



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 09:07 AM UTC

PDB ID : 7CJJ / pdb_00007cjj
Title : Photosystem II structure in the S2 state
Authors : Li, H.; Shen, J.-R.; Suga, M.
Deposited on : 2020-07-11
Resolution : 2.40 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

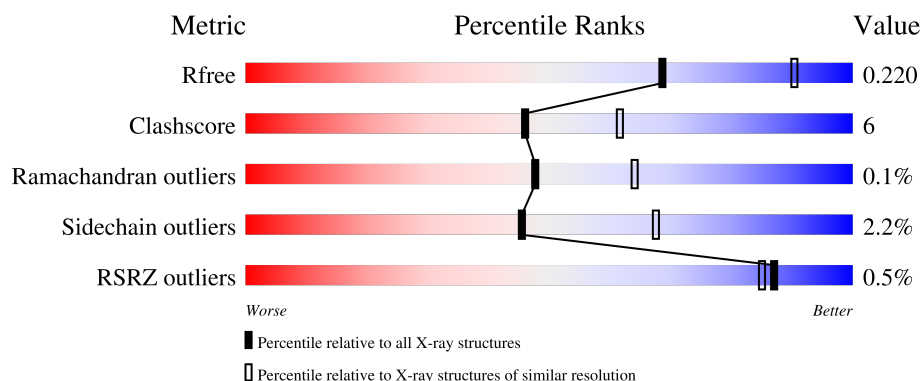
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	86% 11% .
1	a	344	% 86% 10% .
2	B	505	90% 9%
2	b	505	% 89% 10% .
3	C	455	90% 9% .

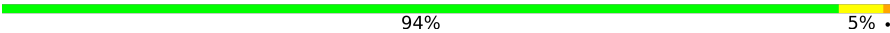
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Mol	Chain	Length	Quality of chain
3	c	455	 89% 11%
4	D	342	 90% 9%
4	d	342	 90% 9%
5	E	84	 73% 24% 3%
5	e	84	 85% 10% 5%
6	F	44	 64% 14% 22%
6	f	44	 64% 7% 29%
7	H	65	 89% 5% 6%
7	h	65	 86% 12% 2%
8	I	38	 89% 8%
8	i	38	 89% 11%
9	J	39	 92% 5% 3%
9	j	39	 87% 13% 3%
10	K	37	 78% 19%
10	k	37	 86% 11%
11	L	37	 86% 11% 3%
11	l	37	 89% 8%
12	M	36	 81% 11% 8%
12	m	36	 75% 17% 8%
13	O	244	 88% 11%
13	o	244	 89% 10%
14	T	32	 84% 6% 10%
14	t	32	 81% 12% 7%
15	U	104	 84% 8% 8%
15	u	104	 88% 6% 6%

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Mol	Chain	Length	Quality of chain
16	V	137	 94% 5% .
16	v	137	 91% 8% .
17	X	40	 82% 12% 5%
17	x	40	 90% 5% 5%
18	Y	30	 77% 20% .
18	y	30	 77% 17% . .
19	Z	62	 84% 15% .
19	z	62	 82% 18%
20	R	34	 94% 6%

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	403	X	-	-	-
23	CLA	A	404	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	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	C	514	X	-	-	-
23	CLA	C	515	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	D	404	X	-	-	-
23	CLA	a	403	X	-	-	-
23	CLA	a	404	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	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	c	514	X	-	-	-
23	CLA	c	515	X	-	-	-

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

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 53612 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	18	0
			2773	1805	459	494	15			
1	a	334	Total	C	N	O	S	0	19	0
			2781	1811	460	495	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	see sequence details	UNP P51765
a	279	PRO	ARG	see sequence details	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	10	0
			4050	2650	677	710	13			
2	b	504	Total	C	N	O	S	0	4	0
			3998	2622	665	698	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	5	0
			3522	2300	589	620	13			
3	c	455	Total	C	N	O	S	0	3	0
			3543	2316	592	622	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	see sequence details	UNP D0VWR7
C	20	SER	-	see sequence details	UNP D0VWR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	see sequence details	UNP D0VWR7
C	22	PHE	-	see sequence details	UNP D0VWR7
c	19	ASN	-	see sequence details	UNP D0VWR7
c	20	SER	-	see sequence details	UNP D0VWR7
c	21	ILE	-	see sequence details	UNP D0VWR7
c	22	PHE	-	see sequence details	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	4	0
			2764	1828	454	470	12			
4	d	341	Total	C	N	O	S	0	4	0
			2755	1823	453	467	12			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
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	see sequence details	UNP P19054
K	39	TRP	VAL	see sequence details	UNP P19054
k	33	LEU	PHE	see sequence details	UNP P19054
k	39	TRP	VAL	see sequence details	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	1	0
			304	203	48	53			
11	l	36	Total	C	N	O	0	1	0
			304	203	48	53			

- 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	0	0
			269	179	40	49	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	see sequence details	UNP P12312
m	8	LEU	PHE	see sequence details	UNP P12312

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	3	0
			1886	1177	318	386	5			
13	o	243	Total	C	N	O	S	0	2	0
			1879	1173	317	384	5			

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

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

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

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

- 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	0	0
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

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

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

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).

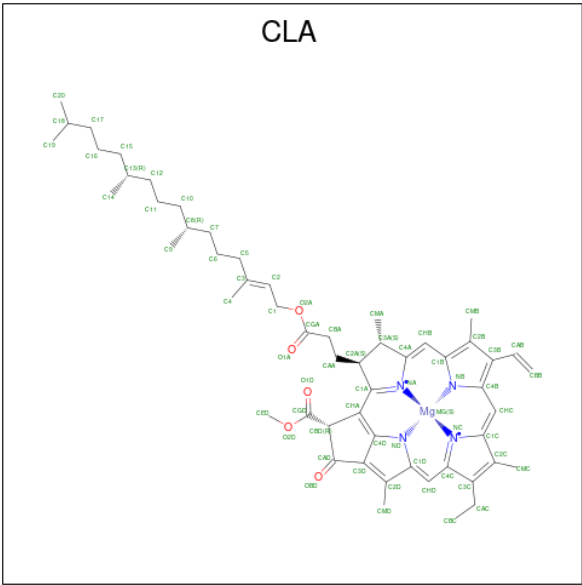
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	1	Total	Cl	0	0
			1	1		
22	C	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	a	1	Total	Cl	0	0
			1	1		
22	c	1	Total	Cl	0	0
			1	1		

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



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

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

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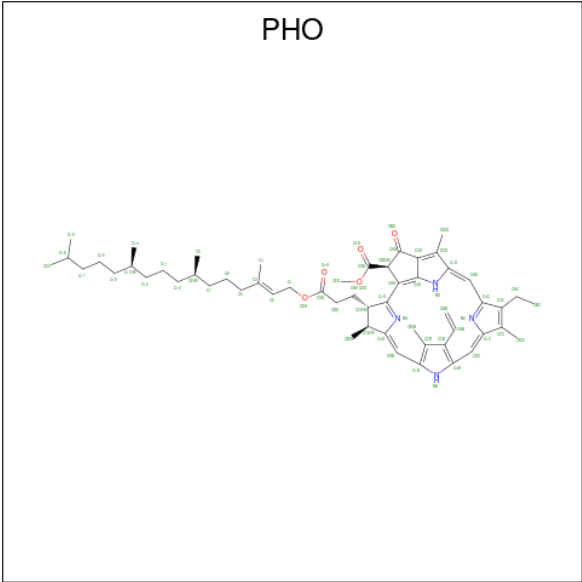
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N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

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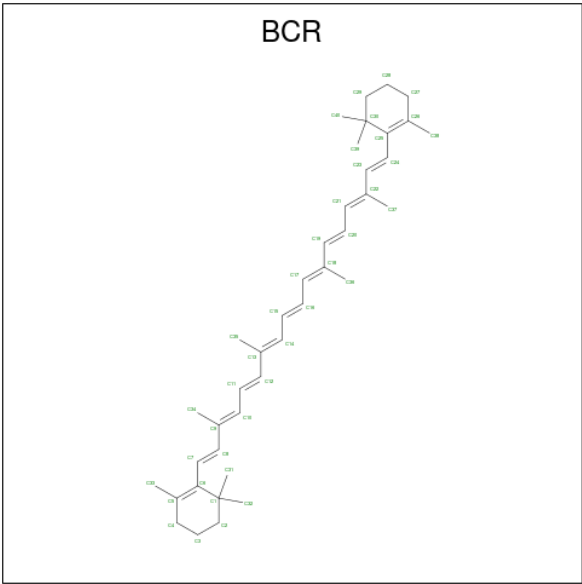
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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



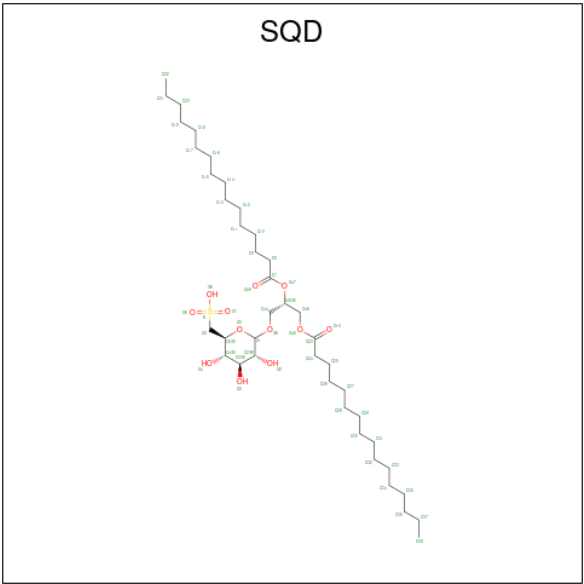
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



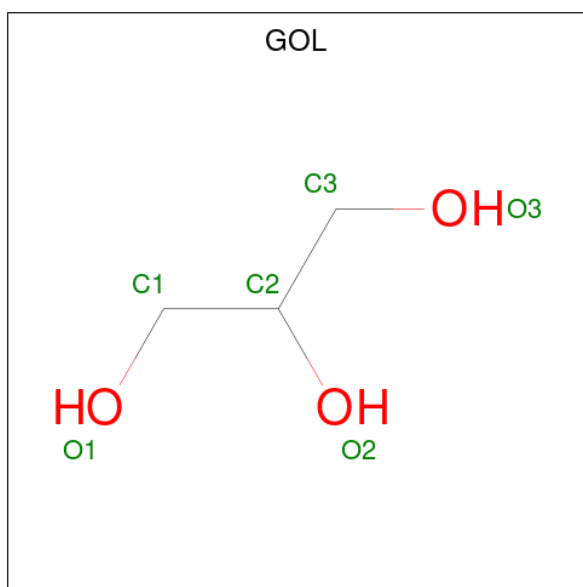
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total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

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



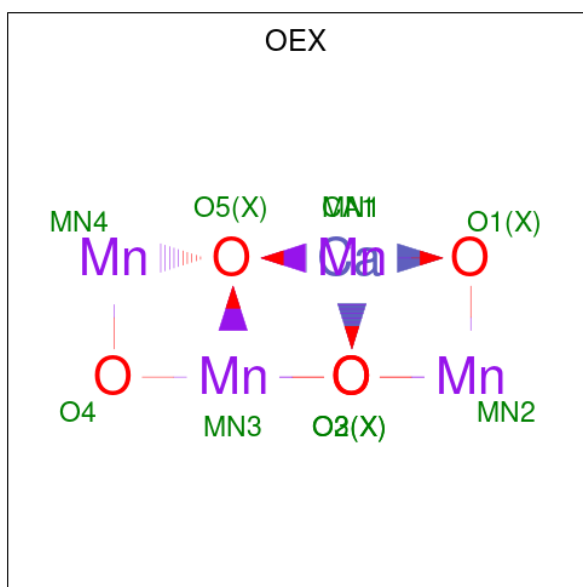
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	B	1	Total	C	O	S	0	0
			54	41	12	1		
26	D	1	Total	C	O	S	0	0
			43	30	12	1		
26	L	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	0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

- Molecule 27 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



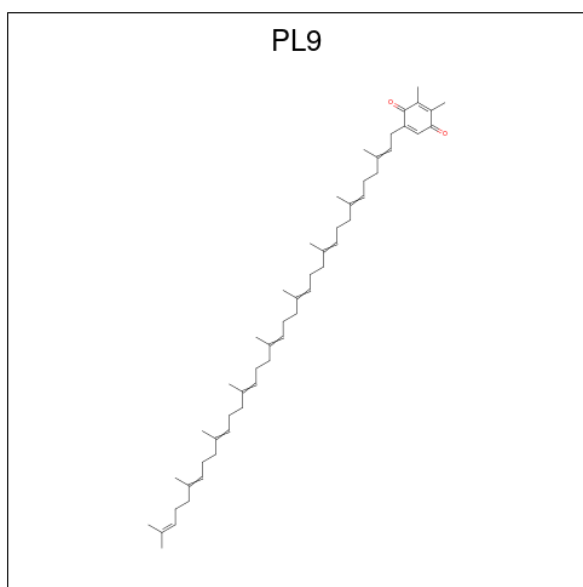
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	0
			6	3	3		
27	O	1	Total	C	O	0	0
			6	3	3		
27	a	1	Total	C	O	0	0
			6	3	3		
27	b	1	Total	C	O	0	0
			6	3	3		
27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

- Molecule 28 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	1
			110	106	4		

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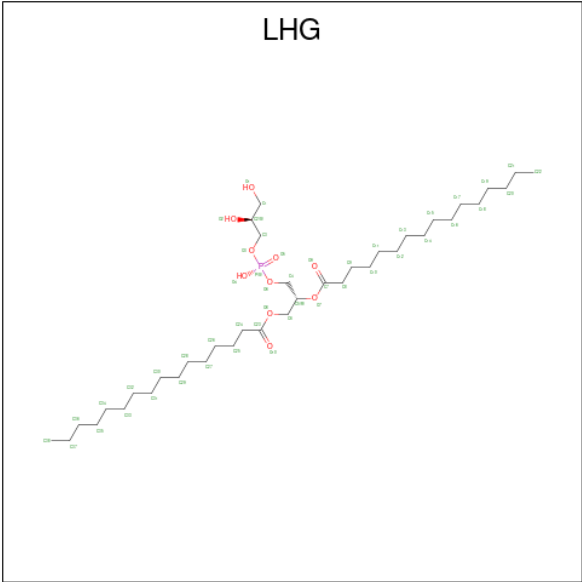
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	D	1	Total	C	O	0	0
			55	53	2		
29	a	1	Total	C	O	0	1
			110	106	4		
29	d	1	Total	C	O	0	0
			55	53	2		

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

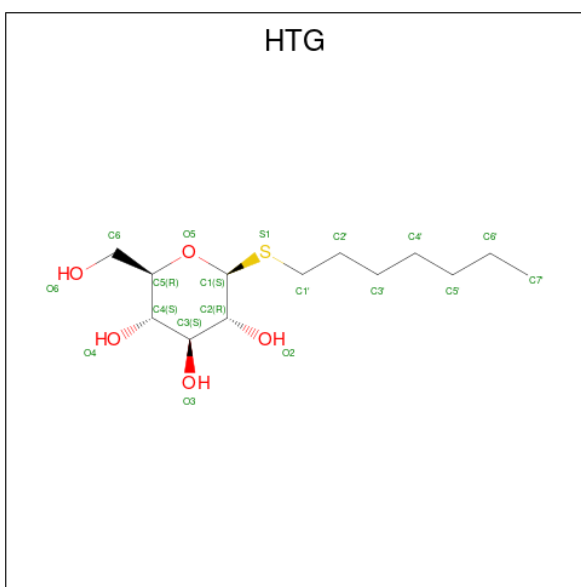
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			28	23	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	C	1	Total	C	O	0	0
			34	29	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	I	1	Total	C	O	0	0
			40	35	5		
30	J	1	Total	C		0	0
			10	10			
30	X	1	Total	C	O	0	0
			18	16	2		
30	a	1	Total	C	O	0	0
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

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



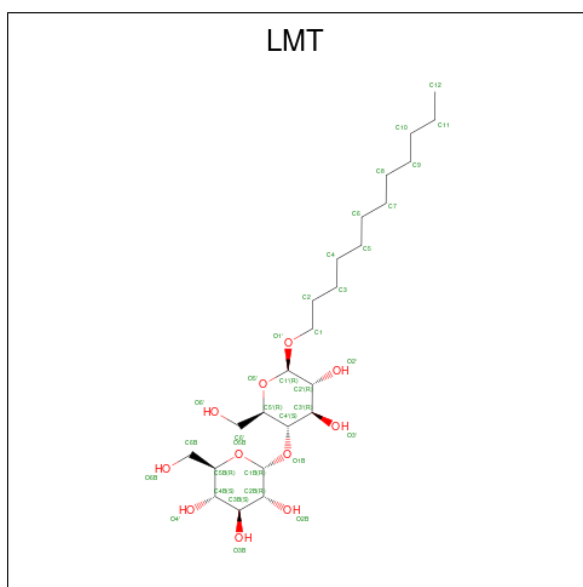
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	E	1	Total	C	O	P	0	0
			42	31	10	1		
31	L	1	Total	C	O	P	0	0
			49	38	10	1		
31	a	1	Total	C	O	P	0	0
			42	31	10	1		
31	b	1	Total	C	O	P	0	0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

- Molecule 32 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C₁₃H₂₆O₅S).



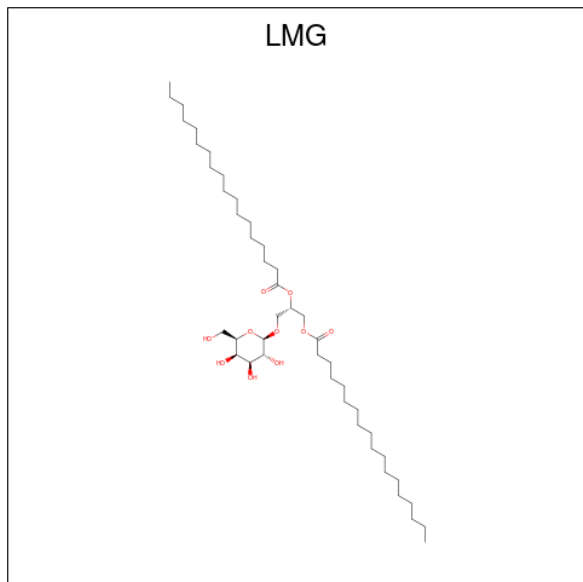
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total 19	C 13	O 5	S 1	0	0
32	B	1	Total 19	C 13	O 5	S 1	0	0
32	B	1	Total 19	C 13	O 5	S 1	0	0
32	C	1	Total 19	C 13	O 5	S 1	0	0
32	D	1	Total 16	C 10	O 5	S 1	0	0
32	V	1	Total 11	C 6	O 5		0	0
32	b	1	Total 19	C 13	O 5	S 1	0	0
32	b	1	Total 19	C 13	O 5	S 1	0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

- Molecule 33 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



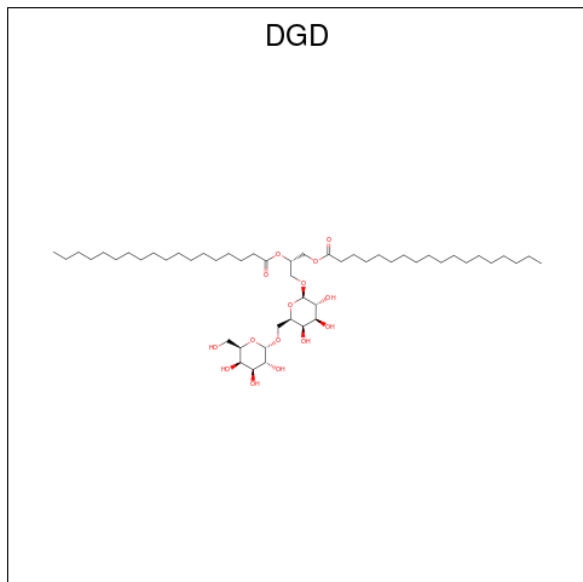
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	B	1	Total 35	C 24	O 11	0	0
33	B	1	Total 25	C 19	O 6	0	0
33	B	1	Total 26	C 19	O 7	0	0
33	C	1	Total 35	C 24	O 11	0	0
33	D	1	Total 35	C 24	O 11	0	0
33	F	1	Total 35	C 24	O 11	0	0
33	M	1	Total 35	C 24	O 11	0	0
33	M	1	Total 35	C 24	O 11	0	0
33	a	1	Total 35	C 24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

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



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

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



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

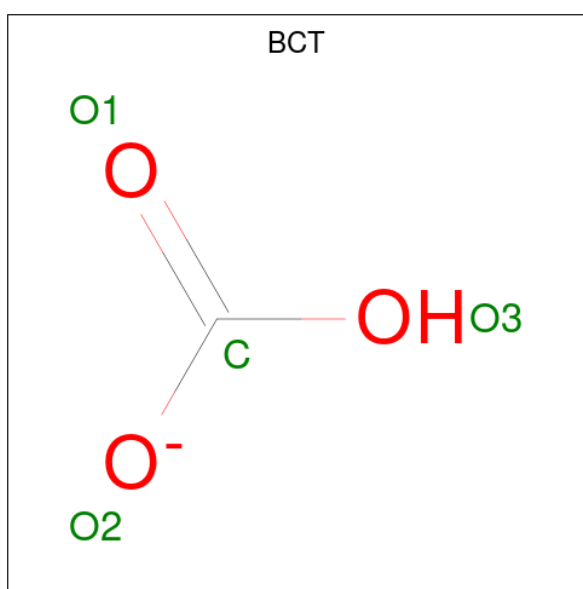
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	C	1	Total	Ca	0	0
			1	1		
36	F	1	Total	Ca	0	0
			1	1		

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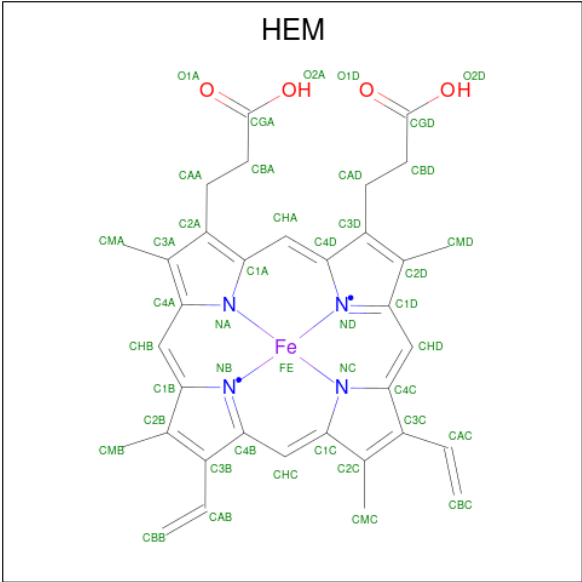
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	O	1	Total	Ca	0	0
			1	1		
36	a	1	Total	Ca	0	0
			1	1		
36	c	2	Total	Ca	0	0
			2	2		
36	o	1	Total	Ca	0	0
			1	1		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	D	1	Total	C	O	0	1
			8	2	6		
37	d	1	Total	C	O	0	1
			8	2	6		

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).

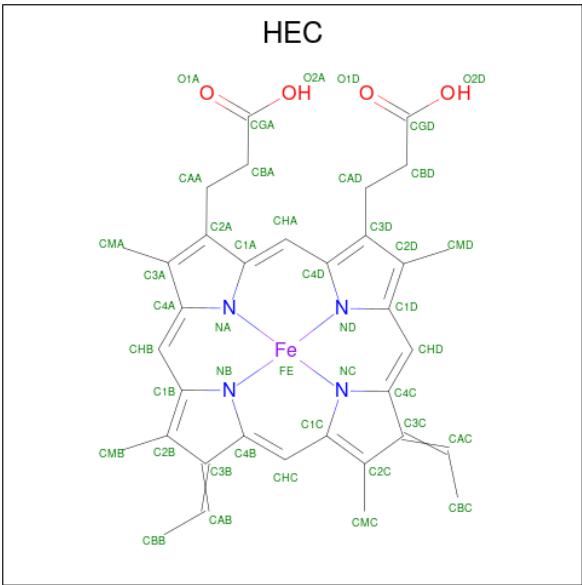


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
38	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
38	e	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- 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	147	Total	O	0	11
			157	157		
41	B	218	Total	O	0	0
			218	218		
41	C	188	Total	O	0	4
			191	191		
41	D	124	Total	O	0	2
			126	126		
41	E	24	Total	O	0	0
			24	24		
41	F	8	Total	O	0	0
			8	8		
41	H	28	Total	O	0	0
			28	28		
41	I	4	Total	O	0	0
			4	4		
41	J	6	Total	O	0	0
			6	6		
41	K	8	Total	O	0	0
			8	8		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	L	8	Total O 8 8	0	0
41	M	18	Total O 18 18	0	0
41	O	118	Total O 118 118	0	0
41	T	14	Total O 14 14	0	0
41	U	56	Total O 56 56	0	0
41	V	95	Total O 95 95	0	0
41	X	10	Total O 10 10	0	0
41	Y	1	Total O 1 1	0	0
41	R	1	Total O 1 1	0	0
41	a	139	Total O 150 150	0	12
41	b	220	Total O 220 220	0	0
41	c	169	Total O 172 172	0	4
41	d	129	Total O 129 129	0	0
41	e	15	Total O 15 15	0	0
41	f	5	Total O 5 5	0	0
41	h	22	Total O 22 22	0	0
41	i	1	Total O 1 1	0	0
41	j	4	Total O 4 4	0	0
41	k	5	Total O 5 5	0	0
41	l	8	Total O 8 8	0	0
41	m	10	Total O 10 10	0	0

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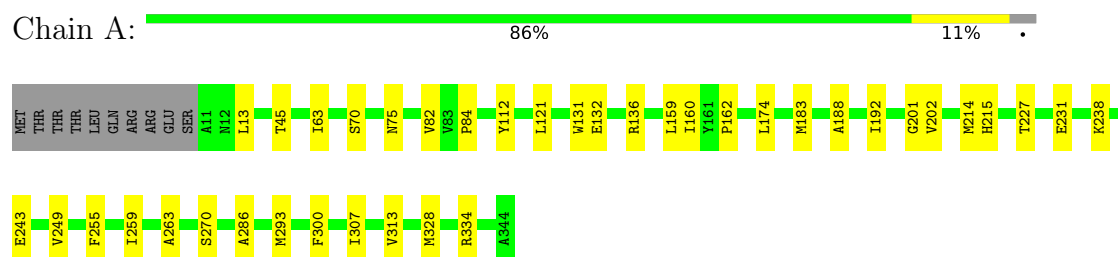
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	o	99	Total 99	O 99	0	0
41	t	10	Total 10	O 10	0	0
41	u	68	Total 68	O 68	0	0
41	v	57	Total 57	O 57	0	0
41	x	10	Total 10	O 10	0	0
41	y	4	Total 4	O 4	0	0

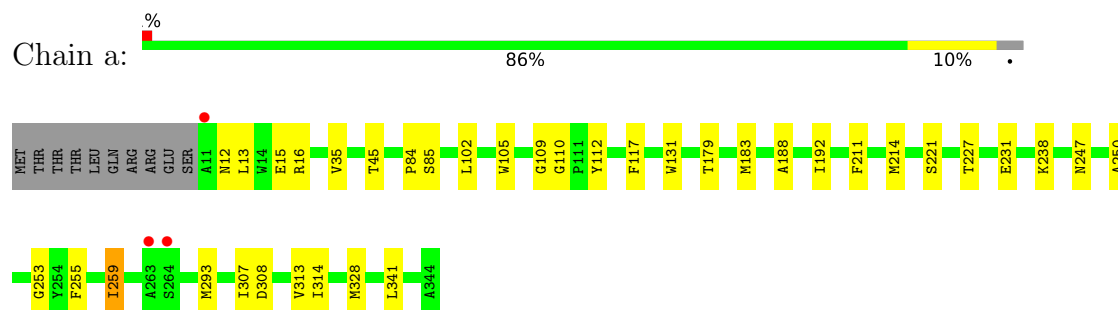
3 Residue-property plots

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.

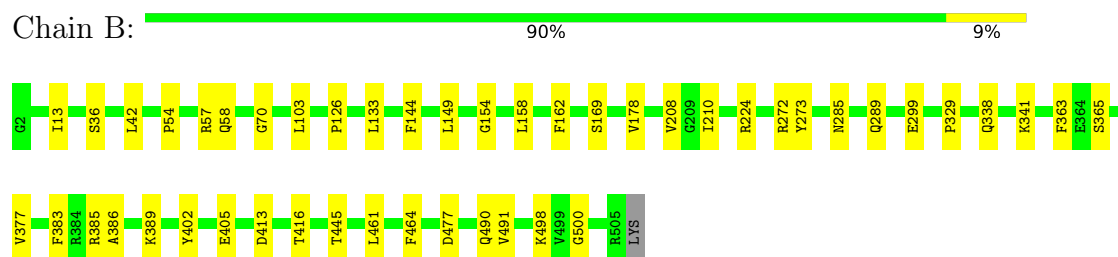
• Molecule 1: Photosystem II protein D1



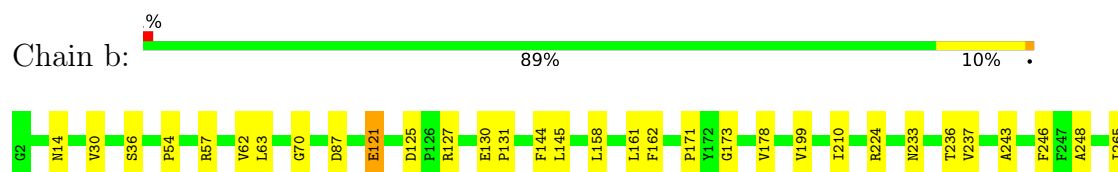
• Molecule 1: Photosystem II protein D1



• Molecule 2: Photosystem II CP47 reaction center protein

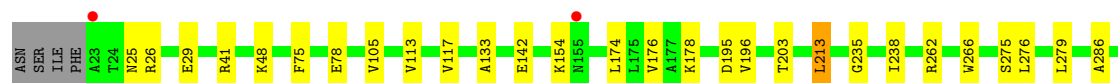
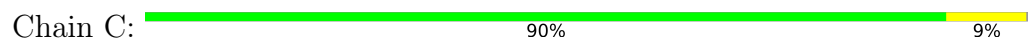


• Molecule 2: Photosystem II CP47 reaction center protein

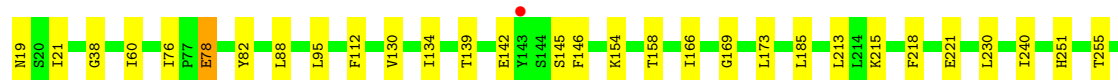
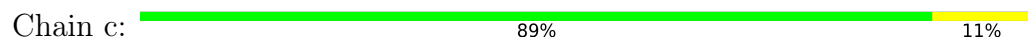




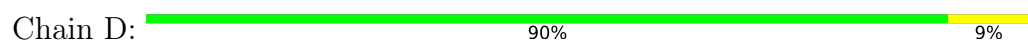
• Molecule 3: Photosystem II CP43 reaction center protein



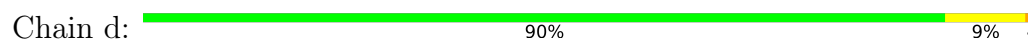
• Molecule 3: Photosystem II CP43 reaction center protein



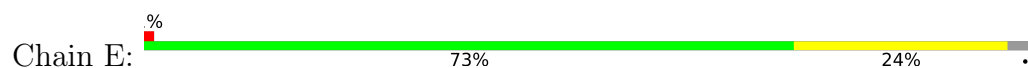
• Molecule 4: Photosystem II D2 protein



• Molecule 4: Photosystem II D2 protein

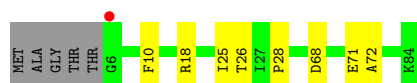
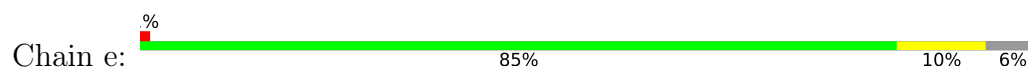


• Molecule 5: Cytochrome b559 subunit alpha





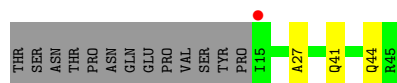
- Molecule 5: Cytochrome b559 subunit alpha



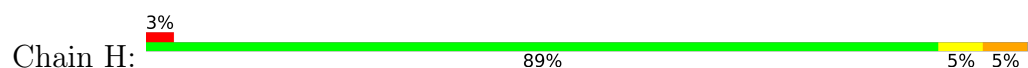
- Molecule 6: Cytochrome b559 subunit beta



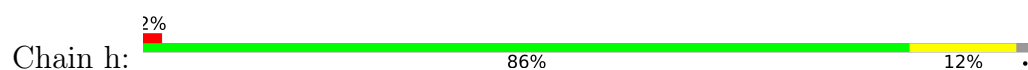
- Molecule 6: Cytochrome b559 subunit beta



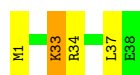
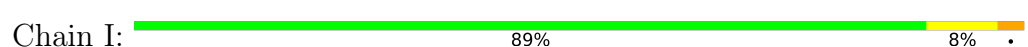
- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I

Chain i:  89% 11%



- Molecule 9: Photosystem II reaction center protein J

Chain J:  3% 92% 5%



- Molecule 9: Photosystem II reaction center protein J

Chain j:  3% 87% 13%



- Molecule 10: Photosystem II reaction center protein K

Chain K:  78% 19%



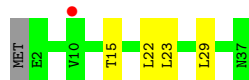
- Molecule 10: Photosystem II reaction center protein K

Chain k:  86% 11%



- Molecule 11: Photosystem II reaction center protein L

Chain L:  3% 86% 11%



- Molecule 11: Photosystem II reaction center protein L

Chain l:  89% 8%



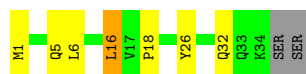
- Molecule 12: Photosystem II reaction center protein M

Chain M:  81% 11% 8%



- Molecule 12: Photosystem II reaction center protein M

Chain m:  75% 17% 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  88% 11% 1%



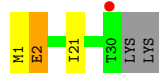
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  89% 10% 1%



- Molecule 14: Photosystem II reaction center protein T

Chain T:  3% 84% 6% 6%



- Molecule 14: Photosystem II reaction center protein T

Chain t:  3% 81% 12% 6%



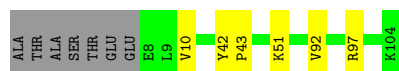
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  84% 8% 8%

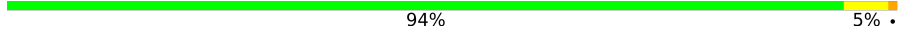


- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  88% 6% 7%



- Molecule 16: Cytochrome c-550

Chain V:  94% 5% .



- Molecule 16: Cytochrome c-550

Chain v:  91% 8% .



- Molecule 17: Photosystem II reaction center protein X

Chain X:  82% 12% 5%



- Molecule 17: Photosystem II reaction center protein X

Chain x:  90% 5% 5%



- Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:  7% 77% 20% .



- Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:  77% 17% . .



- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  84% 15% .



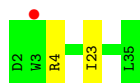
- Molecule 19: Photosystem II reaction center protein Z

Chain z:  3% 82% 18%



- Molecule 20: Photosystem II protein Y

Chain R:  3% 94% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	125.75Å 231.63Å 288.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.90 – 2.40 39.90 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.7 (39.90-2.40) 82.1 (39.90-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.168 , 0.218 0.169 , 0.220	Depositor DCC
R_{free} test set	16450 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 78.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	53612	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.35	0/2861	0.53	0/3897
1	a	0.32	0/2869	0.51	0/3908
2	B	0.33	0/4190	0.50	0/5708
2	b	0.31	0/4138	0.49	0/5640
3	C	0.29	0/3635	0.47	0/4948
3	c	0.27	0/3657	0.45	0/4978
4	D	0.35	0/2861	0.52	0/3897
4	d	0.32	0/2852	0.50	0/3885
5	E	0.26	0/687	0.46	0/936
5	e	0.27	0/667	0.45	0/908
6	F	0.28	0/284	0.45	0/387
6	f	0.23	0/257	0.45	0/349
7	H	0.27	0/530	0.49	0/723
7	h	0.27	0/519	0.48	0/708
8	I	0.24	0/311	0.38	0/419
8	i	0.27	0/311	0.42	0/419
9	J	0.27	0/278	0.46	0/376
9	j	0.25	0/283	0.41	0/383
10	K	0.25	0/303	0.44	0/416
10	k	0.27	0/303	0.48	0/416
11	L	0.40	0/311	0.50	0/423
11	l	0.33	0/311	0.53	0/423
12	M	0.40	0/261	0.52	0/357
12	m	0.32	0/262	0.49	0/357
13	O	0.32	0/1917	0.49	0/2599
13	o	0.29	0/1910	0.48	0/2589
14	T	0.35	0/257	0.46	0/349
14	t	0.34	0/257	0.43	0/349
15	U	0.33	0/776	0.54	0/1052
15	u	0.29	0/785	0.51	0/1064
16	V	0.31	0/1085	0.46	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.27	0/1085	0.44	0/1473
17	X	0.23	0/284	0.37	0/384
17	x	0.20	0/284	0.37	0/384
18	Y	0.19	0/216	0.38	0/289
18	y	0.22	0/216	0.38	0/289
19	Z	0.20	0/490	0.37	0/669
19	z	0.21	0/490	0.34	0/669
20	R	0.20	0/279	0.37	0/383
All	All	0.31	0/43272	0.48	0/58876

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	2773	0	2626	27	0
1	a	2781	0	2636	28	0
2	B	4050	0	3894	35	0
2	b	3998	0	3852	39	0
3	C	3522	0	3429	32	0
3	c	3543	0	3451	34	0
4	D	2764	0	2656	28	0
4	d	2755	0	2650	23	0
5	E	668	0	652	15	0
5	e	648	0	634	5	0
6	F	275	0	282	6	0
6	f	250	0	261	3	0
7	H	517	0	542	7	0
7	h	506	0	529	8	0
8	I	314	0	328	3	0
8	i	314	0	328	2	0
9	J	272	0	279	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	277	0	284	3	0
10	K	293	0	305	5	0
10	k	293	0	305	3	0
11	L	304	0	314	4	0
11	l	304	0	314	3	0
12	M	268	0	283	3	0
12	m	269	0	288	6	0
13	O	1886	0	1856	17	0
13	o	1879	0	1850	13	0
14	T	258	0	261	2	0
14	t	258	0	261	3	0
15	U	765	0	767	5	0
15	u	774	0	773	3	0
16	V	1064	0	1073	6	0
16	v	1064	0	1073	9	0
17	X	281	0	312	4	0
17	x	281	0	312	3	0
18	Y	215	0	246	4	0
18	y	215	0	246	4	0
19	Z	479	0	516	5	0
19	z	479	0	516	4	0
20	R	273	0	305	2	0
21	A	2	0	0	0	0
21	a	2	0	0	0	0
22	A	1	0	0	0	0
22	C	1	0	0	0	0
22	a	1	0	0	0	0
22	c	1	0	0	0	0
23	A	260	0	288	14	0
23	B	1040	0	1152	33	0
23	C	845	0	936	36	0
23	D	130	0	144	4	0
23	a	260	0	288	12	0
23	b	1040	0	1152	36	0
23	c	845	0	936	45	0
23	d	130	0	144	5	0
24	A	128	0	148	2	0
24	a	128	0	148	2	0
25	A	40	0	56	2	0
25	B	160	0	224	14	0
25	C	80	0	112	5	0
25	D	40	0	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	H	40	0	56	3	0
25	K	40	0	56	1	0
25	T	40	0	56	8	0
25	Y	40	0	56	2	0
25	a	40	0	56	1	0
25	b	120	0	168	11	0
25	c	80	0	112	7	0
25	d	40	0	56	4	0
25	h	40	0	56	5	0
25	k	80	0	112	4	0
26	A	108	0	155	3	0
26	B	54	0	78	3	0
26	D	43	0	53	3	0
26	L	54	0	78	1	0
26	a	108	0	155	4	0
26	f	43	0	53	3	0
27	A	6	0	8	0	0
27	B	18	0	24	1	0
27	C	6	0	8	0	0
27	O	6	0	8	0	0
27	a	6	0	8	1	0
27	b	12	0	16	1	0
27	c	12	0	16	1	0
27	v	6	0	8	1	0
28	A	20	0	0	0	0
28	a	20	0	0	0	0
29	A	110	0	160	13	0
29	D	55	0	80	3	0
29	a	110	0	160	12	0
29	d	55	0	80	1	0
30	A	28	0	0	0	0
30	B	33	0	0	0	0
30	C	34	0	0	0	0
30	D	57	0	0	0	0
30	I	40	0	0	0	0
30	J	10	0	0	0	0
30	X	18	0	0	0	0
30	a	30	0	0	0	0
30	b	33	0	0	0	0
30	c	32	0	0	1	0
30	d	71	0	0	0	0
30	i	40	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	j	10	0	0	0	0
30	l	10	0	0	0	0
30	m	10	0	0	0	0
31	A	49	0	74	4	0
31	D	98	0	148	6	0
31	E	42	0	57	5	0
31	L	49	0	74	3	0
31	a	42	0	57	3	0
31	b	49	0	74	0	0
31	d	147	0	222	13	0
32	B	57	0	78	6	0
32	C	19	0	26	0	0
32	D	16	0	17	2	0
32	V	11	0	10	0	0
32	b	57	0	78	2	0
32	c	19	0	26	1	0
32	h	16	0	17	1	0
33	B	86	0	116	1	0
33	C	35	0	46	1	0
33	D	35	0	46	2	0
33	F	35	0	46	1	0
33	M	70	0	92	3	0
33	a	70	0	92	4	0
33	b	50	0	70	1	0
33	e	35	0	46	0	0
33	m	35	0	46	0	0
34	C	153	0	216	10	0
34	D	51	0	72	0	0
34	M	51	0	72	2	0
34	Z	37	0	44	2	0
34	a	51	0	72	4	0
34	c	102	0	144	0	0
34	d	51	0	72	4	0
34	m	51	0	72	0	0
34	z	39	0	48	2	0
35	C	186	0	246	12	0
35	H	62	0	82	1	0
35	c	186	0	246	4	0
35	h	62	0	82	0	0
36	C	1	0	0	0	0
36	F	1	0	0	0	0
36	O	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	a	1	0	0	0	0
36	c	2	0	0	0	0
36	o	1	0	0	0	0
37	D	8	0	0	0	0
37	d	8	0	0	0	0
38	E	43	0	30	3	0
38	e	43	0	30	4	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	V	43	0	30	2	0
40	v	43	0	30	1	0
41	A	157	0	0	0	0
41	B	218	0	0	4	0
41	C	191	0	0	2	0
41	D	126	0	0	1	0
41	E	24	0	0	1	0
41	F	8	0	0	1	0
41	H	28	0	0	1	0
41	I	4	0	0	0	0
41	J	6	0	0	0	0
41	K	8	0	0	0	0
41	L	8	0	0	0	0
41	M	18	0	0	0	0
41	O	118	0	0	1	0
41	R	1	0	0	0	0
41	T	14	0	0	0	0
41	U	56	0	0	1	0
41	V	95	0	0	0	0
41	X	10	0	0	0	0
41	Y	1	0	0	0	0
41	a	150	0	0	1	0
41	b	220	0	0	2	0
41	c	172	0	0	6	0
41	d	129	0	0	0	0
41	e	15	0	0	1	0
41	f	5	0	0	1	0
41	h	22	0	0	0	0
41	i	1	0	0	0	0
41	j	4	0	0	0	0
41	k	5	0	0	1	0
41	l	8	0	0	0	0
41	m	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	o	99	0	0	0	0
41	t	10	0	0	0	0
41	u	68	0	0	0	0
41	v	57	0	0	1	0
41	x	10	0	0	0	0
41	y	4	0	0	1	0
All	All	53612	0	52351	600	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 6.

The worst 5 of 600 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)
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.42	1.02
1:a:250:ALA:HA	2:b:491:VAL:HG11	1.53	0.88
23:c:515:CLA:HBB1	25:c:516:BCR:H24C	1.58	0.84
4:d:192:THR:HG23	23:d:402:CLA:HBC2	1.60	0.83
2:b:121:GLU:HG2	7:h:4:ARG:HG2	1.63	0.81

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	349/344 (102%)	345 (99%)	3 (1%)	1 (0%)	36	50
1	a	350/344 (102%)	345 (99%)	4 (1%)	1 (0%)	36	50
2	B	512/505 (101%)	506 (99%)	6 (1%)	0	100	100
2	b	506/505 (100%)	496 (98%)	10 (2%)	0	100	100
3	C	454/455 (100%)	447 (98%)	5 (1%)	2 (0%)	30	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	c	456/455 (100%)	445 (98%)	10 (2%)	1 (0%)	43	58
4	D	344/342 (101%)	334 (97%)	10 (3%)	0	100	100
4	d	343/342 (100%)	331 (96%)	12 (4%)	0	100	100
5	E	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
5	e	77/84 (92%)	74 (96%)	3 (4%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	29/44 (66%)	29 (100%)	0	0	100	100
7	H	63/65 (97%)	61 (97%)	2 (3%)	0	100	100
7	h	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
8	I	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	i	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
9	J	36/39 (92%)	32 (89%)	3 (8%)	1 (3%)	4	3
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	32/36 (89%)	30 (94%)	2 (6%)	0	100	100
13	O	244/244 (100%)	236 (97%)	7 (3%)	1 (0%)	30	43
13	o	243/244 (100%)	238 (98%)	5 (2%)	0	100	100
14	T	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	94/104 (90%)	91 (97%)	3 (3%)	0	100	100
15	u	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
16	V	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	129 (96%)	6 (4%)	0	100	100
17	X	36/40 (90%)	36 (100%)	0	0	100	100
17	x	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
18	Y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
18	y	27/30 (90%)	25 (93%)	2 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	7	10
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	5286/5384 (98%)	5165 (98%)	113 (2%)	8 (0%)	48	58

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416	SER
13	O	61	GLN
19	z	30	PRO

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	286/279 (102%)	283 (99%)	3 (1%)	68	84
1	a	287/279 (103%)	285 (99%)	2 (1%)	76	88
2	B	412/403 (102%)	409 (99%)	3 (1%)	76	88
2	b	406/403 (101%)	394 (97%)	12 (3%)	36	58
3	C	357/356 (100%)	351 (98%)	6 (2%)	53	74
3	c	359/356 (101%)	351 (98%)	8 (2%)	45	67
4	D	281/277 (101%)	277 (99%)	4 (1%)	59	79
4	d	280/277 (101%)	274 (98%)	6 (2%)	47	69
5	E	73/73 (100%)	72 (99%)	1 (1%)	59	79
5	e	70/73 (96%)	69 (99%)	1 (1%)	59	79
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	25/38 (66%)	25 (100%)	0	100	100
7	H	55/54 (102%)	50 (91%)	5 (9%)	9	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	h	54/54 (100%)	52 (96%)	2 (4%)	30	51
8	I	34/34 (100%)	33 (97%)	1 (3%)	37	60
8	i	34/34 (100%)	34 (100%)	0	100	100
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	26/27 (96%)	24 (92%)	2 (8%)	12	20
10	K	30/30 (100%)	27 (90%)	3 (10%)	7	11
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	11
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	30/32 (94%)	30 (100%)	0	100	100
12	m	30/32 (94%)	28 (93%)	2 (7%)	15	26
13	O	209/207 (101%)	205 (98%)	4 (2%)	50	71
13	o	208/207 (100%)	203 (98%)	5 (2%)	43	65
14	T	26/28 (93%)	25 (96%)	1 (4%)	29	49
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	83/89 (93%)	80 (96%)	3 (4%)	31	52
15	u	84/89 (94%)	83 (99%)	1 (1%)	63	81
16	V	117/117 (100%)	115 (98%)	2 (2%)	53	74
16	v	117/117 (100%)	114 (97%)	3 (3%)	40	63
17	X	31/33 (94%)	30 (97%)	1 (3%)	34	56
17	x	31/33 (94%)	31 (100%)	0	100	100
18	Y	22/23 (96%)	22 (100%)	0	100	100
18	y	22/23 (96%)	19 (86%)	3 (14%)	3	5
19	Z	52/52 (100%)	48 (92%)	4 (8%)	12	20
19	z	52/52 (100%)	49 (94%)	3 (6%)	18	32
20	R	29/29 (100%)	29 (100%)	0	100	100
All	All	4392/4403 (100%)	4298 (98%)	94 (2%)	45	69

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	145	SER
7	h	56	ASP

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Mol	Chain	Res	Type
3	c	279	LEU
4	d	144	ILE
10	k	17	ILE

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

Mol	Chain	Res	Type
3	c	28	GLN
3	c	415	ASN
19	z	58	ASN
13	o	196	GLN
3	c	373	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	$\# Z > 2$
14	FME	t	1	14	8,9,10	0.65	0	8,9,11	1.44	2 (25%)
14	FME	T	1	14	8,9,10	0.67	0	8,9,11	1.15	1 (12%)
12	FME	M	1	12	8,9,10	0.64	0	8,9,11	1.46	3 (37%)
12	FME	m	1	12	8,9,10	0.65	0	8,9,11	1.19	1 (12%)
8	FME	i	1	8	8,9,10	0.63	0	8,9,11	0.88	0
8	FME	I	1	8	8,9,10	0.67	0	8,9,11	1.09	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	t	1	14	-	0/7/9/11	-
14	FME	T	1	14	-	0/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
8	FME	I	1	8	-	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	-2.77	117.65	124.77
12	M	1	FME	CA-N-CN	-2.68	118.70	122.82
14	t	1	FME	O-C-CA	-2.60	118.08	124.77
14	t	1	FME	CA-N-CN	-2.42	119.10	122.82
12	M	1	FME	O-C-CA	-2.25	118.99	124.77

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 224 ligands modelled in this entry, 17 are monoatomic and 18 are unknown - leaving 189 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
31	LHG	d	406	-	48,48,48	0.91	2 (4%)	51,54,54	1.13	5 (9%)
23	CLA	c	509	41	69,73,73	2.08	19 (27%)	82,113,113	2.72	30 (36%)
23	CLA	C	505	-	69,73,73	2.02	20 (28%)	82,113,113	2.71	29 (35%)
23	CLA	b	603	-	69,73,73	2.06	20 (28%)	82,113,113	2.77	32 (39%)
23	CLA	C	510	-	69,73,73	1.99	20 (28%)	82,113,113	2.72	28 (34%)
26	SQD	D	413	-	41,43,54	1.09	2 (4%)	51,54,65	1.83	10 (19%)
23	CLA	A	404	41	69,73,73	2.00	20 (28%)	82,113,113	2.80	33 (40%)
28	OEX	A	412[B]	41,1,3	0,15,15	-	-	-	-	-
23	CLA	b	610	41	69,73,73	1.98	18 (26%)	82,113,113	2.72	32 (39%)
23	CLA	b	611	-	69,73,73	1.95	20 (28%)	82,113,113	2.71	30 (36%)
40	HEC	v	202	16	46,50,50	1.88	5 (10%)	58,82,82	1.87	7 (12%)
31	LHG	E	101	-	41,41,48	1.05	2 (4%)	44,47,54	1.07	2 (4%)
24	PHO	A	406	-	58,69,69	2.67	12 (20%)	55,99,99	2.86	16 (29%)
27	GOL	B	626	-	5,5,5	0.92	0	5,5,5	1.21	0
33	LMT	B	627	-	36,36,36	0.43	0	47,47,47	1.14	4 (8%)
25	BCR	Y	101	-	41,41,41	0.99	1 (2%)	56,56,56	1.86	14 (25%)
34	LMG	C	502	-	51,51,55	0.93	2 (3%)	59,59,63	1.03	2 (3%)
33	LMT	M	102	-	36,36,36	0.43	0	47,47,47	0.94	3 (6%)
23	CLA	C	509	41	69,73,73	1.98	19 (27%)	82,113,113	2.65	29 (35%)
31	LHG	d	407	-	48,48,48	0.90	2 (4%)	51,54,54	1.01	4 (7%)
23	CLA	b	605	-	69,73,73	1.99	21 (30%)	82,113,113	2.80	32 (39%)
32	HTG	D	411	-	16,16,19	0.97	2 (12%)	20,21,24	1.22	1 (5%)
31	LHG	A	416	-	48,48,48	0.88	2 (4%)	51,54,54	1.24	5 (9%)
23	CLA	c	510	-	69,73,73	2.09	21 (30%)	82,113,113	2.72	30 (36%)
23	CLA	d	402	-	69,73,73	1.88	19 (27%)	82,113,113	2.67	34 (41%)
23	CLA	B	616	-	69,73,73	2.00	19 (27%)	82,113,113	2.73	31 (37%)
23	CLA	B	614	-	69,73,73	1.99	18 (26%)	82,113,113	2.90	32 (39%)
35	DGD	h	103	-	63,63,67	0.91	3 (4%)	77,77,81	1.06	4 (5%)
33	LMT	a	412	-	36,36,36	0.65	1 (2%)	47,47,47	1.31	5 (10%)
33	LMT	e	101	-	36,36,36	0.53	1 (2%)	47,47,47	0.94	3 (6%)
25	BCR	B	619	-	41,41,41	1.07	1 (2%)	56,56,56	1.37	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	508	-	69,73,73	2.05	20 (28%)	82,113,113	2.64	30 (36%)
28	OEX	a	413[A]	41,1,3	0,15,15	-	-	-		
34	LMG	C	521	-	51,51,55	0.99	2 (3%)	59,59,63	1.03	3 (5%)
34	LMG	M	101	-	51,51,55	1.03	2 (3%)	59,59,63	1.08	3 (5%)
25	BCR	h	102	-	41,41,41	1.06	1 (2%)	56,56,56	1.41	9 (16%)
27	GOL	b	623	-	5,5,5	0.99	0	5,5,5	1.19	1 (20%)
37	BCT	d	401[B]	21	3,3,3	0.50	0	2,3,3	1.50	0
23	CLA	b	612	-	69,73,73	1.98	18 (26%)	82,113,113	2.78	30 (36%)
25	BCR	c	516	-	41,41,41	1.04	1 (2%)	56,56,56	1.46	6 (10%)
34	LMG	d	411	39	51,51,55	0.92	2 (3%)	59,59,63	0.92	1 (1%)
25	BCR	b	619	-	41,41,41	1.20	2 (4%)	56,56,56	1.64	12 (21%)
29	PL9	A	413[A]	-	55,55,55	0.67	2 (3%)	68,69,69	2.01	22 (32%)
27	GOL	b	627	-	5,5,5	1.00	0	5,5,5	1.10	1 (20%)
25	BCR	C	517	-	41,41,41	1.04	1 (2%)	56,56,56	1.59	10 (17%)
23	CLA	d	403	-	69,73,73	2.09	22 (31%)	82,113,113	2.76	32 (39%)
31	LHG	D	408	-	48,48,48	0.92	2 (4%)	51,54,54	1.08	4 (7%)
35	DGD	c	519	-	63,63,67	0.87	2 (3%)	77,77,81	1.01	4 (5%)
23	CLA	B	606	-	69,73,73	2.00	21 (30%)	82,113,113	2.77	31 (37%)
23	CLA	C	513	3	69,73,73	2.06	22 (31%)	82,113,113	2.60	29 (35%)
32	HTG	c	523	-	19,19,19	0.91	2 (10%)	23,24,24	1.17	1 (4%)
25	BCR	k	102	-	41,41,41	1.08	1 (2%)	56,56,56	1.68	12 (21%)
27	GOL	O	302	-	5,5,5	0.93	0	5,5,5	1.06	0
33	LMT	B	630	-	26,26,36	0.51	1 (3%)	31,31,47	1.02	2 (6%)
33	LMT	M	103	-	36,36,36	0.52	0	47,47,47	1.09	3 (6%)
23	CLA	a	405	41	69,73,73	1.92	20 (28%)	82,113,113	2.71	32 (39%)
23	CLA	b	607	41	69,73,73	2.01	19 (27%)	82,113,113	2.70	32 (39%)
34	LMG	C	522	-	51,51,55	1.04	3 (5%)	59,59,63	1.39	7 (11%)
34	LMG	m	101	-	51,51,55	0.89	2 (3%)	59,59,63	1.10	3 (5%)
26	SQD	L	102	-	52,54,54	0.98	2 (3%)	62,65,65	1.62	10 (16%)
38	HEM	e	102	5,6	50,50,50	1.55	8 (16%)	67,82,82	1.61	11 (16%)
23	CLA	c	512	-	69,73,73	1.95	19 (27%)	82,113,113	2.65	33 (40%)
34	LMG	z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.10	3 (6%)
23	CLA	A	403	-	69,73,73	1.93	19 (27%)	82,113,113	2.72	33 (40%)
23	CLA	C	515	-	69,73,73	2.02	20 (28%)	82,113,113	2.69	29 (35%)
23	CLA	B	601	41	69,73,73	2.08	20 (28%)	82,113,113	2.66	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LMT	b	626	-	25,25,36	0.57	1 (4%)	30,30,47	1.13	3 (10%)
25	BCR	a	408	-	41,41,41	1.06	1 (2%)	56,56,56	1.49	10 (17%)
37	BCT	D	401[B]	21	3,3,3	0.53	0	2,3,3	0.65	0
29	PL9	A	413[B]	-	55,55,55	0.65	2 (3%)	68,69,69	2.01	22 (32%)
32	HTG	b	624	-	19,19,19	0.94	2 (10%)	23,24,24	1.33	5 (21%)
23	CLA	b	609	-	69,73,73	2.00	21 (30%)	82,113,113	2.64	30 (36%)
23	CLA	b	608	-	69,73,73	2.06	21 (30%)	82,113,113	2.69	34 (41%)
32	HTG	B	624	-	19,19,19	1.02	2 (10%)	23,24,24	1.33	3 (13%)
35	DGD	C	520	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	4 (5%)
23	CLA	c	506	41	69,73,73	2.08	21 (30%)	82,113,113	2.70	33 (40%)
29	PL9	a	414[A]	-	55,55,55	0.66	2 (3%)	68,69,69	2.04	20 (29%)
25	BCR	C	516	-	41,41,41	1.05	1 (2%)	56,56,56	1.59	10 (17%)
25	BCR	B	631	-	41,41,41	1.08	1 (2%)	56,56,56	1.46	11 (19%)
25	BCR	H	101	-	41,41,41	1.09	1 (2%)	56,56,56	1.54	10 (17%)
26	SQD	a	409	-	52,54,54	0.93	2 (3%)	62,65,65	1.65	12 (19%)
35	DGD	c	518	-	63,63,67	0.91	2 (3%)	77,77,81	1.09	5 (6%)
23	CLA	B	609	-	69,73,73	2.00	19 (27%)	82,113,113	2.69	26 (31%)
23	CLA	B	604	-	69,73,73	2.00	19 (27%)	82,113,113	2.63	29 (35%)
35	DGD	C	518	-	63,63,67	0.85	2 (3%)	77,77,81	1.14	5 (6%)
33	LMT	B	629	-	25,25,36	0.42	0	30,30,47	1.10	2 (6%)
34	LMG	Z	101	-	37,37,55	1.01	3 (8%)	45,45,63	1.49	6 (13%)
23	CLA	c	513	3	69,73,73	1.98	19 (27%)	82,113,113	2.70	32 (39%)
32	HTG	h	101	-	16,16,19	1.06	1 (6%)	20,21,24	1.90	6 (30%)
33	LMT	C	526	-	36,36,36	0.52	1 (2%)	47,47,47	1.14	3 (6%)
23	CLA	A	405	41	69,73,73	2.02	18 (26%)	82,113,113	2.66	29 (35%)
25	BCR	D	405	-	41,41,41	1.02	1 (2%)	56,56,56	1.81	16 (28%)
23	CLA	B	608	-	69,73,73	1.96	20 (28%)	82,113,113	2.67	31 (37%)
24	PHO	A	415	-	58,69,69	2.70	13 (22%)	55,99,99	3.06	16 (29%)
23	CLA	b	601	41	69,73,73	2.09	20 (28%)	82,113,113	2.69	30 (36%)
23	CLA	c	507	-	69,73,73	2.06	19 (27%)	82,113,113	2.63	29 (35%)
40	HEC	V	201	16	46,50,50	1.89	6 (13%)	58,82,82	1.77	7 (12%)
23	CLA	A	407	-	69,73,73	2.04	20 (28%)	82,113,113	2.75	31 (37%)
33	LMT	m	103	-	36,36,36	0.45	0	47,47,47	1.07	3 (6%)
28	OEX	A	412[A]	41,1,3	0,15,15	-	-	-	-	-
28	OEX	a	413[B]	41,1,3	0,15,15	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	612	-	69,73,73	1.90	18 (26%)	82,113,113	2.81	28 (34%)
25	BCR	T	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.76	17 (30%)
29	PL9	d	405	-	55,55,55	0.70	2 (3%)	68,69,69	1.58	15 (22%)
27	GOL	c	502	-	5,5,5	1.09	0	5,5,5	0.97	0
23	CLA	B	602	-	69,73,73	2.06	19 (27%)	82,113,113	2.74	34 (41%)
26	SQD	A	409	-	52,54,54	0.89	2 (3%)	62,65,65	2.03	11 (17%)
33	LMT	b	620	-	25,25,36	0.52	0	30,30,47	0.60	0
32	HTG	B	621	-	19,19,19	0.91	1 (5%)	23,24,24	1.54	4 (17%)
23	CLA	D	403	-	69,73,73	1.98	19 (27%)	82,113,113	2.80	32 (39%)
25	BCR	K	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.46	8 (14%)
32	HTG	b	622	-	19,19,19	0.94	1 (5%)	23,24,24	1.44	2 (8%)
35	DGD	c	520	-	63,63,67	0.88	3 (4%)	77,77,81	1.06	7 (9%)
26	SQD	f	101	-	41,43,54	1.08	2 (4%)	51,54,65	1.25	5 (9%)
23	CLA	b	602	-	69,73,73	2.07	20 (28%)	82,113,113	2.78	34 (41%)
31	LHG	a	419	-	41,41,48	1.05	2 (4%)	44,47,54	0.97	2 (4%)
26	SQD	B	620	-	52,54,54	0.95	2 (3%)	62,65,65	1.49	9 (14%)
34	LMG	c	521	-	51,51,55	0.92	2 (3%)	59,59,63	1.07	5 (8%)
31	LHG	D	407	-	48,48,48	0.90	3 (6%)	51,54,54	1.00	3 (5%)
35	DGD	C	519	-	63,63,67	0.88	3 (4%)	77,77,81	1.17	5 (6%)
32	HTG	V	202	-	11,11,19	0.19	0	15,15,24	1.20	1 (6%)
27	GOL	C	524	-	5,5,5	1.14	0	5,5,5	1.17	1 (20%)
23	CLA	b	606	-	69,73,73	1.93	19 (27%)	82,113,113	2.81	32 (39%)
23	CLA	b	616	-	69,73,73	1.97	19 (27%)	82,113,113	2.84	33 (40%)
23	CLA	c	504	-	69,73,73	1.99	19 (27%)	82,113,113	2.61	30 (36%)
23	CLA	B	610	41	69,73,73	2.04	20 (28%)	82,113,113	2.73	33 (40%)
23	CLA	c	515	-	69,73,73	2.09	21 (30%)	82,113,113	2.72	31 (37%)
29	PL9	D	406	-	55,55,55	0.70	2 (3%)	68,69,69	1.67	19 (27%)
26	SQD	a	411	-	52,54,54	0.99	2 (3%)	62,65,65	1.21	7 (11%)
24	PHO	a	416	-	58,69,69	2.81	12 (20%)	55,99,99	3.14	15 (27%)
23	CLA	C	504	-	69,73,73	2.00	19 (27%)	82,113,113	2.63	28 (34%)
23	CLA	c	514	-	69,73,73	2.04	19 (27%)	82,113,113	2.66	33 (40%)
32	HTG	B	622	-	19,19,19	0.79	1 (5%)	23,24,24	1.25	1 (4%)
38	HEM	E	102	5,6	50,50,50	1.56	7 (14%)	67,82,82	1.63	17 (25%)
37	BCT	d	401[A]	21	3,3,3	0.43	0	2,3,3	1.94	1 (50%)
33	LMT	a	418	-	36,36,36	0.49	1 (2%)	47,47,47	0.98	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	k	101	-	41,41,41	1.09	1 (2%)	56,56,56	1.60	12 (21%)
23	CLA	C	507	-	69,73,73	2.00	19 (27%)	82,113,113	2.61	30 (36%)
23	CLA	a	404	41	69,73,73	2.03	19 (27%)	82,113,113	2.67	33 (40%)
23	CLA	c	505	-	69,73,73	2.01	19 (27%)	82,113,113	2.68	31 (37%)
23	CLA	C	512	-	69,73,73	2.02	20 (28%)	82,113,113	2.65	29 (35%)
23	CLA	b	614	-	69,73,73	1.97	20 (28%)	82,113,113	2.75	31 (37%)
23	CLA	C	508	-	69,73,73	2.04	20 (28%)	82,113,113	2.66	34 (41%)
23	CLA	B	603	-	69,73,73	1.99	20 (28%)	82,113,113	2.75	30 (36%)
25	BCR	b	617	-	41,41,41	1.13	1 (2%)	56,56,56	1.49	8 (14%)
31	LHG	d	408	-	48,48,48	0.90	2 (4%)	51,54,54	1.12	5 (9%)
23	CLA	D	404	-	69,73,73	2.03	19 (27%)	82,113,113	2.72	33 (40%)
29	PL9	a	414[B]	-	55,55,55	0.68	2 (3%)	68,69,69	1.96	18 (26%)
25	BCR	B	617	-	41,41,41	1.09	2 (4%)	56,56,56	1.16	5 (8%)
23	CLA	B	607	41	69,73,73	1.99	18 (26%)	82,113,113	2.68	31 (37%)
25	BCR	A	408	-	41,41,41	1.11	2 (4%)	56,56,56	1.39	7 (12%)
23	CLA	B	611	-	69,73,73	1.99	20 (28%)	82,113,113	2.74	32 (39%)
23	CLA	B	613	-	69,73,73	1.95	17 (24%)	82,113,113	2.71	28 (34%)
23	CLA	B	615	-	69,73,73	1.94	17 (24%)	82,113,113	2.74	31 (37%)
23	CLA	C	514	-	69,73,73	2.05	20 (28%)	82,113,113	2.61	31 (37%)
25	BCR	c	517	-	41,41,41	1.08	1 (2%)	56,56,56	1.60	11 (19%)
23	CLA	b	604	-	69,73,73	1.96	19 (27%)	82,113,113	2.66	31 (37%)
24	PHO	a	406	-	58,69,69	2.72	13 (22%)	55,99,99	2.86	14 (25%)
23	CLA	a	407	-	69,73,73	1.98	19 (27%)	82,113,113	2.74	33 (40%)
26	SQD	A	411	-	52,54,54	1.00	2 (3%)	62,65,65	1.26	8 (12%)
27	GOL	a	410	-	5,5,5	0.93	0	5,5,5	1.12	1 (20%)
25	BCR	B	618	-	41,41,41	0.93	1 (2%)	56,56,56	1.59	13 (23%)
32	HTG	b	621	-	19,19,19	0.95	1 (5%)	23,24,24	1.31	4 (17%)
23	CLA	a	403	-	69,73,73	1.98	20 (28%)	82,113,113	2.74	34 (41%)
23	CLA	b	615	-	69,73,73	1.97	17 (24%)	82,113,113	2.67	29 (35%)
27	GOL	B	623	-	5,5,5	0.89	0	5,5,5	1.12	1 (20%)
32	HTG	C	523	-	19,19,19	0.85	1 (5%)	23,24,24	1.28	2 (8%)
35	DGD	H	102	-	63,63,67	0.85	3 (4%)	77,77,81	1.07	7 (9%)
23	CLA	C	506	41	69,73,73	1.99	21 (30%)	82,113,113	2.65	35 (42%)
27	GOL	B	628	-	5,5,5	1.09	0	5,5,5	0.98	0
33	LMT	D	402	-	36,36,36	0.56	1 (2%)	47,47,47	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	503	-	69,73,73	2.02	21 (30%)	82,113,113	2.63	32 (39%)
23	CLA	B	605	-	69,73,73	2.06	18 (26%)	82,113,113	2.77	30 (36%)
25	BCR	b	618	-	41,41,41	1.03	1 (2%)	56,56,56	1.49	11 (19%)
27	GOL	c	527	-	5,5,5	0.85	0	5,5,5	1.15	1 (20%)
31	LHG	L	101	-	48,48,48	0.90	3 (6%)	51,54,54	1.17	5 (9%)
34	LMG	a	417	-	51,51,55	0.92	2 (3%)	59,59,63	1.20	7 (11%)
23	CLA	b	613	-	69,73,73	1.97	18 (26%)	82,113,113	2.68	31 (37%)
25	BCR	d	404	-	41,41,41	1.21	2 (4%)	56,56,56	1.84	14 (25%)
27	GOL	A	410	-	5,5,5	1.14	0	5,5,5	0.98	0
23	CLA	c	511	-	69,73,73	2.09	20 (28%)	82,113,113	2.70	29 (35%)
34	LMG	D	412	39	51,51,55	0.88	3 (5%)	59,59,63	1.08	5 (8%)
23	CLA	C	511	-	69,73,73	2.07	20 (28%)	82,113,113	2.67	29 (35%)
37	BCT	D	401[A]	21	3,3,3	0.54	0	2,3,3	0.93	0
34	LMG	c	522	-	51,51,55	0.97	2 (3%)	59,59,63	1.21	6 (10%)
27	GOL	v	201	-	5,5,5	1.26	1 (20%)	5,5,5	0.91	0
31	LHG	b	628	-	48,48,48	0.94	2 (4%)	51,54,54	1.07	3 (5%)
33	LMT	F	101	-	36,36,36	0.55	1 (2%)	47,47,47	1.20	5 (10%)
23	CLA	C	503	-	69,73,73	1.99	19 (27%)	82,113,113	2.74	32 (39%)

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
31	LHG	d	406	-	-	20/53/53/53	-
23	CLA	c	509	41	1/1/15/20	10/39/115/115	-
23	CLA	C	505	-	1/1/15/20	4/39/115/115	-
23	CLA	b	603	-	1/1/15/20	7/39/115/115	-
23	CLA	C	510	-	1/1/15/20	5/39/115/115	-
26	SQD	D	413	-	-	12/38/58/69	0/1/1/1
23	CLA	A	404	41	1/1/15/20	2/39/115/115	-
23	CLA	b	610	41	1/1/15/20	7/39/115/115	-
23	CLA	b	611	-	1/1/15/20	3/39/115/115	-
40	HEC	v	202	16	-	6/14/54/54	-
31	LHG	E	101	-	-	16/46/46/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PHO	A	406	-	-	1/37/103/103	0/5/6/6
27	GOL	B	626	-	-	3/4/4/4	-
33	LMT	B	627	-	-	9/21/61/61	0/2/2/2
25	BCR	Y	101	-	-	5/29/63/63	0/2/2/2
34	LMG	C	502	-	-	24/46/66/70	0/1/1/1
33	LMT	M	102	-	-	6/21/61/61	0/2/2/2
23	CLA	C	509	41	1/1/15/20	6/39/115/115	-
31	LHG	d	407	-	-	23/53/53/53	-
23	CLA	b	605	-	1/1/15/20	6/39/115/115	-
32	HTG	D	411	-	-	2/7/27/30	0/1/1/1
31	LHG	A	416	-	-	16/53/53/53	-
23	CLA	c	510	-	1/1/15/20	8/39/115/115	-
23	CLA	d	402	-	1/1/15/20	3/39/115/115	-
23	CLA	B	616	-	1/1/15/20	8/39/115/115	-
23	CLA	B	614	-	1/1/15/20	9/39/115/115	-
35	DGD	h	103	-	-	12/51/91/95	0/2/2/2
33	LMT	a	412	-	-	7/21/61/61	0/2/2/2
33	LMT	e	101	-	-	9/21/61/61	0/2/2/2
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
23	CLA	c	508	-	1/1/15/20	10/39/115/115	-
34	LMG	C	521	-	-	13/46/66/70	0/1/1/1
34	LMG	M	101	-	-	21/46/66/70	0/1/1/1
25	BCR	h	102	-	-	0/29/63/63	0/2/2/2
27	GOL	b	623	-	-	2/4/4/4	-
23	CLA	b	612	-	1/1/15/20	5/39/115/115	-
25	BCR	c	516	-	-	0/29/63/63	0/2/2/2
34	LMG	d	411	39	-	8/46/66/70	0/1/1/1
25	BCR	b	619	-	-	4/29/63/63	0/2/2/2
29	PL9	A	413[A]	-	-	16/53/73/73	0/1/1/1
27	GOL	b	627	-	-	0/4/4/4	-
25	BCR	C	517	-	-	3/29/63/63	0/2/2/2
23	CLA	d	403	-	1/1/15/20	5/39/115/115	-
31	LHG	D	408	-	-	11/53/53/53	-
35	DGD	c	519	-	-	17/51/91/95	0/2/2/2
23	CLA	B	606	-	1/1/15/20	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	513	3	1/1/15/20	3/39/115/115	-
32	HTG	c	523	-	-	4/10/30/30	0/1/1/1
25	BCR	k	102	-	-	5/29/63/63	0/2/2/2
27	GOL	O	302	-	-	4/4/4/4	-
33	LMT	B	630	-	-	8/17/38/61	0/1/1/2
33	LMT	M	103	-	-	8/21/61/61	0/2/2/2
23	CLA	a	405	41	-	8/39/115/115	-
23	CLA	b	607	41	1/1/15/20	3/39/115/115	-
34	LMG	C	522	-	-	12/46/66/70	0/1/1/1
34	LMG	m	101	-	-	9/46/66/70	0/1/1/1
26	SQD	L	102	-	-	17/49/69/69	0/1/1/1
38	HEM	e	102	5,6	-	9/14/54/54	-
23	CLA	c	512	-	1/1/15/20	8/39/115/115	-
34	LMG	z	101	-	-	7/34/54/70	0/1/1/1
23	CLA	A	403	-	1/1/15/20	3/39/115/115	-
23	CLA	C	515	-	1/1/15/20	9/39/115/115	-
23	CLA	B	601	41	1/1/15/20	9/39/115/115	-
33	LMT	b	626	-	-	9/17/37/61	0/1/1/2
25	BCR	a	408	-	-	0/29/63/63	0/2/2/2
29	PL9	A	413[B]	-	-	16/53/73/73	0/1/1/1
32	HTG	b	624	-	-	2/10/30/30	0/1/1/1
23	CLA	b	609	-	1/1/15/20	10/39/115/115	-
23	CLA	b	608	-	1/1/15/20	5/39/115/115	-
32	HTG	B	624	-	-	5/10/30/30	0/1/1/1
35	DGD	C	520	-	-	8/51/91/95	0/2/2/2
23	CLA	c	506	41	1/1/15/20	4/39/115/115	-
29	PL9	a	414[A]	-	-	18/53/73/73	0/1/1/1
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
25	BCR	B	631	-	-	4/29/63/63	0/2/2/2
25	BCR	H	101	-	-	1/29/63/63	0/2/2/2
26	SQD	a	409	-	-	12/49/69/69	0/1/1/1
35	DGD	c	518	-	-	19/51/91/95	0/2/2/2
23	CLA	B	609	-	1/1/15/20	6/39/115/115	-
23	CLA	B	604	-	1/1/15/20	7/39/115/115	-
35	DGD	C	518	-	-	17/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMT	B	629	-	-	4/17/37/61	0/1/1/2
34	LMG	Z	101	-	-	10/31/51/70	0/1/1/1
23	CLA	c	513	3	1/1/15/20	6/39/115/115	-
32	HTG	h	101	-	-	2/7/27/30	0/1/1/1
33	LMT	C	526	-	-	8/21/61/61	0/2/2/2
23	CLA	A	405	41	-	5/39/115/115	-
25	BCR	D	405	-	-	8/29/63/63	0/2/2/2
23	CLA	B	608	-	-	2/39/115/115	-
24	PHO	A	415	-	-	2/37/103/103	0/5/6/6
23	CLA	b	601	41	1/1/15/20	16/39/115/115	-
23	CLA	c	507	-	1/1/15/20	4/39/115/115	-
40	HEC	V	201	16	-	6/14/54/54	-
23	CLA	A	407	-	1/1/15/20	8/39/115/115	-
33	LMT	m	103	-	-	6/21/61/61	0/2/2/2
23	CLA	B	612	-	1/1/15/20	7/39/115/115	-
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
29	PL9	d	405	-	-	7/53/73/73	0/1/1/1
27	GOL	c	502	-	-	0/4/4/4	-
23	CLA	B	602	-	1/1/15/20	10/39/115/115	-
26	SQD	A	409	-	-	13/49/69/69	0/1/1/1
33	LMT	b	620	-	-	6/17/37/61	0/1/1/2
32	HTG	B	621	-	-	4/10/30/30	0/1/1/1
23	CLA	D	403	-	1/1/15/20	6/39/115/115	-
25	BCR	K	101	-	-	0/29/63/63	0/2/2/2
32	HTG	b	622	-	-	2/10/30/30	0/1/1/1
35	DGD	c	520	-	-	10/51/91/95	0/2/2/2
26	SQD	f	101	-	-	14/38/58/69	0/1/1/1
23	CLA	b	602	-	1/1/15/20	5/39/115/115	-
31	LHG	a	419	-	-	18/46/46/53	-
26	SQD	B	620	-	-	19/49/69/69	0/1/1/1
34	LMG	c	521	-	-	6/46/66/70	0/1/1/1
31	LHG	D	407	-	-	15/53/53/53	-
35	DGD	C	519	-	-	16/51/91/95	0/2/2/2
32	HTG	V	202	-	-	1/2/19/30	0/1/1/1
27	GOL	C	524	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	606	-	1/1/15/20	9/39/115/115	-
23	CLA	b	616	-	1/1/15/20	9/39/115/115	-
23	CLA	c	504	-	1/1/15/20	6/39/115/115	-
23	CLA	B	610	41	1/1/15/20	6/39/115/115	-
23	CLA	c	515	-	1/1/15/20	11/39/115/115	-
29	PL9	D	406	-	-	7/53/73/73	0/1/1/1
26	SQD	a	411	-	-	17/49/69/69	0/1/1/1
24	PHO	a	416	-	-	5/37/103/103	0/5/6/6
23	CLA	C	504	-	-	9/39/115/115	-
23	CLA	c	514	-	1/1/15/20	8/39/115/115	-
32	HTG	B	622	-	-	5/10/30/30	0/1/1/1
38	HEM	E	102	5,6	-	5/14/54/54	-
33	LMT	a	418	-	-	4/21/61/61	0/2/2/2
25	BCR	k	101	-	-	4/29/63/63	0/2/2/2
23	CLA	C	507	-	1/1/15/20	8/39/115/115	-
23	CLA	a	404	41	1/1/15/20	8/39/115/115	-
23	CLA	c	505	-	1/1/15/20	1/39/115/115	-
23	CLA	C	512	-	1/1/15/20	9/39/115/115	-
23	CLA	b	614	-	1/1/15/20	11/39/115/115	-
23	CLA	C	508	-	1/1/15/20	11/39/115/115	-
23	CLA	B	603	-	1/1/15/20	5/39/115/115	-
25	BCR	b	617	-	-	4/29/63/63	0/2/2/2
31	LHG	d	408	-	-	9/53/53/53	-
23	CLA	D	404	-	1/1/15/20	9/39/115/115	-
29	PL9	a	414[B]	-	-	17/53/73/73	0/1/1/1
25	BCR	B	617	-	-	0/29/63/63	0/2/2/2
23	CLA	B	607	41	1/1/15/20	3/39/115/115	-
25	BCR	A	408	-	-	0/29/63/63	0/2/2/2
23	CLA	B	611	-	1/1/15/20	2/39/115/115	-
23	CLA	B	613	-	1/1/15/20	9/39/115/115	-
23	CLA	B	615	-	1/1/15/20	7/39/115/115	-
23	CLA	C	514	-	1/1/15/20	16/39/115/115	-
25	BCR	c	517	-	-	0/29/63/63	0/2/2/2
23	CLA	b	604	-	1/1/15/20	11/39/115/115	-
24	PHO	a	406	-	-	4/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	a	407	-	1/1/15/20	12/39/115/115	-
26	SQD	A	411	-	-	14/49/69/69	0/1/1/1
27	GOL	a	410	-	-	4/4/4/4	-
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
32	HTG	b	621	-	-	5/10/30/30	0/1/1/1
23	CLA	a	403	-	1/1/15/20	5/39/115/115	-
23	CLA	b	615	-	1/1/15/20	11/39/115/115	-
27	GOL	B	623	-	-	2/4/4/4	-
32	HTG	C	523	-	-	2/10/30/30	0/1/1/1
35	DGD	H	102	-	-	15/51/91/95	0/2/2/2
23	CLA	C	506	41	1/1/15/20	7/39/115/115	-
27	GOL	B	628	-	-	0/4/4/4	-
33	LMT	D	402	-	-	10/21/61/61	0/2/2/2
23	CLA	c	503	-	1/1/15/20	5/39/115/115	-
23	CLA	B	605	-	1/1/15/20	9/39/115/115	-
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
27	GOL	c	527	-	-	0/4/4/4	-
31	LHG	L	101	-	-	16/53/53/53	-
34	LMG	a	417	-	-	12/46/66/70	0/1/1/1
23	CLA	b	613	-	1/1/15/20	2/39/115/115	-
25	BCR	d	404	-	-	5/29/63/63	0/2/2/2
27	GOL	A	410	-	-	3/4/4/4	-
23	CLA	c	511	-	1/1/15/20	12/39/115/115	-
34	LMG	D	412	39	-	9/46/66/70	0/1/1/1
23	CLA	C	511	-	1/1/15/20	4/39/115/115	-
34	LMG	c	522	-	-	9/46/66/70	0/1/1/1
27	GOL	v	201	-	-	2/4/4/4	-
31	LHG	b	628	-	-	13/53/53/53	-
33	LMT	F	101	-	-	5/21/61/61	0/2/2/2
23	CLA	C	503	-	1/1/15/20	5/39/115/115	-

The worst 5 of 1585 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	416	PHO	C1B-C2B	10.03	1.50	1.39
24	a	406	PHO	C1D-C2D	8.92	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	415	PHO	C1D-C2D	8.82	1.49	1.39
24	A	406	PHO	C1D-C2D	8.81	1.49	1.39
24	A	406	PHO	C1B-C2B	8.75	1.49	1.39

The worst 5 of 2904 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	415	PHO	C2D-C1D-ND	12.52	118.48	109.43
24	a	416	PHO	C2D-C1D-ND	12.34	118.35	109.43
23	B	614	CLA	C1D-ND-C4D	-10.41	99.01	106.31
24	a	406	PHO	C2D-C1D-ND	10.34	116.91	109.43
23	b	605	CLA	C1D-ND-C4D	-10.34	99.05	106.31

5 of 66 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	403	CLA	ND
23	A	404	CLA	ND
23	A	407	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND

5 of 1336 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	605	CLA	C6-C7-C8-C9
23	B	609	CLA	C1A-C2A-CAA-CBA
23	B	609	CLA	C3A-C2A-CAA-CBA
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D

There are no ring outliers.

154 monomers are involved in 364 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	d	406	LHG	3	0
23	c	509	CLA	3	0
23	C	505	CLA	4	0
23	b	603	CLA	3	0
23	C	510	CLA	4	0
26	D	413	SQD	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	404	CLA	4	0
23	b	610	CLA	2	0
40	v	202	HEC	1	0
31	E	101	LHG	5	0
24	A	406	PHO	1	0
27	B	626	GOL	1	0
25	Y	101	BCR	2	0
34	C	502	LMG	4	0
33	M	102	LMT	2	0
23	C	509	CLA	1	0
31	d	407	LHG	3	0
23	b	605	CLA	10	0
32	D	411	HTG	2	0
31	A	416	LHG	4	0
23	c	510	CLA	4	0
23	d	402	CLA	2	0
23	B	616	CLA	4	0
23	B	614	CLA	2	0
33	a	412	LMT	1	0
25	B	619	BCR	5	0
23	c	508	CLA	3	0
34	C	521	LMG	3	0
34	M	101	LMG	2	0
25	h	102	BCR	5	0
23	b	612	CLA	2	0
25	c	516	BCR	5	0
34	d	411	LMG	4	0
25	b	619	BCR	6	0
29	A	413[A]	PL9	5	0
27	b	627	GOL	1	0
25	C	517	BCR	3	0
23	d	403	CLA	3	0
31	D	408	LHG	3	0
35	c	519	DGD	1	0
23	B	606	CLA	2	0
23	C	513	CLA	1	0
32	c	523	HTG	1	0
25	k	102	BCR	2	0
33	M	103	LMT	1	0
23	a	405	CLA	2	0
34	C	522	LMG	3	0
26	L	102	SQD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	e	102	HEM	4	0
23	c	512	CLA	5	0
34	z	101	LMG	2	0
23	A	403	CLA	3	0
23	C	515	CLA	1	0
23	B	601	CLA	4	0
33	b	626	LMT	1	0
25	a	408	BCR	1	0
29	A	413[B]	PL9	8	0
32	b	624	HTG	1	0
23	b	609	CLA	2	0
23	b	608	CLA	1	0
32	B	624	HTG	1	0
35	C	520	DGD	2	0
23	c	506	CLA	2	0
29	a	414[A]	PL9	3	0
25	C	516	BCR	2	0
25	B	631	BCR	5	0
25	H	101	BCR	3	0
26	a	409	SQD	3	0
35	c	518	DGD	2	0
23	B	604	CLA	3	0
35	C	518	DGD	5	0
33	B	629	LMT	1	0
34	Z	101	LMG	2	0
23	c	513	CLA	4	0
32	h	101	HTG	1	0
33	C	526	LMT	1	0
23	A	405	CLA	4	0
25	D	405	BCR	1	0
24	A	415	PHO	1	0
23	b	601	CLA	1	0
23	c	507	CLA	7	0
40	V	201	HEC	2	0
23	A	407	CLA	4	0
23	B	612	CLA	3	0
25	T	101	BCR	8	0
29	d	405	PL9	1	0
27	c	502	GOL	1	0
23	B	602	CLA	2	0
26	A	409	SQD	3	0
32	B	621	HTG	3	0

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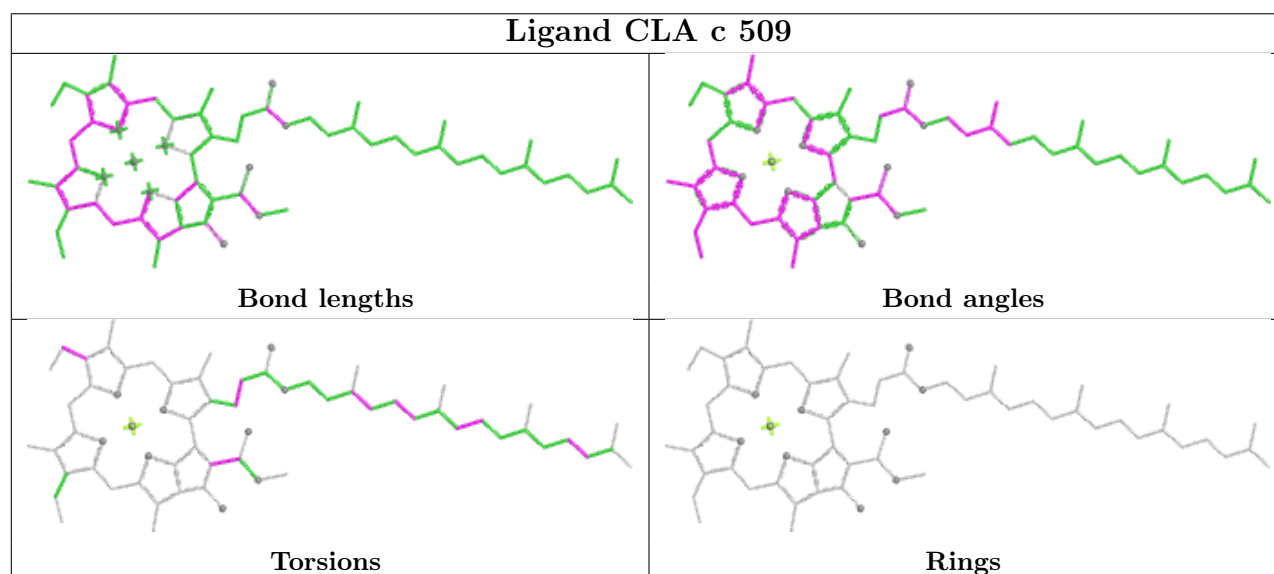
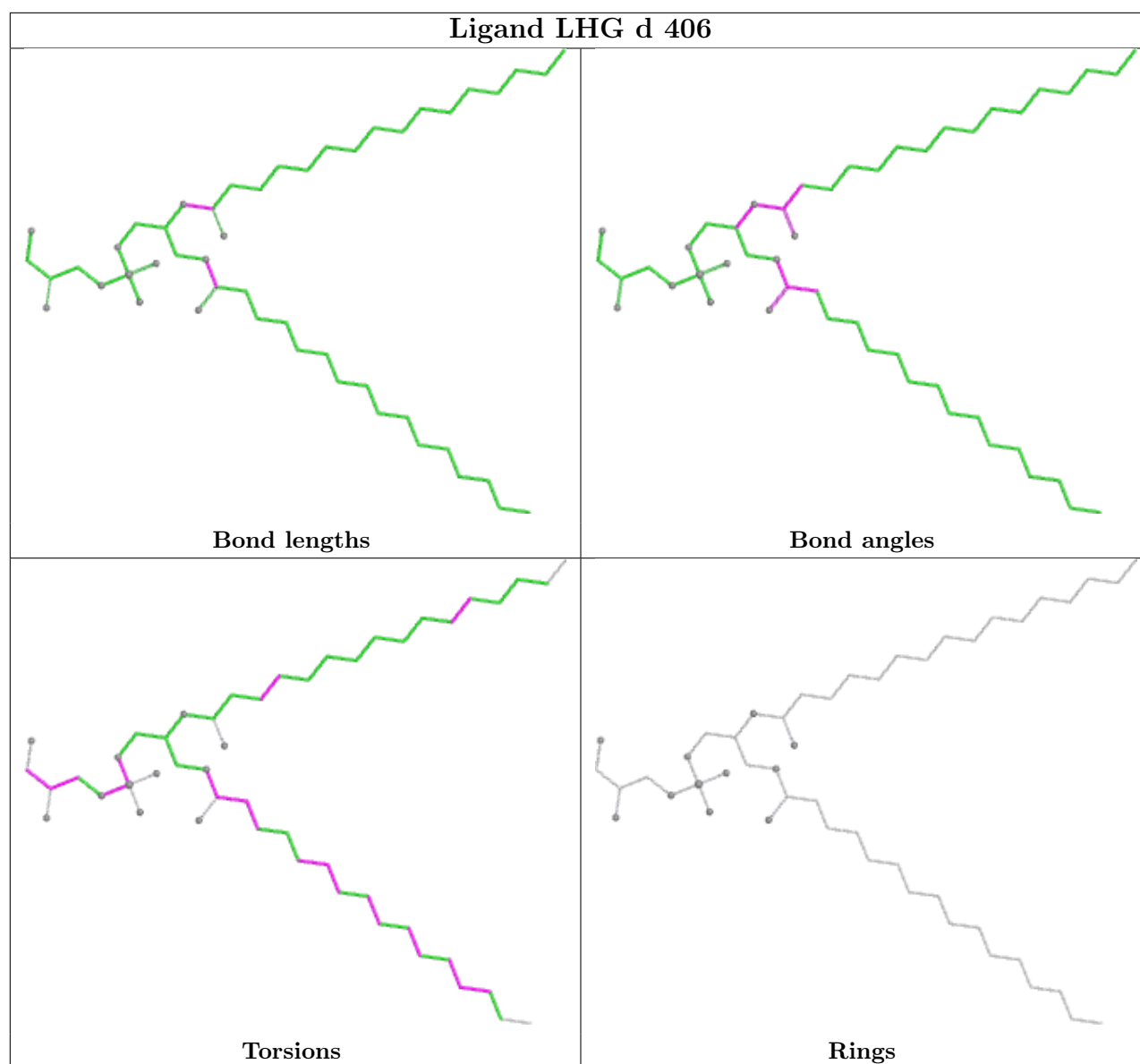
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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25	K	101	BCR	1	0
35	c	520	DGD	2	0
26	f	101	SQD	3	0
23	b	602	CLA	2	0
31	a	419	LHG	3	0
26	B	620	SQD	3	0
31	D	407	LHG	3	0
35	C	519	DGD	5	0
23	b	606	CLA	3	0
23	b	616	CLA	3	0
23	c	504	CLA	3	0
23	B	610	CLA	1	0
23	c	515	CLA	4	0
29	D	406	PL9	3	0
26	a	411	SQD	1	0
24	a	416	PHO	1	0
23	C	504	CLA	7	0
23	c	514	CLA	6	0
32	B	622	HTG	2	0
38	E	102	HEM	3	0
33	a	418	LMT	3	0
25	k	101	BCR	2	0
23	C	507	CLA	2	0
23	a	404	CLA	6	0
23	c	505	CLA	7	0
23	C	512	CLA	5	0
23	b	614	CLA	1	0
23	C	508	CLA	6	0
23	B	603	CLA	1	0
25	b	617	BCR	1	0
31	d	408	LHG	7	0
23	D	404	CLA	2	0
29	a	414[B]	PL9	9	0
25	B	617	BCR	1	0
23	B	607	CLA	3	0
25	A	408	BCR	2	0
23	B	613	CLA	4	0
23	B	615	CLA	2	0
23	C	514	CLA	1	0
25	c	517	BCR	2	0
23	b	604	CLA	7	0

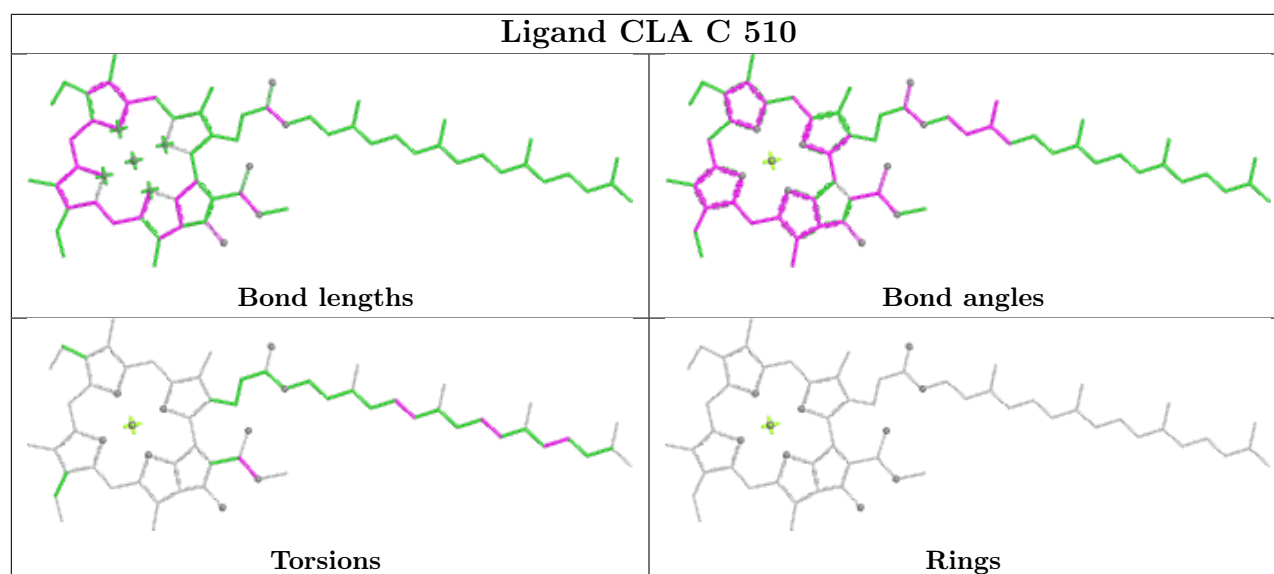
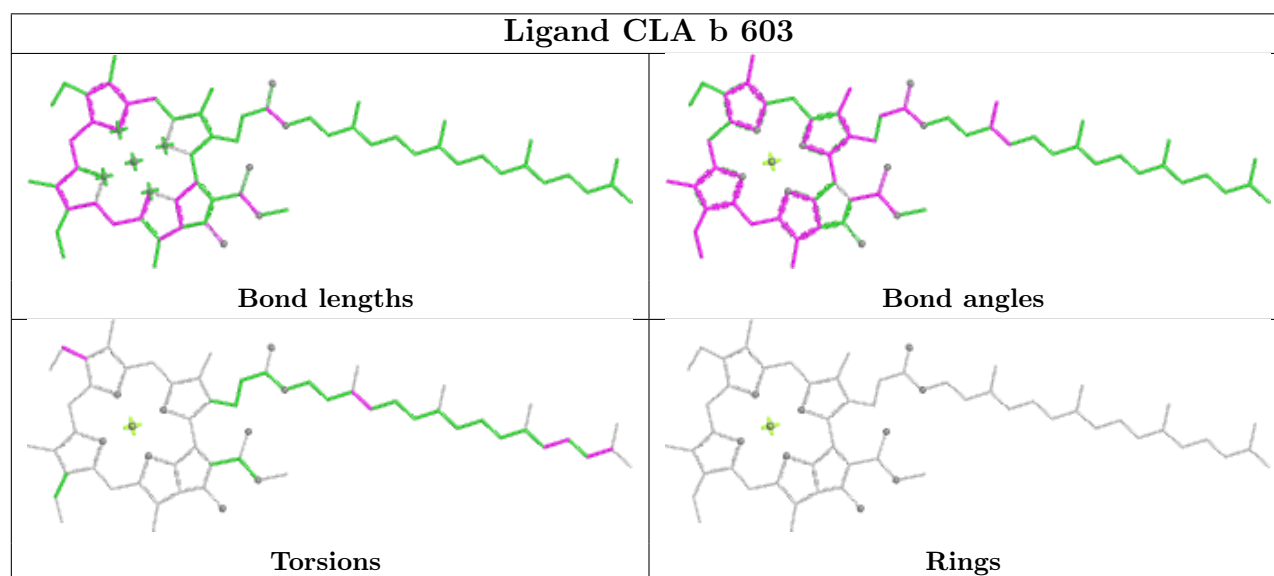
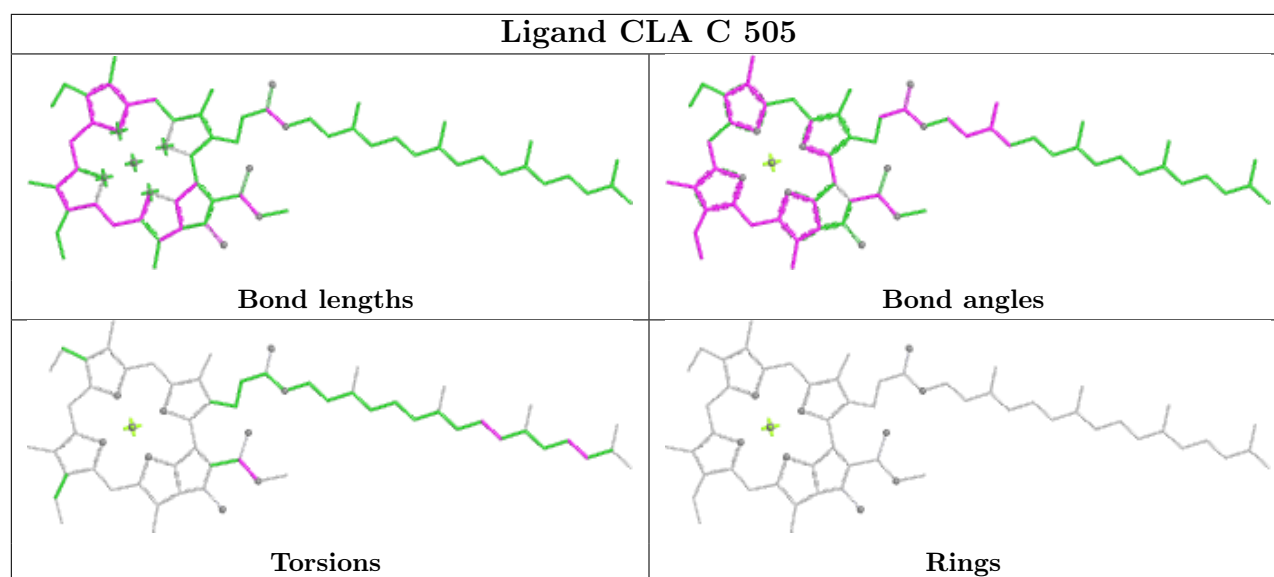
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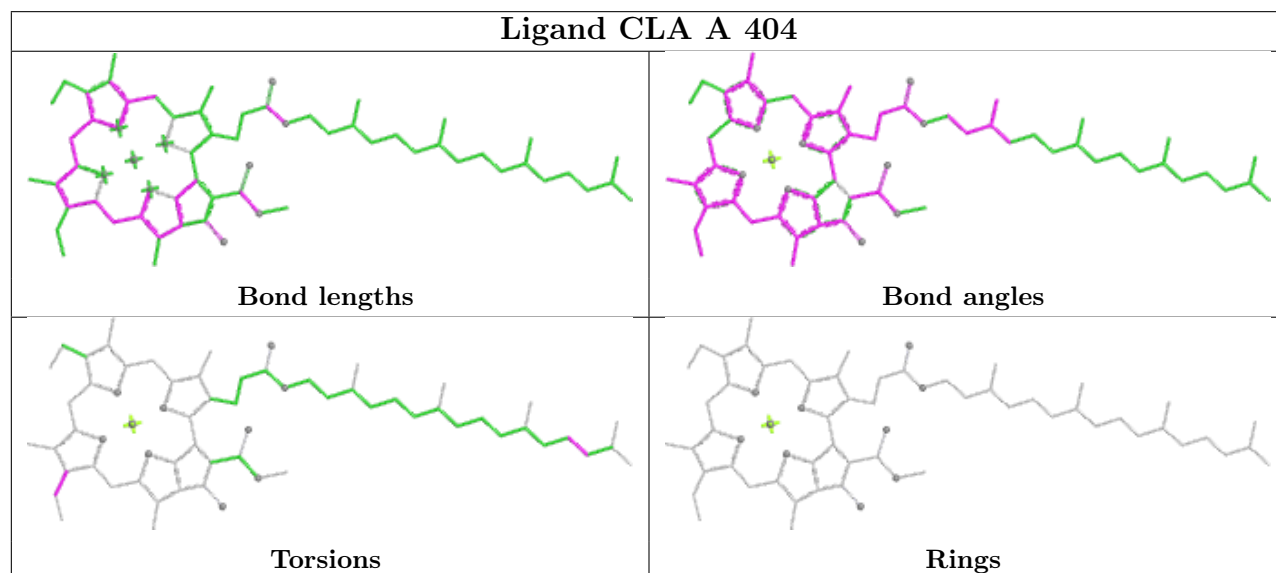
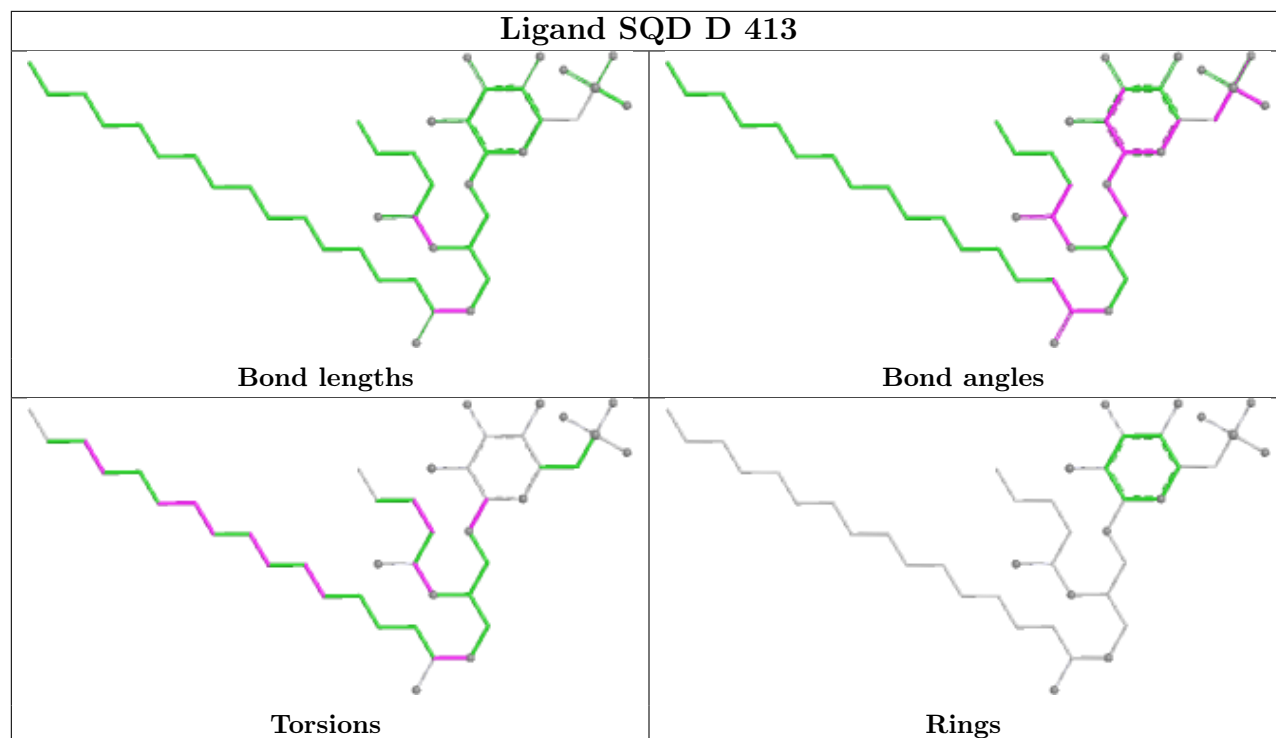
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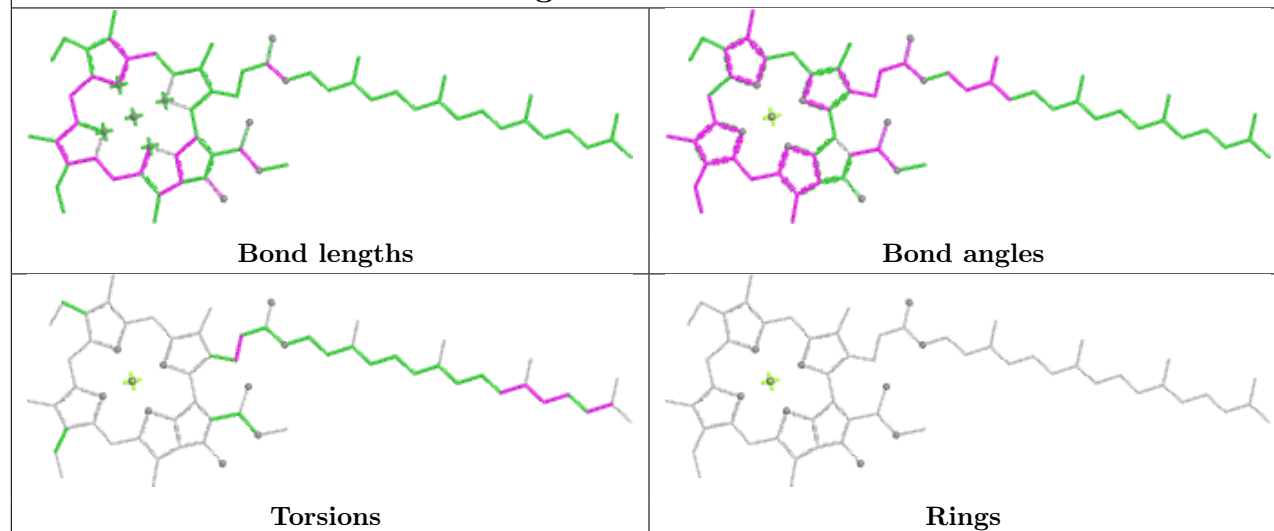
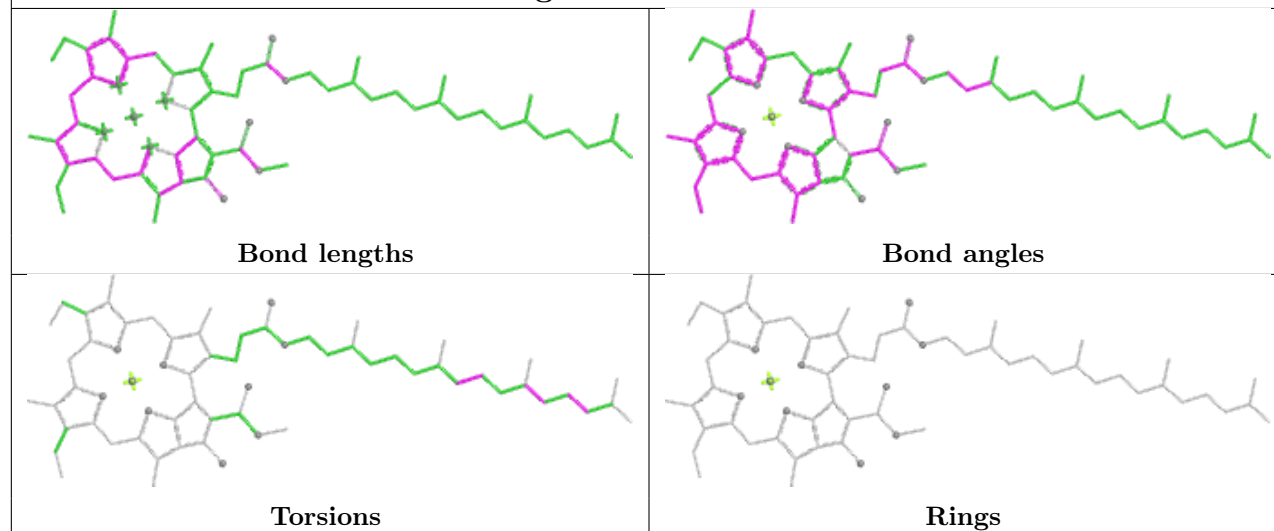
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	a	406	PHO	1	0
23	a	407	CLA	3	0
27	a	410	GOL	1	0
25	B	618	BCR	4	0
32	b	621	HTG	1	0
23	a	403	CLA	2	0
23	b	615	CLA	2	0
35	H	102	DGD	1	0
23	C	506	CLA	3	0
33	D	402	LMT	2	0
23	c	503	CLA	3	0
23	B	605	CLA	4	0
25	b	618	BCR	4	0
31	L	101	LHG	3	0
34	a	417	LMG	4	0
23	b	613	CLA	4	0
25	d	404	BCR	4	0
23	c	511	CLA	1	0
23	C	511	CLA	3	0
27	v	201	GOL	1	0
33	F	101	LMT	1	0
23	C	503	CLA	3	0

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

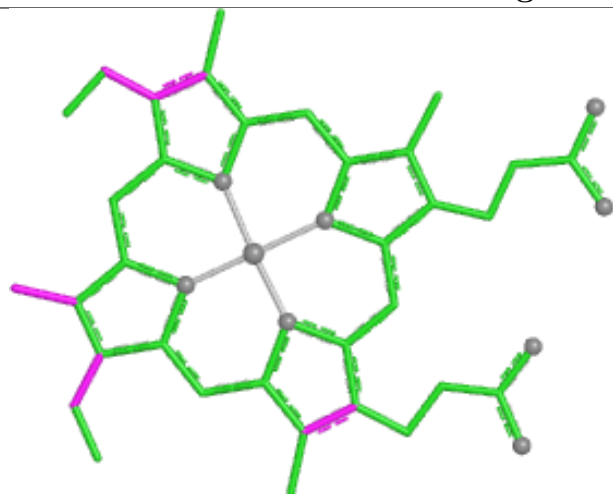




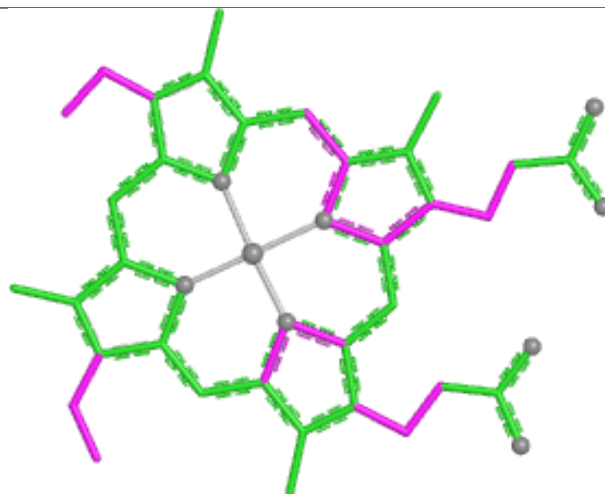


Ligand CLA b 610**Ligand CLA b 611**

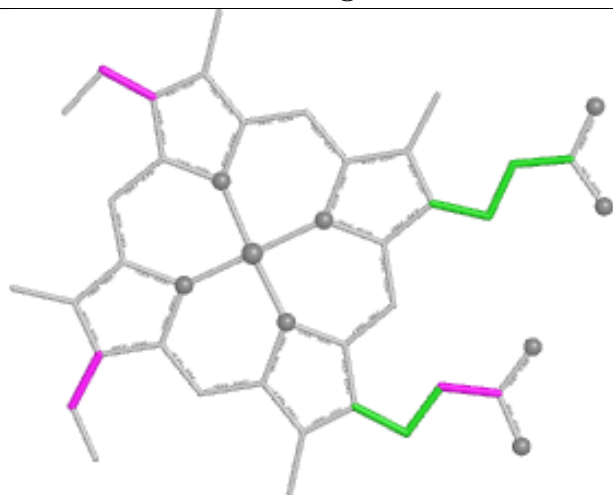
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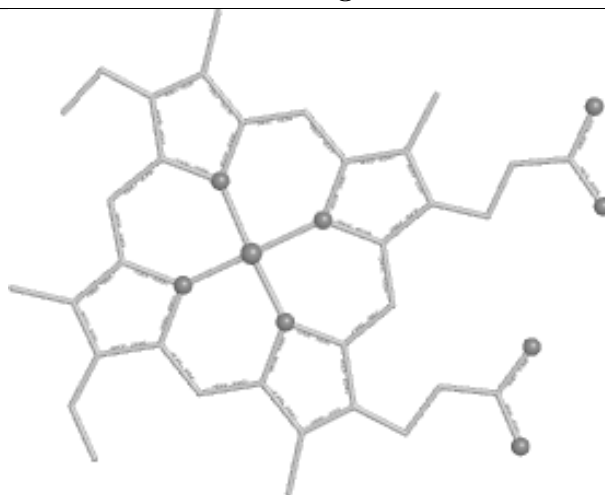
Bond lengths



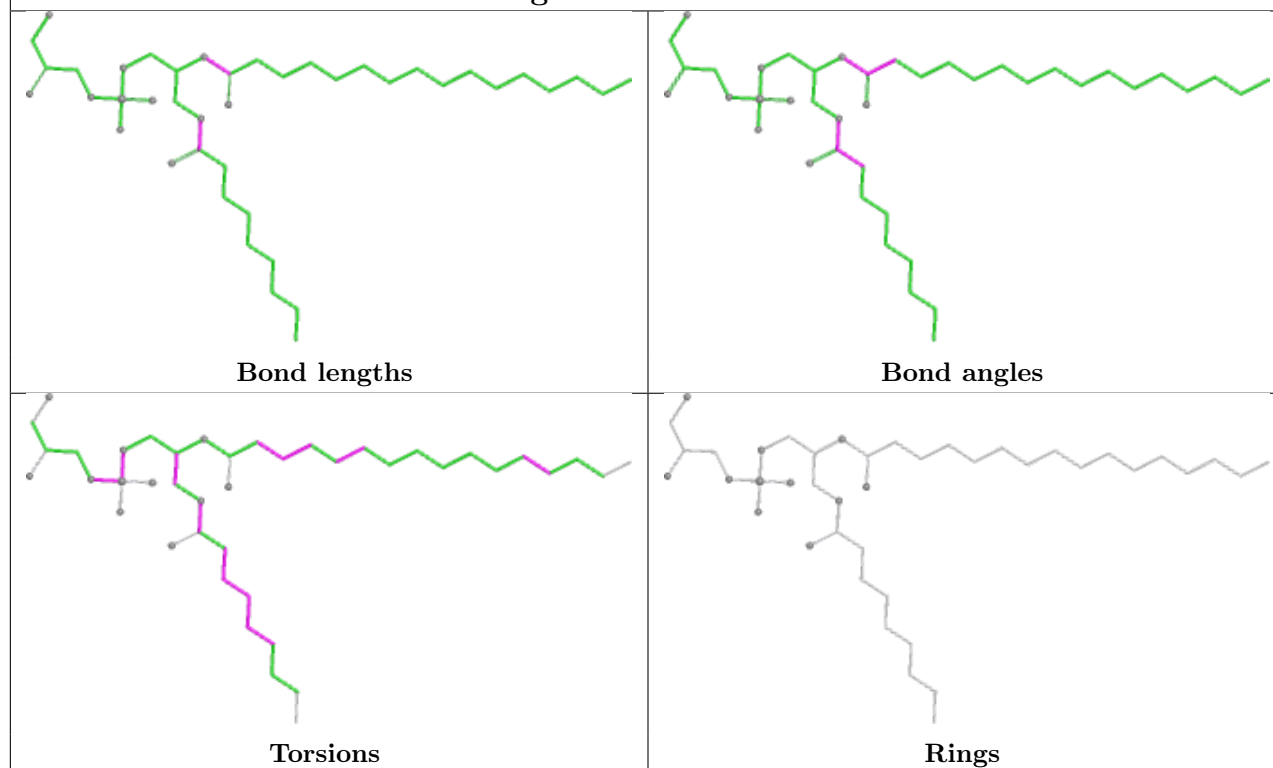
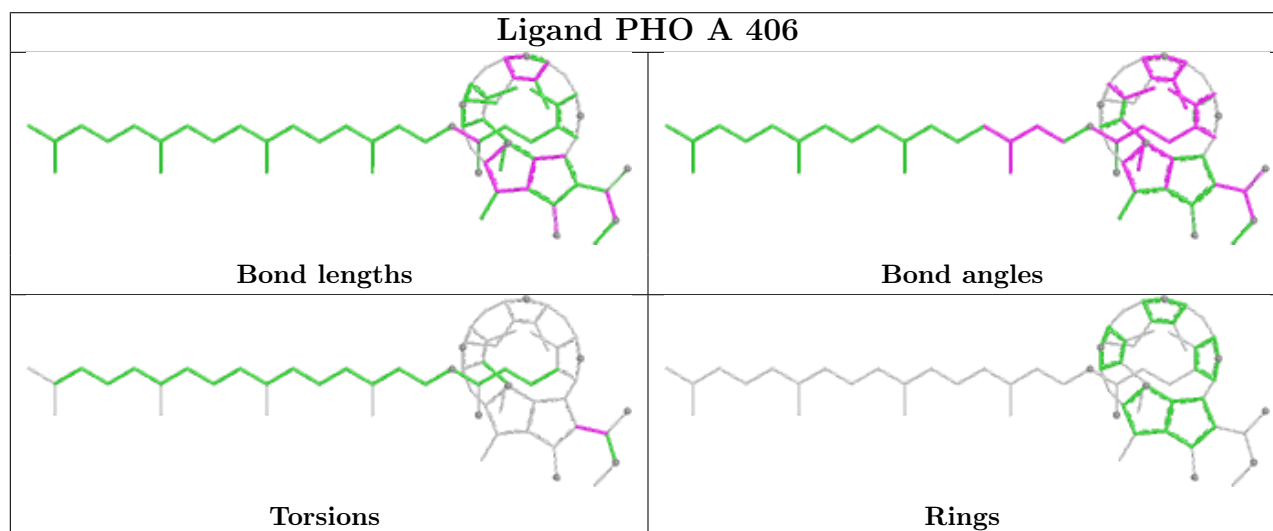
Bond angles

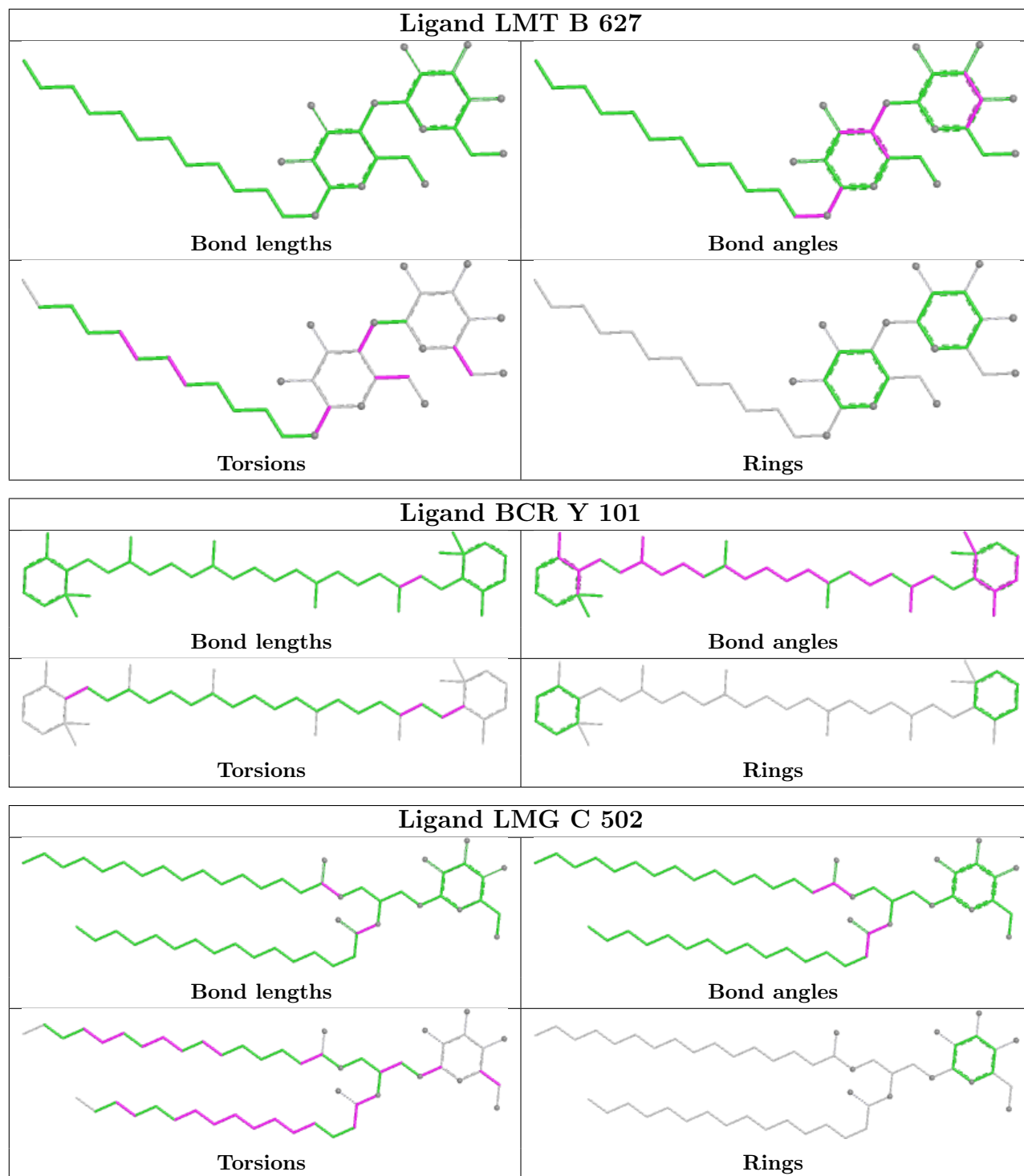


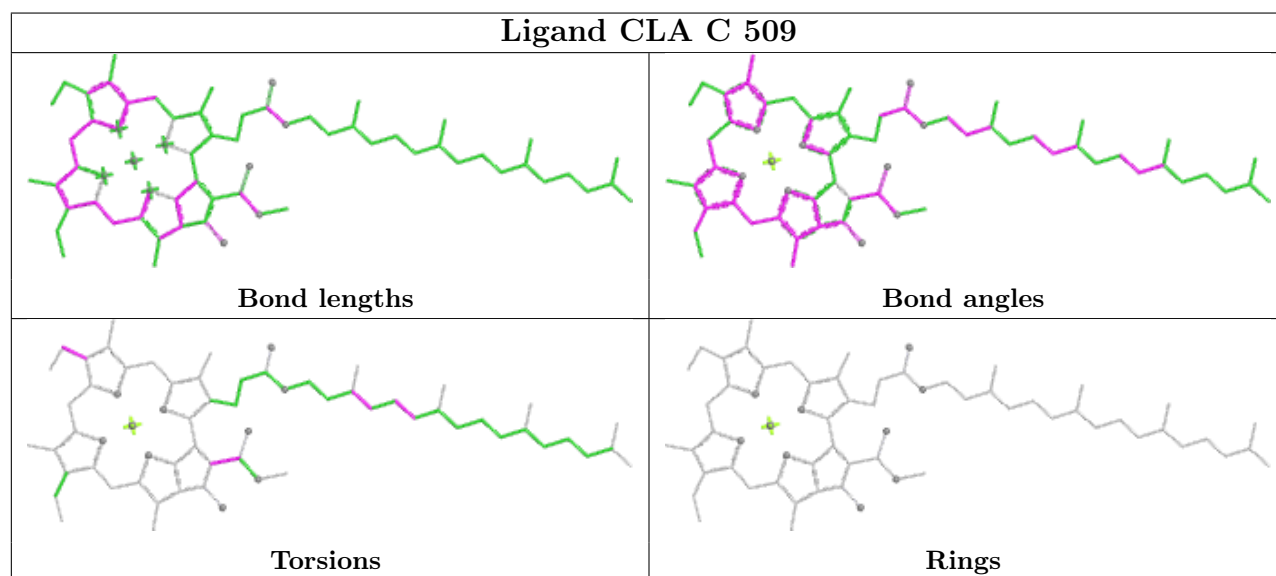
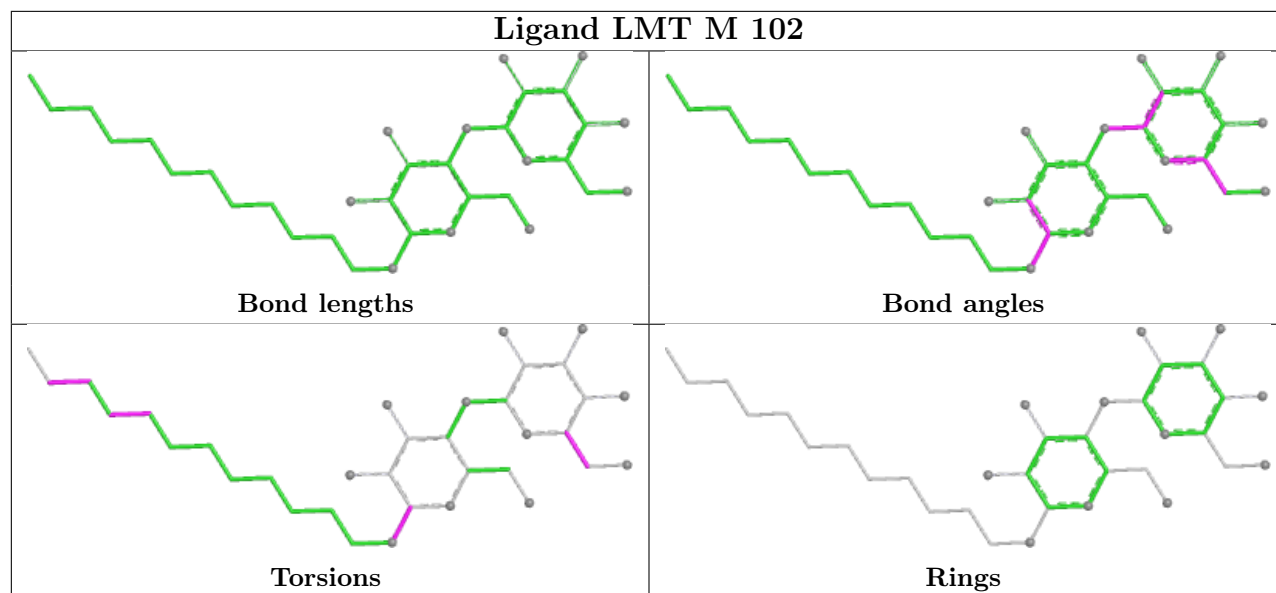
Torsions

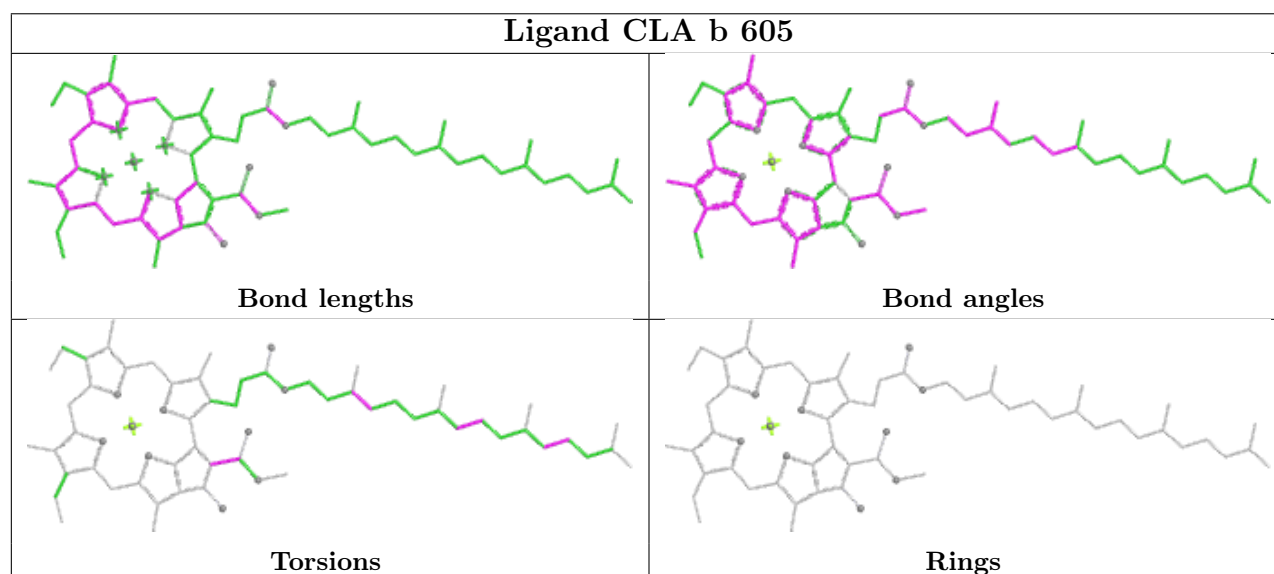
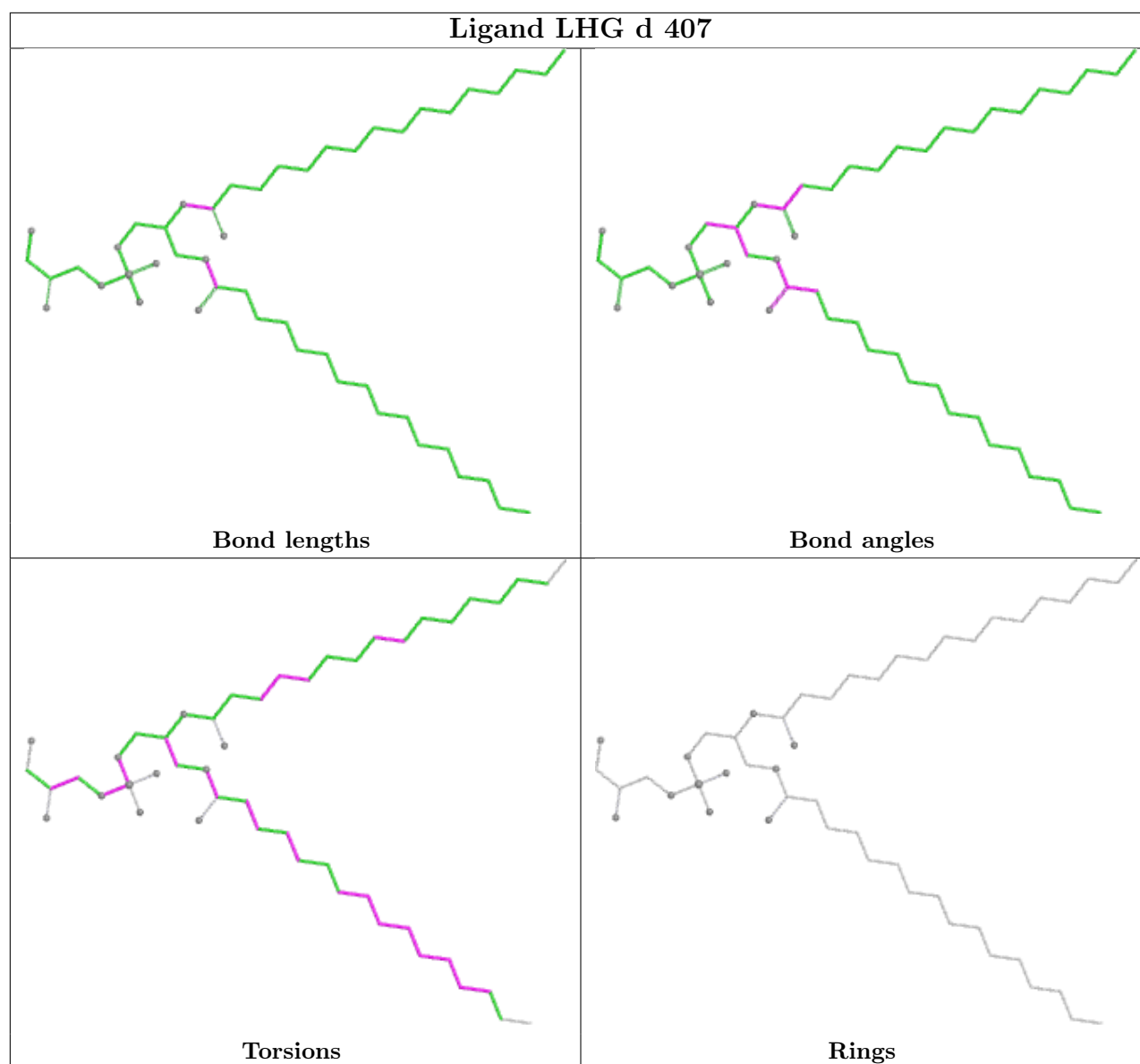


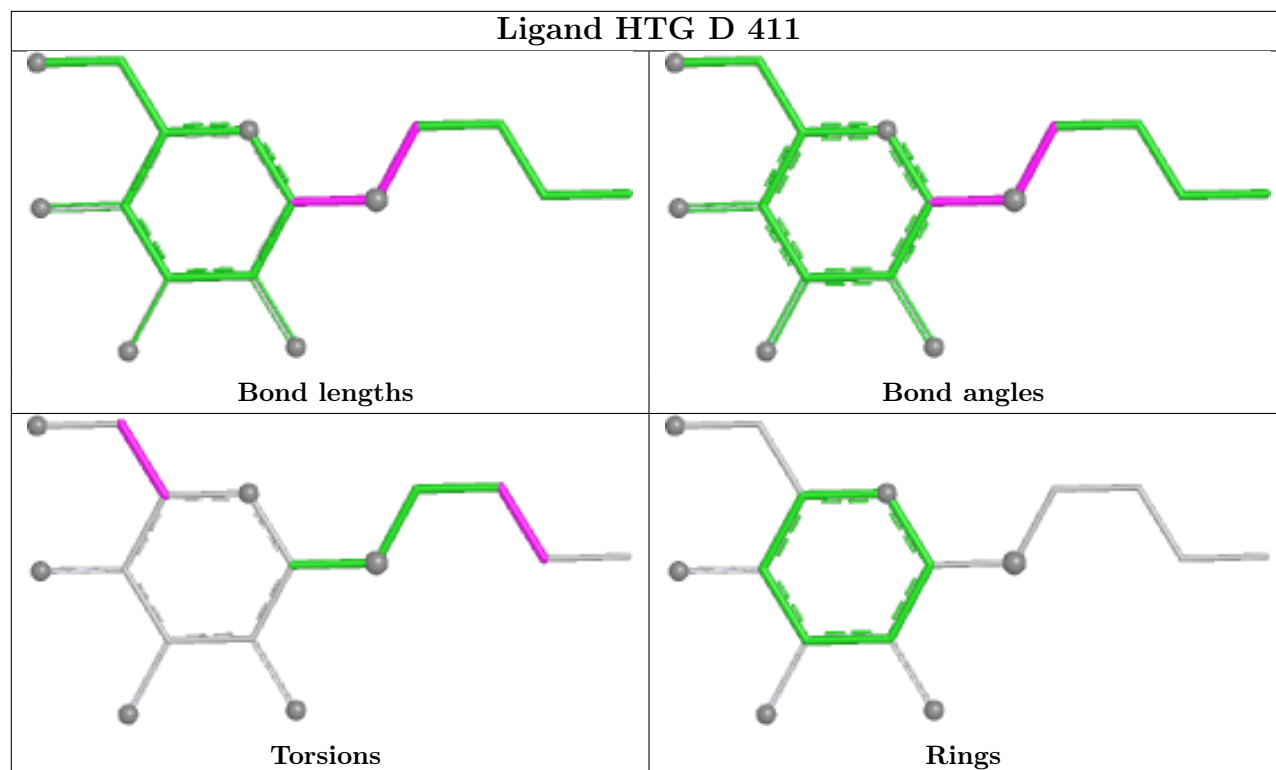
Rings

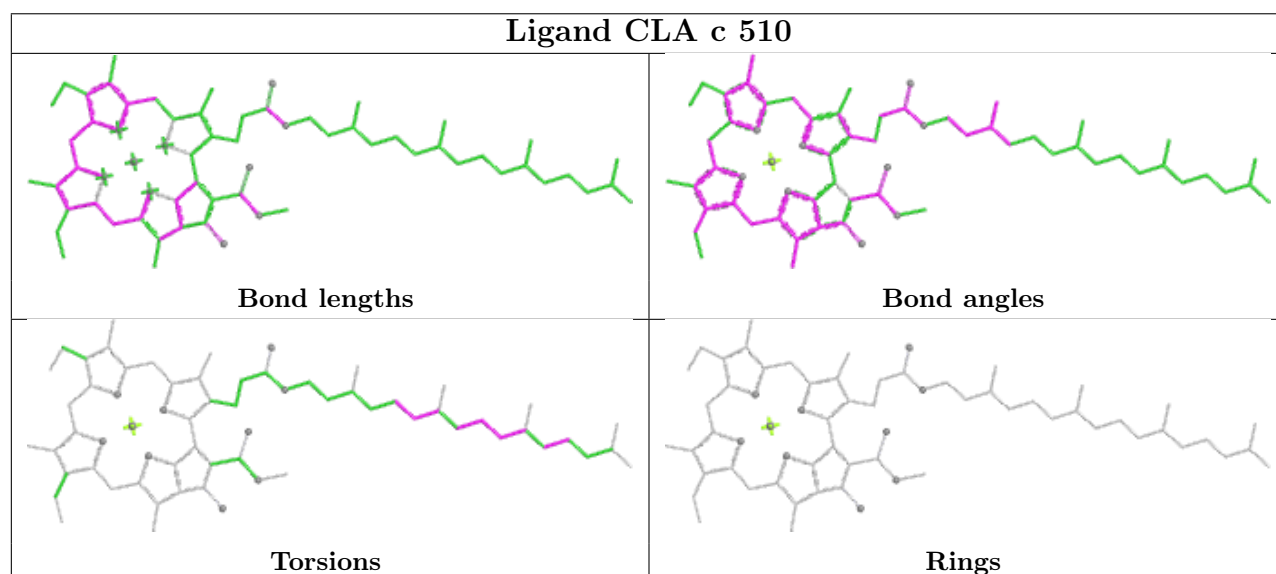
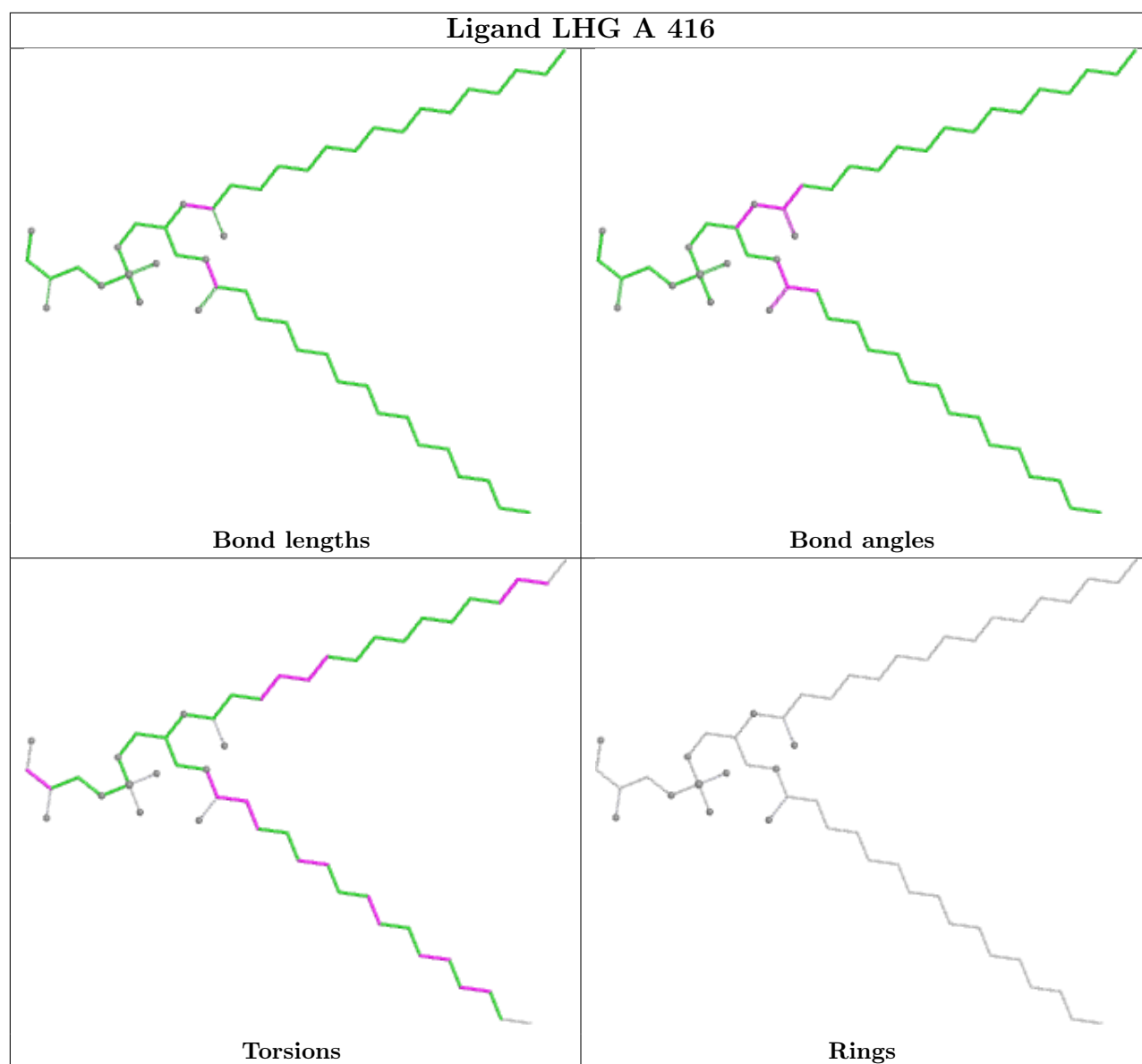
Ligand LHG E 101**Ligand PHO A 406**

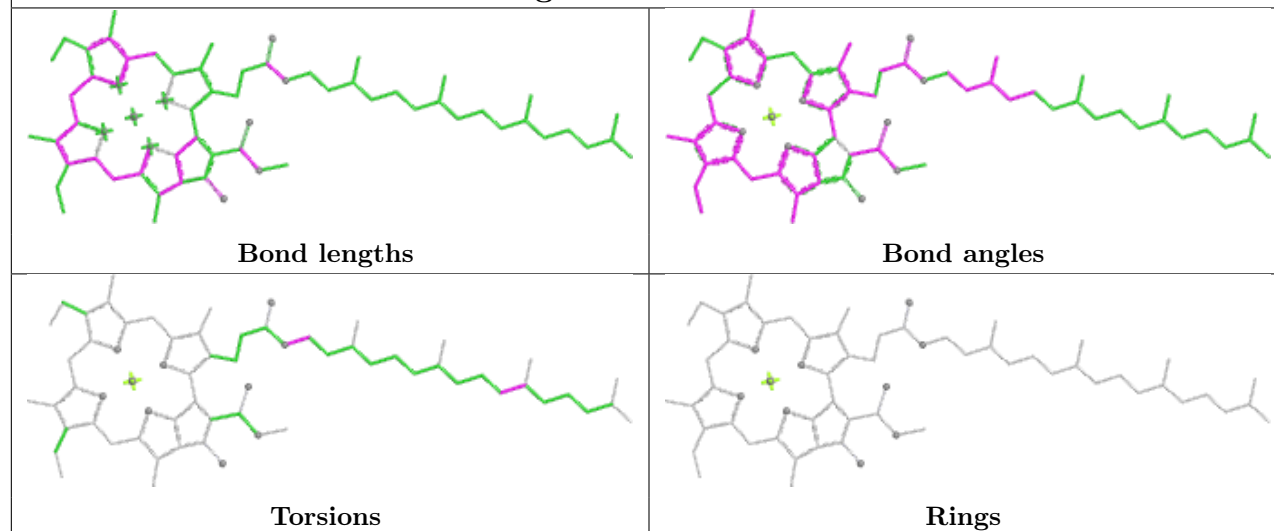
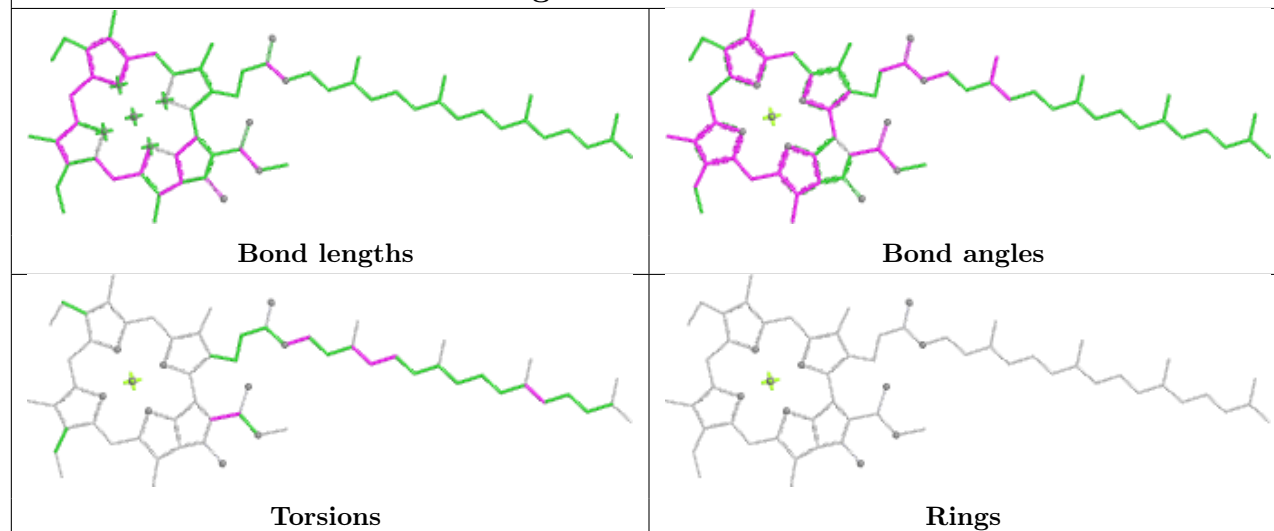
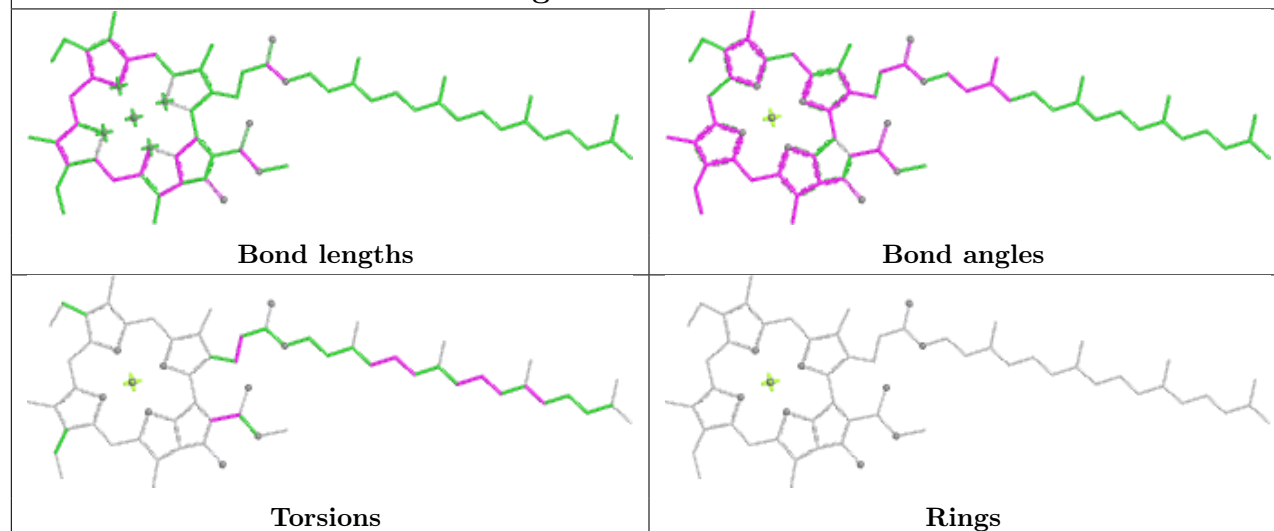


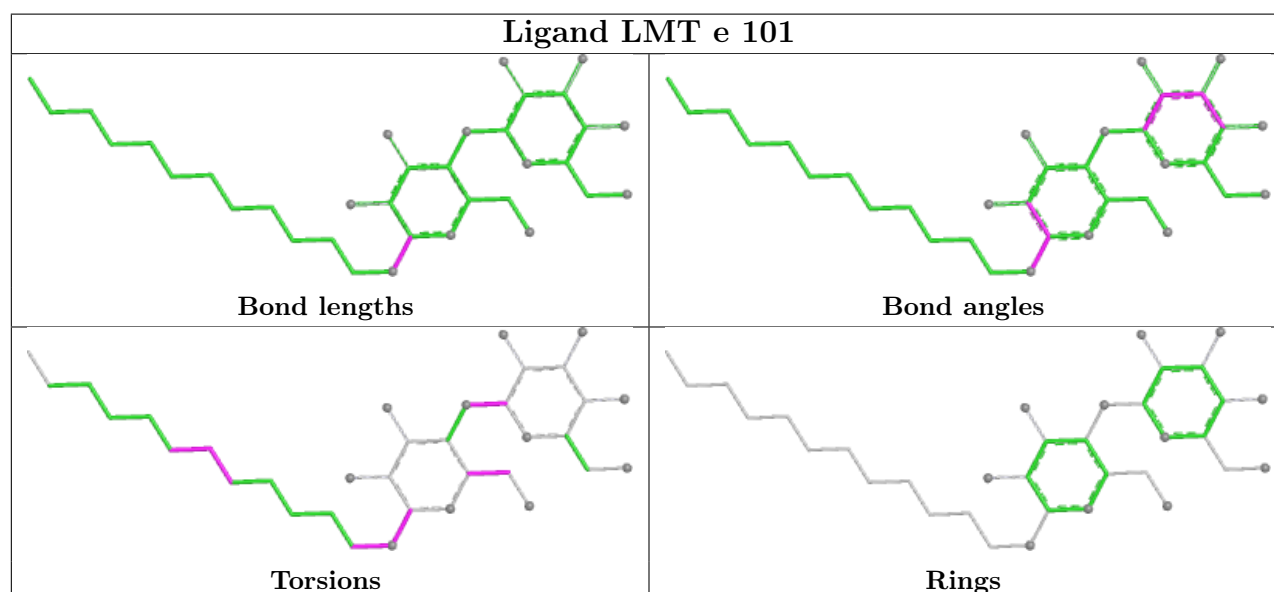
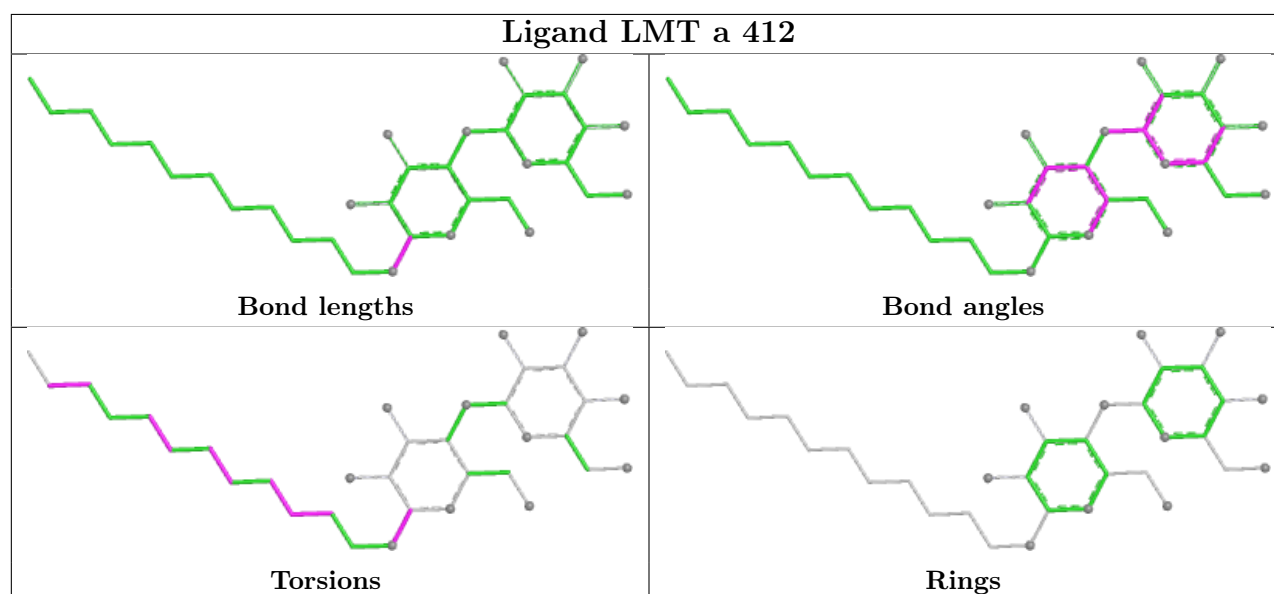
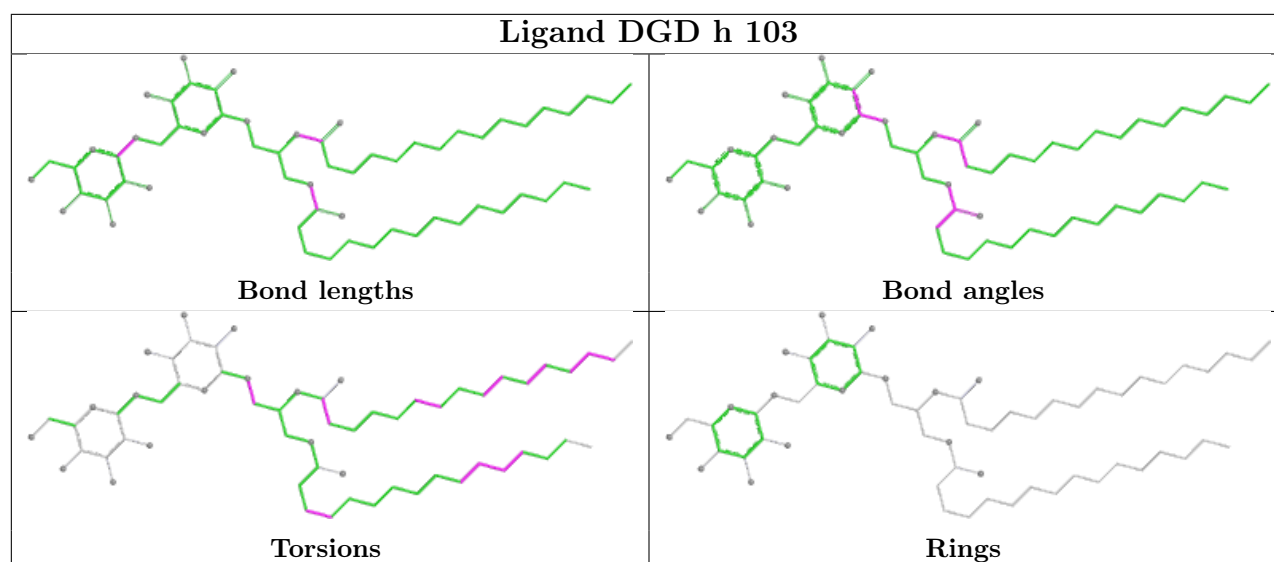


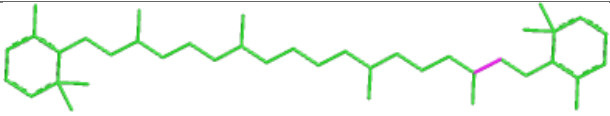
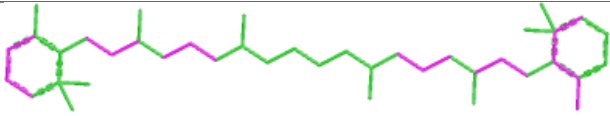
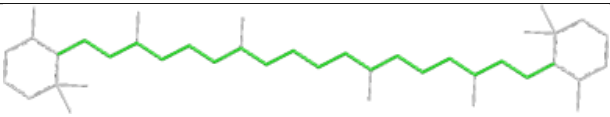
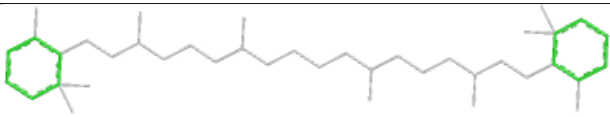
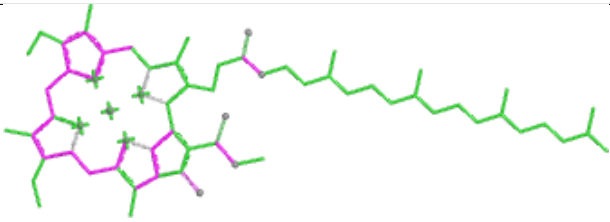
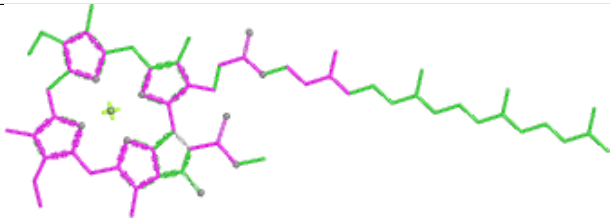
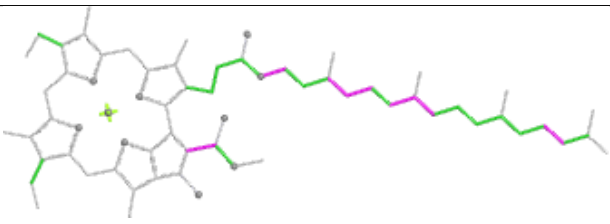
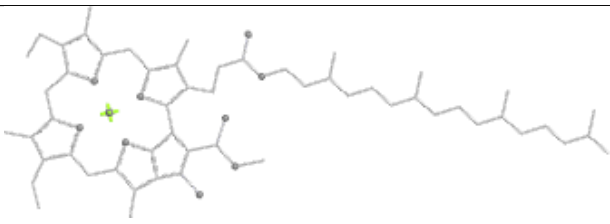
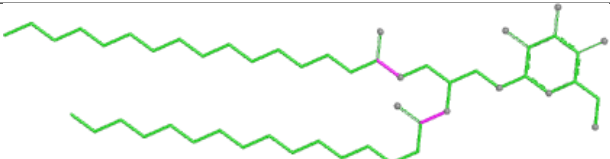
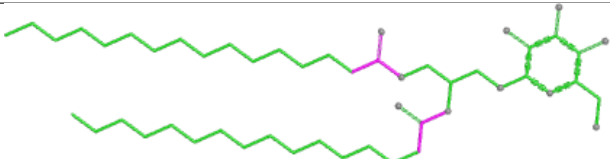
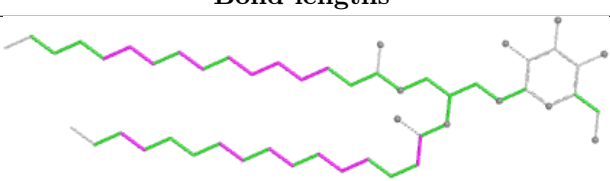
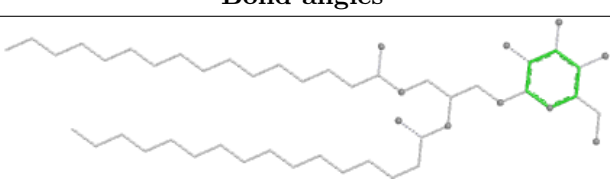


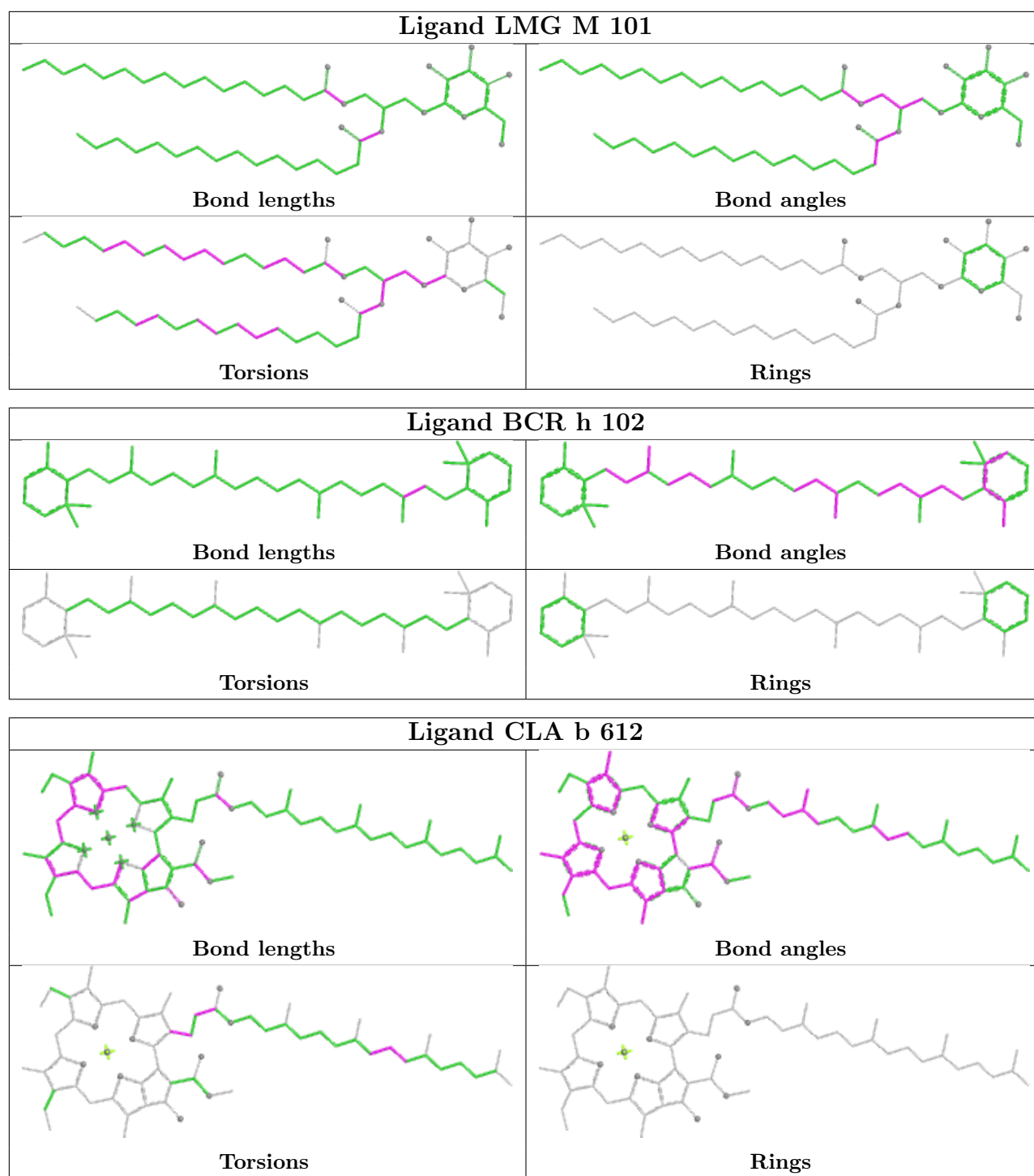


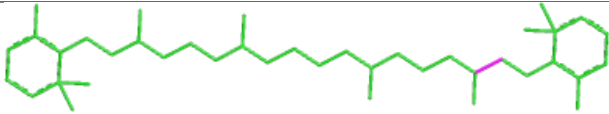
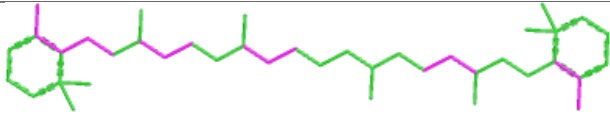
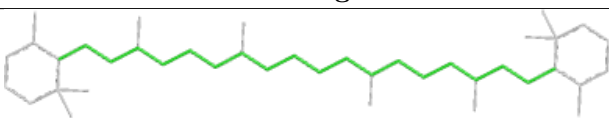
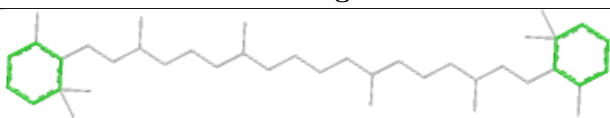


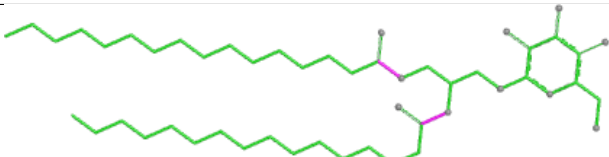
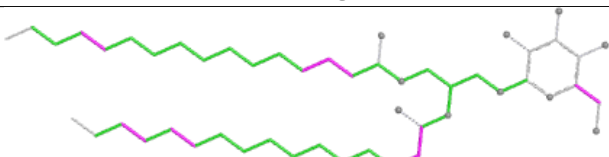
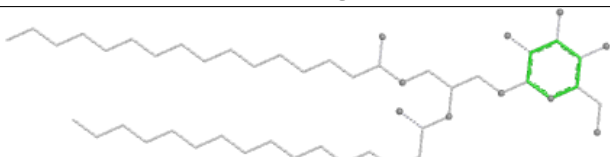
Ligand CLA d 402**Ligand CLA B 616****Ligand CLA B 614**

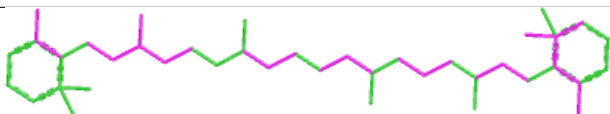
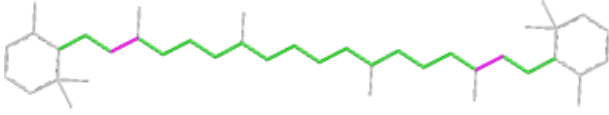
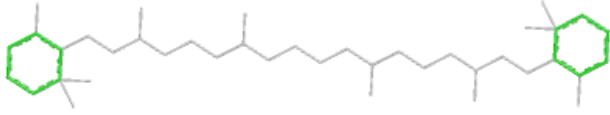


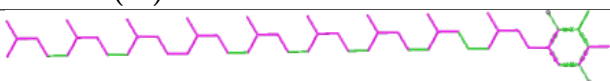
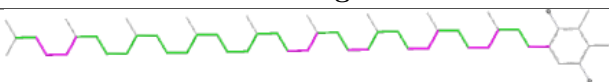
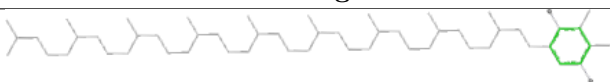
Ligand BCR B 619	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA c 508	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG C 521	
 Bond lengths	 Bond angles
 Torsions	 Rings

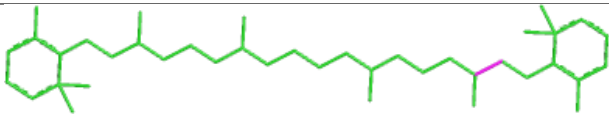
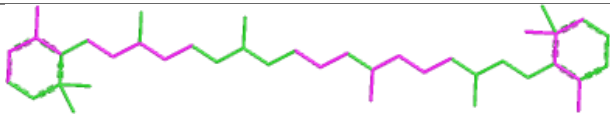
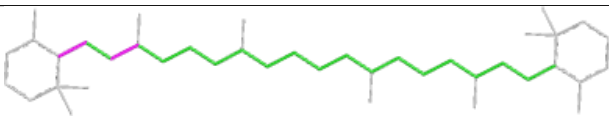
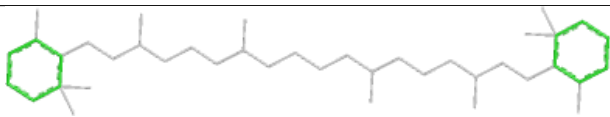


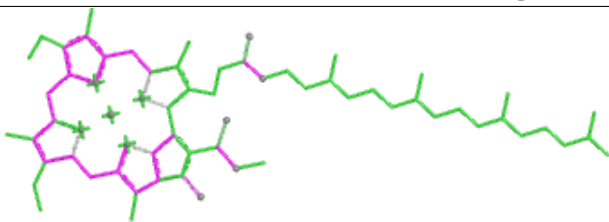
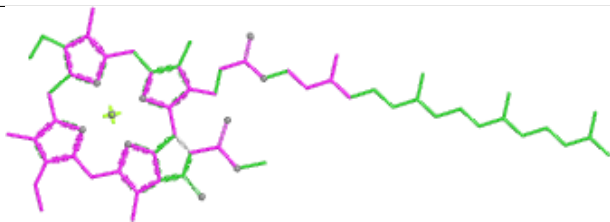
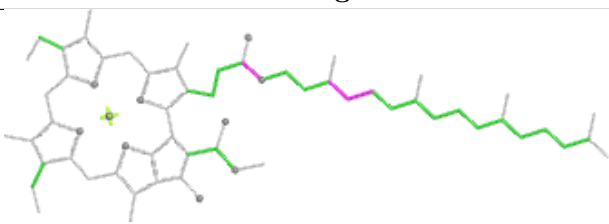
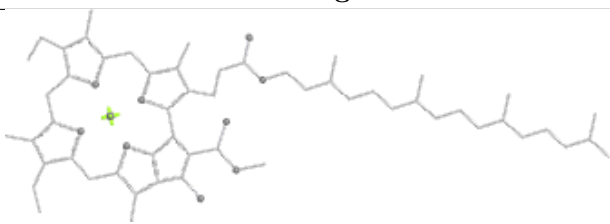
Ligand BCR c 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

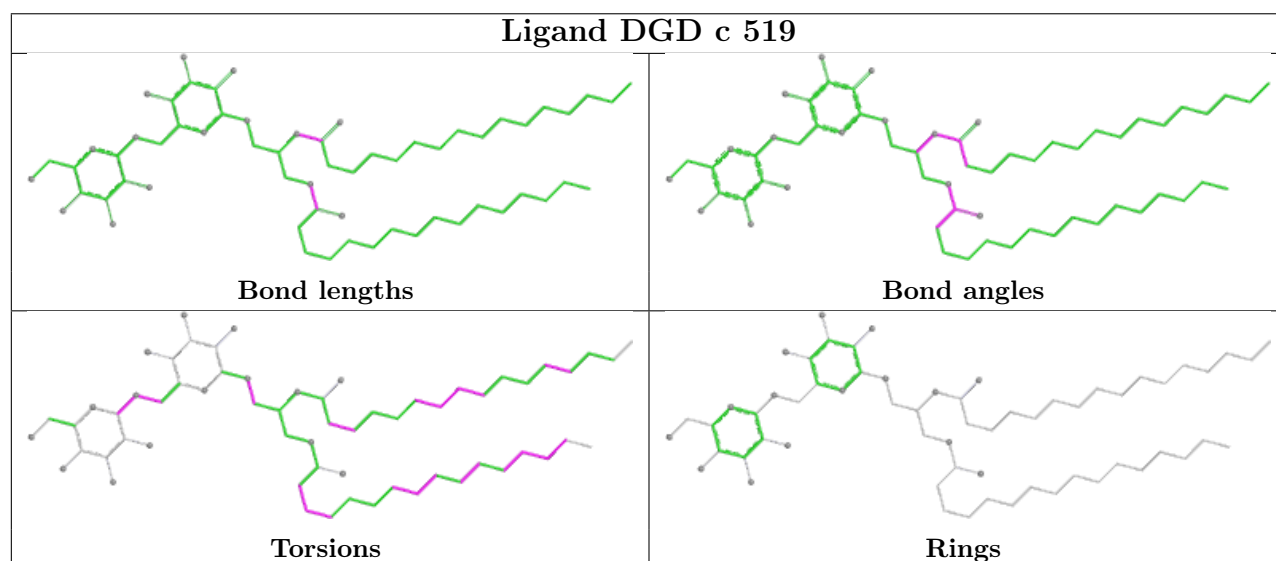
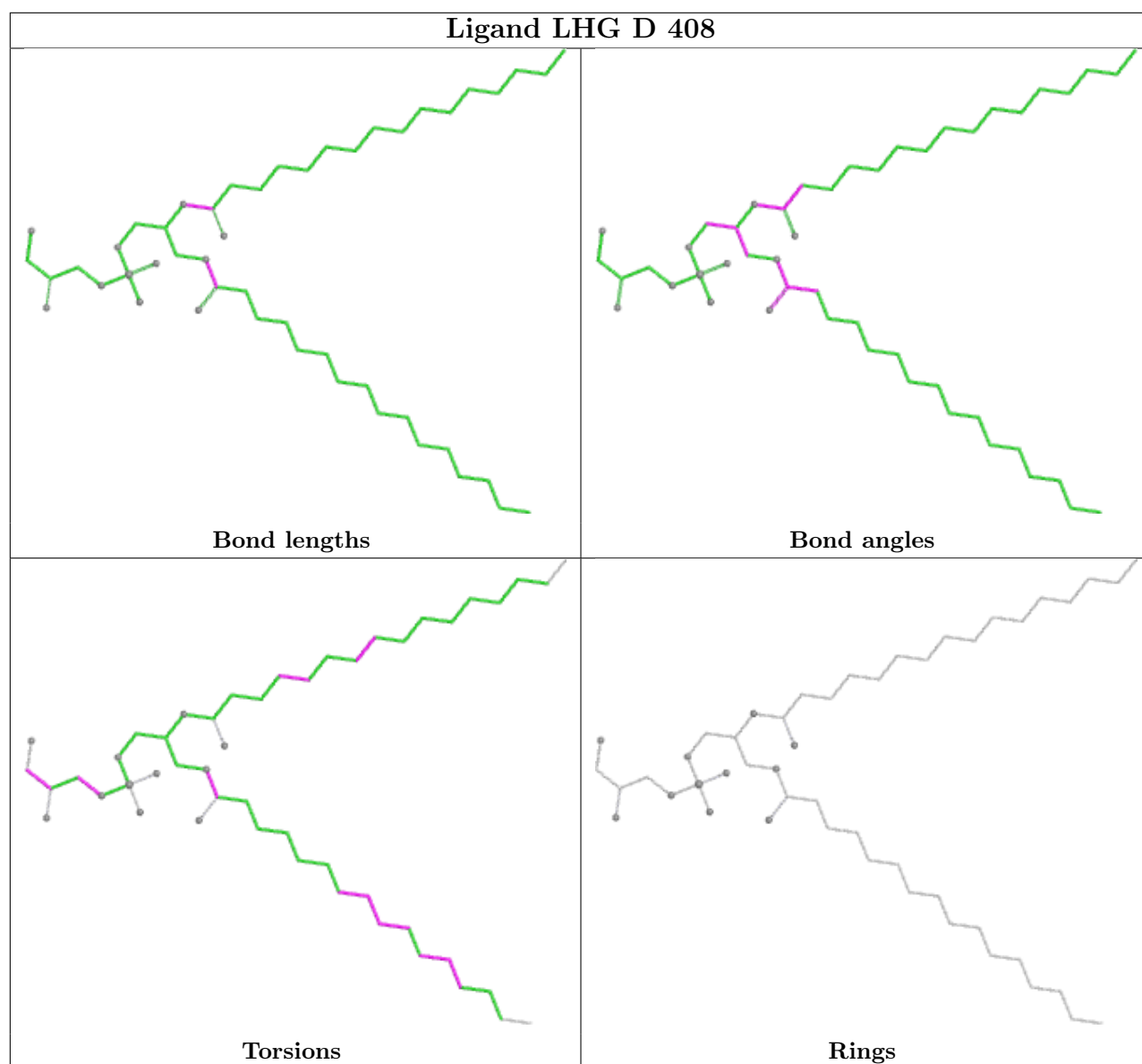
Ligand LMG d 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

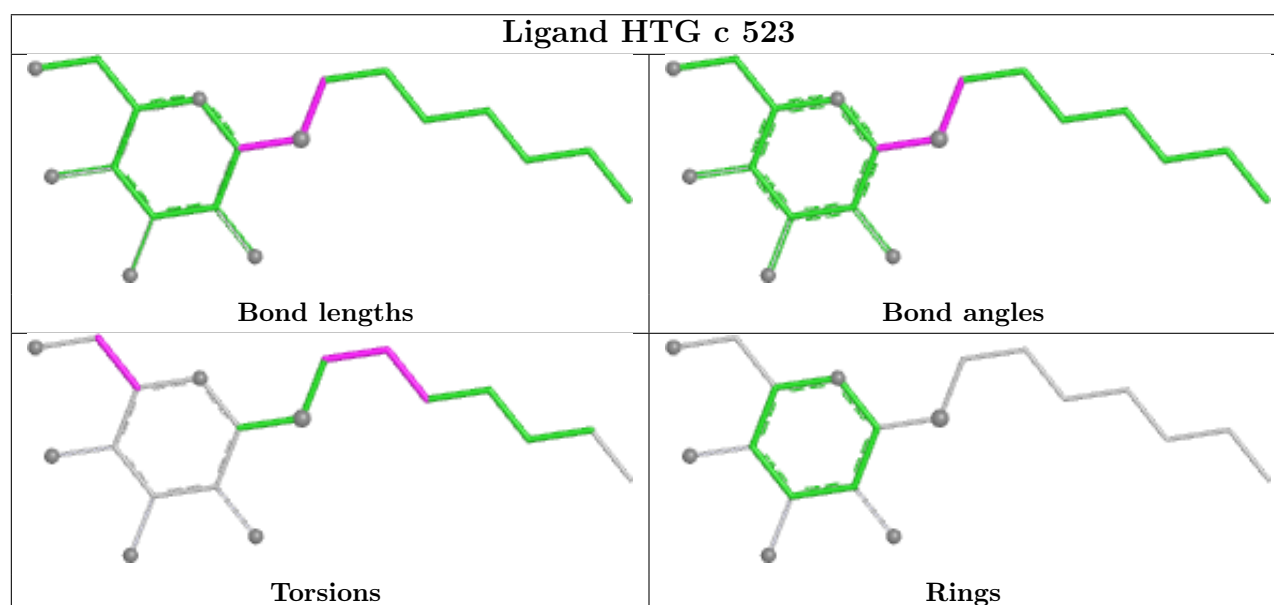
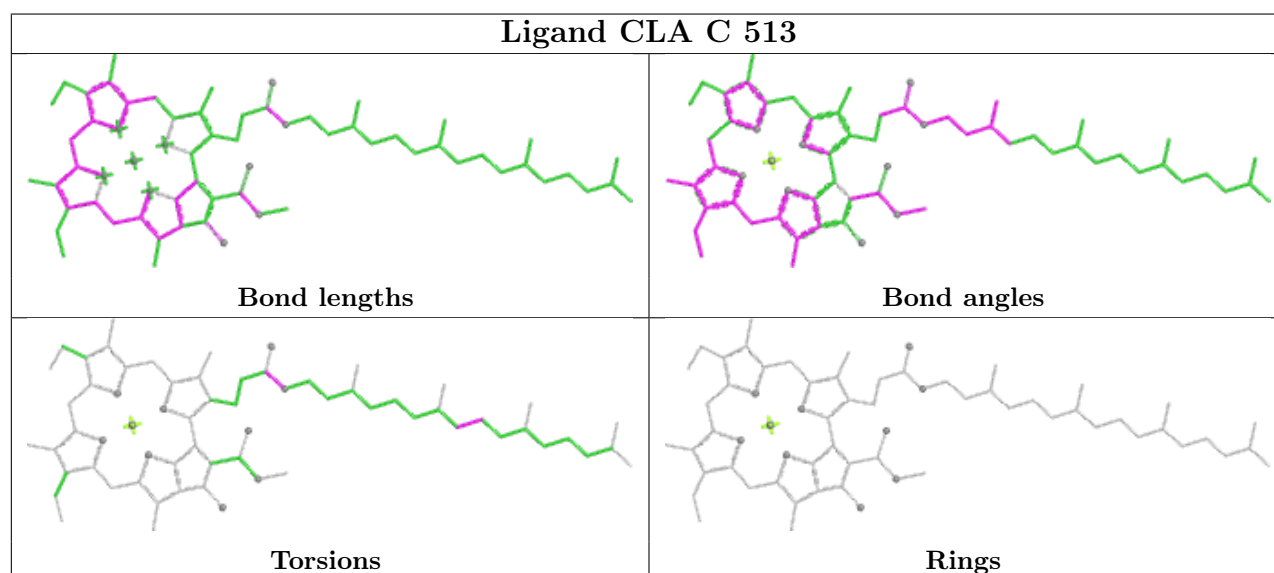
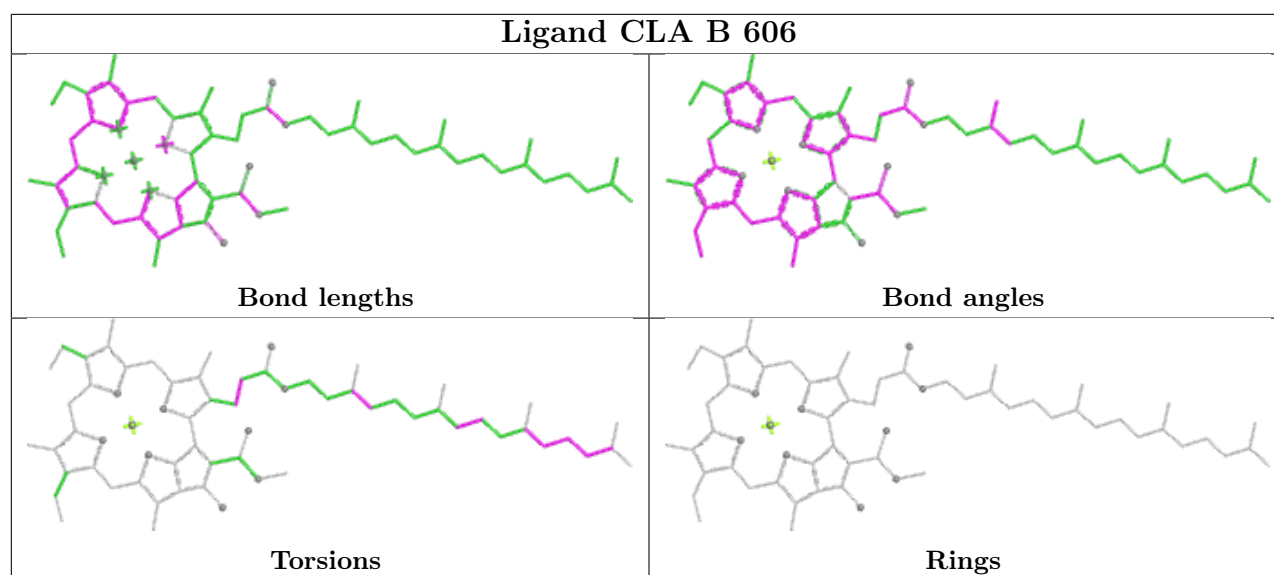
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Bond lengths	Bond angles
	
Torsions	Rings

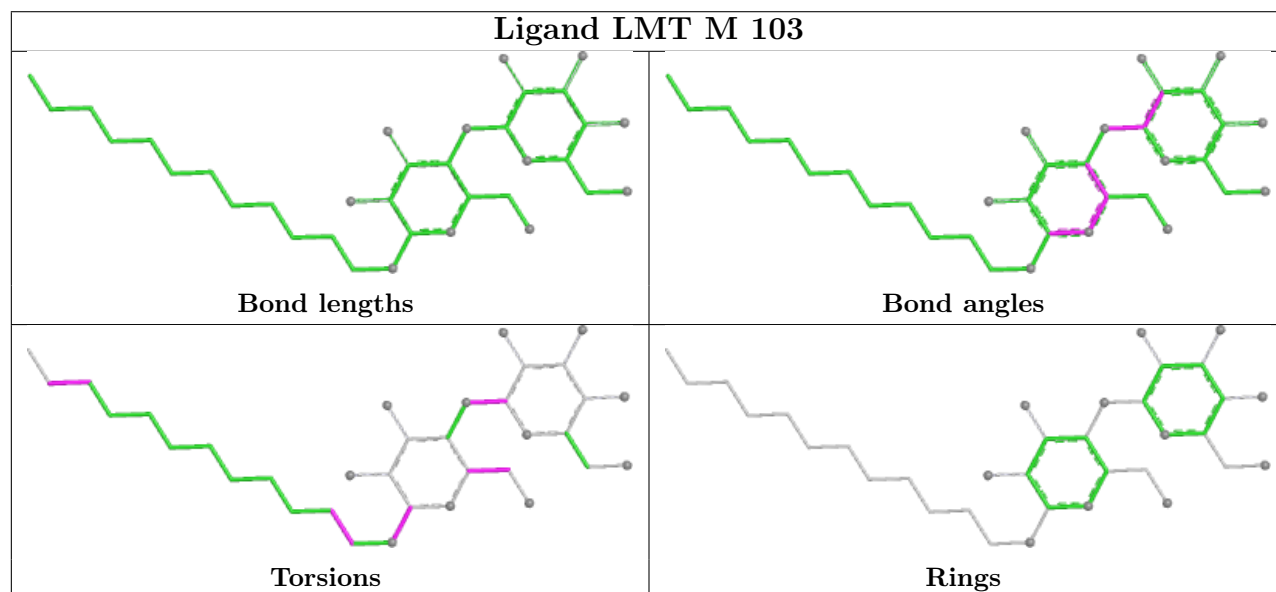
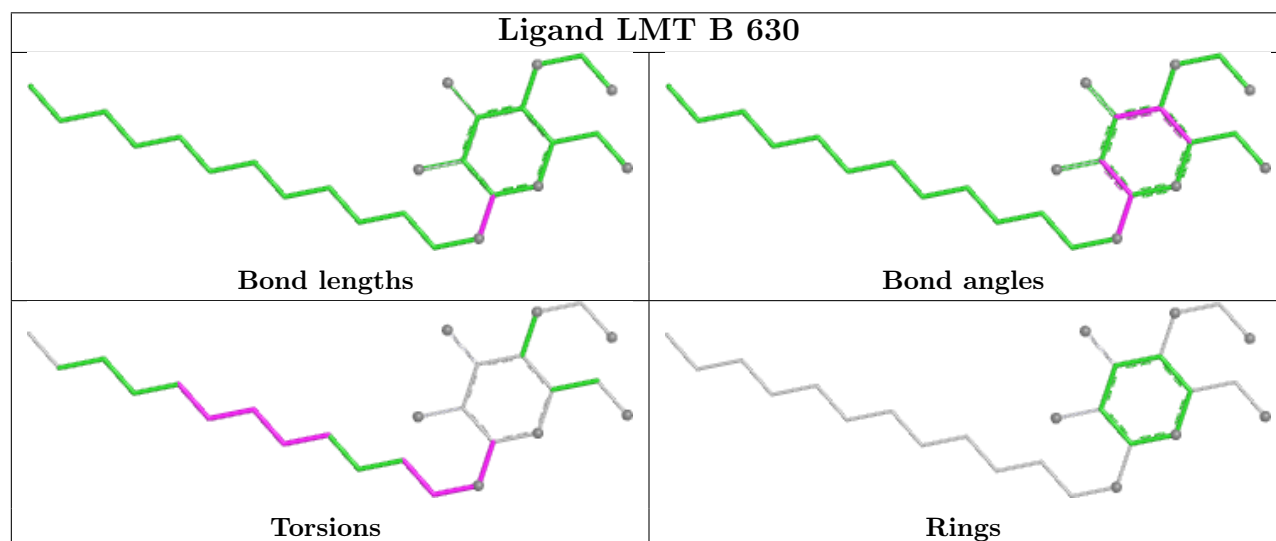
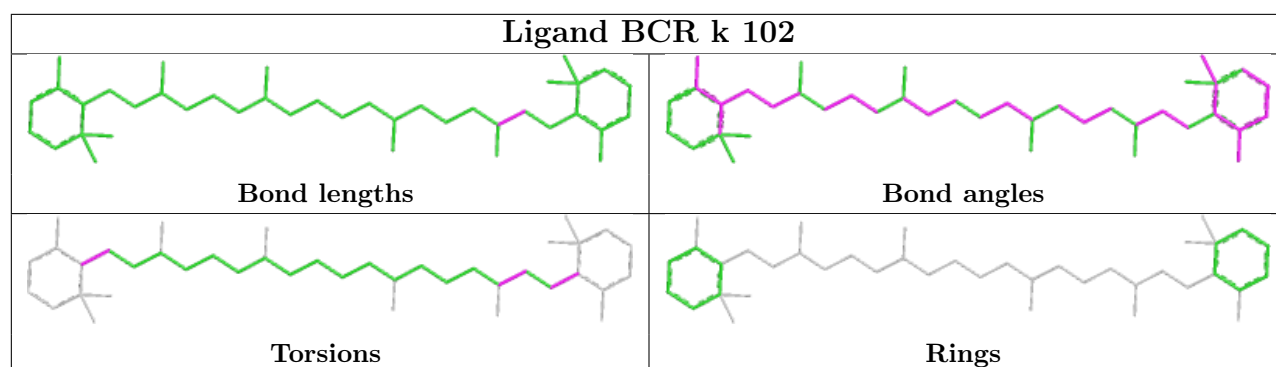
Ligand PL9 A 413 (A)	
	
Bond lengths	Bond angles
	
Torsions	Rings

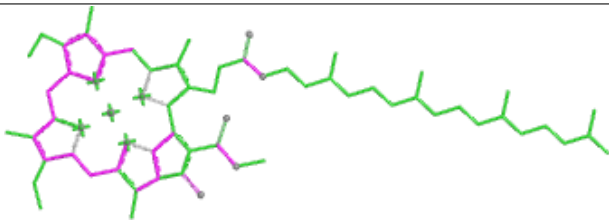
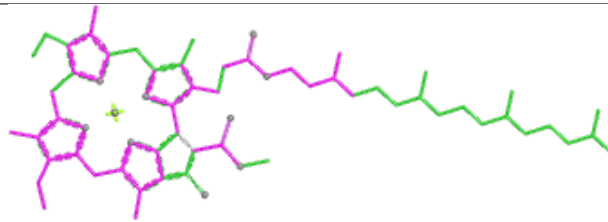
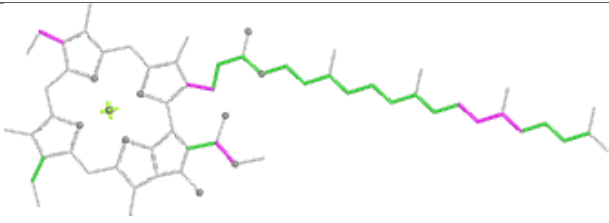
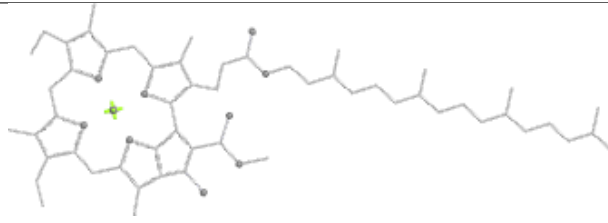
Ligand BCR C 517	
	
Bond lengths	Bond angles
	
Torsions	Rings

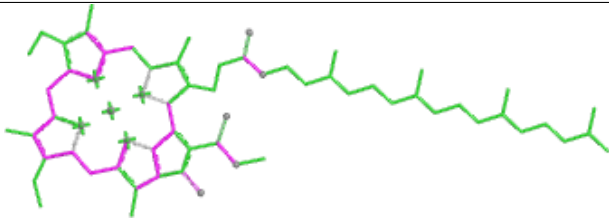
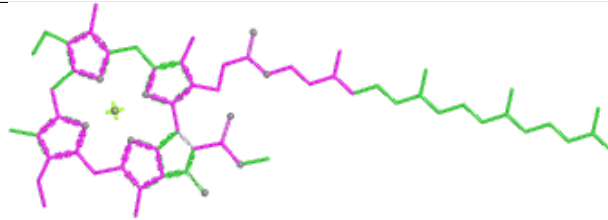
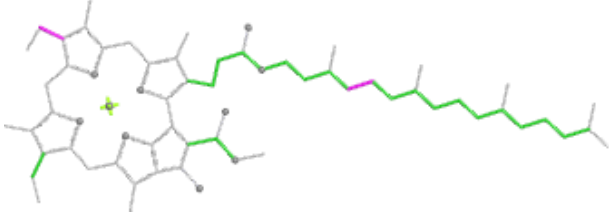
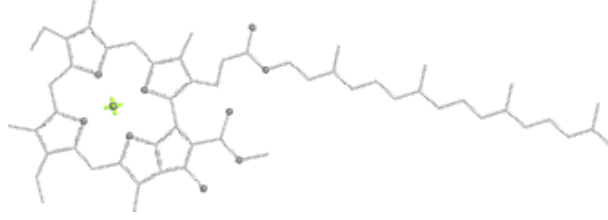
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Bond lengths	Bond angles
	
Torsions	Rings

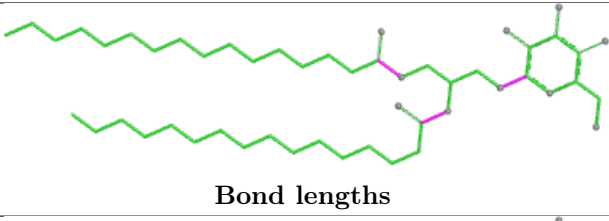
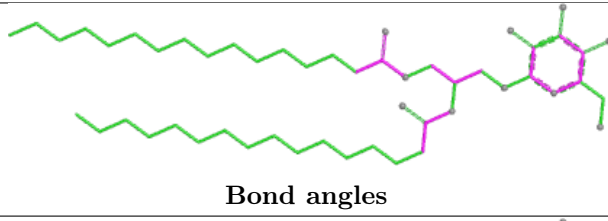
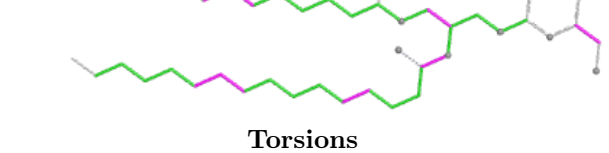


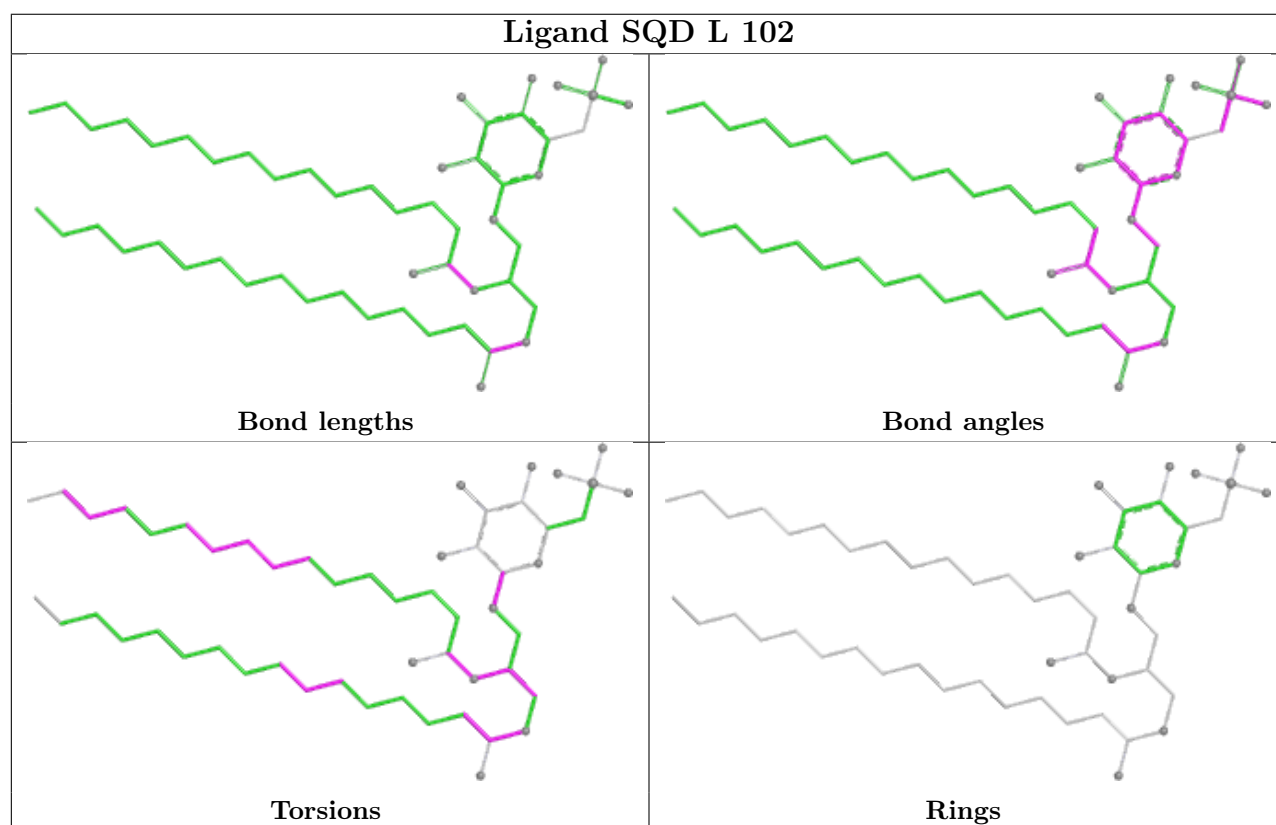
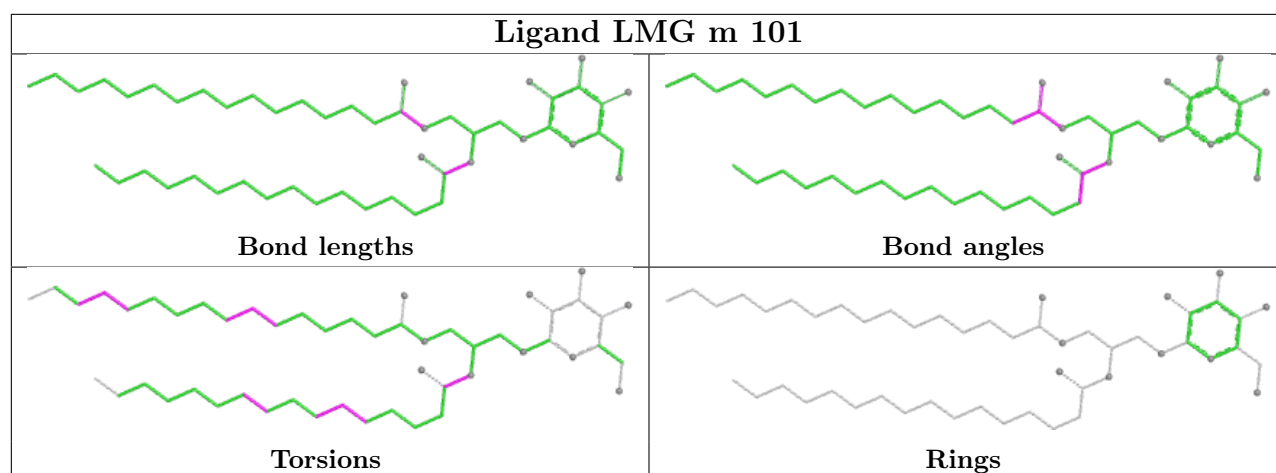




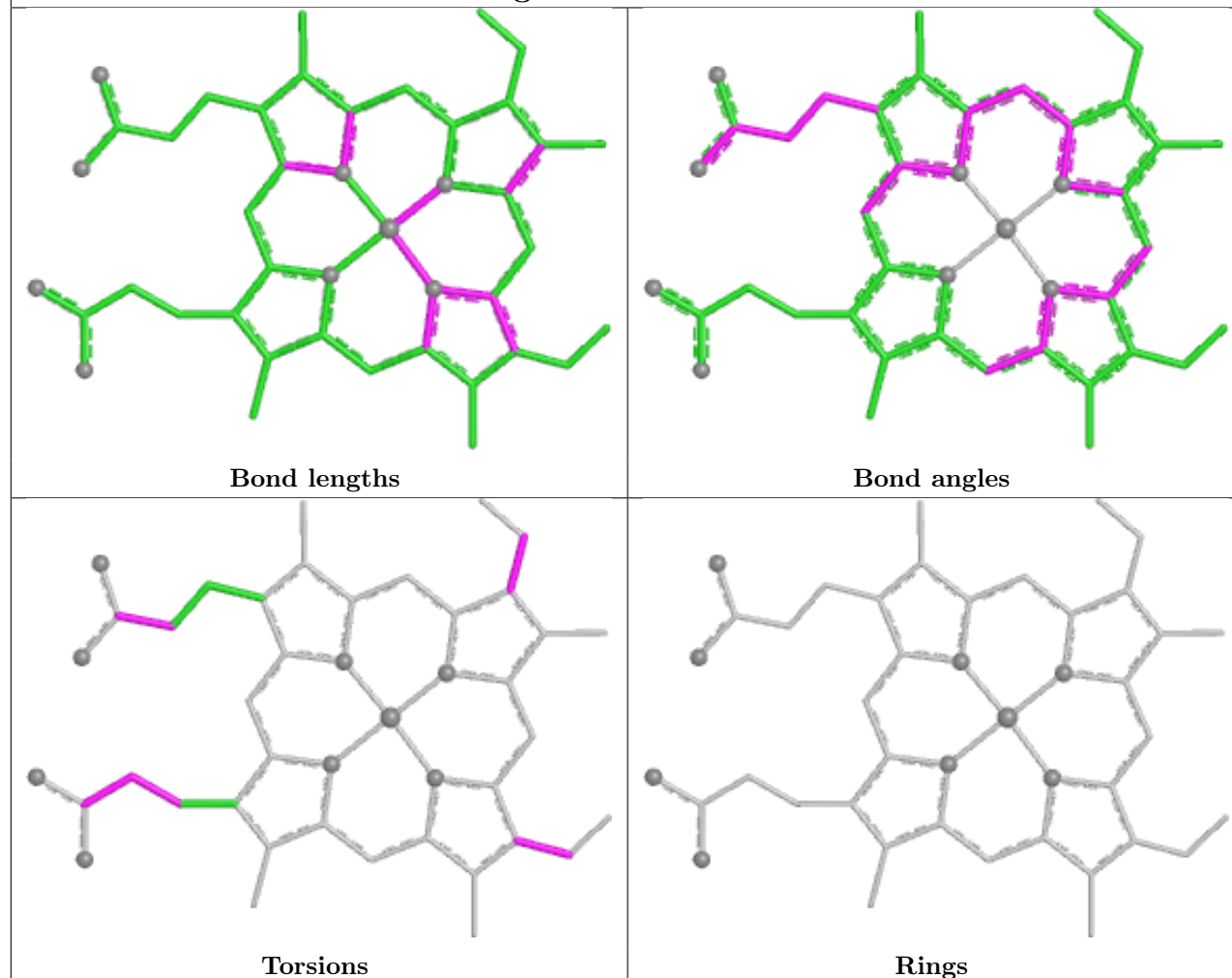
Ligand CLA a 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

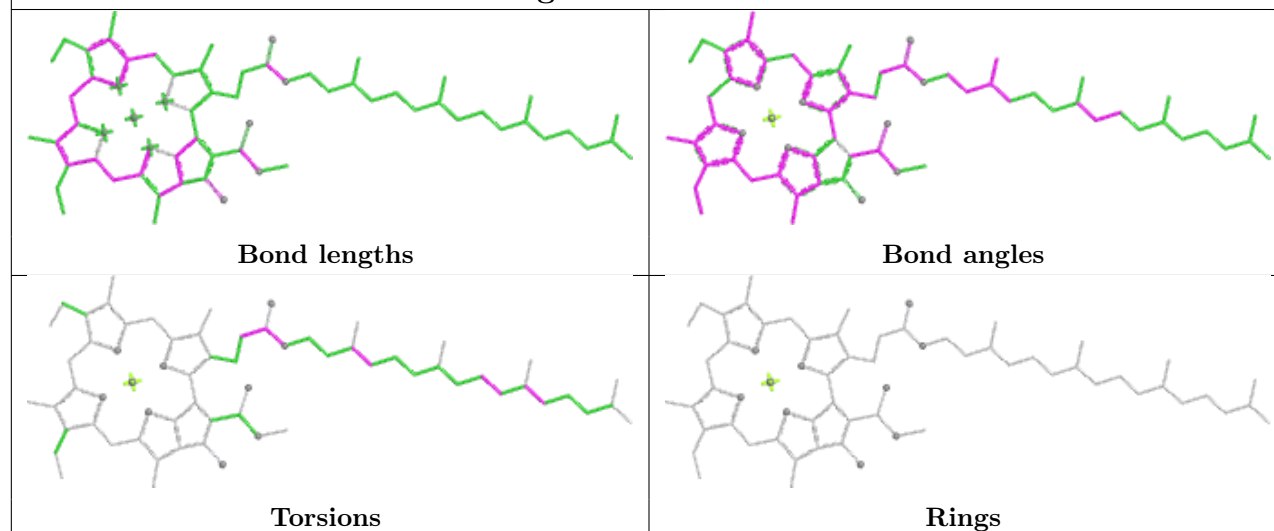
Ligand LMG C 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

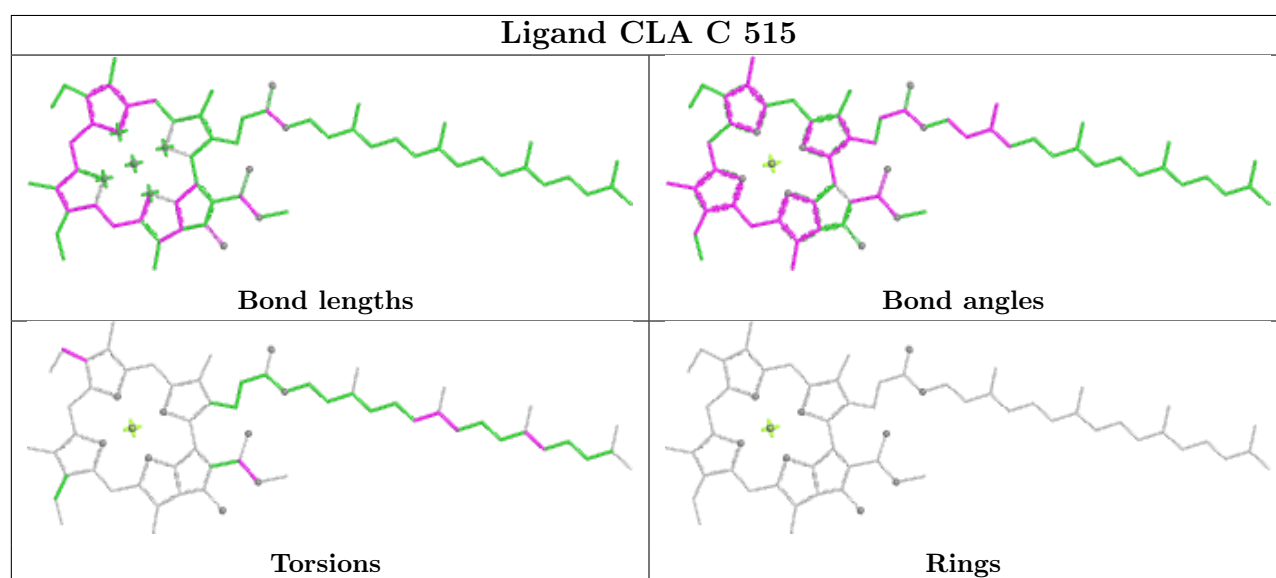
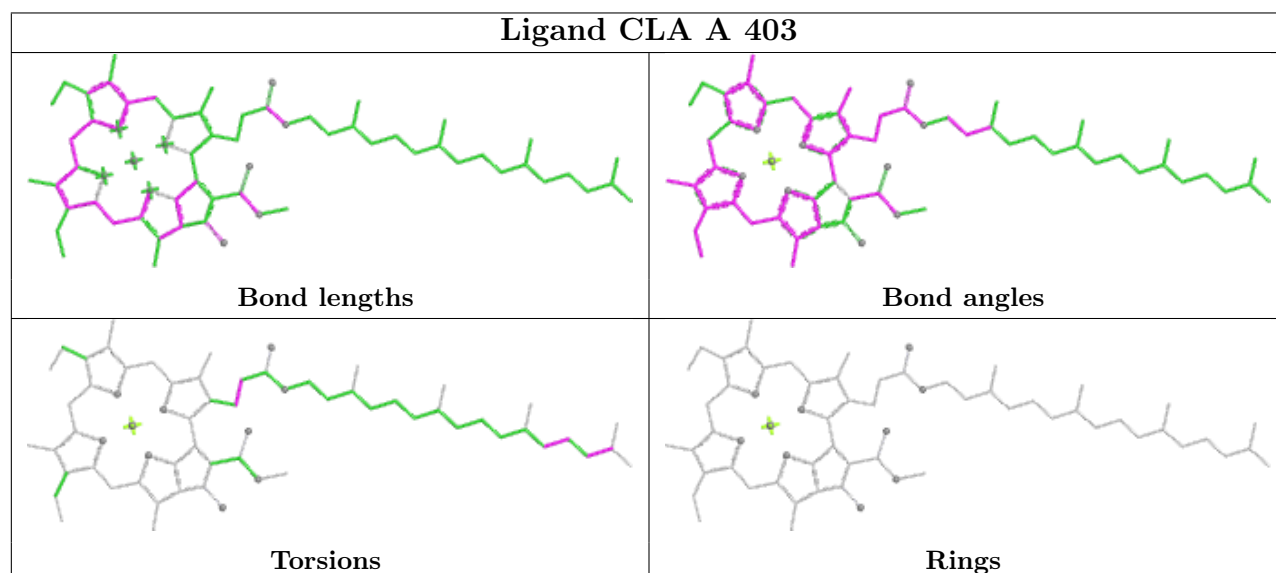
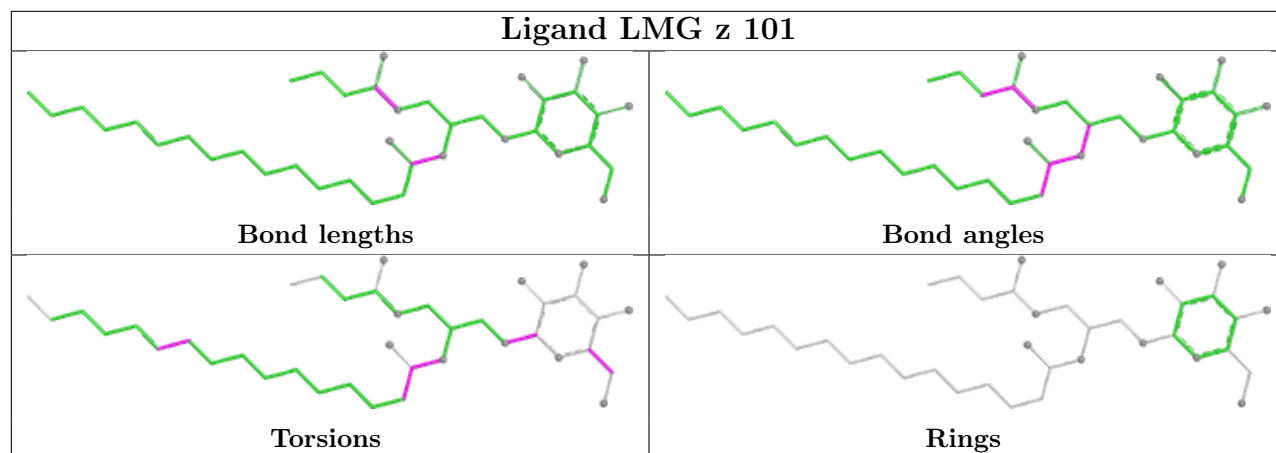


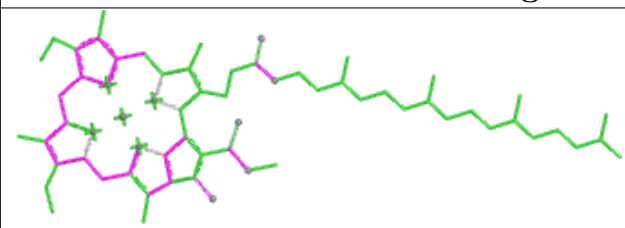
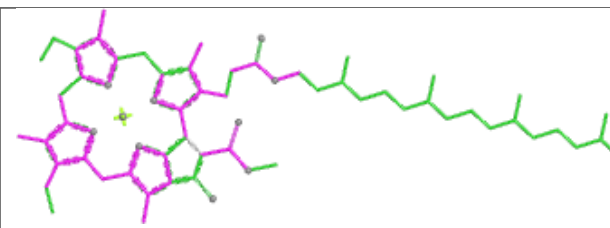
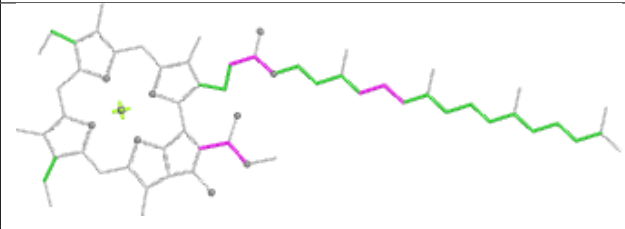
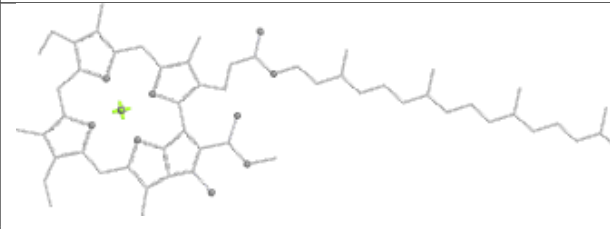
Ligand HEM e 102

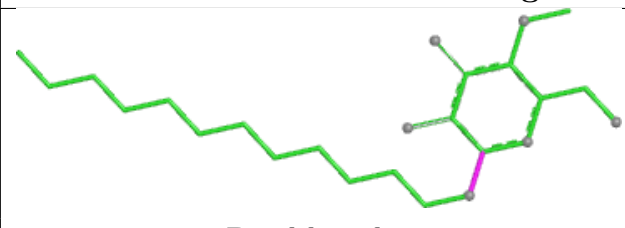
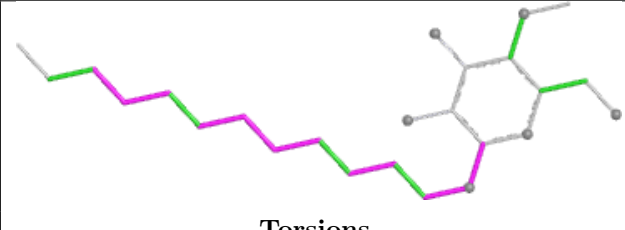
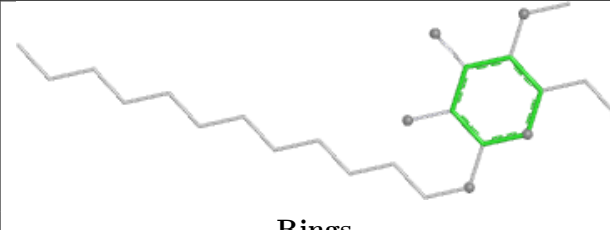


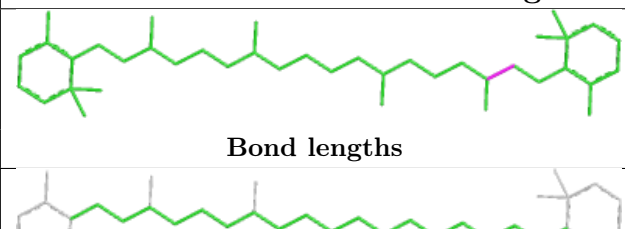
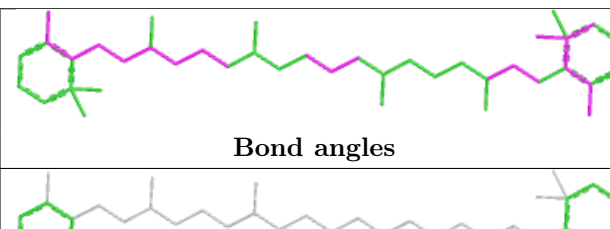
Ligand CLA c 512

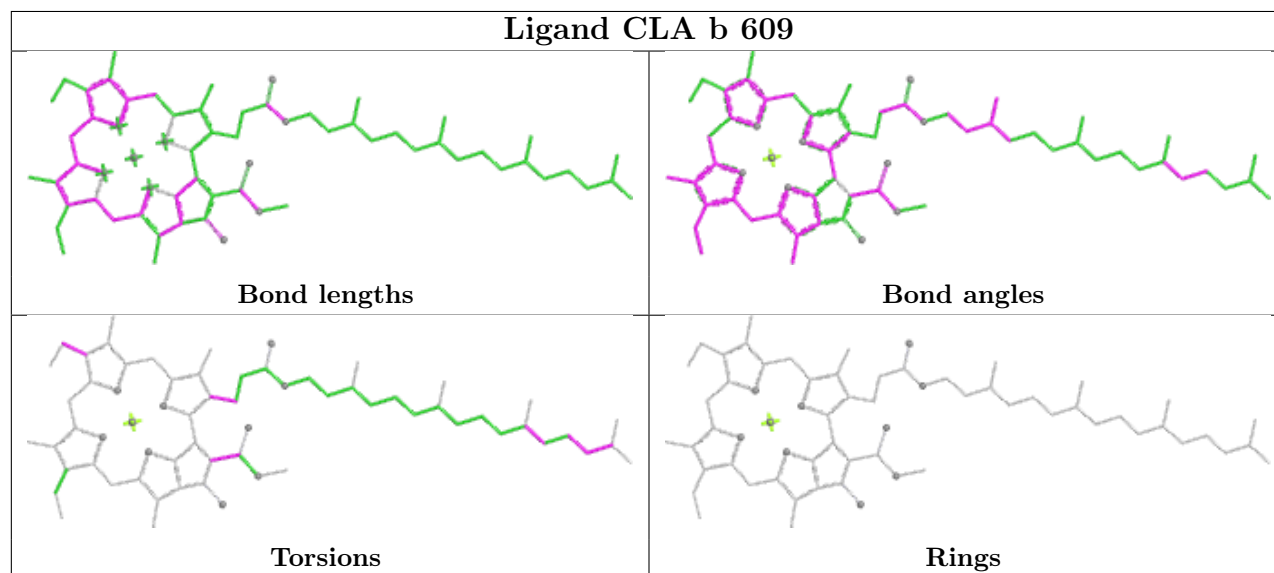
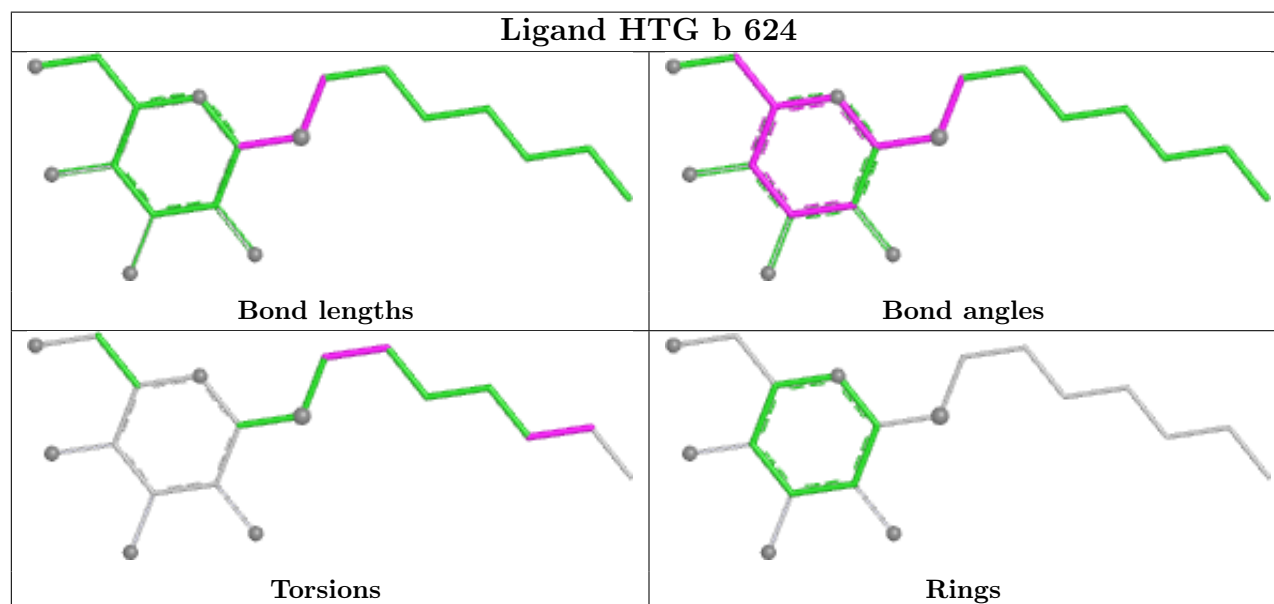
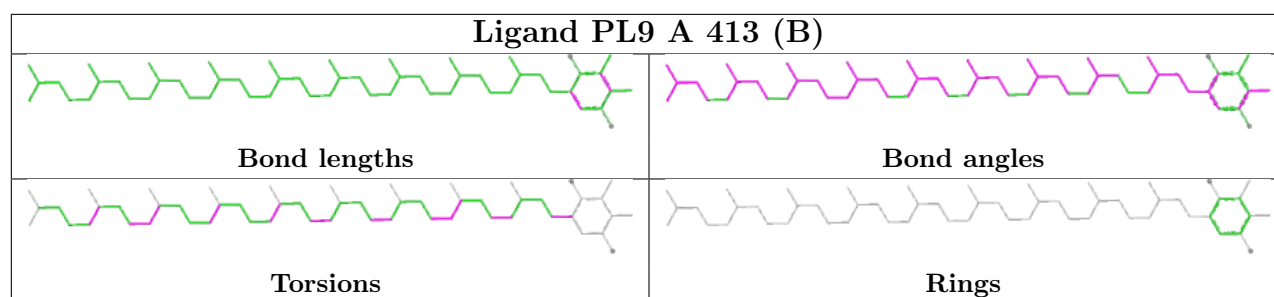


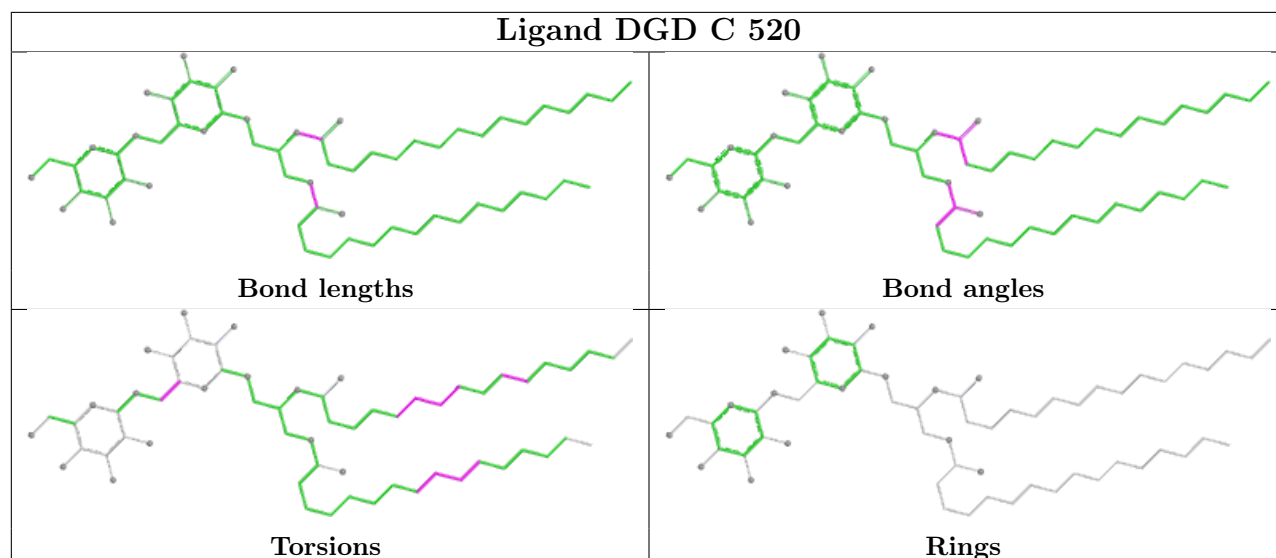
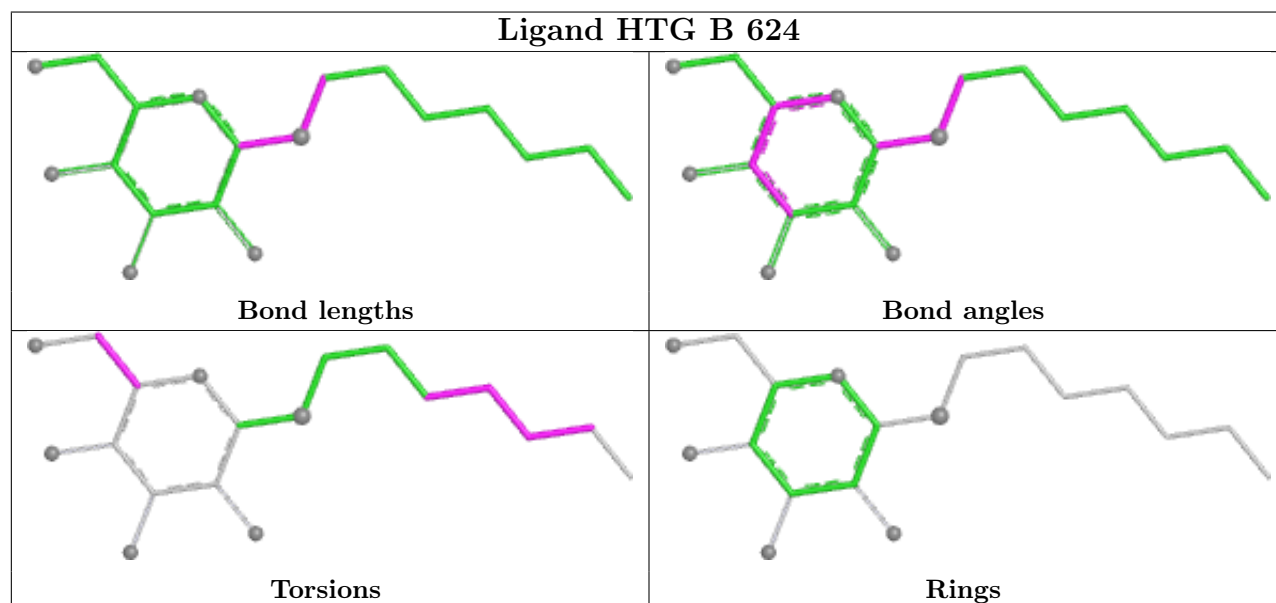
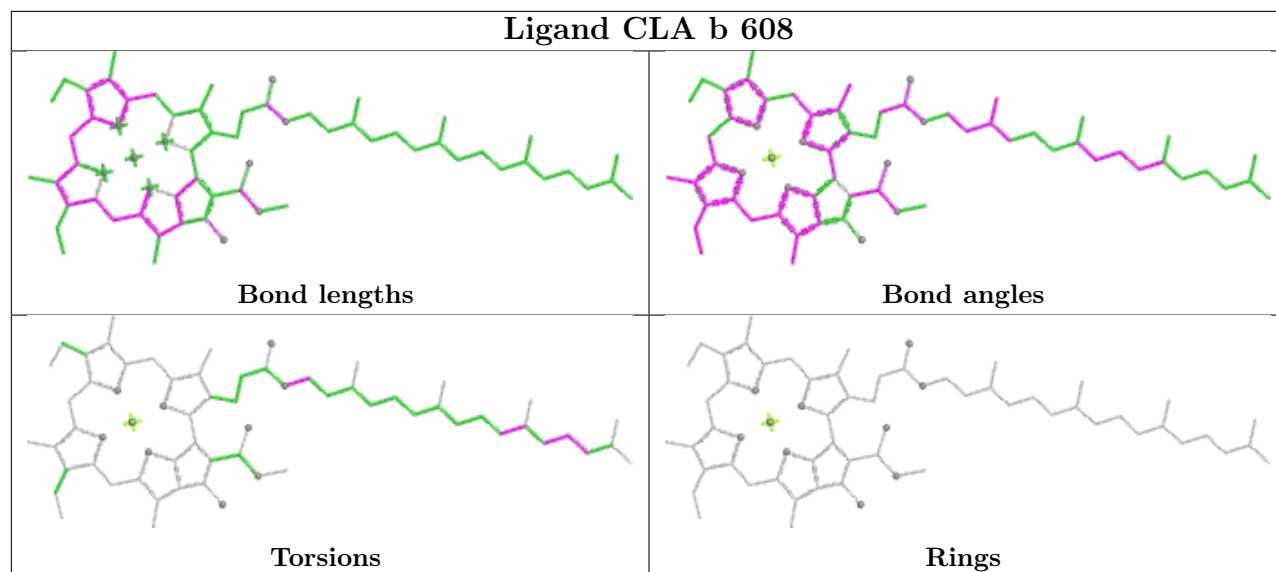


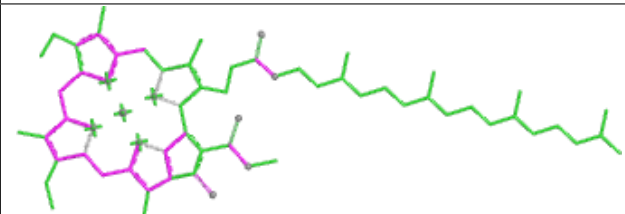
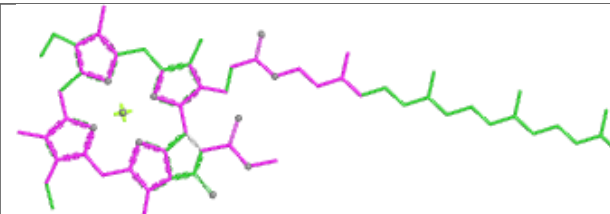
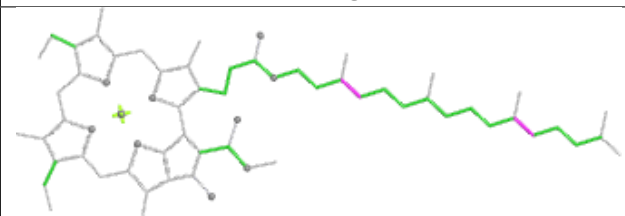
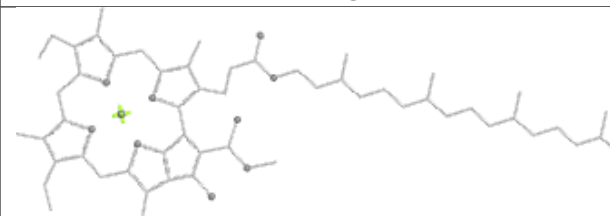
Ligand CLA B 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

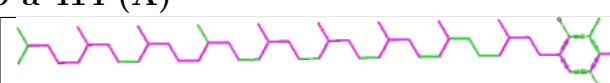
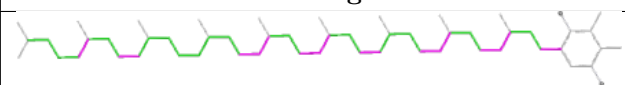
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Bond lengths	Bond angles
	
Torsions	Rings

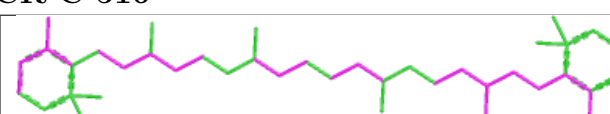
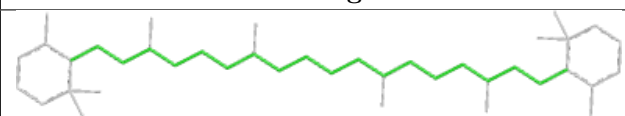
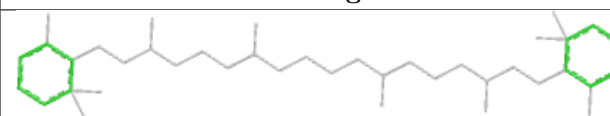
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Bond lengths	Bond angles
	
Torsions	Rings

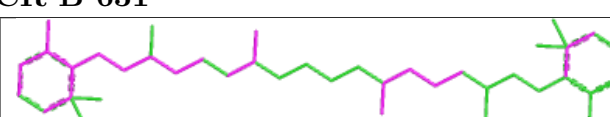
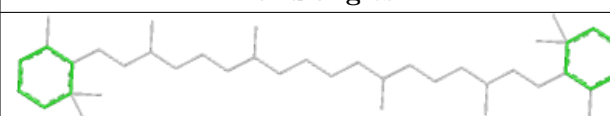


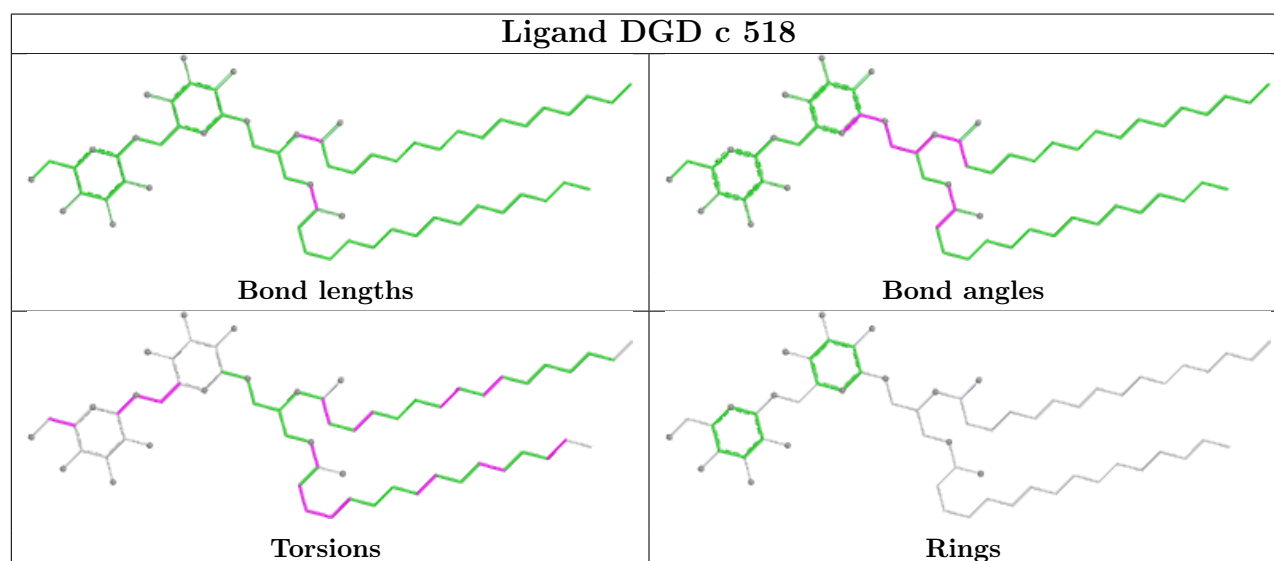
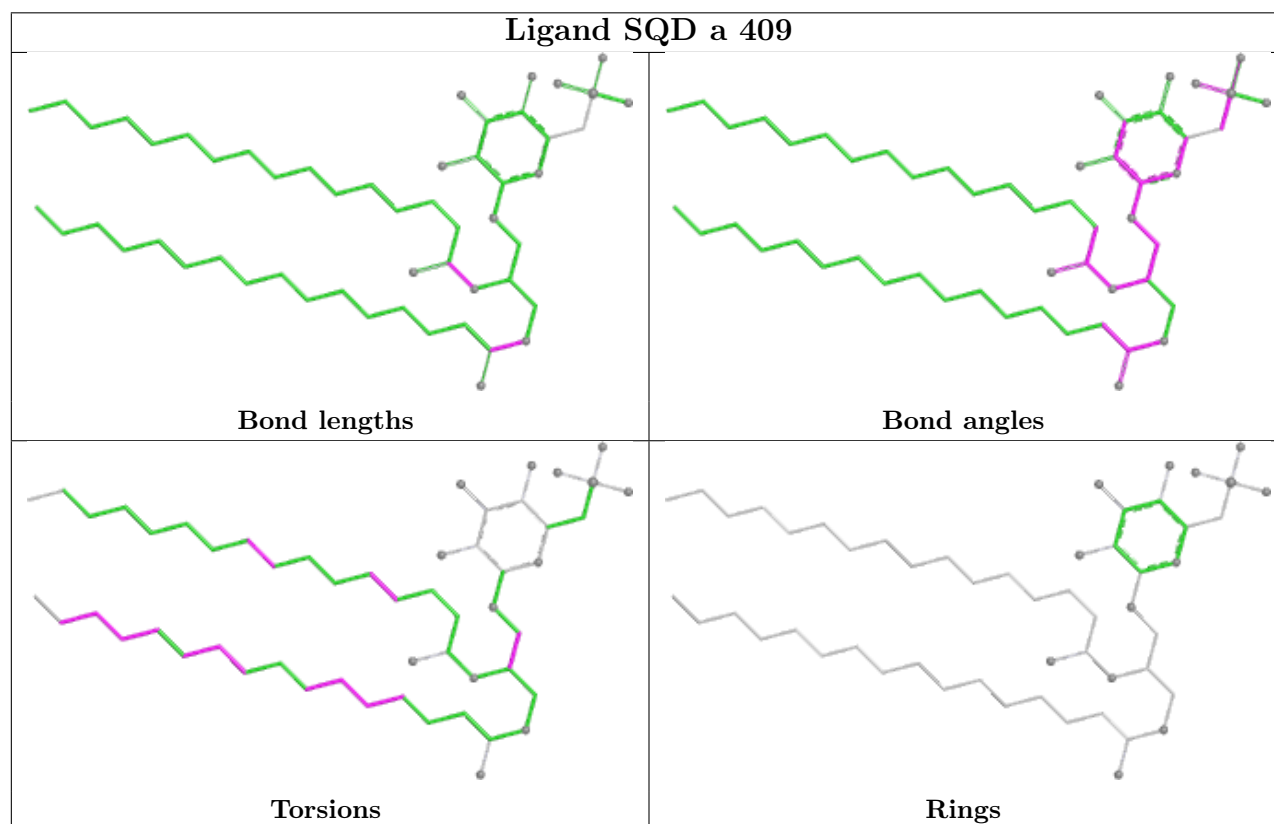
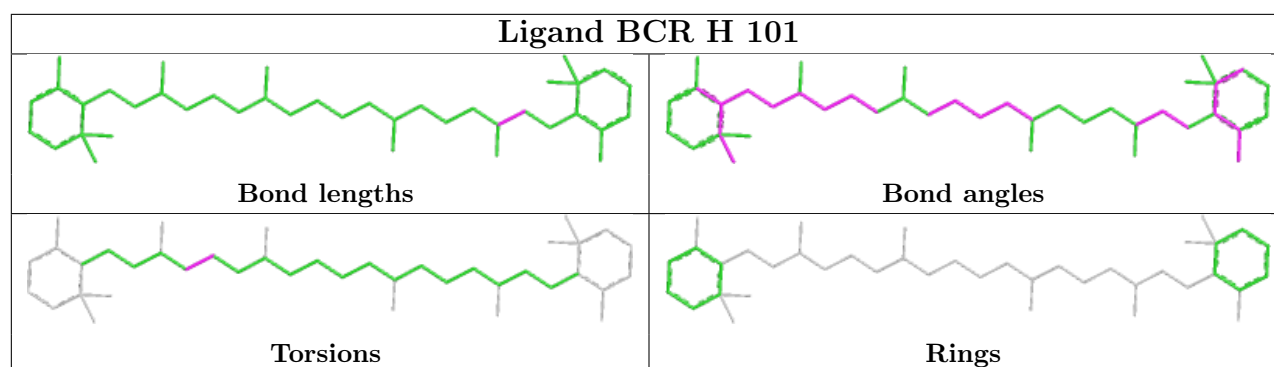


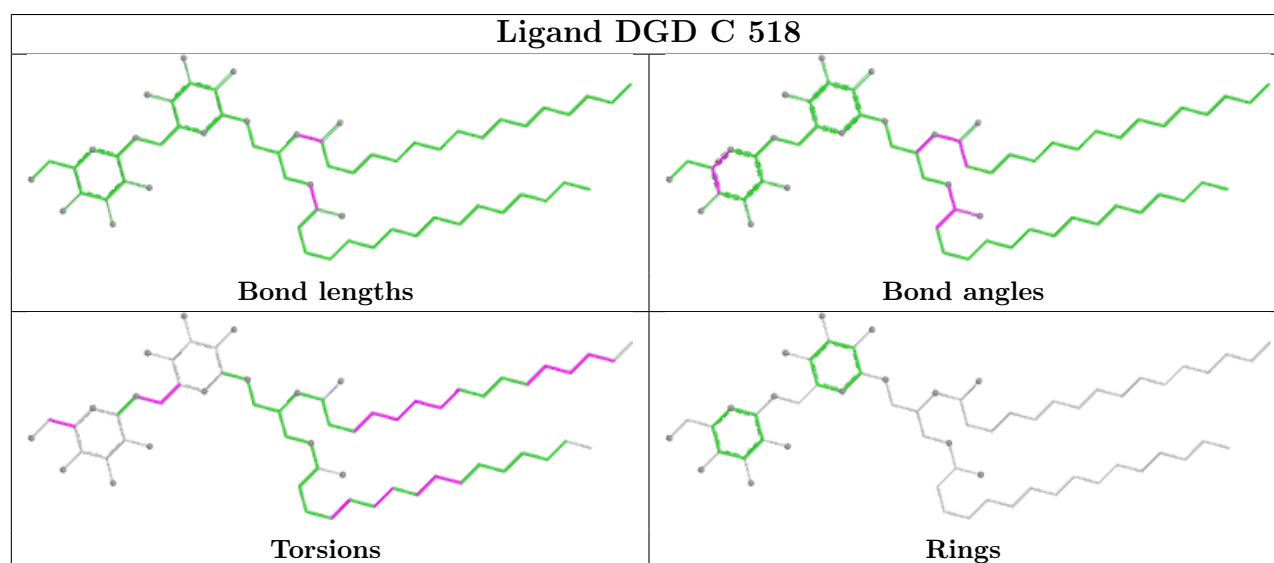
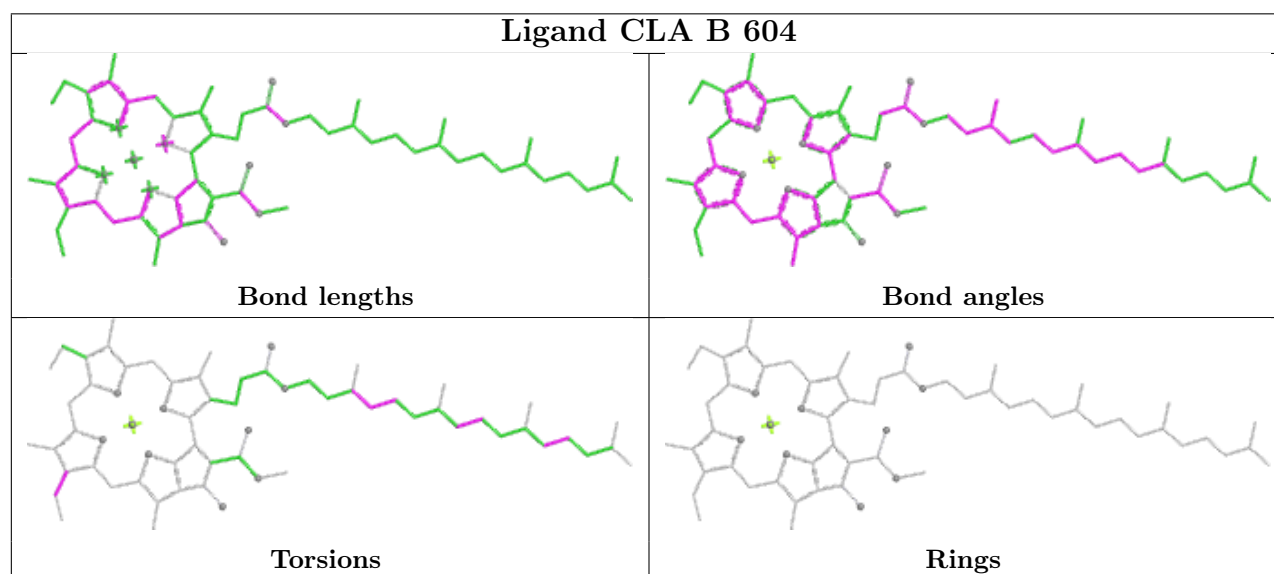
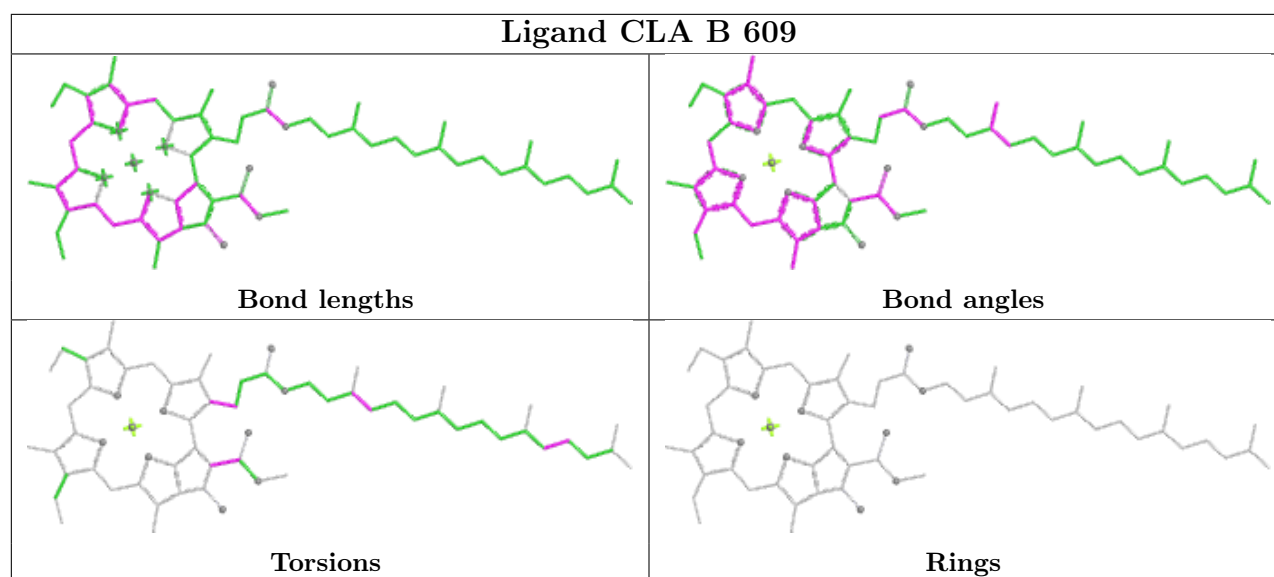
Ligand CLA c 506	
	
Bond lengths	Bond angles
	
Torsions	Rings

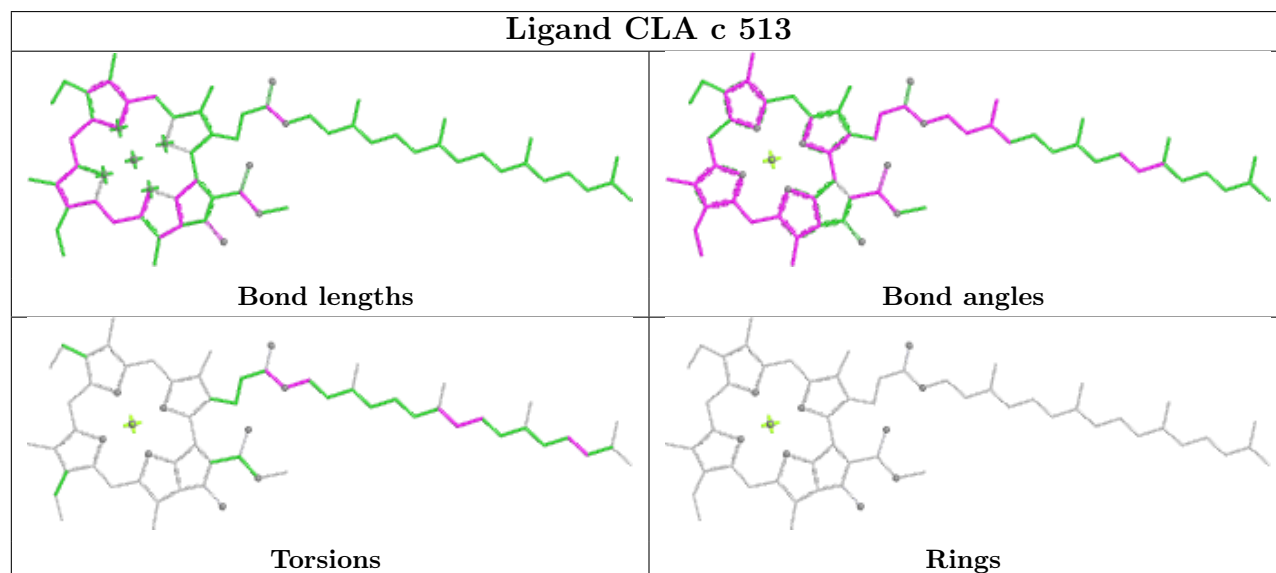
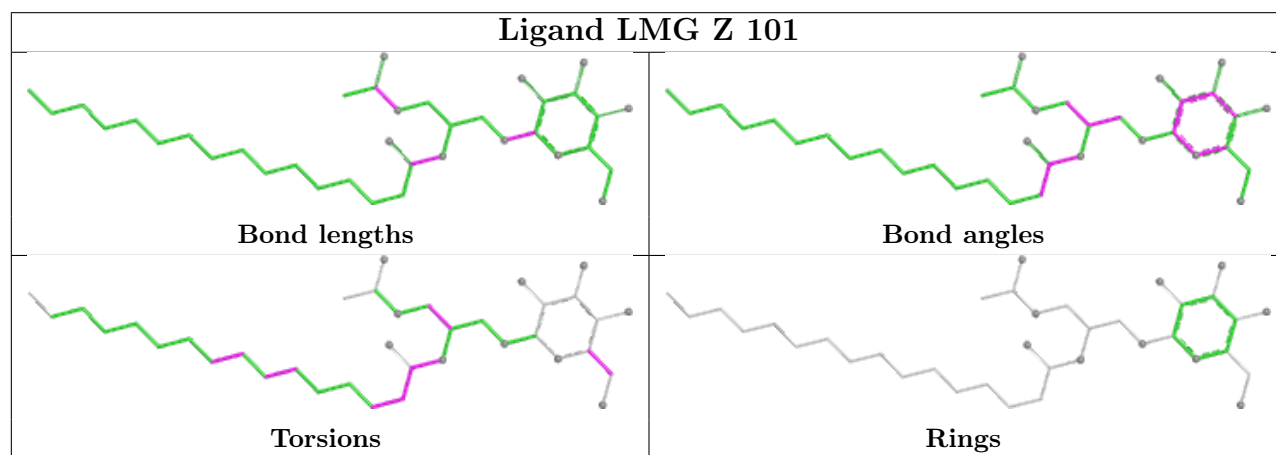
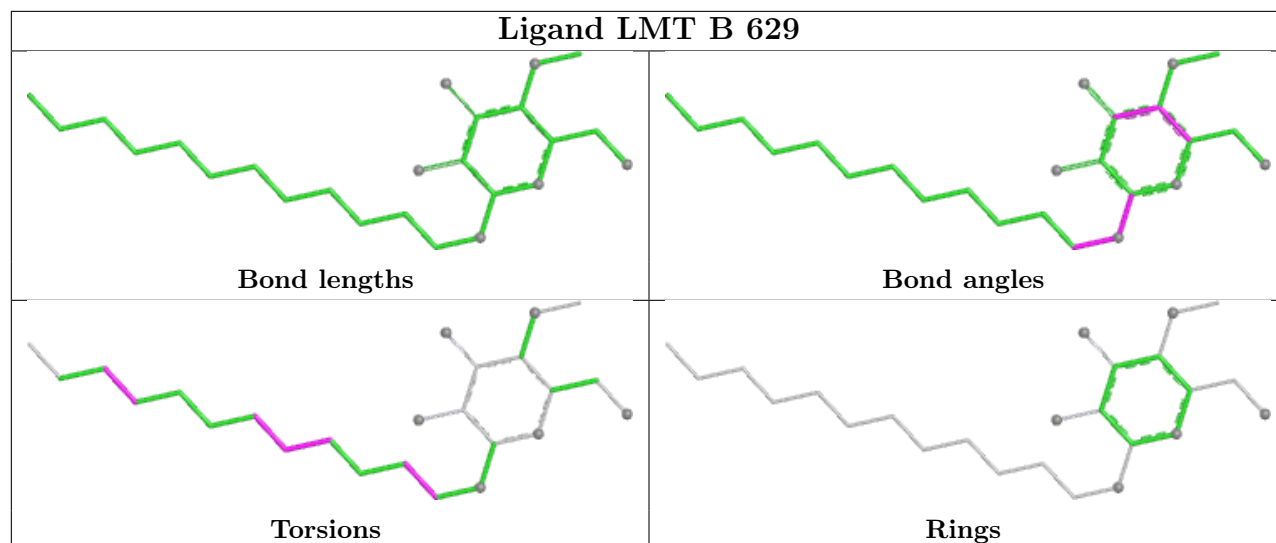
Ligand PL9 a 414 (A)	
	
Bond lengths	Bond angles
	
Torsions	Rings

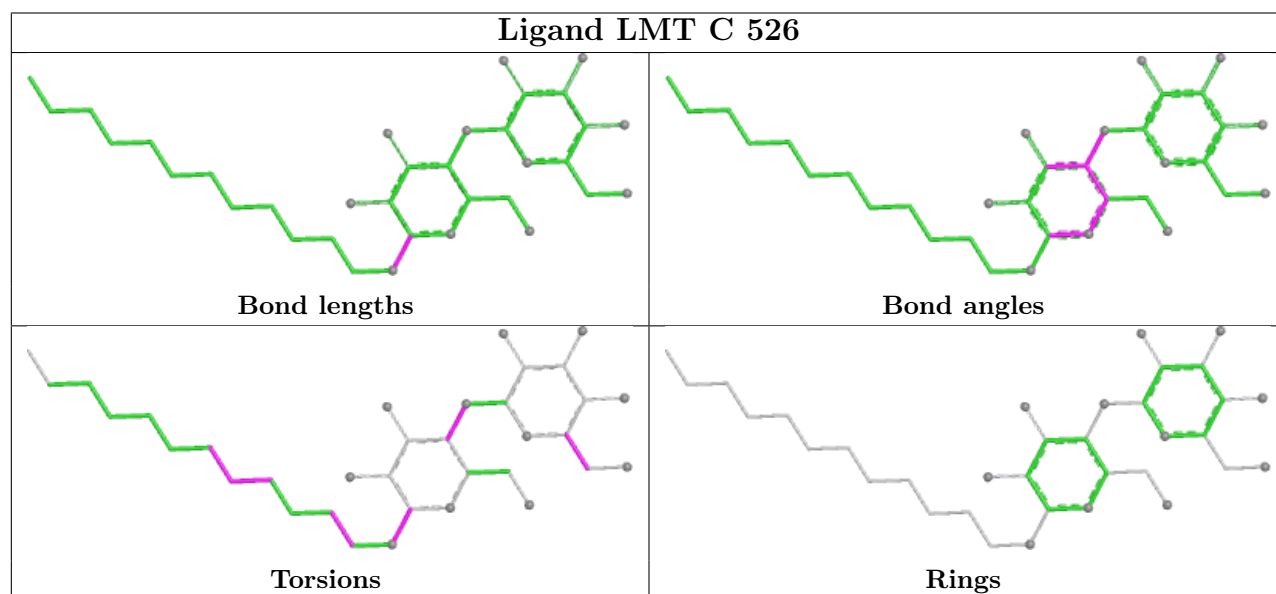
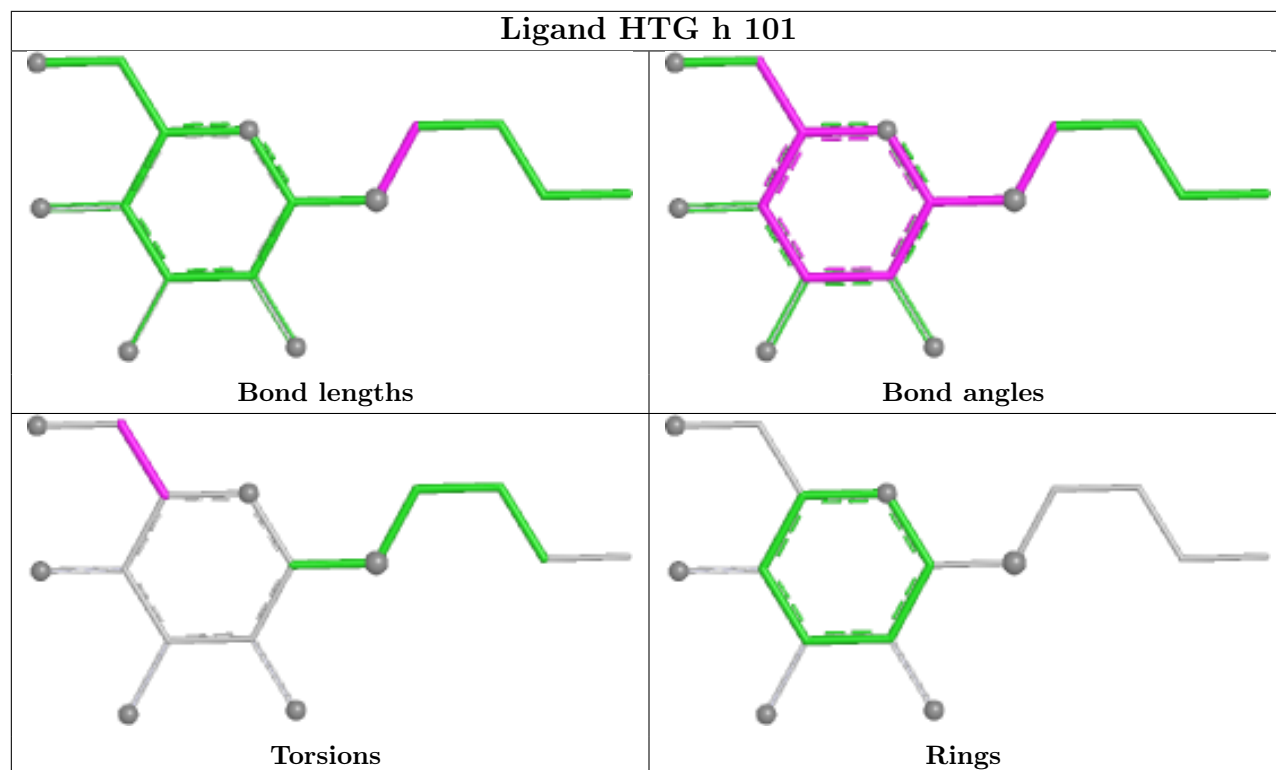
Ligand BCR C 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

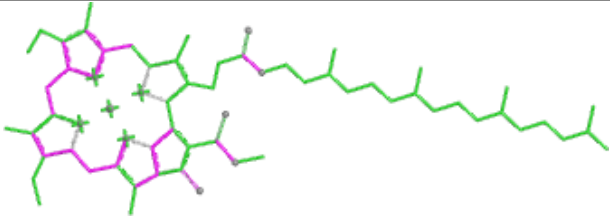
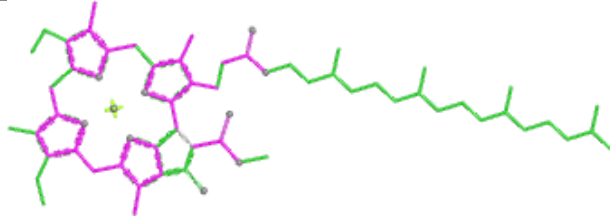
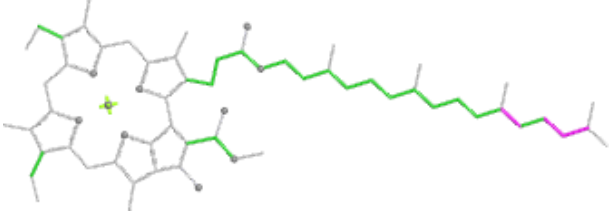
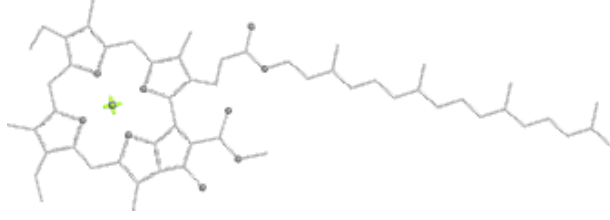
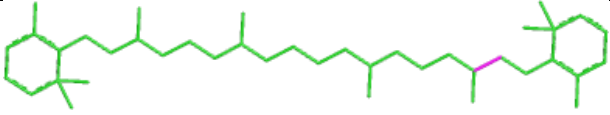
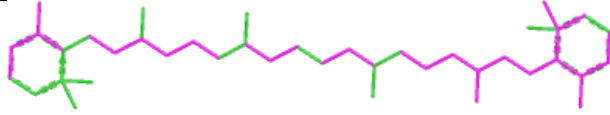
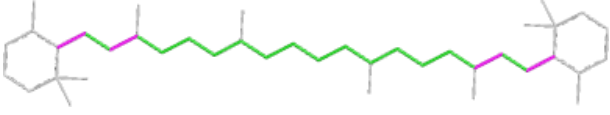
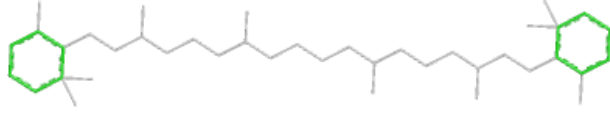
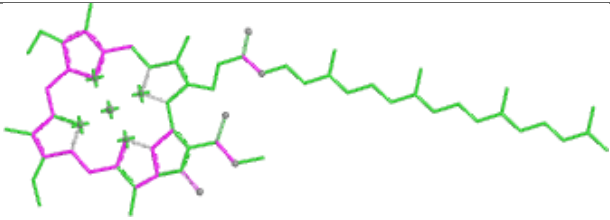
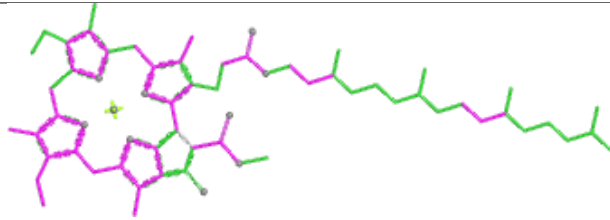
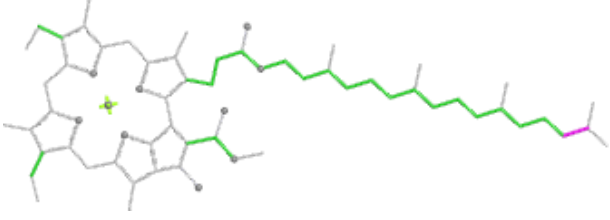
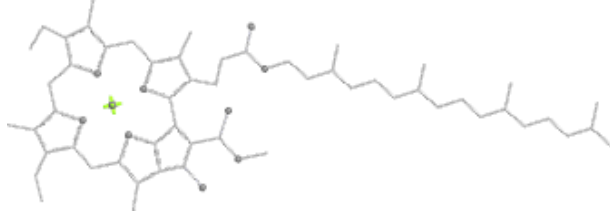
Ligand BCR B 631	
	
Bond lengths	Bond angles
	
Torsions	Rings

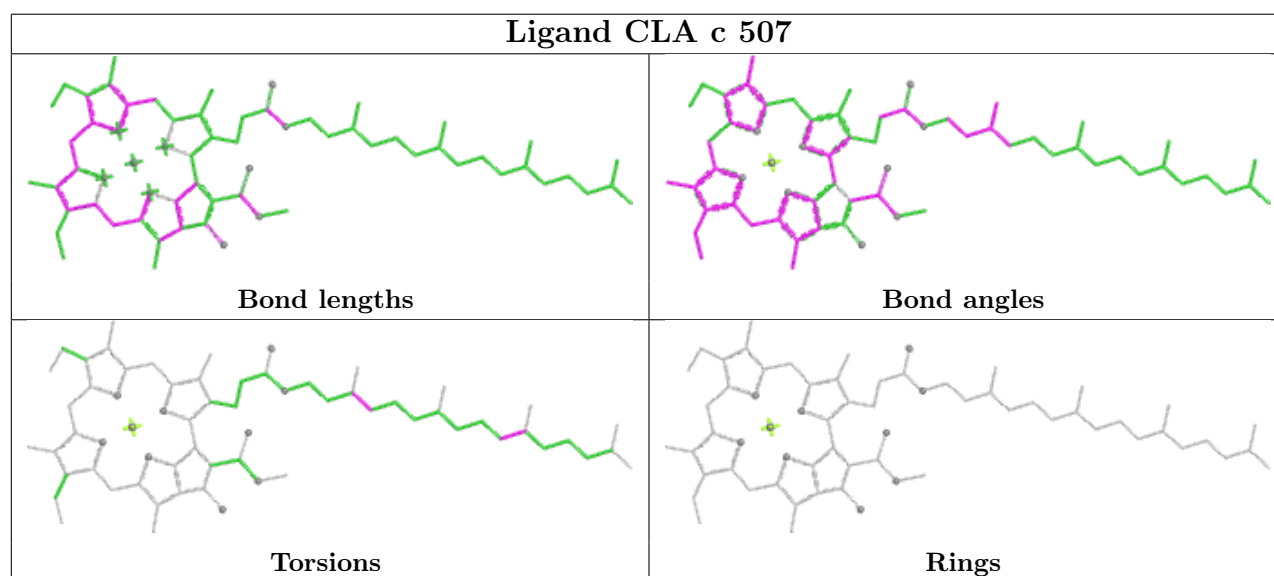
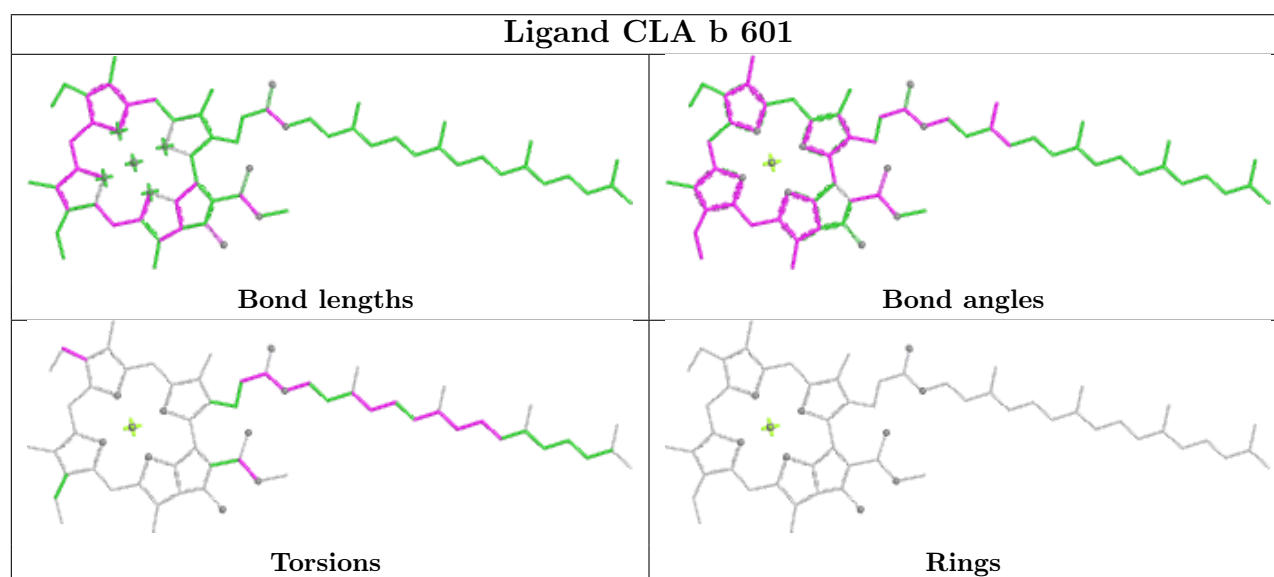
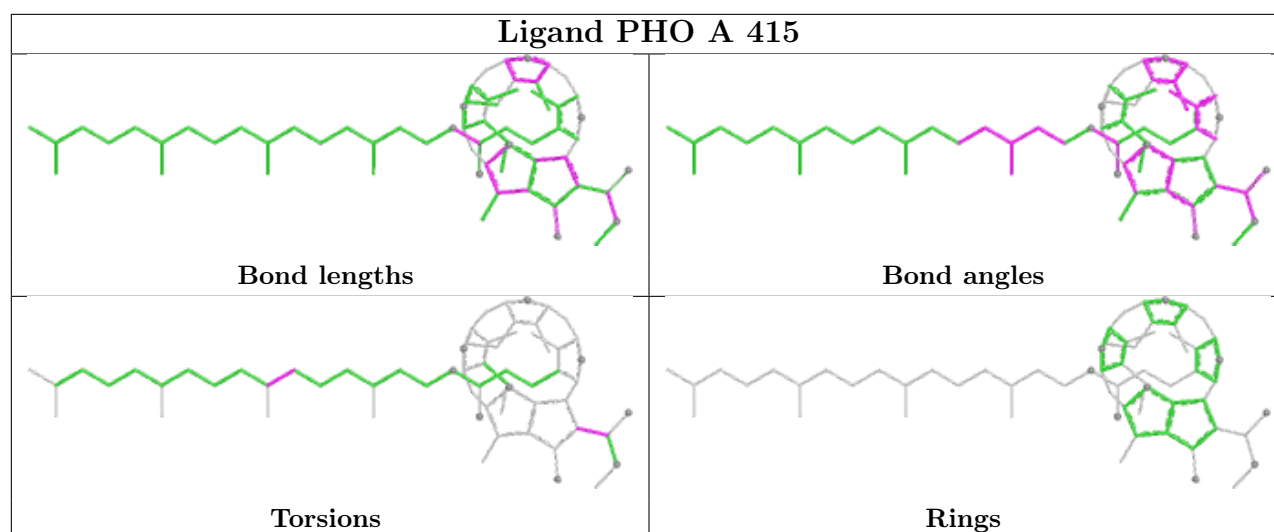




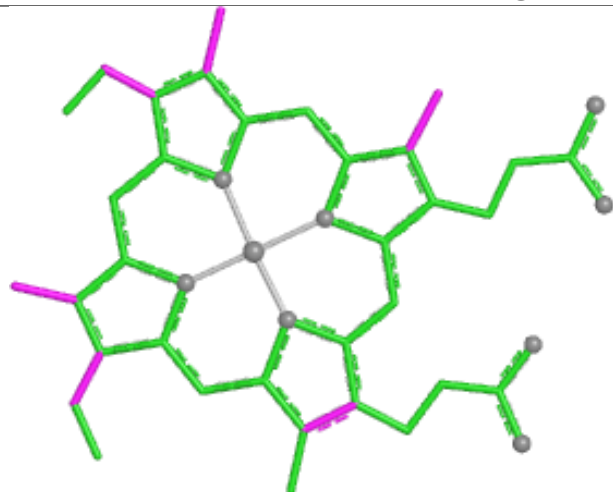




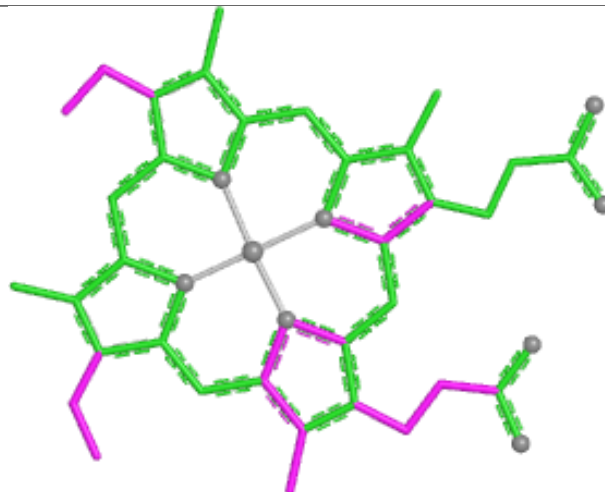
Ligand CLA A 405	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR D 405	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 608	
 Bond lengths	 Bond angles
 Torsions	 Rings



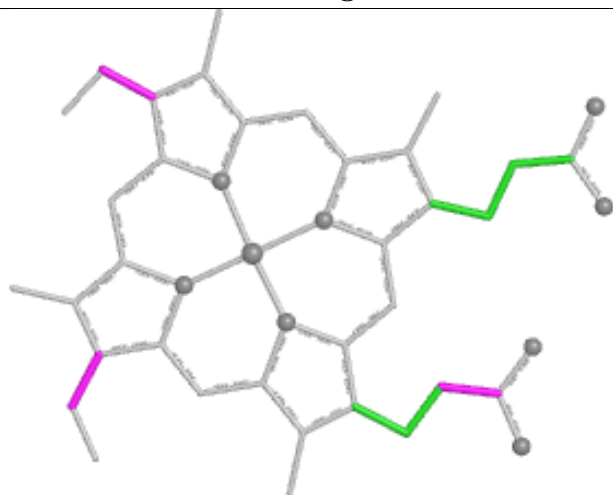
Ligand HEC V 201



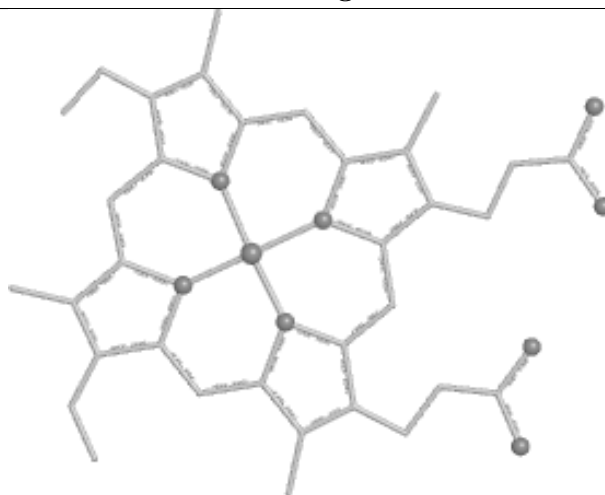
Bond lengths



Bond angles

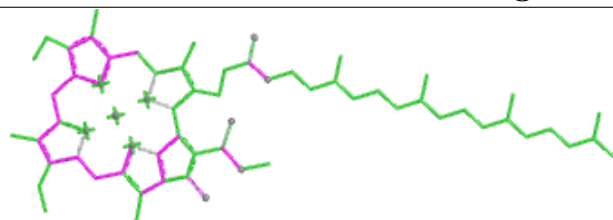


Torsions

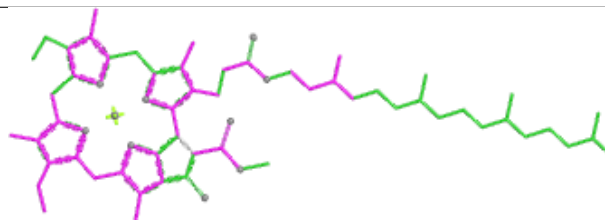


Rings

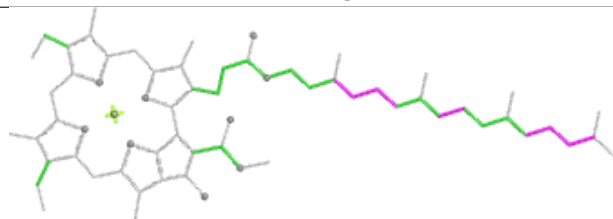
Ligand CLA A 407



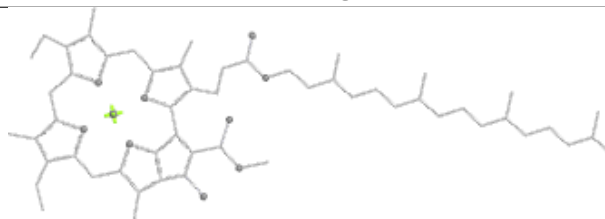
Bond lengths



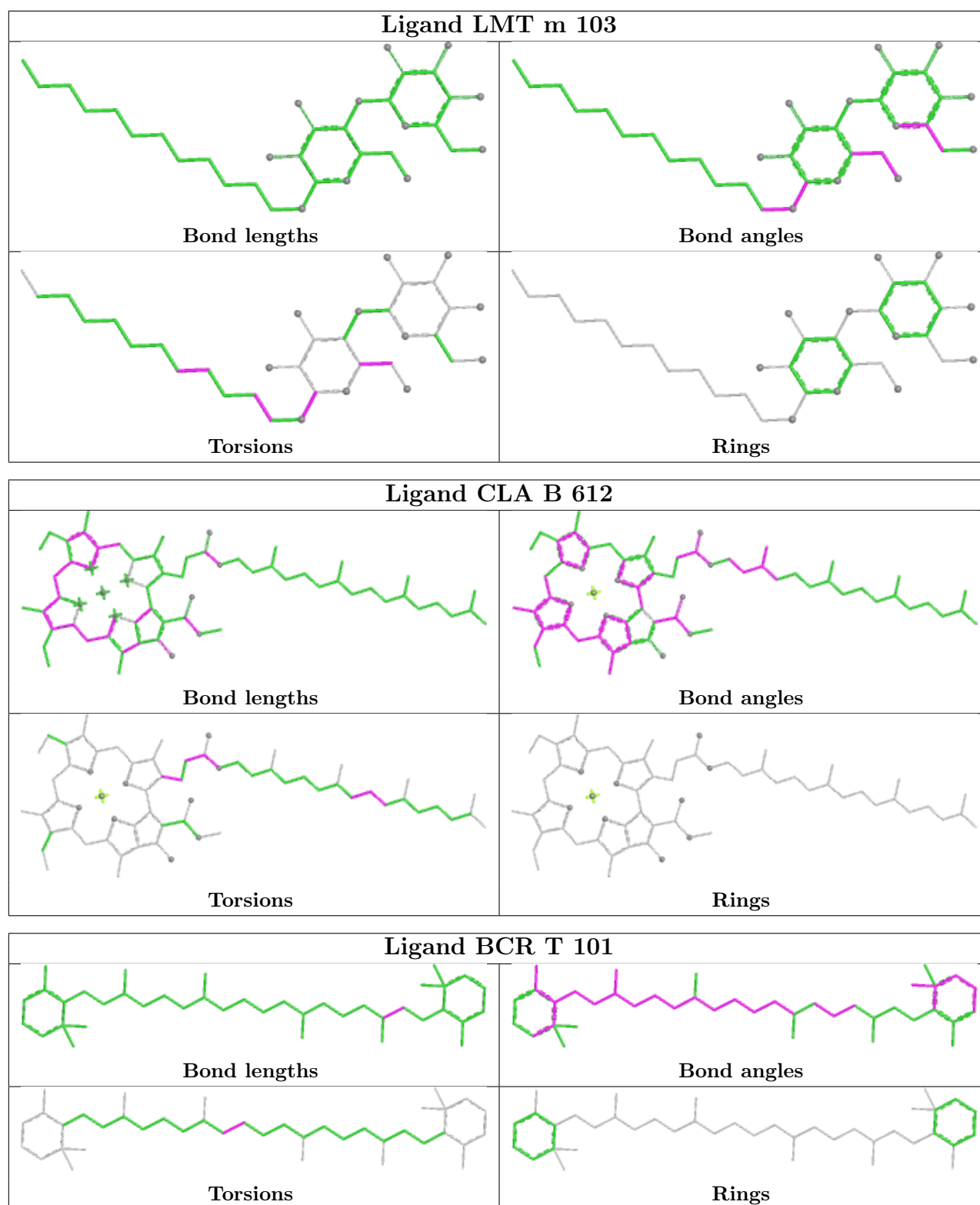
Bond angles

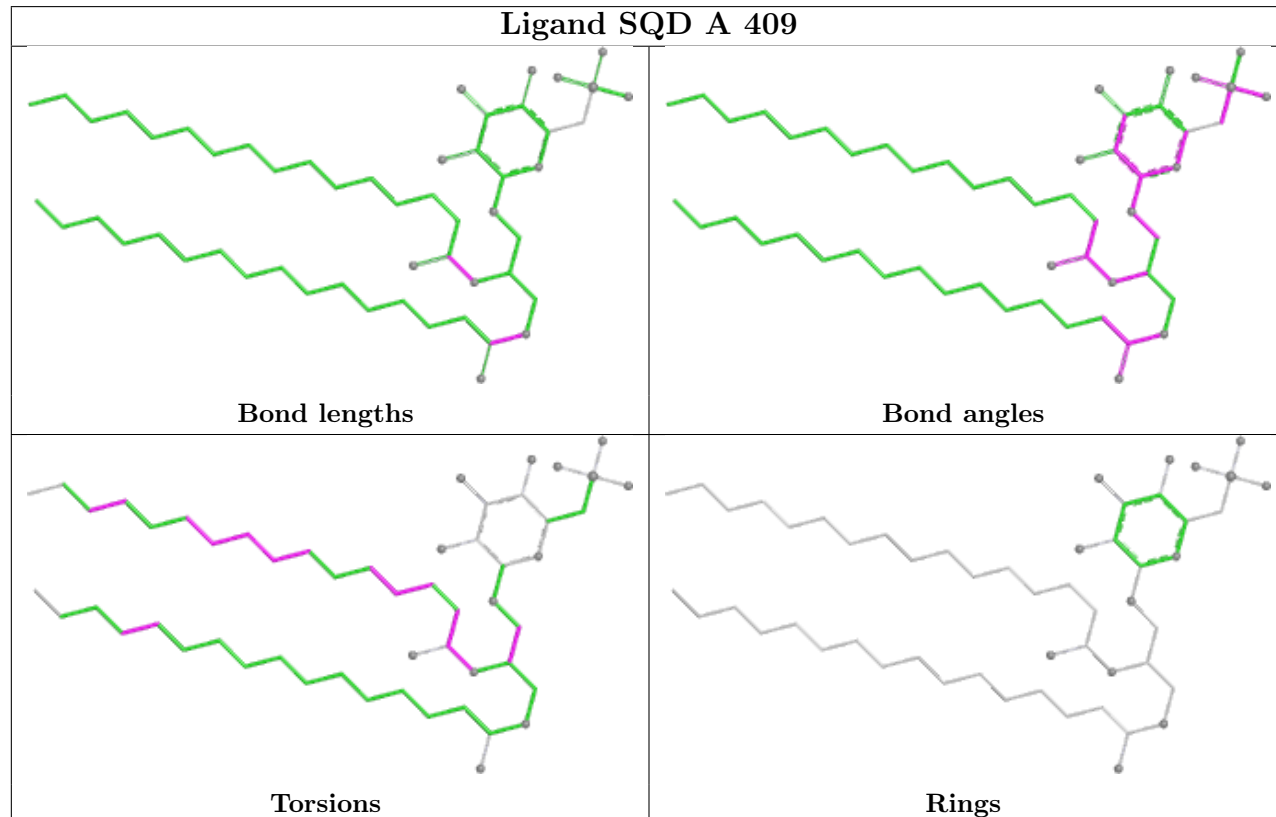
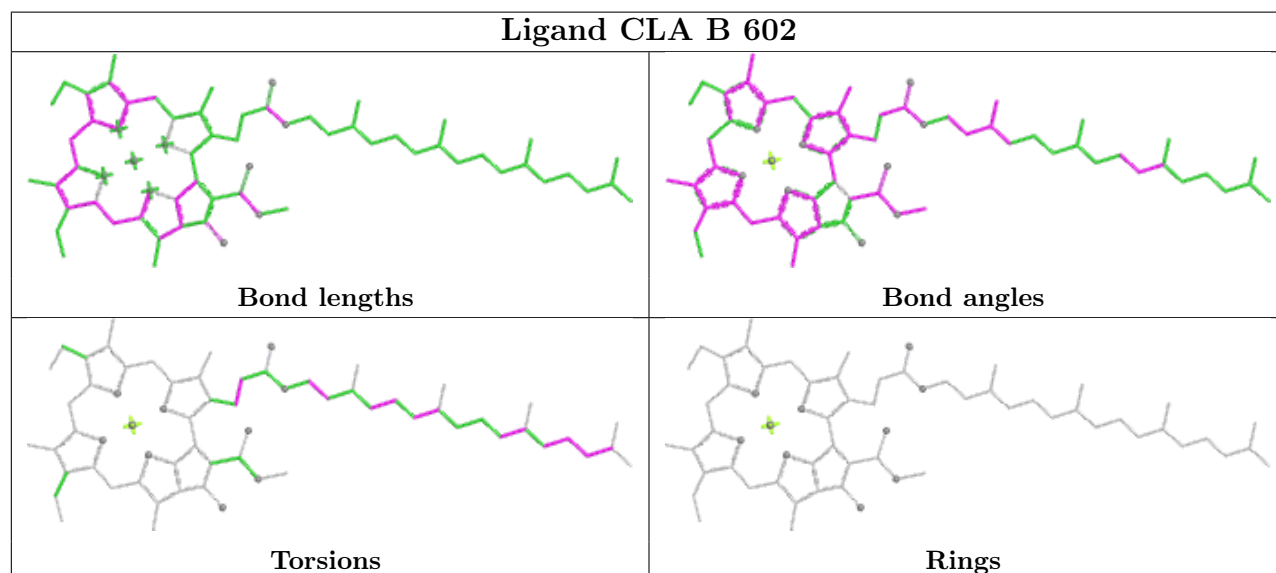
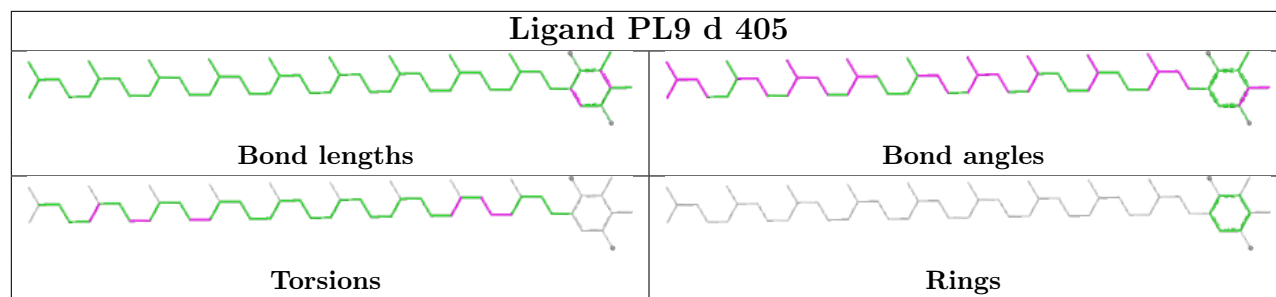


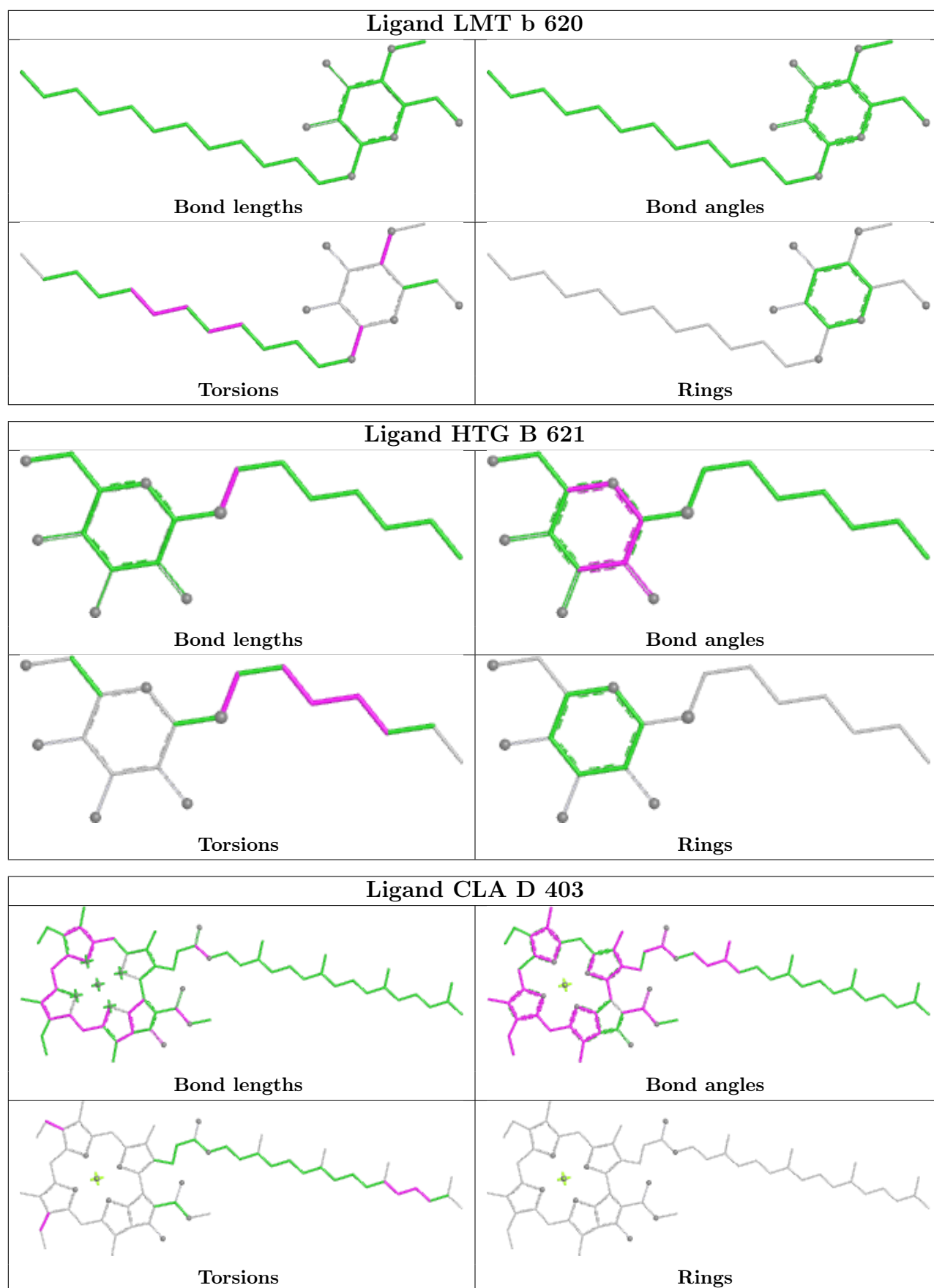
Torsions

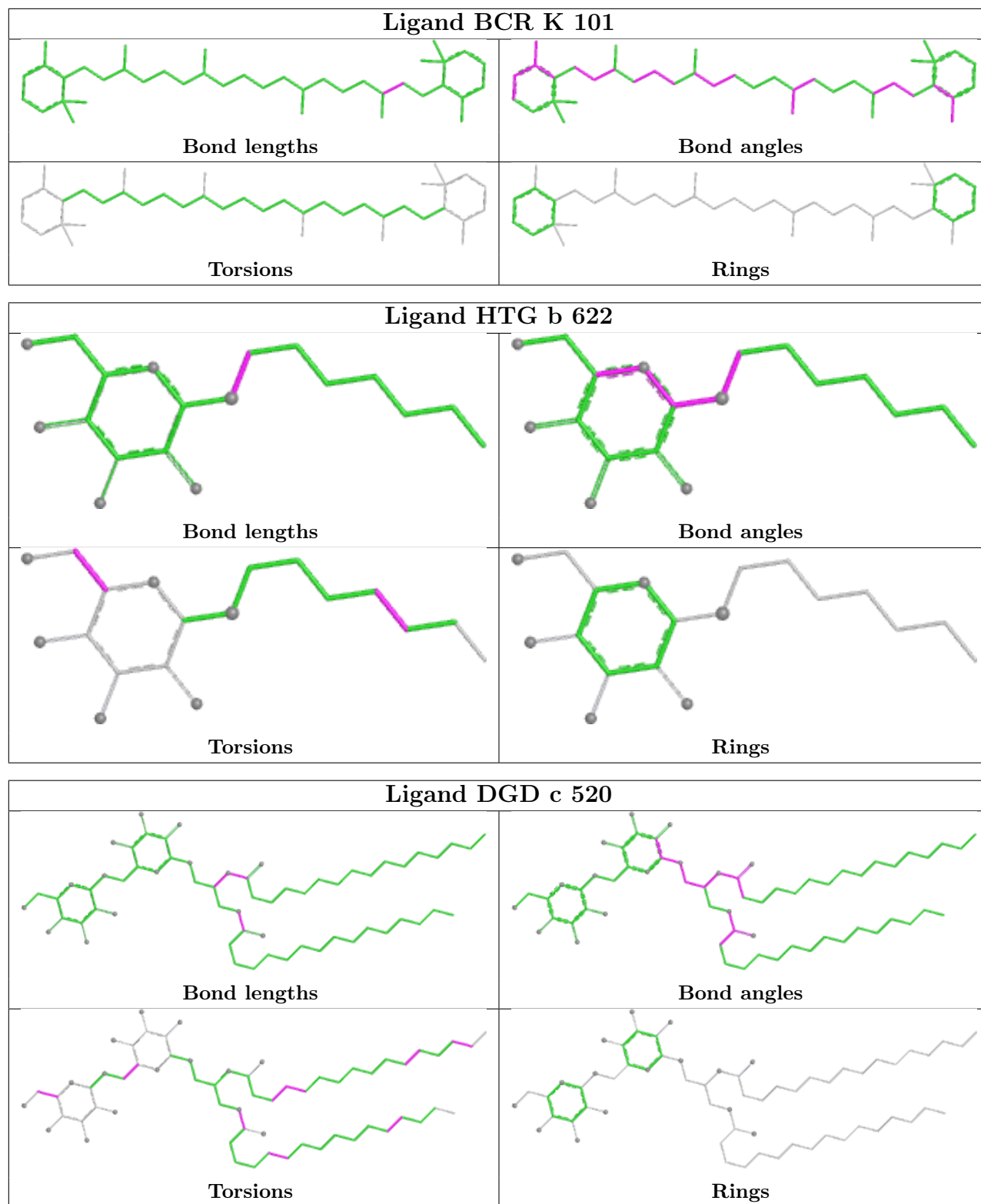


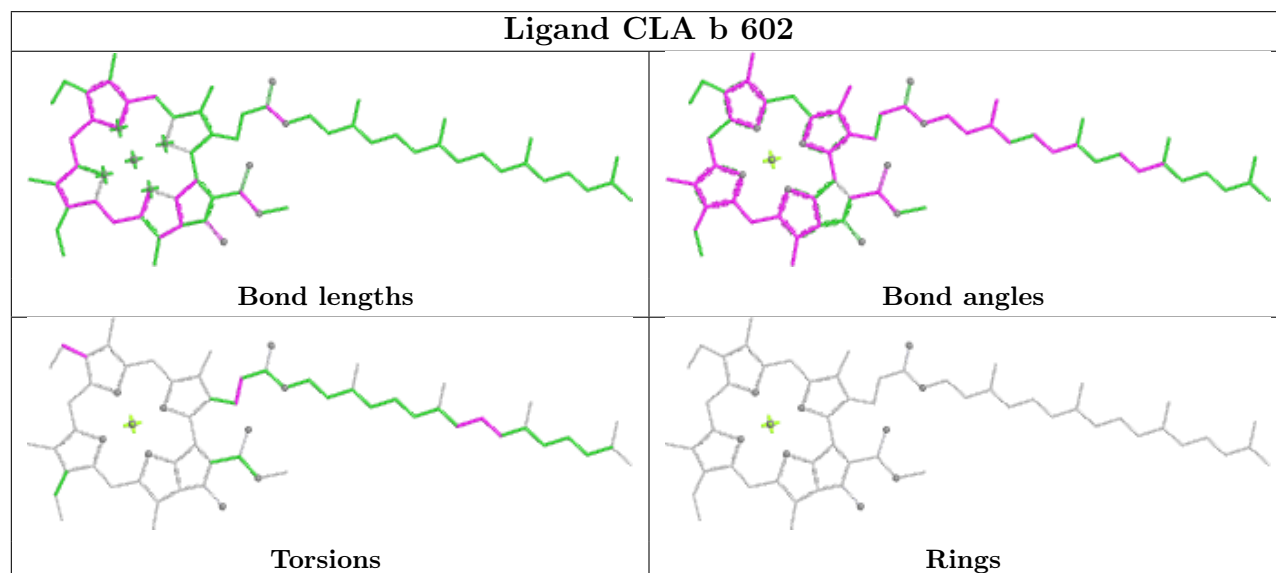
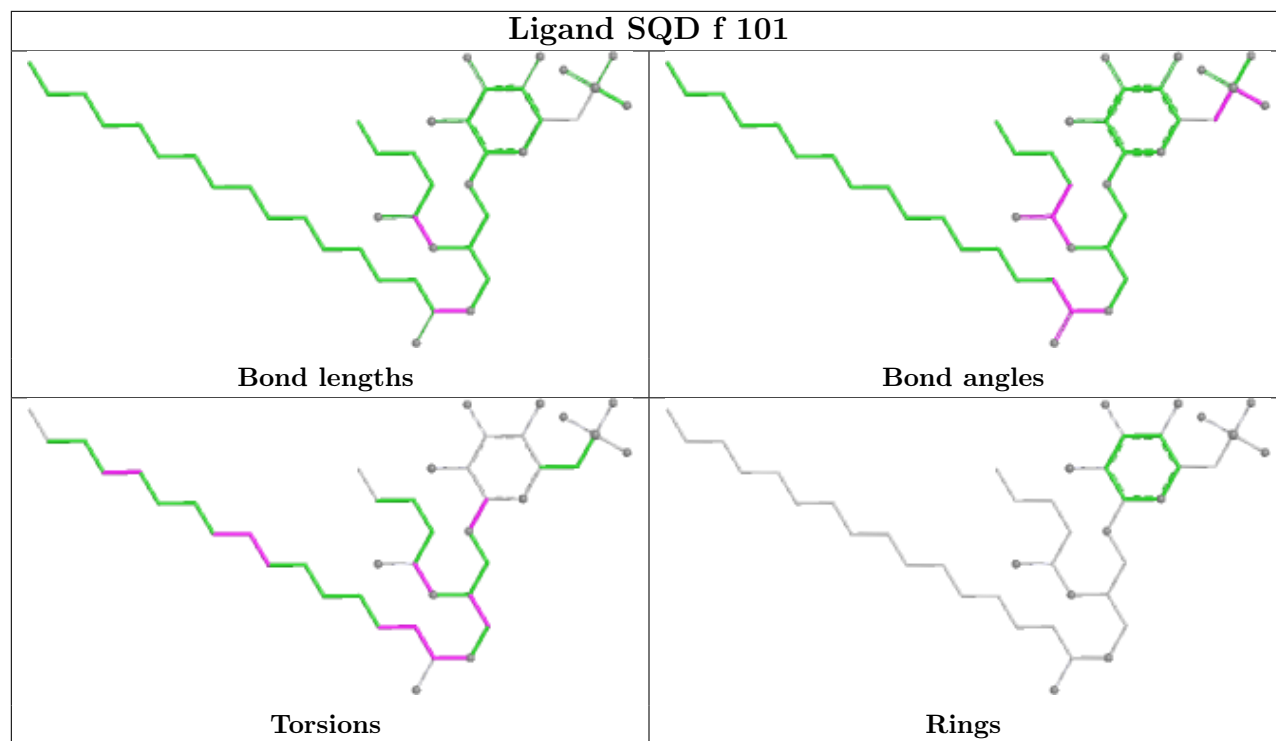
Rings

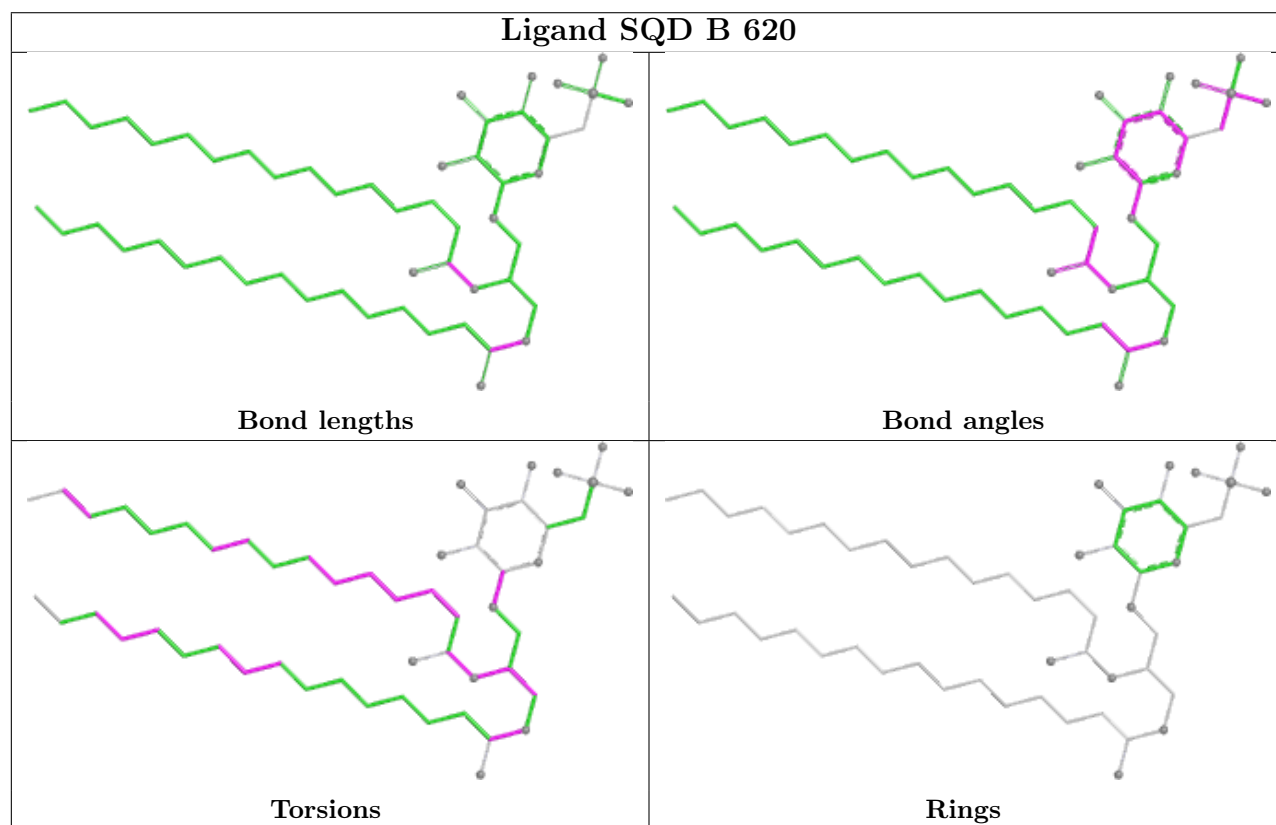
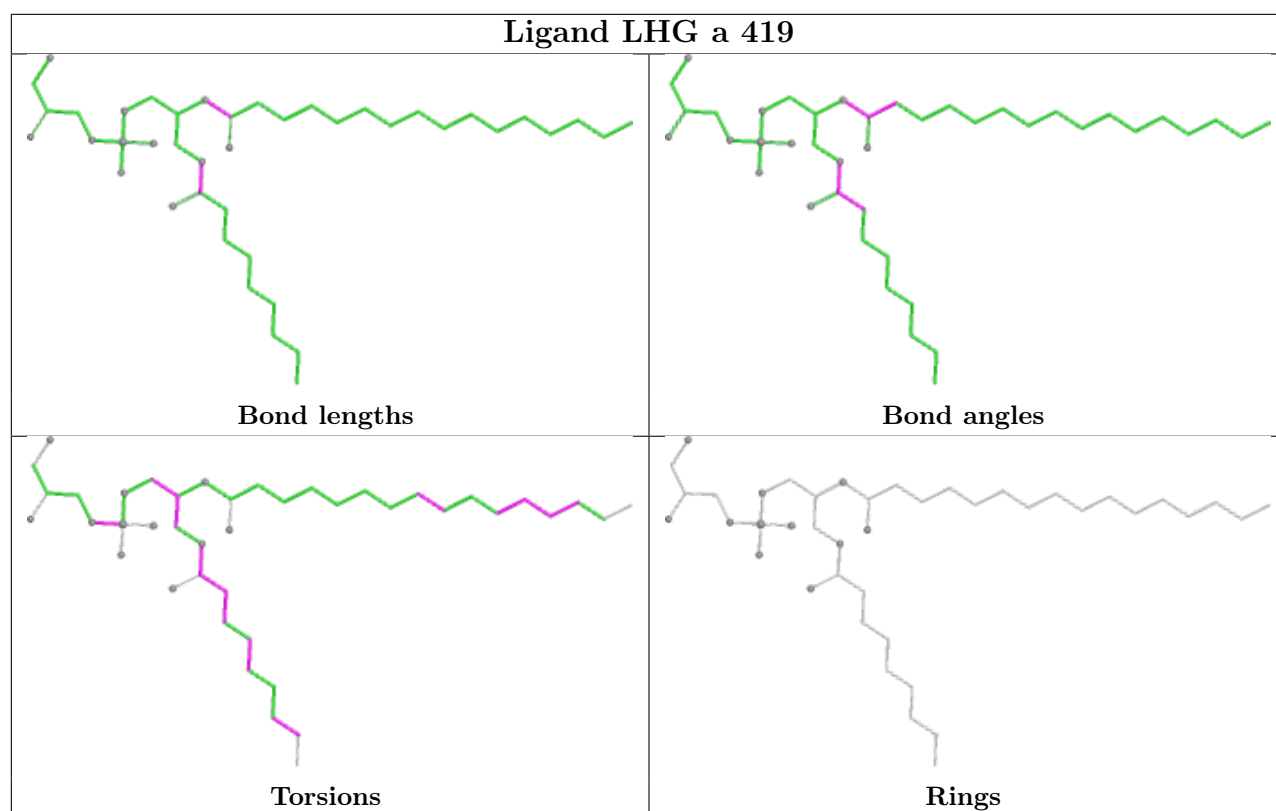


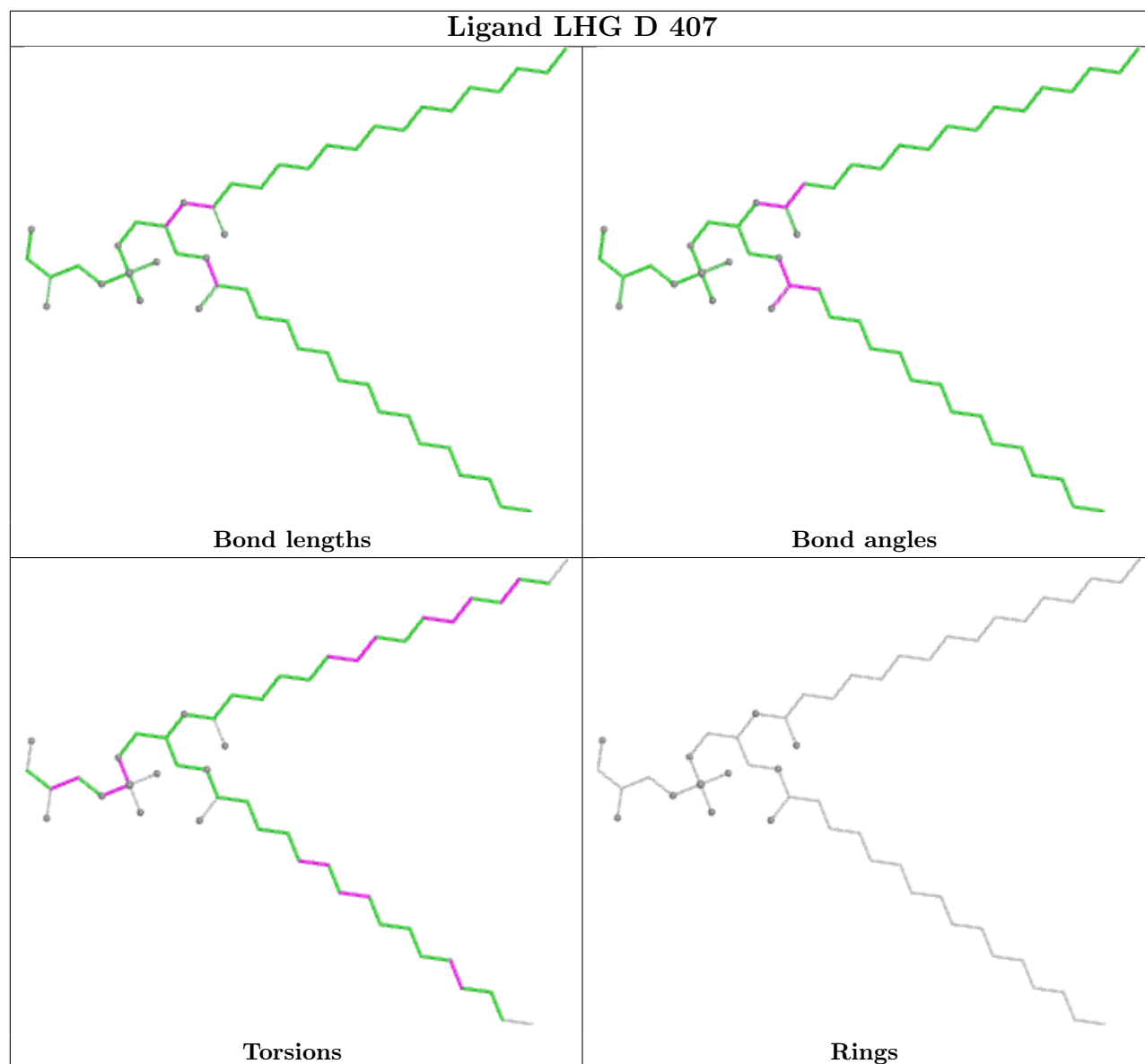
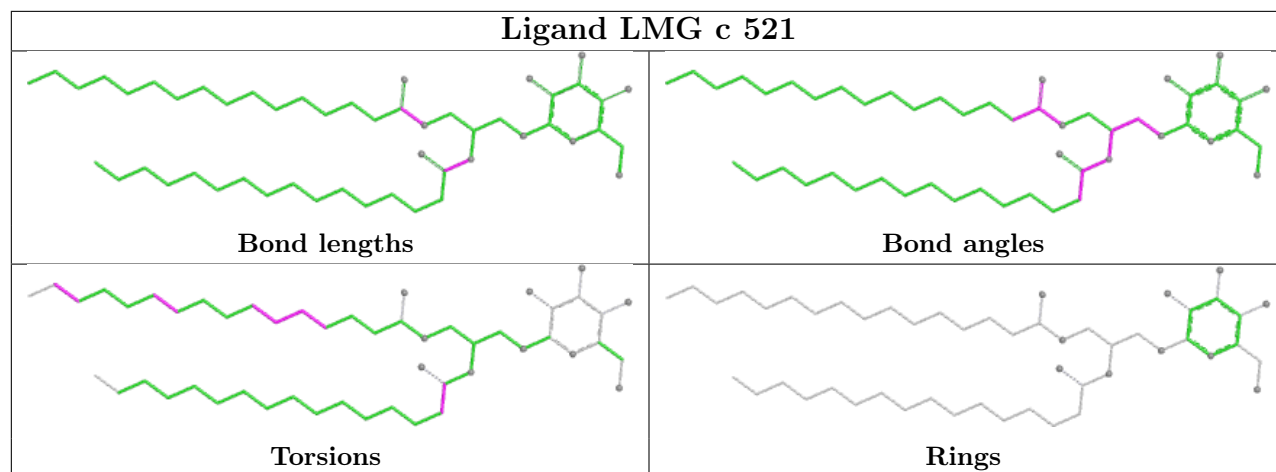


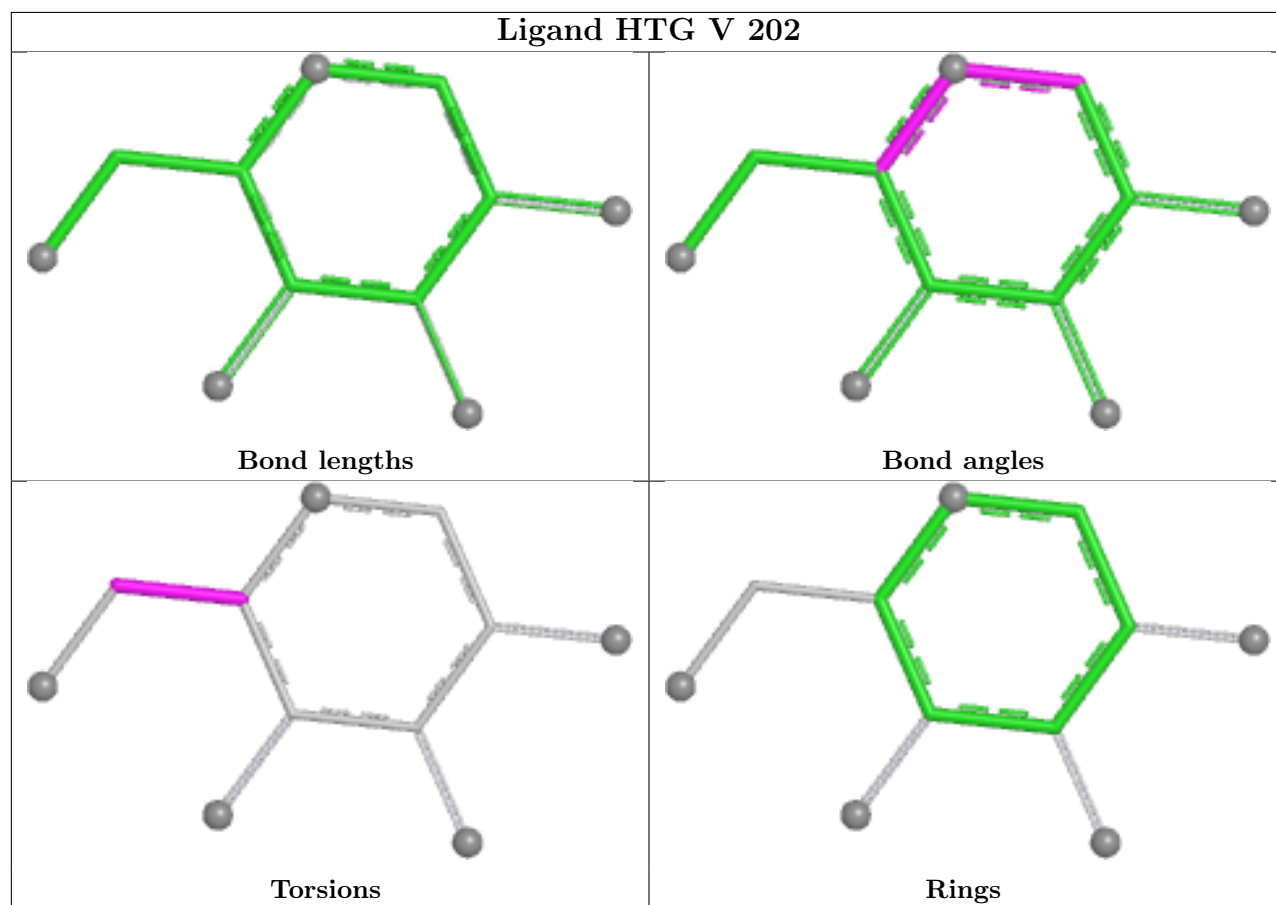
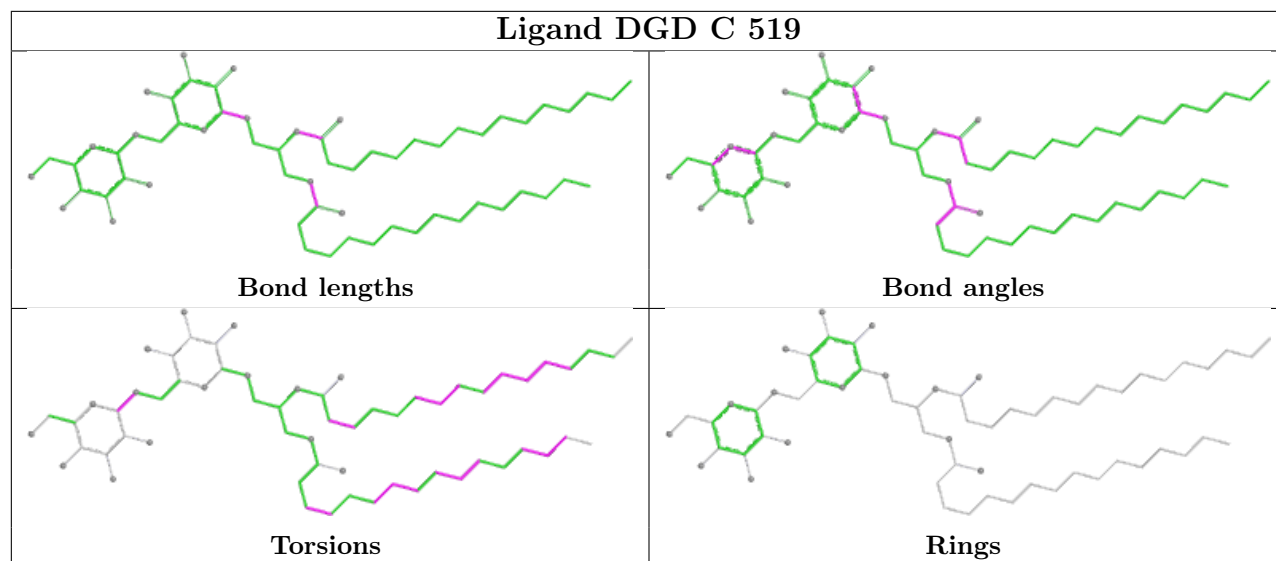


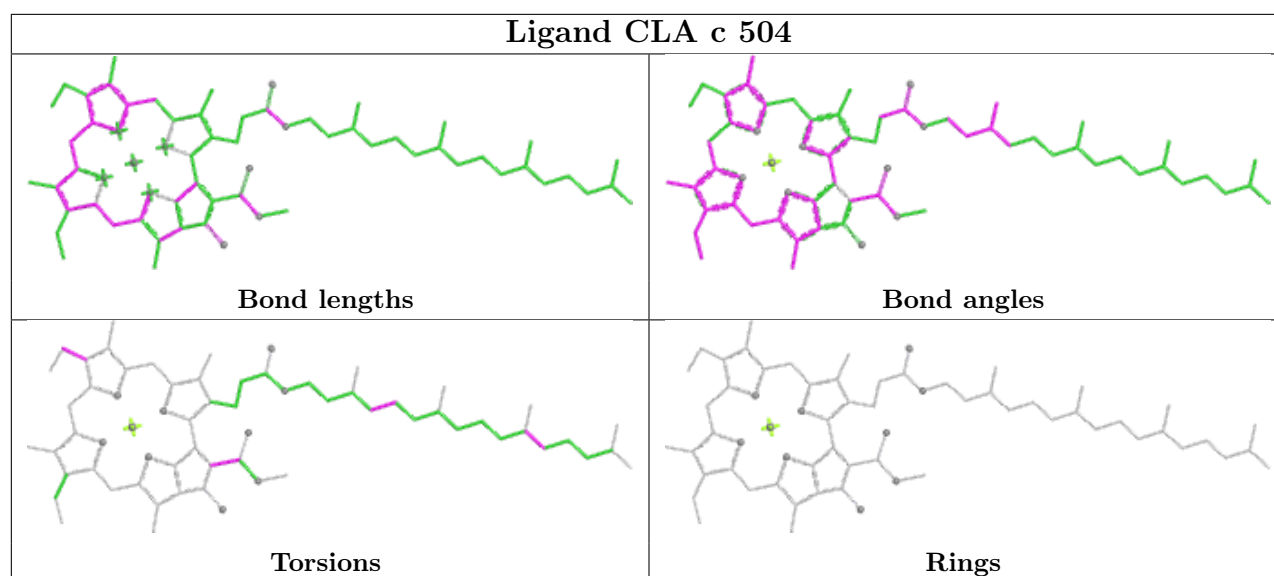
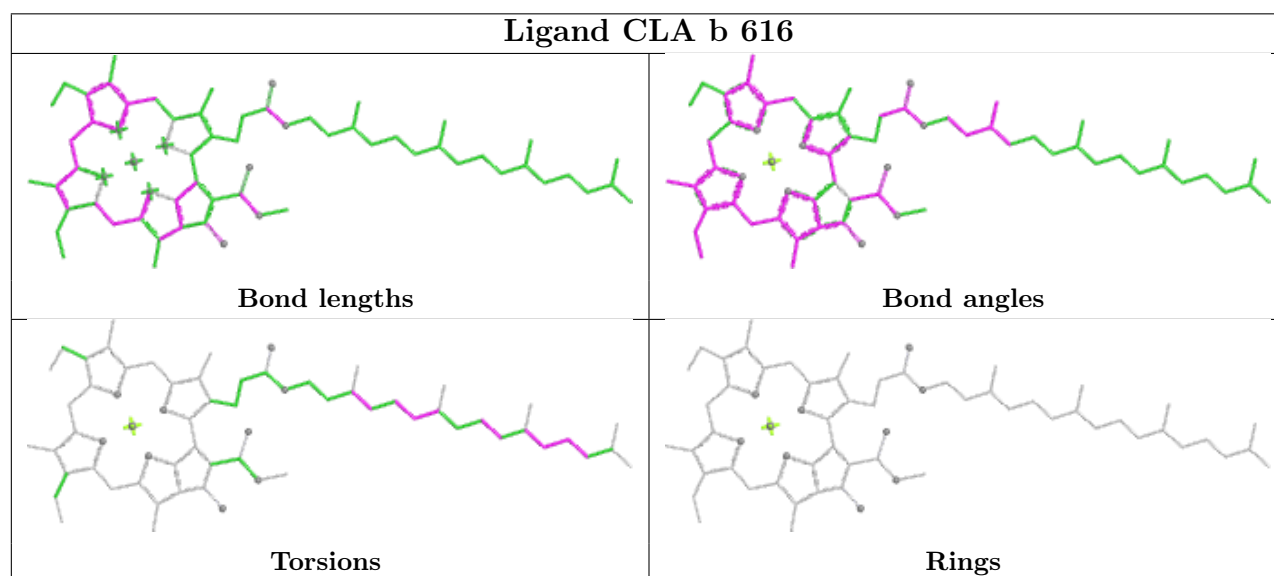
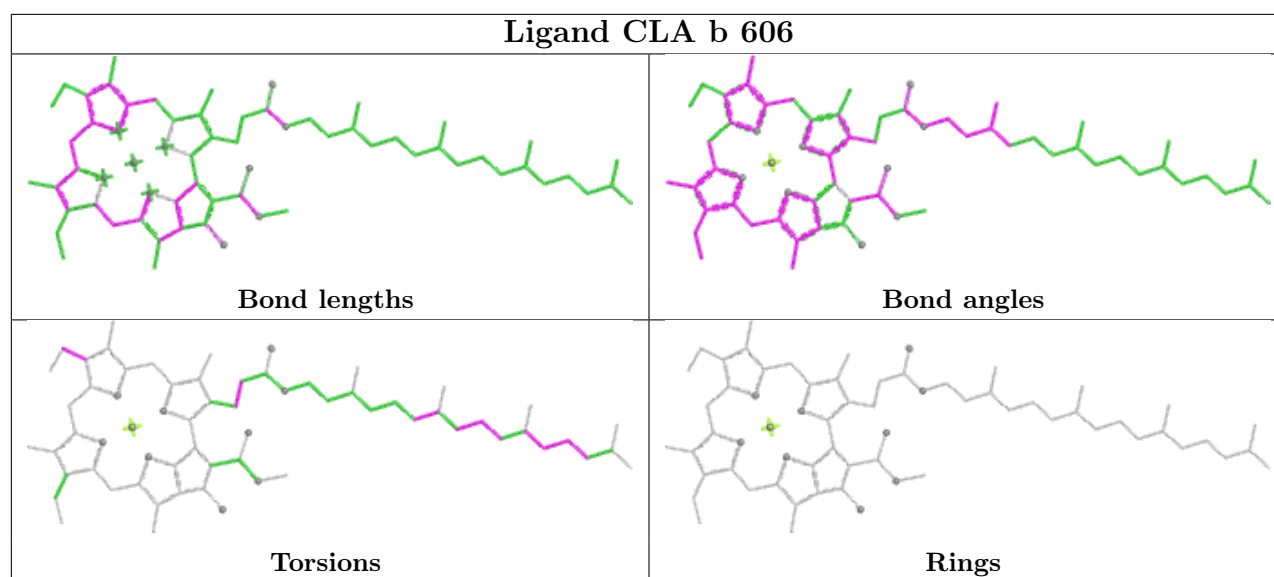


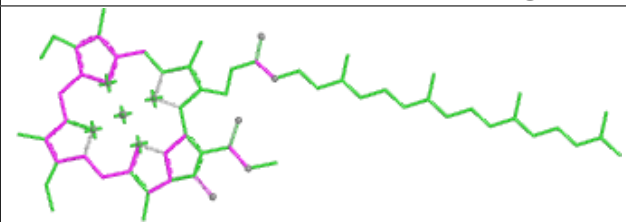
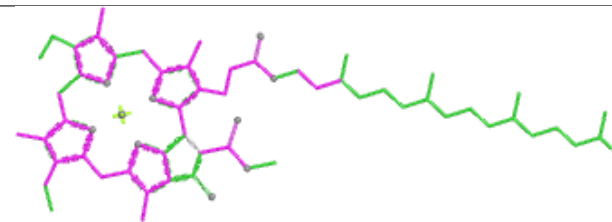
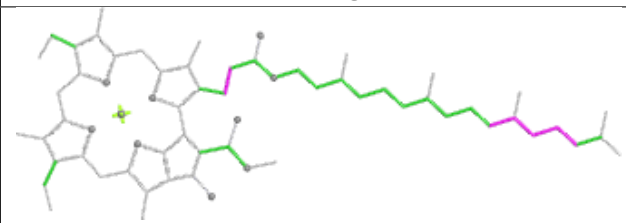
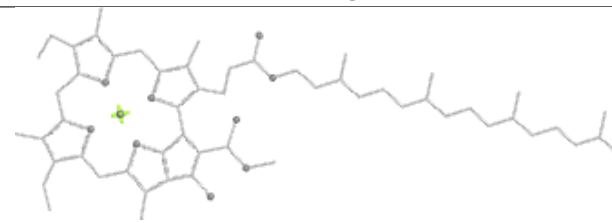


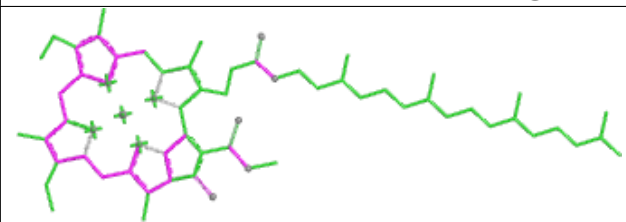
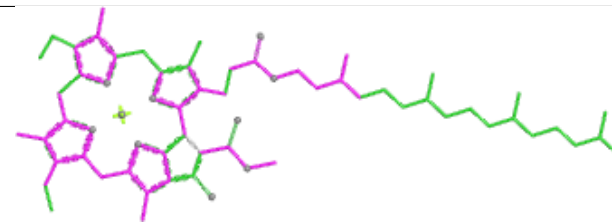
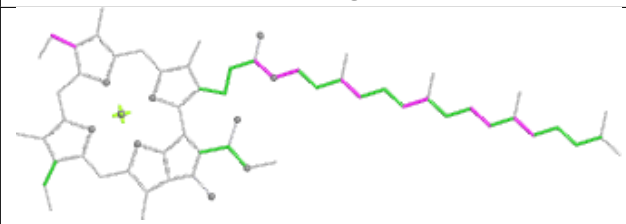
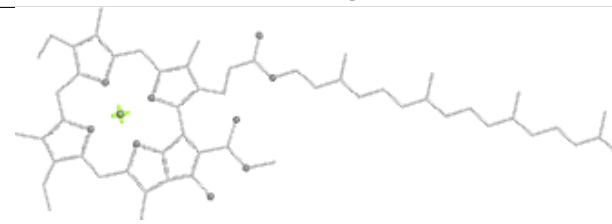


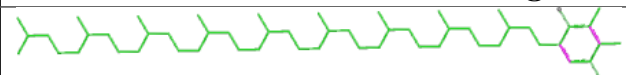
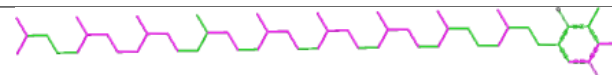
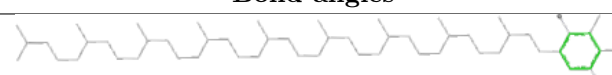


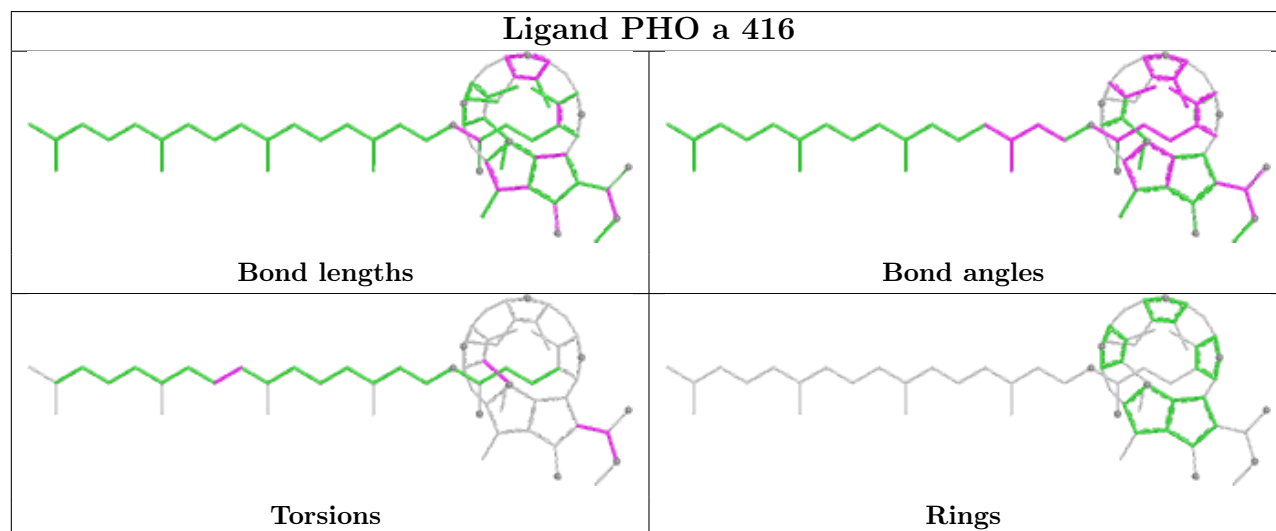
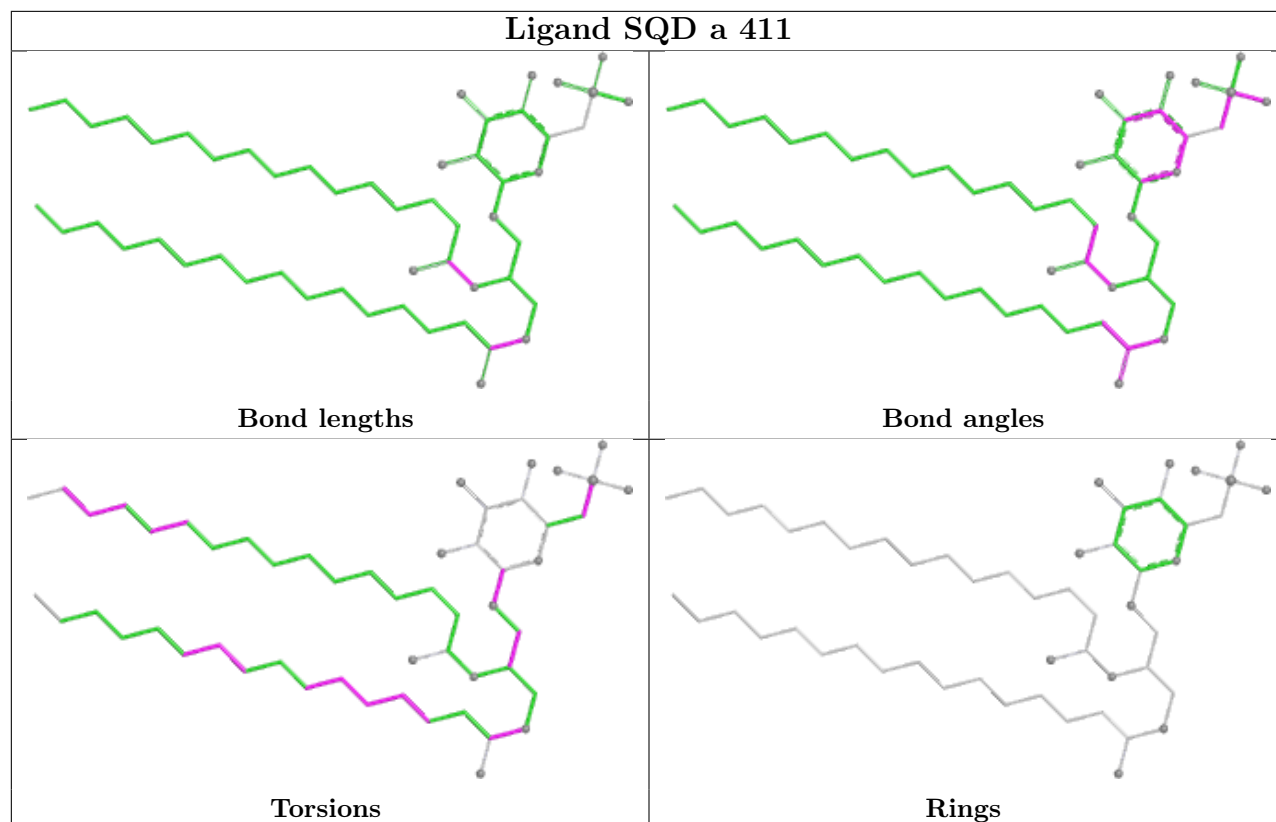


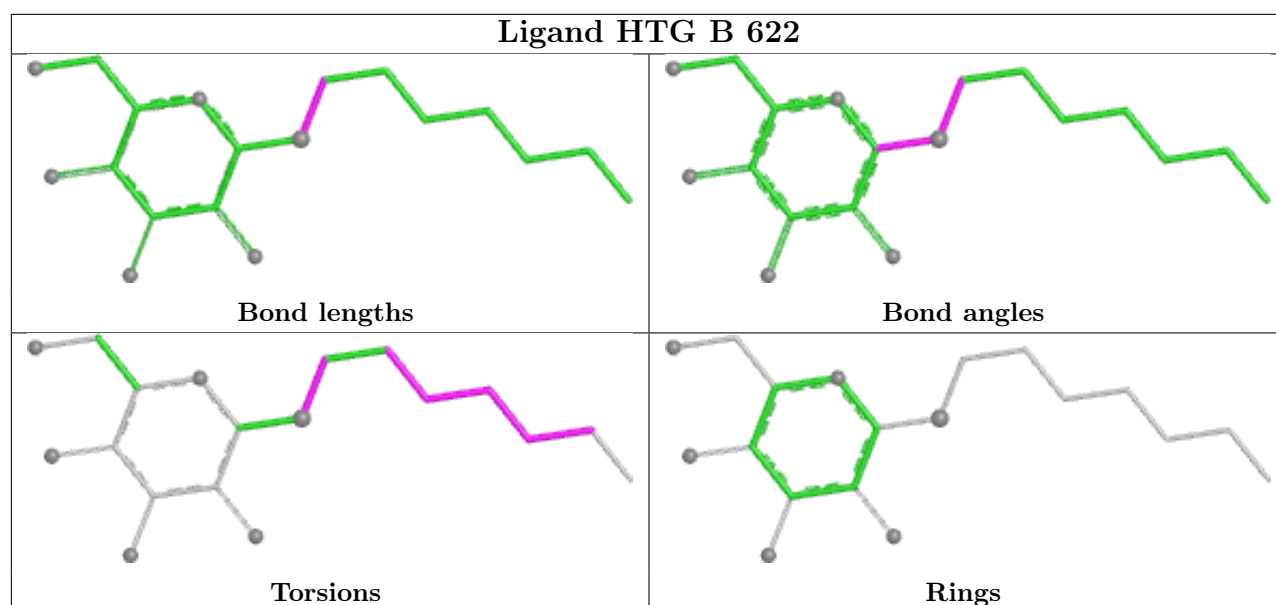
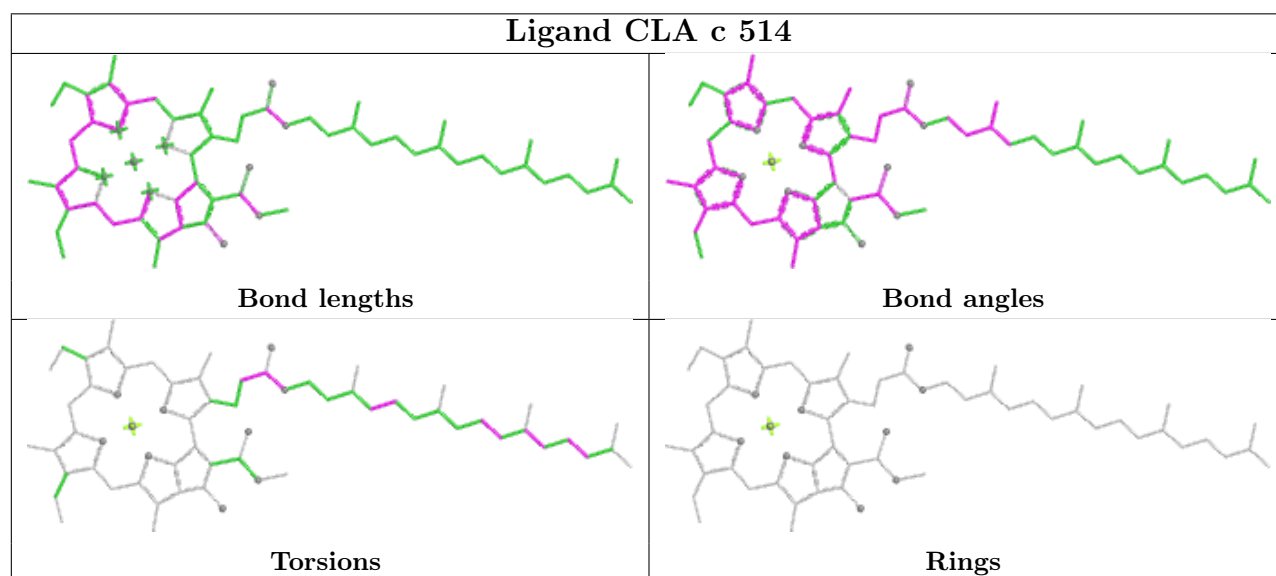
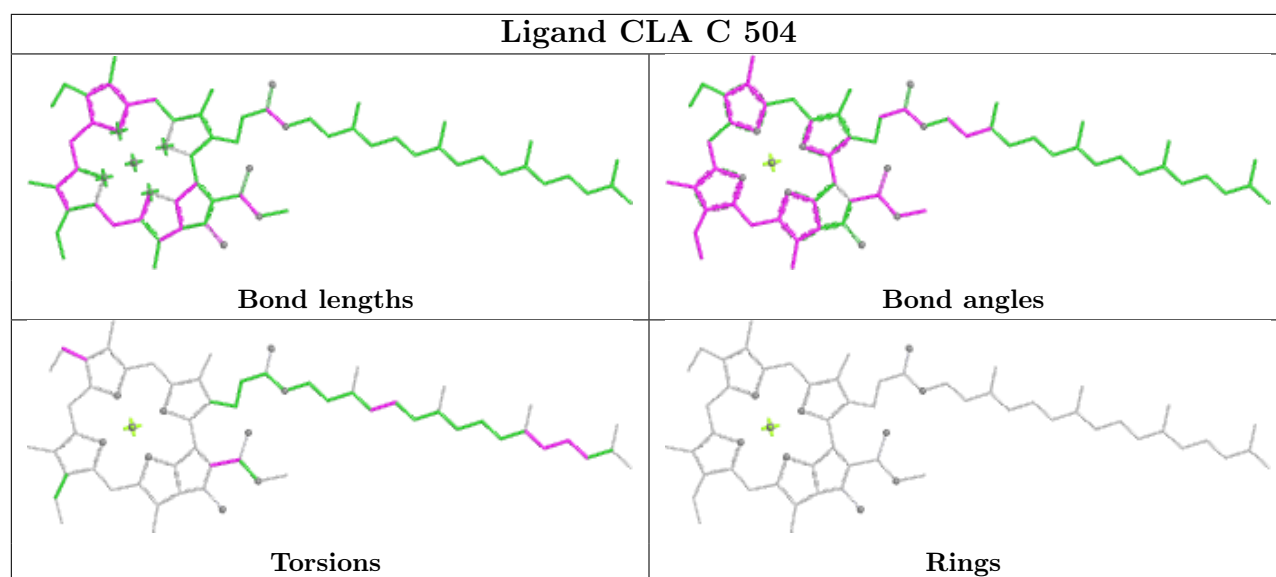


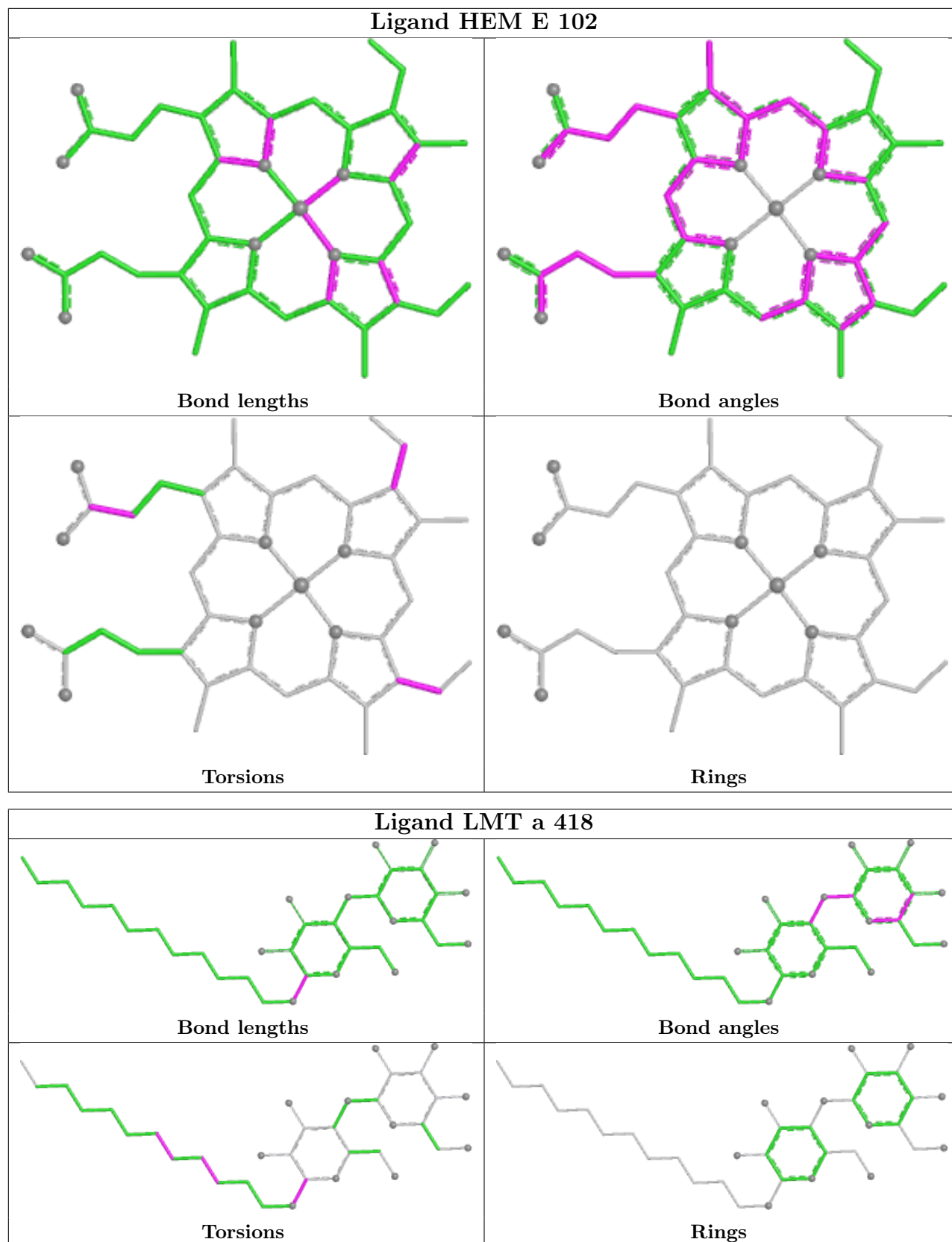
Ligand CLA B 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

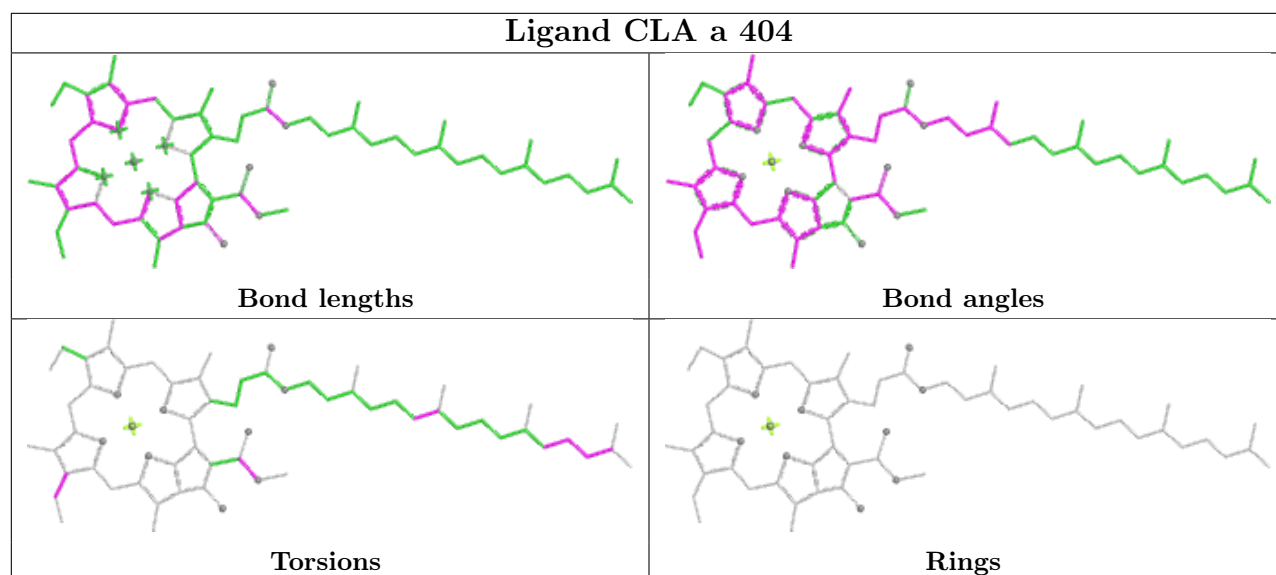
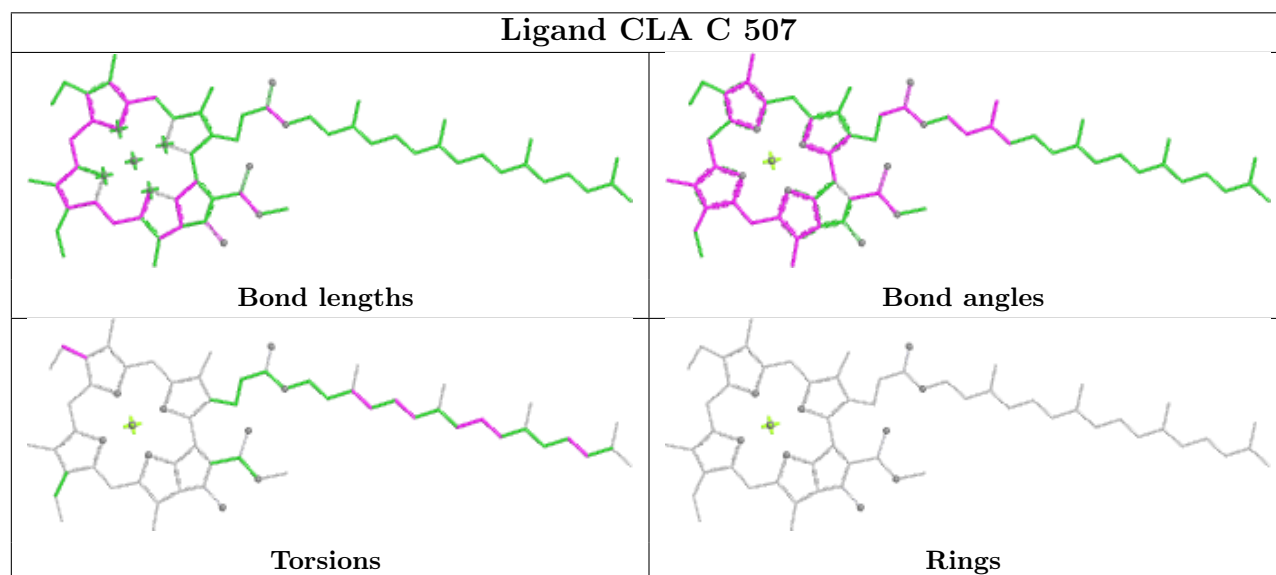
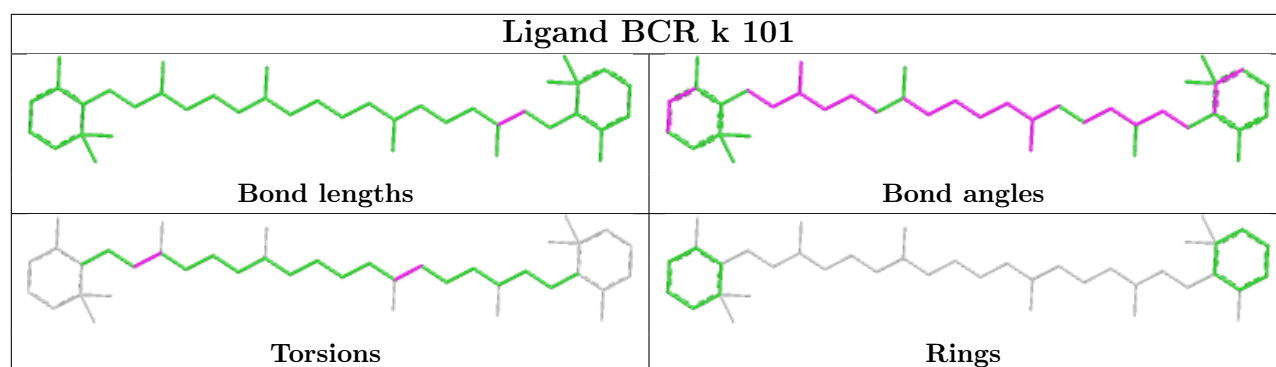
Ligand CLA c 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

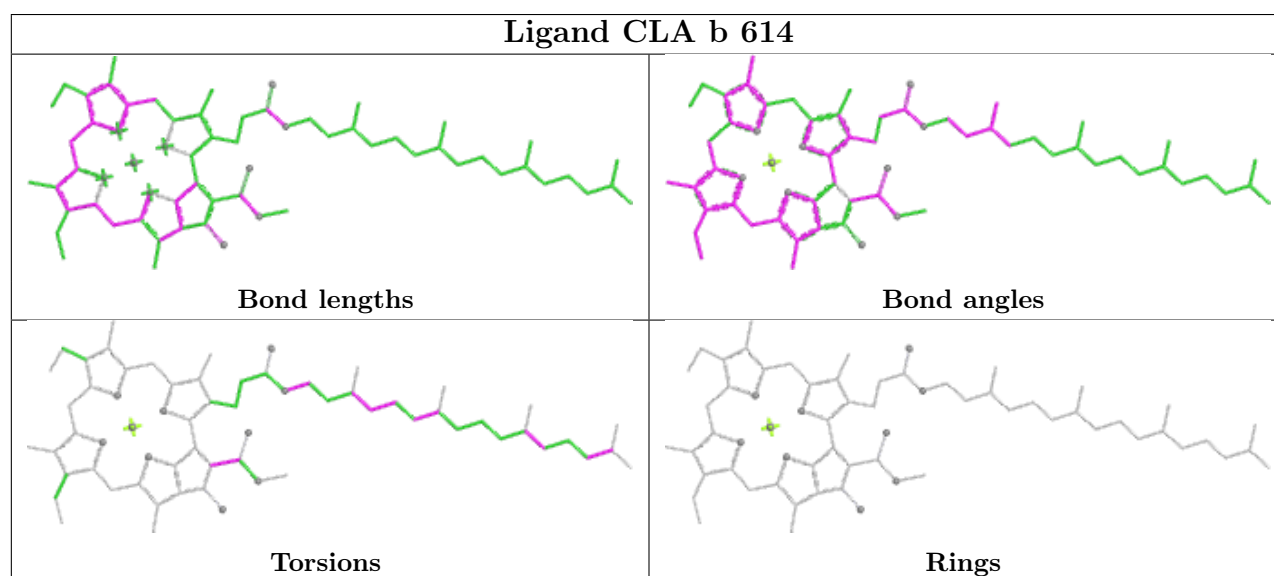
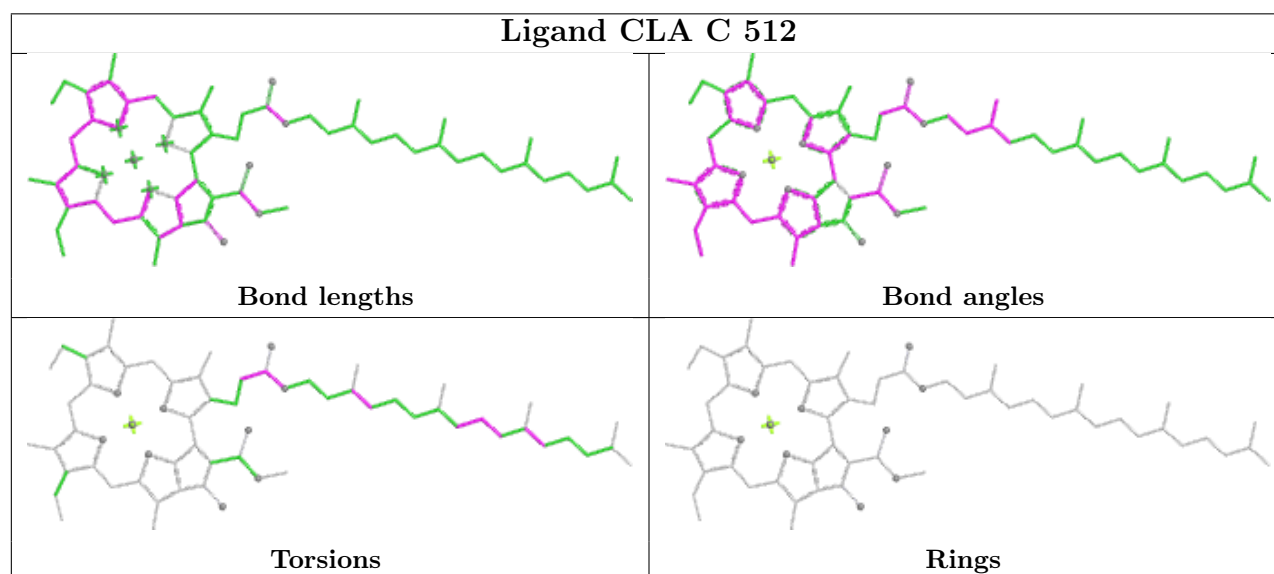
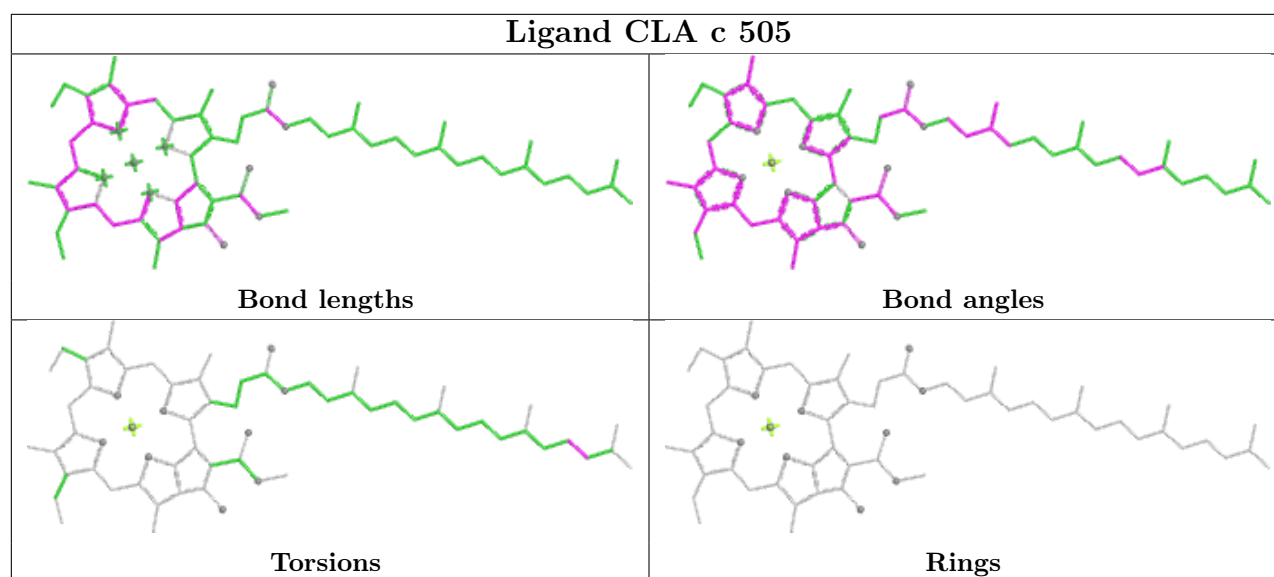
Ligand PL9 D 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

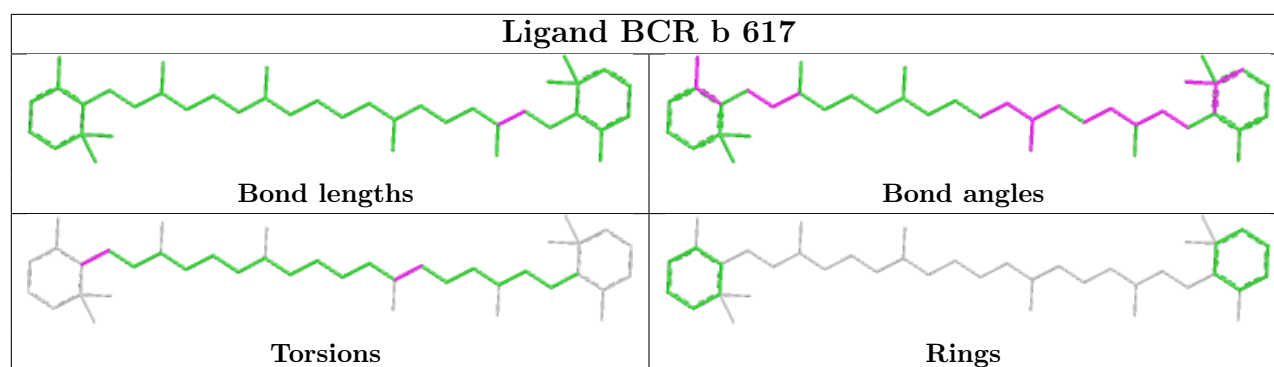
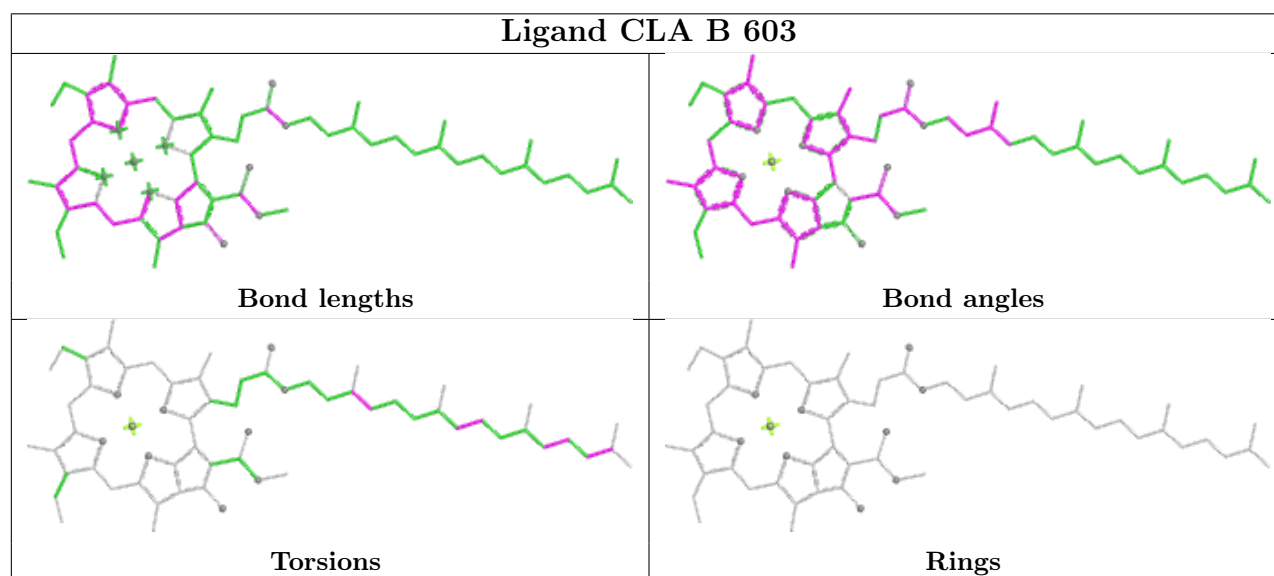
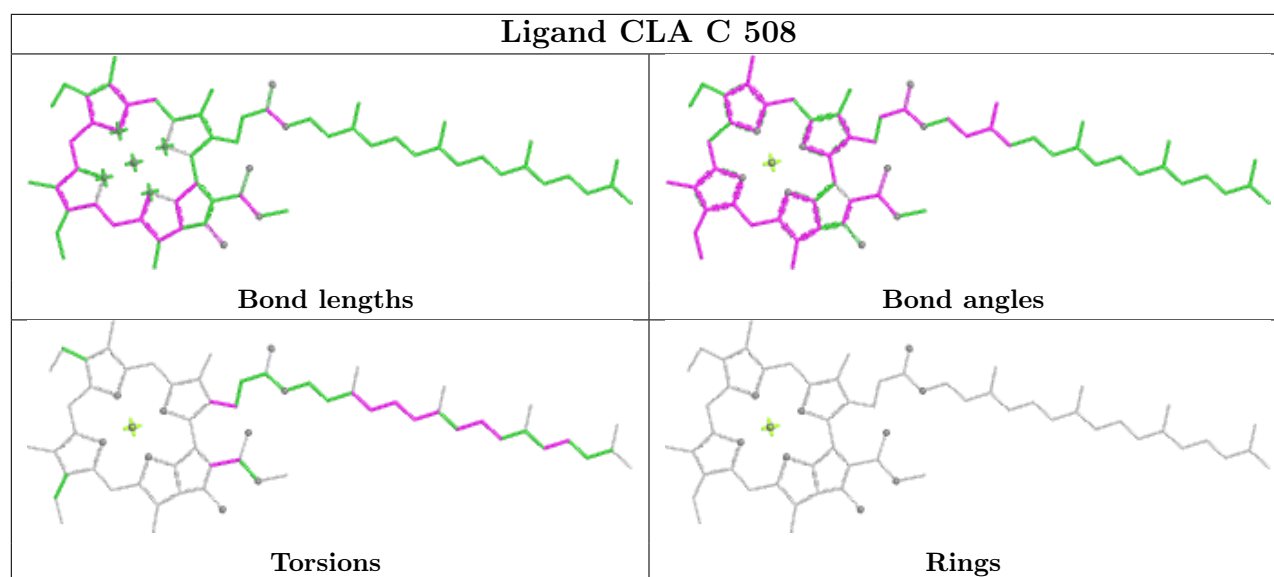


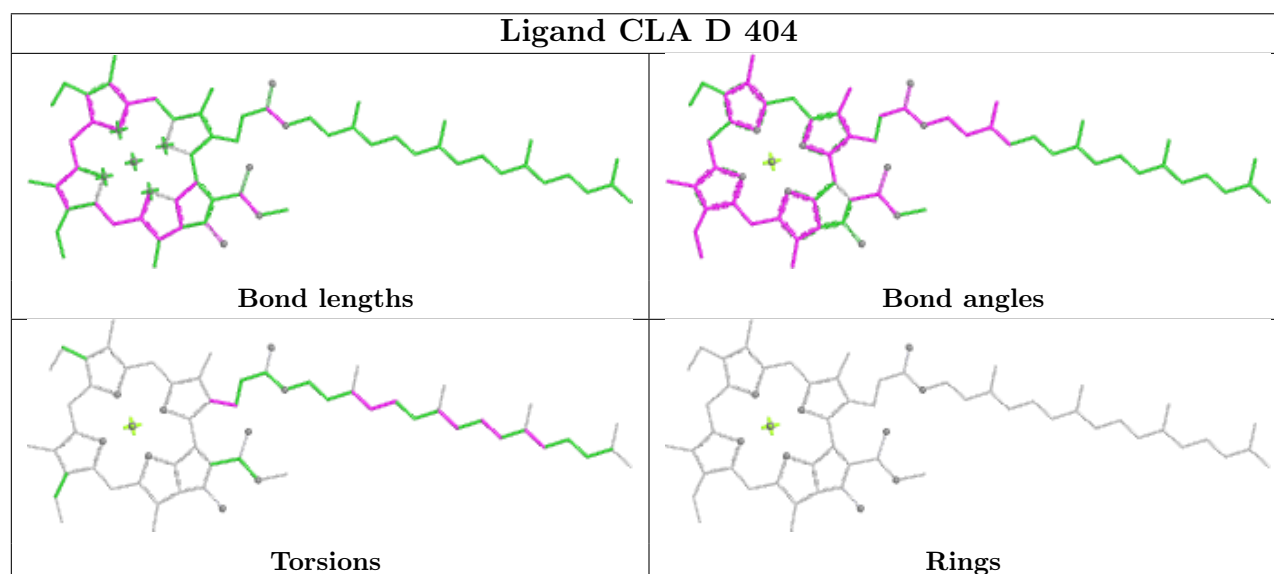
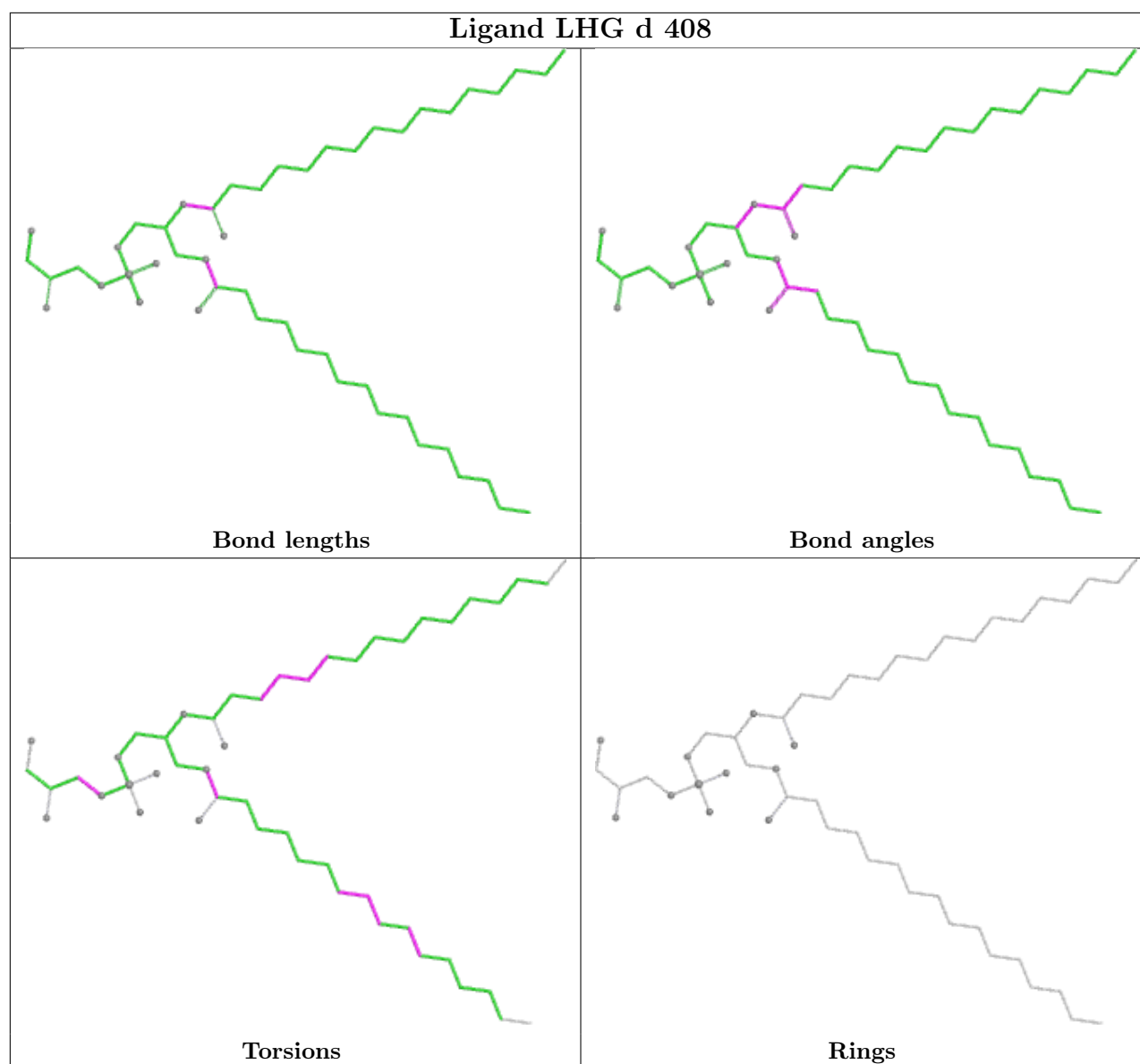


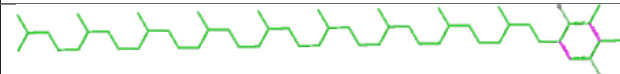
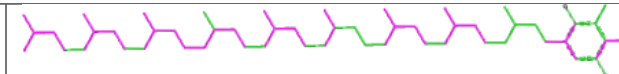
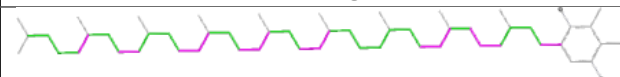
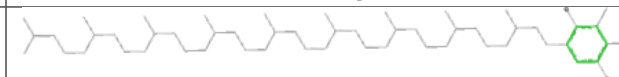
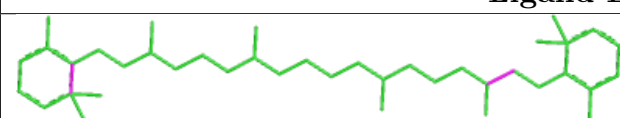
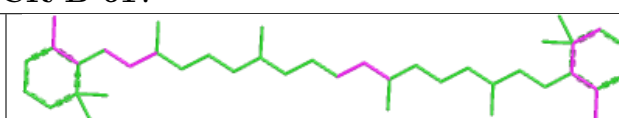
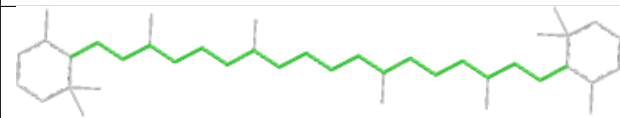
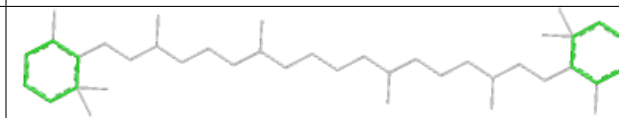
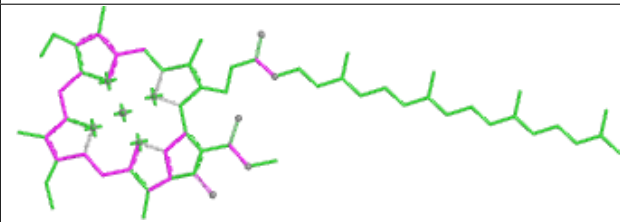
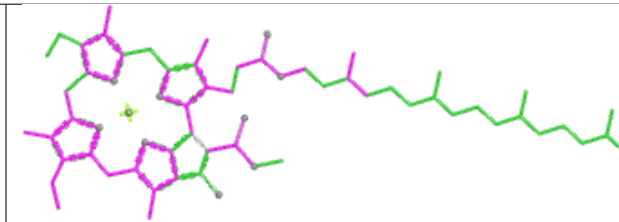
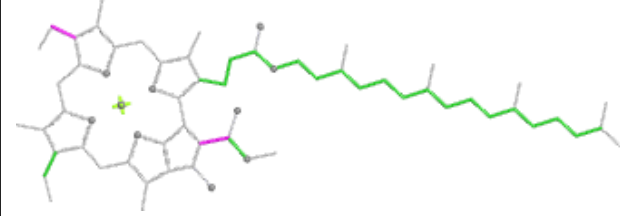
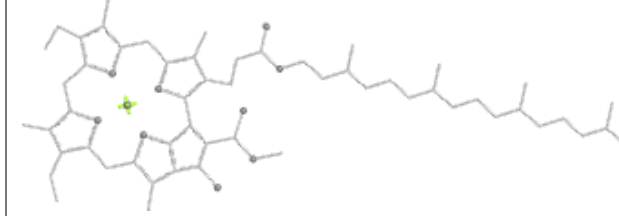
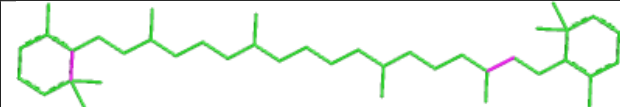
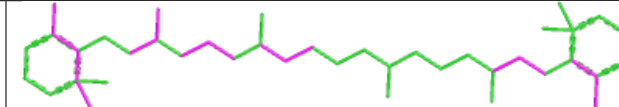
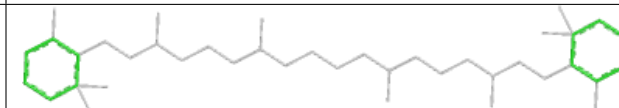


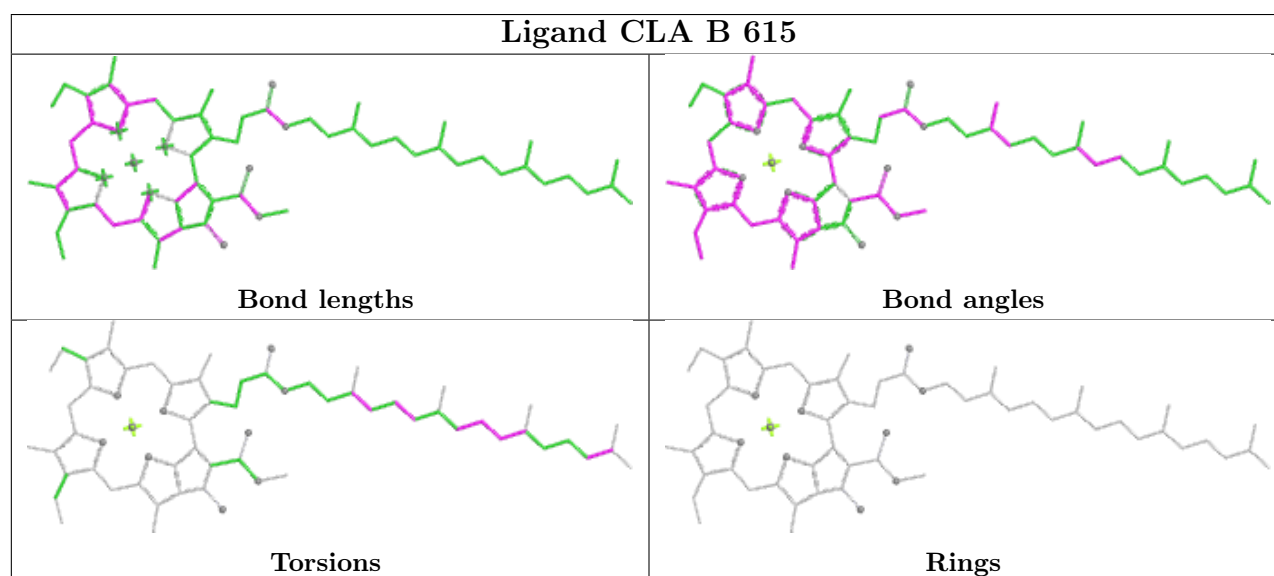
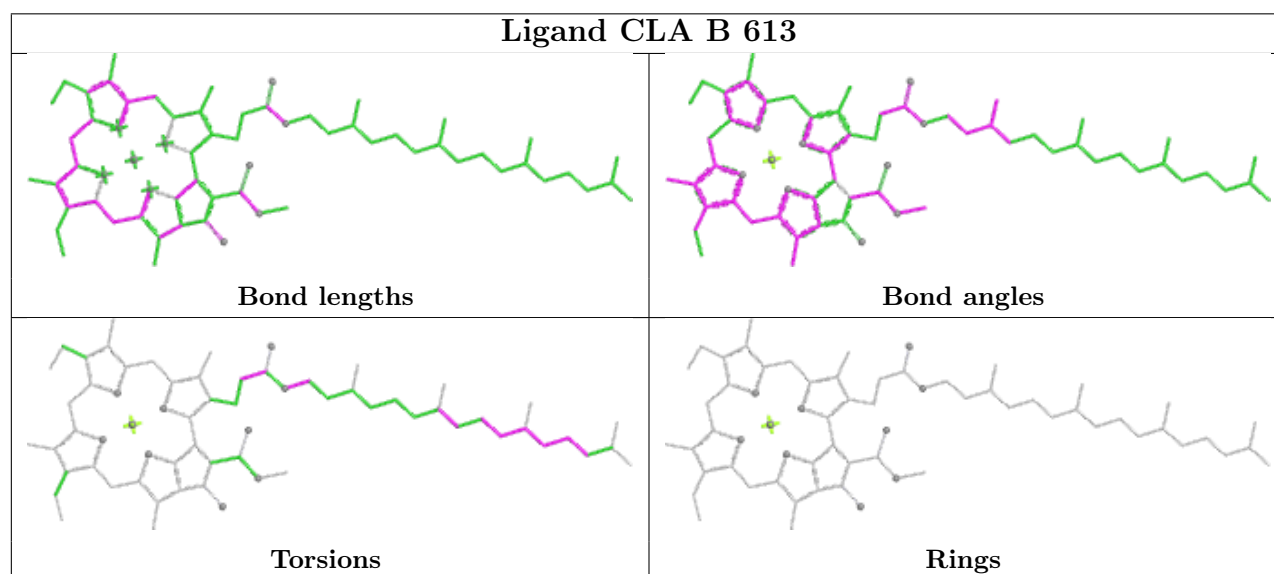
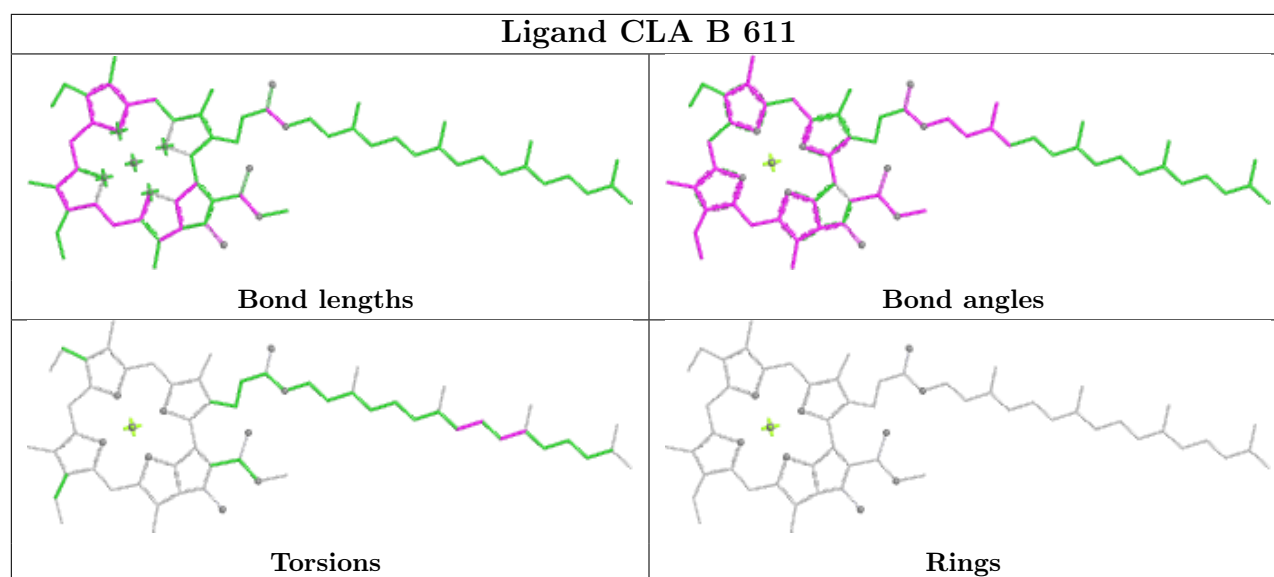


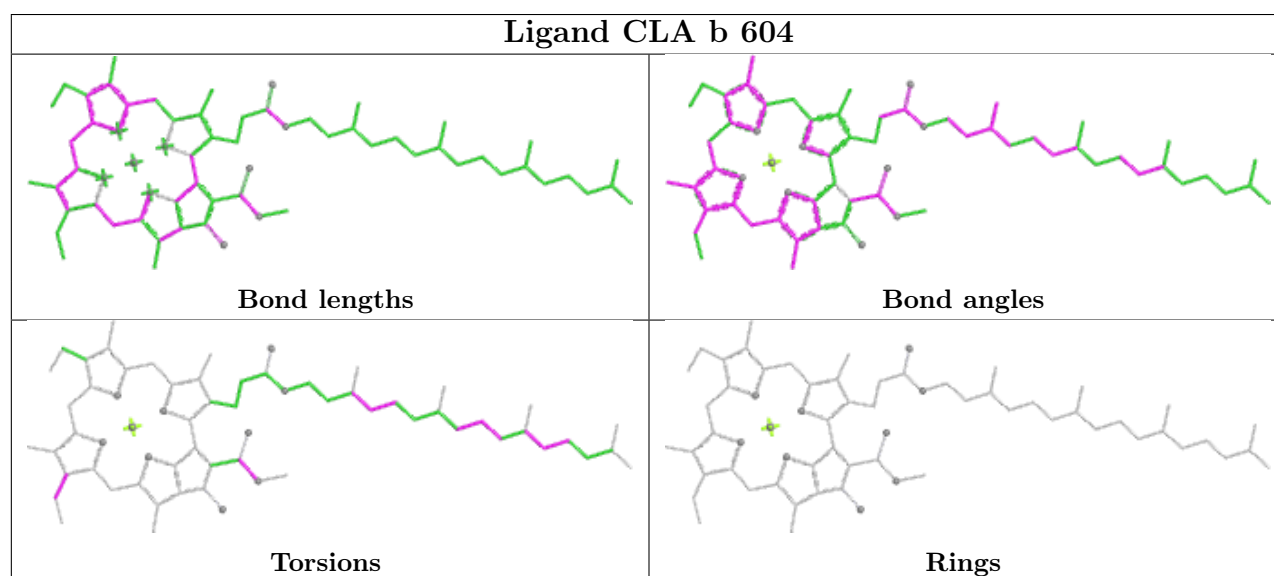
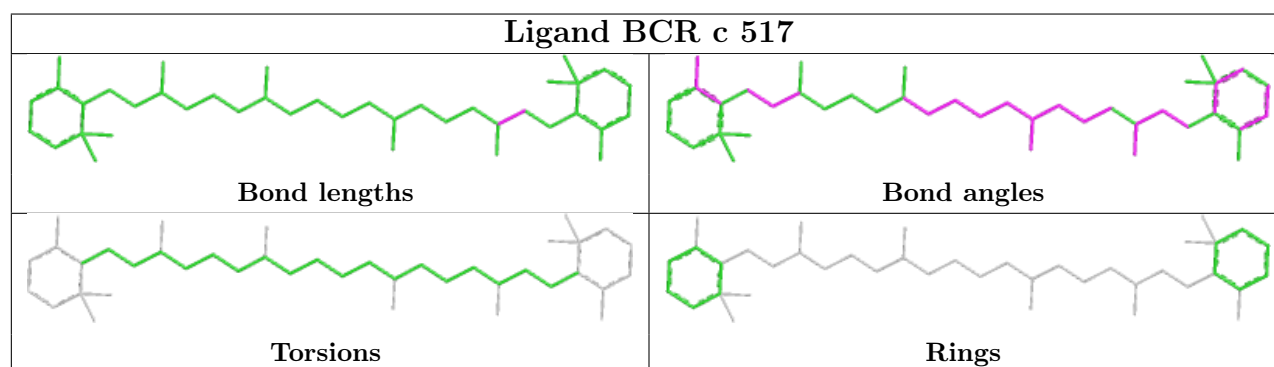
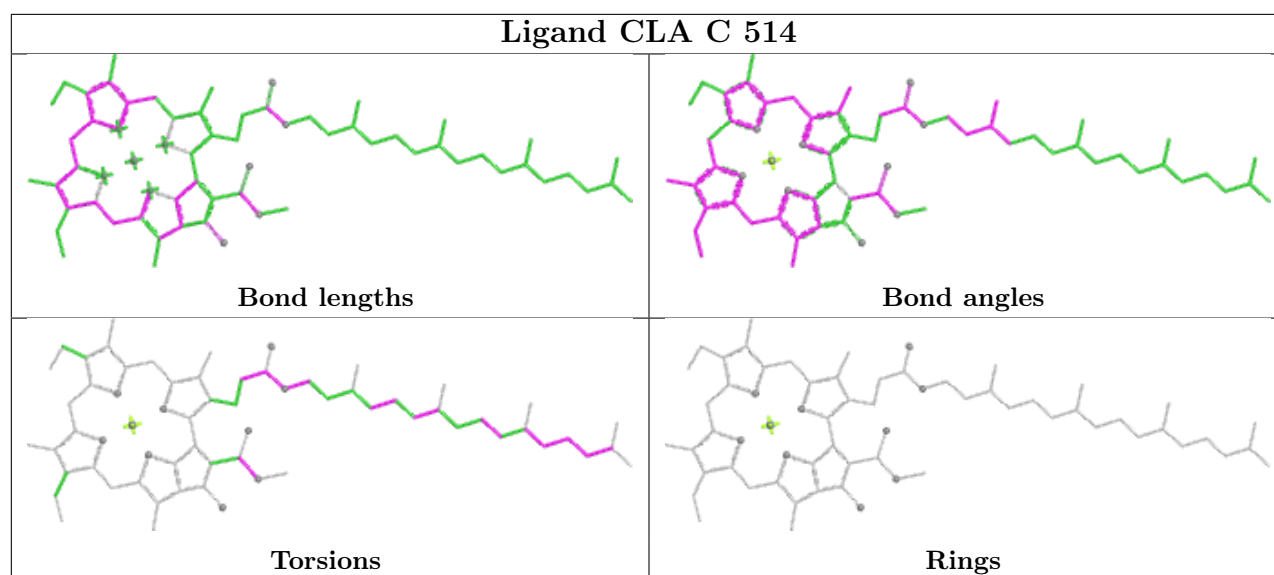


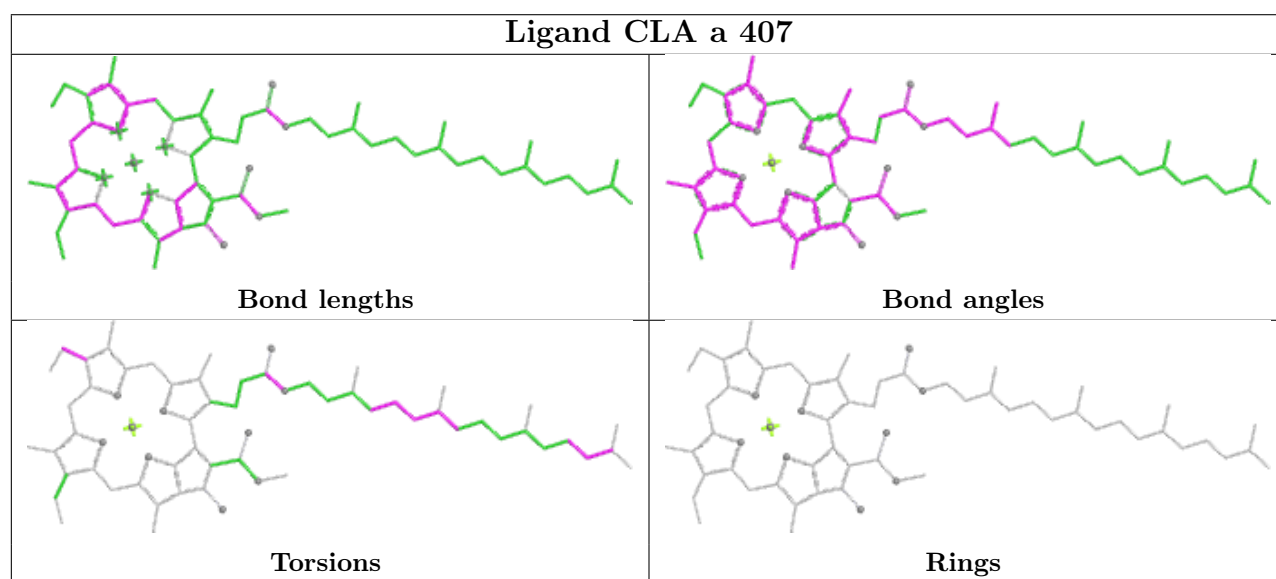
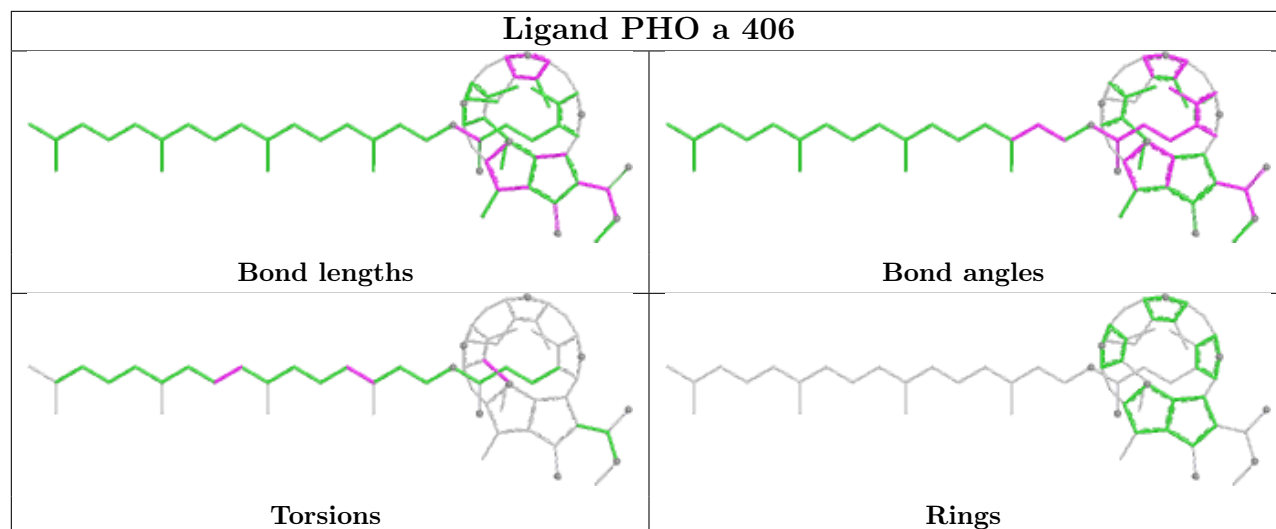


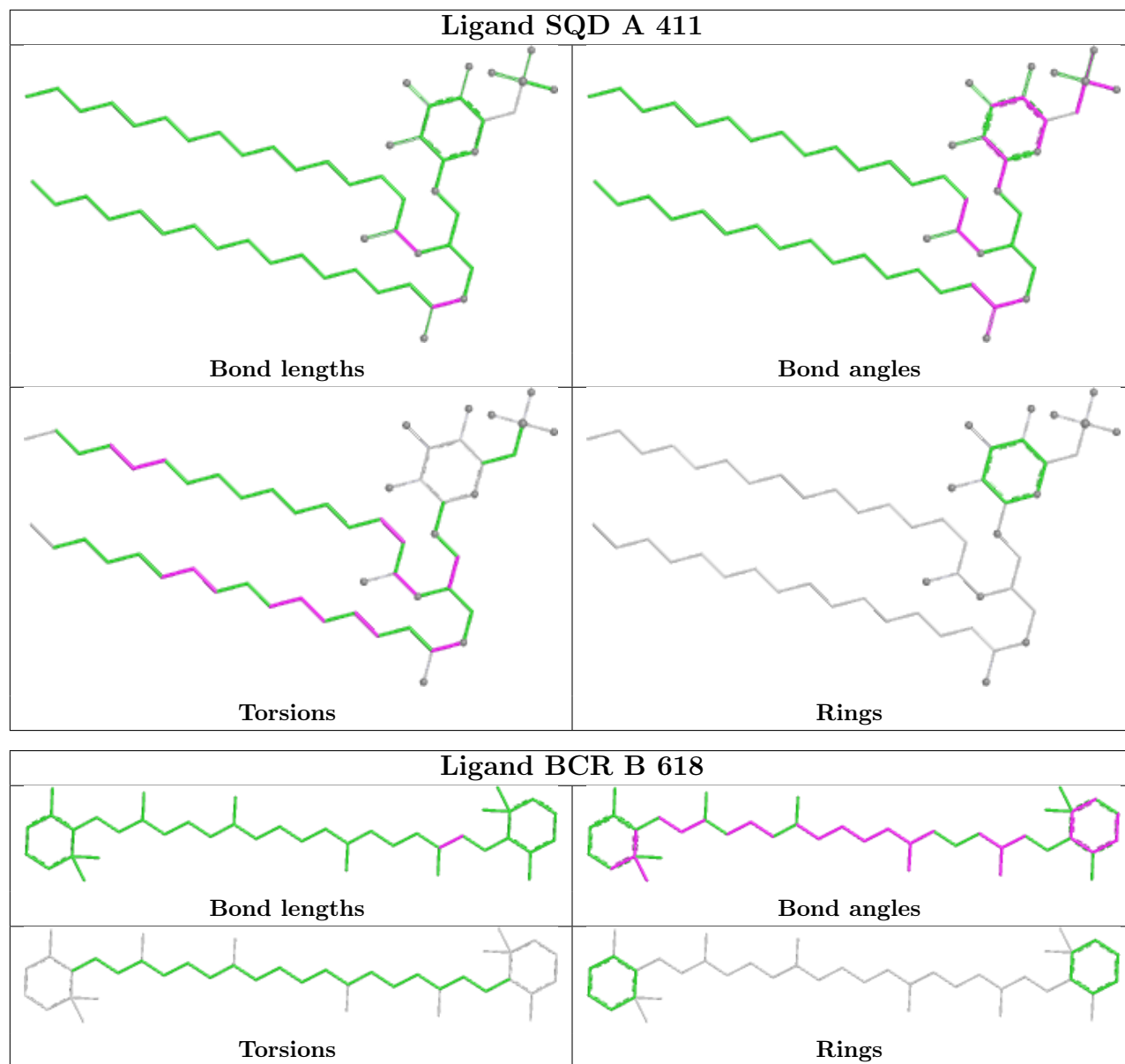


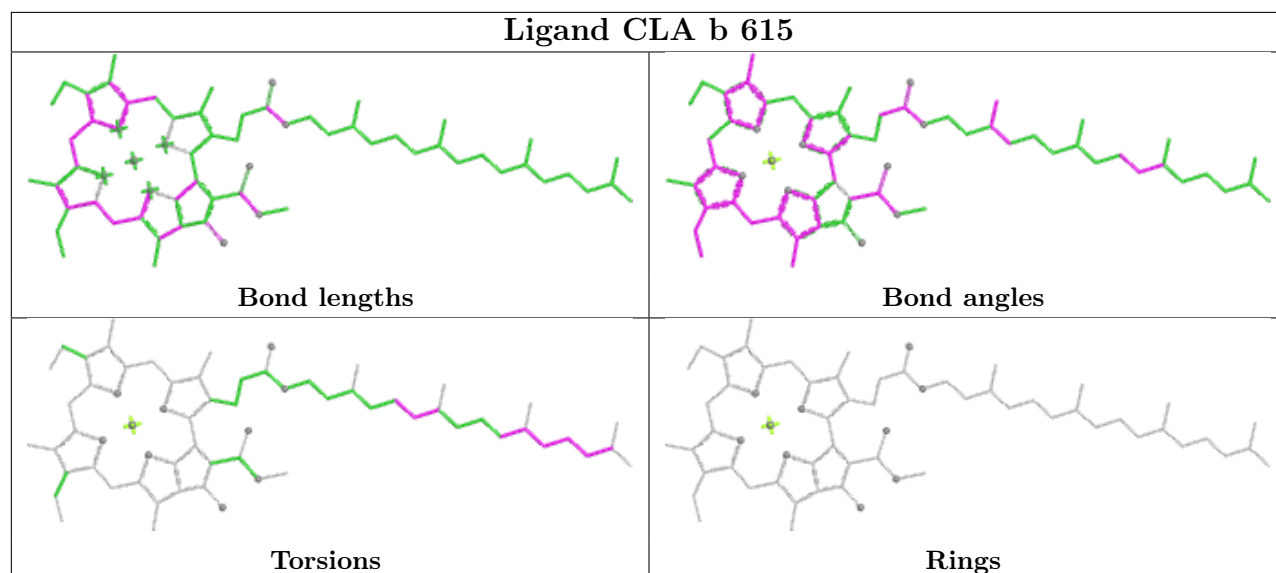
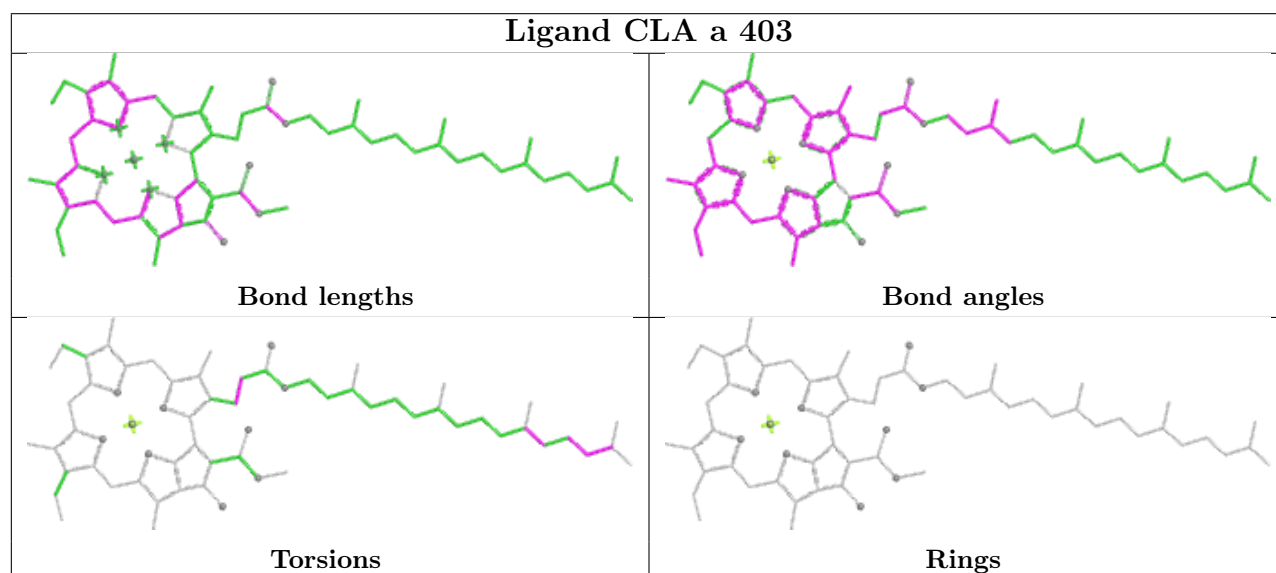
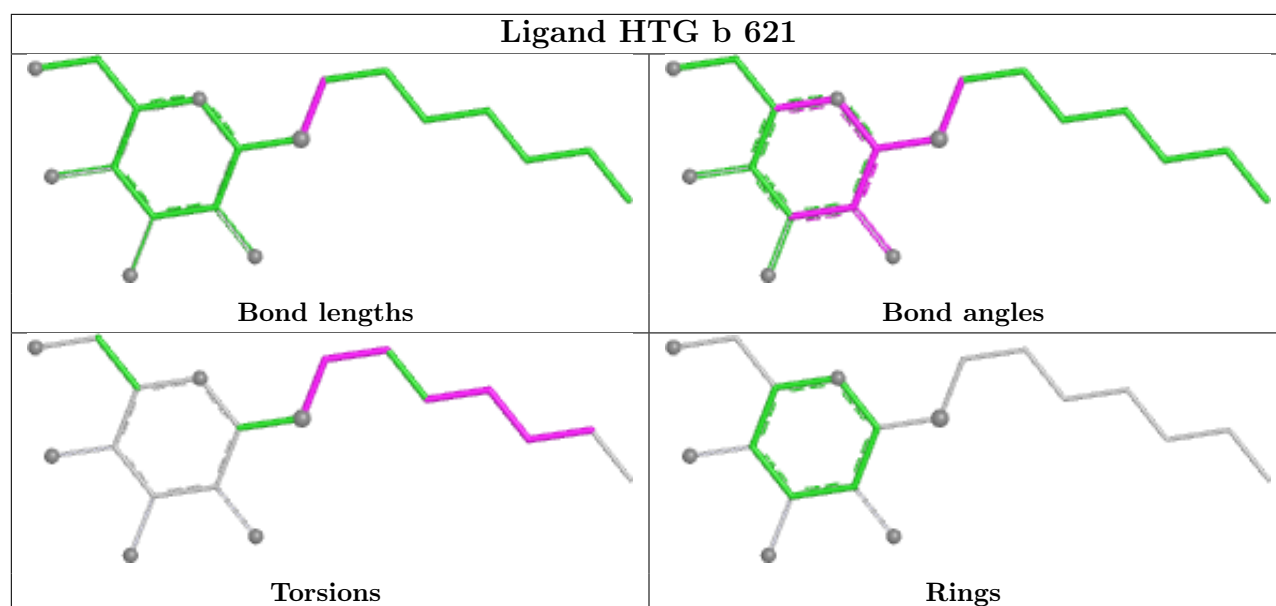
Ligand PL9 a 414 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 617	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 607	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR A 408	
 Bond lengths	 Bond angles
 Torsions	 Rings

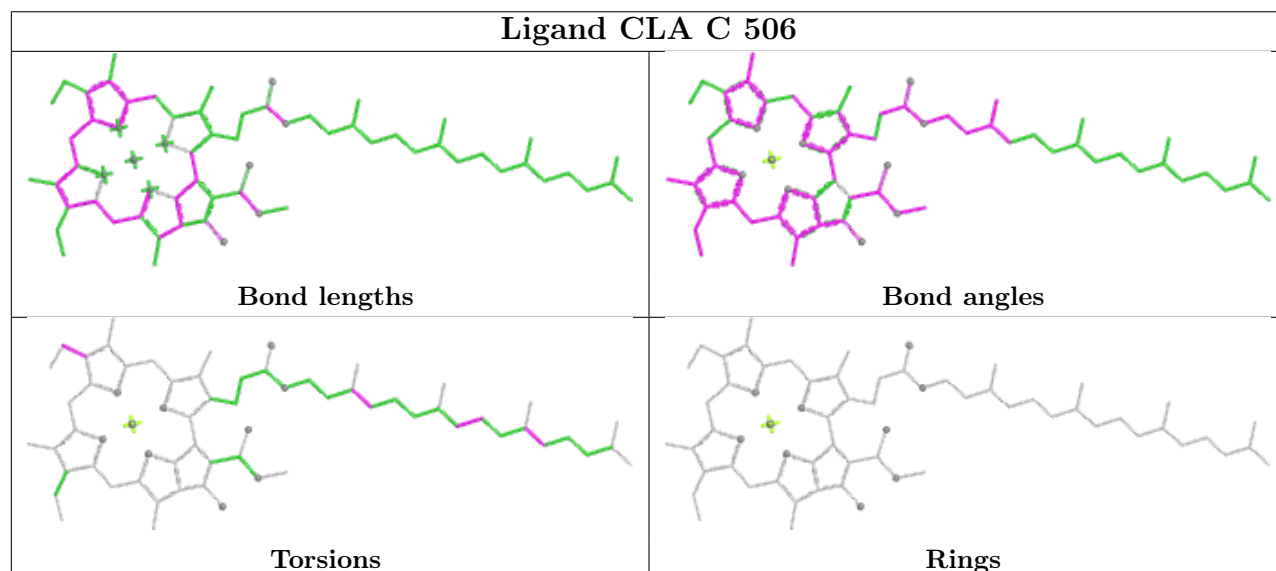
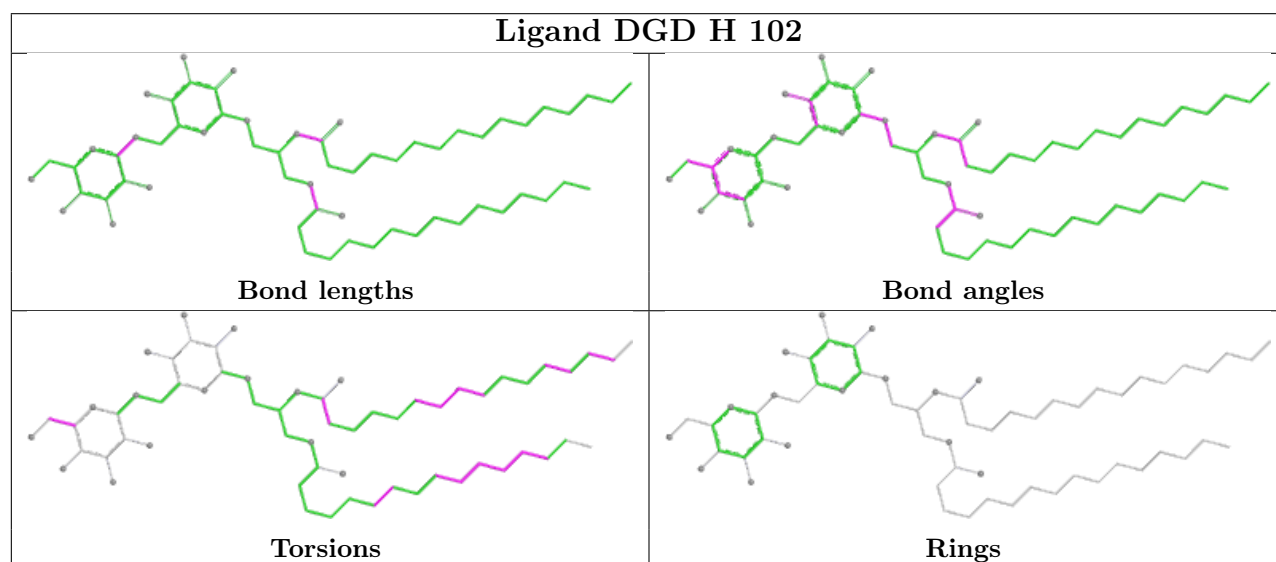
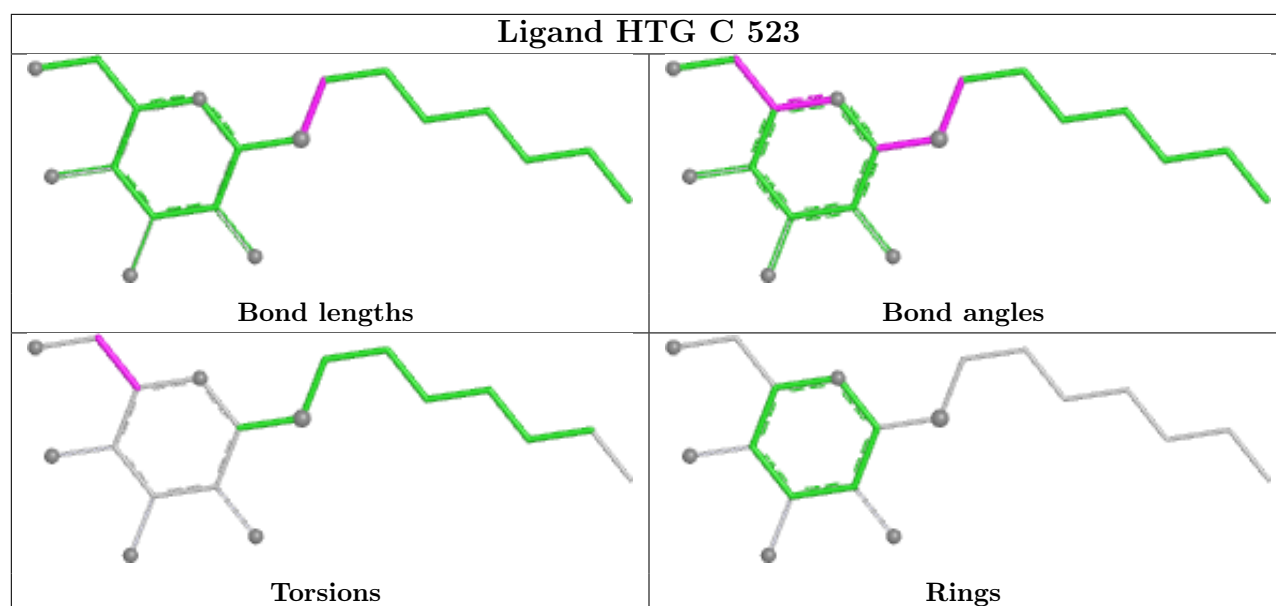


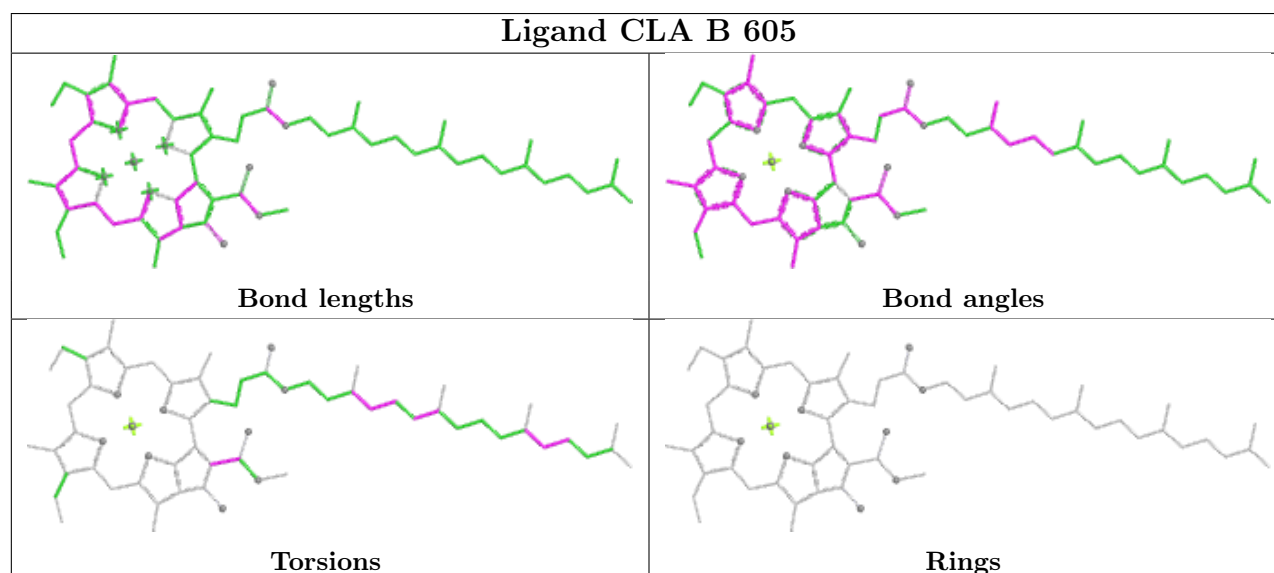
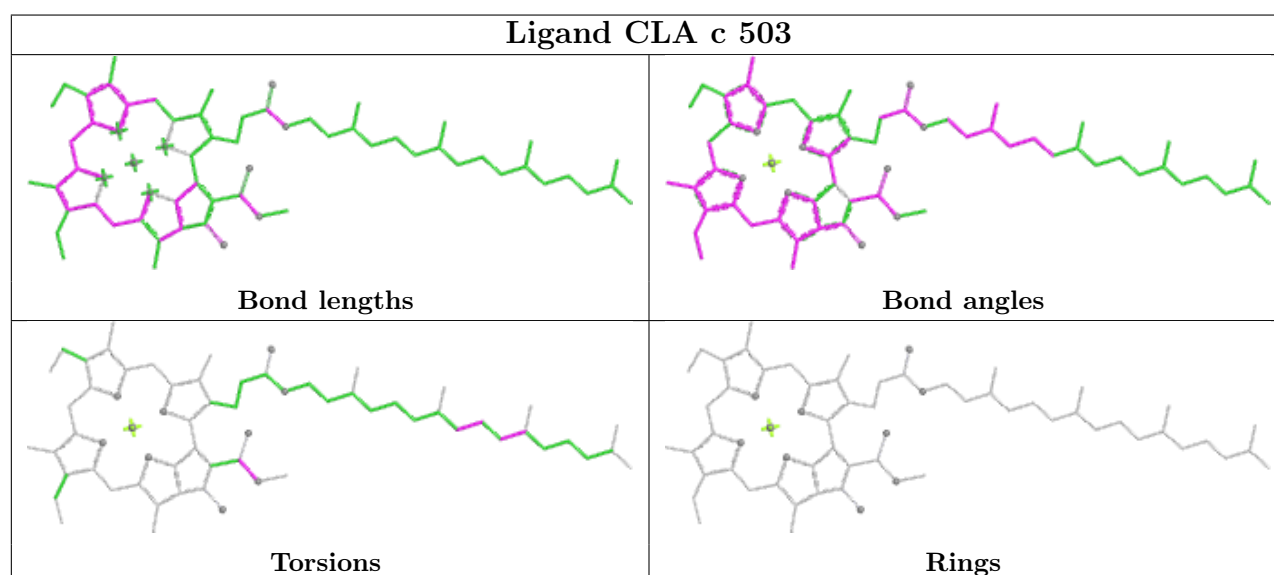
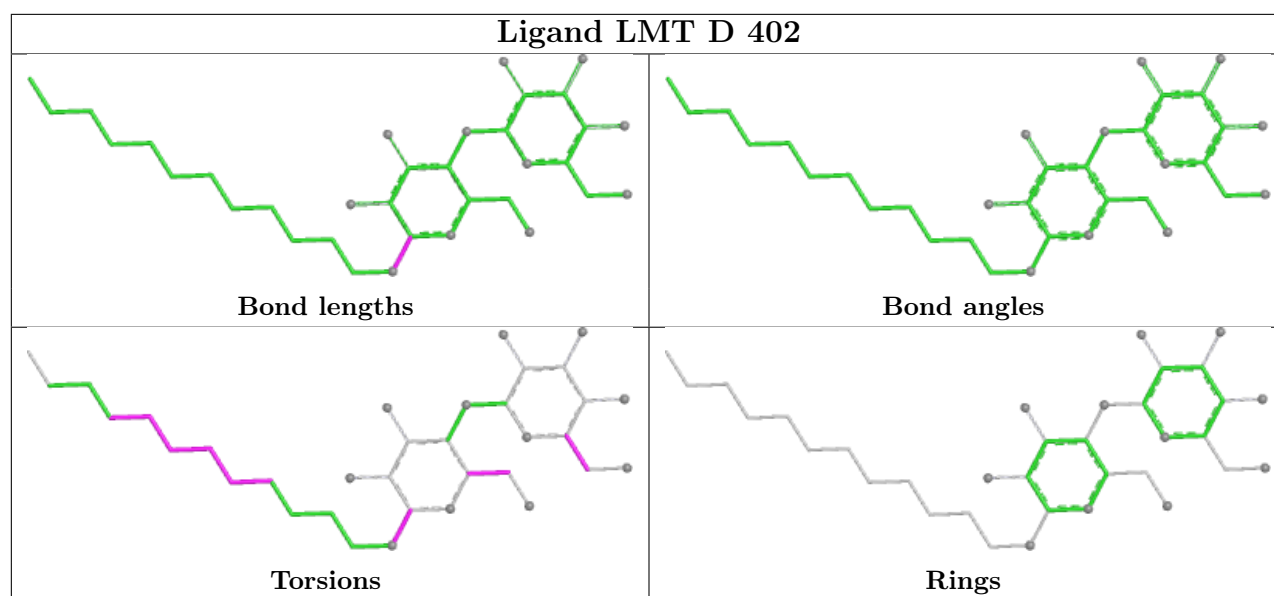


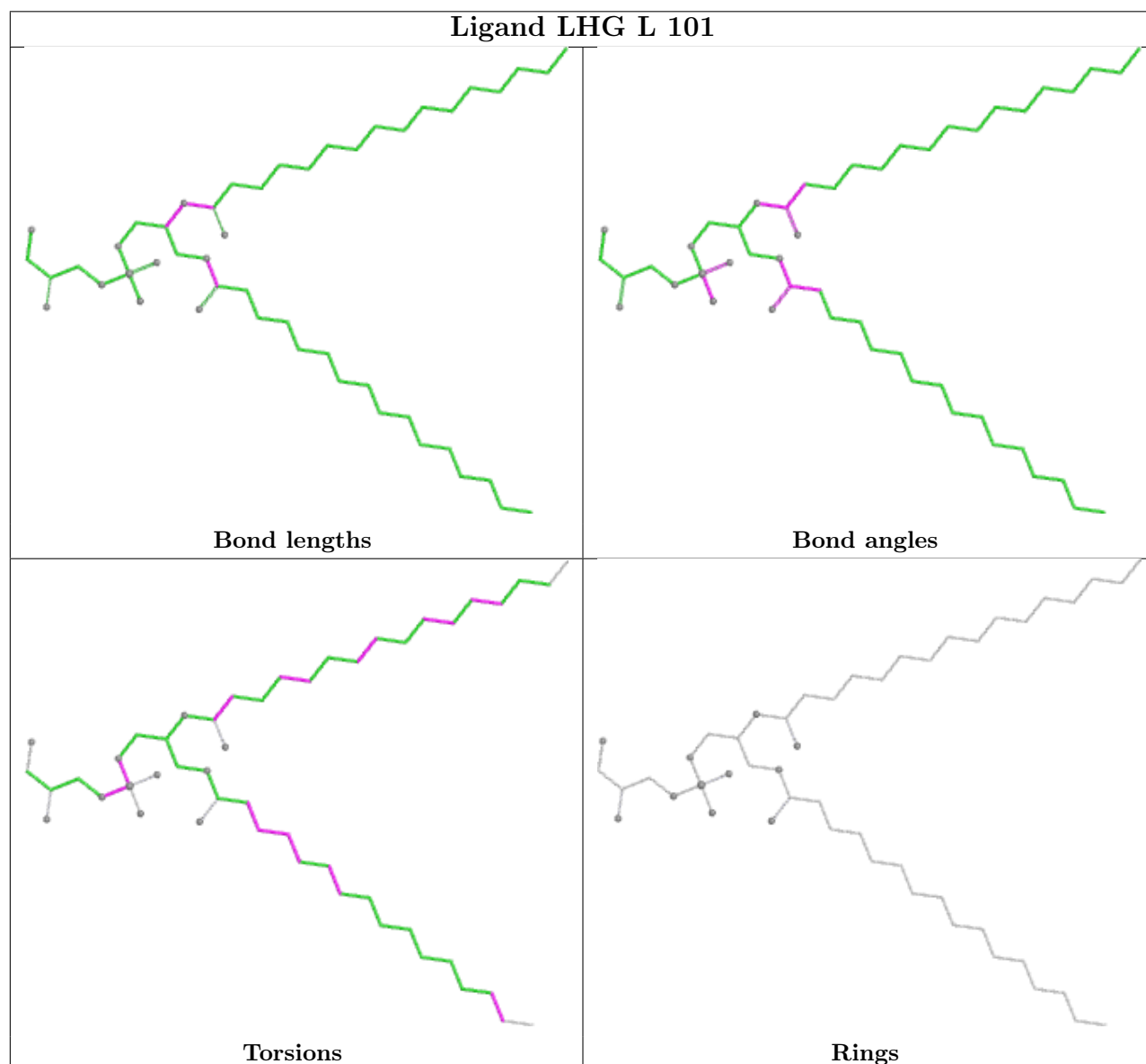
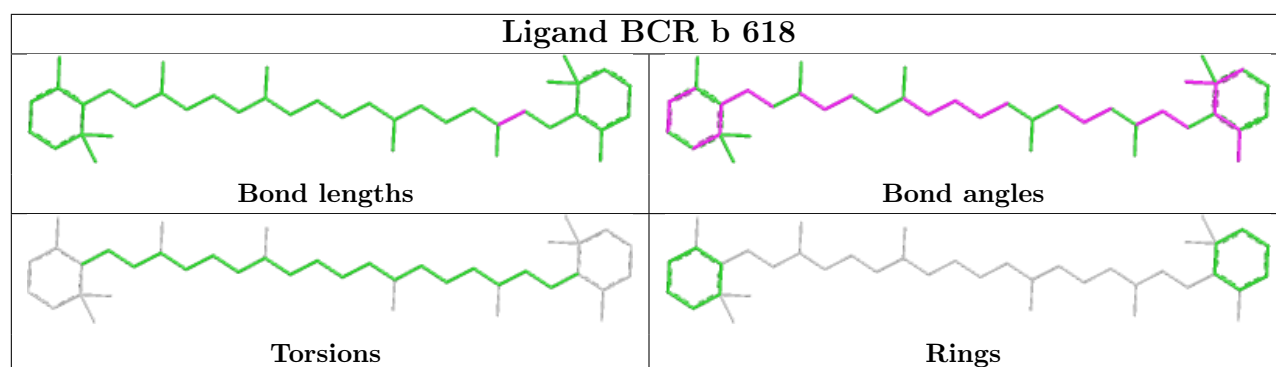


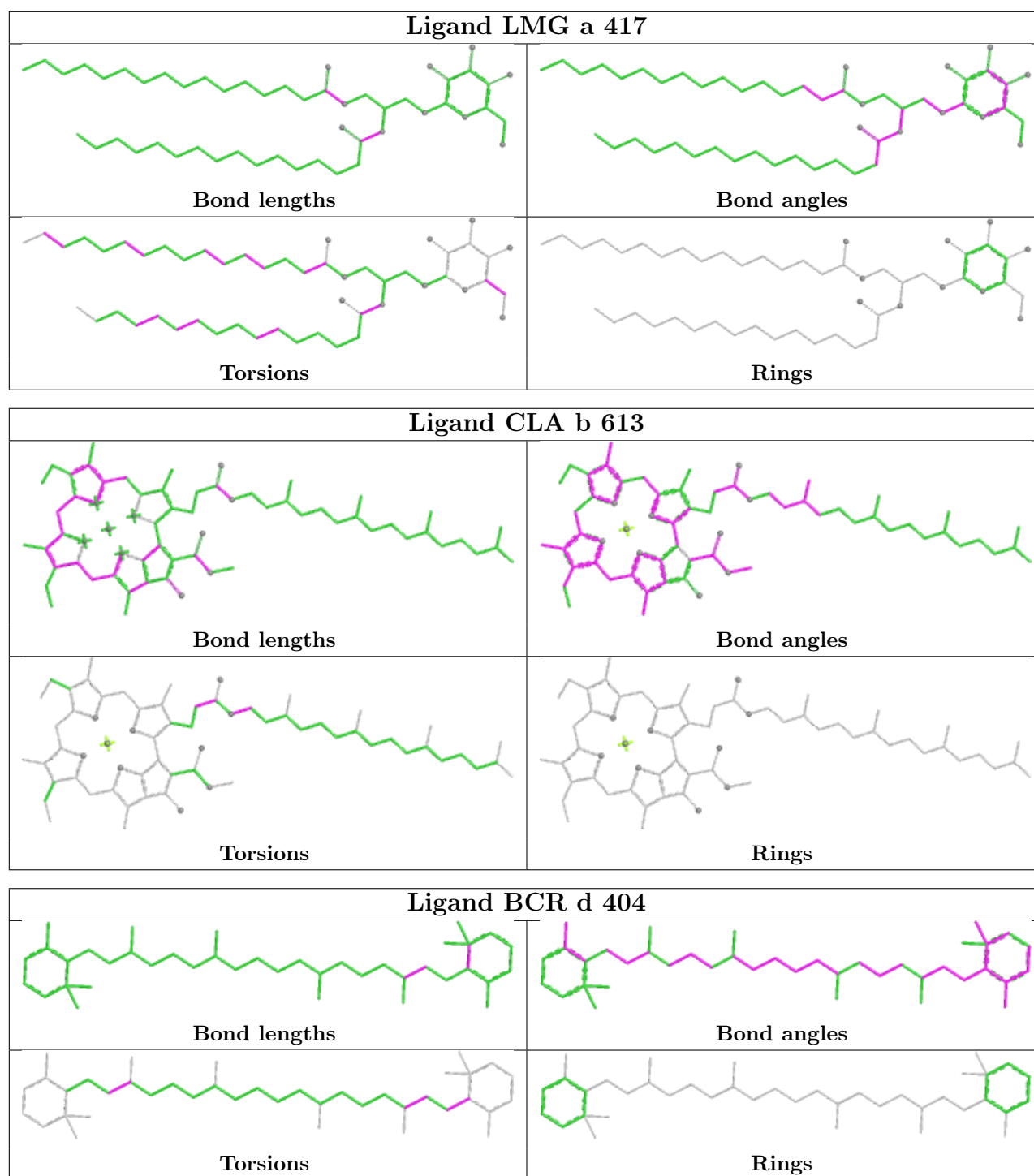




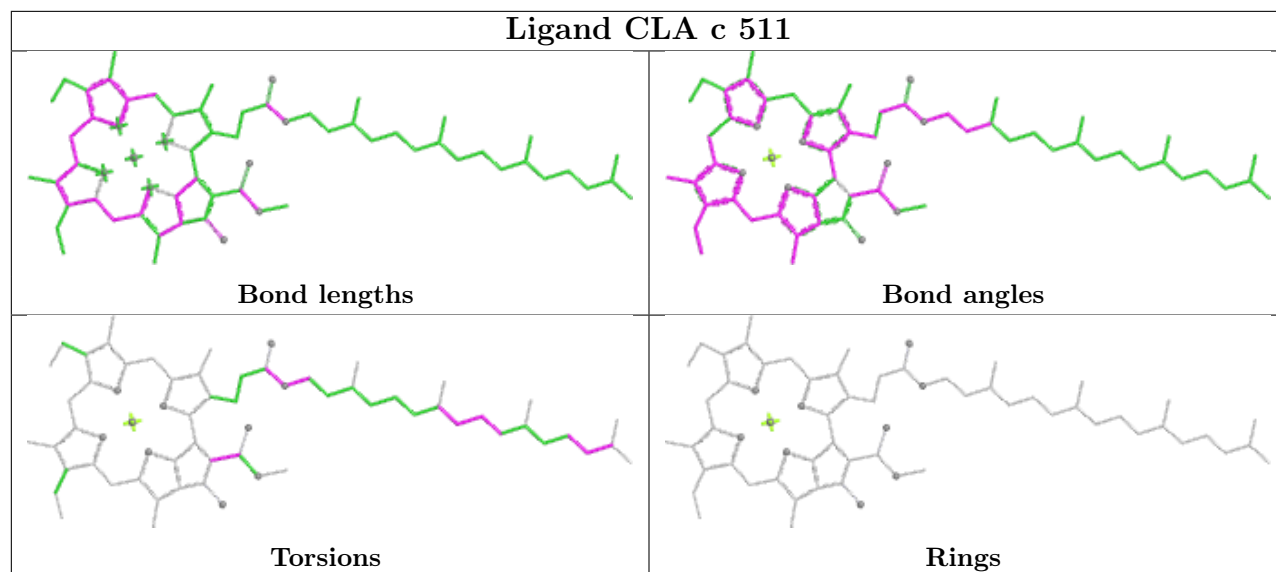




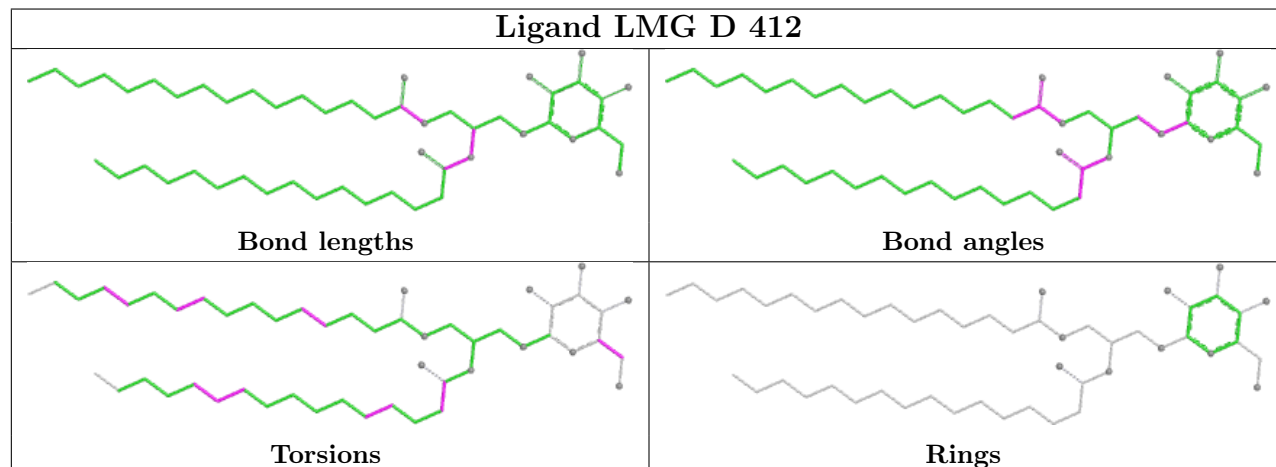




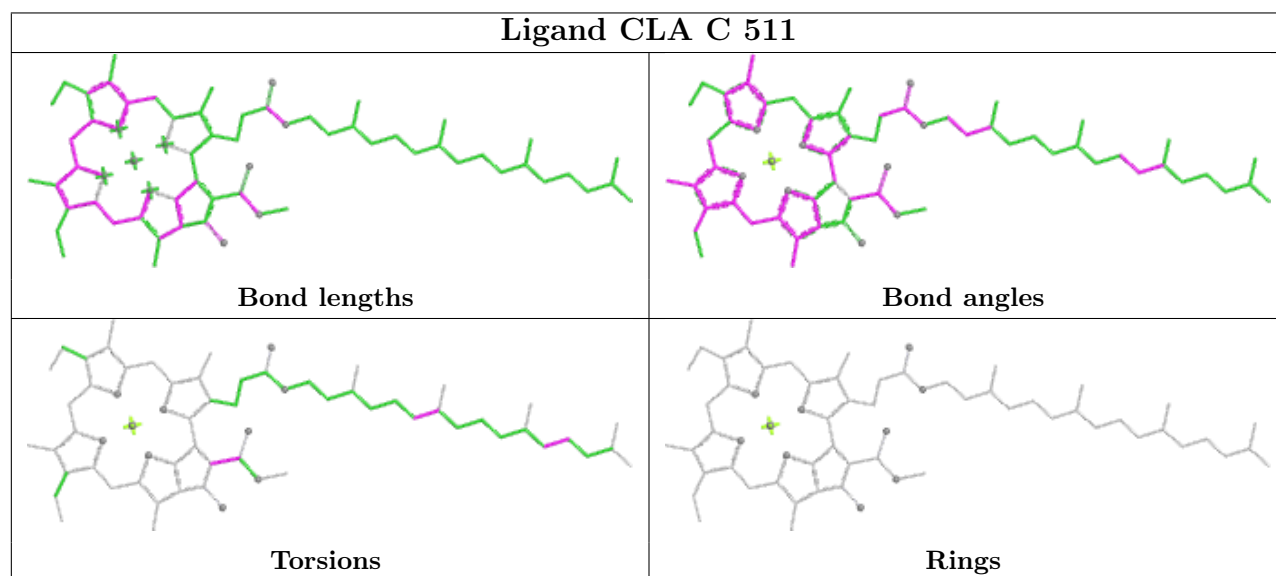
Ligand CLA c 511

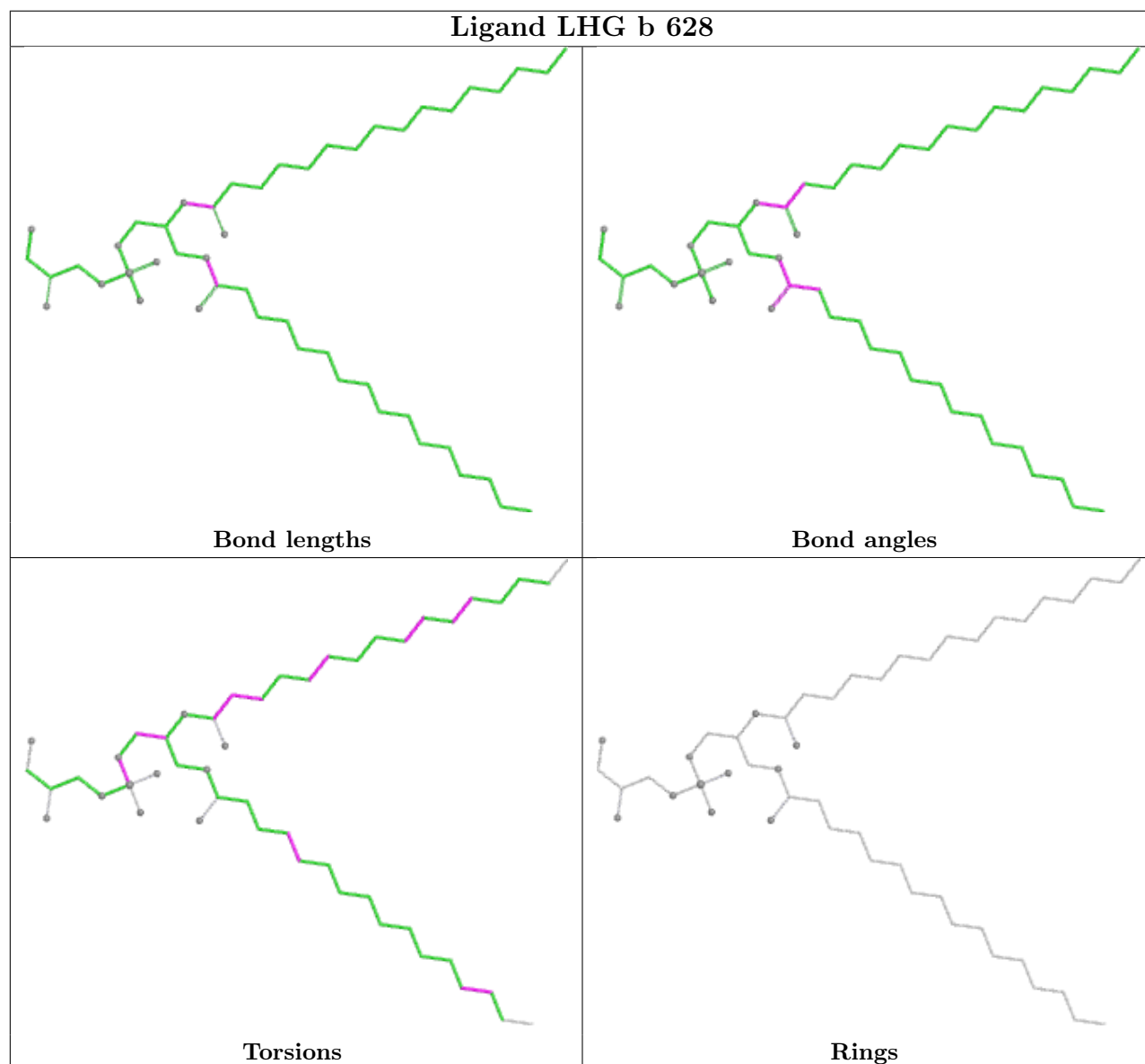
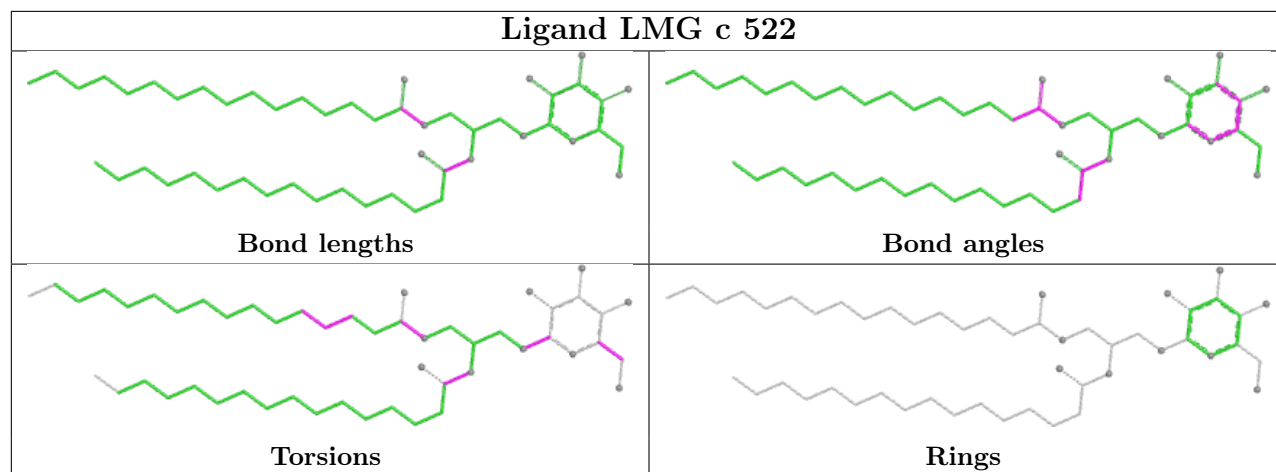


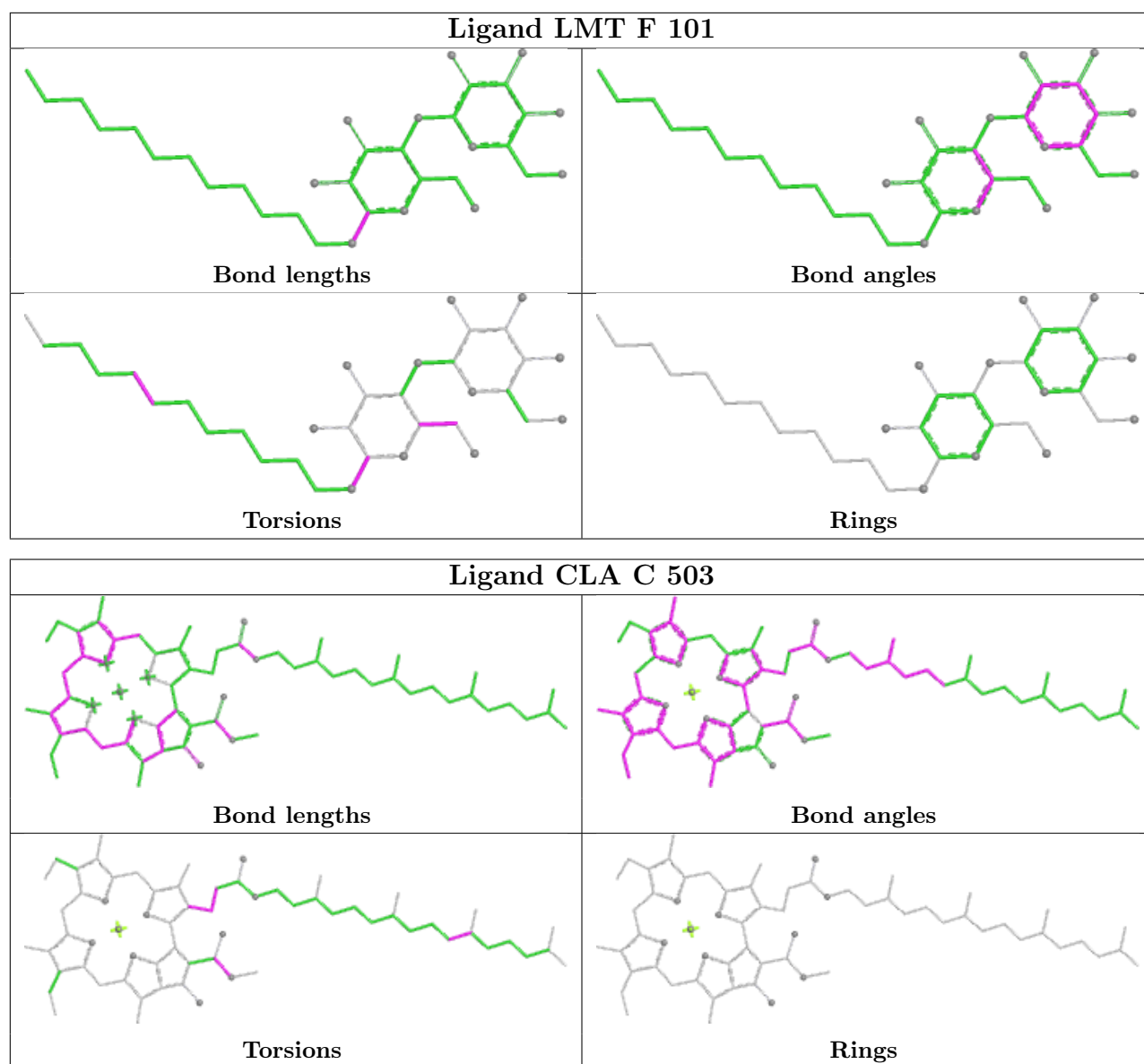
Ligand LMG D 412



Ligand CLA C 511







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%)	-0.60	0 100 100	20, 43, 67, 128	18 (5%)
1	a	334/344 (97%)	-0.57	3 (0%) 81 78	21, 47, 75, 110	19 (5%)
2	B	504/505 (99%)	-0.52	0 100 100	21, 49, 81, 127	10 (1%)
2	b	504/505 (99%)	-0.39	4 (0%) 82 80	23, 52, 92, 158	4 (0%)
3	C	451/455 (99%)	-0.38	2 (0%) 88 86	21, 56, 81, 156	5 (1%)
3	c	455/455 (100%)	-0.38	1 (0%) 91 89	24, 64, 86, 133	3 (0%)
4	D	342/342 (100%)	-0.57	0 100 100	22, 45, 68, 139	4 (1%)
4	d	341/342 (99%)	-0.63	0 100 100	23, 50, 73, 129	4 (1%)
5	E	81/84 (96%)	-0.15	1 (1%) 76 73	34, 70, 96, 139	1 (1%)
5	e	79/84 (94%)	-0.10	1 (1%) 75 71	59, 74, 116, 157	0
6	F	34/44 (77%)	-0.09	1 (2%) 53 50	50, 62, 85, 108	0
6	f	31/44 (70%)	-0.12	1 (3%) 50 46	58, 67, 92, 144	0
7	H	64/65 (98%)	-0.06	2 (3%) 51 47	29, 59, 81, 133	1 (1%)
7	h	64/65 (98%)	-0.07	1 (1%) 70 66	52, 65, 91, 105	0
8	I	37/38 (97%)	-0.13	0 100 100	49, 60, 124, 148	0
8	i	37/38 (97%)	-0.21	0 100 100	52, 60, 114, 145	0
9	J	38/39 (97%)	-0.16	1 (2%) 57 53	50, 70, 131, 177	0
9	j	39/39 (100%)	0.05	1 (2%) 57 53	58, 73, 125, 165	0
10	K	37/37 (100%)	-0.33	0 100 100	58, 67, 89, 113	0
10	k	37/37 (100%)	-0.31	0 100 100	66, 73, 95, 113	0
11	L	36/37 (97%)	-0.28	1 (2%) 55 51	20, 41, 93, 140	1 (2%)
11	l	36/37 (97%)	-0.29	0 100 100	20, 42, 105, 134	1 (2%)
12	M	32/36 (88%)	-0.41	0 100 100	21, 44, 73, 146	1 (3%)
12	m	33/36 (91%)	-0.57	0 100 100	38, 44, 82, 132	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.37	0 100 100	25, 60, 113, 178	3 (1%)
13	o	243/244 (99%)	-0.26	0 100 100	26, 61, 119, 171	2 (0%)
14	T	29/32 (90%)	-0.59	1 (3%) 48 44	38, 43, 83, 104	0
14	t	29/32 (90%)	-0.57	1 (3%) 48 44	38, 46, 74, 139	0
15	U	96/104 (92%)	-0.52	0 100 100	44, 56, 88, 92	0
15	u	97/104 (93%)	-0.52	0 100 100	48, 61, 80, 129	0
16	V	137/137 (100%)	-0.55	0 100 100	43, 55, 80, 112	0
16	v	137/137 (100%)	-0.39	0 100 100	50, 69, 103, 131	0
17	X	38/40 (95%)	-0.06	0 100 100	54, 69, 91, 110	0
17	x	38/40 (95%)	-0.03	0 100 100	60, 74, 124, 157	0
18	Y	29/30 (96%)	0.29	2 (6%) 23 19	67, 89, 136, 169	0
18	y	29/30 (96%)	0.14	0 100 100	75, 87, 113, 116	0
19	Z	62/62 (100%)	-0.08	0 100 100	69, 83, 138, 186	0
19	z	62/62 (100%)	0.31	2 (3%) 50 46	76, 95, 137, 185	0
20	R	34/34 (100%)	0.94	1 (2%) 53 50	91, 106, 138, 142	0
All	All	5283/5384 (98%)	-0.40	27 (0%) 87 85	20, 55, 99, 186	77 (1%)

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	5.7
14	t	30	THR	3.7
7	h	65	LEU	3.2
1	a	264[A]	SER	3.2
3	C	23	ALA	3.1

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	0.08	46,67,72,75	0
12	FME	M	1	10/11	0.96	0.10	31,59,83,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	FME	T	1	10/11	0.97	0.07	39,48,63,64	0
8	FME	i	1	10/11	0.97	0.05	52,62,75,81	0
12	FME	m	1	10/11	0.97	0.06	38,52,79,90	0
14	FME	t	1	10/11	0.97	0.07	35,44,61,70	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
33	LMT	F	101	35/35	0.65	0.20	105,152,164,167	0
33	LMT	C	526	35/35	0.66	0.17	93,147,159,160	0
33	LMT	e	101	35/35	0.67	0.18	121,173,177,179	0
30	UNL	A	414	28/-	0.73	0.19	88,103,120,121	0
30	UNL	j	101	10/-	0.73	0.27	81,90,102,103	0
32	HTG	D	411	16/19	0.73	0.14	82,116,129,129	0
32	HTG	b	622	19/19	0.74	0.15	86,138,148,150	0
33	LMT	a	418	35/35	0.75	0.16	113,144,152,153	0
33	LMT	a	412	35/35	0.75	0.19	63,131,144,146	0
30	UNL	J	101	10/-	0.78	0.27	69,84,88,90	0
33	LMT	D	402	35/35	0.78	0.20	75,130,140,142	0
32	HTG	c	523	19/19	0.78	0.14	119,131,139,141	0
30	UNL	m	102	10/-	0.79	0.20	59,67,88,90	0
30	UNL	C	527	34/-	0.79	0.18	83,110,123,129	0
26	SQD	f	101	43/54	0.80	0.16	111,129,159,160	0
30	UNL	i	101	40/-	0.81	0.19	72,97,151,154	0
30	UNL	a	415	30/-	0.81	0.15	100,110,133,140	0
34	LMG	C	522	51/55	0.81	0.18	76,125,159,161	0
30	UNL	I	101	40/-	0.82	0.20	74,108,148,149	0
30	UNL	c	526	32/-	0.83	0.18	91,111,125,129	0
32	HTG	B	622	19/19	0.83	0.17	79,89,99,100	0
32	HTG	C	523	19/19	0.83	0.15	108,122,132,133	0
33	LMT	m	103	35/35	0.83	0.14	59,97,109,113	0
33	LMT	M	103	35/35	0.83	0.15	75,140,160,163	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	LMG	c	522	51/55	0.83	0.17	80,125,151,152	0
30	UNL	b	625	33/-	0.84	0.17	65,94,146,147	0
33	LMT	B	627	35/35	0.84	0.14	68,112,127,131	0
34	LMG	Z	101	37/55	0.84	0.15	73,129,162,169	0
31	LHG	a	419	42/49	0.84	0.14	86,136,170,174	0
33	LMT	b	626	25/35	0.85	0.14	46,70,129,135	0
31	LHG	E	101	42/49	0.85	0.16	74,114,131,133	0
36	CA	F	102	1/1	0.85	0.10	103,103,103,103	0
32	HTG	h	101	16/19	0.86	0.12	99,134,140,142	0
30	UNL	B	625	33/-	0.87	0.15	56,105,148,152	0
30	UNL	d	410	36/-	0.87	0.16	72,92,117,120	0
32	HTG	b	621	19/19	0.87	0.15	61,78,111,112	0
33	LMT	b	620	25/35	0.87	0.16	90,129,147,148	0
27	GOL	B	626	6/6	0.87	0.20	82,99,100,103	0
30	UNL	D	410	40/-	0.87	0.17	52,87,126,132	0
30	UNL	l	101	10/-	0.87	0.17	63,74,83,85	0
27	GOL	B	628	6/6	0.87	0.16	90,102,105,109	0
27	GOL	O	302	6/6	0.87	0.10	78,84,85,85	0
27	GOL	c	527	6/6	0.87	0.19	105,109,114,116	0
26	SQD	a	411	54/54	0.87	0.12	63,89,126,130	0
33	LMT	B	630	26/35	0.88	0.15	78,117,140,143	0
32	HTG	V	202	11/19	0.88	0.12	109,114,122,124	0
26	SQD	D	413	43/54	0.88	0.14	70,105,125,136	0
23	CLA	b	601	65/65	0.88	0.12	58,80,119,128	0
33	LMT	B	629	25/35	0.88	0.14	56,79,132,133	0
26	SQD	B	620	54/54	0.89	0.13	60,89,121,127	0
23	CLA	B	601	65/65	0.89	0.12	54,73,118,127	0
33	LMT	M	102	35/35	0.89	0.11	54,105,130,138	0
29	PL9	A	413[A]	55/55	0.89	0.22	89,97,103,104	55
29	PL9	A	413[B]	55/55	0.89	0.22	88,97,104,104	55
26	SQD	A	411	54/54	0.89	0.13	60,84,125,128	0
34	LMG	z	101	39/55	0.89	0.16	81,136,147,148	0
32	HTG	B	621	19/19	0.89	0.15	72,87,118,120	0
36	CA	O	301	1/1	0.89	0.10	118,118,118,118	0
26	SQD	L	102	54/54	0.90	0.13	55,91,118,119	0
34	LMG	C	521	51/55	0.90	0.14	59,84,115,118	0
27	GOL	b	623	6/6	0.91	0.16	87,92,94,102	0
29	PL9	a	414[A]	55/55	0.91	0.24	93,104,111,112	55
29	PL9	a	414[B]	55/55	0.91	0.24	92,104,111,112	55
27	GOL	c	502	6/6	0.91	0.15	67,70,80,85	0
27	GOL	A	410	6/6	0.91	0.12	65,67,74,83	0
27	GOL	v	201	6/6	0.91	0.17	59,82,83,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	C	515	65/65	0.91	0.12	59,76,108,109	0
34	LMG	a	417	51/55	0.92	0.13	59,90,115,128	0
32	HTG	b	624	19/19	0.92	0.11	64,77,95,104	0
30	UNL	d	409	17/-	0.92	0.15	68,84,106,108	0
23	CLA	c	515	65/65	0.92	0.11	68,85,111,112	0
30	UNL	D	409	17/-	0.92	0.16	60,78,113,114	0
36	CA	o	301	1/1	0.92	0.07	104,104,104,104	0
25	BCR	D	405	40/40	0.93	0.11	48,57,94,99	0
34	LMG	C	502	51/55	0.93	0.12	58,89,113,120	0
25	BCR	d	404	40/40	0.93	0.11	52,64,87,93	0
25	BCR	h	102	40/40	0.93	0.10	50,66,74,75	0
34	LMG	D	412	51/55	0.93	0.12	46,69,108,116	0
31	LHG	A	416	49/49	0.93	0.13	41,61,78,84	0
25	BCR	k	102	40/40	0.93	0.10	58,72,89,92	0
34	LMG	c	521	51/55	0.93	0.13	66,93,123,128	0
23	CLA	C	508	65/65	0.93	0.12	51,69,117,126	0
23	CLA	c	509	65/65	0.93	0.11	55,65,78,87	0
35	DGD	C	519	62/66	0.93	0.11	45,64,116,121	0
30	UNL	d	412	18/-	0.93	0.13	72,81,121,124	0
32	HTG	B	624	19/19	0.93	0.09	63,79,90,90	0
23	CLA	C	506	65/65	0.93	0.11	43,53,92,102	0
25	BCR	c	516	40/40	0.94	0.10	68,85,89,95	0
27	GOL	B	623	6/6	0.94	0.12	79,89,96,98	0
23	CLA	B	616	65/65	0.94	0.11	45,56,134,137	0
23	CLA	c	514	65/65	0.94	0.11	62,80,117,125	0
23	CLA	C	514	65/65	0.94	0.12	55,69,119,122	0
26	SQD	A	409	54/54	0.94	0.11	57,74,105,111	0
34	LMG	M	101	51/55	0.94	0.10	48,69,87,101	0
31	LHG	b	628	49/49	0.94	0.10	42,54,68,80	0
27	GOL	b	627	6/6	0.94	0.16	91,93,95,97	0
25	BCR	B	619	40/40	0.94	0.09	43,55,74,76	0
25	BCR	B	631	40/40	0.94	0.08	36,57,68,70	0
34	LMG	m	101	51/55	0.94	0.11	53,69,98,101	0
25	BCR	C	516	40/40	0.94	0.11	64,80,88,91	0
23	CLA	b	616	65/65	0.94	0.11	41,58,112,116	0
35	DGD	C	520	62/66	0.94	0.10	43,57,92,104	0
26	SQD	a	409	54/54	0.94	0.11	62,81,108,113	0
25	BCR	H	101	40/40	0.94	0.09	47,59,77,80	0
25	BCR	T	101	40/40	0.94	0.07	35,51,63,63	0
23	CLA	c	507	65/65	0.95	0.09	44,57,80,84	0
23	CLA	c	508	65/65	0.95	0.10	56,69,122,127	0
23	CLA	C	510	65/65	0.95	0.10	44,55,118,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	c	510	65/65	0.95	0.09	48,59,116,123	0
30	UNL	X	101	18/-	0.95	0.11	57,74,95,98	0
23	CLA	C	512	65/65	0.95	0.08	47,57,77,83	0
23	CLA	C	513	65/65	0.95	0.09	51,65,83,84	0
23	CLA	d	403	65/65	0.95	0.09	49,60,108,119	0
24	PHO	A	415	64/64	0.95	0.07	36,46,53,54	0
25	BCR	B	618	40/40	0.95	0.08	39,53,64,68	0
23	CLA	C	503	65/65	0.95	0.09	47,56,66,81	0
23	CLA	C	505	65/65	0.95	0.08	48,58,73,76	0
23	CLA	D	404	65/65	0.95	0.10	43,55,120,122	0
23	CLA	B	614	65/65	0.95	0.09	34,44,96,103	0
27	GOL	a	410	6/6	0.95	0.11	60,70,83,86	0
23	CLA	b	606	65/65	0.95	0.09	40,52,114,120	0
31	LHG	D	408	49/49	0.95	0.12	43,60,115,123	0
25	BCR	K	101	40/40	0.95	0.10	57,69,78,81	0
31	LHG	L	101	49/49	0.95	0.10	41,52,63,88	0
23	CLA	b	612	65/65	0.95	0.08	38,47,59,75	0
25	BCR	Y	101	40/40	0.95	0.08	53,67,77,84	0
31	LHG	d	406	49/49	0.95	0.11	50,62,82,94	0
31	LHG	d	408	49/49	0.95	0.12	56,66,109,120	0
25	BCR	b	617	40/40	0.95	0.07	39,49,57,59	0
25	BCR	b	618	40/40	0.95	0.08	39,53,69,75	0
23	CLA	b	614	65/65	0.95	0.09	36,45,103,107	0
29	PL9	D	406	55/55	0.95	0.09	32,44,58,67	0
25	BCR	c	517	40/40	0.95	0.10	54,67,73,75	0
23	CLA	B	606	65/65	0.95	0.09	39,50,95,104	0
35	DGD	c	519	62/66	0.95	0.10	51,73,114,122	0
23	CLA	c	505	65/65	0.95	0.08	52,65,75,81	0
25	BCR	k	101	40/40	0.95	0.10	60,73,84,87	0
23	CLA	c	506	65/65	0.95	0.09	51,59,100,110	0
37	BCT	D	401[A]	4/4	0.95	0.08	57,57,60,62	4
37	BCT	D	401[B]	4/4	0.95	0.08	59,59,61,64	4
37	BCT	d	401[A]	4/4	0.95	0.08	55,59,59,60	4
37	BCT	d	401[B]	4/4	0.95	0.08	53,58,60,67	4
23	CLA	a	407	65/65	0.96	0.10	40,51,124,127	0
23	CLA	B	607	65/65	0.96	0.07	32,42,62,72	0
25	BCR	A	408	40/40	0.96	0.07	35,46,55,56	0
25	BCR	B	617	40/40	0.96	0.06	38,47,58,61	0
23	CLA	b	602	65/65	0.96	0.08	48,56,68,81	0
23	CLA	b	605	65/65	0.96	0.08	36,47,67,70	0
23	CLA	C	507	65/65	0.96	0.08	43,52,86,87	0
23	CLA	b	607	65/65	0.96	0.08	33,43,72,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	BCR	C	517	40/40	0.96	0.08	50,61,74,79	0
31	LHG	D	407	49/49	0.96	0.09	41,50,67,84	0
23	CLA	b	609	65/65	0.96	0.08	49,57,76,98	0
23	CLA	b	610	65/65	0.96	0.09	44,52,66,73	0
23	CLA	B	610	65/65	0.96	0.09	42,50,63,75	0
23	CLA	C	509	65/65	0.96	0.09	48,57,78,86	0
23	CLA	B	611	65/65	0.96	0.07	35,41,60,68	0
25	BCR	a	408	40/40	0.96	0.07	38,48,56,59	0
31	LHG	d	407	49/49	0.96	0.08	39,51,69,80	0
23	CLA	c	503	65/65	0.96	0.08	56,63,75,79	0
23	CLA	c	504	65/65	0.96	0.08	49,58,73,89	0
25	BCR	b	619	40/40	0.96	0.08	46,55,77,86	0
34	LMG	d	411	51/55	0.96	0.10	53,67,107,116	0
23	CLA	C	511	65/65	0.96	0.09	49,58,76,83	0
29	PL9	d	405	55/55	0.96	0.08	36,47,56,65	0
35	DGD	C	518	62/66	0.96	0.10	41,57,98,102	0
23	CLA	A	405	65/65	0.96	0.08	34,46,107,111	0
23	CLA	B	602	65/65	0.96	0.08	40,51,74,84	0
35	DGD	H	102	62/66	0.96	0.08	41,57,76,80	0
35	DGD	c	518	62/66	0.96	0.09	46,59,90,92	0
23	CLA	B	603	65/65	0.96	0.08	38,49,65,68	0
35	DGD	c	520	62/66	0.96	0.09	49,60,97,101	0
35	DGD	h	103	62/66	0.96	0.09	46,62,73,78	0
23	CLA	C	504	65/65	0.96	0.08	44,57,77,85	0
23	CLA	A	407	65/65	0.96	0.09	39,47,109,116	0
23	CLA	c	511	65/65	0.96	0.08	54,63,79,88	0
23	CLA	c	512	65/65	0.96	0.07	52,61,74,79	0
23	CLA	c	513	65/65	0.96	0.09	56,66,80,83	0
23	CLA	a	403	65/65	0.96	0.07	37,43,66,74	0
23	CLA	a	405	65/65	0.96	0.09	40,50,112,117	0
38	HEM	e	102	43/43	0.96	0.08	63,77,113,121	0
39	MG	J	102	1/1	0.96	0.10	56,56,56,56	0
23	CLA	D	403	65/65	0.97	0.07	33,40,57,69	0
23	CLA	B	612	65/65	0.97	0.07	36,44,58,67	0
23	CLA	b	611	65/65	0.97	0.07	38,47,70,82	0
23	CLA	B	613	65/65	0.97	0.07	36,43,86,93	0
27	GOL	C	524	6/6	0.97	0.16	49,58,63,63	0
23	CLA	b	613	65/65	0.97	0.07	34,45,80,86	0
24	PHO	A	406	64/64	0.97	0.06	33,41,49,58	0
23	CLA	a	404	65/65	0.97	0.06	35,43,52,58	0
24	PHO	a	416	64/64	0.97	0.06	40,48,55,63	0
23	CLA	b	615	65/65	0.97	0.07	41,52,73,79	0

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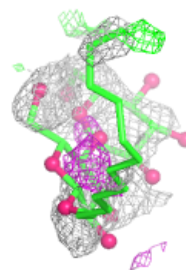
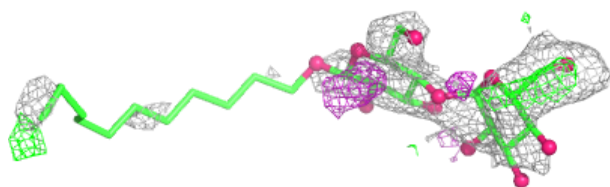
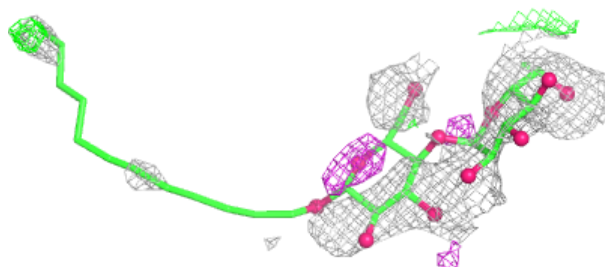
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	A	404	65/65	0.97	0.06	32,40,51,56	0
36	CA	C	525	1/1	0.97	0.11	68,68,68,68	0
23	CLA	B	615	65/65	0.97	0.07	40,47,75,84	0
23	CLA	A	403	65/65	0.97	0.07	34,38,63,71	0
36	CA	a	420	1/1	0.97	0.09	108,108,108,108	0
36	CA	c	525	1/1	0.97	0.04	81,81,81,81	0
23	CLA	B	608	65/65	0.97	0.07	39,49,66,67	0
23	CLA	b	603	65/65	0.97	0.07	41,53,74,81	0
23	CLA	b	604	65/65	0.97	0.08	35,46,105,111	0
23	CLA	B	609	65/65	0.97	0.07	45,54,72,80	0
23	CLA	B	604	65/65	0.97	0.08	34,41,98,103	0
23	CLA	B	605	65/65	0.97	0.07	37,43,59,71	0
23	CLA	b	608	65/65	0.97	0.07	45,53,68,73	0
40	HEC	v	202	43/43	0.97	0.07	53,60,67,72	0
38	HEM	E	102	43/43	0.98	0.07	58,65,82,93	0
23	CLA	d	402	65/65	0.98	0.06	37,44,70,78	0
24	PHO	a	406	64/64	0.98	0.06	35,44,51,58	0
40	HEC	V	201	43/43	0.98	0.07	44,51,55,56	0
36	CA	c	524	1/1	0.98	0.07	75,75,75,75	0
22	CL	c	501	1/1	0.99	0.06	46,46,46,46	0
22	CL	C	501	1/1	0.99	0.03	43,43,43,43	0
22	CL	a	402	1/1	0.99	0.05	46,46,46,46	0
39	MG	j	102	1/1	0.99	0.04	61,61,61,61	0
28	OEX	A	412[A]	10/10	0.99	0.04	42,45,49,49	10
28	OEX	A	412[B]	10/10	0.99	0.04	39,46,51,51	10
28	OEX	a	413[A]	10/10	1.00	0.03	46,48,52,56	10
28	OEX	a	413[B]	10/10	1.00	0.03	44,50,54,54	10
21	FE2	A	401[B]	1/1	1.00	0.04	57,57,57,57	1
21	FE2	a	401[A]	1/1	1.00	0.04	56,56,56,56	1
21	FE2	a	401[B]	1/1	1.00	0.04	63,63,63,63	1
22	CL	A	402	1/1	1.00	0.04	39,39,39,39	0
21	FE2	A	401[A]	1/1	1.00	0.04	54,54,54,54	1

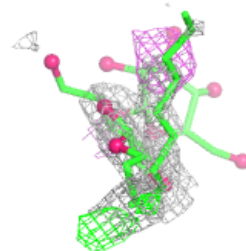
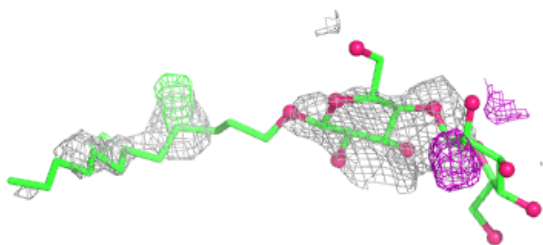
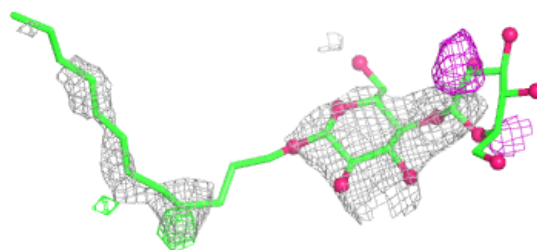
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT 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)

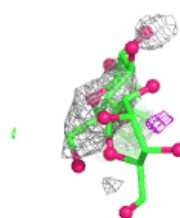
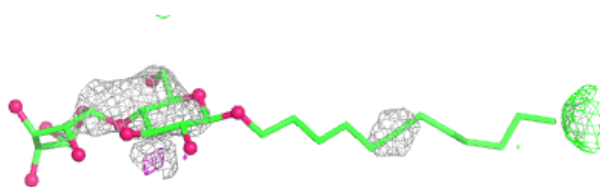
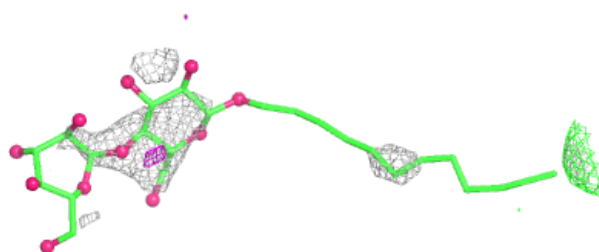
**Electron density around LMT C 526:**

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

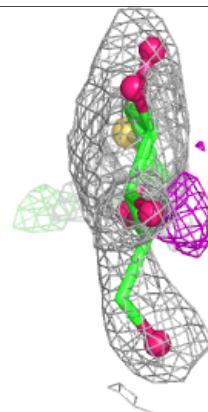
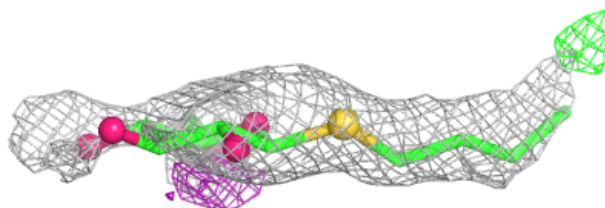
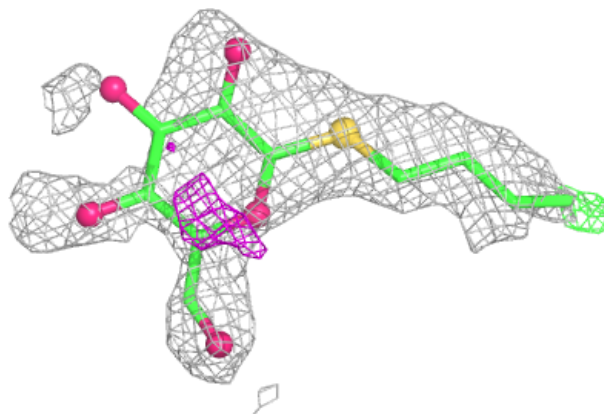


Electron density around LMT e 101:

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

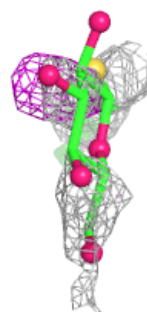
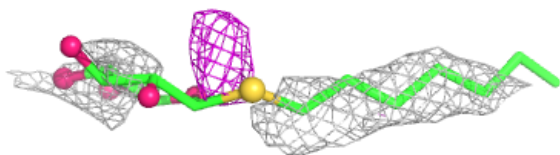
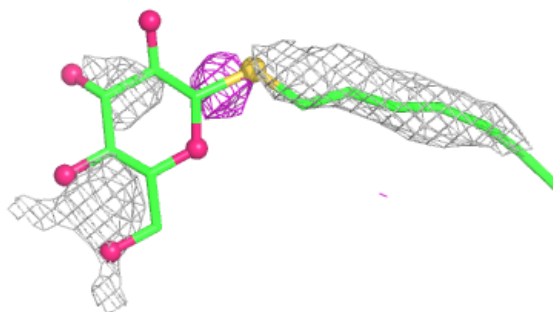
**Electron density around HTG D 411:**

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

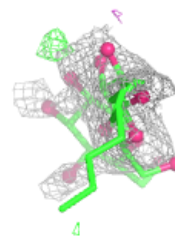
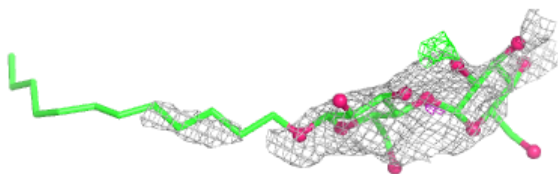
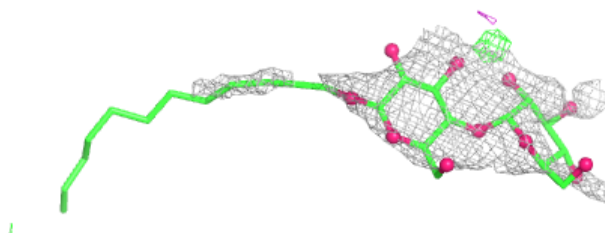


Electron density around HTG b 622:

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

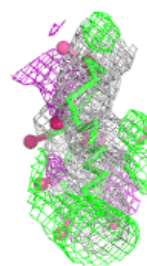
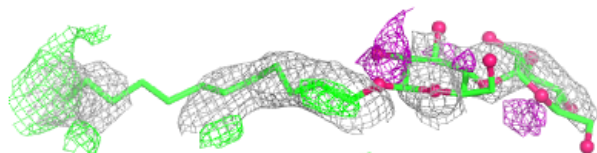
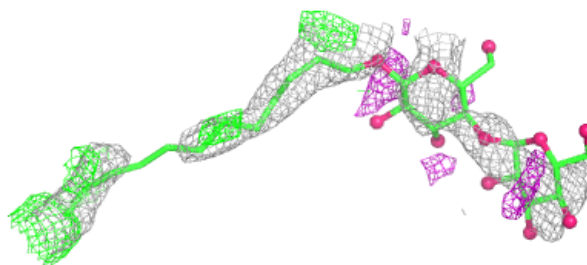
**Electron density around LMT a 418:**

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

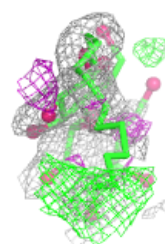
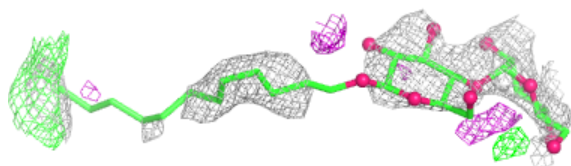
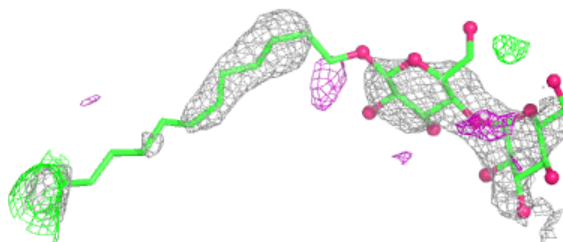


Electron density around LMT a 412:

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

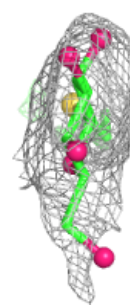
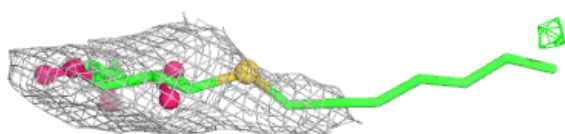
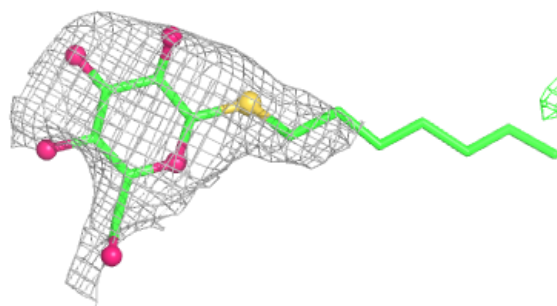
**Electron density around LMT D 402:**

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

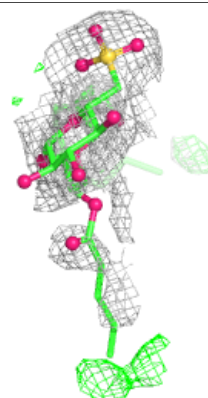
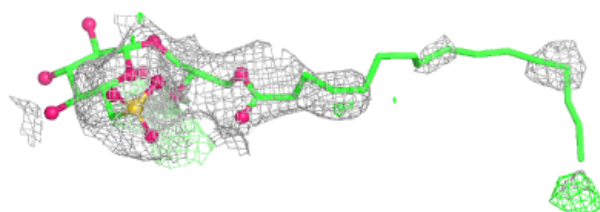
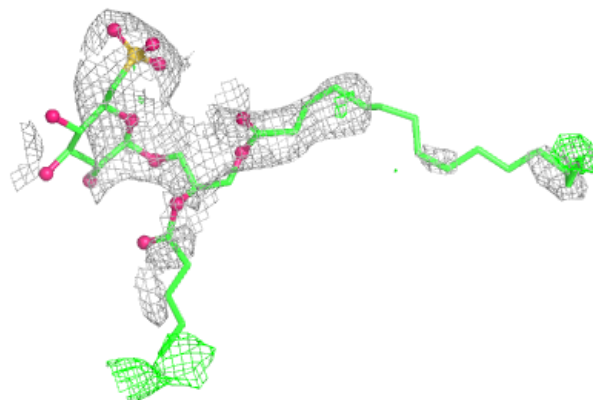


Electron density around HTG c 523:

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

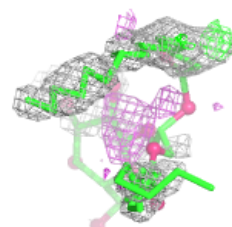
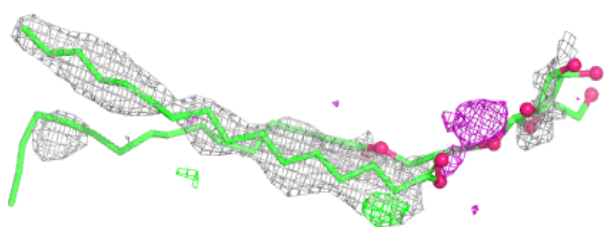
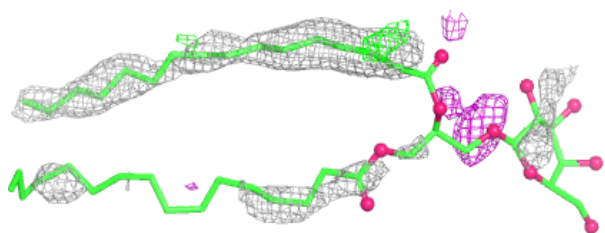
**Electron density around SQD f 101:**

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

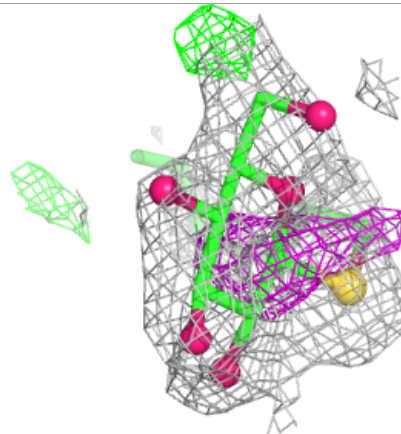
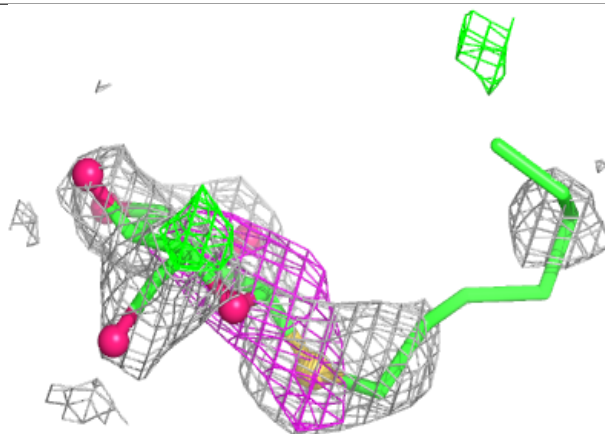
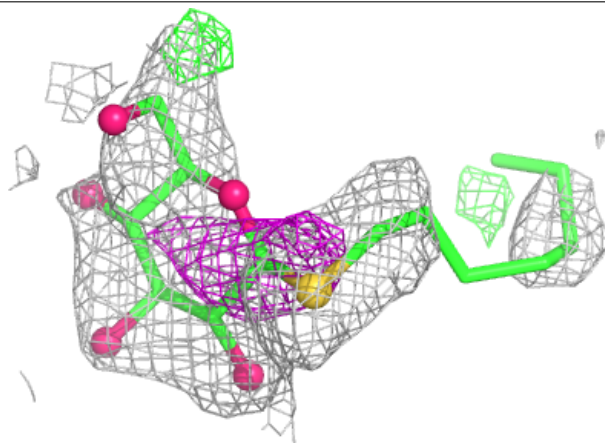


Electron density around LMG C 522:

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

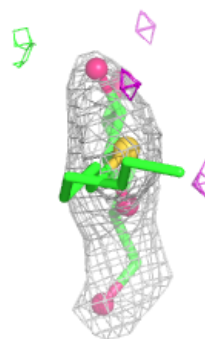
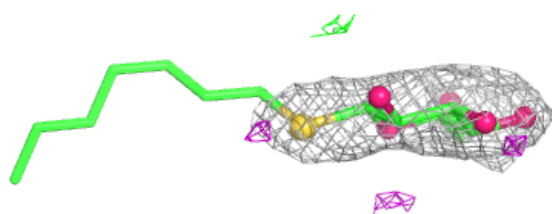
**Electron density around HTG B 622:**

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

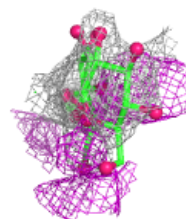
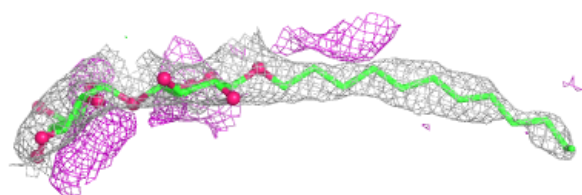
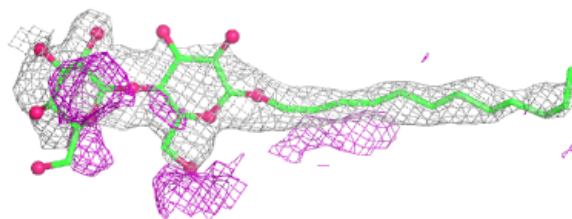


Electron density around HTG C 523:

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

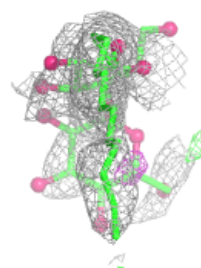
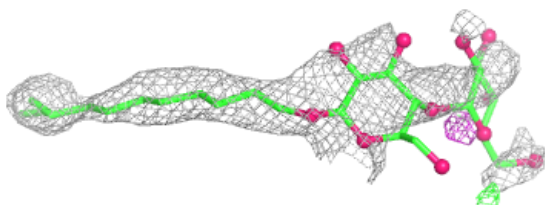
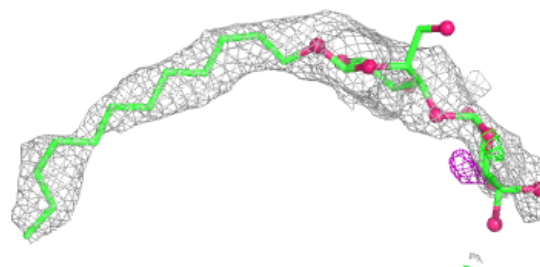
**Electron density around LMT m 103:**

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

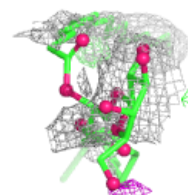
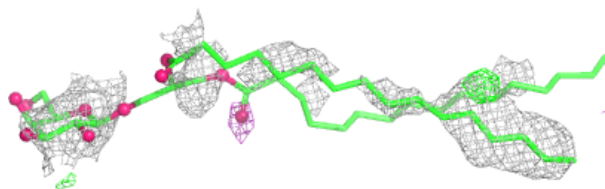
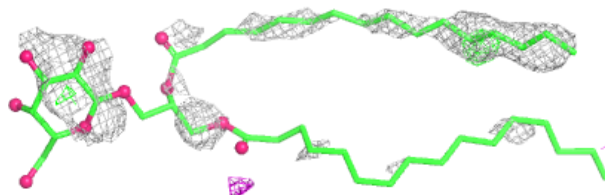


Electron density around LMT M 103:

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

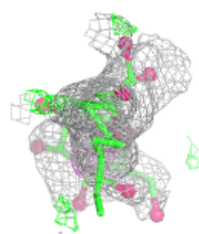
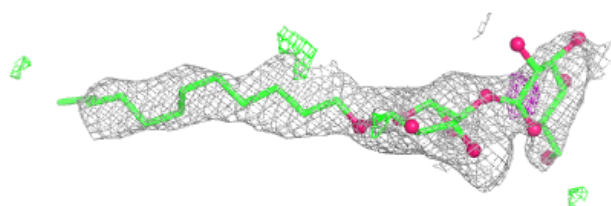
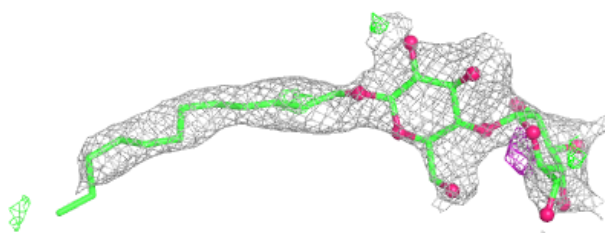
**Electron density around LMG c 522:**

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

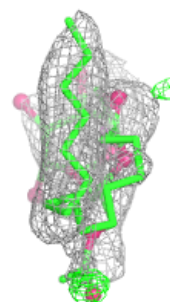
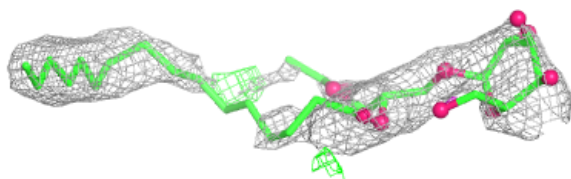
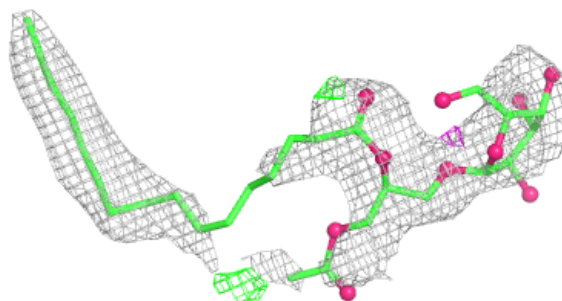


Electron density around LMT B 627:

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

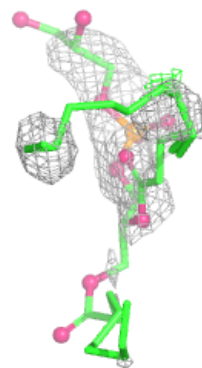
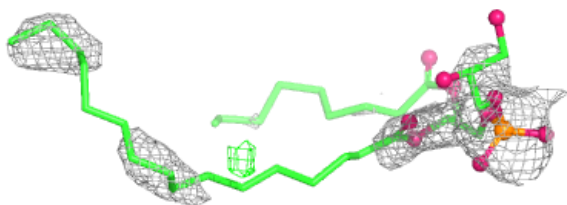
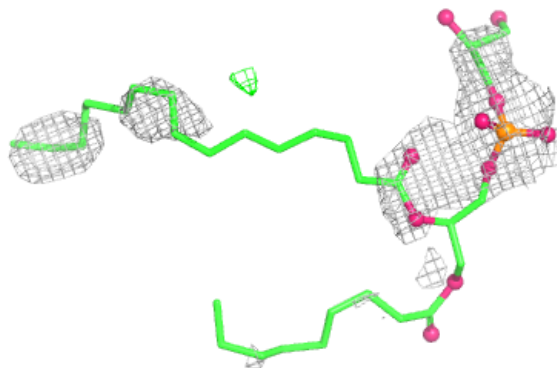
**Electron density around LMG Z 101:**

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

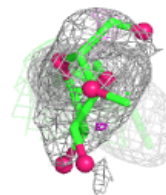
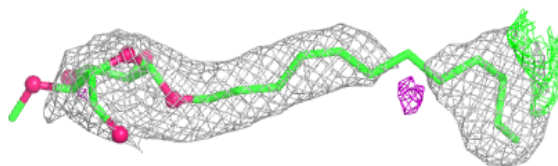
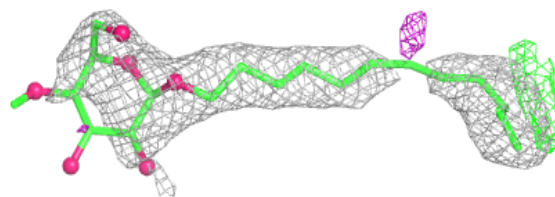


Electron density around LHG a 419:

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

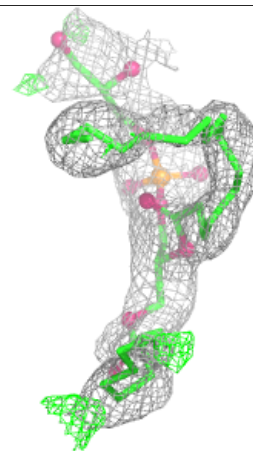
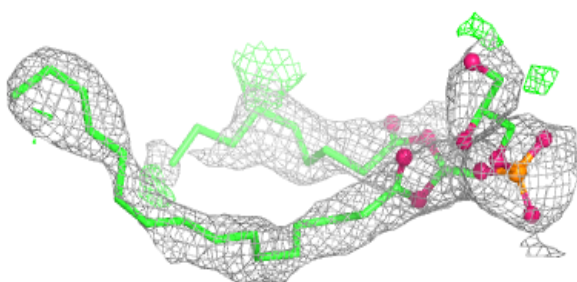
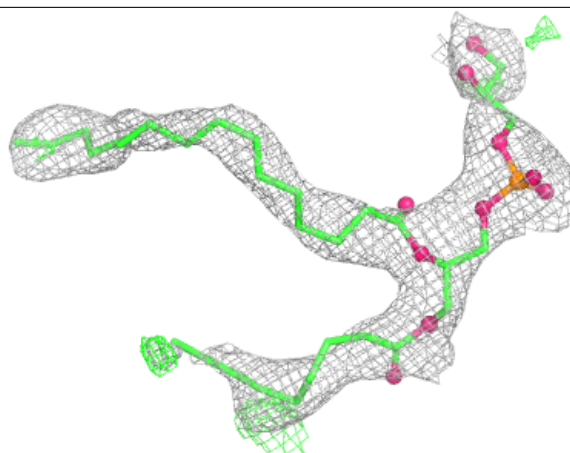
**Electron density around LMT b 626:**

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



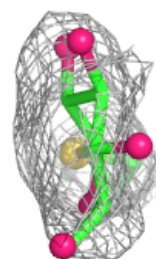
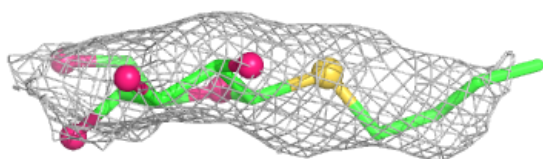
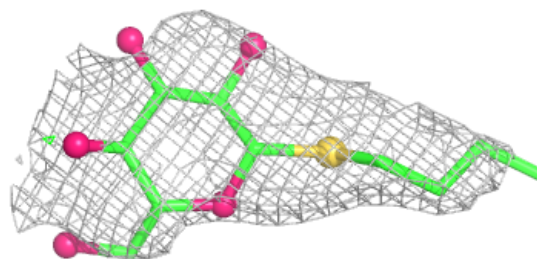
Electron density around LHG E 101:

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

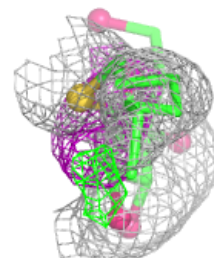
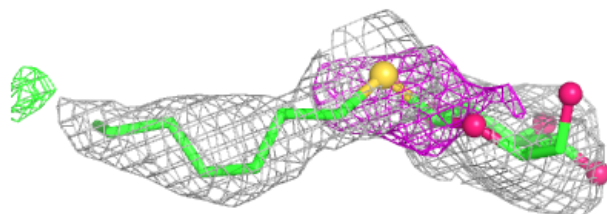
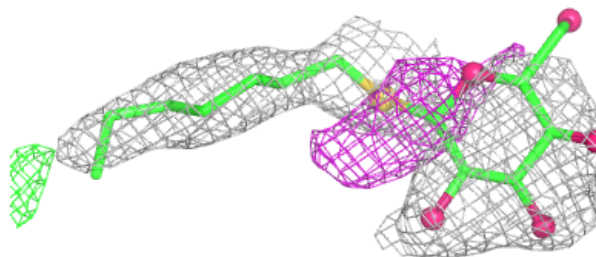


Electron density around HTG h 101:

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

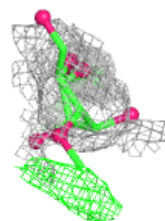
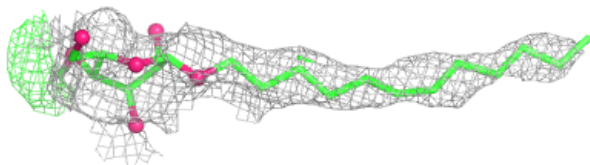
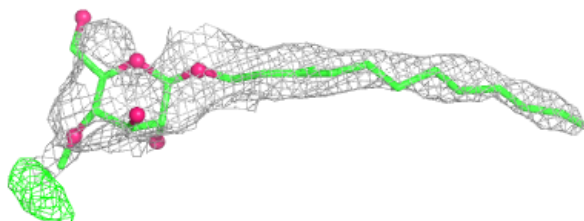
**Electron density around HTG b 621:**

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

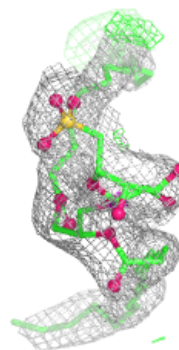
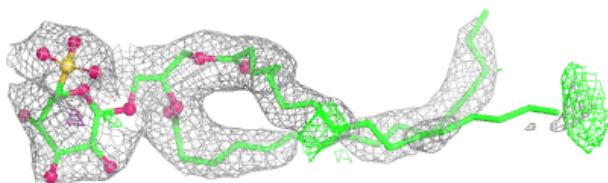
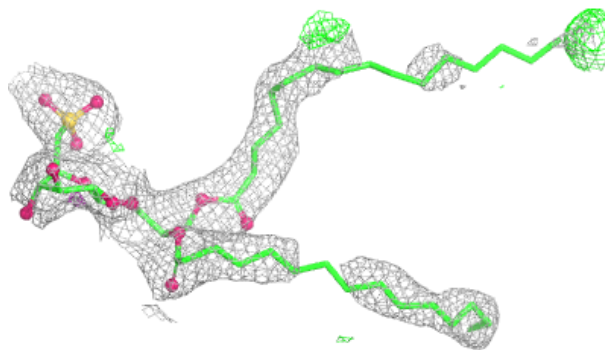


Electron density around LMT b 620:

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

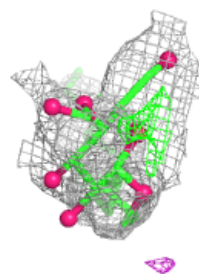
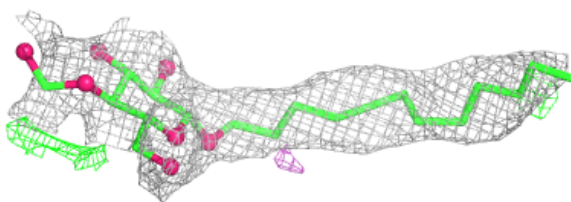
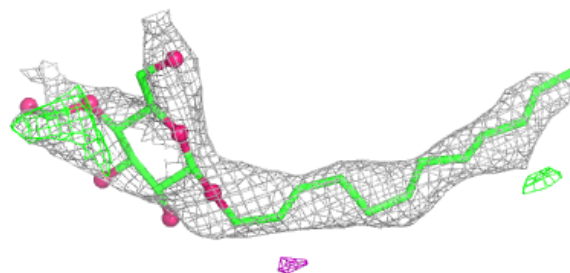
**Electron density around SQD a 411:**

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



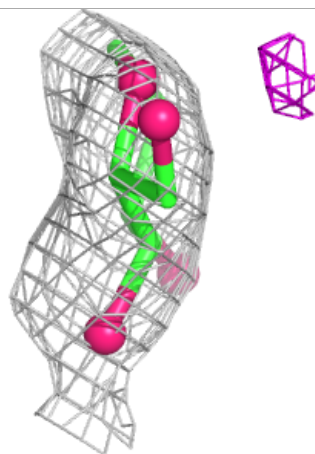
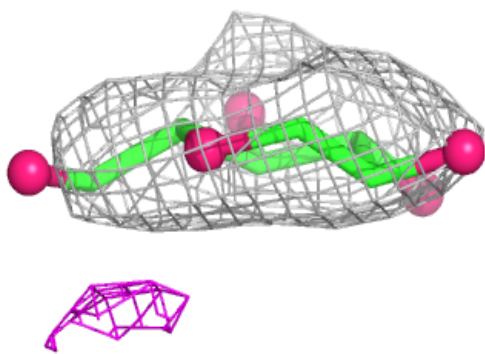
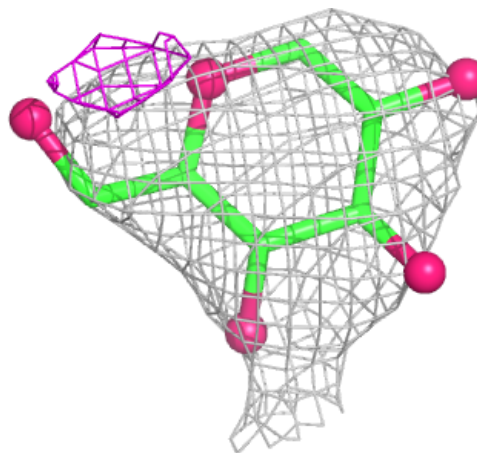
Electron density around LMT B 630:

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



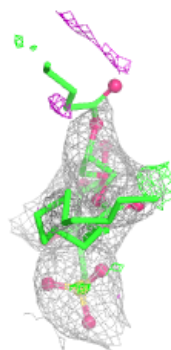
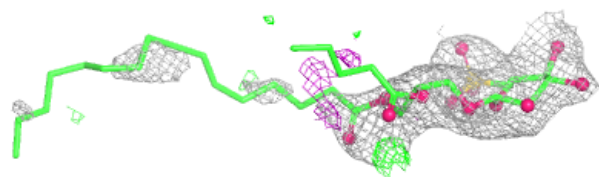
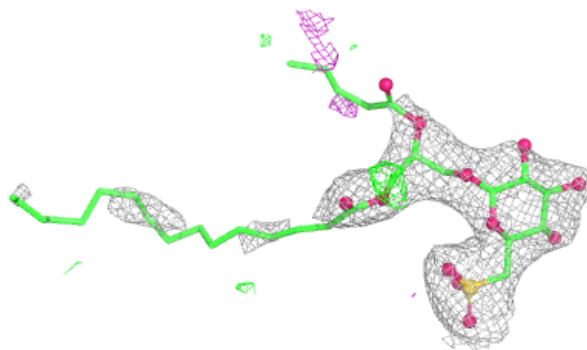
Electron density around HTG V 202:

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



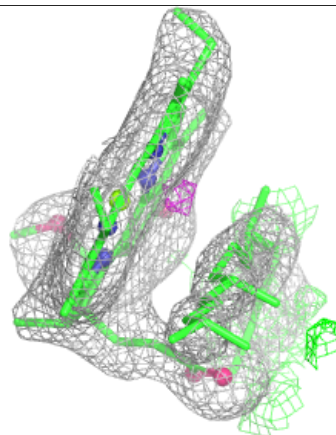
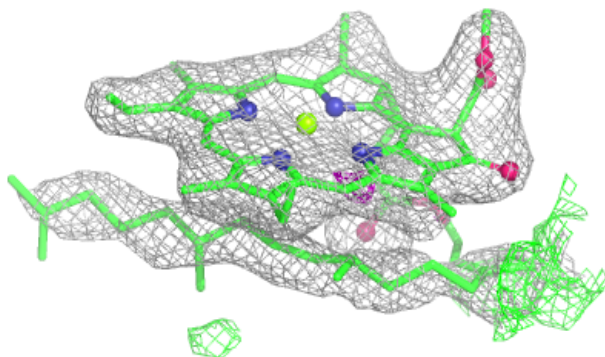
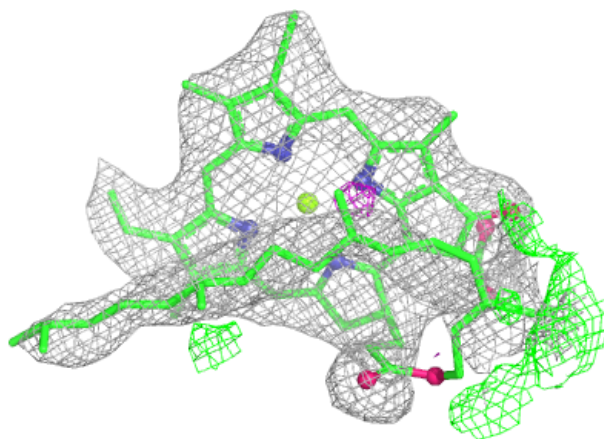
Electron density around SQD D 413:

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



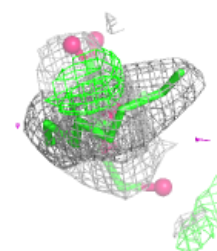
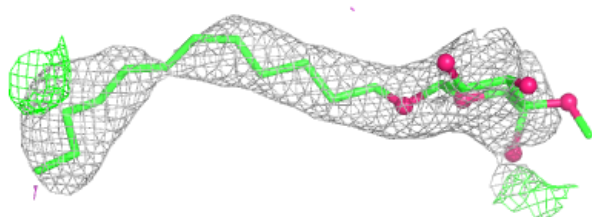
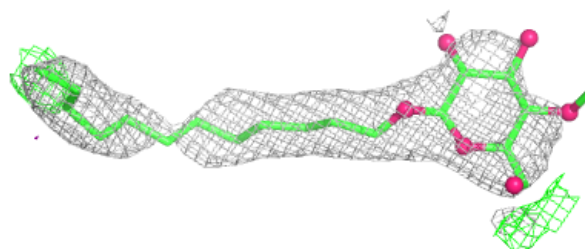
Electron density around CLA b 601:

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

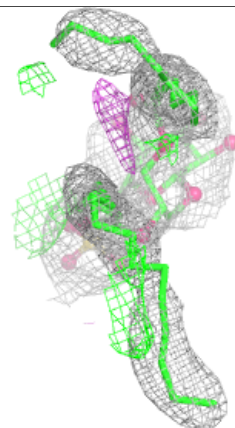
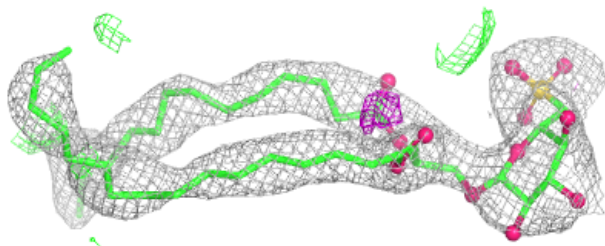
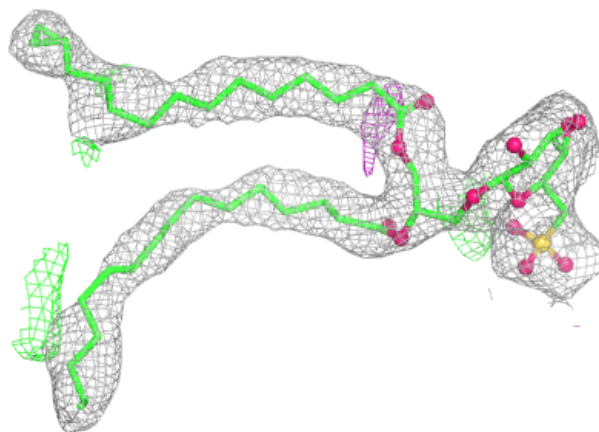


Electron density around LMT B 629:

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

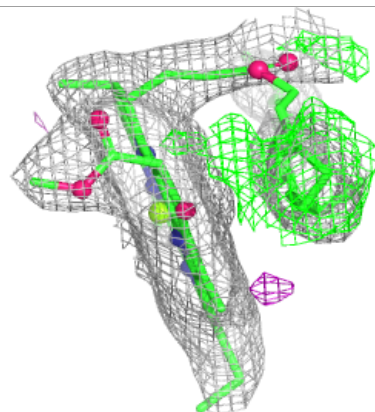
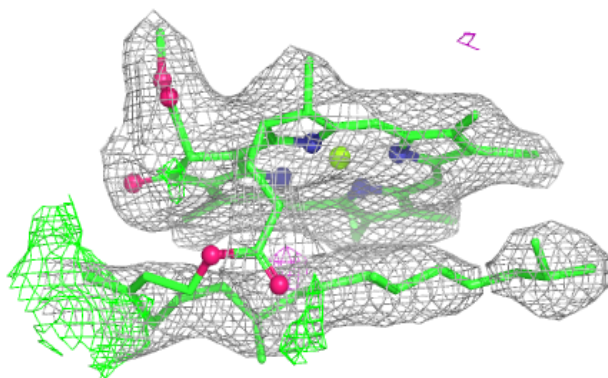
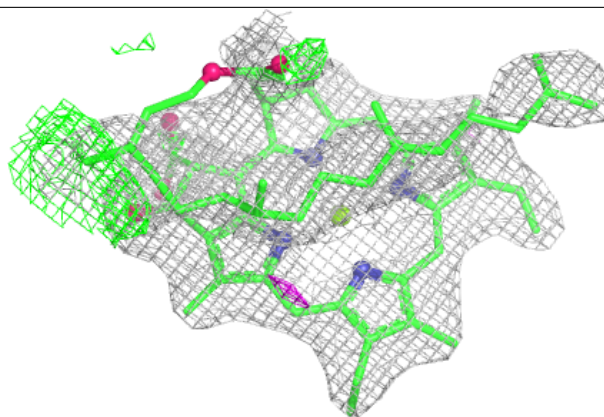
**Electron density around SQD B 620:**

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

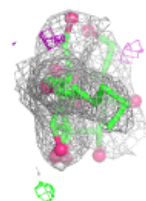
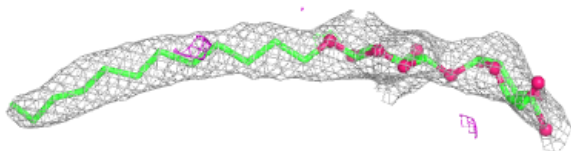
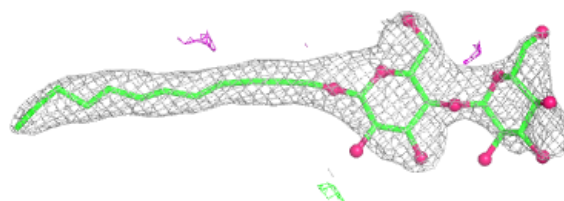


Electron density around CLA B 601:

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

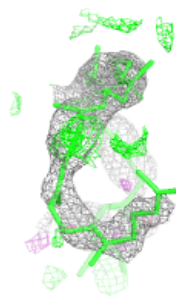
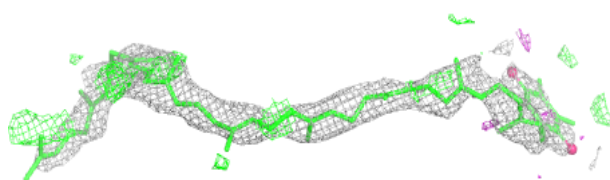
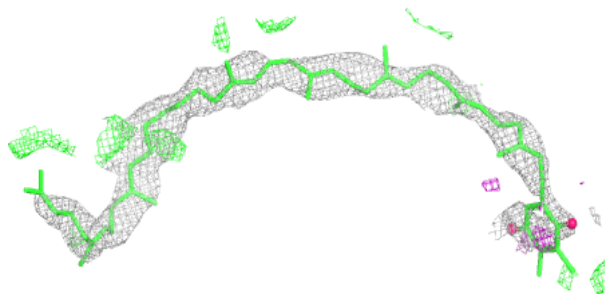
**Electron density around LMT M 102:**

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

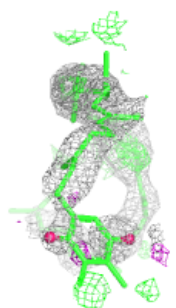
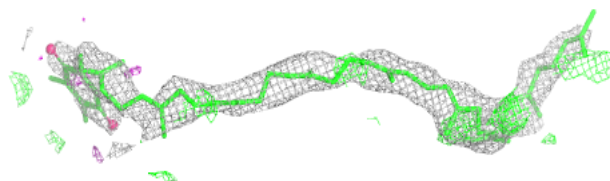
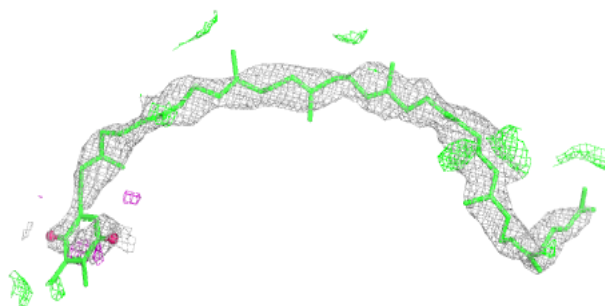


Electron density around PL9 A 413 (A):

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

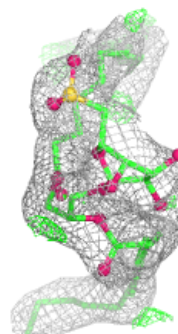
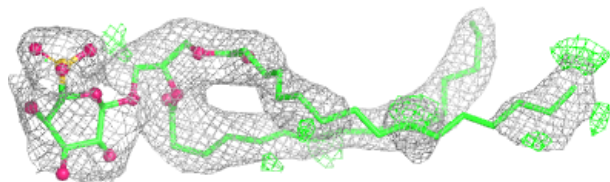
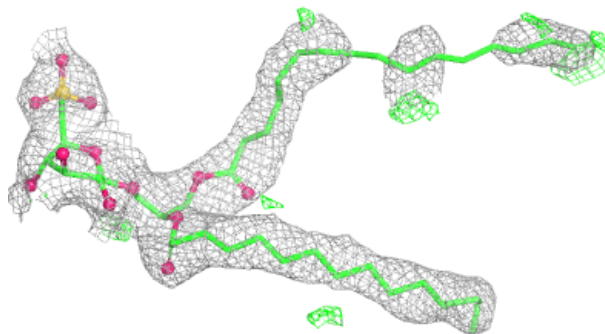
**Electron density around PL9 A 413 (B):**

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

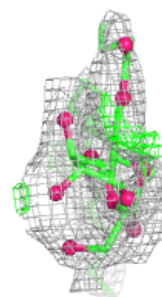
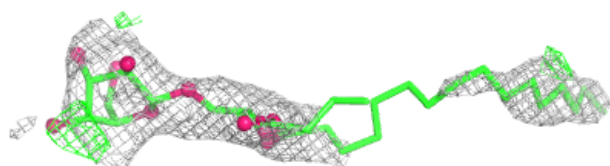
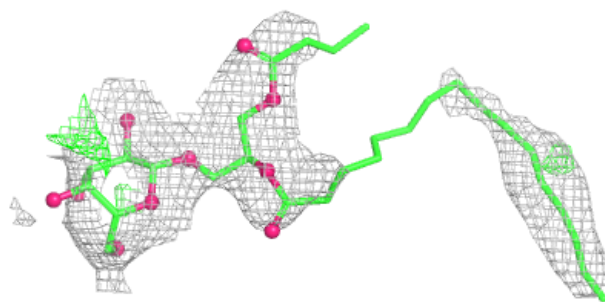


Electron density around SQD A 411:

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

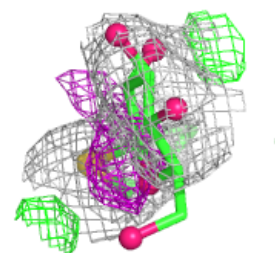
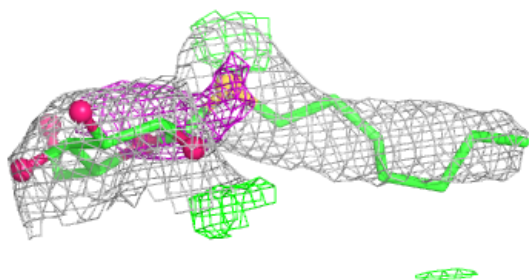
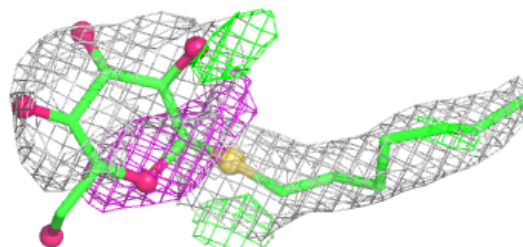
**Electron density around LMG z 101:**

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

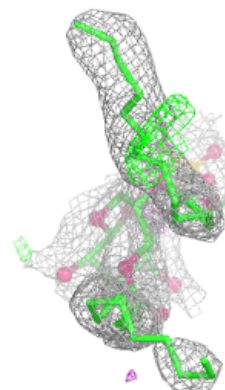
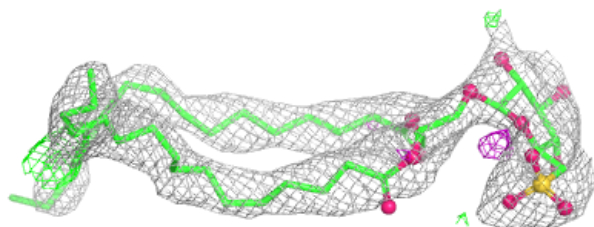
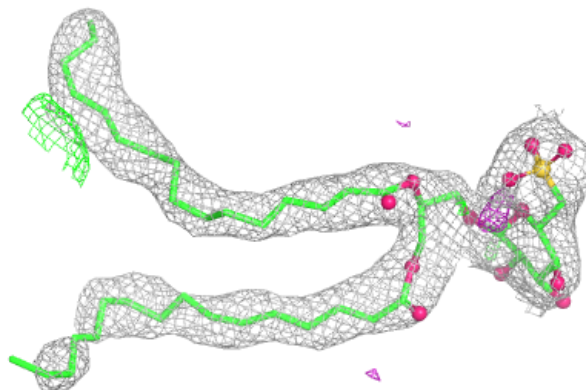


Electron density around HTG B 621:

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

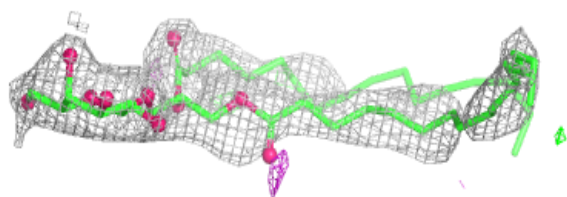
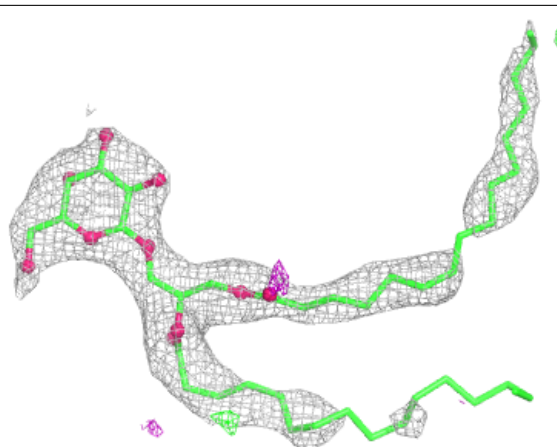
**Electron density around SQD L 102:**

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



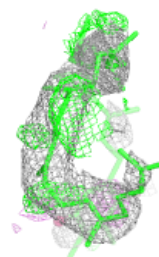
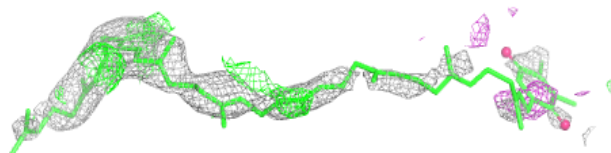
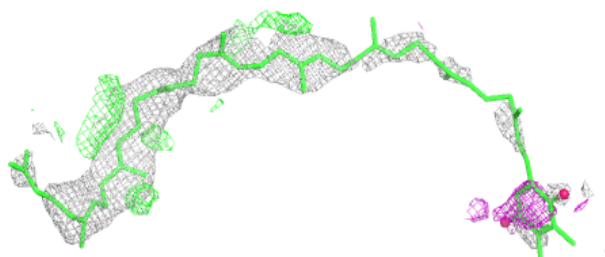
Electron density around LMG C 521:

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

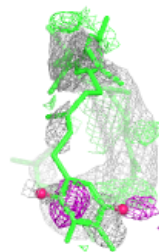
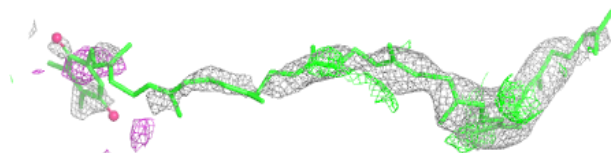
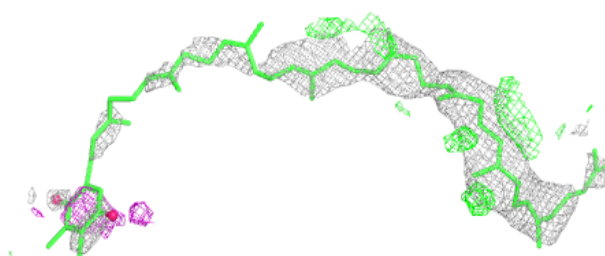


Electron density around PL9 a 414 (A):

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

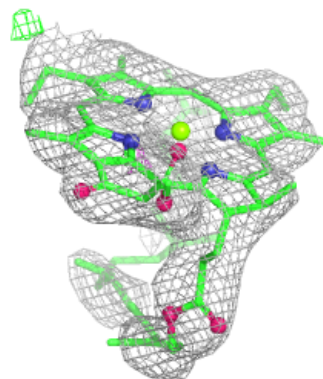
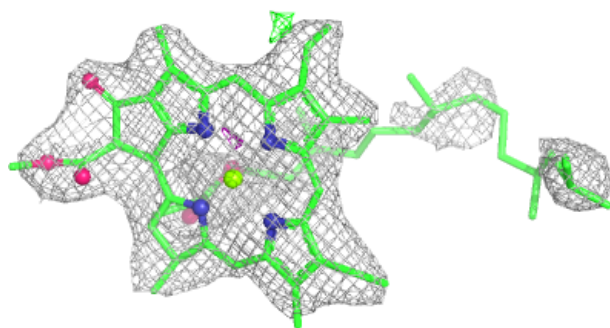
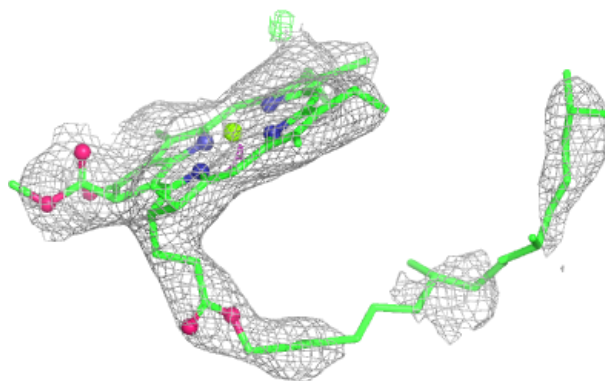
**Electron density around PL9 a 414 (B):**

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

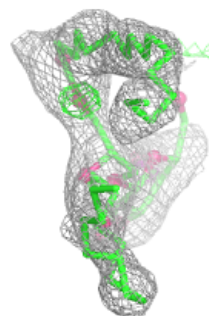
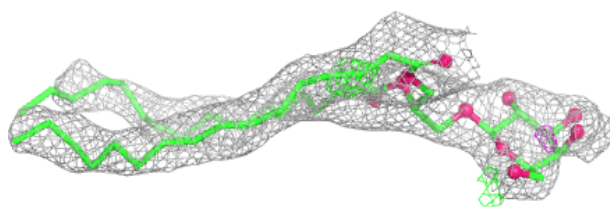


Electron density around CLA C 515:

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

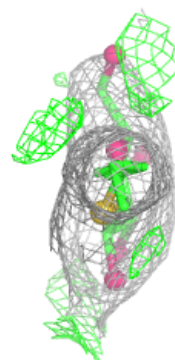
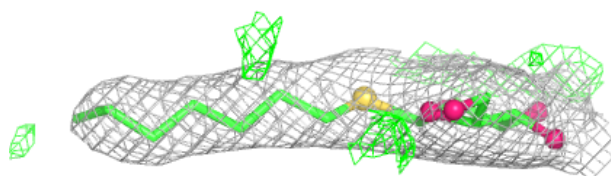
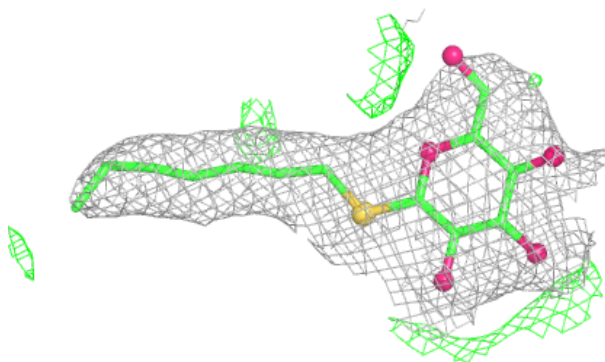
**Electron density around LMG a 417:**

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

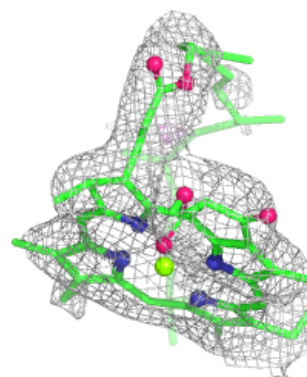
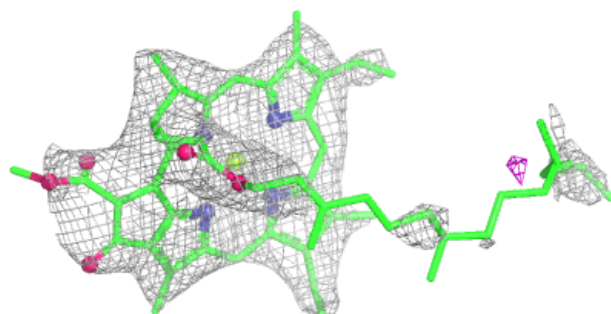
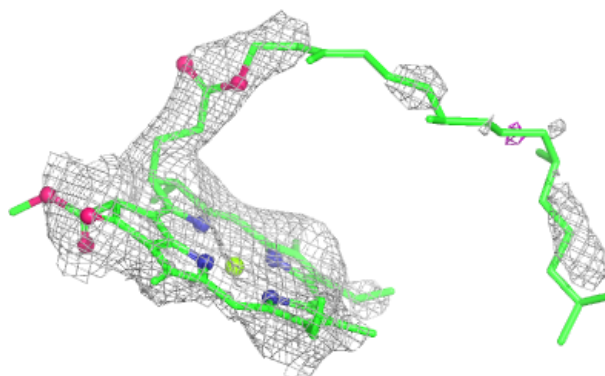


Electron density around HTG b 624:

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

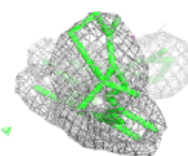
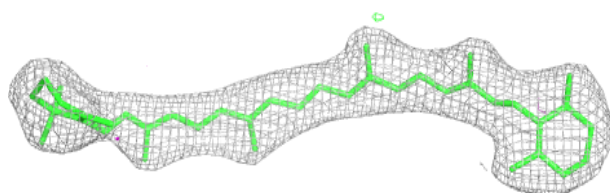
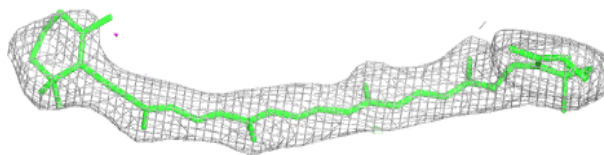
**Electron density around CLA c 515:**

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

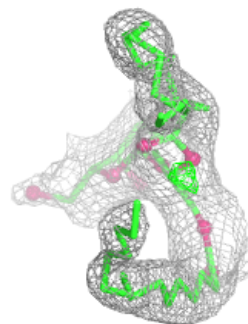
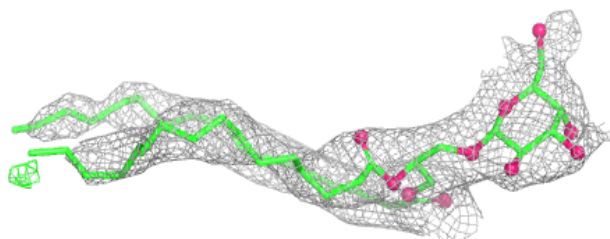
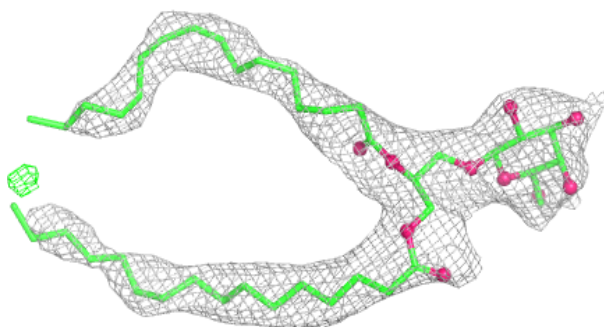


Electron density around BCR D 405:

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

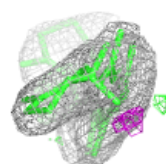
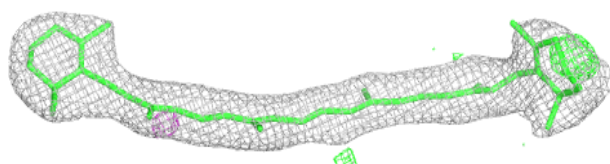
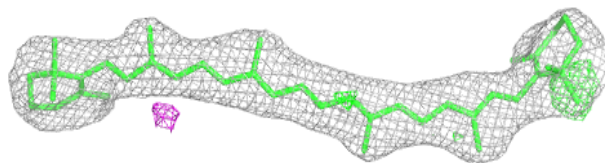
**Electron density around LMG C 502:**

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

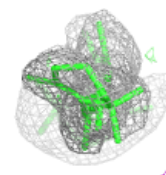
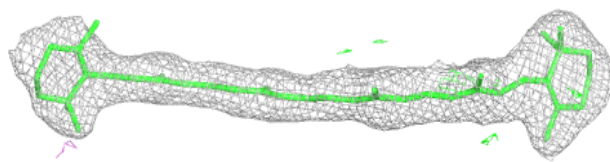
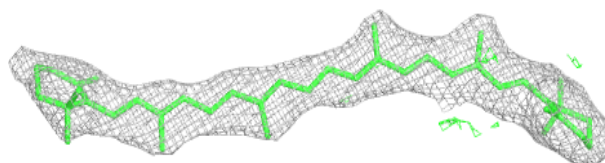


Electron density around BCR d 404:

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

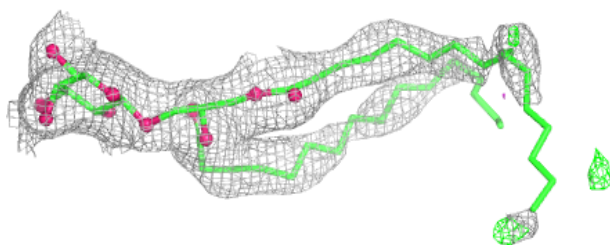
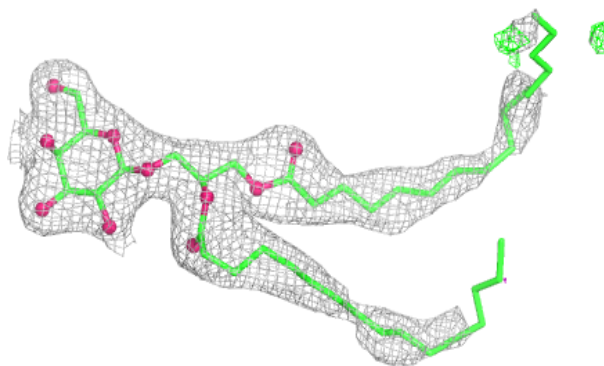
**Electron density around BCR h 102:**

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

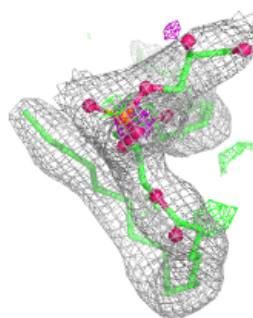
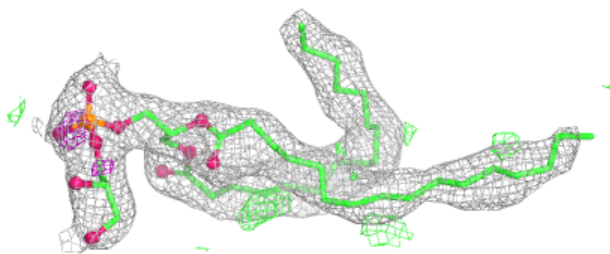
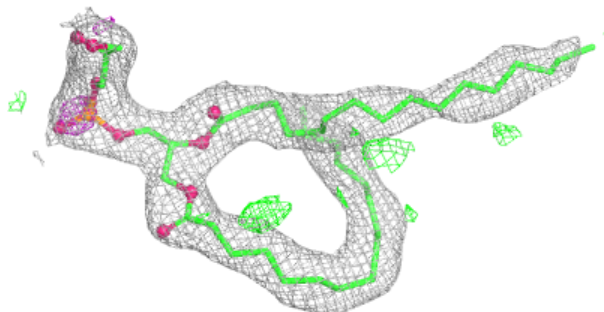


Electron density around LMG D 412:

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

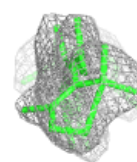
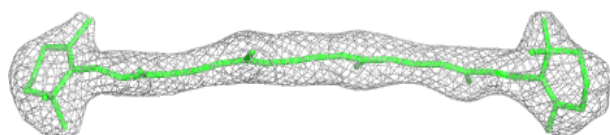
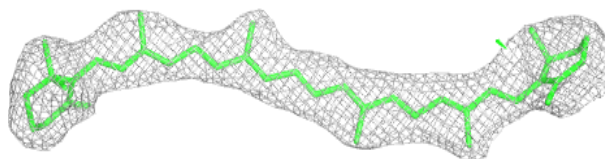
**Electron density around LHG A 416:**

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

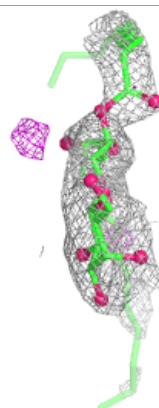
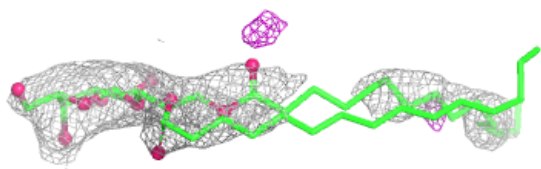
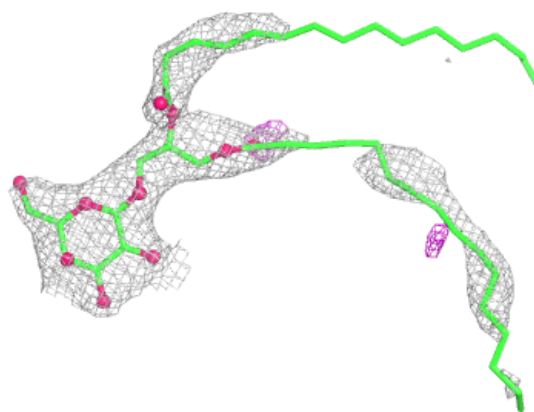


Electron density around BCR k 102:

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

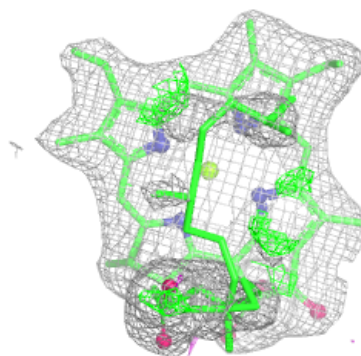
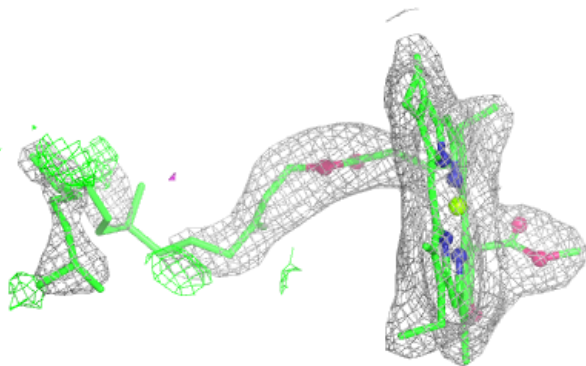
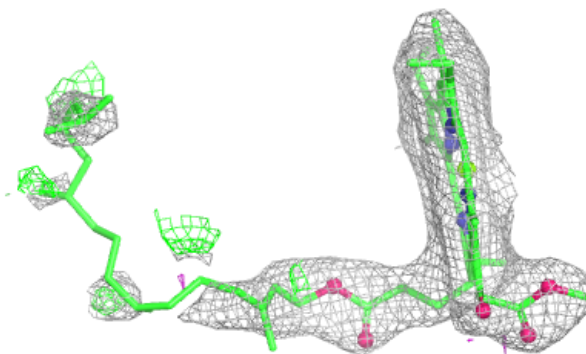
**Electron density around LMG c 521:**

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



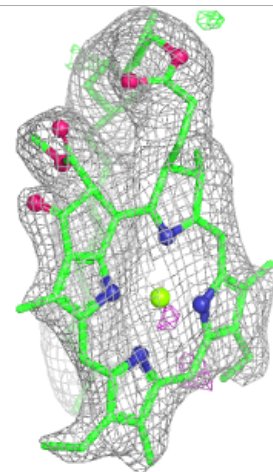
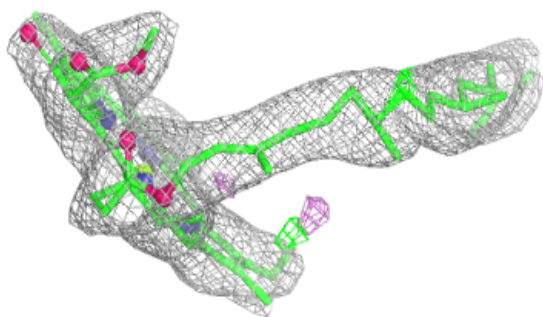
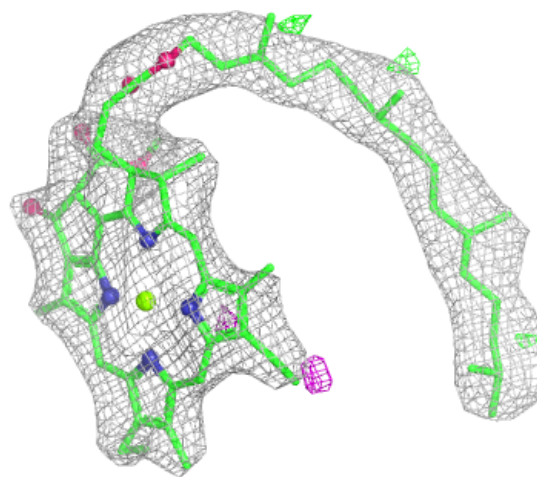
Electron density around CLA C 508:

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



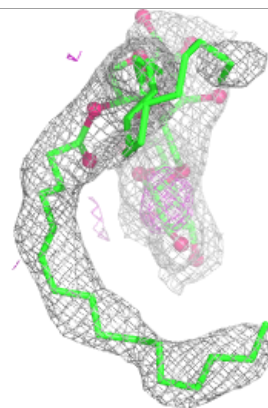
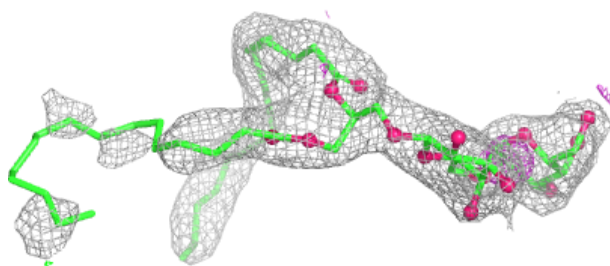
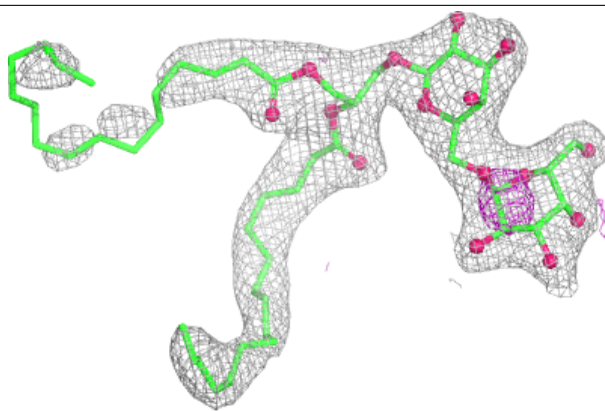
Electron density around CLA c 509:

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

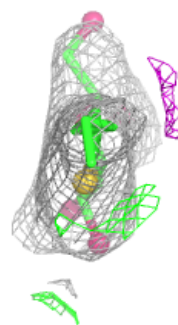
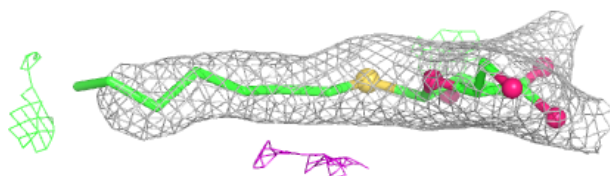
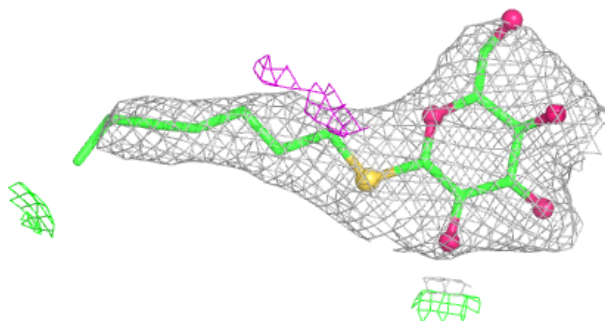


Electron density around DGD C 519:

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

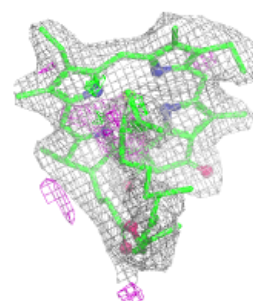
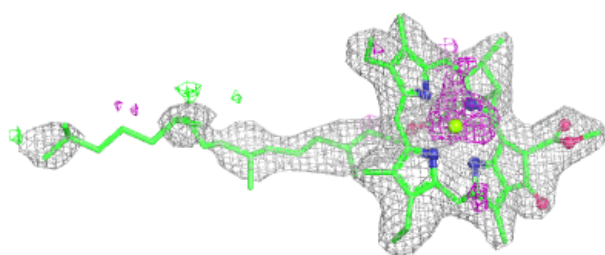
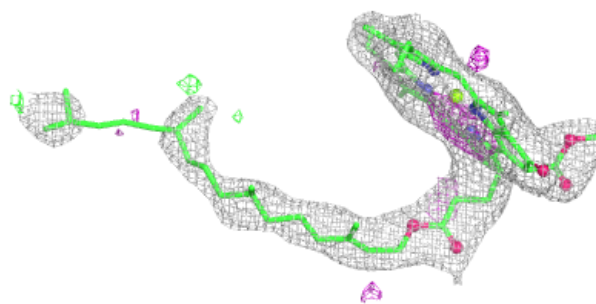
**Electron density around HTG B 624:**

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

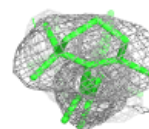
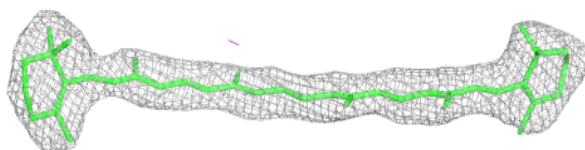
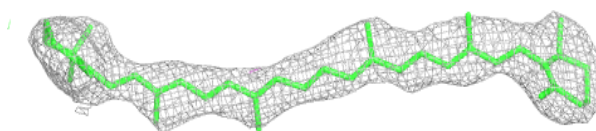


Electron density around CLA C 506:

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

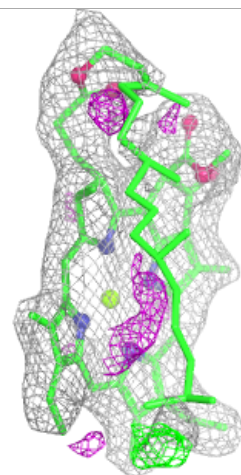
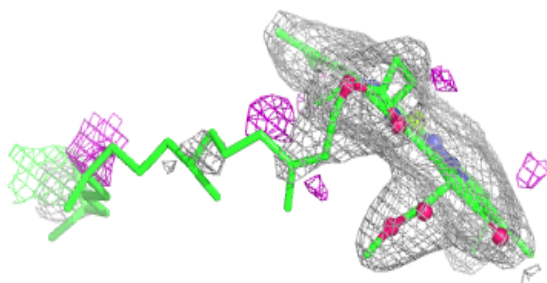
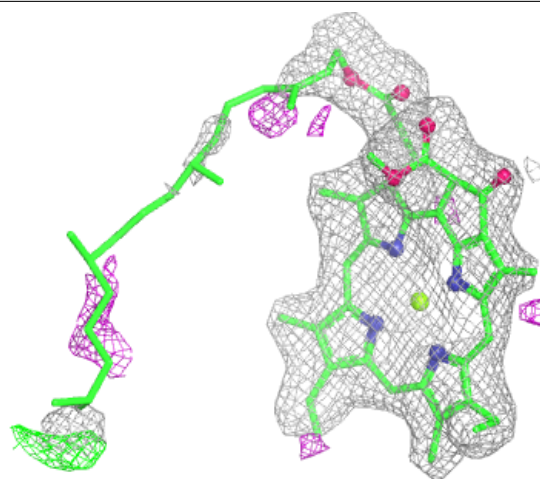
**Electron density around BCR c 516:**

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



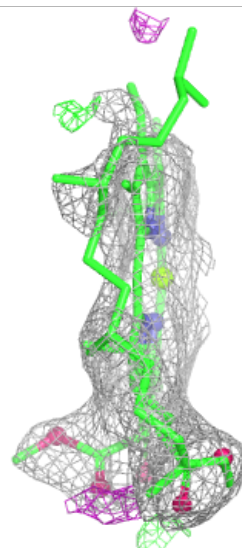
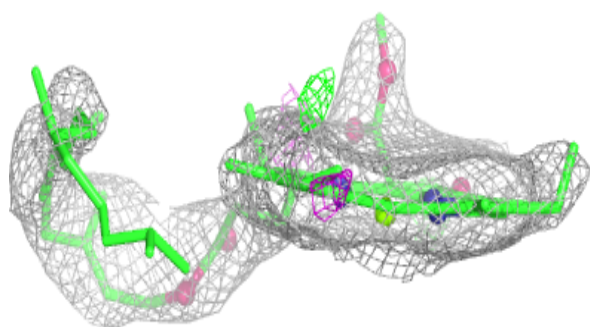
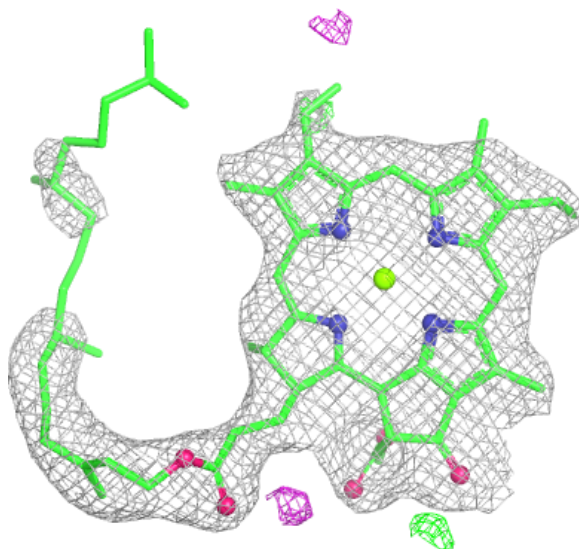
Electron density around CLA B 616:

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



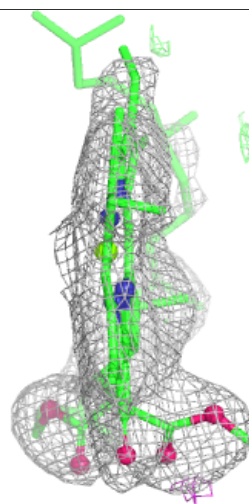
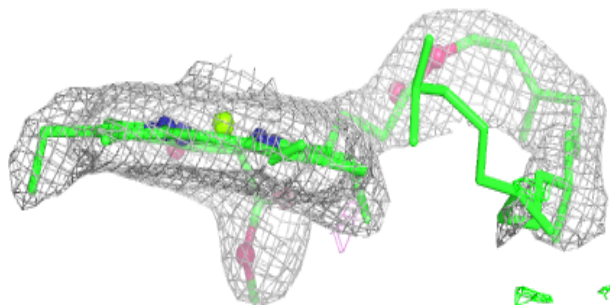
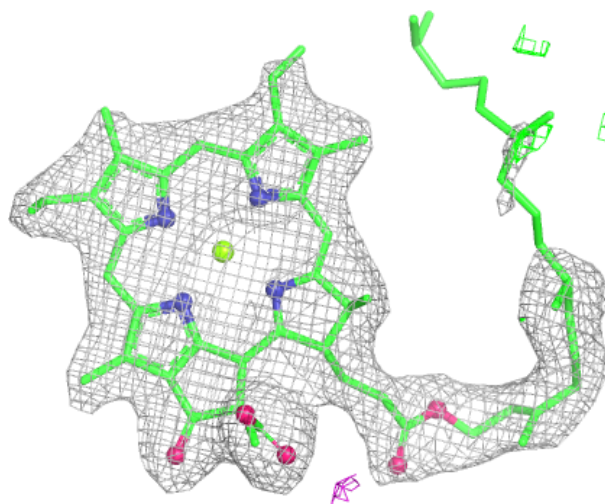
Electron density around CLA c 514:

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



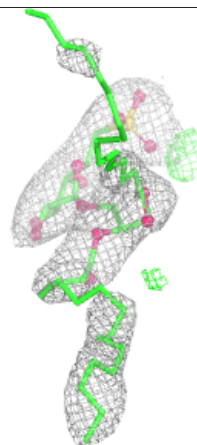
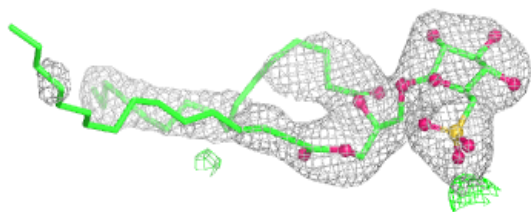
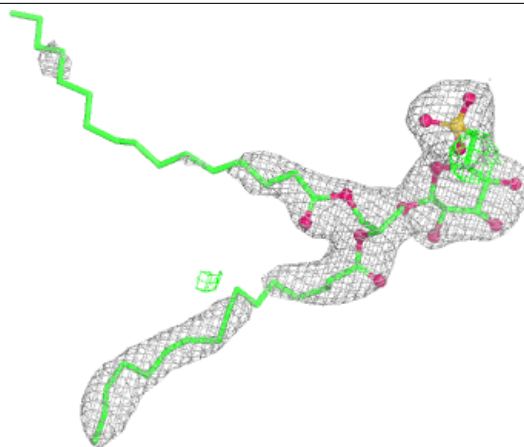
Electron density around CLA C 514:

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



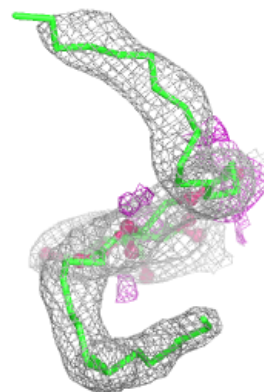
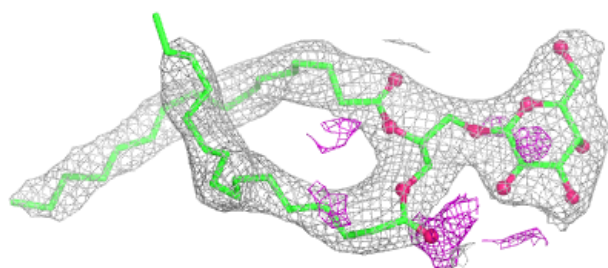
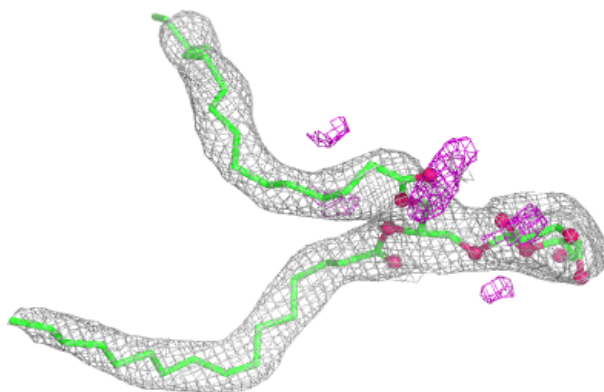
Electron density around SQD A 409:

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



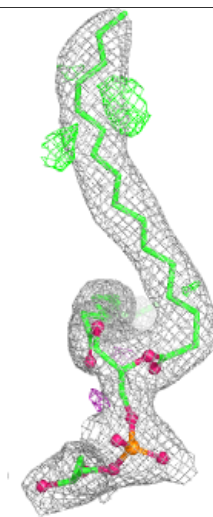
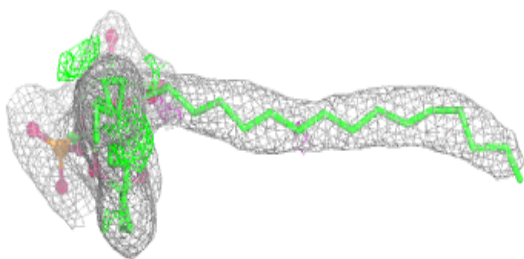
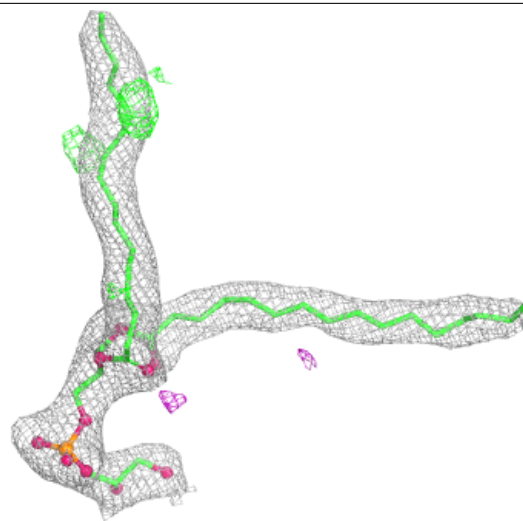
Electron density around LMG M 101:

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



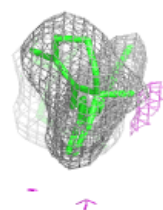
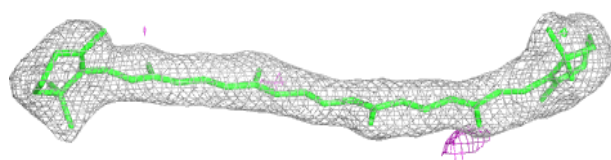
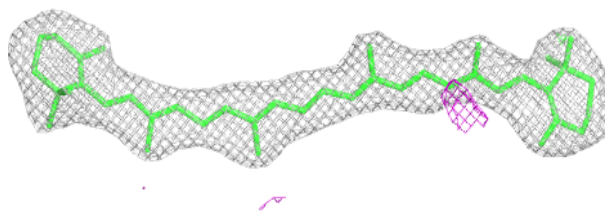
Electron density around LHG b 628:

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

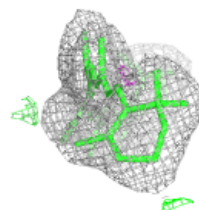
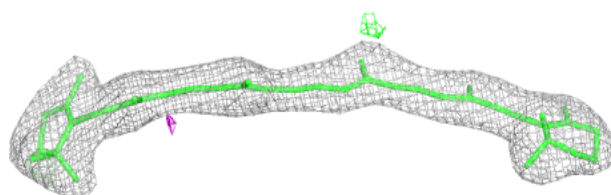
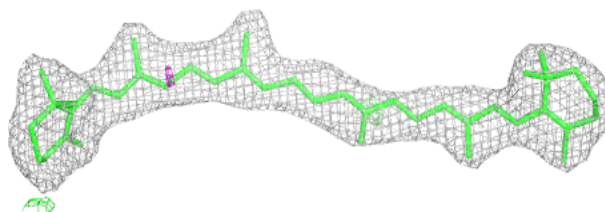


Electron density around BCR B 619:

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

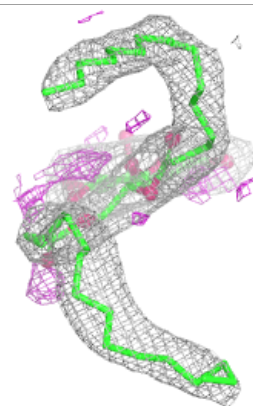
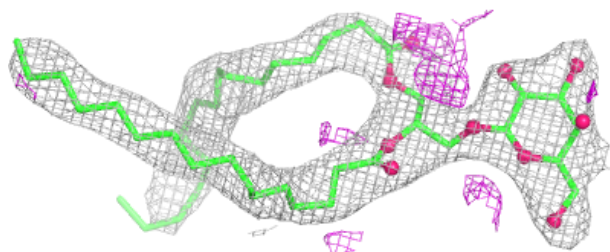
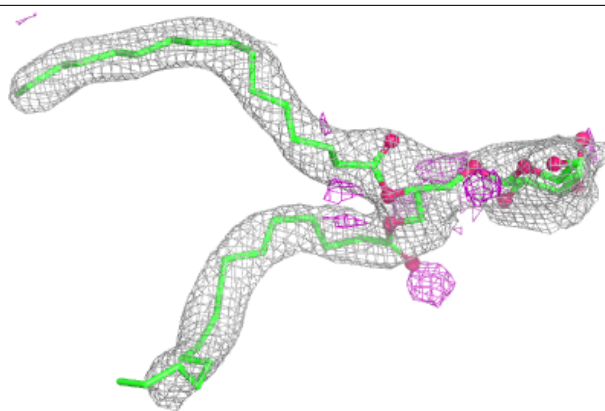
**Electron density around BCR B 631:**

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

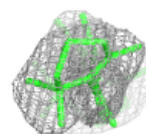
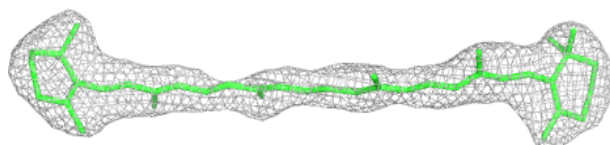
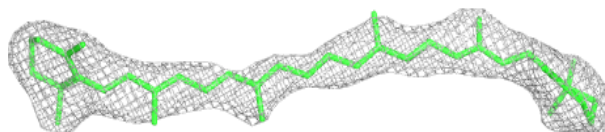


Electron density around LMG m 101:

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

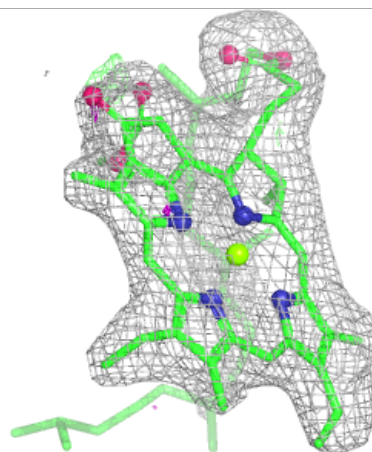
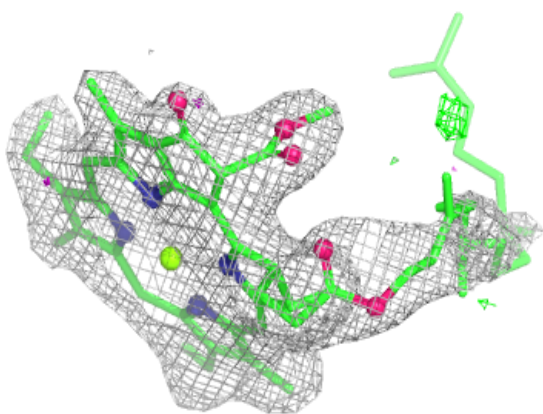
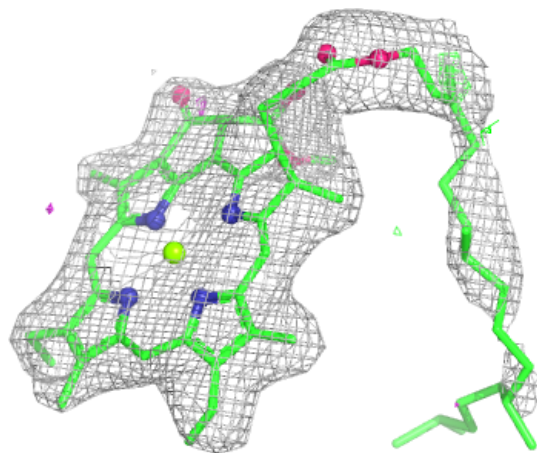
**Electron density around BCR C 516:**

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



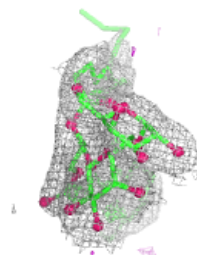
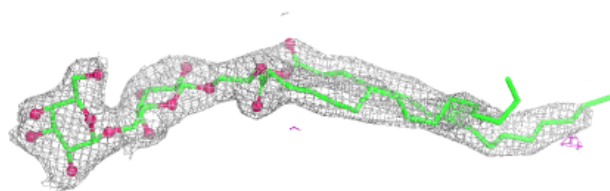
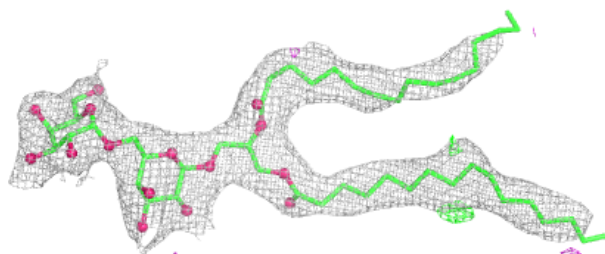
Electron density around CLA b 616:

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

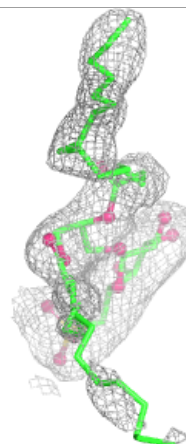
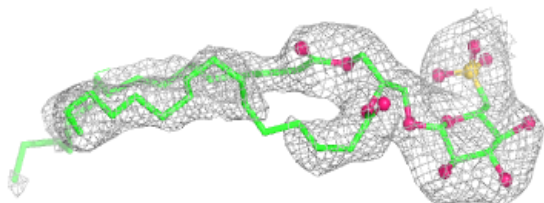
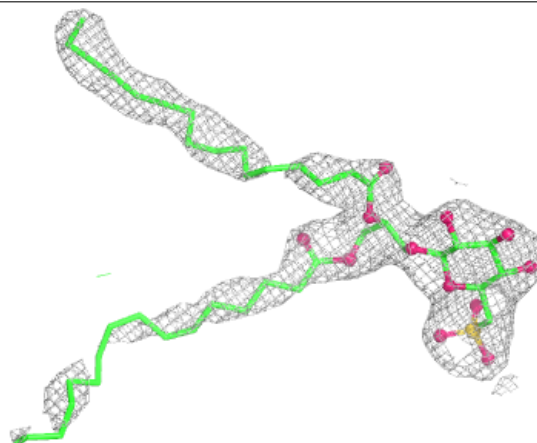


Electron density around DGD C 520:

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

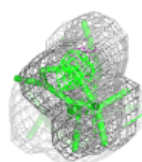
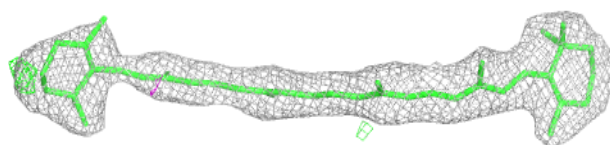
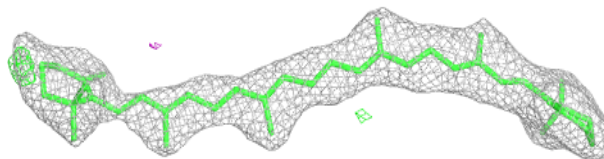
**Electron density around SQD a 409:**

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

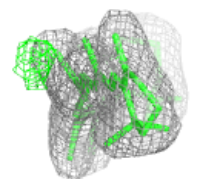
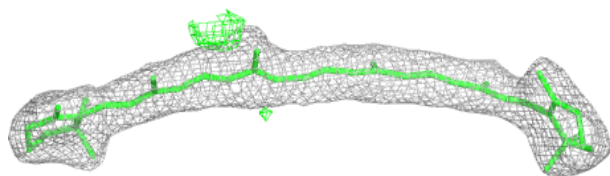
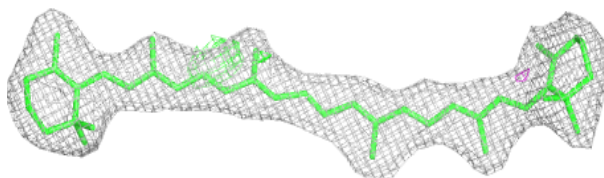


Electron density around BCR H 101:

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

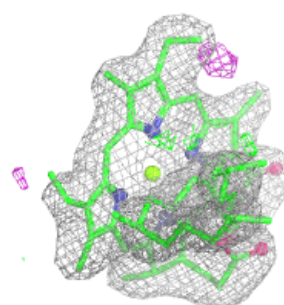
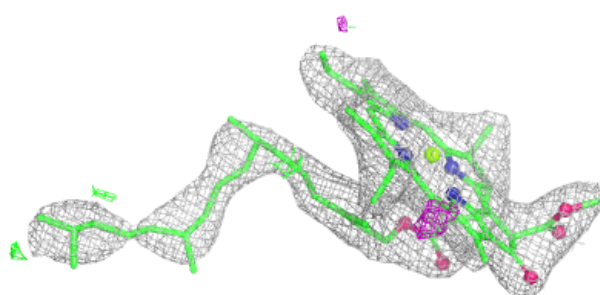
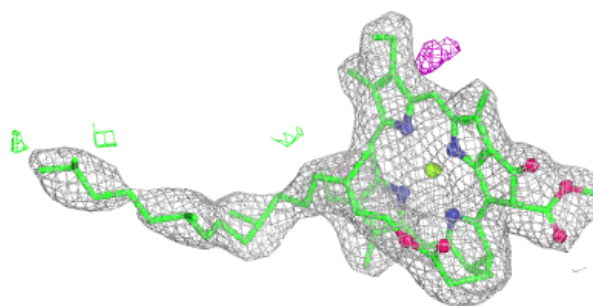
**Electron density around BCR T 101:**

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

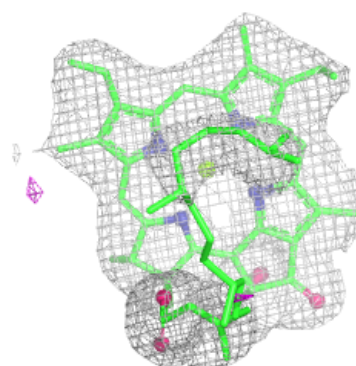
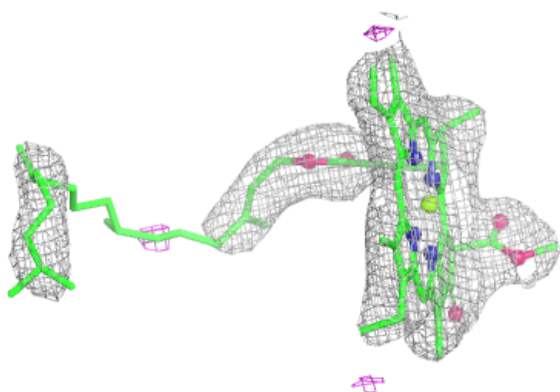
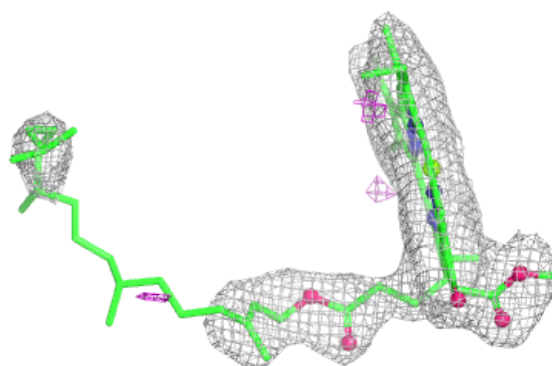


Electron density around CLA c 507:

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

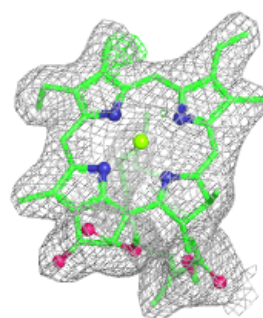
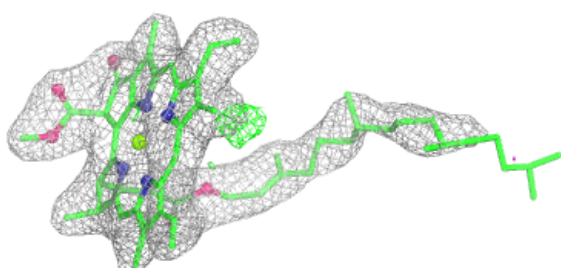
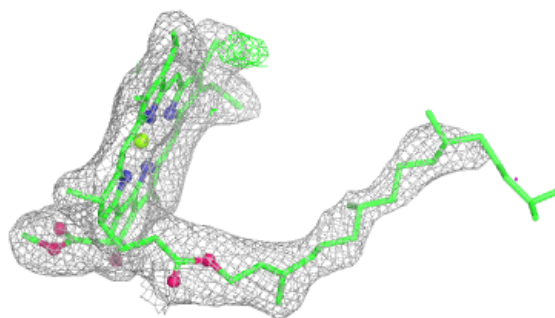
**Electron density around CLA c 508:**

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

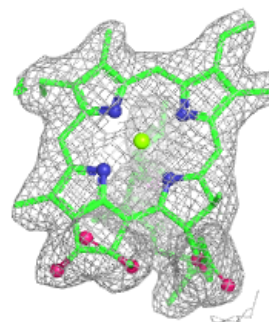
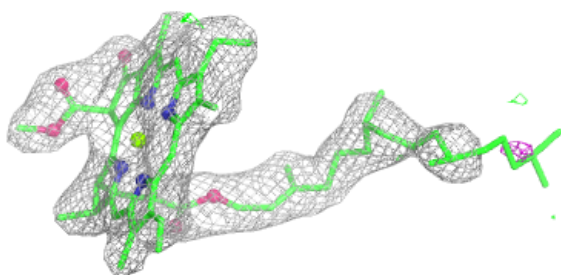
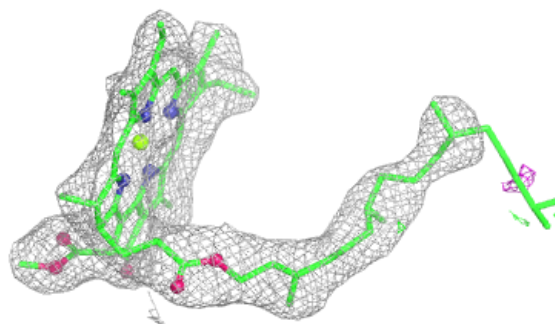


Electron density around CLA C 510:

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

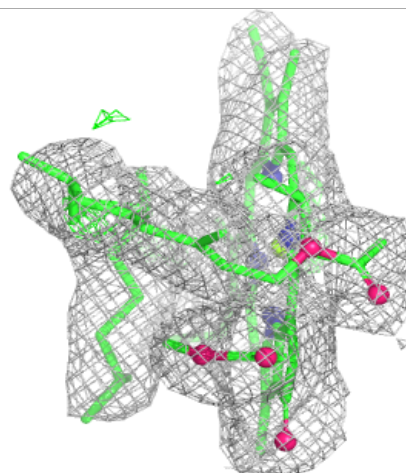
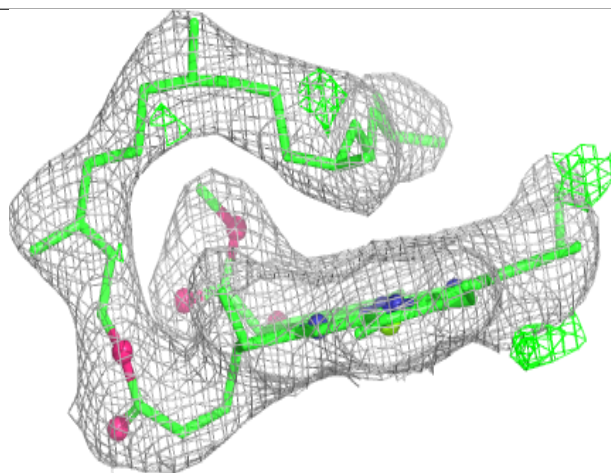
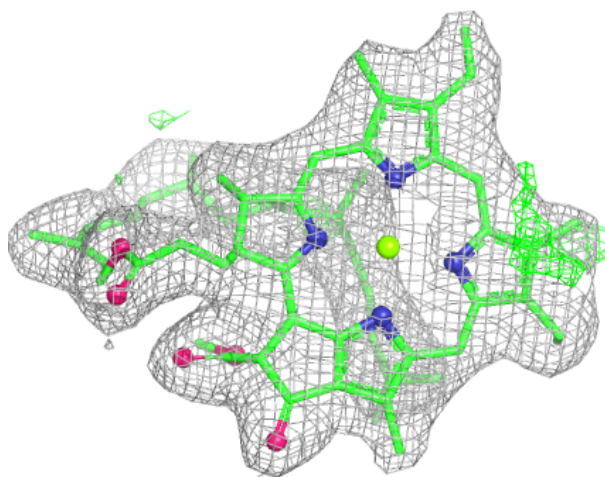
**Electron density around CLA c 510:**

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



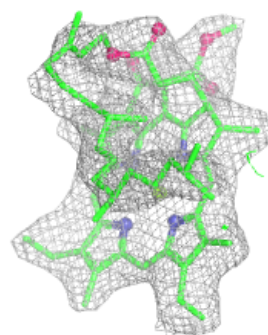
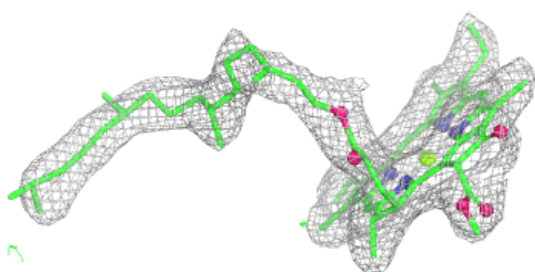
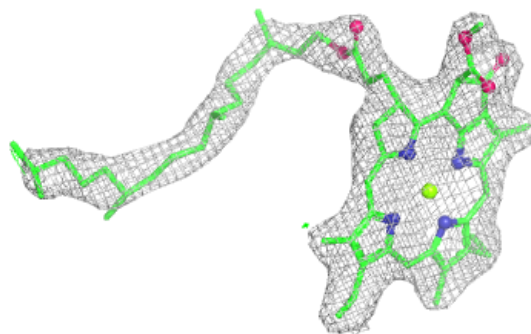
Electron density around CLA C 512:

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

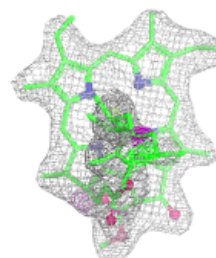
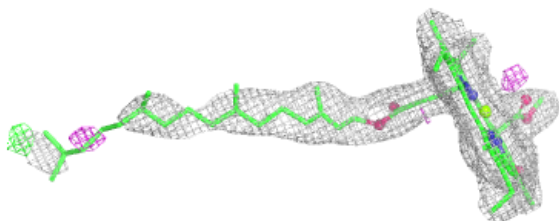
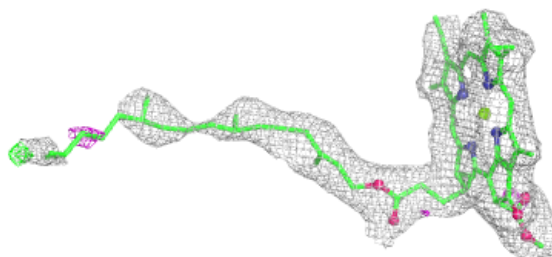


Electron density around CLA C 513:

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

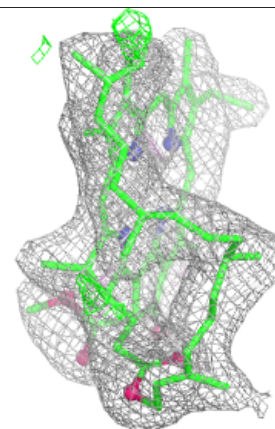
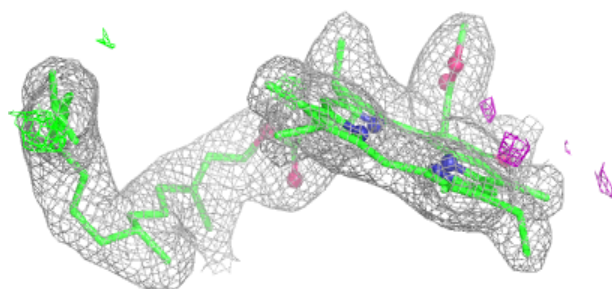
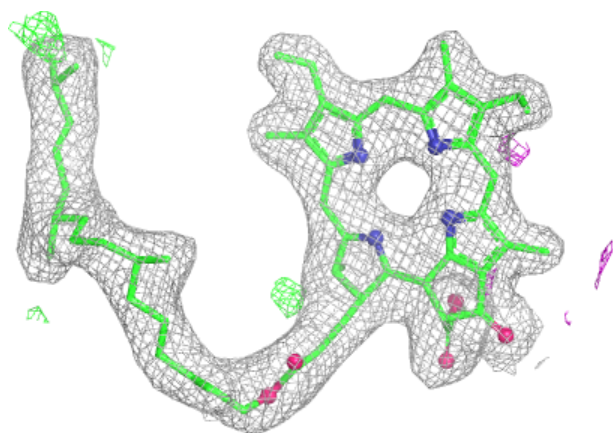
**Electron density around CLA d 403:**

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

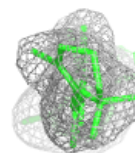
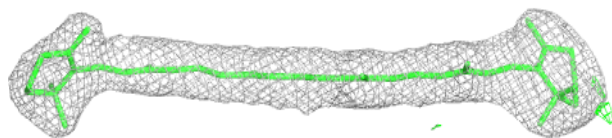
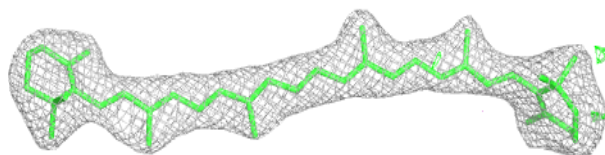


Electron density around PHO A 415:

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

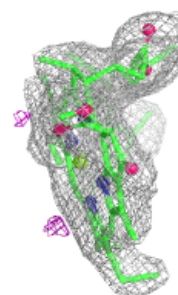
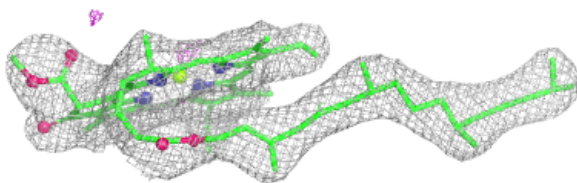
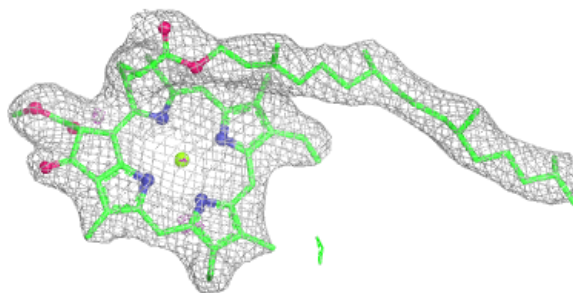
**Electron density around BCR B 618:**

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



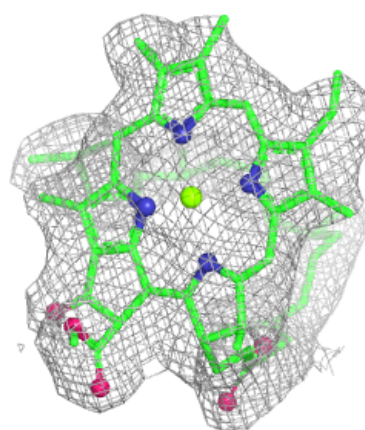
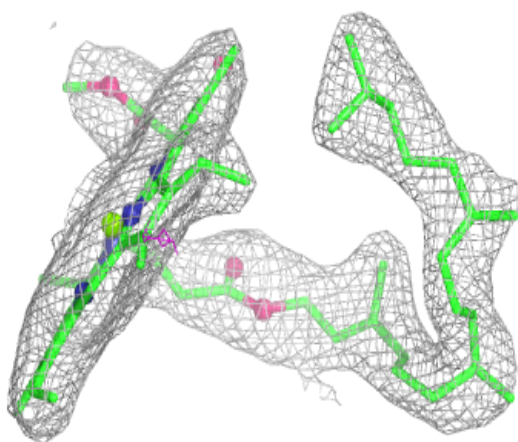
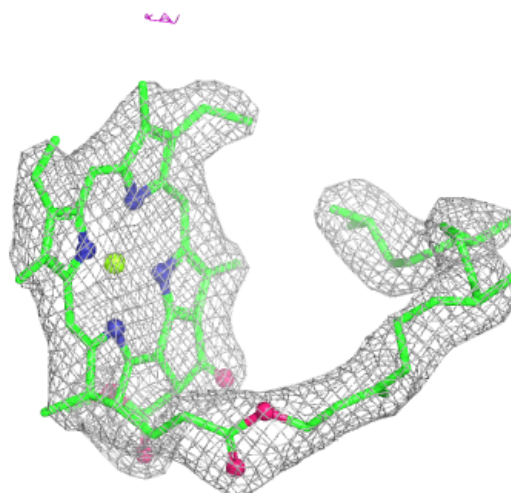
Electron density around CLA C 503:

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



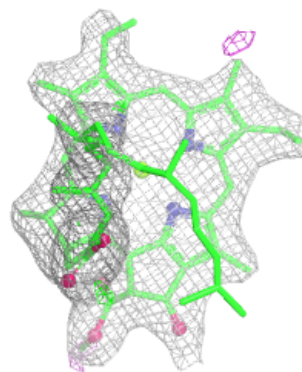
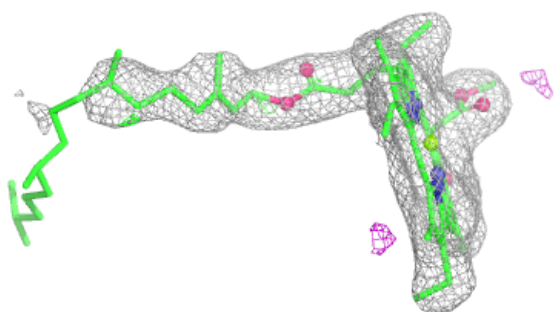
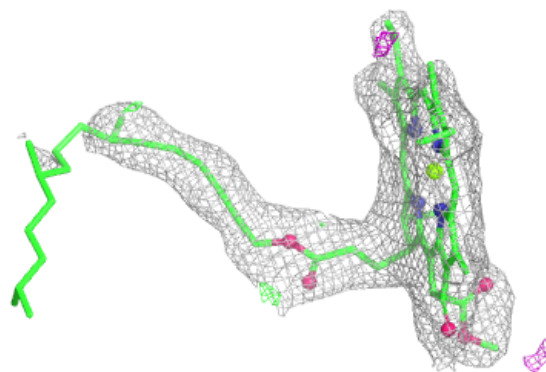
Electron density around CLA C 505:

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

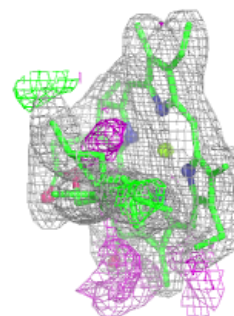
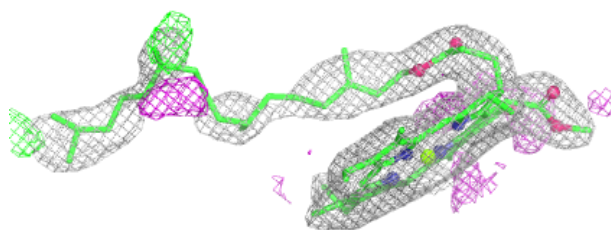
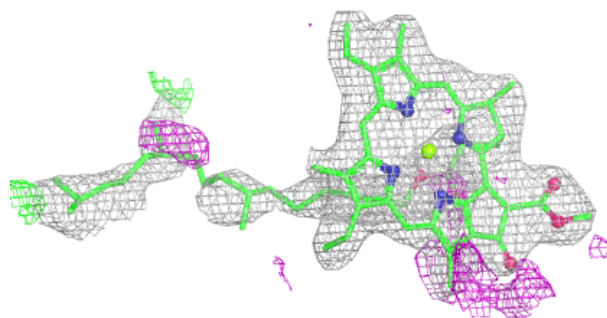


Electron density around CLA D 404:

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

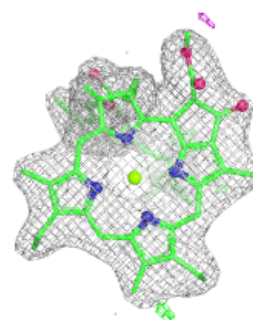
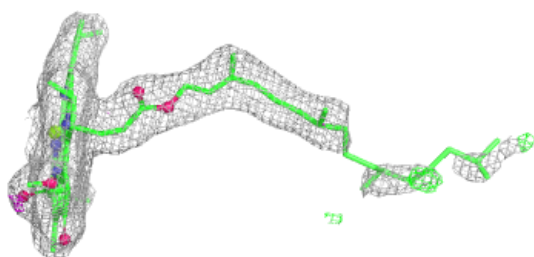
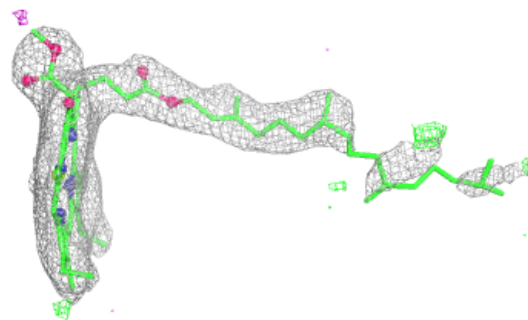
**Electron density around CLA B 614:**

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

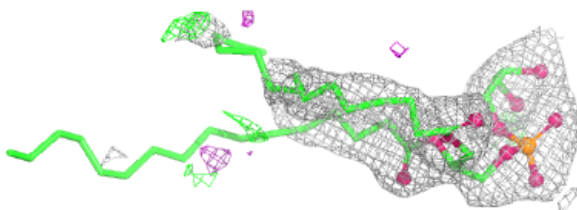
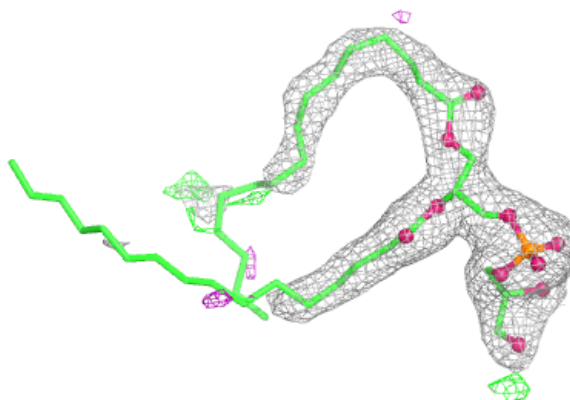


Electron density around CLA b 606:

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

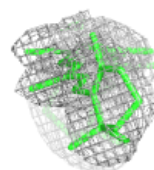
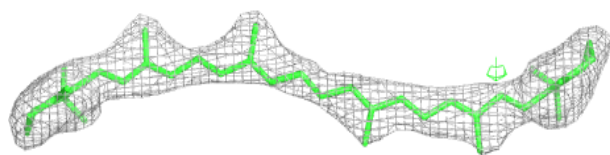
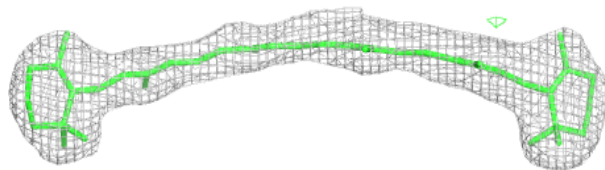
**Electron density around LHG D 408:**

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



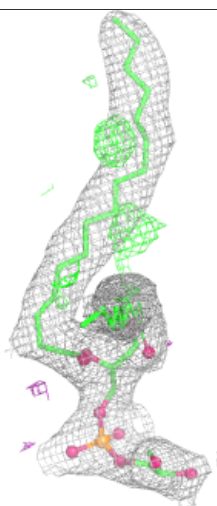
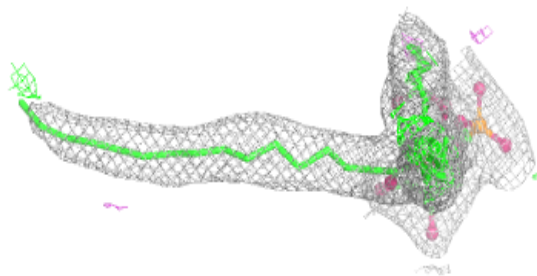
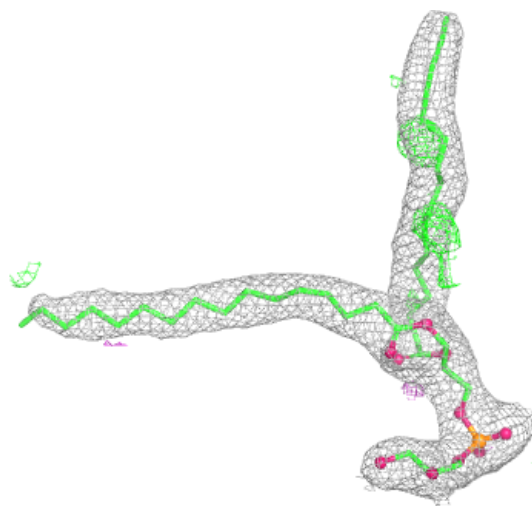
Electron density around BCR K 101:

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



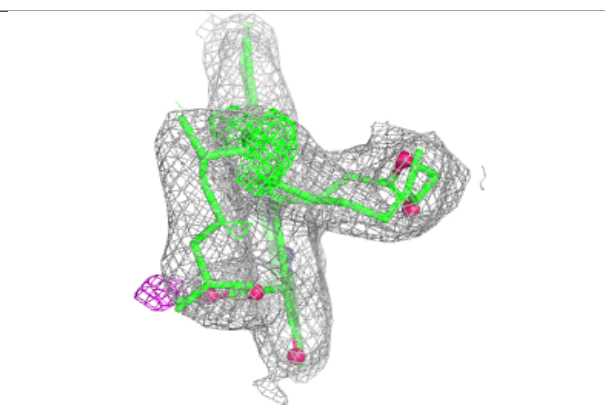
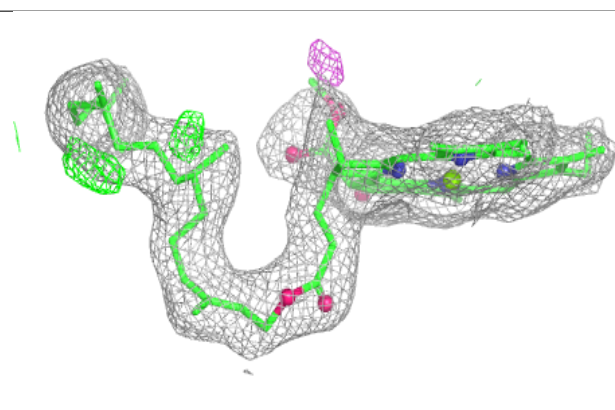
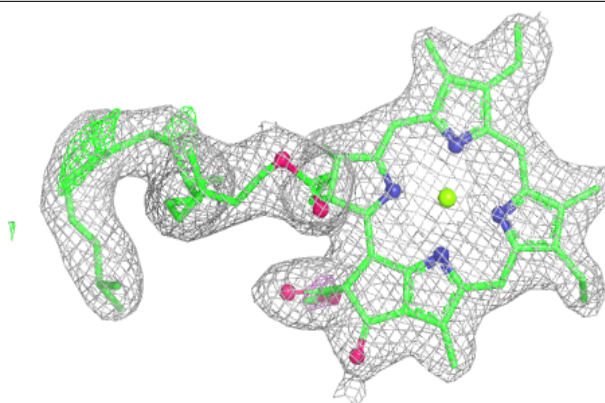
Electron density around LHG L 101:

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

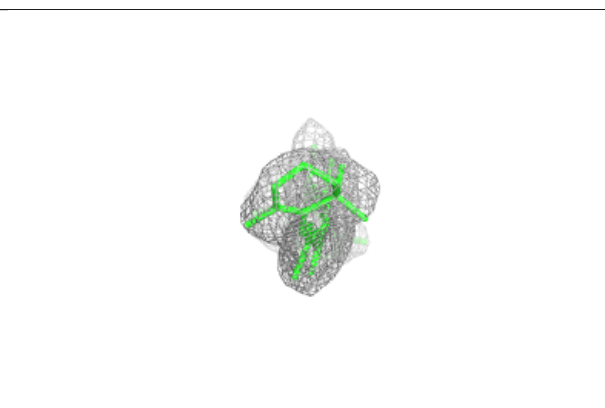
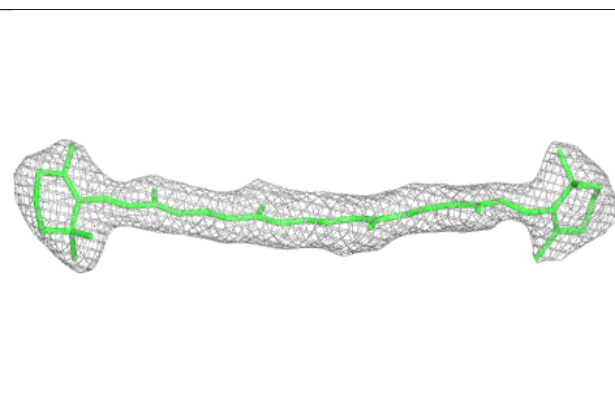
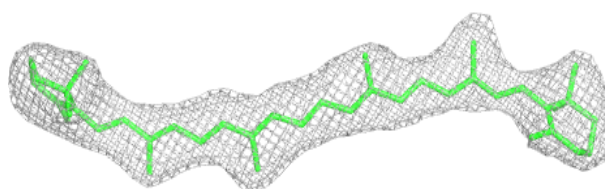


Electron density around CLA b 612:

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

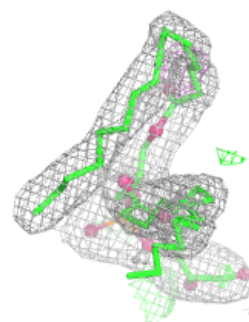
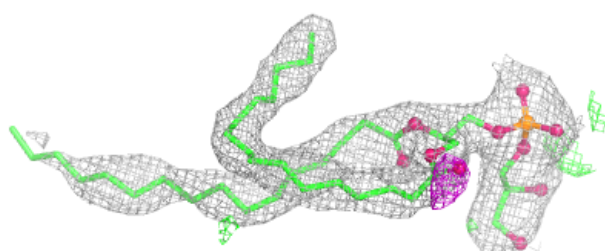
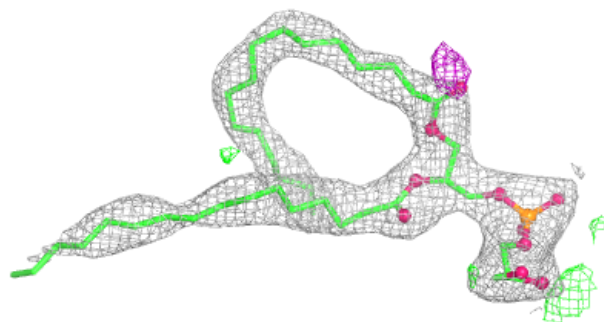
**Electron density around BCR Y 101:**

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

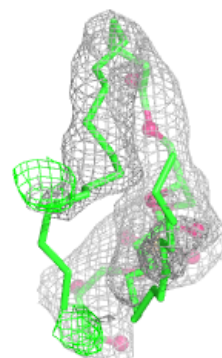
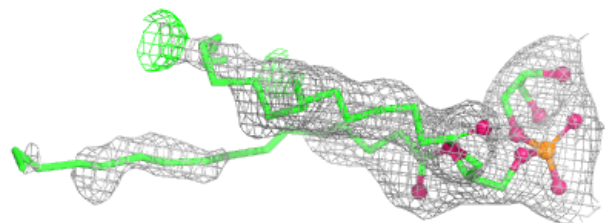
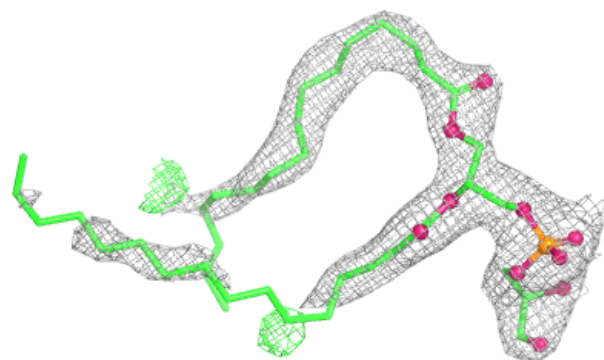


Electron density around LHG d 406:

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

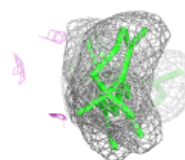
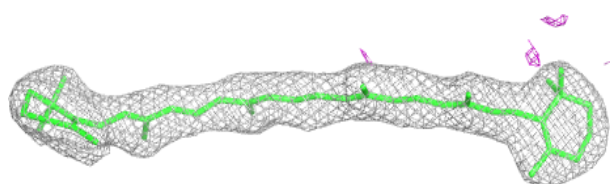
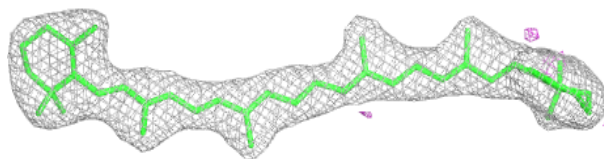
**Electron density around LHG d 408:**

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

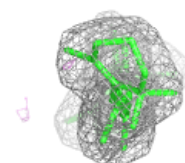
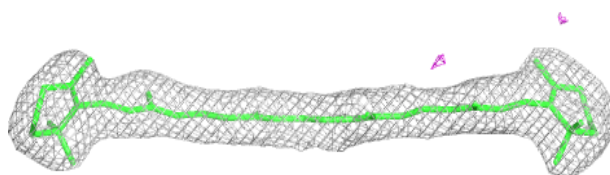
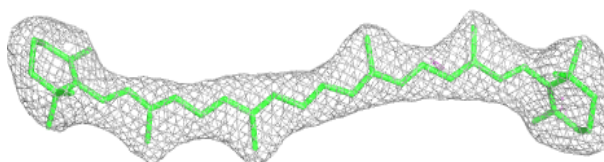


Electron density around BCR b 617:

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

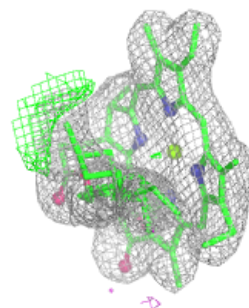
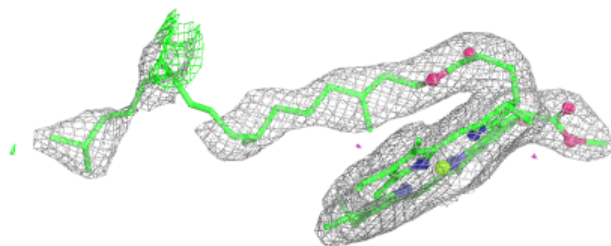
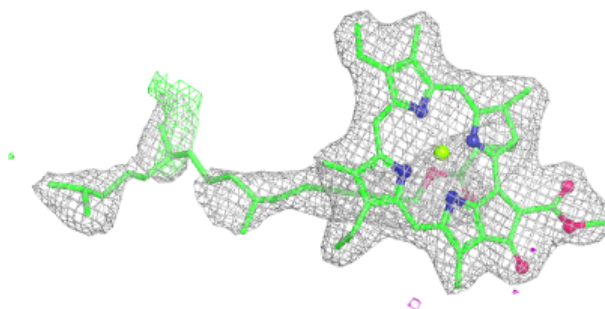
**Electron density around BCR b 618:**

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

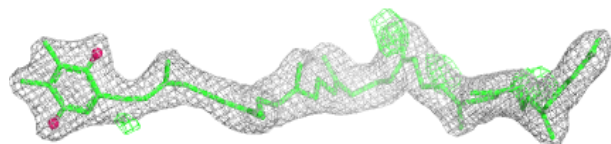
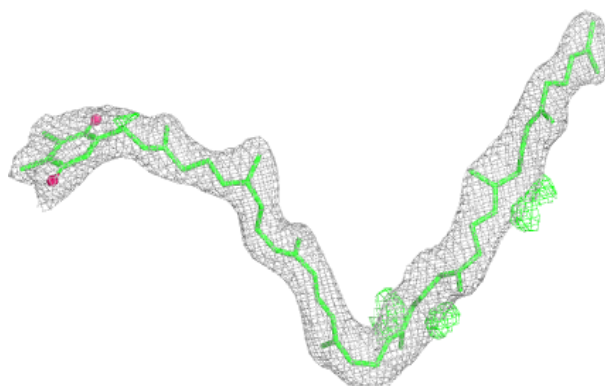


Electron density around CLA b 614:

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

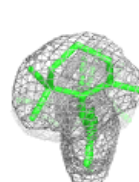
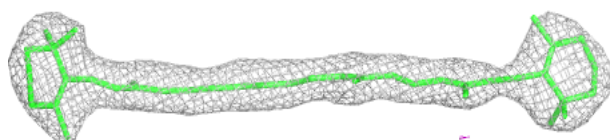
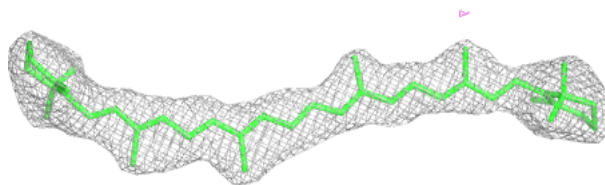
**Electron density around PL9 D 406:**

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

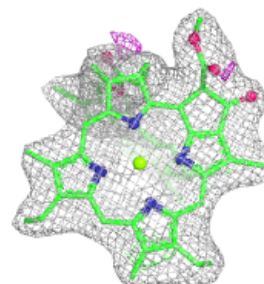
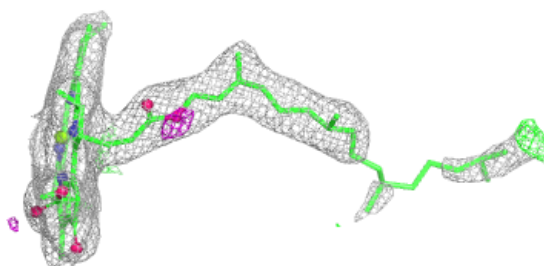
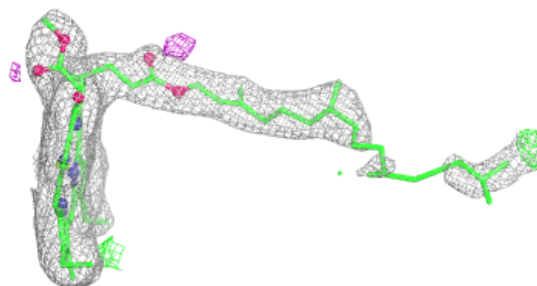


Electron density around BCR c 517:

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

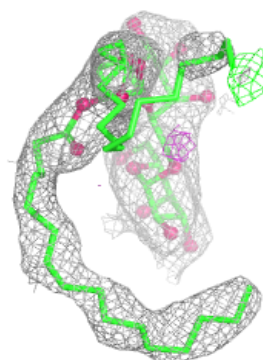
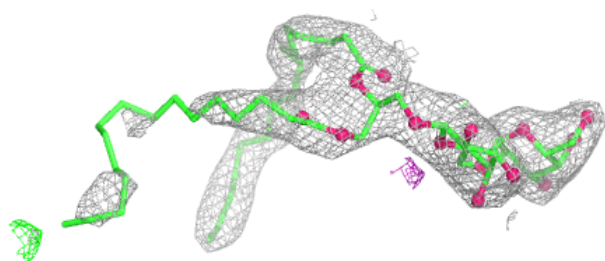
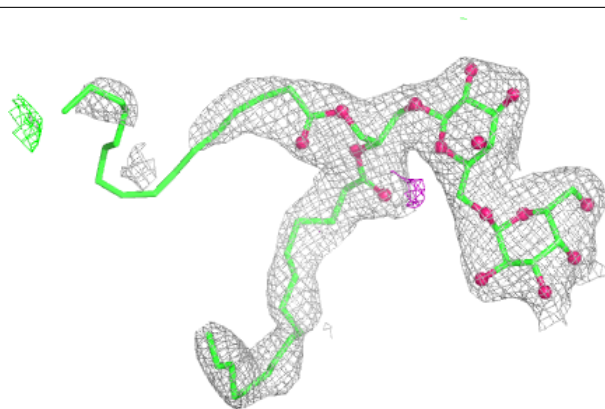
**Electron density around CLA B 606:**

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

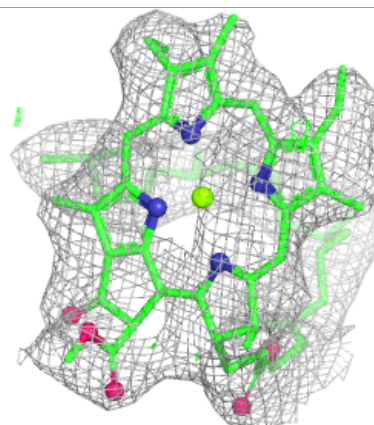
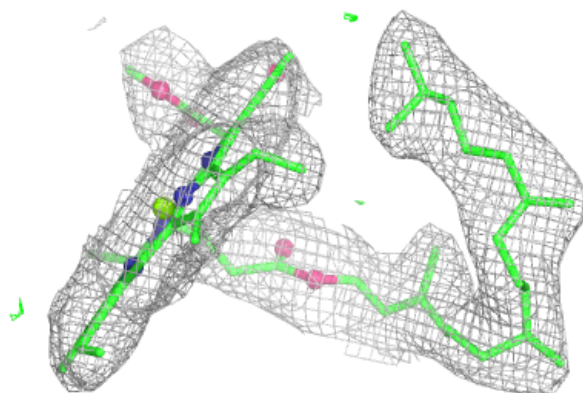
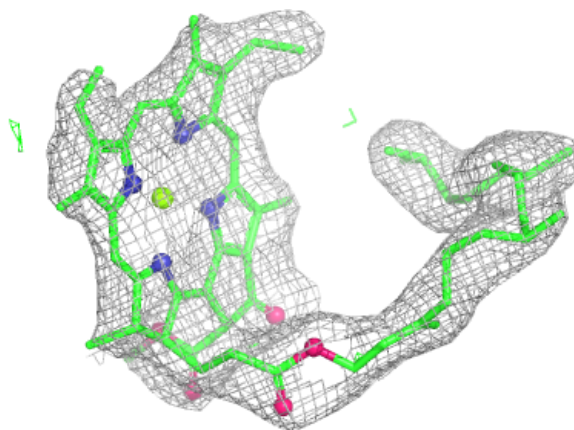


Electron density around DGD c 519:

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

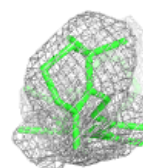
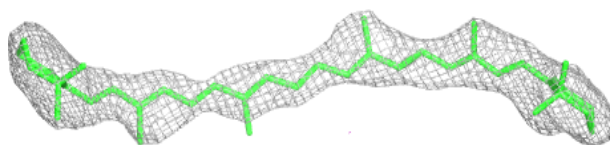
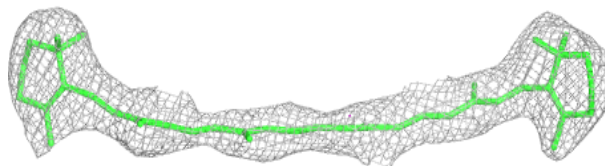
**Electron density around CLA c 505:**

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

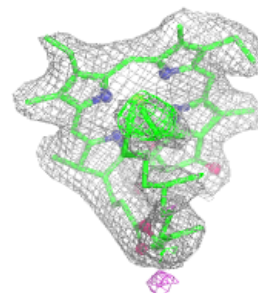
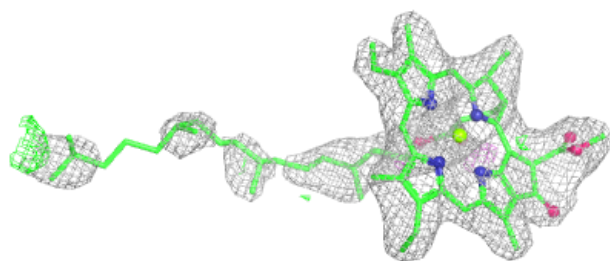
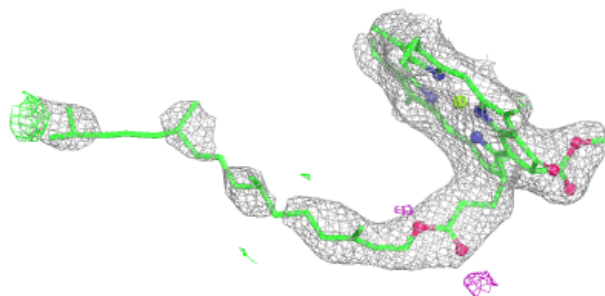


Electron density around BCR k 101:

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

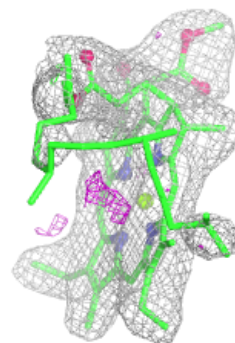
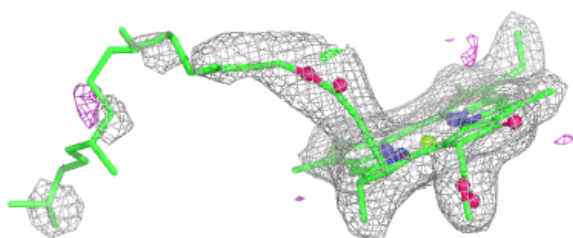
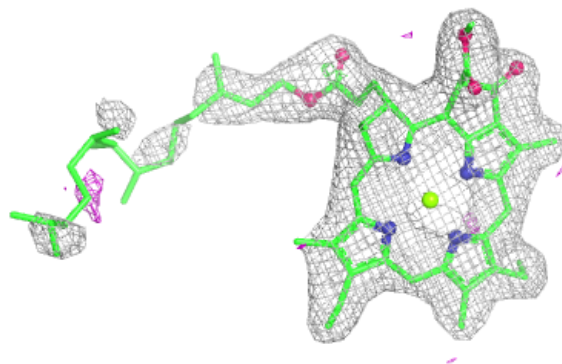
**Electron density around CLA c 506:**

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

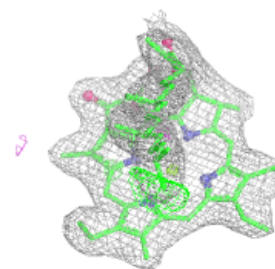
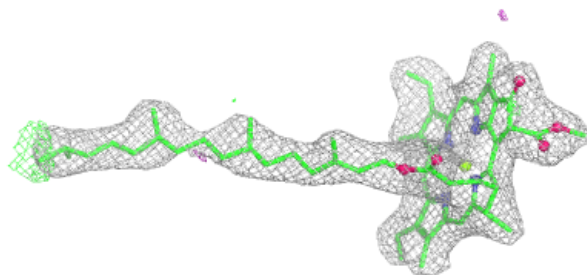
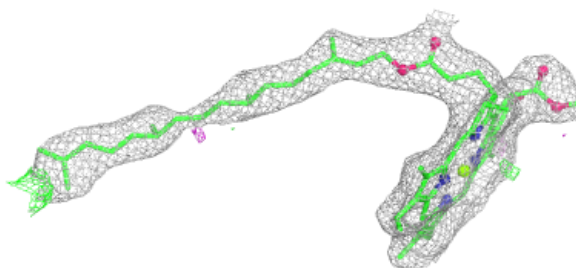


Electron density around CLA a 407:

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

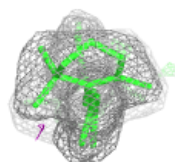
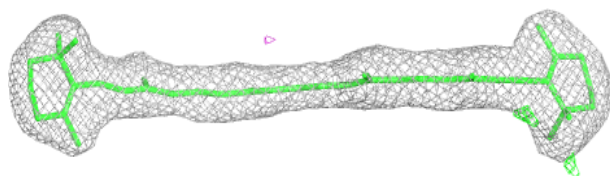
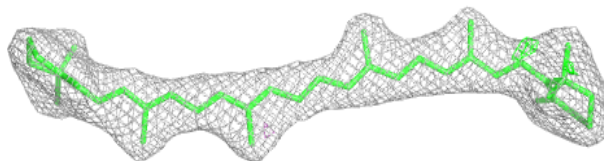
**Electron density around CLA B 607:**

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

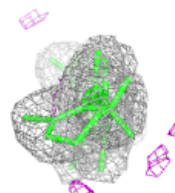
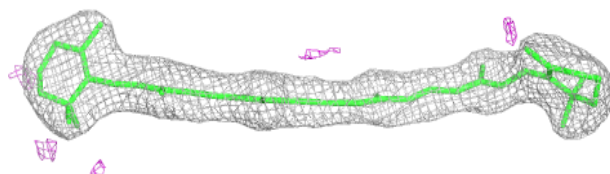
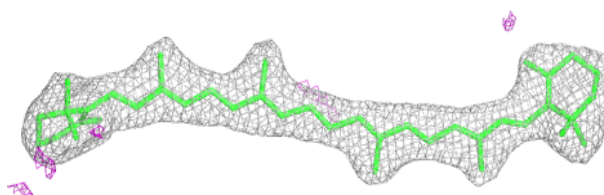


Electron density around BCR A 408:

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

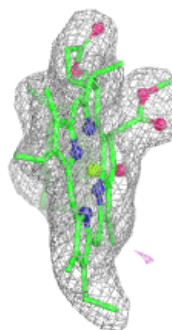
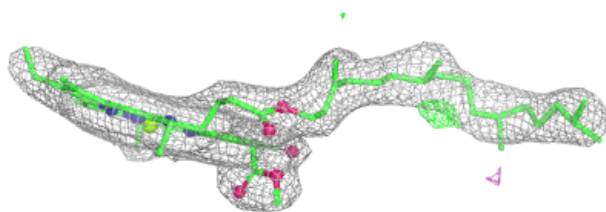
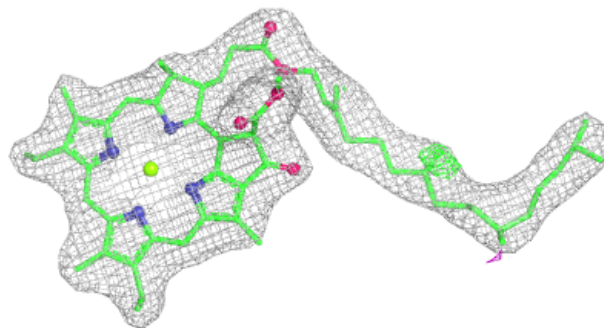
**Electron density around BCR B 617:**

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

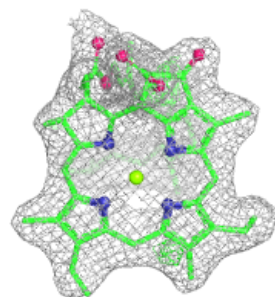
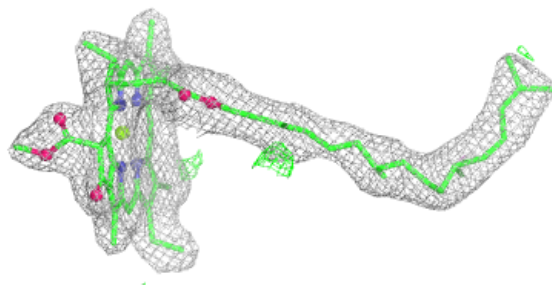
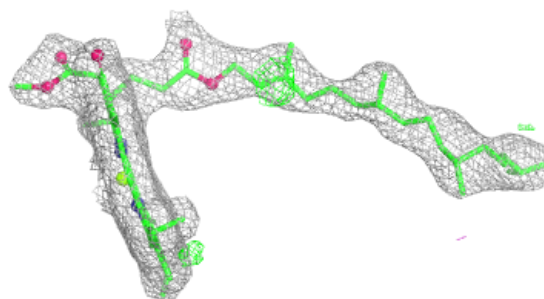


Electron density around CLA b 602:

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

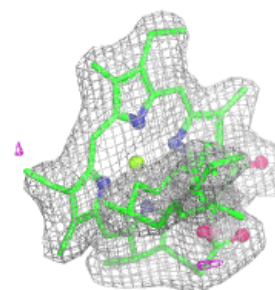
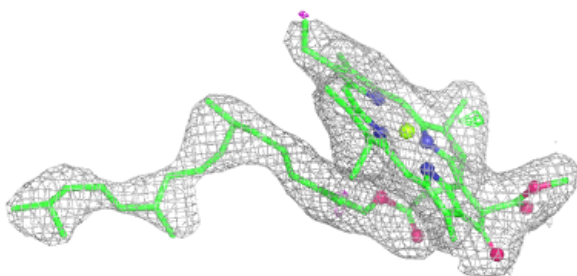
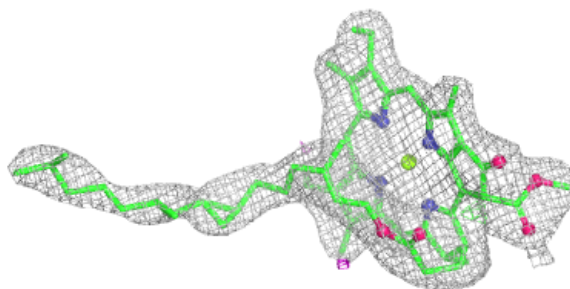
**Electron density around CLA b 605:**

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

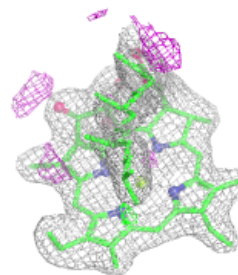
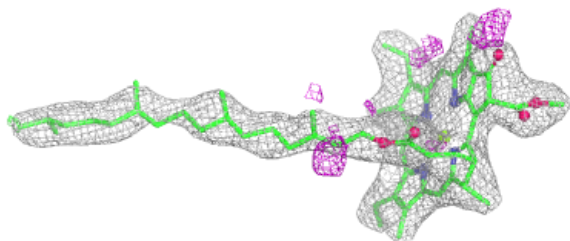
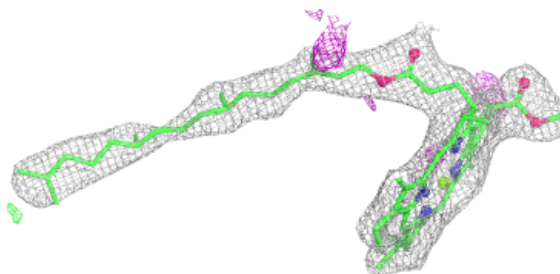


Electron density around CLA C 507:

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

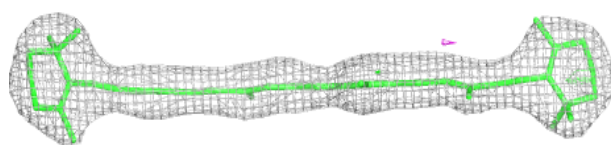
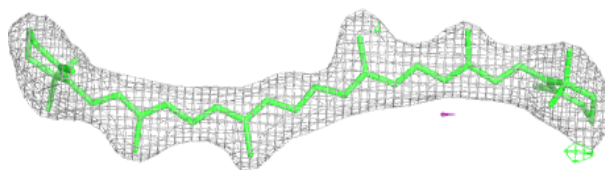
**Electron density around CLA b 607:**

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

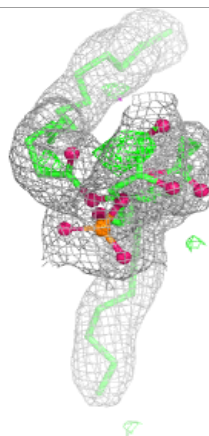
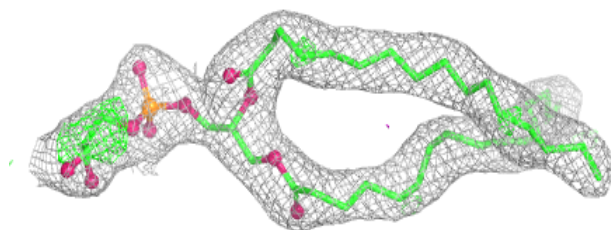
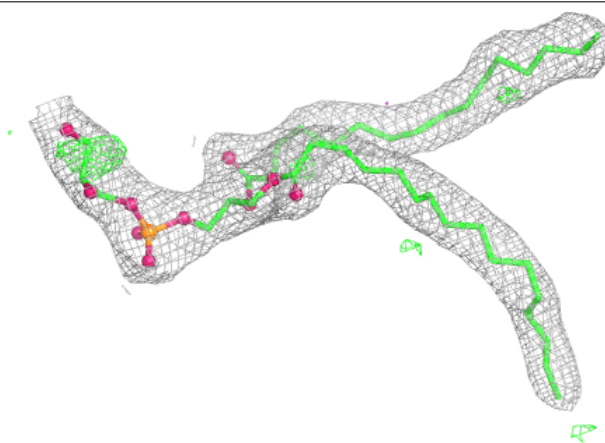


Electron density around BCR C 517:

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

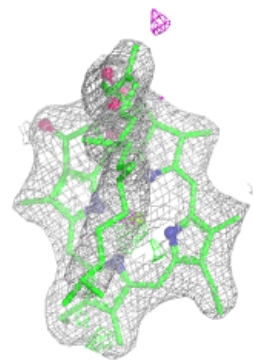
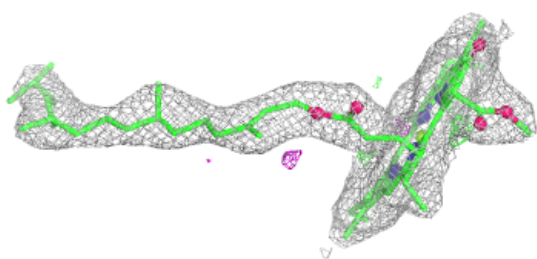
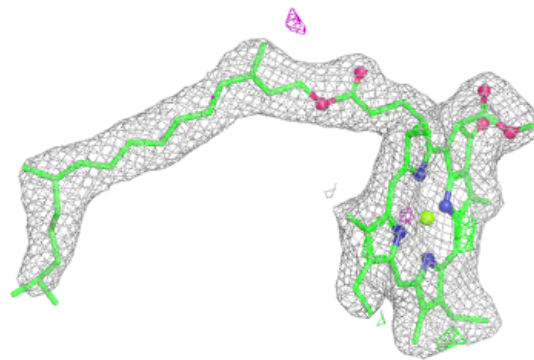
**Electron density around LHG D 407:**

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



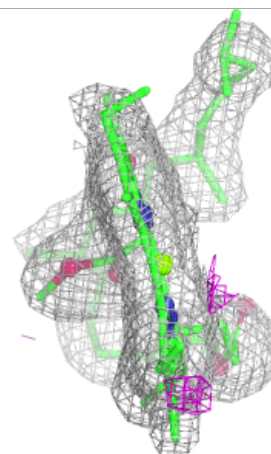
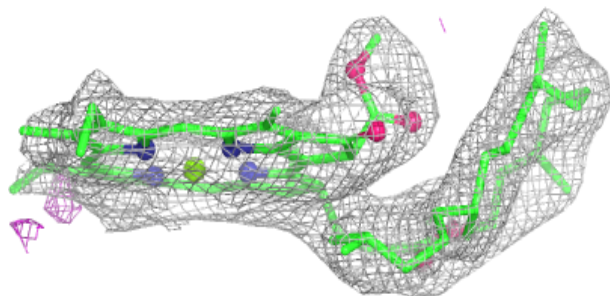
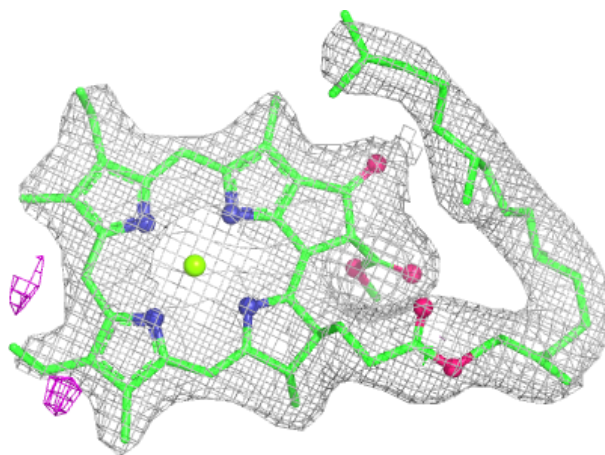
Electron density around CLA b 609:

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



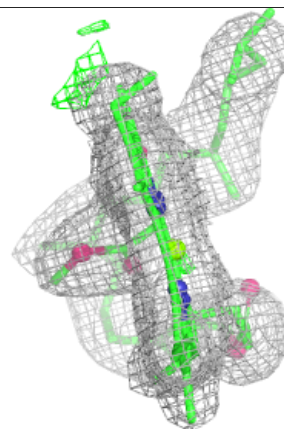
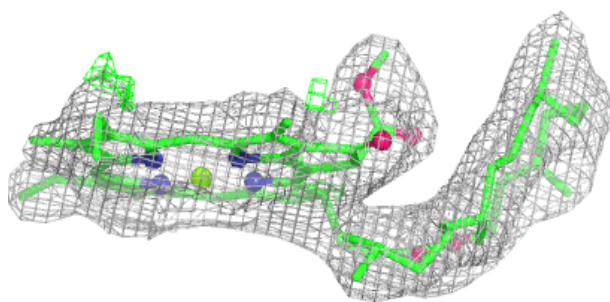
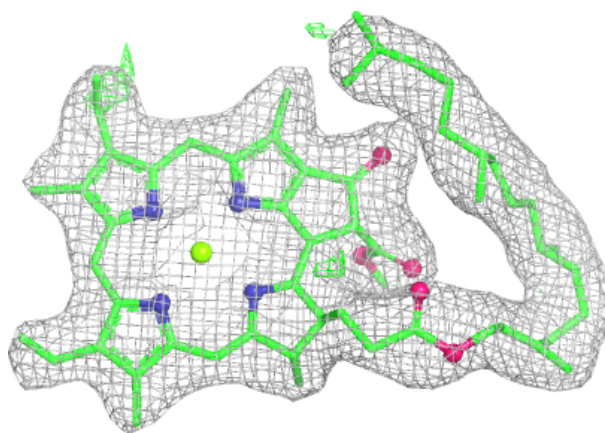
Electron density around CLA b 610:

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



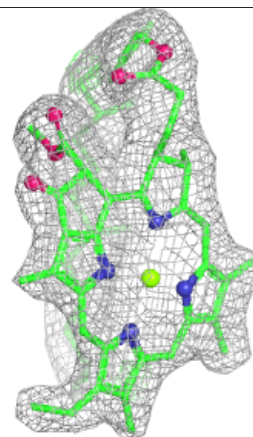
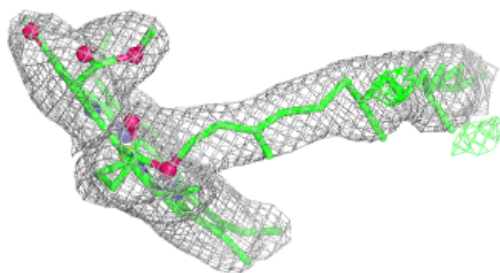
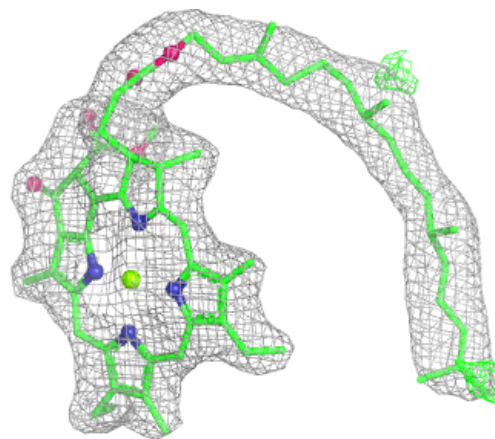
Electron density around CLA B 610:

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



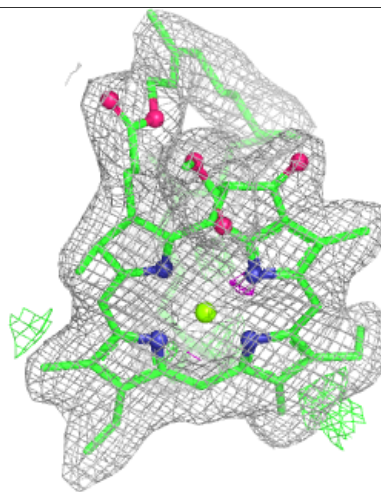
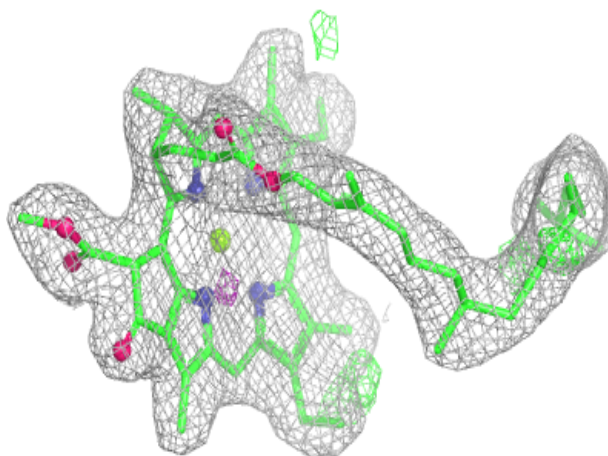
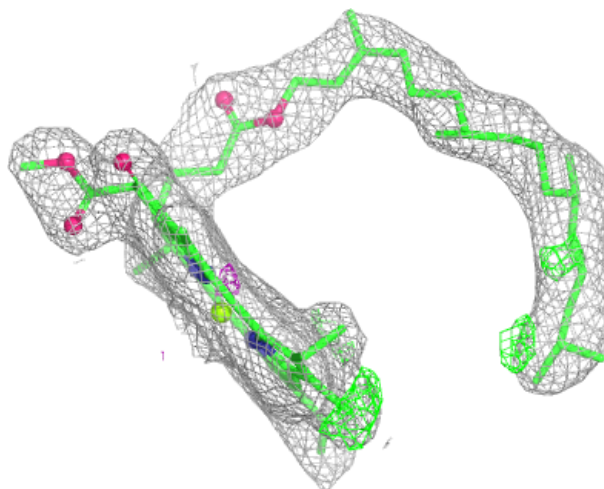
Electron density around CLA C 509:

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



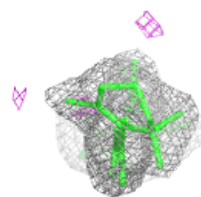
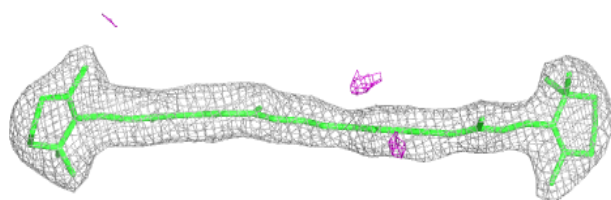
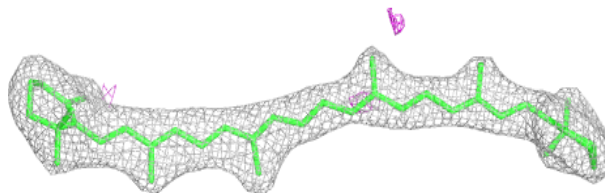
Electron density around CLA B 611:

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



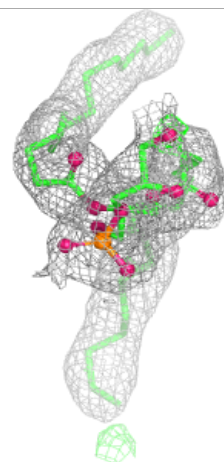
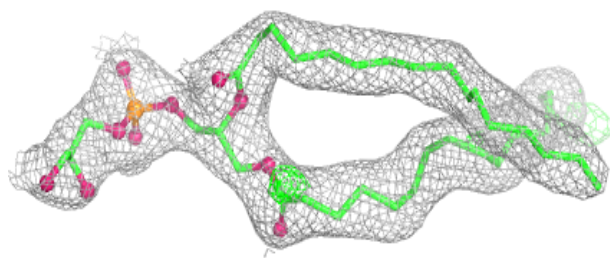
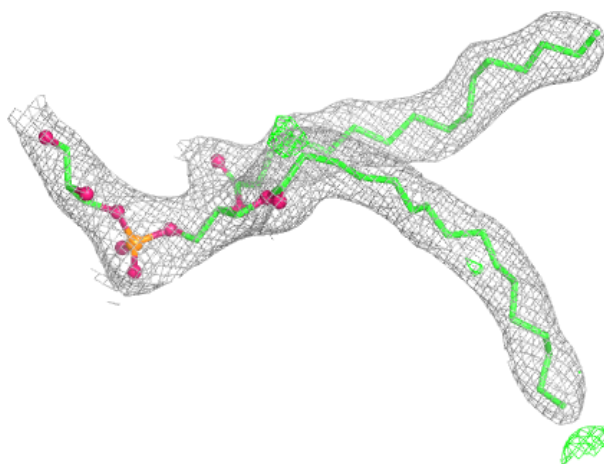
Electron density around BCR a 408:

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



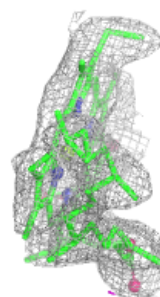
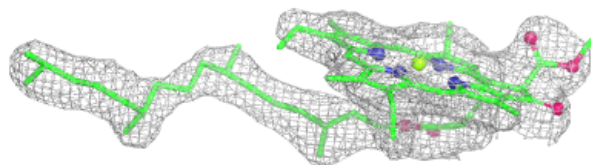
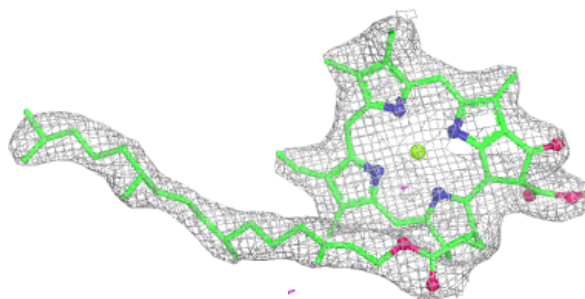
Electron density around LHG d 407:

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

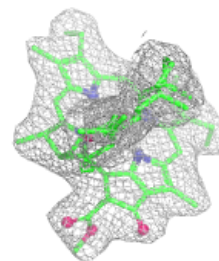
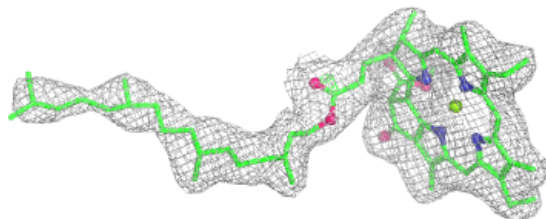
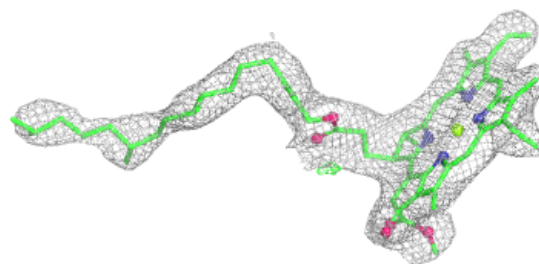


Electron density around CLA c 503:

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

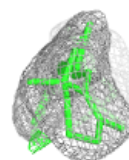
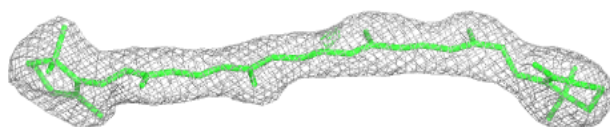
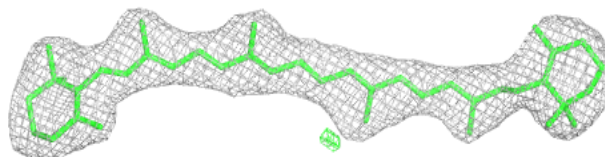
**Electron density around CLA c 504:**

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

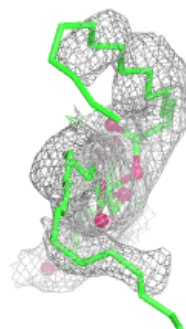
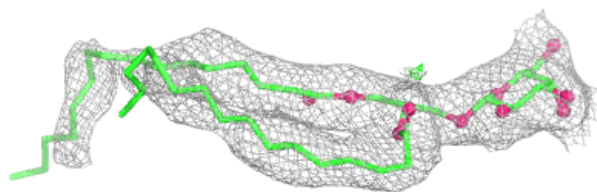
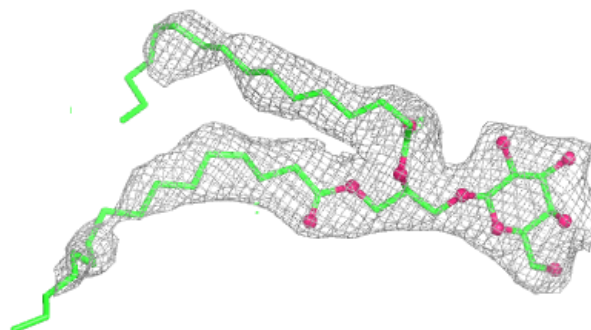


Electron density around BCR b 619:

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

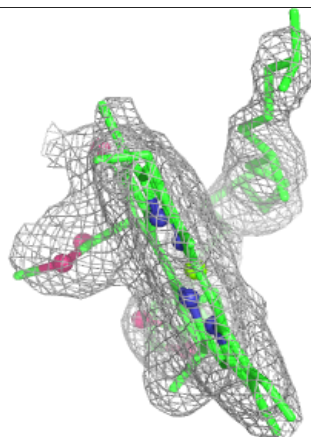
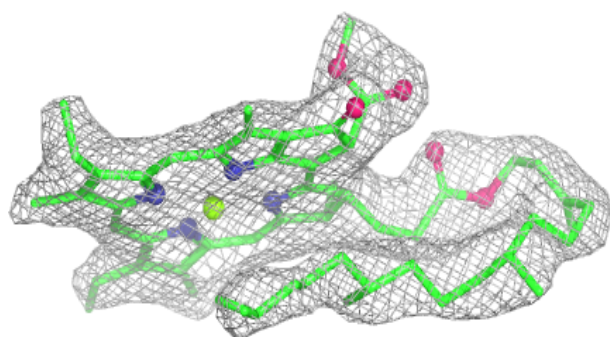
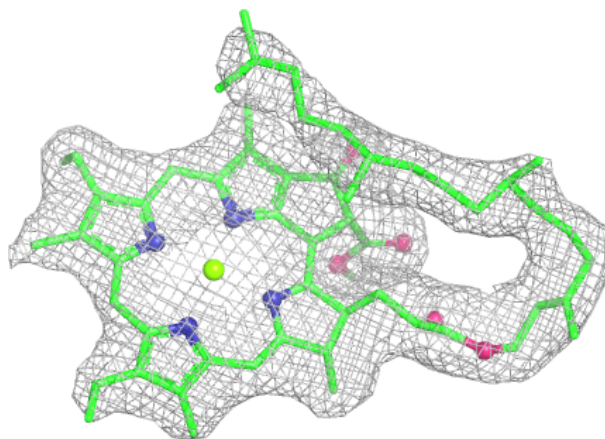
**Electron density around LMG d 411:**

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

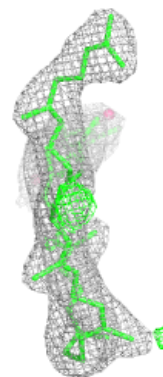
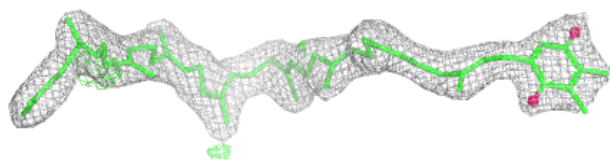
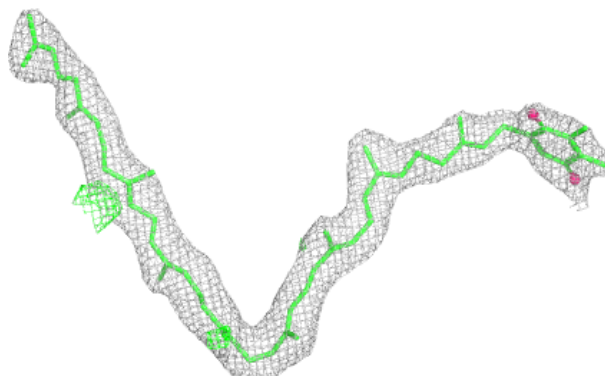


Electron density around CLA C 511:

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

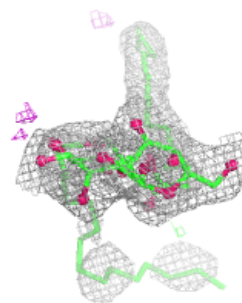
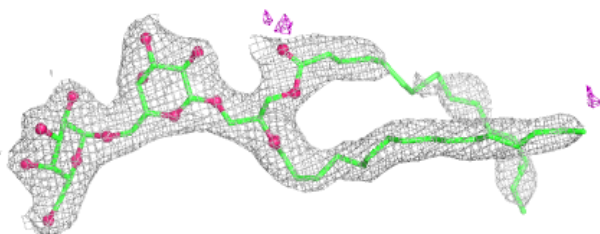
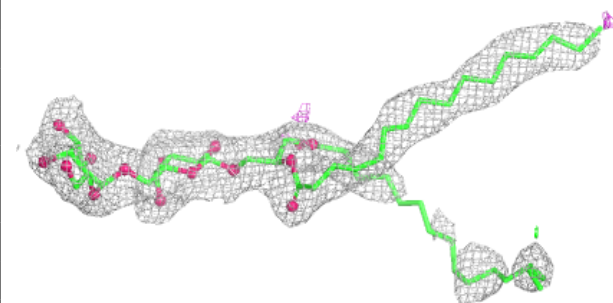
**Electron density around PL9 d 405:**

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

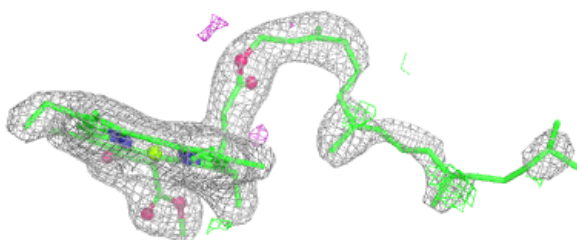
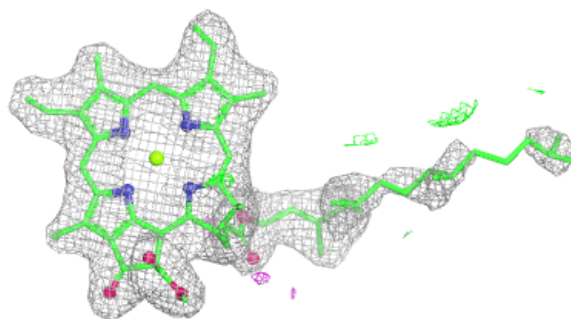


Electron density around DGD C 518:

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

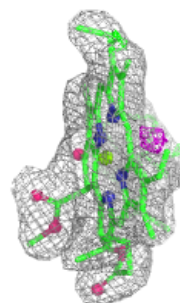
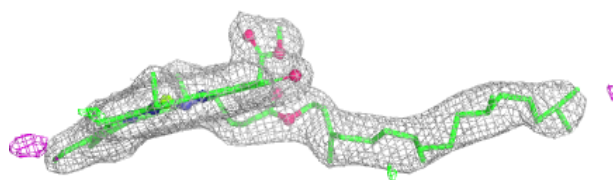
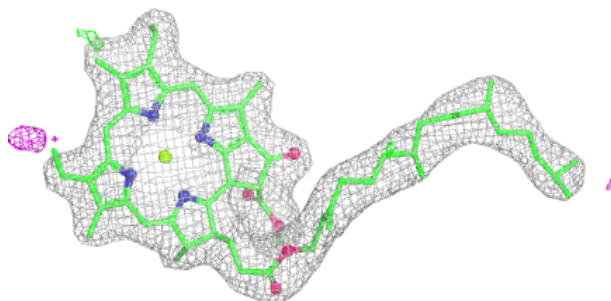
**Electron density around CLA A 405:**

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

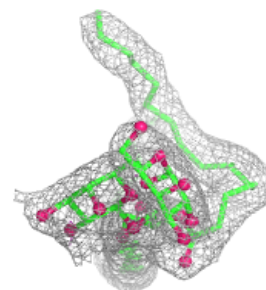
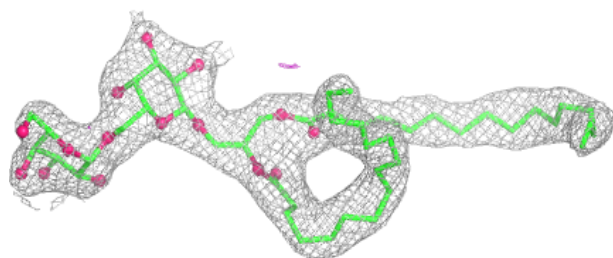
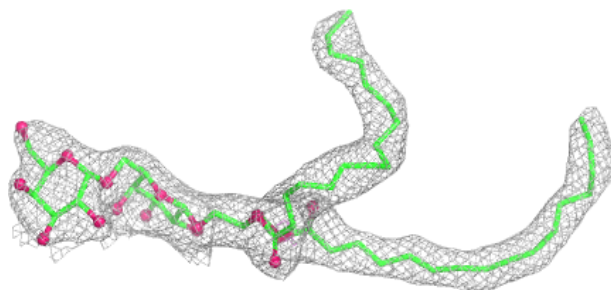


Electron density around CLA B 602:

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

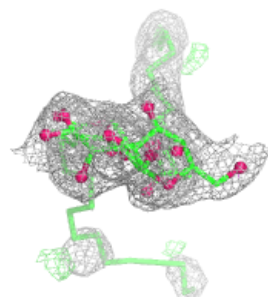
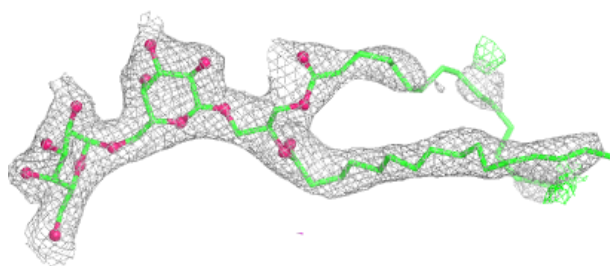
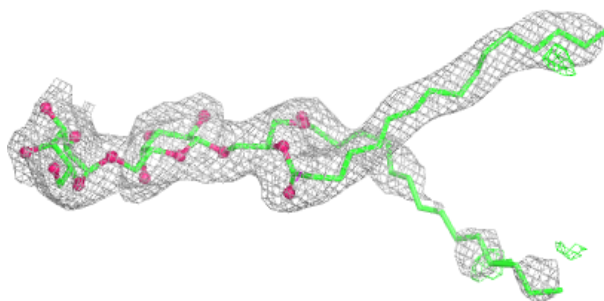
**Electron density around DGD H 102:**

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

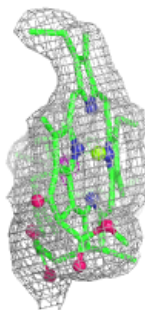
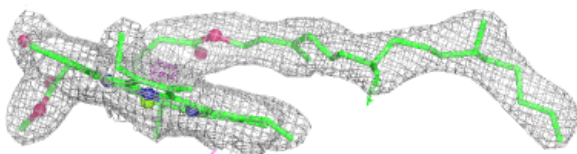
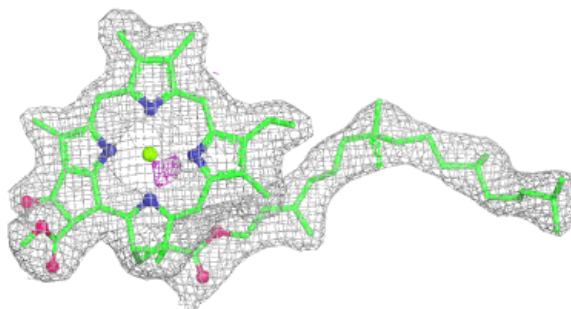


Electron density around DGD c 518:

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

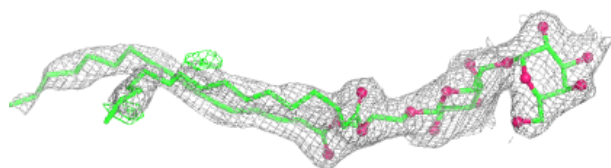
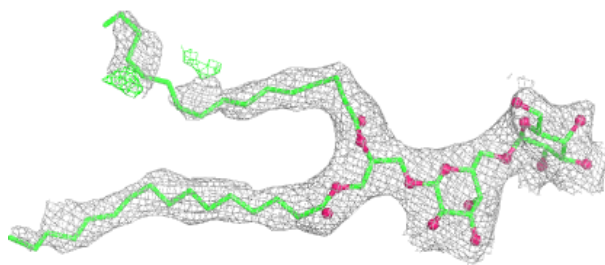
**Electron density around CLA B 603:**

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

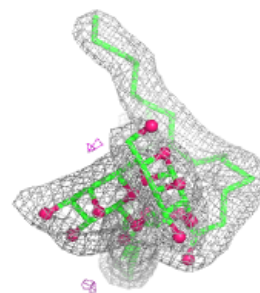
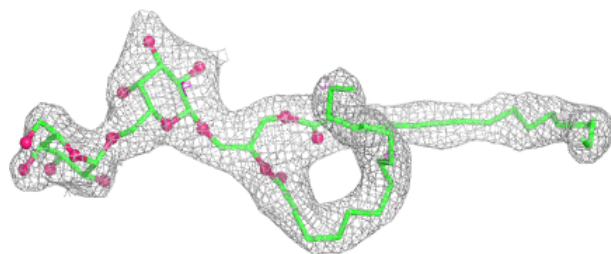
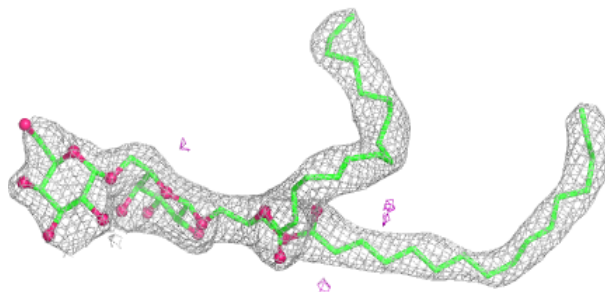


Electron density around DGD c 520:

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

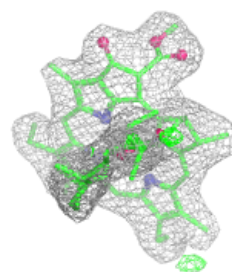
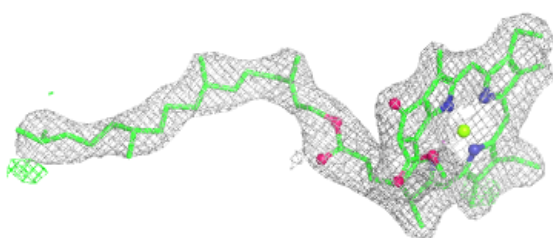
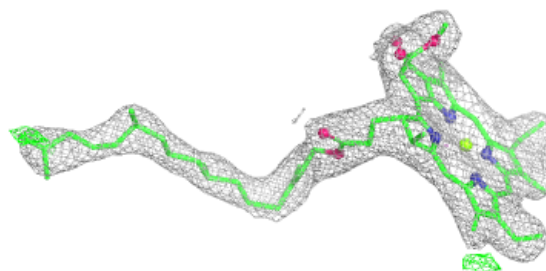
**Electron density around DGD h 103:**

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

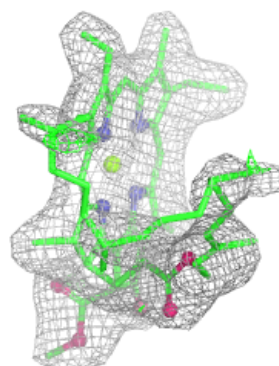
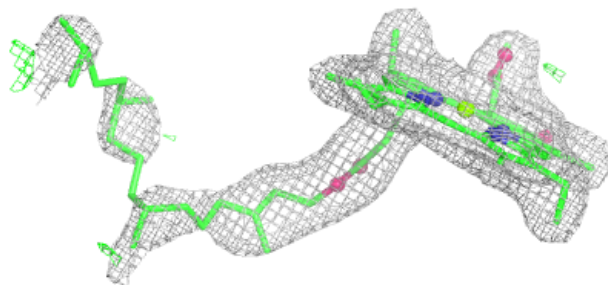
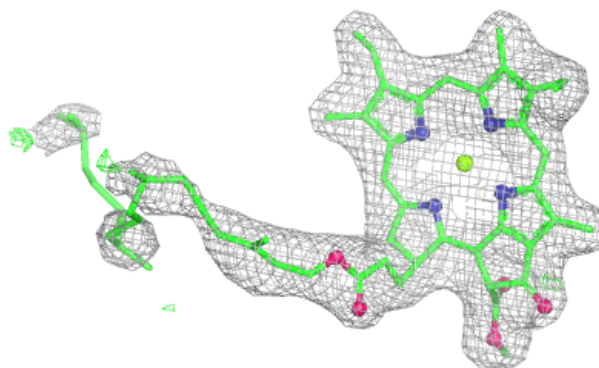


Electron density around CLA C 504:

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

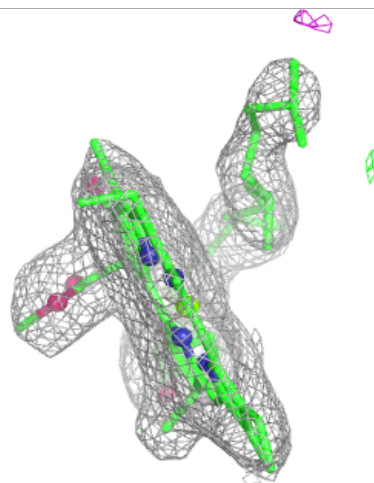
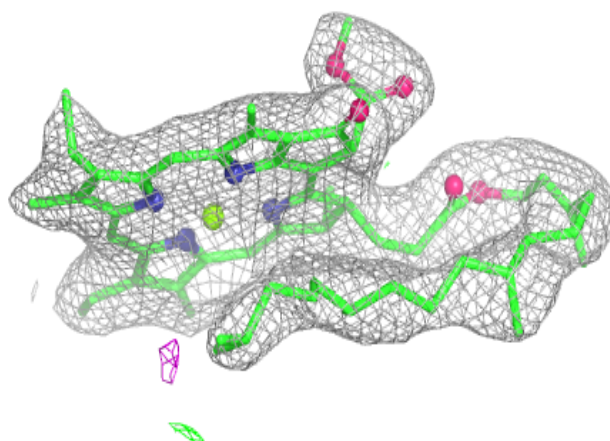
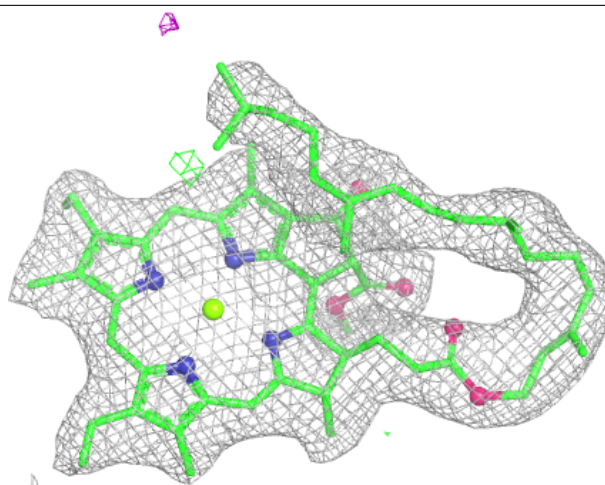
**Electron density around CLA A 407:**

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



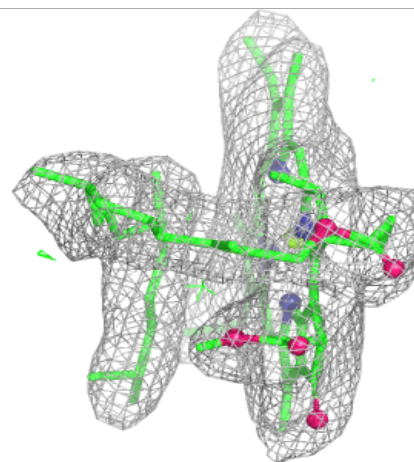
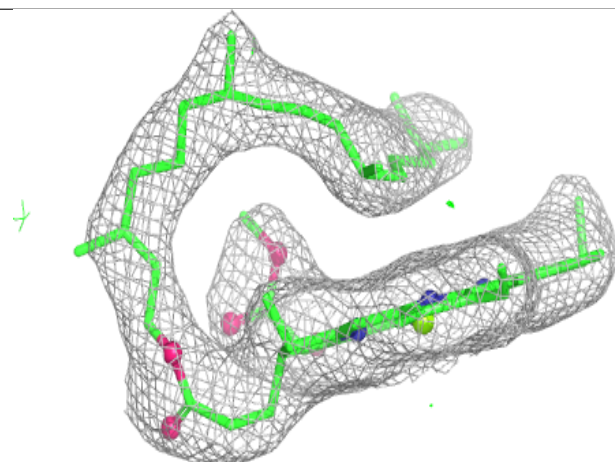
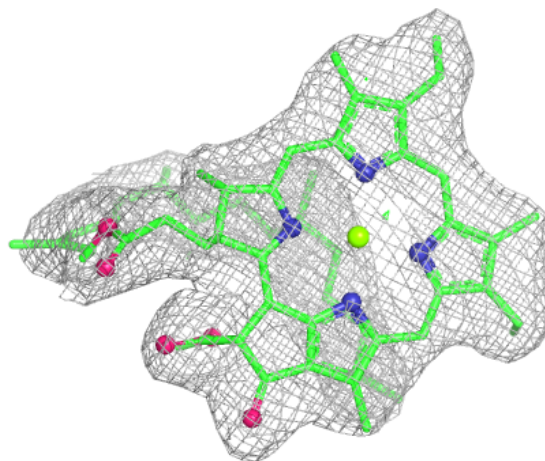
Electron density around CLA c 511:

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



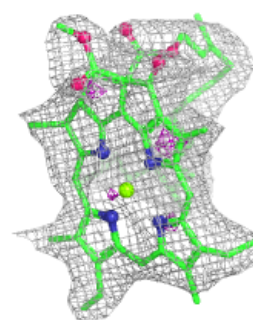
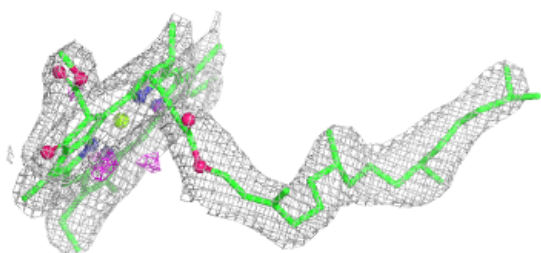
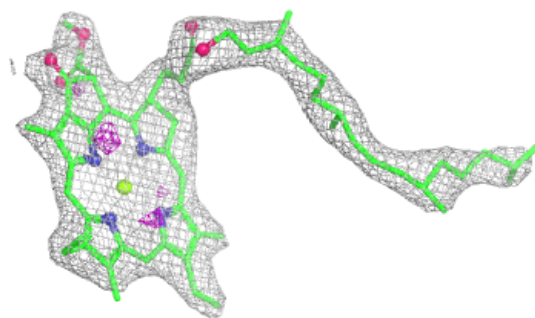
Electron density around CLA c 512:

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

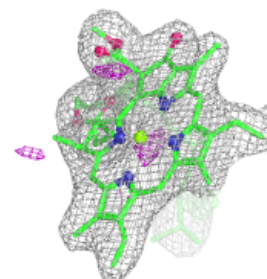
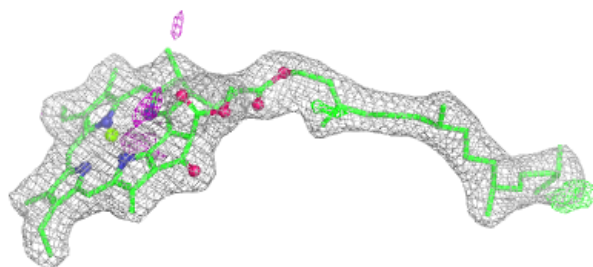
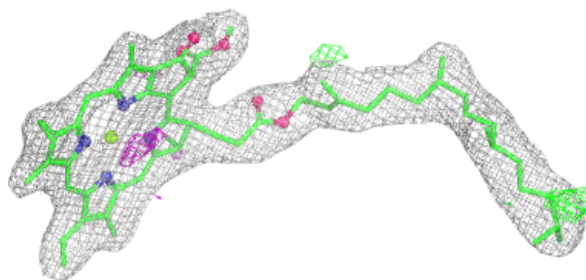


Electron density around CLA c 513:

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

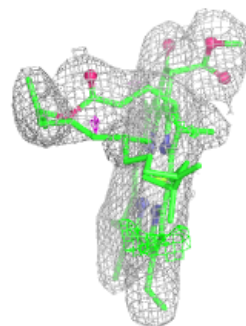
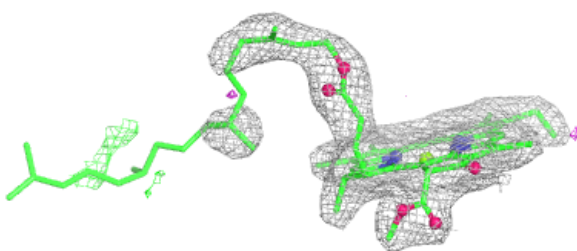
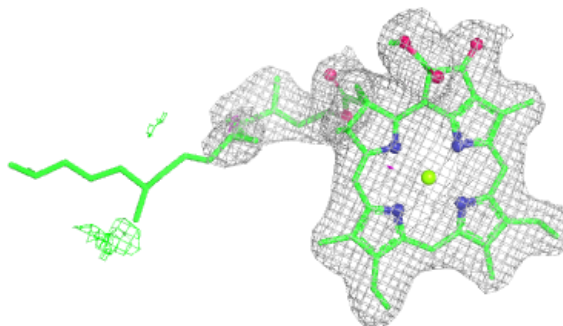
**Electron density around CLA a 403:**

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



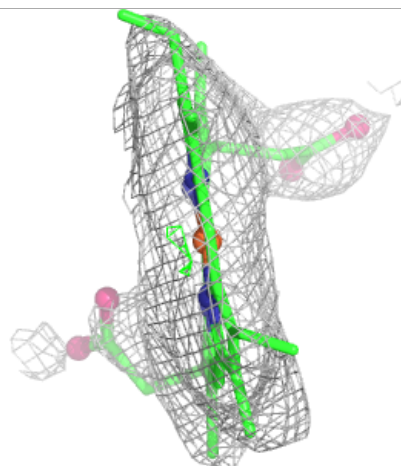
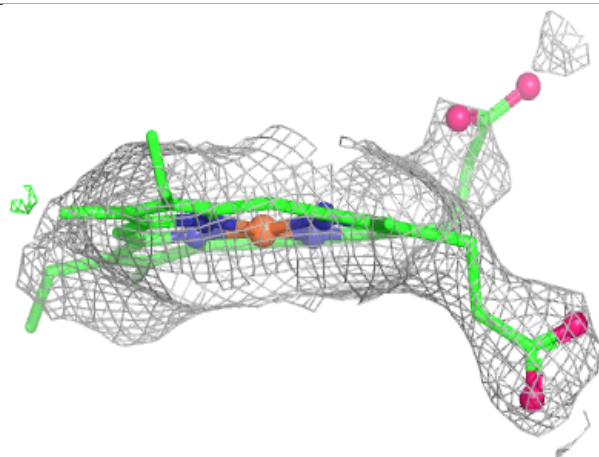
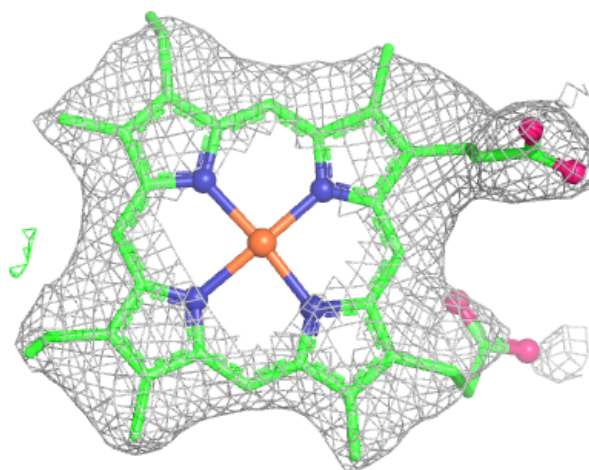
Electron density around CLA a 405:

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



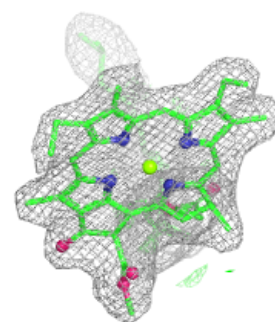
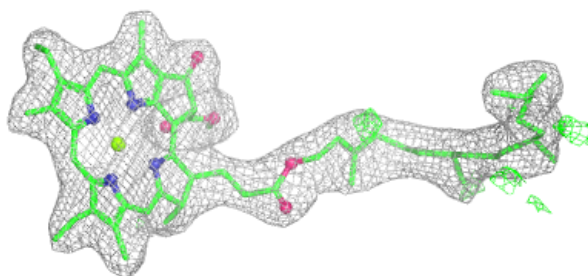
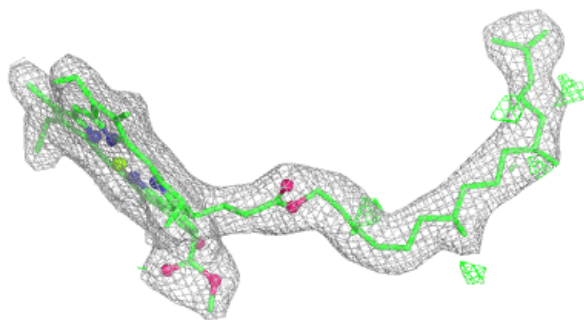
Electron density around HEM e 102:

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

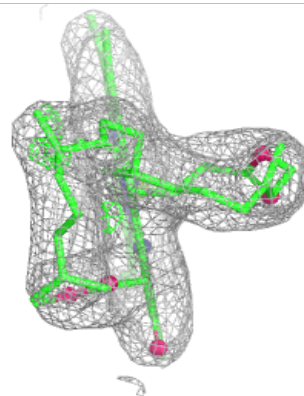
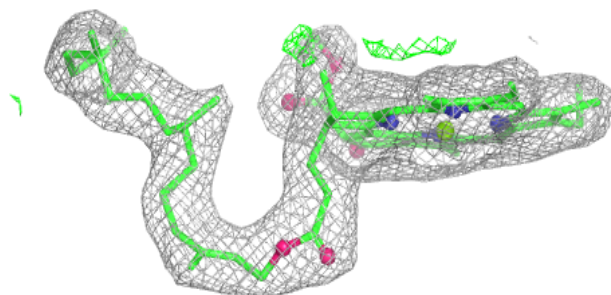
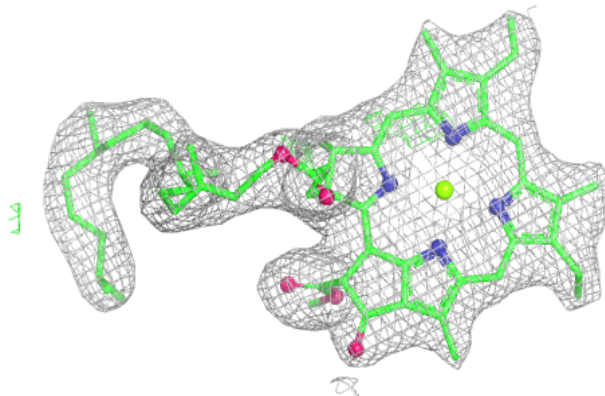


Electron density around CLA D 403:

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

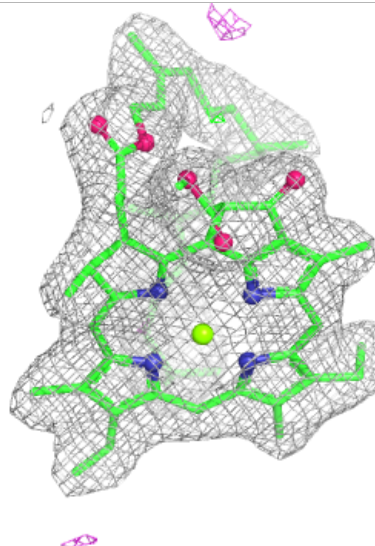
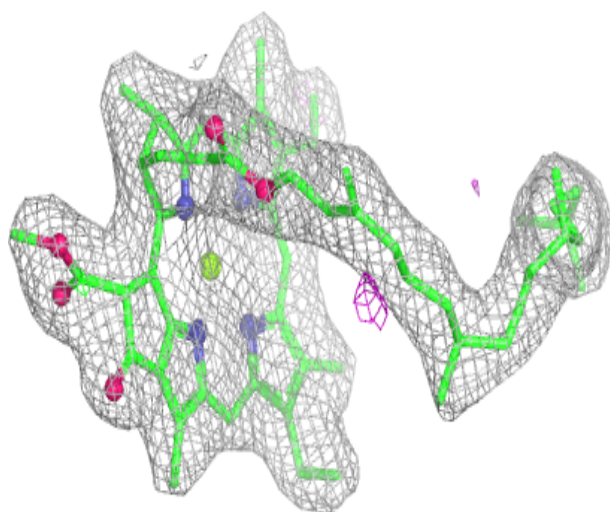
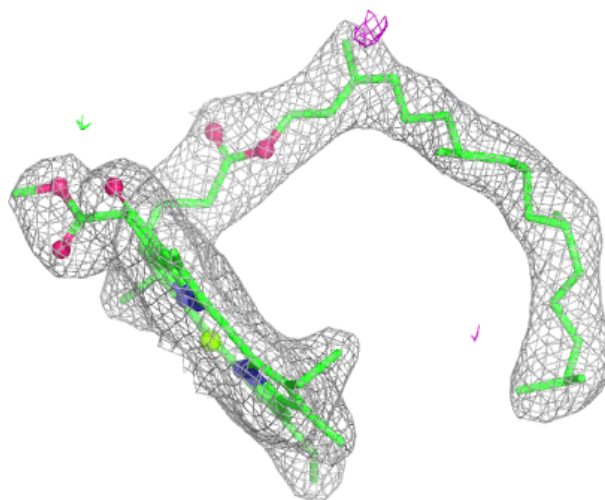
**Electron density around CLA B 612:**

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



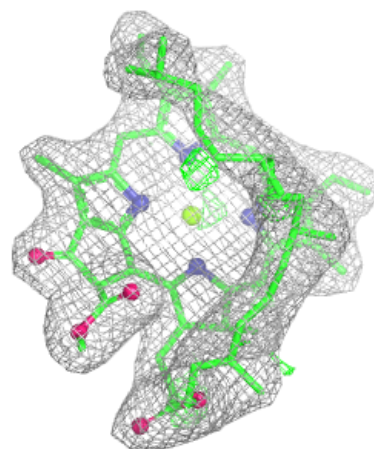
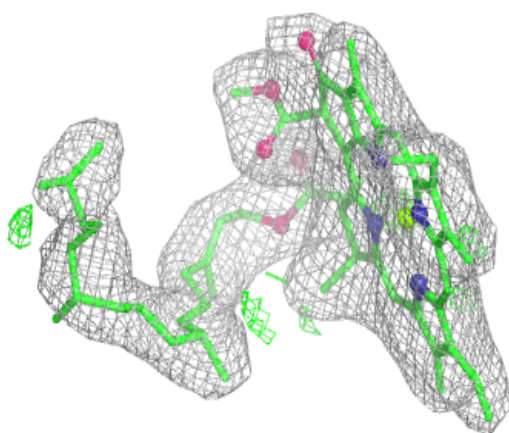
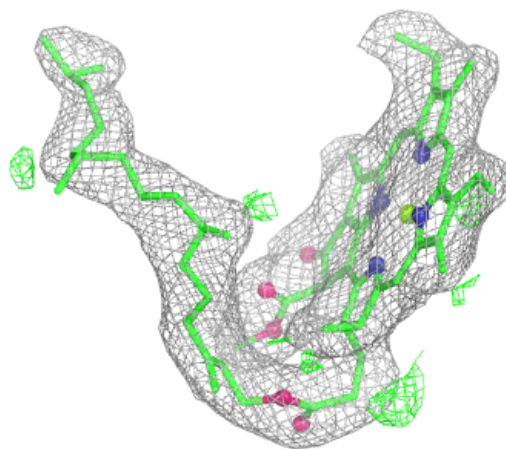
Electron density around CLA b 611:

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



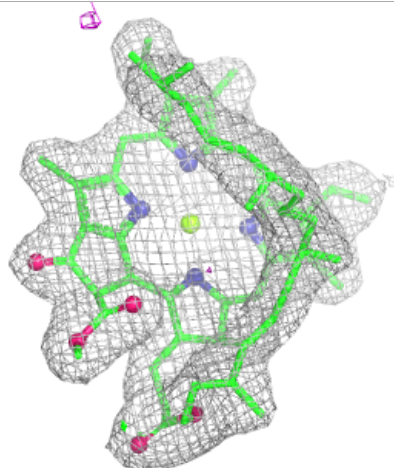
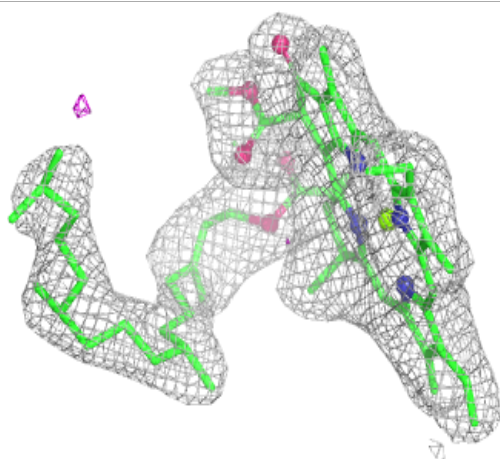
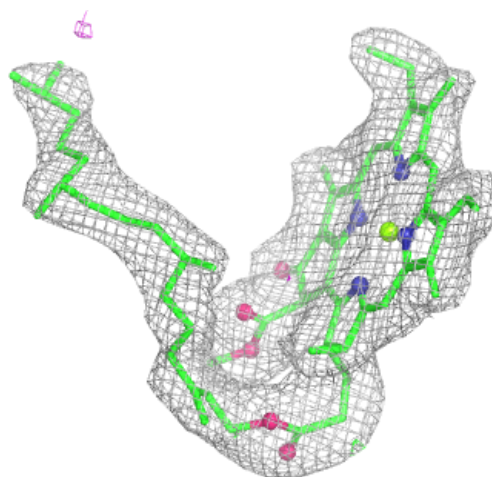
Electron density around CLA B 613:

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



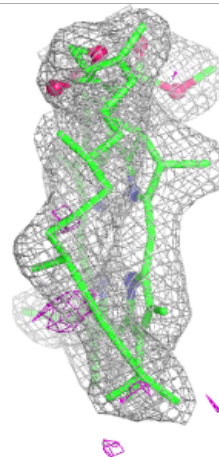
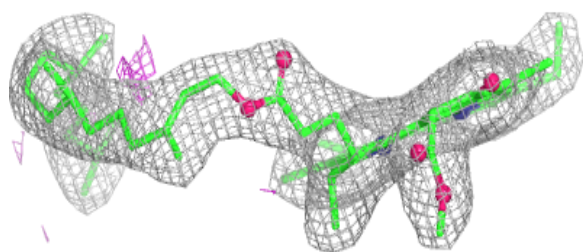
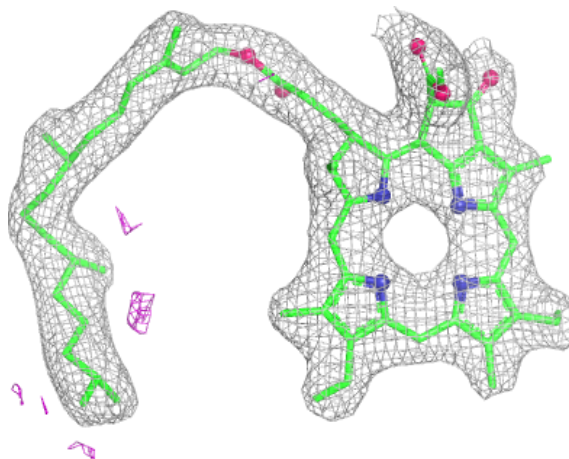
Electron density around CLA b 613:

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



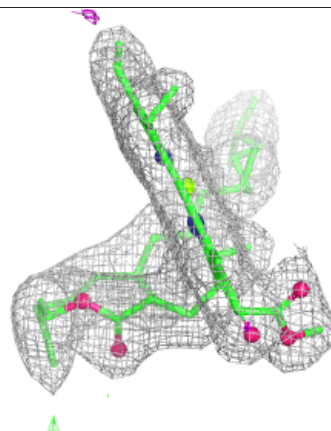
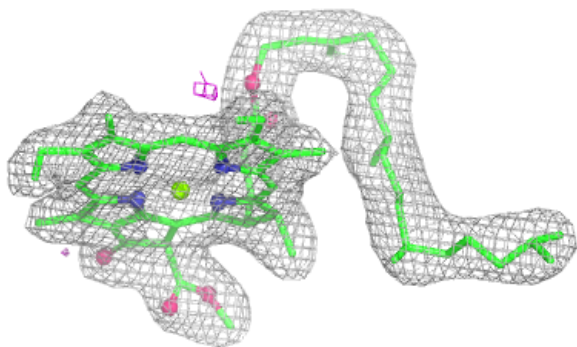
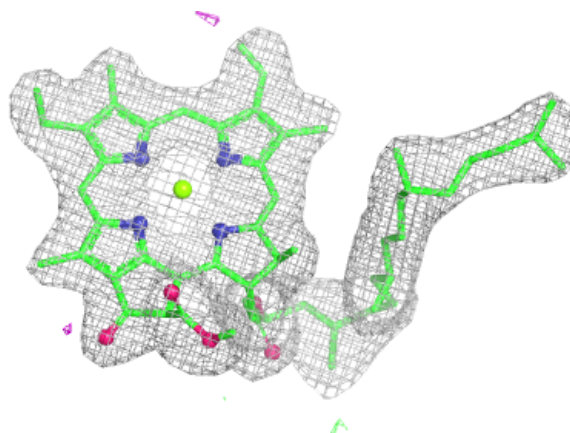
Electron density around PHO A 406:

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



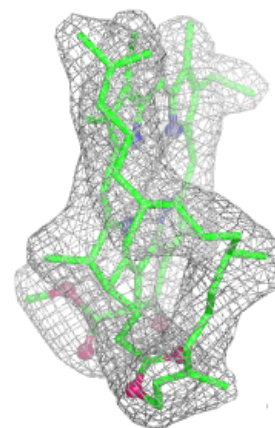
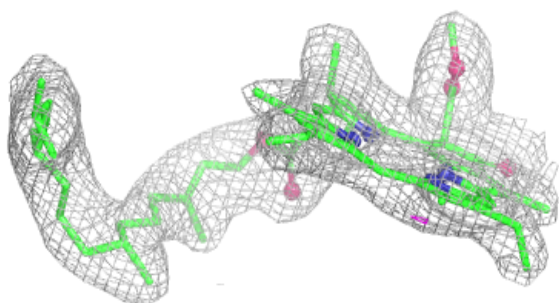
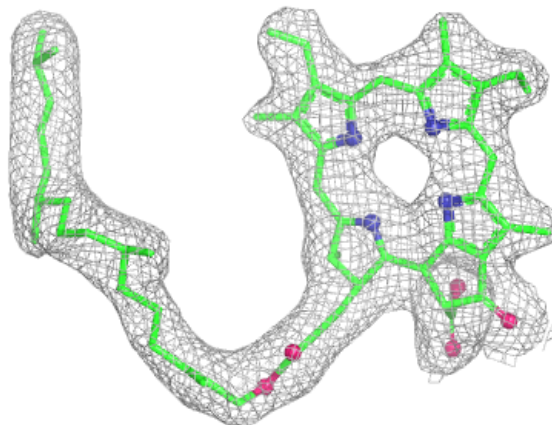
Electron density around CLA a 404:

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



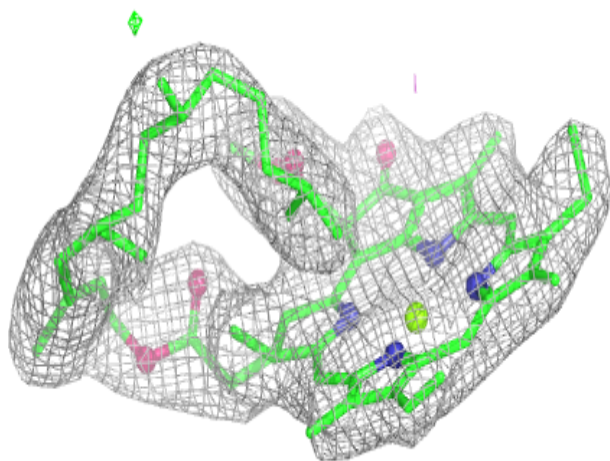
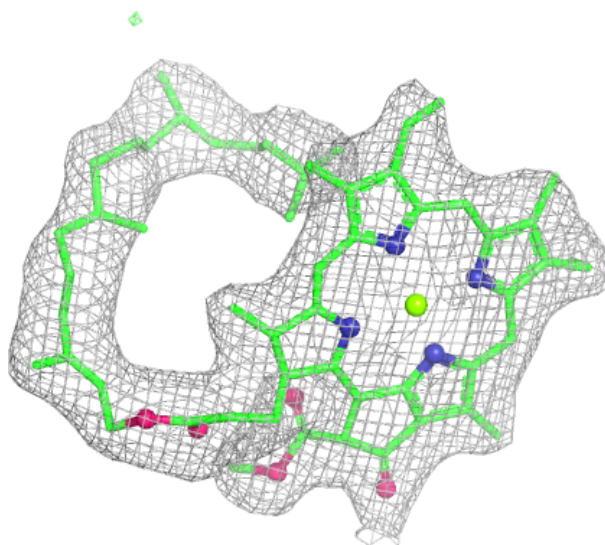
Electron density around PHO a 416:

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



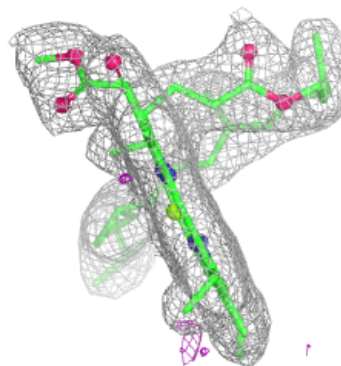
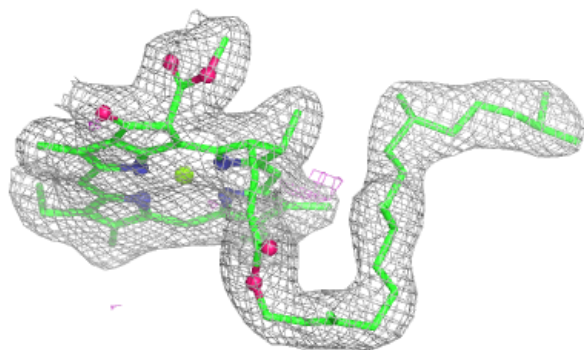
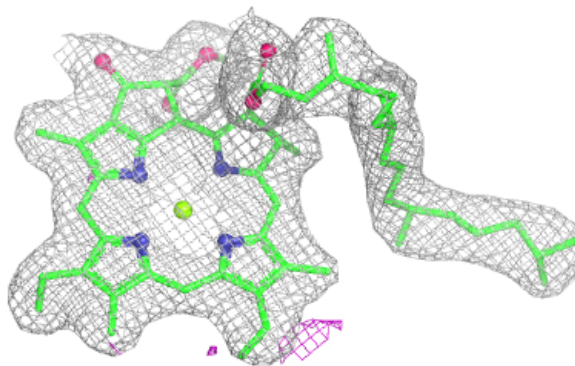
Electron density around CLA b 615:

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



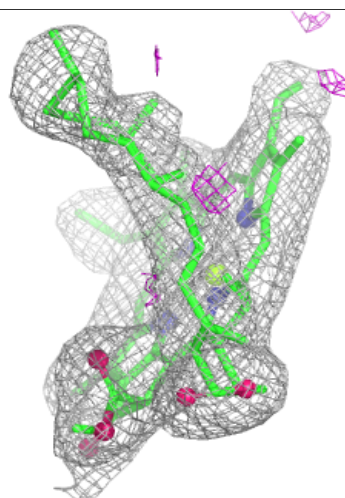
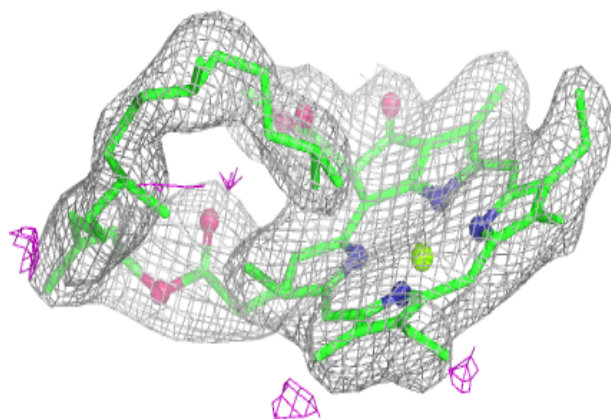
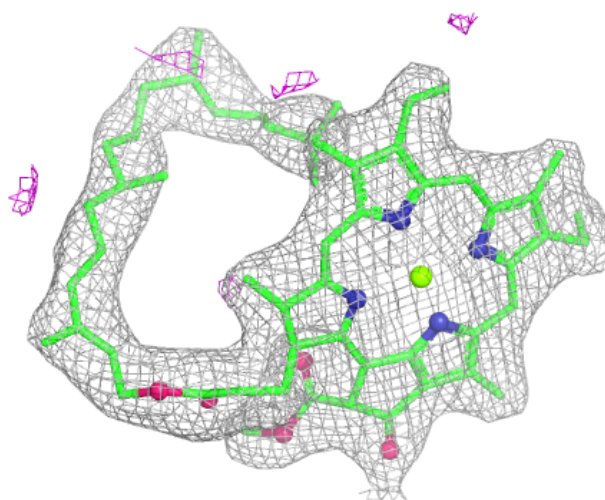
Electron density around CLA A 404:

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



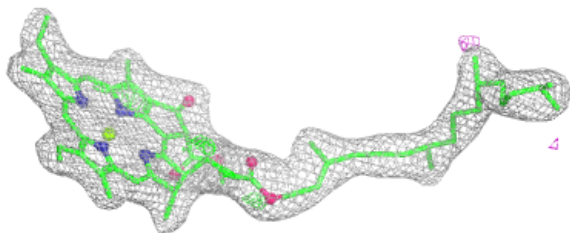
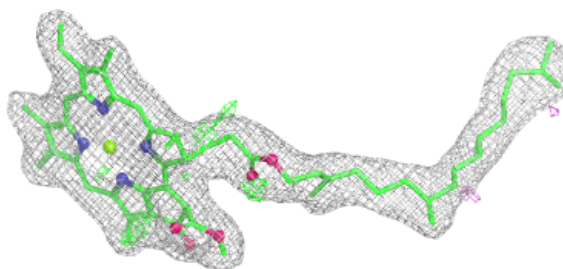
Electron density around CLA B 615:

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

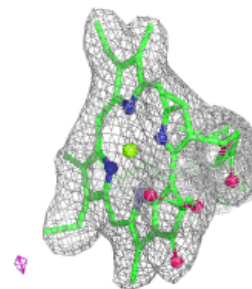
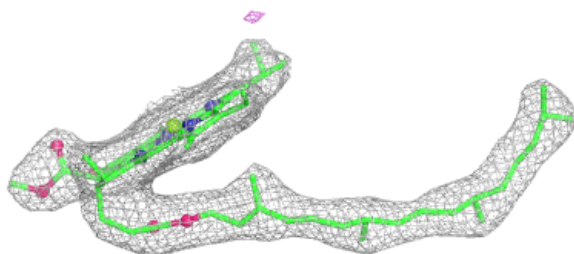
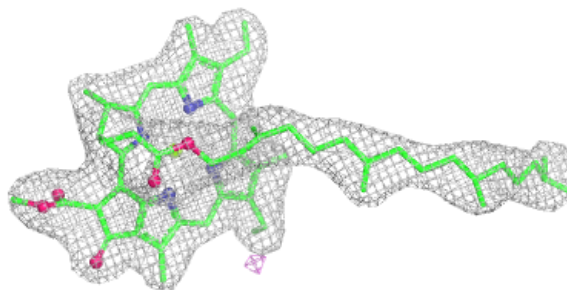


Electron density around CLA A 403:

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

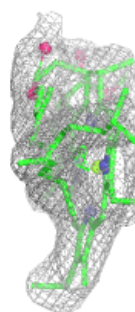
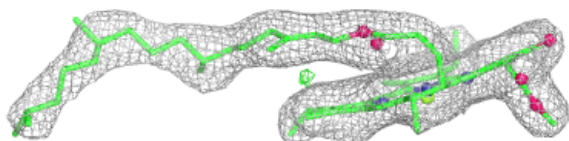
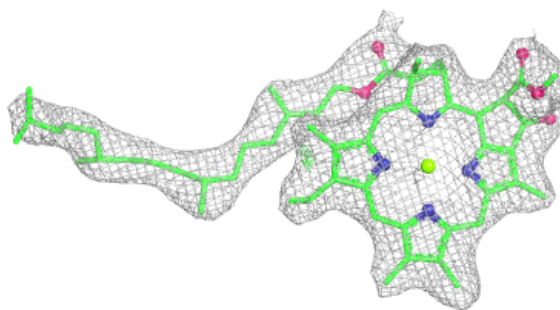
**Electron density around CLA B 608:**

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

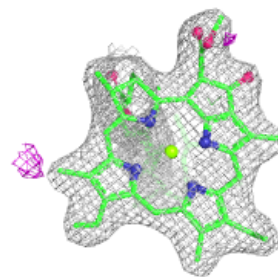
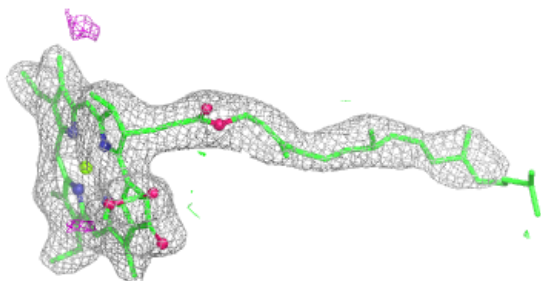
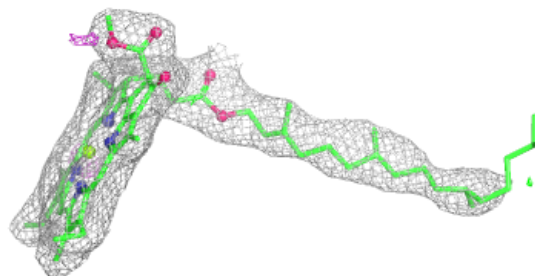


Electron density around CLA b 603:

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

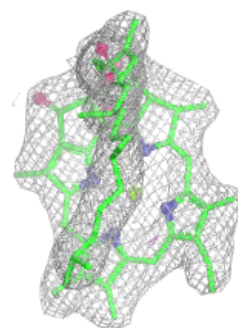
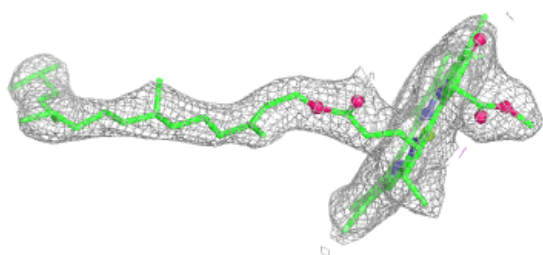
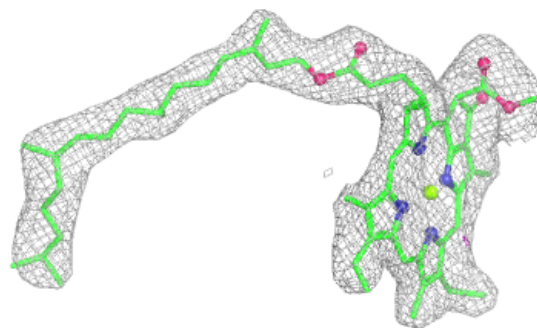
**Electron density around CLA b 604:**

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

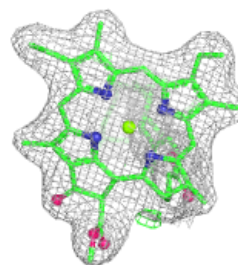
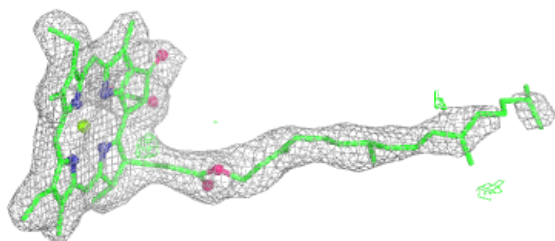
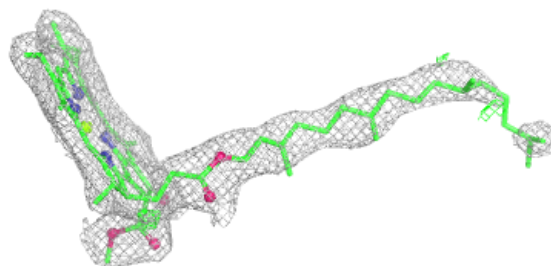


Electron density around CLA B 609:

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

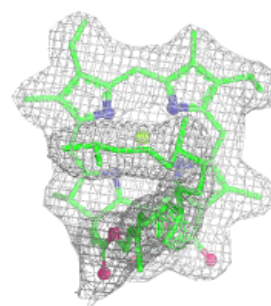
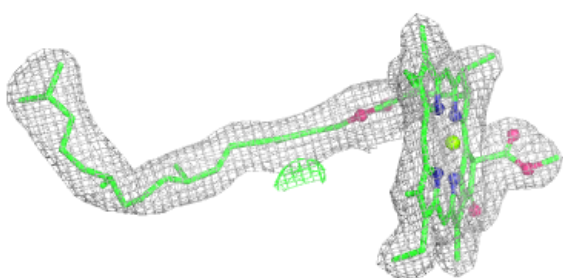
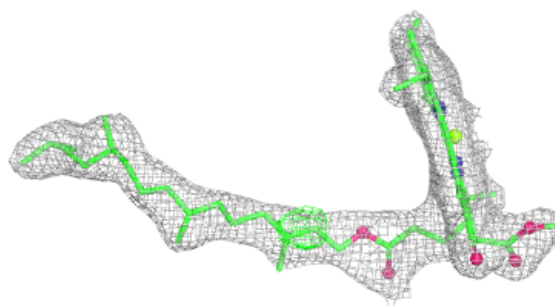
**Electron density around CLA B 604:**

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

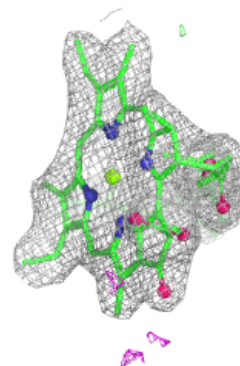
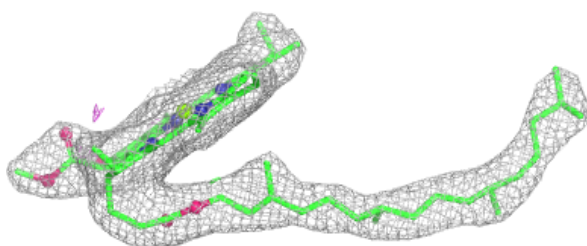
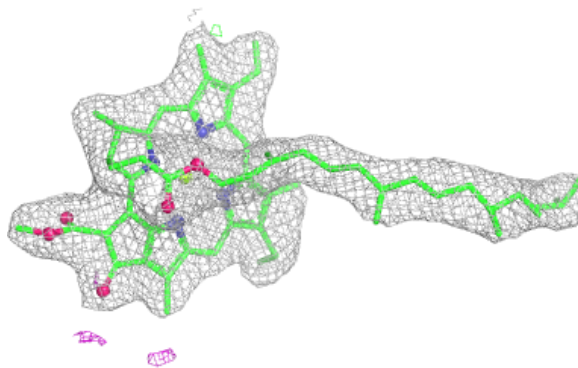


Electron density around CLA B 605:

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

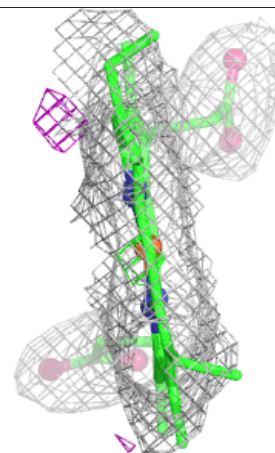
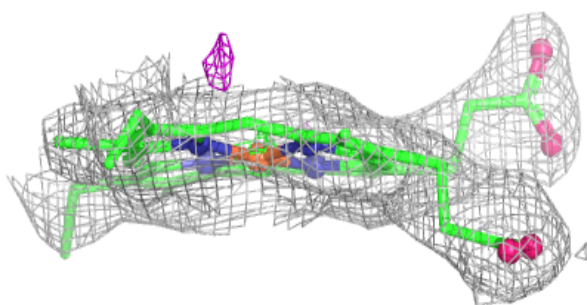
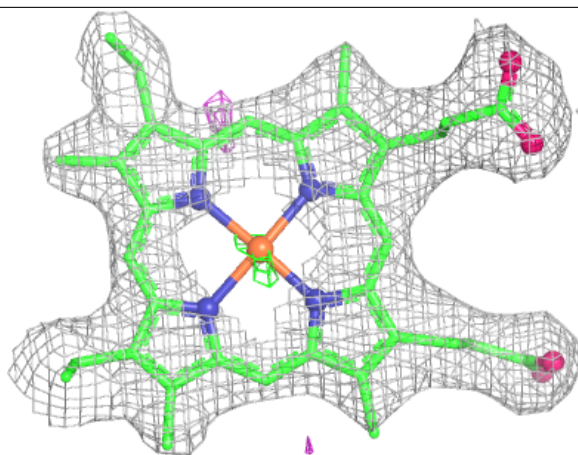
**Electron density around CLA b 608:**

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



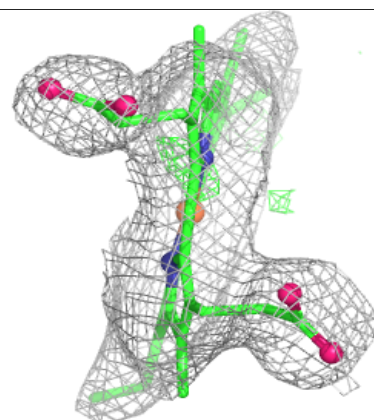
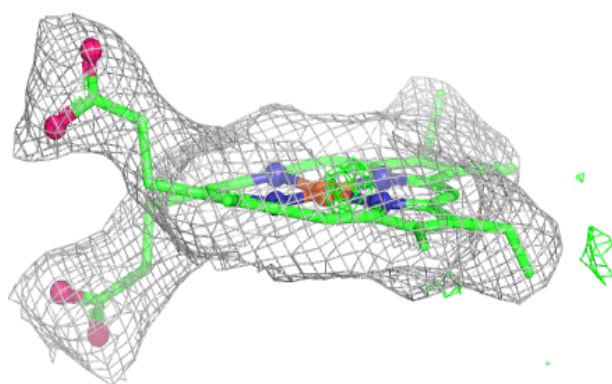
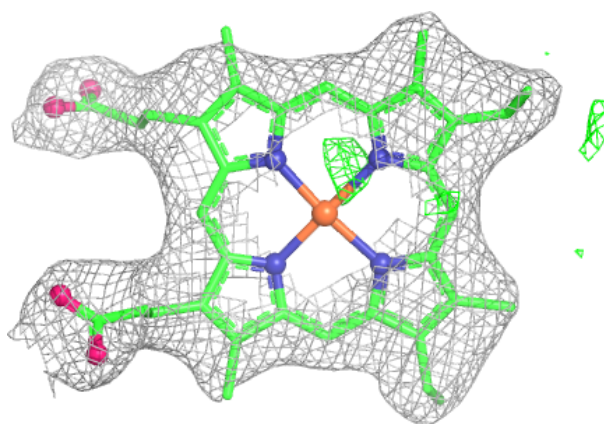
Electron density around HEC v 202:

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

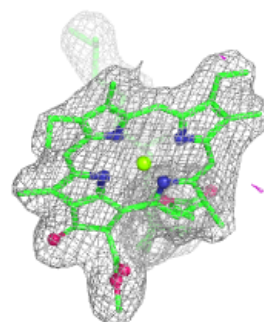
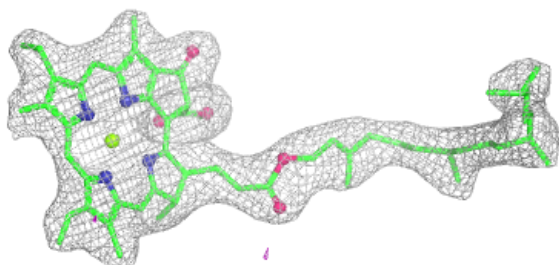
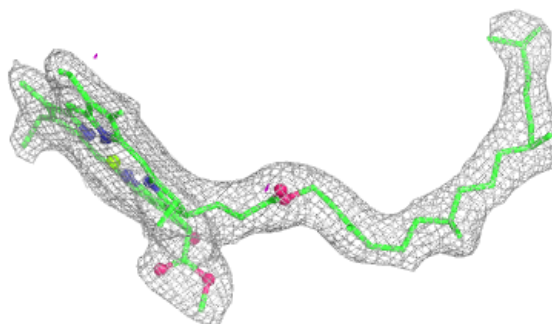


Electron density around HEM E 102:

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

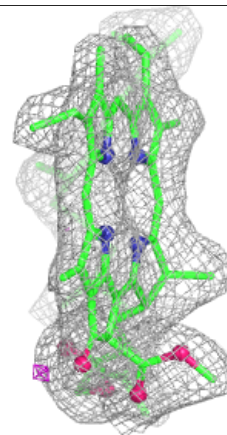
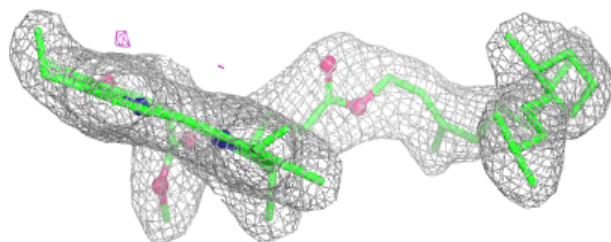
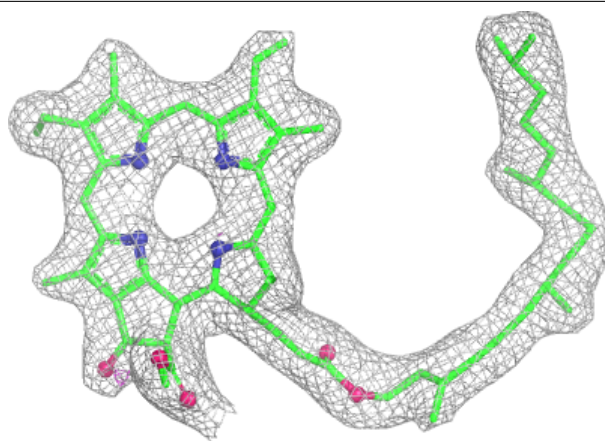
**Electron density around CLA d 402:**

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



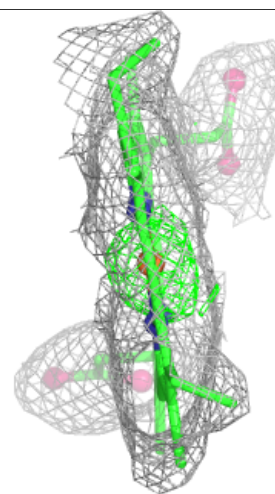
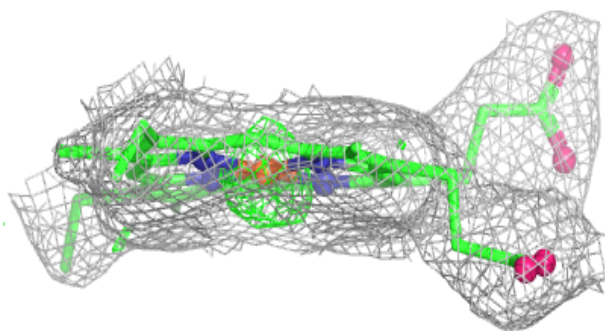
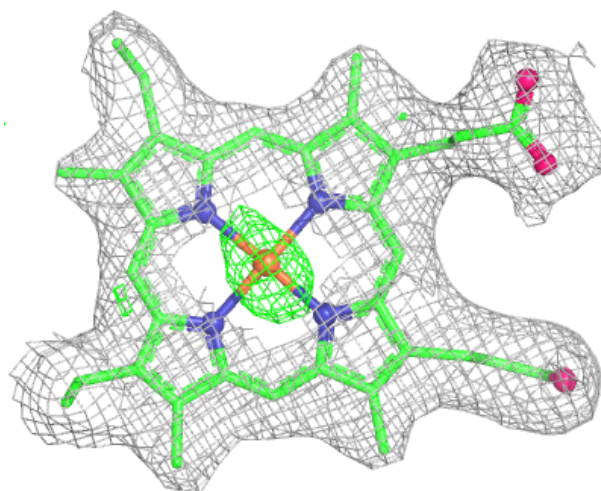
Electron density around PHO a 406:

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



Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.