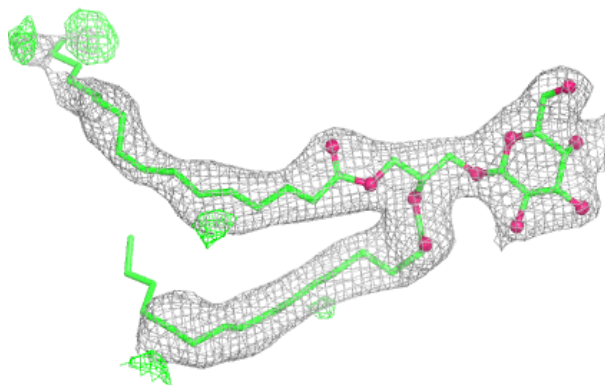


Electron density around LMG m 101:

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

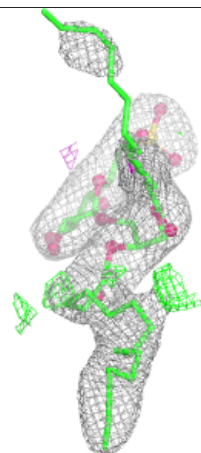
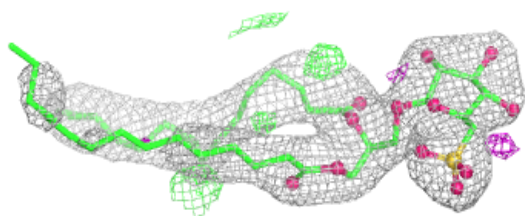
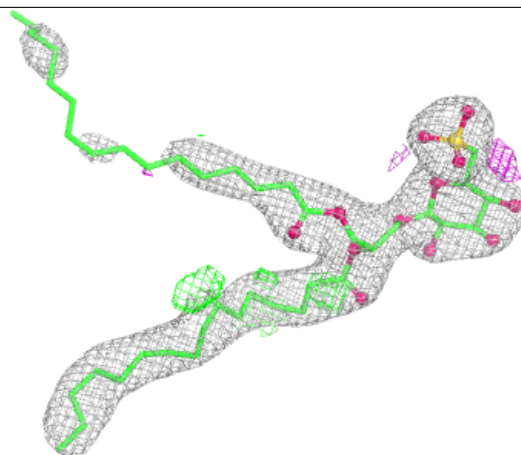
**Electron density around LMG D 413:**

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



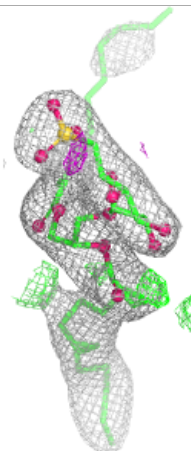
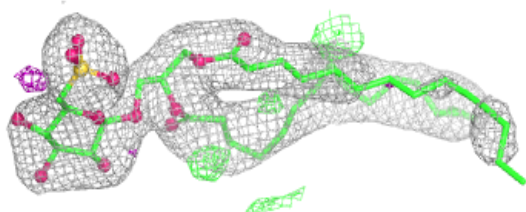
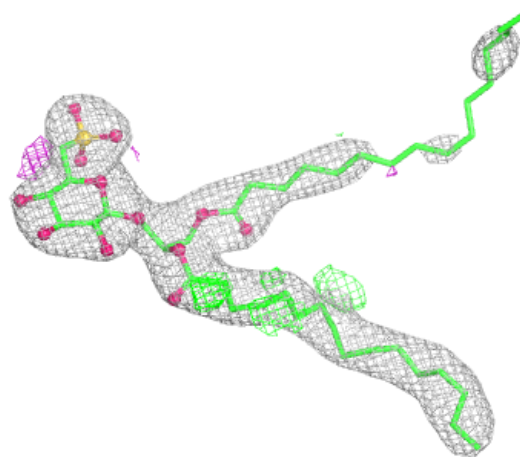
Electron density around SQD C 501 (A):

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



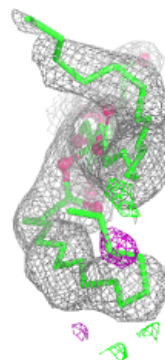
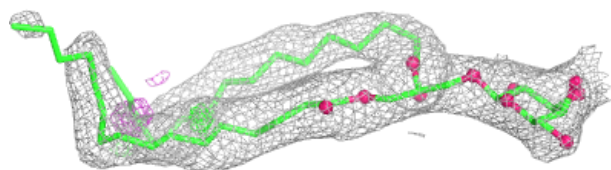
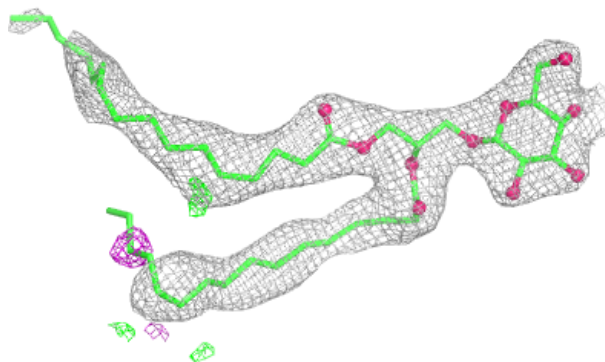
Electron density around SQD C 501 (B):

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



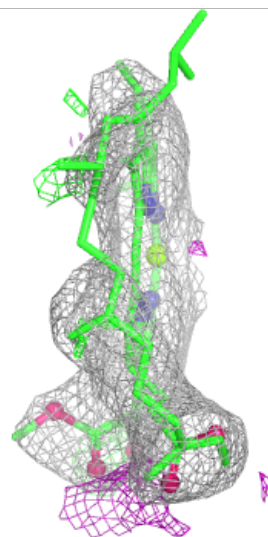
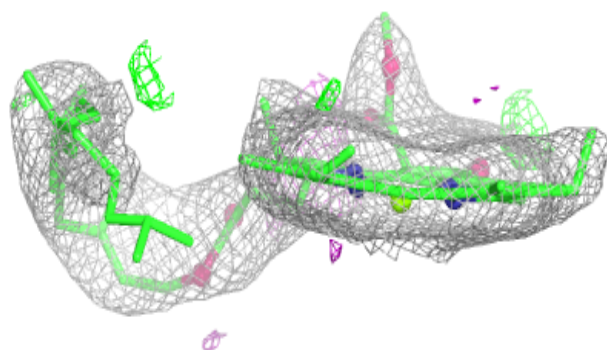
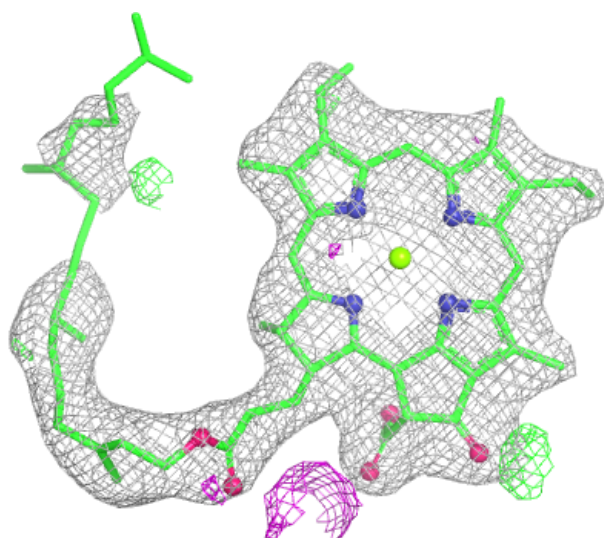
Electron density around LMG d 409:

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



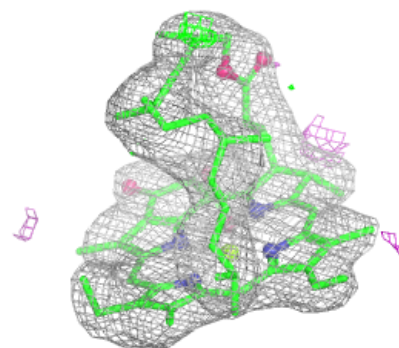
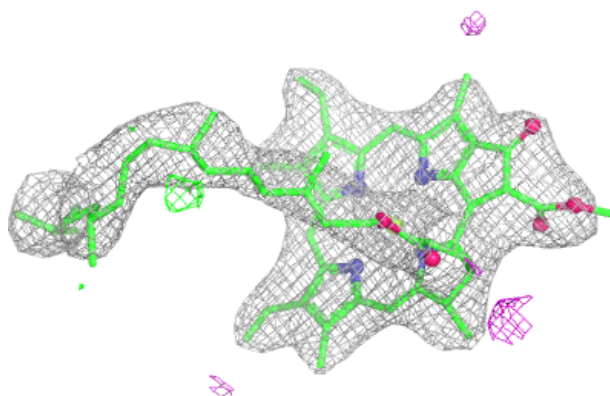
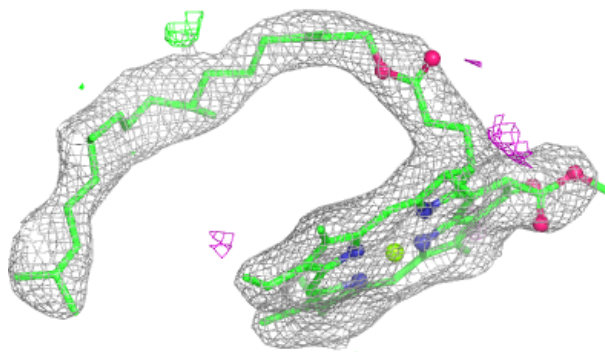
Electron density around CLA c 513:

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

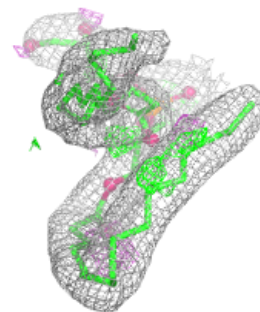
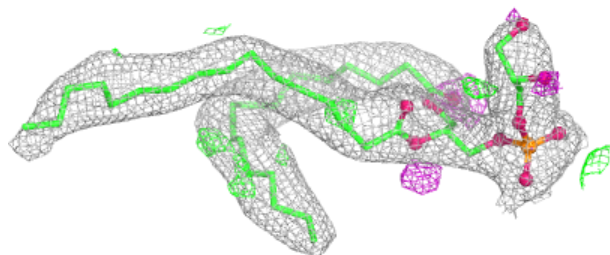
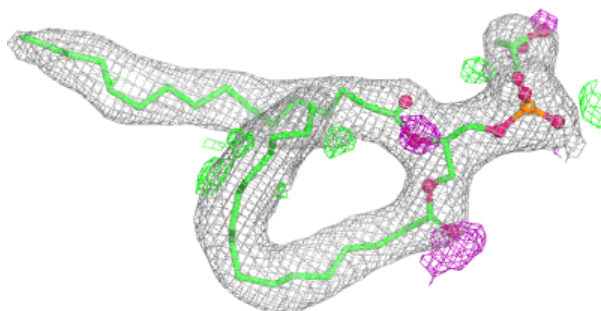


Electron density around CLA C 515:

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

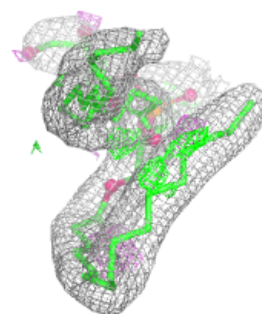
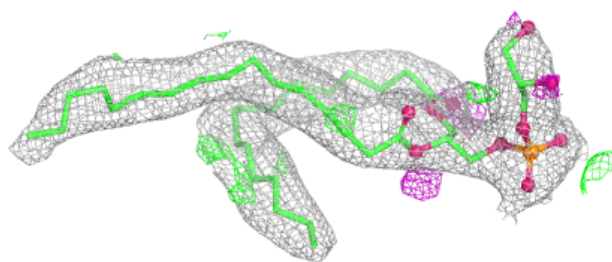
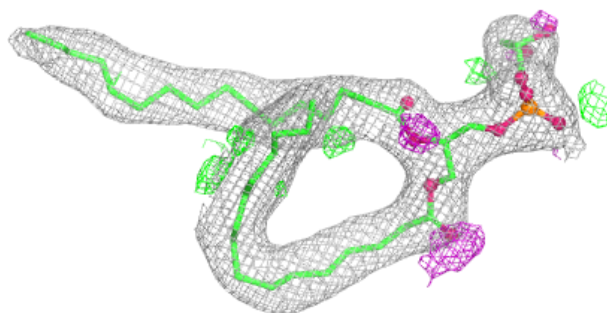
**Electron density around LHG A 416 (A):**

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

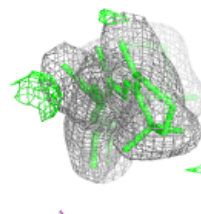
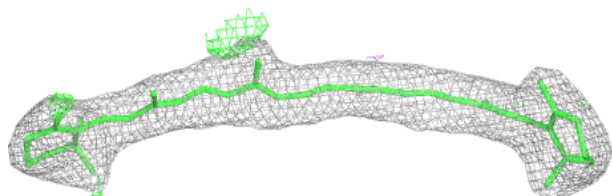
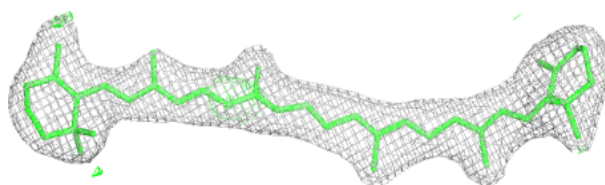


Electron density around LHG A 416 (B):

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

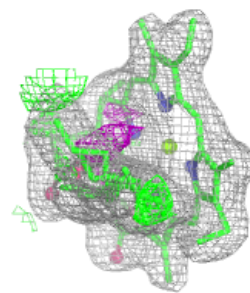
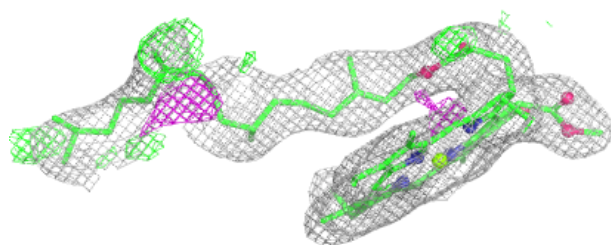
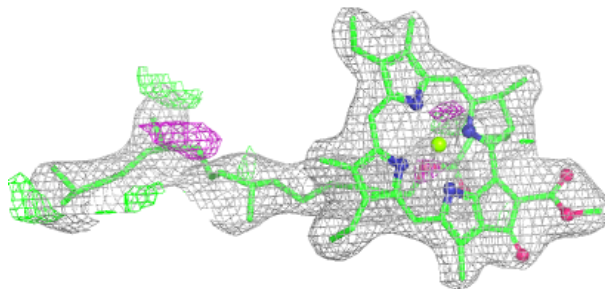
**Electron density around BCR T 102:**

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

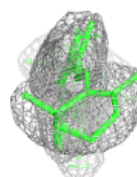
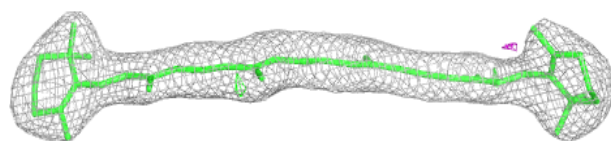
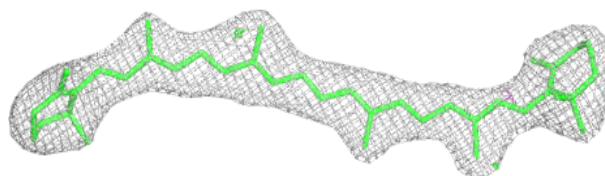


Electron density around CLA B 614:

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

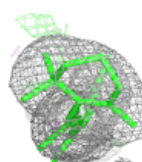
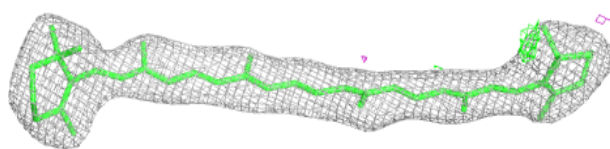
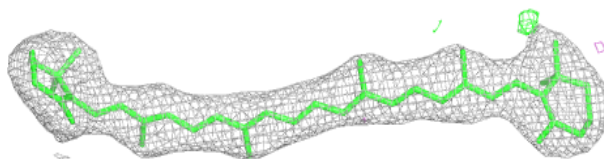
**Electron density around BCR Y 101:**

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

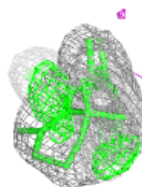
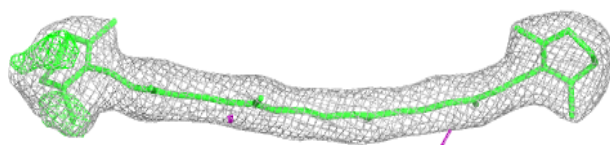
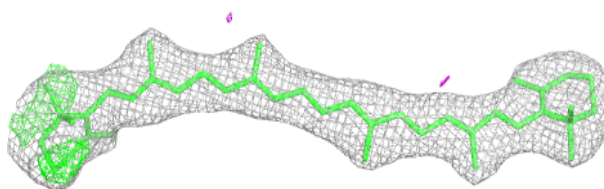


Electron density around BCR c 515:

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

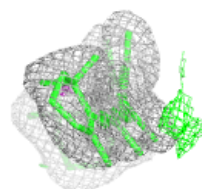
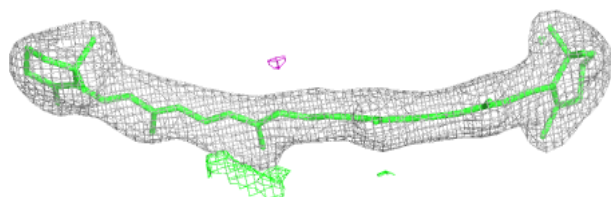
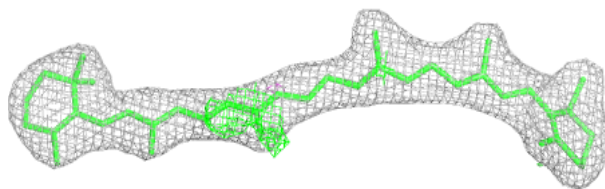
**Electron density around BCR d 403:**

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

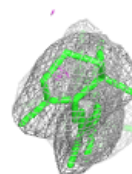
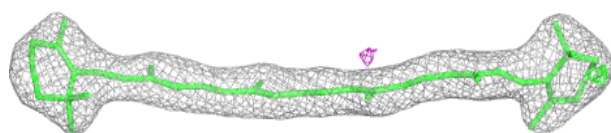
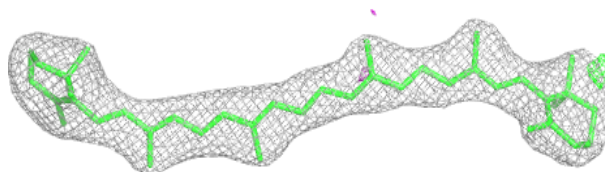


Electron density around BCR t 103:

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

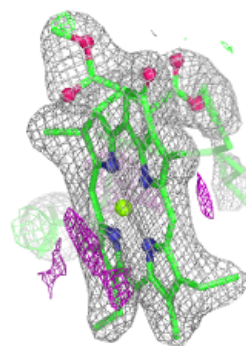
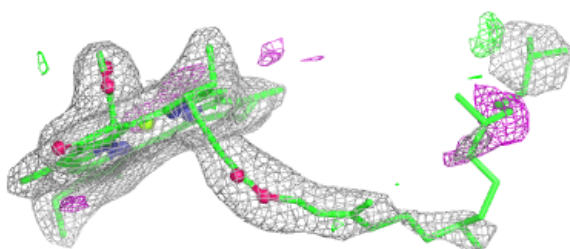
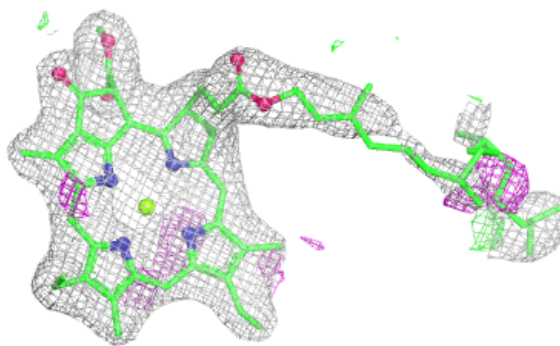
**Electron density around BCR y 101:**

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

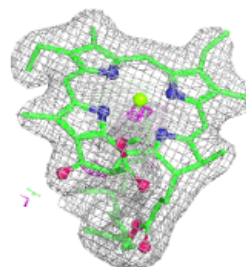
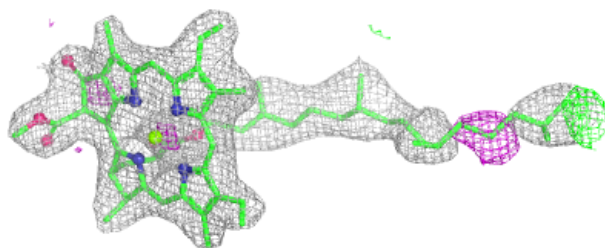
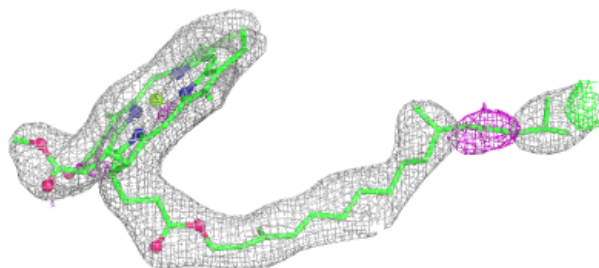


Electron density around CLA a 409:

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

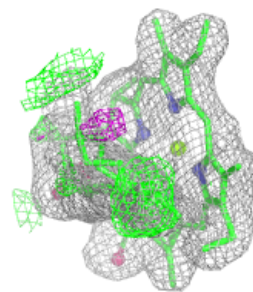
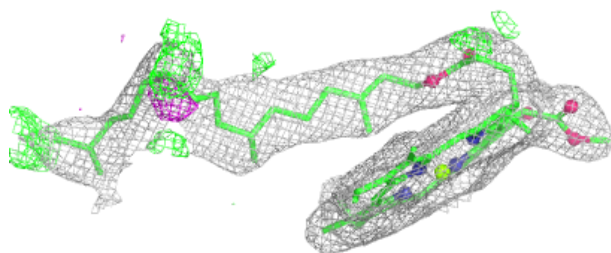
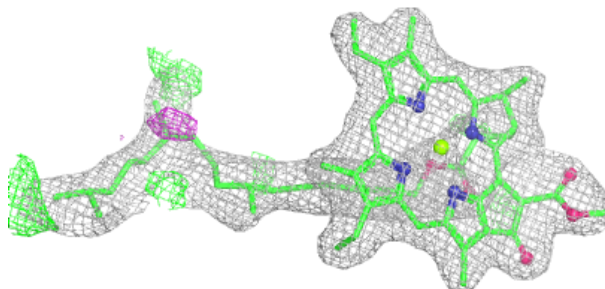
**Electron density around CLA C 506:**

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

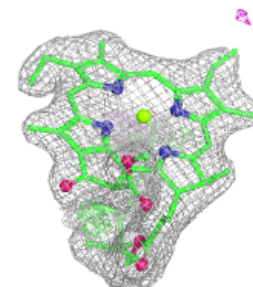
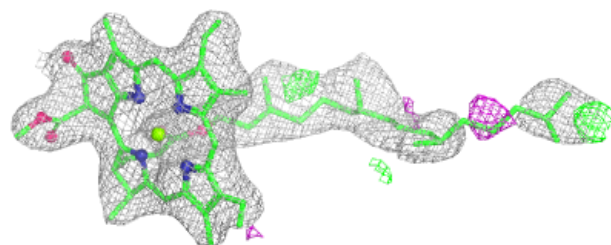
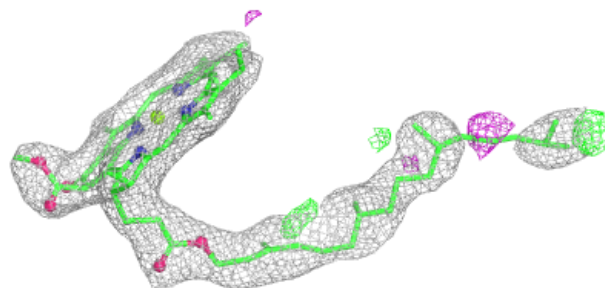


Electron density around CLA b 614:

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

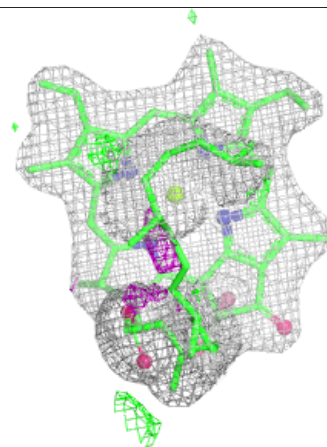
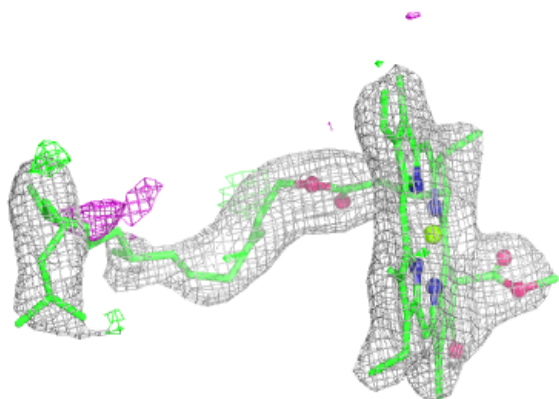
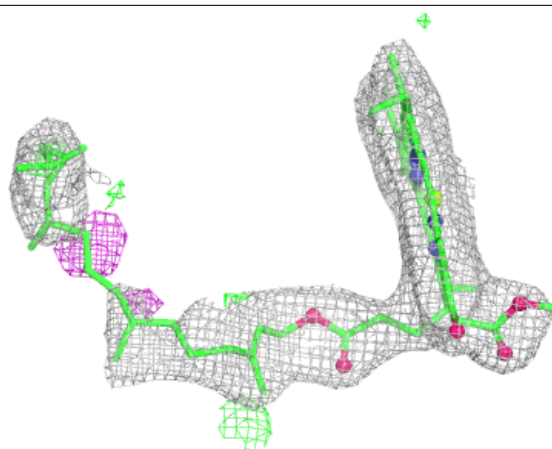
**Electron density around CLA c 505:**

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



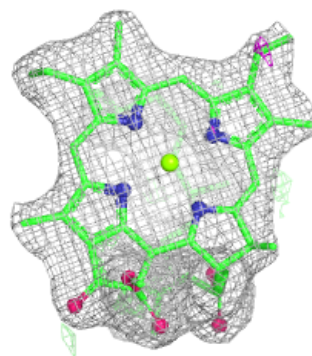
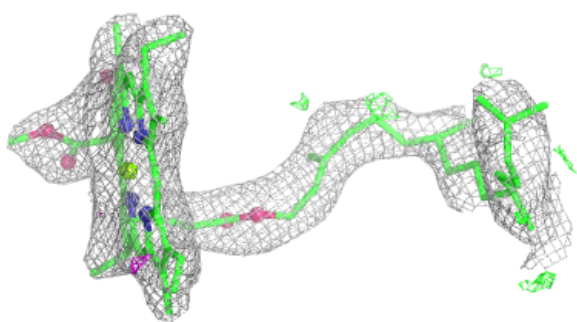
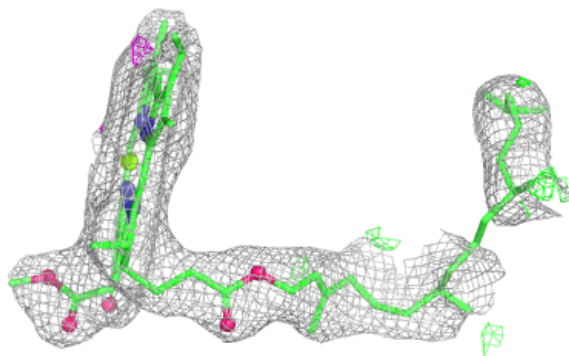
Electron density around CLA c 507:

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



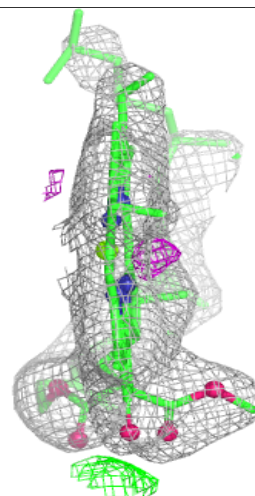
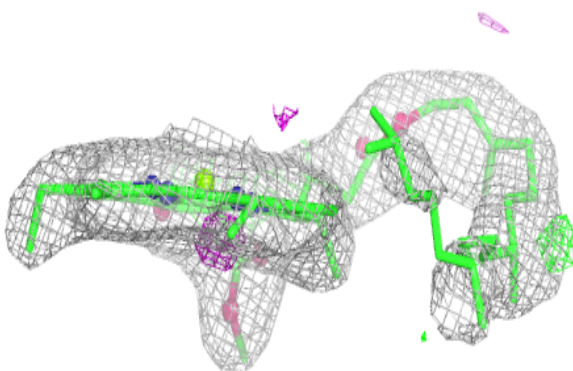
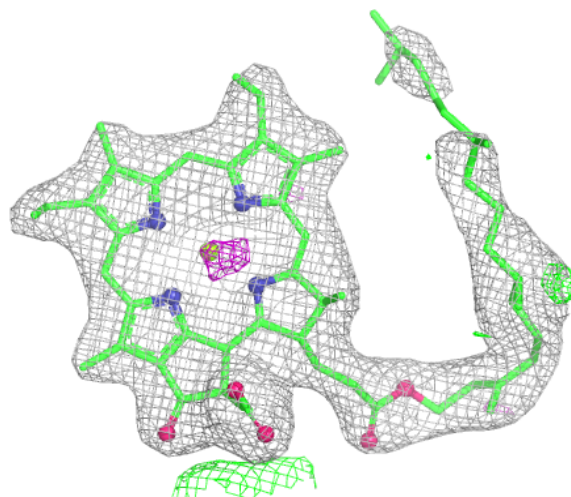
Electron density around CLA C 508:

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



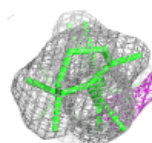
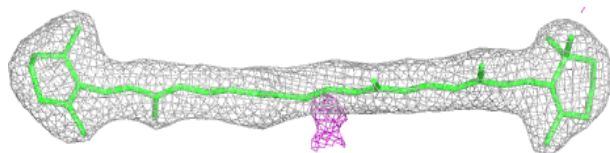
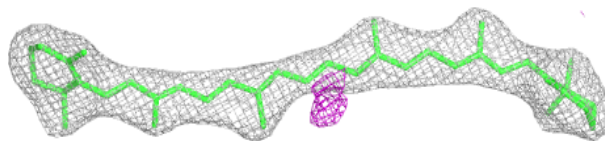
Electron density around CLA C 514:

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



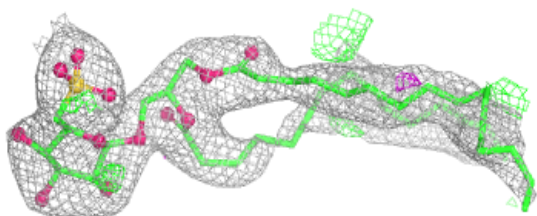
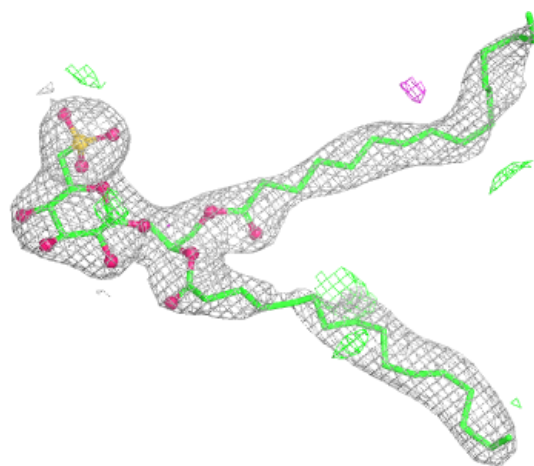
Electron density around BCR C 516:

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



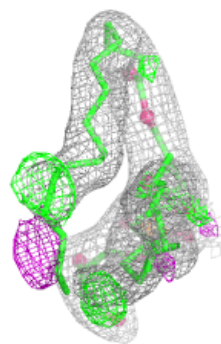
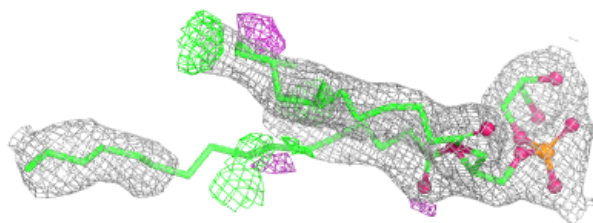
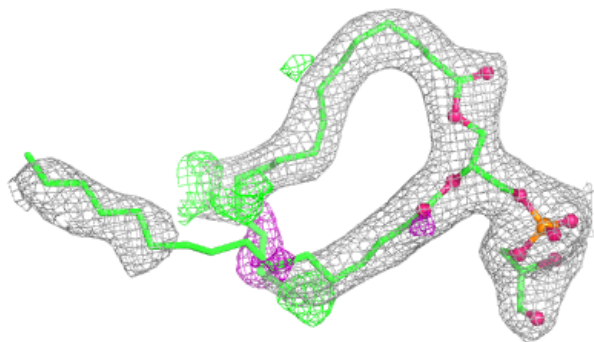
Electron density around SQD a 411 (A):

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

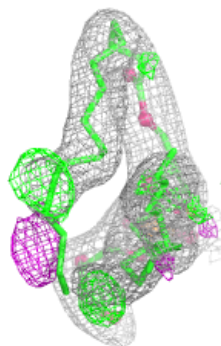
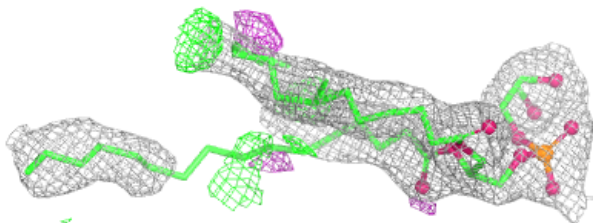
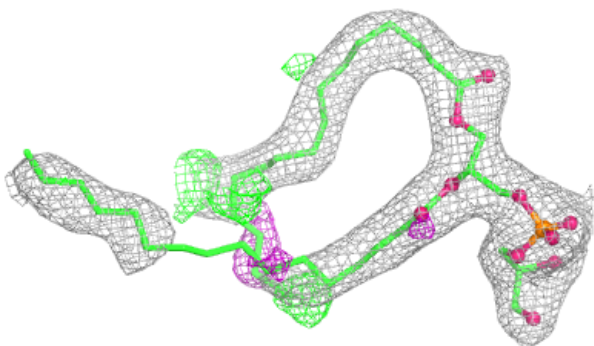


Electron density around LHG D 409 (A):

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

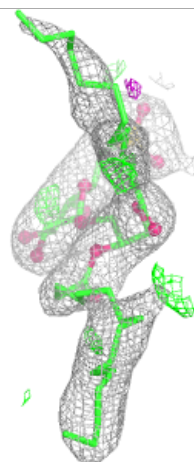
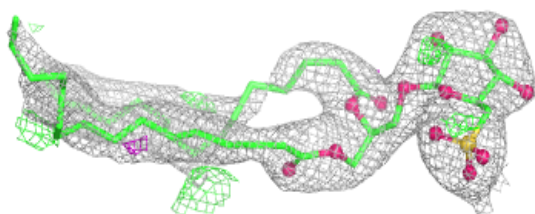
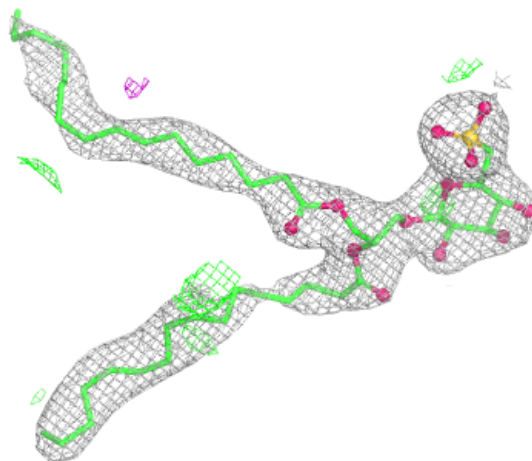
**Electron density around LHG D 409 (B):**

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



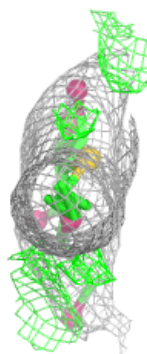
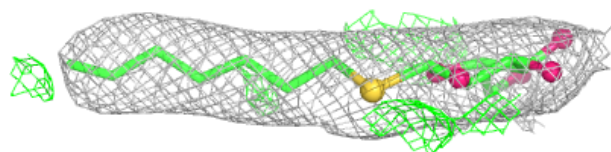
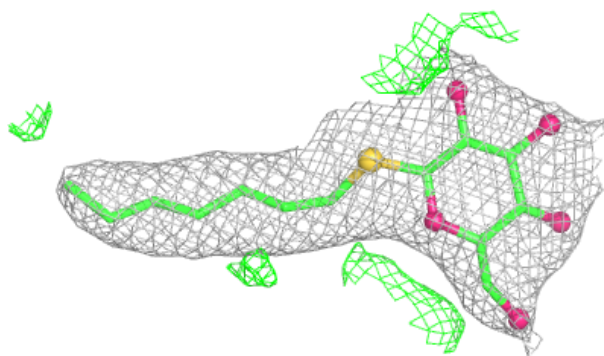
Electron density around SQD a 411 (B):

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

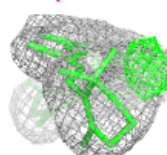
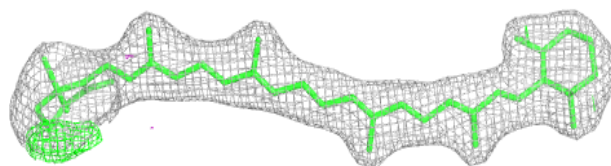
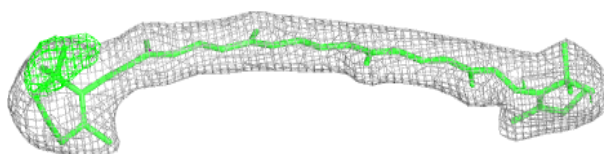


Electron density around HTG b 625:

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

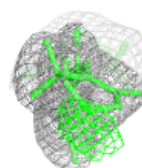
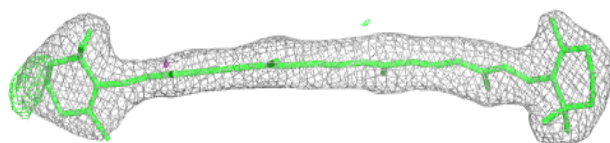
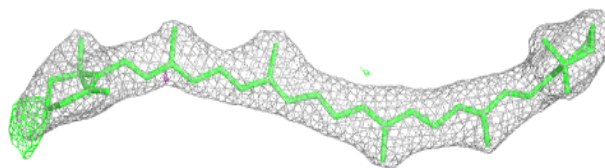
**Electron density around BCR D 406:**

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

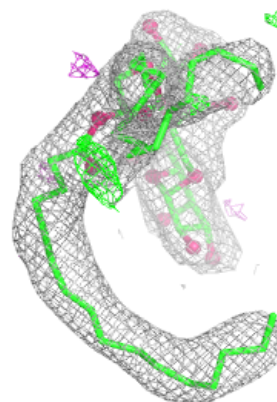
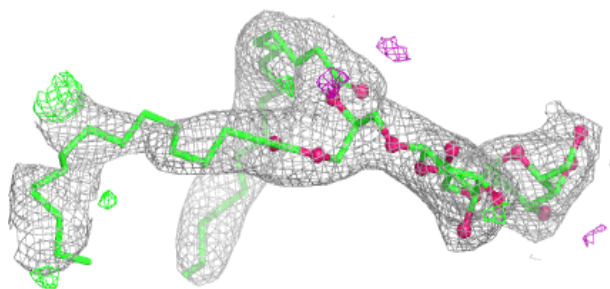
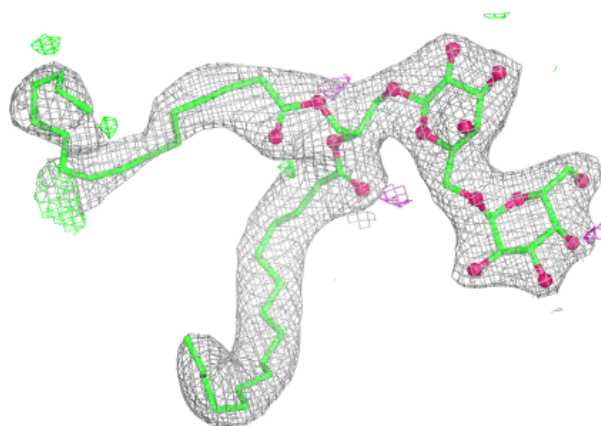


Electron density around BCR H 101:

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

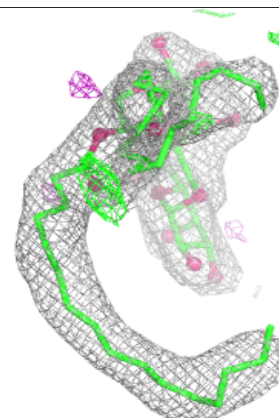
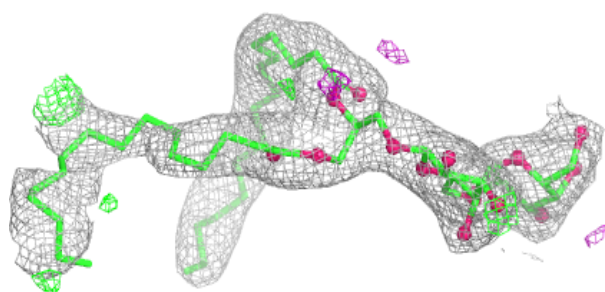
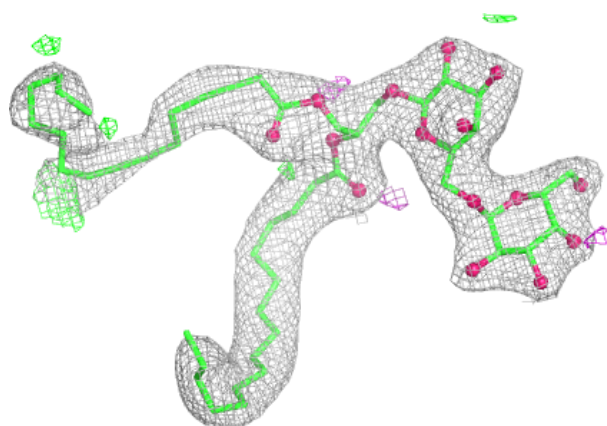
**Electron density around DGD C 519 (A):**

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

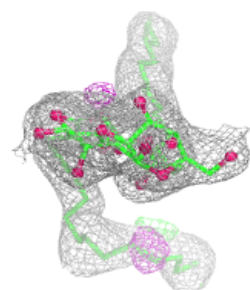
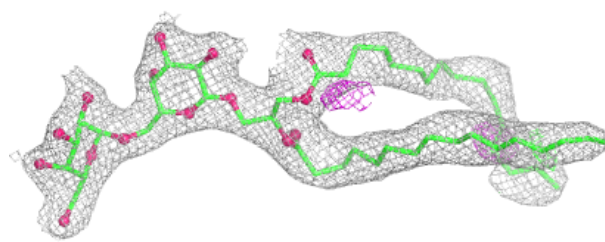
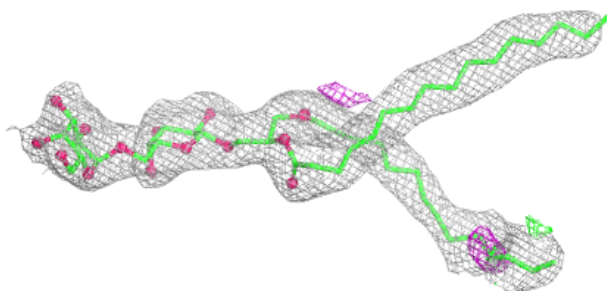


Electron density around DGD C 519 (B):

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

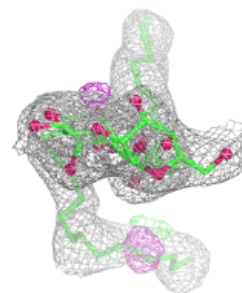
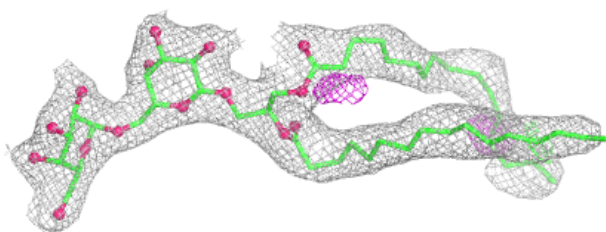
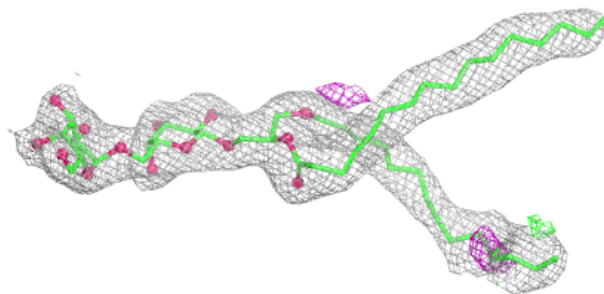
**Electron density around DGD c 517 (A):**

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

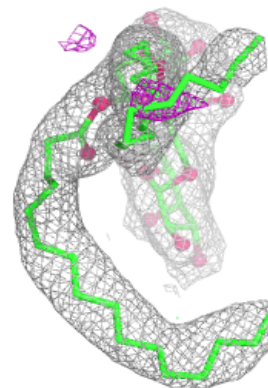
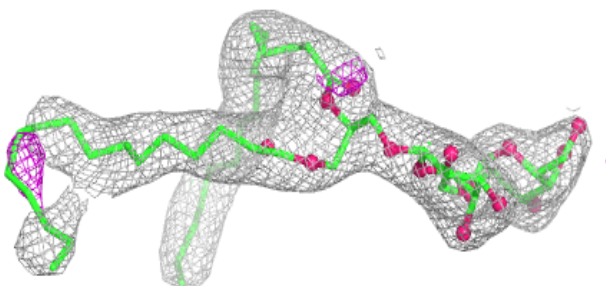
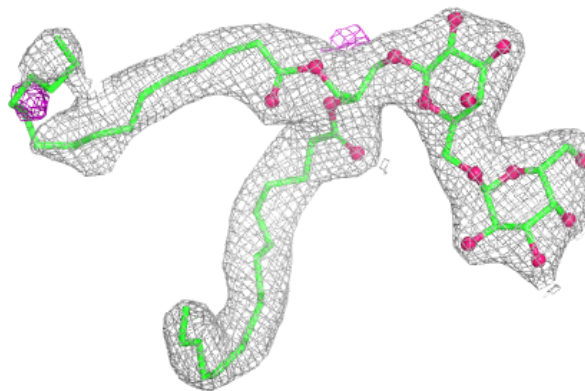


Electron density around DGD c 517 (B):

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

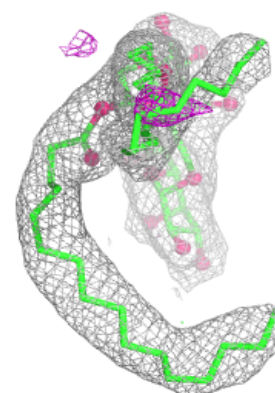
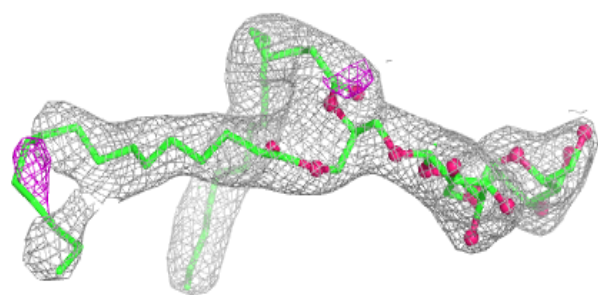
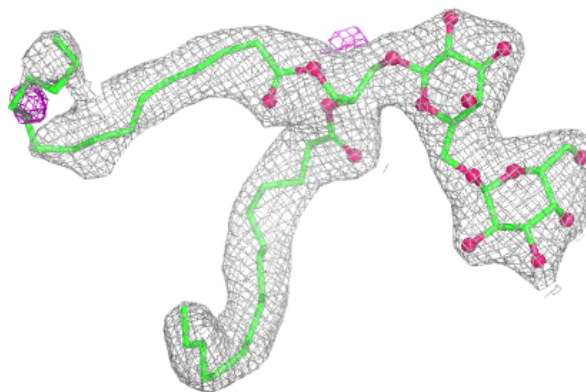
**Electron density around DGD c 518 (A):**

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

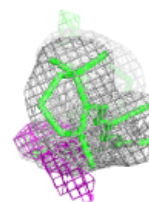
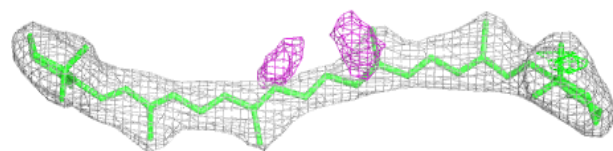
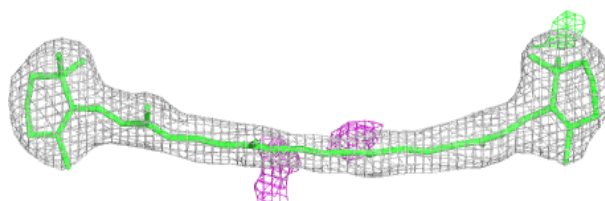


Electron density around DGD c 518 (B):

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

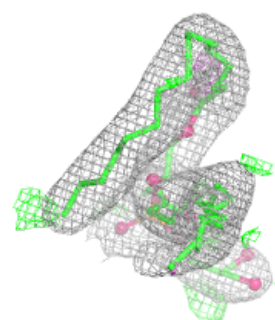
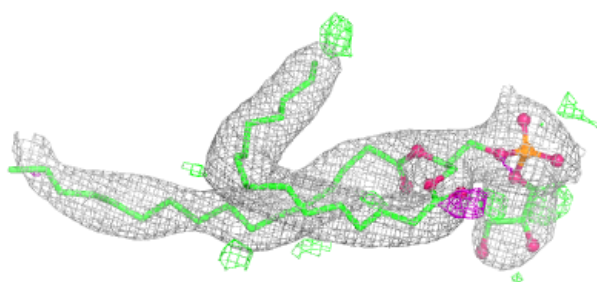
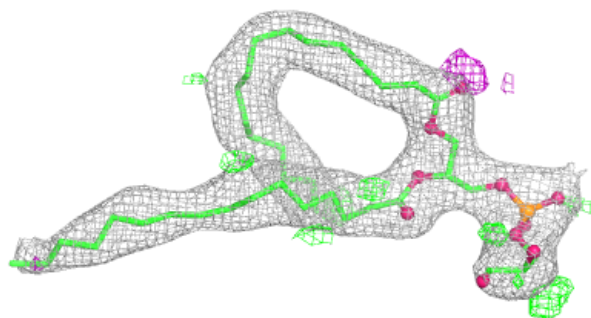
**Electron density around BCR K 102:**

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

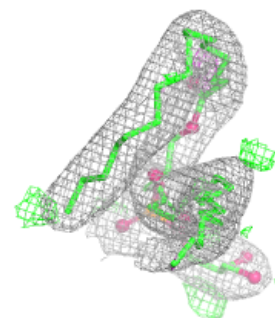
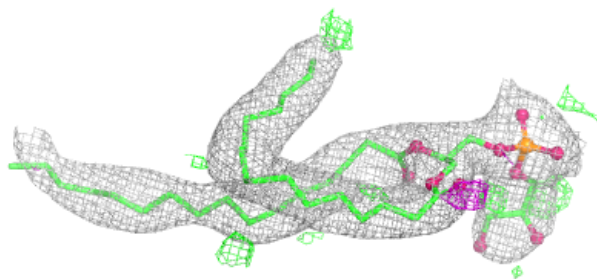
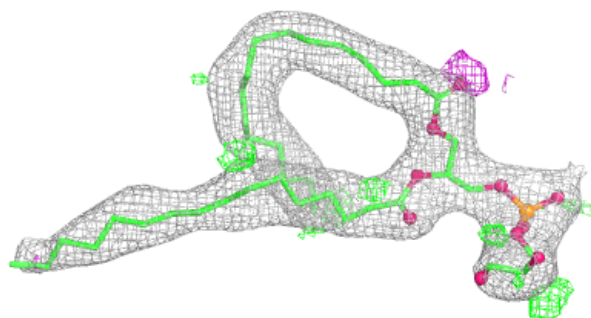


Electron density around LHG d 411 (A):

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

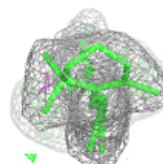
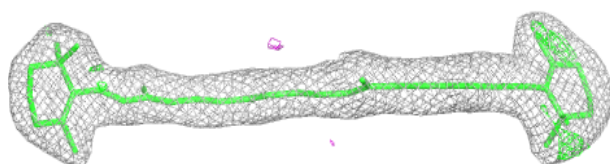
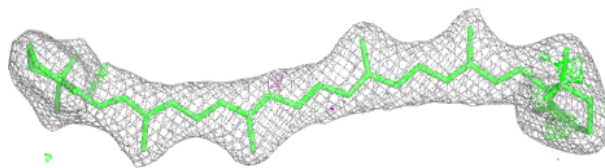
**Electron density around LHG d 411 (B):**

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

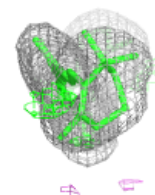
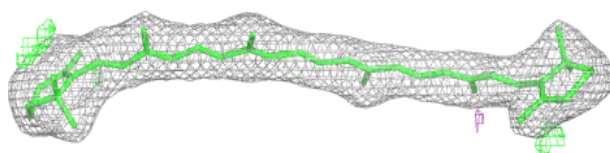
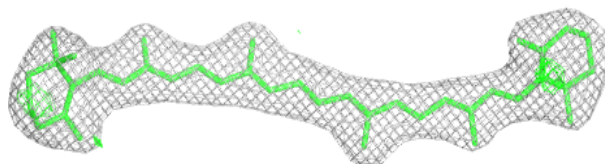


Electron density around BCR A 408:

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

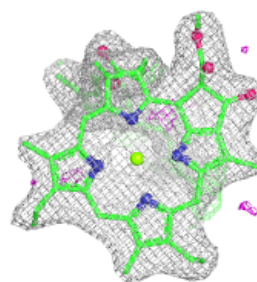
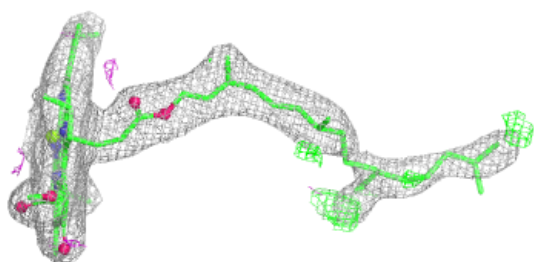
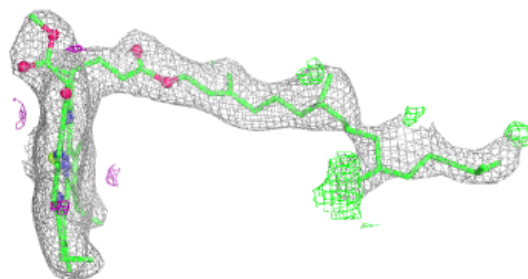
**Electron density around BCR B 619:**

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

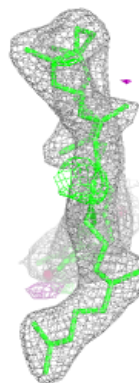
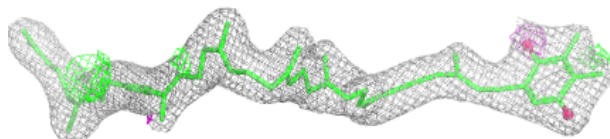
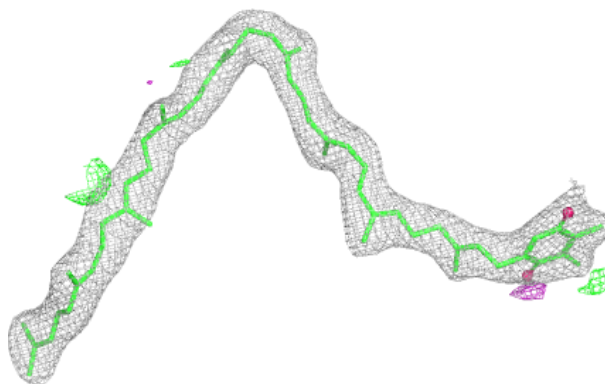


Electron density around CLA b 606:

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

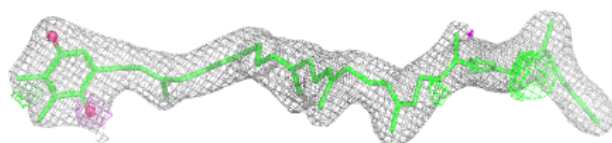
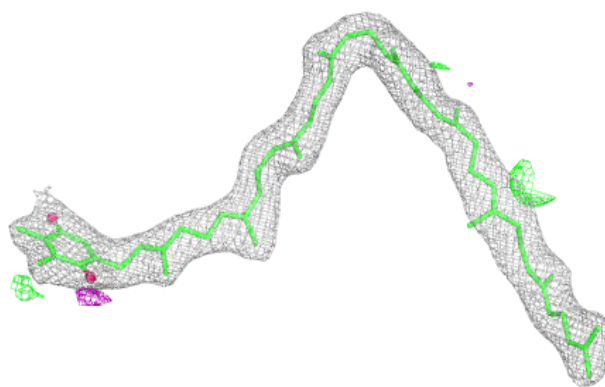
**Electron density around PL9 D 407 (A):**

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

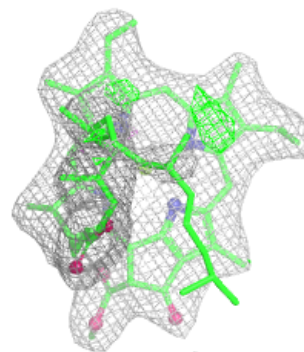
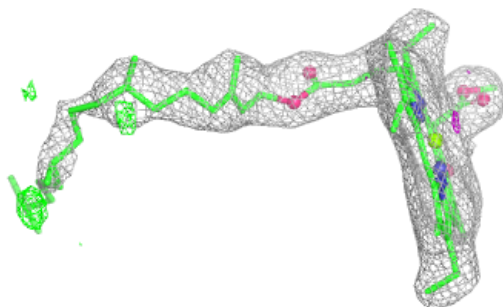
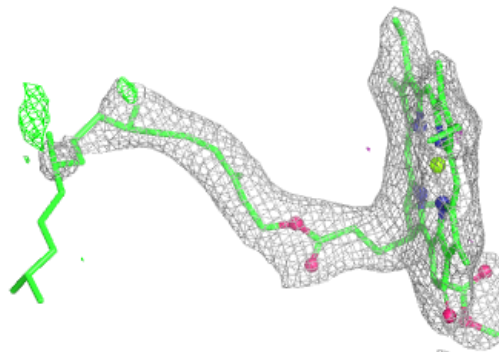


Electron density around PL9 D 407 (B):

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

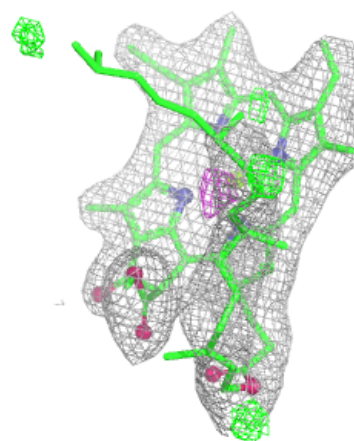
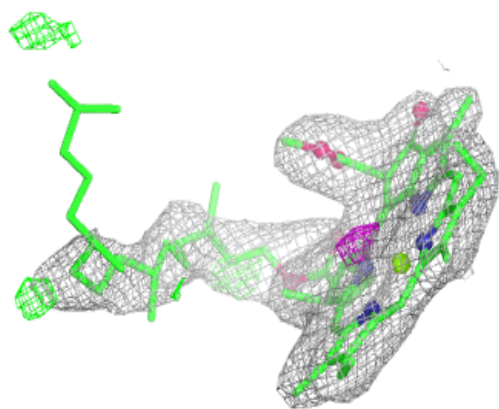
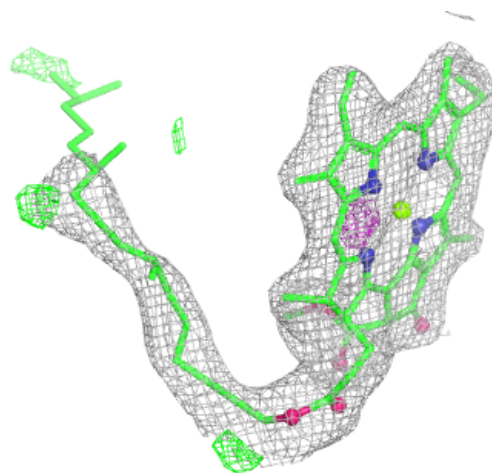
**Electron density around CLA D 405:**

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



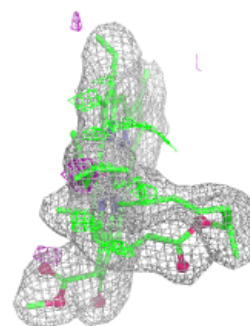
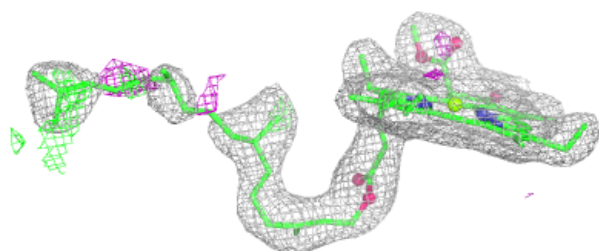
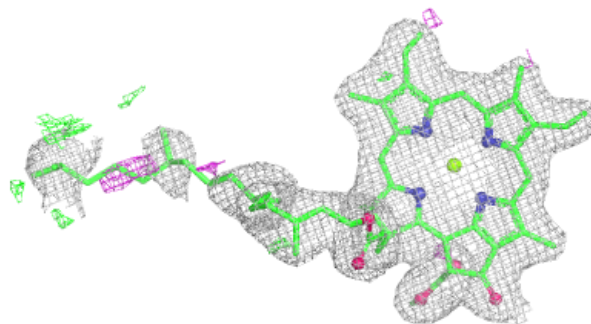
Electron density around CLA b 616:

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

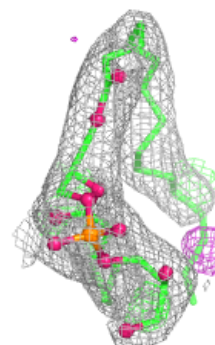
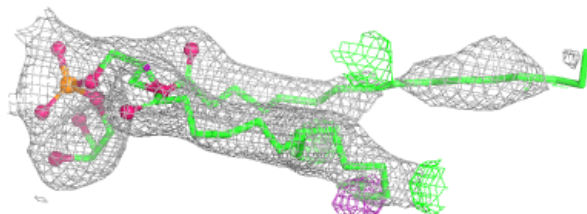
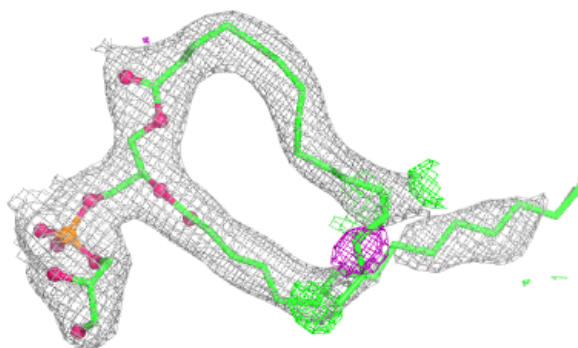


Electron density around CLA a 407 (A):

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

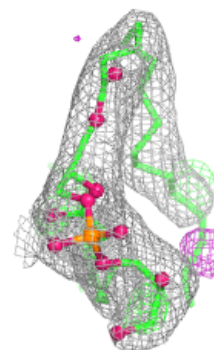
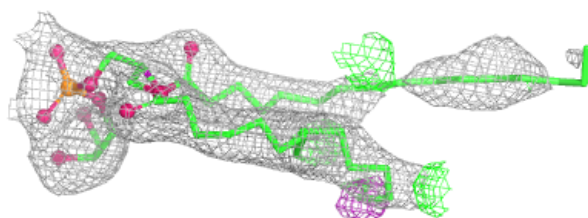
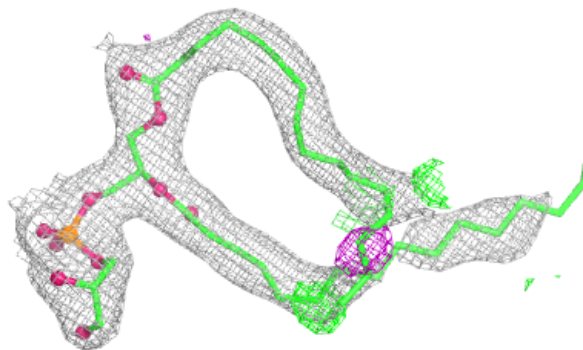
**Electron density around LHG d 406 (A):**

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

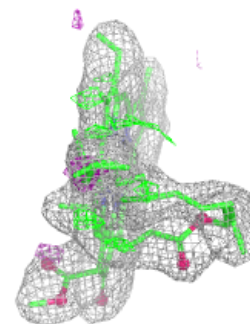
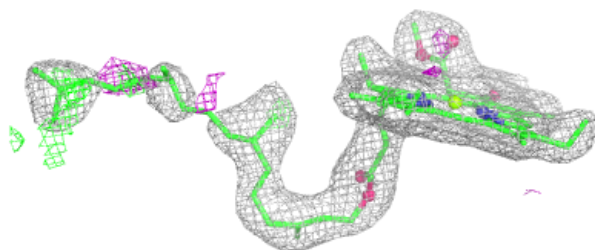
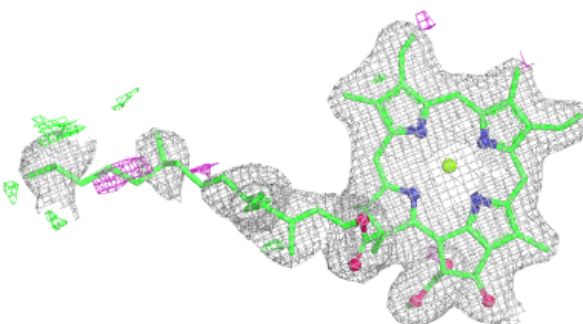


Electron density around LHG d 406 (B):

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

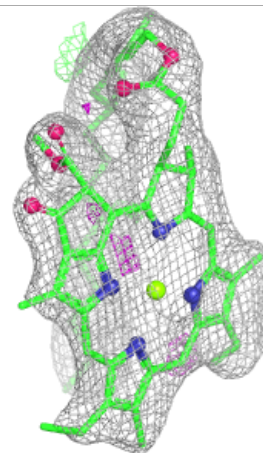
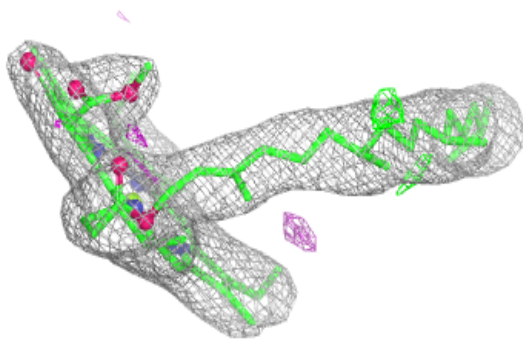
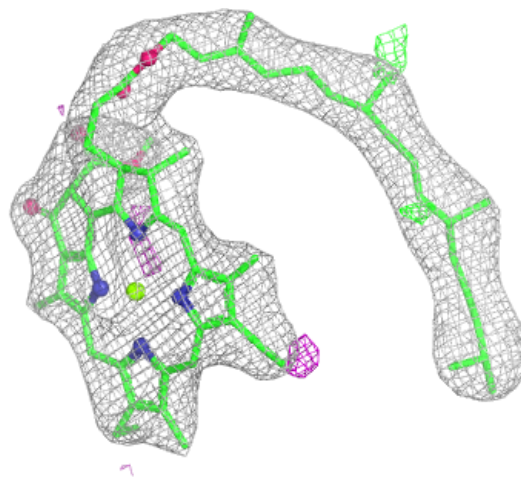
**Electron density around CLA a 407 (B):**

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



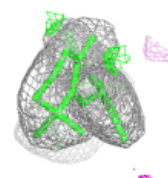
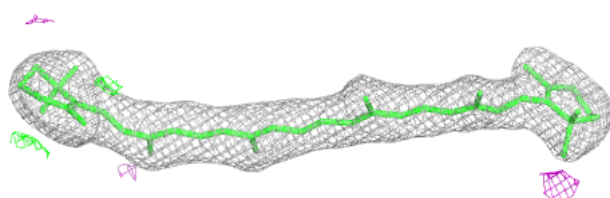
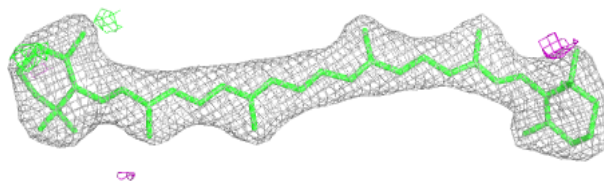
Electron density around CLA c 508:

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

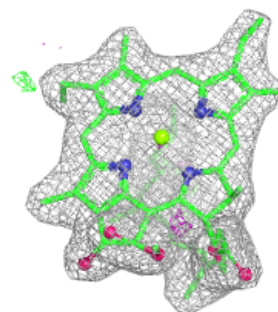
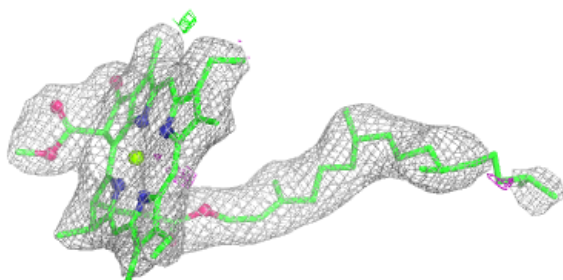
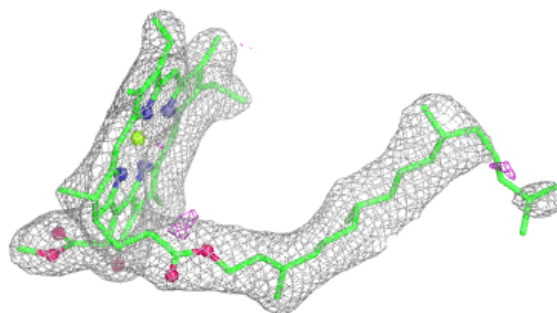


Electron density around BCR b 619:

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

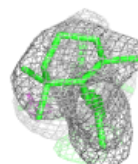
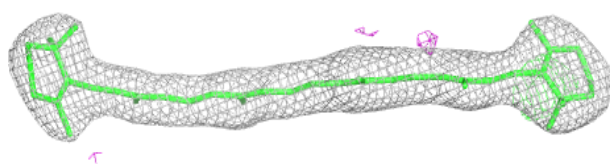
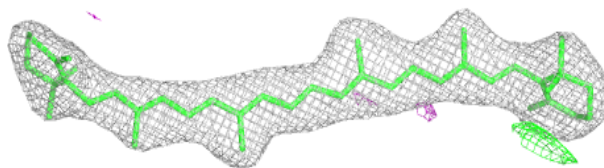
**Electron density around CLA c 509:**

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

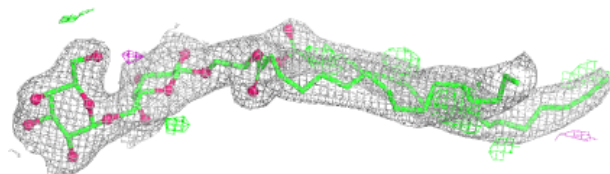
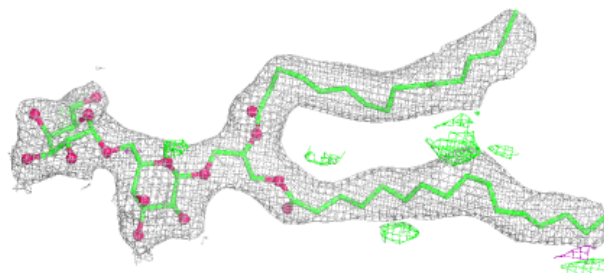


Electron density around BCR c 516:

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

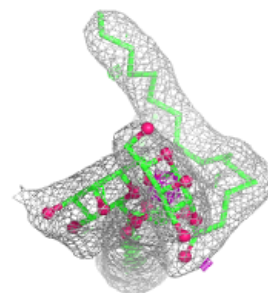
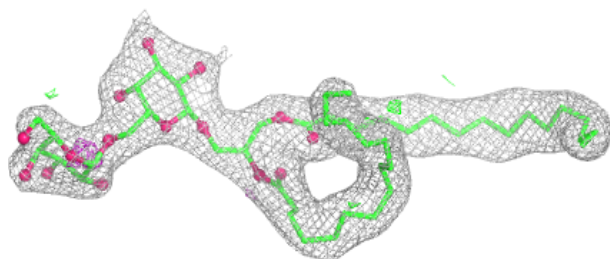
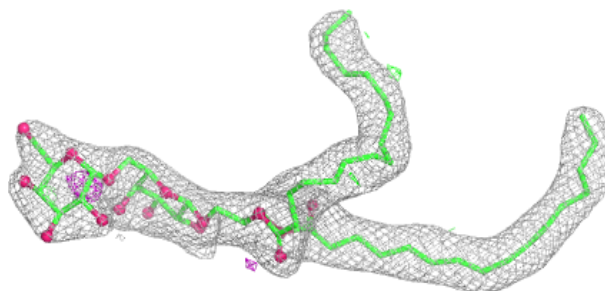
**Electron density around DGD C 520:**

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

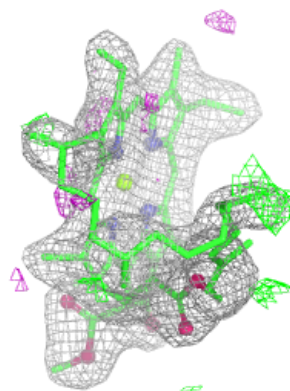
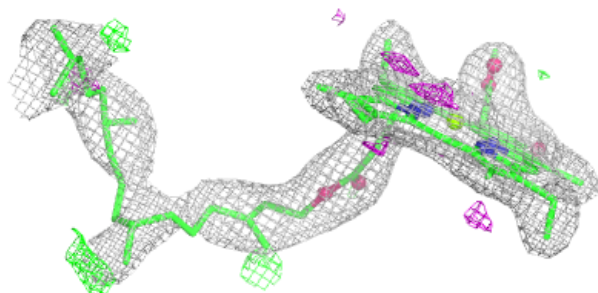
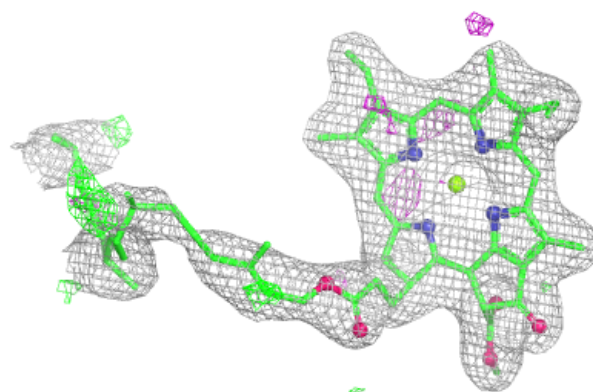


Electron density around DGD H 102:

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

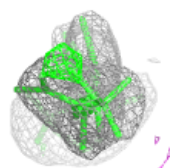
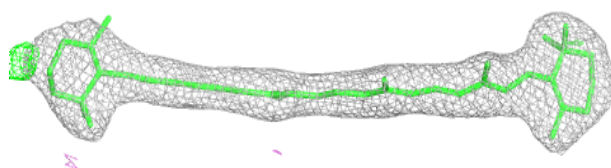
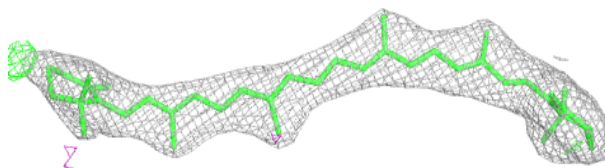
**Electron density around CLA A 407:**

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

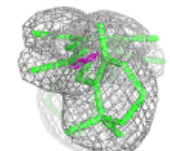
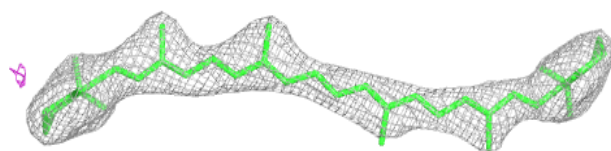
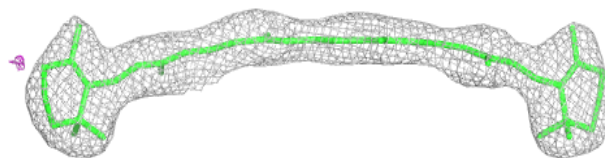


Electron density around BCR h 101:

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

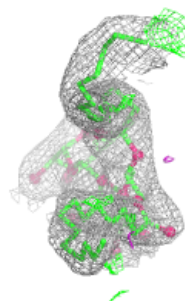
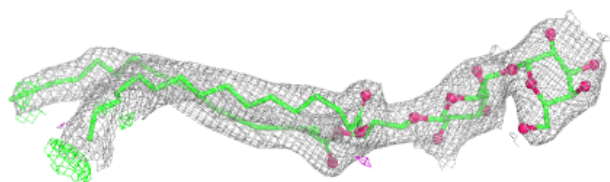
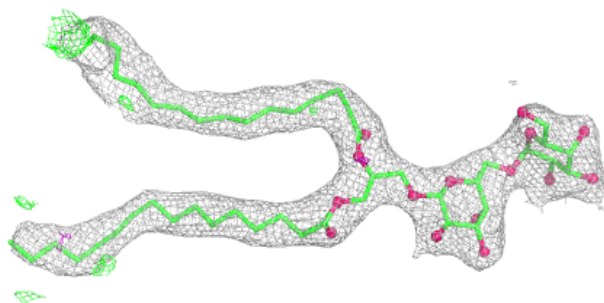
**Electron density around BCR k 101:**

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

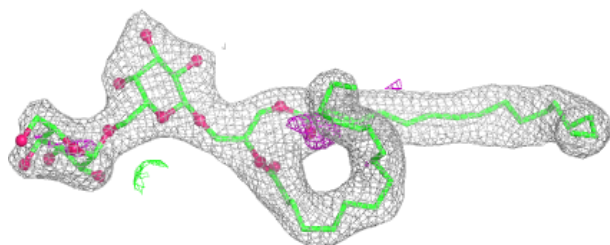
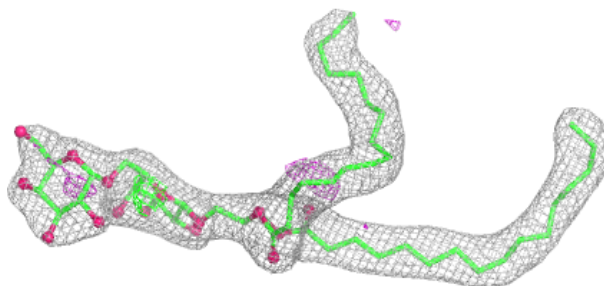


Electron density around DGD c 519:

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

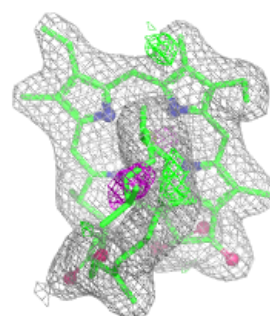
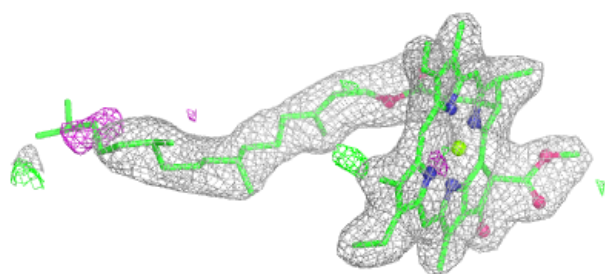
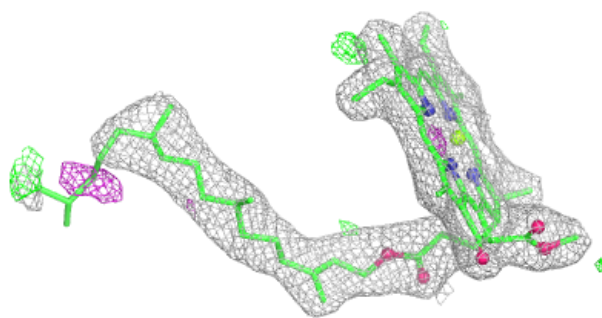
**Electron density around DGD h 102:**

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

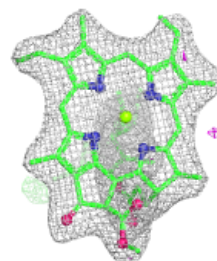
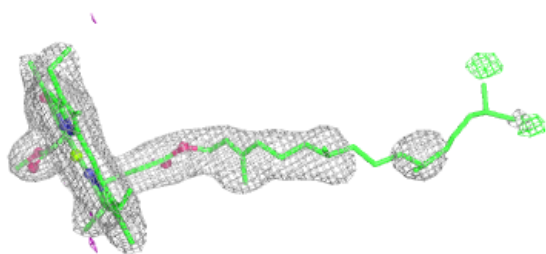
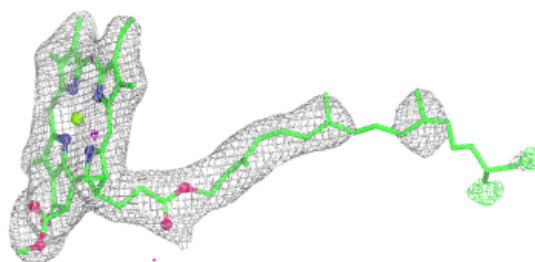


Electron density around CLA C 510:

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

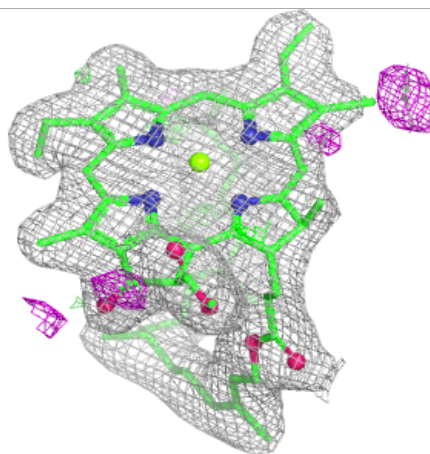
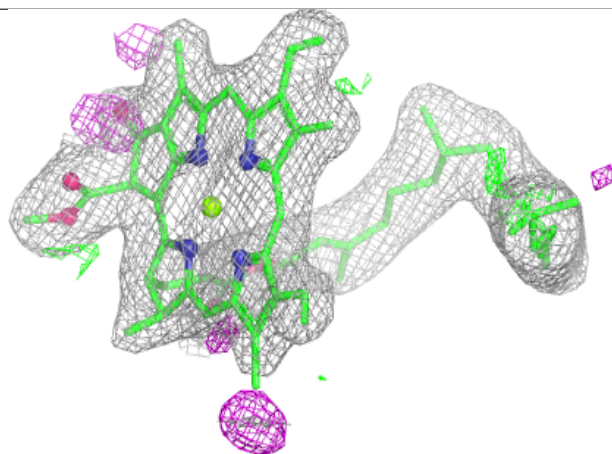
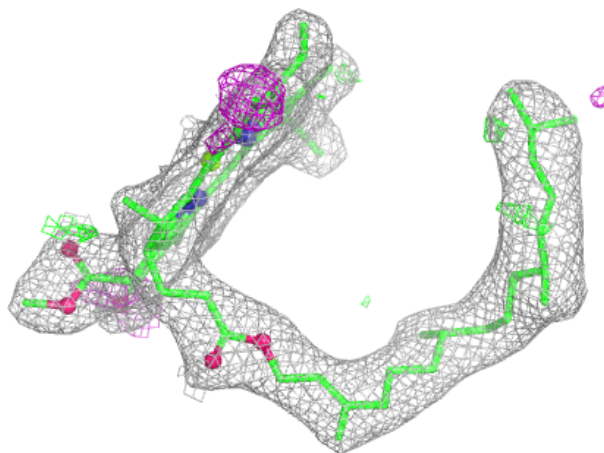
**Electron density around CLA d 402:**

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



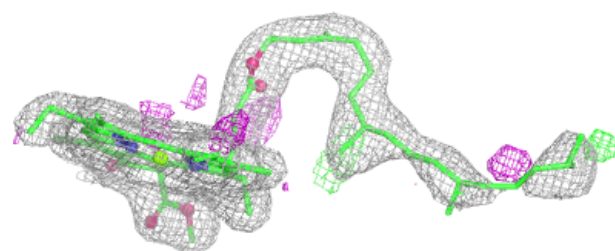
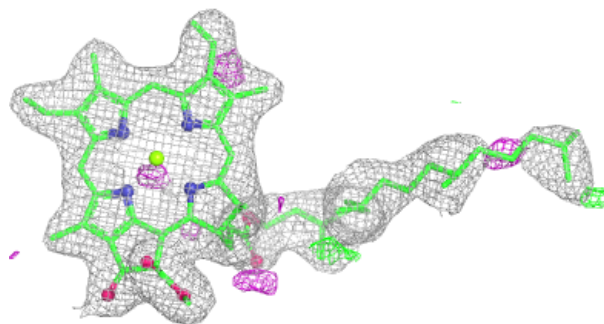
Electron density around CLA B 611:

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

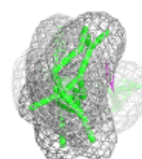
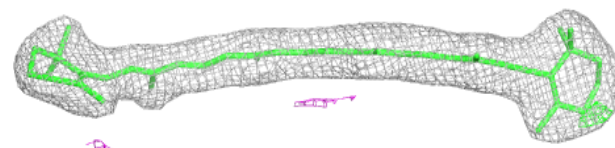
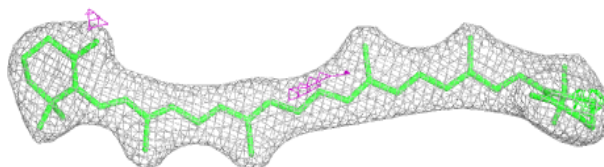


Electron density around CLA A 406 (A):

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

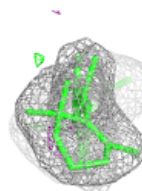
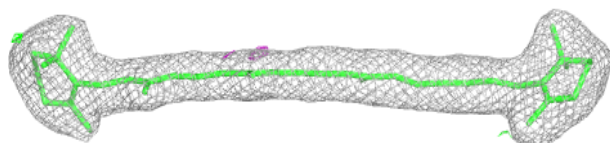
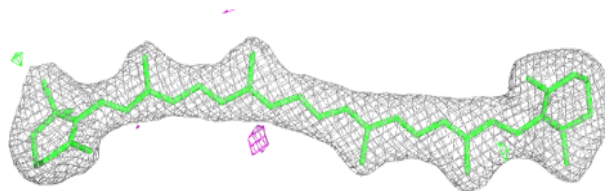
**Electron density around BCR B 617:**

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



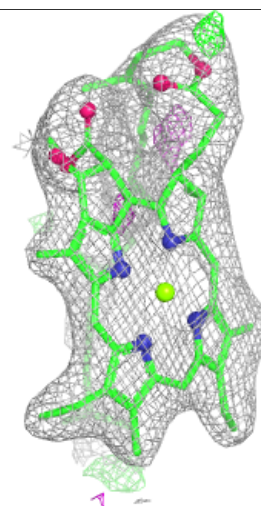
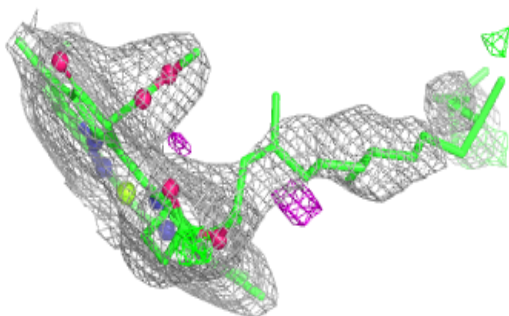
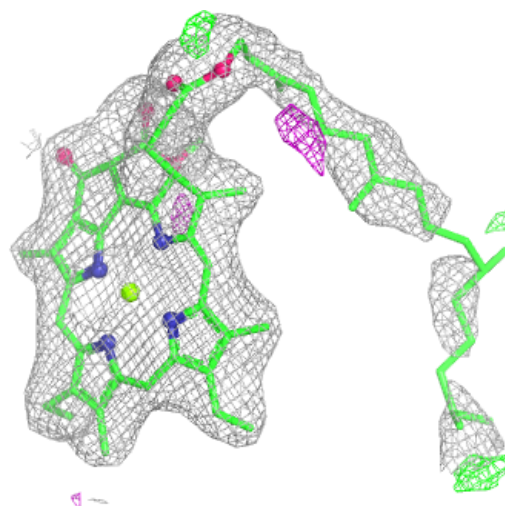
Electron density around BCR B 618:

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



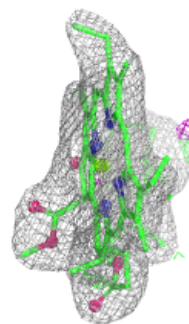
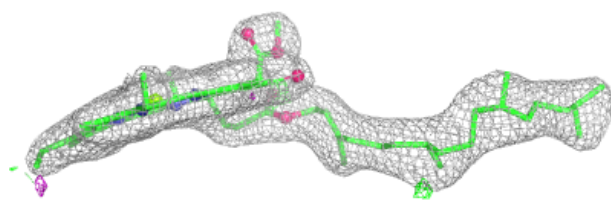
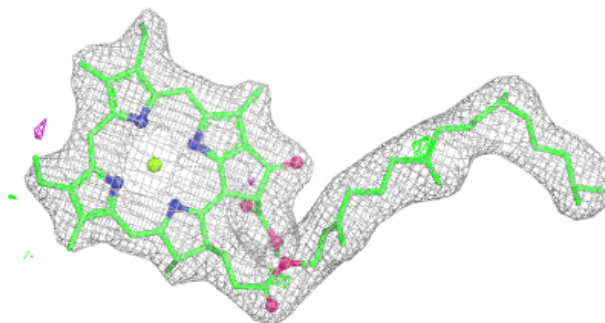
Electron density around CLA B 616:

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

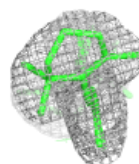
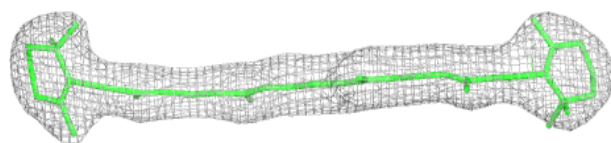
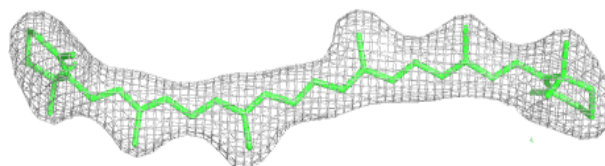


Electron density around CLA b 602:

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

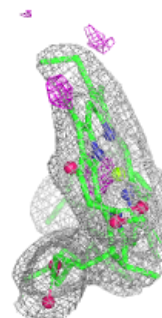
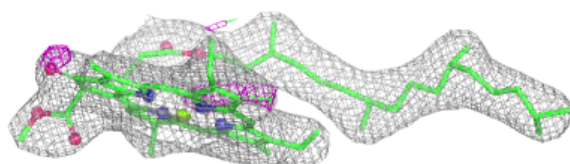
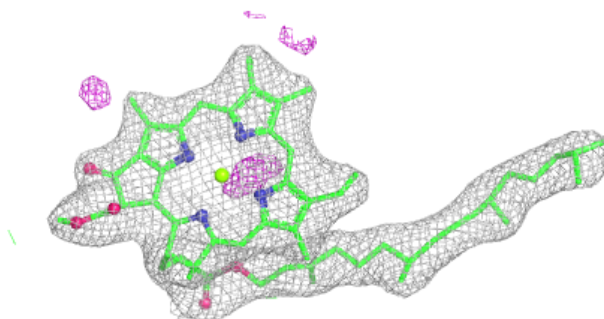
**Electron density around BCR C 517:**

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

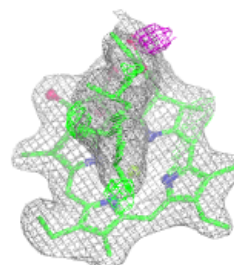
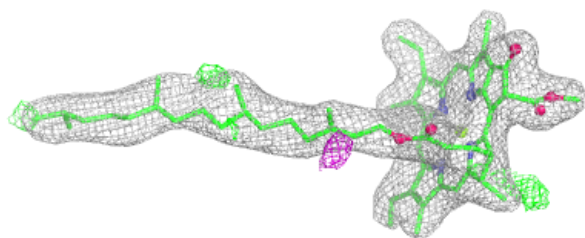
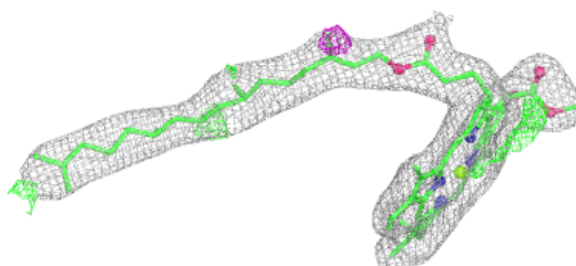


Electron density around CLA C 503:

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

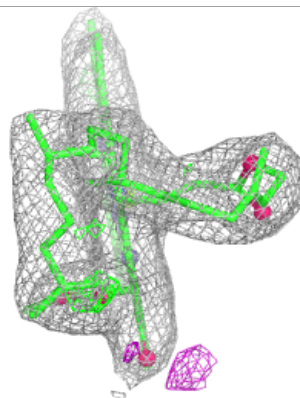
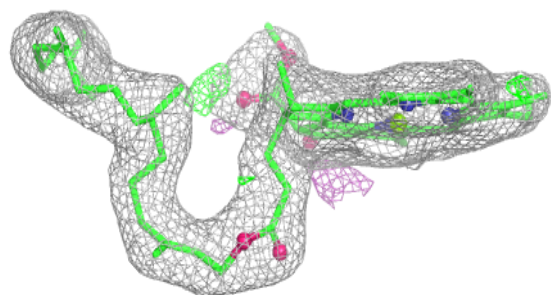
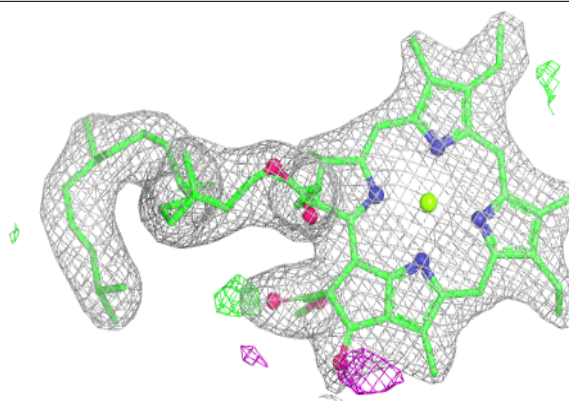
**Electron density around CLA b 607:**

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

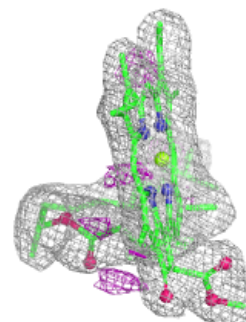
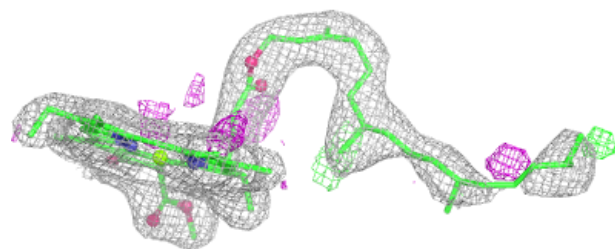
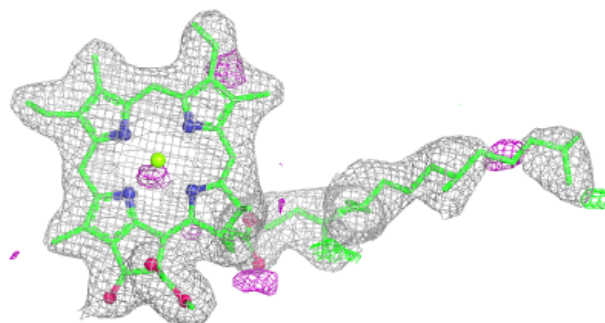


Electron density around CLA b 612:

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

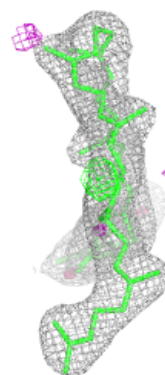
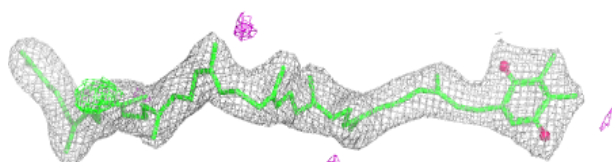
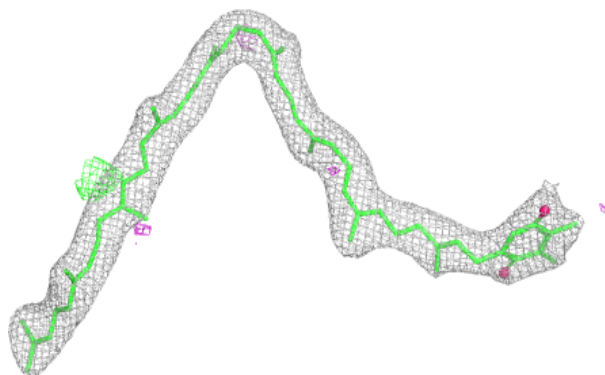
**Electron density around CLA A 406 (B):**

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

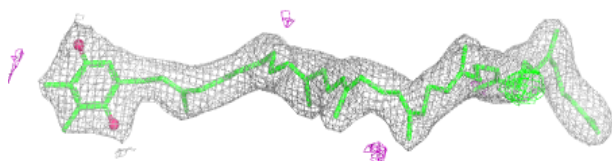
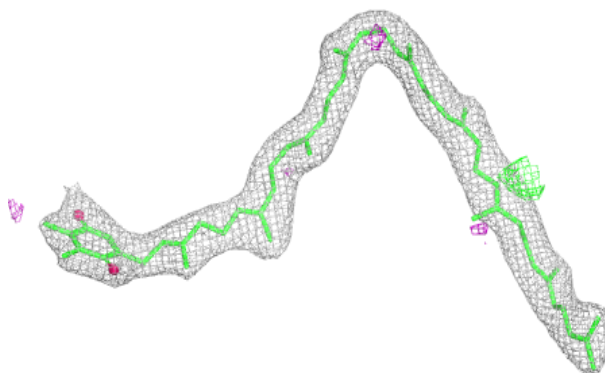


Electron density around PL9 d 404 (A):

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

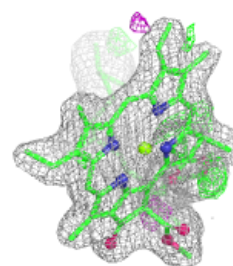
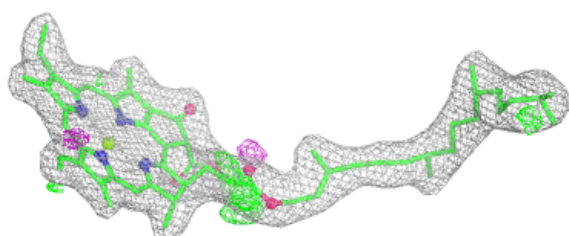
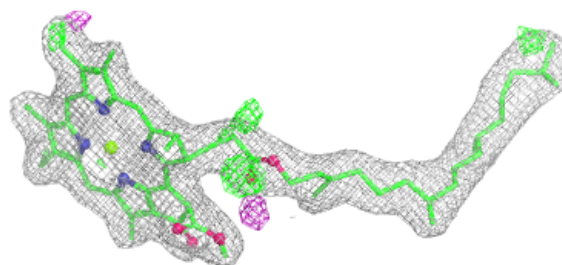
**Electron density around PL9 d 404 (B):**

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

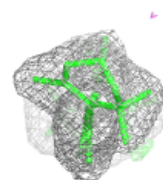
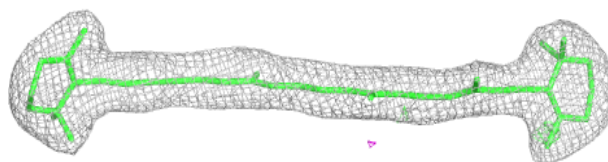
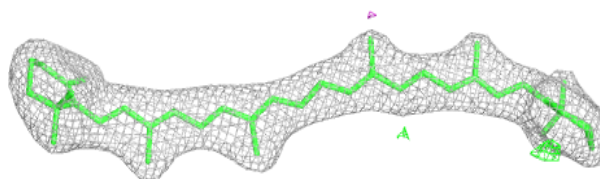


Electron density around CLA A 404 (A):

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

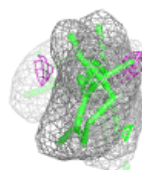
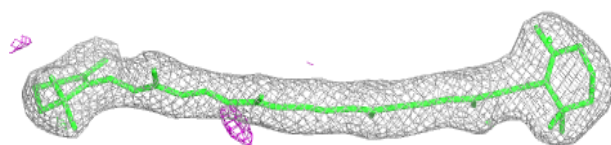
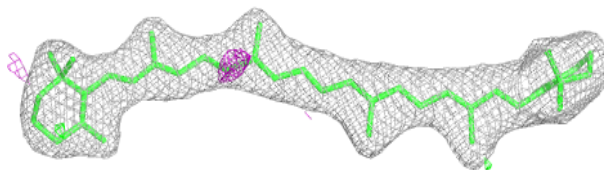
**Electron density around BCR a 410:**

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

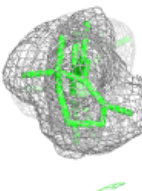
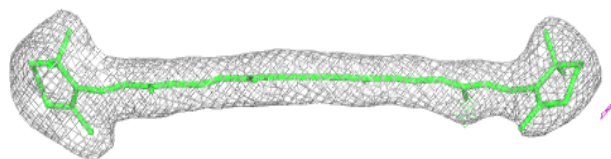
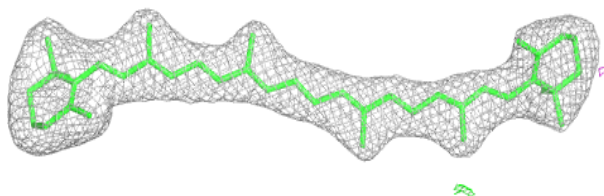


Electron density around BCR b 617:

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

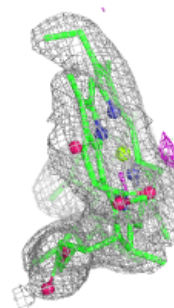
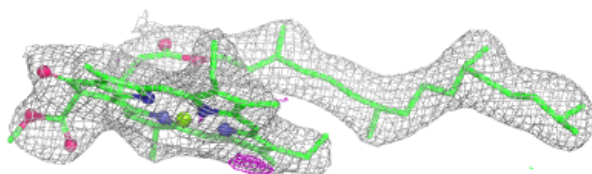
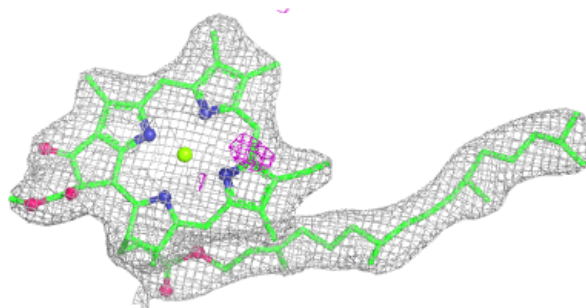
**Electron density around BCR b 618:**

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



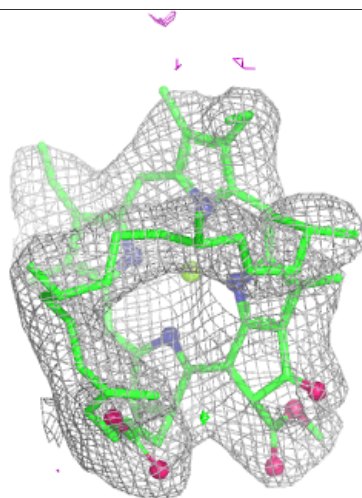
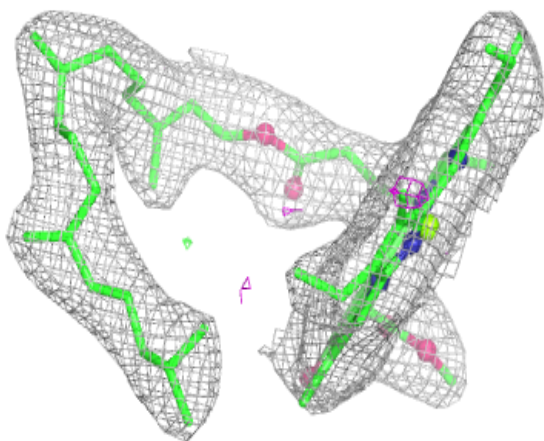
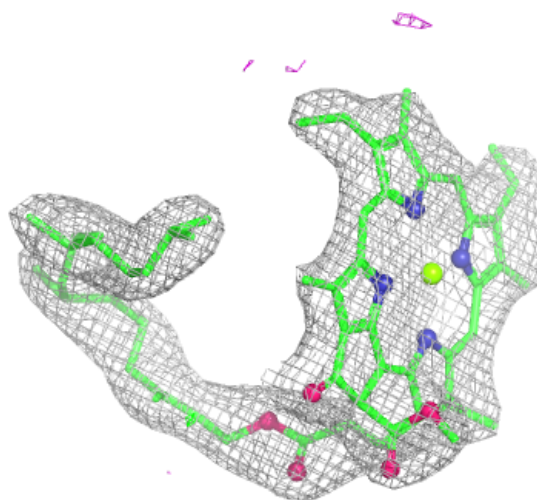
Electron density around CLA c 502:

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



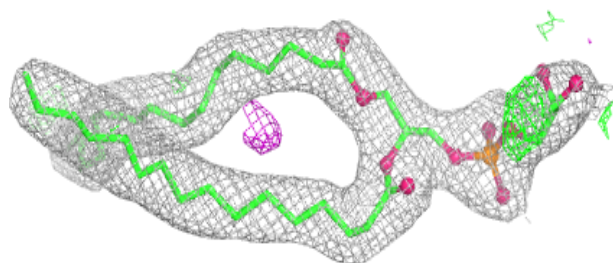
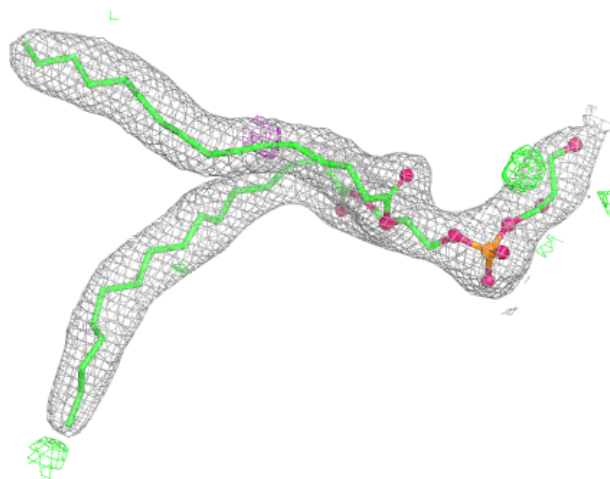
Electron density around CLA c 504:

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



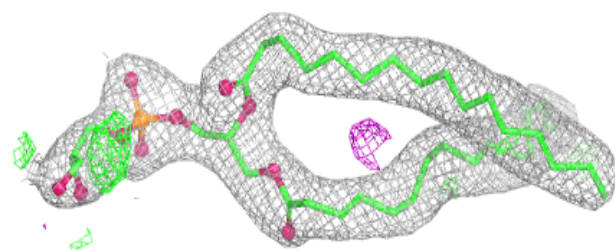
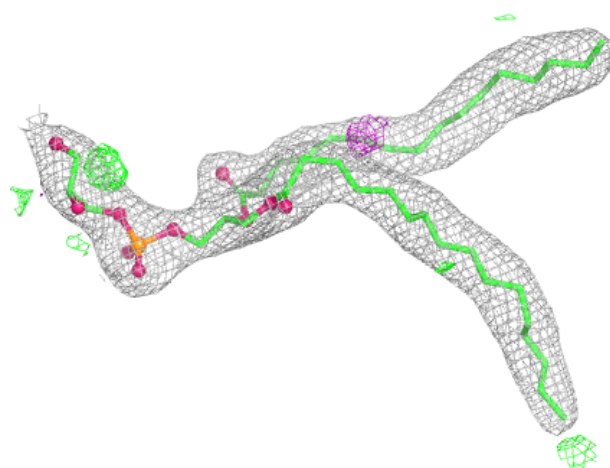
Electron density around LHG D 408 (A):

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



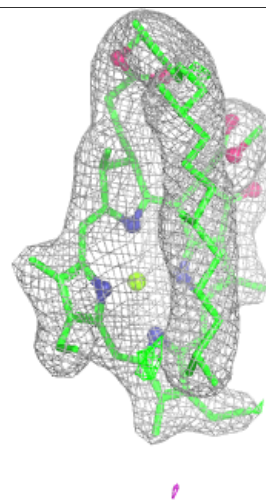
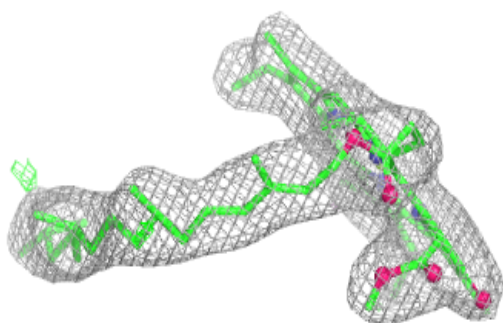
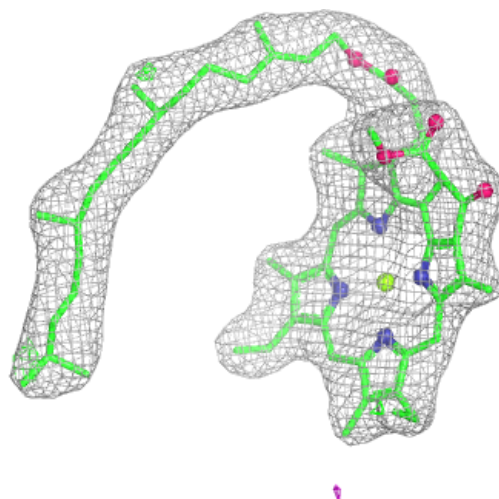
Electron density around LHG D 408 (B):

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



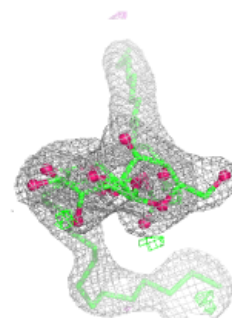
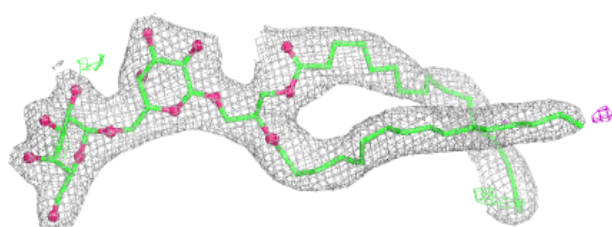
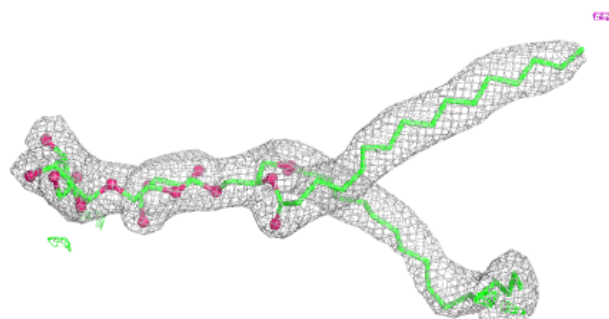
Electron density around CLA C 509:

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

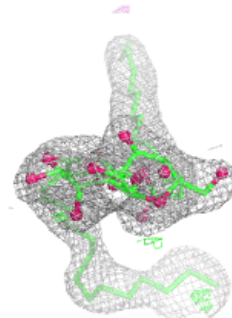
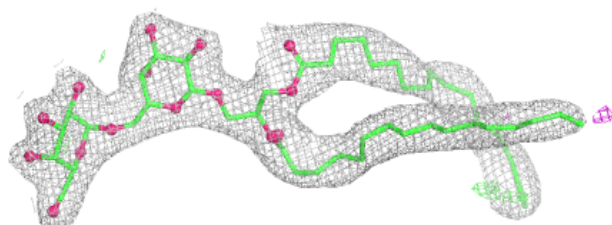
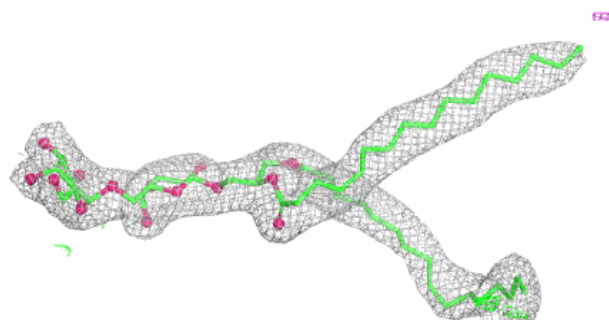


Electron density around DGD C 518 (A):

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

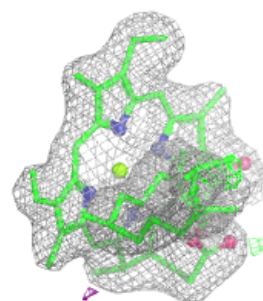
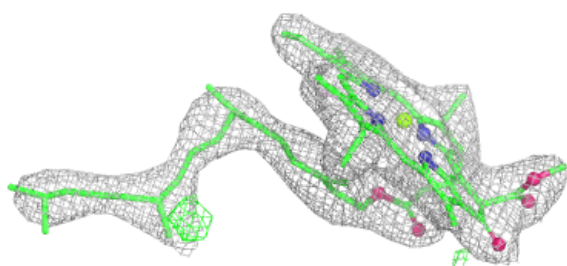
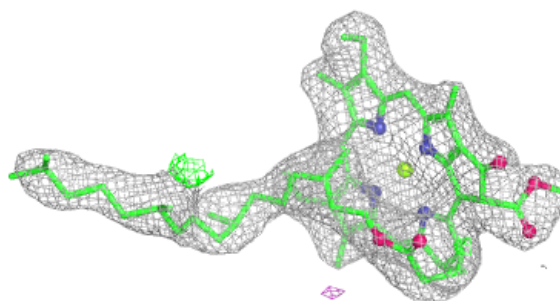
**Electron density around DGD C 518 (B):**

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

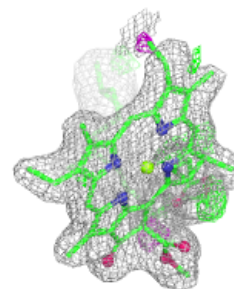
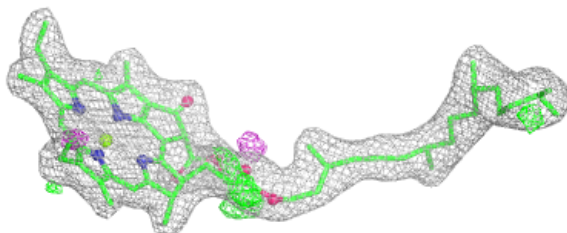
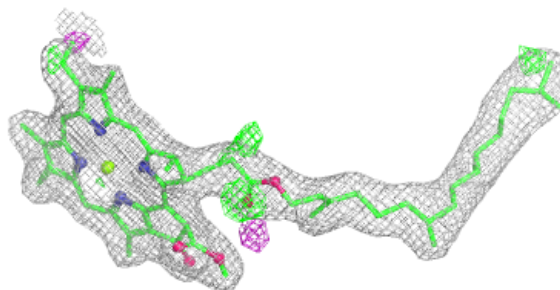


Electron density around CLA c 506:

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

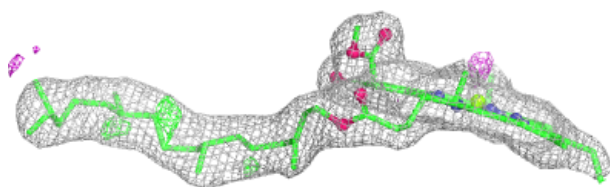
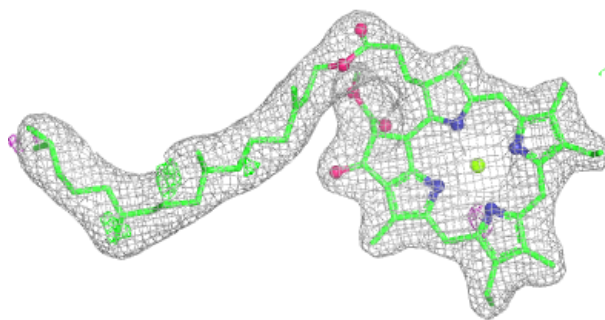
**Electron density around CLA A 404 (B):**

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

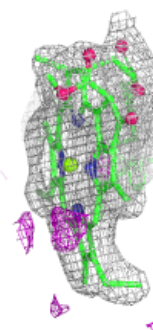
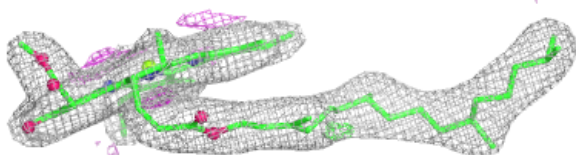
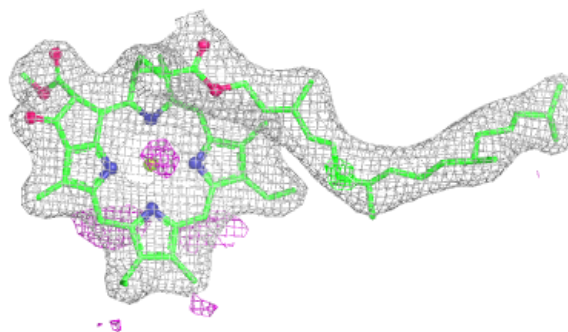


Electron density around CLA B 602:

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

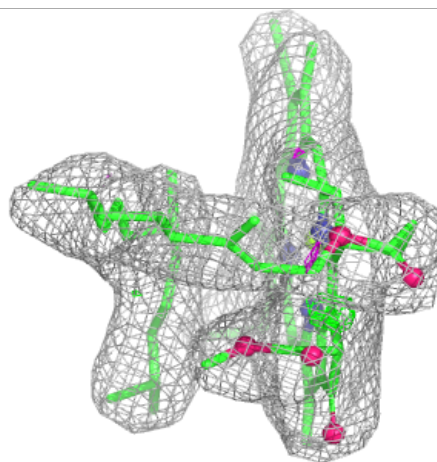
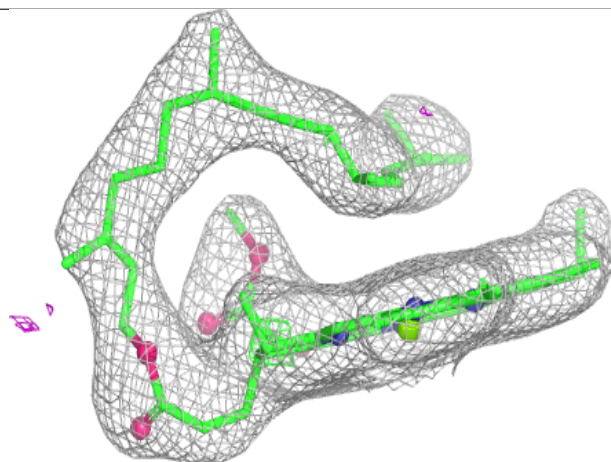
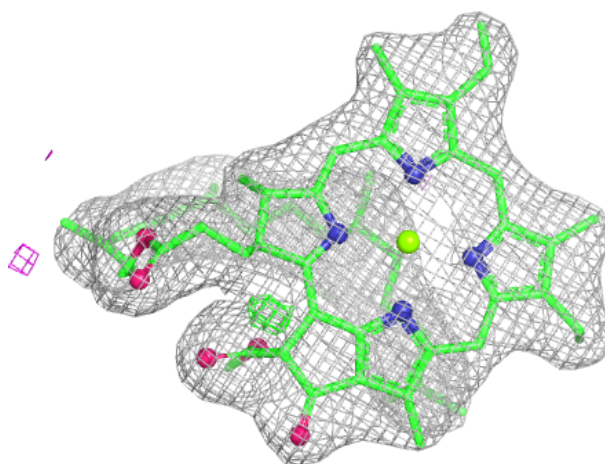
**Electron density around CLA B 603:**

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



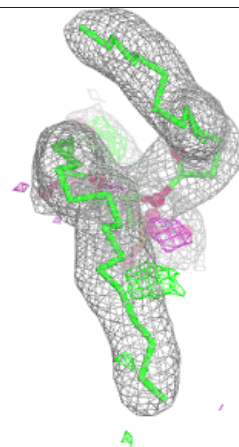
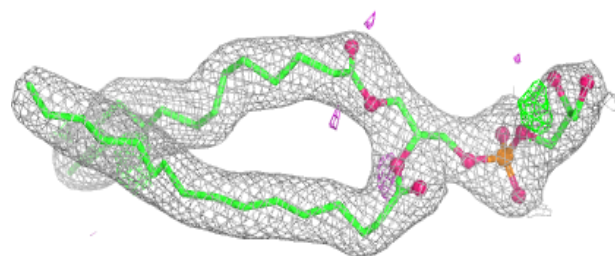
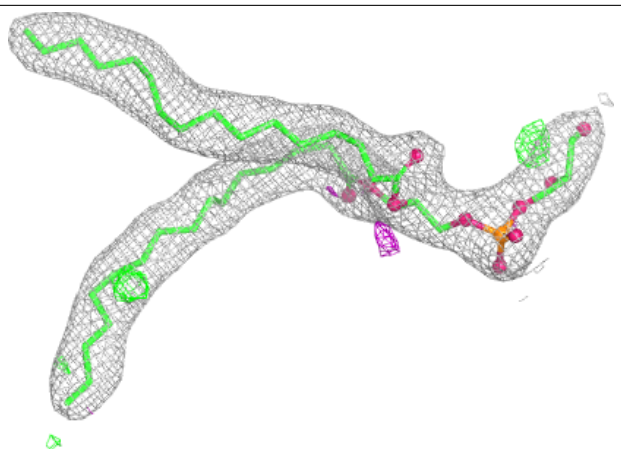
Electron density around CLA c 511:

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



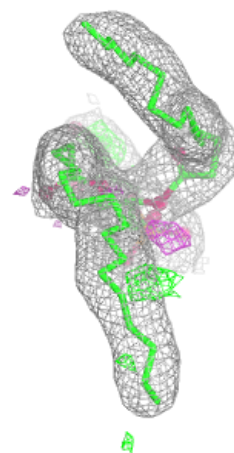
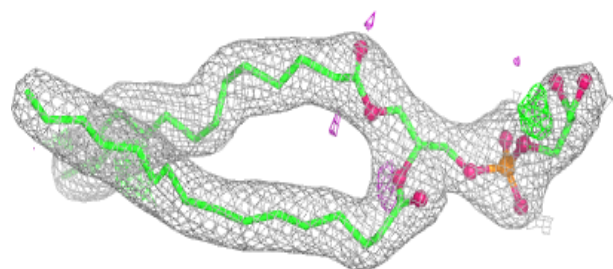
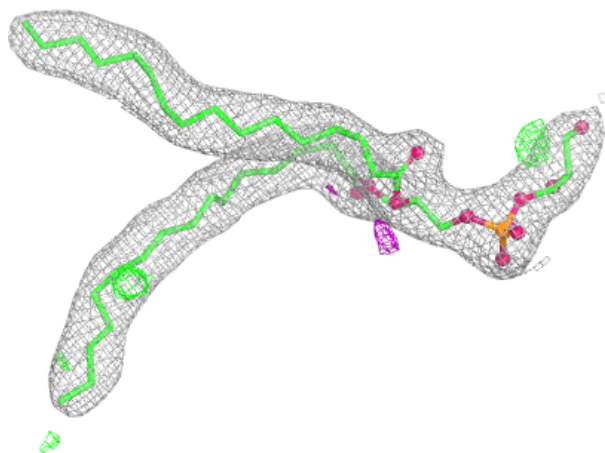
Electron density around LHG d 405 (A):

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



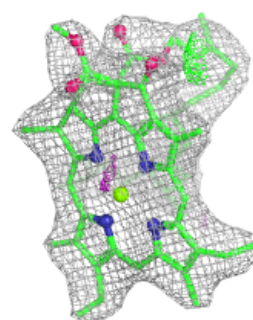
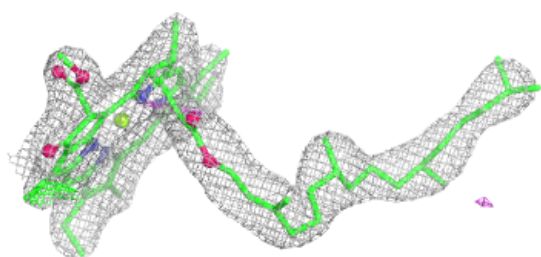
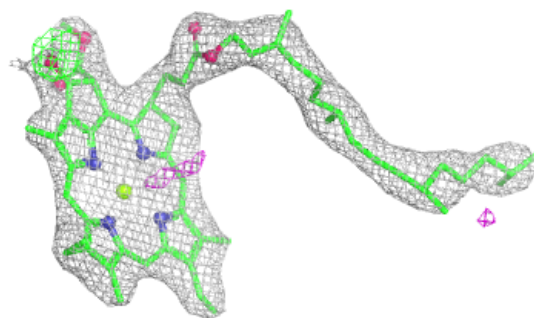
Electron density around LHG d 405 (B):

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

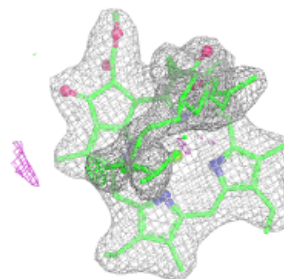
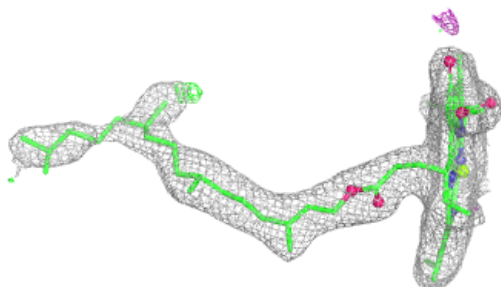
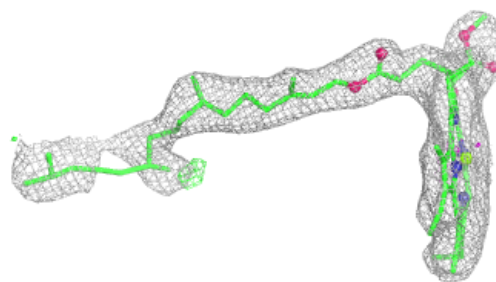


Electron density around CLA c 512:

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

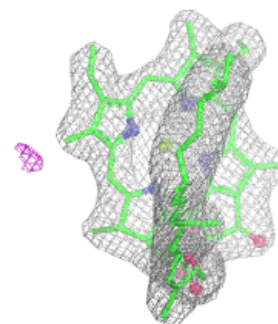
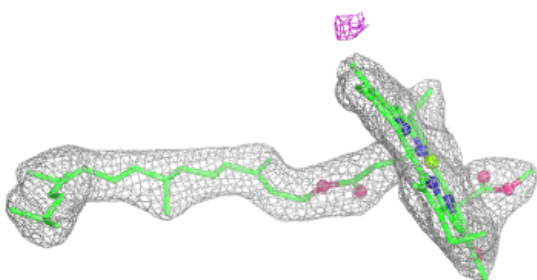
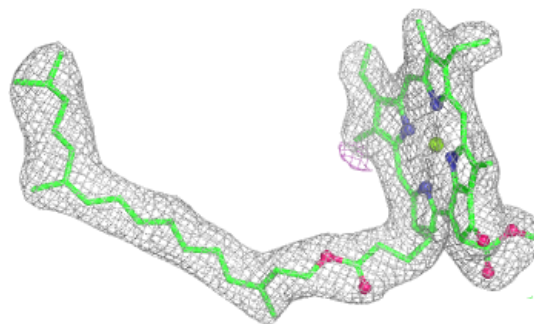
**Electron density around CLA B 606:**

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



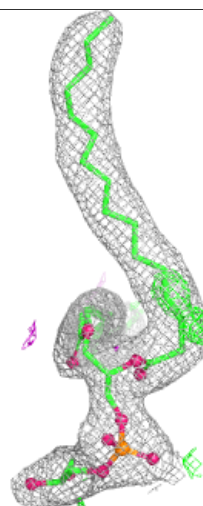
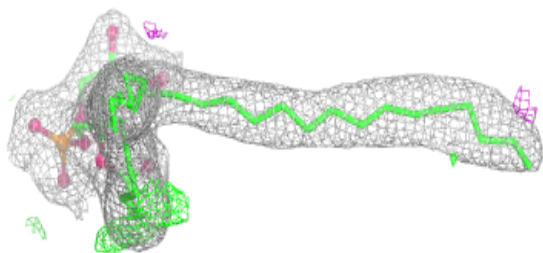
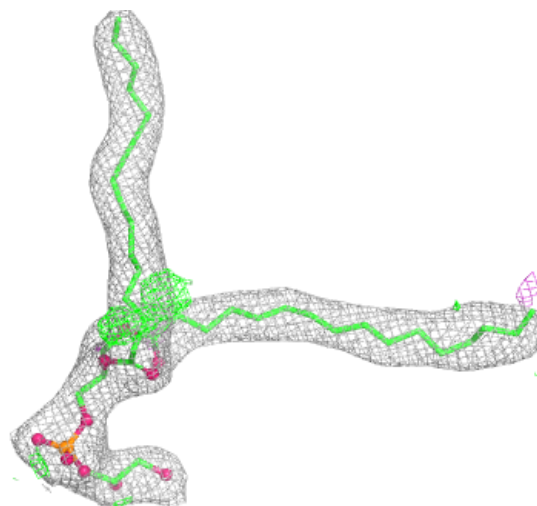
Electron density around CLA B 609:

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



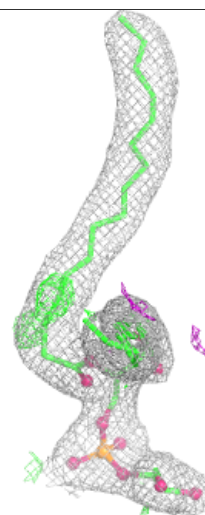
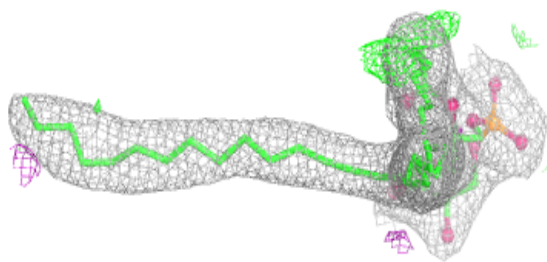
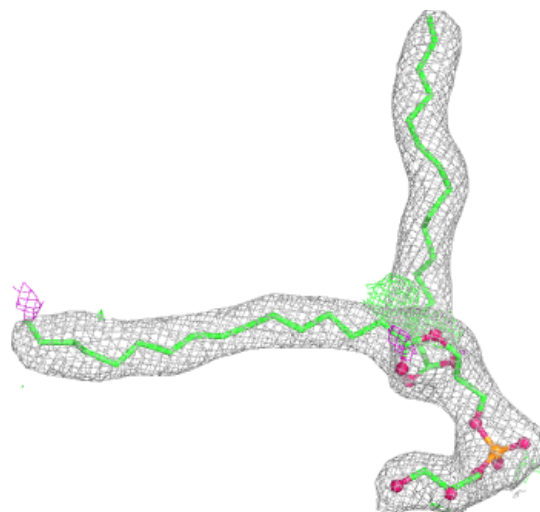
Electron density around LHG 1 802 (A):

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



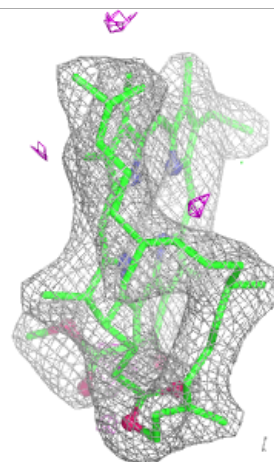
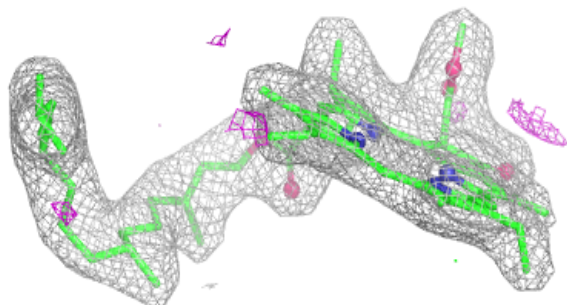
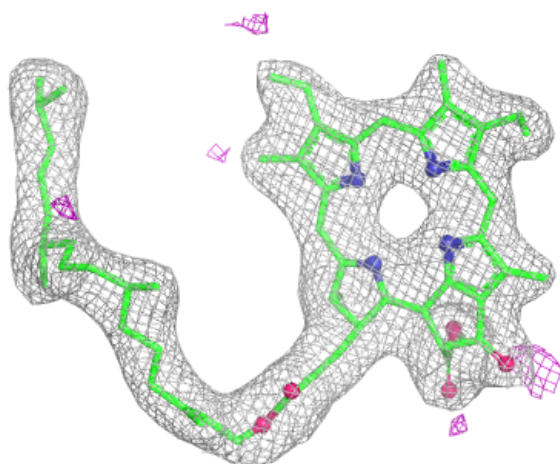
Electron density around LHG 1 802 (B):

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



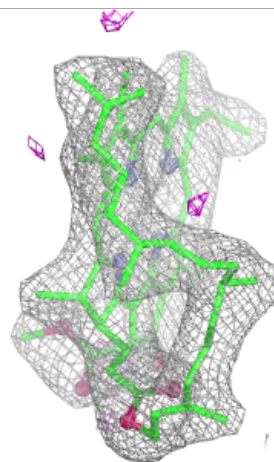
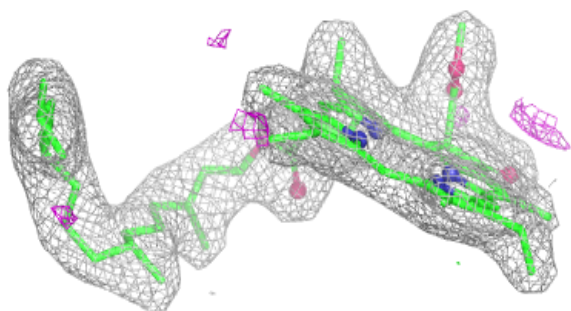
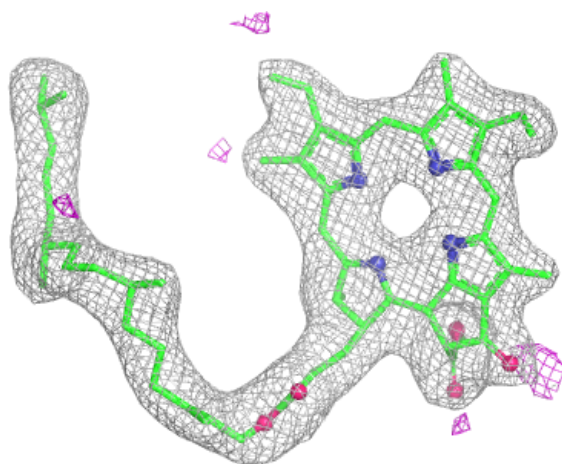
Electron density around PHO D 402 (A):

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



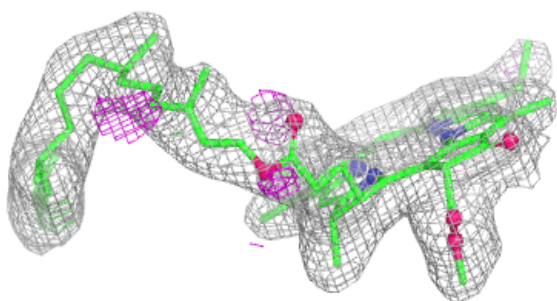
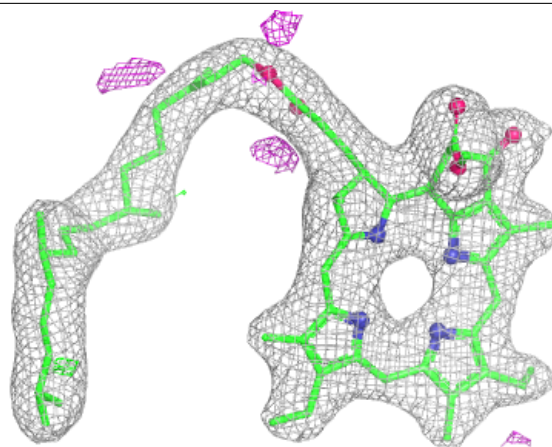
Electron density around PHO D 402 (B):

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



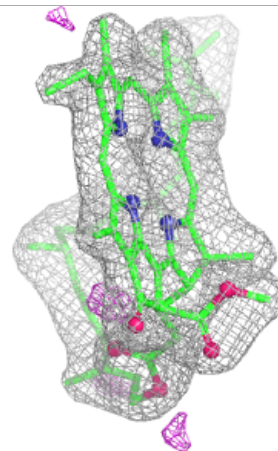
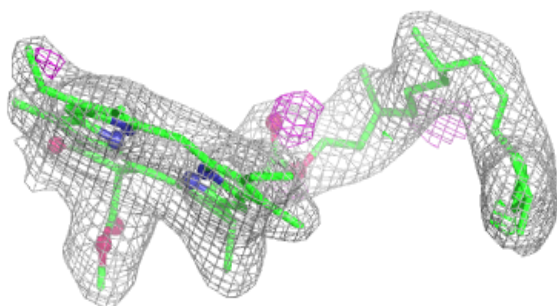
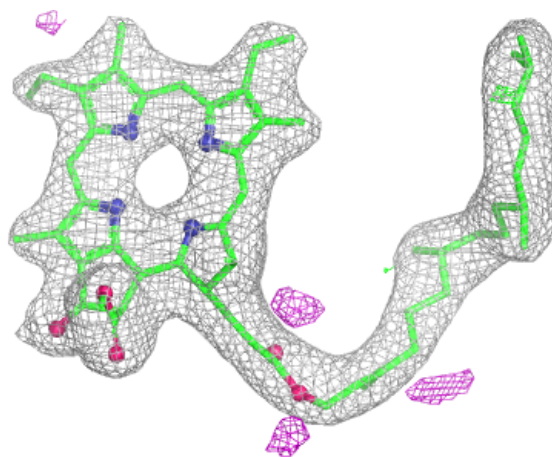
Electron density around PHO a 416 (A):

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



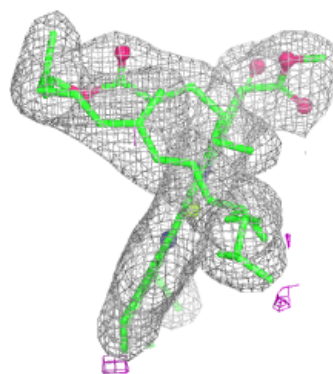
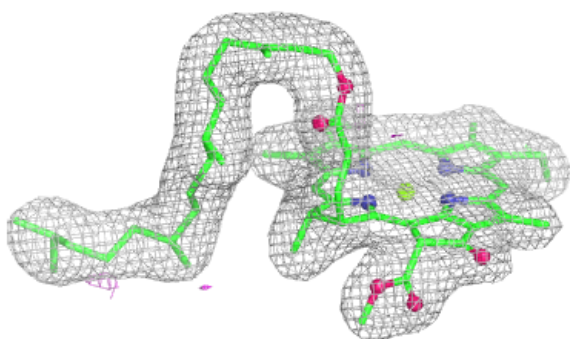
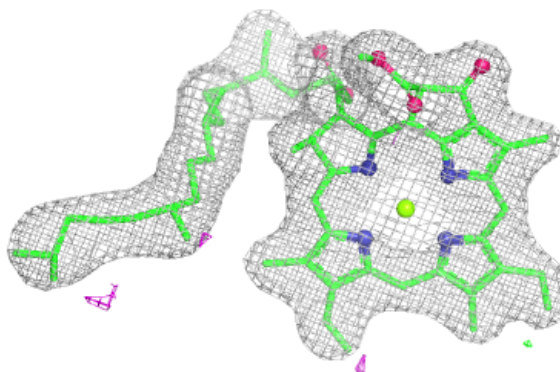
Electron density around PHO a 416 (B):

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

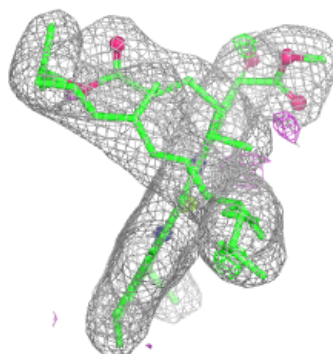
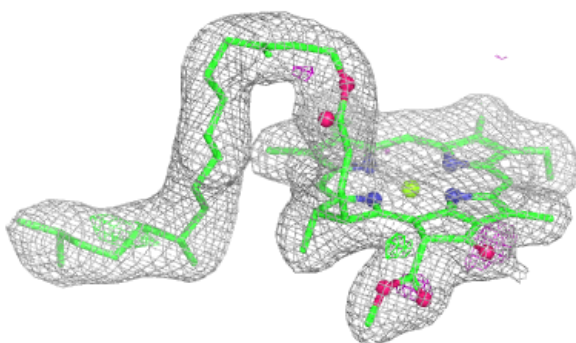
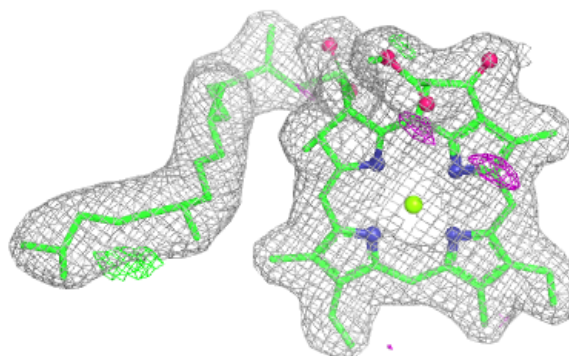


Electron density around CLA a 406 (B):

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

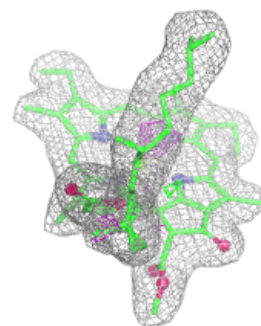
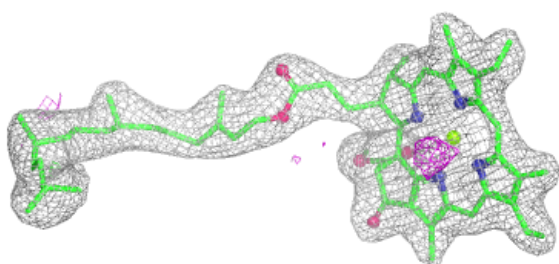
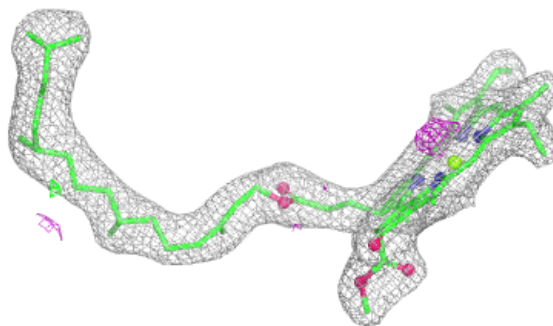
**Electron density around CLA A 405 (A):**

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

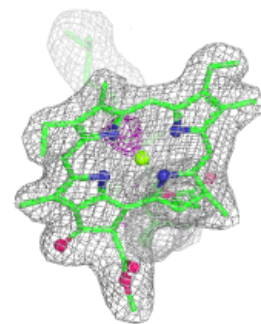
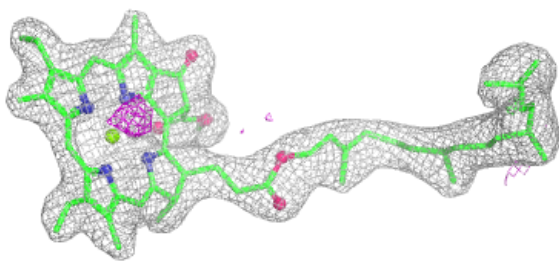
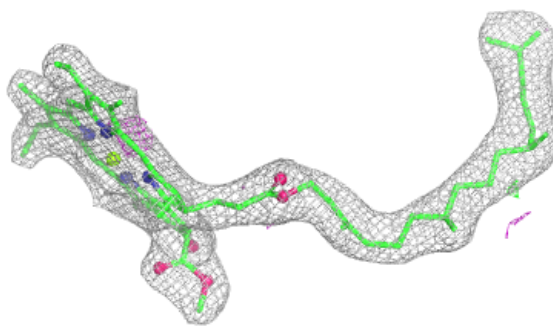


Electron density around CLA d 401 (A):

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

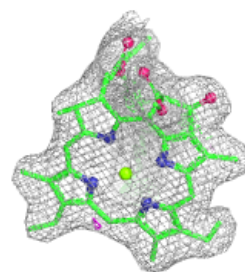
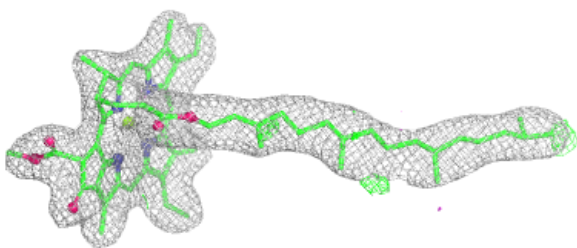
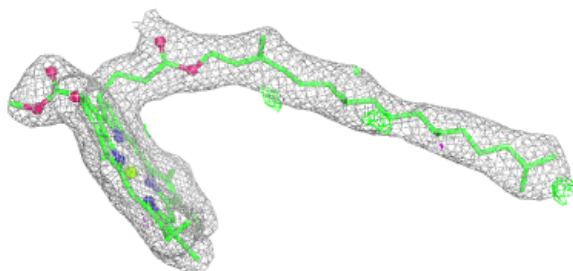
**Electron density around CLA d 401 (B):**

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



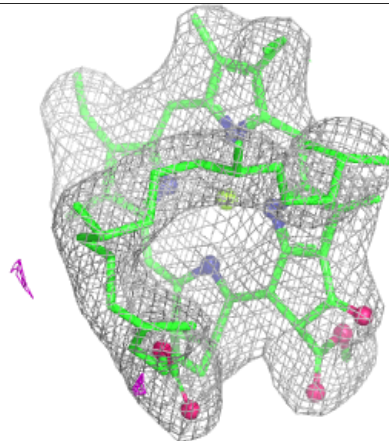
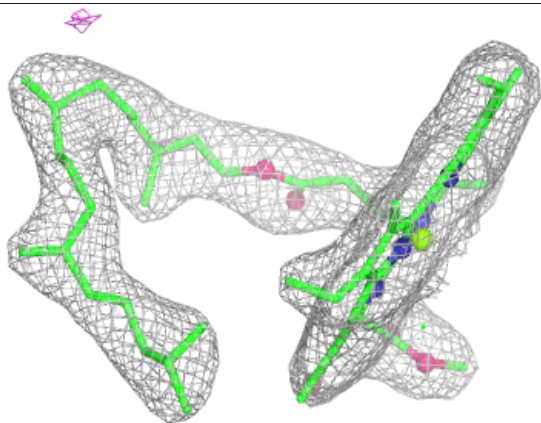
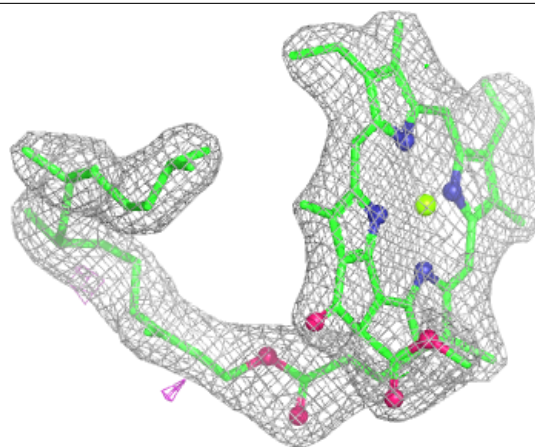
Electron density around CLA B 607:

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



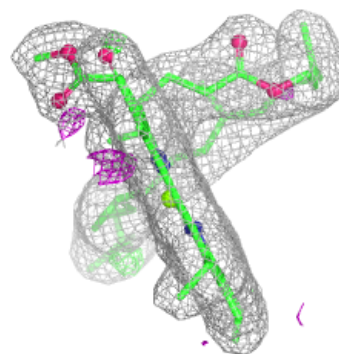
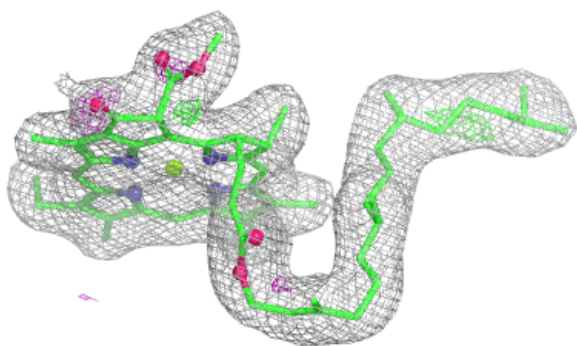
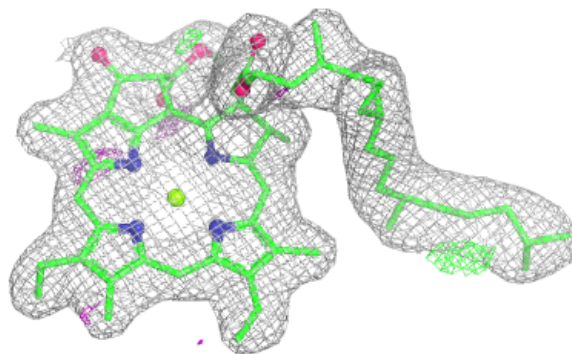
Electron density around CLA C 505:

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

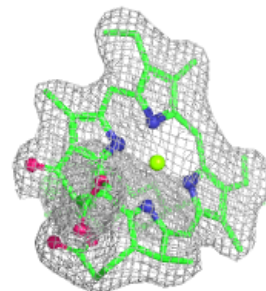
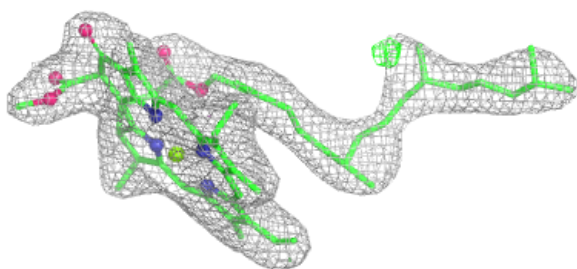
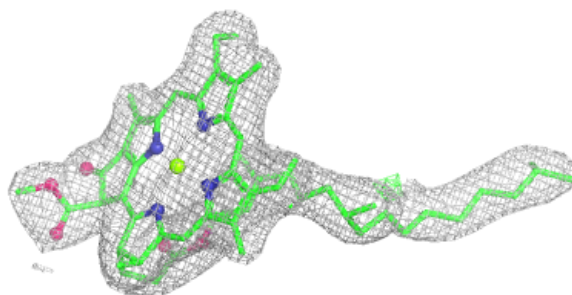


Electron density around CLA A 405 (B):

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

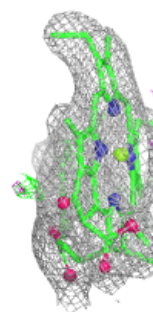
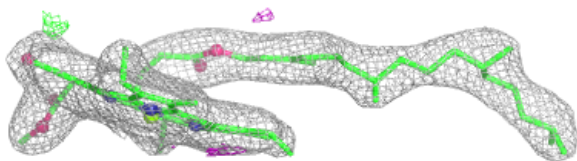
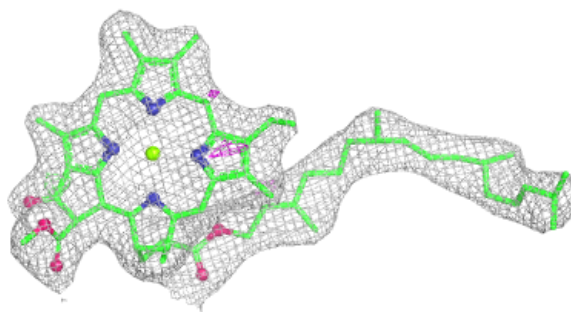
**Electron density around CLA C 507:**

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

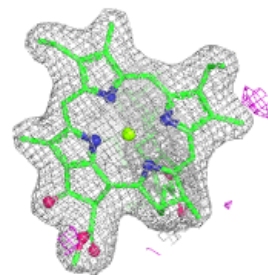
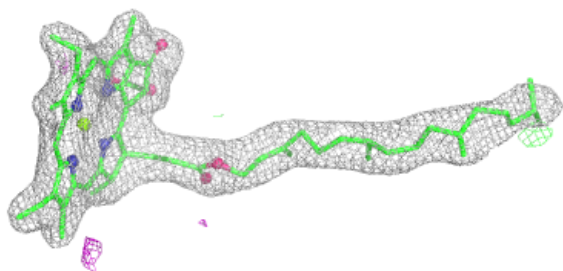
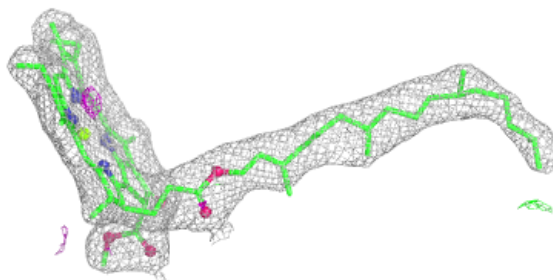


Electron density around CLA b 603:

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

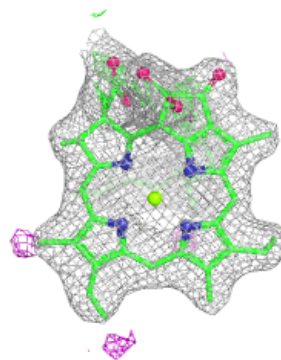
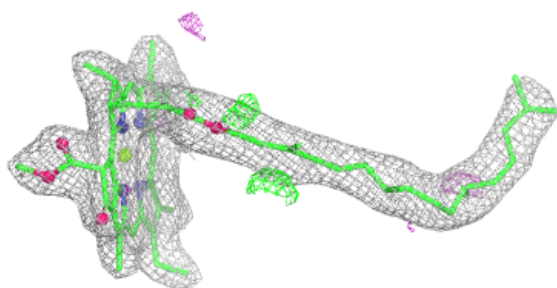
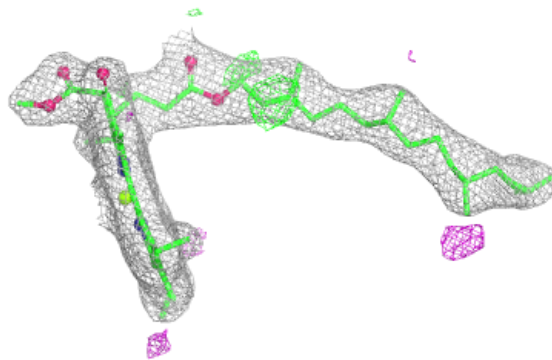
**Electron density around CLA b 604:**

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



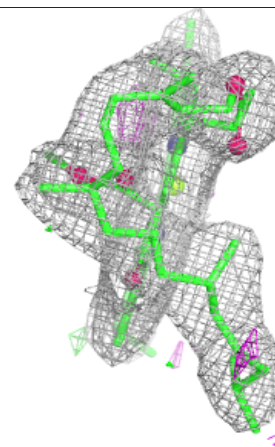
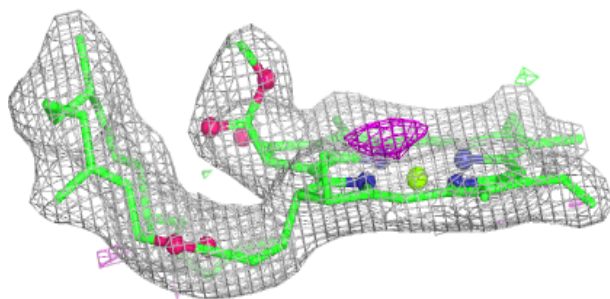
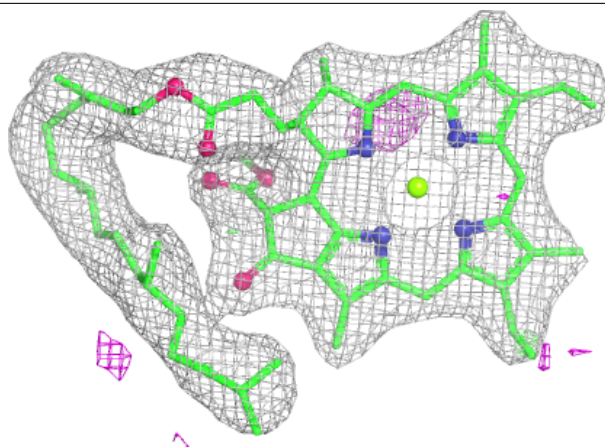
Electron density around CLA b 605:

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



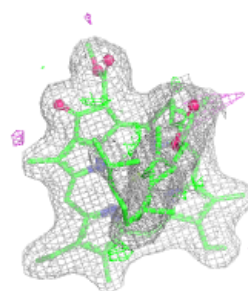
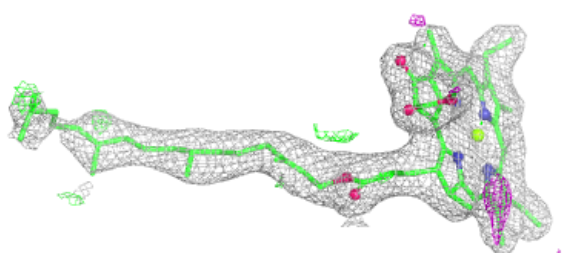
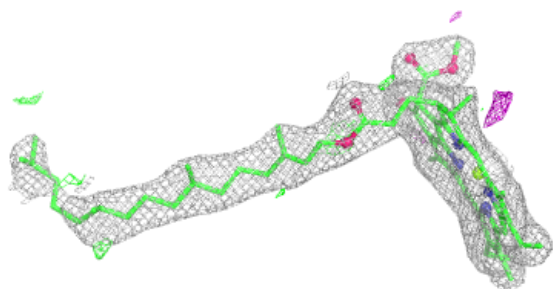
Electron density around CLA B 610:

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

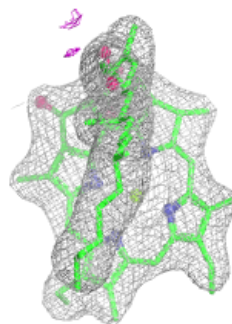
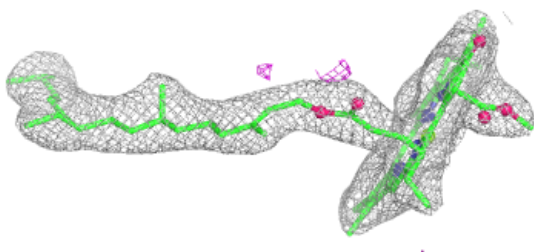
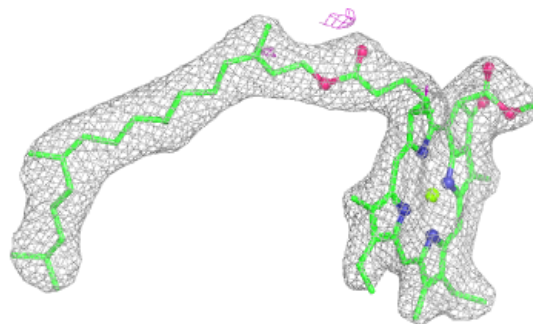


Electron density around CLA B 604:

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

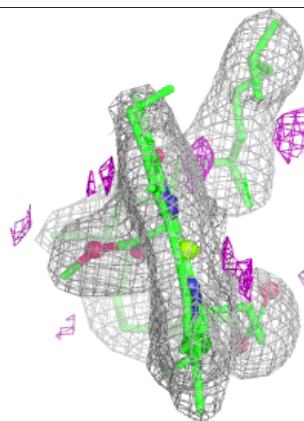
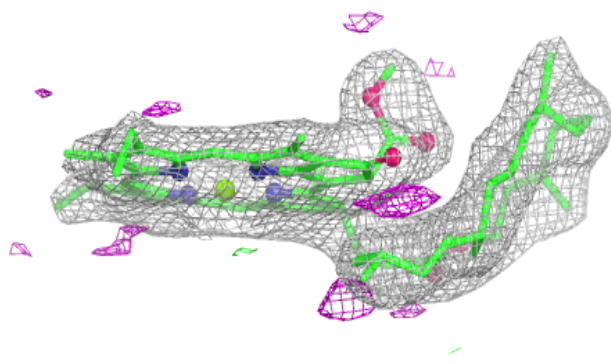
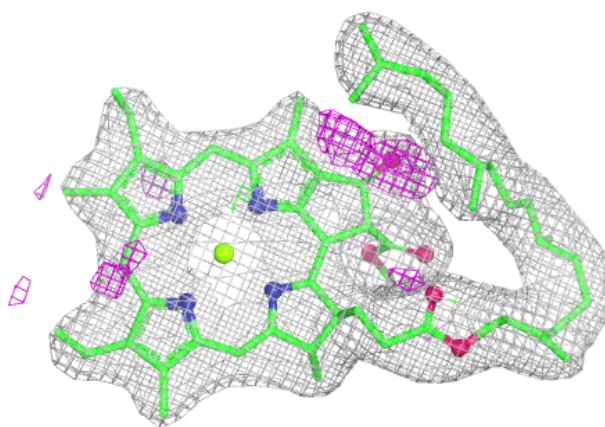
**Electron density around CLA b 609:**

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



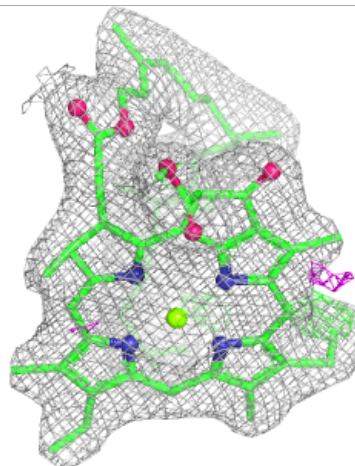
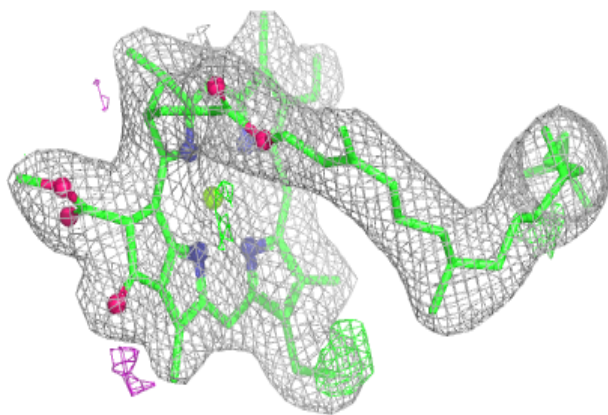
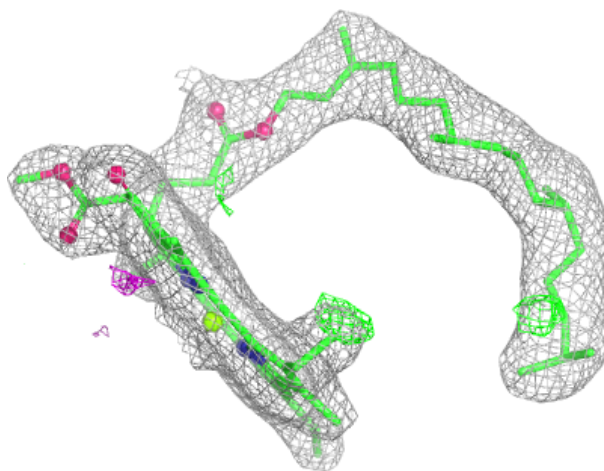
Electron density around CLA b 610:

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



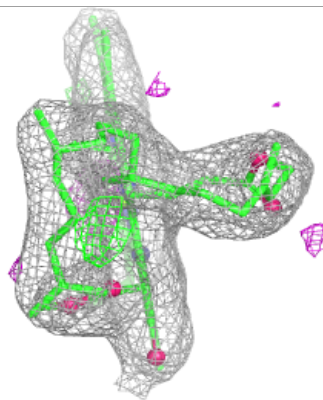
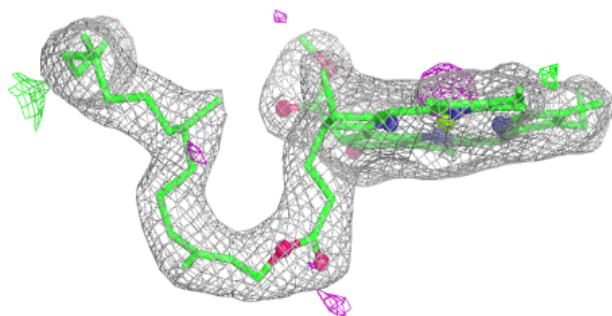
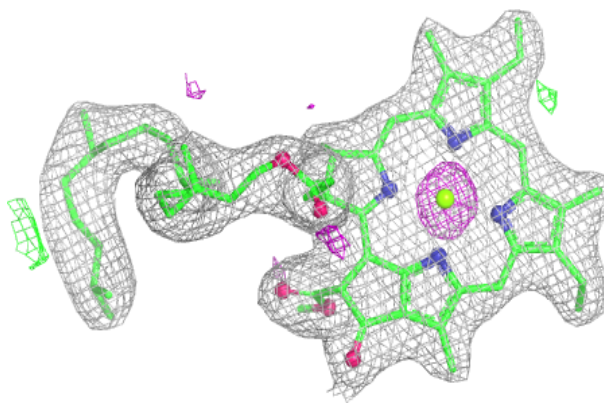
Electron density around CLA b 611:

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



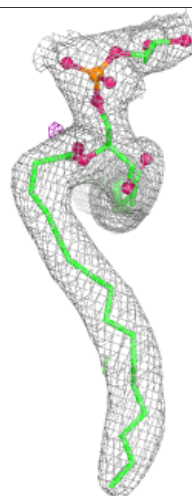
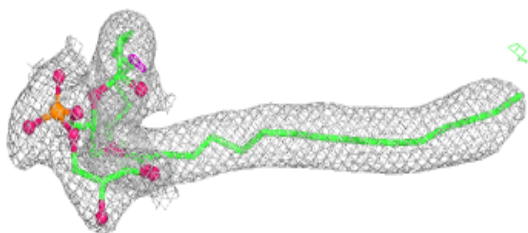
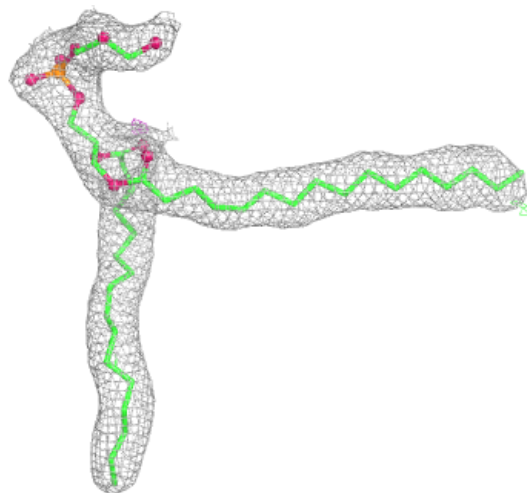
Electron density around CLA B 612:

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



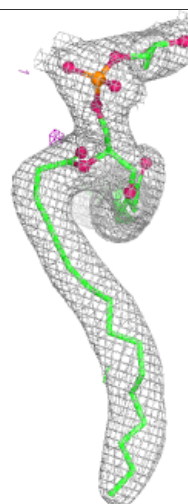
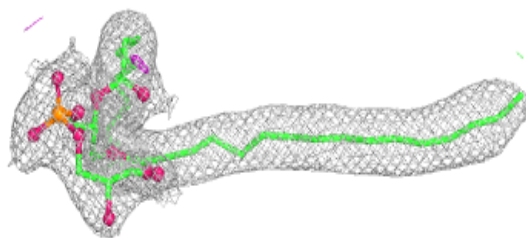
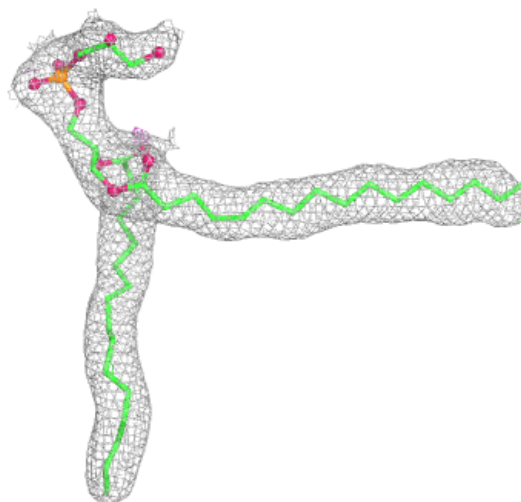
Electron density around LHG L 101 (A):

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



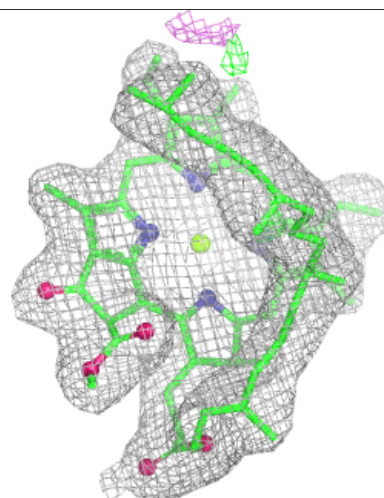
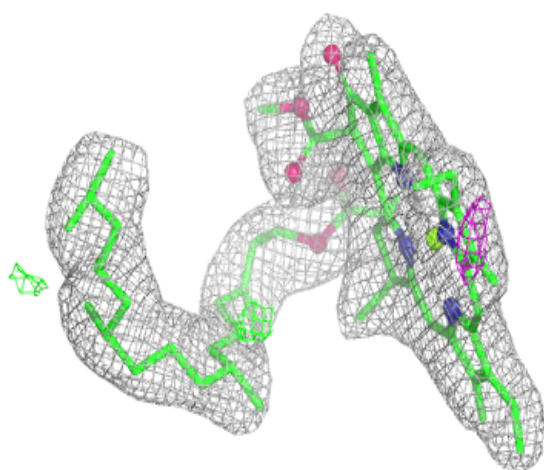
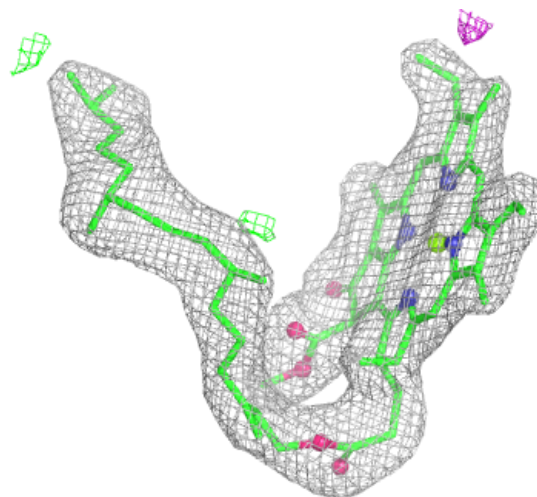
Electron density around LHG L 101 (B):

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



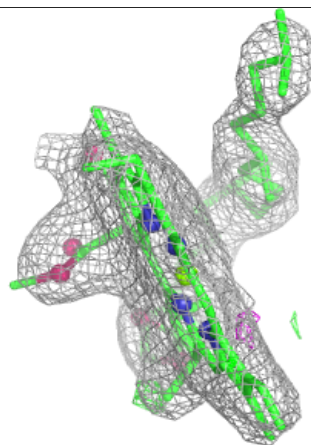
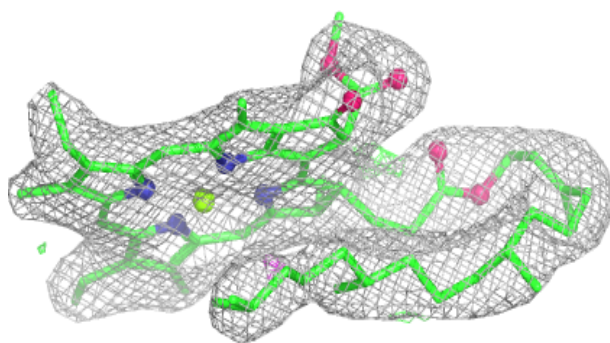
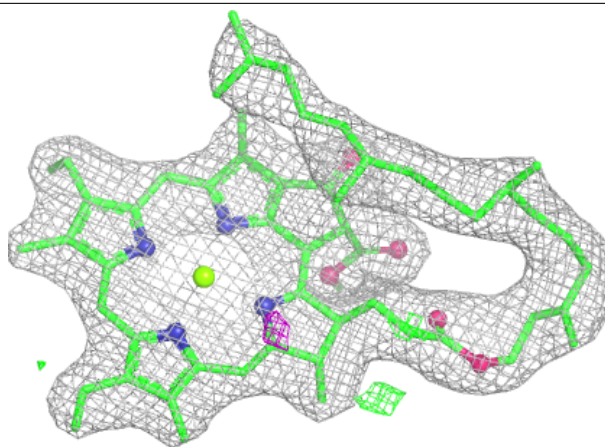
Electron density around CLA b 613:

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



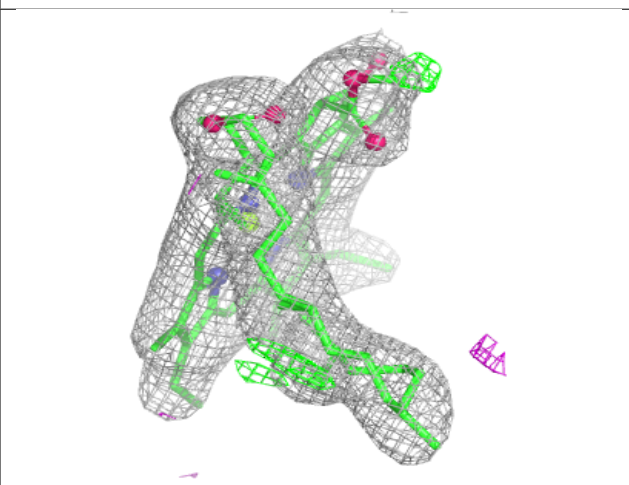
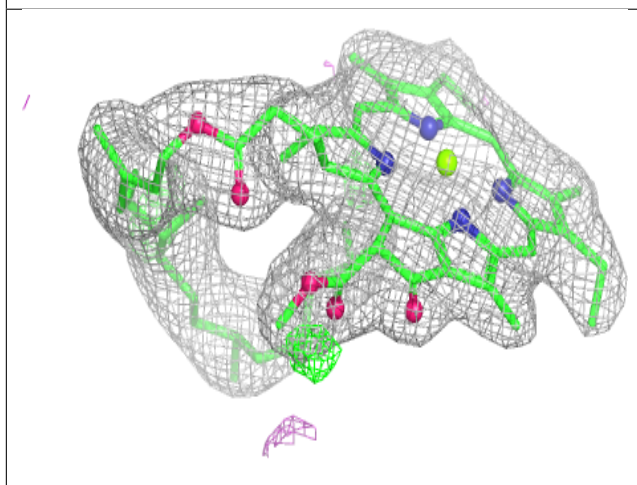
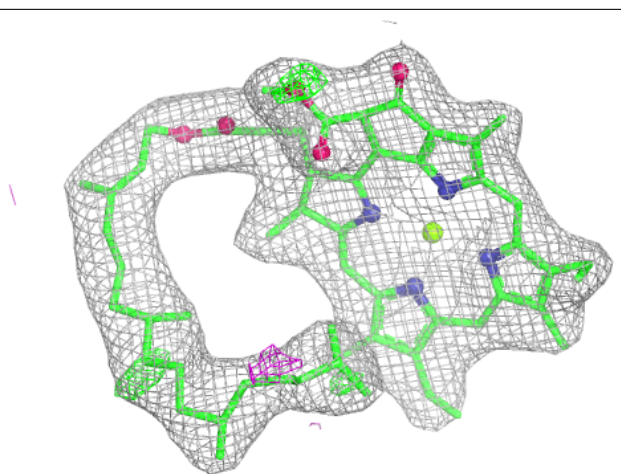
Electron density around CLA C 511:

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



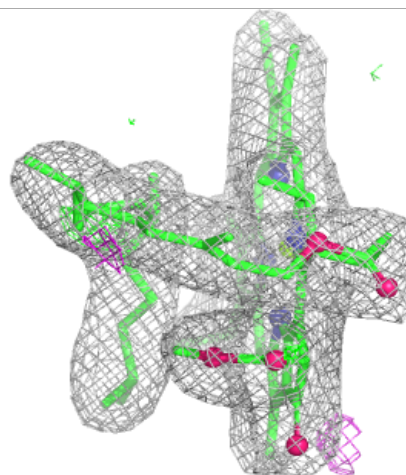
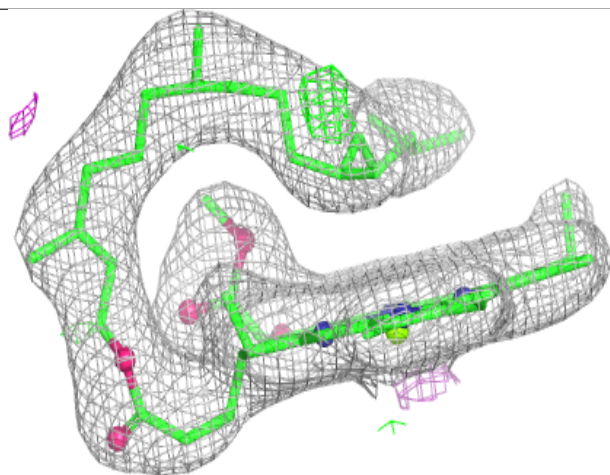
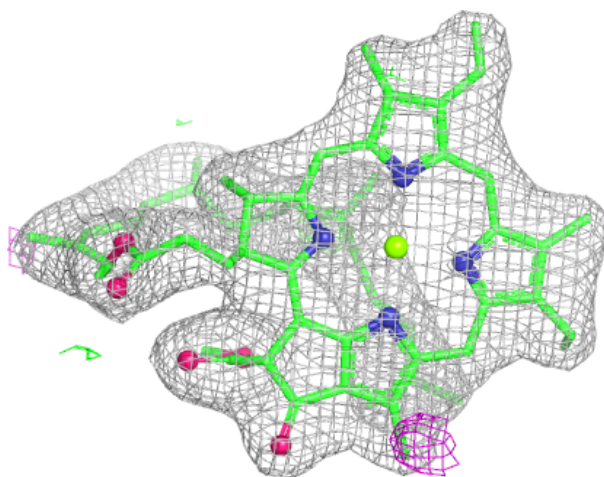
Electron density around CLA b 615:

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



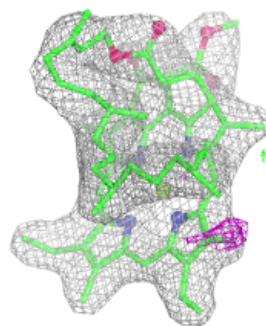
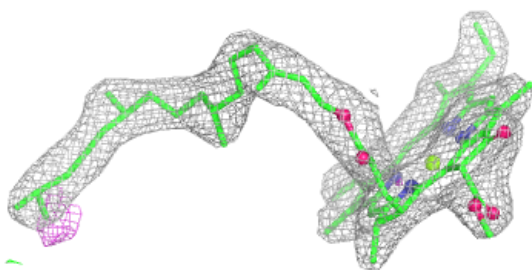
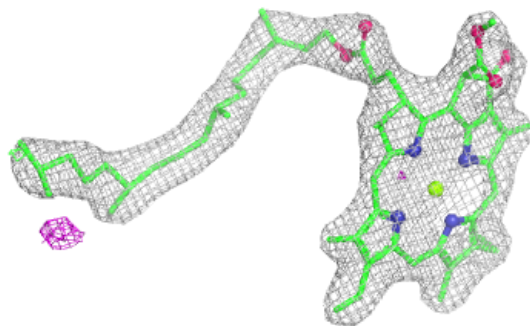
Electron density around CLA C 512:

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

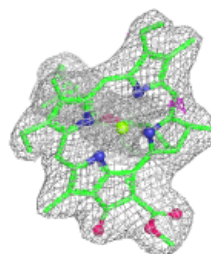
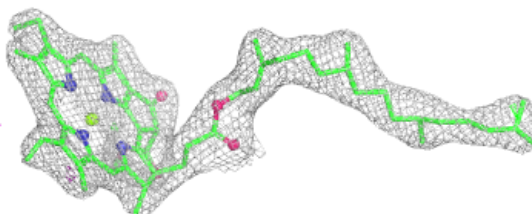
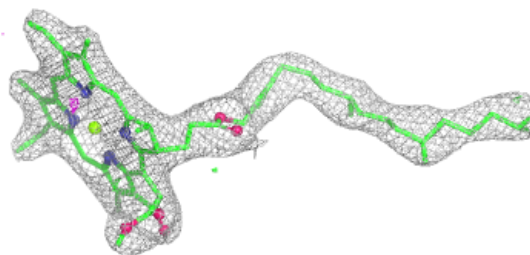


Electron density around CLA C 513:

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

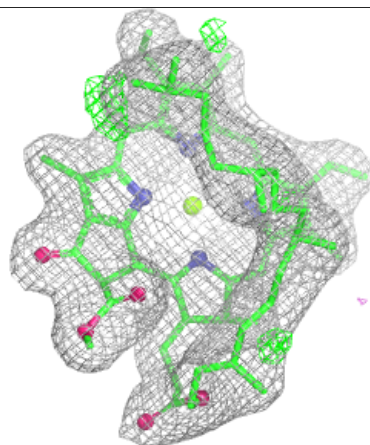
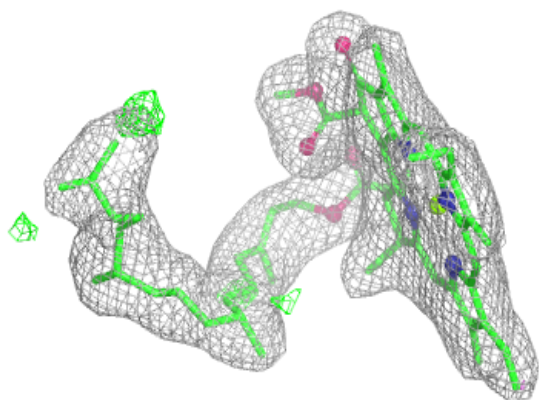
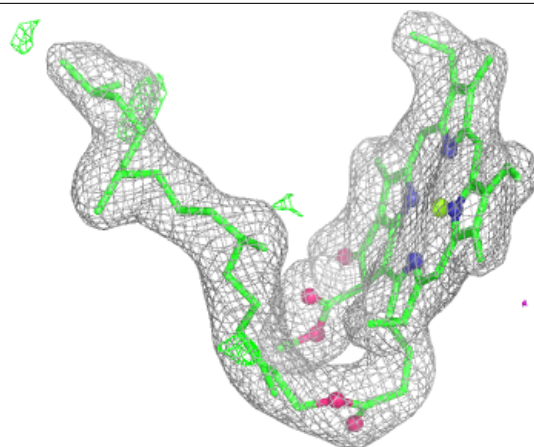
**Electron density around CLA c 503:**

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



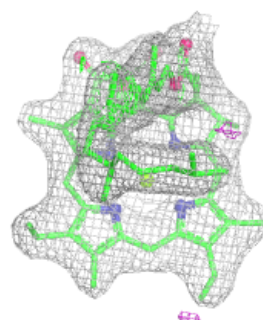
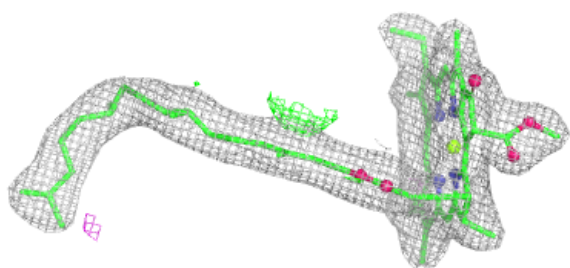
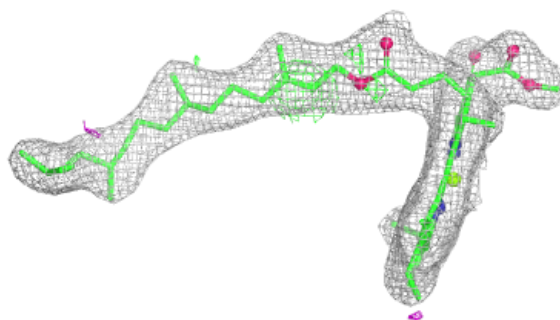
Electron density around CLA B 613:

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

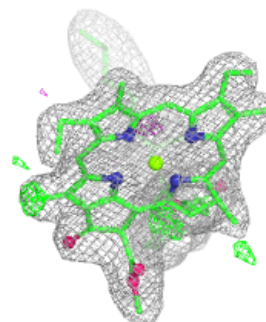
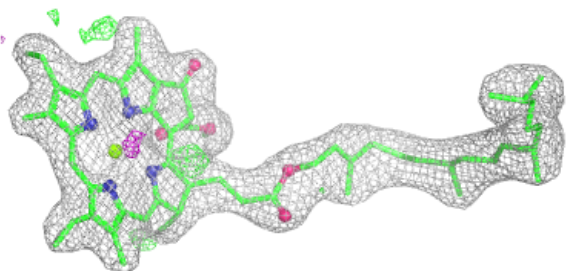
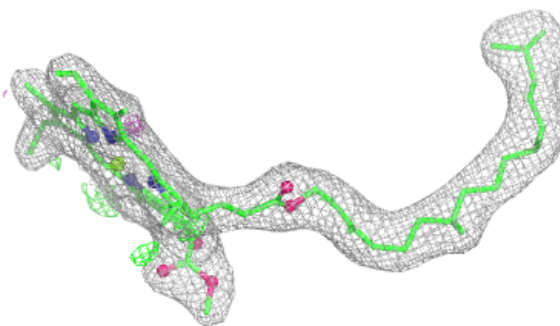


Electron density around CLA B 605:

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

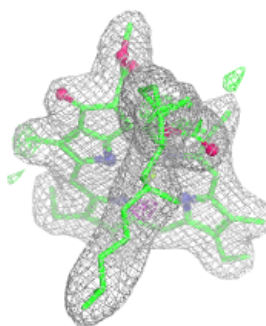
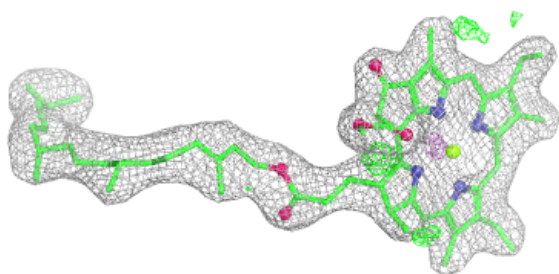
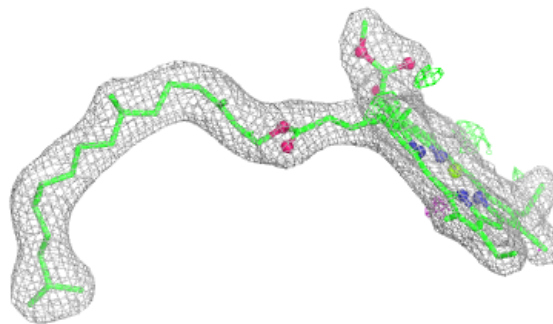
**Electron density around CLA D 404 (A):**

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

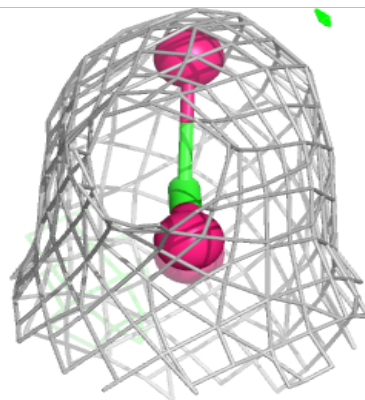
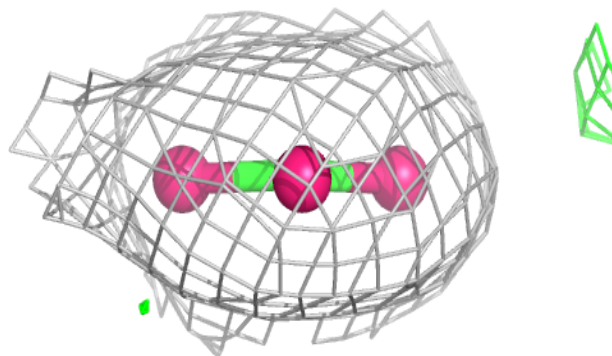
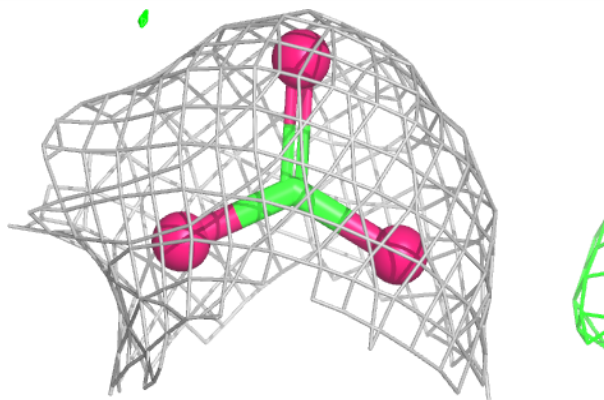


Electron density around CLA D 404 (B):

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

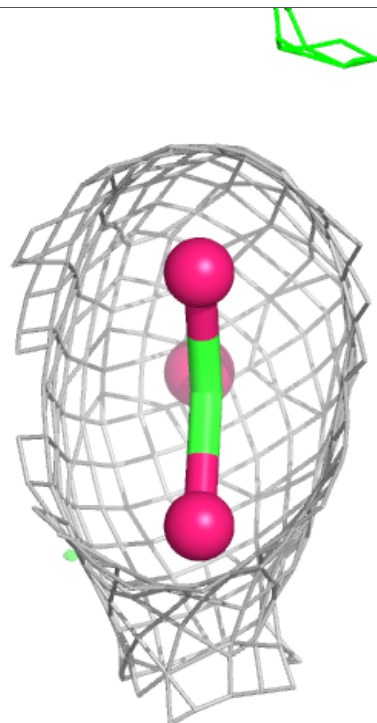
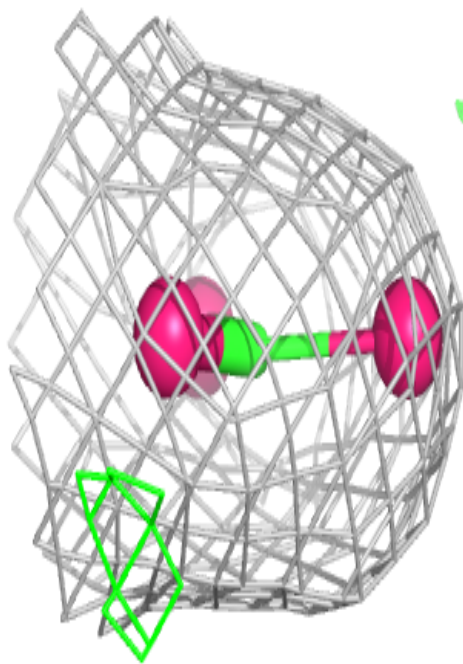
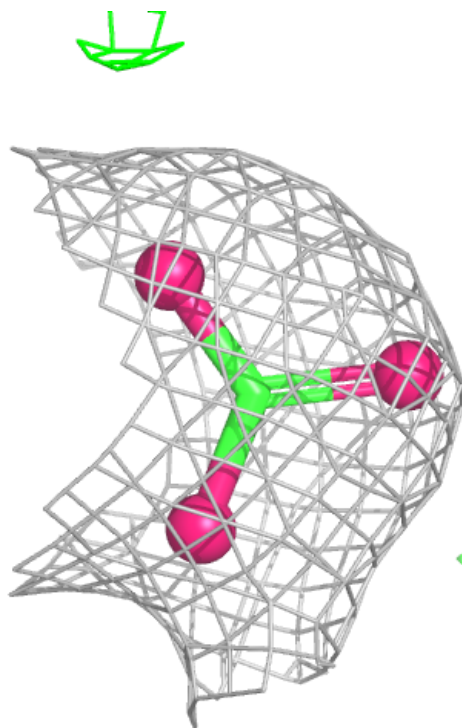
**Electron density around BCT a 404 (A):**

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



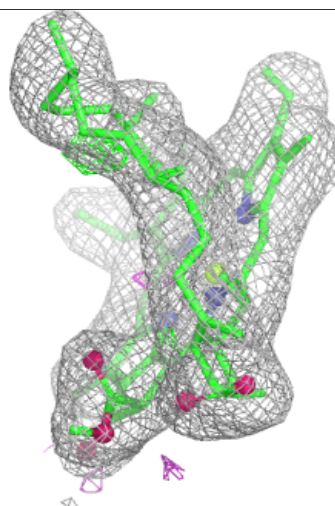
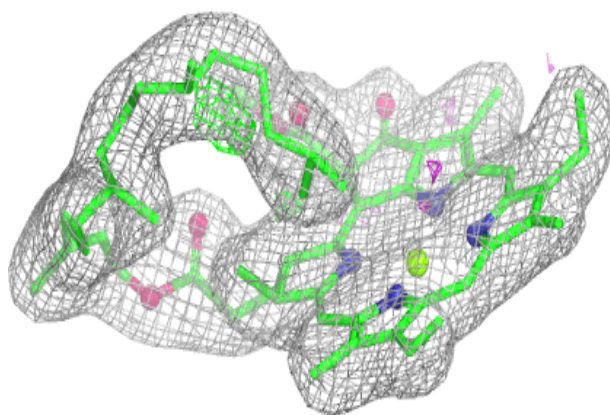
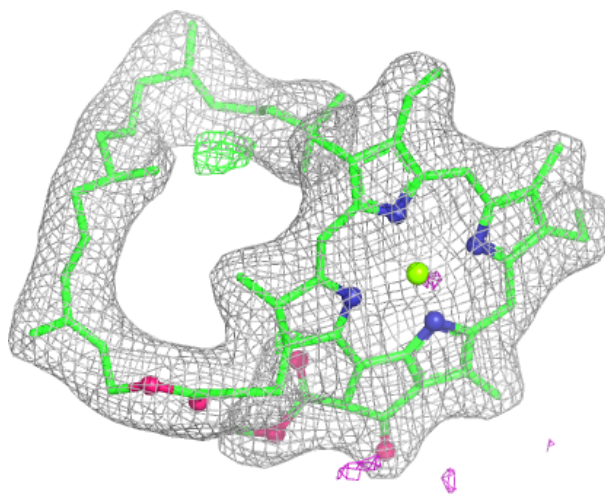
Electron density around BCT a 404 (B):

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



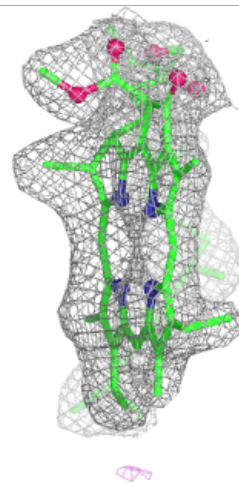
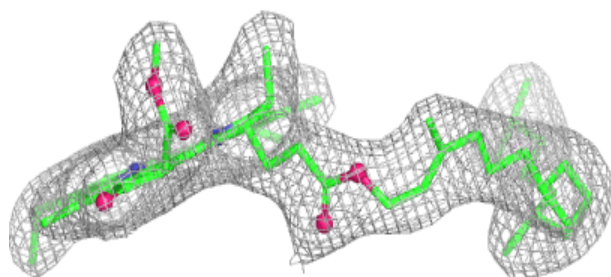
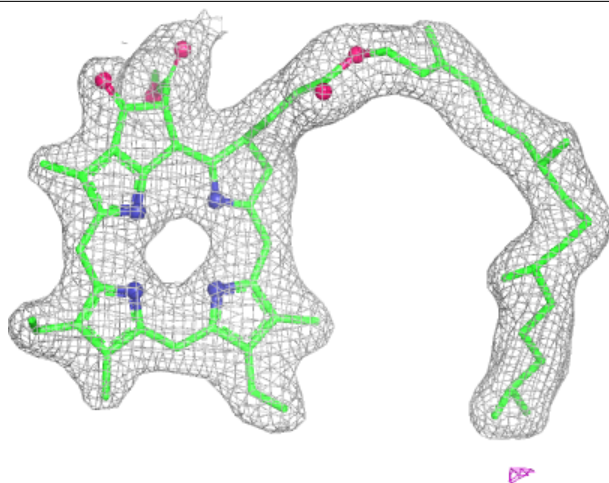
Electron density around CLA B 615:

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



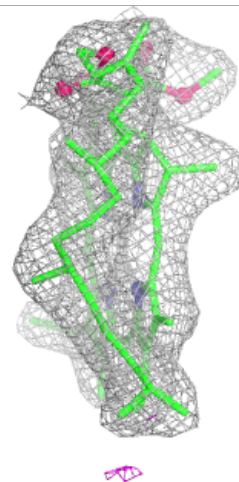
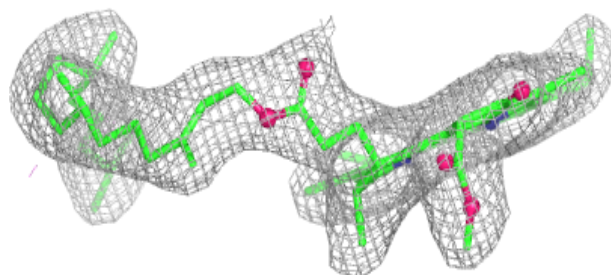
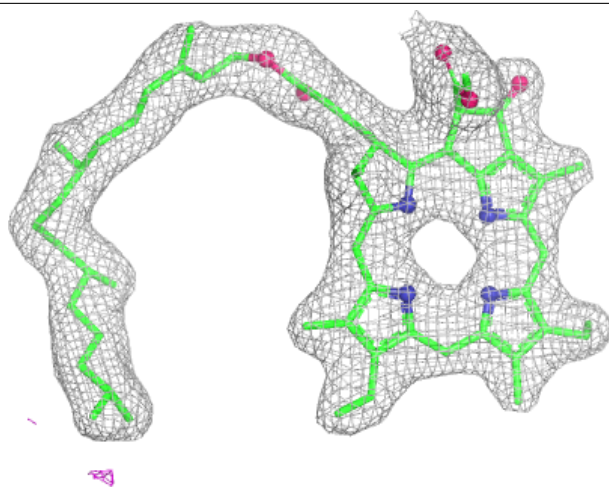
Electron density around PHO D 401 (A):

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



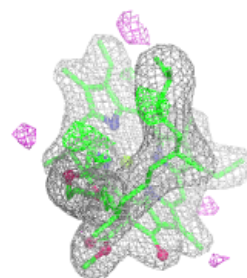
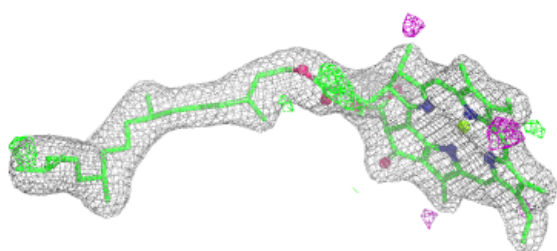
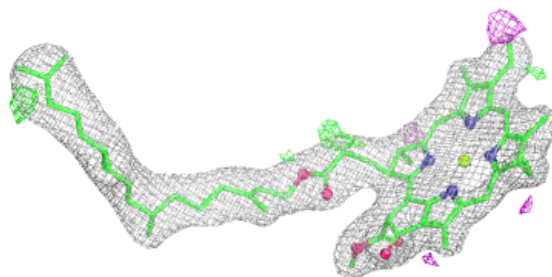
Electron density around PHO D 401 (B):

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



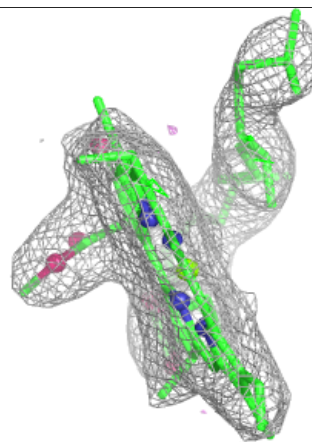
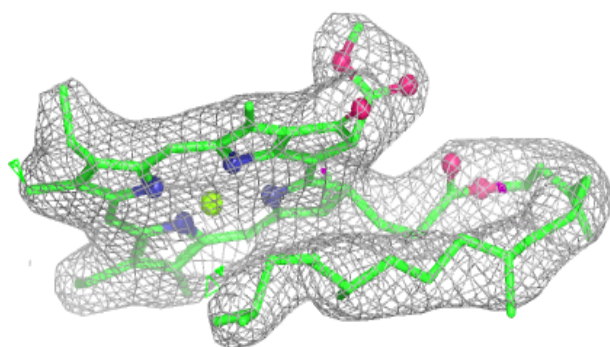
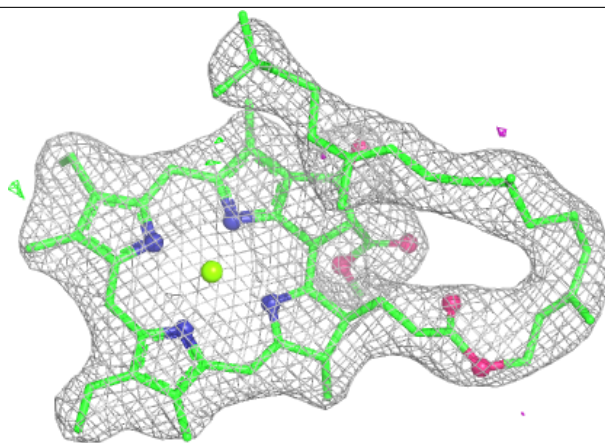
Electron density around CLA a 405 (A):

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



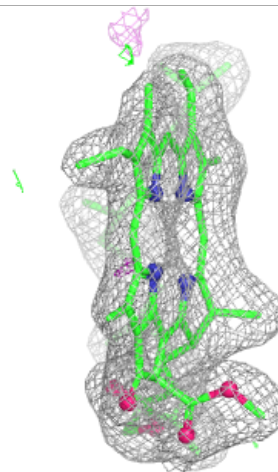
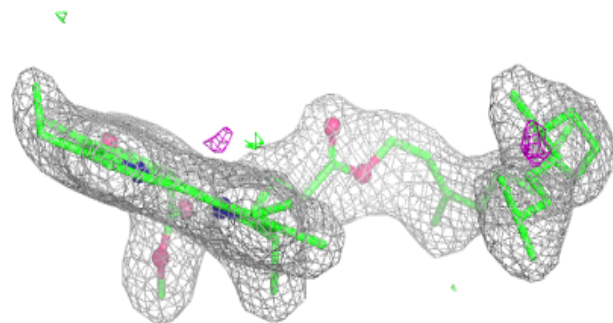
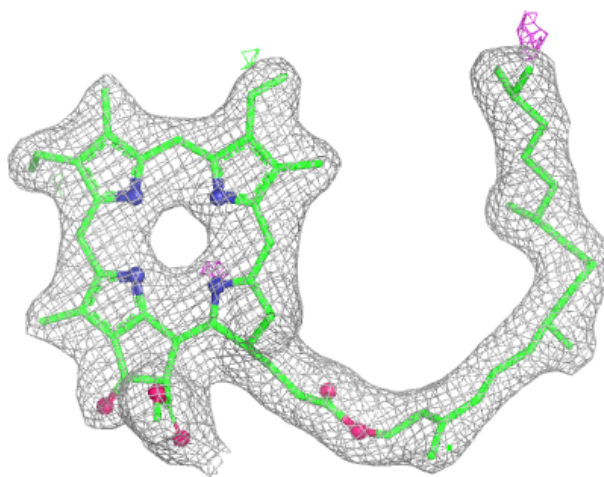
Electron density around CLA c 510:

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



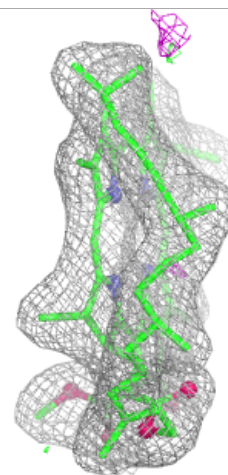
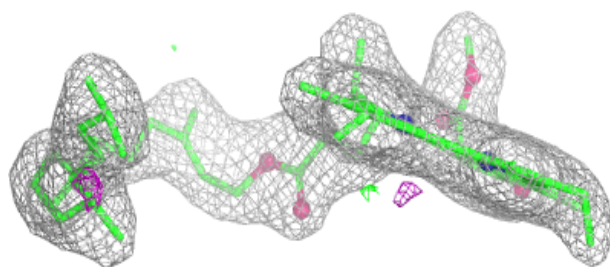
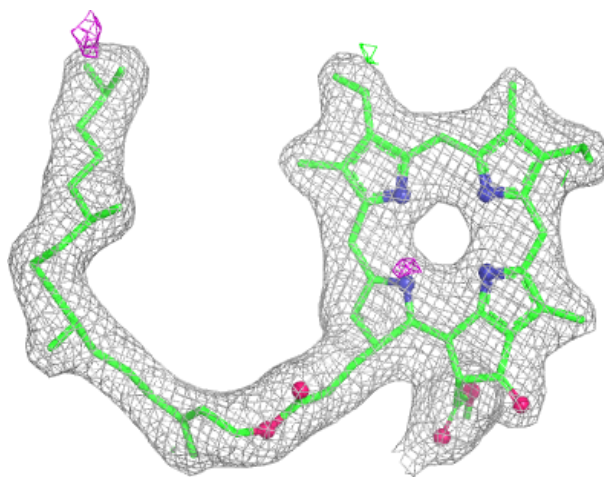
Electron density around PHO a 408 (A):

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



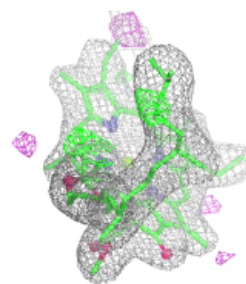
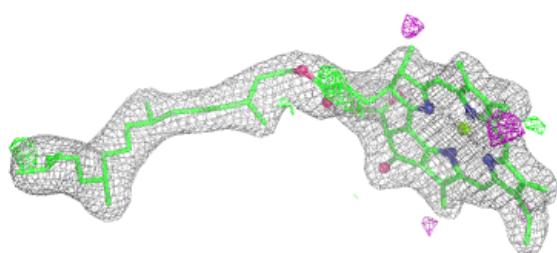
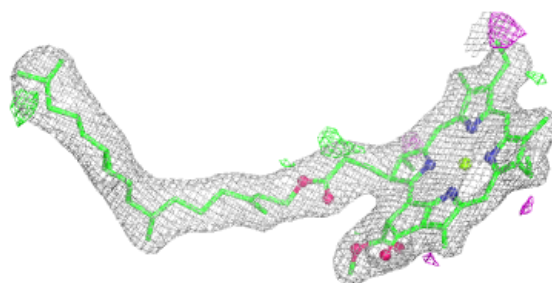
Electron density around PHO a 408 (B):

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

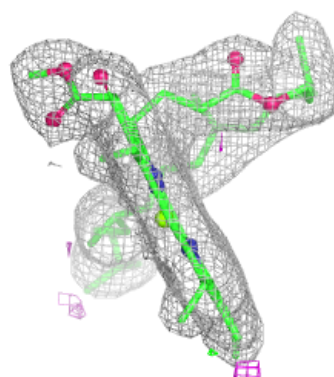
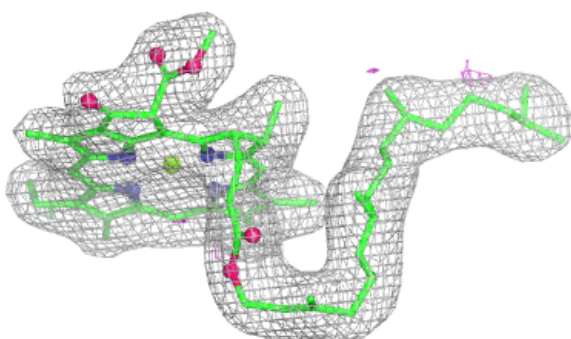
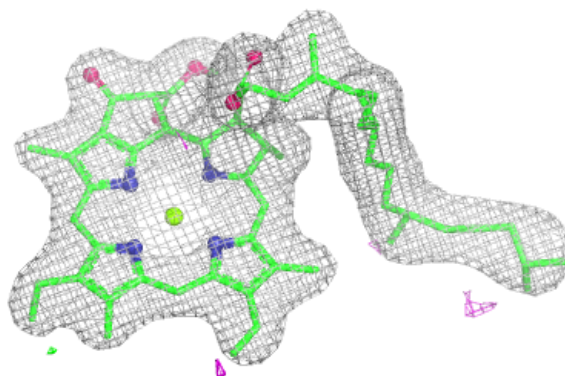


Electron density around CLA a 405 (B):

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

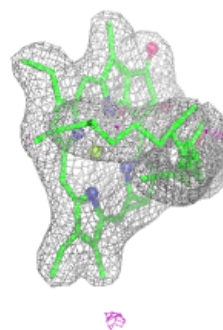
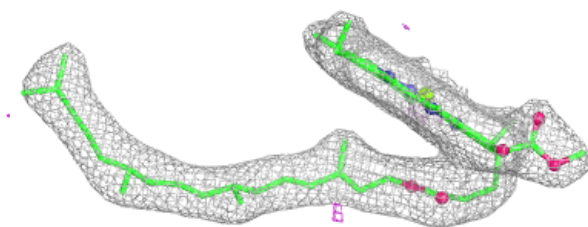
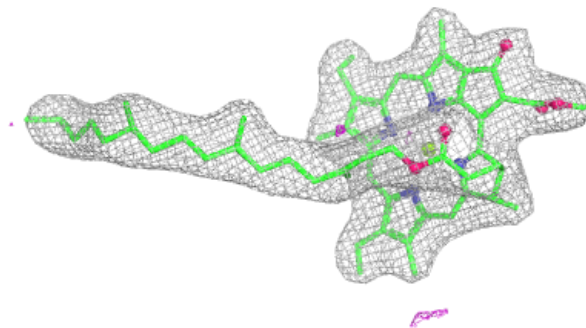
**Electron density around CLA a 406 (A):**

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



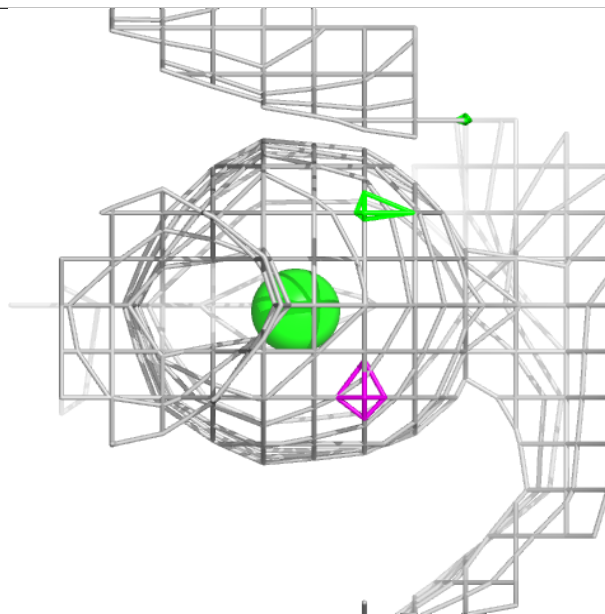
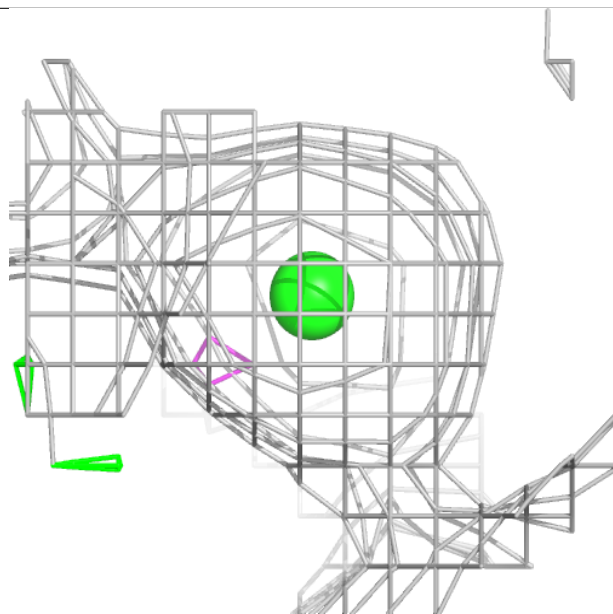
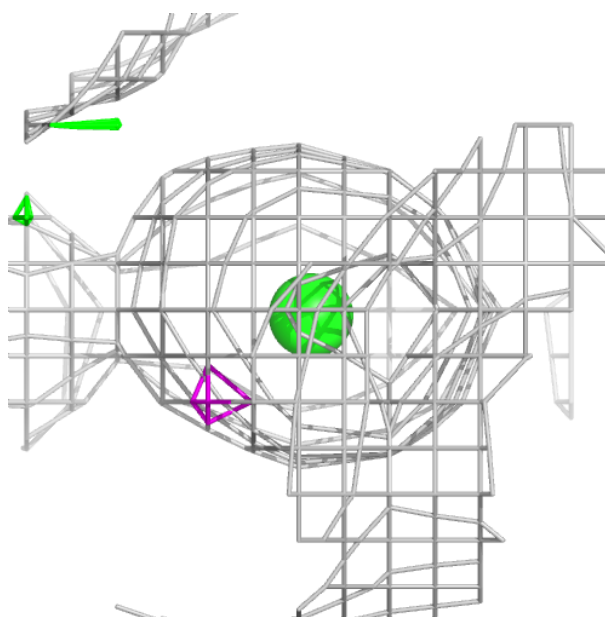
Electron density around CLA B 608:

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



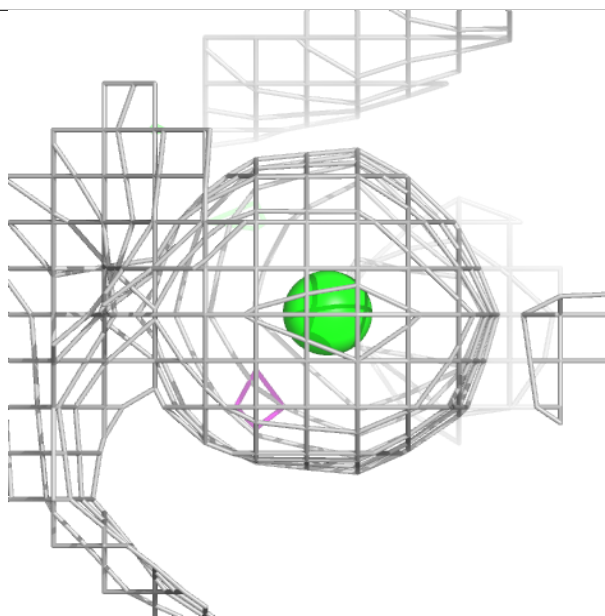
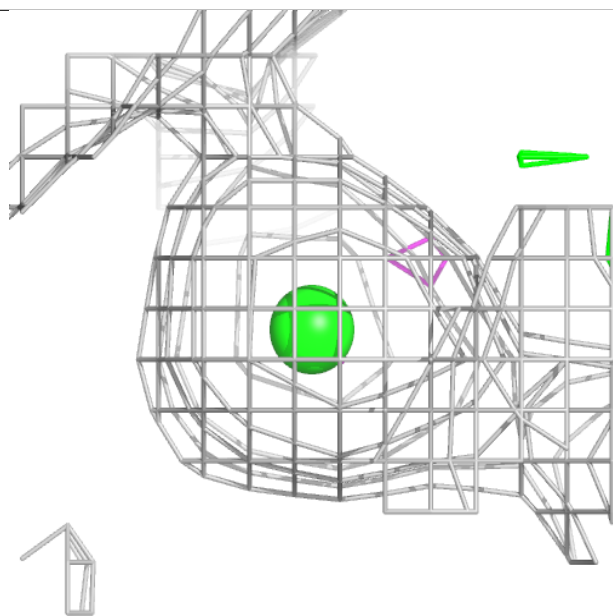
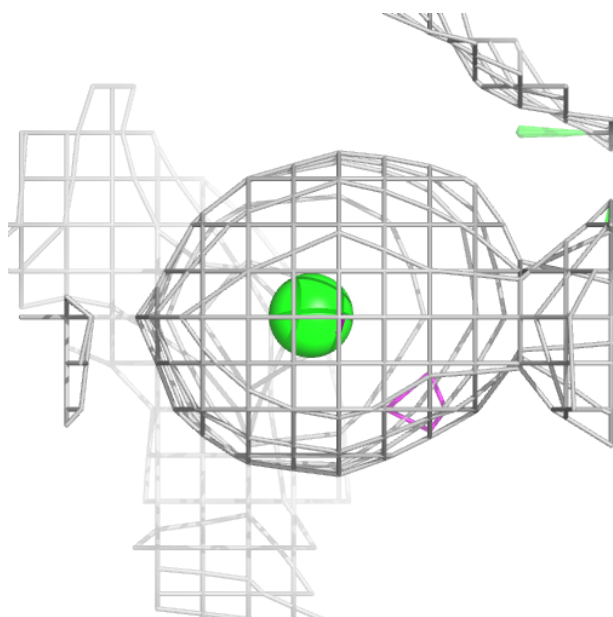
Electron density around CL a 403 (A):

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



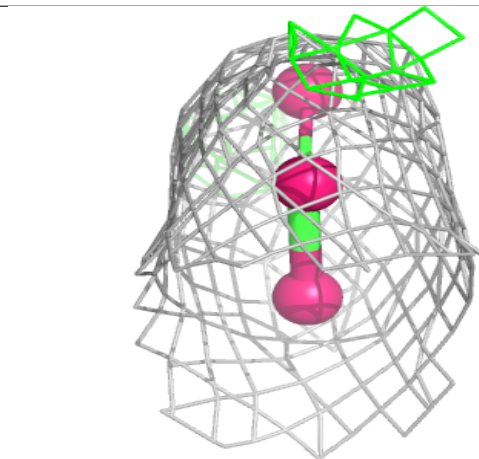
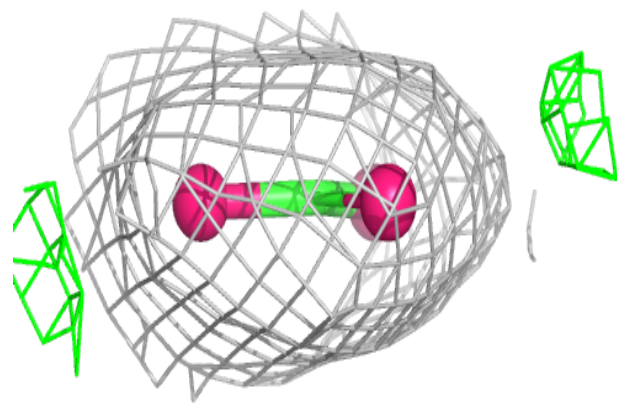
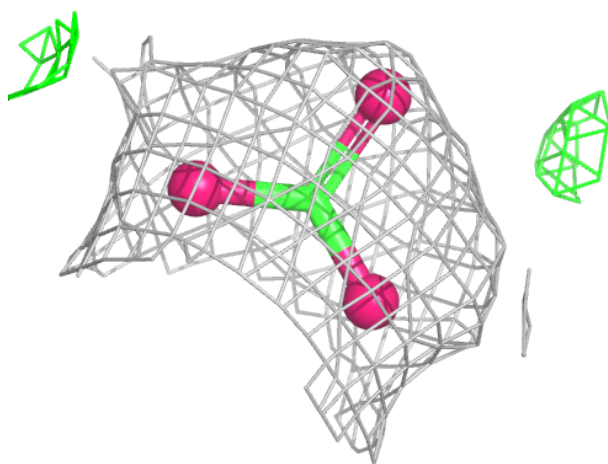
Electron density around CL a 403 (B):

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



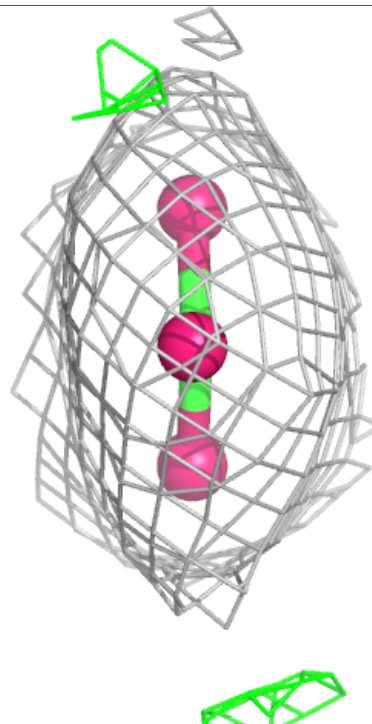
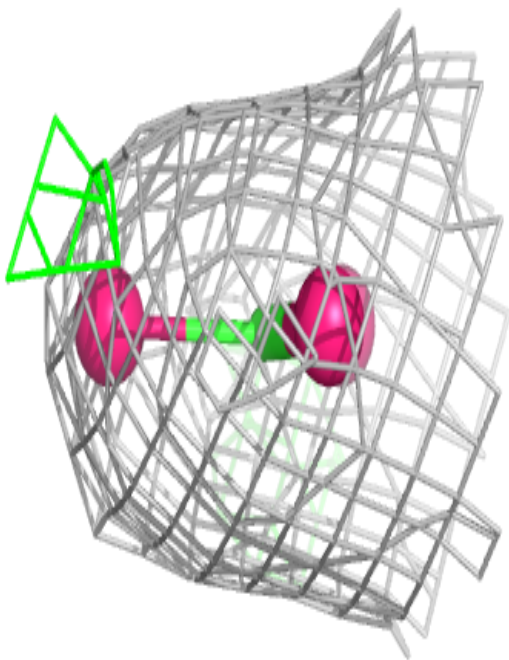
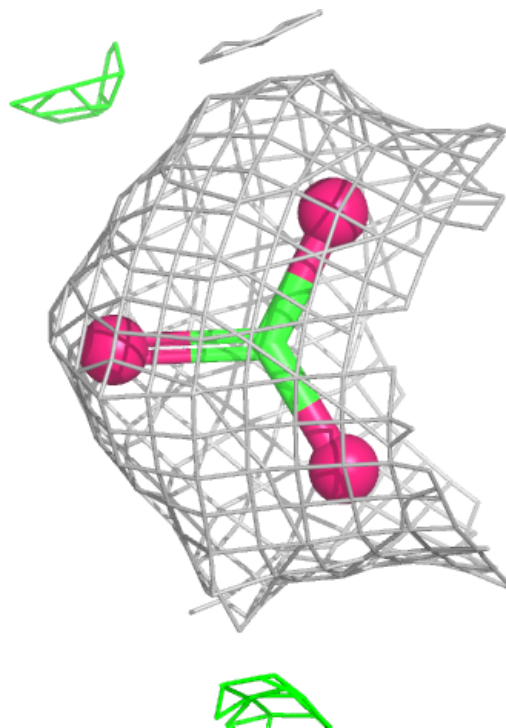
Electron density around BCT A 414 (A):

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



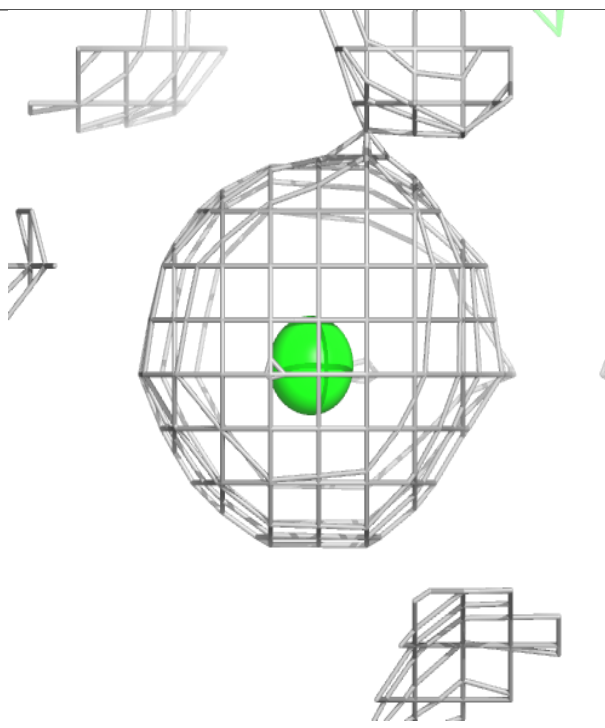
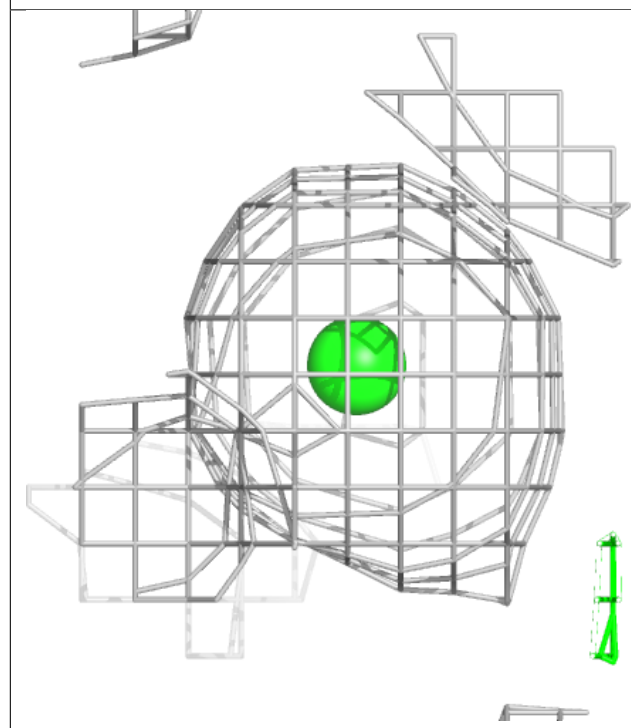
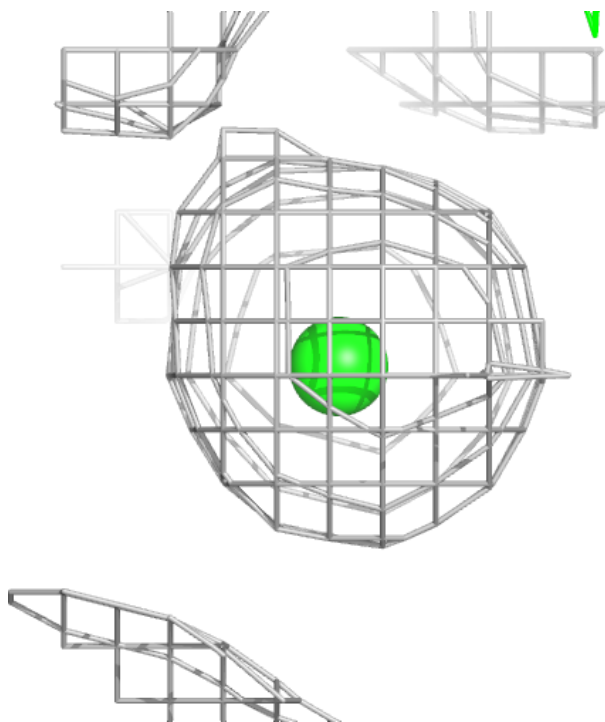
Electron density around BCT A 414 (B):

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



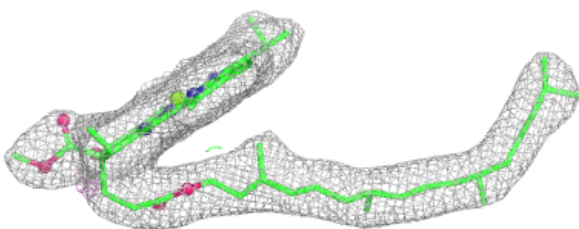
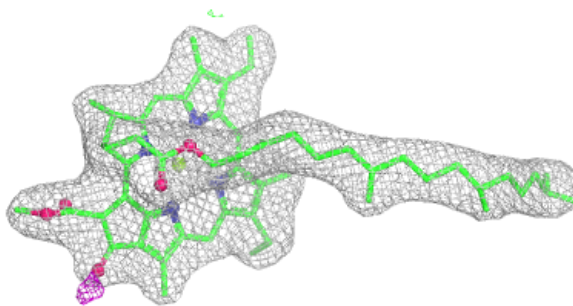
Electron density around CL a 402 (A):

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



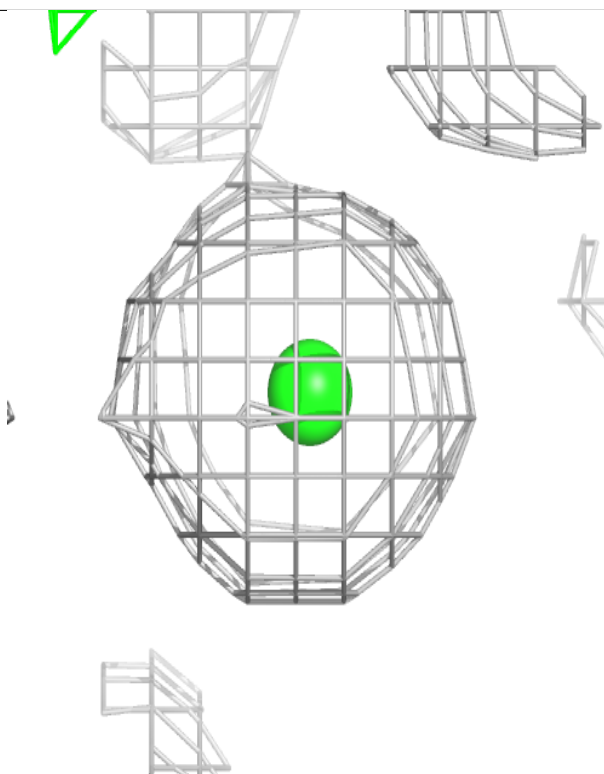
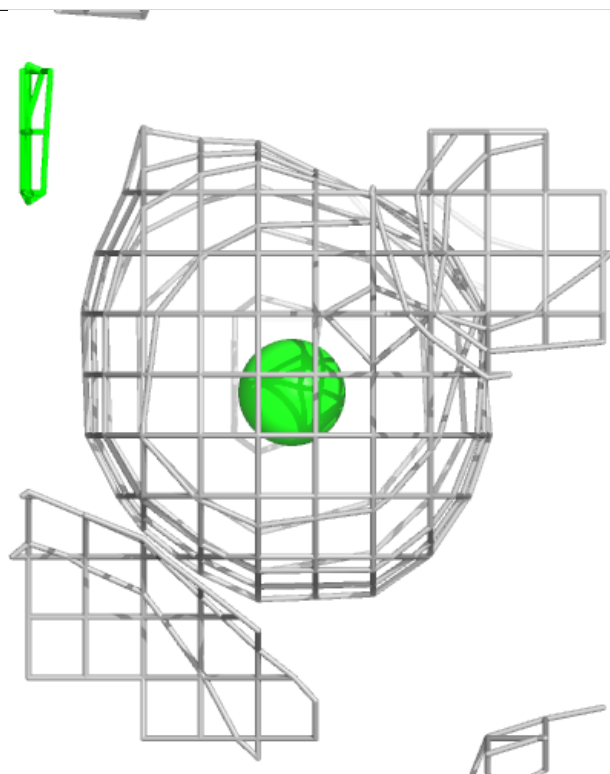
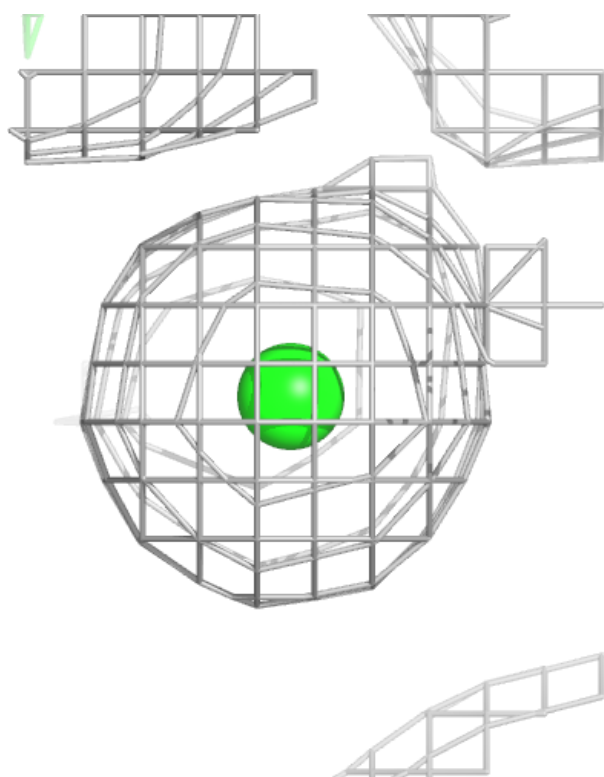
Electron density around CLA b 608:

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



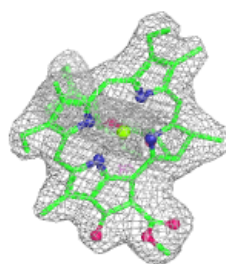
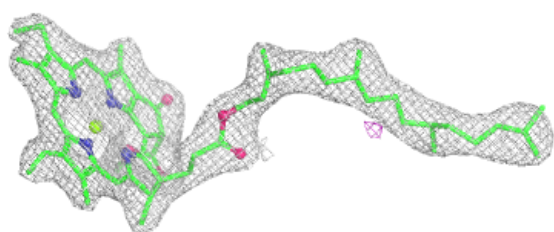
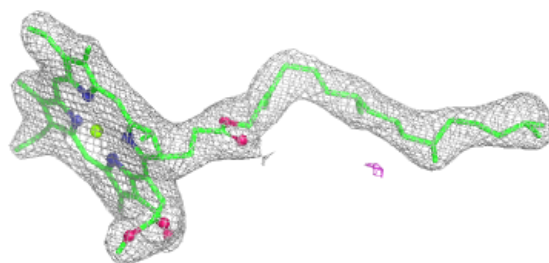
Electron density around CL a 402 (B):

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



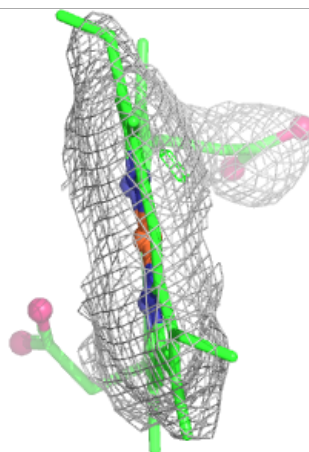
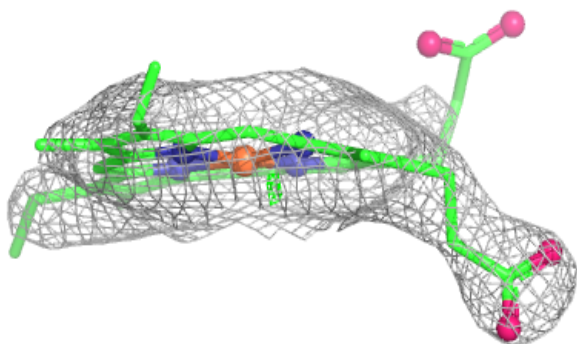
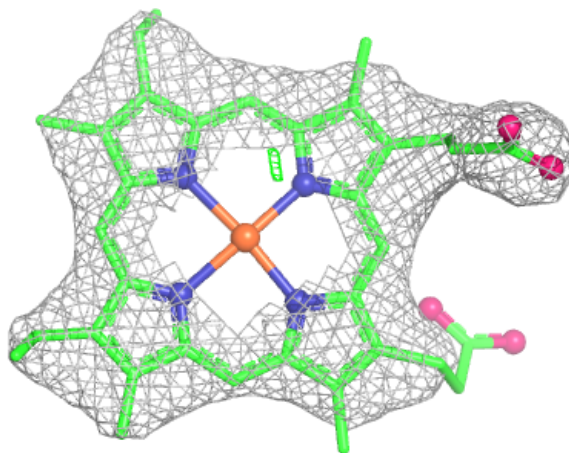
Electron density around CLA C 504:

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



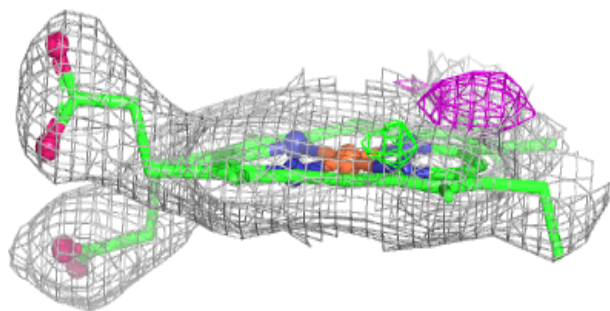
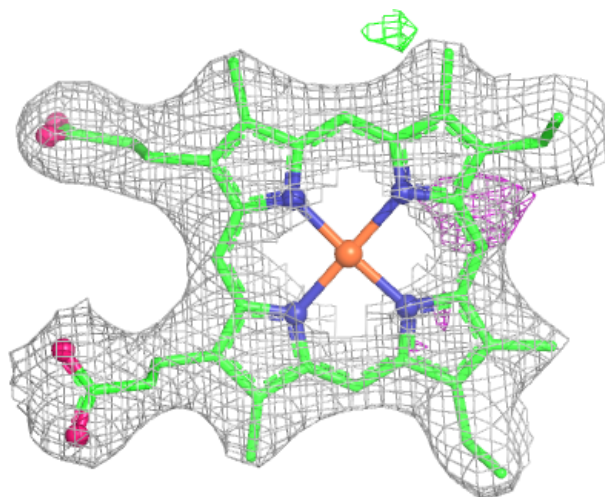
Electron density around HEM f 101:

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



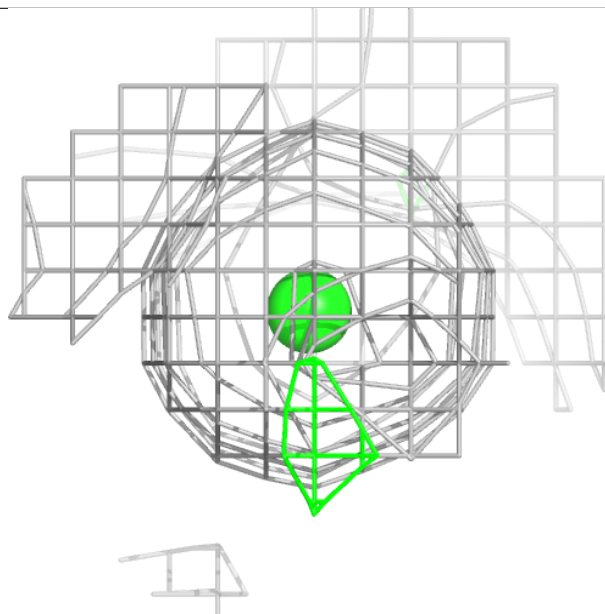
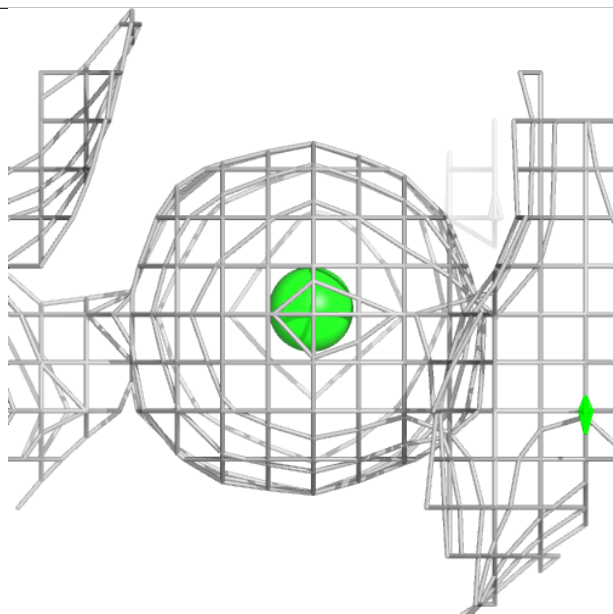
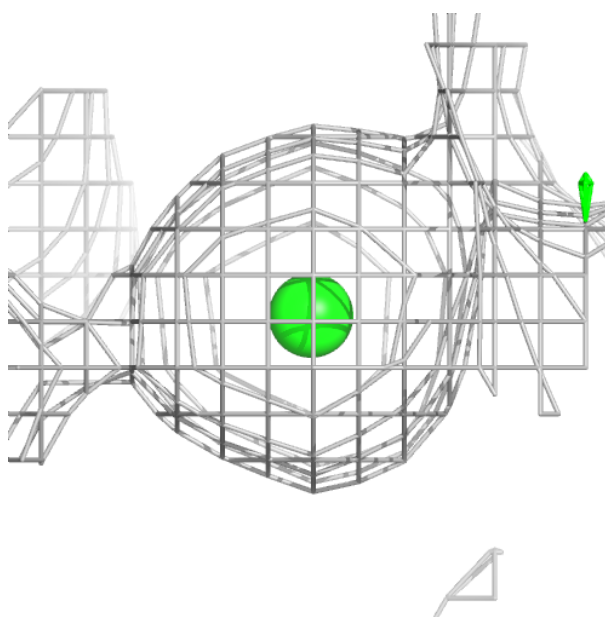
Electron density around HEC v 201:

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



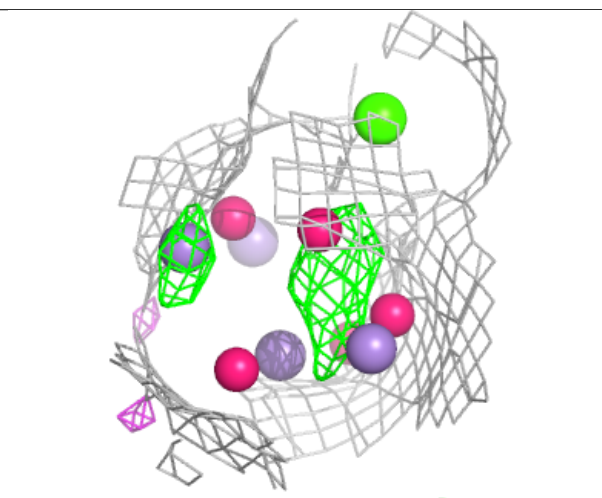
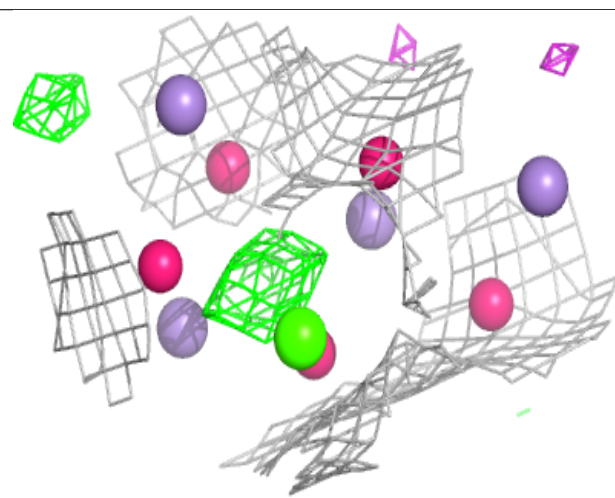
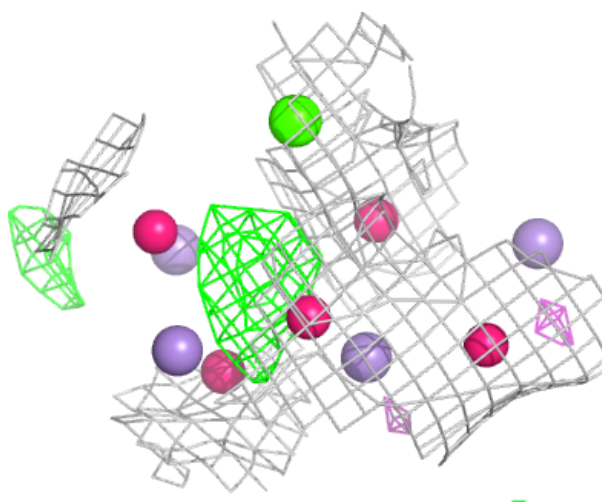
Electron density around CL A 403 (B):

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



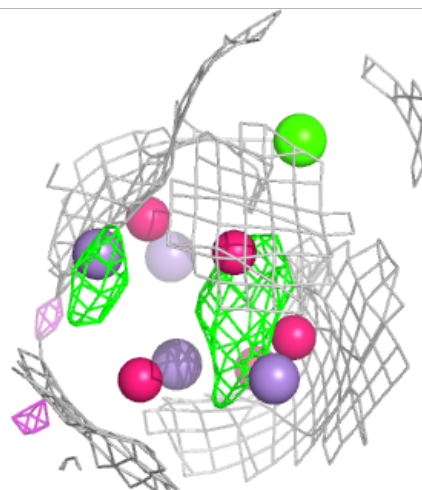
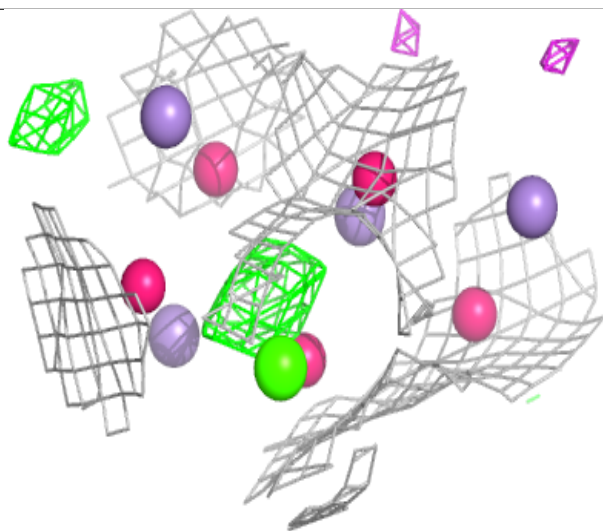
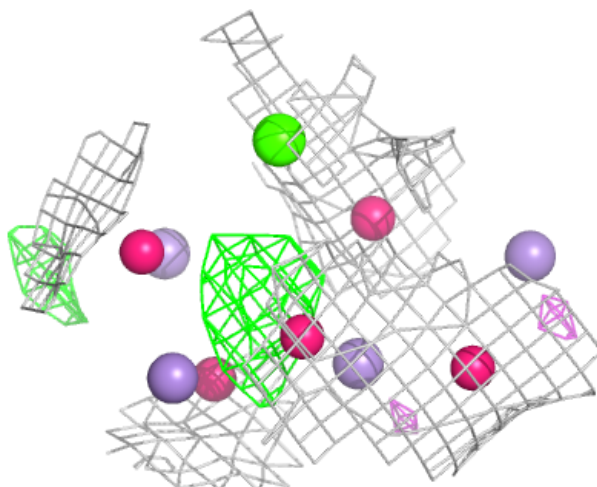
Electron density around OEX A 411 (A):

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



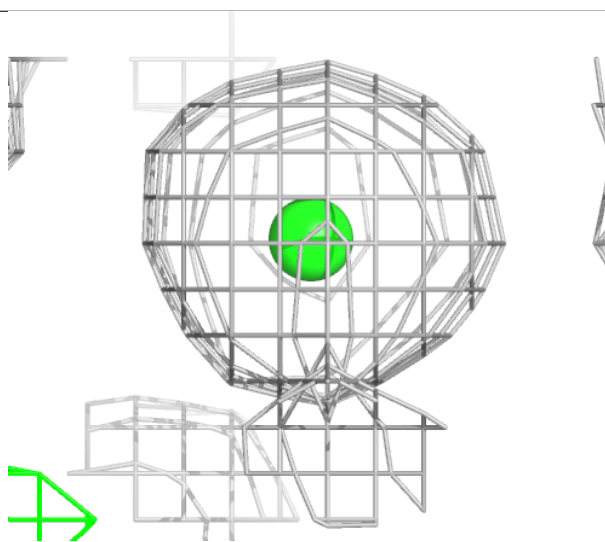
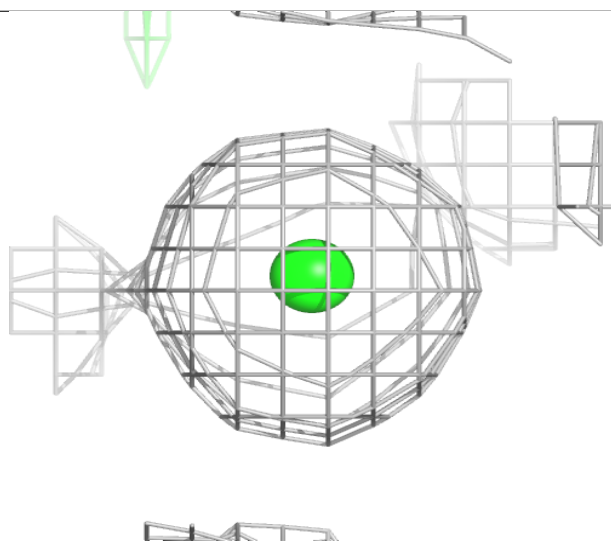
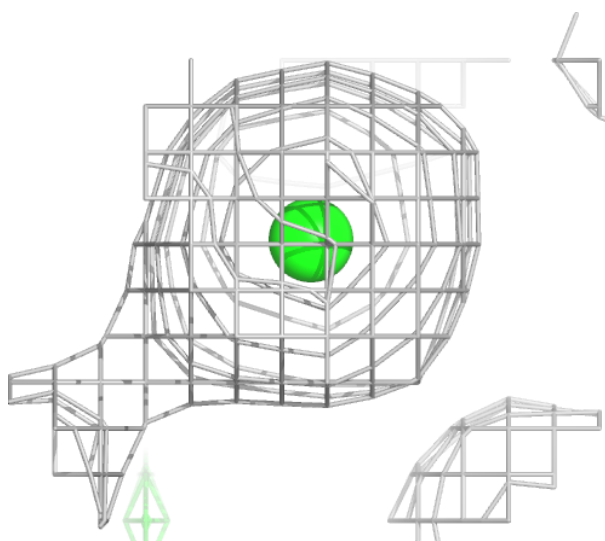
Electron density around OEX A 411 (B):

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



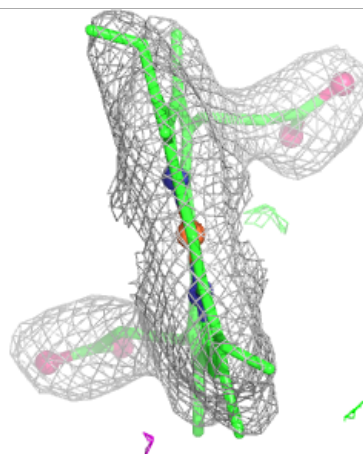
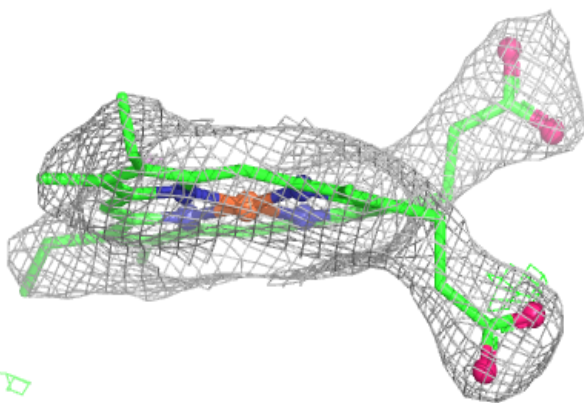
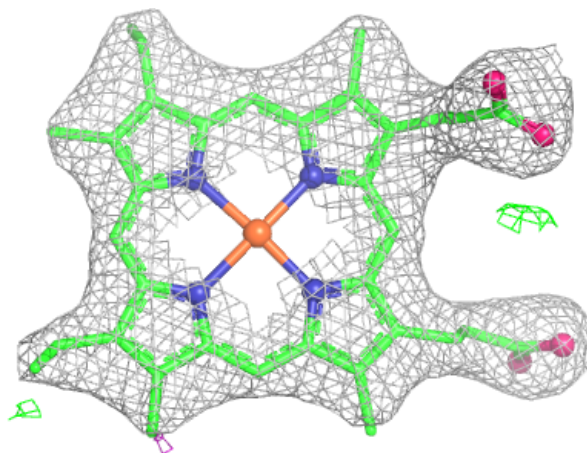
Electron density around CL A 402 (A):

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



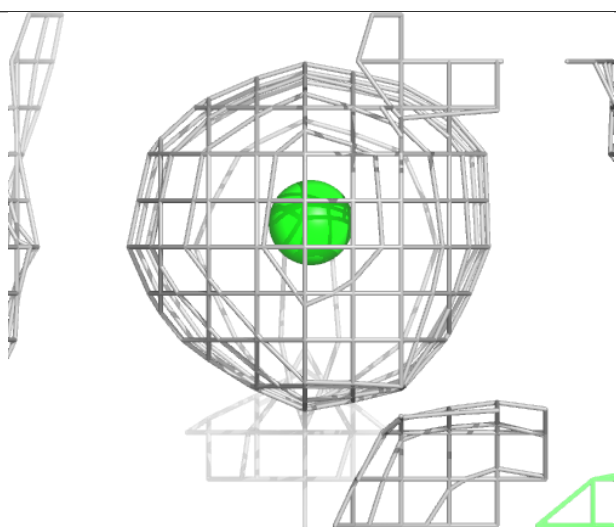
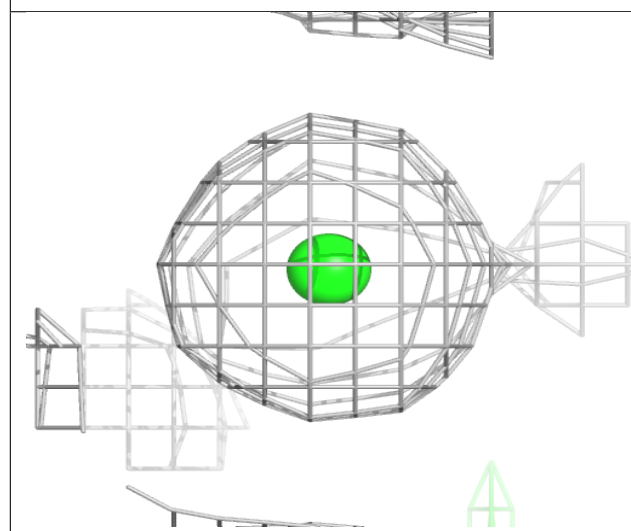
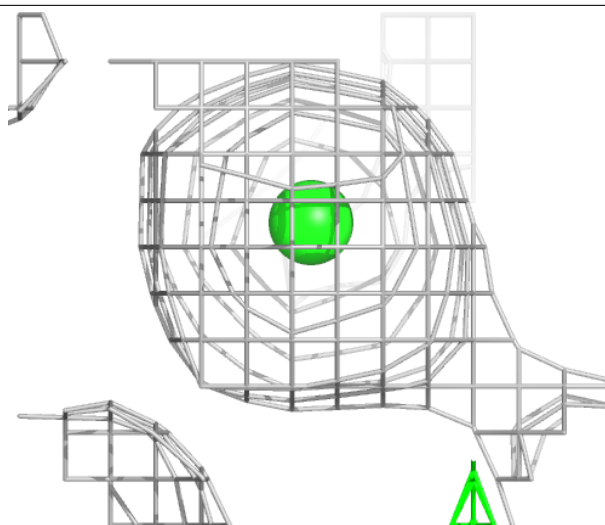
Electron density around HEM F 102:

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



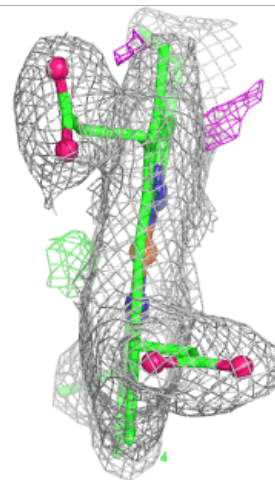
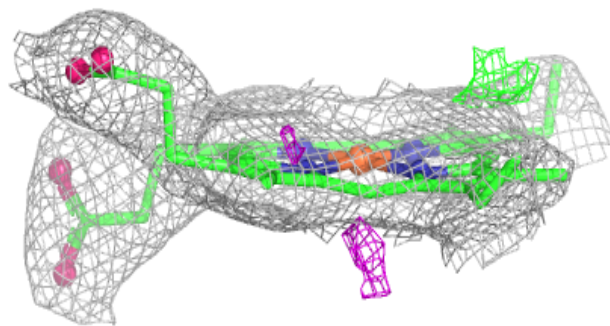
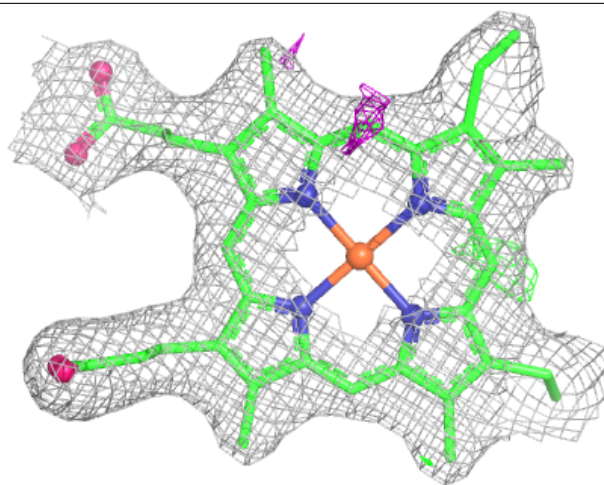
Electron density around CL A 402 (B):

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



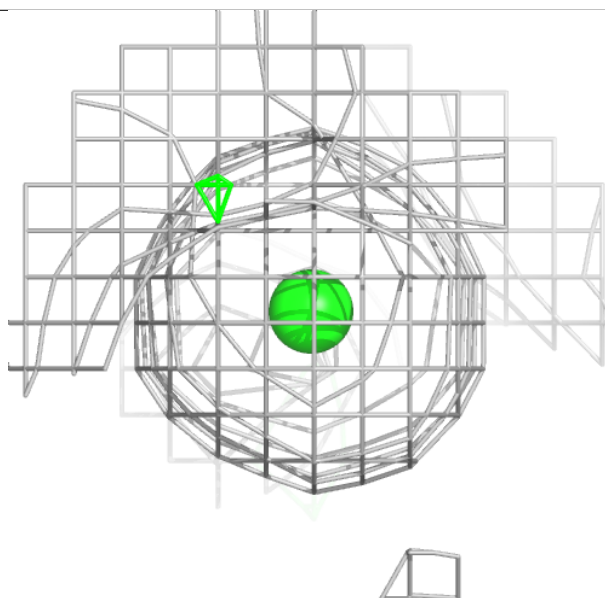
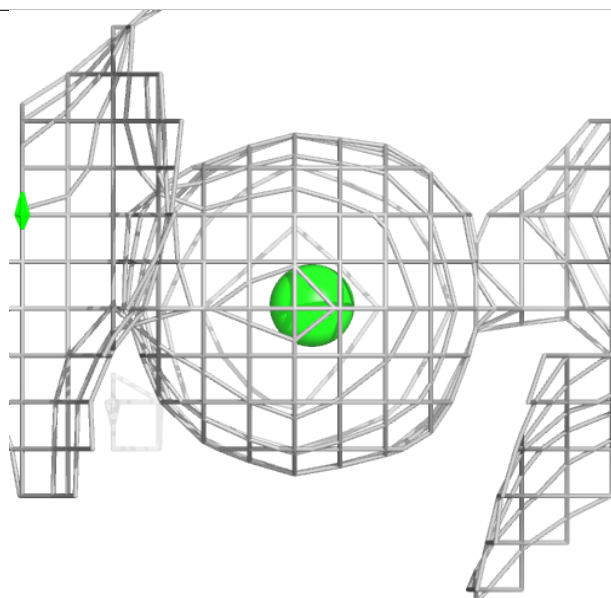
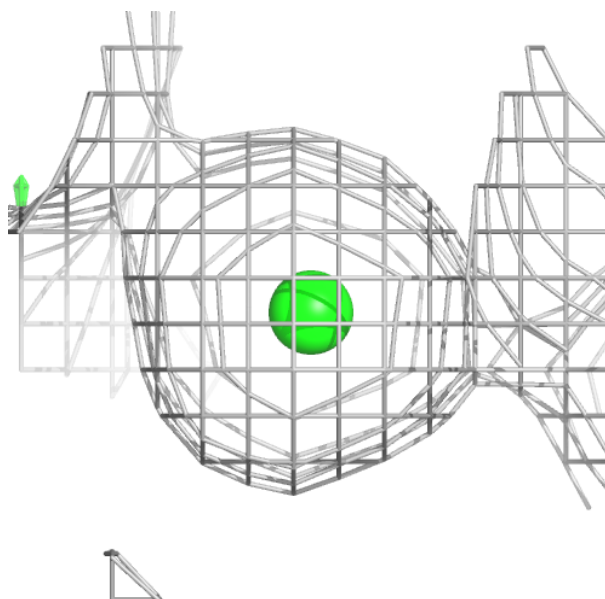
Electron density around HEC V 202:

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



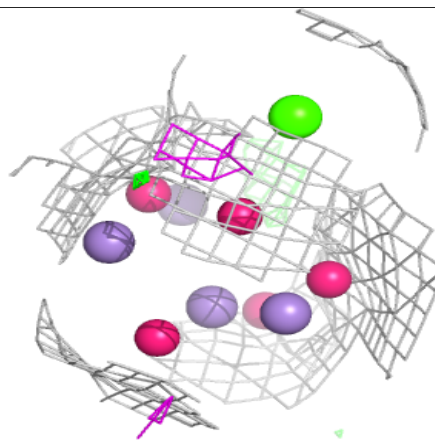
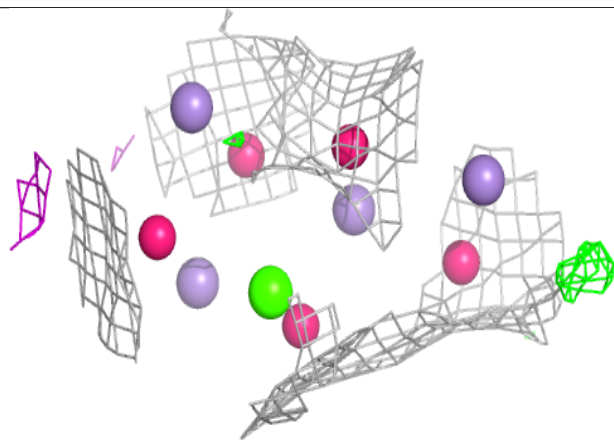
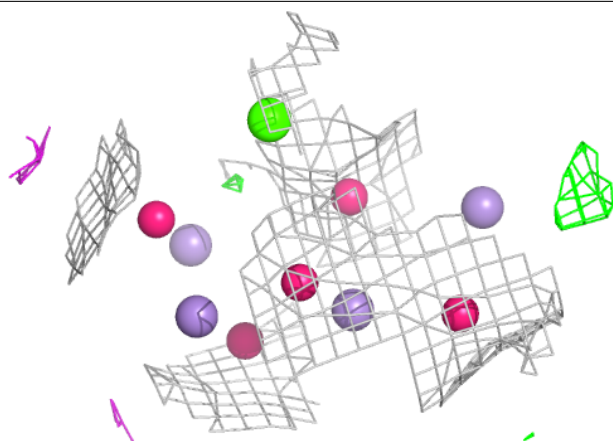
Electron density around CL A 403 (A):

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



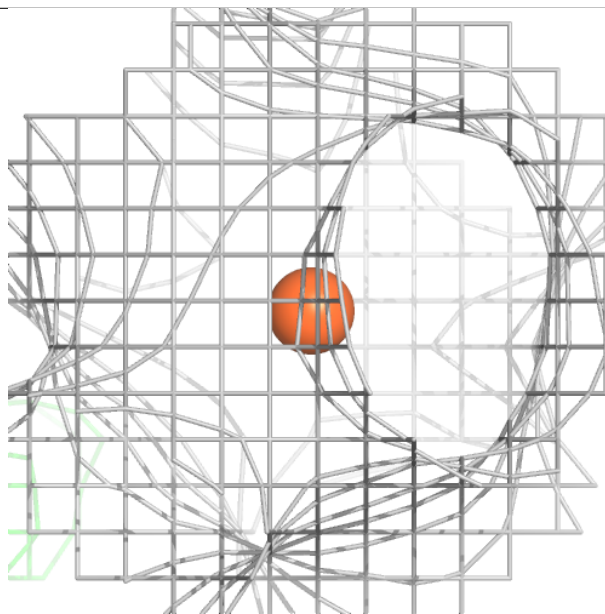
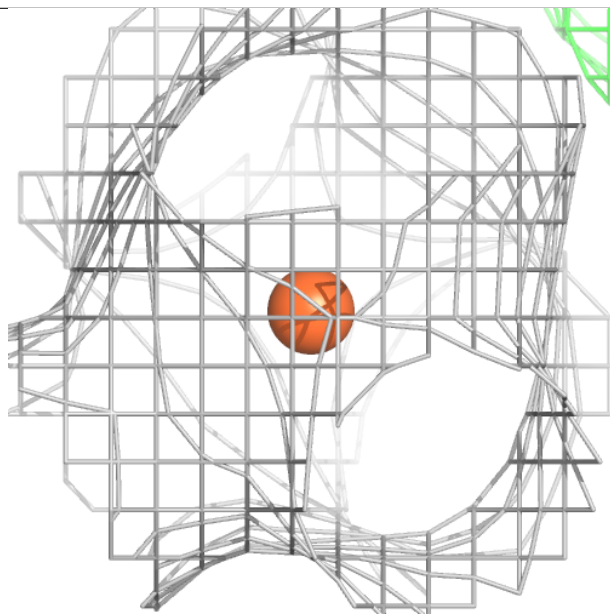
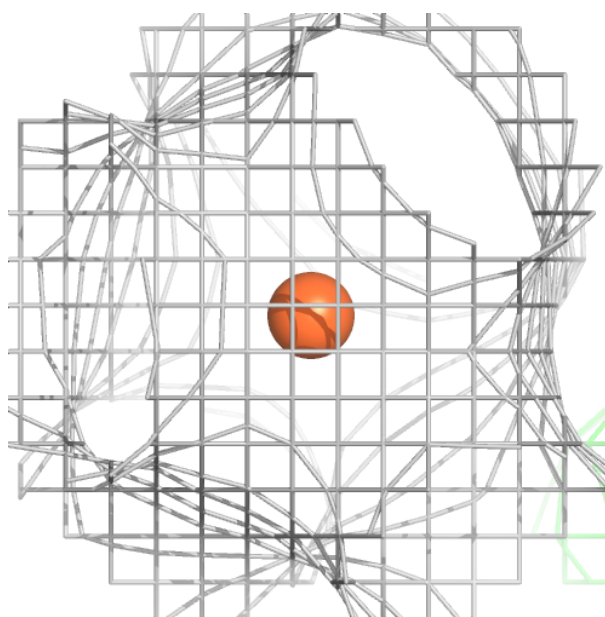
Electron density around OEX a 413 (B):

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



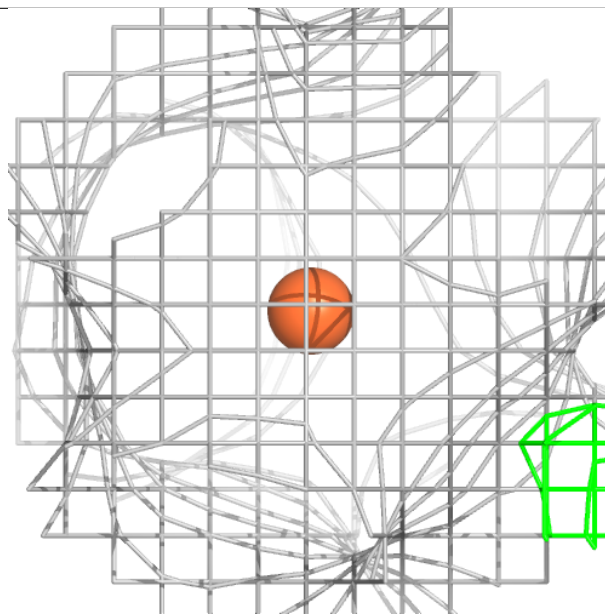
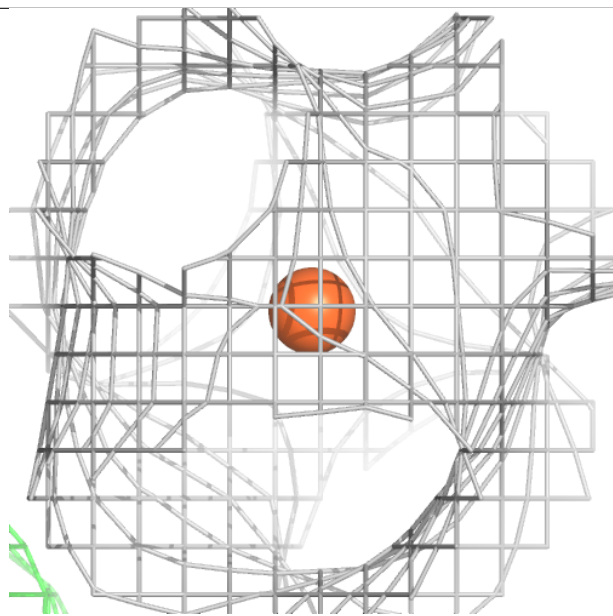
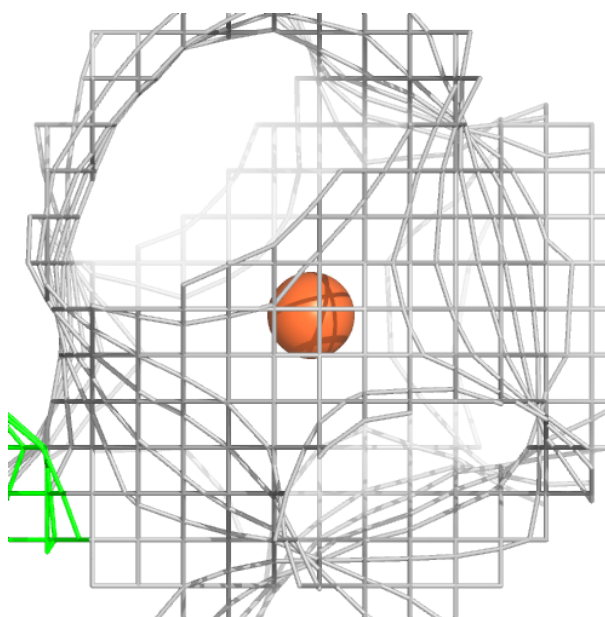
Electron density around FE2 a 401 (A):

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



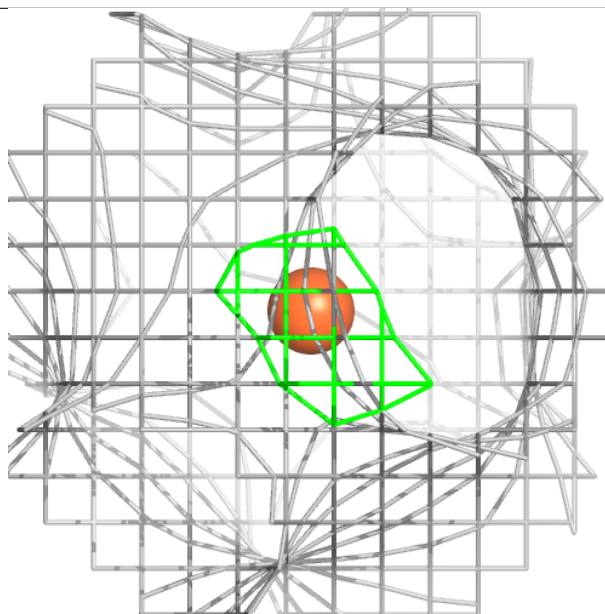
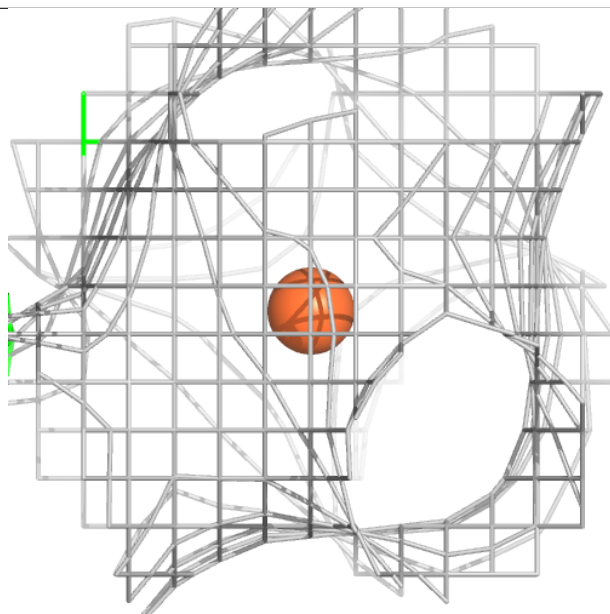
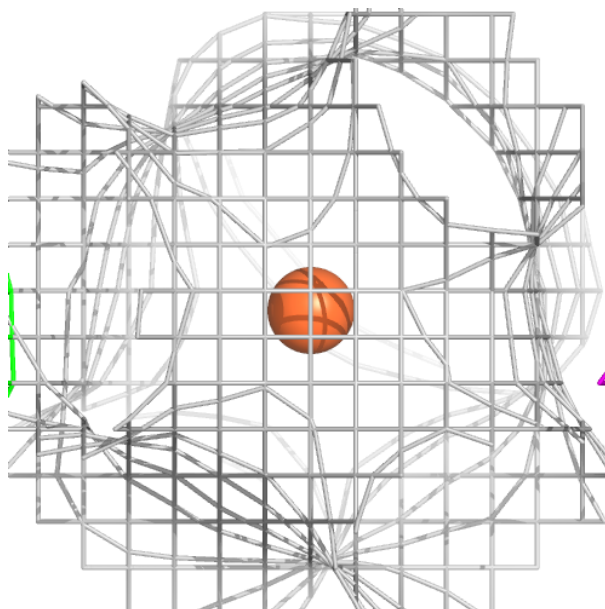
Electron density around FE2 a 401 (B):

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



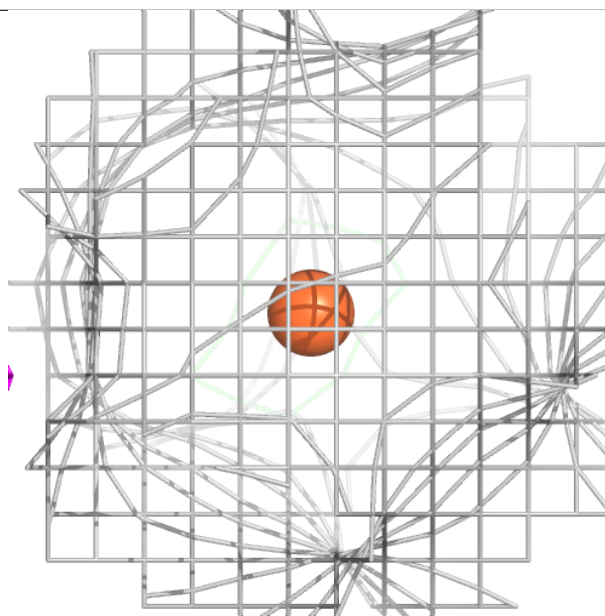
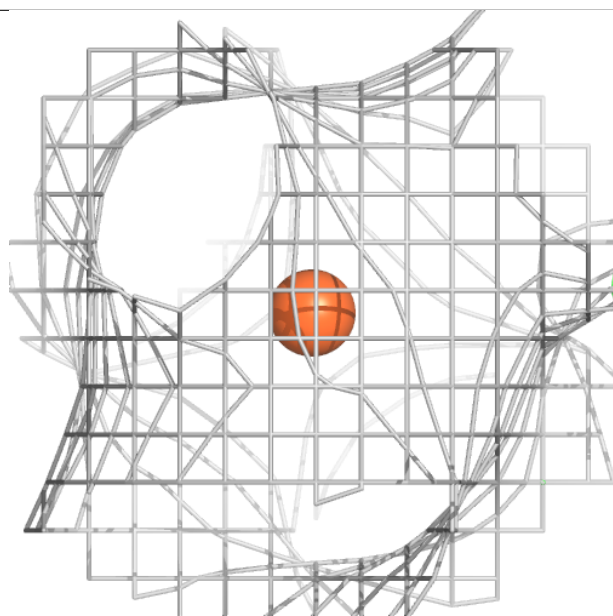
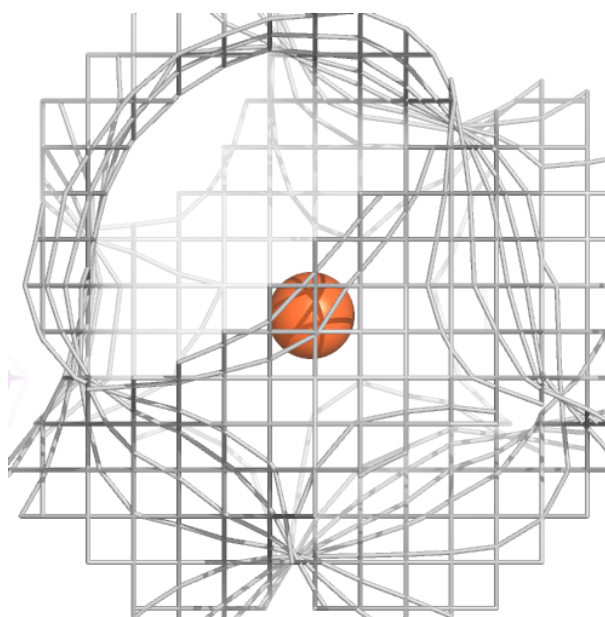
Electron density around FE2 A 401 (A):

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



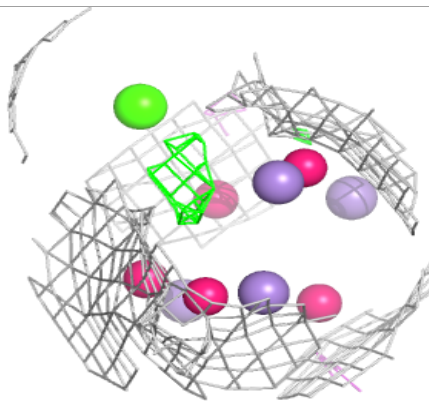
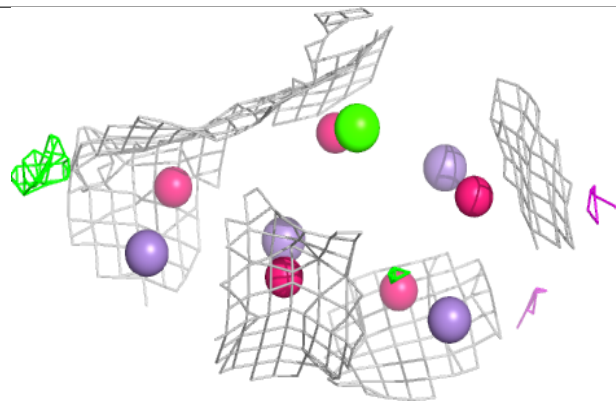
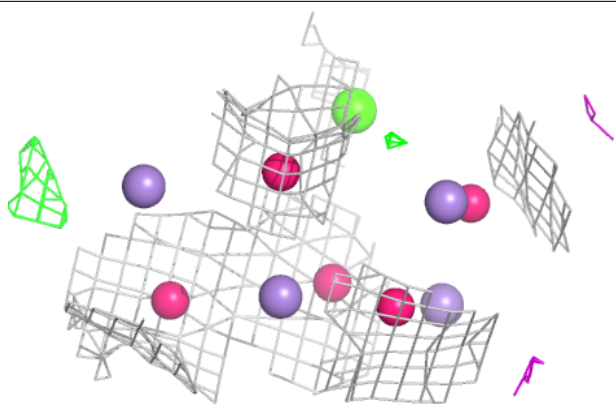
Electron density around FE2 A 401 (B):

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



Electron density around OEX a 413 (A):

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



6.5 Other polymers [i](#)

There are no such residues in this entry.