



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2026 – 09:39 PM UTC

PDB ID : 6JLP / pdb_00006jlp
Title : XFEL structure of cyanobacterial photosystem II (3F state, dataset2)
Authors : Suga, M.; Shen, J.R.
Deposited on : 2019-03-06
Resolution : 2.50 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

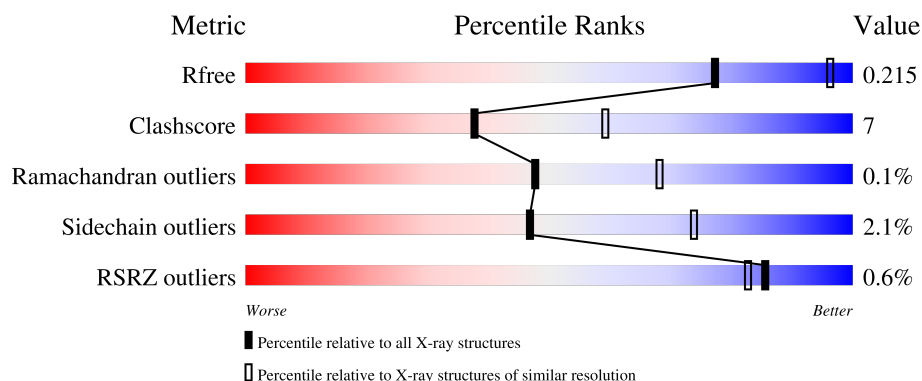
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

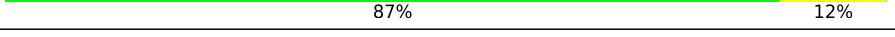
The reported resolution of this entry is 2.50 Å.

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.



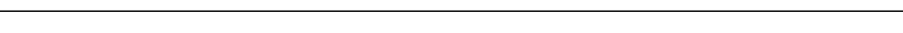
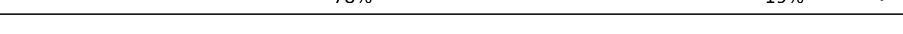
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	
1	a	344	
2	B	505	
2	b	505	
3	C	455	

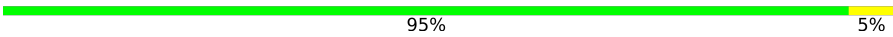
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Mol	Chain	Length	Quality of chain
3	c	455	
4	D	342	
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	404	X	-	-	-
23	CLA	A	405	X	-	-	-
23	CLA	A	407	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	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	B	617	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	C	514	X	-	-	-
23	CLA	D	406	X	-	-	-
23	CLA	D	407	X	-	-	-
23	CLA	a	409	X	-	-	-
23	CLA	a	412	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	b	618	X	-	-	-
23	CLA	b	619	X	-	-	-
23	CLA	b	620	X	-	-	-
23	CLA	b	621	X	-	-	-
23	CLA	b	622	X	-	-	-
23	CLA	b	623	X	-	-	-
23	CLA	b	624	X	-	-	-
23	CLA	b	625	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	c	514	X	-	-	-
23	CLA	c	515	X	-	-	-
23	CLA	c	516	X	-	-	-
23	CLA	c	517	X	-	-	-
23	CLA	d	403	X	-	-	-
23	CLA	d	404	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	d	405	X	-	-	-

2 Entry composition

There are 42 unique types of molecules in this entry. The entry contains 55697 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	54	0
			3024	1969	499	538	18			
1	a	334	Total	C	N	O	S	0	56	0
			3020	1970	497	535	18			

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
			4021	2639	667	702	13			
2	b	503	Total	C	N	O	S	0	12	0
			4022	2644	664	701	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	14	0
			3553	2322	592	626	13			
3	c	455	Total	C	N	O	S	0	20	0
			3641	2382	606	639	14			

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	341	Total	C	N	O	S	0	16	0
			2849	1884	469	483	13			
4	d	341	Total	C	N	O	S	0	16	0
			2849	1884	469	483	13			

- 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	2	0
			668	436	107	125			
5	e	81	Total	C	N	O	0	2	0
			670	439	107	124			

- 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	32	Total	C	N	O	S	0	0	0
			257	175	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	1	0
			519	346	85	86	2			
7	h	65	Total	C	N	O	S	0	0	0
			511	341	82	86	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
			280	187	43	48	2			

- 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	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			
11	l	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	1	0
			274	184	40	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	8	0
			1903	1191	315	392	5			
13	o	243	Total	C	N	O	S	0	5	0
			1891	1183	315	388	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	1	0
			264	185	36	41	2			
14	t	30	Total	C	N	O	S	0	1	0
			264	185	36	41	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O		0	0	0
			774	491	129	154				
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	2	0
			1085	689	181	211	4			
16	v	137	Total	C	N	O	S	0	1	0
			1077	684	178	211	4			

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	39	Total	C	N	O		0	0	0
			287	191	46	50				
18	x	38	Total	C	N	O		0	0	0
			281	188	45	48				

- 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	30	Total	C	N	O		98	0	0
			239	163	41	35				

- 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
			1	1		

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

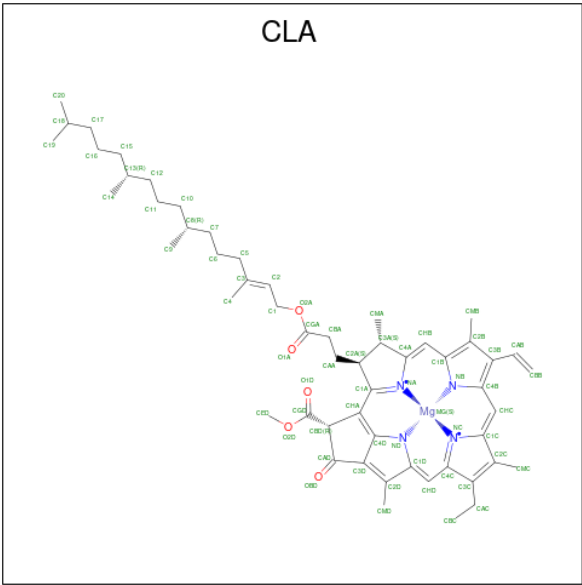
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	2
			4	4		
22	U	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	a	2	Total	Cl	0	2
			4	4		
22	v	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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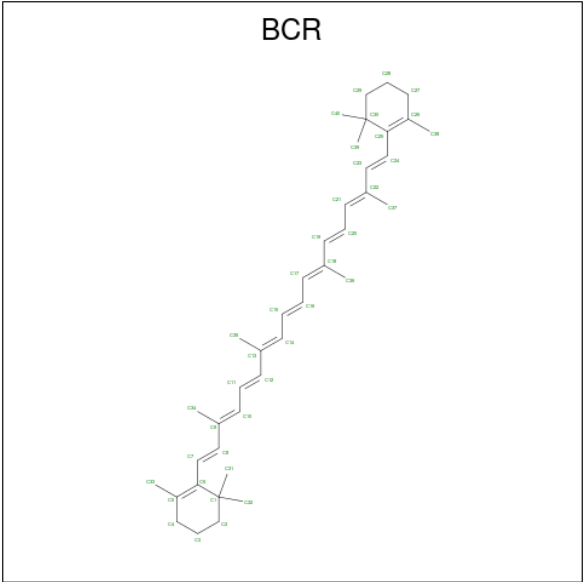
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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

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



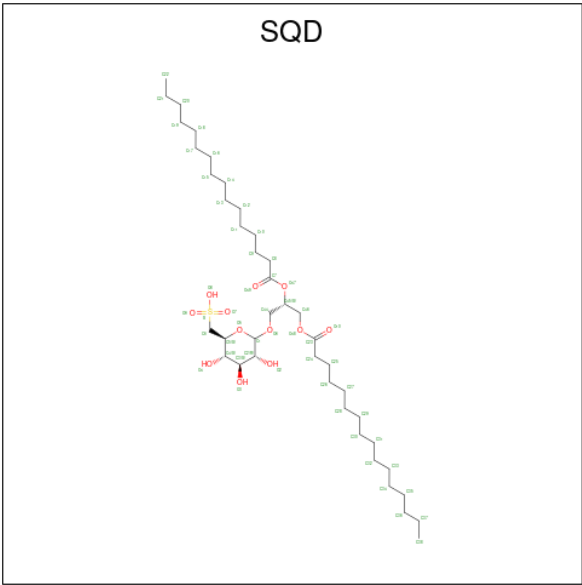
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	T	1	Total C 40 40	0	0
24	Y	1	Total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

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

- Molecule 25 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



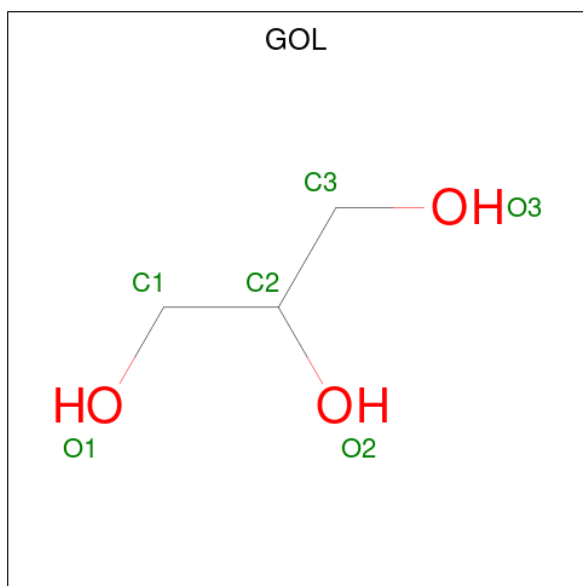
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O S 54 41 12 1	0	0
25	A	1	Total C O S 54 41 12 1	0	0
25	B	1	Total C O S 54 41 12 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	F	1	Total	C	O	S	0	0
			43	30	12	1		
25	L	1	Total	C	O	S	0	0
			54	41	12	1		
25	a	1	Total	C	O	S	0	0
			54	41	12	1		
25	a	1	Total	C	O	S	0	0
			54	41	12	1		
25	f	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 26 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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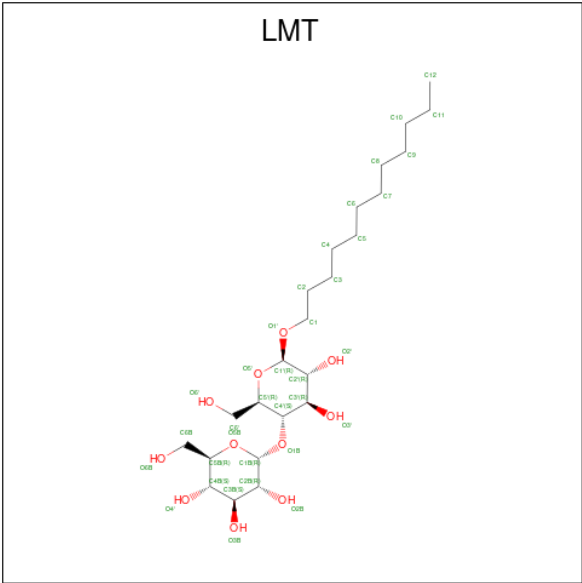
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	B	1	Total	C	O	0	0
			6	3	3		
26	B	1	Total	C	O	0	0
			6	3	3		
26	C	1	Total	C	O	0	0
			6	3	3		
26	C	1	Total	C	O	0	0
			6	3	3		
26	D	1	Total	C	O	0	0
			6	3	3		
26	F	1	Total	C	O	0	0
			6	3	3		
26	O	1	Total	C	O	0	0
			6	3	3		
26	T	1	Total	C	O	0	0
			6	3	3		
26	T	1	Total	C	O	0	0
			6	3	3		
26	V	1	Total	C	O	0	0
			6	3	3		
26	V	1	Total	C	O	0	0
			6	3	3		
26	V	1	Total	C	O	0	0
			6	3	3		
26	V	1	Total	C	O	0	0
			6	3	3		
26	V	1	Total	C	O	0	0
			6	3	3		
26	a	1	Total	C	O	0	0
			6	3	3		
26	a	1	Total	C	O	0	0
			6	3	3		
26	b	1	Total	C	O	0	0
			6	3	3		
26	b	1	Total	C	O	0	0
			6	3	3		
26	b	1	Total	C	O	0	0
			6	3	3		
26	b	1	Total	C	O	0	0
			6	3	3		
26	b	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	c	1	Total	C	O	0	0
			6	3	3		
26	c	1	Total	C	O	0	0
			6	3	3		
26	c	1	Total	C	O	0	0
			6	3	3		
26	f	1	Total	C	O	0	0
			6	3	3		
26	t	1	Total	C	O	0	0
			6	3	3		
26	v	1	Total	C	O	0	0
			6	3	3		
26	v	1	Total	C	O	0	0
			6	3	3		
26	v	1	Total	C	O	0	0
			6	3	3		

- Molecule 27 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



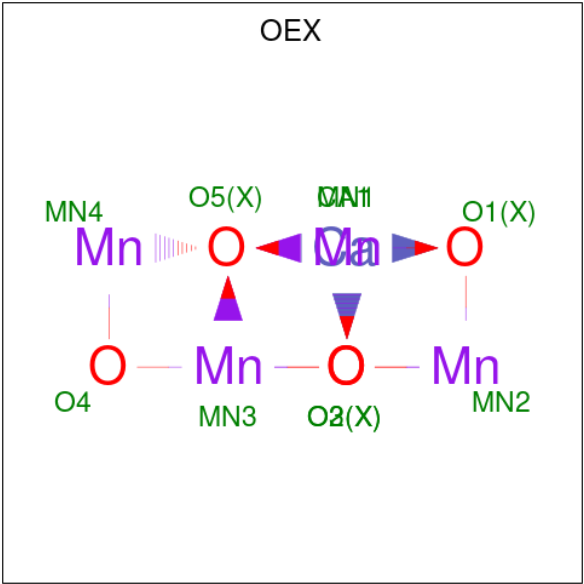
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			35	24	11		
27	C	1	Total	C	O	0	0
			35	24	11		
27	D	1	Total	C	O	0	0
			35	24	11		

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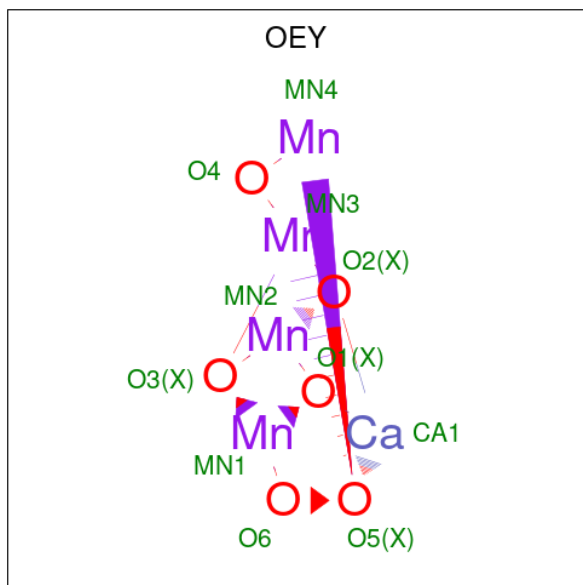
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	F	1	Total	C	O	0	0
			35	24	11		
27	M	1	Total	C	O	0	0
			35	24	11		
27	M	1	Total	C	O	0	0
			35	24	11		
27	M	1	Total	C	O	0	0
			35	24	11		
27	T	1	Total	C	O	0	0
			25	19	6		
27	a	1	Total	C	O	0	0
			35	24	11		
27	a	1	Total	C	O	0	0
			35	24	11		
27	b	1	Total	C	O	0	0
			25	19	6		
27	e	1	Total	C	O	0	0
			35	24	11		
27	m	1	Total	C	O	0	0
			35	24	11		
27	t	1	Total	C	O	0	0
			25	19	6		

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



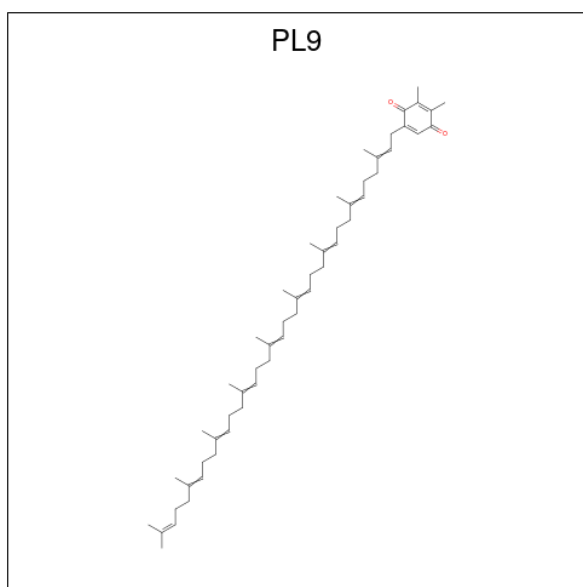
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
28	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 29 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: CaMn_4O_6).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	Ca	Mn	O	0	1
			11	1	4	6		
29	a	1	Total	Ca	Mn	O	0	1
			11	1	4	6		

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



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

- Molecule 31 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			28	23	5		
31	B	1	Total	C	O	0	0
			33	28	5		
31	D	2	Total	C	O	0	0
			57	51	6		
31	I	1	Total	C	O	0	0
			40	35	5		
31	J	1	Total	C		0	0
			10	10			
31	K	1	Total	C	O	0	0
			34	29	5		
31	M	1	Total	C		0	0
			10	10			
31	X	1	Total	C	O	0	0
			18	16	2		

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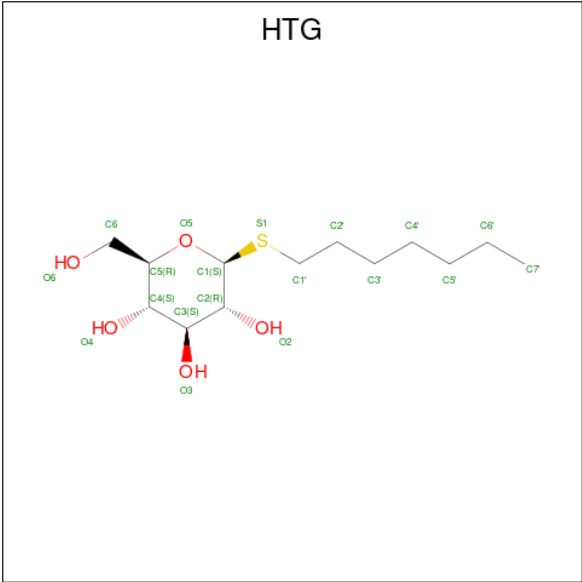
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	a	1	Total C O 30 25 5	0	0
31	b	1	Total C O 33 28 5	0	0
31	c	1	Total C O 32 27 5	0	0
31	d	3	Total C O 71 63 8	0	0
31	i	1	Total C O 40 35 5	0	0
31	j	1	Total C 10 10	0	0
31	m	1	Total C 10 10	0	0

- Molecule 32 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

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



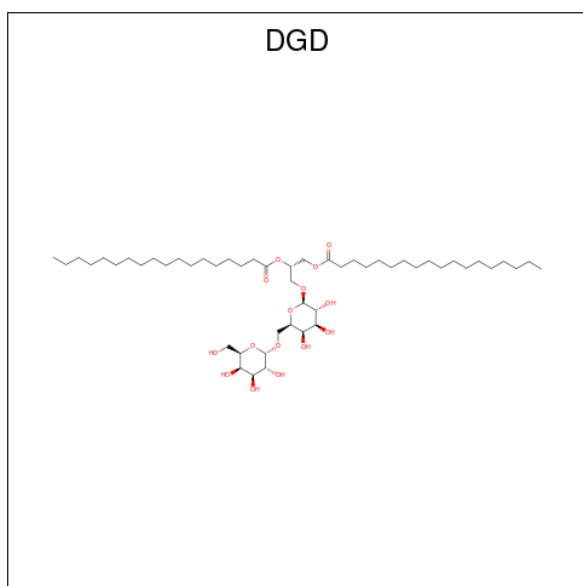
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	C	1	Total	C	O	S	0	0
			19	13	5	1		
33	C	1	Total	C	O	S	0	0
			19	13	5	1		
33	D	1	Total	C	O	S	0	0
			16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

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

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



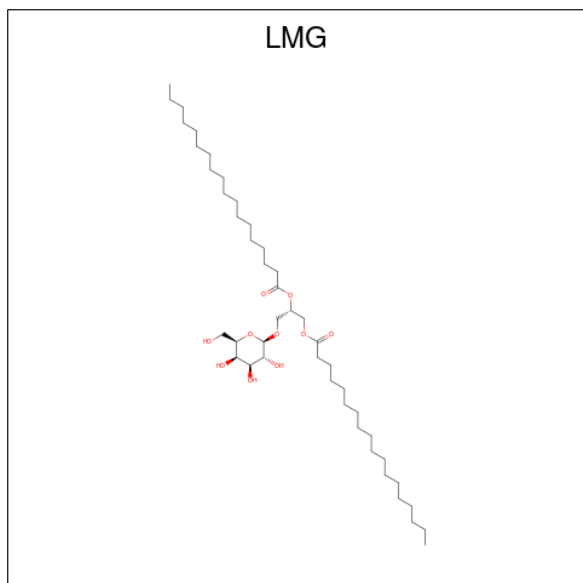
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total	C	O		0	0
			62	47	15			
34	C	1	Total	C	O		0	0
			62	47	15			
34	C	1	Total	C	O		0	0
			62	47	15			
34	C	1	Total	C	O		0	0
			62	47	15			
34	D	1	Total	C	O		0	0
			52	42	10			
34	c	1	Total	C	O		0	0
			62	47	15			
34	c	1	Total	C	O		0	0
			62	47	15			
34	c	1	Total	C	O		0	0
			62	47	15			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	d	1	Total	C	O	0	0
			62	47	15		
34	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 35 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



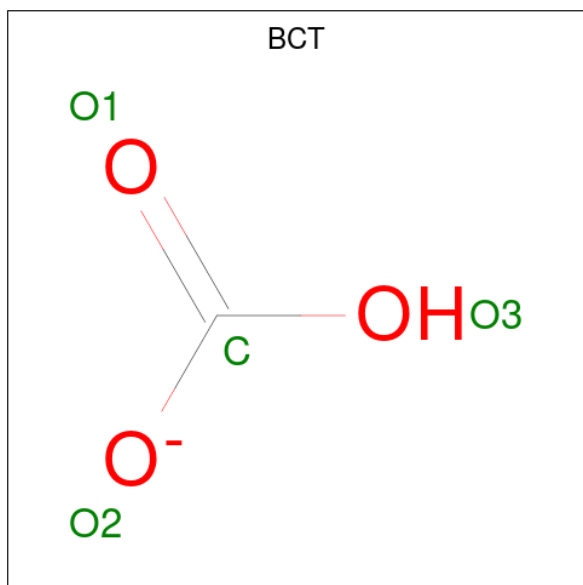
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	C	1	Total	C	O	0	0
			51	41	10		
35	C	1	Total	C	O	0	0
			51	41	10		
35	C	1	Total	C	O	0	0
			51	41	10		
35	D	1	Total	C	O	0	0
			51	41	10		
35	M	1	Total	C	O	0	0
			51	41	10		
35	Z	1	Total	C	O	0	0
			37	27	10		
35	a	1	Total	C	O	0	0
			51	41	10		
35	b	1	Total	C	O	0	0
			51	41	10		
35	c	1	Total	C	O	0	0
			51	41	10		

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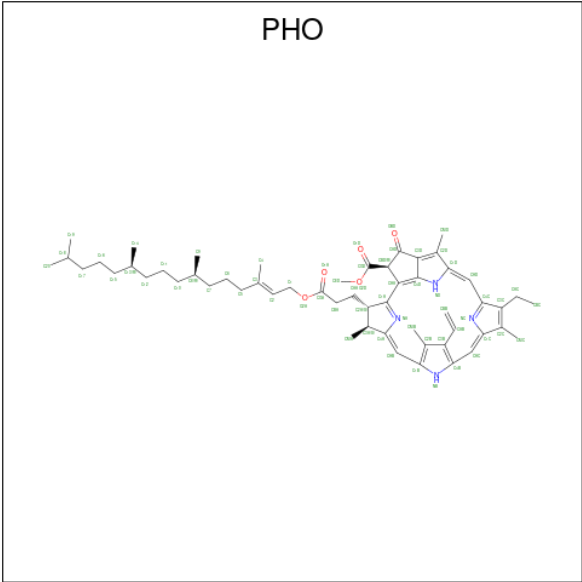
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	c	1	Total	C	O	0	0
			51	41	10		
35	d	1	Total	C	O	0	0
			51	41	10		
35	z	1	Total	C	O	0	0
			39	29	10		

- Molecule 36 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-).



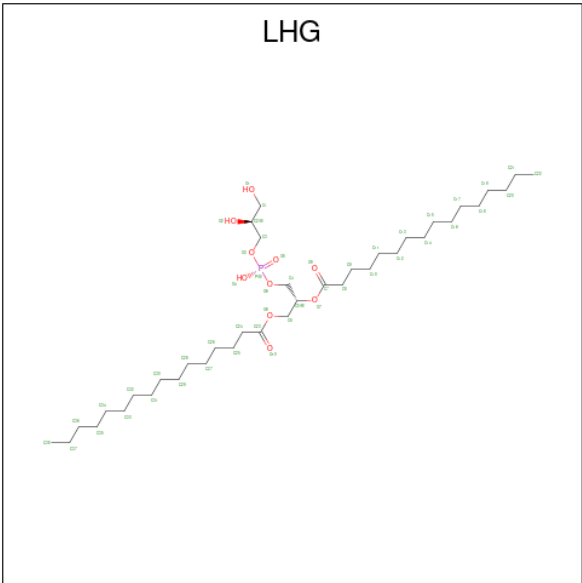
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	D	1	Total	C	O	0	1
			8	2	6		
36	d	1	Total	C	O	0	1
			8	2	6		

- Molecule 37 is PHEOPHYTIN A (CCD ID: PHO) (formula: $\text{C}_{55}\text{H}_{74}\text{N}_4\text{O}_5$).



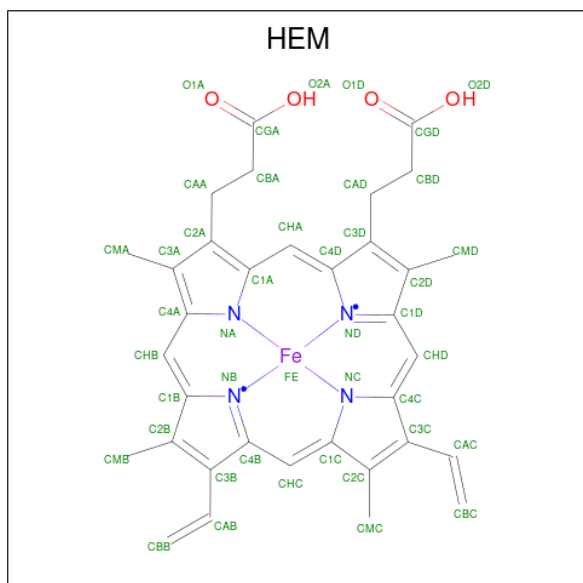
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	D	1	Total	C	N	O	0	0
			64	55	4	5		
37	D	1	Total	C	N	O	0	1
			128	110	8	10		
37	a	1	Total	C	N	O	0	0
			64	55	4	5		
37	d	1	Total	C	N	O	0	1
			128	110	8	10		

- Molecule 38 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



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

- Molecule 39 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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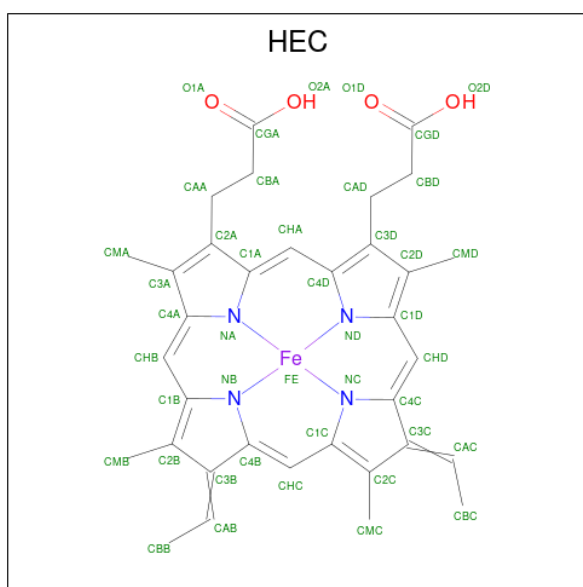
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
39	e	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 40 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 41 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄).



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

- Molecule 42 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	A	160	Total	O	0	14
			172	172		
42	B	286	Total	O	0	4
			290	290		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	C	218	Total 222	O 222	0	5
42	D	146	Total 150	O 150	0	5
42	E	34	Total 35	O 35	0	1
42	F	11	Total 11	O 11	0	0
42	H	40	Total 40	O 40	0	0
42	I	6	Total 6	O 6	0	0
42	J	10	Total 10	O 10	0	0
42	K	9	Total 9	O 9	0	0
42	L	15	Total 16	O 16	0	1
42	M	23	Total 23	O 23	0	0
42	O	180	Total 182	O 182	0	2
42	T	16	Total 17	O 17	0	1
42	U	79	Total 79	O 79	0	0
42	V	122	Total 124	O 124	0	2
42	Y	4	Total 4	O 4	0	0
42	X	10	Total 10	O 10	0	0
42	Z	1	Total 1	O 1	0	0
42	a	146	Total 155	O 155	0	12
42	b	259	Total 262	O 262	0	3
42	c	204	Total 209	O 209	0	6
42	d	142	Total 145	O 145	0	3

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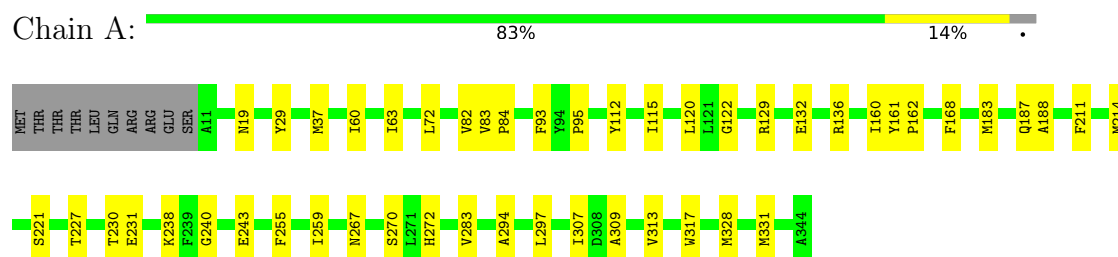
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	e	18	Total 18	O 18	0	0
42	f	7	Total 7	O 7	0	0
42	h	44	Total 44	O 44	0	0
42	i	4	Total 4	O 4	0	0
42	j	7	Total 7	O 7	0	0
42	k	7	Total 7	O 7	0	0
42	l	8	Total 8	O 8	0	0
42	m	13	Total 13	O 13	0	0
42	o	154	Total 154	O 154	0	0
42	t	16	Total 16	O 16	0	0
42	u	93	Total 93	O 93	0	0
42	v	79	Total 80	O 80	0	1
42	y	2	Total 2	O 2	0	0
42	x	6	Total 6	O 6	0	0

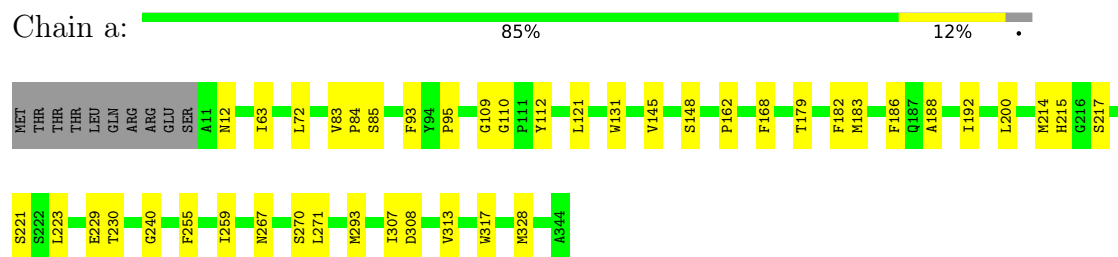
3 Residue-property plots [i](#)

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

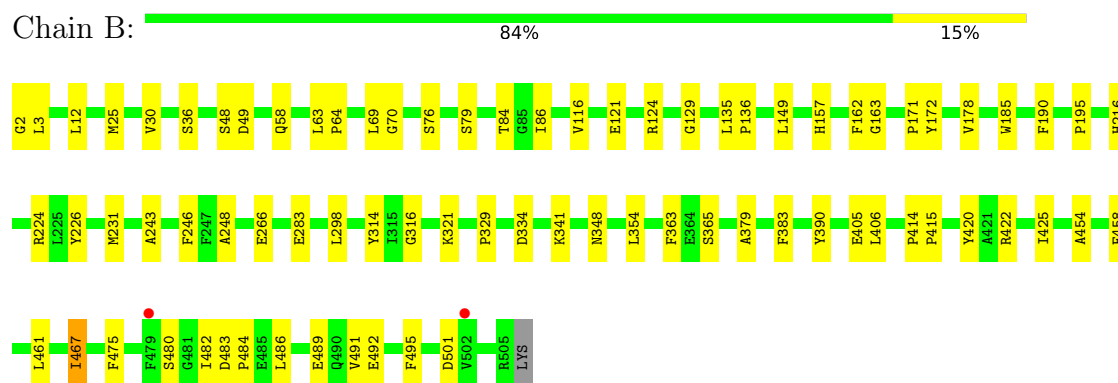
- Molecule 1: Photosystem II protein D1



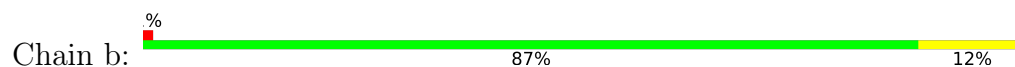
- Molecule 1: Photosystem II protein D1

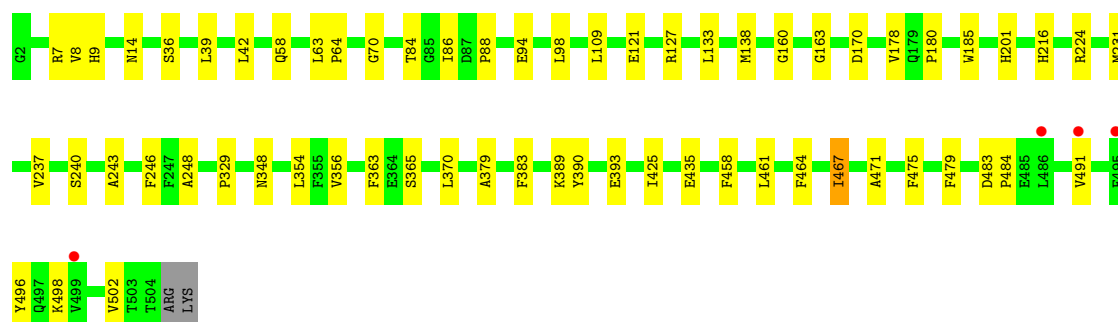


- Molecule 2: Photosystem II CP47 reaction center protein



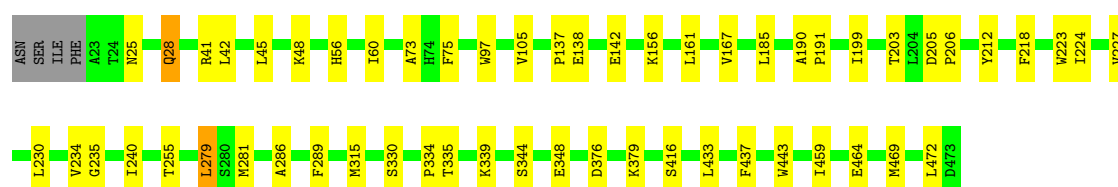
- Molecule 2: Photosystem II CP47 reaction center protein





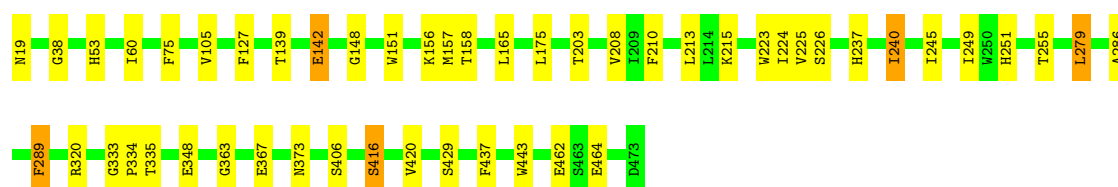
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 87% 12%



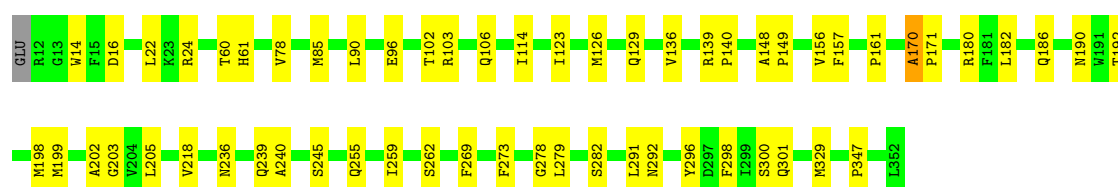
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 89% 10%



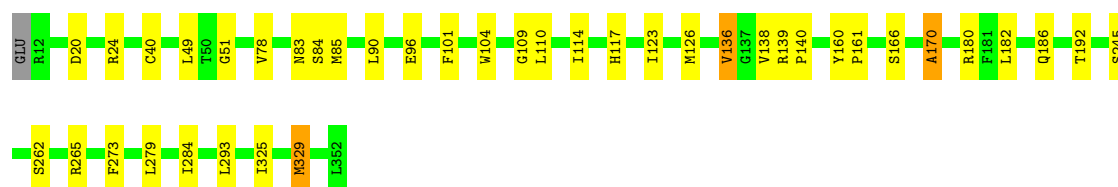
• Molecule 4: Photosystem II D2 protein

Chain D: 83% 17%

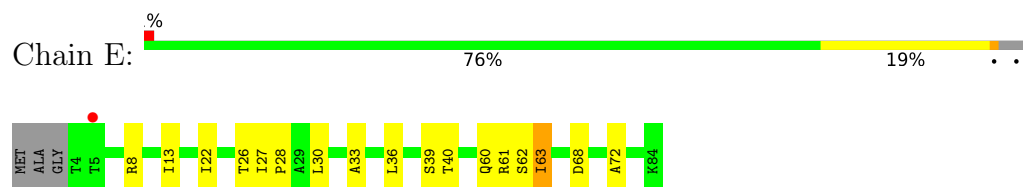


• Molecule 4: Photosystem II D2 protein

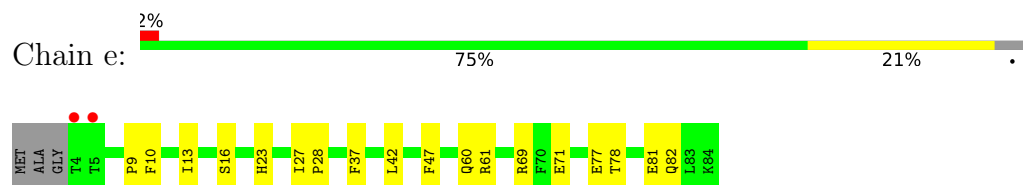
Chain d: 88% 11%



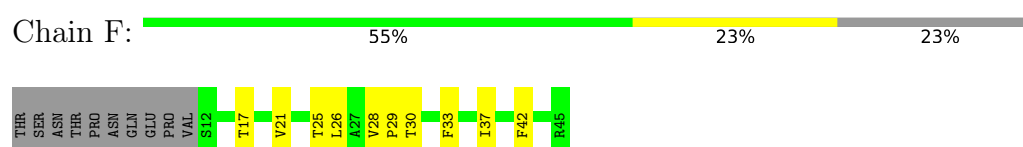
- Molecule 5: Cytochrome b559 subunit alpha



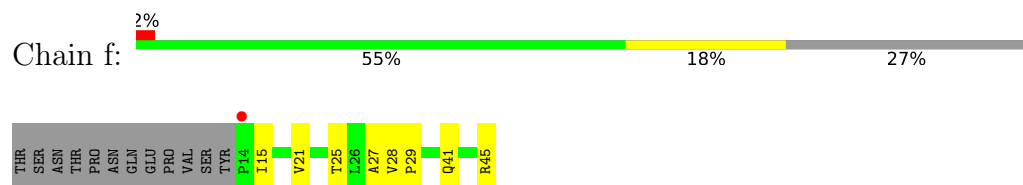
- Molecule 5: Cytochrome b559 subunit alpha



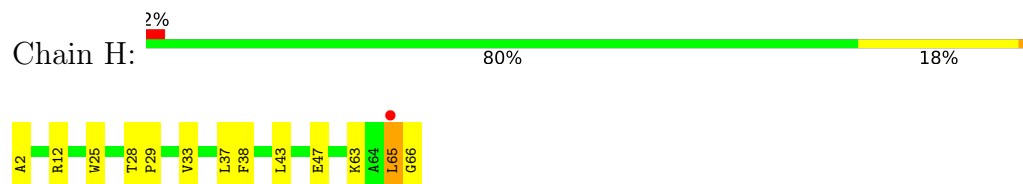
- Molecule 6: Cytochrome b559 subunit beta



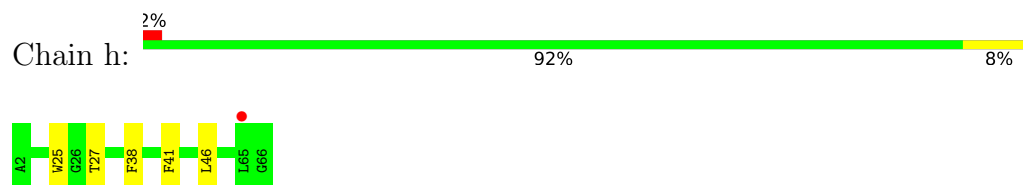
- Molecule 6: Cytochrome b559 subunit beta



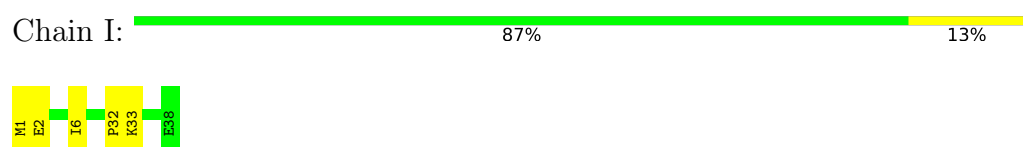
- Molecule 7: Photosystem II reaction center protein H



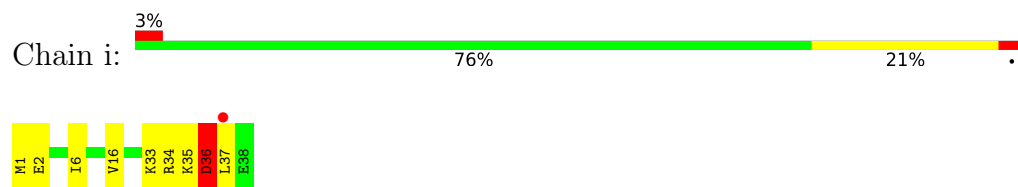
- Molecule 7: Photosystem II reaction center protein H



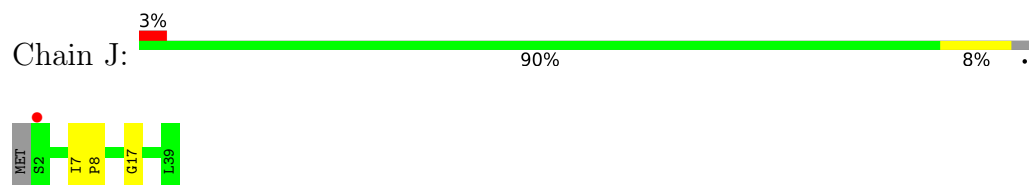
- Molecule 8: Photosystem II reaction center protein I



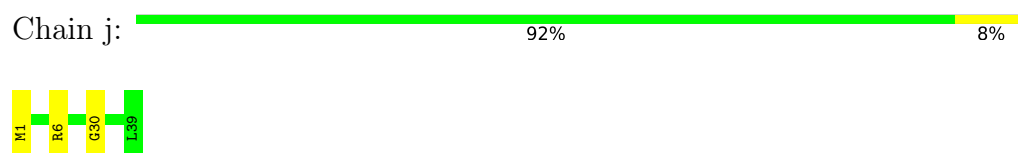
- Molecule 8: Photosystem II reaction center protein I



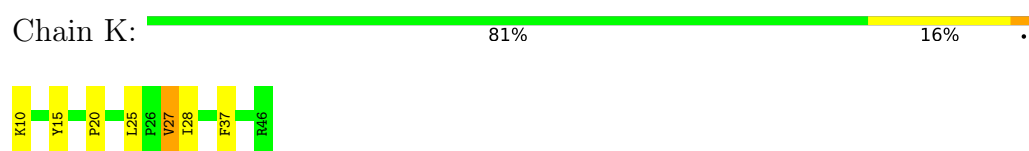
- Molecule 9: Photosystem II reaction center protein J



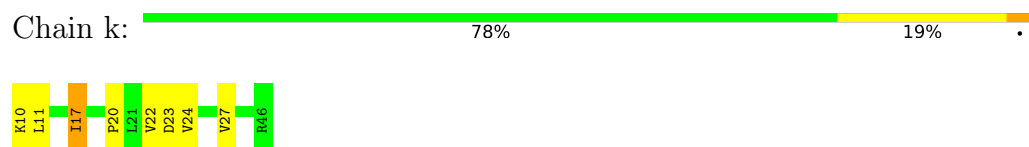
- Molecule 9: Photosystem II reaction center protein J



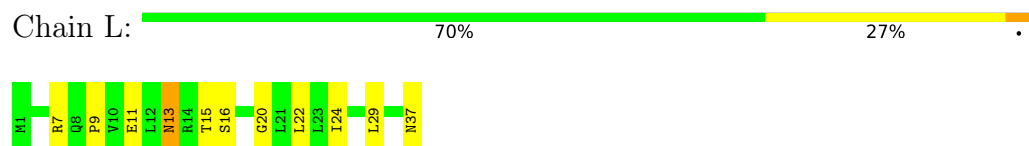
- Molecule 10: Photosystem II reaction center protein K



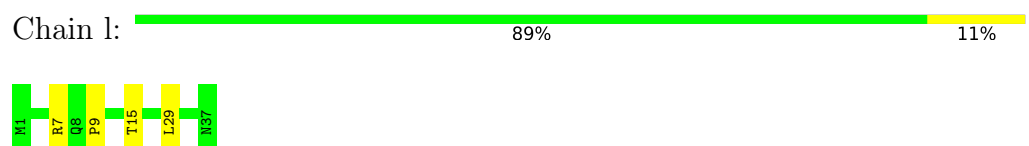
- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



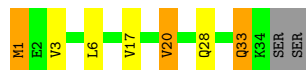
- Molecule 12: Photosystem II reaction center protein M

Chain M:  56% 28% 11% 6%



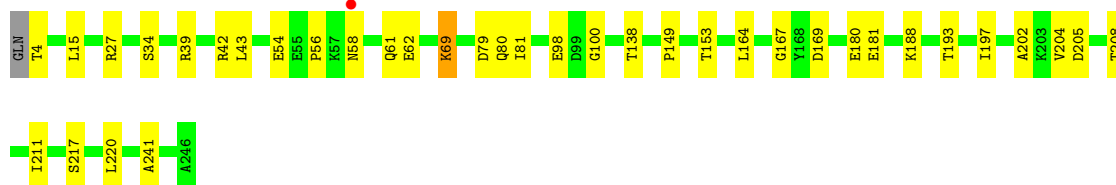
- Molecule 12: Photosystem II reaction center protein M

Chain m:  75% 11% 8% 6%



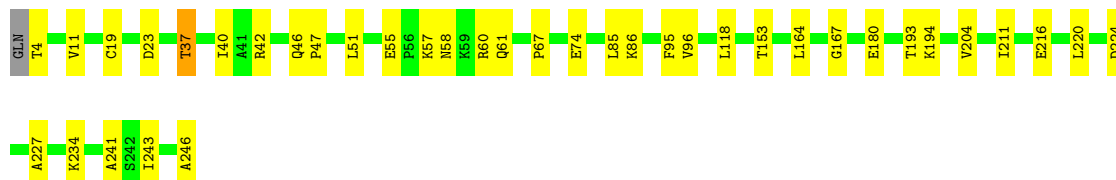
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  84% 15%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  84% 15%



- Molecule 14: Photosystem II reaction center protein T

Chain T:  3% 69% 22% 6%



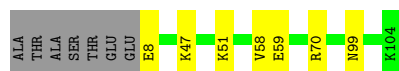
- Molecule 14: Photosystem II reaction center protein T

Chain t:  3% 78% 12% 6%



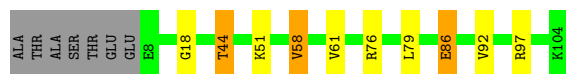
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  87% 7% 7%

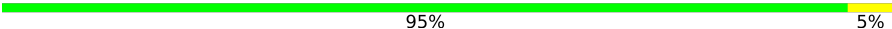


- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  84% 7% 7%



- Molecule 16: Cytochrome c-550

Chain V:  95% 5%



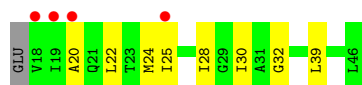
- Molecule 16: Cytochrome c-550

Chain v:  81% 19%



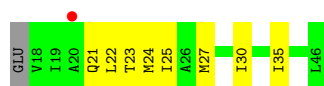
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:  13% 70% 27%



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:  3% 70% 27%

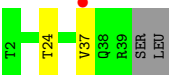
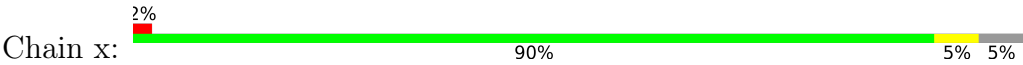


- Molecule 18: Photosystem II reaction center protein X

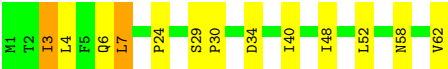
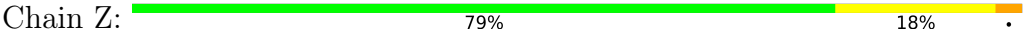
Chain X:  85% 12%



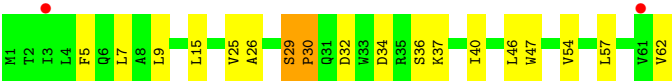
- Molecule 18: Photosystem II reaction center protein X



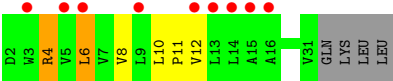
• Molecule 19: Photosystem II reaction center protein Z



• Molecule 19: Photosystem II reaction center protein Z



• Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	122.04Å 228.84Å 286.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.50 19.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.99-2.50) 99.7 (19.99-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.151 , 0.211 0.157 , 0.215	Depositor DCC
R_{free} test set	14865 reflections (2.76%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 93.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	55697	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.52	0/3126	0.81	1/4257 (0.0%)
1	a	0.53	0/3128	0.81	2/4260 (0.0%)
2	B	0.52	0/4191	0.83	2/5709 (0.0%)
2	b	0.52	0/4198	0.84	4/5720 (0.1%)
3	C	0.46	0/3678	0.83	0/5007
3	c	0.47	0/3774	0.79	2/5135 (0.0%)
4	D	0.55	0/2952	0.81	3/4021 (0.1%)
4	d	0.54	0/2952	0.84	5/4021 (0.1%)
5	E	0.45	0/693	0.84	0/944
5	e	0.43	0/695	0.83	0/948
6	F	0.55	0/284	0.80	0/387
6	f	0.55	0/265	0.80	0/360
7	H	0.46	0/535	0.80	0/728
7	h	0.43	0/524	0.84	0/713
8	I	0.48	0/311	0.80	0/419
8	i	0.48	0/311	0.79	0/419
9	J	0.46	0/278	0.73	0/376
9	j	0.45	0/286	0.79	0/386
10	K	0.48	0/303	0.85	0/416
10	k	0.49	0/303	0.86	0/416
11	L	0.55	0/319	0.74	0/433
11	l	0.51	0/319	0.68	0/433
12	M	0.62	0/270	1.11	2/368 (0.5%)
12	m	0.61	0/262	1.01	2/357 (0.6%)
13	O	0.47	0/1958	0.78	0/2654
13	o	0.45	0/1937	0.82	2/2625 (0.1%)
14	T	0.57	0/266	0.78	0/362
14	t	0.60	0/266	0.77	0/362
15	U	0.50	0/785	0.76	0/1064
15	u	0.48	0/785	0.74	0/1064
16	V	0.49	0/1109	0.79	0/1502

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.46	0/1098	0.83	1/1488 (0.1%)
17	Y	0.48	0/216	0.82	0/289
17	y	0.46	0/216	0.80	0/289
18	X	0.47	0/290	0.77	0/392
18	x	0.46	0/284	0.76	0/384
19	Z	0.39	0/490	0.77	0/669
19	z	0.40	0/490	0.83	0/669
20	R	0.34	0/245	0.70	0/338
All	All	0.50	0/44392	0.82	26/60384 (0.0%)

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	170	ALA	CA-C-N	-6.88	112.90	119.85
4	d	170	ALA	C-N-CA	-6.88	112.90	119.85
4	d	160	TYR	CA-C-N	-6.44	113.05	119.56
4	d	160	TYR	C-N-CA	-6.44	113.05	119.56
4	d	262	SER	N-CA-C	-6.22	106.66	114.56

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	3024	0	2877	41	0
1	a	3020	0	2883	36	0
2	B	4021	0	3898	64	0
2	b	4022	0	3908	45	0
3	C	3553	0	3474	39	0
3	c	3641	0	3569	33	0
4	D	2849	0	2741	46	0
4	d	2849	0	2741	35	0
5	E	668	0	658	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	e	670	0	664	12	0
6	F	275	0	282	8	0
6	f	257	0	269	5	0
7	H	519	0	545	14	0
7	h	511	0	532	8	0
8	I	314	0	328	2	0
8	i	314	0	328	5	0
9	J	272	0	279	2	0
9	j	280	0	291	2	0
10	K	293	0	305	7	0
10	k	293	0	305	6	0
11	L	309	0	327	10	0
11	l	309	0	327	4	0
12	M	274	0	299	13	0
12	m	269	0	288	6	0
13	O	1903	0	1886	22	0
13	o	1891	0	1870	23	0
14	T	264	0	267	6	0
14	t	264	0	267	5	0
15	U	774	0	773	3	0
15	u	774	0	773	7	0
16	V	1085	0	1095	4	0
16	v	1077	0	1082	16	0
17	Y	215	0	246	6	0
17	y	215	0	246	6	0
18	X	287	0	317	5	0
18	x	281	0	312	2	0
19	Z	479	0	516	7	0
19	z	479	0	516	12	0
20	R	239	0	262	5	0
21	A	2	0	0	0	0
21	a	1	0	0	0	0
22	A	4	0	0	0	0
22	U	1	0	0	0	0
22	a	4	0	0	0	0
22	v	1	0	0	0	0
23	A	260	0	288	17	0
23	B	1040	0	1152	44	0
23	C	845	0	936	40	0
23	D	130	0	144	5	0
23	a	195	0	216	9	0
23	b	1040	0	1152	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	c	845	0	936	40	0
23	d	195	0	216	6	0
24	A	40	0	56	1	0
24	B	120	0	168	11	0
24	C	40	0	56	2	0
24	D	40	0	56	5	0
24	H	40	0	56	3	0
24	K	80	0	112	8	0
24	T	40	0	56	5	0
24	Y	40	0	56	5	0
24	a	40	0	56	2	0
24	b	120	0	168	7	0
24	c	80	0	112	6	0
24	d	40	0	56	3	0
24	h	40	0	56	5	0
24	k	80	0	112	5	0
24	t	40	0	56	6	0
25	A	108	0	156	7	0
25	B	54	0	78	1	0
25	F	43	0	53	2	0
25	L	54	0	78	2	0
25	a	108	0	156	1	0
25	f	43	0	53	4	0
26	A	12	0	16	1	0
26	B	36	0	48	1	0
26	C	12	0	16	1	0
26	D	6	0	8	2	0
26	F	6	0	8	0	0
26	O	6	0	8	0	0
26	T	12	0	16	4	0
26	V	30	0	40	0	0
26	a	12	0	16	1	0
26	b	30	0	40	1	0
26	c	18	0	24	2	0
26	f	6	0	8	1	0
26	t	6	0	8	1	0
26	v	18	0	24	2	0
27	A	35	0	46	2	0
27	C	35	0	46	2	0
27	D	35	0	46	0	0
27	F	35	0	46	1	0
27	M	105	0	138	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	T	25	0	35	1	0
27	a	70	0	92	4	0
27	b	25	0	35	1	0
27	e	35	0	46	0	0
27	m	35	0	46	2	0
27	t	25	0	35	0	0
28	A	10	0	0	0	0
28	a	10	0	0	0	0
29	A	11	0	0	1	0
29	a	11	0	0	1	0
30	A	110	0	160	7	0
30	D	110	0	160	5	0
30	a	110	0	160	16	0
30	d	110	0	160	3	0
31	A	28	0	0	0	0
31	B	33	0	0	0	0
31	D	57	0	0	0	0
31	I	40	0	0	0	0
31	J	10	0	0	0	0
31	K	34	0	0	0	0
31	M	10	0	0	0	0
31	X	18	0	0	0	0
31	a	30	0	0	0	0
31	b	33	0	0	0	0
31	c	32	0	0	0	0
31	d	71	0	0	0	0
31	i	40	0	0	0	0
31	j	10	0	0	0	0
31	m	10	0	0	0	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	F	1	0	0	0	0
32	O	1	0	0	0	0
32	b	1	0	0	0	0
32	c	2	0	0	0	0
32	f	1	0	0	0	0
32	o	1	0	0	0	0
33	B	76	0	104	2	0
33	C	38	0	52	1	0
33	D	16	0	17	3	0
33	V	19	0	26	1	0
33	b	95	0	130	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	c	38	0	52	1	0
33	d	16	0	17	2	0
33	o	19	0	26	2	0
34	B	62	0	82	2	0
34	C	186	0	246	9	0
34	D	52	0	71	5	0
34	c	186	0	246	4	0
34	d	62	0	82	6	0
34	h	62	0	82	1	0
35	C	153	0	216	7	0
35	D	51	0	72	2	0
35	M	51	0	72	3	0
35	Z	37	0	44	2	0
35	a	51	0	72	3	0
35	b	51	0	72	6	0
35	c	102	0	144	1	0
35	d	51	0	72	2	0
35	z	39	0	48	7	0
36	D	8	0	0	0	0
36	d	8	0	0	0	0
37	D	192	0	222	7	0
37	a	64	0	74	0	0
37	d	128	0	148	4	0
38	D	147	0	222	13	0
38	E	42	0	57	0	0
38	L	49	0	74	2	0
38	a	42	0	57	5	0
38	b	49	0	74	3	0
38	d	147	0	222	6	0
39	F	43	0	30	2	0
39	e	43	0	30	3	0
40	J	1	0	0	0	0
40	j	1	0	0	0	0
41	V	43	0	30	0	0
41	v	43	0	30	0	0
42	A	172	0	0	4	0
42	B	290	0	0	2	0
42	C	222	0	0	2	0
42	D	150	0	0	1	0
42	E	35	0	0	0	0
42	F	11	0	0	0	0
42	H	40	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	I	6	0	0	0	0
42	J	10	0	0	0	0
42	K	9	0	0	1	0
42	L	16	0	0	0	0
42	M	23	0	0	0	0
42	O	182	0	0	3	0
42	T	17	0	0	1	0
42	U	79	0	0	2	0
42	V	124	0	0	0	0
42	X	10	0	0	1	0
42	Y	4	0	0	0	0
42	Z	1	0	0	0	0
42	a	155	0	0	2	0
42	b	262	0	0	5	0
42	c	209	0	0	0	0
42	d	145	0	0	1	0
42	e	18	0	0	0	0
42	f	7	0	0	1	0
42	h	44	0	0	0	0
42	i	4	0	0	0	0
42	j	7	0	0	0	0
42	k	7	0	0	1	0
42	l	8	0	0	0	0
42	m	13	0	0	1	0
42	o	154	0	0	2	0
42	t	16	0	0	0	0
42	u	93	0	0	3	0
42	v	80	0	0	0	0
42	x	6	0	0	0	0
42	y	2	0	0	0	0
All	All	55697	0	54238	747	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 7.

The worst 5 of 747 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)
1:A:214[A]:MET:HG2	30:A:416[A]:PL9:H102	1.48	0.93
29:A:415[B]:OEY:O6	29:A:415[B]:OEY:O5	1.90	0.89
29:a:418[B]:OEY:O6	29:a:418[B]:OEY:O5	1.89	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:D:404:GOL:H11	12:M:1:FME:HG2	1.61	0.81
35:a:415:LMG:H221	34:c:519:DGD:HA82	1.62	0.80

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	385/344 (112%)	378 (98%)	6 (2%)	1 (0%)	36	55
1	a	385/344 (112%)	377 (98%)	7 (2%)	1 (0%)	36	55
2	B	512/505 (101%)	506 (99%)	6 (1%)	0	100	100
2	b	513/505 (102%)	498 (97%)	14 (3%)	1 (0%)	43	63
3	C	461/455 (101%)	446 (97%)	13 (3%)	2 (0%)	30	49
3	c	473/455 (104%)	455 (96%)	16 (3%)	2 (0%)	30	49
4	D	355/342 (104%)	344 (97%)	11 (3%)	0	100	100
4	d	355/342 (104%)	345 (97%)	10 (3%)	0	100	100
5	E	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
5	e	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
6	F	32/44 (73%)	31 (97%)	1 (3%)	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	64/65 (98%)	60 (94%)	4 (6%)	0	100	100
7	h	63/65 (97%)	57 (90%)	6 (10%)	0	100	100
8	I	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	i	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	4	6
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	34 (92%)	3 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/36 (92%)	33 (100%)	0	0	100	100
12	m	32/36 (89%)	32 (100%)	0	0	100	100
13	O	249/244 (102%)	239 (96%)	10 (4%)	0	100	100
13	o	246/244 (101%)	236 (96%)	10 (4%)	0	100	100
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	29/32 (91%)	29 (100%)	0	0	100	100
15	U	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
15	u	95/104 (91%)	91 (96%)	4 (4%)	0	100	100
16	V	136/137 (99%)	131 (96%)	5 (4%)	0	100	100
16	v	135/137 (98%)	129 (96%)	6 (4%)	0	100	100
17	Y	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
17	y	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
18	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
18	x	36/40 (90%)	34 (94%)	2 (6%)	0	100	100
19	Z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
19	z	60/62 (97%)	57 (95%)	2 (3%)	1 (2%)	7	13
20	R	28/34 (82%)	27 (96%)	1 (4%)	0	100	100
All	All	5431/5384 (101%)	5261 (97%)	161 (3%)	9 (0%)	48	63

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
2	b	127	ARG
3	c	416[A]	SER
3	c	416[B]	SER

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	312/279 (112%)	312 (100%)	0	100	100
1	a	312/279 (112%)	311 (100%)	1 (0%)	86	94
2	B	412/403 (102%)	407 (99%)	5 (1%)	63	83
2	b	413/403 (102%)	405 (98%)	8 (2%)	50	76
3	C	361/356 (101%)	354 (98%)	7 (2%)	50	76
3	c	371/356 (104%)	361 (97%)	10 (3%)	39	67
4	D	290/277 (105%)	288 (99%)	2 (1%)	76	89
4	d	290/277 (105%)	288 (99%)	2 (1%)	76	89
5	E	74/73 (101%)	73 (99%)	1 (1%)	59	81
5	e	74/73 (101%)	73 (99%)	1 (1%)	59	81
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	26/38 (68%)	25 (96%)	1 (4%)	29	56
7	H	55/54 (102%)	54 (98%)	1 (2%)	51	77
7	h	54/54 (100%)	54 (100%)	0	100	100
8	I	34/34 (100%)	33 (97%)	1 (3%)	37	65
8	i	34/34 (100%)	33 (97%)	1 (3%)	37	65
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	27/27 (100%)	26 (96%)	1 (4%)	30	57
10	K	30/30 (100%)	29 (97%)	1 (3%)	33	61
10	k	30/30 (100%)	28 (93%)	2 (7%)	15	31
11	L	36/35 (103%)	34 (94%)	2 (6%)	19	39
11	l	36/35 (103%)	35 (97%)	1 (3%)	38	66
12	M	31/32 (97%)	28 (90%)	3 (10%)	8	17
12	m	30/32 (94%)	28 (93%)	2 (7%)	15	31
13	O	214/207 (103%)	209 (98%)	5 (2%)	44	72
13	o	211/207 (102%)	205 (97%)	6 (3%)	38	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	T	27/28 (96%)	25 (93%)	2 (7%)	13	27
14	t	27/28 (96%)	25 (93%)	2 (7%)	13	27
15	U	84/89 (94%)	80 (95%)	4 (5%)	23	46
15	u	84/89 (94%)	80 (95%)	4 (5%)	23	46
16	V	119/117 (102%)	118 (99%)	1 (1%)	73	88
16	v	118/117 (101%)	115 (98%)	3 (2%)	42	69
17	Y	22/23 (96%)	20 (91%)	2 (9%)	9	19
17	y	22/23 (96%)	20 (91%)	2 (9%)	9	19
18	X	32/33 (97%)	32 (100%)	0	100	100
18	x	31/33 (94%)	31 (100%)	0	100	100
19	Z	52/52 (100%)	47 (90%)	5 (10%)	8	17
19	z	52/52 (100%)	48 (92%)	4 (8%)	12	25
20	R	25/29 (86%)	23 (92%)	2 (8%)	11	24
All	All	4506/4403 (102%)	4411 (98%)	95 (2%)	47	74

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	279	LEU
11	l	15	THR
3	c	416[A]	SER
5	e	71	GLU
13	o	23	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	497	GLN
13	o	124	ASN
3	c	155	ASN
4	d	186	GLN
13	o	147	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
12	FME	m	1	12	8,9,10	0.66	0	8,9,11	1.05	1 (12%)
8	FME	I	1	8	8,9,10	0.76	0	8,9,11	1.28	2 (25%)
14	FME	T	1	14	8,9,10	0.69	0	8,9,11	1.52	3 (37%)
14	FME	t	1	14	8,9,10	0.88	0	8,9,11	1.95	4 (50%)
8	FME	i	1	8	8,9,10	0.71	0	8,9,11	1.36	2 (25%)
12	FME	M	1	12	8,9,10	0.76	0	8,9,11	1.29	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
12	FME	m	1	12	-	3/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
14	FME	T	1	14	-	0/7/9/11	-
14	FME	t	1	14	-	1/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
12	FME	M	1	12	-	2/7/9/11	-

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	CA-N-CN	-3.11	118.04	122.82
14	T	1	FME	CA-N-CN	-2.72	118.64	122.82
14	t	1	FME	O-C-CA	-2.67	117.90	124.77
12	M	1	FME	CA-N-CN	-2.47	119.02	122.82
14	T	1	FME	O-C-CA	-2.34	118.74	124.77

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 266 ligands modelled in this entry, 24 are monoatomic and 18 are unknown - leaving 224 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	$\# Z > 2$
36	BCT	d	401[B]	21	3,3,3	0.52	0	2,3,3	0.85	0
23	CLA	B	612	-	69,73,73	2.02	20 (28%)	82,113,113	2.65	30 (36%)
23	CLA	b	613	-	69,73,73	2.04	20 (28%)	82,113,113	2.65	29 (35%)
25	SQD	A	412	-	52,54,54	0.97	2 (3%)	62,65,65	1.13	4 (6%)
27	LMT	F	101	-	36,36,36	0.50	0	47,47,47	1.01	2 (4%)
38	LHG	d	409	-	48,48,48	0.87	3 (6%)	51,54,54	1.02	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	a	409	-	69,73,73	2.07	19 (27%)	82,113,113	2.67	31 (37%)
26	GOL	O	301	-	5,5,5	0.38	0	5,5,5	0.38	0
38	LHG	D	413	-	48,48,48	0.95	2 (4%)	51,54,54	1.16	5 (9%)
23	CLA	C	502	-	69,73,73	2.03	20 (28%)	82,113,113	2.69	30 (36%)
35	LMG	d	416	40	51,51,55	0.89	2 (3%)	59,59,63	1.11	6 (10%)
23	CLA	C	504	-	69,73,73	2.08	20 (28%)	82,113,113	2.65	30 (36%)
25	SQD	f	102	-	41,43,54	1.13	2 (4%)	51,54,65	1.41	7 (13%)
26	GOL	a	402	-	5,5,5	0.40	0	5,5,5	0.23	0
33	HTG	B	623	-	19,19,19	0.98	1 (5%)	23,24,24	1.79	4 (17%)
41	HEC	v	205	16	46,50,50	1.72	10 (21%)	58,82,82	1.67	11 (18%)
27	LMT	C	521	-	36,36,36	0.49	0	47,47,47	1.07	3 (6%)
27	LMT	D	405	-	36,36,36	0.46	0	47,47,47	1.01	1 (2%)
26	GOL	C	525	-	5,5,5	0.45	0	5,5,5	0.64	0
30	PL9	A	416[A]	-	55,55,55	0.64	2 (3%)	68,69,69	1.79	21 (30%)
24	BCR	B	619	-	41,41,41	1.03	1 (2%)	56,56,56	1.52	12 (21%)
26	GOL	T	101	-	5,5,5	0.44	0	5,5,5	0.20	0
38	LHG	a	420	-	41,41,48	1.02	2 (4%)	44,47,54	1.00	3 (6%)
33	HTG	B	622	-	19,19,19	0.80	1 (5%)	23,24,24	1.62	3 (13%)
37	PHO	D	403[A]	-	58,69,69	2.78	15 (25%)	55,99,99	2.92	15 (27%)
26	GOL	t	103	-	5,5,5	0.50	0	5,5,5	0.21	0
23	CLA	D	407	-	69,73,73	2.03	21 (30%)	82,113,113	2.68	32 (39%)
23	CLA	A	405	42	69,73,73	2.00	19 (27%)	82,113,113	2.81	32 (39%)
23	CLA	B	613	-	69,73,73	1.95	19 (27%)	82,113,113	2.66	30 (36%)
26	GOL	D	404	-	5,5,5	0.46	0	5,5,5	0.46	0
35	LMG	a	415	-	51,51,55	0.91	2 (3%)	59,59,63	1.19	6 (10%)
30	PL9	D	409[B]	-	55,55,55	0.66	2 (3%)	68,69,69	1.77	19 (27%)
30	PL9	A	416[B]	-	55,55,55	0.66	2 (3%)	68,69,69	1.80	22 (32%)
25	SQD	F	104	-	41,43,54	1.11	2 (4%)	51,54,65	1.60	10 (19%)
23	CLA	b	620	-	69,73,73	1.96	19 (27%)	82,113,113	2.61	32 (39%)
35	LMG	c	523	-	51,51,55	0.95	2 (3%)	59,59,63	1.23	7 (11%)
26	GOL	A	411	-	5,5,5	0.42	0	5,5,5	0.27	0
37	PHO	D	403[B]	-	58,69,69	2.82	14 (24%)	55,99,99	2.74	13 (23%)
38	LHG	D	412	-	48,48,48	0.92	3 (6%)	51,54,54	0.83	2 (3%)
23	CLA	C	506	-	69,73,73	2.01	19 (27%)	82,113,113	2.62	29 (35%)
24	BCR	K	103	-	41,41,41	1.04	1 (2%)	56,56,56	1.52	12 (21%)
24	BCR	T	103	-	41,41,41	1.03	1 (2%)	56,56,56	1.78	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LMT	m	102	-	36,36,36	0.47	0	47,47,47	1.06	3 (6%)
27	LMT	A	413	-	36,36,36	0.57	1 (2%)	47,47,47	1.32	7 (14%)
38	LHG	D	411	-	48,48,48	0.88	2 (4%)	51,54,54	1.05	3 (5%)
36	BCT	d	401[A]	-	3,3,3	0.54	0	2,3,3	0.85	0
28	OEX	A	414[A]	1,42,3	0,15,15	-	-	-		
24	BCR	d	406	-	41,41,41	1.10	1 (2%)	56,56,56	1.64	11 (19%)
23	CLA	d	403	42	69,73,73	2.03	18 (26%)	82,113,113	2.70	32 (39%)
23	CLA	B	602	42	69,73,73	2.05	21 (30%)	82,113,113	2.69	31 (37%)
33	HTG	b	601	-	19,19,19	0.96	1 (5%)	23,24,24	1.12	2 (8%)
34	DGD	D	410	-	52,52,67	1.04	3 (5%)	60,60,81	1.19	5 (8%)
26	GOL	B	627	-	5,5,5	0.44	0	5,5,5	0.48	0
38	LHG	L	101	-	48,48,48	0.92	2 (4%)	51,54,54	1.11	6 (11%)
34	DGD	C	517	-	63,63,67	0.89	2 (3%)	77,77,81	1.08	8 (10%)
23	CLA	c	515	3	69,73,73	1.96	20 (28%)	82,113,113	2.63	30 (36%)
26	GOL	v	202	-	5,5,5	0.38	0	5,5,5	0.42	0
35	LMG	M	101	-	51,51,55	0.92	2 (3%)	59,59,63	1.09	4 (6%)
25	SQD	L	102	-	52,54,54	0.98	2 (3%)	62,65,65	1.58	11 (17%)
26	GOL	B	628	-	5,5,5	0.38	0	5,5,5	0.37	0
23	CLA	c	506	-	69,73,73	2.04	19 (27%)	82,113,113	2.52	28 (34%)
26	GOL	B	633	-	5,5,5	0.42	0	5,5,5	0.47	0
35	LMG	D	417	40	51,51,55	0.93	2 (3%)	59,59,63	0.98	4 (6%)
23	CLA	B	607	-	69,73,73	2.01	19 (27%)	82,113,113	2.72	31 (37%)
26	GOL	b	605	-	5,5,5	0.39	0	5,5,5	0.30	0
23	CLA	c	507	-	69,73,73	2.00	20 (28%)	82,113,113	2.70	29 (35%)
25	SQD	A	409	-	52,54,54	0.92	2 (3%)	62,65,65	1.43	9 (14%)
33	HTG	B	630	-	19,19,19	0.97	2 (10%)	23,24,24	1.21	1 (4%)
24	BCR	c	518	-	41,41,41	1.04	1 (2%)	56,56,56	1.59	11 (19%)
33	HTG	D	416	-	16,16,19	0.99	2 (12%)	20,21,24	1.25	1 (5%)
25	SQD	a	405	-	52,54,54	1.01	2 (3%)	62,65,65	1.14	4 (6%)
26	GOL	T	102	-	5,5,5	0.41	0	5,5,5	0.32	0
23	CLA	C	508	42	69,73,73	2.00	20 (28%)	82,113,113	2.63	31 (37%)
26	GOL	V	202	-	5,5,5	0.39	0	5,5,5	0.43	0
37	PHO	D	402	-	58,69,69	2.73	13 (22%)	55,99,99	3.05	18 (32%)
23	CLA	c	511	42	69,73,73	2.04	18 (26%)	82,113,113	2.72	28 (34%)
23	CLA	C	511	-	69,73,73	2.11	20 (28%)	82,113,113	2.64	33 (40%)
30	PL9	D	409[A]	-	55,55,55	0.65	2 (3%)	68,69,69	1.67	19 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	A	404	-	69,73,73	2.01	20 (28%)	82,113,113	2.70	32 (39%)
23	CLA	B	609	-	69,73,73	2.05	21 (30%)	82,113,113	2.60	33 (40%)
24	BCR	K	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.46	8 (14%)
35	LMG	C	501	-	51,51,55	0.94	2 (3%)	59,59,63	1.17	7 (11%)
37	PHO	d	402[A]	-	58,69,69	2.76	13 (22%)	55,99,99	3.03	15 (27%)
23	CLA	b	621	-	69,73,73	1.99	20 (28%)	82,113,113	2.72	33 (40%)
27	LMT	M	104	-	36,36,36	0.55	0	47,47,47	1.01	3 (6%)
36	BCT	D	401[B]	21	3,3,3	0.51	0	2,3,3	0.93	0
25	SQD	a	414	-	52,54,54	0.92	2 (3%)	62,65,65	1.50	11 (17%)
38	LHG	d	411	-	48,48,48	0.93	2 (4%)	51,54,54	1.14	4 (7%)
33	HTG	c	525	-	19,19,19	0.93	2 (10%)	23,24,24	1.35	3 (13%)
23	CLA	B	614	-	69,73,73	2.05	19 (27%)	82,113,113	2.63	31 (37%)
23	CLA	b	617	-	69,73,73	2.05	19 (27%)	82,113,113	2.56	33 (40%)
24	BCR	B	620	-	41,41,41	1.08	1 (2%)	56,56,56	1.56	10 (17%)
23	CLA	c	516	-	69,73,73	2.04	20 (28%)	82,113,113	2.76	30 (36%)
23	CLA	b	612	-	69,73,73	2.00	20 (28%)	82,113,113	2.74	32 (39%)
24	BCR	B	618	-	41,41,41	1.06	1 (2%)	56,56,56	1.44	8 (14%)
26	GOL	v	201	-	5,5,5	0.39	0	5,5,5	0.32	0
33	HTG	C	522	-	19,19,19	0.92	2 (10%)	23,24,24	1.34	2 (8%)
35	LMG	b	629	-	51,51,55	0.91	2 (3%)	59,59,63	1.09	3 (5%)
37	PHO	d	402[B]	-	58,69,69	2.78	14 (24%)	55,99,99	2.91	15 (27%)
24	BCR	c	527	-	41,41,41	1.06	1 (2%)	56,56,56	1.64	10 (17%)
23	CLA	a	410	42	69,73,73	1.99	19 (27%)	82,113,113	2.70	32 (39%)
33	HTG	o	301	-	19,19,19	1.04	1 (5%)	23,24,24	1.24	1 (4%)
27	LMT	a	404	-	36,36,36	0.58	1 (2%)	47,47,47	1.24	5 (10%)
26	GOL	c	501	-	5,5,5	0.44	0	5,5,5	0.46	0
34	DGD	c	520	-	63,63,67	0.89	2 (3%)	77,77,81	1.00	4 (5%)
24	BCR	t	102	-	41,41,41	1.01	1 (2%)	56,56,56	1.59	14 (25%)
26	GOL	f	101	32	5,5,5	0.32	0	5,5,5	0.43	0
23	CLA	C	507	-	69,73,73	2.03	19 (27%)	82,113,113	2.56	30 (36%)
26	GOL	F	103	32	5,5,5	0.38	0	5,5,5	0.30	0
33	HTG	V	207	-	19,19,19	0.95	2 (10%)	23,24,24	1.30	4 (17%)
28	OEX	a	417[A]	1,42,3	0,15,15	-	-	-	-	-
33	HTG	b	608	-	19,19,19	0.99	2 (10%)	23,24,24	1.02	1 (4%)
23	CLA	A	406	42	69,73,73	1.97	20 (28%)	82,113,113	2.70	33 (40%)
23	CLA	B	606	-	69,73,73	2.03	20 (28%)	82,113,113	2.70	29 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	619	42	69,73,73	2.02	21 (30%)	82,113,113	2.63	32 (39%)
34	DGD	d	408	-	63,63,67	0.95	3 (4%)	77,77,81	1.30	7 (9%)
27	LMT	M	105	-	36,36,36	0.48	0	47,47,47	0.89	1 (2%)
34	DGD	h	102	-	63,63,67	0.90	3 (4%)	77,77,81	0.98	6 (7%)
23	CLA	c	513	-	69,73,73	2.07	20 (28%)	82,113,113	2.68	31 (37%)
27	LMT	t	101	-	25,25,36	0.52	0	30,30,47	0.85	1 (3%)
24	BCR	a	413	-	41,41,41	1.10	1 (2%)	56,56,56	1.45	9 (16%)
23	CLA	C	503	-	69,73,73	2.02	20 (28%)	82,113,113	2.56	29 (35%)
24	BCR	C	515	-	41,41,41	1.05	1 (2%)	56,56,56	1.65	10 (17%)
33	HTG	B	629	-	19,19,19	0.94	1 (5%)	23,24,24	1.28	1 (4%)
23	CLA	c	517	-	69,73,73	2.05	20 (28%)	82,113,113	2.62	33 (40%)
39	HEM	F	102	6,5	50,50,50	1.55	6 (12%)	67,82,82	1.73	15 (22%)
23	CLA	B	617	-	69,73,73	1.99	19 (27%)	82,113,113	2.68	30 (36%)
24	BCR	Y	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.69	11 (19%)
23	CLA	A	407	-	69,73,73	2.03	21 (30%)	82,113,113	2.70	35 (42%)
23	CLA	C	512	3	69,73,73	2.08	20 (28%)	82,113,113	2.62	29 (35%)
23	CLA	b	625	-	69,73,73	2.00	20 (28%)	82,113,113	2.71	29 (35%)
23	CLA	c	510	-	69,73,73	2.00	19 (27%)	82,113,113	2.62	33 (40%)
34	DGD	B	632	-	63,63,67	0.90	2 (3%)	77,77,81	1.10	6 (7%)
26	GOL	b	606	-	5,5,5	0.38	0	5,5,5	0.29	0
30	PL9	a	416[B]	-	55,55,55	0.65	2 (3%)	68,69,69	1.85	22 (32%)
26	GOL	V	201	-	5,5,5	0.37	0	5,5,5	0.31	0
26	GOL	b	602	-	5,5,5	0.39	0	5,5,5	0.65	0
38	LHG	E	101	-	41,41,48	1.03	2 (4%)	44,47,54	1.16	4 (9%)
36	BCT	D	401[A]	21	3,3,3	0.51	0	2,3,3	1.09	0
23	CLA	C	505	42	69,73,73	2.05	19 (27%)	82,113,113	2.66	32 (39%)
23	CLA	b	611	-	69,73,73	2.06	20 (28%)	82,113,113	2.65	31 (37%)
34	DGD	C	516	-	63,63,67	0.87	2 (3%)	77,77,81	1.11	6 (7%)
24	BCR	b	627	-	41,41,41	1.02	1 (2%)	56,56,56	1.31	7 (12%)
39	HEM	e	101	6,5	50,50,50	1.54	8 (16%)	67,82,82	1.61	12 (17%)
24	BCR	h	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.42	8 (14%)
24	BCR	k	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.68	12 (21%)
23	CLA	b	610	42	69,73,73	2.09	21 (30%)	82,113,113	2.62	30 (36%)
23	CLA	b	618	-	69,73,73	1.99	18 (26%)	82,113,113	2.71	31 (37%)
27	LMT	e	102	-	36,36,36	0.50	1 (2%)	47,47,47	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	LMG	C	519	-	51,51,55	0.96	2 (3%)	59,59,63	1.06	5 (8%)
23	CLA	d	405	-	69,73,73	2.03	19 (27%)	82,113,113	2.69	33 (40%)
23	CLA	D	406	-	69,73,73	1.99	18 (26%)	82,113,113	2.76	30 (36%)
26	GOL	b	604	-	5,5,5	0.35	0	5,5,5	0.26	0
23	CLA	B	604	-	69,73,73	2.07	19 (27%)	82,113,113	2.69	30 (36%)
23	CLA	b	624	-	69,73,73	2.00	18 (26%)	82,113,113	2.64	31 (37%)
35	LMG	Z	101	-	37,37,55	0.98	3 (8%)	45,45,63	1.34	6 (13%)
35	LMG	z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.19	3 (6%)
23	CLA	B	603	-	69,73,73	2.03	20 (28%)	82,113,113	2.73	34 (41%)
26	GOL	B	626	-	5,5,5	0.39	0	5,5,5	0.51	0
38	LHG	b	634	-	48,48,48	0.95	2 (4%)	51,54,54	1.05	2 (3%)
33	HTG	b	607	-	19,19,19	0.94	1 (5%)	23,24,24	1.63	4 (17%)
30	PL9	d	407[B]	-	55,55,55	0.67	3 (5%)	68,69,69	1.67	20 (29%)
33	HTG	b	632	-	19,19,19	1.07	2 (10%)	23,24,24	1.87	5 (21%)
41	HEC	V	206	16	46,50,50	1.73	11 (23%)	58,82,82	1.77	15 (25%)
24	BCR	b	626	-	41,41,41	1.09	1 (2%)	56,56,56	1.56	9 (16%)
26	GOL	a	401	-	5,5,5	0.40	0	5,5,5	0.49	0
23	CLA	b	622	-	69,73,73	2.04	21 (30%)	82,113,113	2.62	31 (37%)
37	PHO	a	411	-	58,69,69	2.78	13 (22%)	55,99,99	2.79	16 (29%)
23	CLA	c	514	-	69,73,73	2.05	19 (27%)	82,113,113	2.65	31 (37%)
26	GOL	c	502	-	5,5,5	0.44	0	5,5,5	0.45	0
23	CLA	B	605	-	69,73,73	1.93	20 (28%)	82,113,113	2.60	29 (35%)
30	PL9	a	416[A]	-	55,55,55	0.63	2 (3%)	68,69,69	1.93	21 (30%)
23	CLA	B	616	-	69,73,73	2.04	19 (27%)	82,113,113	2.61	29 (35%)
35	LMG	C	520	-	51,51,55	0.97	2 (3%)	59,59,63	1.09	5 (8%)
23	CLA	d	404	-	69,73,73	1.97	19 (27%)	82,113,113	2.73	32 (39%)
24	BCR	b	628	-	41,41,41	1.07	2 (4%)	56,56,56	1.26	6 (10%)
33	HTG	d	414	-	16,16,19	1.09	2 (12%)	20,21,24	1.66	2 (10%)
23	CLA	b	616	42	69,73,73	2.01	20 (28%)	82,113,113	2.63	31 (37%)
23	CLA	B	608	42	69,73,73	1.99	19 (27%)	82,113,113	2.68	32 (39%)
23	CLA	B	610	-	69,73,73	2.03	18 (26%)	82,113,113	2.63	30 (36%)
23	CLA	C	513	-	69,73,73	2.05	20 (28%)	82,113,113	2.64	30 (36%)
23	CLA	c	505	-	69,73,73	1.97	19 (27%)	82,113,113	2.61	32 (39%)
24	BCR	H	101	-	41,41,41	1.11	1 (2%)	56,56,56	1.55	9 (16%)
26	GOL	B	625	-	5,5,5	0.42	0	5,5,5	0.52	0
27	LMT	b	630	-	25,25,36	0.53	0	30,30,47	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	OEY	a	418[B]	1,42,3	0,16,16	-	-	-		
34	DGD	C	518	-	63,63,67	0.91	2 (3%)	77,77,81	1.02	7 (9%)
27	LMT	M	102	-	36,36,36	0.43	0	47,47,47	0.84	0
23	CLA	B	611	42	69,73,73	2.08	20 (28%)	82,113,113	2.71	34 (41%)
34	DGD	c	521	-	63,63,67	0.85	2 (3%)	77,77,81	1.06	3 (3%)
23	CLA	C	509	-	69,73,73	2.07	20 (28%)	82,113,113	2.68	29 (35%)
23	CLA	c	509	-	69,73,73	2.05	20 (28%)	82,113,113	2.60	31 (37%)
35	LMG	c	522	-	51,51,55	0.91	2 (3%)	59,59,63	1.18	5 (8%)
24	BCR	D	408	-	41,41,41	1.05	1 (2%)	56,56,56	1.79	11 (19%)
24	BCR	k	102	-	41,41,41	1.08	1 (2%)	56,56,56	1.72	12 (21%)
26	GOL	B	624	-	5,5,5	0.40	0	5,5,5	0.33	0
34	DGD	c	519	-	63,63,67	0.84	2 (3%)	77,77,81	1.10	6 (7%)
26	GOL	v	203	-	5,5,5	0.38	0	5,5,5	0.25	0
26	GOL	C	524	-	5,5,5	0.37	0	5,5,5	0.69	0
26	GOL	A	410	-	5,5,5	0.36	0	5,5,5	0.57	0
23	CLA	b	615	-	69,73,73	2.01	20 (28%)	82,113,113	2.72	29 (35%)
26	GOL	V	204	-	5,5,5	0.41	0	5,5,5	0.25	0
33	HTG	c	524	-	19,19,19	0.98	2 (10%)	23,24,24	1.47	2 (8%)
23	CLA	C	514	-	69,73,73	2.03	21 (30%)	82,113,113	2.61	31 (37%)
23	CLA	c	508	42	69,73,73	2.00	18 (26%)	82,113,113	2.72	32 (39%)
26	GOL	c	528	-	5,5,5	0.42	0	5,5,5	0.37	0
25	SQD	B	621	-	52,54,54	0.96	2 (3%)	62,65,65	1.33	6 (9%)
23	CLA	c	512	-	69,73,73	2.05	19 (27%)	82,113,113	2.63	32 (39%)
27	LMT	T	104	-	25,25,36	0.56	1 (4%)	30,30,47	0.97	1 (3%)
27	LMT	a	419	-	36,36,36	0.44	0	47,47,47	0.83	1 (2%)
30	PL9	d	407[A]	-	55,55,55	0.67	2 (3%)	68,69,69	1.55	13 (19%)
23	CLA	b	623	-	69,73,73	1.98	18 (26%)	82,113,113	2.74	31 (37%)
38	LHG	d	410	-	48,48,48	0.89	2 (4%)	51,54,54	0.97	3 (5%)
26	GOL	b	603	-	5,5,5	0.38	0	5,5,5	0.18	0
26	GOL	V	205	-	5,5,5	0.35	0	5,5,5	0.24	0
29	OEY	A	415[B]	1,42,3	0,16,16	-	-	-		
23	CLA	b	614	-	69,73,73	1.99	20 (28%)	82,113,113	2.76	31 (37%)
24	BCR	A	408	-	41,41,41	1.09	1 (2%)	56,56,56	1.27	6 (10%)
23	CLA	C	510	-	69,73,73	2.06	20 (28%)	82,113,113	2.65	32 (39%)
33	HTG	C	523	-	19,19,19	0.93	1 (5%)	23,24,24	1.67	4 (17%)
26	GOL	V	203	-	5,5,5	0.36	0	5,5,5	0.46	0
23	CLA	B	615	-	69,73,73	2.04	17 (24%)	82,113,113	2.78	31 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	HTG	b	631	-	19,19,19	0.83	1 (5%)	23,24,24	1.27	3 (13%)
23	CLA	a	412	-	69,73,73	2.03	19 (27%)	82,113,113	2.68	33 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	612	-	1/1/15/20	3/39/115/115	-
23	CLA	b	613	-	1/1/15/20	4/39/115/115	-
25	SQD	A	412	-	-	14/49/69/69	0/1/1/1
27	LMT	F	101	-	-	4/21/61/61	0/2/2/2
38	LHG	d	409	-	-	14/53/53/53	-
23	CLA	a	409	-	1/1/15/20	4/39/115/115	-
26	GOL	O	301	-	-	0/4/4/4	-
38	LHG	D	413	-	-	17/53/53/53	-
23	CLA	C	502	-	1/1/15/20	7/39/115/115	-
35	LMG	d	416	40	-	10/46/66/70	0/1/1/1
23	CLA	C	504	-	1/1/15/20	1/39/115/115	-
25	SQD	f	102	-	-	14/38/58/69	0/1/1/1
26	GOL	a	402	-	-	2/4/4/4	-
33	HTG	B	623	-	-	3/10/30/30	0/1/1/1
41	HEC	v	205	16	-	6/14/54/54	-
27	LMT	C	521	-	-	9/21/61/61	0/2/2/2
27	LMT	D	405	-	-	11/21/61/61	0/2/2/2
26	GOL	C	525	-	-	1/4/4/4	-
30	PL9	A	416[A]	-	-	10/53/73/73	0/1/1/1
24	BCR	B	619	-	-	0/29/63/63	0/2/2/2
26	GOL	T	101	-	-	0/4/4/4	-
38	LHG	a	420	-	-	17/46/46/53	-
33	HTG	B	622	-	-	5/10/30/30	0/1/1/1
37	PHO	D	403[A]	-	-	0/37/103/103	0/5/6/6
26	GOL	t	103	-	-	0/4/4/4	-
23	CLA	D	407	-	1/1/15/20	5/39/115/115	-
23	CLA	A	405	42	1/1/15/20	5/39/115/115	-
23	CLA	B	613	-	1/1/15/20	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	GOL	D	404	-	-	2/4/4/4	-
35	LMG	a	415	-	-	19/46/66/70	0/1/1/1
30	PL9	D	409[B]	-	-	7/53/73/73	0/1/1/1
30	PL9	A	416[B]	-	-	11/53/73/73	0/1/1/1
25	SQD	F	104	-	-	13/38/58/69	0/1/1/1
23	CLA	b	620	-	1/1/15/20	8/39/115/115	-
35	LMG	c	523	-	-	5/46/66/70	0/1/1/1
26	GOL	A	411	-	-	2/4/4/4	-
37	PHO	D	403[B]	-	-	2/37/103/103	0/5/6/6
38	LHG	D	412	-	-	11/53/53/53	-
23	CLA	C	506	-	1/1/15/20	8/39/115/115	-
24	BCR	K	103	-	-	2/29/63/63	0/2/2/2
24	BCR	T	103	-	-	1/29/63/63	0/2/2/2
27	LMT	m	102	-	-	6/21/61/61	0/2/2/2
27	LMT	A	413	-	-	6/21/61/61	0/2/2/2
38	LHG	D	411	-	-	14/53/53/53	-
24	BCR	d	406	-	-	8/29/63/63	0/2/2/2
23	CLA	d	403	42	1/1/15/20	5/39/115/115	-
23	CLA	B	602	42	1/1/15/20	13/39/115/115	-
33	HTG	b	601	-	-	3/10/30/30	0/1/1/1
34	DGD	D	410	-	-	19/47/67/95	0/1/1/2
26	GOL	B	627	-	-	4/4/4/4	-
38	LHG	L	101	-	-	13/53/53/53	-
34	DGD	C	517	-	-	14/51/91/95	0/2/2/2
23	CLA	c	515	3	1/1/15/20	5/39/115/115	-
26	GOL	v	202	-	-	3/4/4/4	-
35	LMG	M	101	-	-	8/46/66/70	0/1/1/1
25	SQD	L	102	-	-	23/49/69/69	0/1/1/1
26	GOL	B	628	-	-	1/4/4/4	-
23	CLA	c	506	-	1/1/15/20	4/39/115/115	-
26	GOL	B	633	-	-	0/4/4/4	-
35	LMG	D	417	40	-	10/46/66/70	0/1/1/1
23	CLA	B	607	-	1/1/15/20	6/39/115/115	-
26	GOL	b	605	-	-	2/4/4/4	-
23	CLA	c	507	-	1/1/15/20	2/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	SQD	A	409	-	-	12/49/69/69	0/1/1/1
33	HTG	B	630	-	-	1/10/30/30	0/1/1/1
24	BCR	c	518	-	-	4/29/63/63	0/2/2/2
33	HTG	D	416	-	-	0/7/27/30	0/1/1/1
25	SQD	a	405	-	-	12/49/69/69	0/1/1/1
26	GOL	T	102	-	-	2/4/4/4	-
23	CLA	C	508	42	1/1/15/20	7/39/115/115	-
26	GOL	V	202	-	-	3/4/4/4	-
37	PHO	D	402	-	-	2/37/103/103	0/5/6/6
23	CLA	c	511	42	1/1/15/20	8/39/115/115	-
23	CLA	C	511	-	1/1/15/20	8/39/115/115	-
30	PL9	D	409[A]	-	-	7/53/73/73	0/1/1/1
23	CLA	A	404	-	1/1/15/20	4/39/115/115	-
23	CLA	B	609	-	-	1/39/115/115	-
24	BCR	K	101	-	-	2/29/63/63	0/2/2/2
35	LMG	C	501	-	-	17/46/66/70	0/1/1/1
37	PHO	d	402[A]	-	-	1/37/103/103	0/5/6/6
23	CLA	b	621	-	1/1/15/20	4/39/115/115	-
27	LMT	M	104	-	-	9/21/61/61	0/2/2/2
25	SQD	a	414	-	-	11/49/69/69	0/1/1/1
38	LHG	d	411	-	-	16/53/53/53	-
33	HTG	c	525	-	-	0/10/30/30	0/1/1/1
23	CLA	B	614	-	1/1/15/20	8/39/115/115	-
23	CLA	b	617	-	-	2/39/115/115	-
24	BCR	B	620	-	-	0/29/63/63	0/2/2/2
23	CLA	c	516	-	1/1/15/20	7/39/115/115	-
23	CLA	b	612	-	1/1/15/20	5/39/115/115	-
24	BCR	B	618	-	-	2/29/63/63	0/2/2/2
26	GOL	v	201	-	-	2/4/4/4	-
33	HTG	C	522	-	-	0/10/30/30	0/1/1/1
35	LMG	b	629	-	-	10/46/66/70	0/1/1/1
37	PHO	d	402[B]	-	-	1/37/103/103	0/5/6/6
24	BCR	c	527	-	-	0/29/63/63	0/2/2/2
23	CLA	a	410	42	-	4/39/115/115	-
33	HTG	o	301	-	-	3/10/30/30	0/1/1/1
27	LMT	a	404	-	-	5/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	GOL	c	501	-	-	2/4/4/4	-
34	DGD	c	520	-	-	18/51/91/95	0/2/2/2
24	BCR	t	102	-	-	3/29/63/63	0/2/2/2
26	GOL	f	101	32	-	3/4/4/4	-
23	CLA	C	507	-	1/1/15/20	10/39/115/115	-
26	GOL	F	103	32	-	0/4/4/4	-
33	HTG	V	207	-	-	4/10/30/30	0/1/1/1
33	HTG	b	608	-	-	0/10/30/30	0/1/1/1
23	CLA	A	406	42	-	4/39/115/115	-
23	CLA	B	606	-	1/1/15/20	4/39/115/115	-
23	CLA	b	619	42	1/1/15/20	5/39/115/115	-
34	DGD	d	408	-	-	24/51/91/95	0/2/2/2
27	LMT	M	105	-	-	7/21/61/61	0/2/2/2
34	DGD	h	102	-	-	9/51/91/95	0/2/2/2
23	CLA	c	513	-	1/1/15/20	16/39/115/115	-
27	LMT	t	101	-	-	7/17/37/61	0/1/1/2
24	BCR	a	413	-	-	0/29/63/63	0/2/2/2
23	CLA	C	503	-	-	7/39/115/115	-
24	BCR	C	515	-	-	6/29/63/63	0/2/2/2
33	HTG	B	629	-	-	1/10/30/30	0/1/1/1
23	CLA	c	517	-	1/1/15/20	5/39/115/115	-
39	HEM	F	102	6,5	-	8/14/54/54	-
23	CLA	B	617	-	1/1/15/20	8/39/115/115	-
24	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
23	CLA	A	407	-	1/1/15/20	10/39/115/115	-
23	CLA	C	512	3	1/1/15/20	3/39/115/115	-
23	CLA	b	625	-	1/1/15/20	7/39/115/115	-
23	CLA	c	510	-	1/1/15/20	15/39/115/115	-
34	DGD	B	632	-	-	11/51/91/95	0/2/2/2
26	GOL	b	606	-	-	4/4/4/4	-
30	PL9	a	416[B]	-	-	14/53/73/73	0/1/1/1
26	GOL	V	201	-	-	2/4/4/4	-
26	GOL	b	602	-	-	0/4/4/4	-
38	LHG	E	101	-	-	18/46/46/53	-
23	CLA	C	505	42	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	611	-	1/1/15/20	3/39/115/115	-
34	DGD	C	516	-	-	16/51/91/95	0/2/2/2
24	BCR	b	627	-	-	0/29/63/63	0/2/2/2
39	HEM	e	101	6,5	-	8/14/54/54	-
24	BCR	h	101	-	-	1/29/63/63	0/2/2/2
24	BCR	k	101	-	-	0/29/63/63	0/2/2/2
23	CLA	b	610	42	1/1/15/20	13/39/115/115	-
23	CLA	b	618	-	1/1/15/20	3/39/115/115	-
27	LMT	e	102	-	-	9/21/61/61	0/2/2/2
35	LMG	C	519	-	-	9/46/66/70	0/1/1/1
23	CLA	d	405	-	1/1/15/20	7/39/115/115	-
23	CLA	D	406	-	1/1/15/20	3/39/115/115	-
26	GOL	b	604	-	-	3/4/4/4	-
23	CLA	B	604	-	1/1/15/20	6/39/115/115	-
23	CLA	b	624	-	1/1/15/20	4/39/115/115	-
35	LMG	Z	101	-	-	15/31/51/70	0/1/1/1
35	LMG	z	101	-	-	15/34/54/70	0/1/1/1
23	CLA	B	603	-	1/1/15/20	5/39/115/115	-
26	GOL	B	626	-	-	2/4/4/4	-
38	LHG	b	634	-	-	19/53/53/53	-
33	HTG	b	607	-	-	1/10/30/30	0/1/1/1
30	PL9	d	407[B]	-	-	7/53/73/73	0/1/1/1
33	HTG	b	632	-	-	4/10/30/30	0/1/1/1
41	HEC	V	206	16	-	6/14/54/54	-
24	BCR	b	626	-	-	2/29/63/63	0/2/2/2
26	GOL	a	401	-	-	1/4/4/4	-
23	CLA	b	622	-	1/1/15/20	4/39/115/115	-
37	PHO	a	411	-	-	2/37/103/103	0/5/6/6
23	CLA	c	514	-	1/1/15/20	8/39/115/115	-
26	GOL	c	502	-	-	2/4/4/4	-
23	CLA	B	605	-	1/1/15/20	1/39/115/115	-
30	PL9	a	416[A]	-	-	14/53/73/73	0/1/1/1
23	CLA	B	616	-	1/1/15/20	9/39/115/115	-
35	LMG	C	520	-	-	11/46/66/70	0/1/1/1
23	CLA	d	404	-	1/1/15/20	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	b	628	-	-	0/29/63/63	0/2/2/2
33	HTG	d	414	-	-	0/7/27/30	0/1/1/1
23	CLA	b	616	42	1/1/15/20	3/39/115/115	-
23	CLA	B	608	42	1/1/15/20	5/39/115/115	-
23	CLA	B	610	-	1/1/15/20	9/39/115/115	-
23	CLA	C	513	-	1/1/15/20	11/39/115/115	-
23	CLA	c	505	-	1/1/15/20	4/39/115/115	-
24	BCR	H	101	-	-	1/29/63/63	0/2/2/2
26	GOL	B	625	-	-	2/4/4/4	-
27	LMT	b	630	-	-	3/17/37/61	0/1/1/2
34	DGD	C	518	-	-	9/51/91/95	0/2/2/2
27	LMT	M	102	-	-	7/21/61/61	0/2/2/2
23	CLA	B	611	42	1/1/15/20	3/39/115/115	-
34	DGD	c	521	-	-	13/51/91/95	0/2/2/2
23	CLA	C	509	-	1/1/15/20	3/39/115/115	-
23	CLA	c	509	-	1/1/15/20	2/39/115/115	-
35	LMG	c	522	-	-	17/46/66/70	0/1/1/1
24	BCR	D	408	-	-	6/29/63/63	0/2/2/2
24	BCR	k	102	-	-	6/29/63/63	0/2/2/2
26	GOL	B	624	-	-	0/4/4/4	-
34	DGD	c	519	-	-	14/51/91/95	0/2/2/2
26	GOL	v	203	-	-	2/4/4/4	-
26	GOL	C	524	-	-	1/4/4/4	-
26	GOL	A	410	-	-	1/4/4/4	-
23	CLA	b	615	-	1/1/15/20	7/39/115/115	-
26	GOL	V	204	-	-	1/4/4/4	-
33	HTG	c	524	-	-	3/10/30/30	0/1/1/1
23	CLA	C	514	-	1/1/15/20	9/39/115/115	-
23	CLA	c	508	42	1/1/15/20	5/39/115/115	-
26	GOL	c	528	-	-	0/4/4/4	-
25	SQD	B	621	-	-	24/49/69/69	0/1/1/1
23	CLA	c	512	-	1/1/15/20	2/39/115/115	-
27	LMT	T	104	-	-	7/17/37/61	0/1/1/2
27	LMT	a	419	-	-	4/21/61/61	0/2/2/2
30	PL9	d	407[A]	-	-	8/53/73/73	0/1/1/1
23	CLA	b	623	-	1/1/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	LHG	d	410	-	-	11/53/53/53	-
26	GOL	b	603	-	-	0/4/4/4	-
26	GOL	V	205	-	-	4/4/4/4	-
23	CLA	b	614	-	1/1/15/20	6/39/115/115	-
24	BCR	A	408	-	-	4/29/63/63	0/2/2/2
23	CLA	C	510	-	1/1/15/20	11/39/115/115	-
33	HTG	C	523	-	-	3/10/30/30	0/1/1/1
26	GOL	V	203	-	-	1/4/4/4	-
23	CLA	B	615	-	1/1/15/20	17/39/115/115	-
33	HTG	b	631	-	-	3/10/30/30	0/1/1/1
23	CLA	a	412	-	1/1/15/20	10/39/115/115	-

The worst 5 of 1639 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	a	411	PHO	C1B-C2B	9.31	1.49	1.39
37	d	402[B]	PHO	C1B-C2B	9.22	1.49	1.39
37	D	403[B]	PHO	C1B-C2B	9.17	1.49	1.39
37	D	402	PHO	C1D-C2D	8.92	1.49	1.39
37	D	403[B]	PHO	C1D-C2D	8.83	1.49	1.39

The worst 5 of 2985 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	d	402[B]	PHO	C2D-C1D-ND	11.47	117.72	109.43
37	a	411	PHO	C2D-C1D-ND	11.26	117.57	109.43
37	D	403[A]	PHO	C2D-C1D-ND	11.24	117.56	109.43
37	d	402[A]	PHO	C2D-C1D-ND	10.79	117.23	109.43
37	D	402	PHO	C2D-C1D-ND	10.71	117.17	109.43

5 of 65 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404	CLA	ND
23	A	405	CLA	ND
23	A	407	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND

5 of 1359 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	602	CLA	C11-C10-C8-C9
23	B	607	CLA	C4B-C3B-CAB-CBB
23	B	610	CLA	C2B-C3B-CAB-CBB
23	B	610	CLA	C4B-C3B-CAB-CBB
23	B	615	CLA	CAD-CBD-CGD-O1D

There are no ring outliers.

175 monomers are involved in 410 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	b	613	CLA	2	0
25	A	412	SQD	2	0
27	F	101	LMT	1	0
38	d	409	LHG	3	0
23	a	409	CLA	3	0
38	D	413	LHG	6	0
23	C	502	CLA	2	0
35	d	416	LMG	2	0
23	C	504	CLA	3	0
25	f	102	SQD	4	0
33	B	623	HTG	1	0
27	C	521	LMT	2	0
30	A	416[A]	PL9	3	0
24	B	619	BCR	4	0
26	T	101	GOL	2	0
38	a	420	LHG	5	0
33	B	622	HTG	1	0
37	D	403[A]	PHO	1	0
26	t	103	GOL	1	0
23	D	407	CLA	1	0
23	A	405	CLA	6	0
23	B	613	CLA	2	0
26	D	404	GOL	2	0
35	a	415	LMG	3	0
30	D	409[B]	PL9	4	0
30	A	416[B]	PL9	4	0
25	F	104	SQD	2	0
23	b	620	CLA	1	0
26	A	411	GOL	1	0
37	D	403[B]	PHO	2	0
38	D	412	LHG	4	0
23	C	506	CLA	4	0
24	K	103	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	T	103	BCR	5	0
27	m	102	LMT	2	0
27	A	413	LMT	2	0
38	D	411	LHG	3	0
24	d	406	BCR	3	0
23	d	403	CLA	2	0
23	B	602	CLA	1	0
33	b	601	HTG	1	0
34	D	410	DGD	5	0
26	B	627	GOL	1	0
38	L	101	LHG	2	0
34	C	517	DGD	4	0
23	c	515	CLA	2	0
35	M	101	LMG	3	0
25	L	102	SQD	2	0
23	c	506	CLA	3	0
35	D	417	LMG	2	0
23	B	607	CLA	5	0
23	c	507	CLA	4	0
25	A	409	SQD	5	0
24	c	518	BCR	2	0
33	D	416	HTG	3	0
25	a	405	SQD	1	0
26	T	102	GOL	2	0
23	C	508	CLA	5	0
37	D	402	PHO	4	0
23	c	511	CLA	4	0
23	C	511	CLA	4	0
30	D	409[A]	PL9	1	0
23	A	404	CLA	5	0
23	B	609	CLA	1	0
24	K	101	BCR	6	0
35	C	501	LMG	5	0
37	d	402[A]	PHO	1	0
23	b	621	CLA	1	0
27	M	104	LMT	1	0
38	d	411	LHG	3	0
23	b	617	CLA	1	0
24	B	620	BCR	3	0
23	c	516	CLA	3	0
23	b	612	CLA	4	0
24	B	618	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	v	201	GOL	2	0
33	C	522	HTG	1	0
35	b	629	LMG	6	0
37	d	402[B]	PHO	3	0
24	c	527	BCR	4	0
23	a	410	CLA	4	0
33	o	301	HTG	2	0
27	a	404	LMT	3	0
34	c	520	DGD	2	0
24	t	102	BCR	6	0
26	f	101	GOL	1	0
23	C	507	CLA	5	0
33	V	207	HTG	1	0
33	b	608	HTG	1	0
23	A	406	CLA	7	0
23	B	606	CLA	8	0
23	b	619	CLA	4	0
34	d	408	DGD	6	0
27	M	105	LMT	4	0
34	h	102	DGD	1	0
23	c	513	CLA	2	0
24	a	413	BCR	2	0
23	C	503	CLA	3	0
24	C	515	BCR	2	0
23	c	517	CLA	5	0
39	F	102	HEM	2	0
23	B	617	CLA	6	0
24	Y	101	BCR	5	0
23	A	407	CLA	1	0
23	C	512	CLA	4	0
23	b	625	CLA	2	0
23	c	510	CLA	4	0
34	B	632	DGD	2	0
30	a	416[B]	PL9	7	0
23	b	611	CLA	2	0
34	C	516	DGD	4	0
24	b	627	BCR	3	0
39	e	101	HEM	3	0
24	h	101	BCR	5	0
24	k	101	BCR	3	0
23	b	610	CLA	2	0
23	b	618	CLA	3	0

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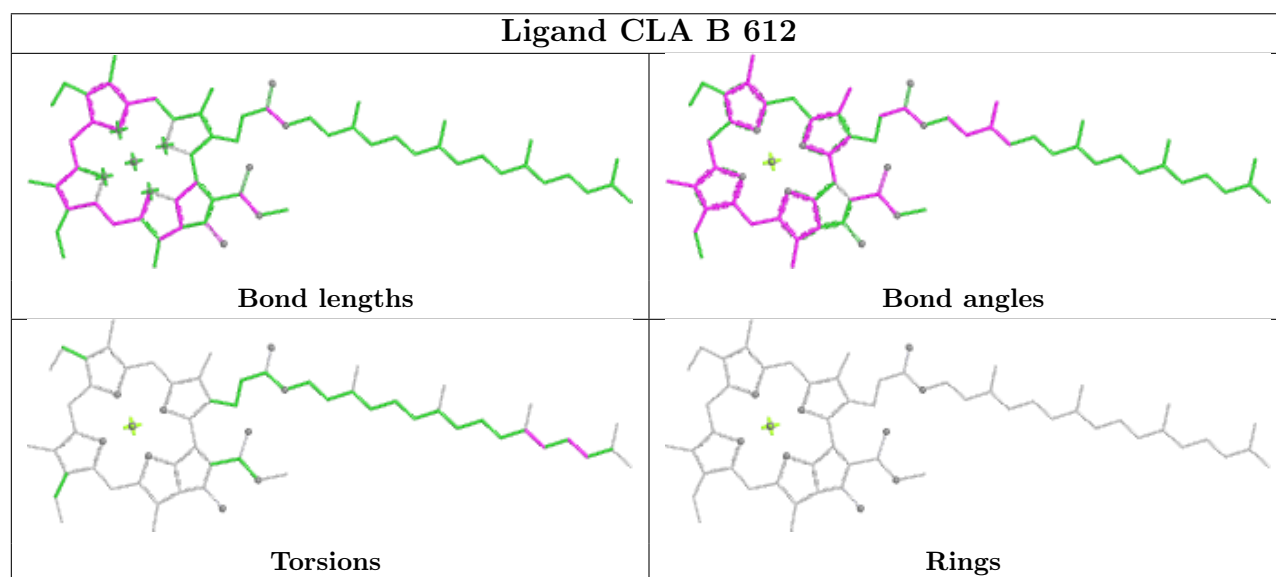
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	C	519	LMG	2	0
23	D	406	CLA	4	0
26	b	604	GOL	1	0
23	B	604	CLA	4	0
23	b	624	CLA	6	0
35	Z	101	LMG	2	0
35	z	101	LMG	7	0
23	B	603	CLA	4	0
38	b	634	LHG	3	0
33	b	607	HTG	1	0
30	d	407[B]	PL9	2	0
33	b	632	HTG	1	0
24	b	626	BCR	3	0
26	a	401	GOL	1	0
23	b	622	CLA	5	0
23	c	514	CLA	6	0
26	c	502	GOL	1	0
23	B	605	CLA	2	0
30	a	416[A]	PL9	9	0
23	B	616	CLA	3	0
23	d	404	CLA	4	0
24	b	628	BCR	1	0
33	d	414	HTG	2	0
23	b	616	CLA	2	0
23	B	608	CLA	3	0
23	B	610	CLA	3	0
23	C	513	CLA	8	0
23	c	505	CLA	2	0
24	H	101	BCR	3	0
27	b	630	LMT	1	0
29	a	418[B]	OEY	1	0
34	C	518	DGD	2	0
27	M	102	LMT	1	0
23	B	611	CLA	3	0
34	c	521	DGD	1	0
23	C	509	CLA	4	0
23	c	509	CLA	9	0
35	c	522	LMG	1	0
24	D	408	BCR	5	0
24	k	102	BCR	2	0
34	c	519	DGD	1	0
26	C	524	GOL	1	0

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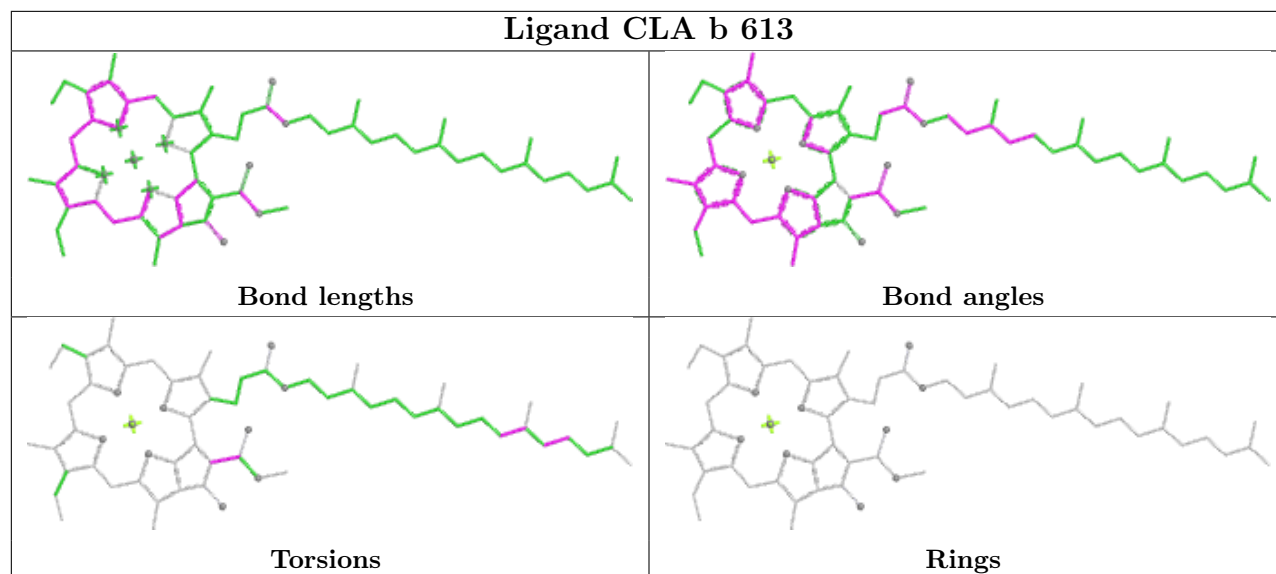
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	c	524	HTG	1	0
23	C	514	CLA	7	0
23	c	508	CLA	1	0
26	c	528	GOL	1	0
25	B	621	SQD	1	0
23	c	512	CLA	5	0
27	T	104	LMT	1	0
27	a	419	LMT	1	0
30	d	407[A]	PL9	1	0
23	b	623	CLA	3	0
29	A	415[B]	OEY	1	0
23	b	614	CLA	3	0
24	A	408	BCR	1	0
23	C	510	CLA	2	0
23	B	615	CLA	7	0
23	a	412	CLA	2	0

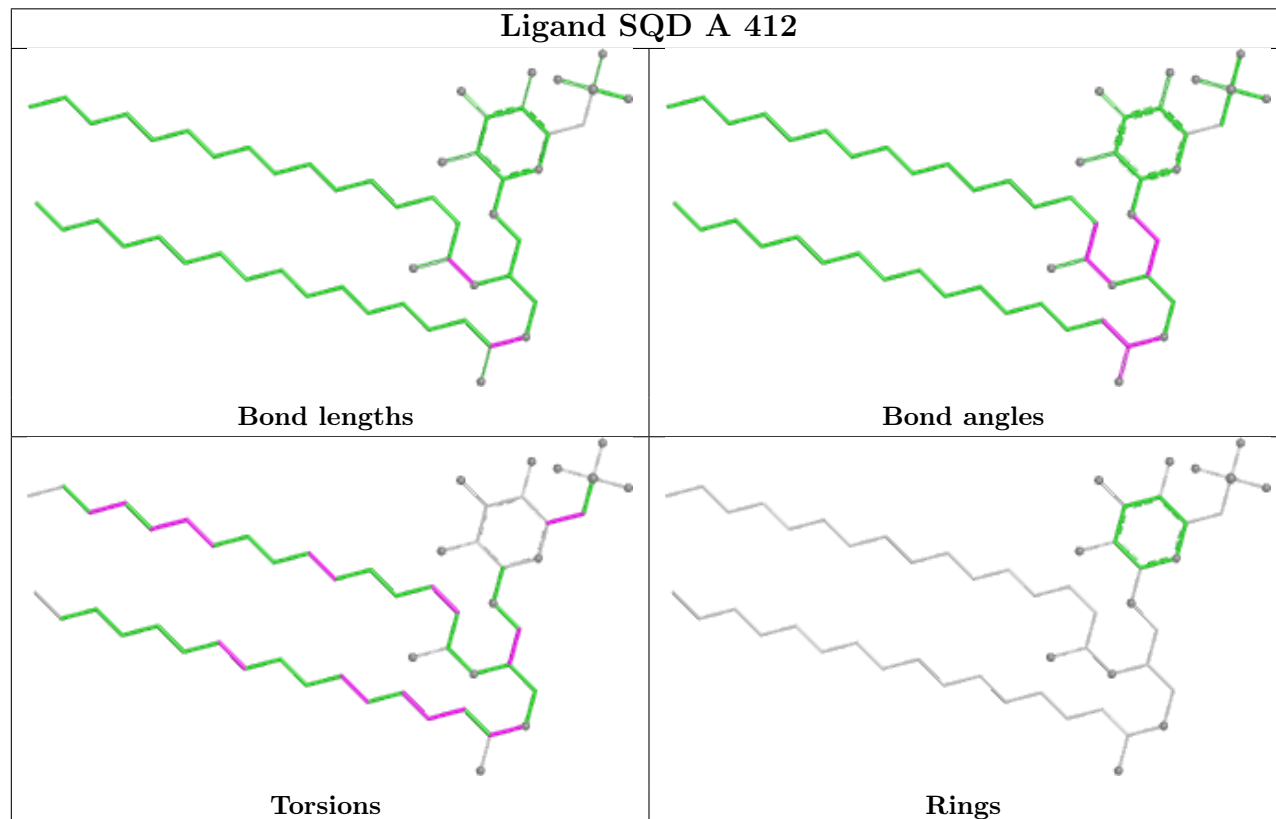
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

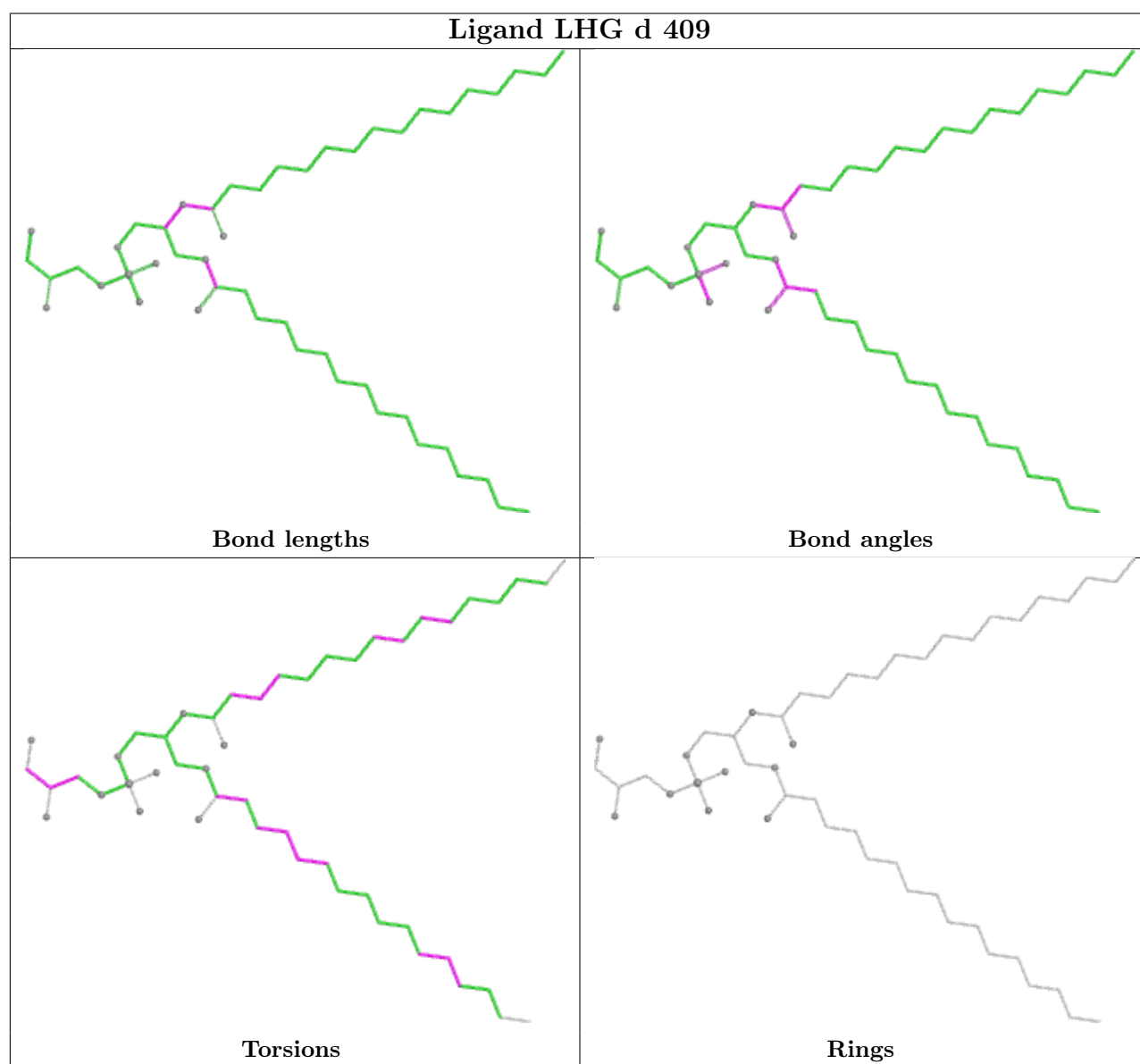
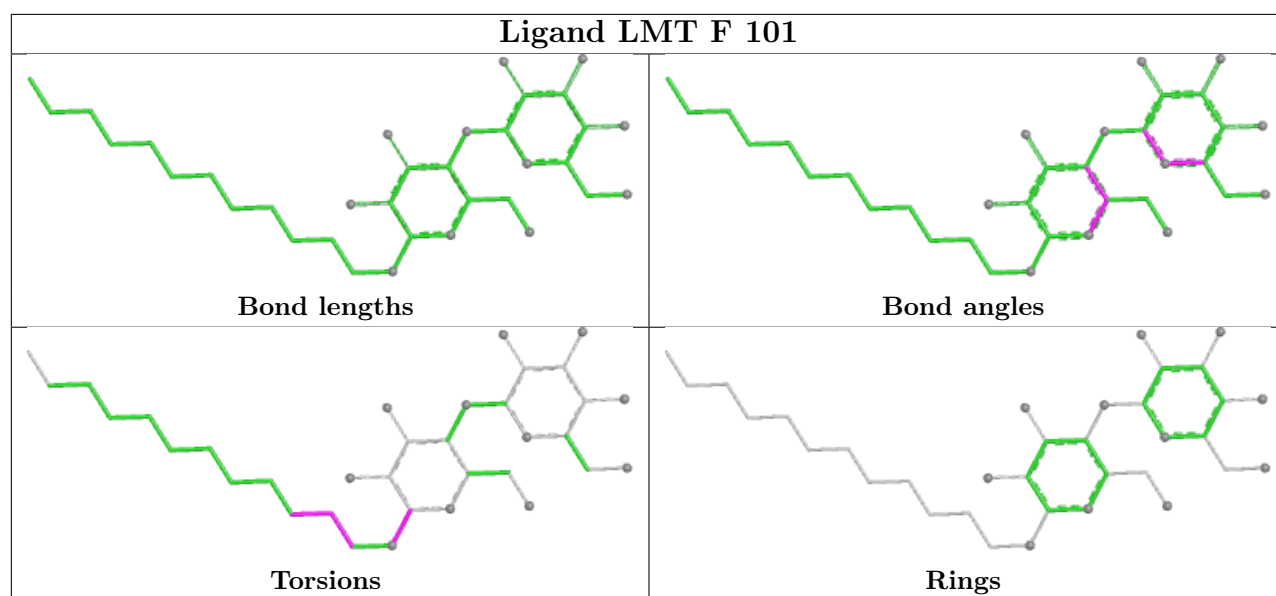


Ligand CLA b 613

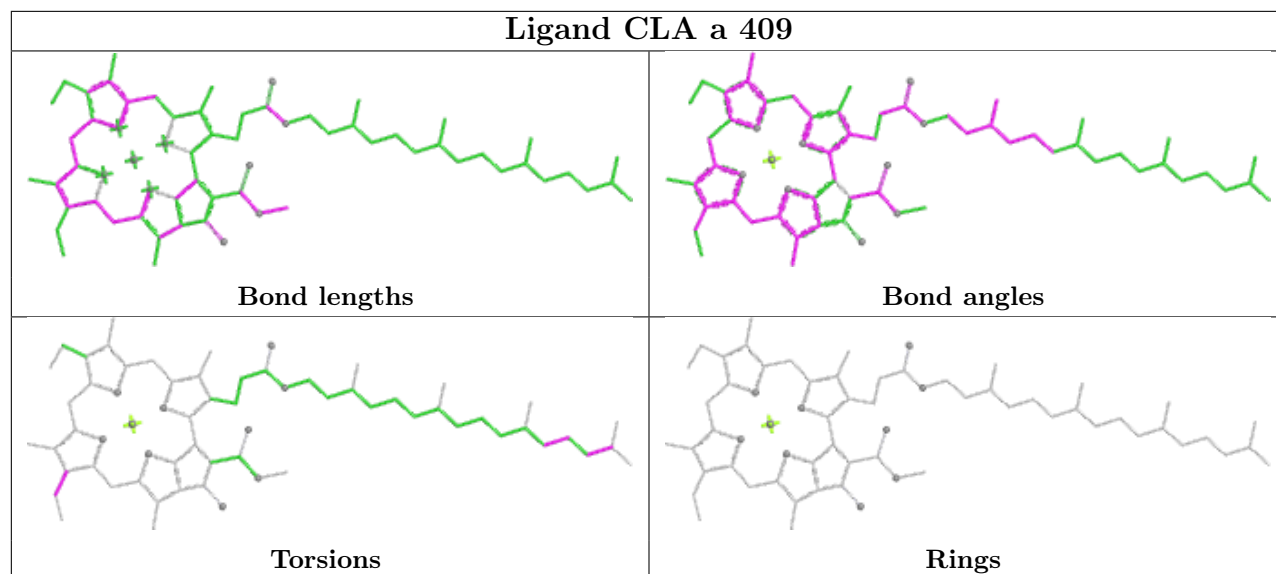


Ligand SQD A 412

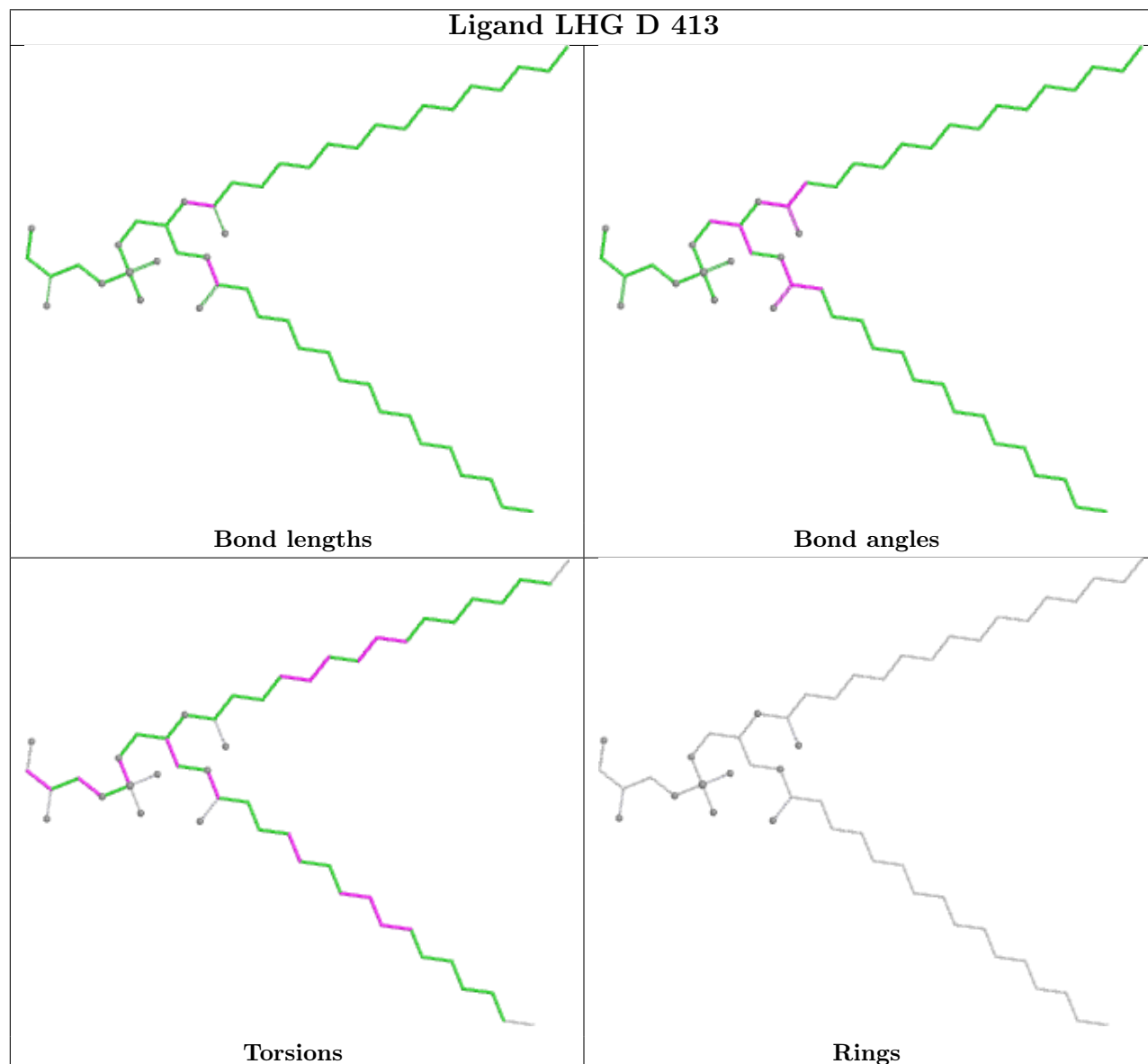


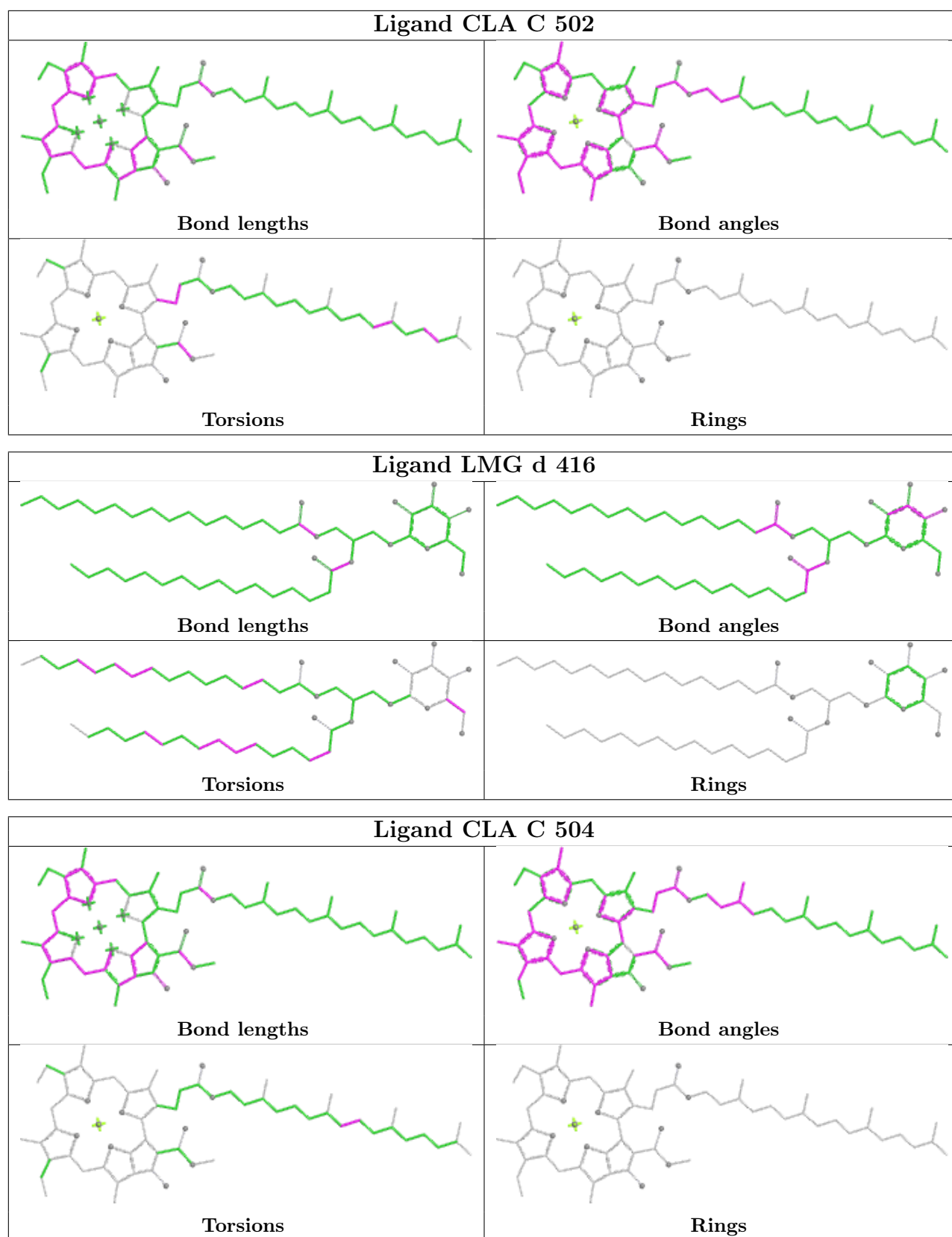


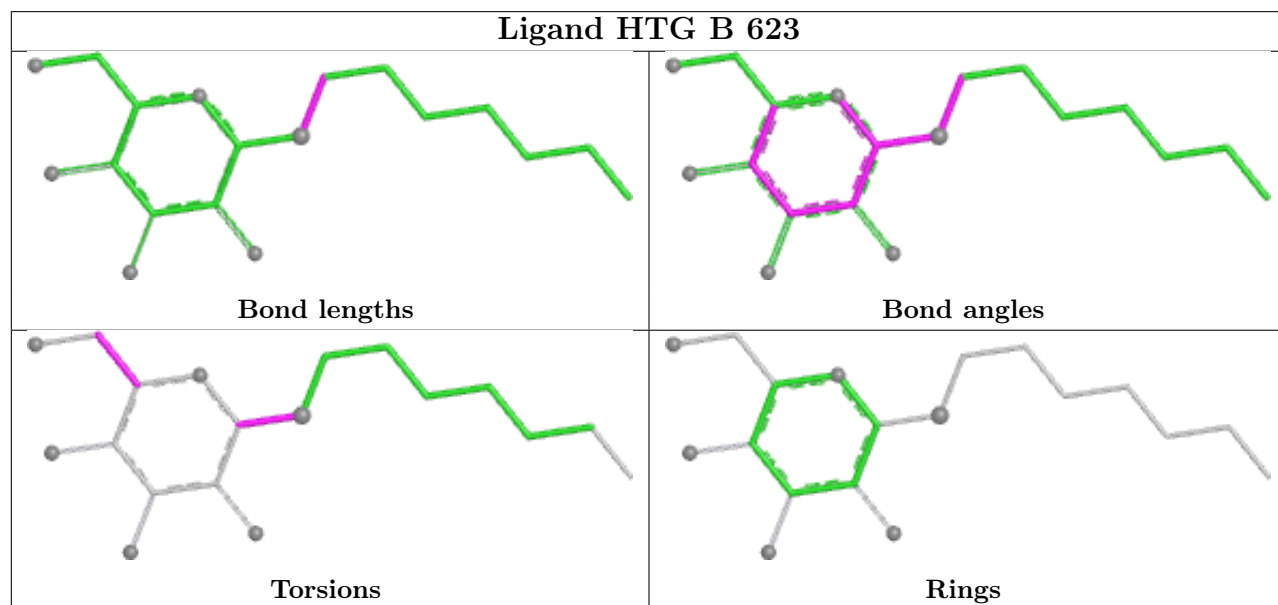
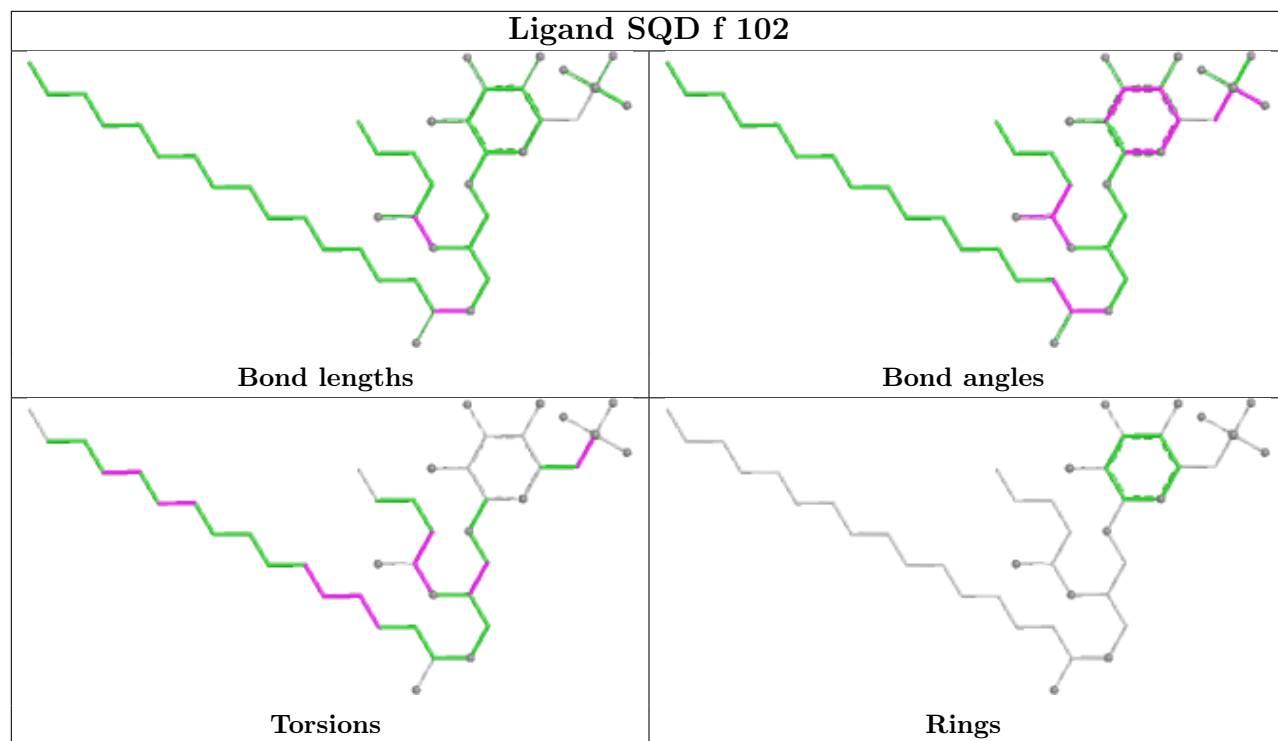
Ligand CLA a 409



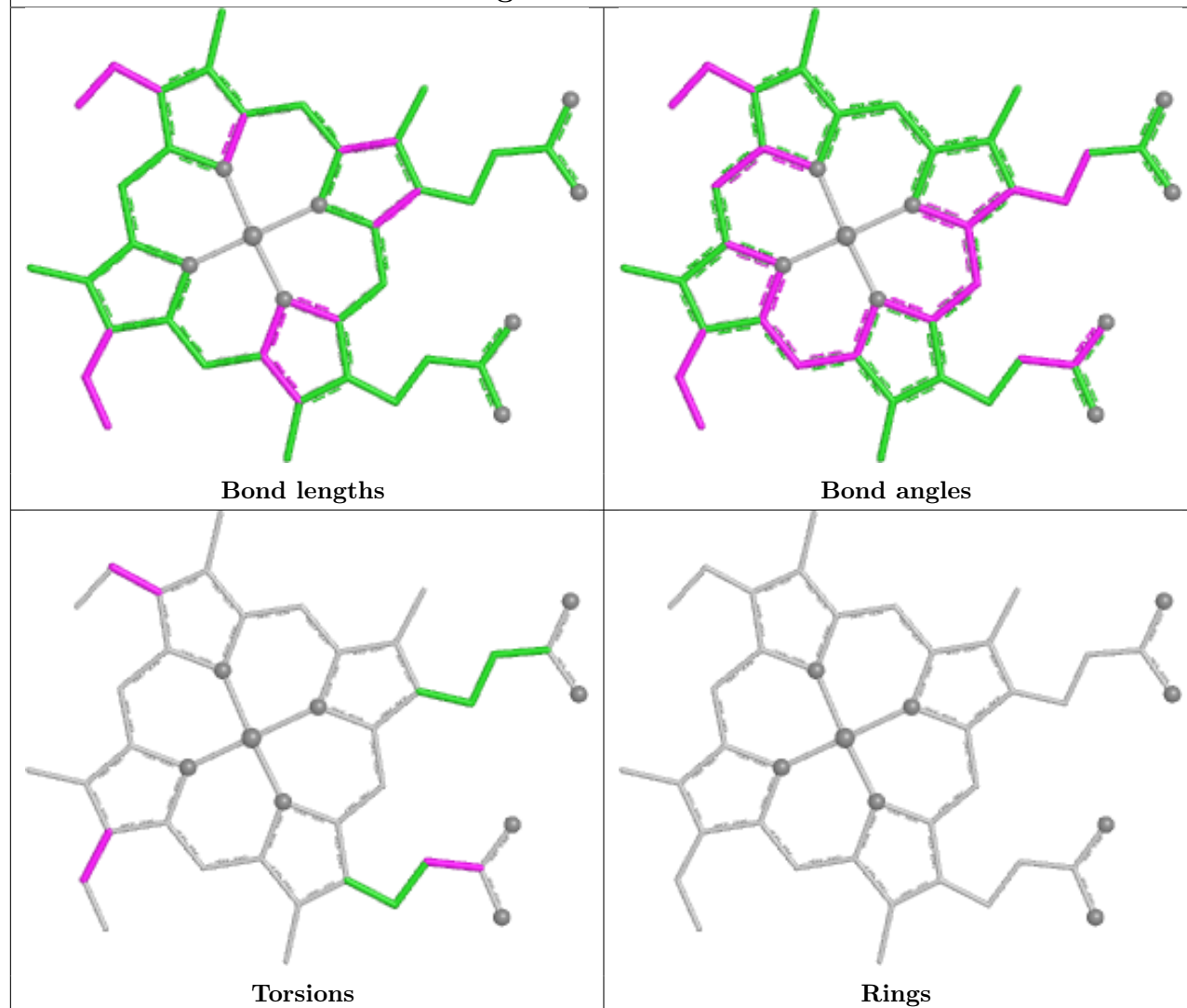
Ligand LHG D 413



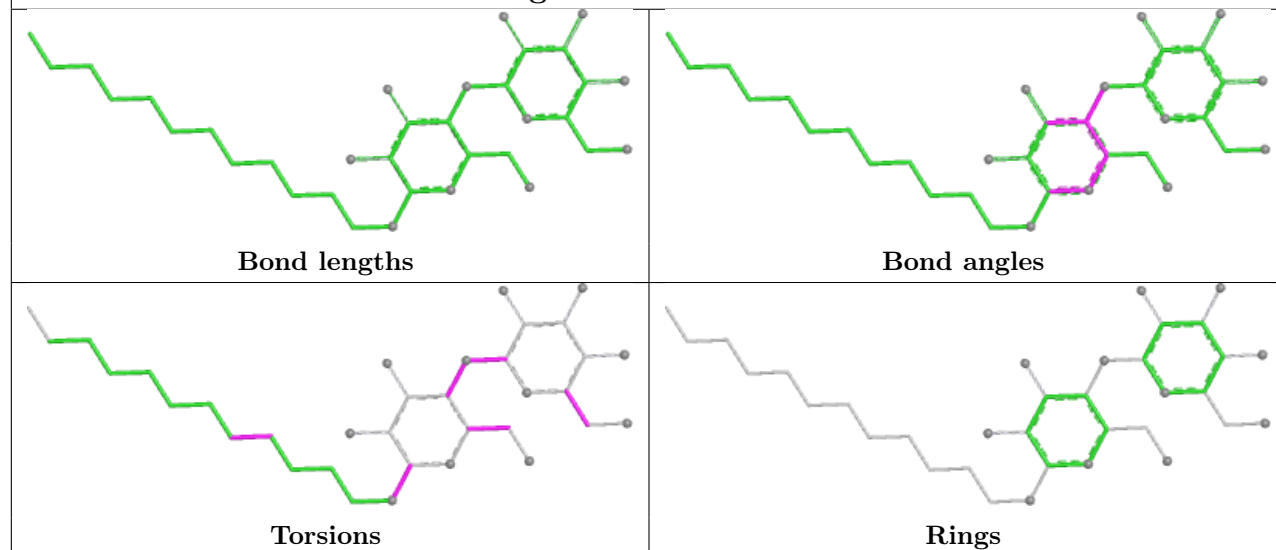


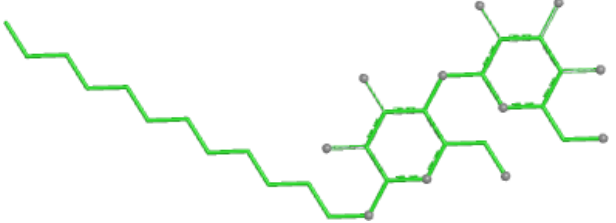
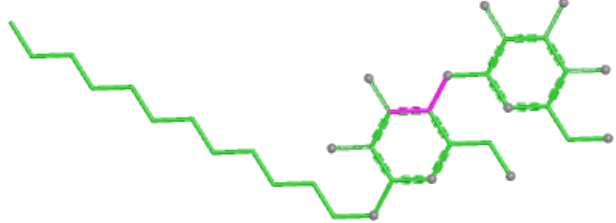
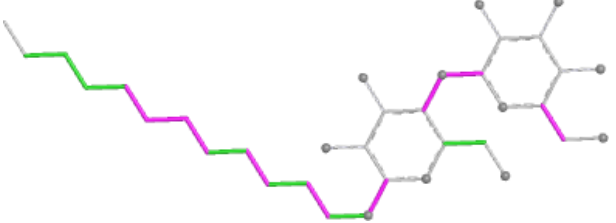
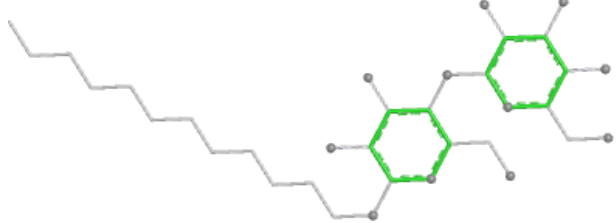
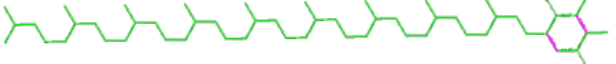
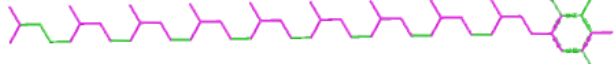
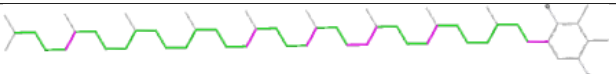
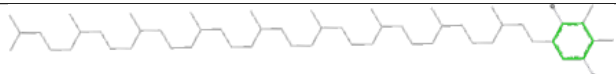
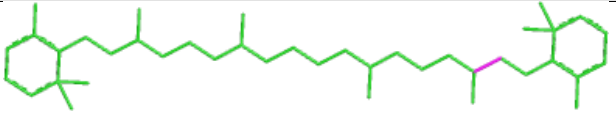
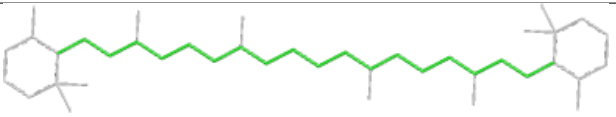
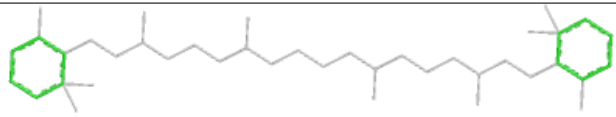


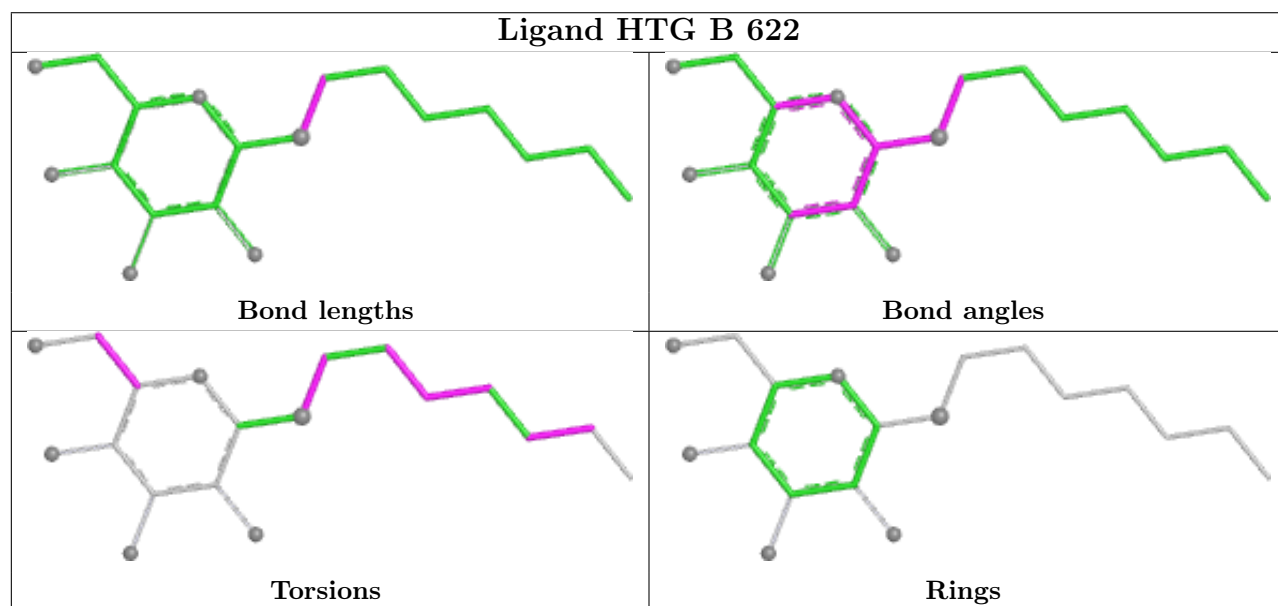
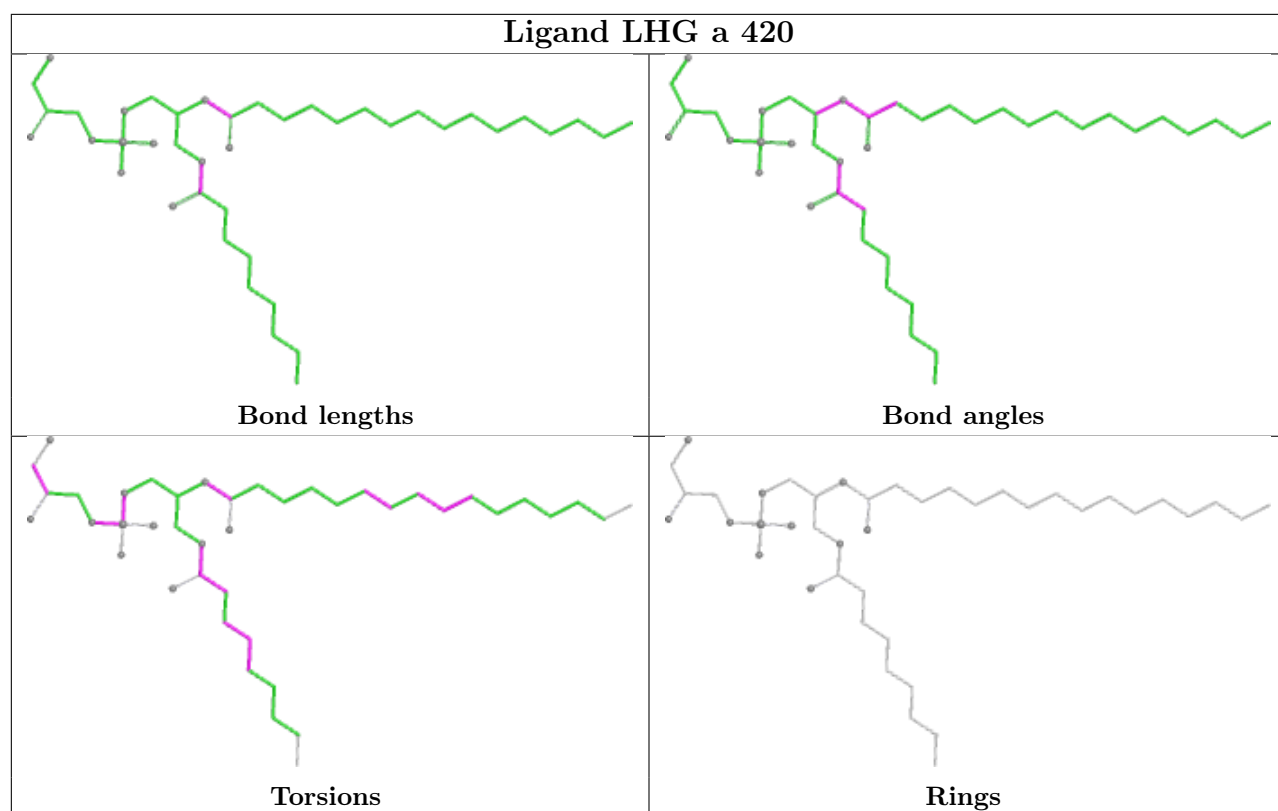
Ligand HEC v 205

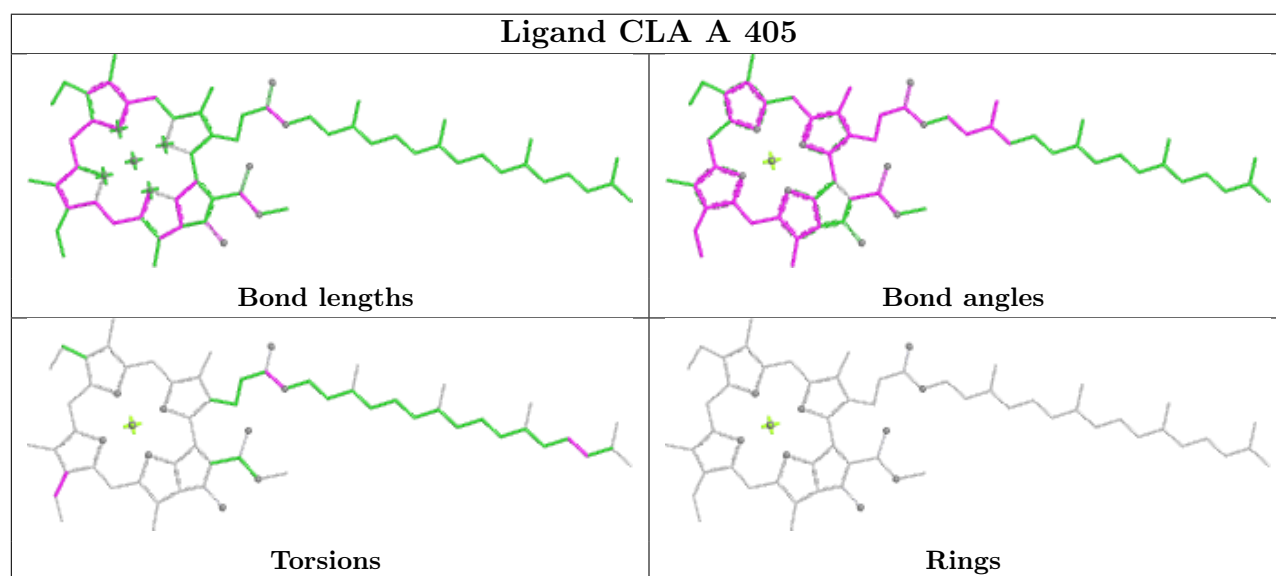
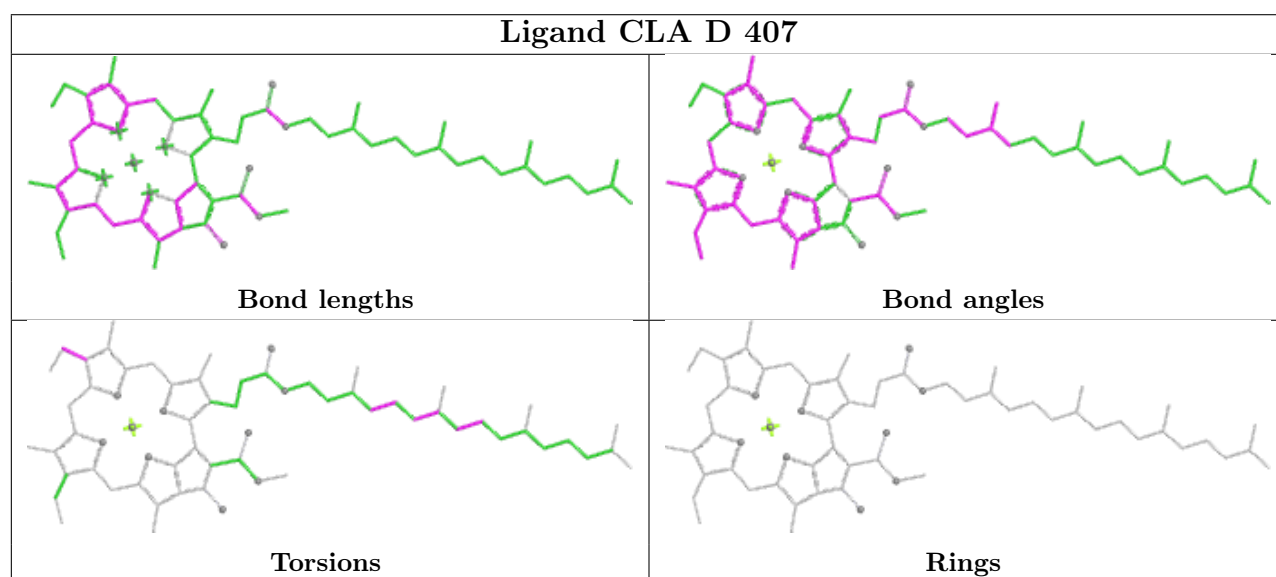
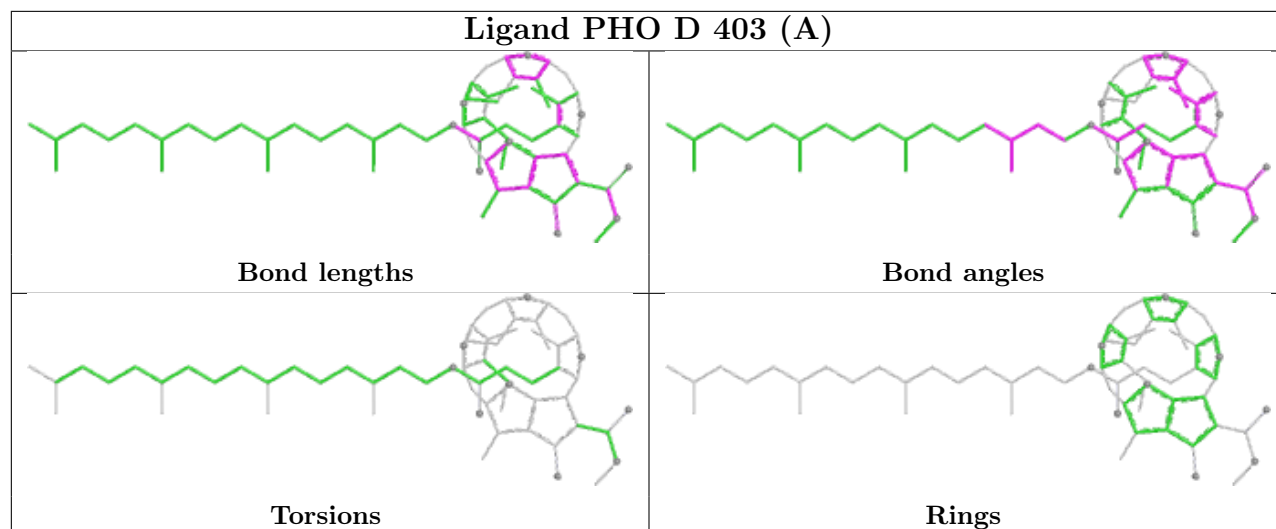


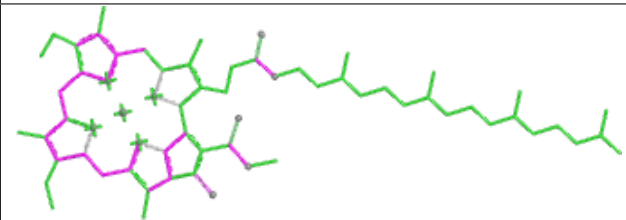
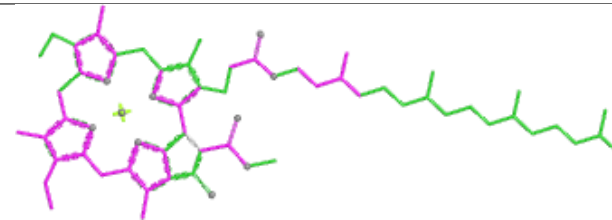
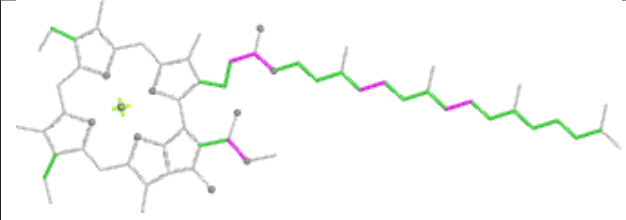
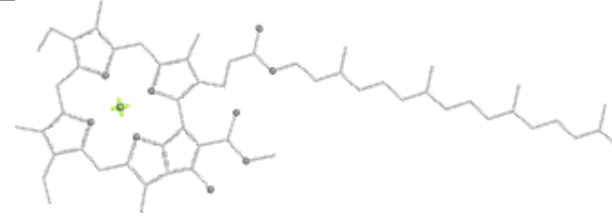
Ligand LMT C 521

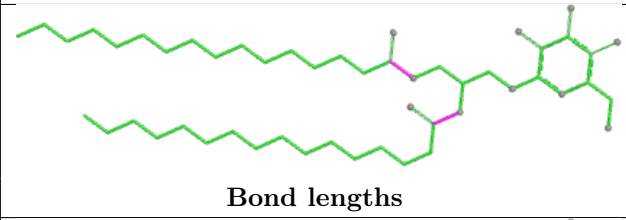
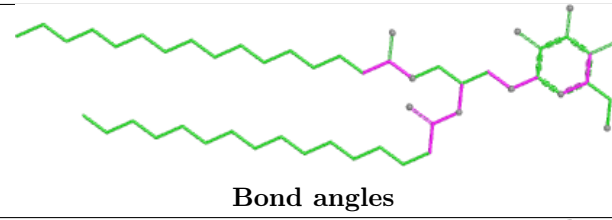
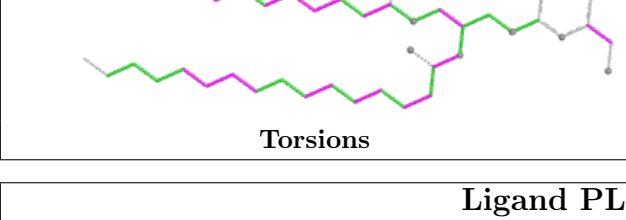


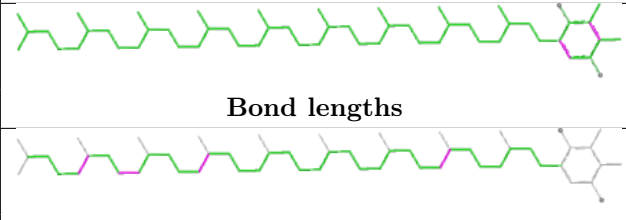
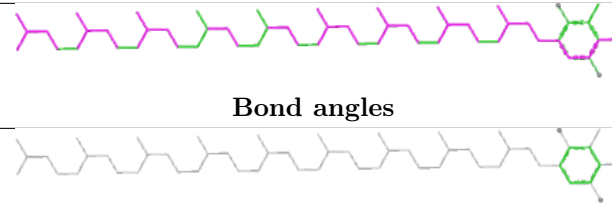
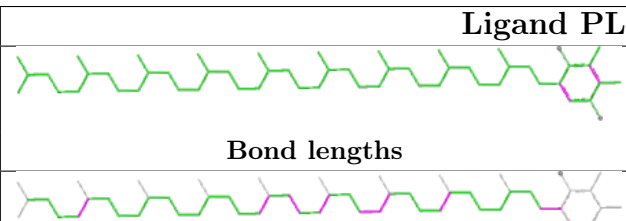
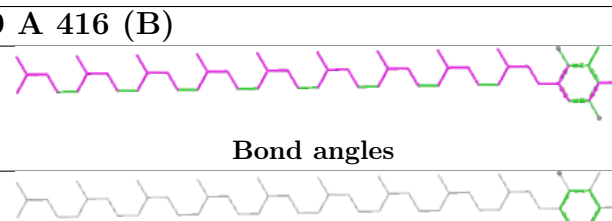
Ligand LMT D 405	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 A 416 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

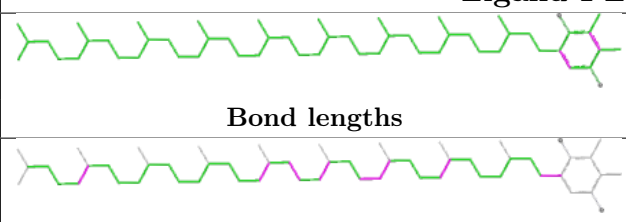
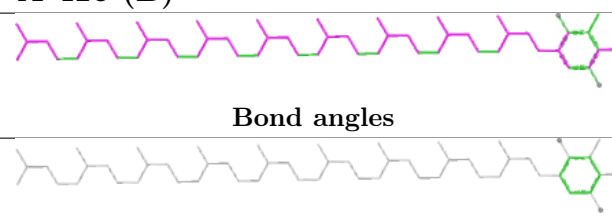
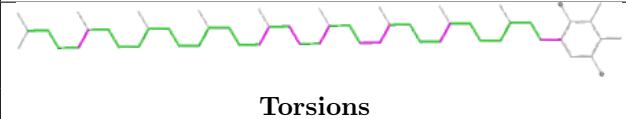
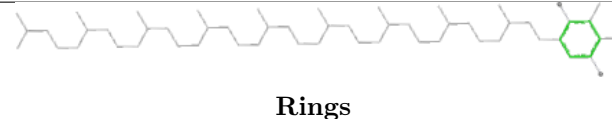


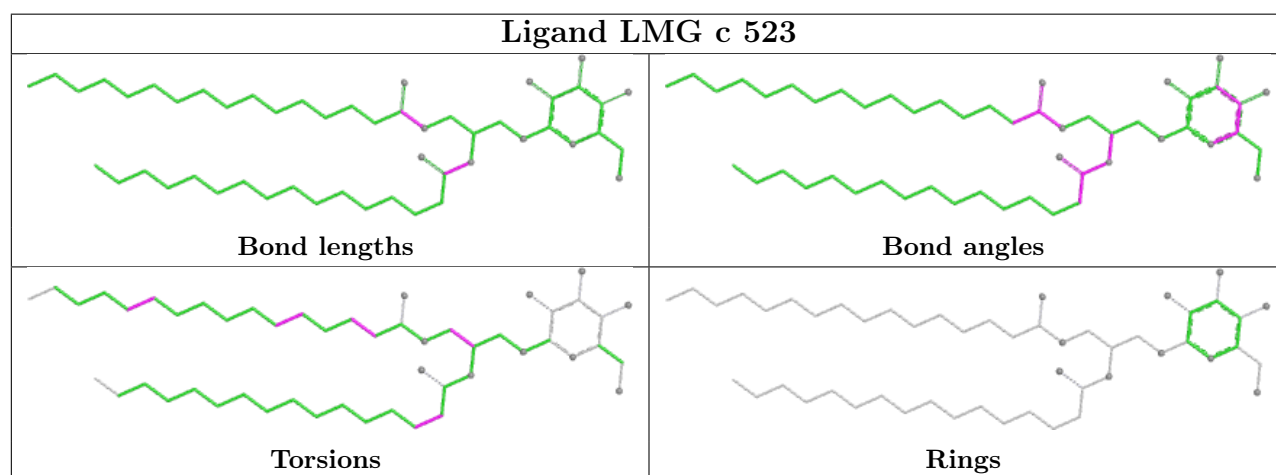
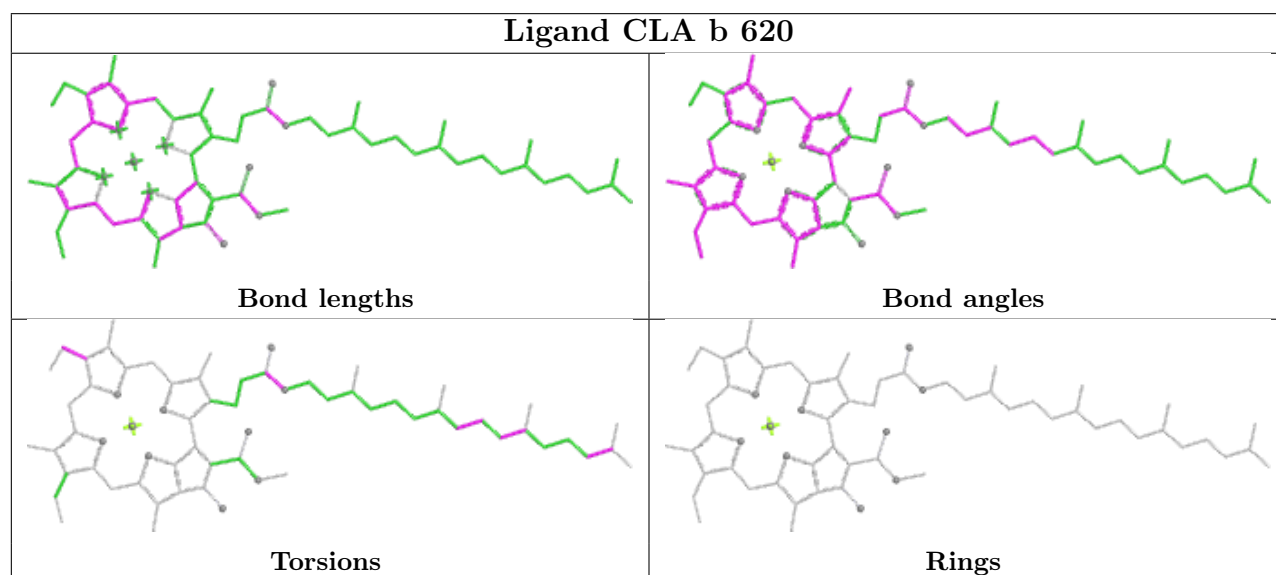
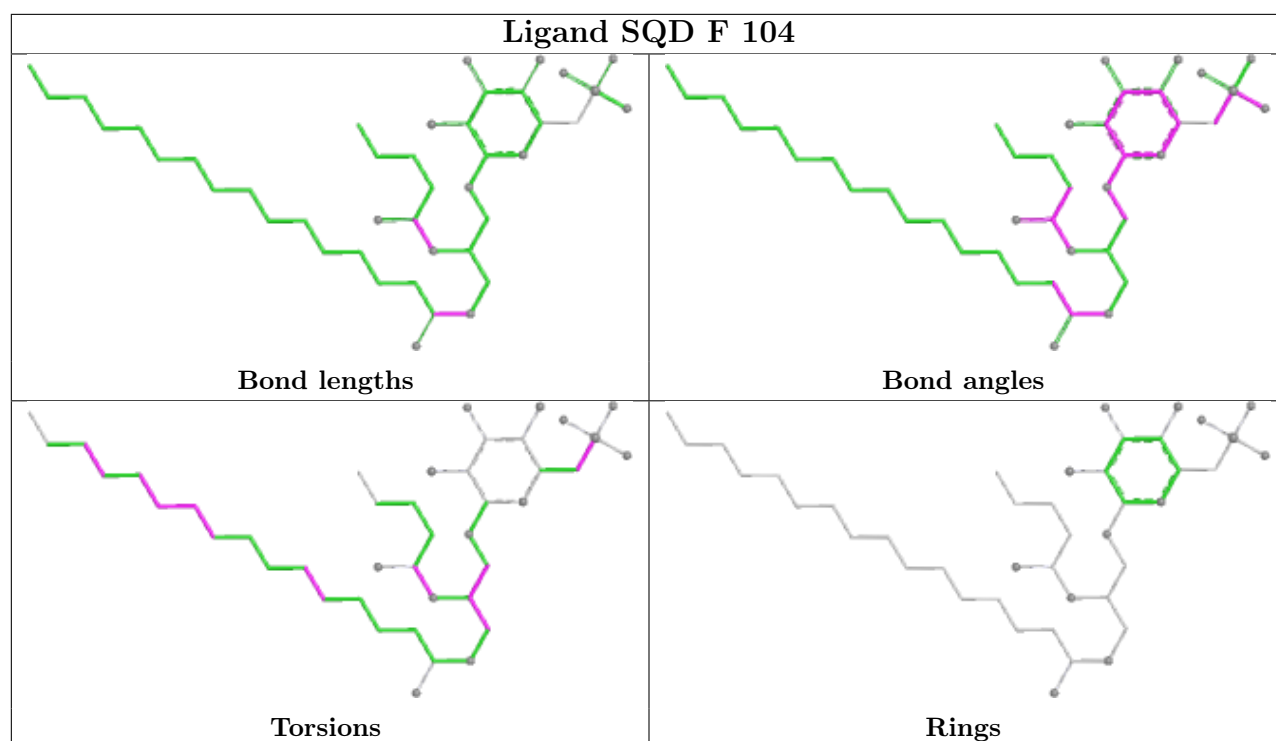


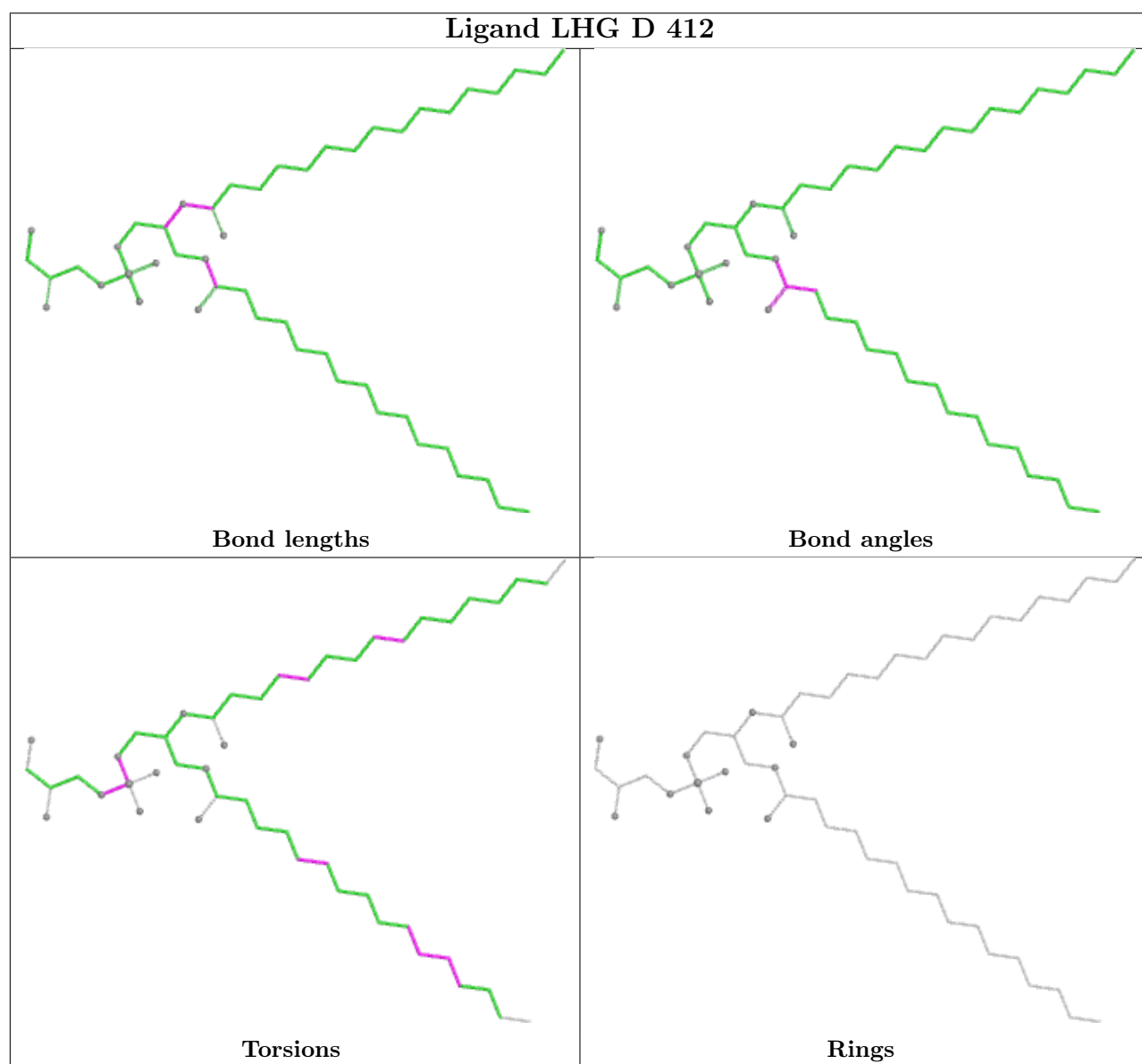
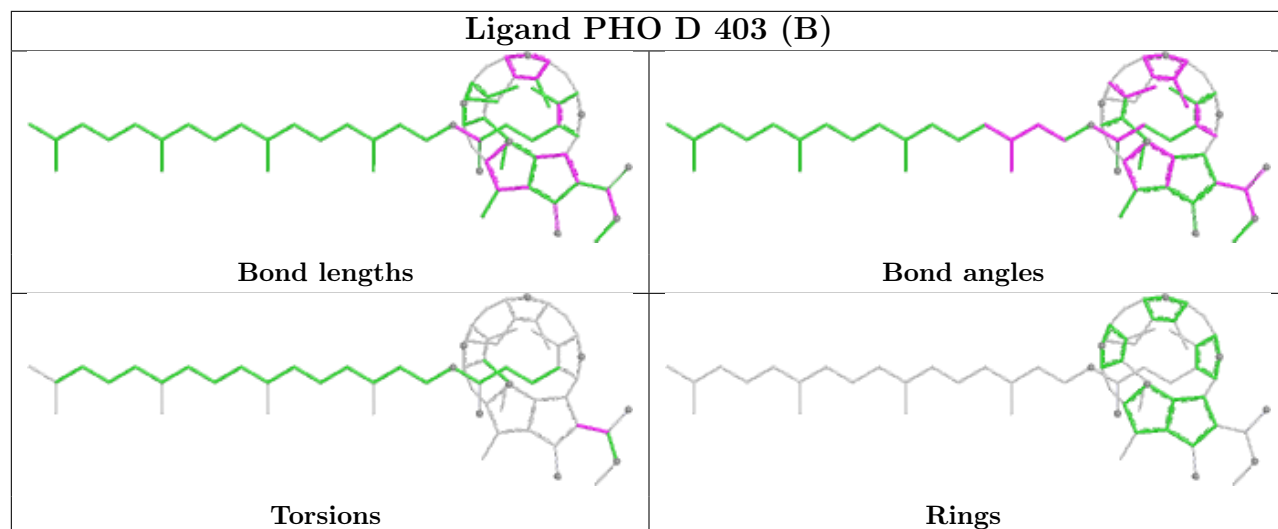
Ligand CLA B 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

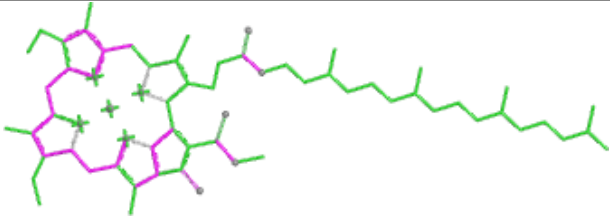
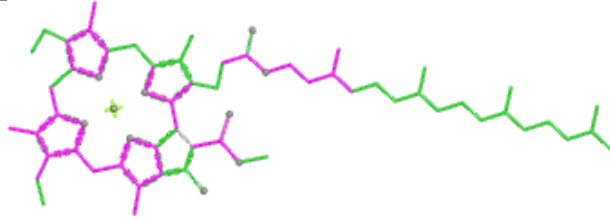
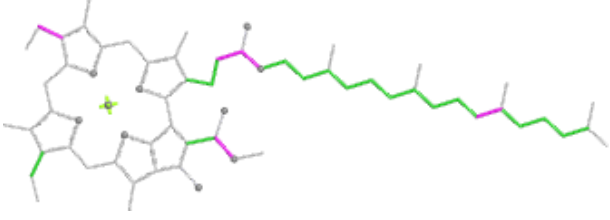
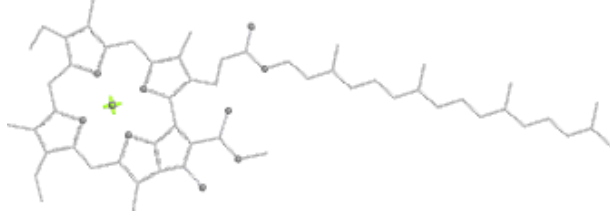
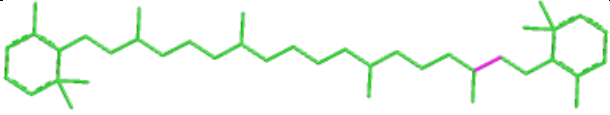
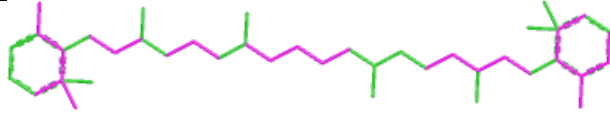
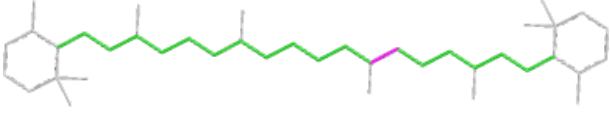
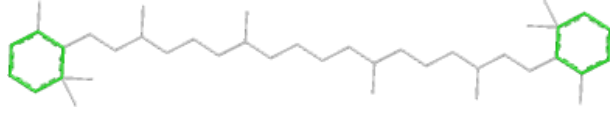
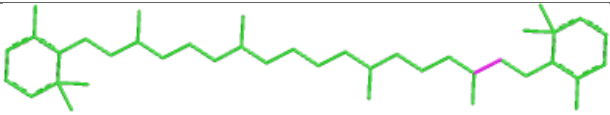
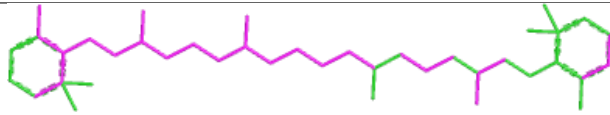
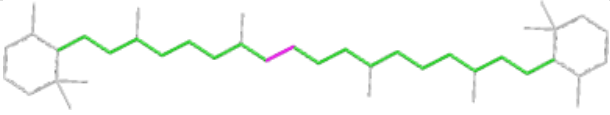
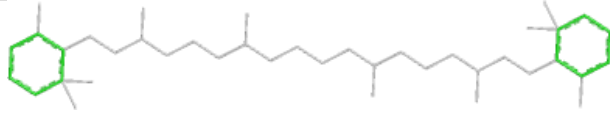
Ligand LMG a 415	
	
Bond lengths	Bond angles
	
Torsions	Rings

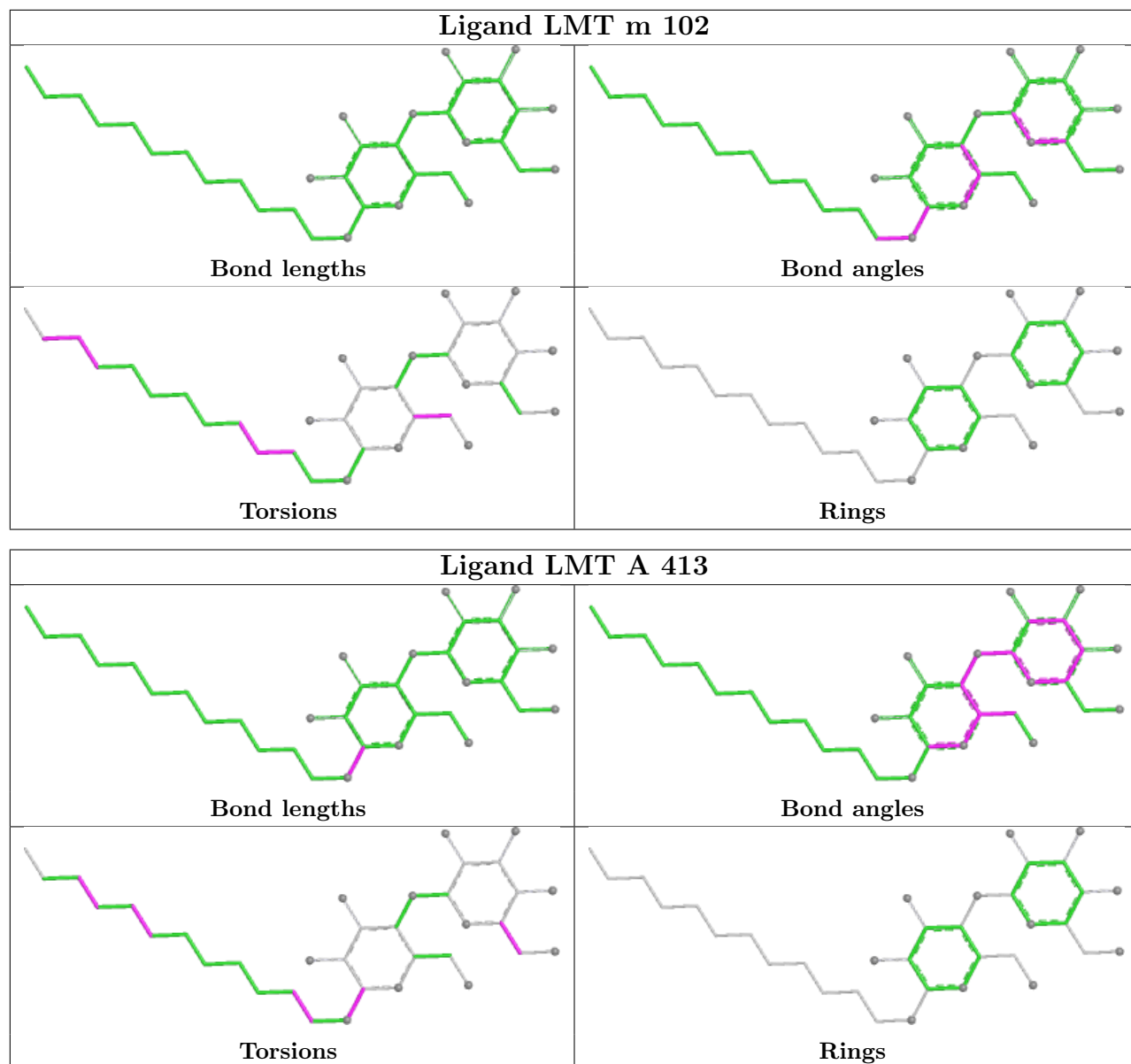
Ligand PL9 D 409 (B)	
	
Bond lengths	Bond angles
	
Torsions	Rings

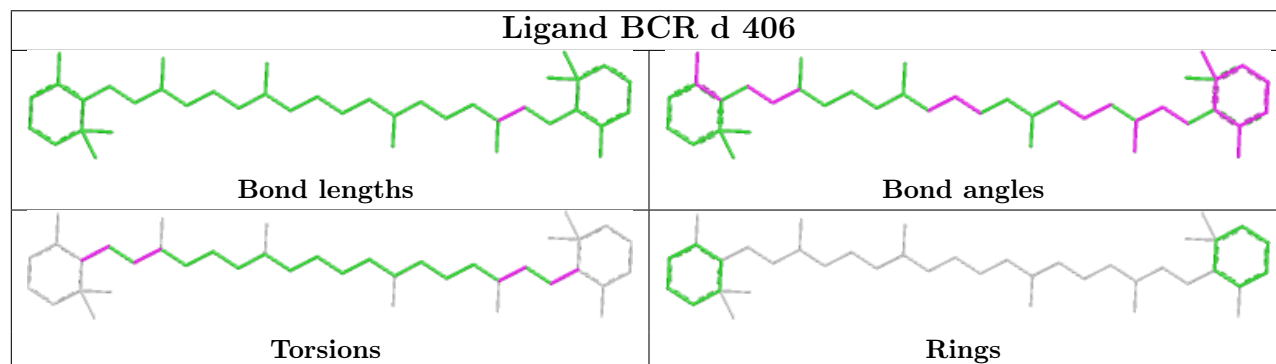
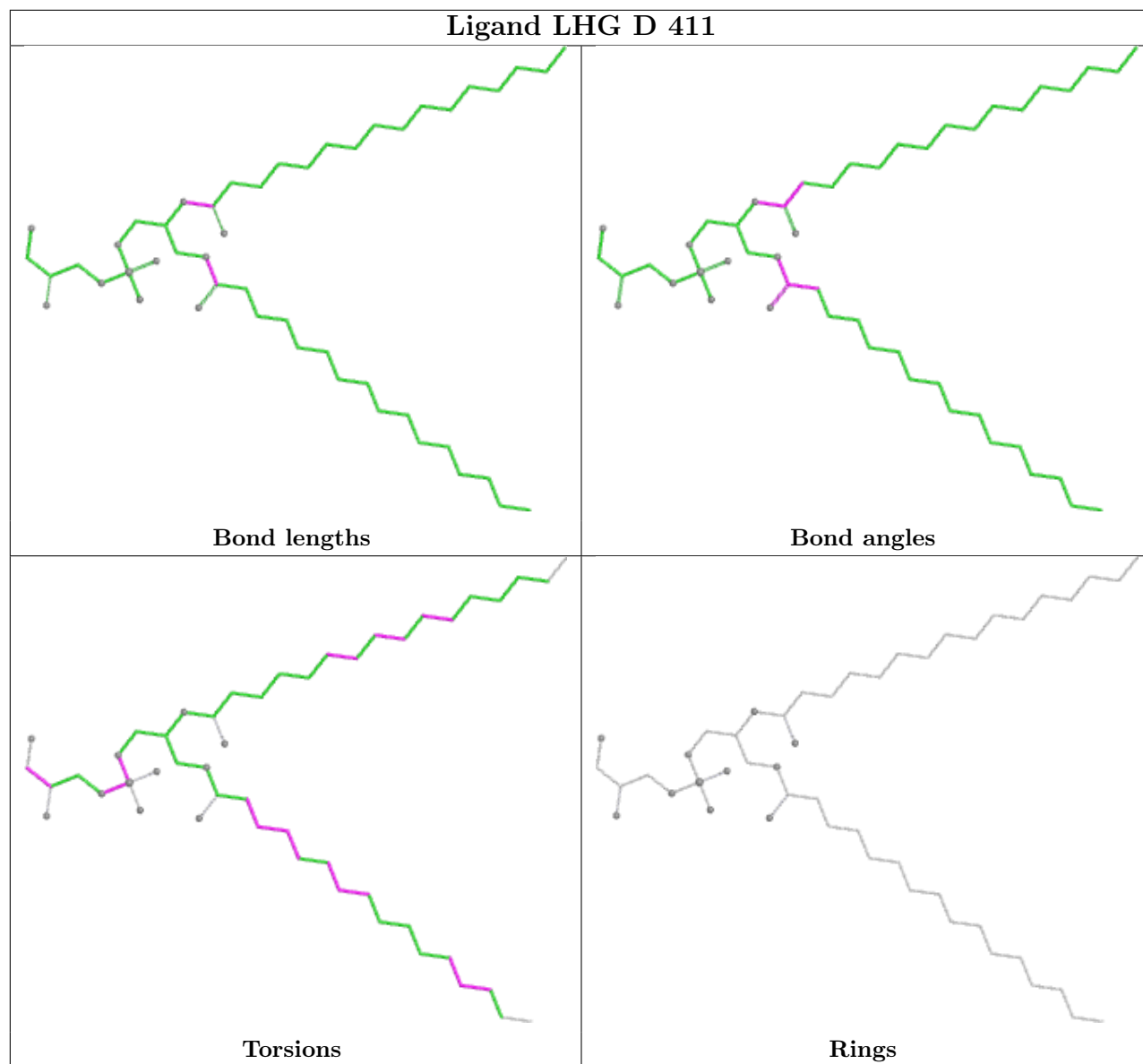
Ligand PL9 A 416 (B)	
	
Bond lengths	Bond angles
	
Torsions	Rings



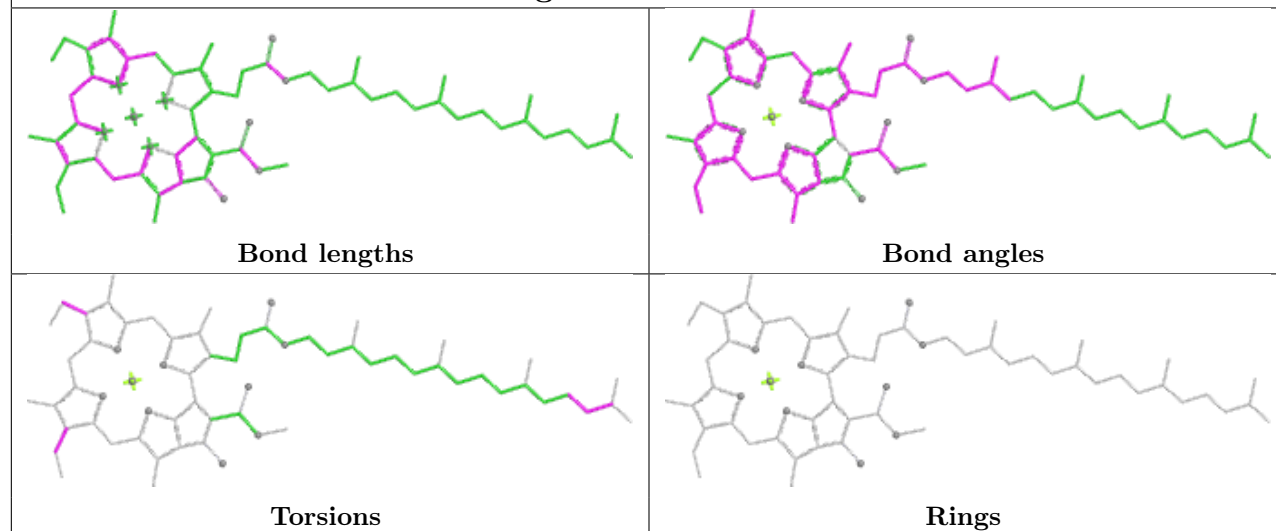


Ligand CLA C 506	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR K 103	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR T 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

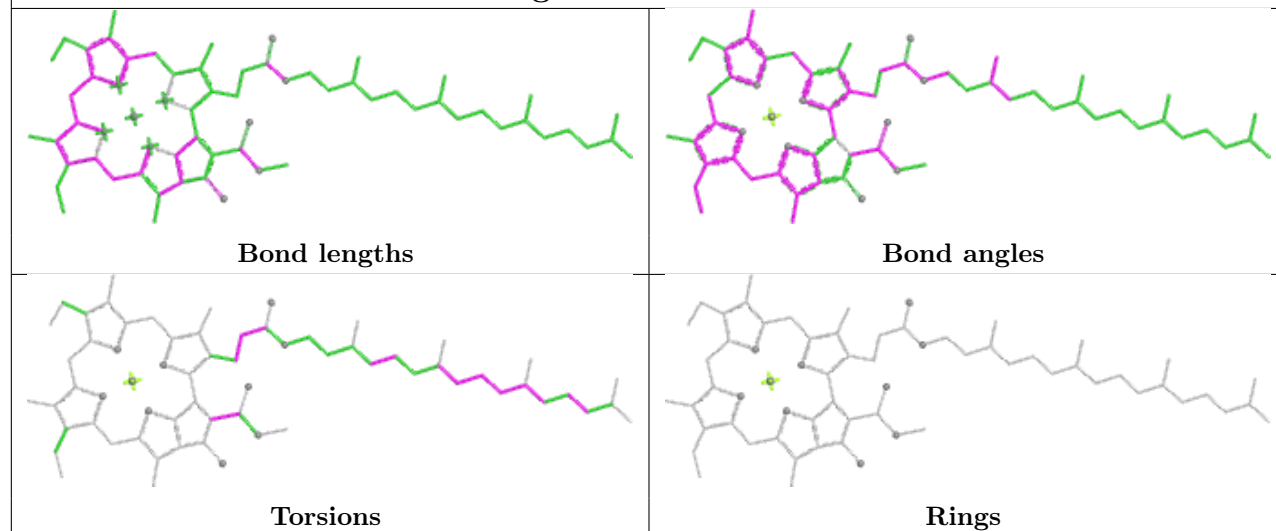




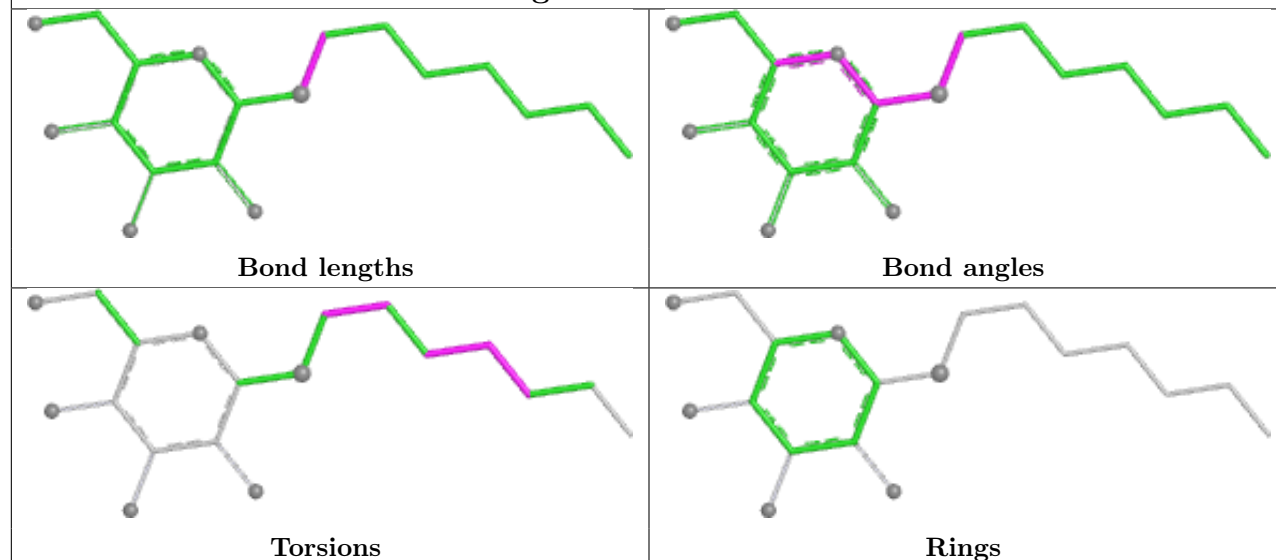
Ligand CLA d 403

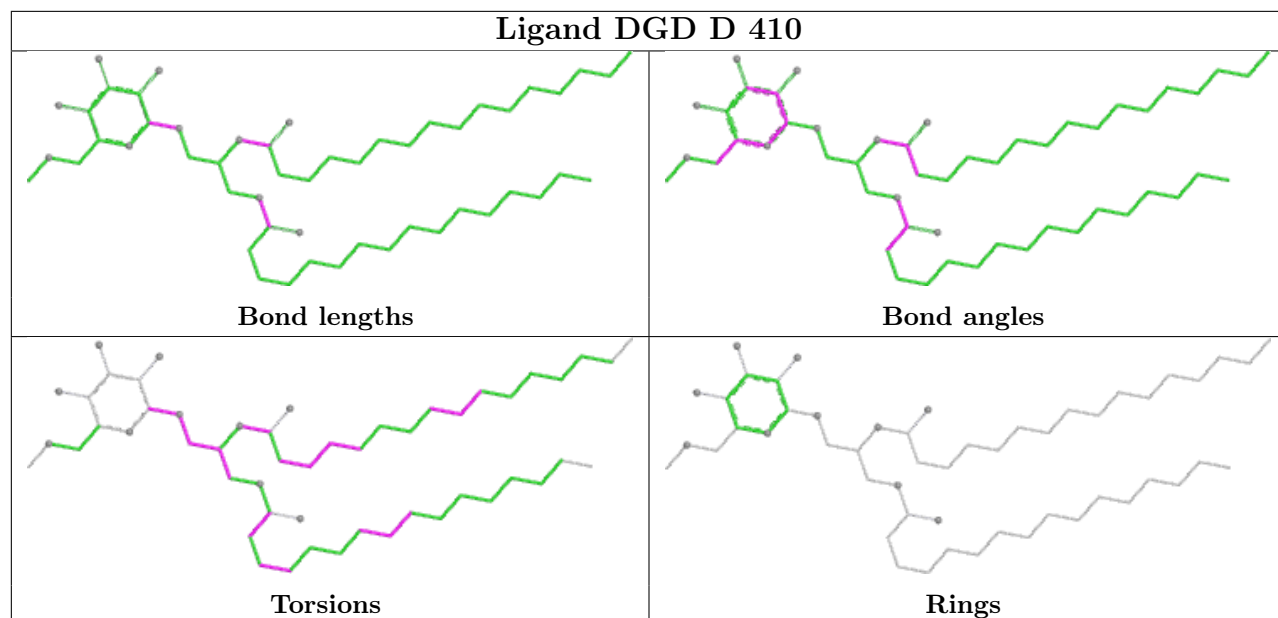


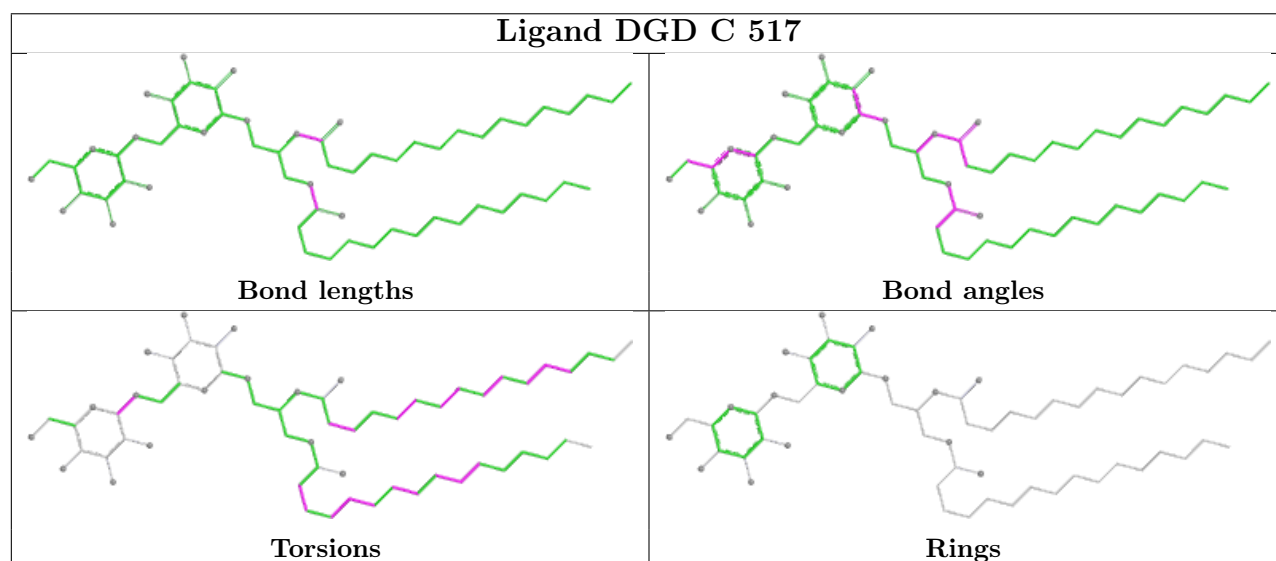
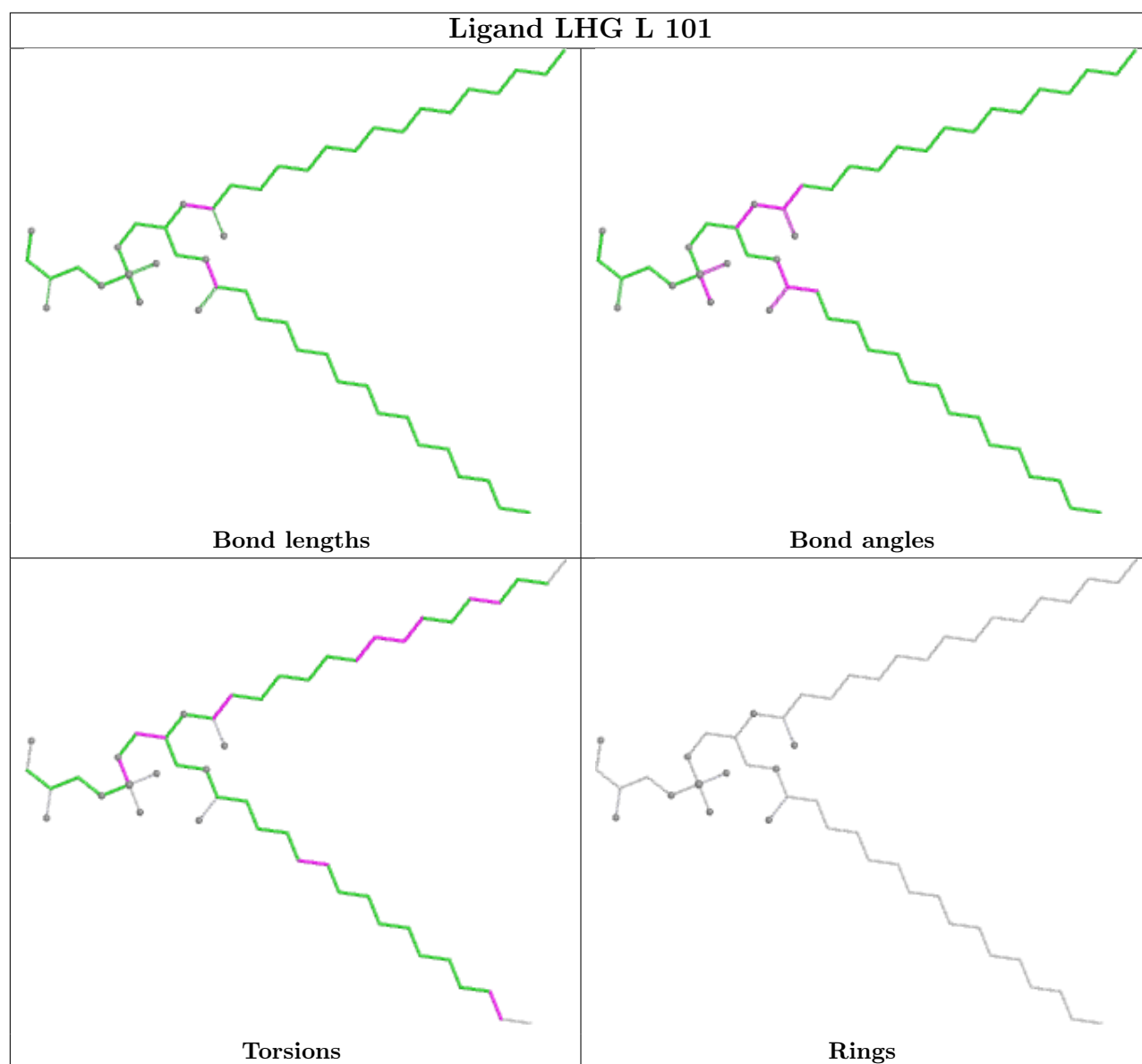
Ligand CLA B 602

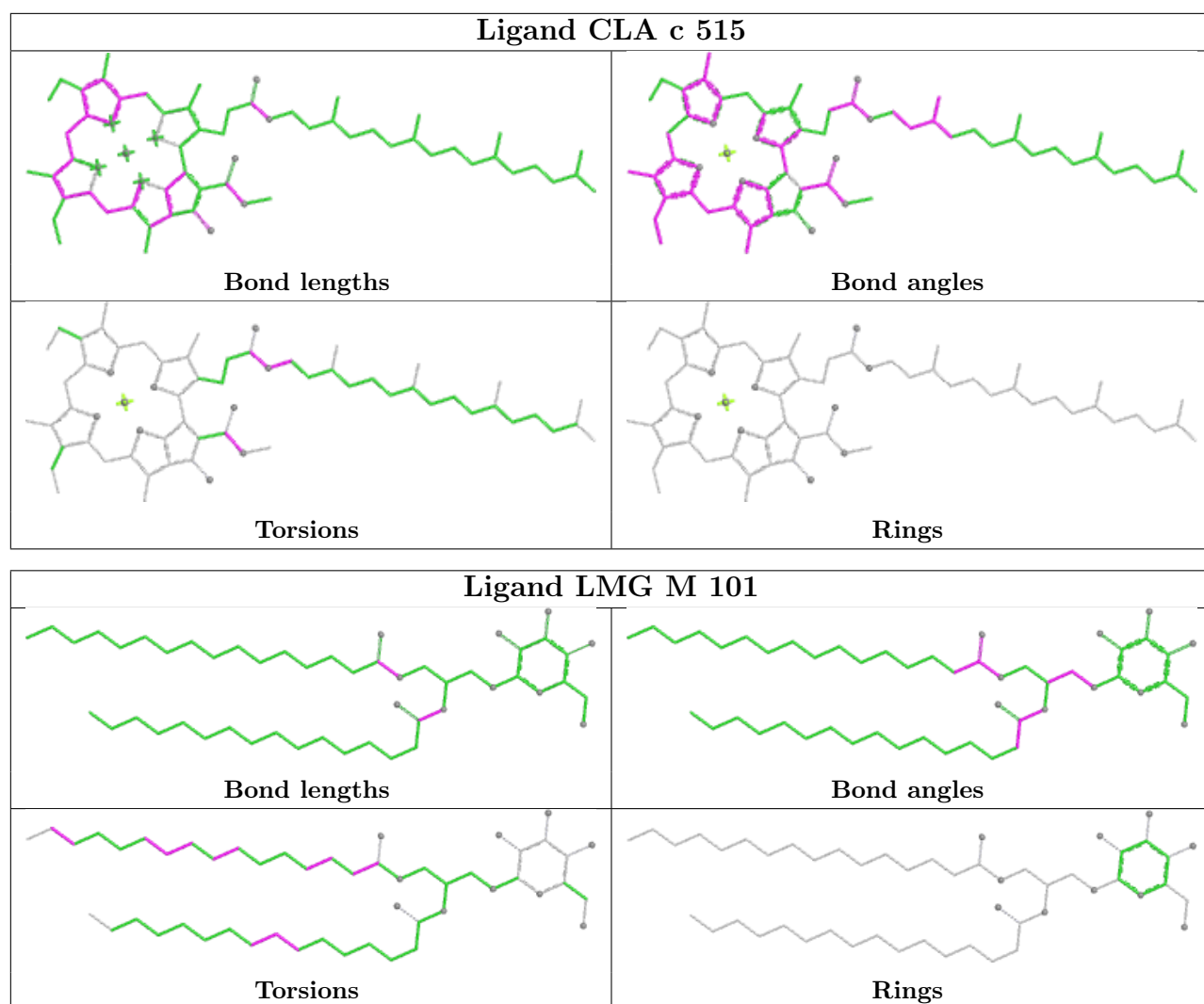


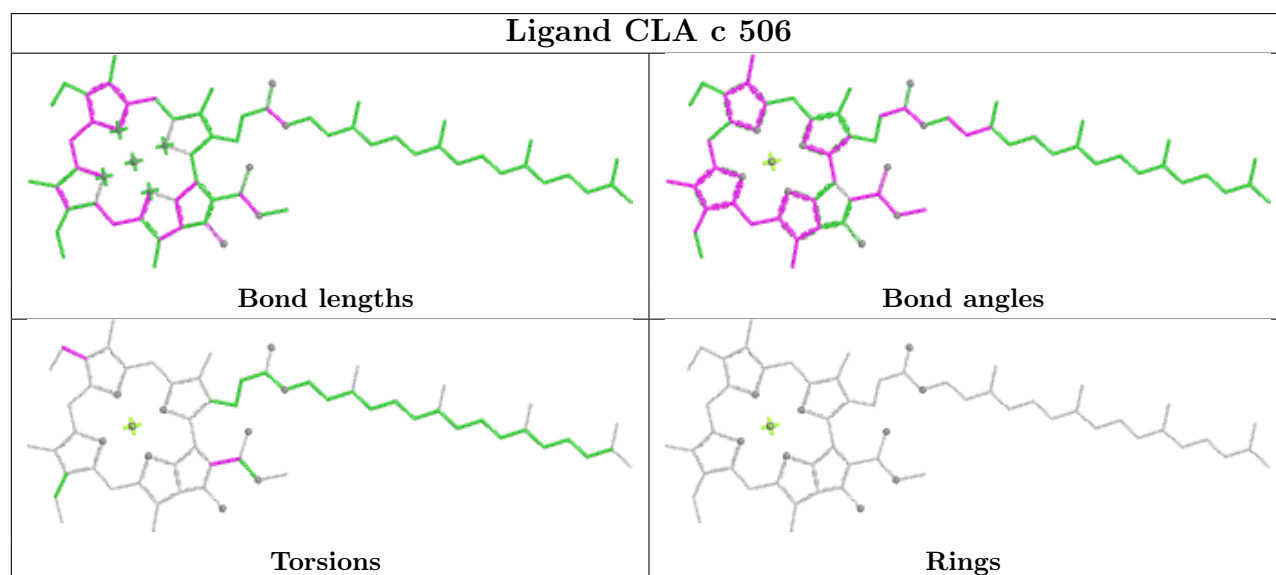
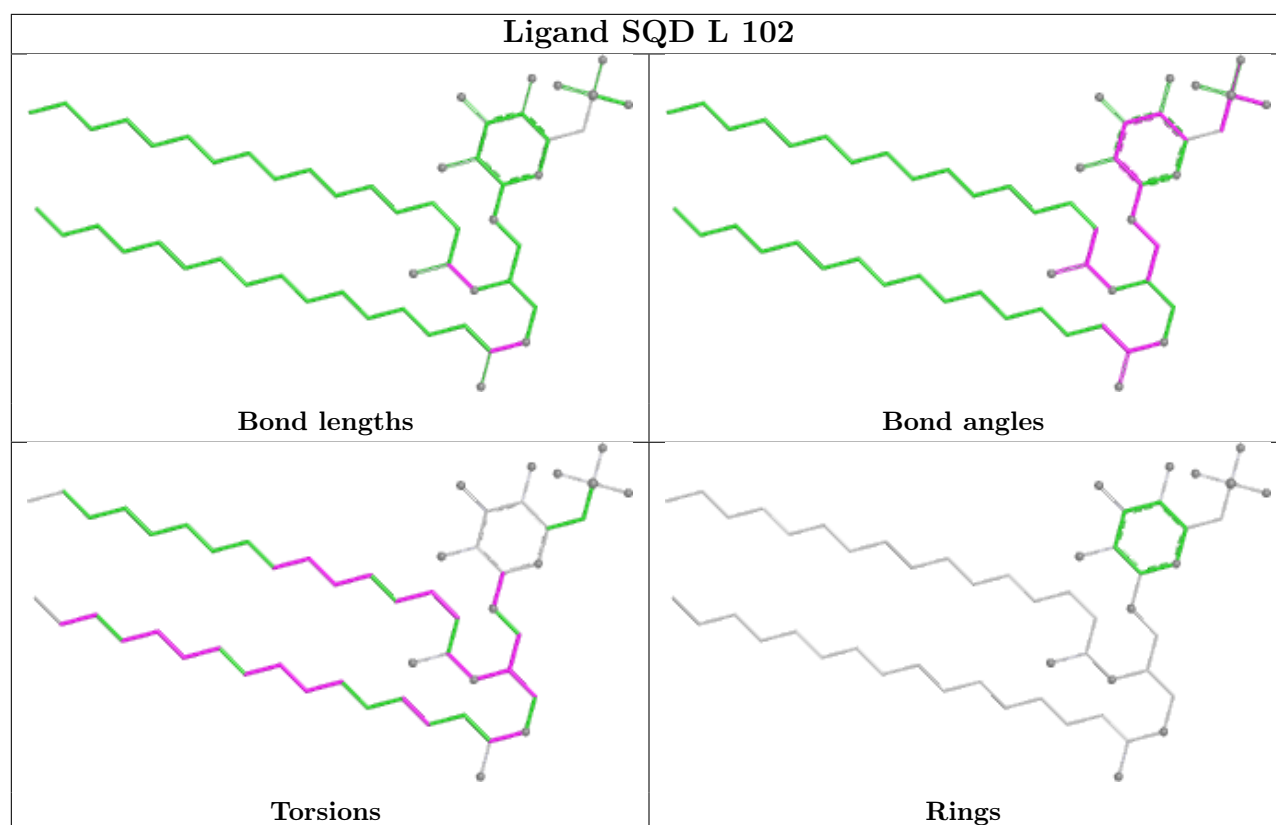
Ligand HTG b 601

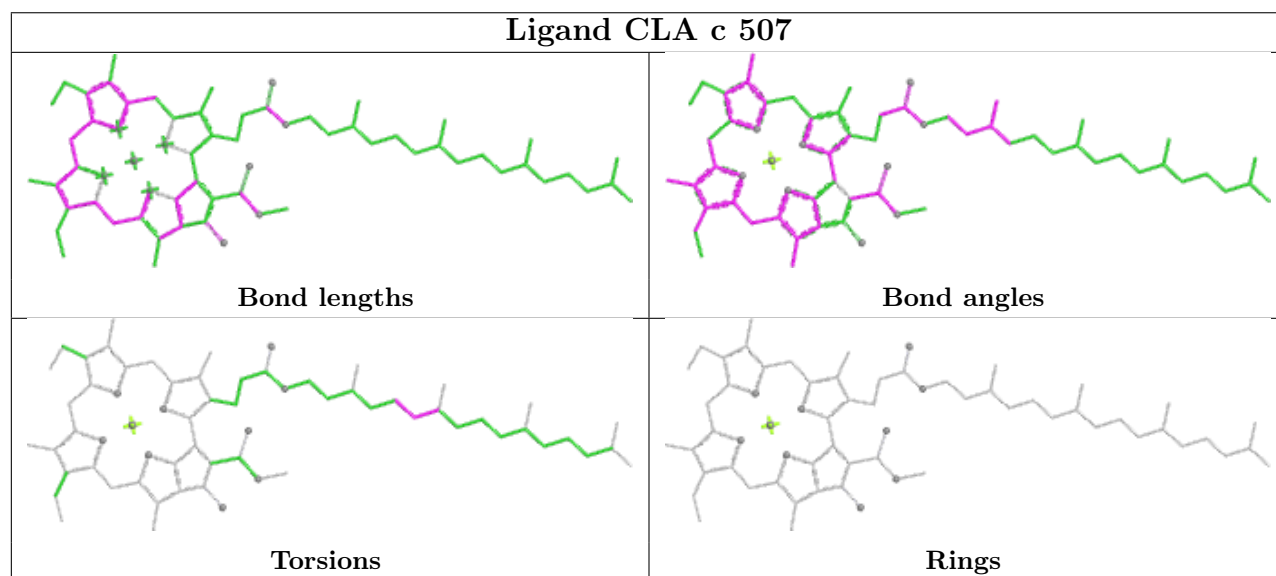
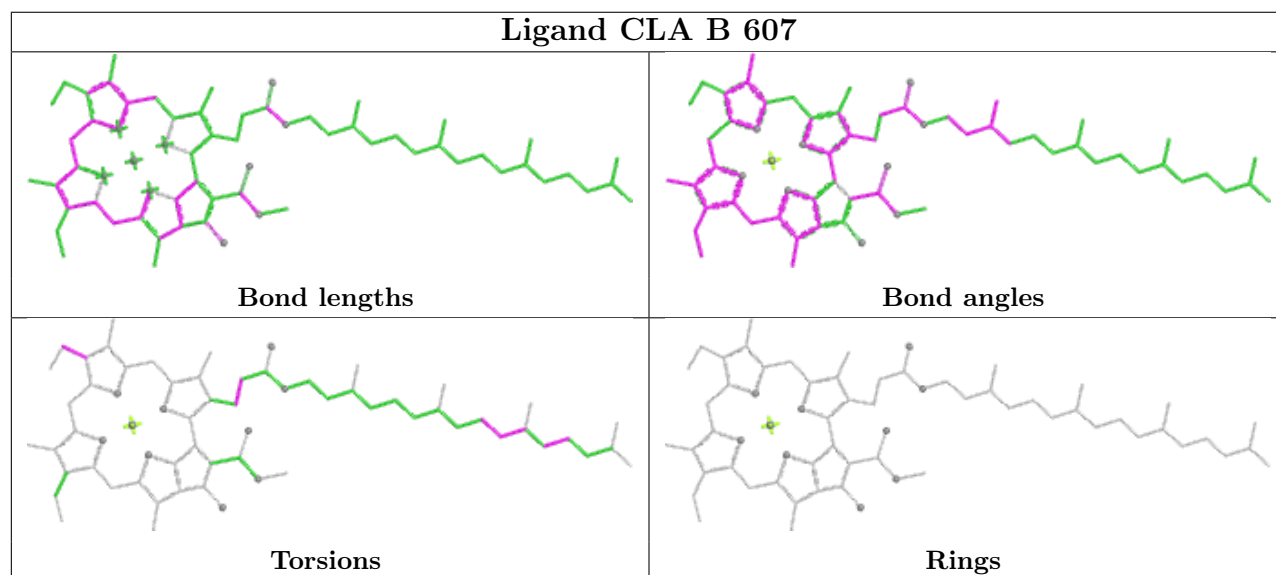
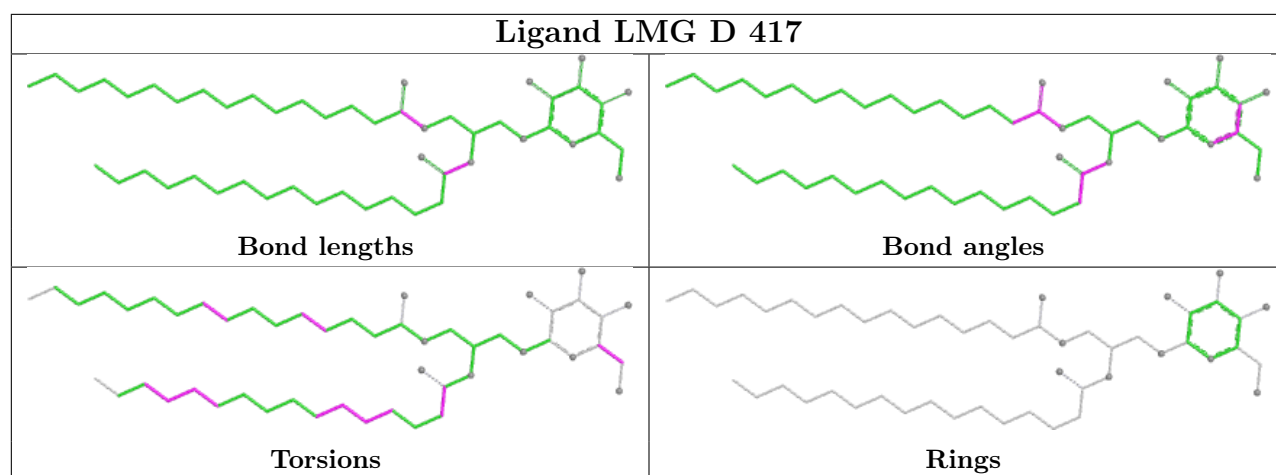


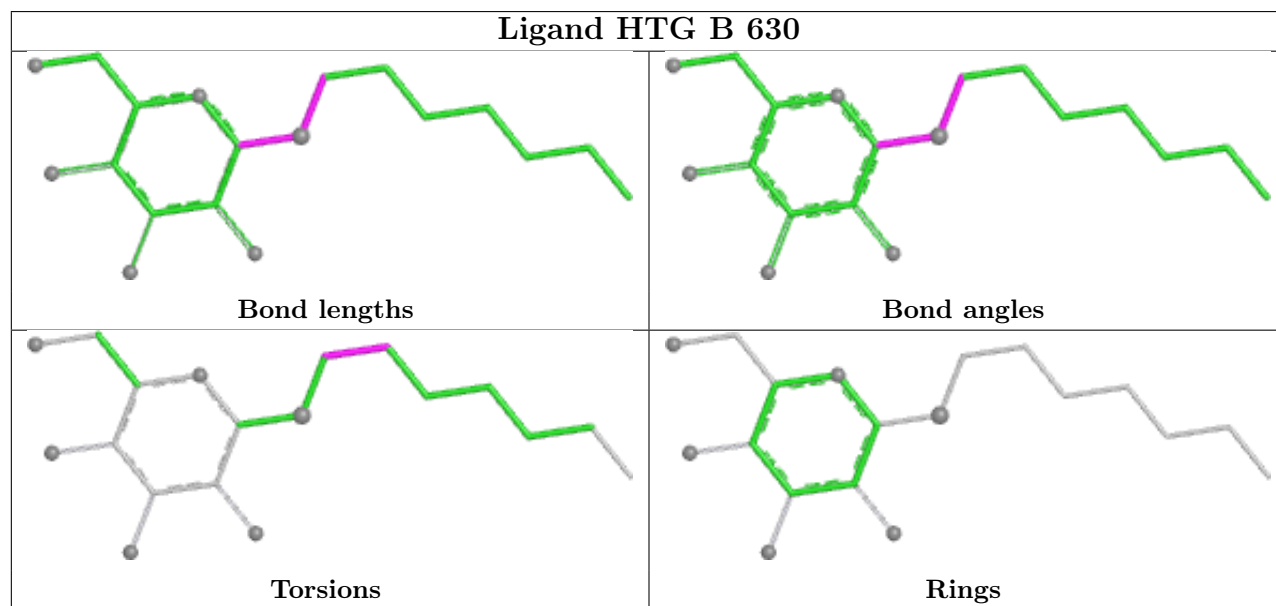
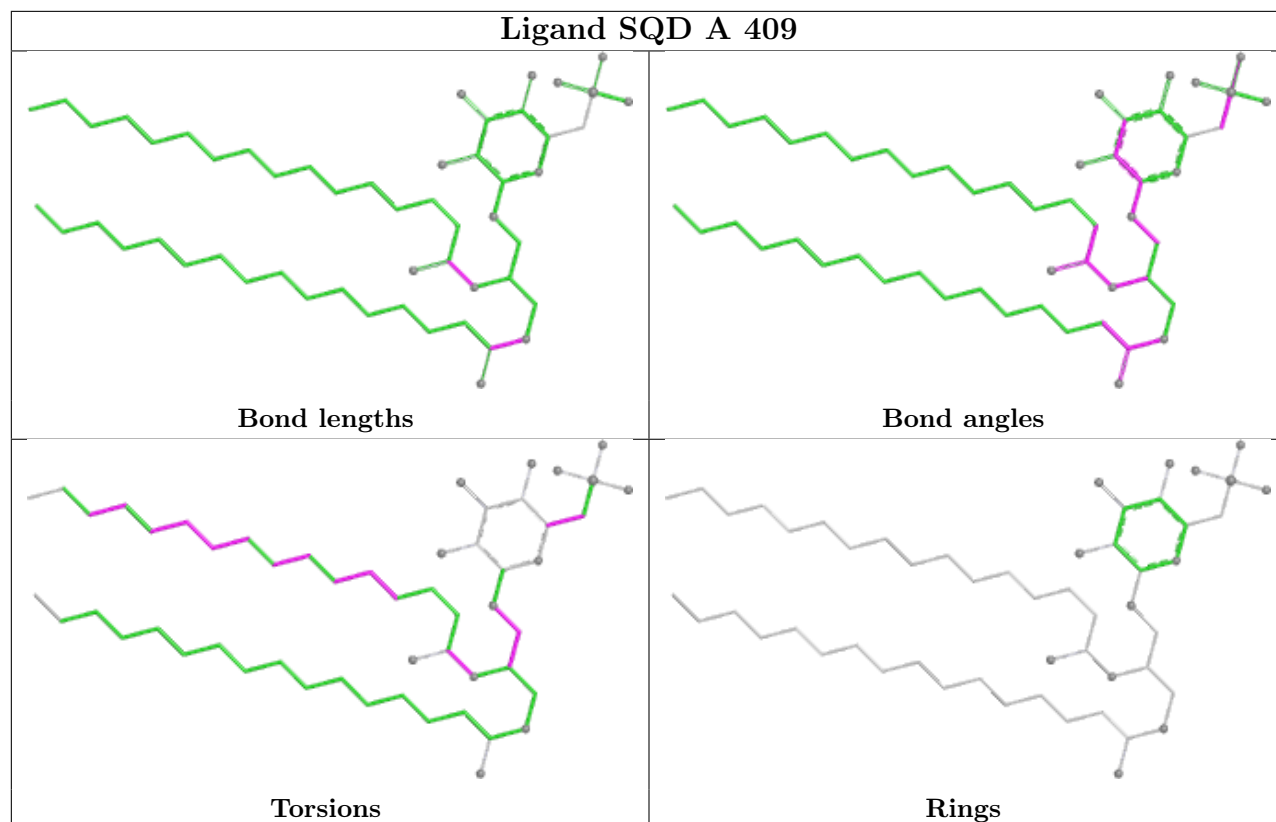


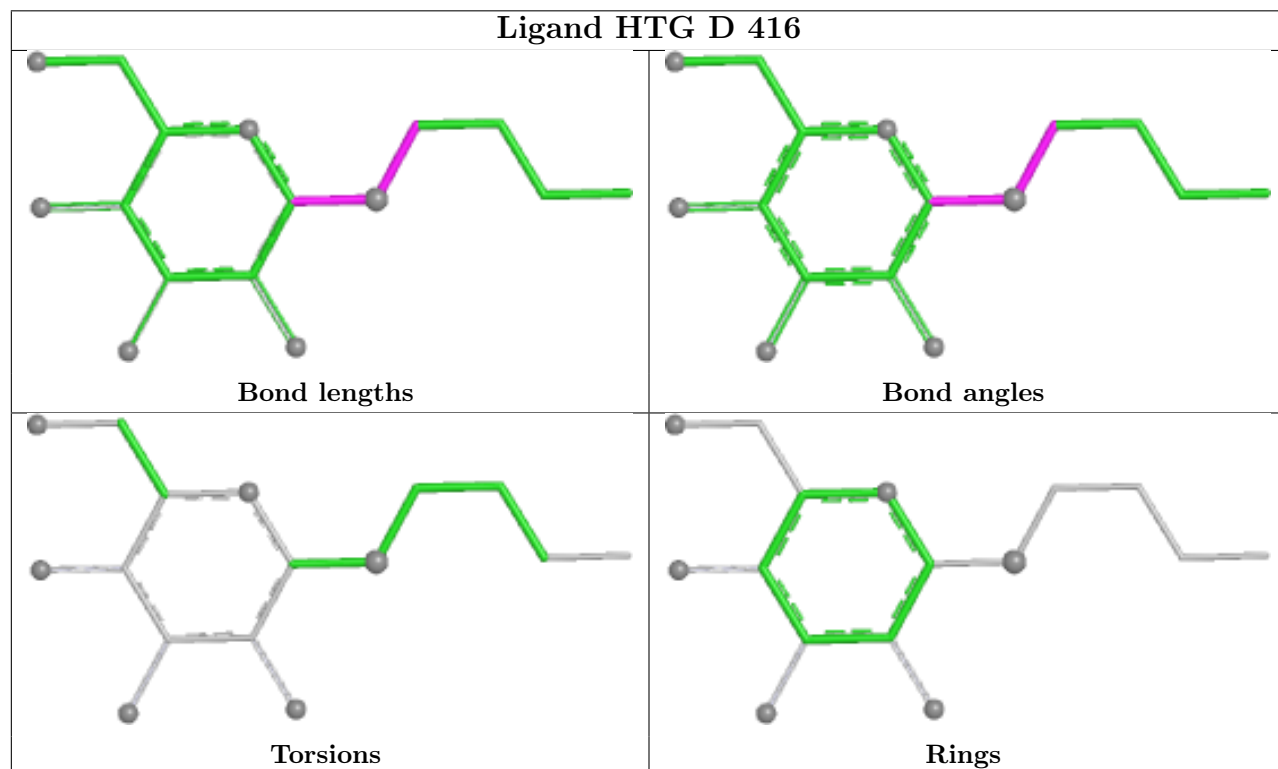
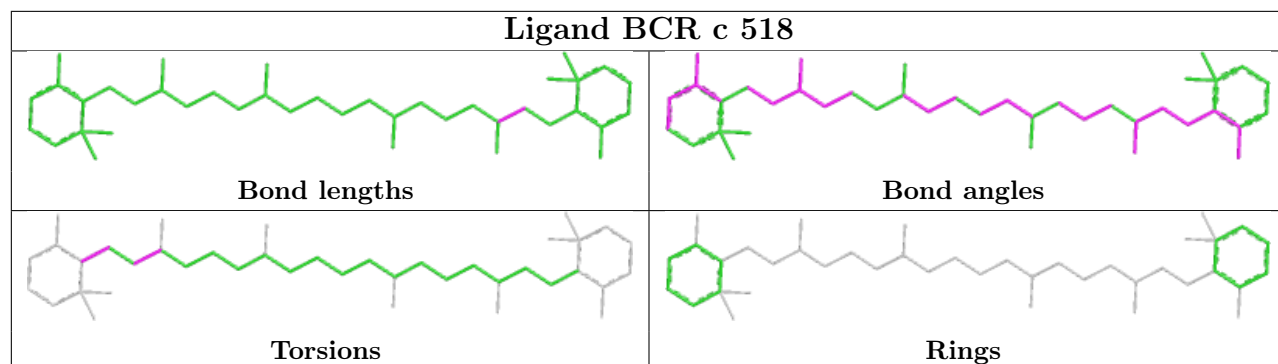


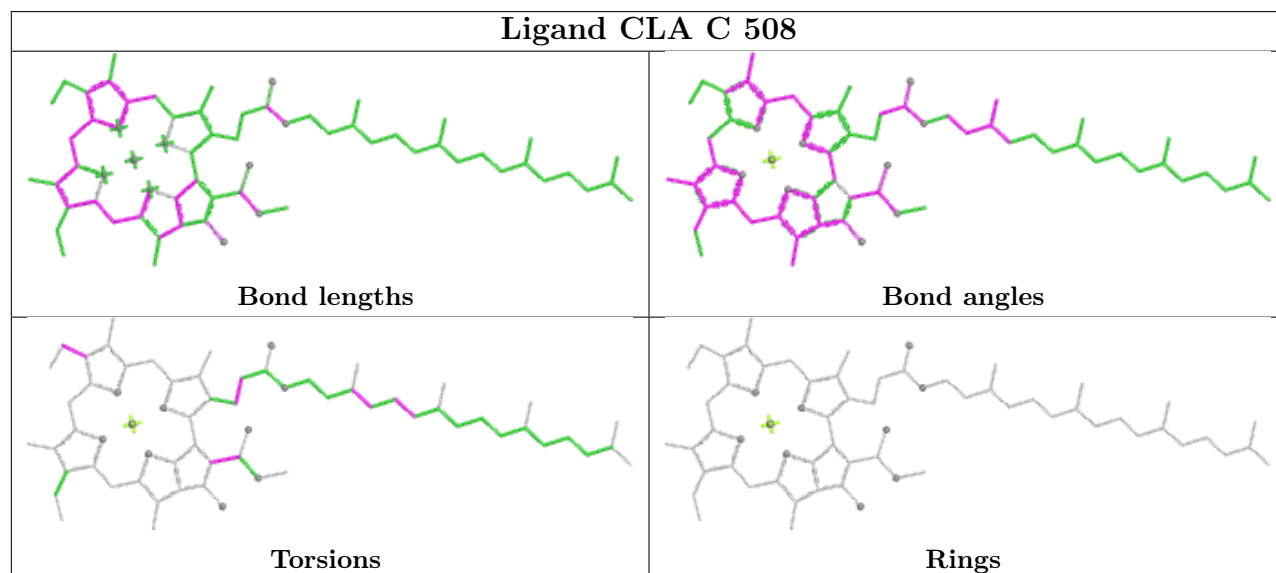
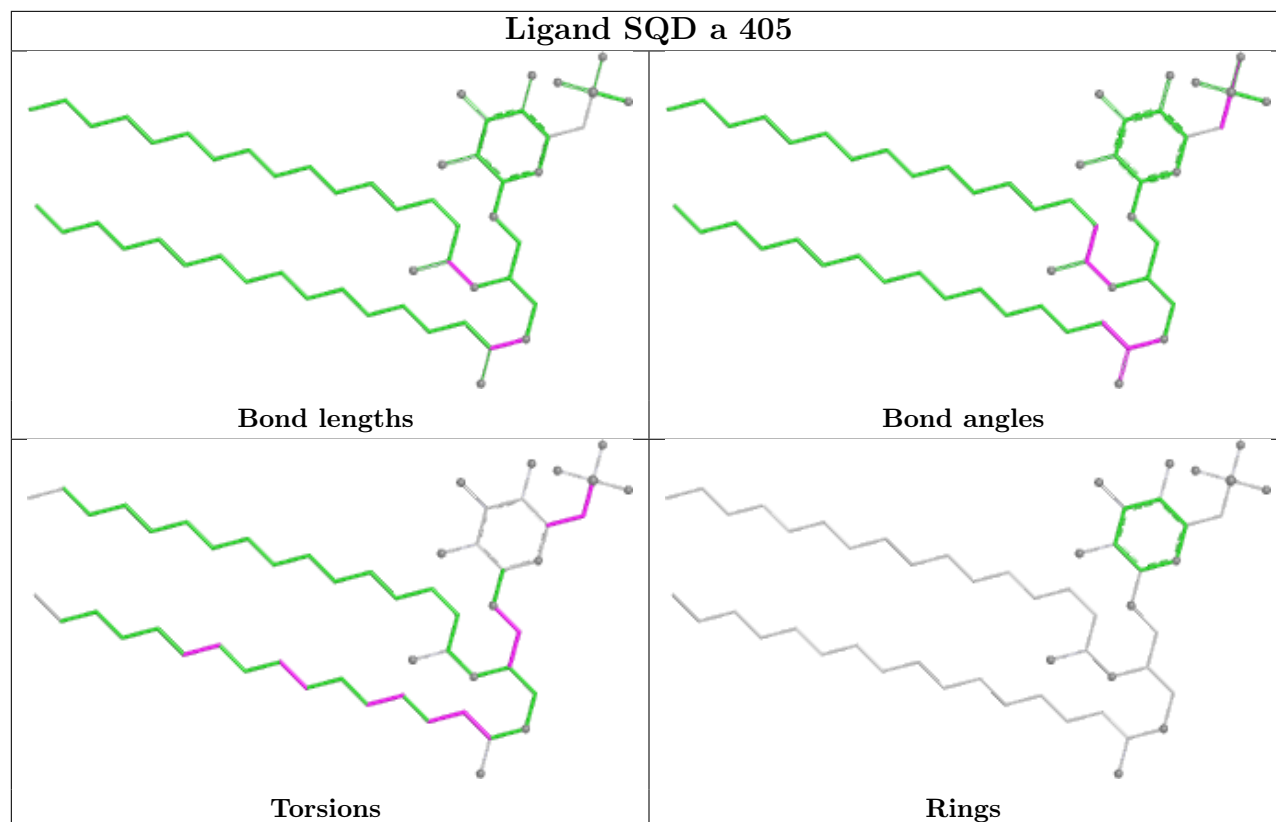


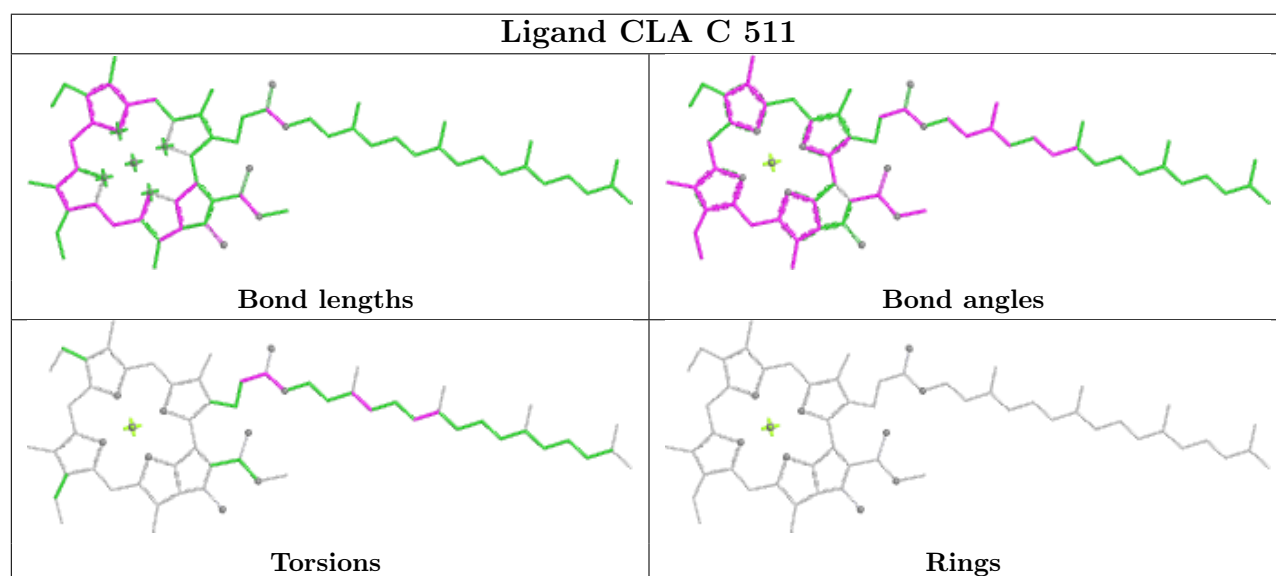
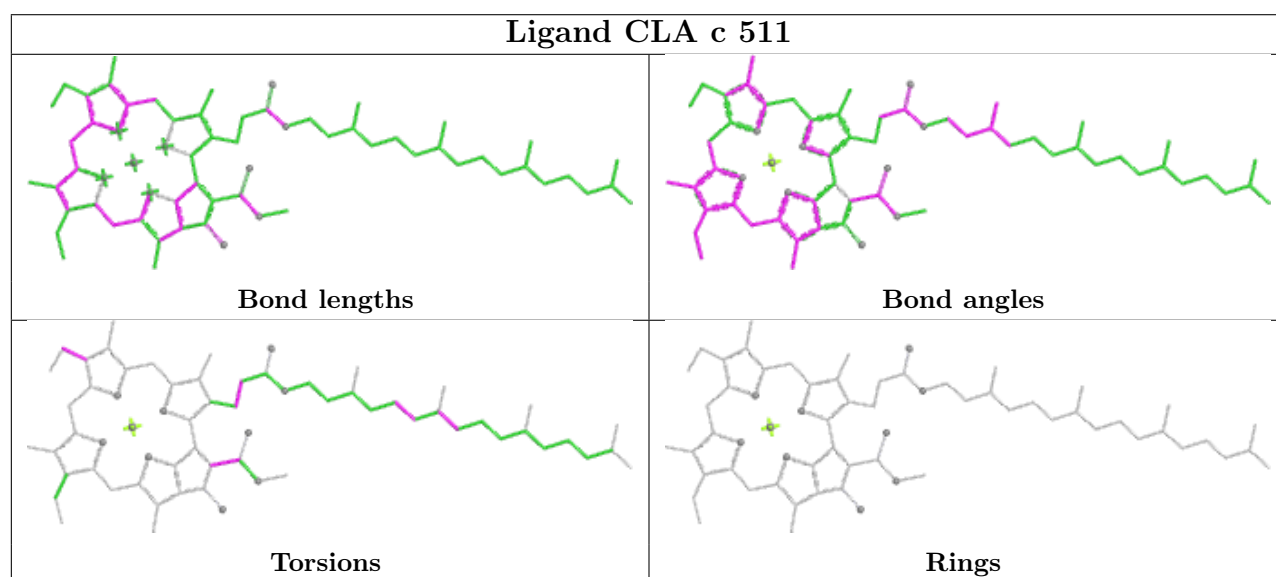
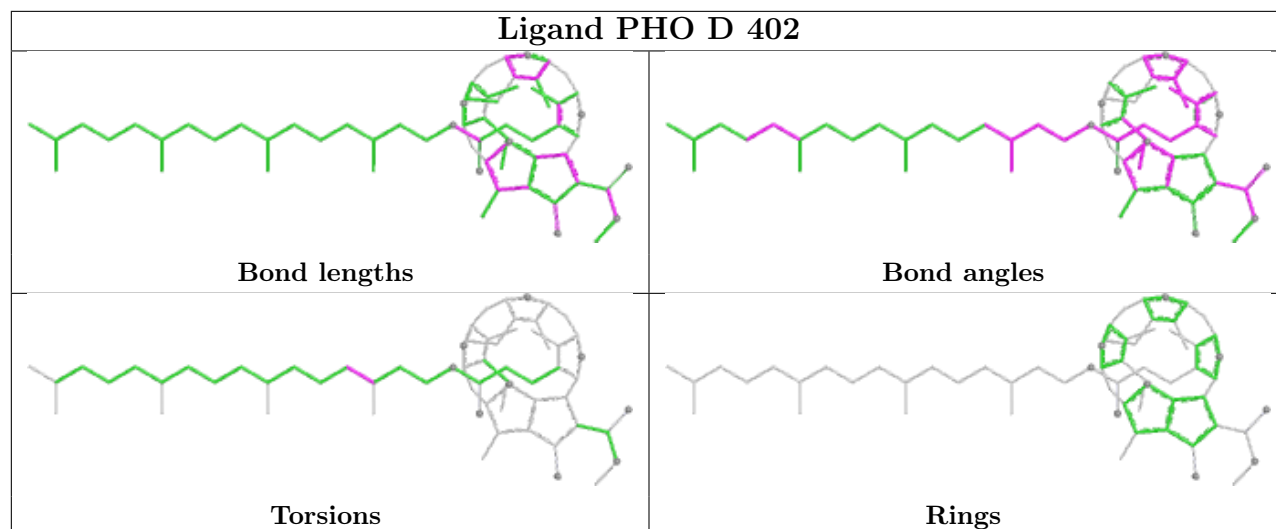


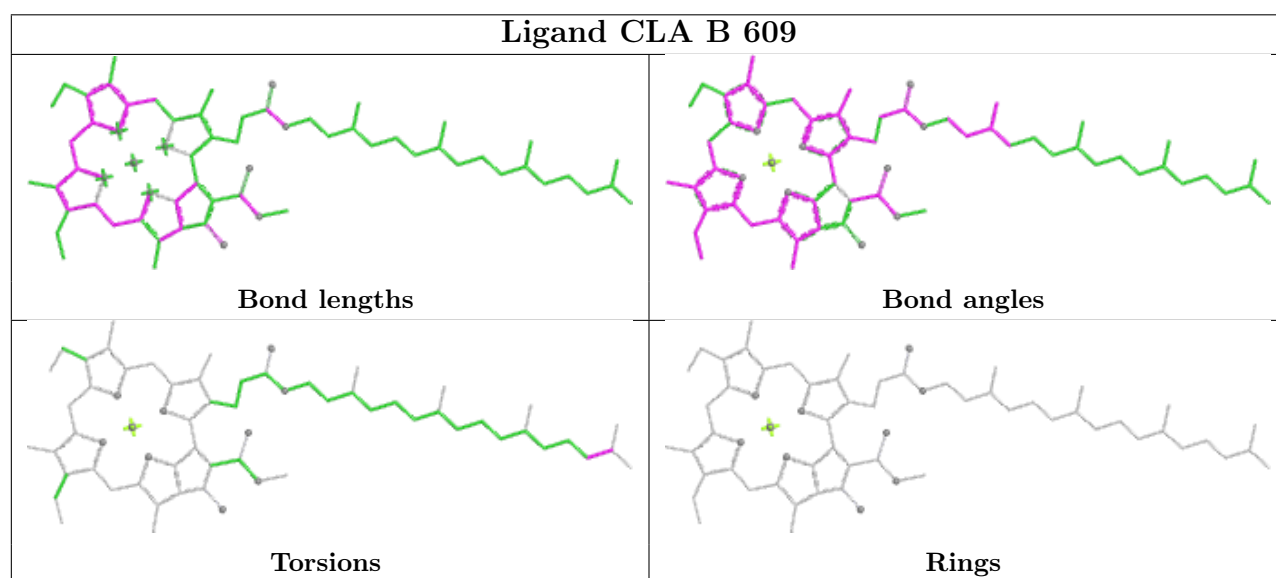
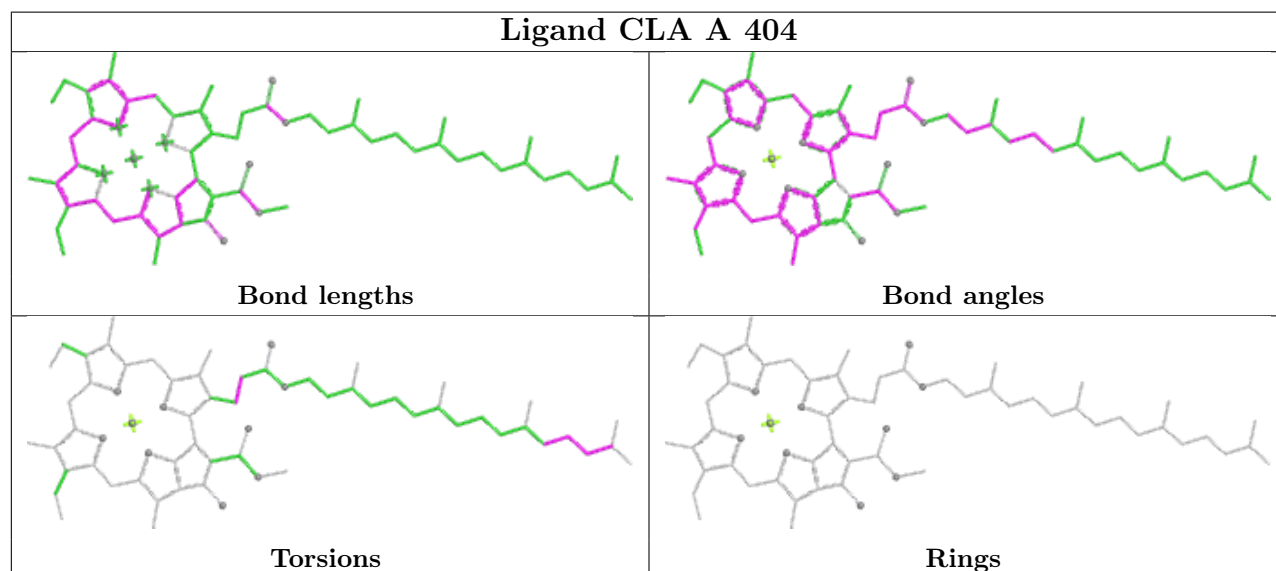
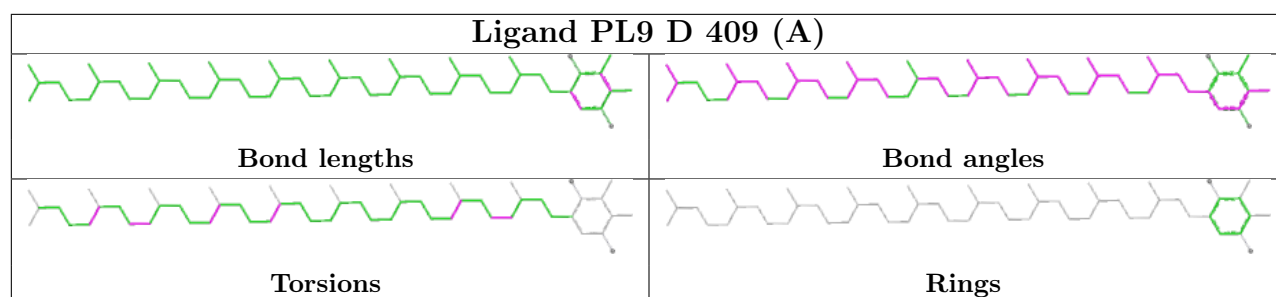


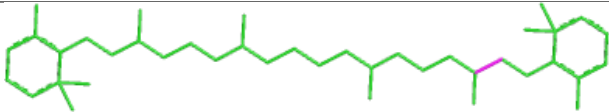
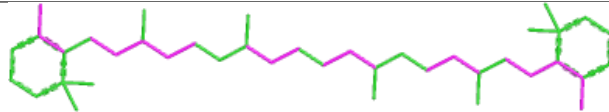
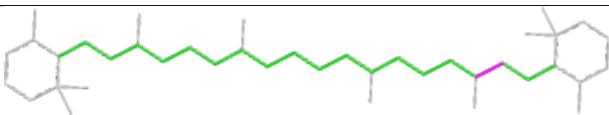
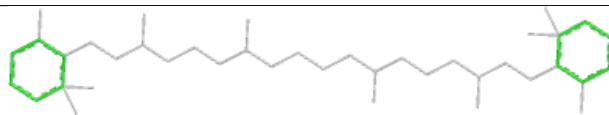


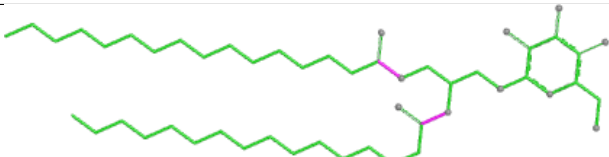
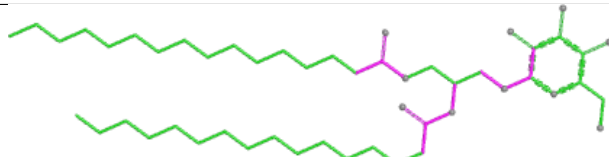
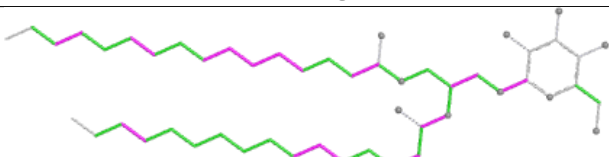
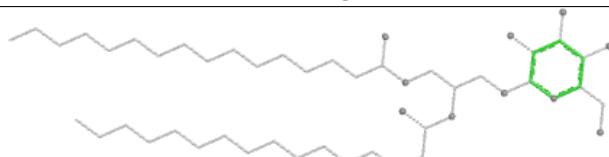


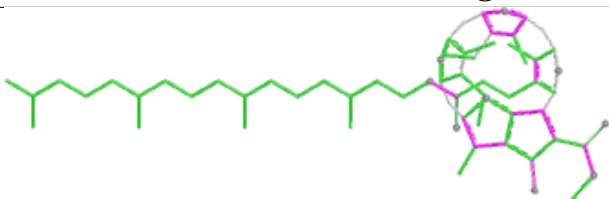
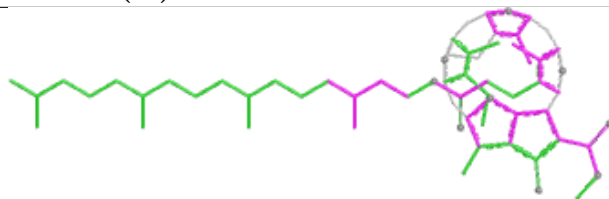
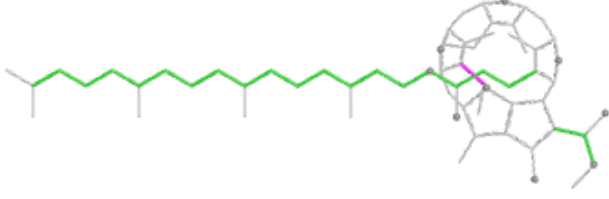
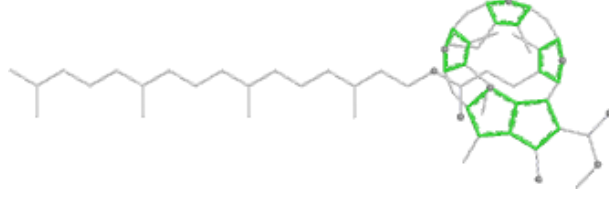


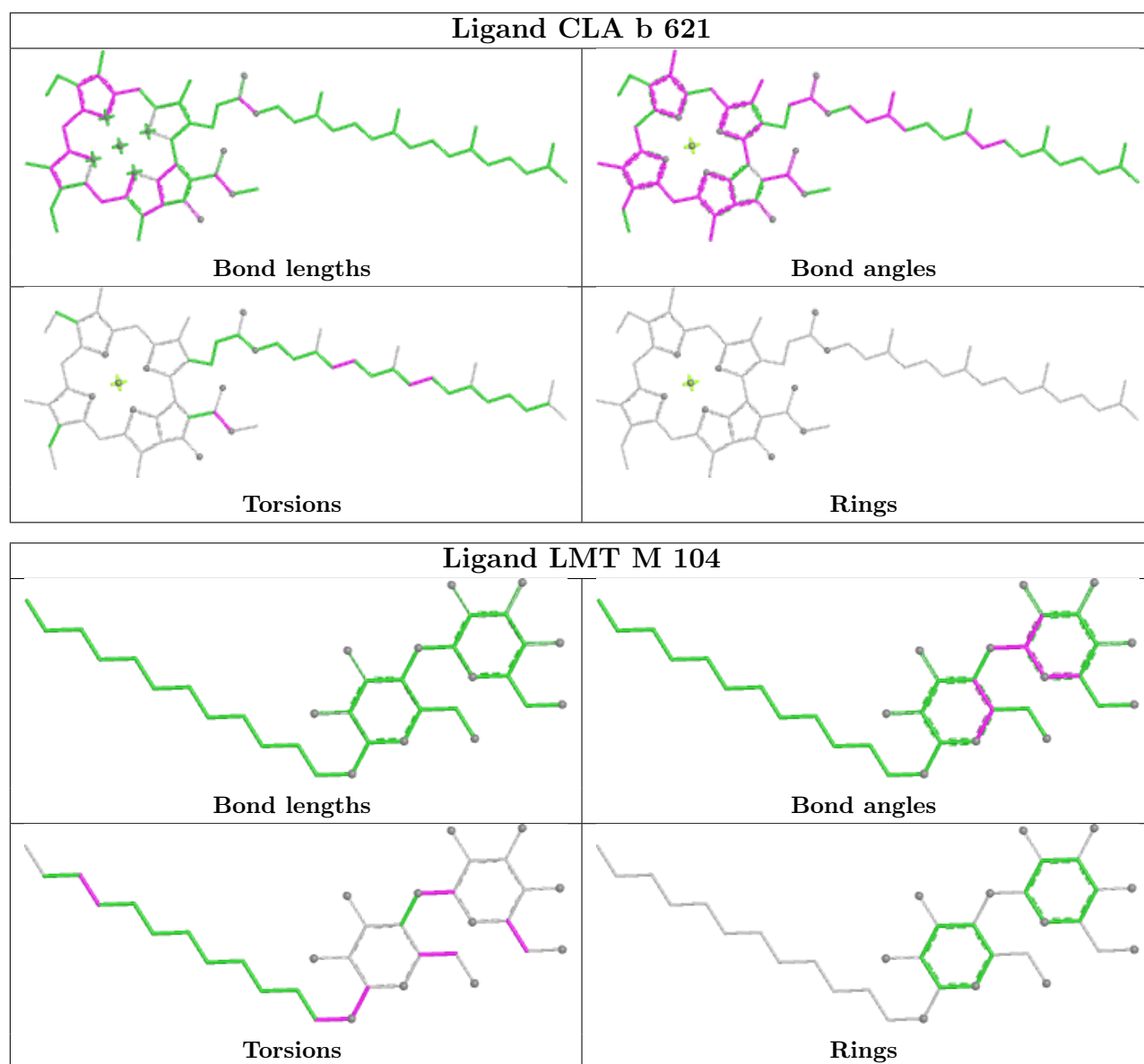


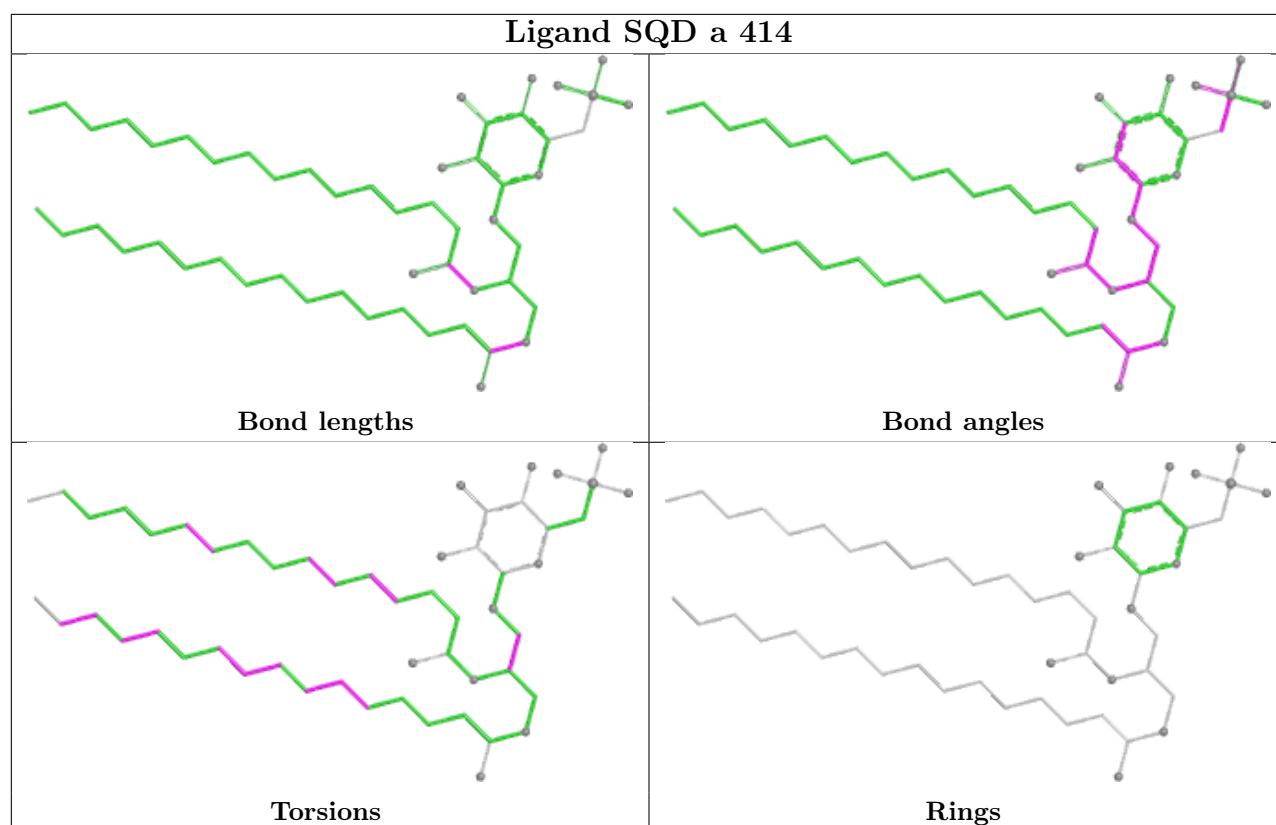


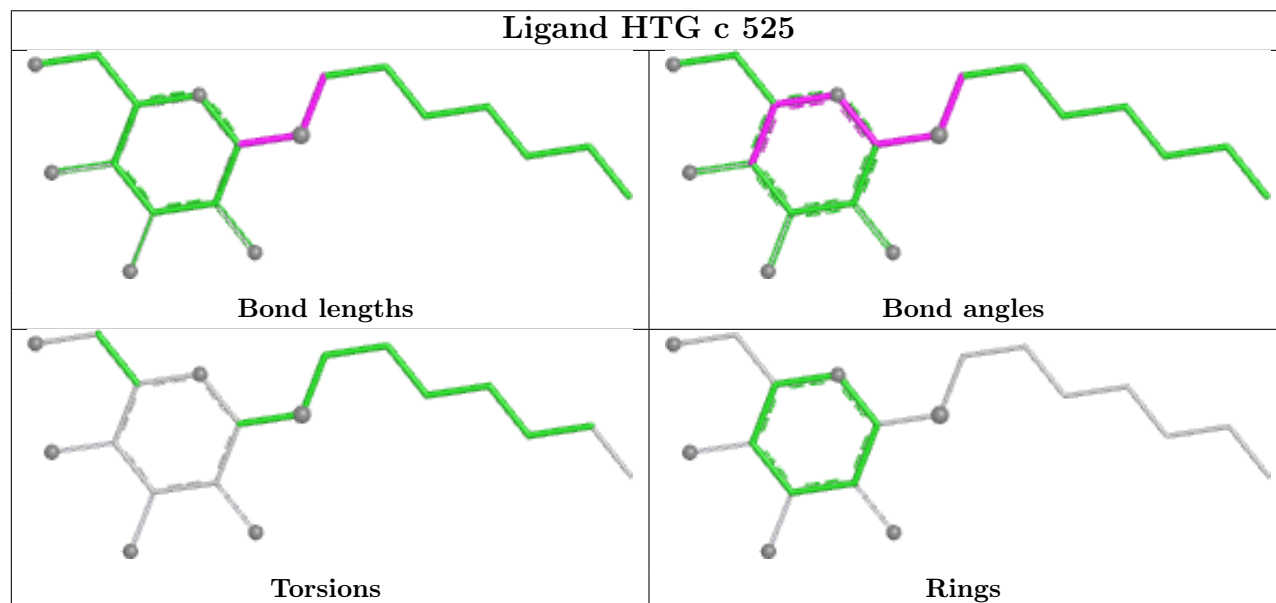
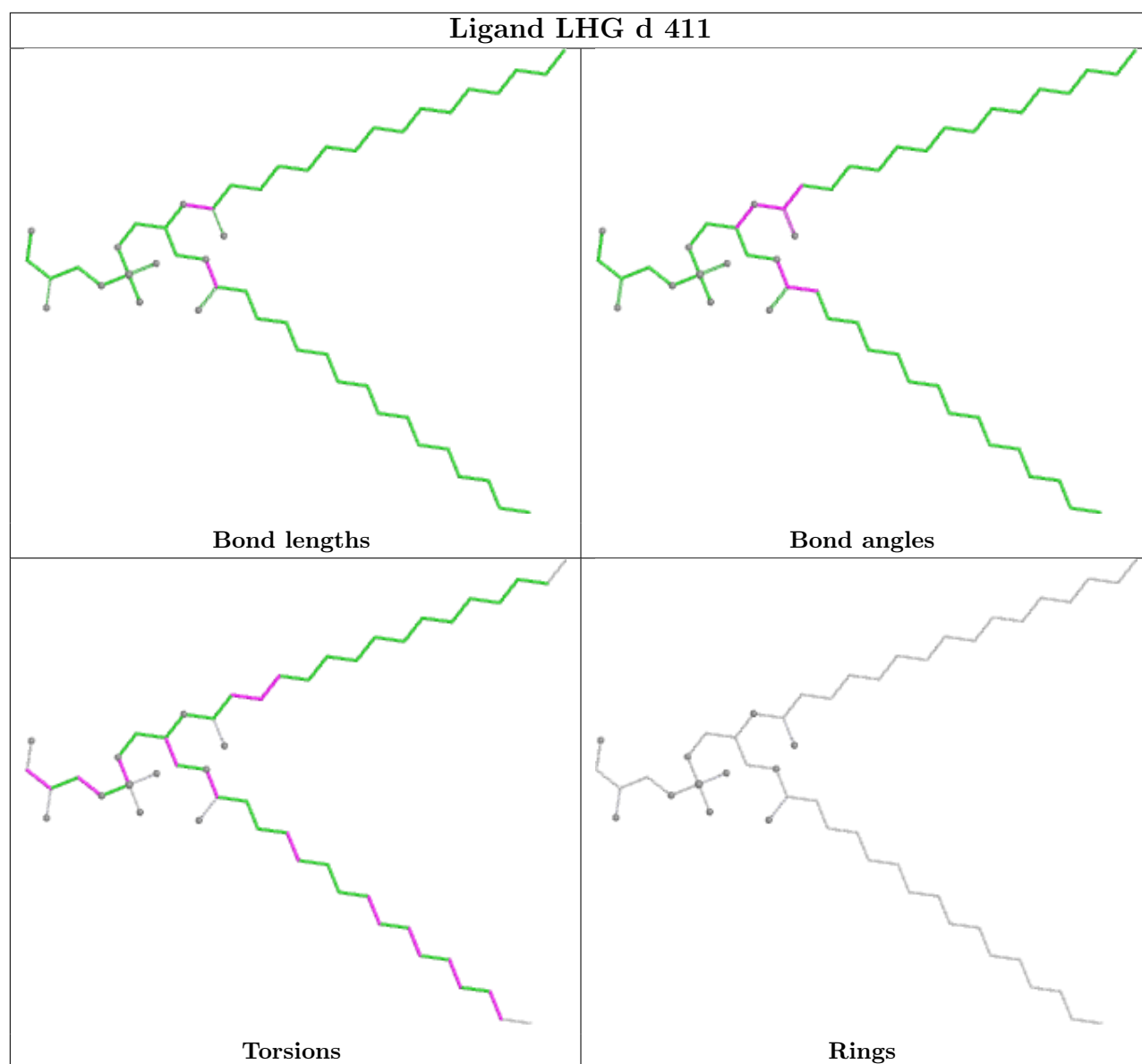
Ligand BCR K 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

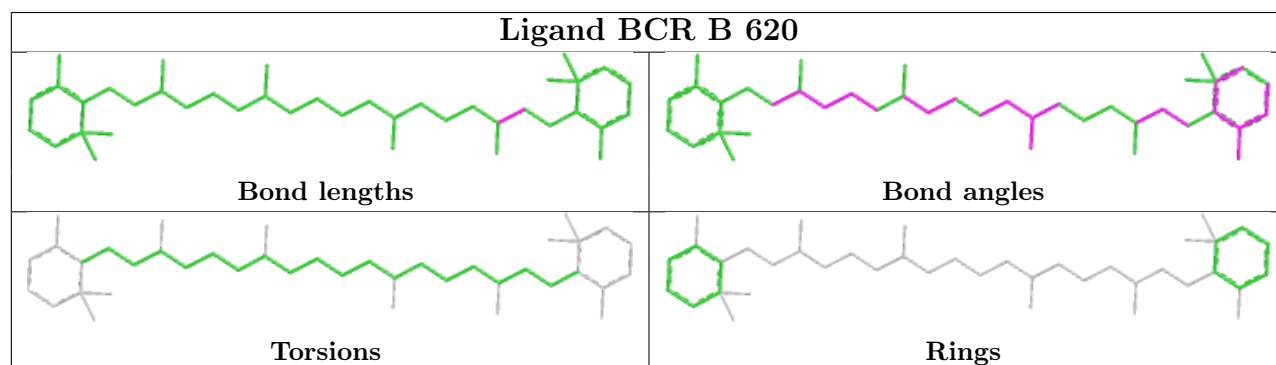
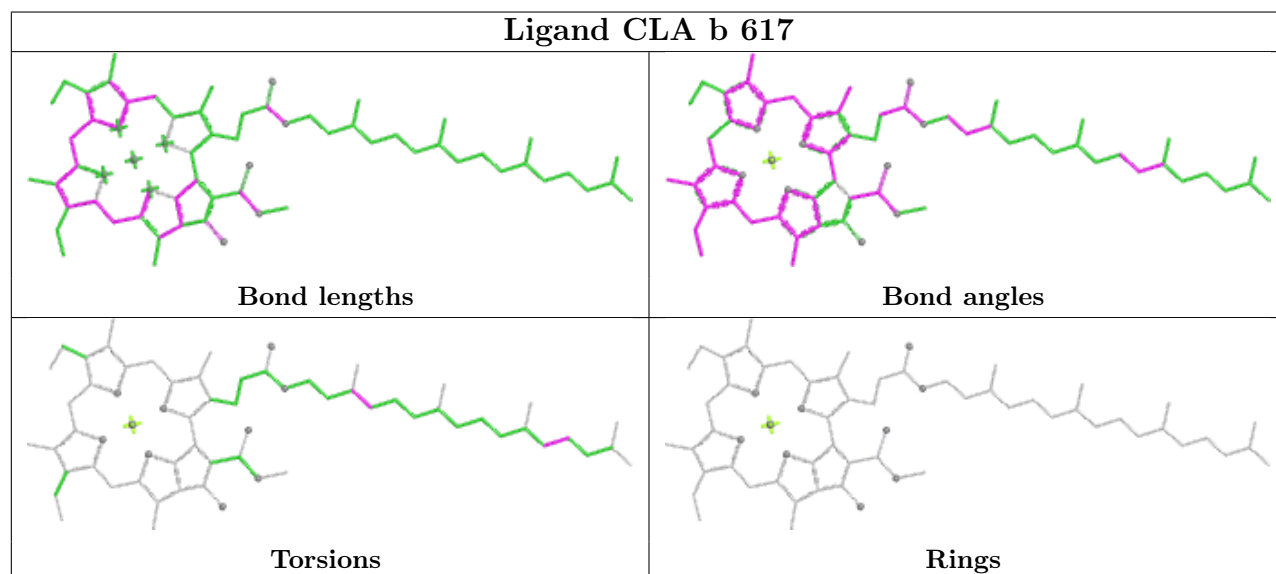
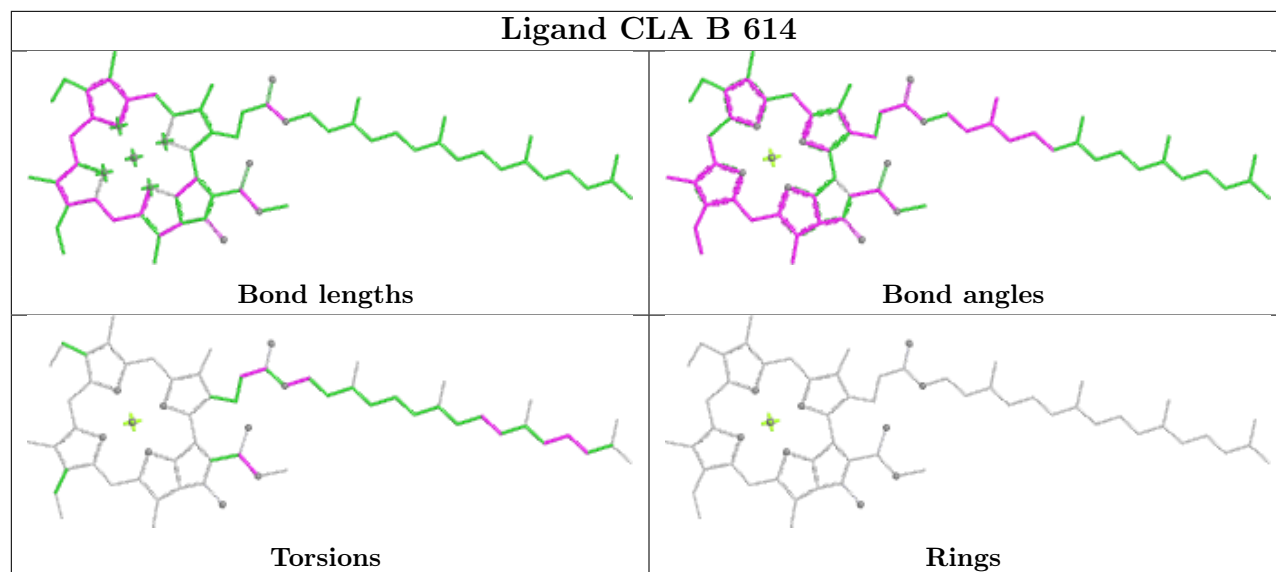
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Bond lengths	Bond angles
	
Torsions	Rings

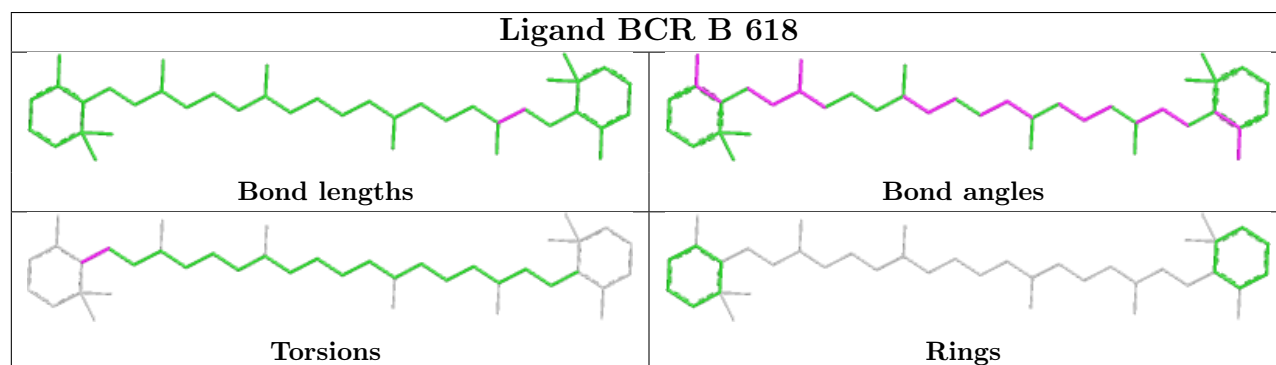
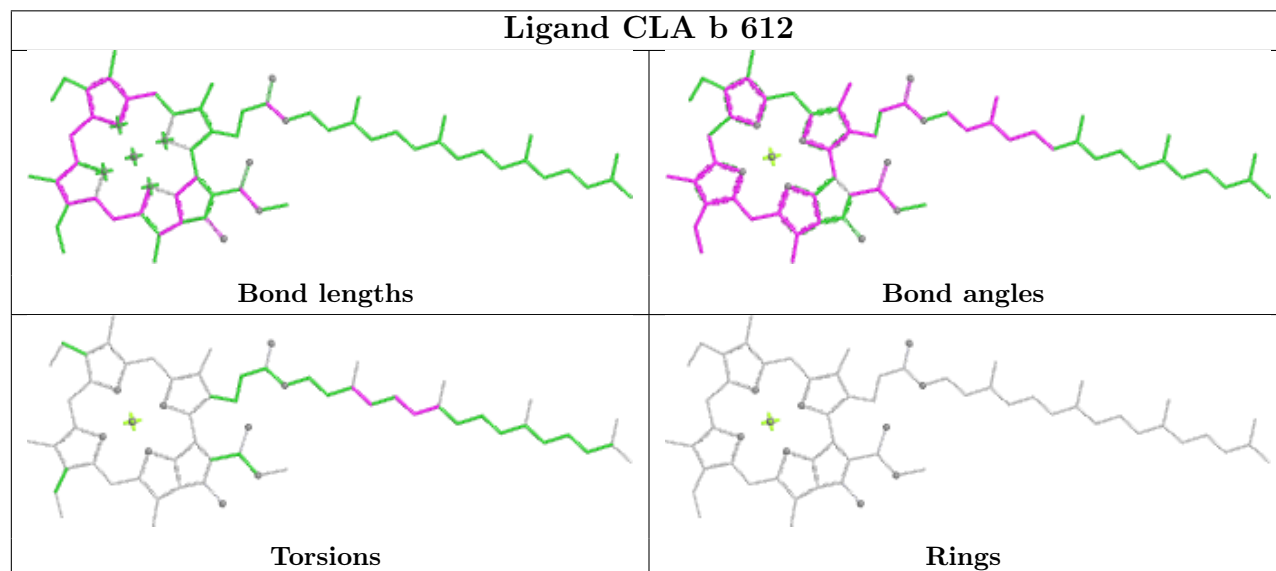
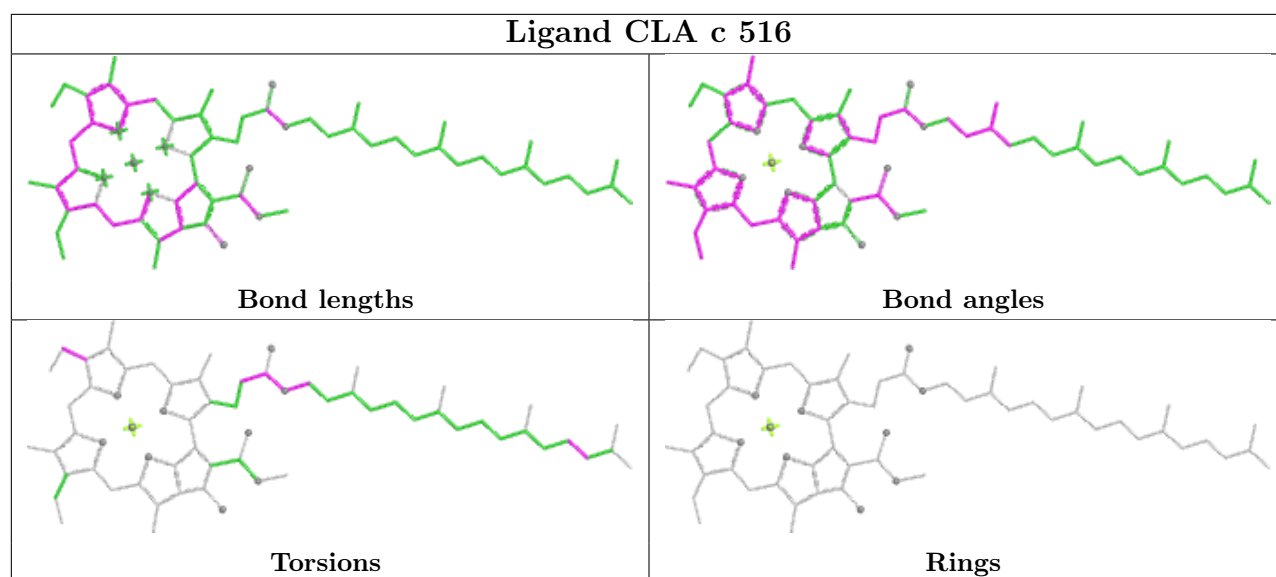
Ligand PHO d 402 (A)	
	
Bond lengths	Bond angles
	
Torsions	Rings

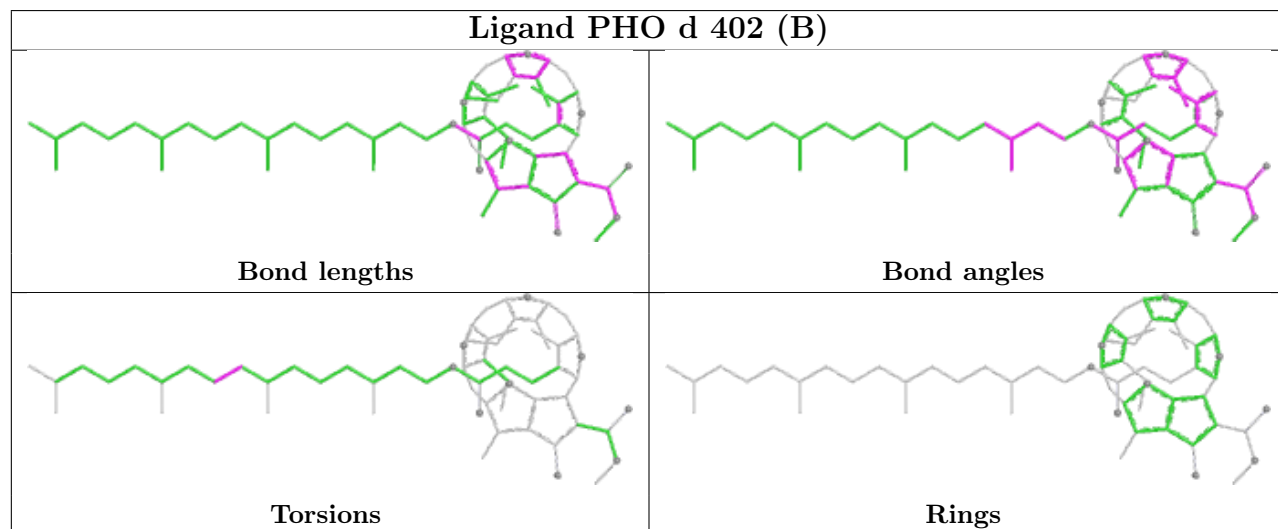
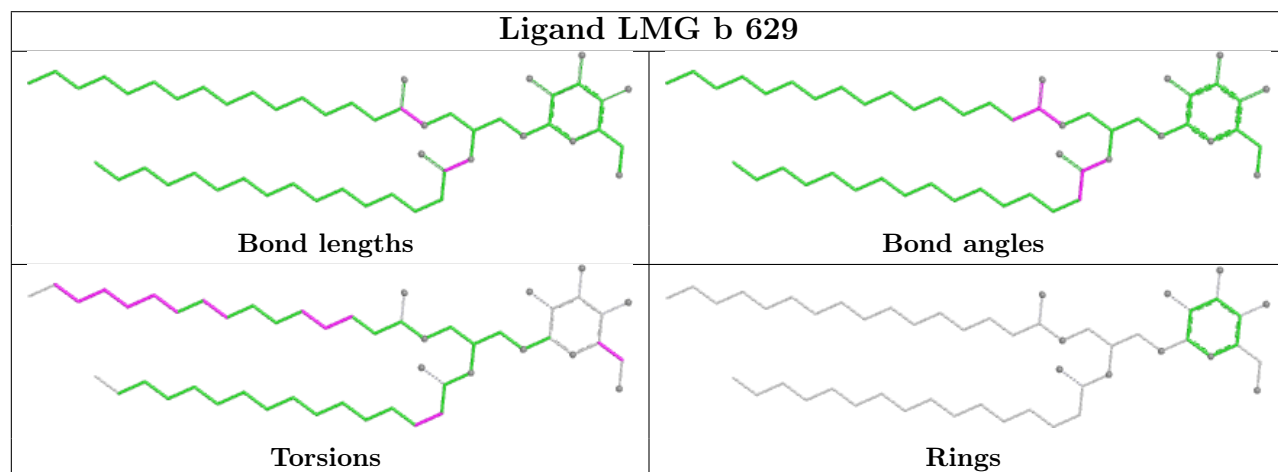
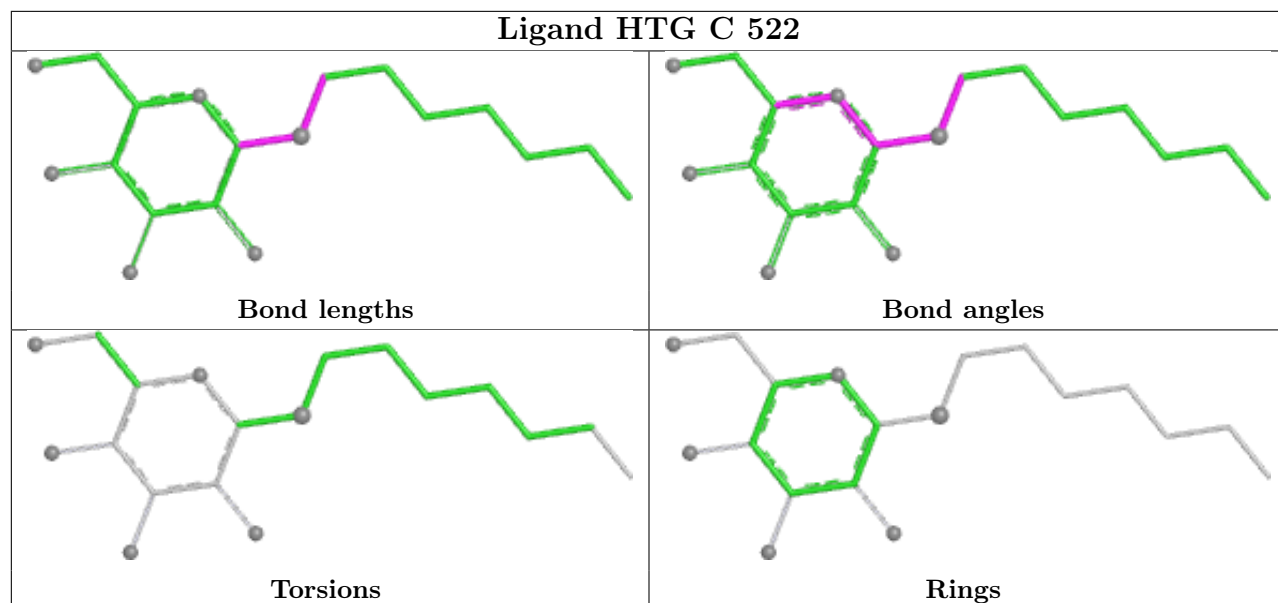


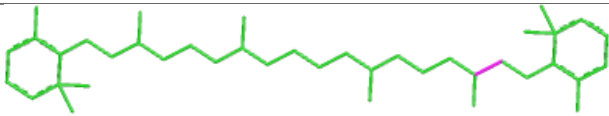
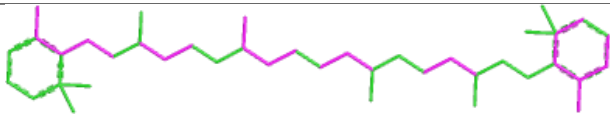
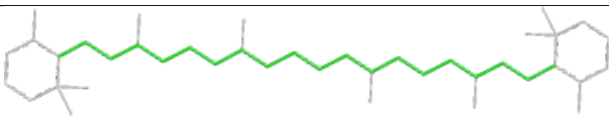
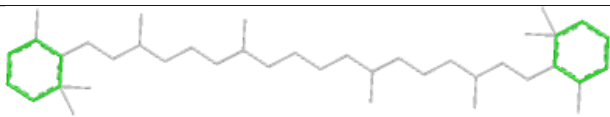


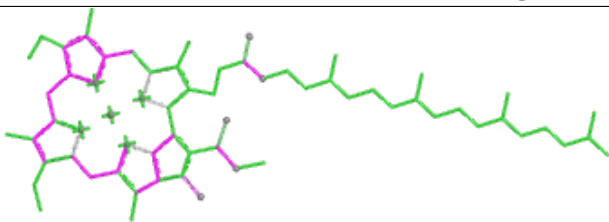
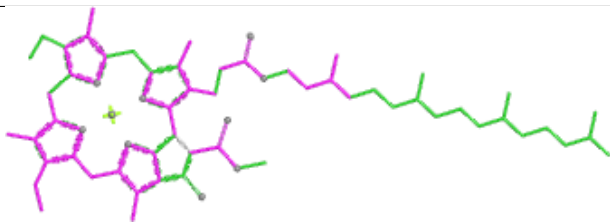
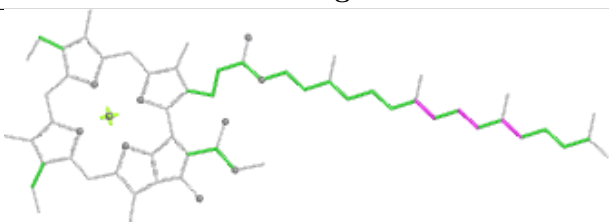
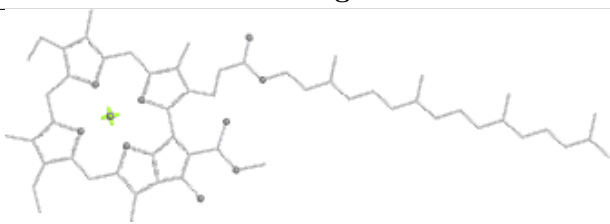


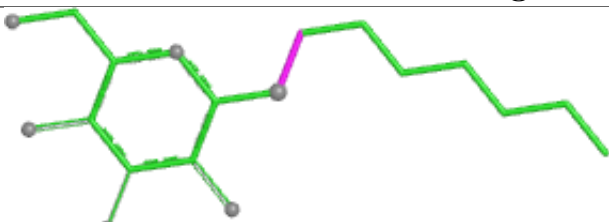
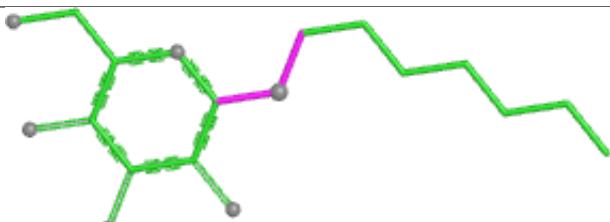
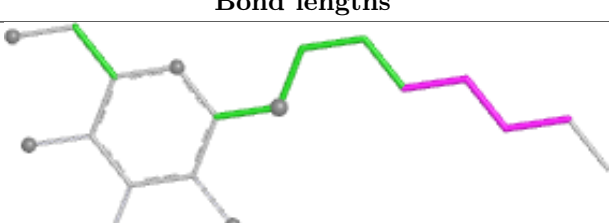
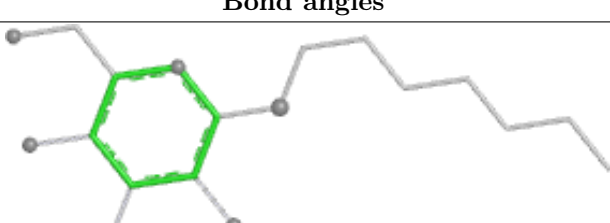


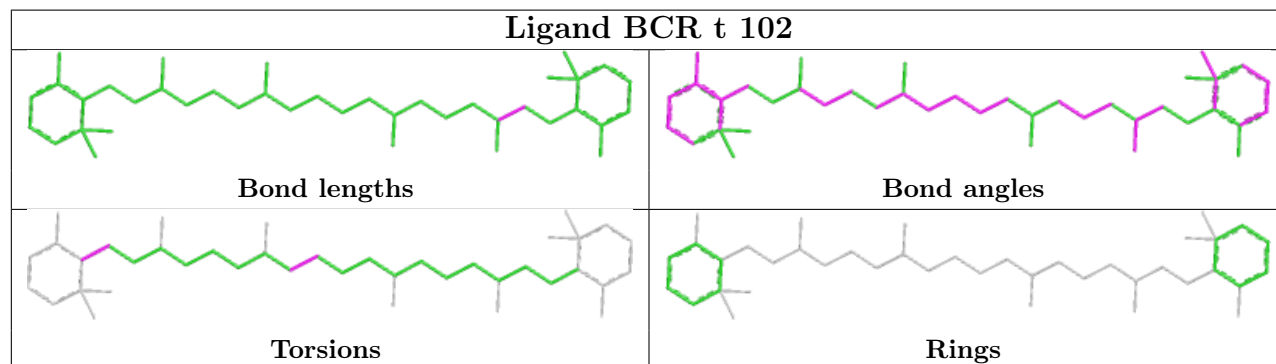
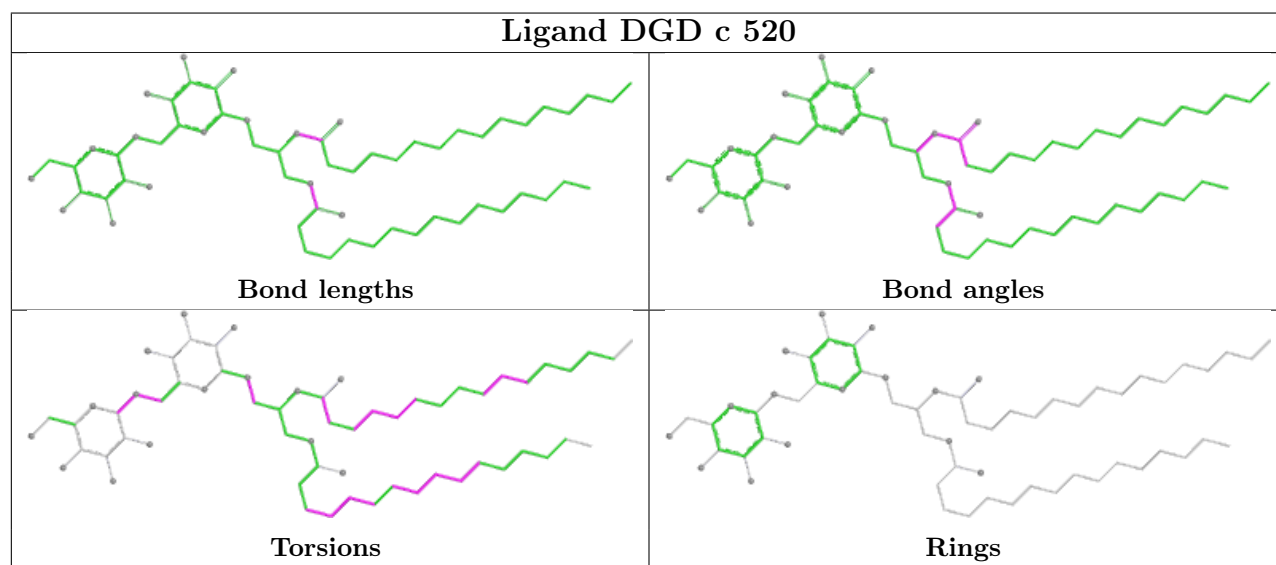
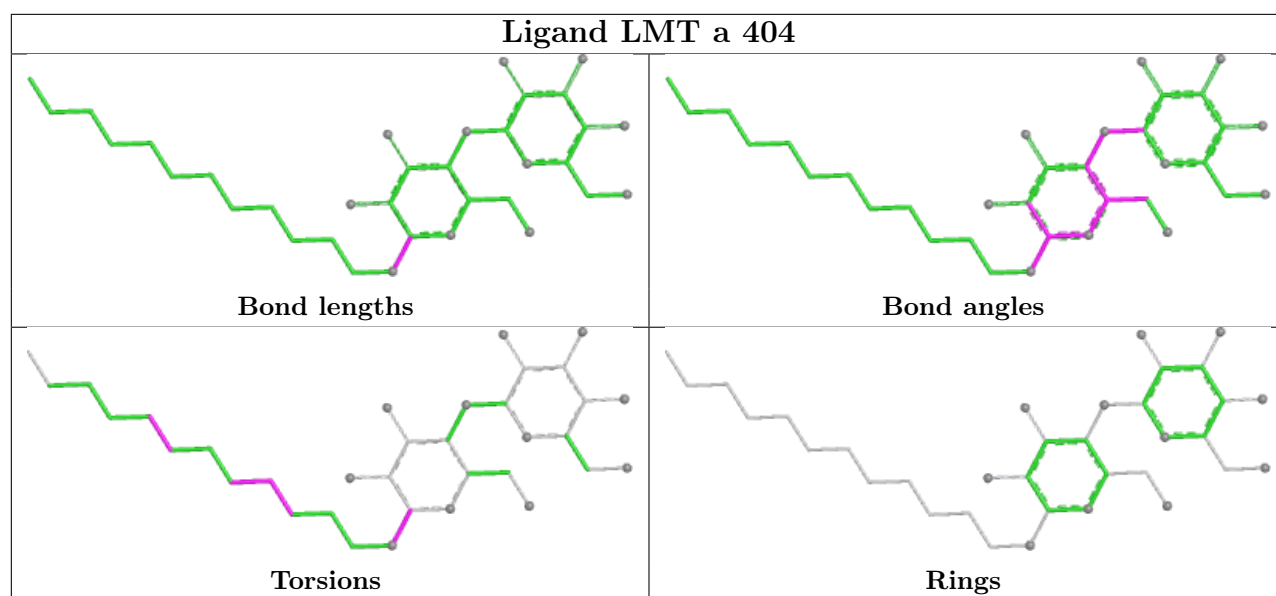


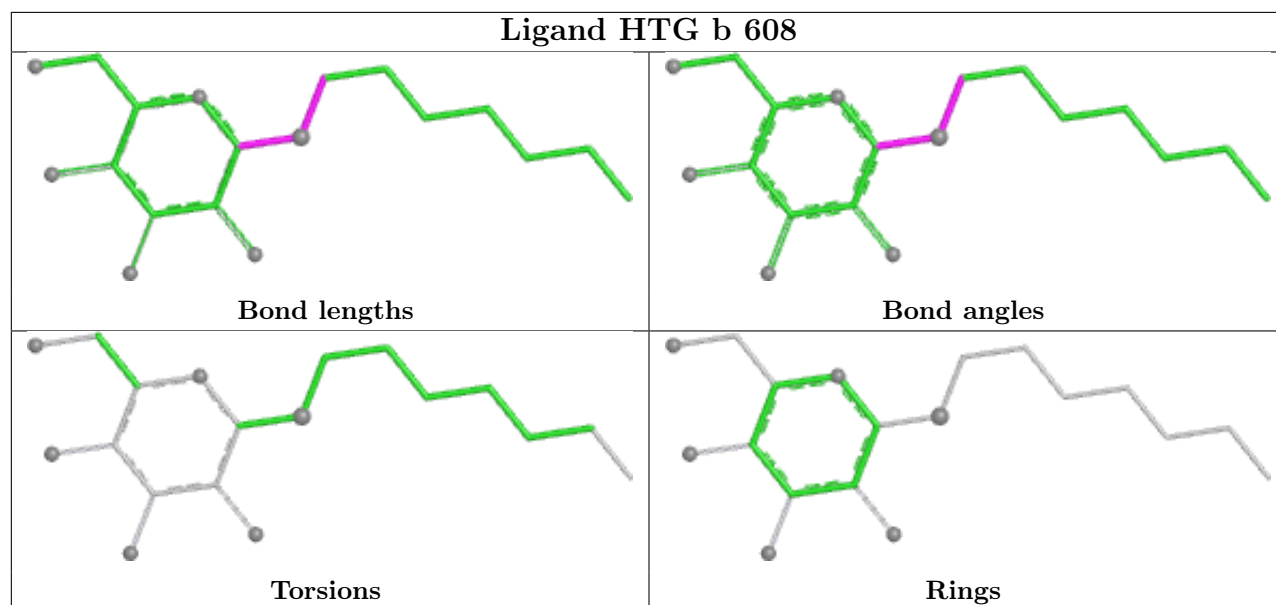
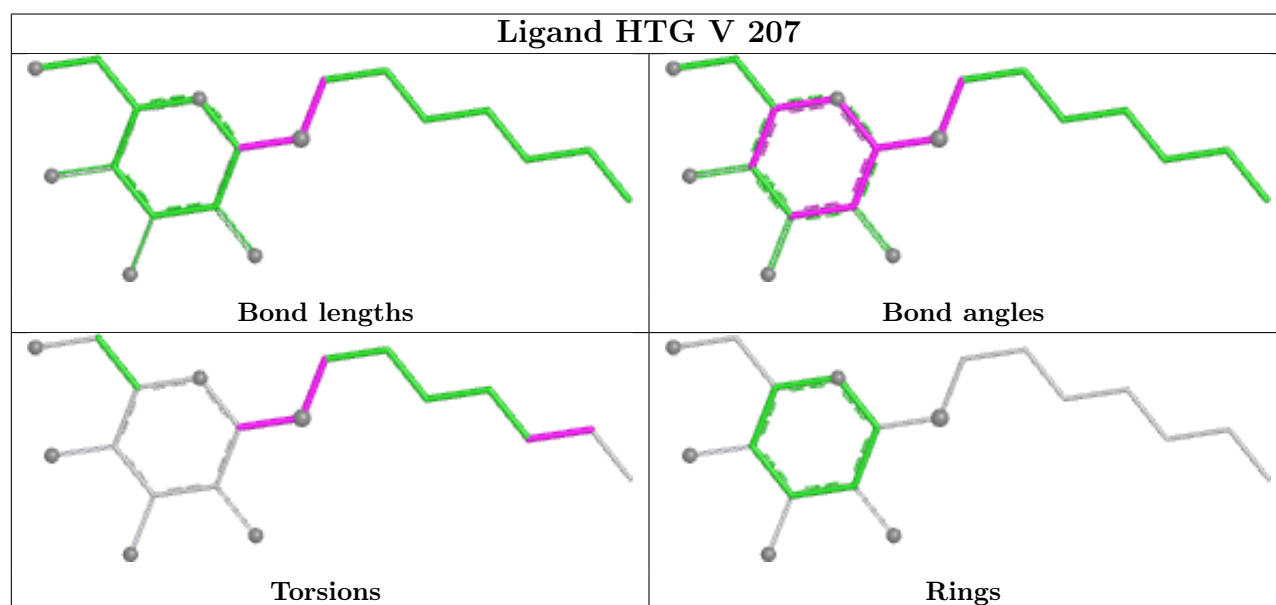
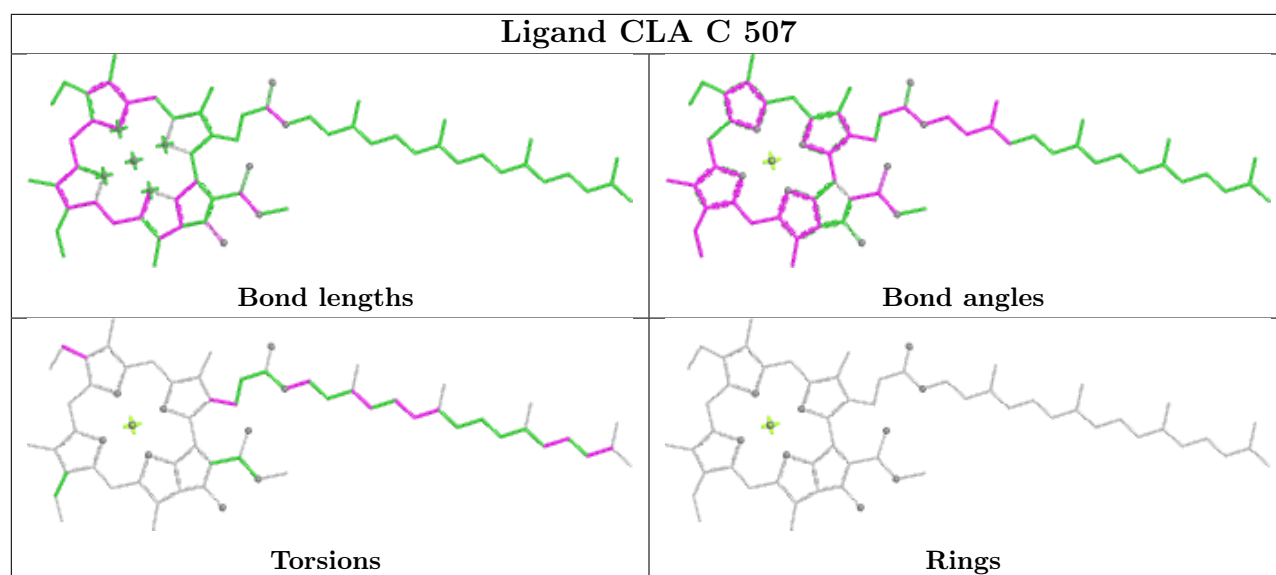


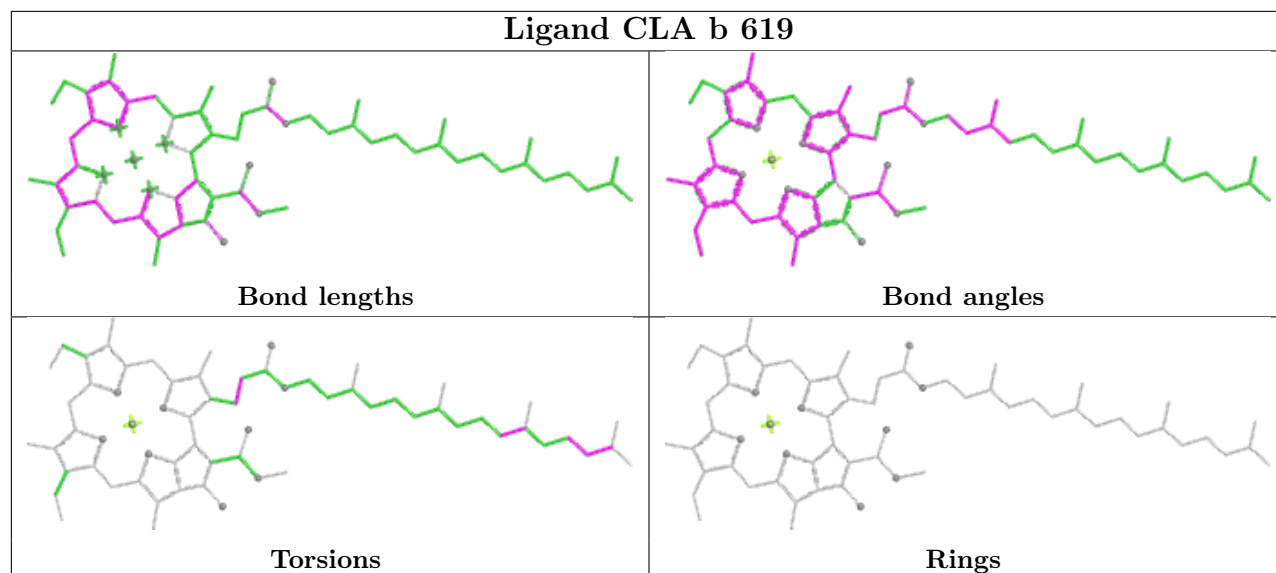
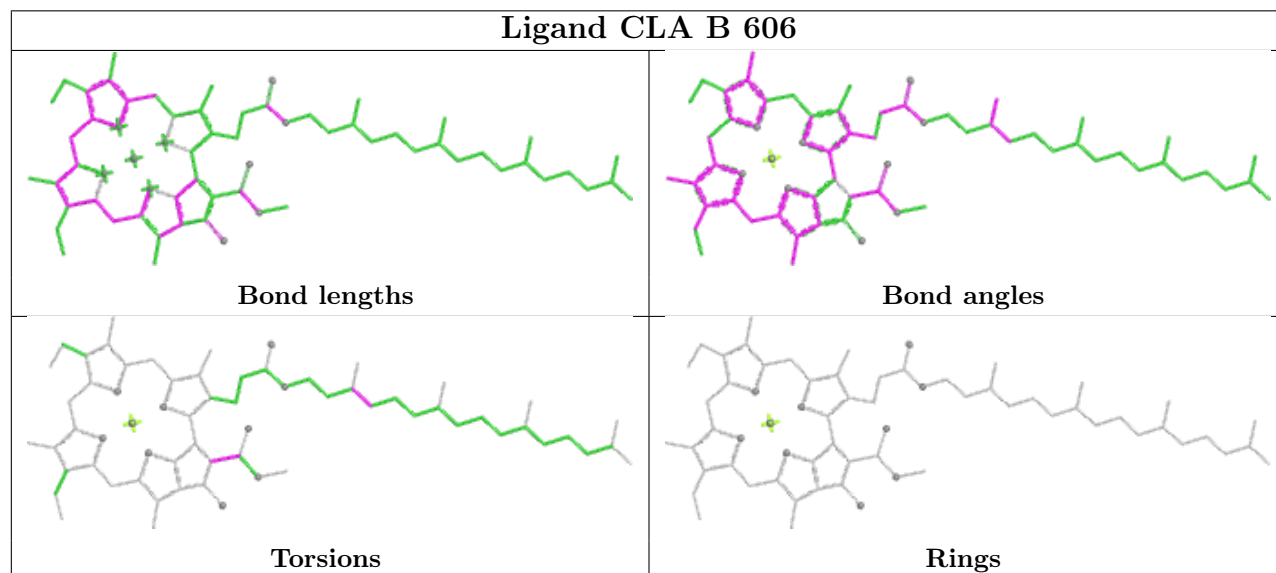
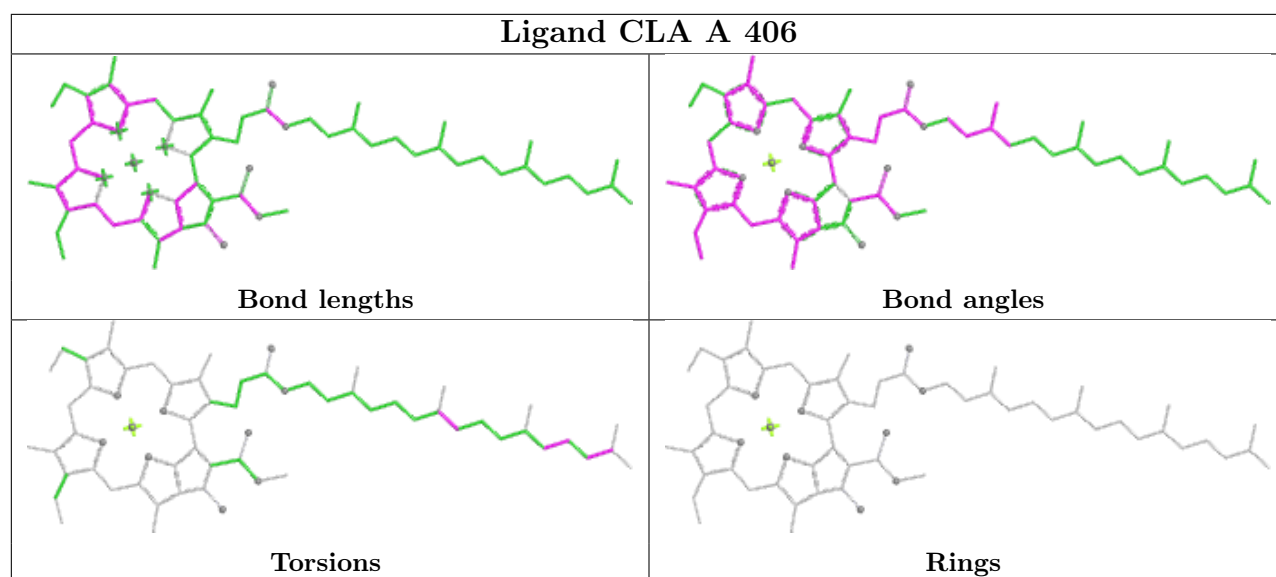
Ligand BCR c 527	
	
Bond lengths	Bond angles
	
Torsions	Rings

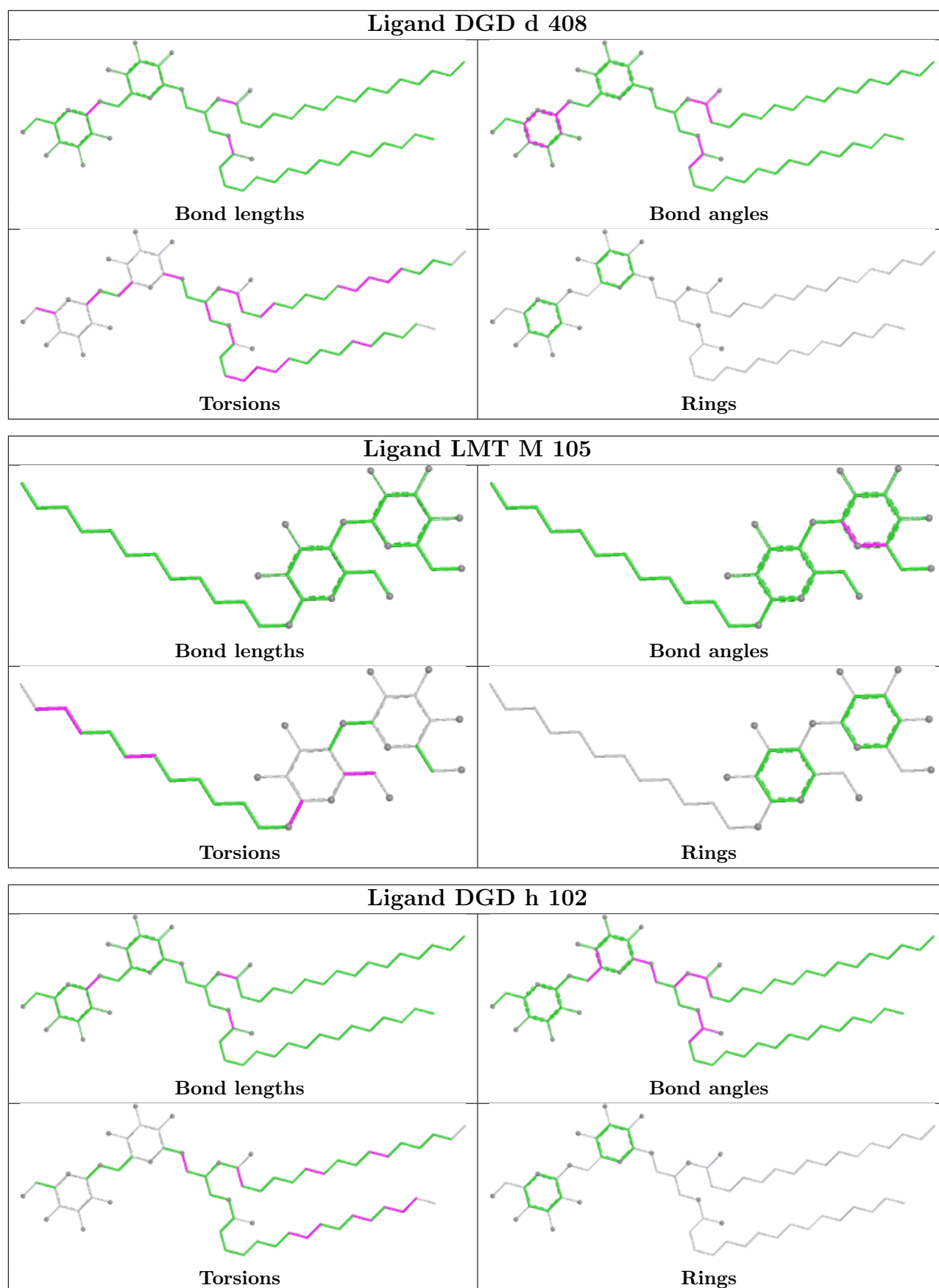
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Bond lengths	Bond angles
	
Torsions	Rings

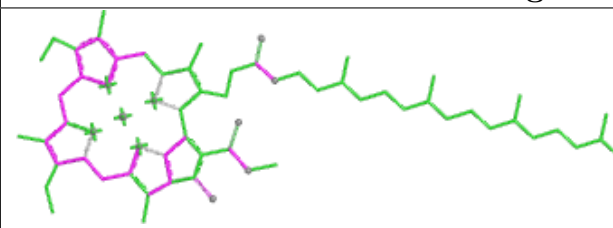
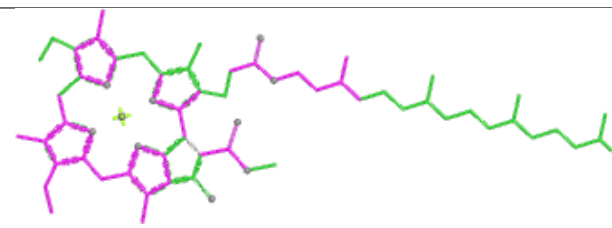
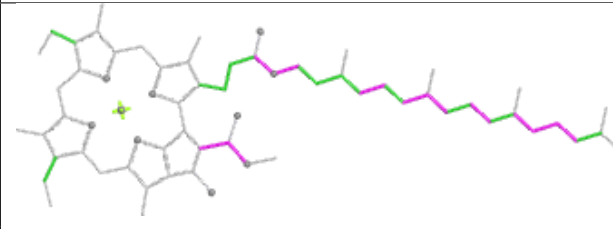
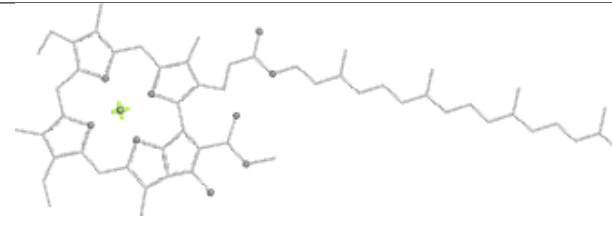
Ligand HTG o 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

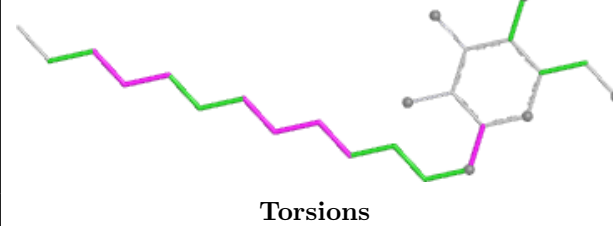
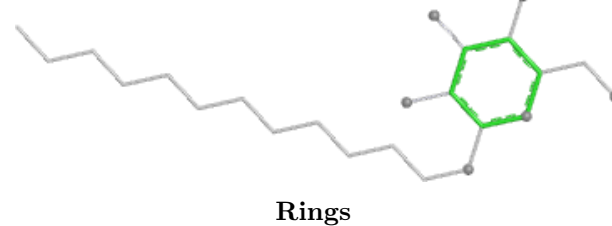


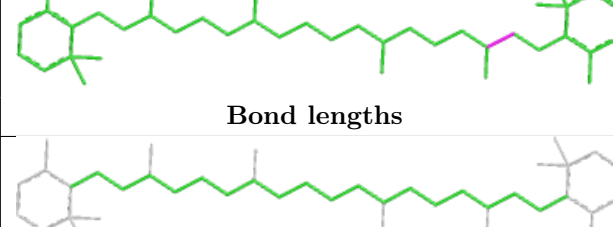
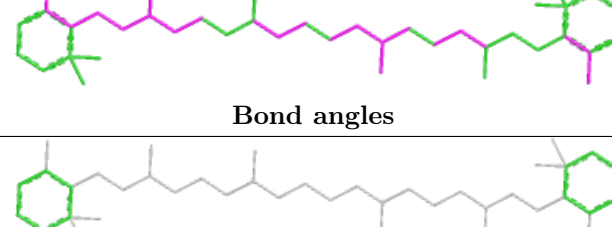


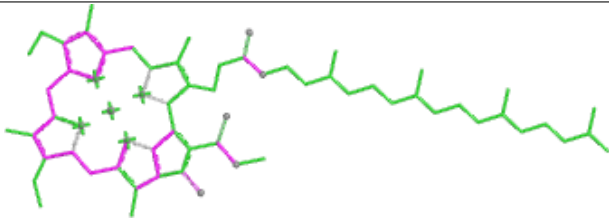
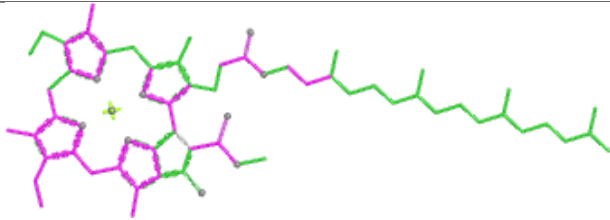
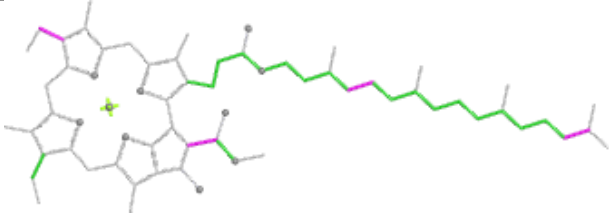
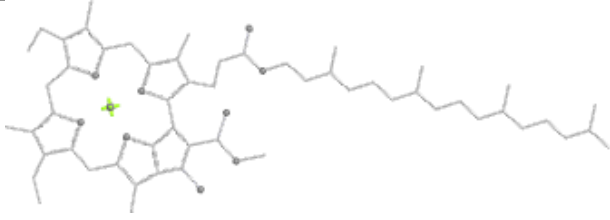


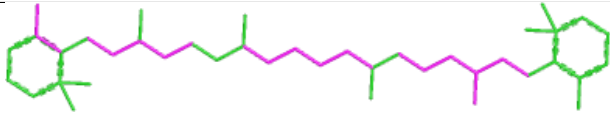
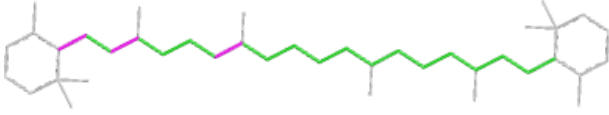
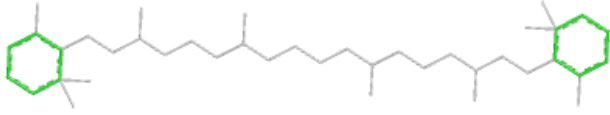


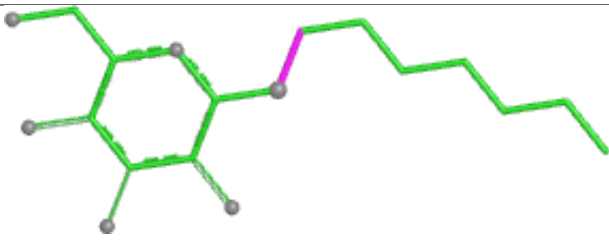
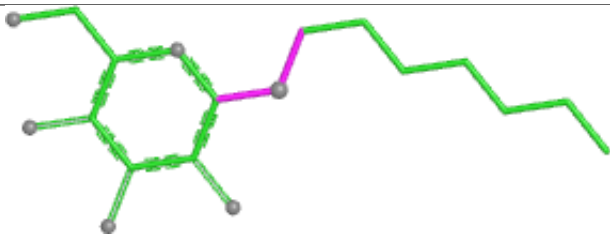
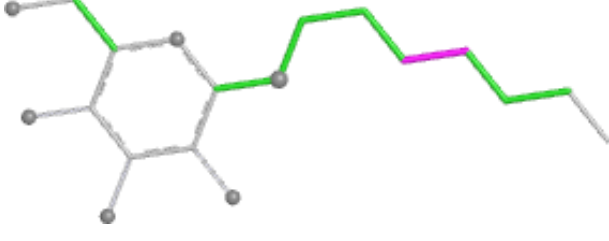
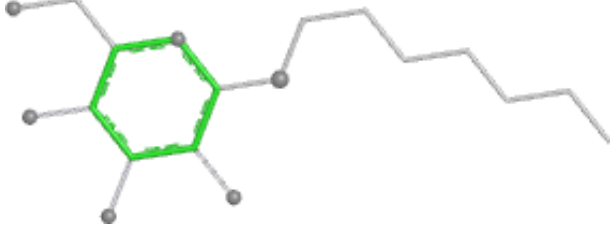
Ligand CLA c 513	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMT t 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

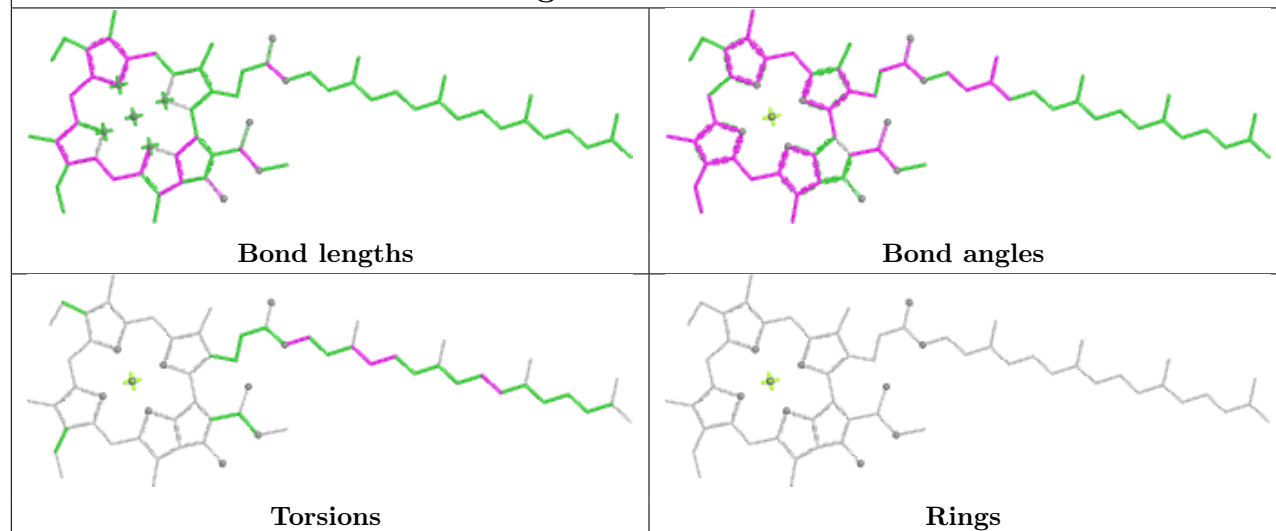
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

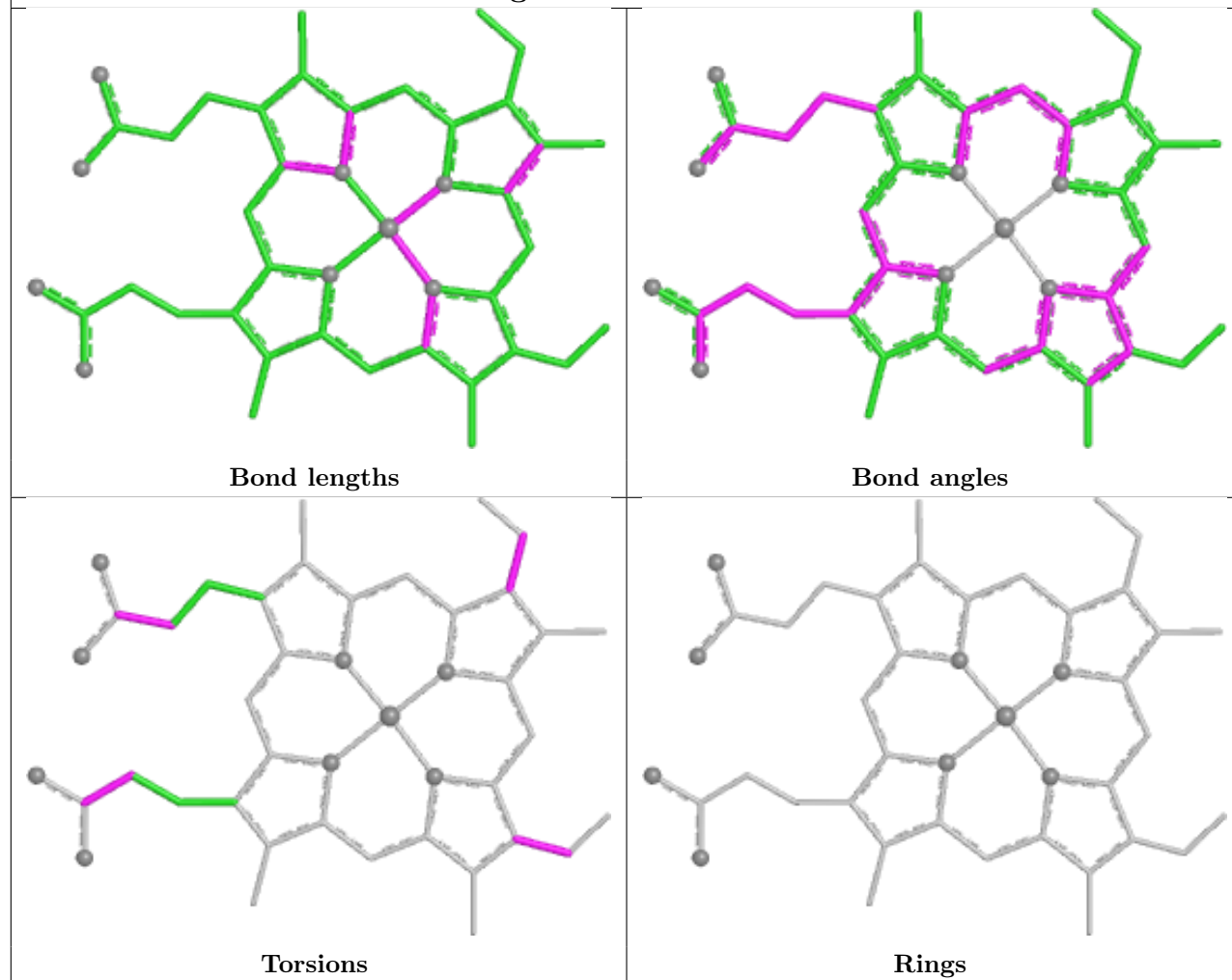
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Bond lengths	Bond angles
	
Torsions	Rings

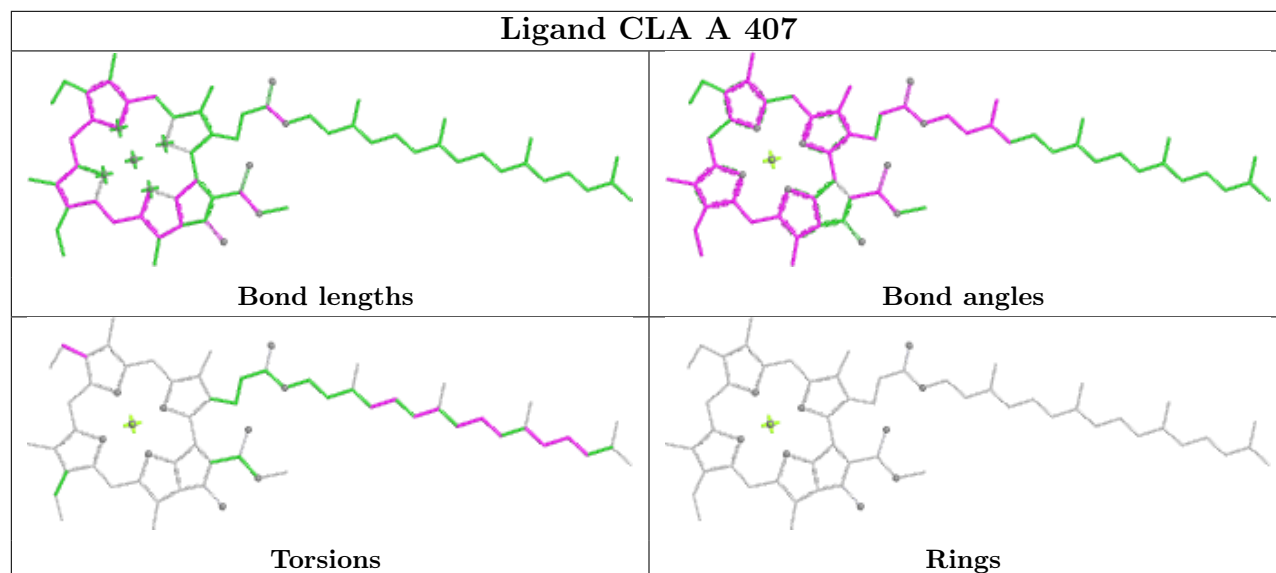
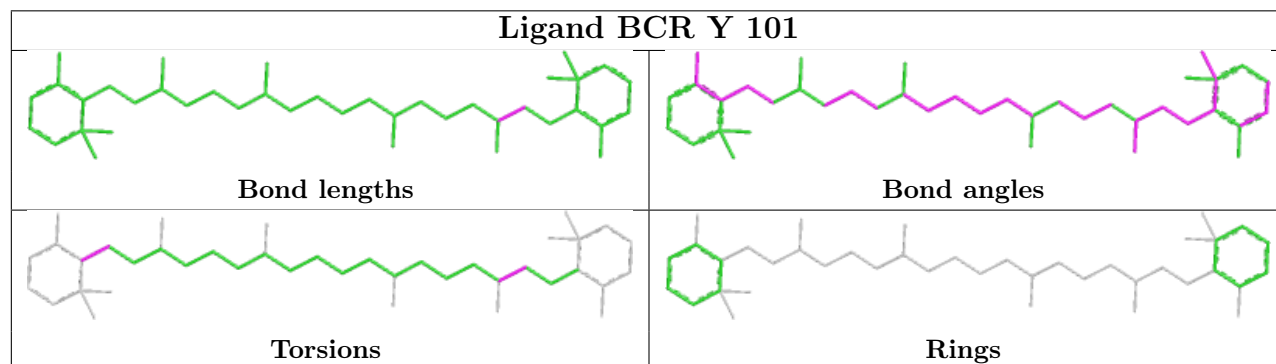
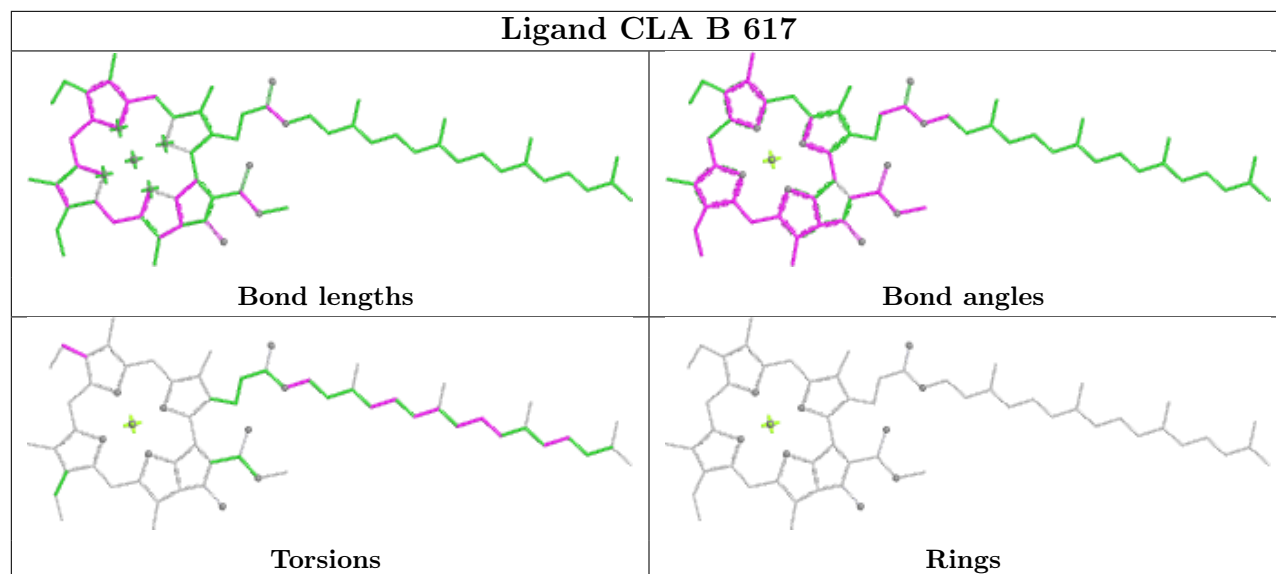
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Bond lengths	Bond angles
	
Torsions	Rings

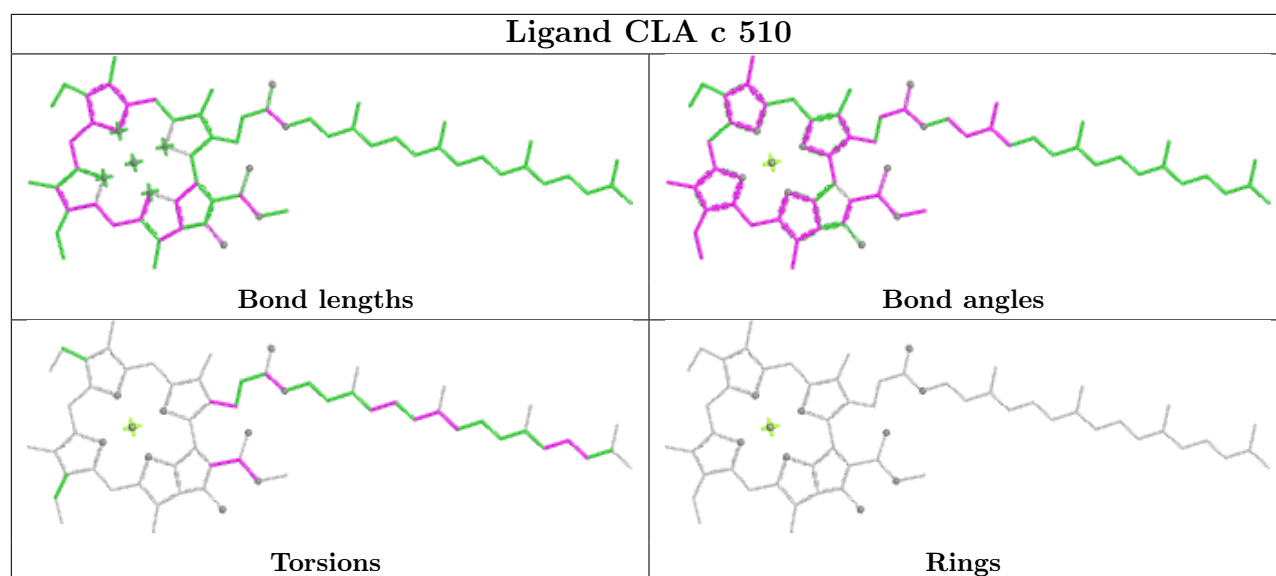
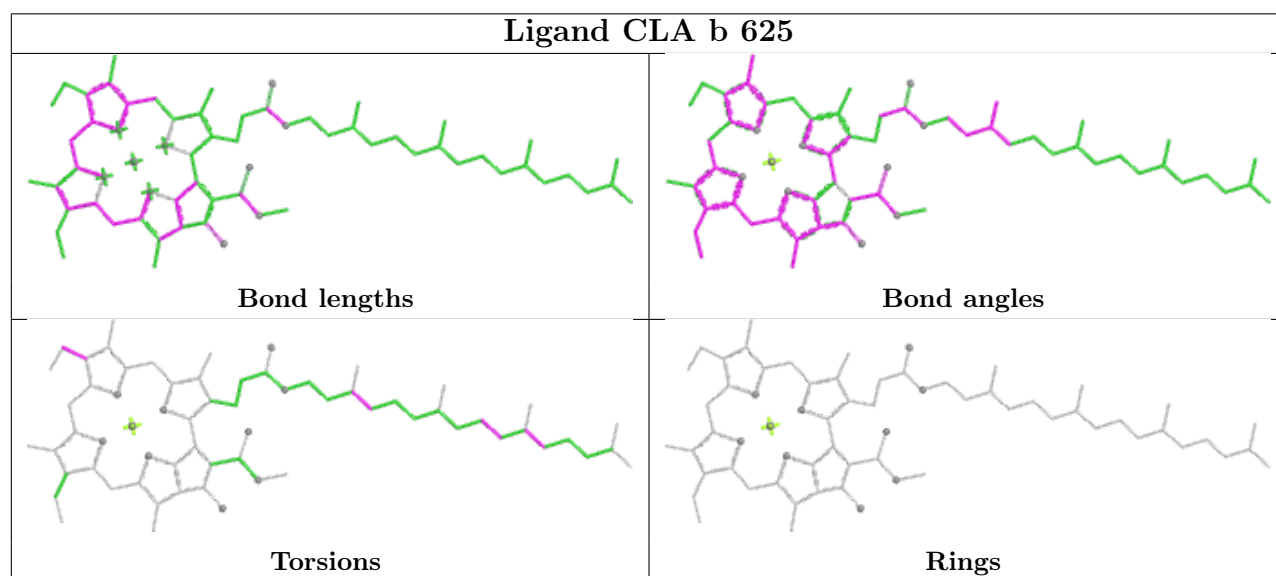
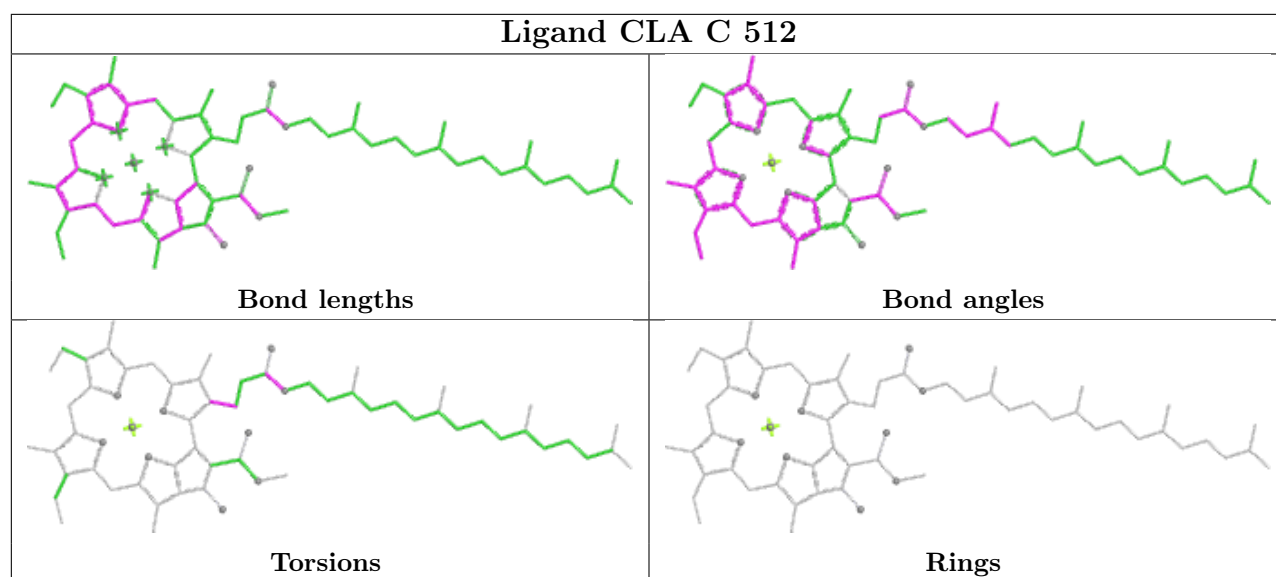
Ligand CLA c 517

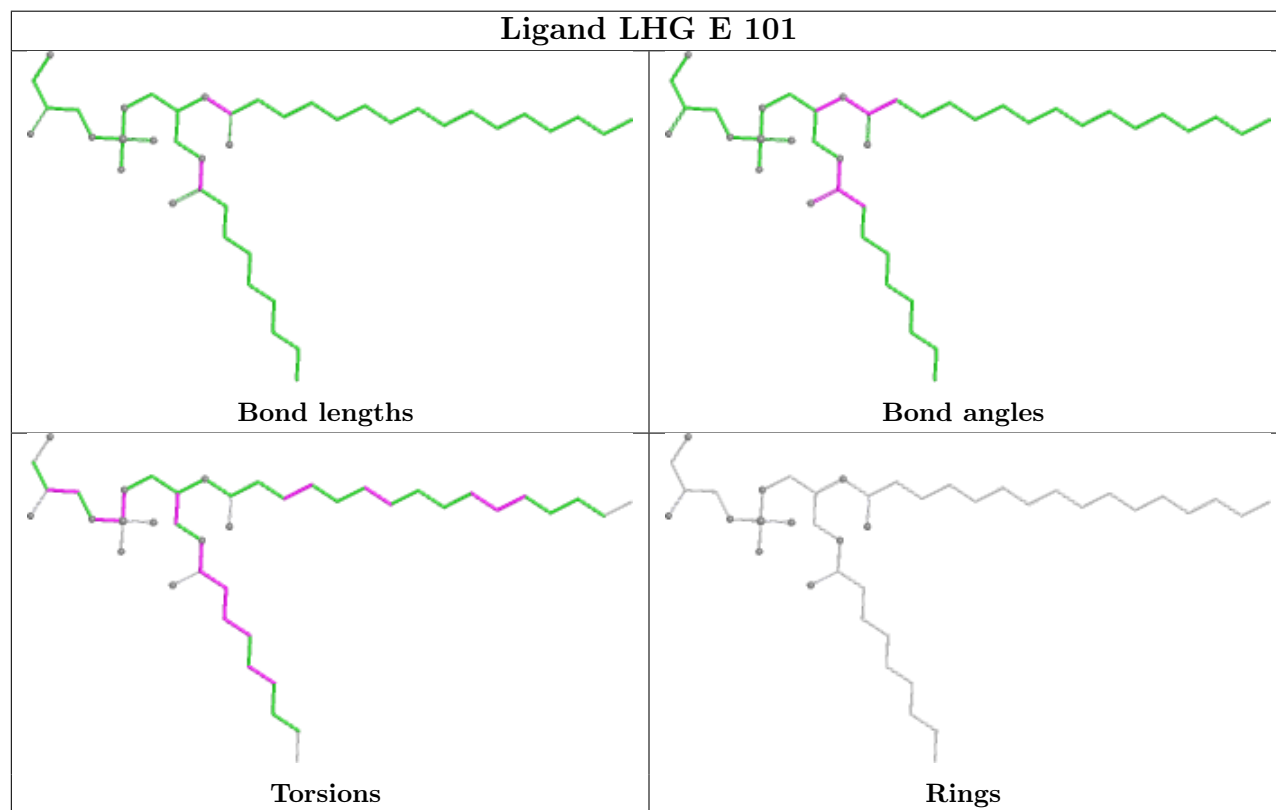
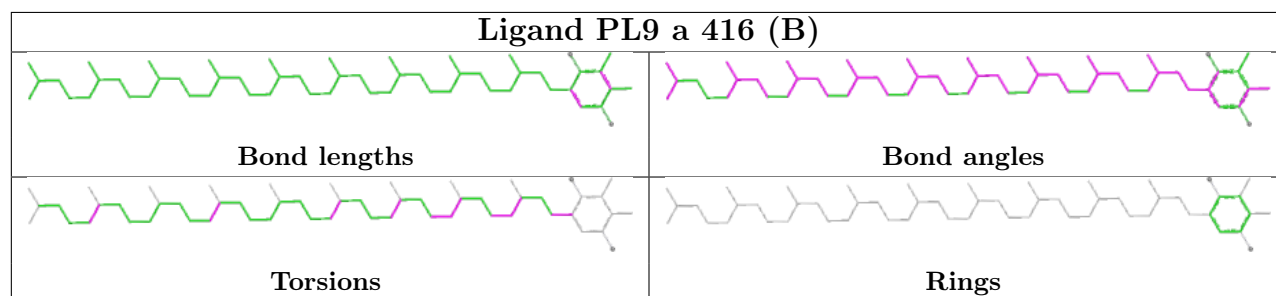
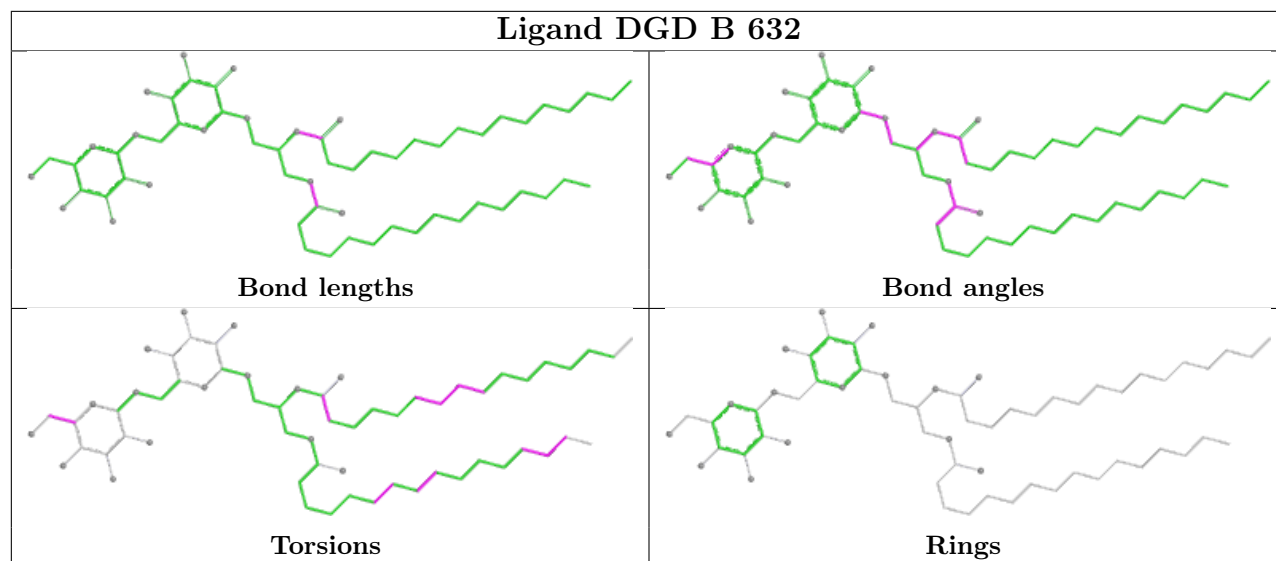


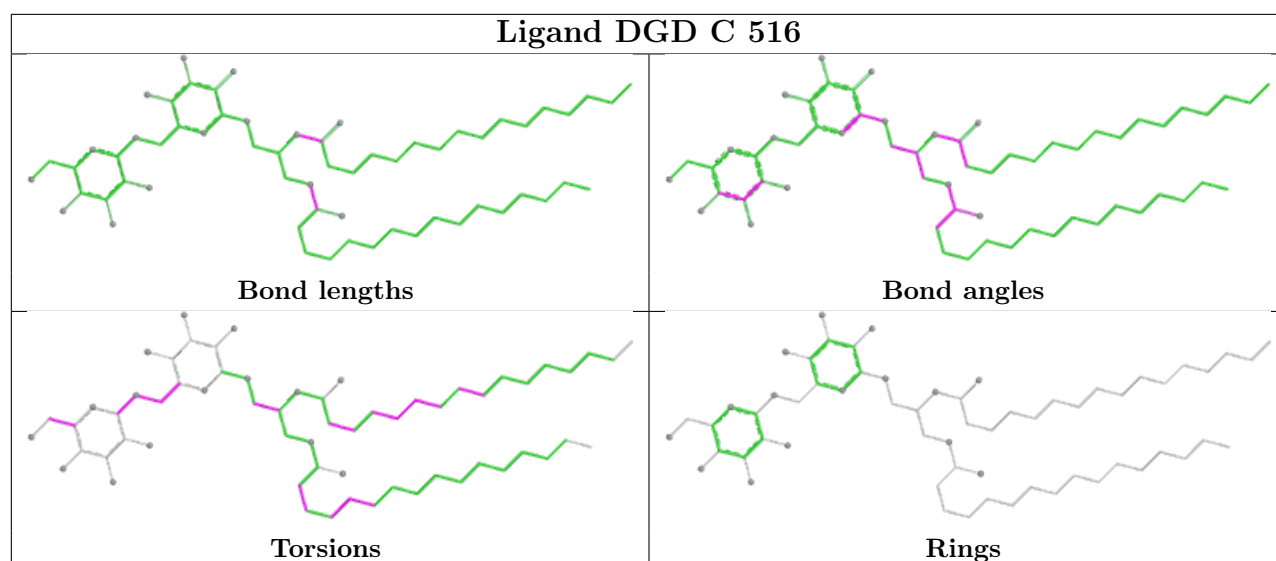
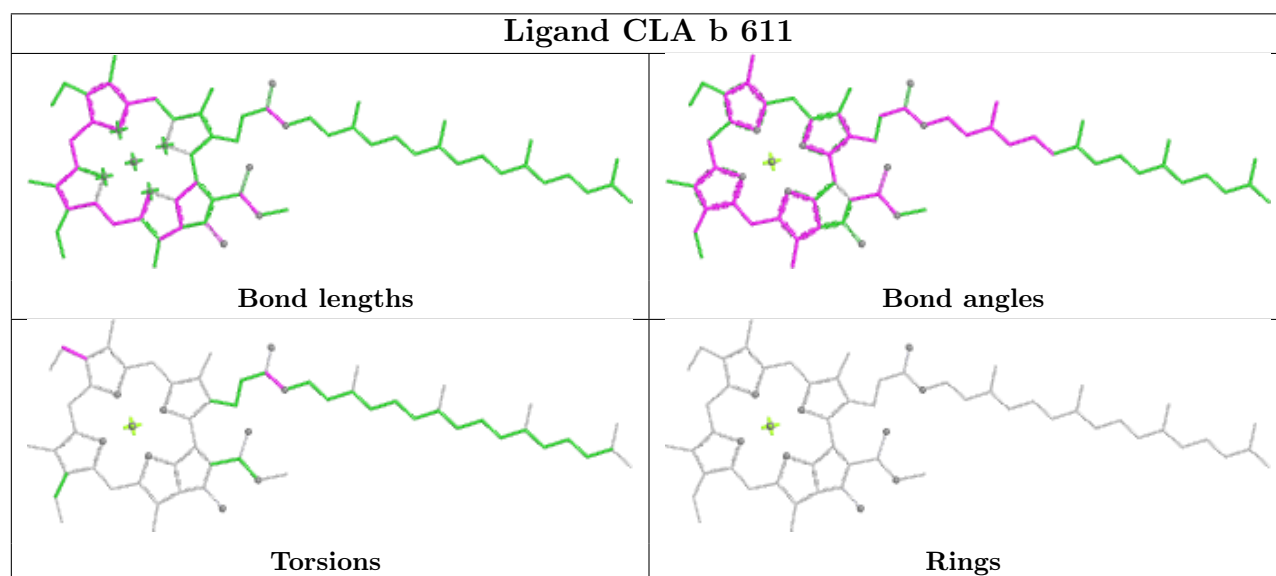
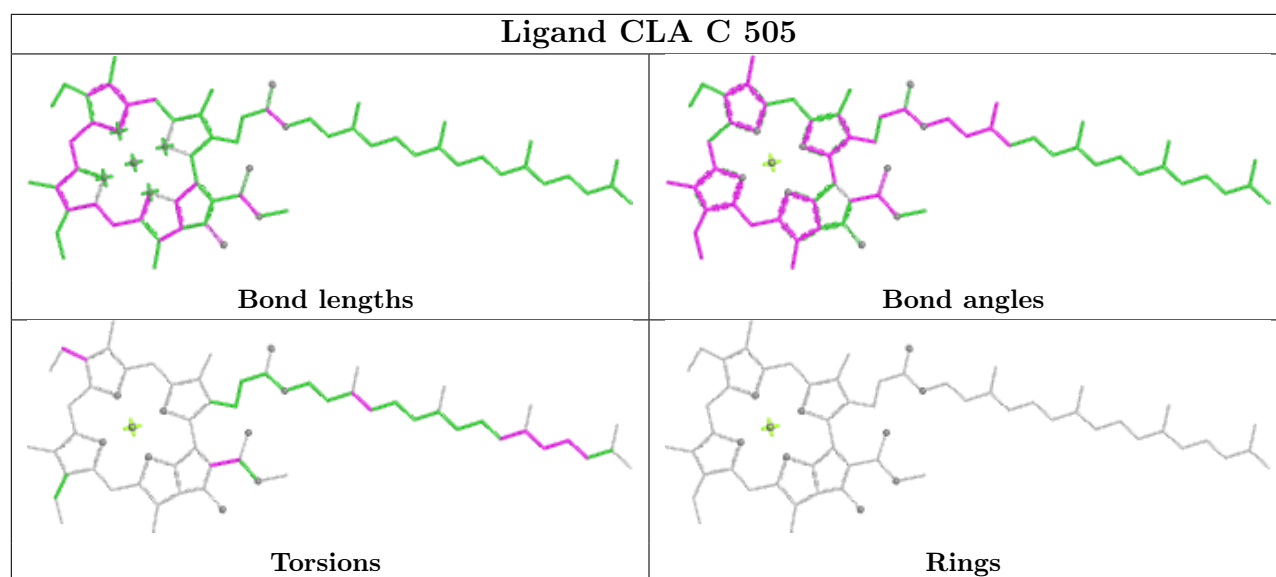
Ligand HEM F 102



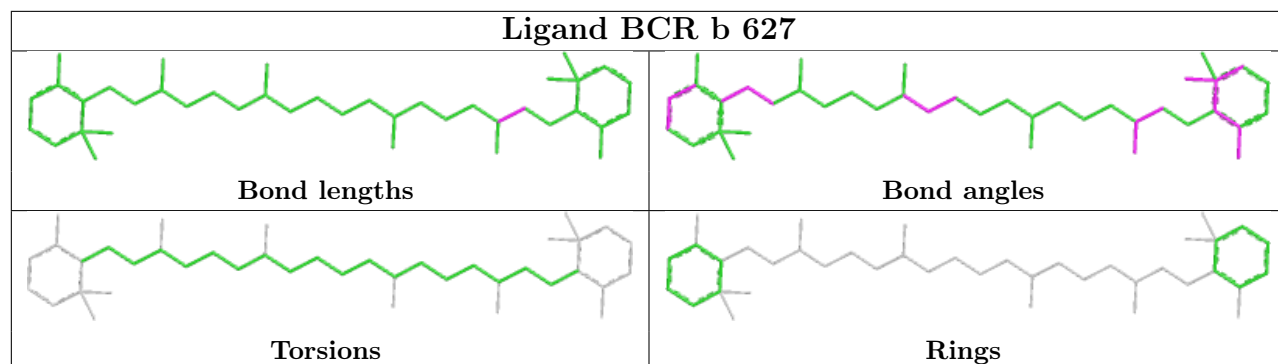




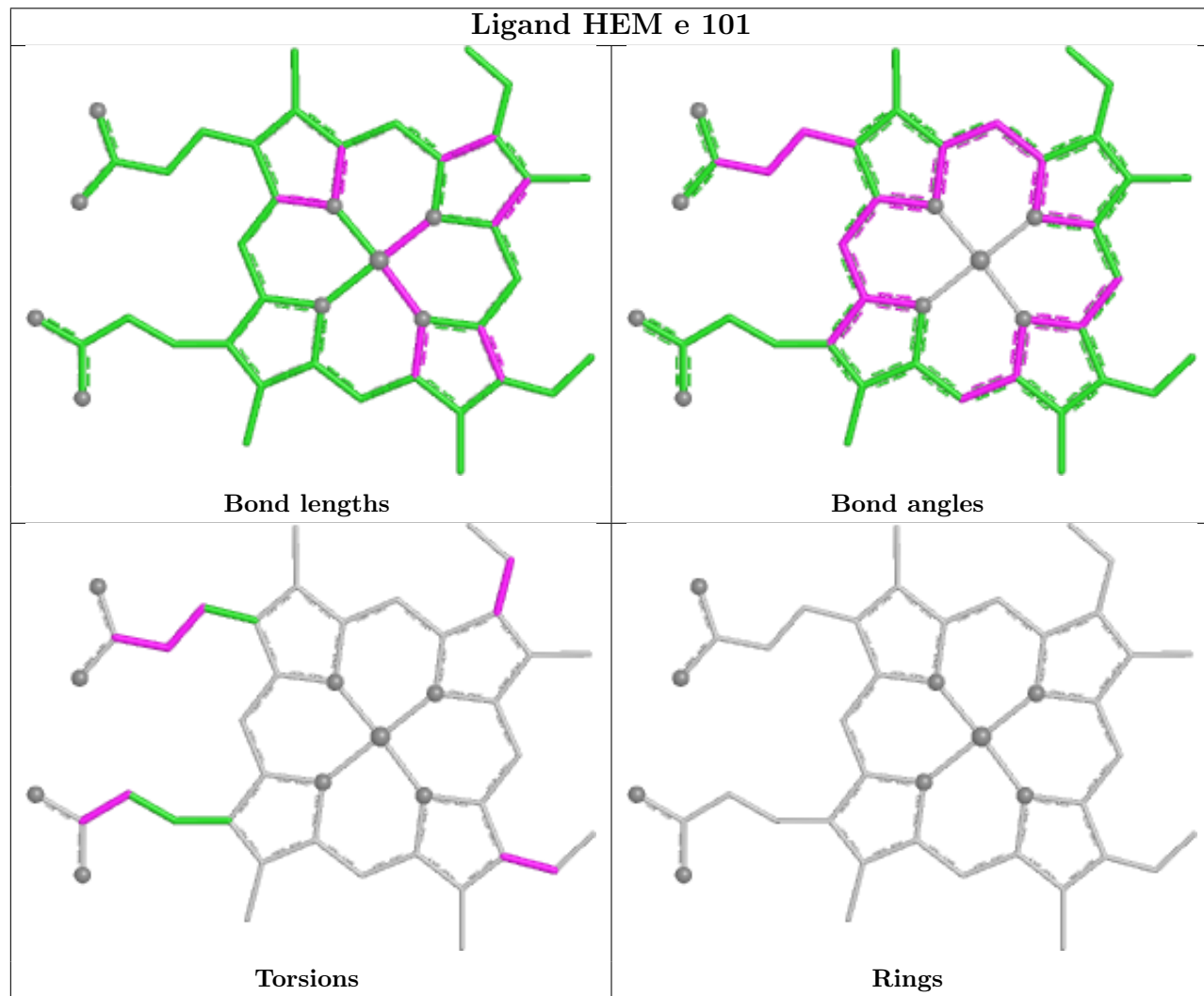


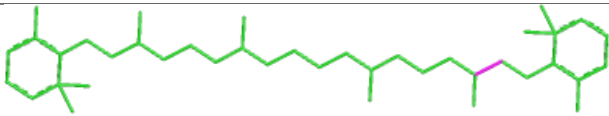
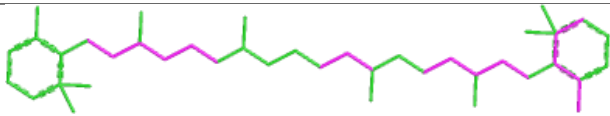
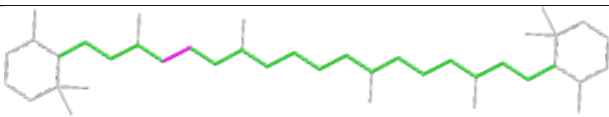
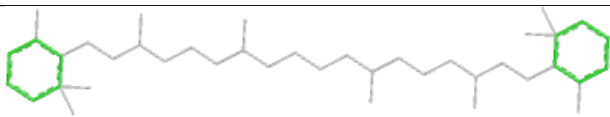


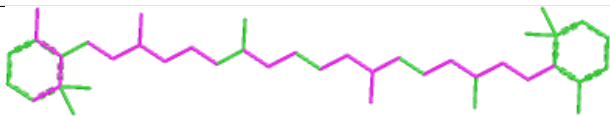
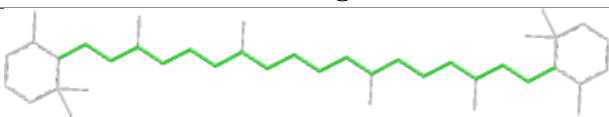
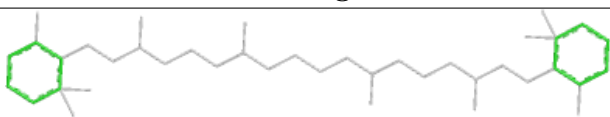
Ligand BCR b 627

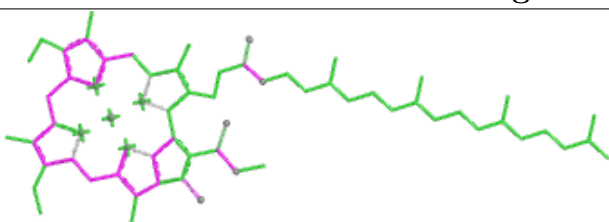
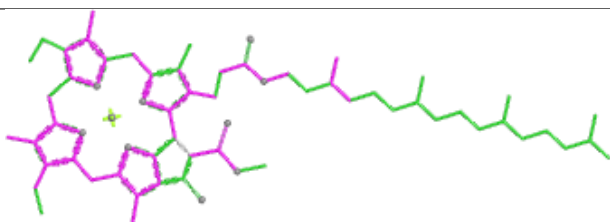
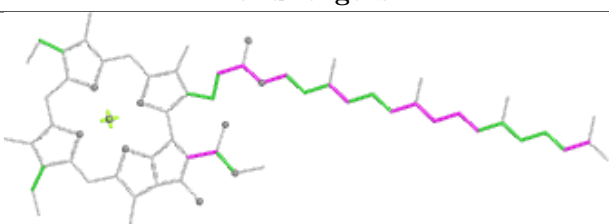
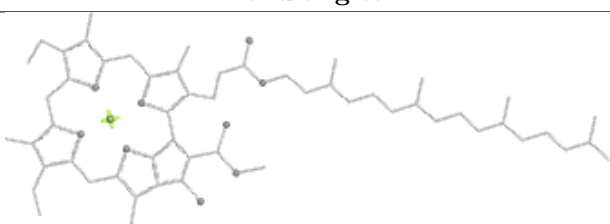


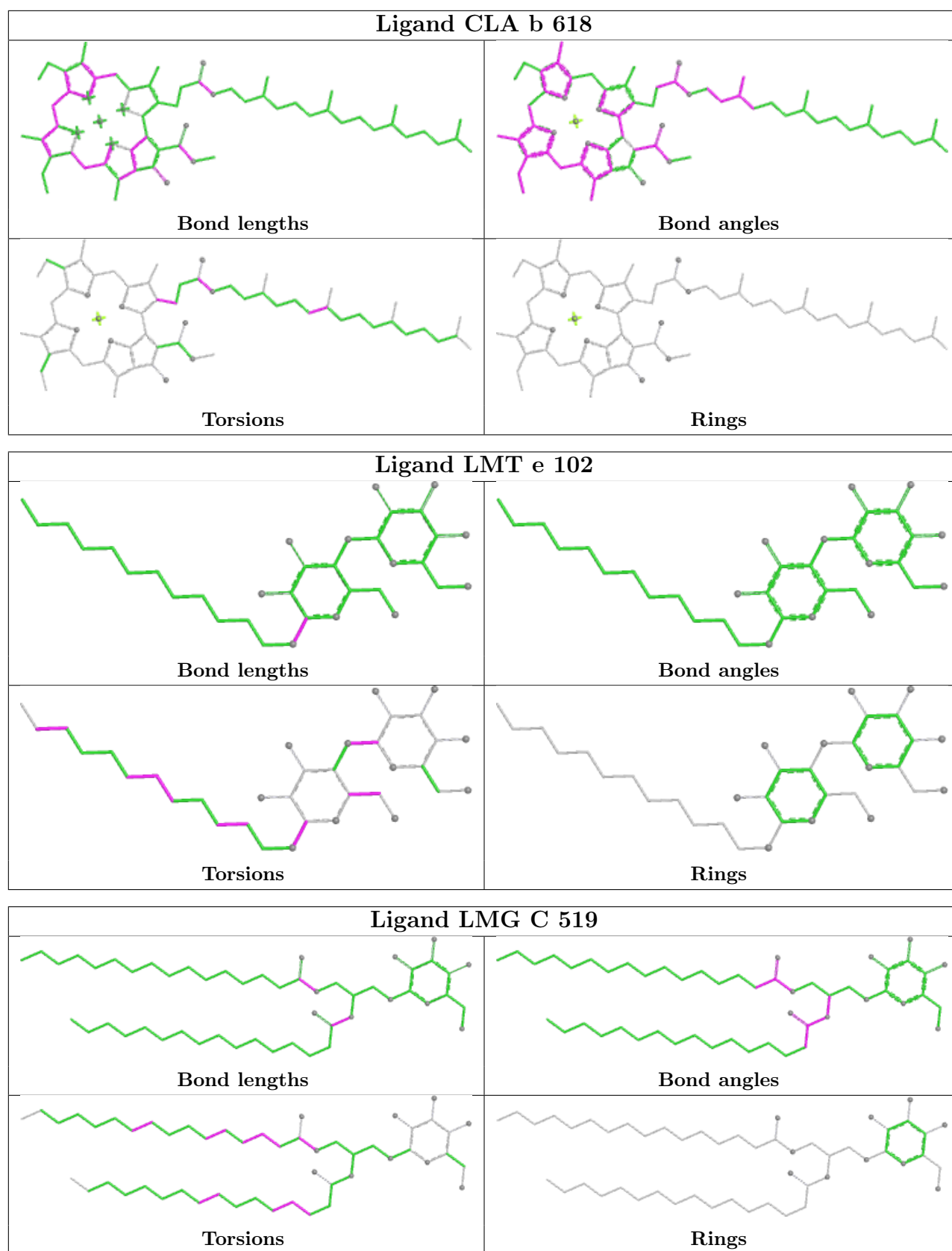
Ligand HEM e 101



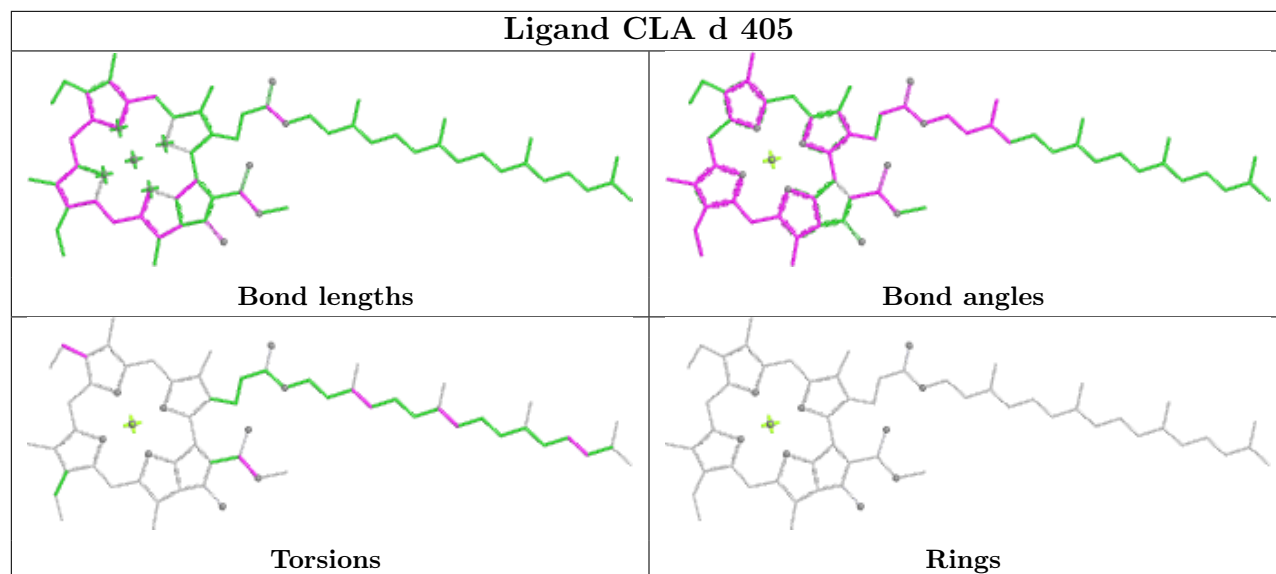
Ligand BCR h 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR k 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

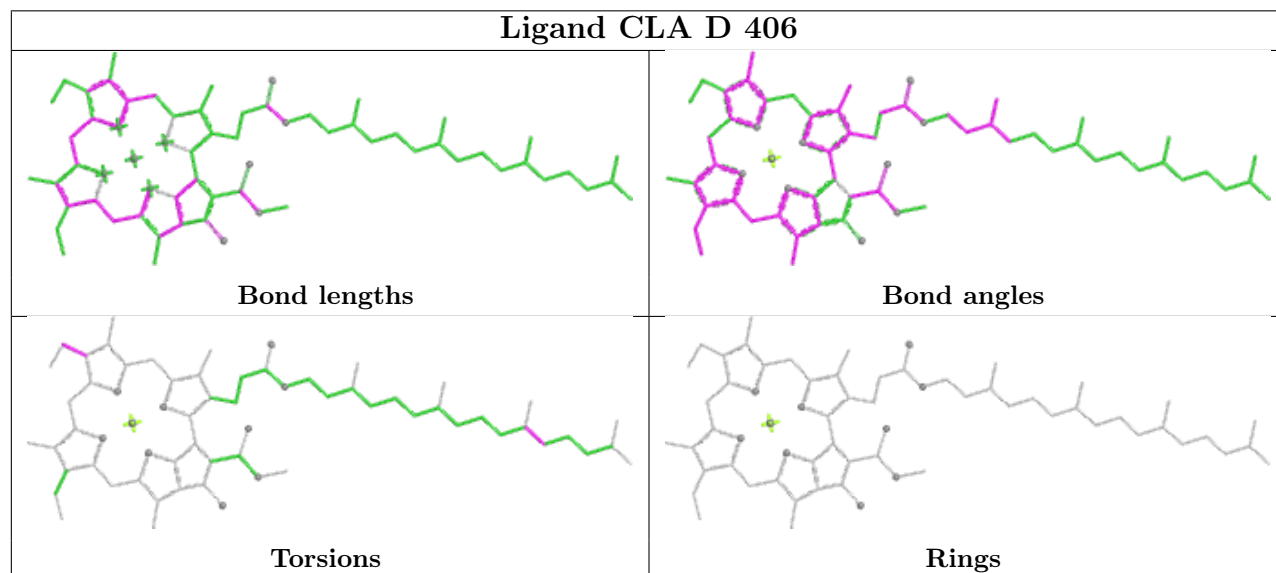
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Bond lengths	Bond angles
	
Torsions	Rings



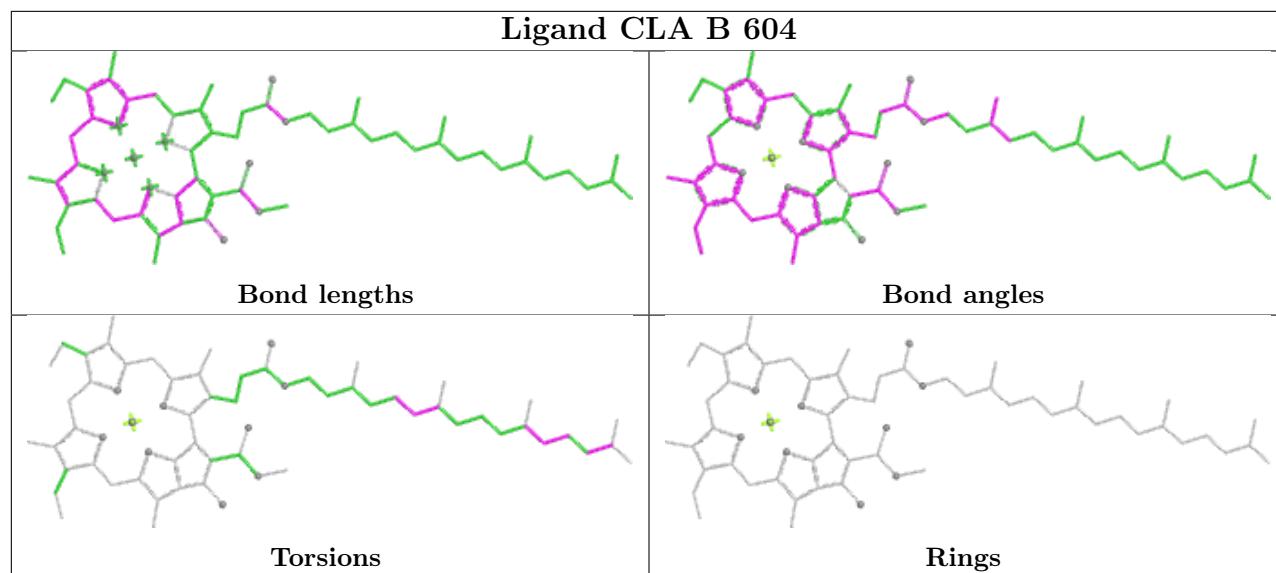
Ligand CLA d 405

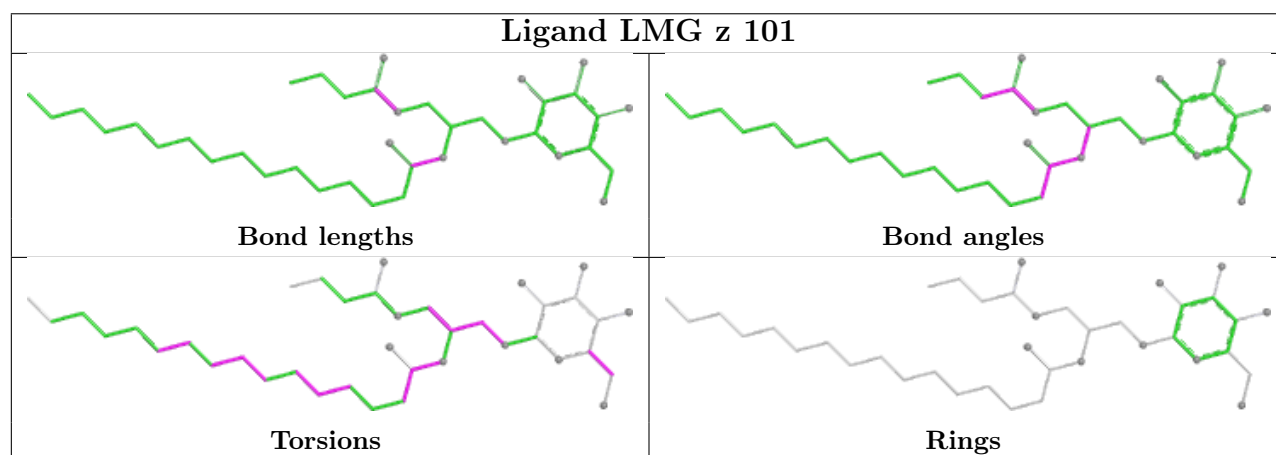
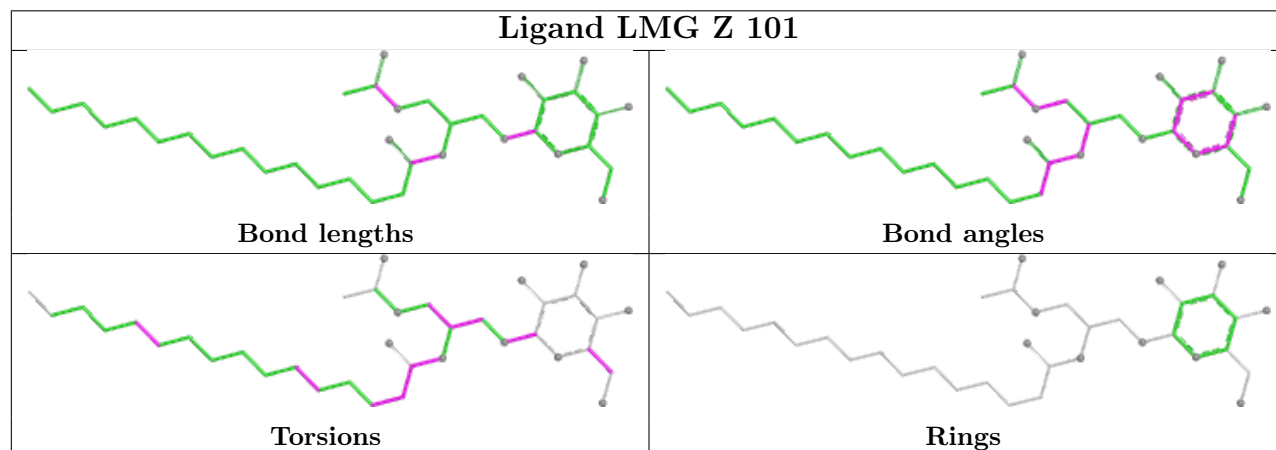
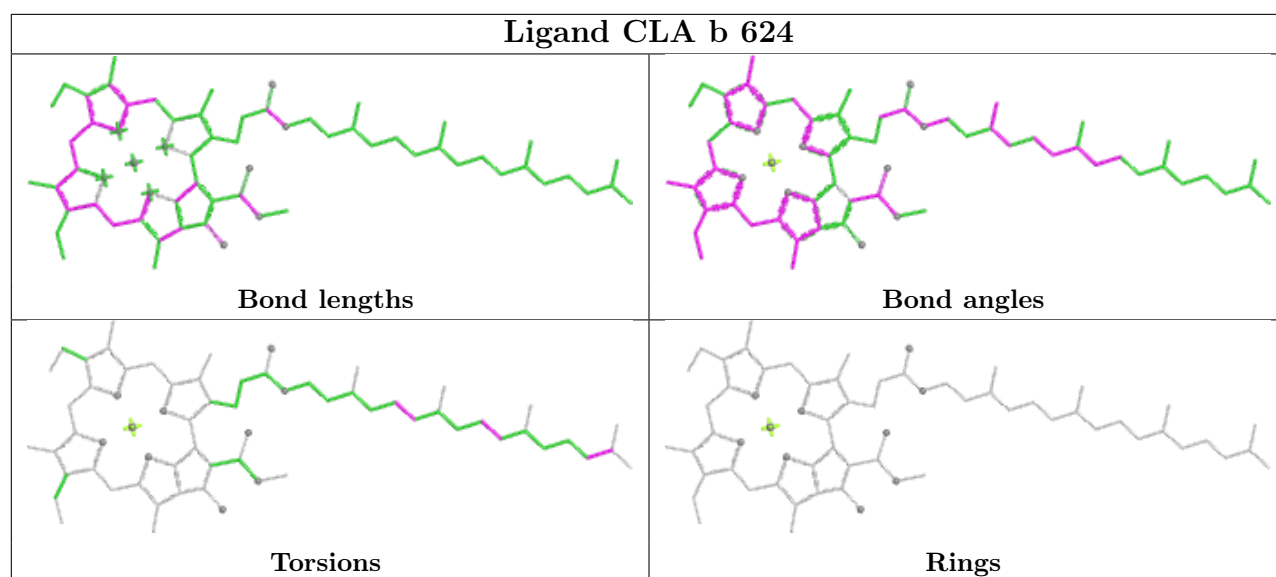


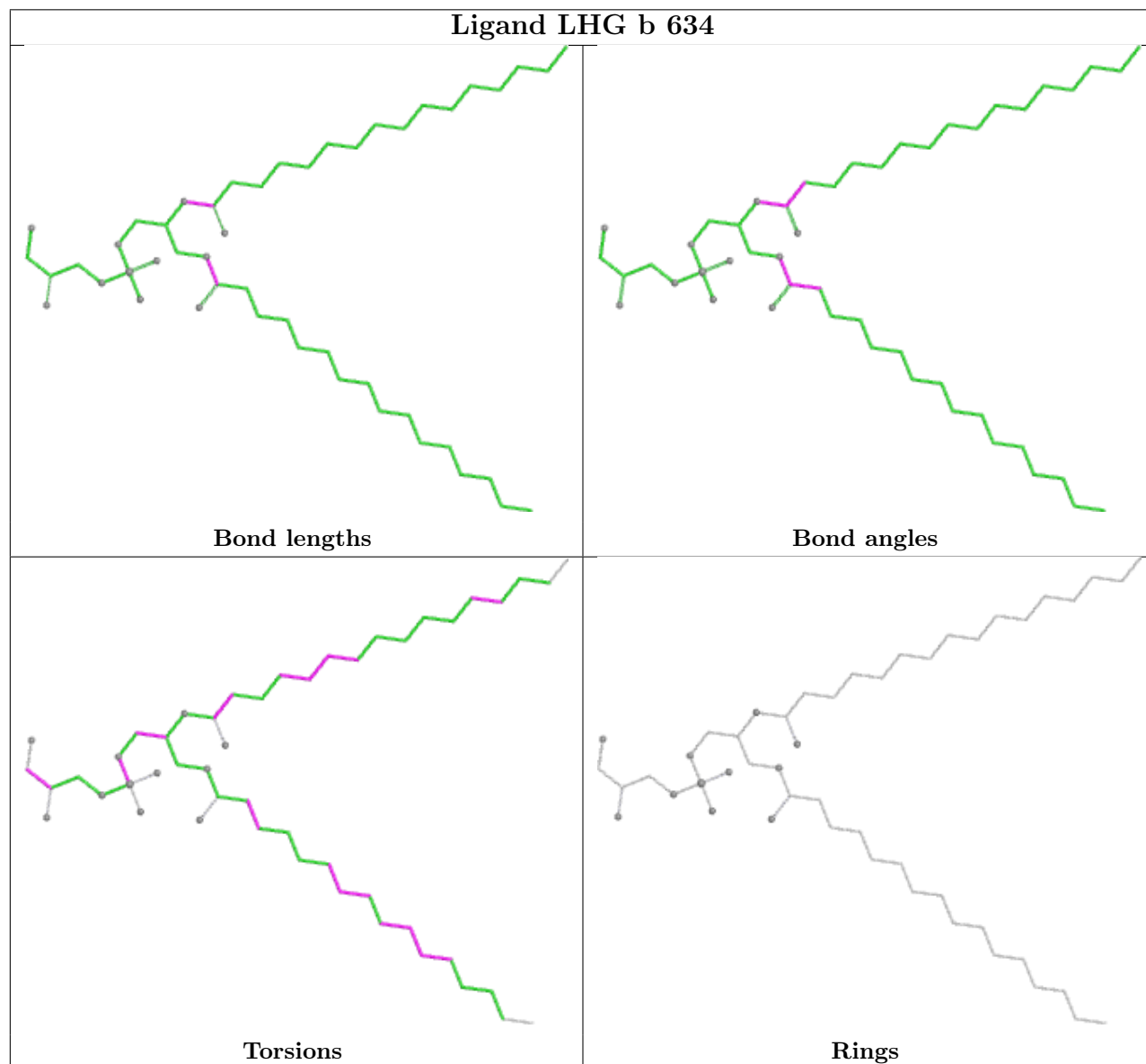
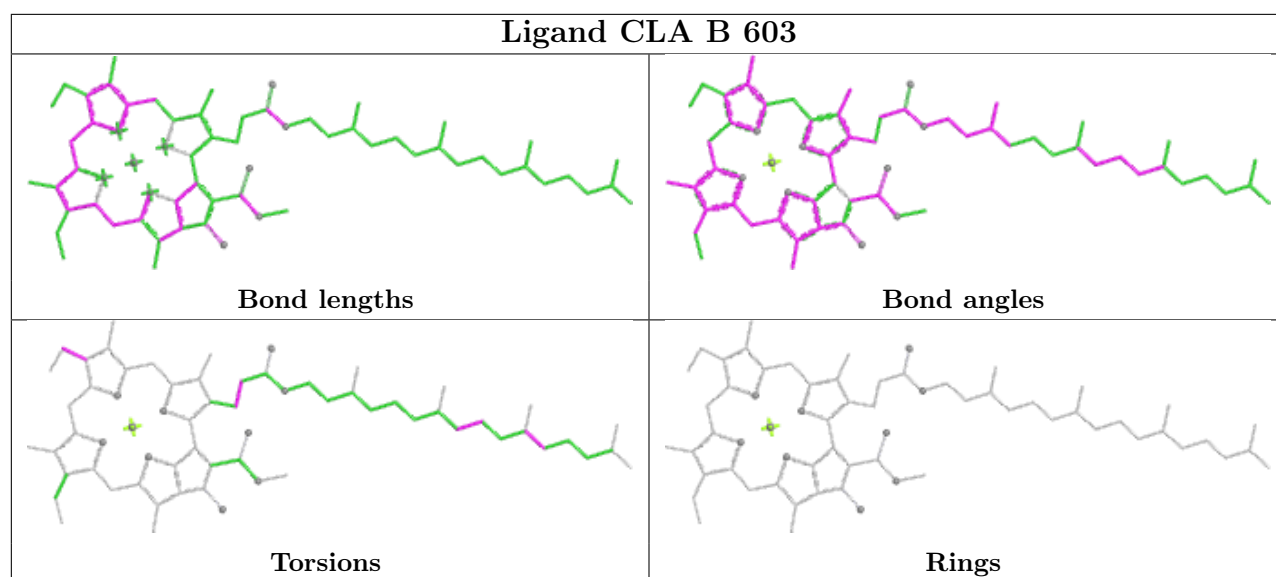
Ligand CLA D 406

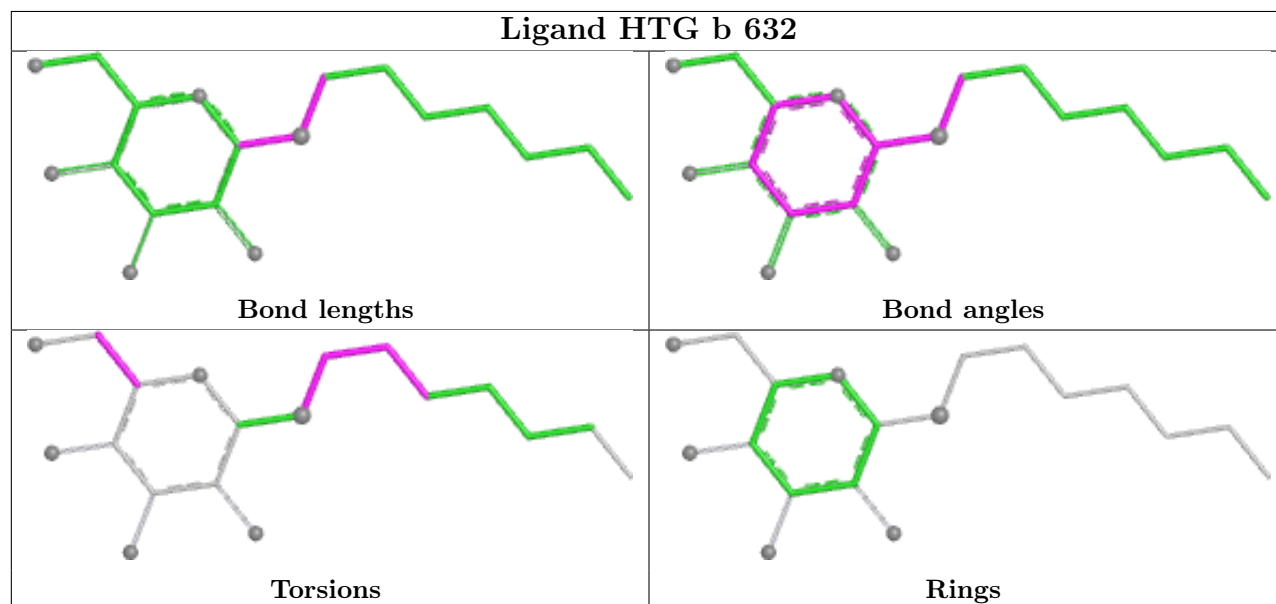
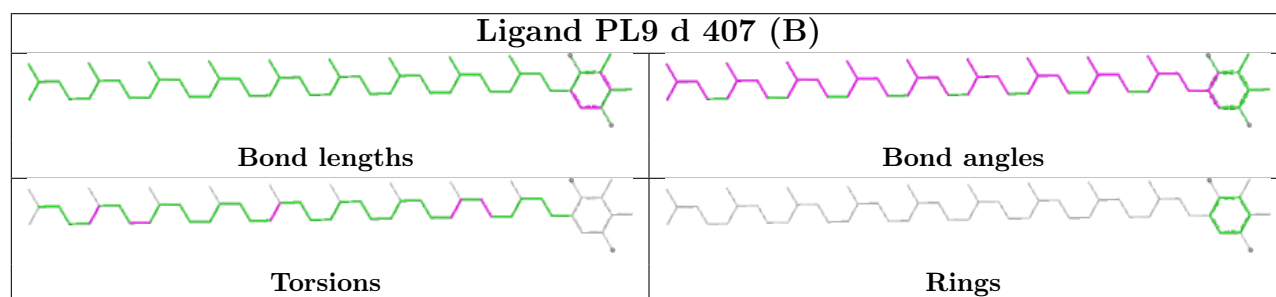
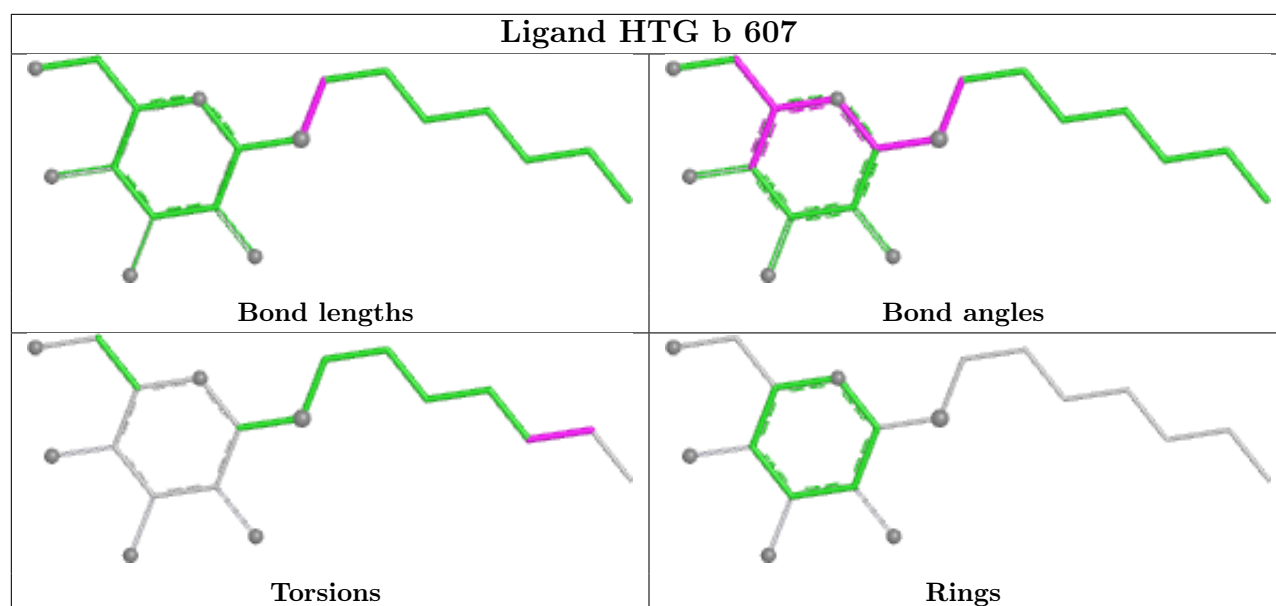


Ligand CLA B 604

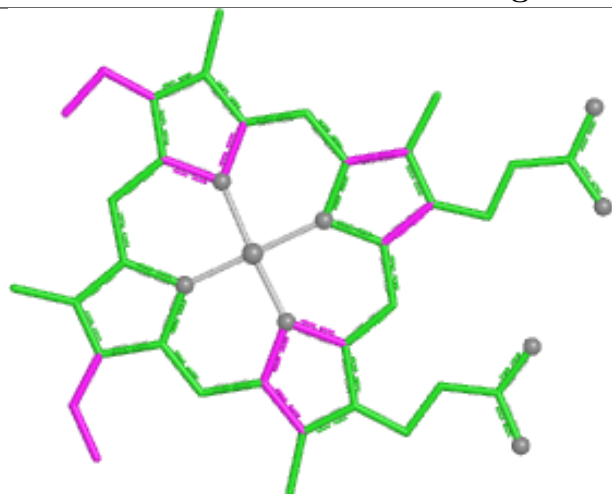




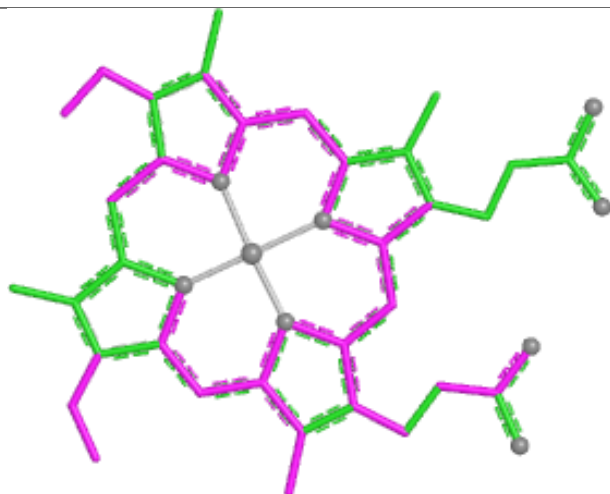




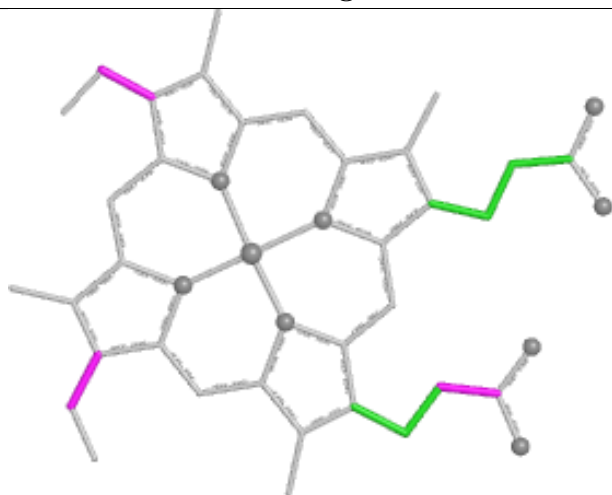
Ligand HEC V 206



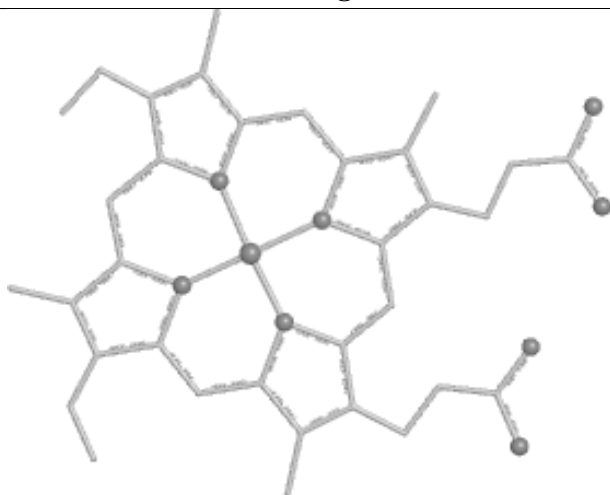
Bond lengths



Bond angles



Torsions

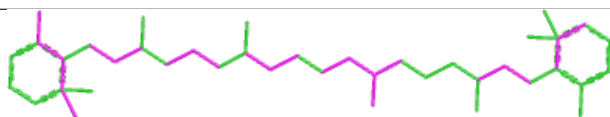


Rings

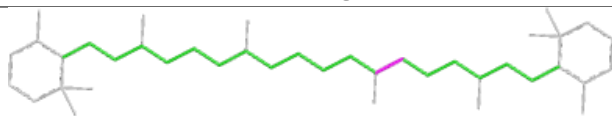
Ligand BCR b 626



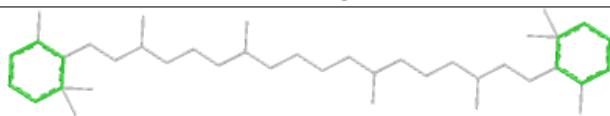
Bond lengths



Bond angles

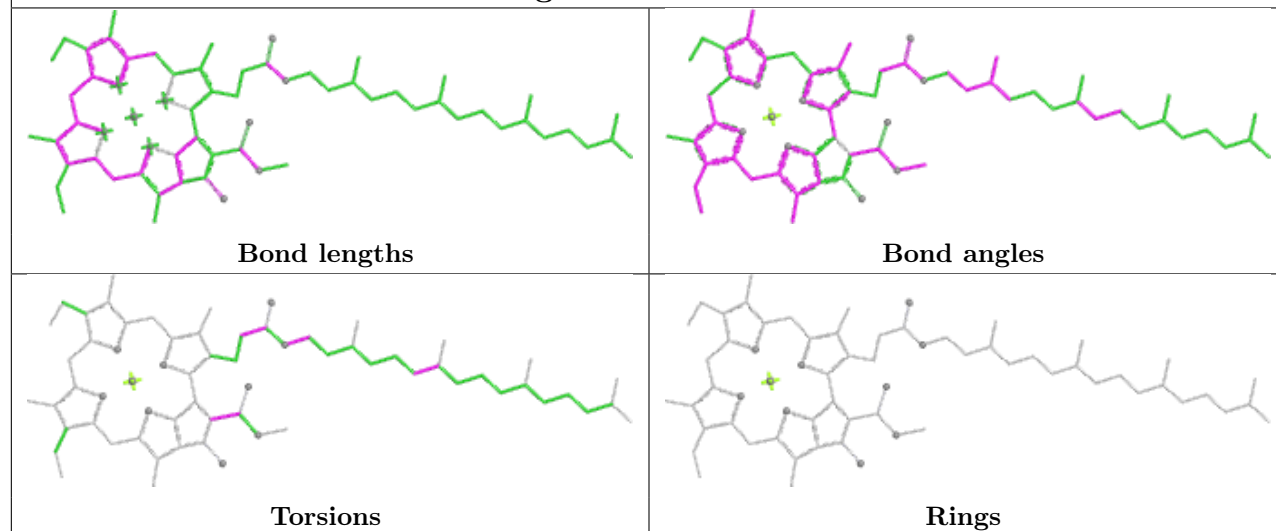


Torsions

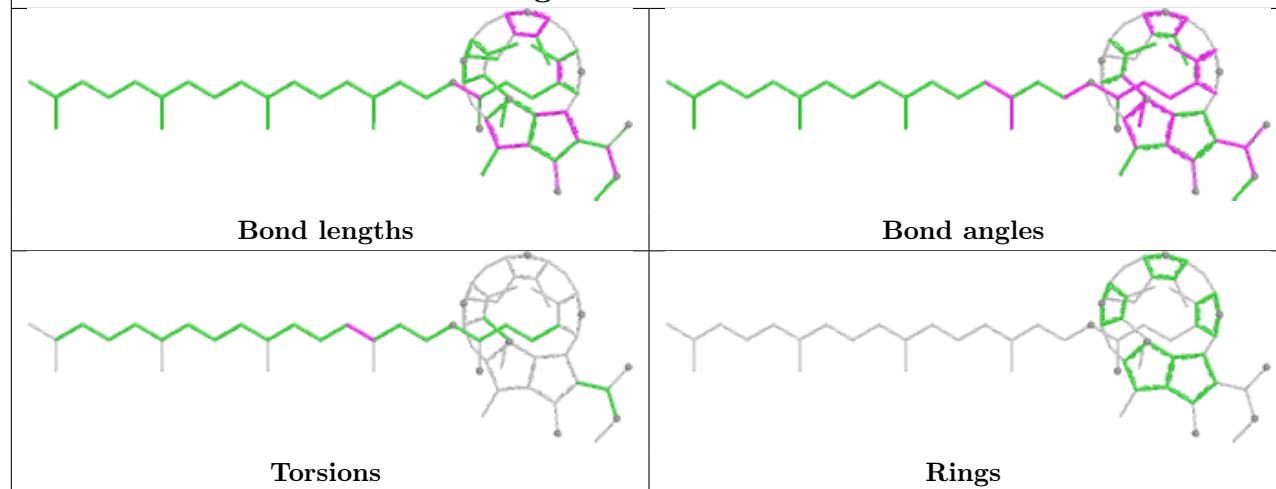


Rings

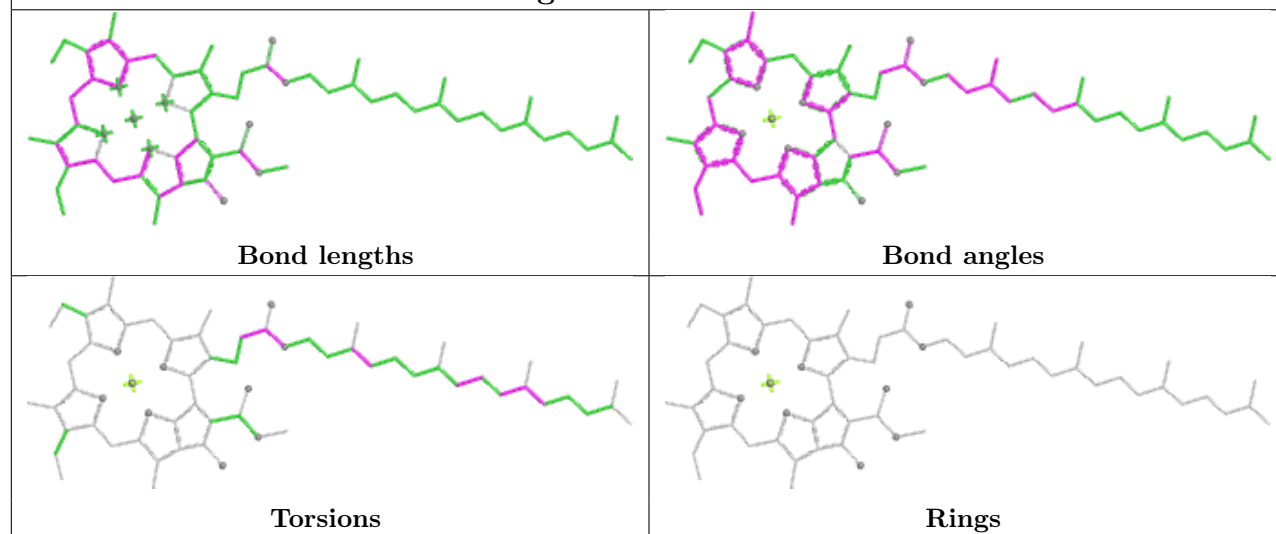
Ligand CLA b 622

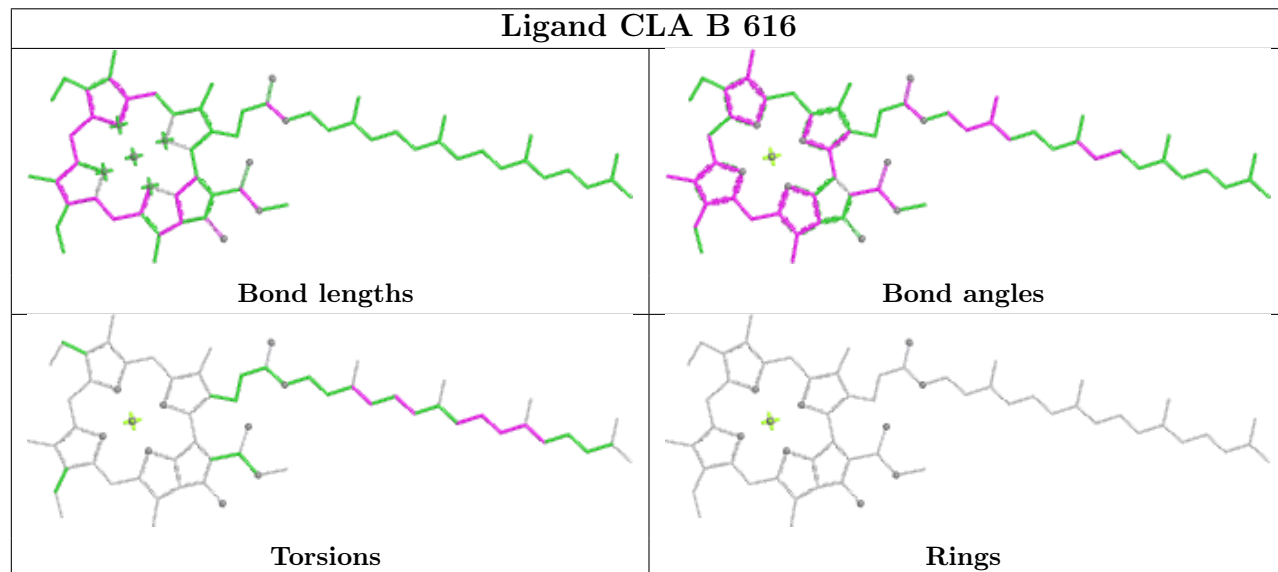
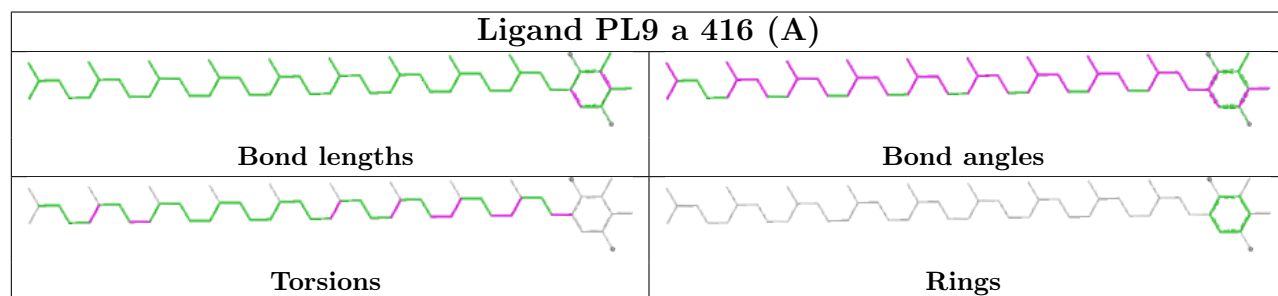
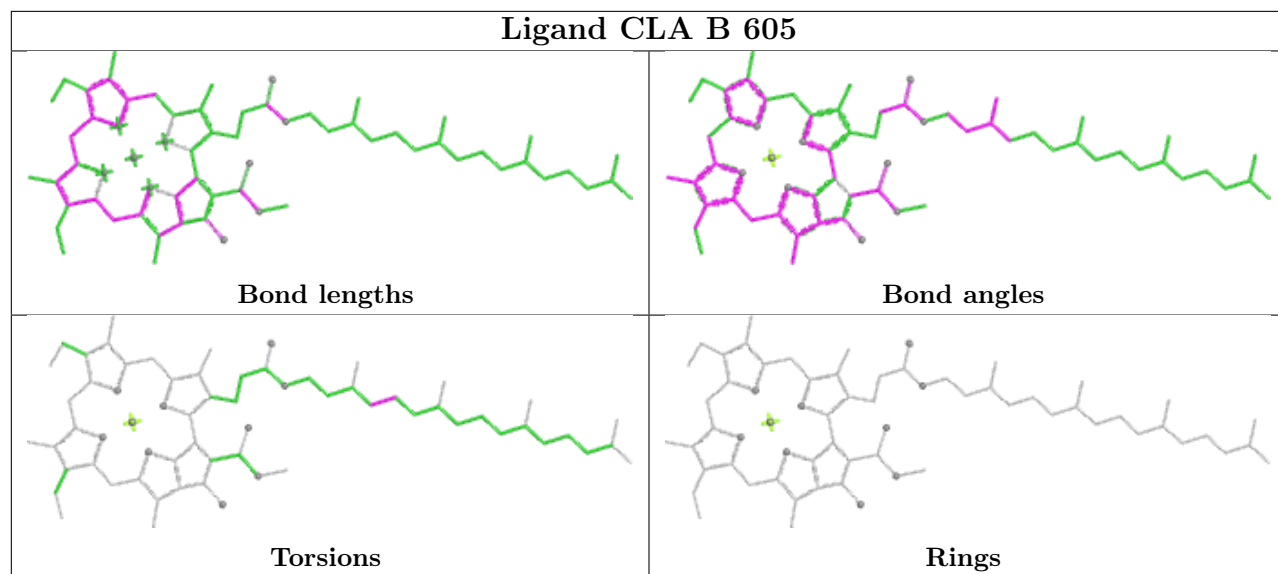


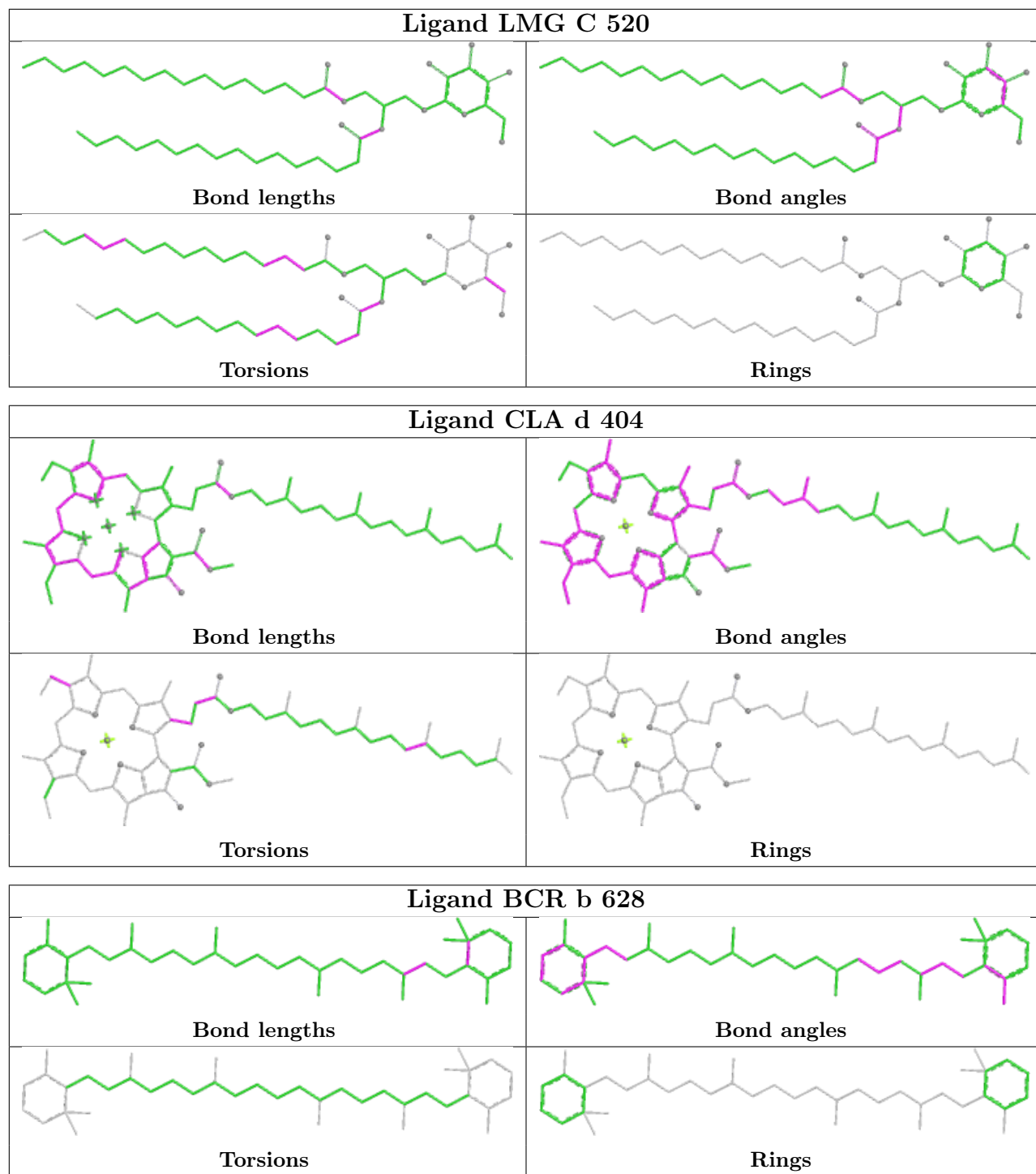
Ligand PHO a 411

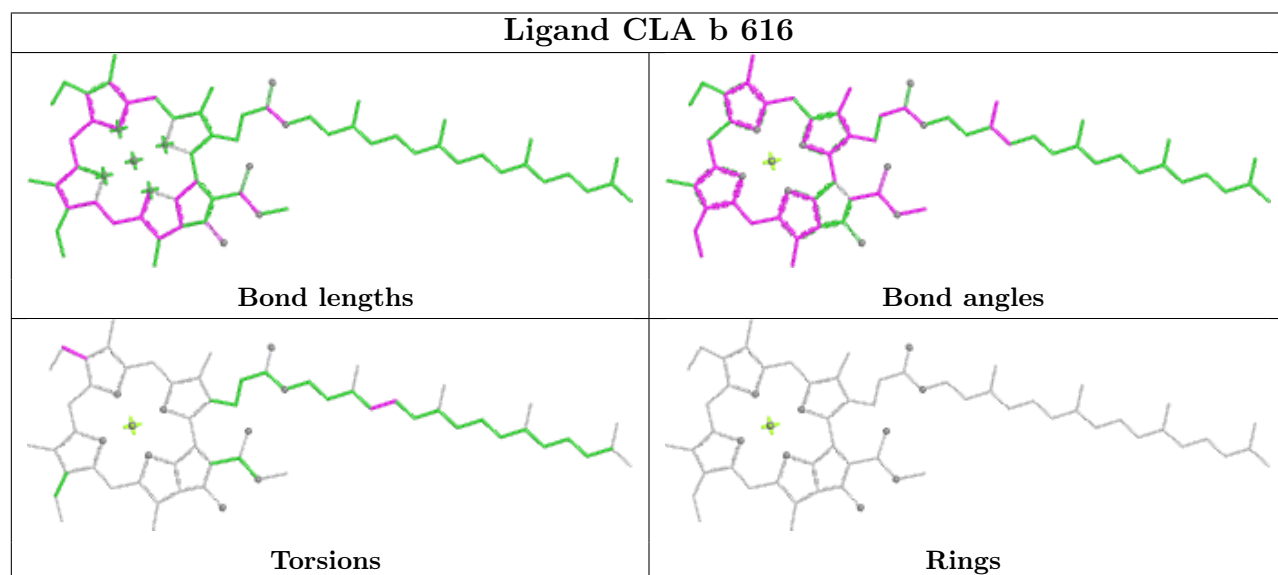
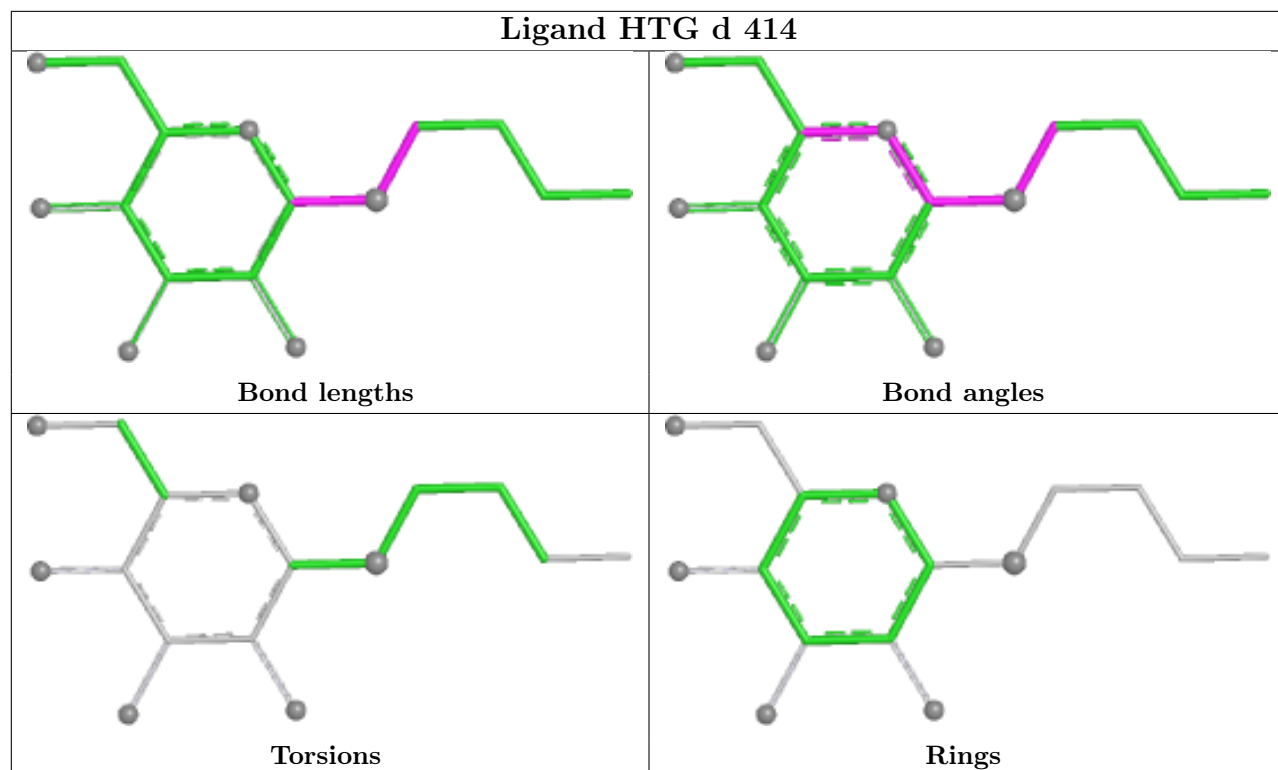


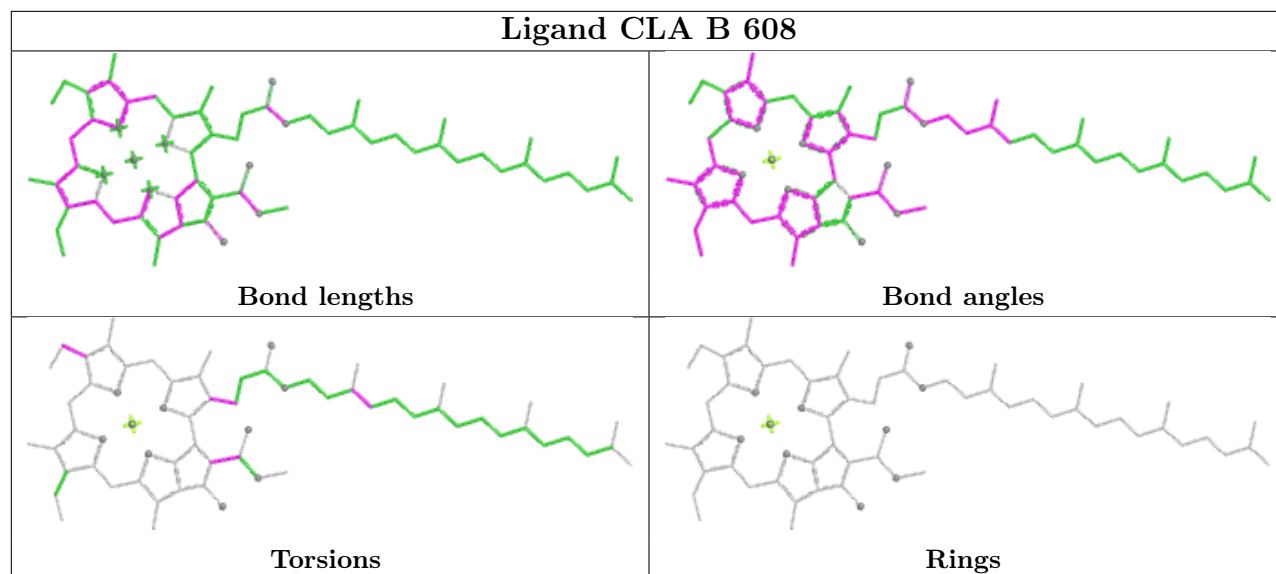
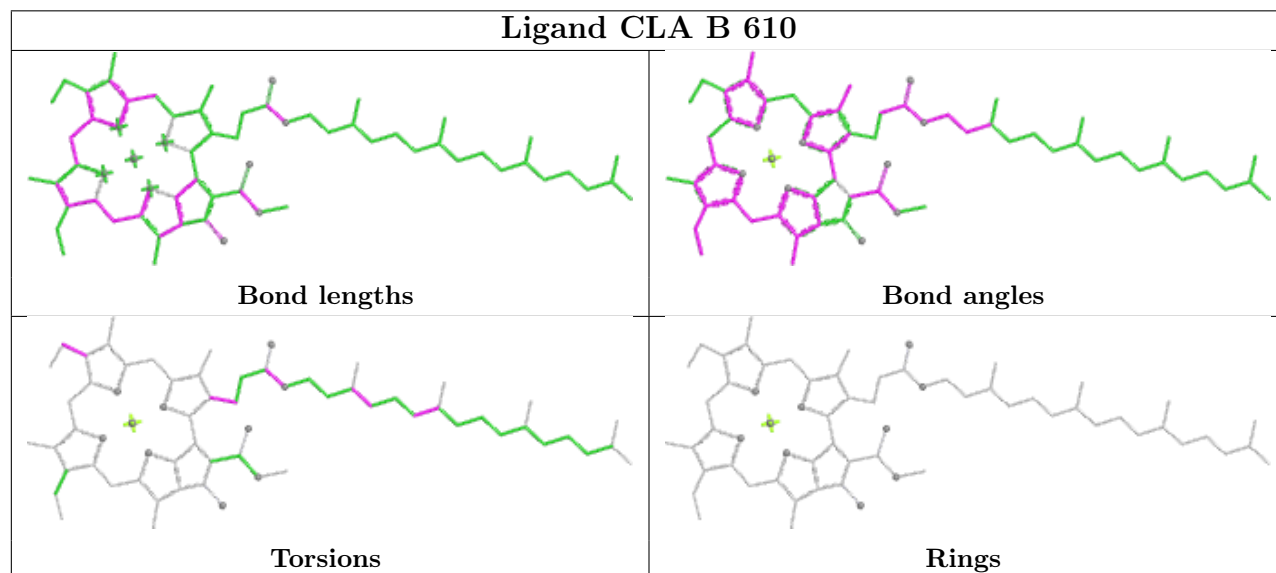
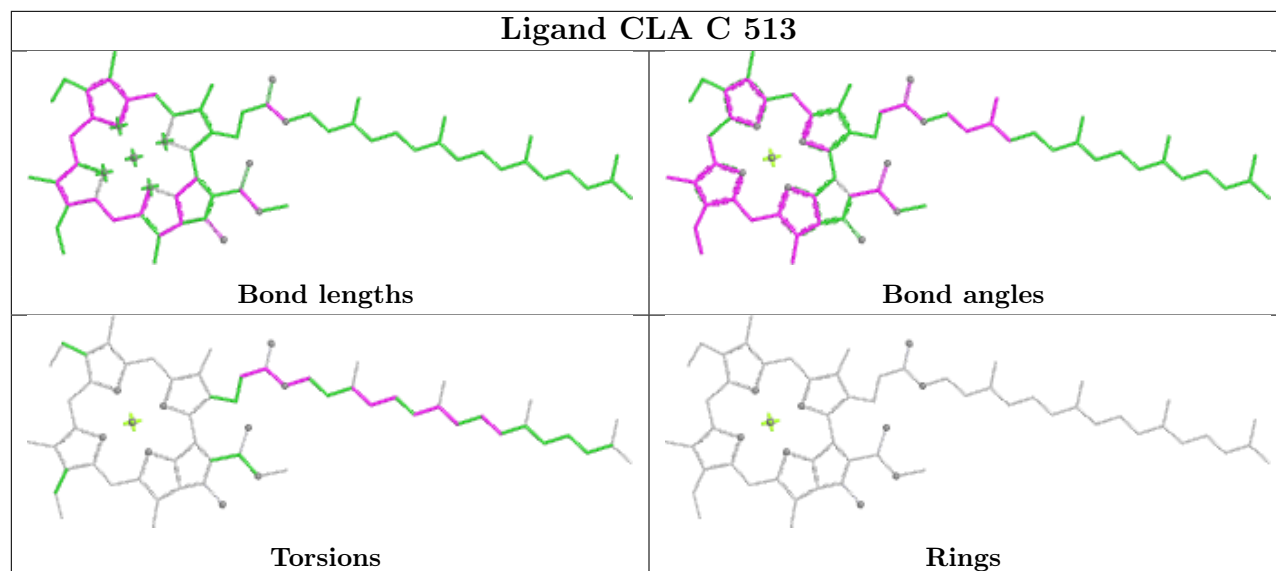
Ligand CLA c 514

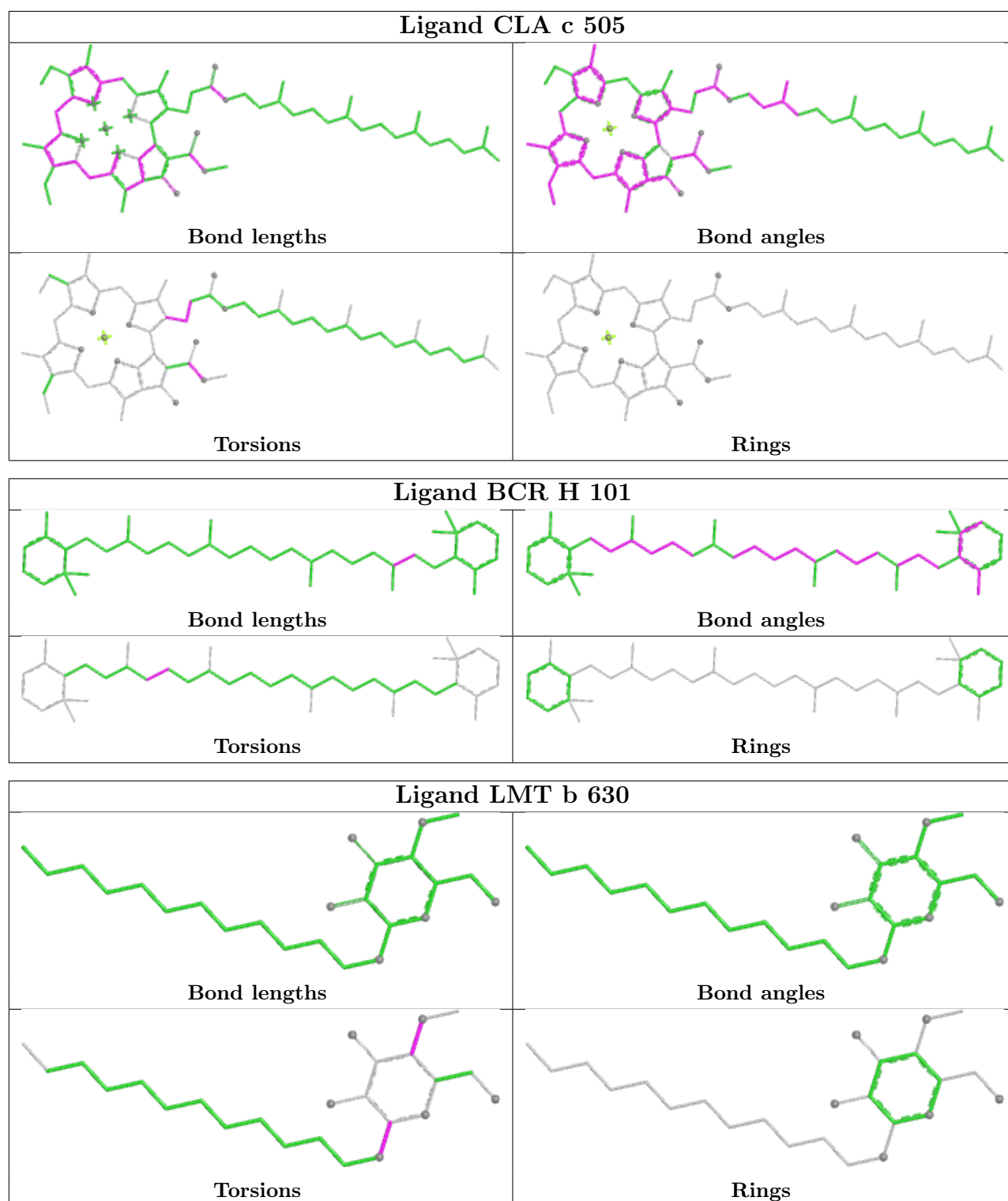


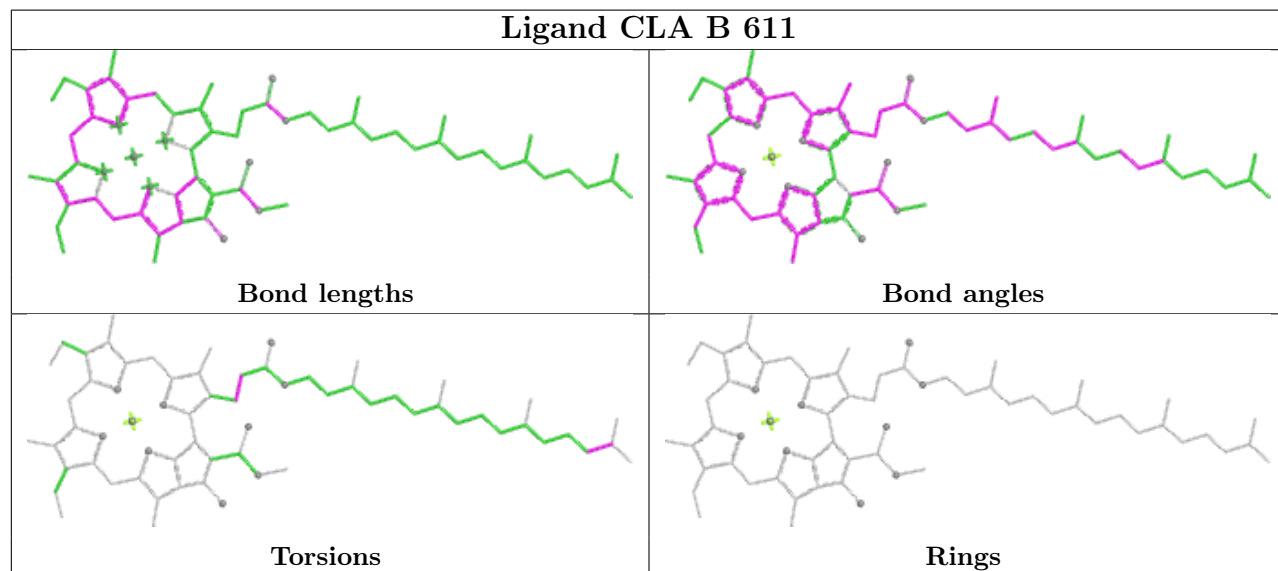
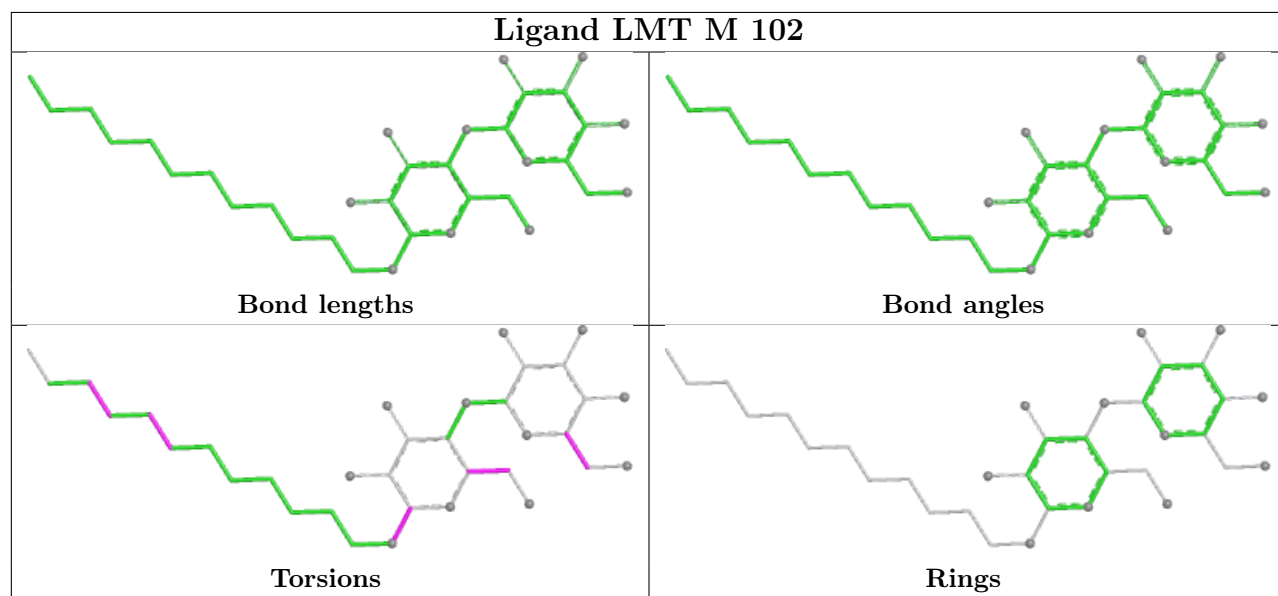
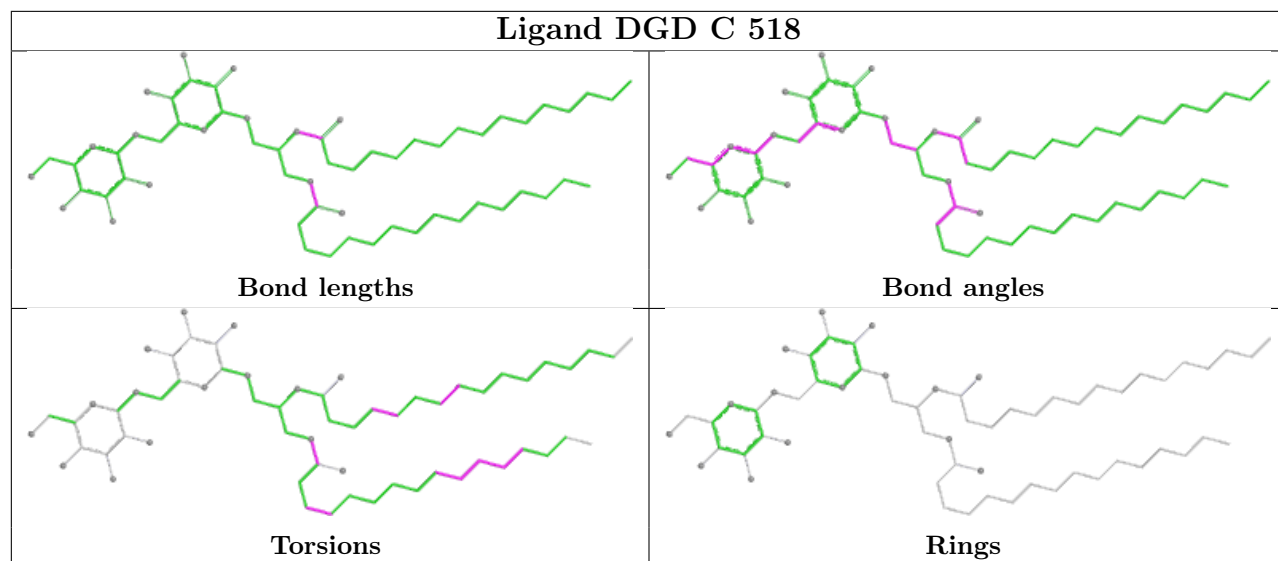


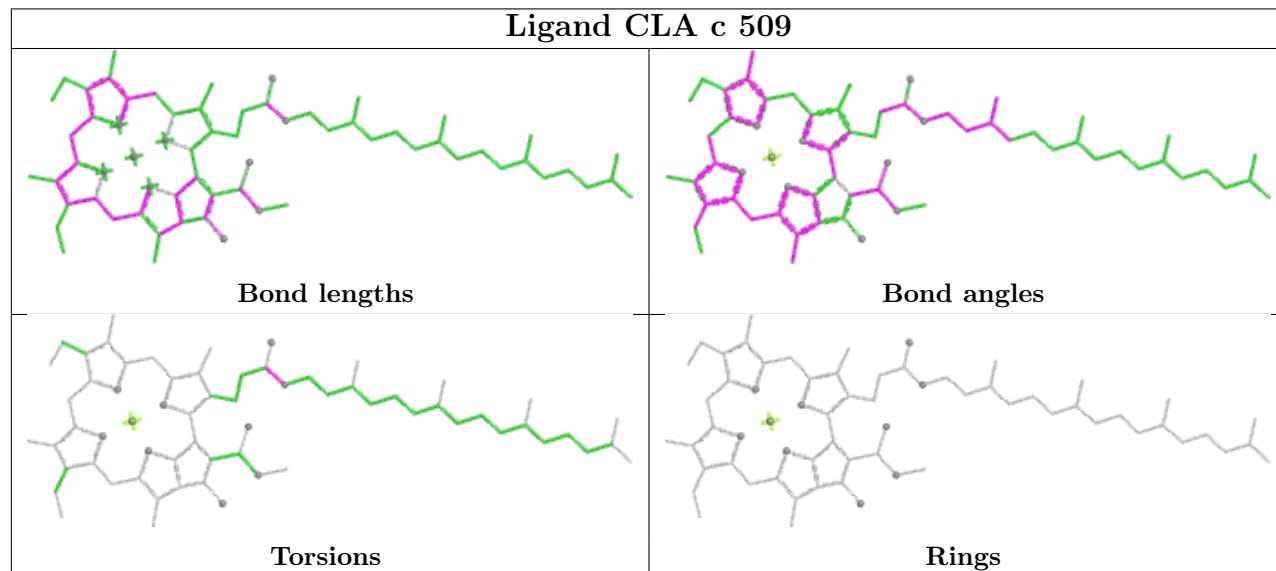
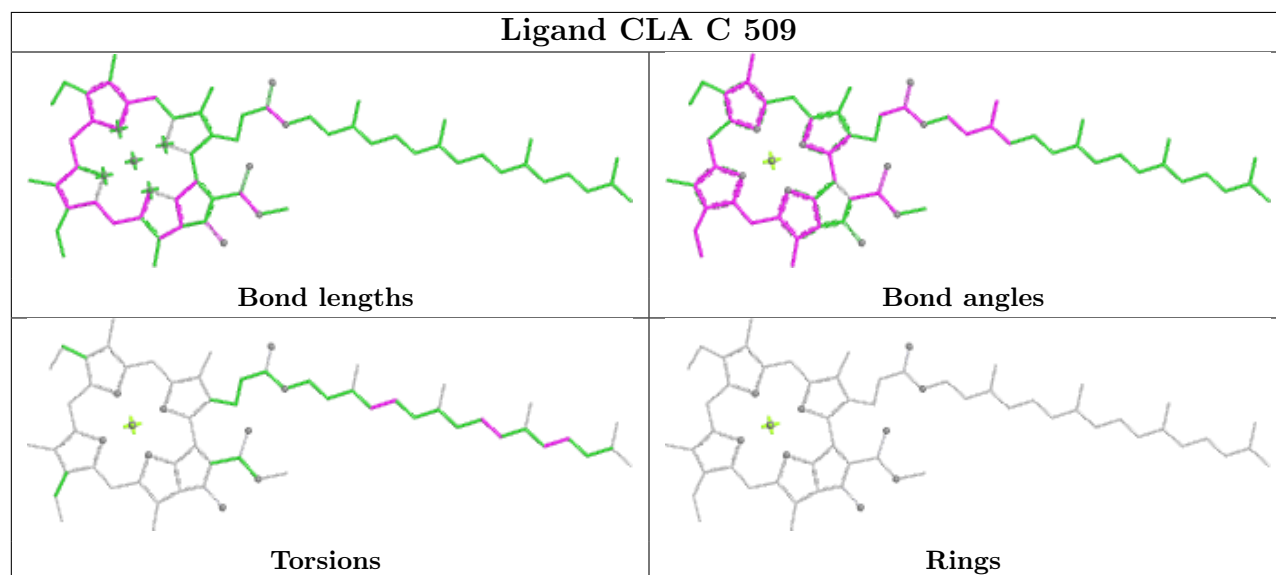
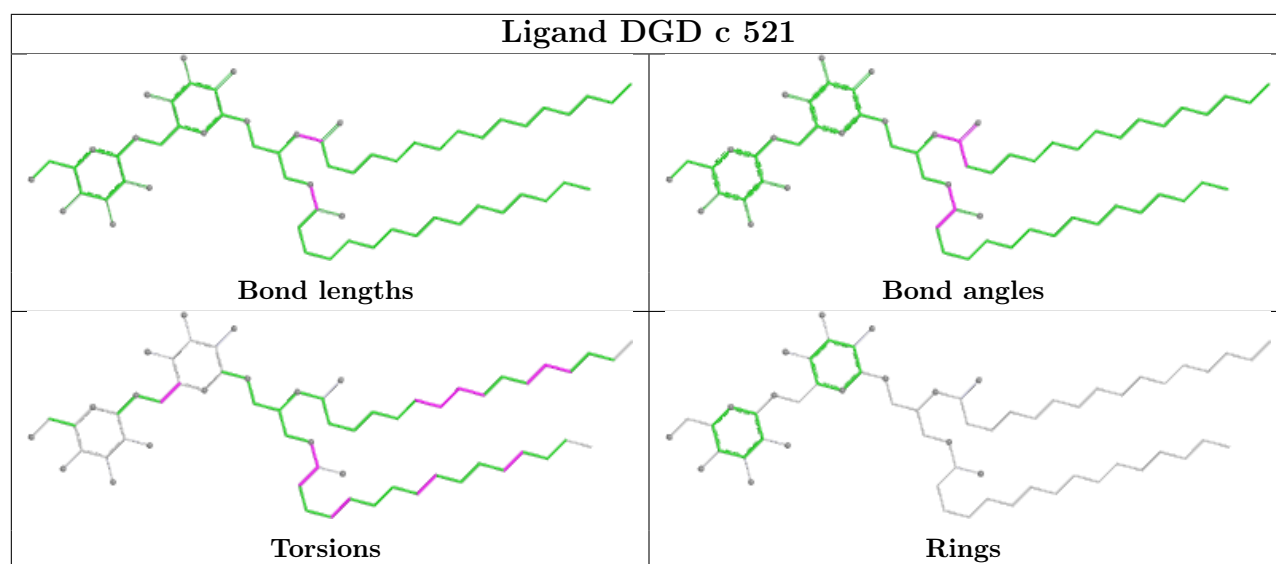


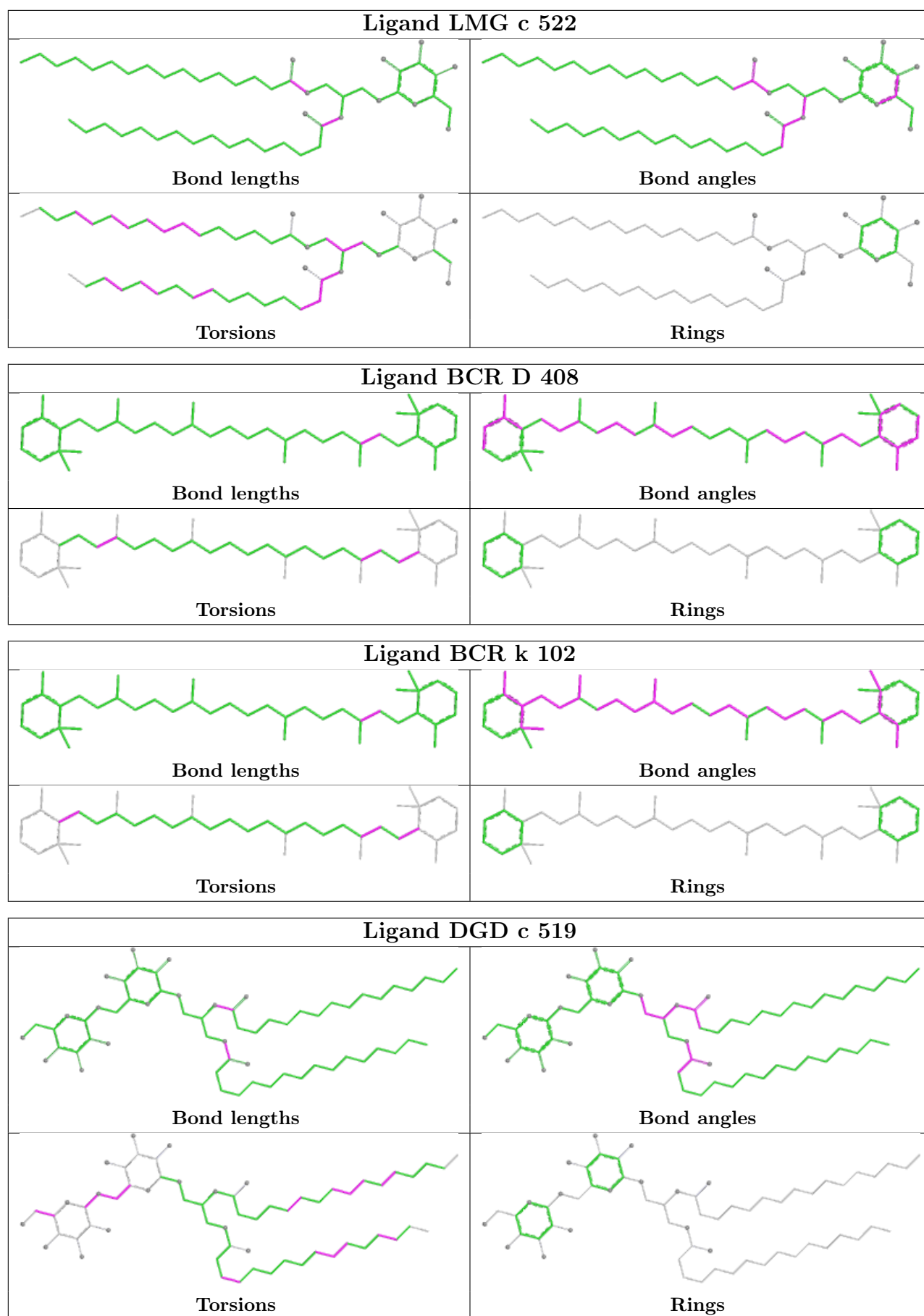


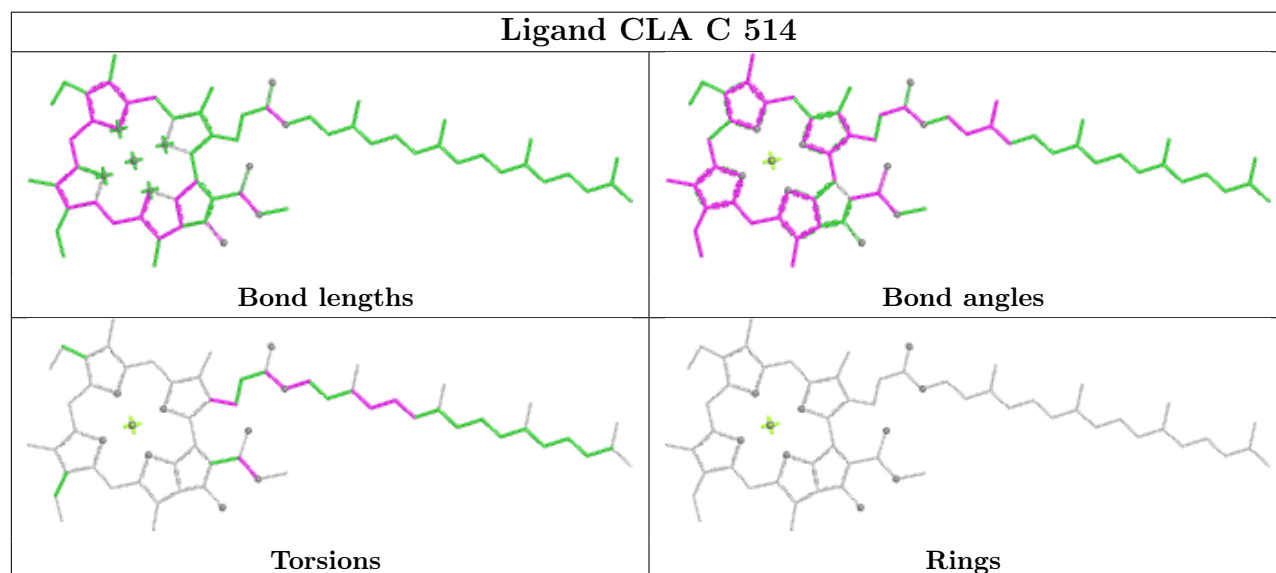
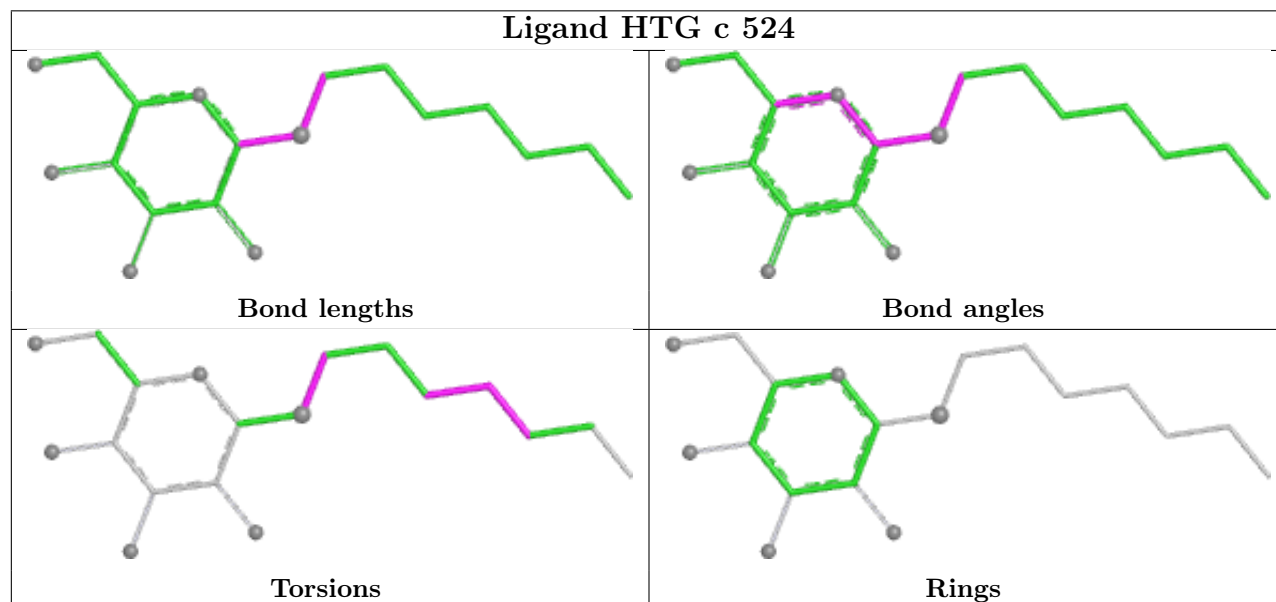
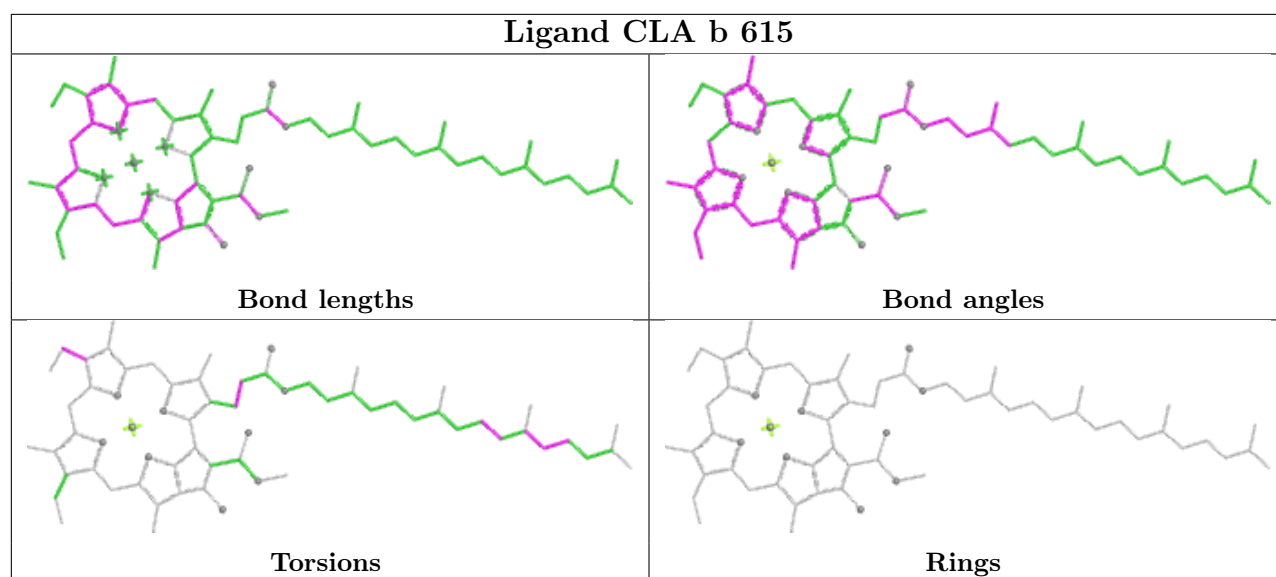
Ligand CLA B 608**Ligand CLA B 610****Ligand CLA C 513**



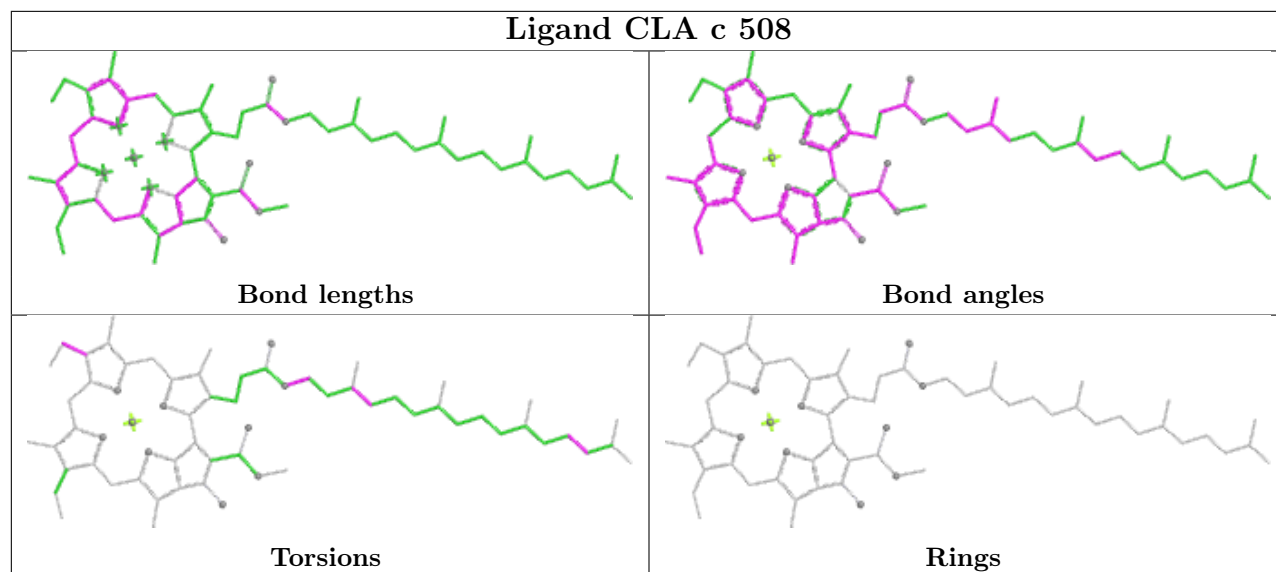




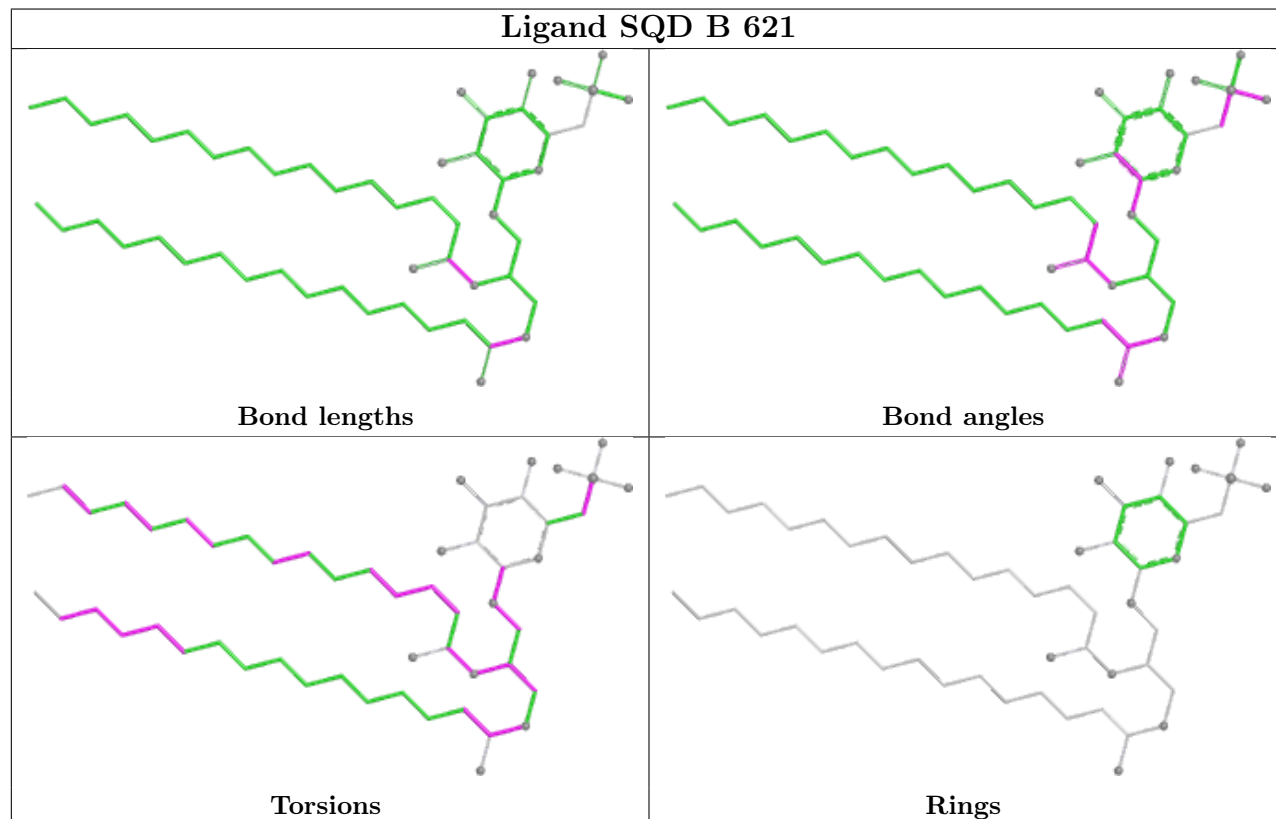


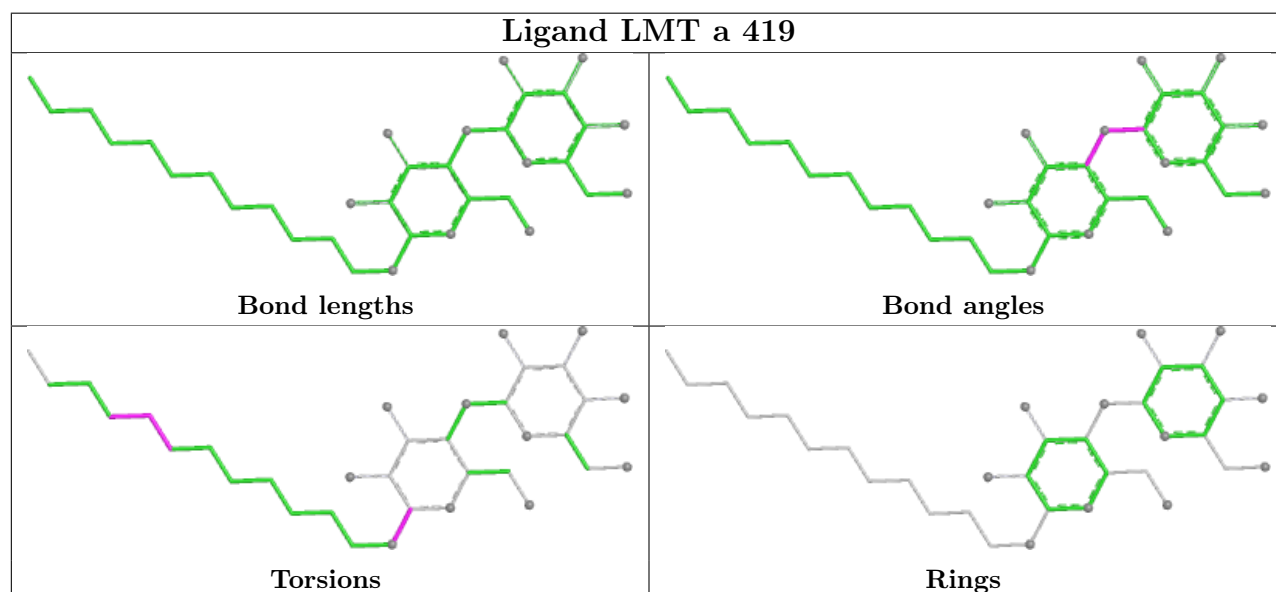
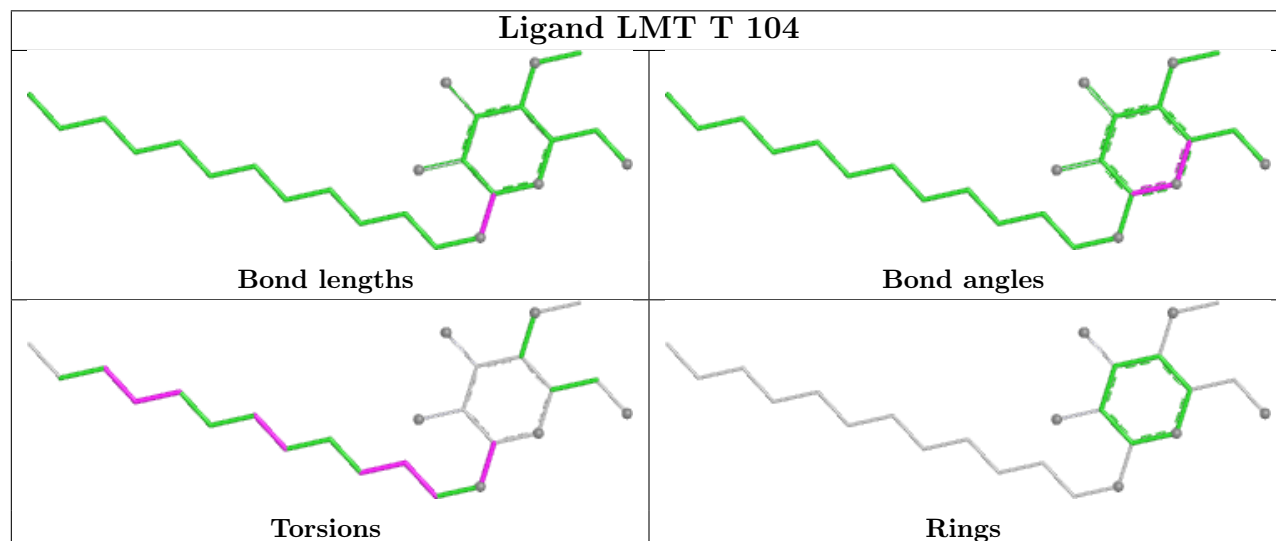
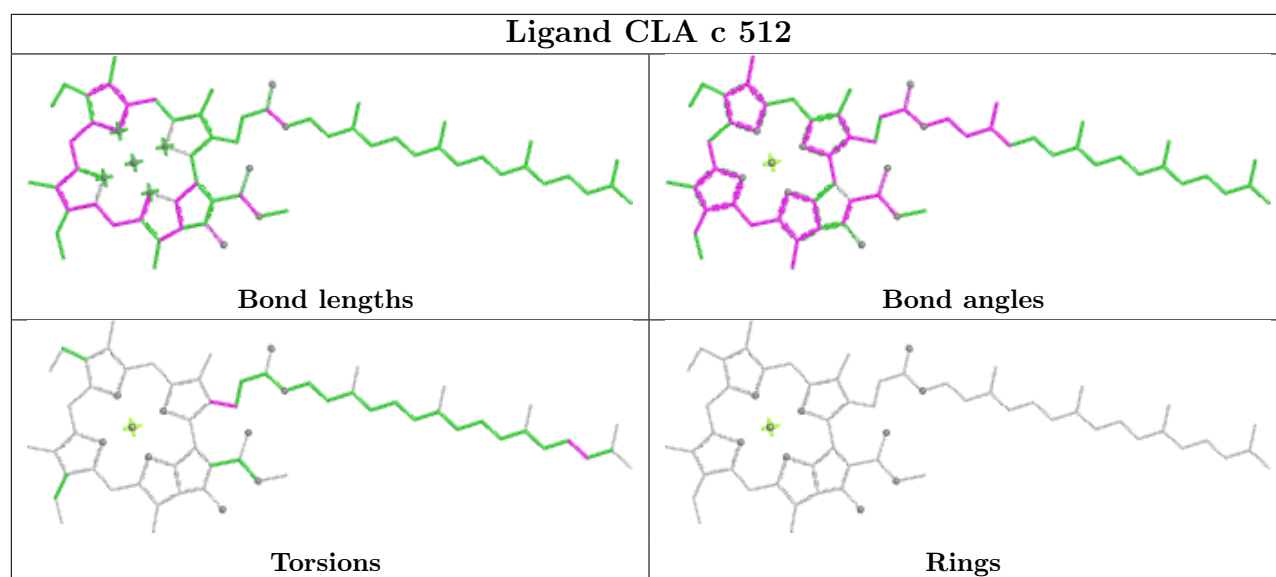


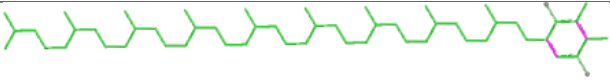
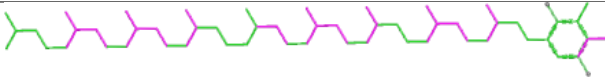
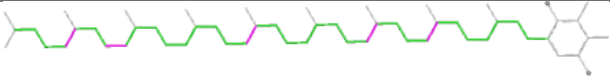
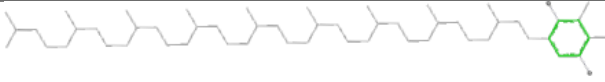
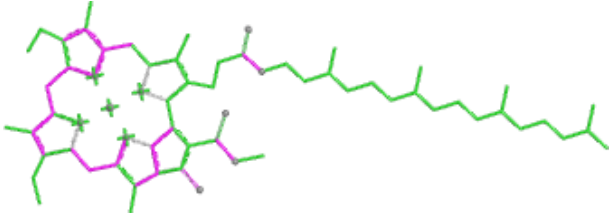
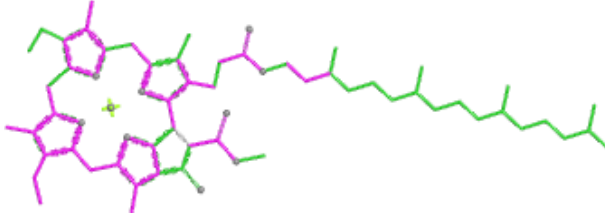
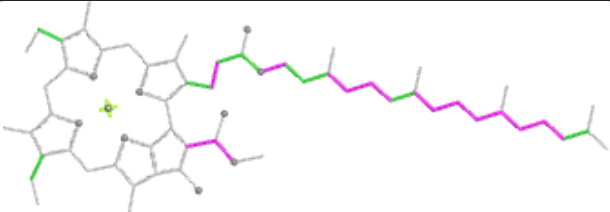
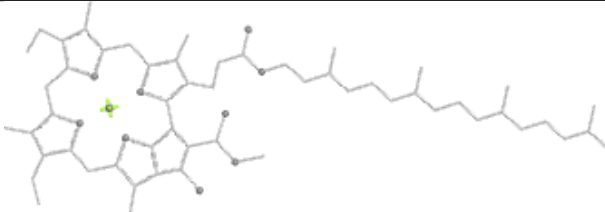
Ligand CLA c 508

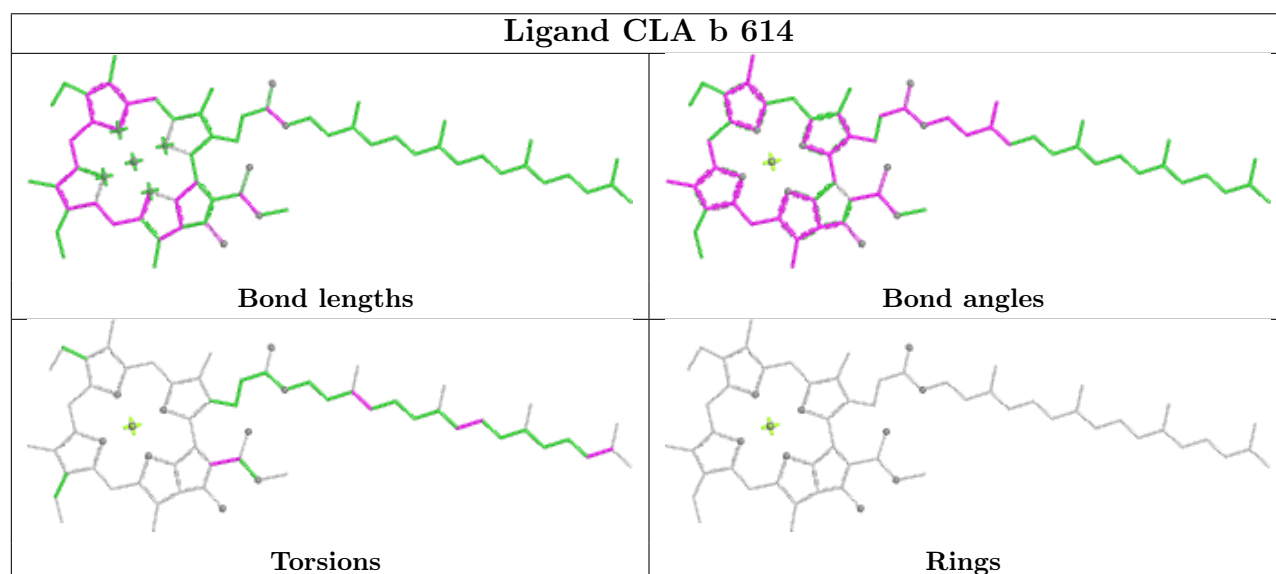
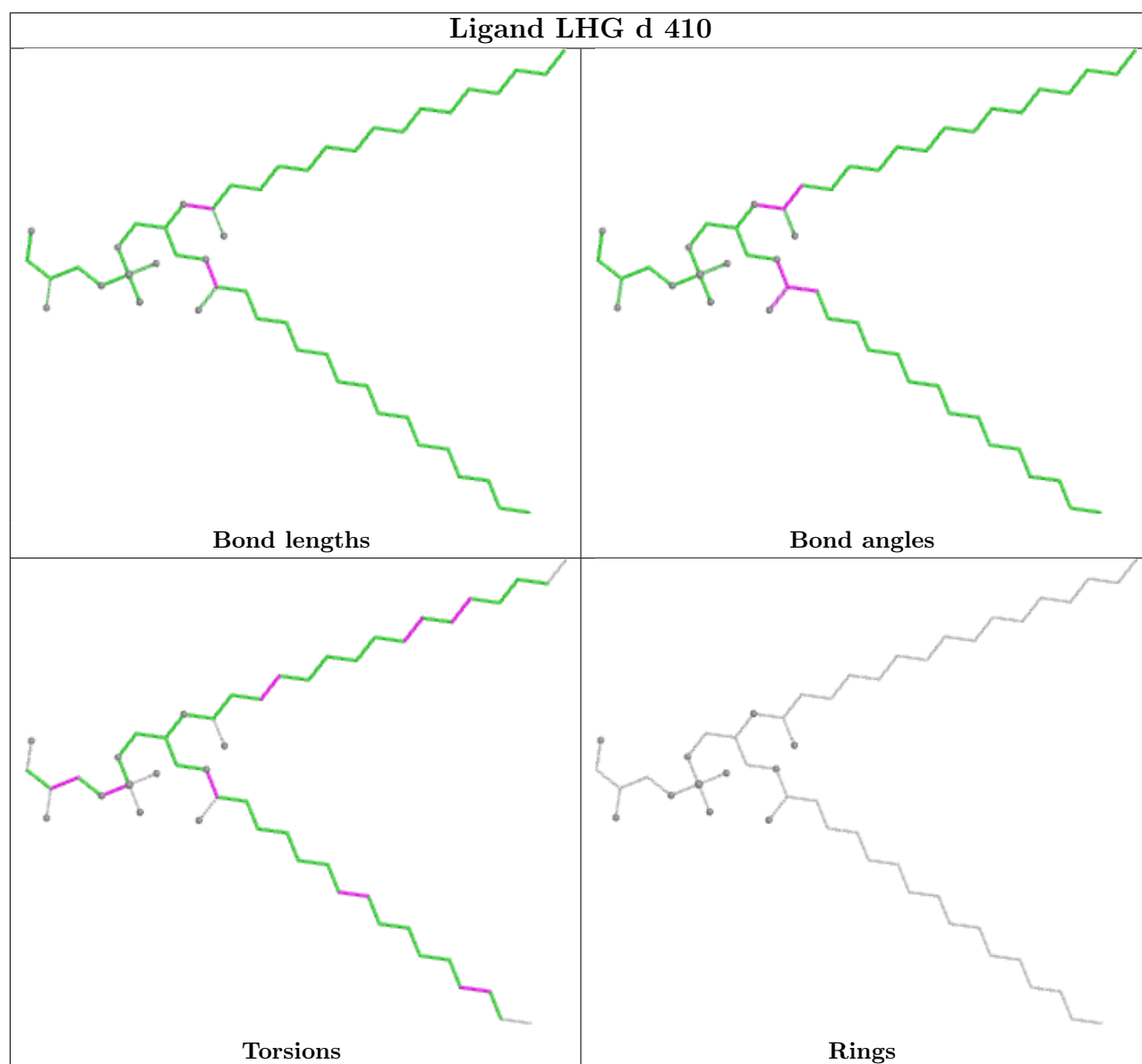


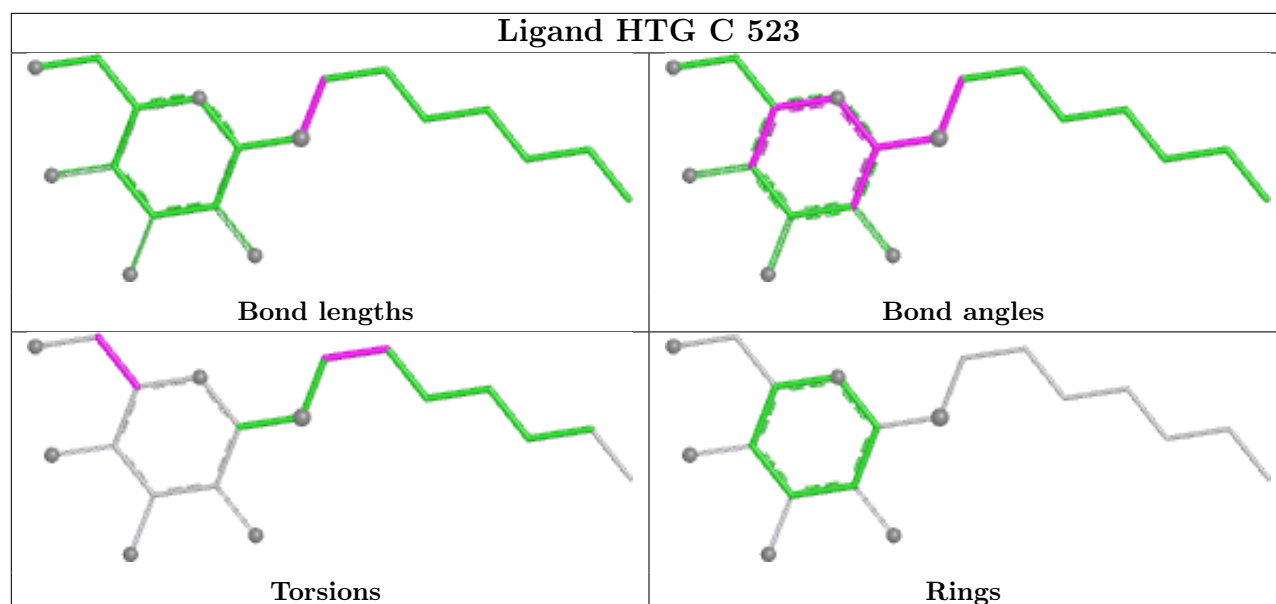
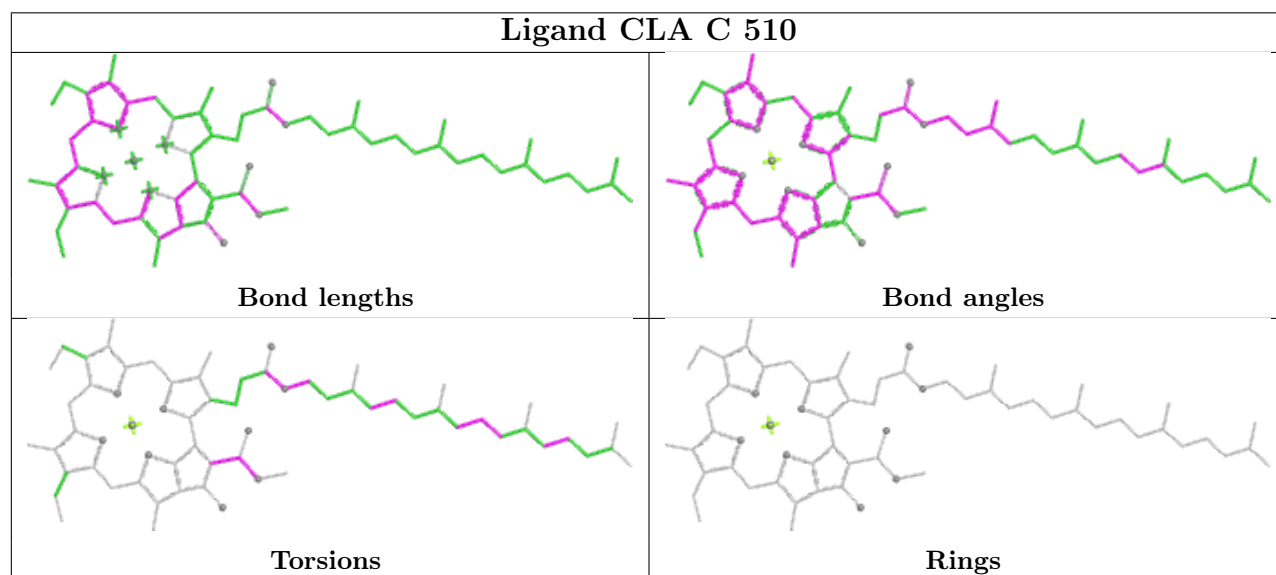
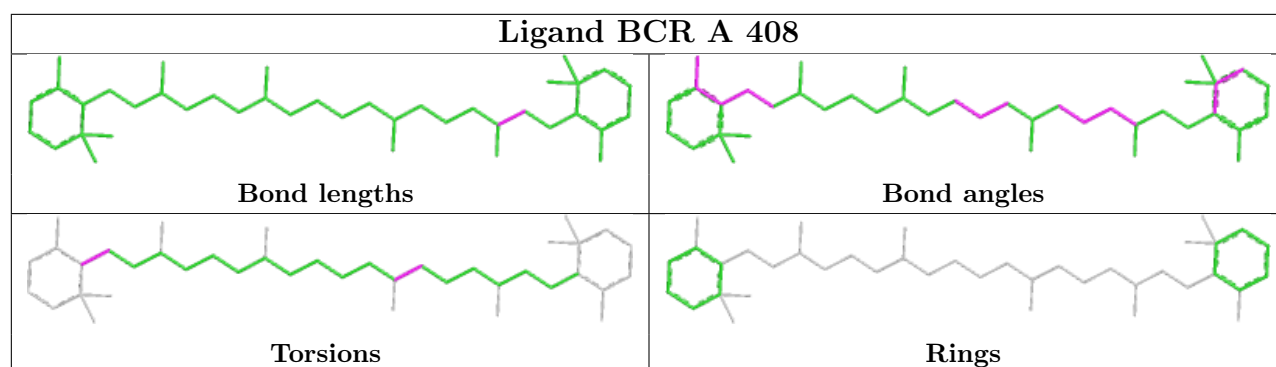
Ligand SQD B 621

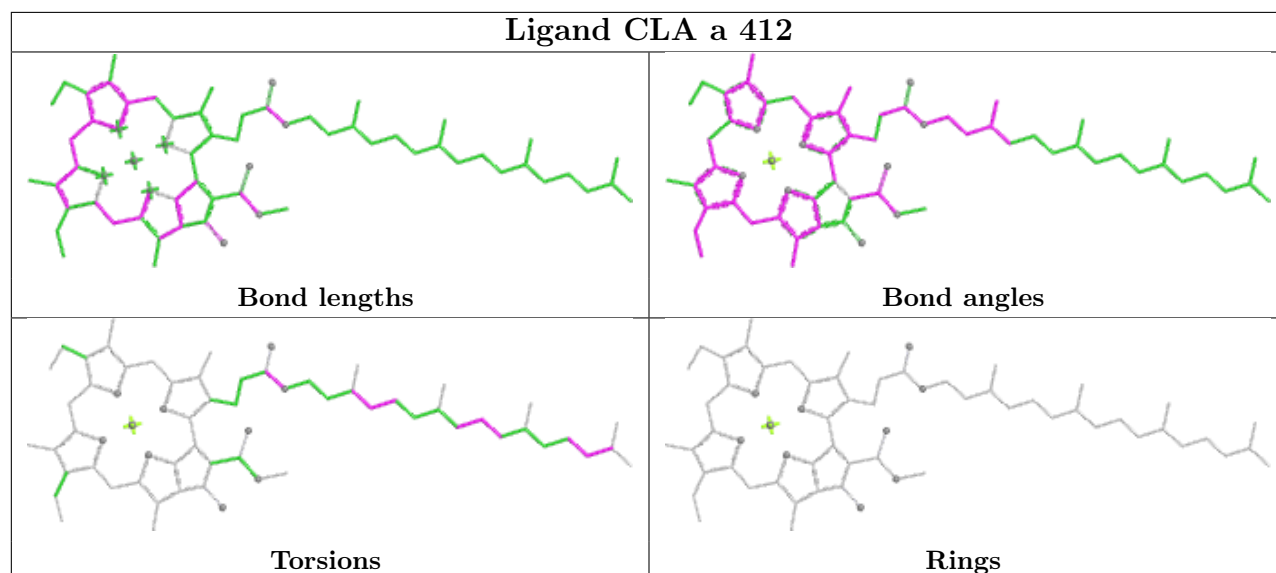
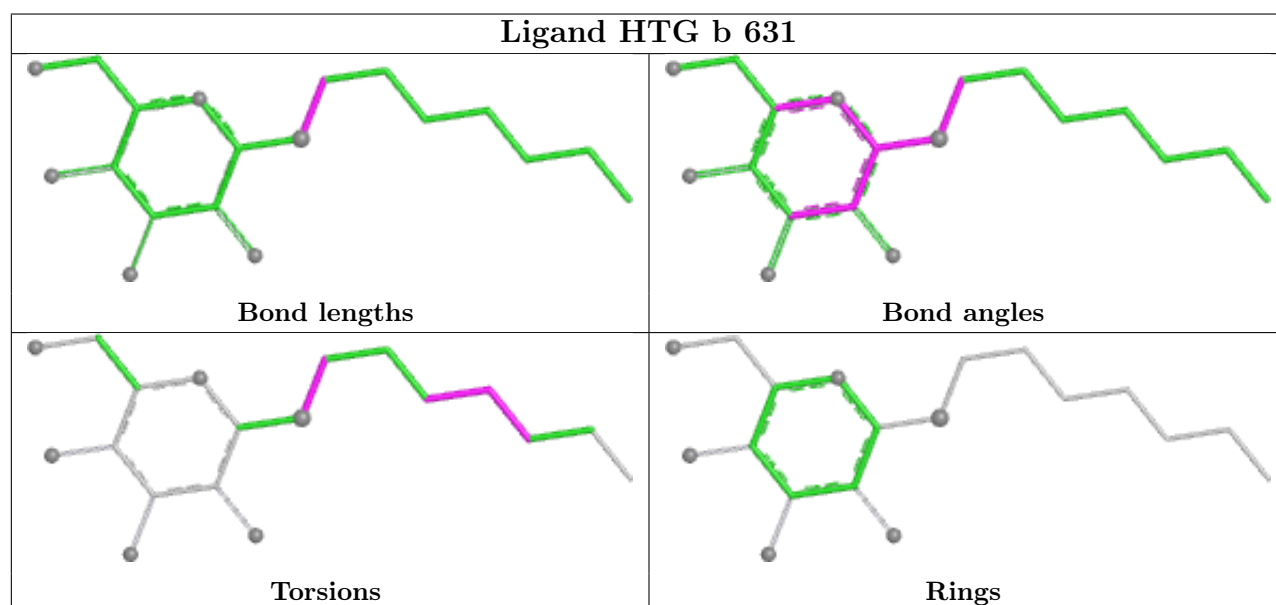
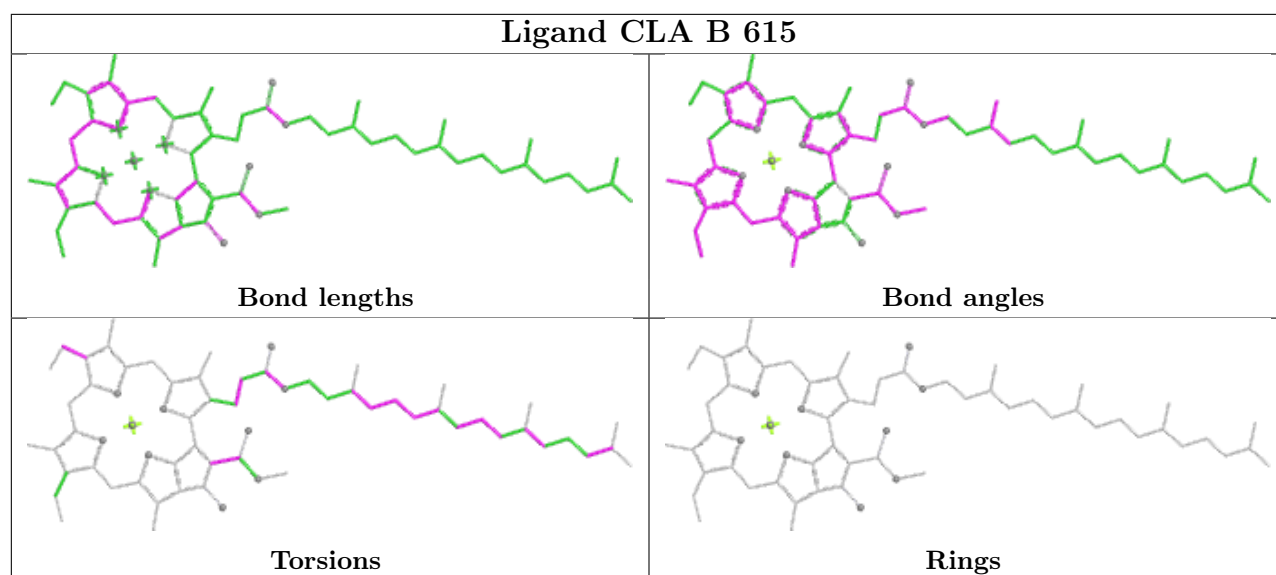




Ligand PL9 d 407 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA b 623	
 Bond lengths	 Bond angles
 Torsions	 Rings







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	-0.62	0 100 100	20, 46, 74, 129	54 (16%)
1	a	334/344 (97%)	-0.64	0 100 100	21, 47, 78, 147	54 (16%)
2	B	504/505 (99%)	-0.58	2 (0%) 88 86	26, 52, 93, 149	10 (1%)
2	b	503/505 (99%)	-0.55	4 (0%) 82 80	31, 52, 91, 202	12 (2%)
3	C	451/455 (99%)	-0.49	0 100 100	24, 62, 91, 136	12 (2%)
3	c	455/455 (100%)	-0.51	0 100 100	23, 66, 87, 123	20 (4%)
4	D	341/342 (99%)	-0.68	0 100 100	22, 48, 77, 143	16 (4%)
4	d	341/342 (99%)	-0.67	0 100 100	24, 50, 71, 112	16 (4%)
5	E	81/84 (96%)	-0.11	1 (1%) 76 73	40, 82, 117, 162	2 (2%)
5	e	81/84 (96%)	-0.18	2 (2%) 58 54	41, 77, 131, 187	2 (2%)
6	F	34/44 (77%)	-0.22	0 100 100	58, 72, 120, 130	0
6	f	32/44 (72%)	-0.36	1 (3%) 51 47	58, 68, 128, 159	0
7	H	65/65 (100%)	-0.41	1 (1%) 72 68	42, 64, 85, 166	1 (1%)
7	h	65/65 (100%)	-0.50	1 (1%) 72 68	52, 65, 85, 169	0
8	I	37/38 (97%)	-0.13	0 100 100	50, 64, 136, 194	0
8	i	37/38 (97%)	-0.32	1 (2%) 56 51	48, 61, 131, 164	0
9	J	38/39 (97%)	0.01	1 (2%) 57 52	63, 79, 167, 195	0
9	j	39/39 (100%)	-0.19	0 100 100	58, 71, 149, 191	0
10	K	37/37 (100%)	-0.30	0 100 100	65, 79, 98, 119	0
10	k	37/37 (100%)	-0.44	0 100 100	62, 75, 97, 119	0
11	L	37/37 (100%)	-0.71	0 100 100	26, 42, 101, 127	1 (2%)
11	l	37/37 (100%)	-0.58	0 100 100	27, 43, 104, 138	1 (2%)
12	M	33/36 (91%)	-0.72	0 100 100	26, 43, 76, 131	1 (3%)
12	m	33/36 (91%)	-0.61	0 100 100	37, 44, 89, 122	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.63	1 (0%) 88 86	31, 58, 101, 145	8 (3%)
13	o	243/244 (99%)	-0.53	0 100 100	32, 61, 115, 178	5 (2%)
14	T	29/32 (90%)	-0.72	1 (3%) 48 43	33, 42, 77, 145	1 (3%)
14	t	29/32 (90%)	-0.67	1 (3%) 48 43	34, 43, 75, 144	1 (3%)
15	U	97/104 (93%)	-0.65	0 100 100	45, 57, 90, 133	0
15	u	97/104 (93%)	-0.64	0 100 100	46, 61, 79, 123	0
16	V	137/137 (100%)	-0.66	0 100 100	24, 59, 83, 114	2 (1%)
16	v	137/137 (100%)	-0.58	0 100 100	25, 70, 103, 132	1 (0%)
17	Y	29/30 (96%)	0.76	4 (13%) 6 5	80, 102, 195, 215	0
17	y	29/30 (96%)	0.17	1 (3%) 48 43	80, 94, 148, 163	0
18	X	39/40 (97%)	-0.13	0 100 100	63, 72, 125, 163	0
18	x	38/40 (95%)	0.10	1 (2%) 57 52	64, 74, 130, 159	0
19	Z	62/62 (100%)	-0.04	0 100 100	82, 99, 136, 151	0
19	z	62/62 (100%)	0.17	2 (3%) 50 46	80, 100, 152, 195	0
20	R	18/34 (52%)	1.86	9 (50%) 0 0	111, 147, 171, 187	0
All	All	5275/5384 (97%)	-0.51	34 (0%) 85 83	20, 57, 109, 215	220 (4%)

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	Y	20	ALA	3.9
20	R	15	ALA	3.4
18	x	37	VAL	3.3
7	H	65	LEU	3.1
17	Y	19	ILE	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
14	FME	t	1	10/11	0.94	0.07	28,39,49,95	0
12	FME	m	1	10/11	0.95	0.09	35,51,97,107	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	0.95	0.07	38,48,56,93	0
8	FME	i	1	10/11	0.97	0.06	41,58,64,68	0
12	FME	M	1	10/11	0.97	0.07	31,47,94,99	0
8	FME	I	1	10/11	0.97	0.06	39,51,61,66	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
27	LMT	F	101	35/35	0.70	0.18	133,171,182,184	0
31	UNL	J	101	10/-	0.72	0.20	70,104,114,115	0
34	DGD	D	410	52/66	0.73	0.14	74,109,157,168	0
34	DGD	d	408	62/66	0.73	0.16	87,130,176,182	0
32	CA	f	103	1/1	0.74	0.07	127,127,127,127	0
31	UNL	j	101	10/-	0.75	0.16	59,89,101,103	0
27	LMT	C	521	35/35	0.75	0.14	103,145,170,173	0
38	LHG	a	420	42/49	0.75	0.12	92,136,181,183	0
31	UNL	M	103	10/-	0.76	0.12	52,63,78,80	0
27	LMT	b	630	25/35	0.76	0.15	85,107,156,159	0
25	SQD	f	102	43/54	0.77	0.15	106,125,157,166	0
31	UNL	K	102	34/-	0.77	0.14	94,127,136,139	0
27	LMT	a	419	35/35	0.77	0.15	98,142,160,162	0
27	LMT	D	405	35/35	0.77	0.13	84,132,152,153	0
31	UNL	m	101	10/-	0.78	0.15	46,60,79,80	0
38	LHG	E	101	42/49	0.78	0.12	89,127,142,147	0
32	CA	b	609	1/1	0.78	0.09	131,131,131,131	0
33	HTG	D	416	16/19	0.79	0.13	70,134,155,156	0
35	LMG	C	520	51/55	0.79	0.13	63,125,134,137	0
27	LMT	e	102	35/35	0.80	0.13	86,136,156,157	0
33	HTG	B	630	19/19	0.80	0.12	58,118,140,169	0
33	HTG	b	608	19/19	0.81	0.12	58,116,151,164	0
31	UNL	I	101	40/-	0.81	0.15	58,93,150,153	0
31	UNL	i	101	40/-	0.81	0.13	50,87,139,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
27	LMT	a	404	35/35	0.81	0.12	55,101,126,145	0
27	LMT	A	413	35/35	0.81	0.13	57,91,114,119	0
33	HTG	V	207	19/19	0.81	0.13	80,105,126,240	0
26	GOL	O	301	6/6	0.82	0.10	81,84,87,87	0
31	UNL	c	526	32/-	0.82	0.13	82,100,140,147	0
31	UNL	a	403	30/-	0.83	0.12	67,93,124,131	0
25	SQD	F	104	43/54	0.83	0.12	91,122,143,145	0
35	LMG	Z	101	37/55	0.83	0.14	67,138,150,151	0
33	HTG	d	414	16/19	0.83	0.11	75,116,122,125	0
31	UNL	A	417	28/-	0.83	0.12	63,89,113,115	0
26	GOL	V	202	6/6	0.84	0.16	88,95,99,99	0
35	LMG	z	101	39/55	0.84	0.13	74,125,149,162	0
31	UNL	d	413	36/-	0.84	0.12	64,85,131,137	0
27	LMT	M	104	35/35	0.84	0.12	44,109,152,157	0
31	UNL	b	633	33/-	0.85	0.14	55,88,143,145	0
35	LMG	c	523	51/55	0.85	0.11	65,117,129,133	0
31	UNL	D	415	40/-	0.85	0.12	62,86,130,137	0
31	UNL	B	631	33/-	0.85	0.14	61,83,134,137	0
33	HTG	c	525	19/19	0.85	0.10	86,116,133,149	0
33	HTG	B	623	19/19	0.86	0.10	85,137,145,176	0
25	SQD	B	621	54/54	0.86	0.11	53,79,156,160	0
33	HTG	C	522	19/19	0.86	0.11	84,94,135,137	0
26	GOL	a	402	6/6	0.86	0.15	103,108,108,109	0
30	PL9	A	416[A]	55/55	0.86	0.14	86,107,117,119	55
30	PL9	A	416[B]	55/55	0.86	0.14	86,107,117,119	55
33	HTG	b	631	19/19	0.86	0.13	66,80,98,102	0
33	HTG	c	524	19/19	0.86	0.11	99,106,117,119	0
25	SQD	L	102	54/54	0.86	0.10	42,76,124,140	0
30	PL9	a	416[B]	55/55	0.87	0.14	92,108,122,124	55
27	LMT	m	102	35/35	0.87	0.10	51,111,129,130	0
35	LMG	C	519	51/55	0.87	0.11	59,102,122,125	0
33	HTG	B	622	19/19	0.87	0.12	63,75,85,91	0
25	SQD	A	412	54/54	0.87	0.11	56,77,134,138	0
33	HTG	b	632	19/19	0.87	0.11	80,134,152,155	0
27	LMT	M	105	35/35	0.87	0.12	50,99,119,121	0
30	PL9	a	416[A]	55/55	0.87	0.14	91,109,122,123	55
33	HTG	C	523	19/19	0.87	0.10	78,110,127,130	0
27	LMT	T	104	25/35	0.88	0.13	44,81,135,142	0
23	CLA	C	514	65/65	0.88	0.10	71,91,120,124	0
27	LMT	t	101	25/35	0.88	0.12	45,80,143,149	0
25	SQD	a	405	54/54	0.88	0.10	50,82,127,132	0
26	GOL	v	201	6/6	0.88	0.13	78,98,103,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	GOL	B	627	6/6	0.89	0.14	58,78,80,82	0
35	LMG	c	522	51/55	0.89	0.10	64,95,120,122	0
31	UNL	X	101	18/-	0.89	0.12	69,87,109,111	0
39	HEM	F	102	43/43	0.89	0.11	59,85,111,234	0
26	GOL	v	202	6/6	0.90	0.12	103,105,109,122	0
26	GOL	b	605	6/6	0.90	0.15	69,87,103,103	0
35	LMG	C	501	51/55	0.90	0.10	62,84,103,107	0
26	GOL	B	626	6/6	0.90	0.11	83,86,88,89	0
26	GOL	c	528	6/6	0.91	0.11	77,90,101,113	0
24	BCR	K	101	40/40	0.91	0.09	64,83,92,94	0
26	GOL	A	411	6/6	0.91	0.10	84,86,91,92	0
25	SQD	A	409	54/54	0.91	0.09	55,98,108,111	0
33	HTG	B	629	19/19	0.91	0.09	48,88,113,116	0
23	CLA	B	602	65/65	0.91	0.10	53,75,112,132	0
26	GOL	C	524	6/6	0.91	0.16	88,89,103,104	0
23	CLA	C	507	65/65	0.91	0.09	59,78,118,125	0
35	LMG	a	415	51/55	0.91	0.09	59,85,101,114	0
27	LMT	M	102	35/35	0.91	0.09	42,101,123,131	0
31	UNL	d	412	17/-	0.91	0.10	62,71,93,94	0
22	CL	v	204	1/1	0.91	0.09	120,120,120,120	0
23	CLA	b	610	65/65	0.91	0.10	53,84,129,138	0
23	CLA	c	517	65/65	0.91	0.09	80,95,105,107	0
26	GOL	c	502	6/6	0.91	0.18	81,89,105,110	0
23	CLA	C	505	65/65	0.92	0.09	47,67,101,108	0
26	GOL	B	633	6/6	0.92	0.08	56,60,61,63	0
34	DGD	C	517	62/66	0.92	0.08	55,74,100,114	0
22	CL	U	201	1/1	0.92	0.15	120,120,120,120	0
26	GOL	b	606	6/6	0.92	0.08	75,87,92,94	0
36	BCT	D	401[A]	4/4	0.92	0.12	76,77,81,89	4
36	BCT	D	401[B]	4/4	0.92	0.12	75,76,81,89	4
38	LHG	D	413	49/49	0.92	0.10	51,78,118,126	0
24	BCR	k	102	40/40	0.92	0.09	57,73,91,92	0
26	GOL	T	101	6/6	0.92	0.14	58,81,84,93	0
32	CA	B	601	1/1	0.92	0.08	131,131,131,131	0
35	LMG	D	417	51/55	0.93	0.09	50,76,125,133	0
26	GOL	T	102	6/6	0.93	0.11	107,116,118,122	0
23	CLA	C	513	65/65	0.93	0.08	71,87,94,97	0
26	GOL	V	205	6/6	0.93	0.11	87,100,106,115	0
25	SQD	a	414	54/54	0.93	0.08	56,83,104,105	0
35	LMG	d	416	51/55	0.93	0.08	53,66,107,118	0
31	UNL	D	414	17/-	0.93	0.08	48,71,87,90	0
24	BCR	K	103	40/40	0.93	0.09	62,74,82,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	UNL	d	415	18/-	0.93	0.10	67,80,109,116	0
26	GOL	A	410	6/6	0.93	0.09	49,56,61,66	0
24	BCR	d	406	40/40	0.93	0.08	52,61,83,87	0
26	GOL	B	624	6/6	0.93	0.09	64,74,77,86	0
26	GOL	t	103	6/6	0.93	0.15	72,88,96,97	0
23	CLA	c	512	65/65	0.94	0.07	47,57,115,122	0
23	CLA	C	511	65/65	0.94	0.07	54,71,85,96	0
24	BCR	D	408	40/40	0.94	0.08	49,68,101,109	0
24	BCR	H	101	40/40	0.94	0.07	47,60,78,78	0
33	HTG	o	301	19/19	0.94	0.08	51,74,87,91	0
34	DGD	C	516	62/66	0.94	0.08	40,56,87,95	0
23	CLA	A	407	65/65	0.94	0.09	42,56,118,126	0
34	DGD	C	518	62/66	0.94	0.07	51,64,88,105	0
23	CLA	B	615	65/65	0.94	0.08	32,45,99,102	0
34	DGD	c	519	62/66	0.94	0.08	42,62,92,96	0
26	GOL	f	101	6/6	0.94	0.10	85,90,93,96	0
30	PL9	D	409[A]	55/55	0.94	0.07	30,43,51,65	55
30	PL9	D	409[B]	55/55	0.94	0.07	30,43,51,61	55
24	BCR	c	527	40/40	0.94	0.08	72,89,97,102	0
23	CLA	a	412	65/65	0.94	0.10	41,55,120,125	0
24	BCR	h	101	40/40	0.94	0.08	48,66,72,78	0
26	GOL	B	628	6/6	0.94	0.15	55,87,89,91	0
35	LMG	b	629	51/55	0.94	0.07	40,54,76,84	0
24	BCR	k	101	40/40	0.94	0.08	59,76,86,87	0
23	CLA	C	509	65/65	0.94	0.08	49,67,135,141	0
26	GOL	F	103	6/6	0.94	0.10	98,110,118,121	0
23	CLA	b	615	65/65	0.94	0.07	39,51,93,95	0
23	CLA	b	623	65/65	0.94	0.07	34,45,91,105	0
23	CLA	b	625	65/65	0.94	0.08	46,59,103,110	0
33	HTG	b	601	19/19	0.94	0.08	49,65,76,77	0
33	HTG	b	607	19/19	0.94	0.07	53,83,94,95	0
23	CLA	c	510	65/65	0.94	0.08	57,75,99,102	0
38	LHG	d	411	49/49	0.94	0.09	47,63,114,118	0
26	GOL	V	203	6/6	0.94	0.10	51,70,86,89	0
23	CLA	b	620	65/65	0.95	0.06	34,48,58,63	0
24	BCR	Y	101	40/40	0.95	0.08	61,79,92,106	0
24	BCR	b	627	40/40	0.95	0.06	32,48,64,70	0
24	BCR	c	518	40/40	0.95	0.07	50,65,74,77	0
23	CLA	C	512	65/65	0.95	0.08	54,76,92,97	0
23	CLA	B	617	65/65	0.95	0.10	45,61,139,140	0
23	CLA	c	507	65/65	0.95	0.07	53,64,74,93	0
23	CLA	c	508	65/65	0.95	0.07	50,64,81,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	DGD	c	520	62/66	0.95	0.07	49,66,111,127	0
34	DGD	c	521	62/66	0.95	0.07	51,61,98,109	0
23	CLA	c	509	65/65	0.95	0.07	45,56,73,77	0
34	DGD	h	102	62/66	0.95	0.07	36,58,75,82	0
24	BCR	t	102	40/40	0.95	0.07	37,52,68,71	0
26	GOL	V	204	6/6	0.95	0.10	70,71,74,75	0
23	CLA	C	508	65/65	0.95	0.08	53,72,85,89	0
23	CLA	c	511	65/65	0.95	0.08	52,65,77,82	0
35	LMG	M	101	51/55	0.95	0.07	39,59,75,91	0
23	CLA	D	407	65/65	0.95	0.08	48,62,108,118	0
23	CLA	c	515	65/65	0.95	0.08	54,71,88,93	0
23	CLA	c	516	65/65	0.95	0.07	64,78,87,94	0
23	CLA	B	607	65/65	0.95	0.07	37,52,91,95	0
30	PL9	d	407[A]	55/55	0.95	0.07	33,45,54,57	55
30	PL9	d	407[B]	55/55	0.95	0.07	35,45,53,58	55
23	CLA	d	405	65/65	0.95	0.08	47,61,114,122	0
24	BCR	A	408	40/40	0.95	0.06	33,46,55,56	0
24	BCR	B	620	40/40	0.95	0.06	43,50,60,77	0
36	BCT	d	401[A]	4/4	0.95	0.09	72,74,75,77	4
36	BCT	d	401[B]	4/4	0.95	0.09	71,74,75,77	4
37	PHO	d	402[A]	64/64	0.95	0.07	37,50,55,59	64
37	PHO	d	402[B]	64/64	0.95	0.07	39,50,55,57	64
38	LHG	D	411	49/49	0.95	0.07	40,52,64,80	0
23	CLA	C	510	65/65	0.95	0.09	54,74,91,95	0
26	GOL	v	203	6/6	0.95	0.10	65,68,73,74	0
23	CLA	C	506	65/65	0.95	0.07	46,59,74,81	0
38	LHG	d	409	49/49	0.95	0.07	40,56,63,69	0
26	GOL	B	625	6/6	0.95	0.10	49,66,85,101	0
23	CLA	b	618	65/65	0.95	0.07	47,55,66,73	0
34	DGD	B	632	62/66	0.96	0.07	43,59,89,105	0
23	CLA	b	614	65/65	0.96	0.06	36,45,58,64	0
23	CLA	C	504	65/65	0.96	0.07	54,67,80,86	0
23	CLA	b	617	65/65	0.96	0.06	44,55,66,69	0
23	CLA	B	614	65/65	0.96	0.06	32,43,62,72	0
23	CLA	b	619	65/65	0.96	0.07	42,54,69,72	0
24	BCR	B	619	40/40	0.96	0.05	36,47,58,66	0
23	CLA	B	603	65/65	0.96	0.06	43,53,60,68	0
24	BCR	C	515	40/40	0.96	0.07	51,63,78,78	0
23	CLA	b	621	65/65	0.96	0.06	36,46,58,63	0
23	CLA	b	622	65/65	0.96	0.06	34,46,55,70	0
23	CLA	B	616	65/65	0.96	0.06	41,52,67,76	0
23	CLA	b	624	65/65	0.96	0.06	42,53,71,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	BCR	T	103	40/40	0.96	0.05	29,49,65,68	0
23	CLA	A	406	65/65	0.96	0.07	35,46,104,109	0
32	CA	F	105	1/1	0.96	0.09	119,119,119,119	0
24	BCR	a	413	40/40	0.96	0.05	34,47,57,60	0
26	GOL	C	525	6/6	0.96	0.08	53,59,63,63	0
26	GOL	D	404	6/6	0.96	0.11	51,61,73,76	0
24	BCR	b	626	40/40	0.96	0.05	33,45,53,54	0
23	CLA	c	505	65/65	0.96	0.07	52,67,76,79	0
24	BCR	b	628	40/40	0.96	0.06	42,55,65,67	0
23	CLA	c	506	65/65	0.96	0.07	51,62,84,87	0
26	GOL	V	201	6/6	0.96	0.09	63,81,87,88	0
23	CLA	a	410	65/65	0.96	0.07	37,49,104,112	0
23	CLA	C	502	65/65	0.96	0.07	51,62,88,93	0
37	PHO	D	403[A]	64/64	0.96	0.06	41,48,54,59	64
37	PHO	D	403[B]	64/64	0.96	0.06	39,48,54,59	64
23	CLA	C	503	65/65	0.96	0.07	48,66,75,83	0
23	CLA	b	611	65/65	0.96	0.06	43,52,62,70	0
26	GOL	a	401	6/6	0.96	0.08	53,59,71,80	0
23	CLA	b	612	65/65	0.96	0.06	42,54,63,67	0
26	GOL	b	602	6/6	0.96	0.08	63,68,78,79	0
38	LHG	L	101	49/49	0.96	0.06	37,50,58,62	0
23	CLA	b	613	65/65	0.96	0.06	34,45,72,79	0
38	LHG	b	634	49/49	0.96	0.06	35,50,62,72	0
23	CLA	c	513	65/65	0.96	0.08	55,68,82,88	0
26	GOL	c	501	6/6	0.96	0.08	55,59,61,62	0
23	CLA	c	514	65/65	0.96	0.06	51,64,72,82	0
39	HEM	e	101	43/43	0.96	0.10	73,94,130,141	0
23	CLA	B	605	65/65	0.97	0.06	33,43,69,75	0
23	CLA	D	406	65/65	0.97	0.06	32,40,65,75	0
22	CL	A	403[A]	1/1	0.97	0.07	44,44,44,44	1
23	CLA	a	409	65/65	0.97	0.06	36,42,50,72	0
23	CLA	B	608	65/65	0.97	0.05	29,43,55,67	0
23	CLA	d	403	65/65	0.97	0.05	34,41,48,51	0
37	PHO	D	402	64/64	0.97	0.05	31,41,49,51	0
23	CLA	d	404	65/65	0.97	0.06	35,43,59,65	0
26	GOL	b	603	6/6	0.97	0.06	60,70,74,75	0
37	PHO	a	411	64/64	0.97	0.05	33,43,54,58	0
26	GOL	b	604	6/6	0.97	0.08	65,84,86,92	0
23	CLA	B	609	65/65	0.97	0.05	40,51,63,66	0
23	CLA	B	610	65/65	0.97	0.06	42,55,66,79	0
38	LHG	D	412	49/49	0.97	0.06	35,46,75,85	0
24	BCR	B	618	40/40	0.97	0.05	31,44,56,59	0

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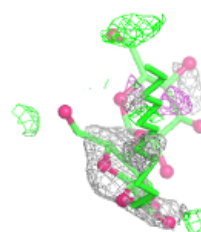
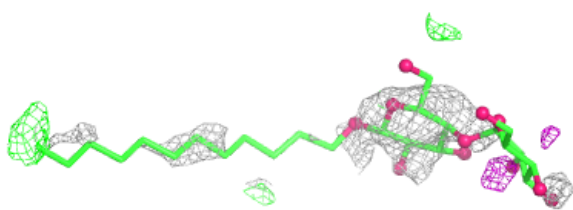
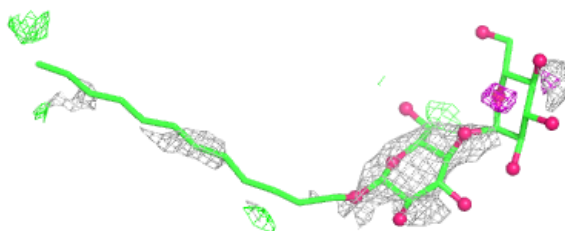
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	B	611	65/65	0.97	0.07	43,55,62,65	0
23	CLA	B	612	65/65	0.97	0.06	34,45,53,61	0
23	CLA	B	613	65/65	0.97	0.06	35,45,55,58	0
22	CL	A	403[B]	1/1	0.97	0.07	44,44,44,44	1
23	CLA	A	404	65/65	0.97	0.06	33,39,50,61	0
38	LHG	d	410	49/49	0.97	0.06	34,46,66,84	0
23	CLA	b	616	65/65	0.97	0.05	29,42,50,53	0
23	CLA	A	405	65/65	0.97	0.05	32,39,46,51	0
23	CLA	B	604	65/65	0.97	0.06	38,52,60,64	0
40	MG	J	102	1/1	0.97	0.06	62,62,62,62	0
41	HEC	v	205	43/43	0.97	0.07	53,63,78,80	0
32	CA	C	526	1/1	0.98	0.07	83,83,83,83	0
23	CLA	B	606	65/65	0.98	0.05	34,44,55,62	0
32	CA	O	302	1/1	0.98	0.04	90,90,90,90	0
22	CL	a	408[B]	1/1	0.98	0.05	46,46,46,46	1
32	CA	c	503	1/1	0.98	0.06	79,79,79,79	0
22	CL	a	408[A]	1/1	0.98	0.05	46,46,46,46	1
41	HEC	V	206	43/43	0.98	0.06	47,53,63,69	0
32	CA	o	302	1/1	0.98	0.03	96,96,96,96	0
22	CL	A	402[A]	1/1	0.99	0.02	40,40,40,40	1
22	CL	A	402[B]	1/1	0.99	0.02	40,40,40,40	1
21	FE2	A	401[A]	1/1	0.99	0.05	72,72,72,72	1
32	CA	c	504	1/1	0.99	0.02	84,84,84,84	0
21	FE2	A	401[B]	1/1	0.99	0.05	73,73,73,73	1
21	FE2	a	406[B]	1/1	0.99	0.04	60,60,60,60	0
28	OEX	A	414[A]	10/10	0.99	0.04	49,56,74,80	10
29	OEY	A	415[B]	11/11	0.99	0.03	49,56,78,79	11
40	MG	j	102	1/1	0.99	0.06	72,72,72,72	0
22	CL	a	407[A]	1/1	0.99	0.04	43,43,43,43	1
22	CL	a	407[B]	1/1	0.99	0.04	46,46,46,46	1
28	OEX	a	417[A]	10/10	1.00	0.02	40,47,52,54	10
29	OEY	a	418[B]	11/11	1.00	0.02	40,46,55,59	11

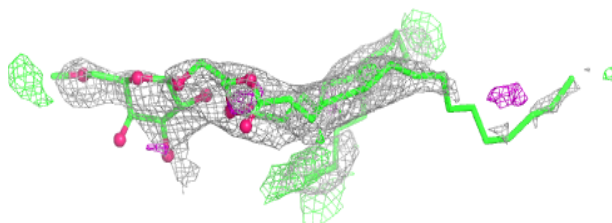
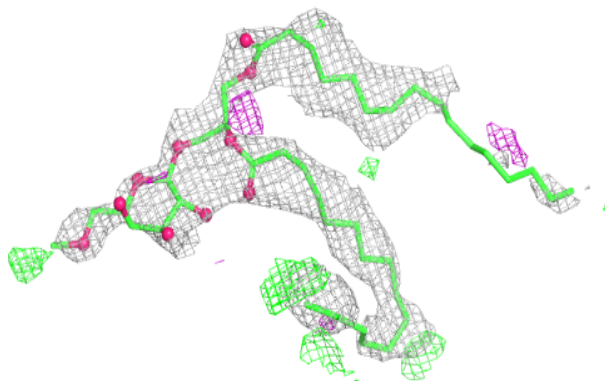
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

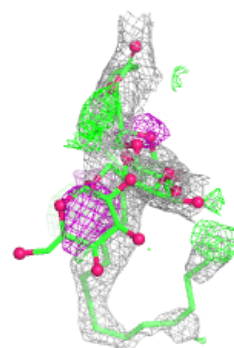
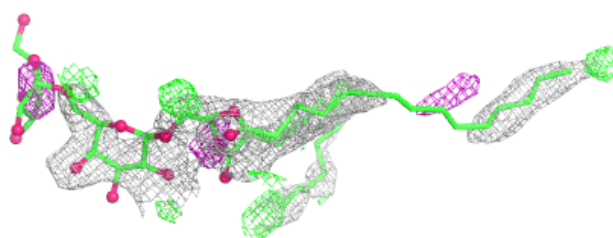
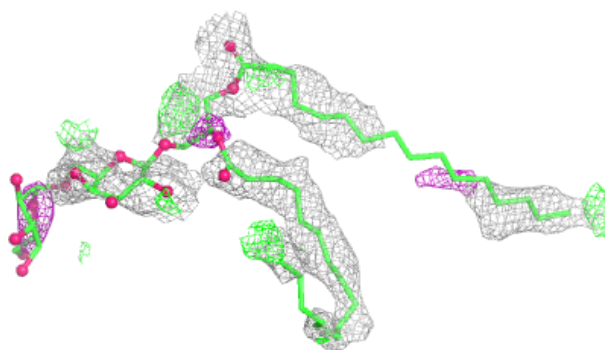
**Electron density around DGD D 410:**

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

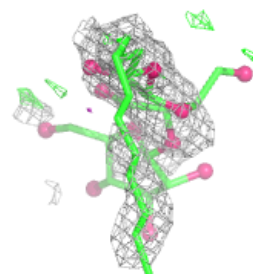
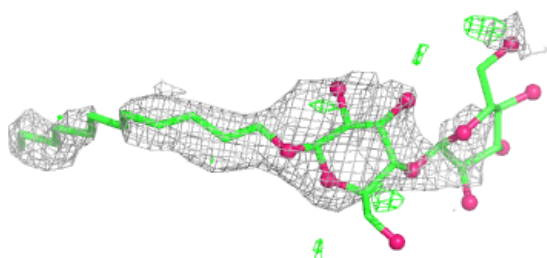
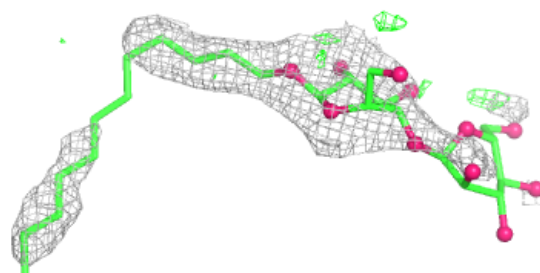


Electron density around DGD d 408:

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

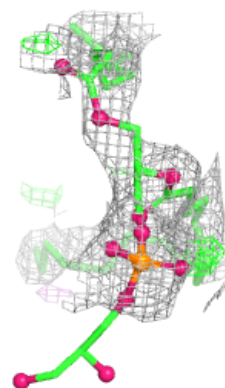
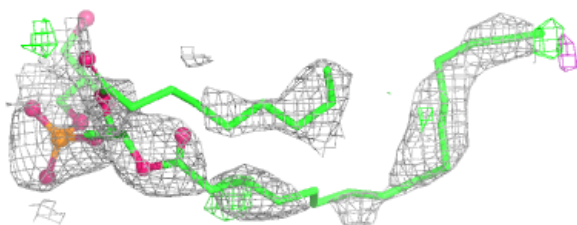
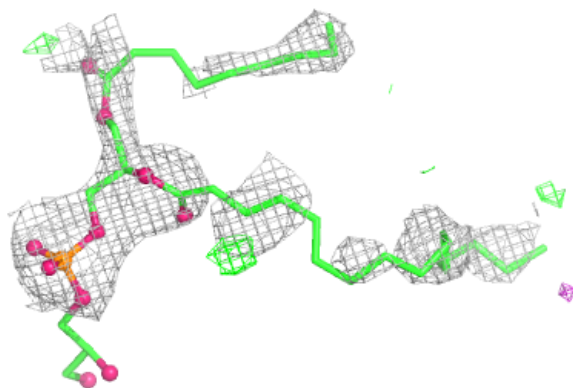
**Electron density around LMT C 521:**

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

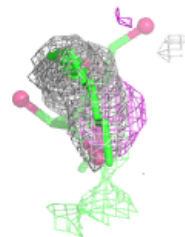
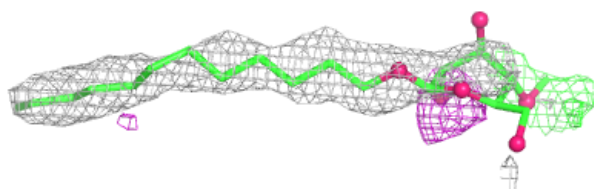
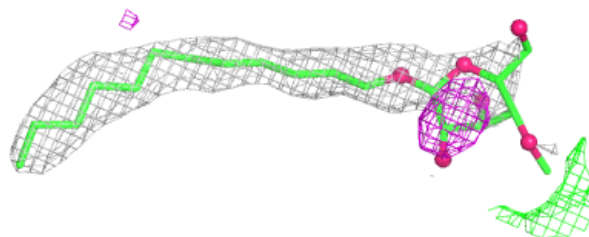


Electron density around LHG a 420:

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

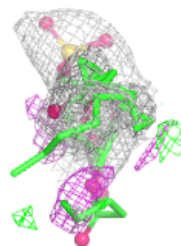
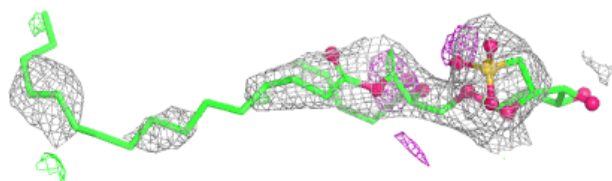
**Electron density around LMT b 630:**

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

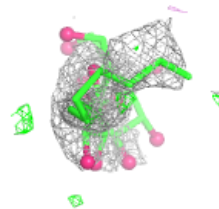
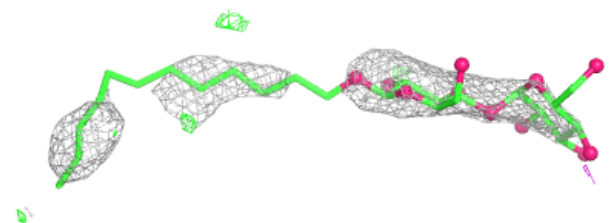
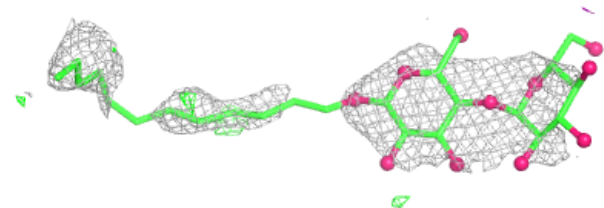


Electron density around SQD f 102:

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

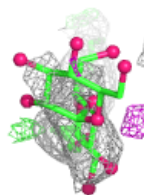
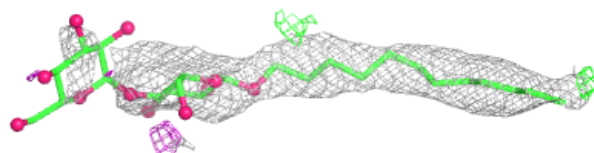
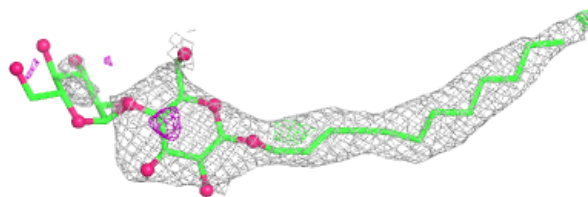
**Electron density around LMT a 419:**

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



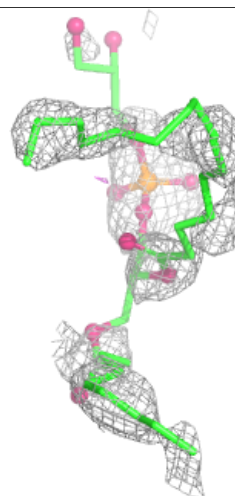
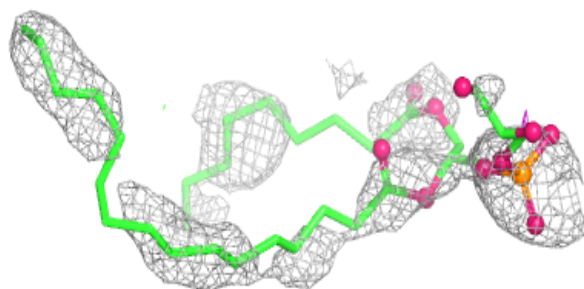
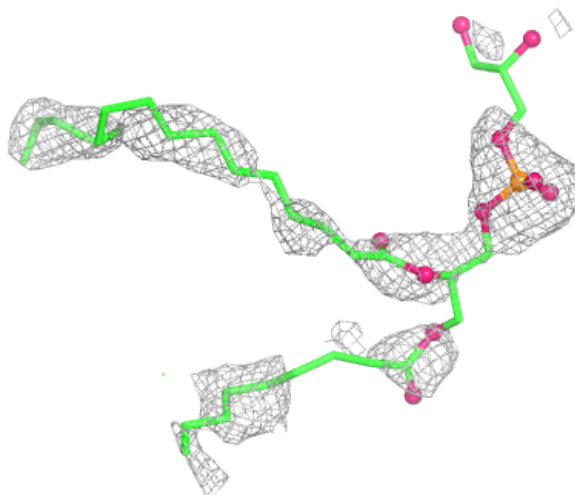
Electron density around LMT D 405:

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



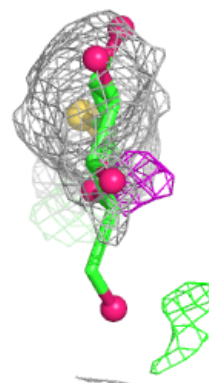
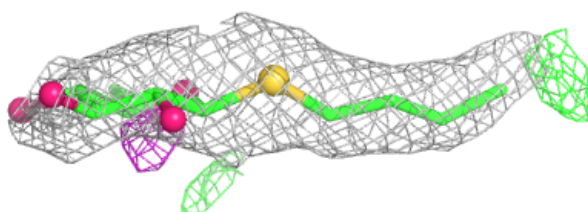
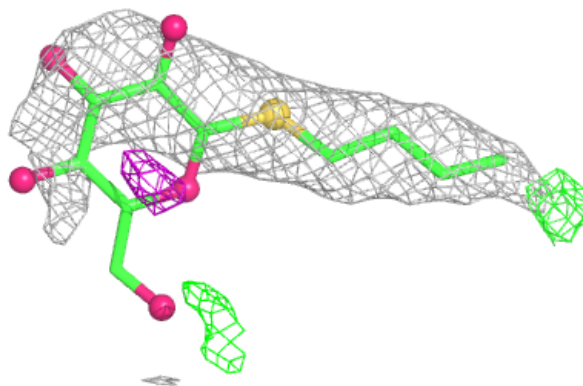
Electron density around LHG E 101:

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

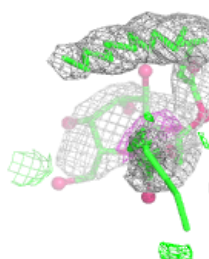
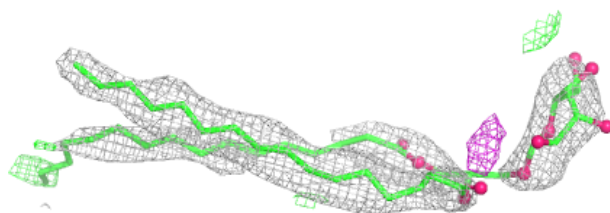
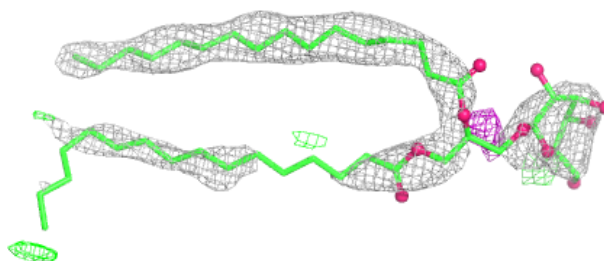


Electron density around HTG D 416:

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

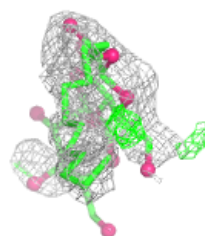
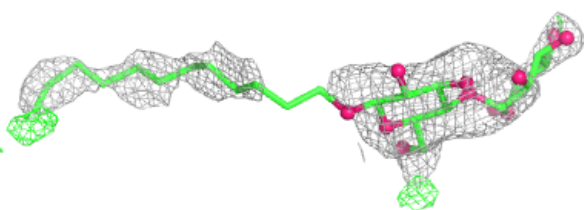
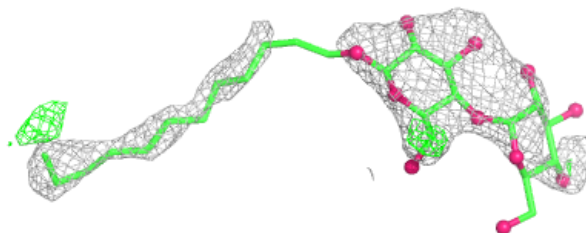
**Electron density around LMG C 520:**

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

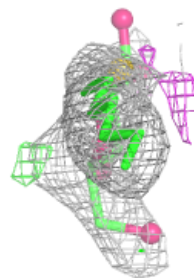
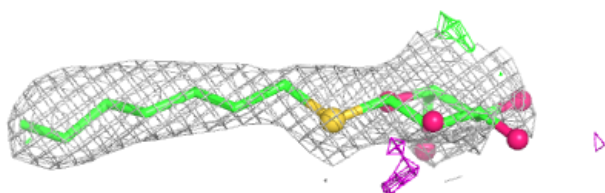
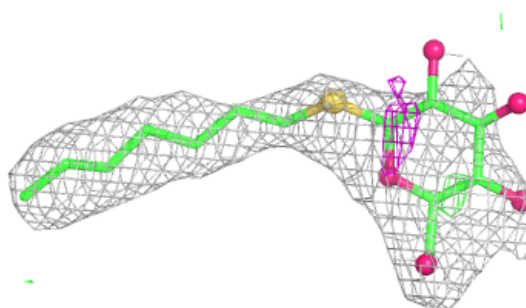


Electron density around LMT e 102:

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

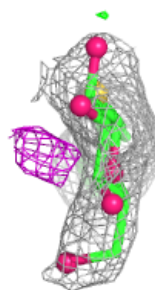
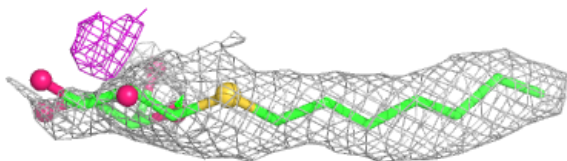
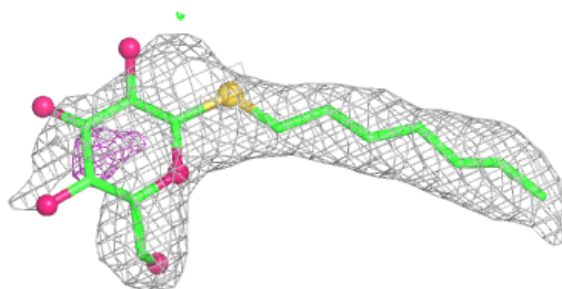
**Electron density around HTG B 630:**

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

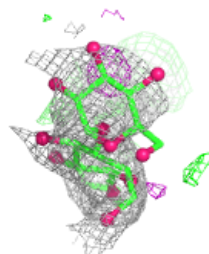
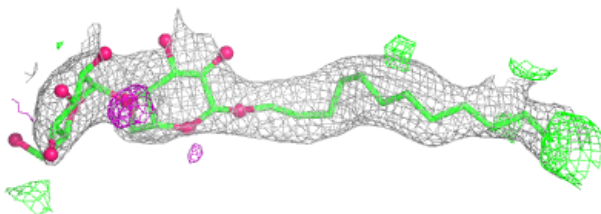
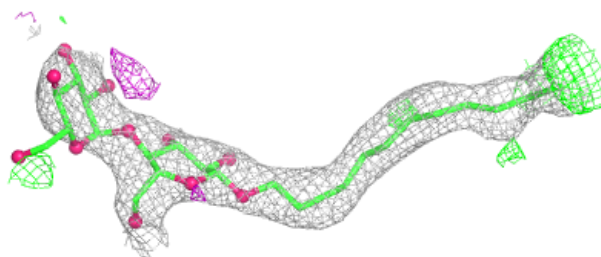


Electron density around HTG b 608:

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

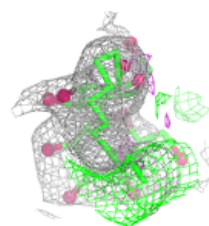
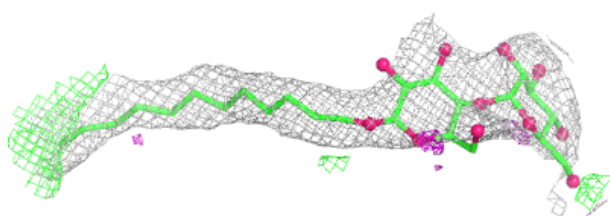
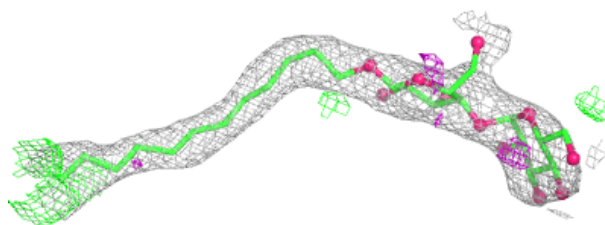
**Electron density around LMT a 404:**

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

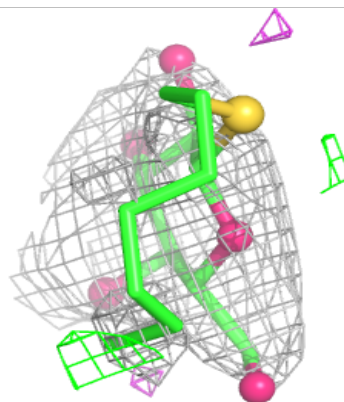
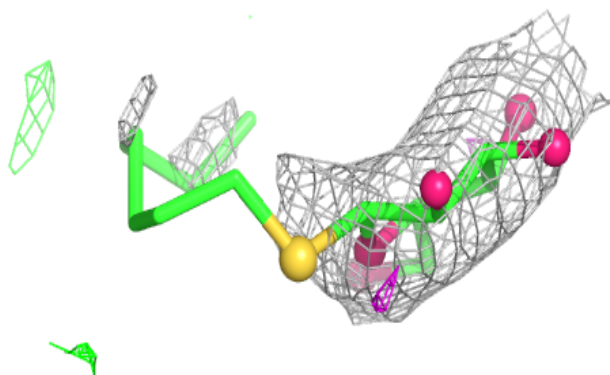
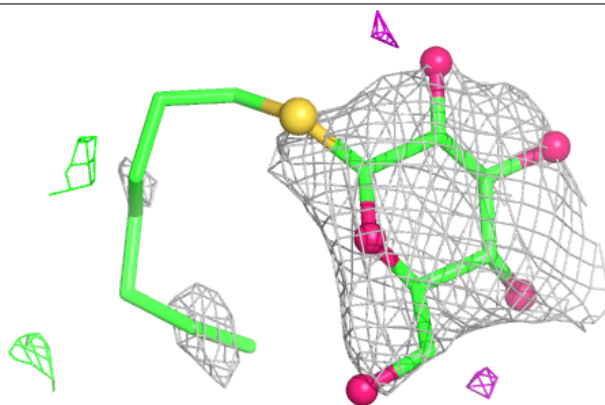


Electron density around LMT A 413:

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

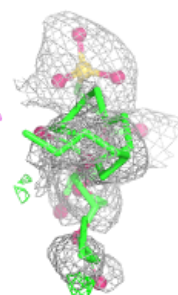
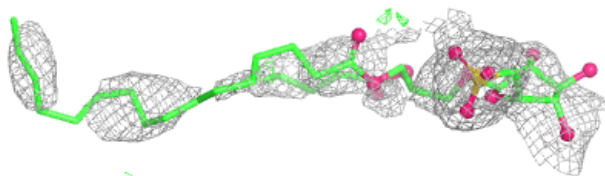
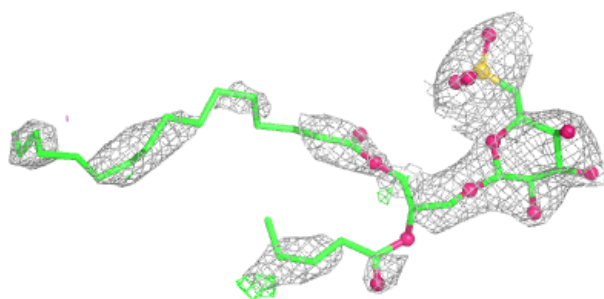
**Electron density around HTG V 207:**

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

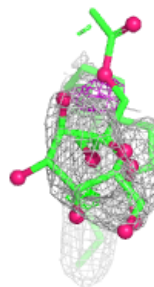
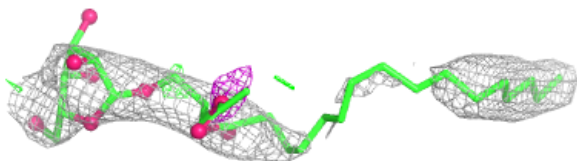
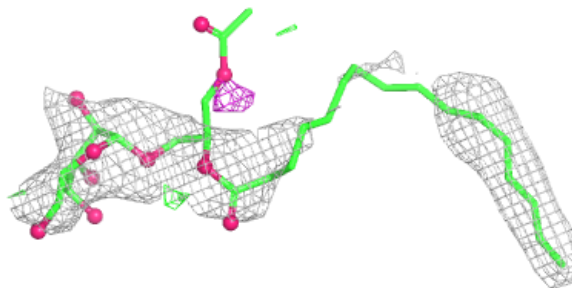


Electron density around SQD F 104:

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

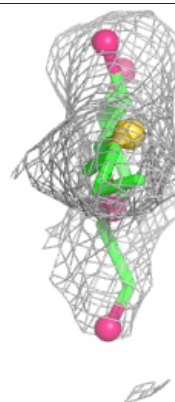
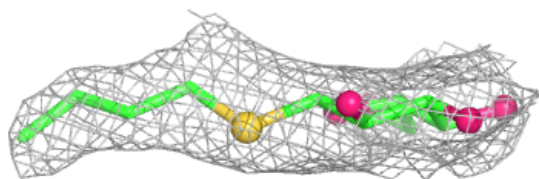
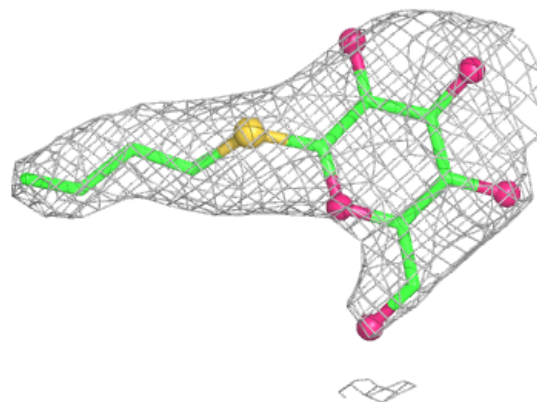
**Electron density around LMG Z 101:**

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

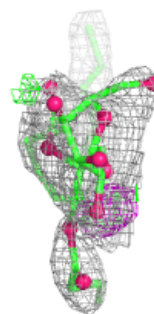
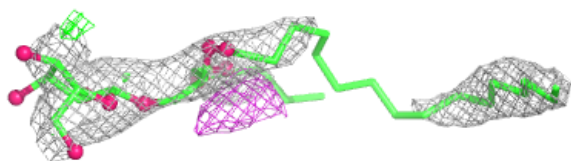
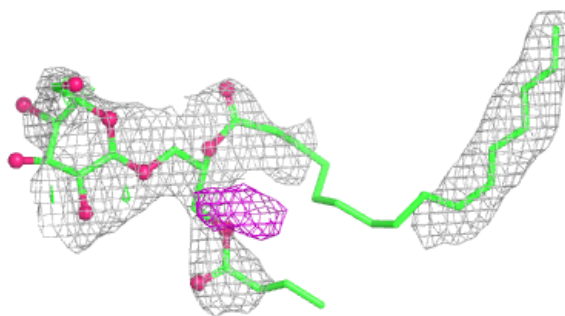


Electron density around HTG d 414:

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

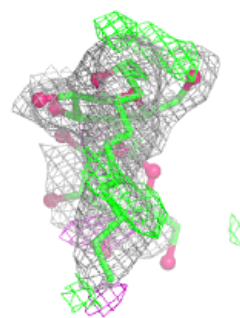
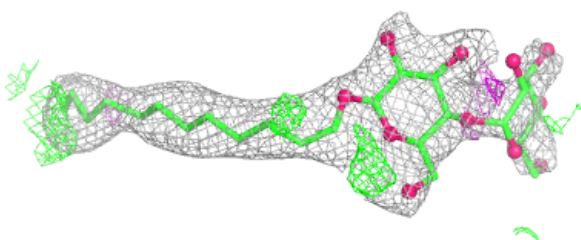
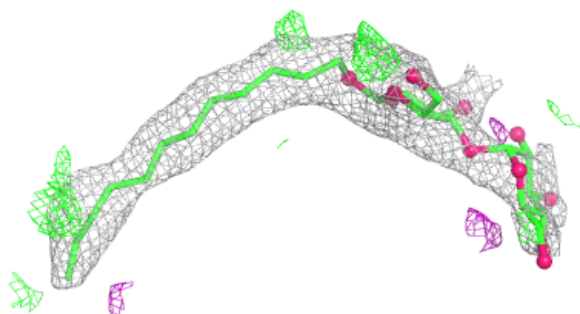
**Electron density around LMG z 101:**

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

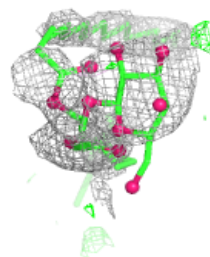
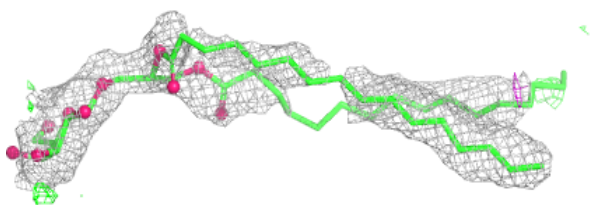
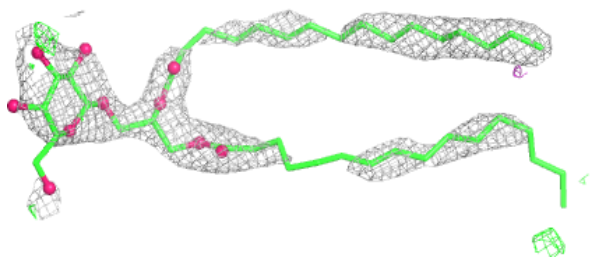


Electron density around LMT M 104:

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

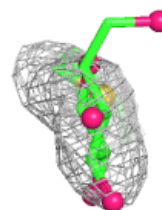
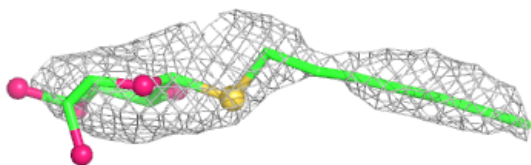
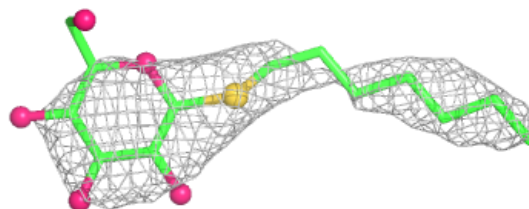
**Electron density around LMG c 523:**

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

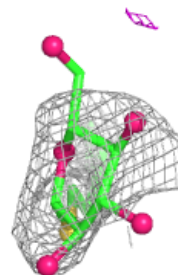
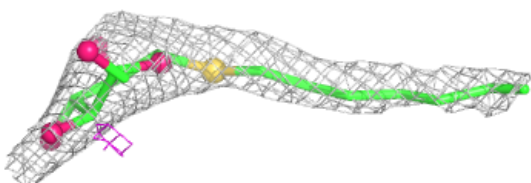
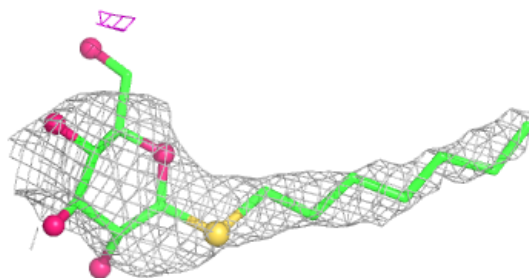


Electron density around HTG c 525:

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

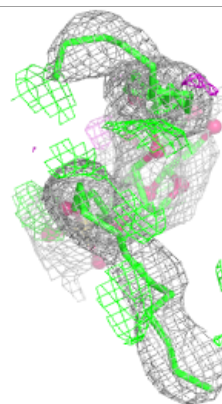
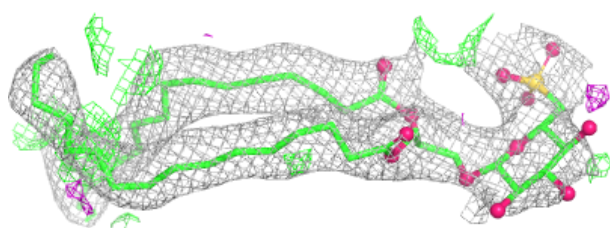
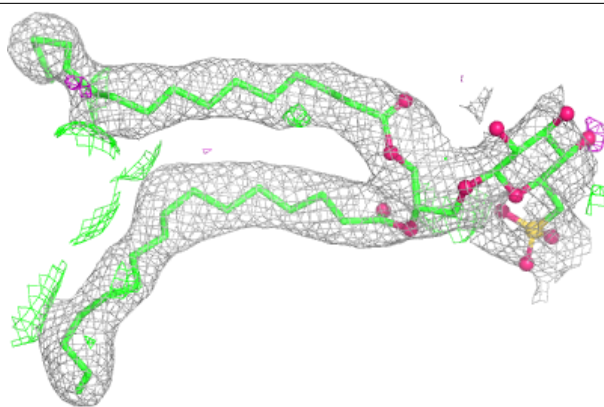
**Electron density around HTG B 623:**

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

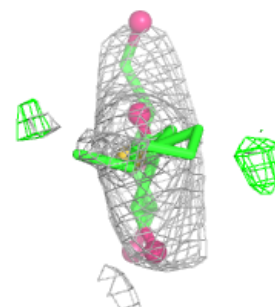
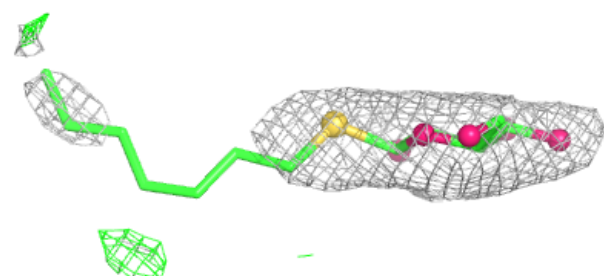
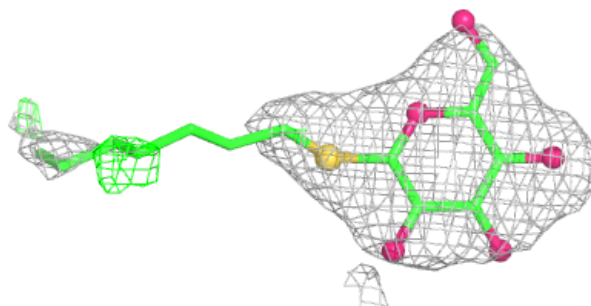


Electron density around SQD B 621:

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

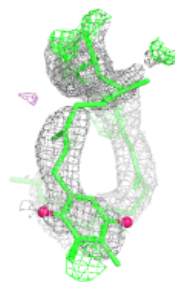
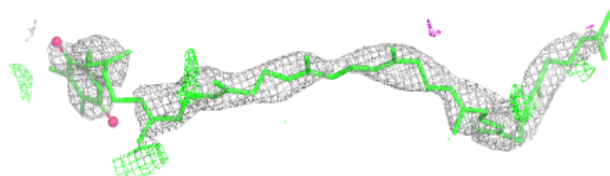
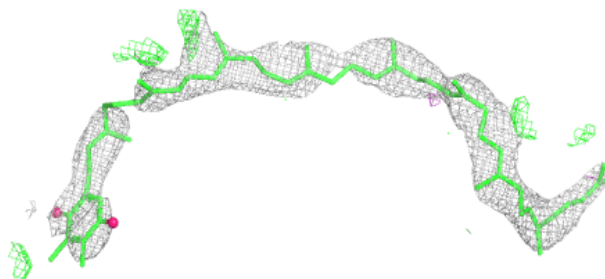
**Electron density around HTG C 522:**

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

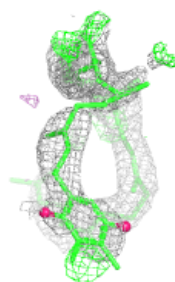
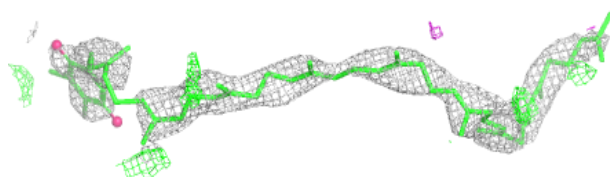
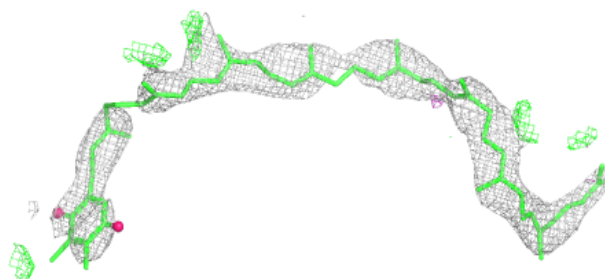


Electron density around PL9 A 416 (A):

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

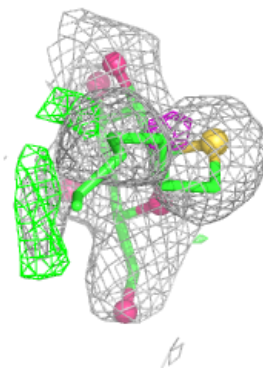
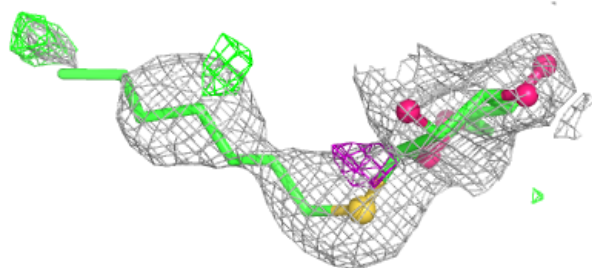
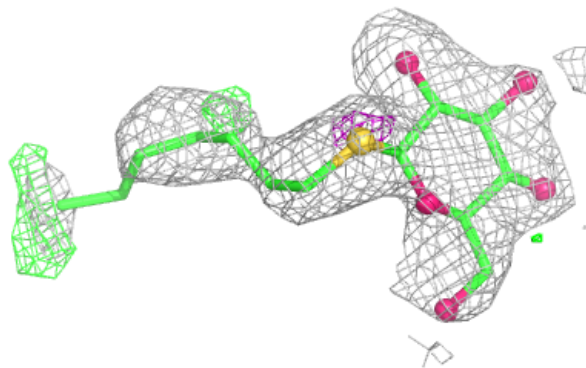
**Electron density around PL9 A 416 (B):**

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

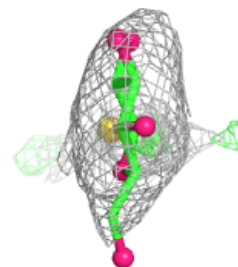
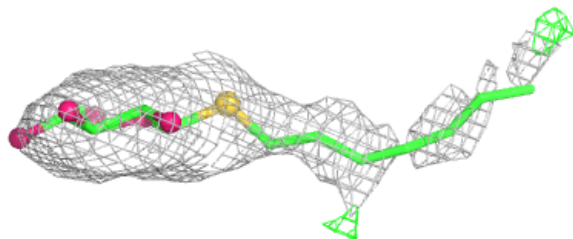
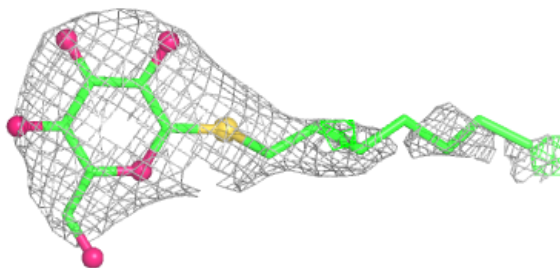


Electron density around HTG b 631:

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

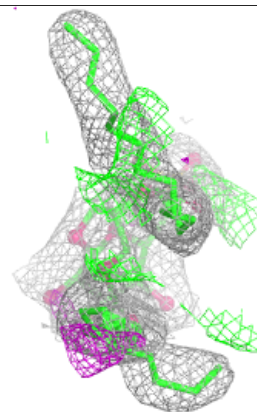
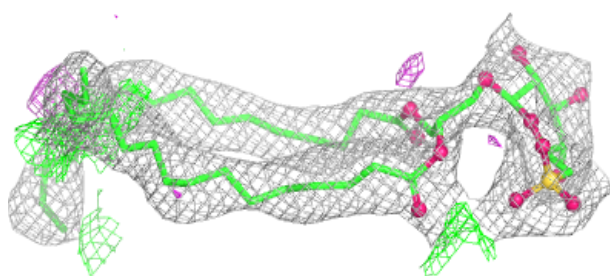
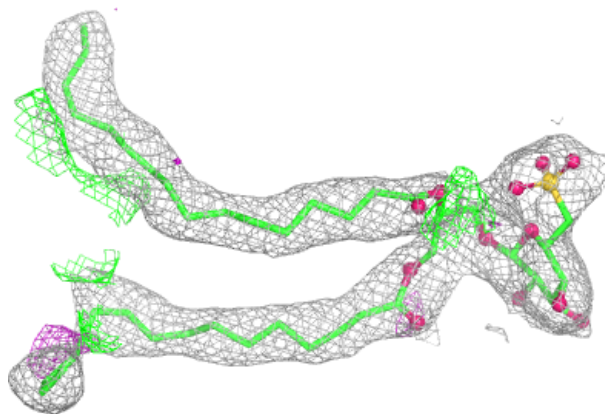
**Electron density around HTG c 524:**

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

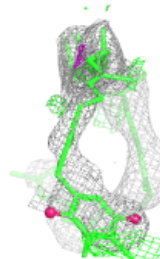
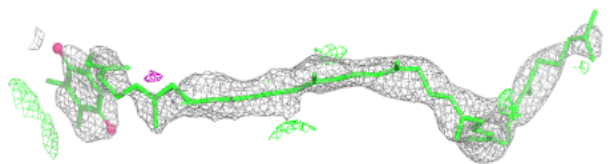
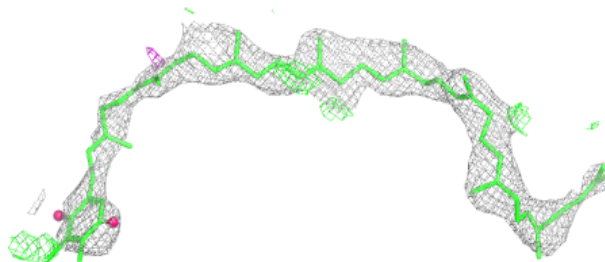


Electron density around SQD L 102:

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

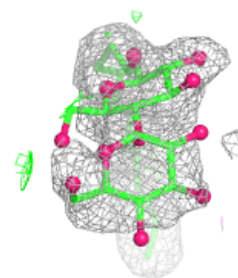
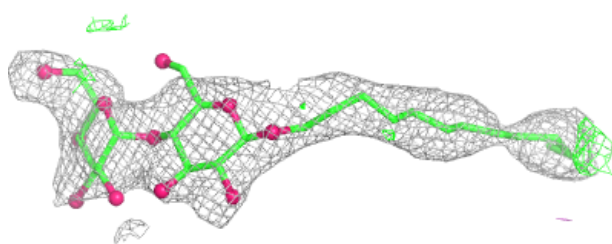
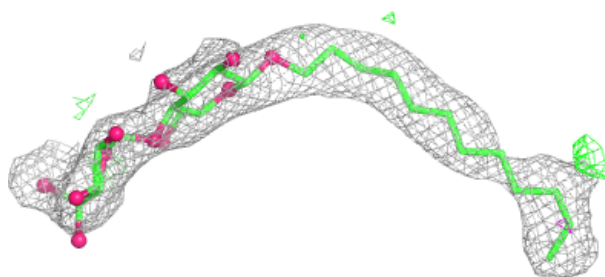
**Electron density around PL9 a 416 (B):**

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

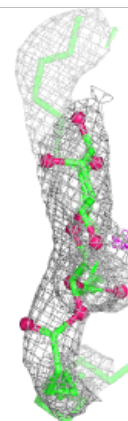
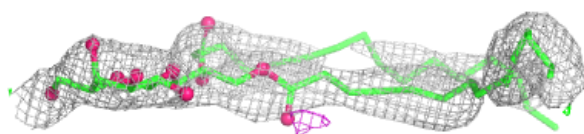
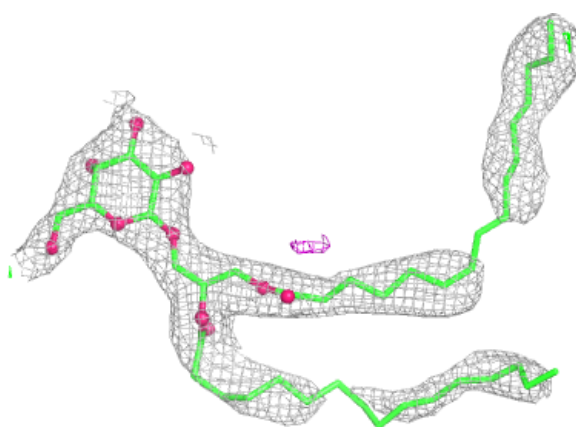


Electron density around LMT m 102:

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

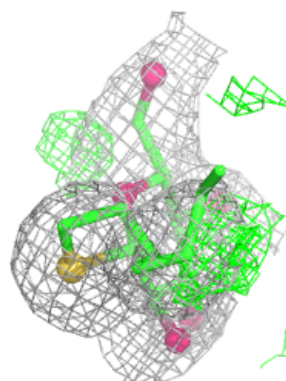
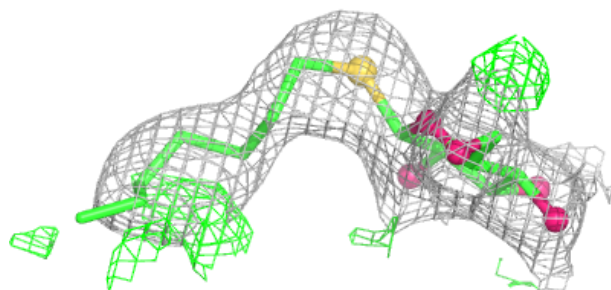
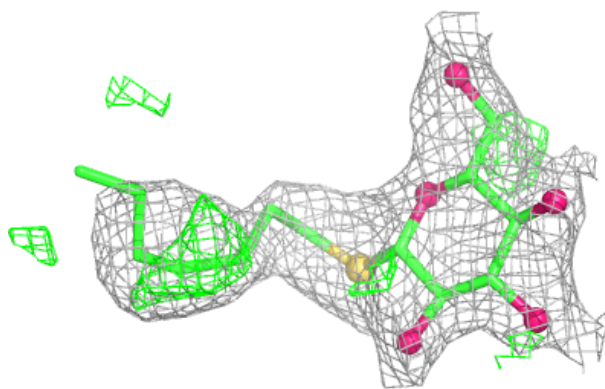
**Electron density around LMG C 519:**

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

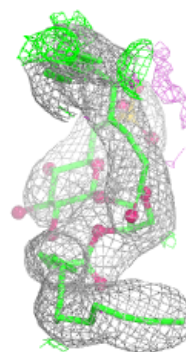
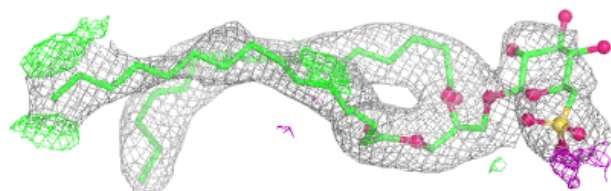
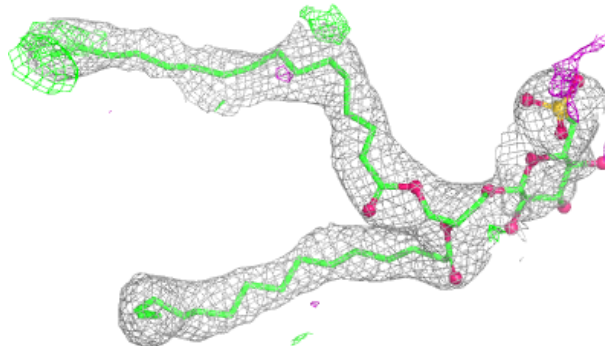


Electron density around HTG B 622:

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

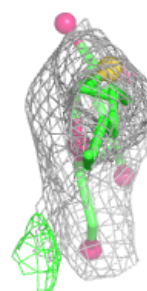
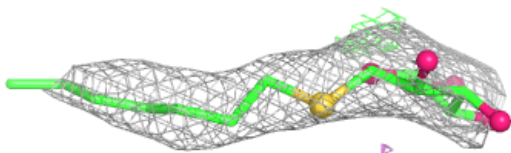
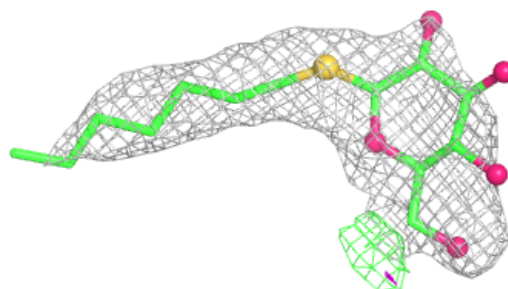
**Electron density around SQD A 412:**

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

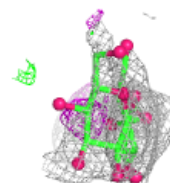
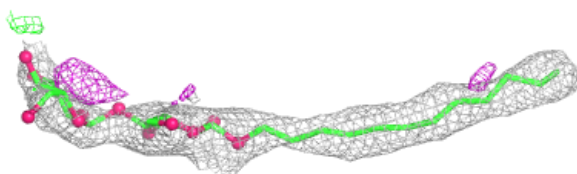
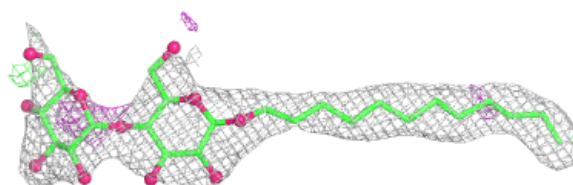


Electron density around HTG b 632:

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

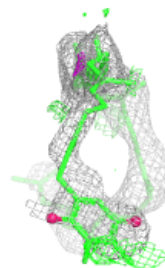
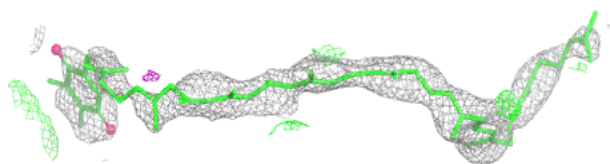
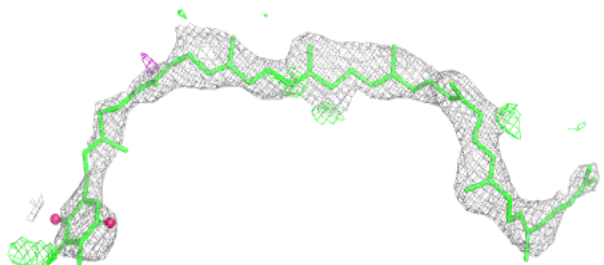
**Electron density around LMT M 105:**

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

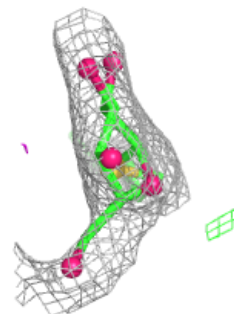
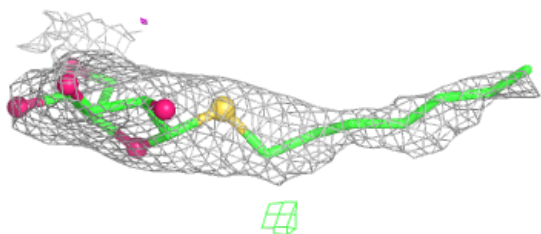
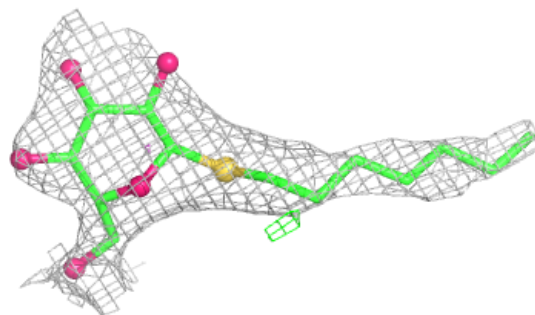


Electron density around PL9 a 416 (A):

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

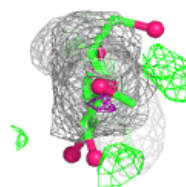
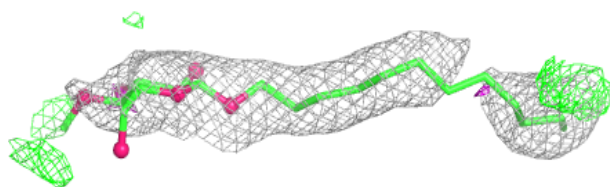
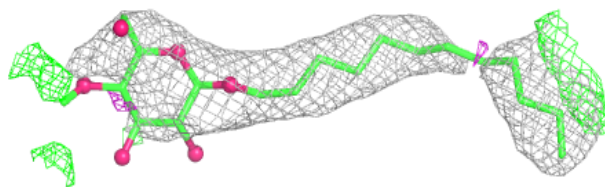
**Electron density around HTG C 523:**

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

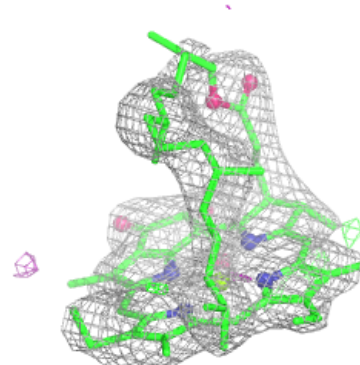
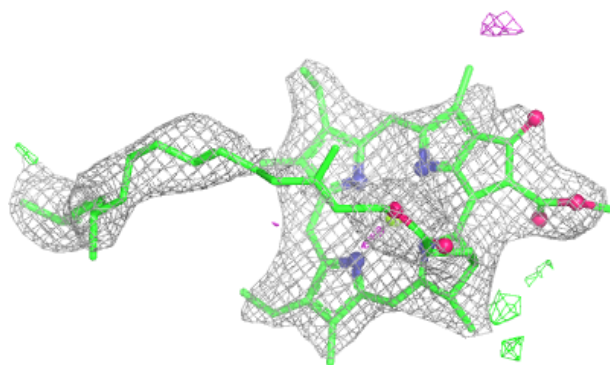
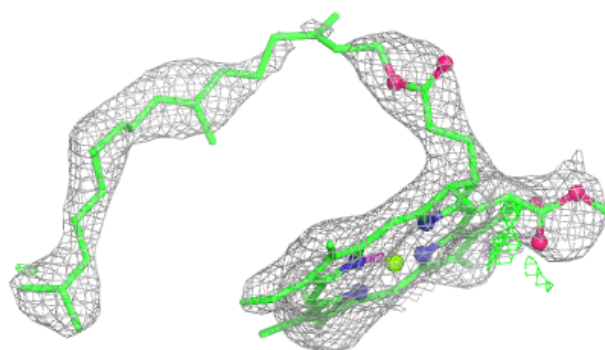


Electron density around LMT T 104:

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

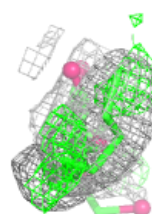
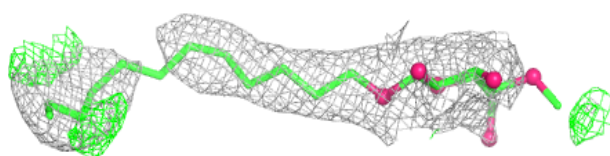
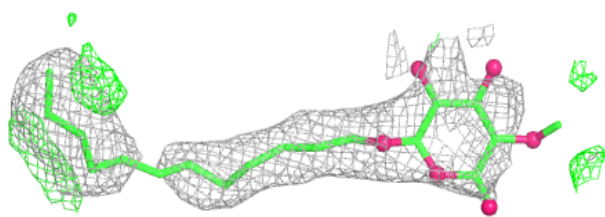
**Electron density around CLA C 514:**

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

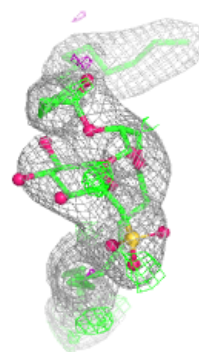
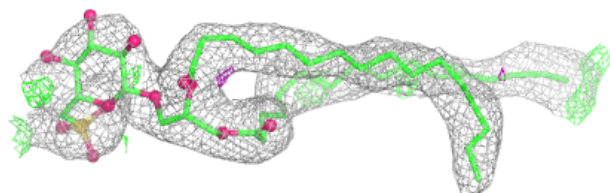
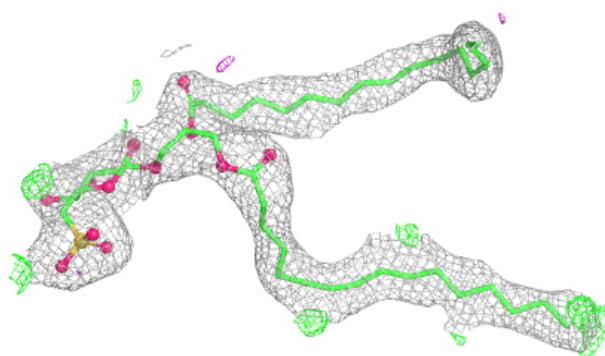


Electron density around LMT t 101:

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

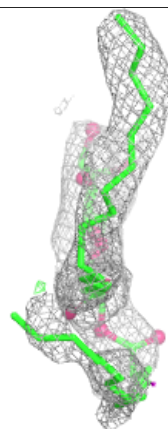
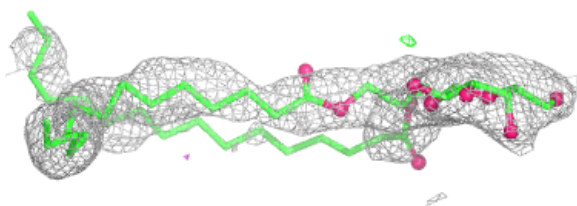
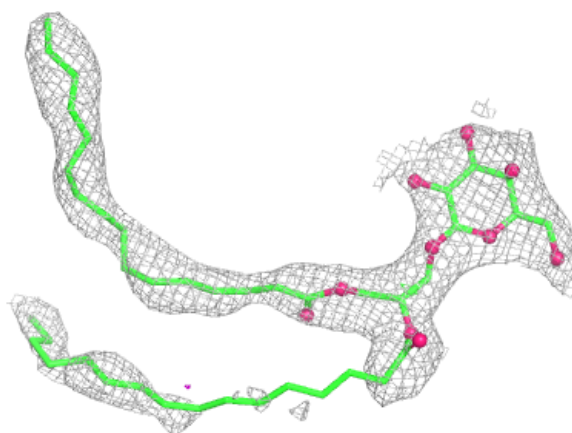
**Electron density around SQD a 405:**

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



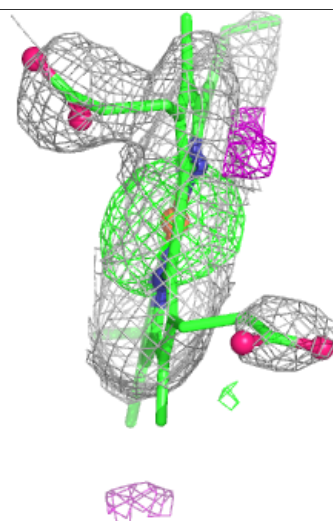
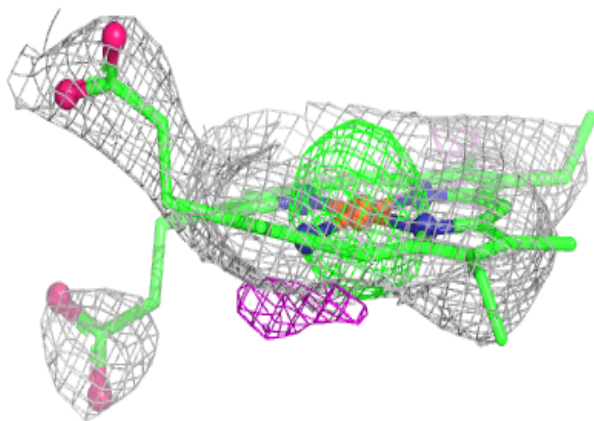
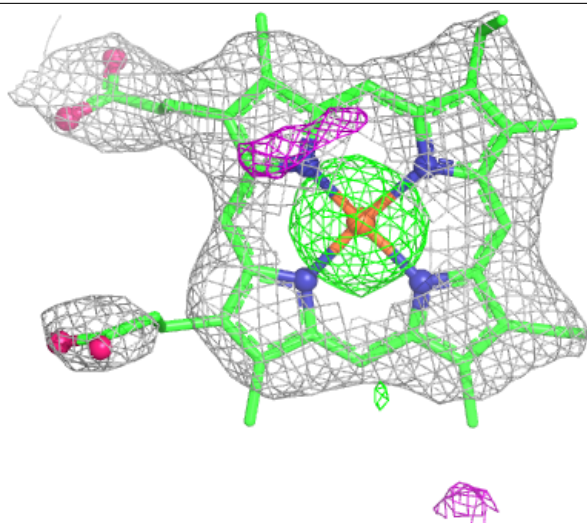
Electron density around LMG c 522:

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



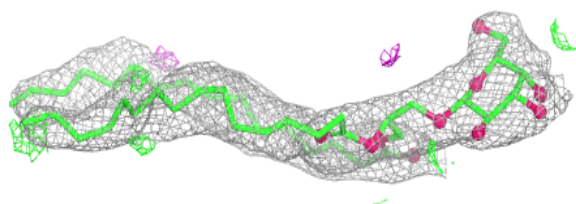
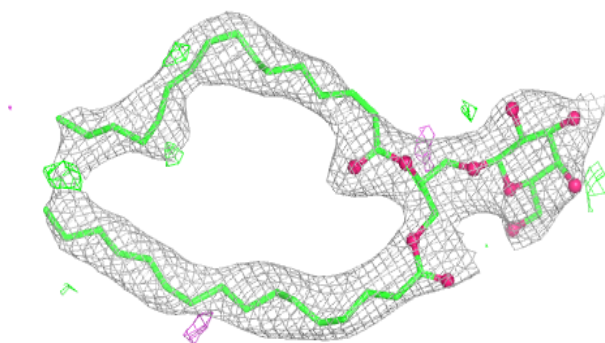
Electron density around HEM F 102:

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

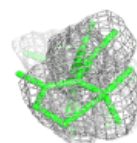
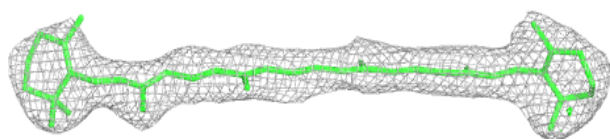
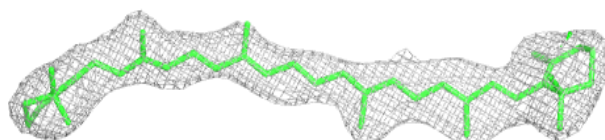


Electron density around LMG C 501:

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

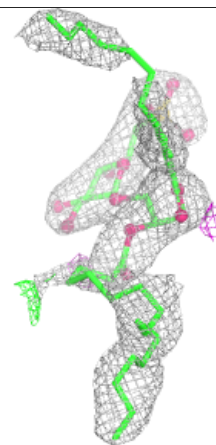
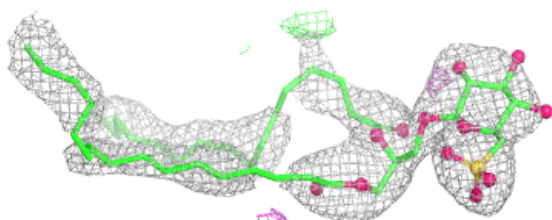
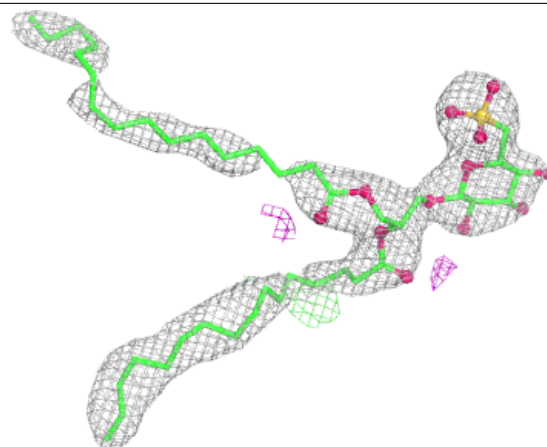
**Electron density around BCR K 101:**

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

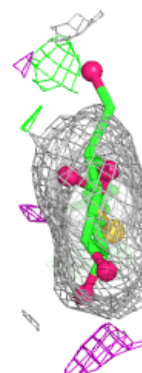
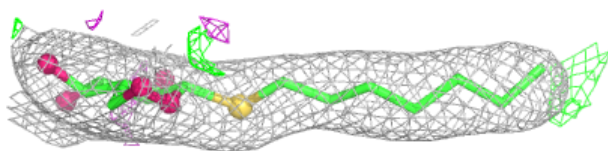
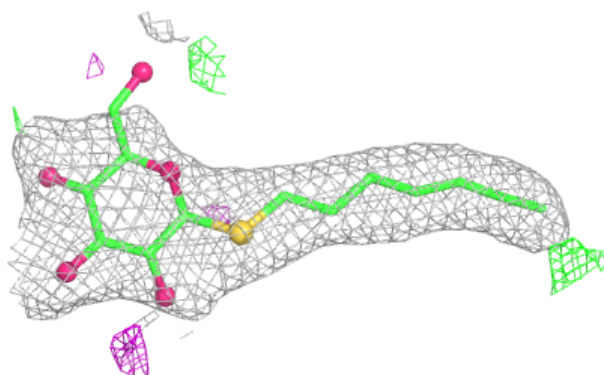


Electron density around SQD A 409:

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

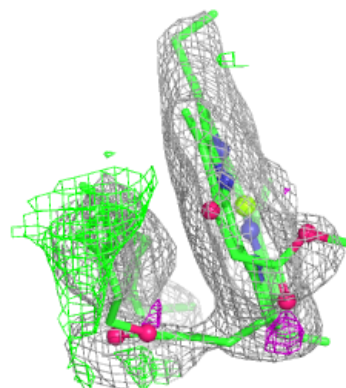
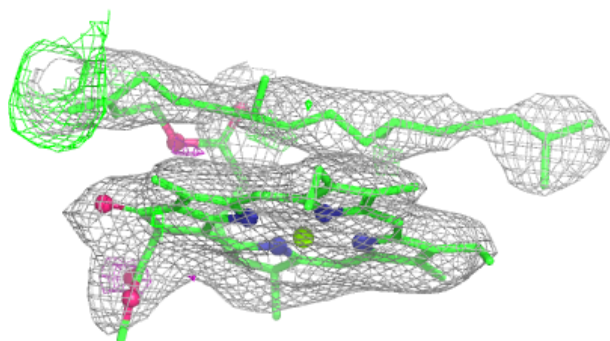
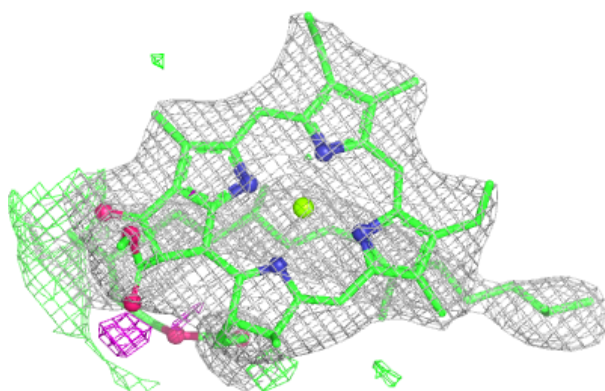
**Electron density around HTG B 629:**

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

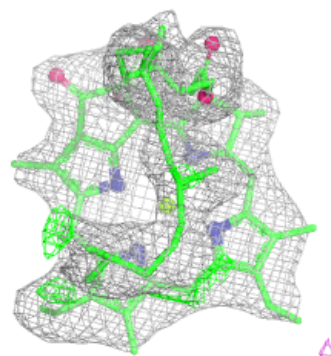
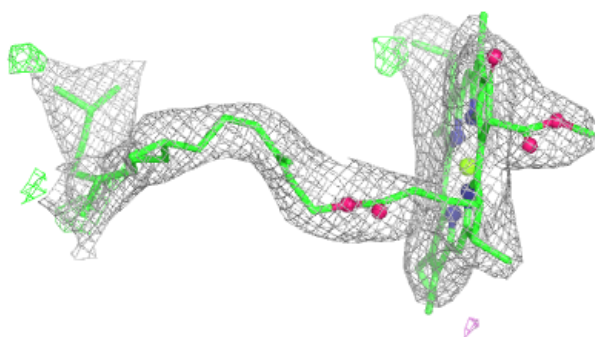
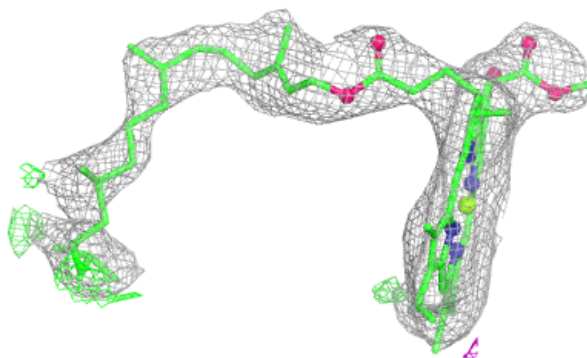


Electron density around CLA B 602:

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

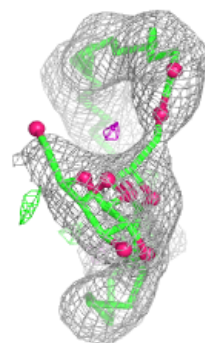
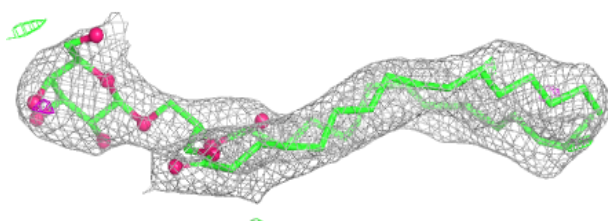
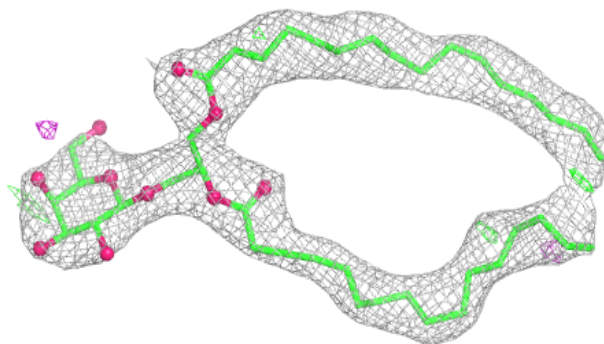
**Electron density around CLA C 507:**

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

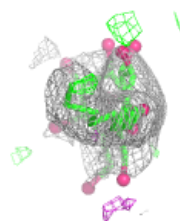
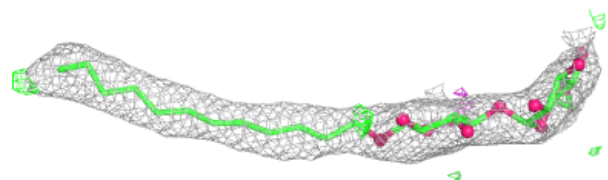
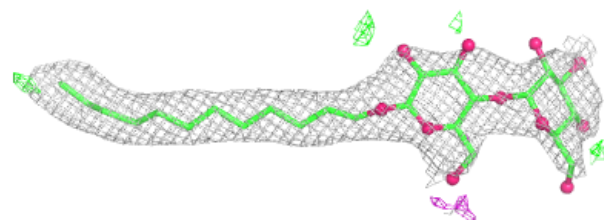


Electron density around LMG a 415:

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

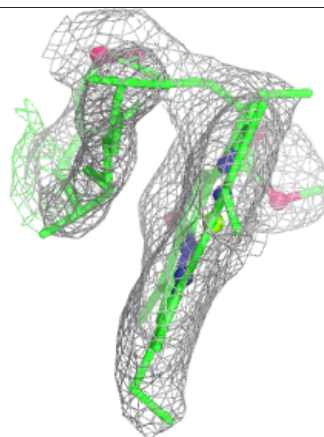
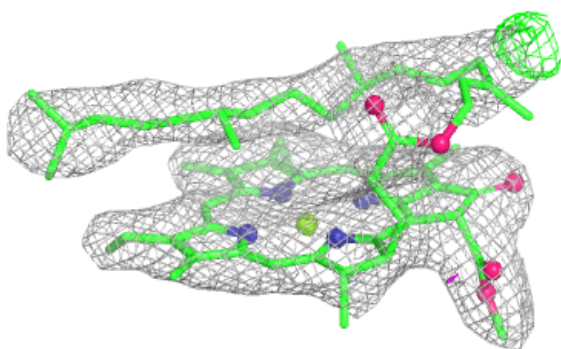
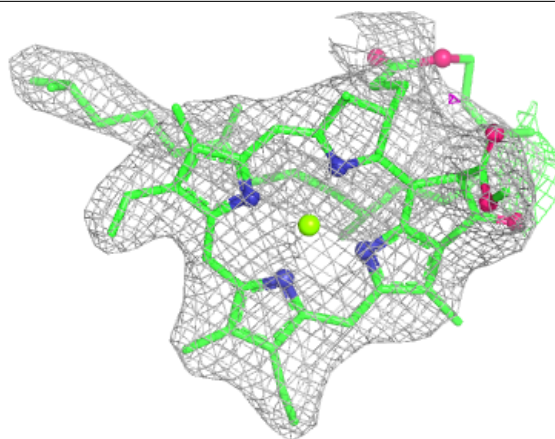
**Electron density around LMT M 102:**

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

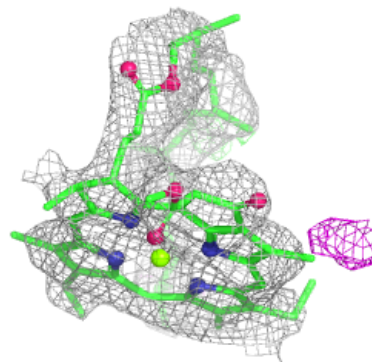
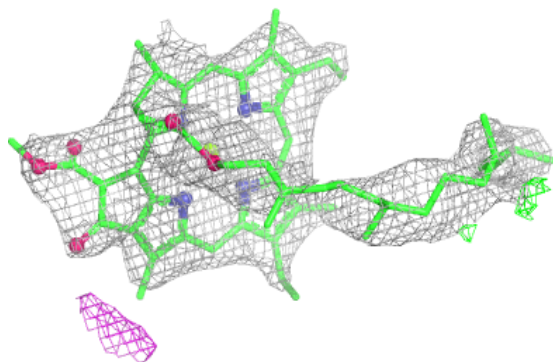
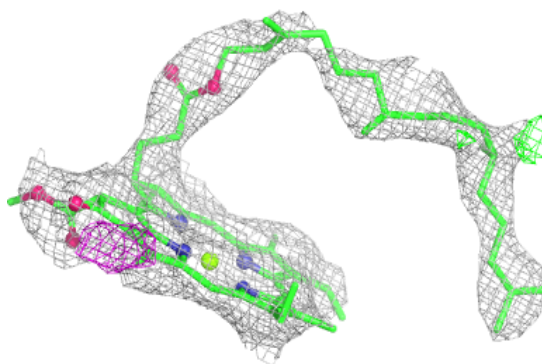


Electron density around CLA b 610:

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

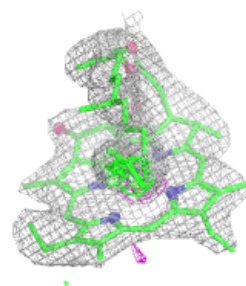
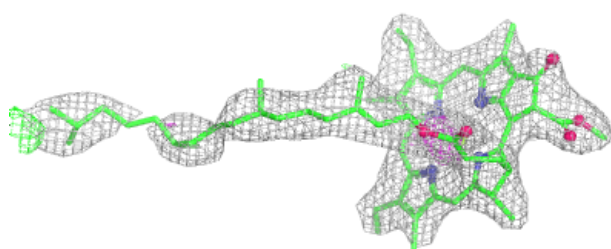
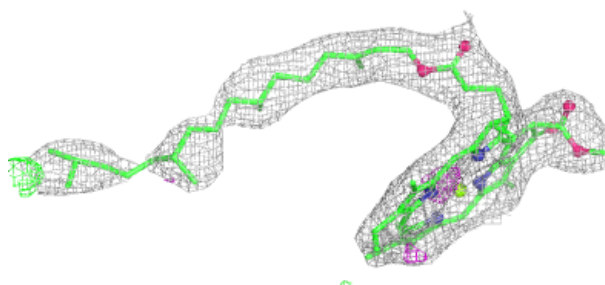
**Electron density around CLA c 517:**

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

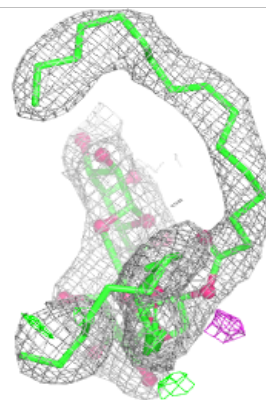
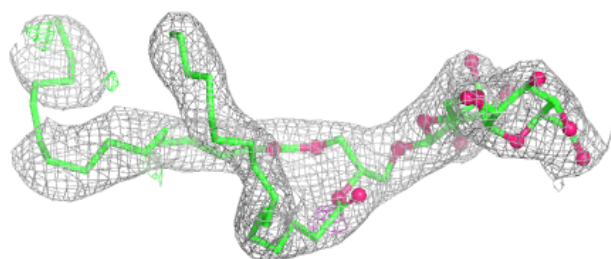
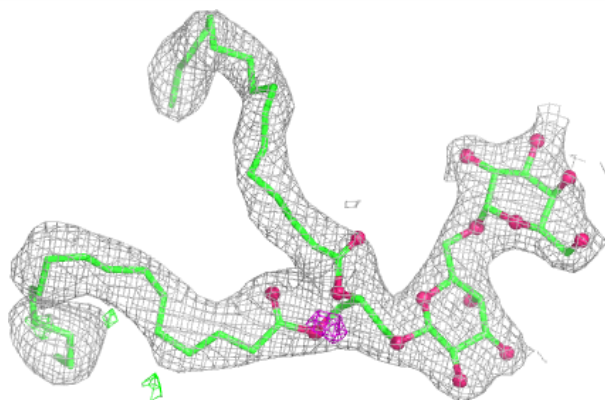


Electron density around CLA C 505:

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

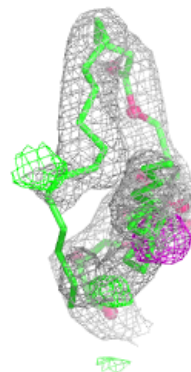
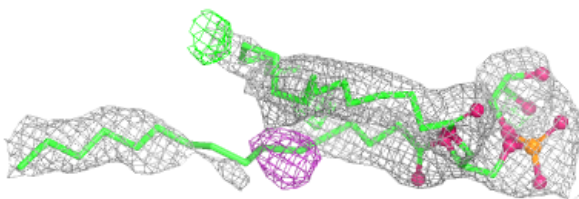
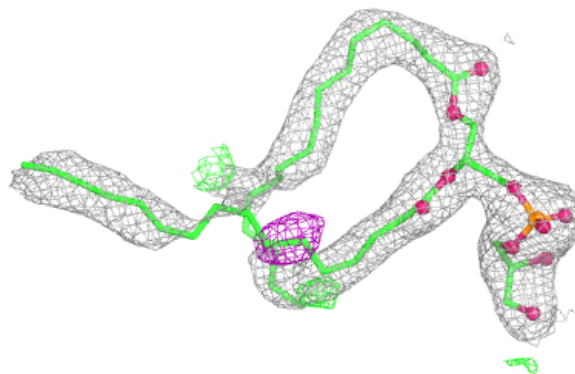
**Electron density around DGD C 517:**

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

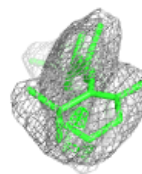
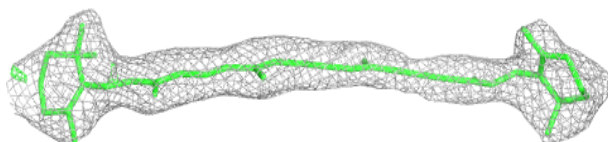
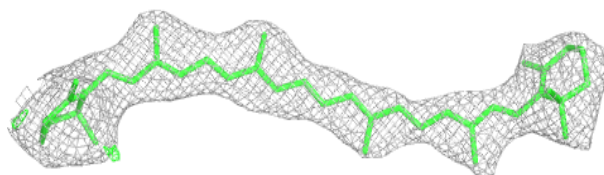


Electron density around LHG D 413:

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

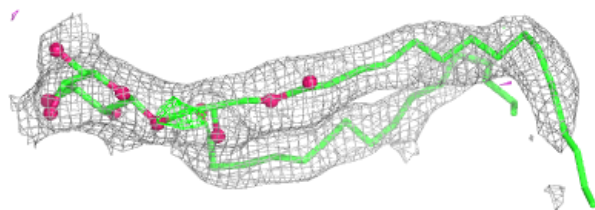
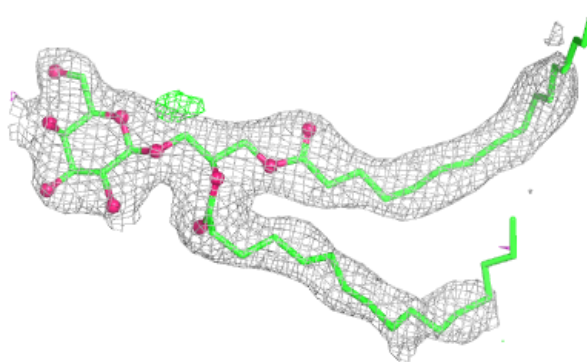
**Electron density around BCR k 102:**

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



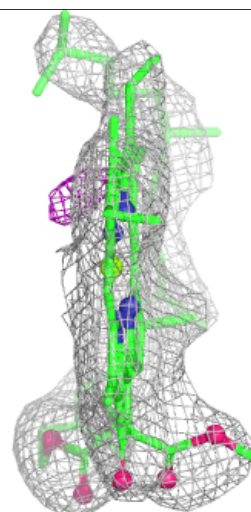
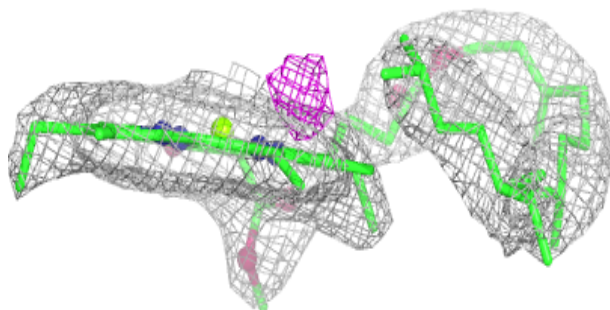
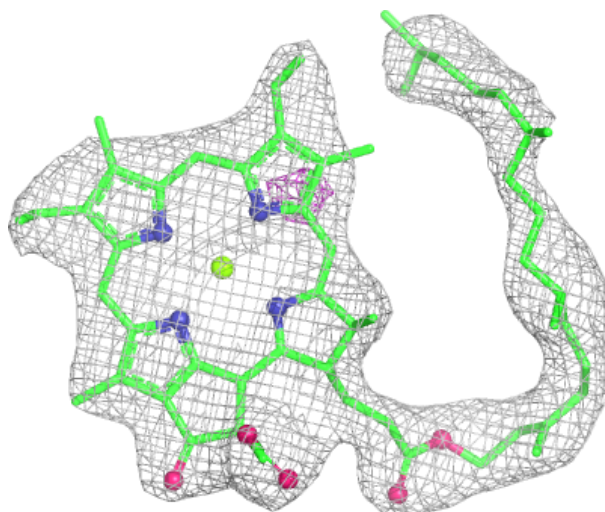
Electron density around LMG D 417:

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



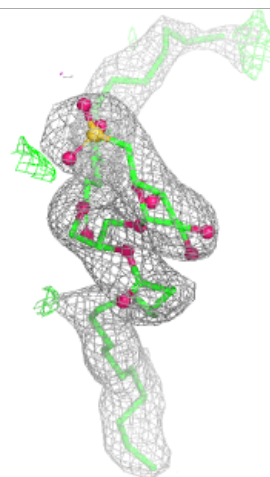
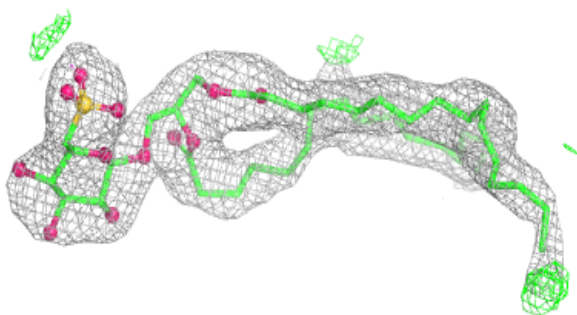
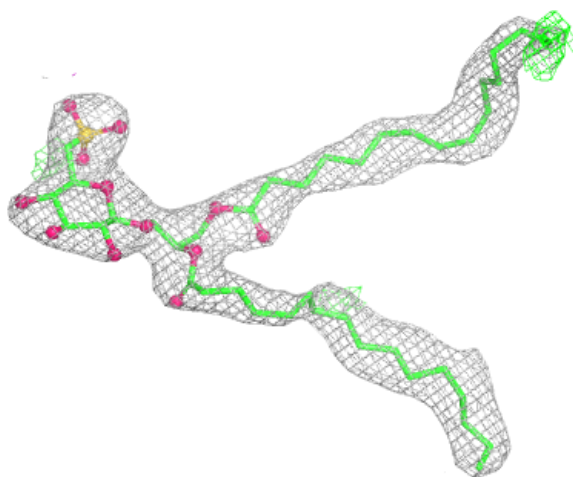
Electron density around CLA C 513:

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



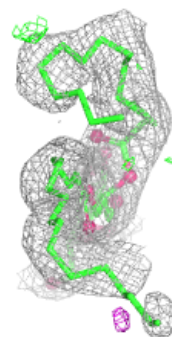
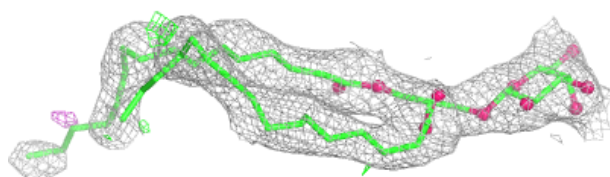
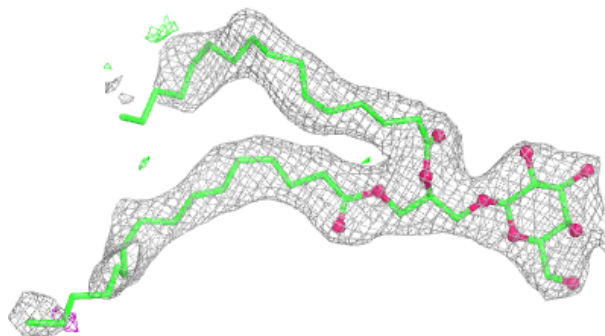
Electron density around SQD a 414:

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

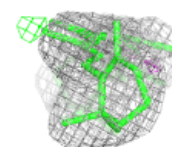
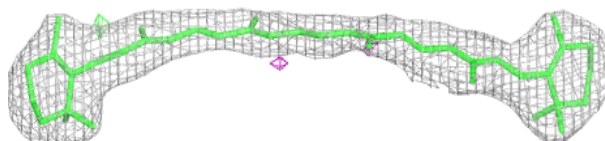


Electron density around LMG d 416:

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

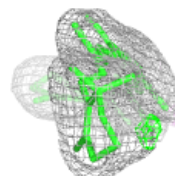
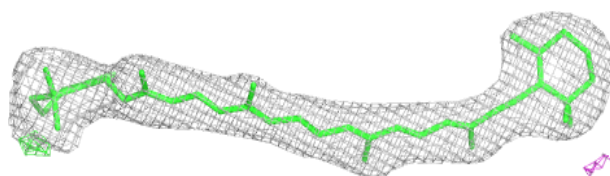
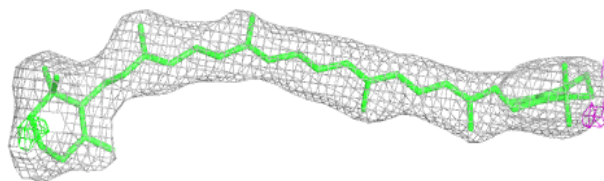
**Electron density around BCR K 103:**

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

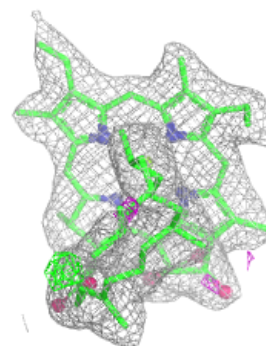
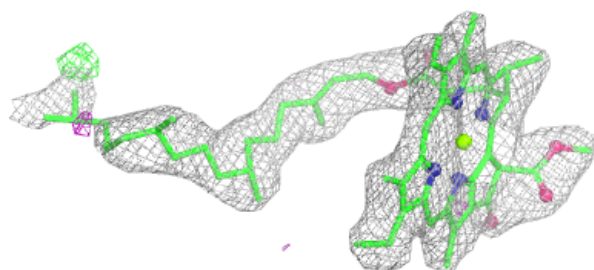
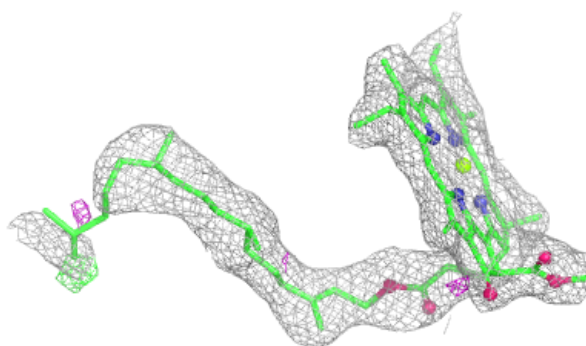


Electron density around BCR d 406:

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

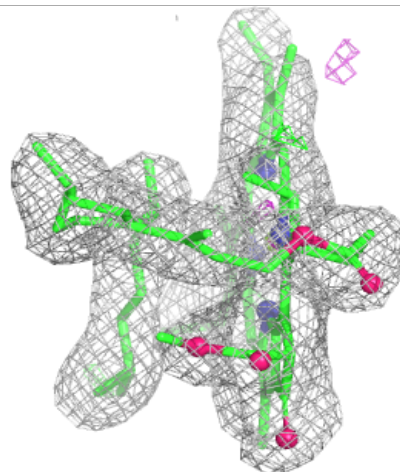
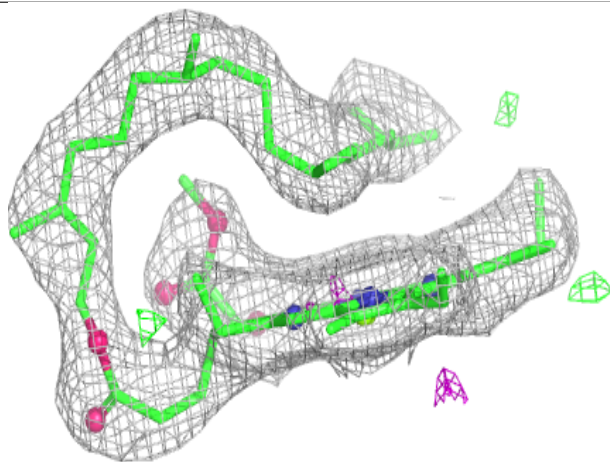
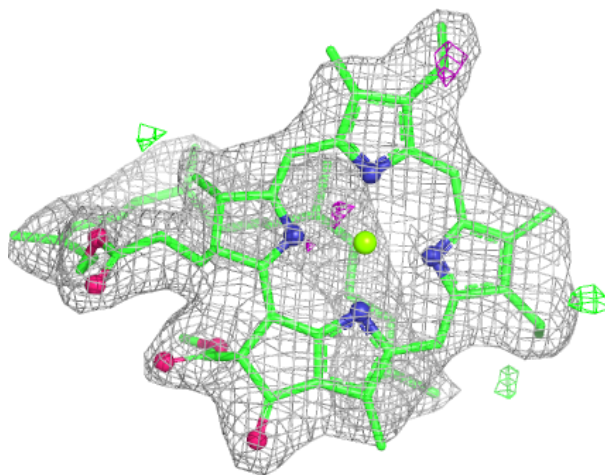
**Electron density around CLA c 512:**

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



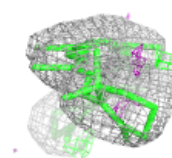
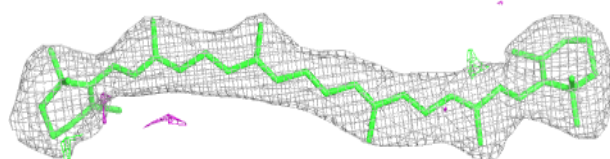
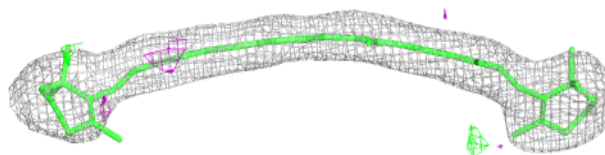
Electron density around CLA C 511:

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

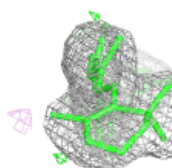
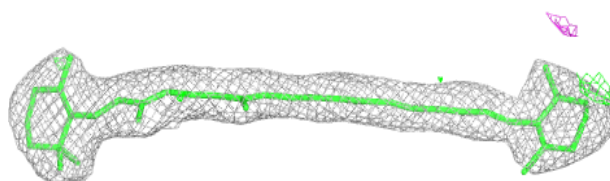
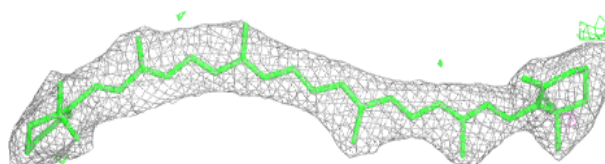


Electron density around BCR D 408:

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

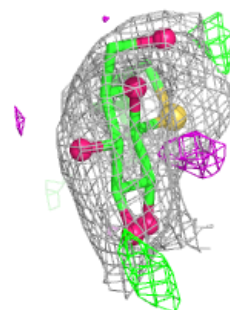
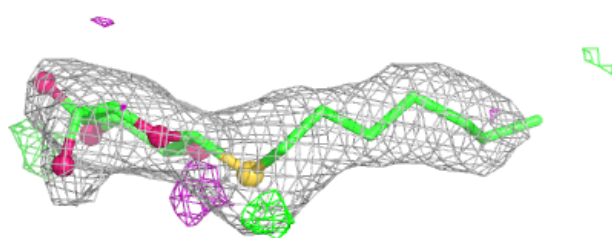
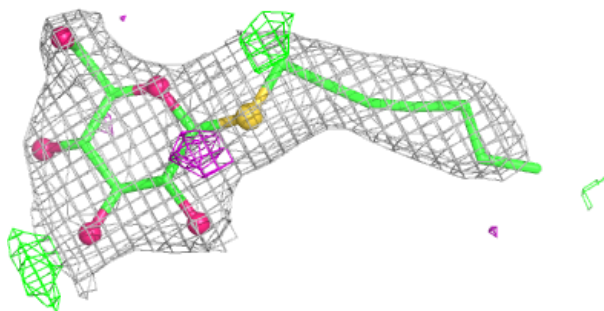
**Electron density around BCR H 101:**

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

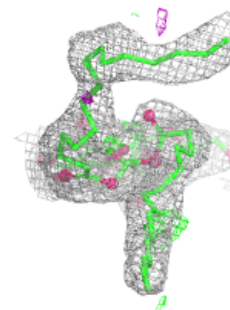
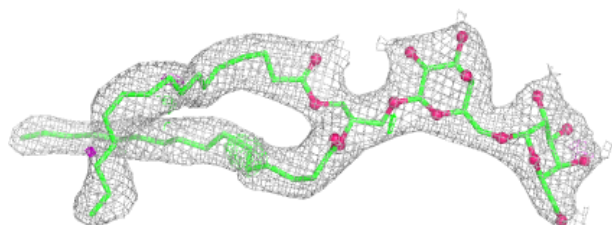
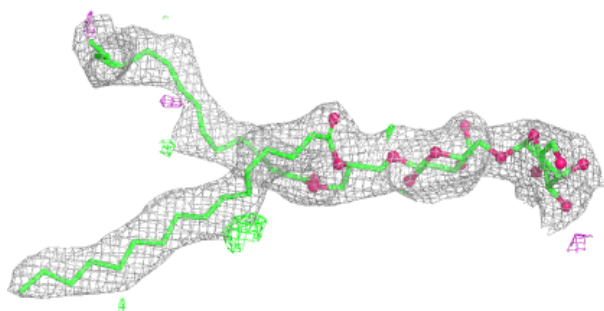


Electron density around HTG O 301:

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

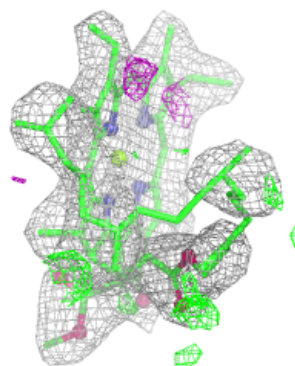
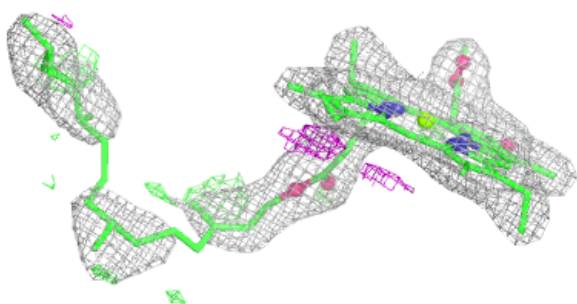
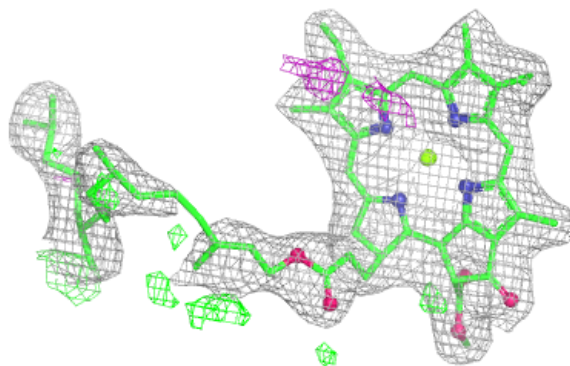
**Electron density around DGD C 516:**

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

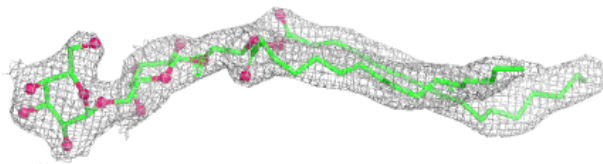
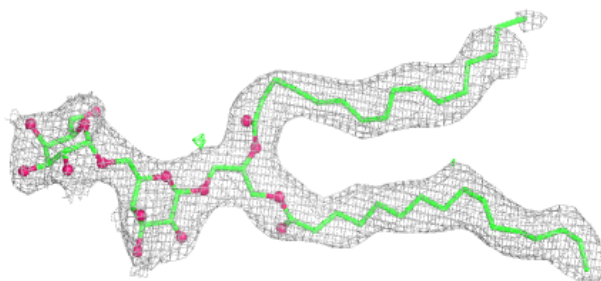


Electron density around CLA A 407:

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

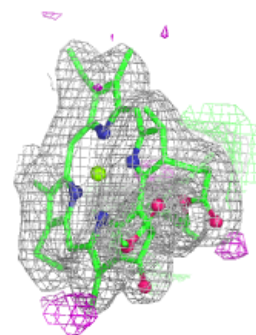
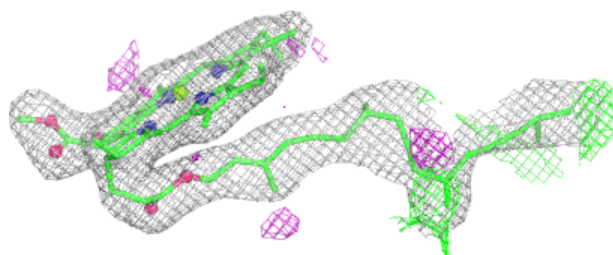
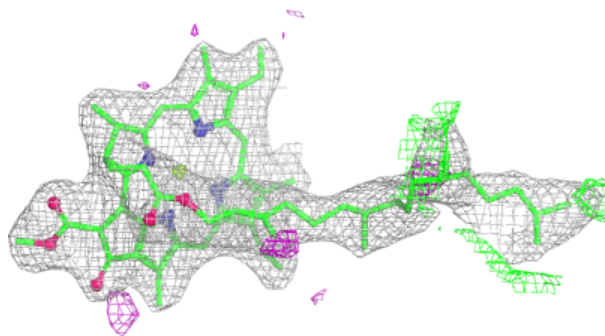
**Electron density around DGD C 518:**

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

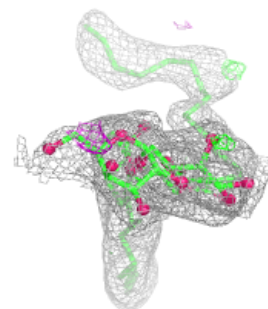
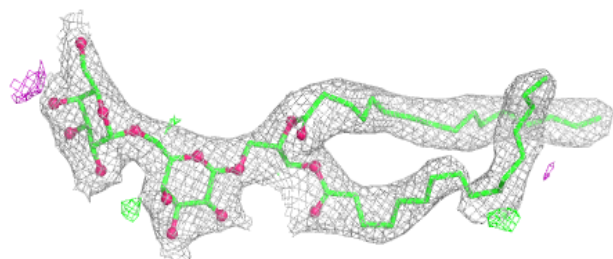
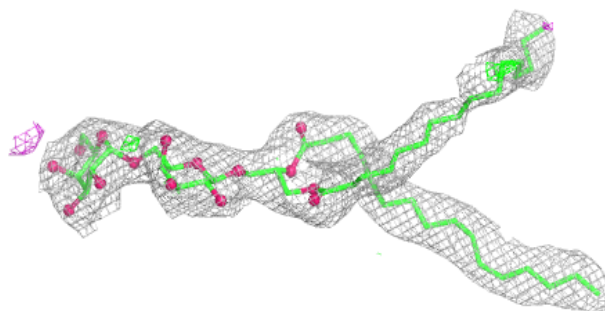


Electron density around CLA B 615:

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

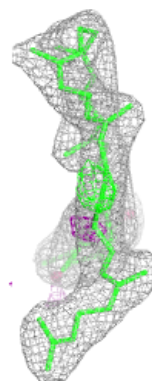
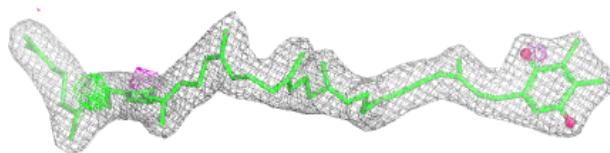
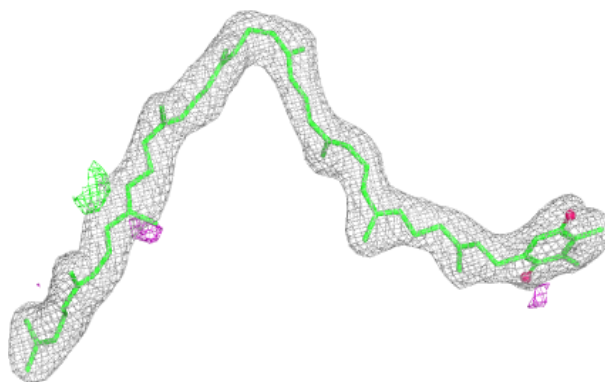
**Electron density around DGD c 519:**

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

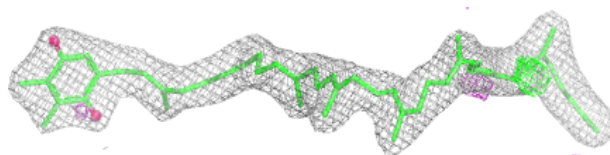
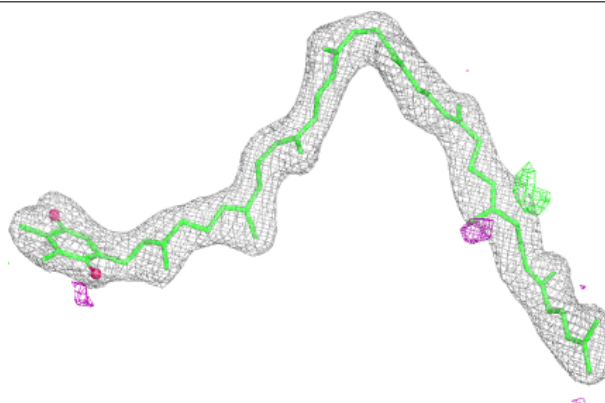


Electron density around PL9 D 409 (A):

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

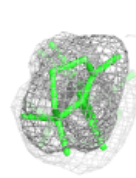
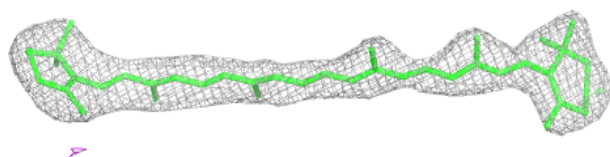
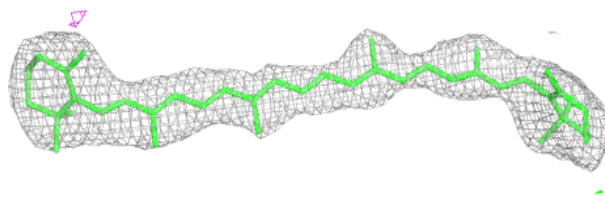
**Electron density around PL9 D 409 (B):**

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

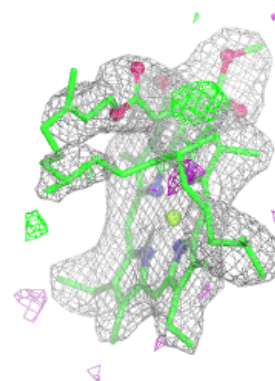
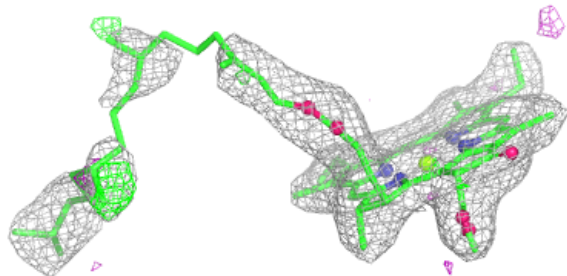
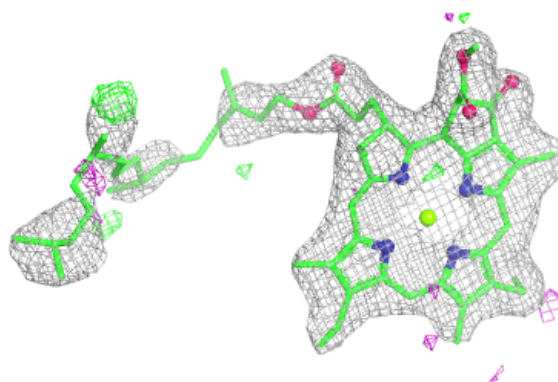


Electron density around BCR c 527:

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

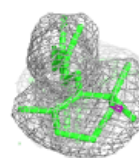
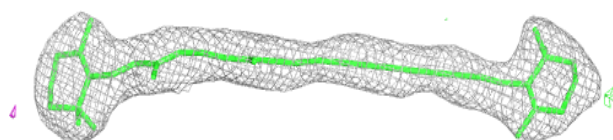
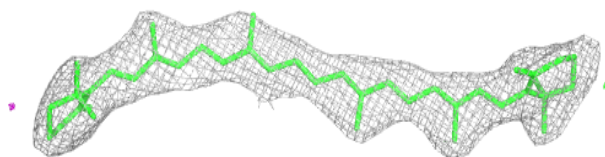
**Electron density around CLA a 412:**

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

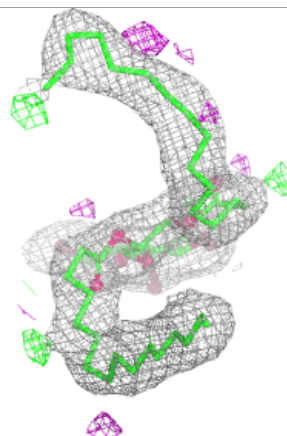
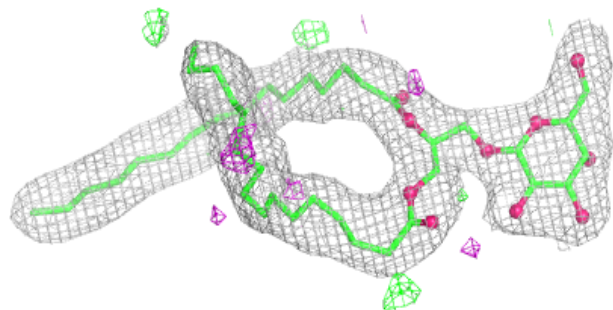
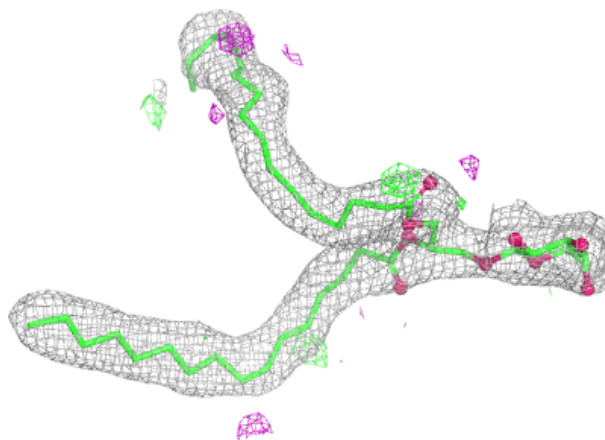


Electron density around BCR h 101:

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

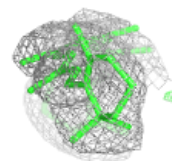
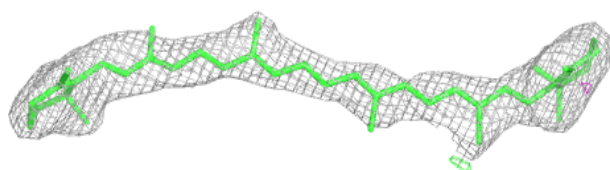
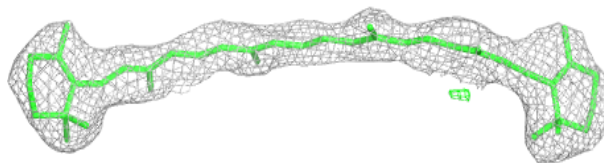
**Electron density around LMG b 629:**

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

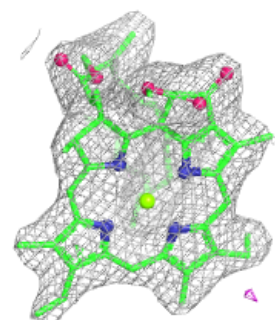
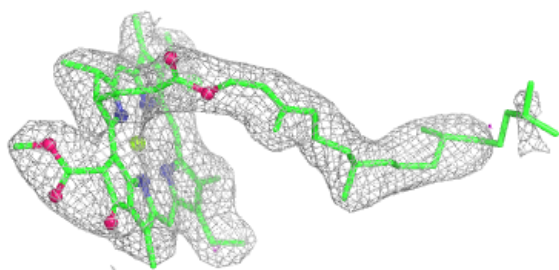
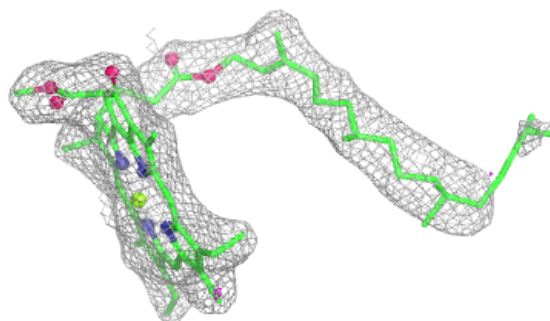


Electron density around BCR k 101:

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

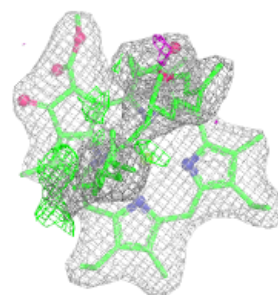
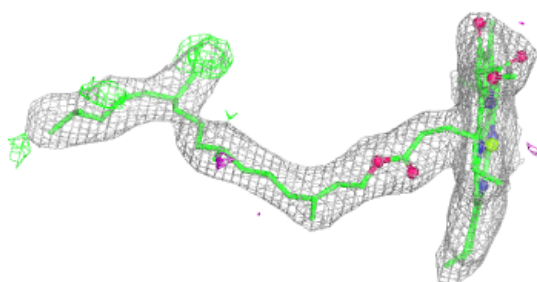
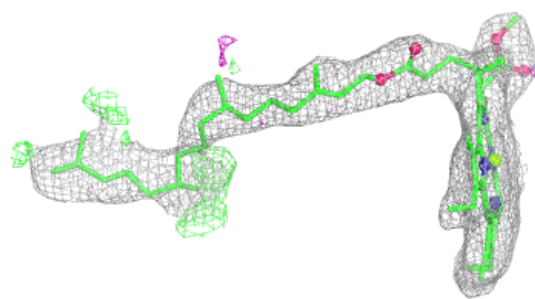
**Electron density around CLA C 509:**

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

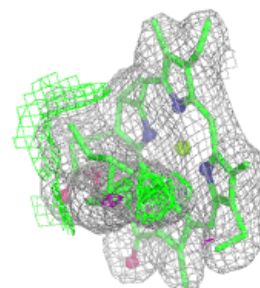
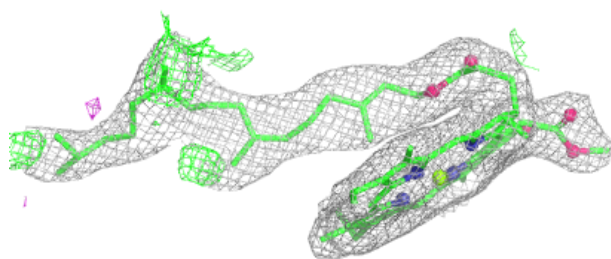
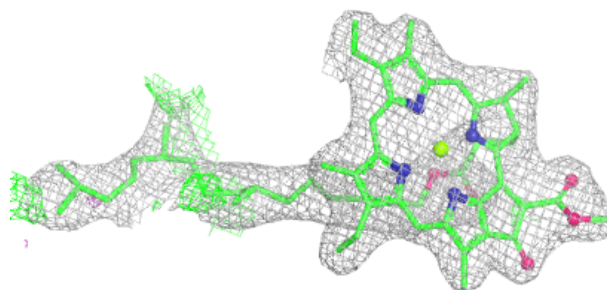


Electron density around CLA b 615:

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

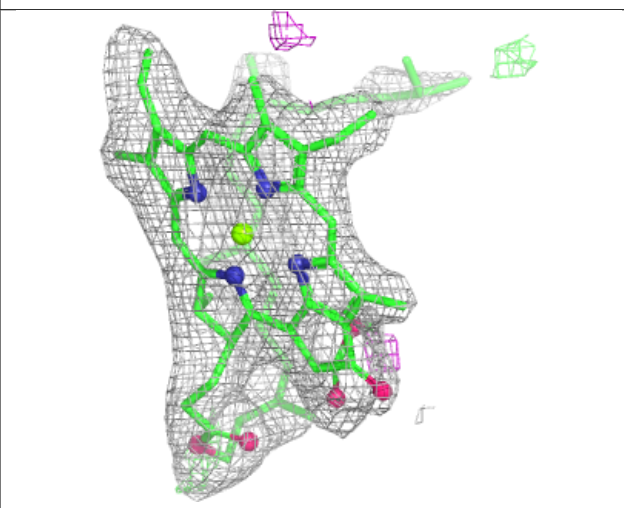
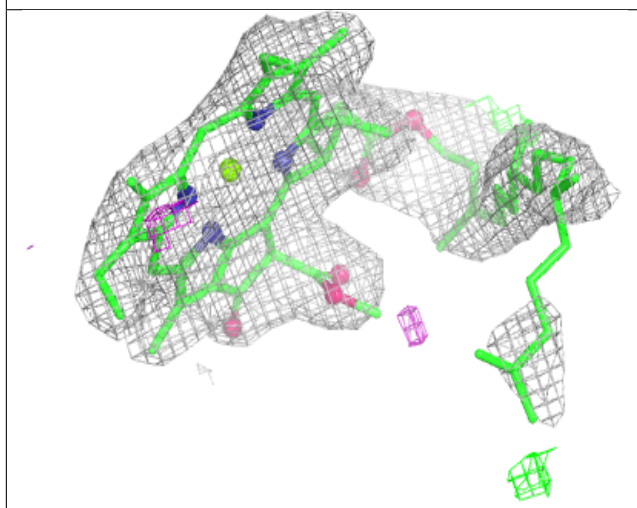
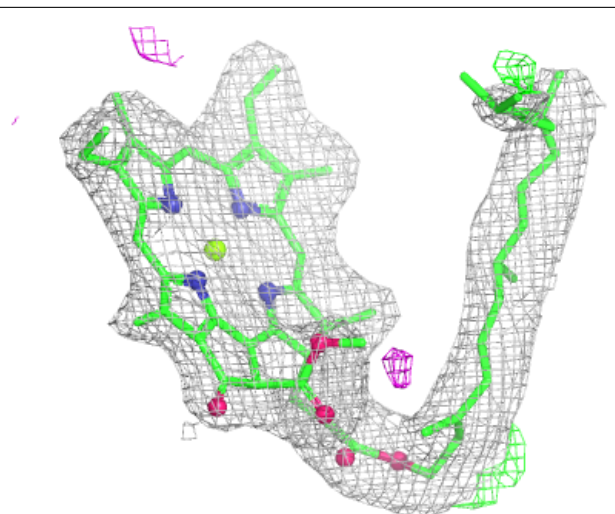
**Electron density around CLA b 623:**

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



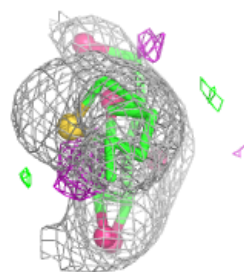
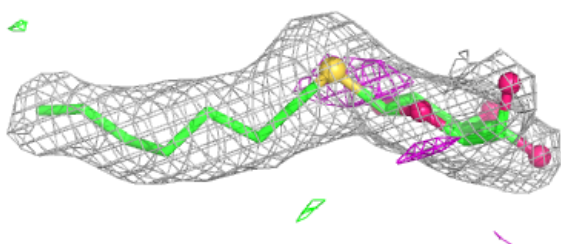
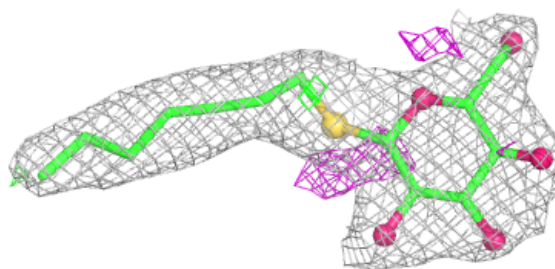
Electron density around CLA b 625:

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

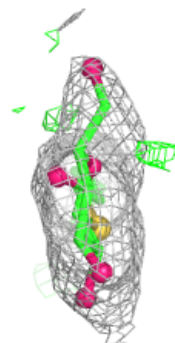
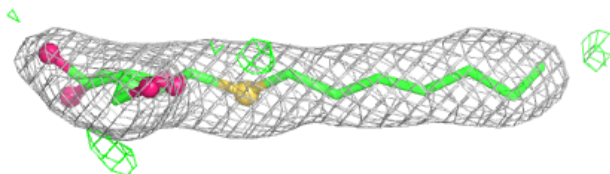
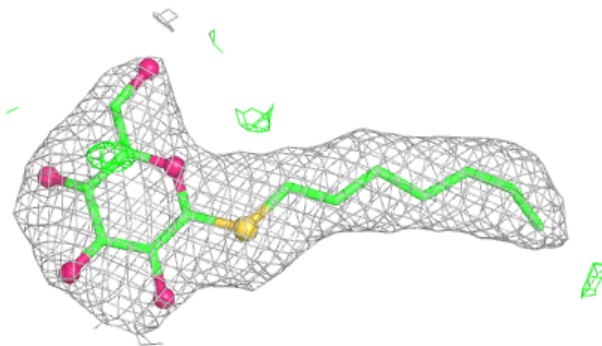


Electron density around HTG b 601:

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

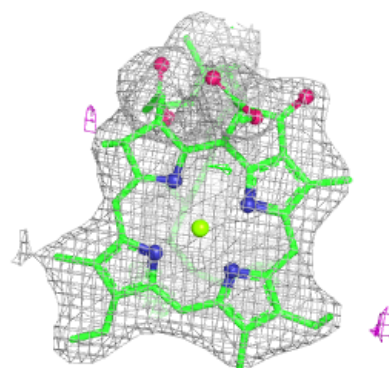
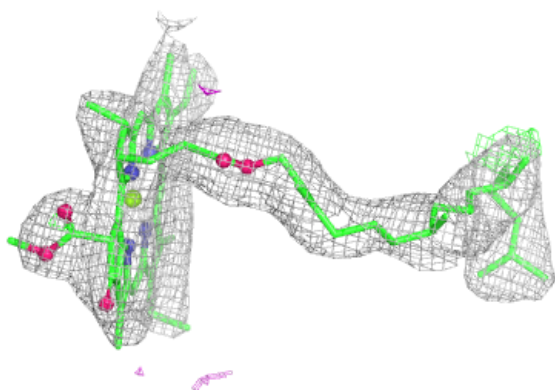
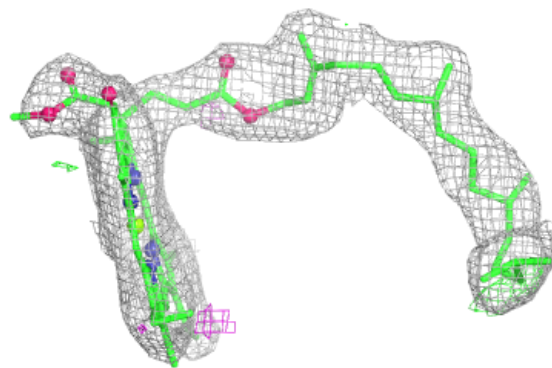
**Electron density around HTG b 607:**

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

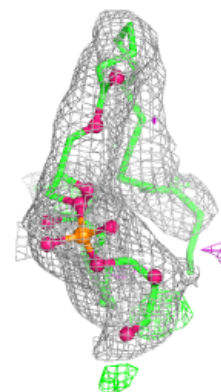
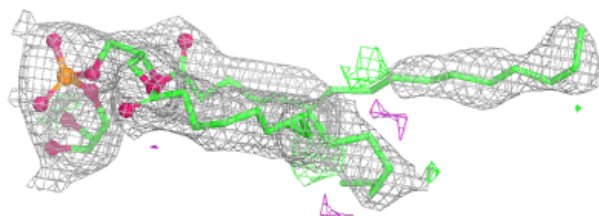
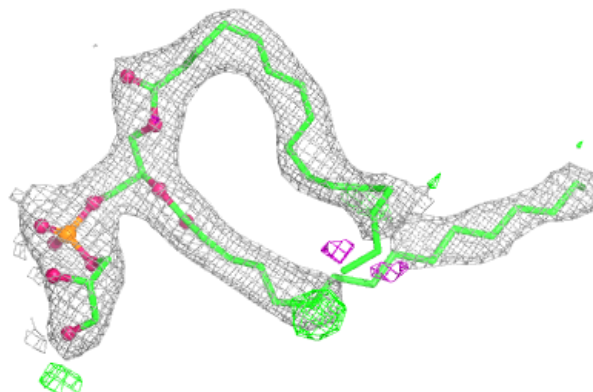


Electron density around CLA c 510:

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

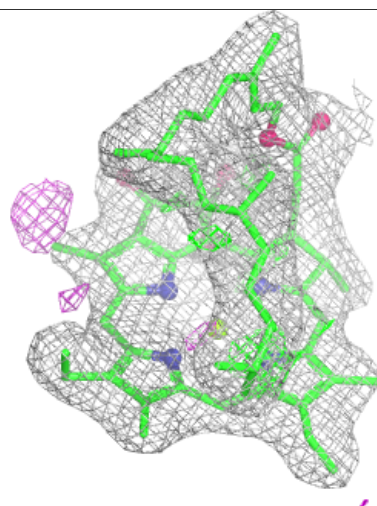
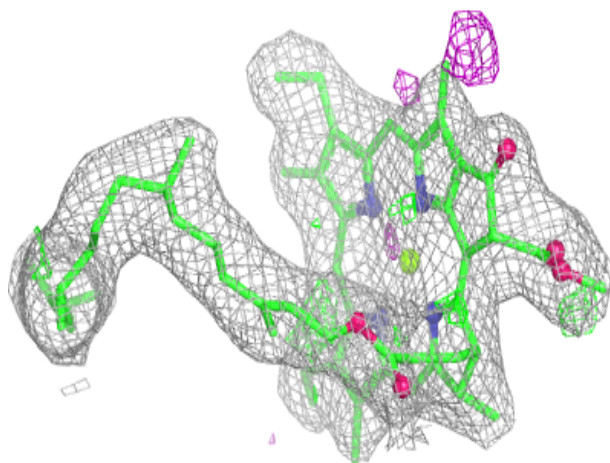
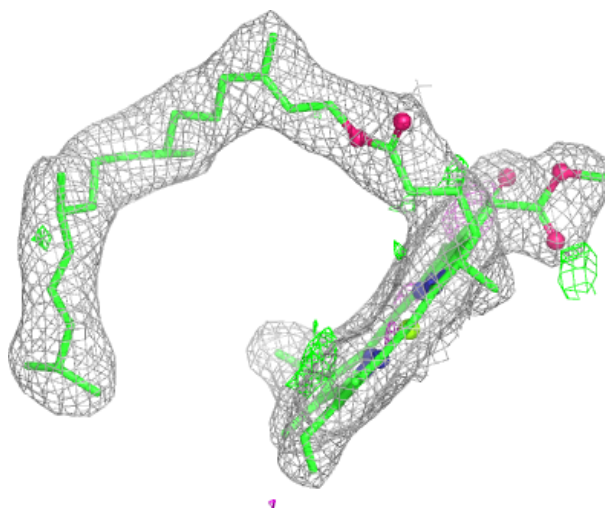
**Electron density around LHG d 411:**

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



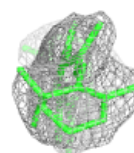
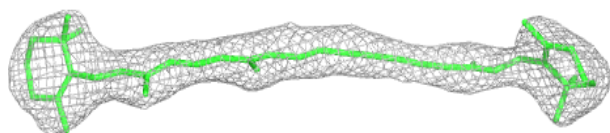
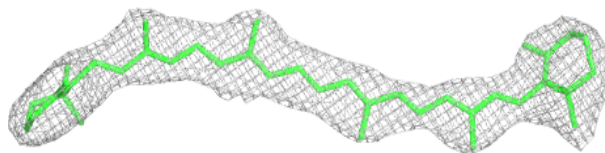
Electron density around CLA b 620:

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

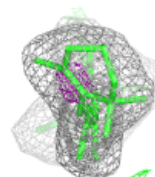
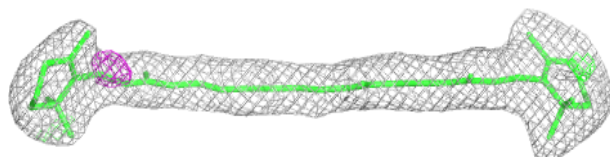
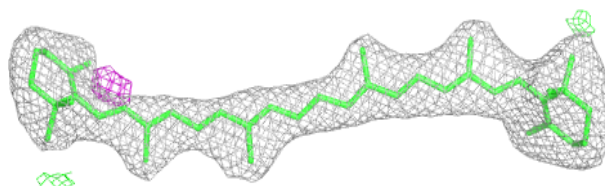


Electron density around BCR Y 101:

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

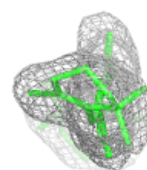
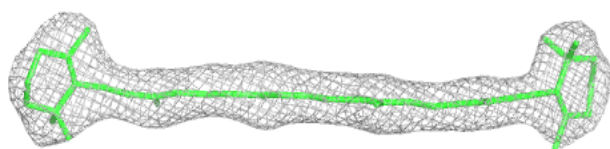
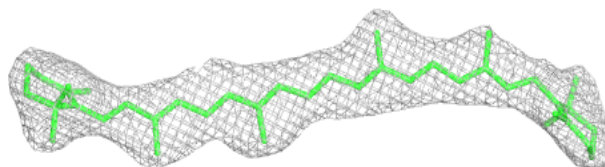
**Electron density around BCR b 627:**

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

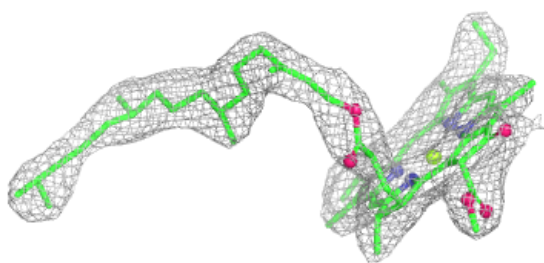
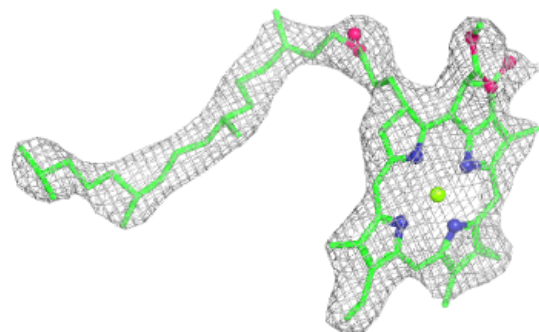


Electron density around BCR c 518:

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

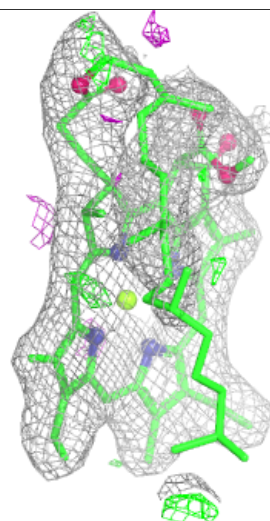
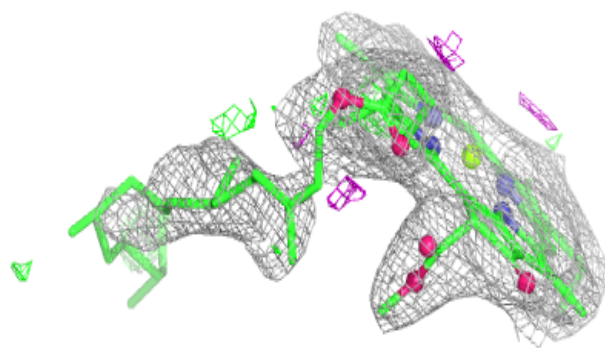
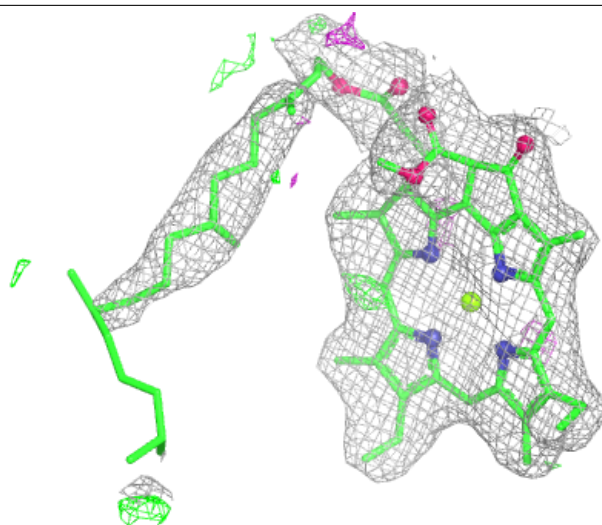
**Electron density around CLA C 512:**

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



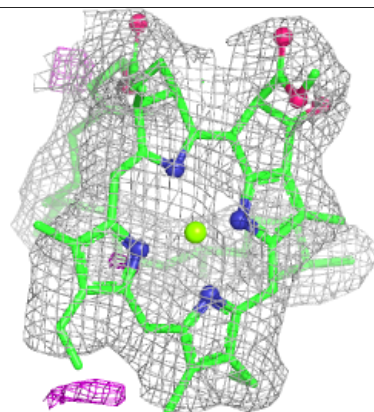
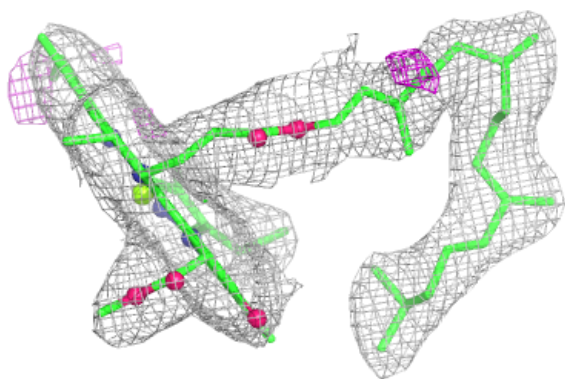
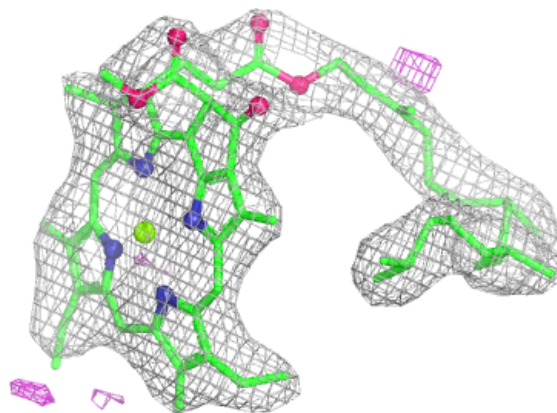
Electron density around CLA B 617:

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

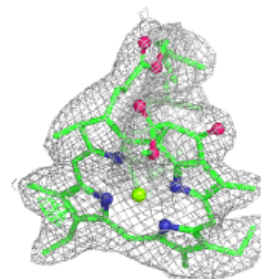
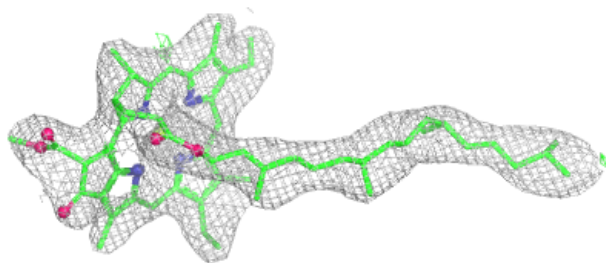
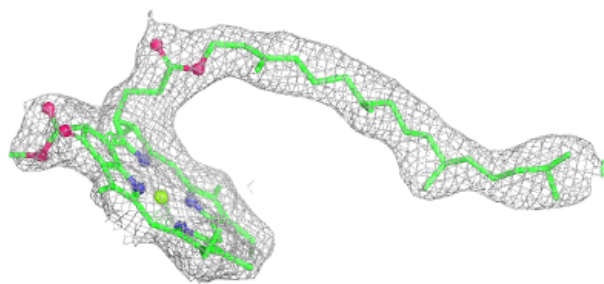


Electron density around CLA c 507:

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

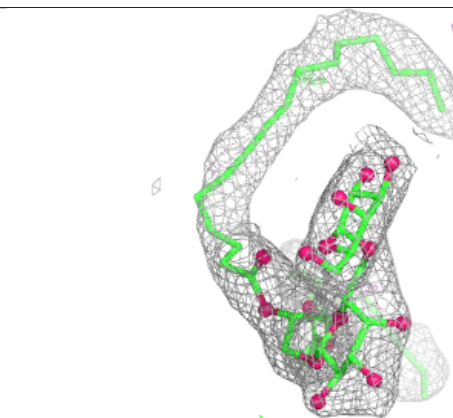
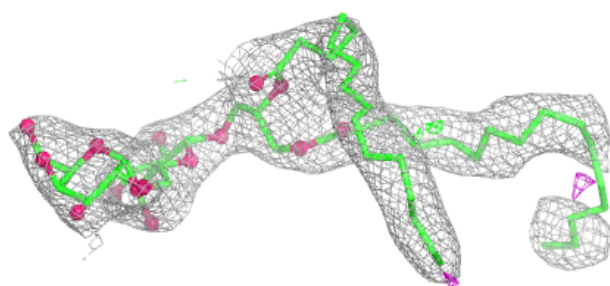
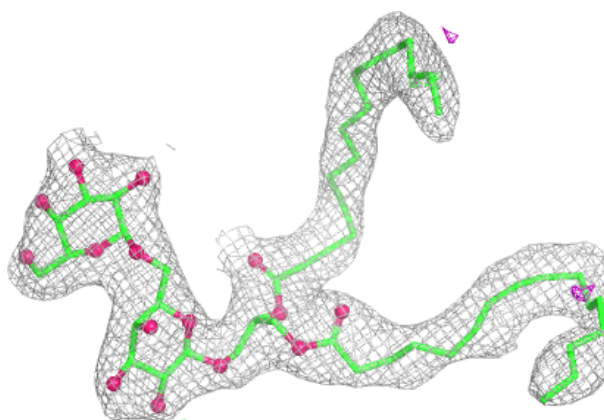
**Electron density around CLA c 508:**

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

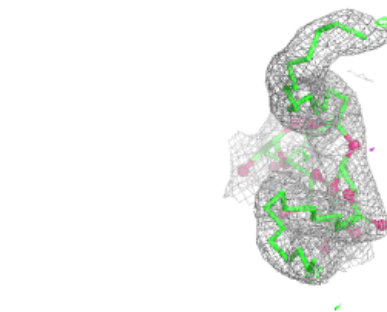
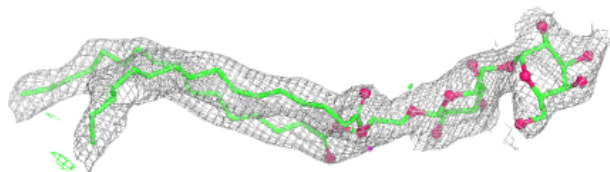
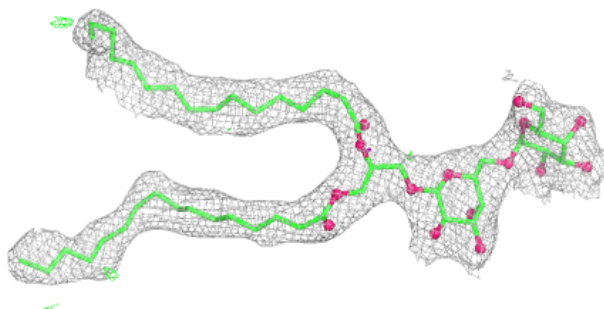


Electron density around DGD c 520:

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

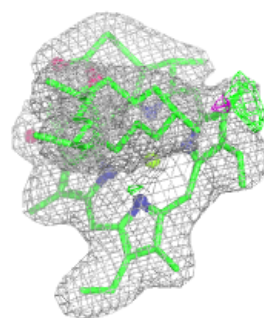
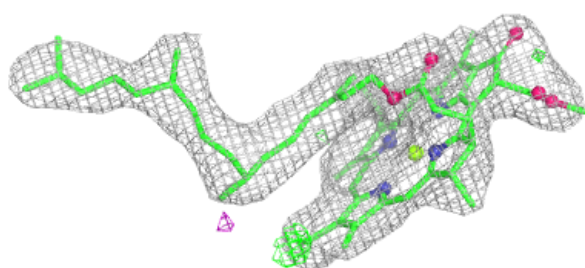
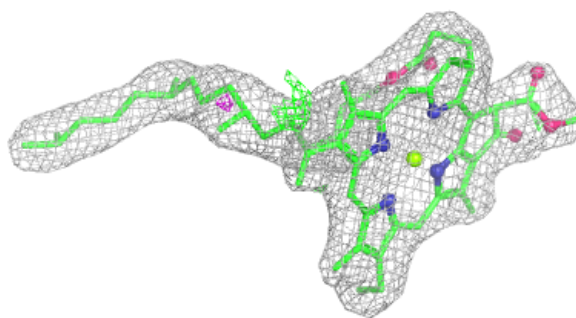
**Electron density around DGD c 521:**

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

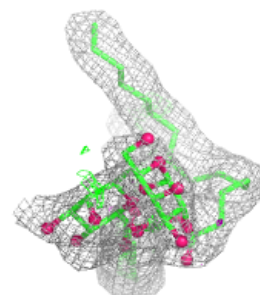
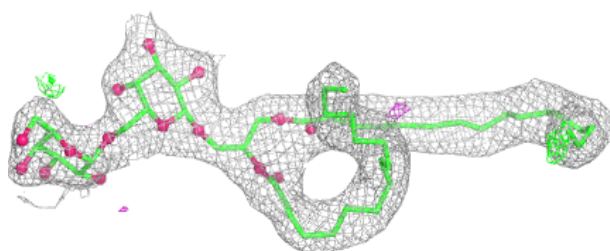
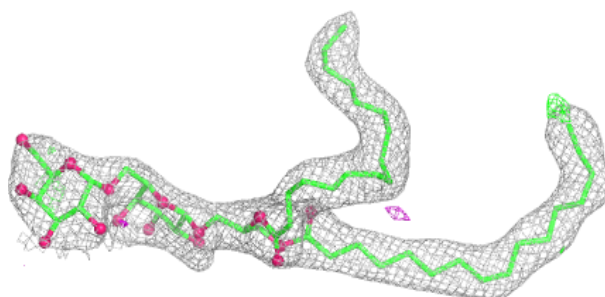


Electron density around CLA c 509:

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

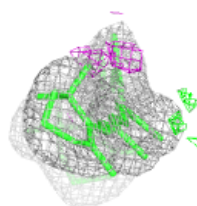
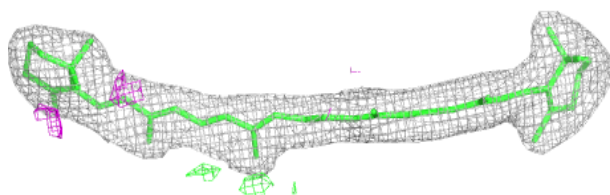
**Electron density around DGD h 102:**

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



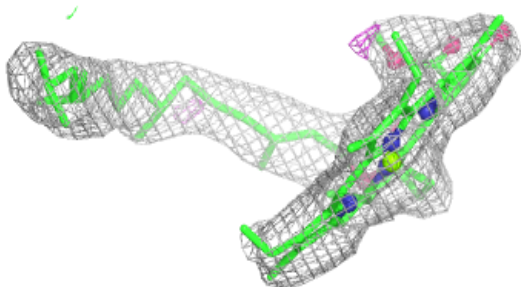
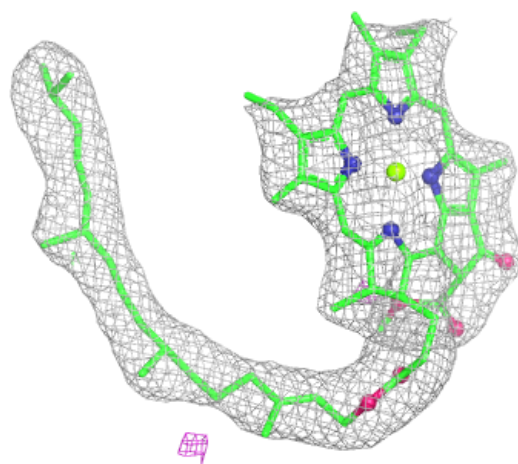
Electron density around BCR t 102:

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



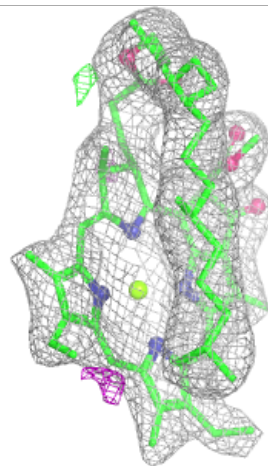
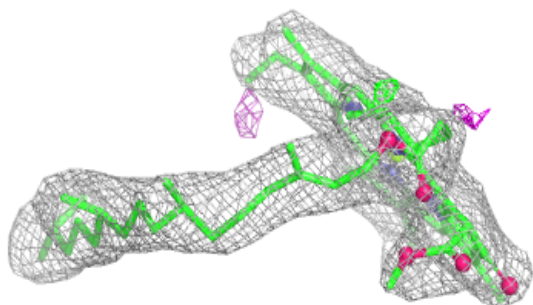
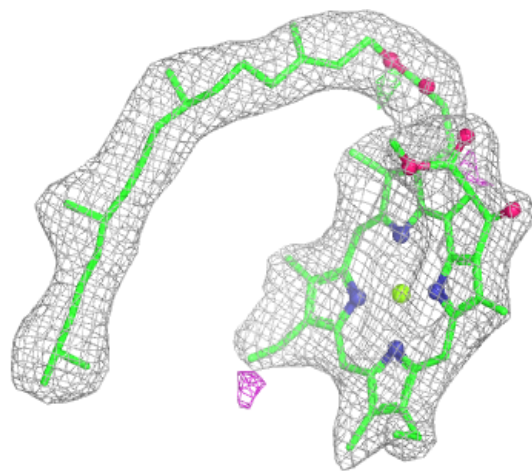
Electron density around CLA C 508:

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



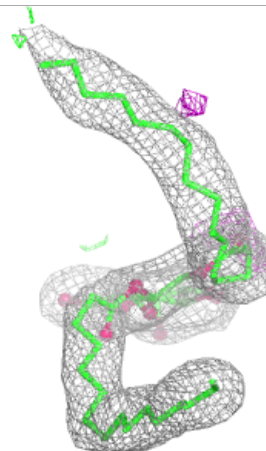
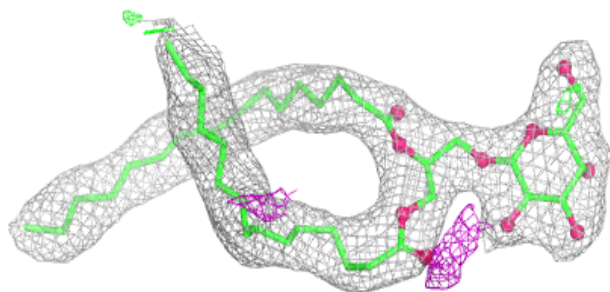
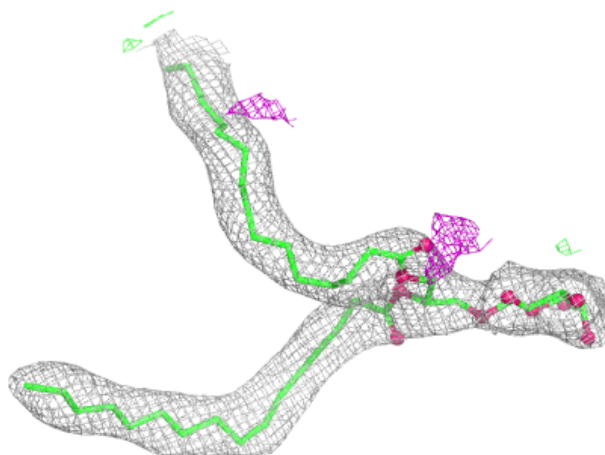
Electron density around CLA c 511:

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



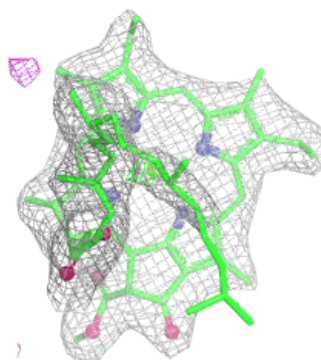
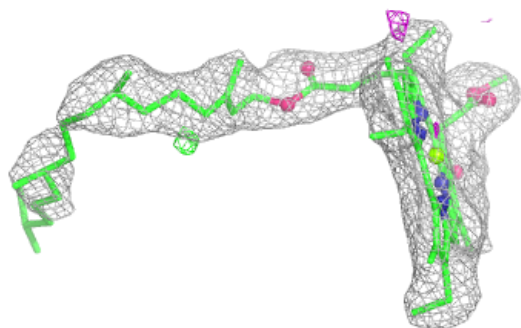
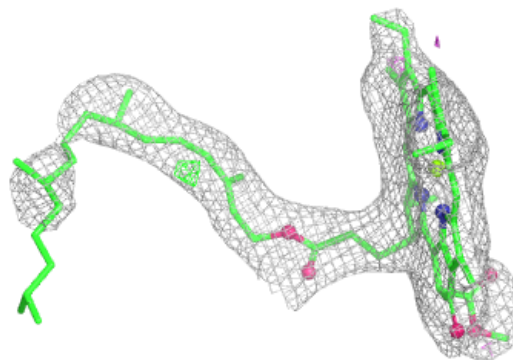
Electron density around LMG M 101:

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

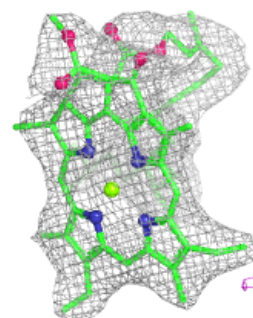
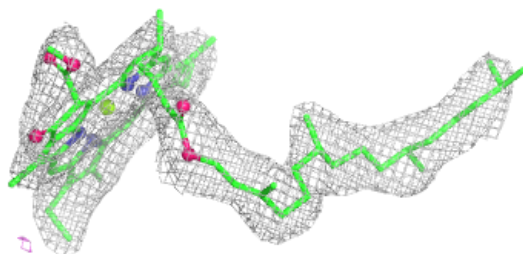
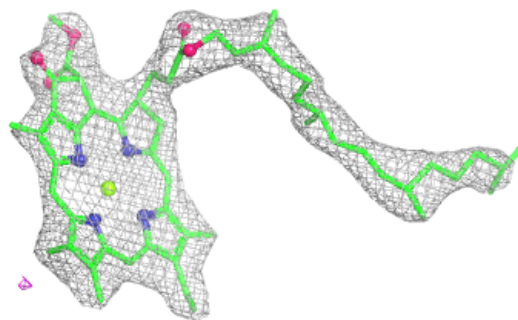


Electron density around CLA D 407:

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

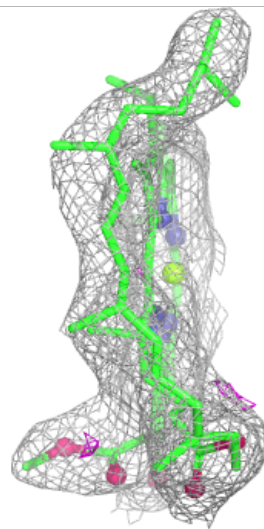
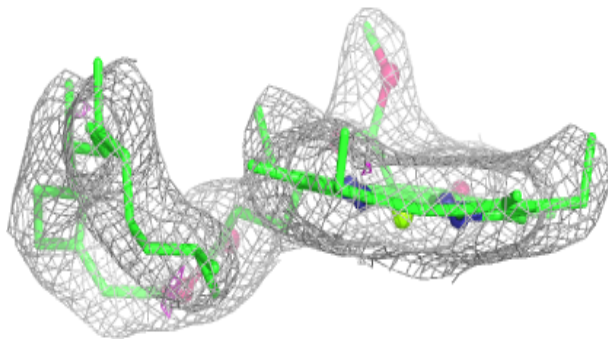
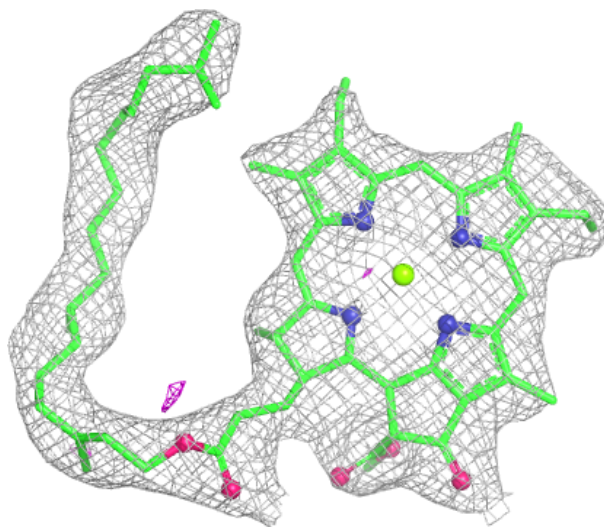
**Electron density around CLA c 515:**

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



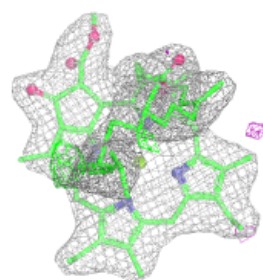
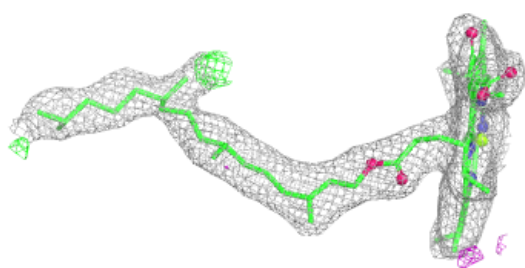
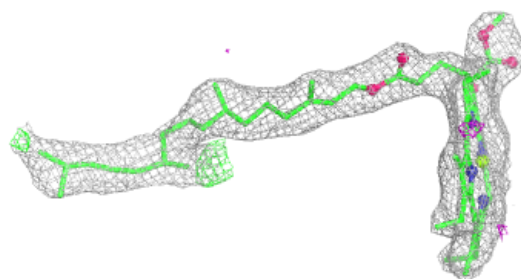
Electron density around CLA c 516:

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

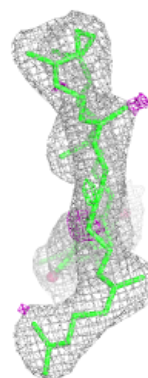
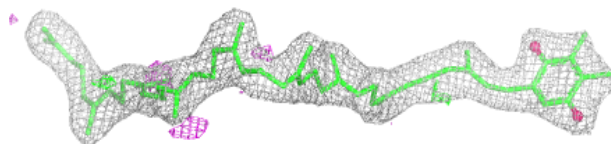
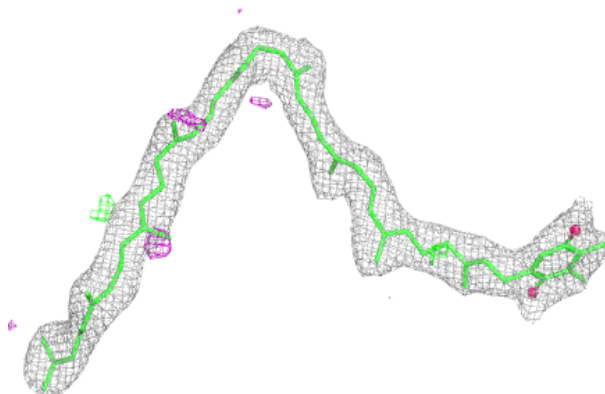


Electron density around CLA B 607:

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

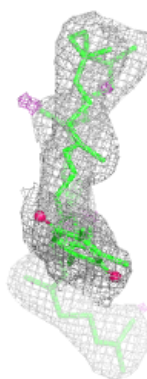
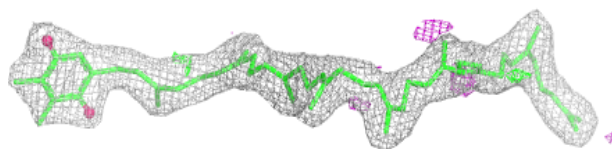
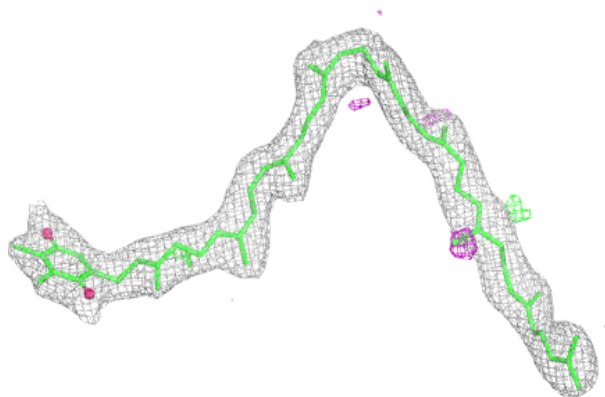
**Electron density around PL9 d 407 (A):**

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

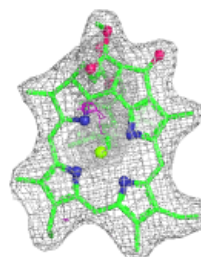
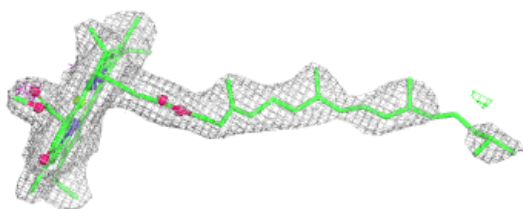
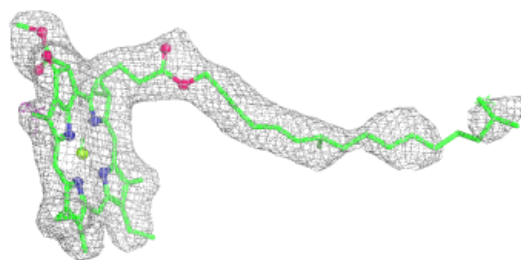


Electron density around PL9 d 407 (B):

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

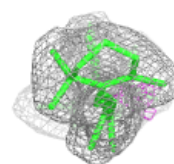
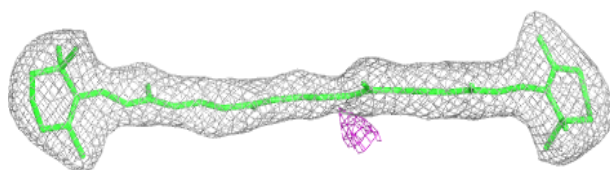
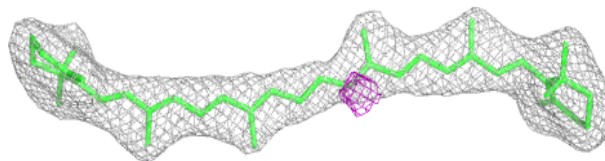
**Electron density around CLA d 405:**

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

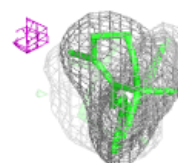
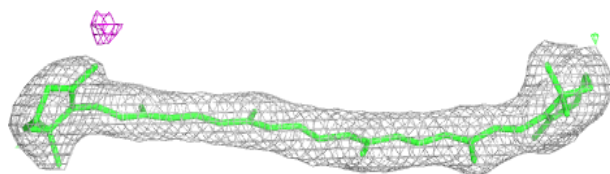
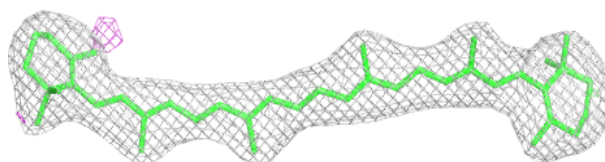


Electron density around BCR A 408:

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

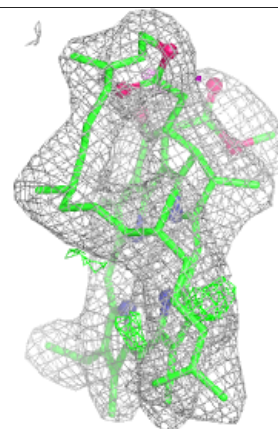
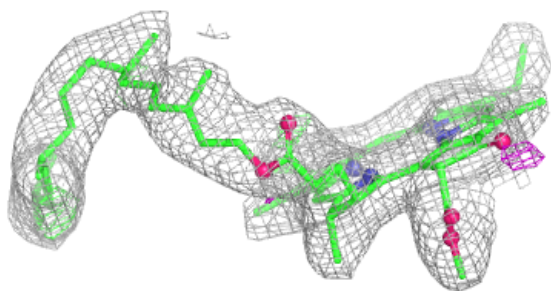
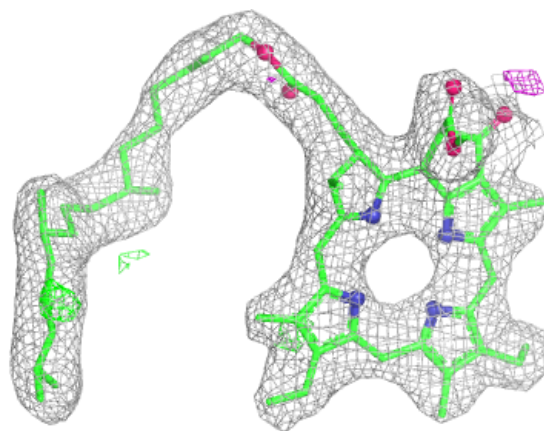
**Electron density around BCR B 620:**

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



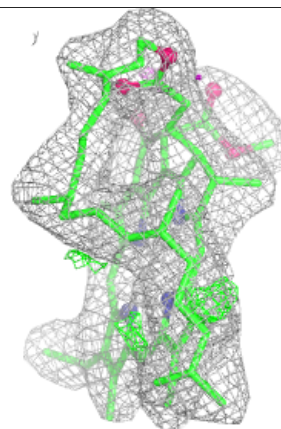
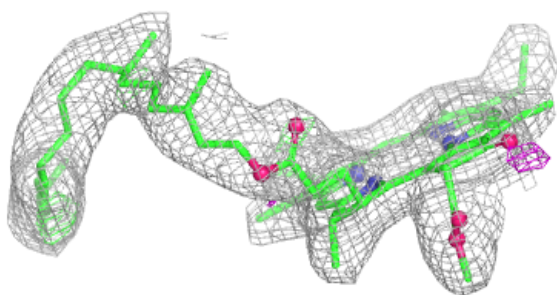
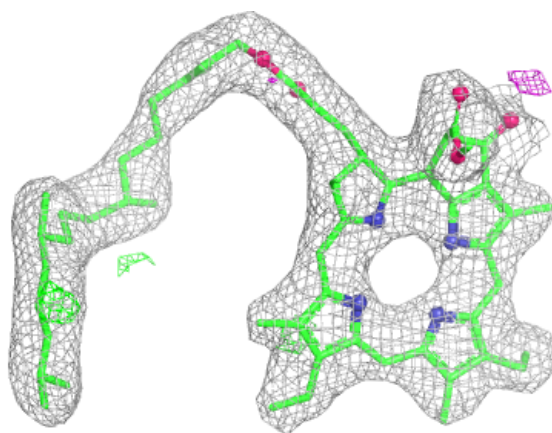
Electron density around PHO d 402 (A):

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

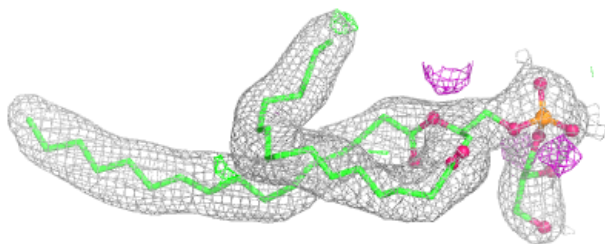
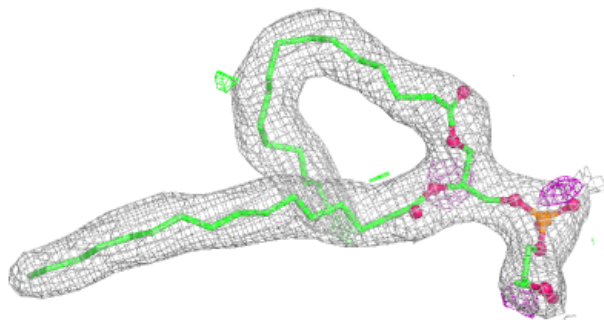


Electron density around PHO d 402 (B):

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

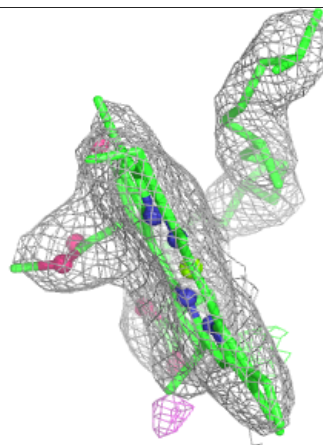
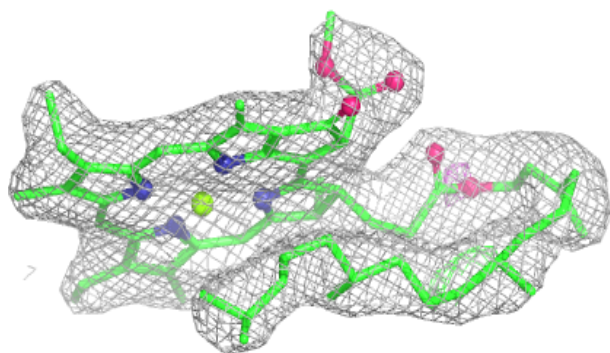
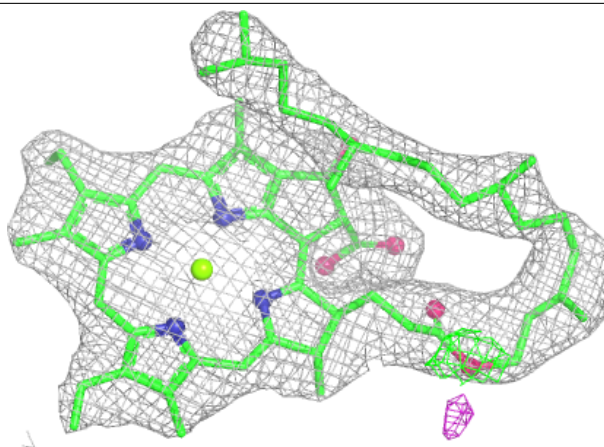
**Electron density around LHG D 411:**

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



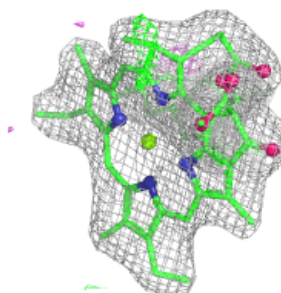
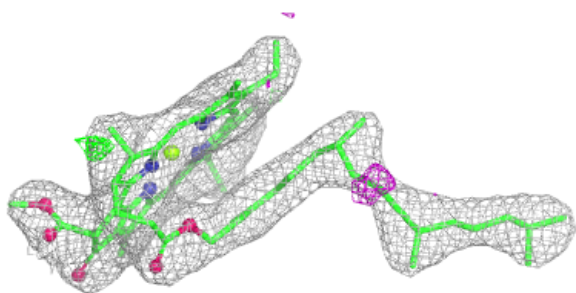
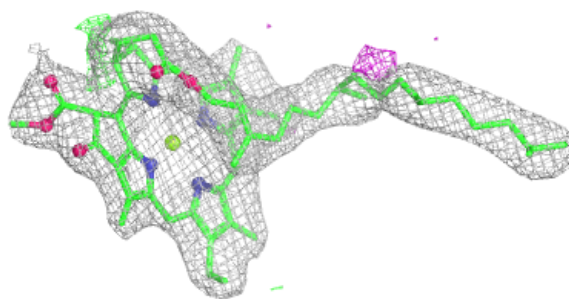
Electron density around CLA C 510:

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

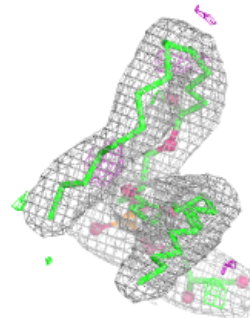
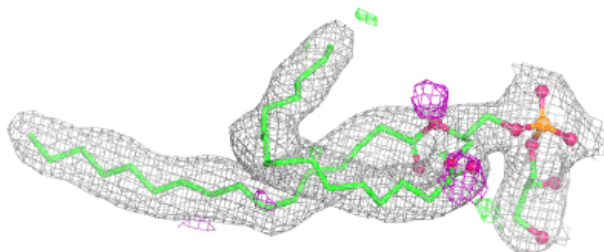
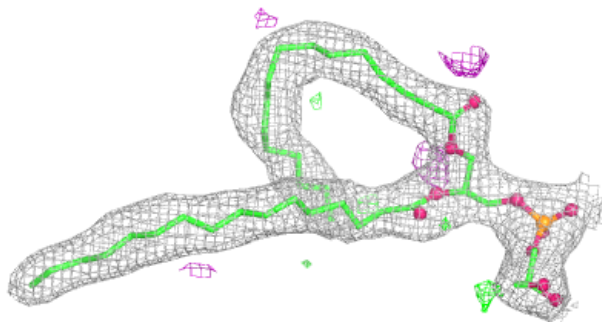


Electron density around CLA C 506:

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

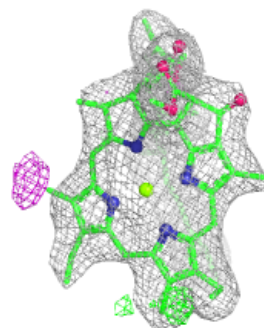
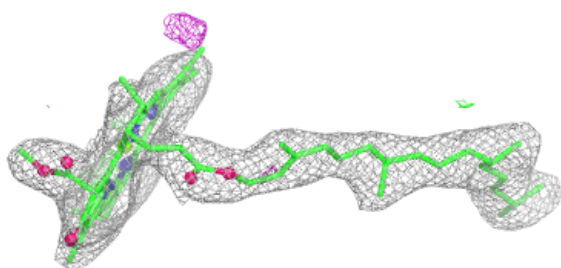
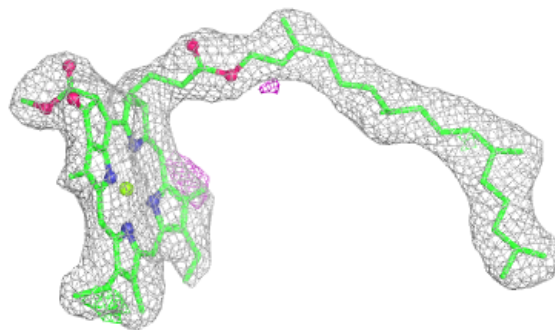
**Electron density around LHG d 409:**

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

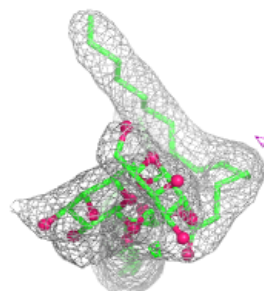
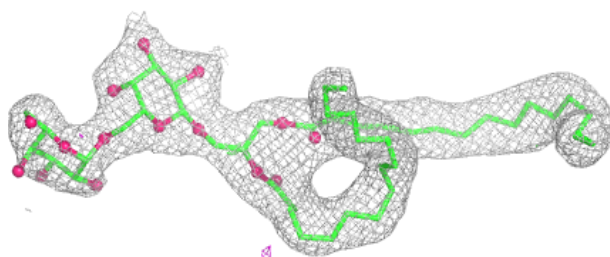
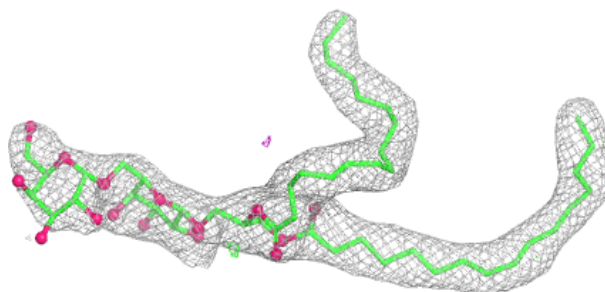


Electron density around CLA b 618:

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

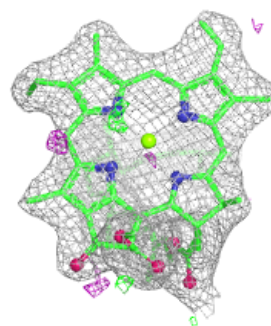
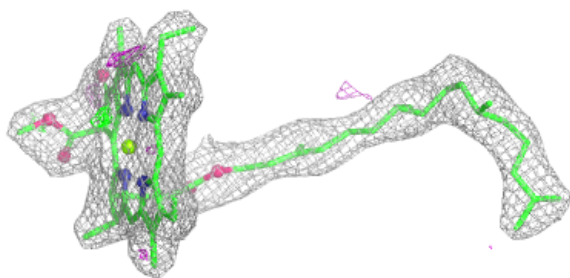
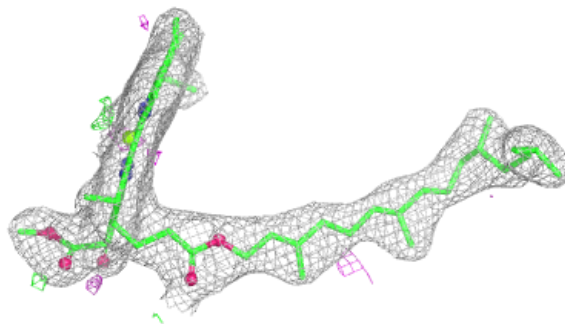
**Electron density around DGD B 632:**

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



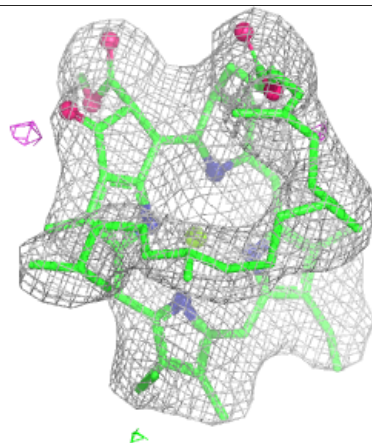
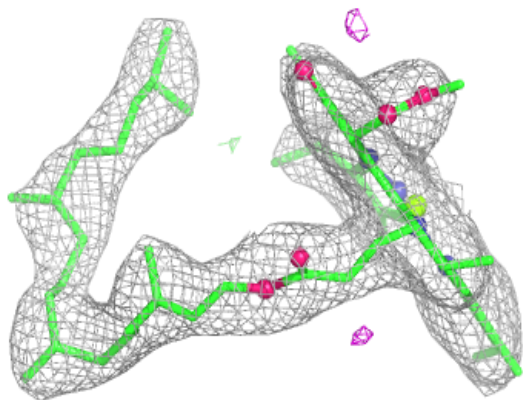
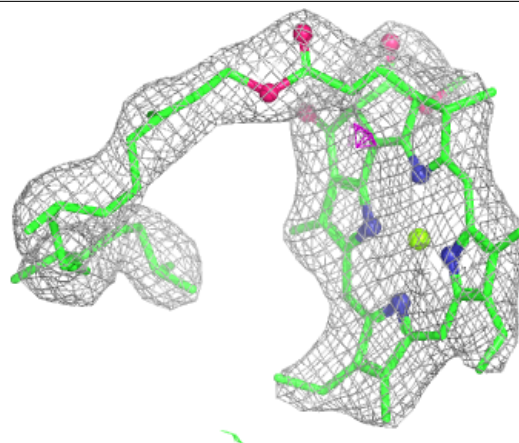
Electron density around CLA b 614:

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



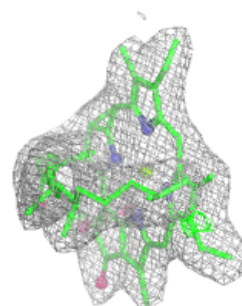
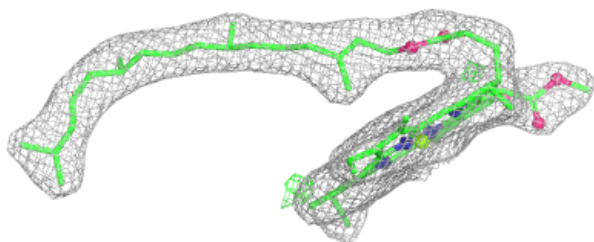
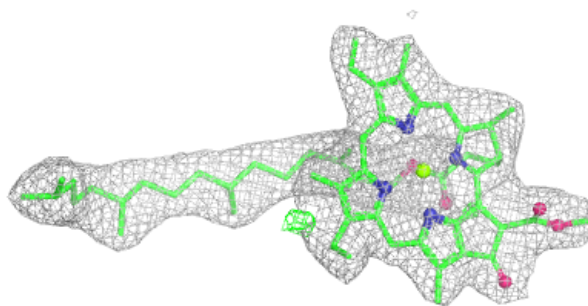
Electron density around CLA C 504:

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



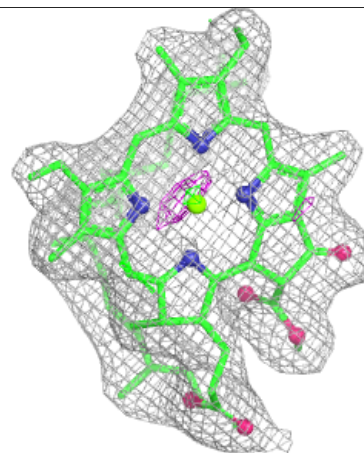
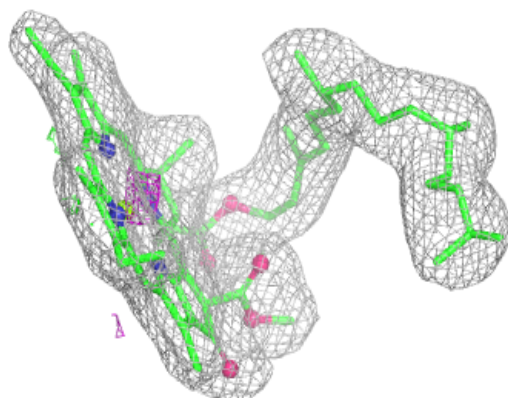
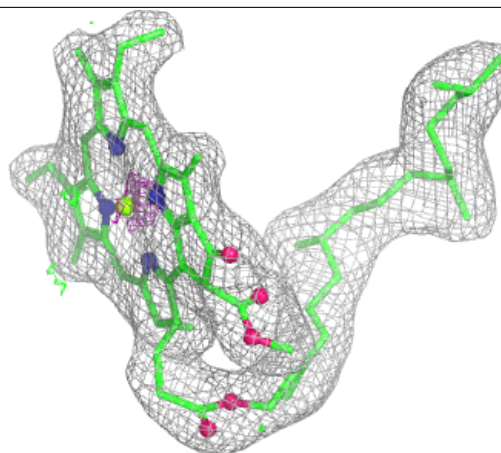
Electron density around CLA b 617:

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



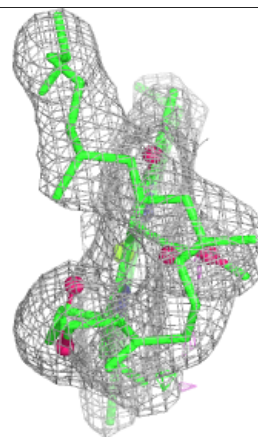
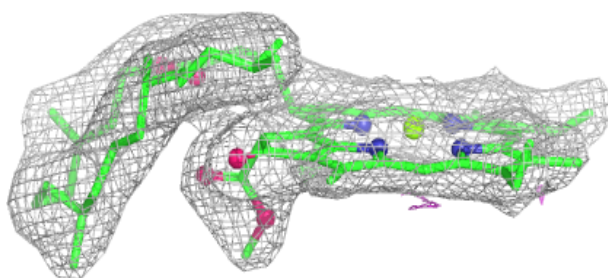
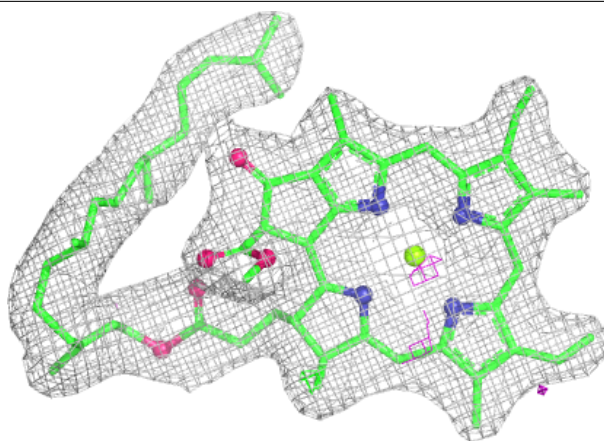
Electron density around CLA B 614:

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

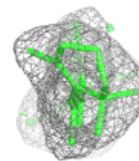
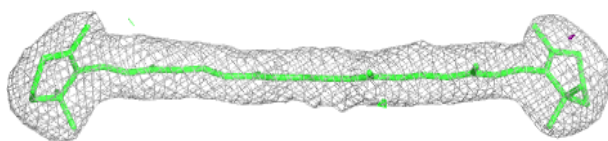
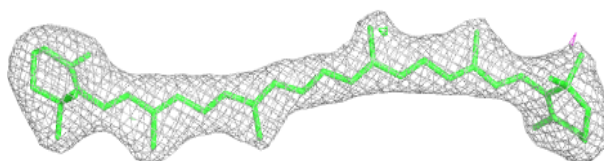


Electron density around CLA b 619:

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

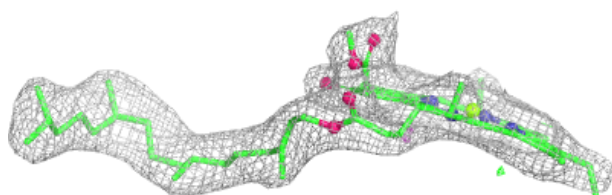
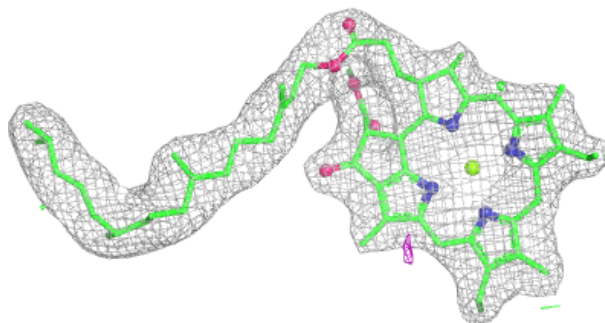
**Electron density around BCR B 619:**

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

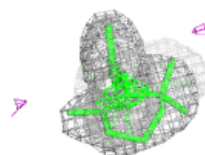
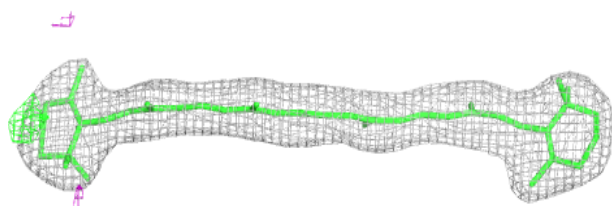
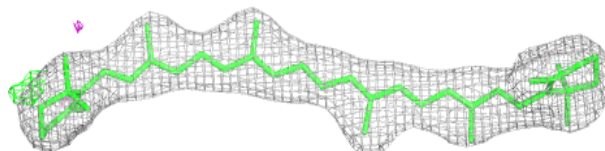


Electron density around CLA B 603:

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

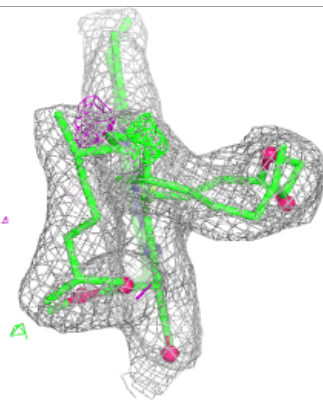
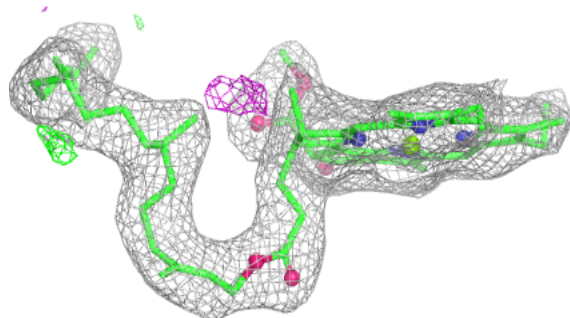
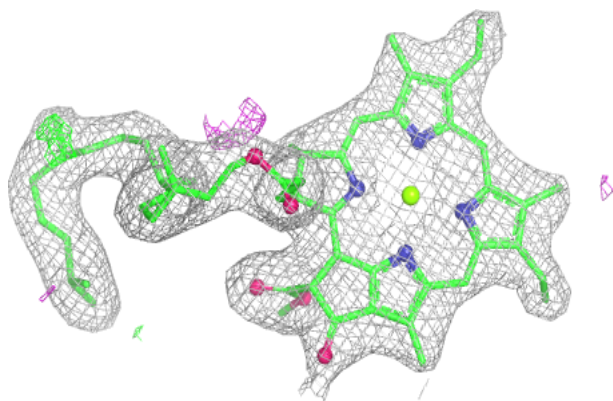
**Electron density around BCR C 515:**

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



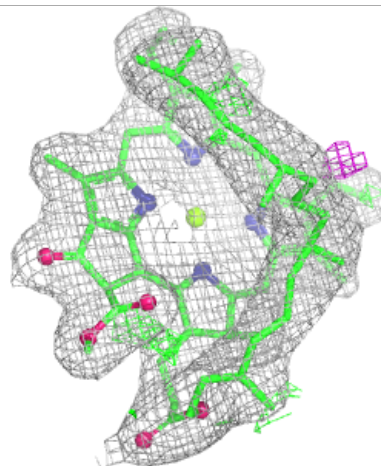
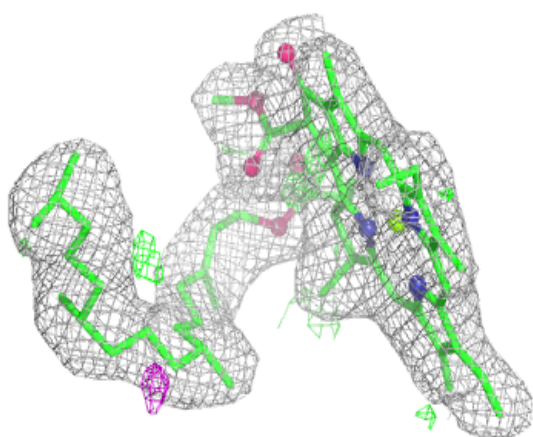
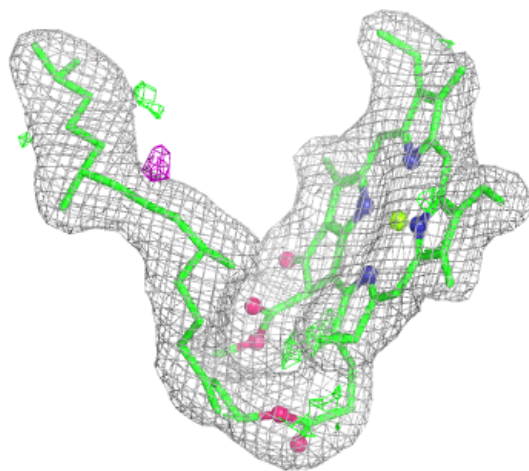
Electron density around CLA b 621:

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



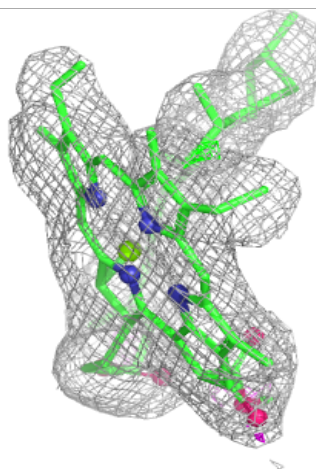
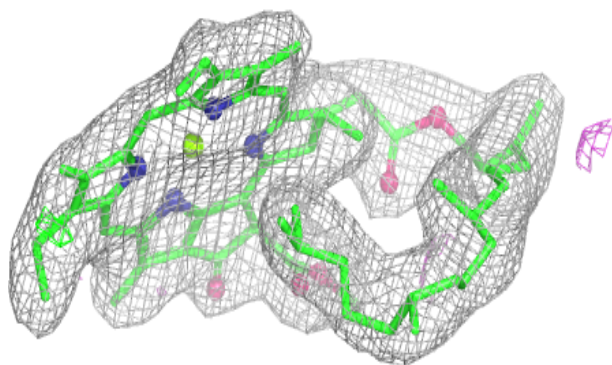
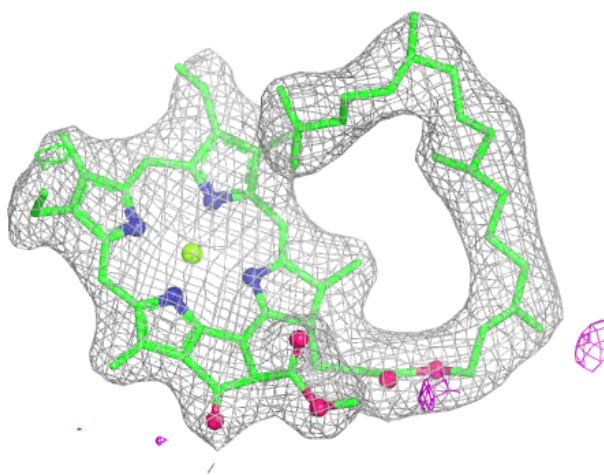
Electron density around CLA b 622:

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



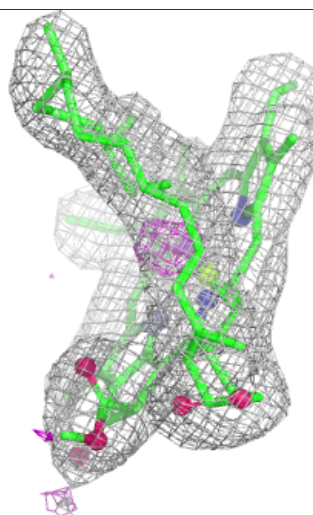
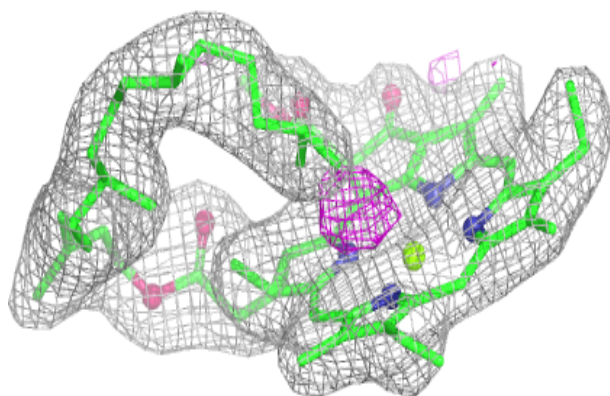
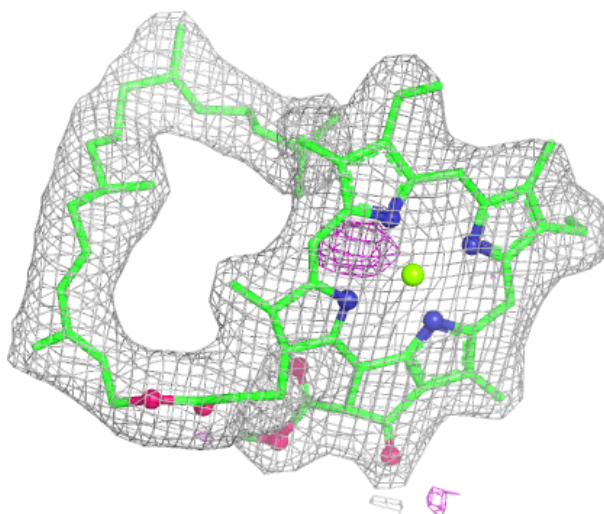
Electron density around CLA B 616:

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



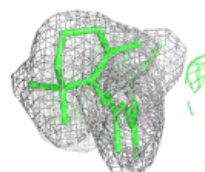
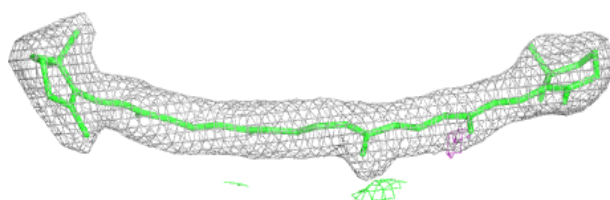
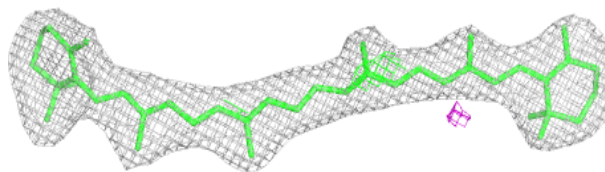
Electron density around CLA b 624:

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

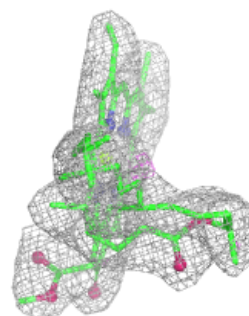
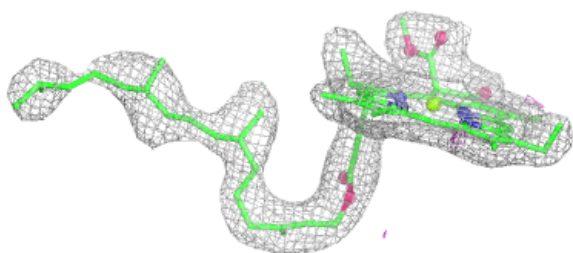
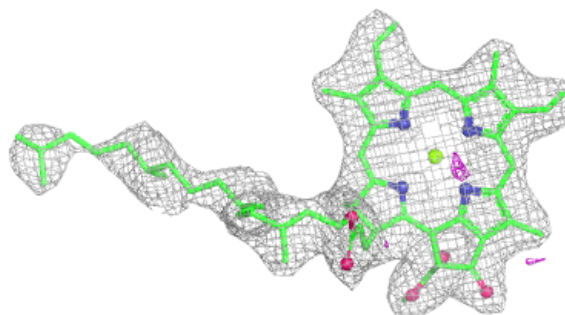


Electron density around BCR T 103:

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

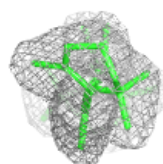
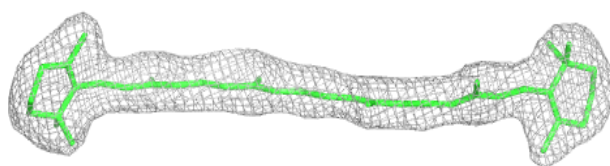
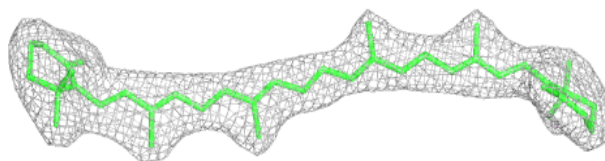
**Electron density around CLA A 406:**

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

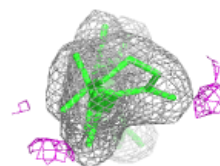
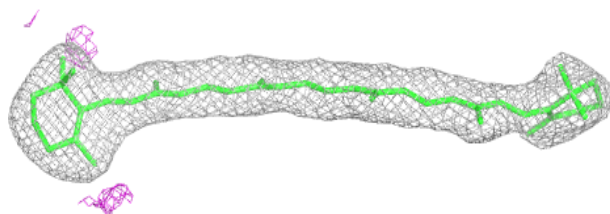
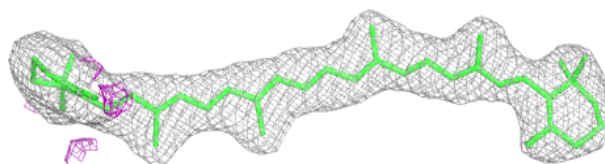


Electron density around BCR a 413:

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

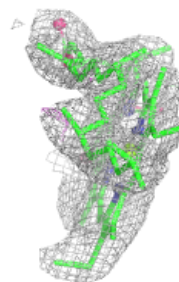
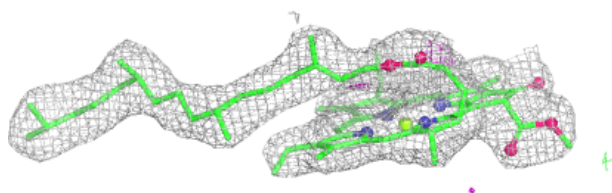
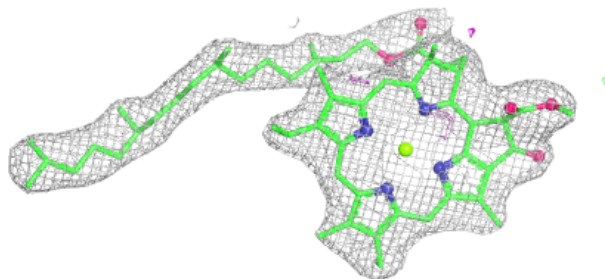
**Electron density around BCR b 626:**

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

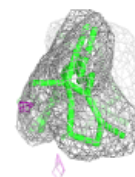
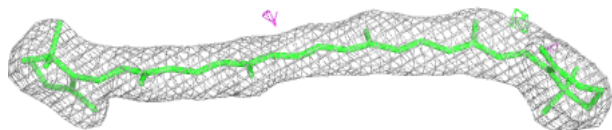
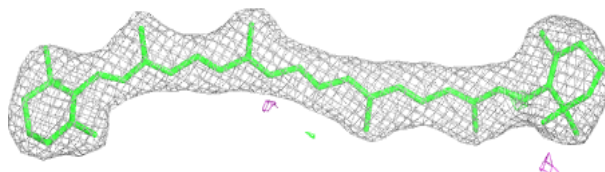


Electron density around CLA c 505:

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

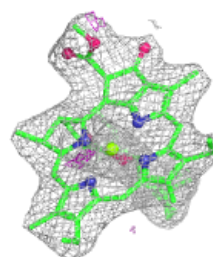
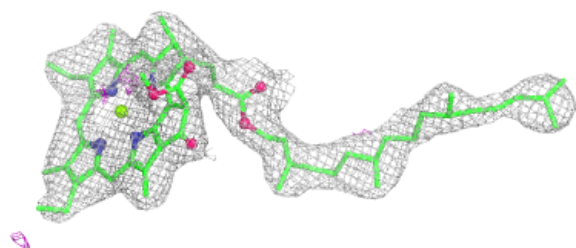
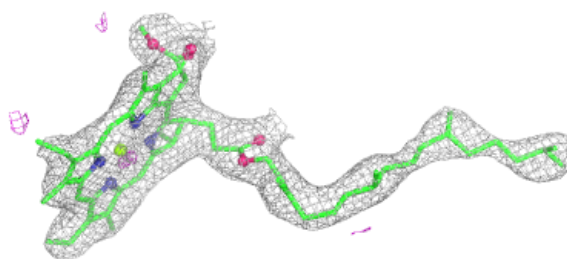
**Electron density around BCR b 628:**

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

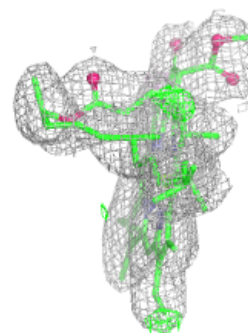
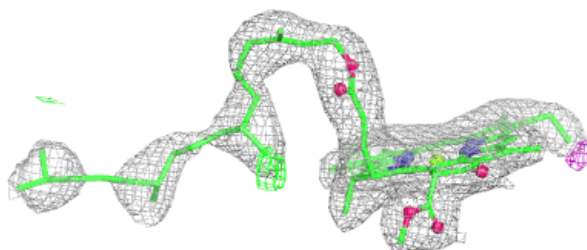
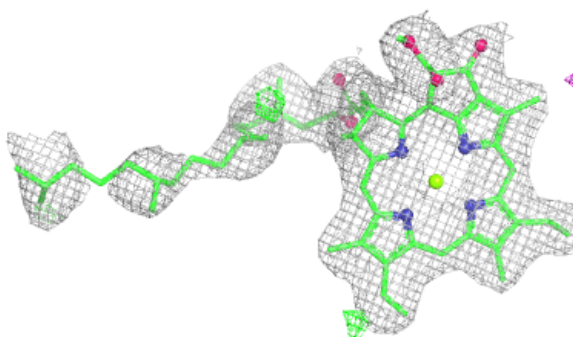


Electron density around CLA c 506:

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

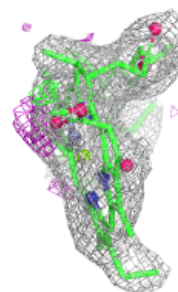
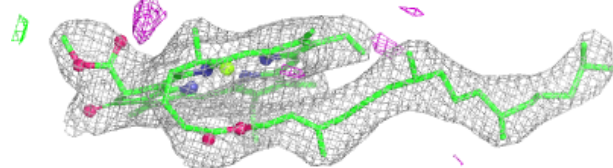
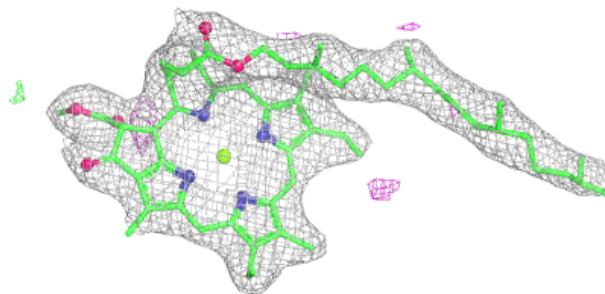
**Electron density around CLA a 410:**

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

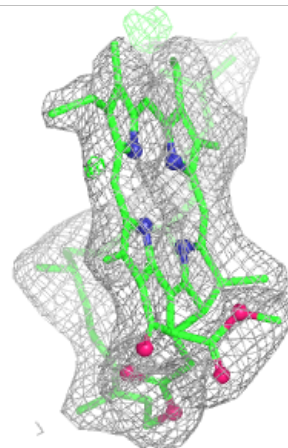
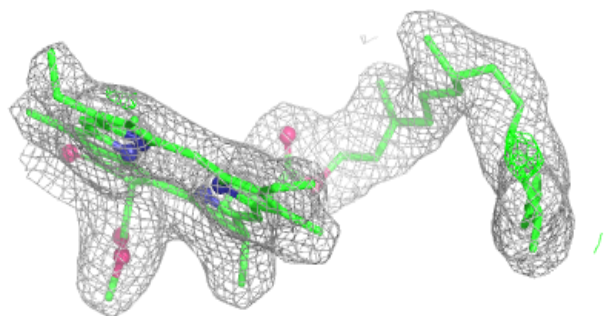
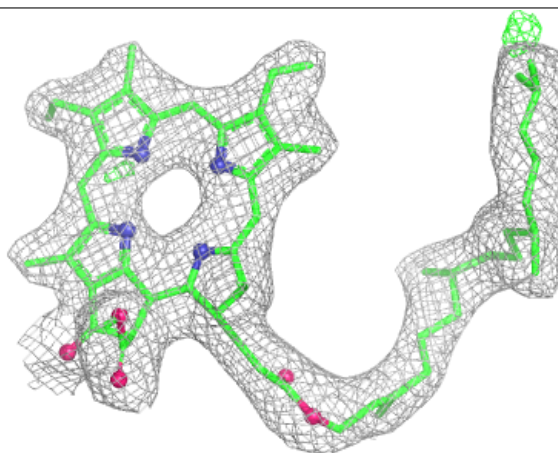


Electron density around CLA C 502:

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

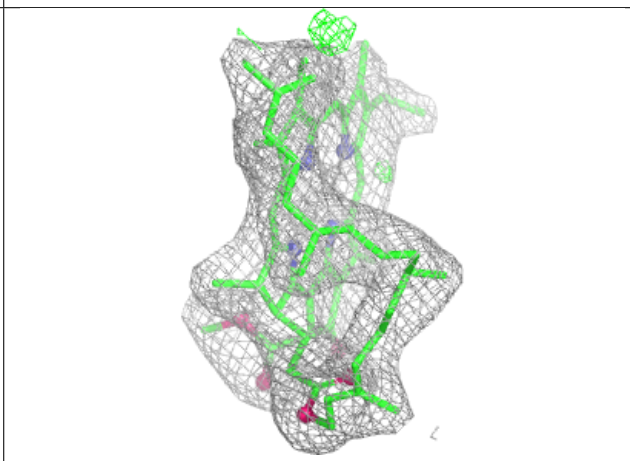
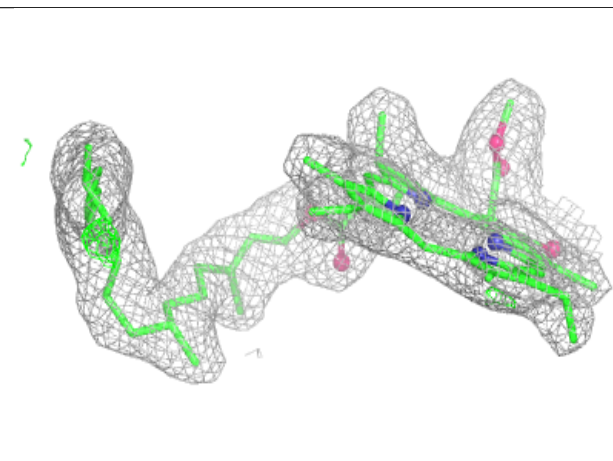
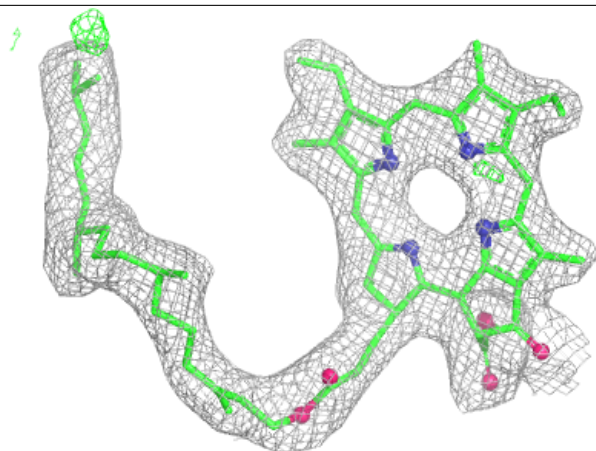
**Electron density around PHO D 403 (A):**

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



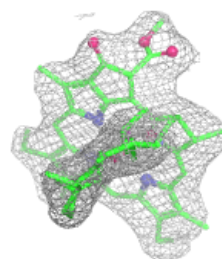
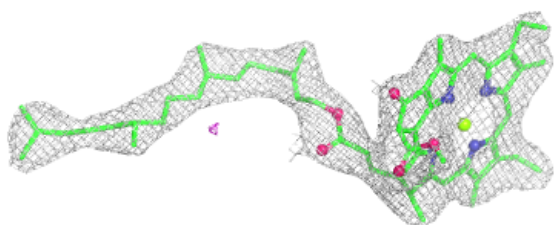
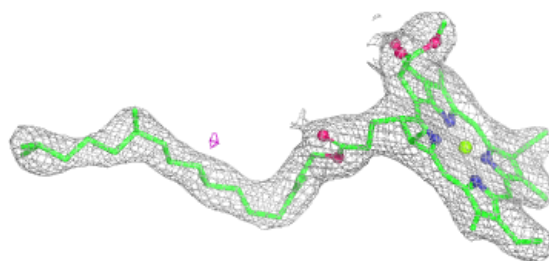
Electron density around PHO D 403 (B):

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

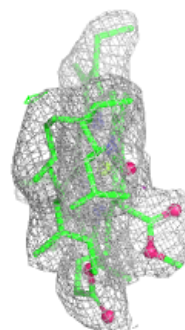
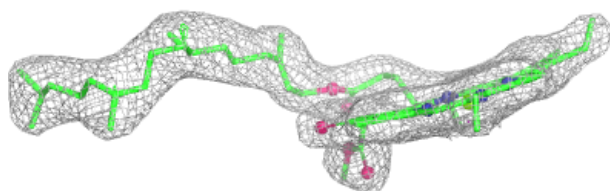
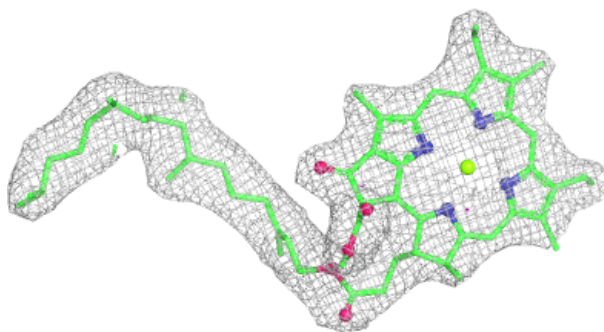


Electron density around CLA C 503:

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

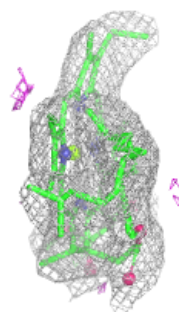
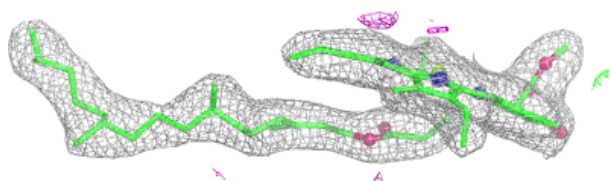
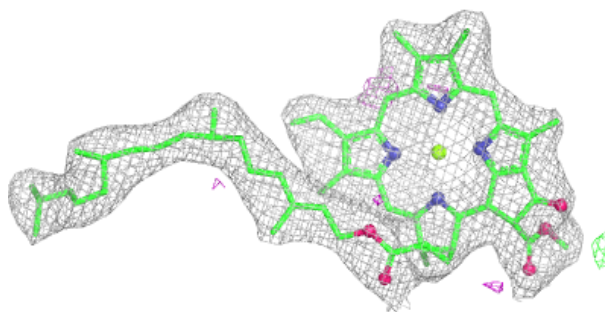
**Electron density around CLA b 611:**

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



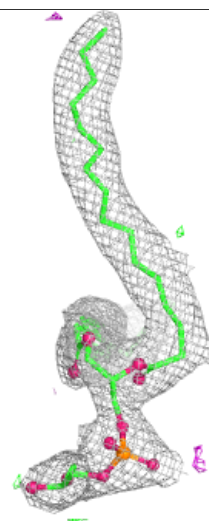
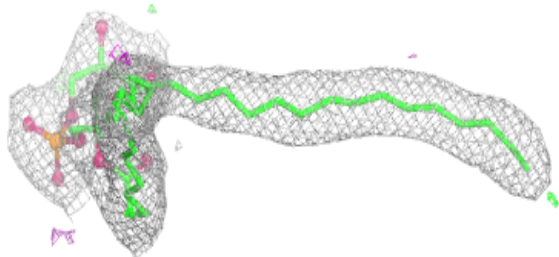
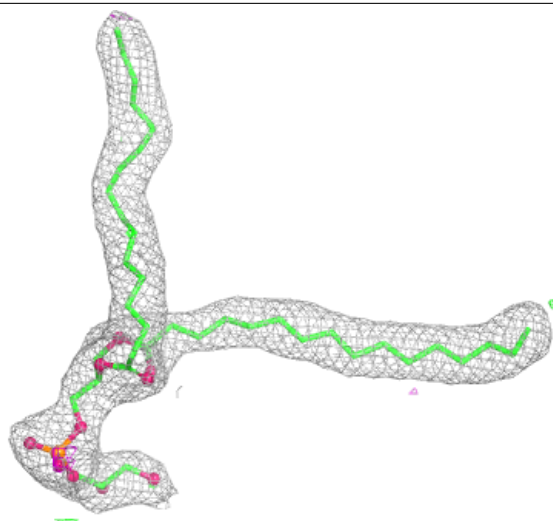
Electron density around CLA b 612:

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



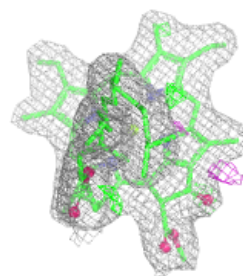
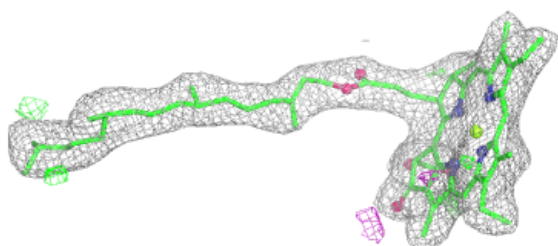
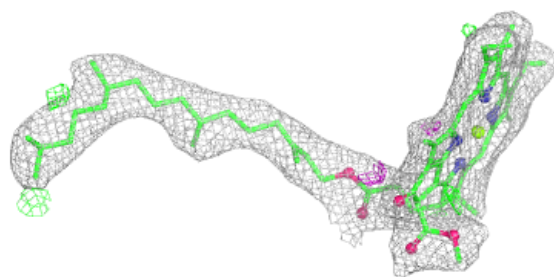
Electron density around LHG L 101:

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



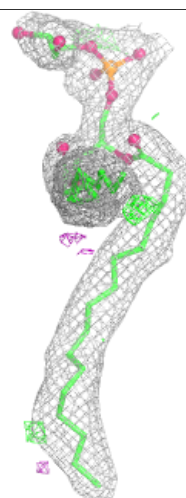
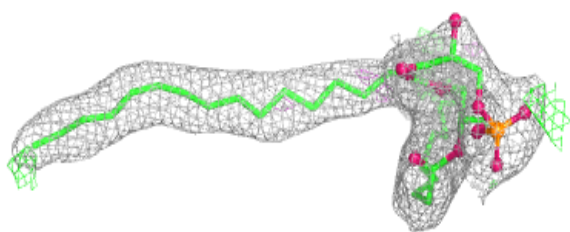
Electron density around CLA b 613:

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



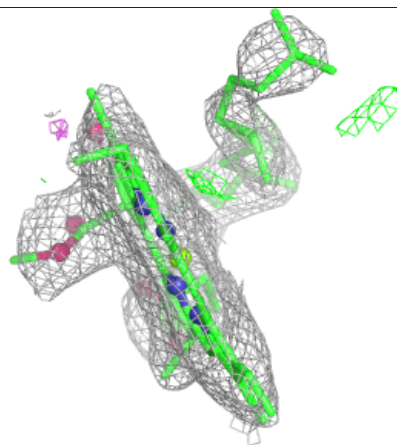
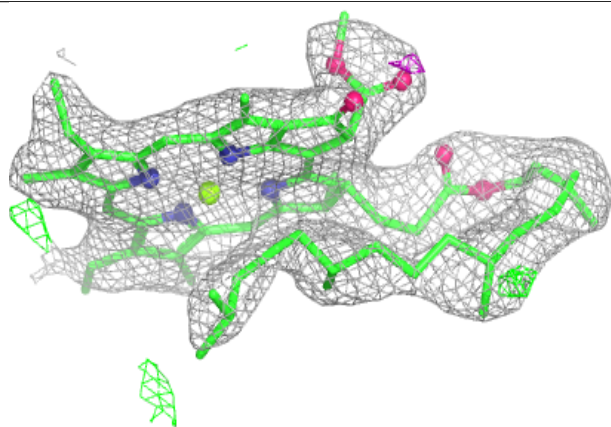
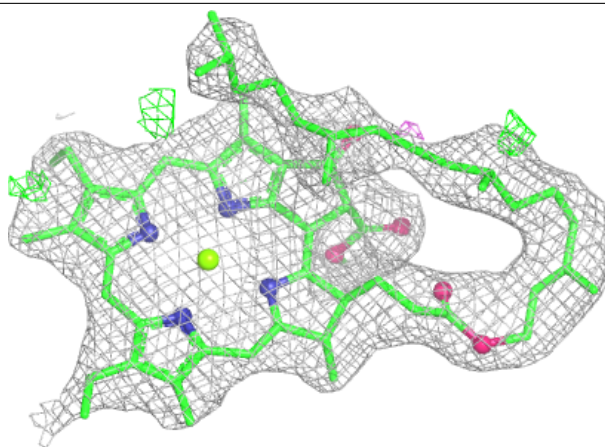
Electron density around LHG b 634:

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



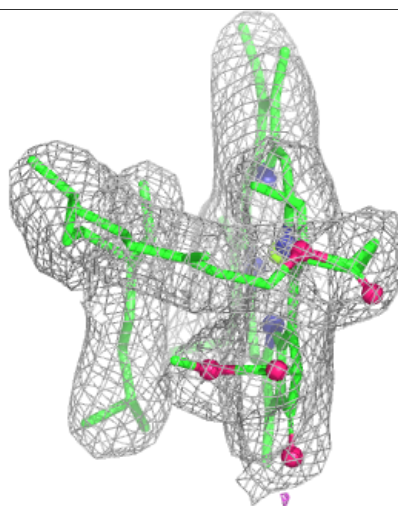
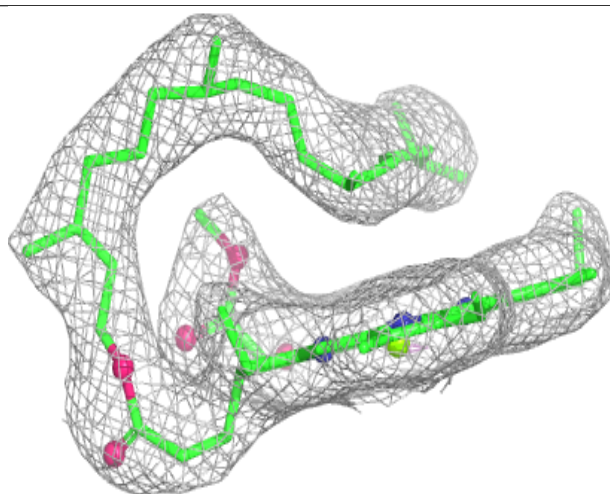
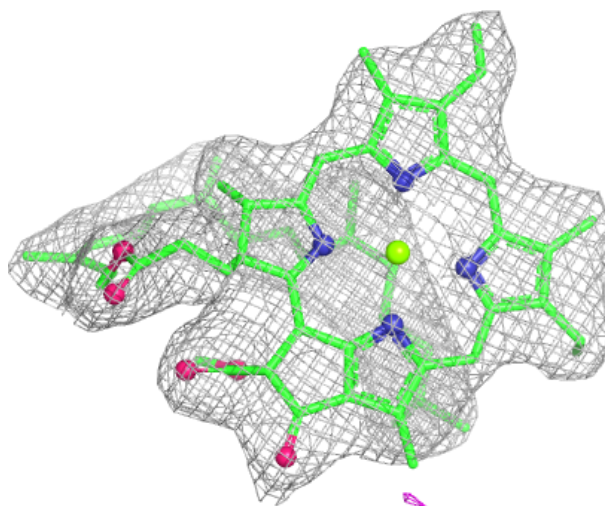
Electron density around CLA c 513:

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



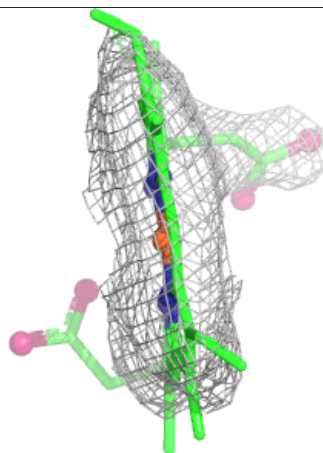
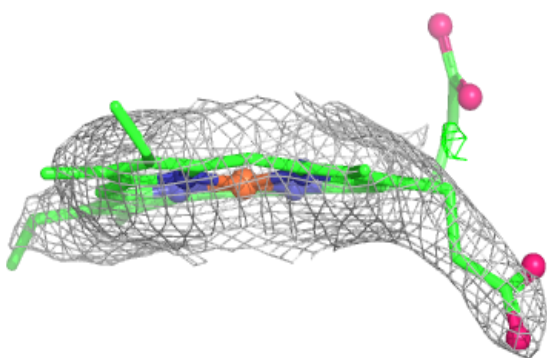
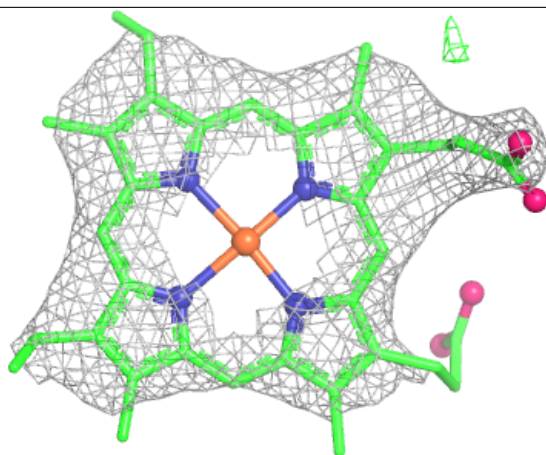
Electron density around CLA c 514:

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



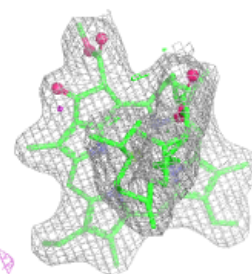
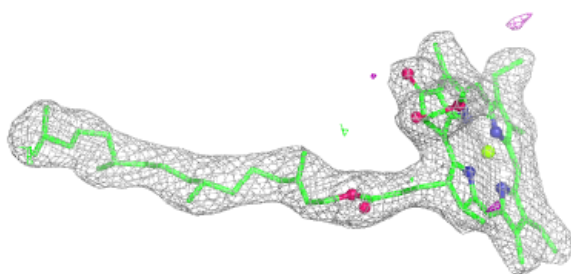
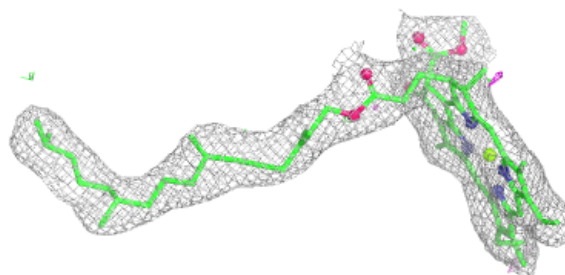
Electron density around HEM e 101:

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

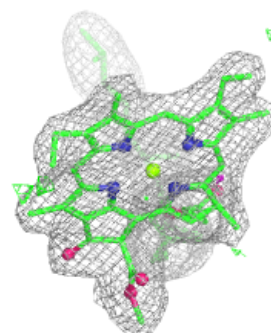
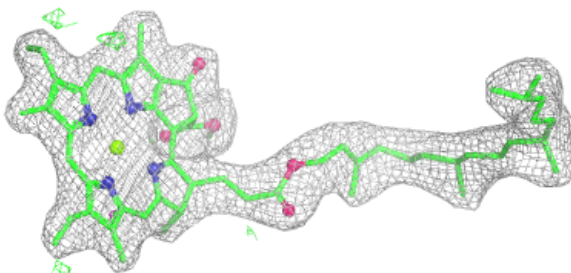
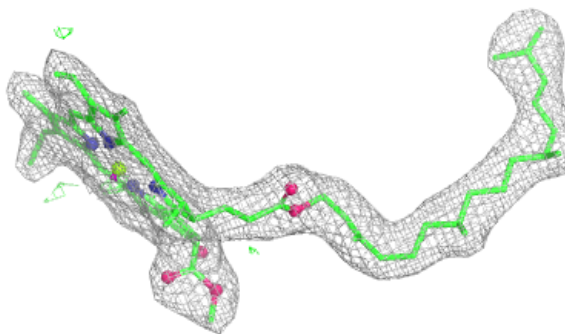


Electron density around CLA B 605:

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

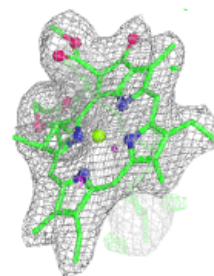
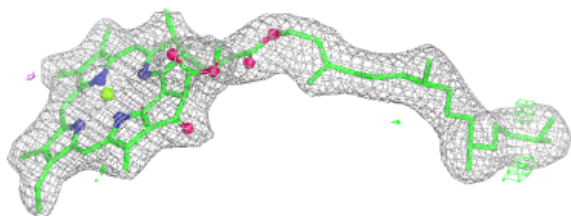
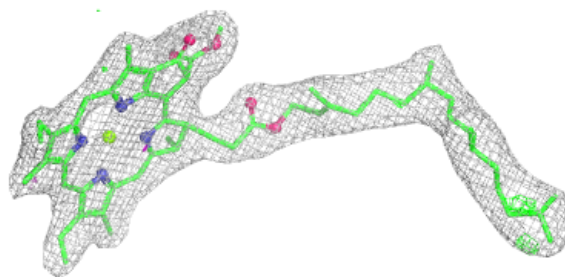
**Electron density around CLA D 406:**

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

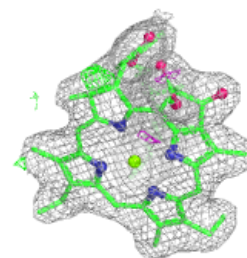
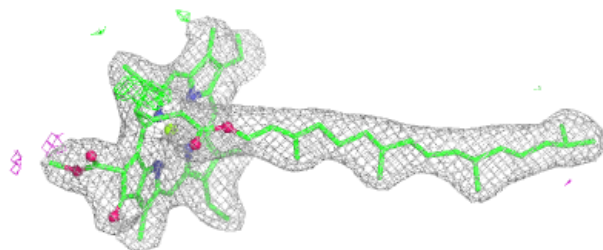
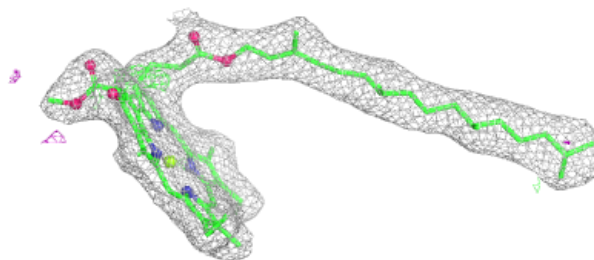


Electron density around CLA a 409:

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

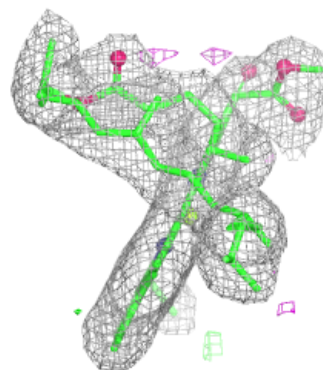
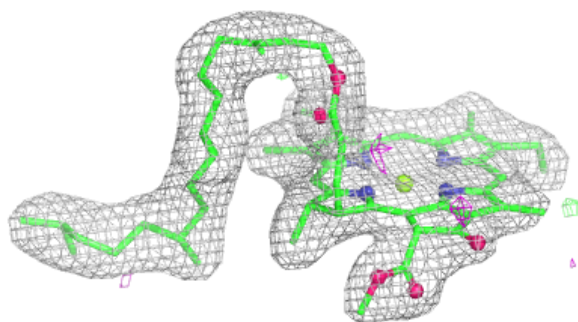
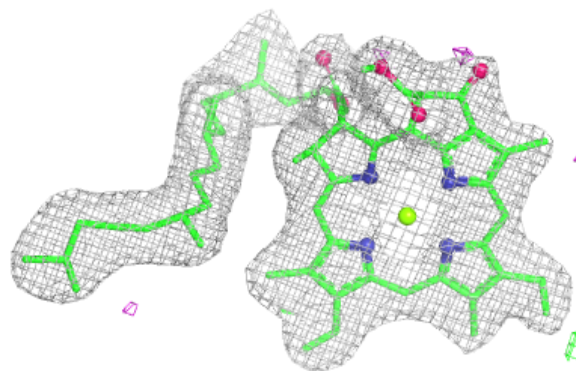
**Electron density around CLA B 608:**

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

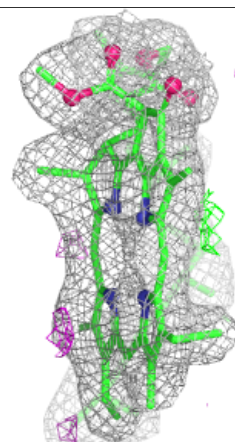
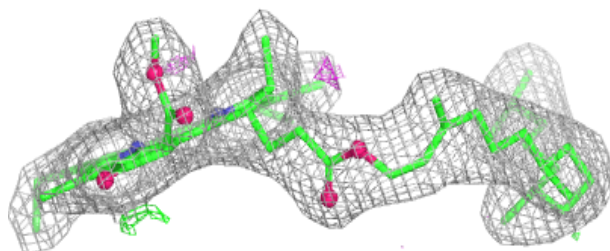
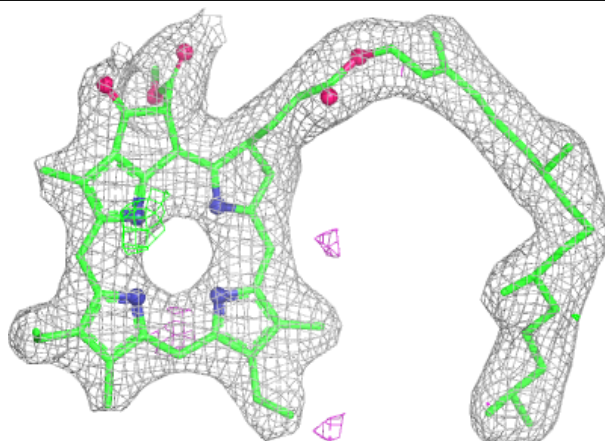


Electron density around CLA d 403:

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

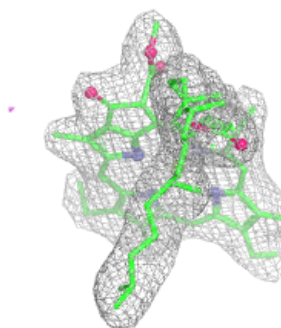
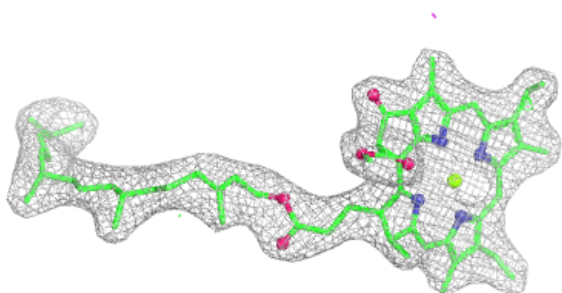
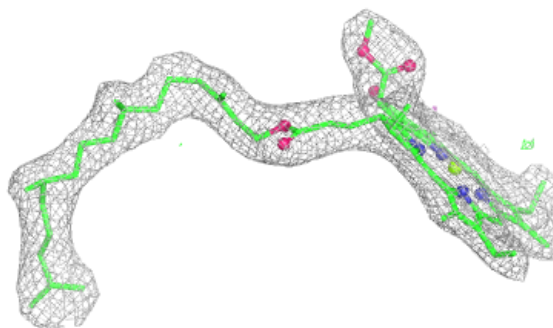
**Electron density around PHO D 402:**

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



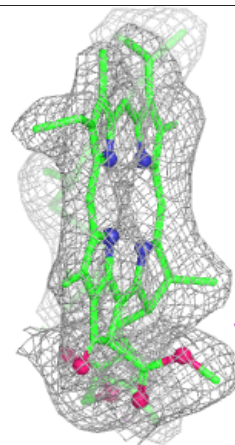
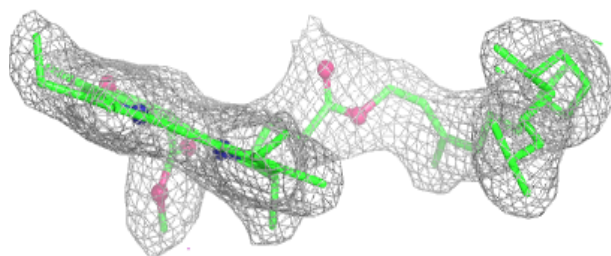
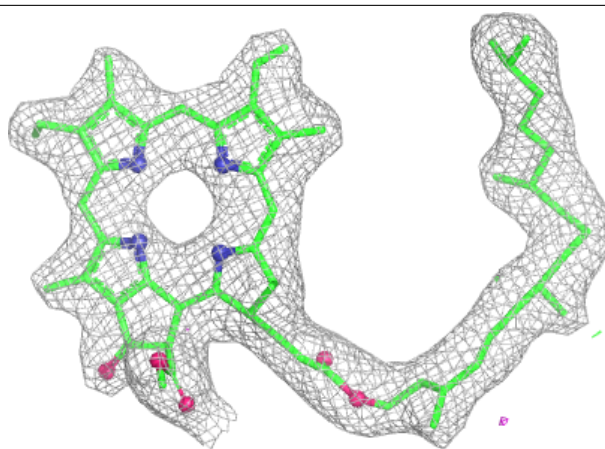
Electron density around CLA d 404:

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



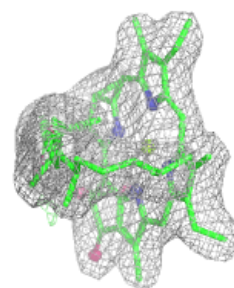
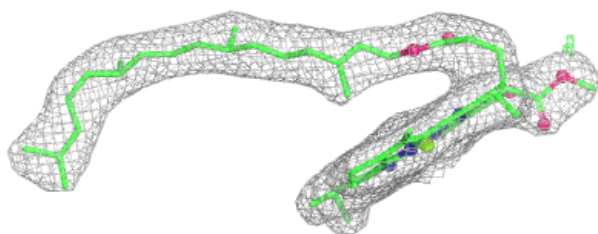
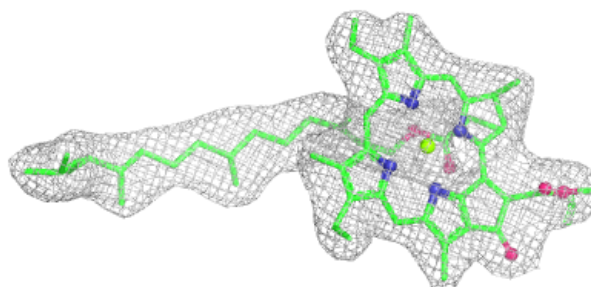
Electron density around PHO a 411:

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

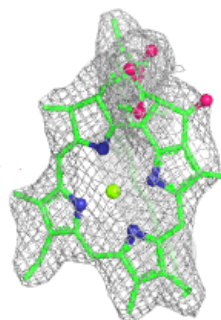
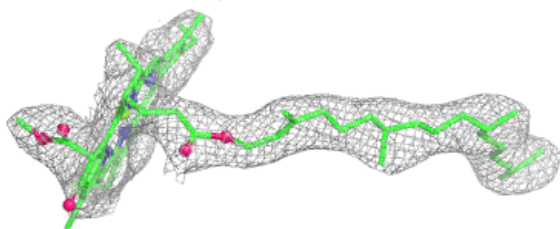
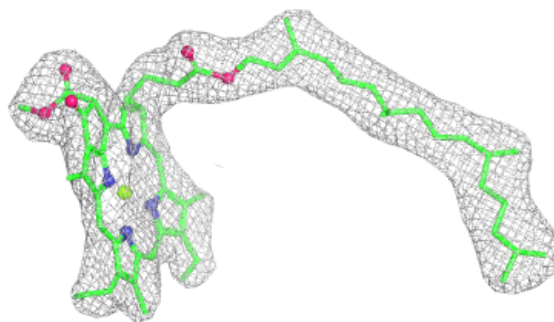


Electron density around CLA B 609:

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

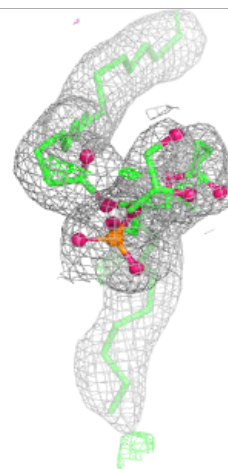
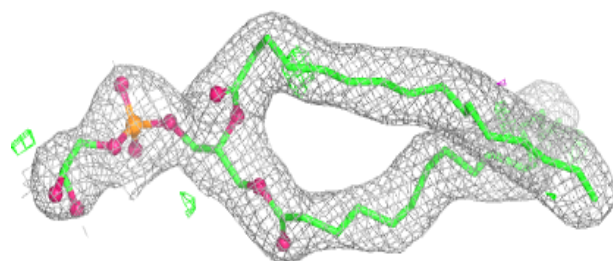
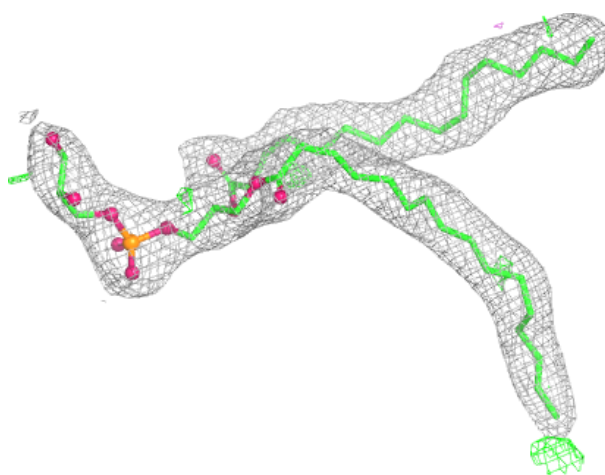
**Electron density around CLA B 610:**

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



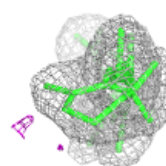
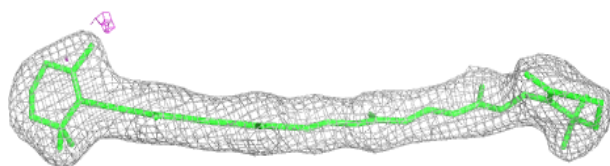
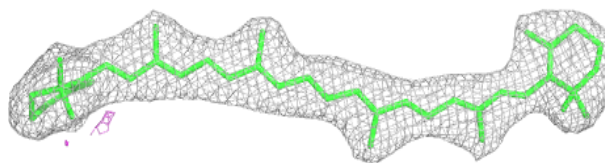
Electron density around LHG D 412:

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



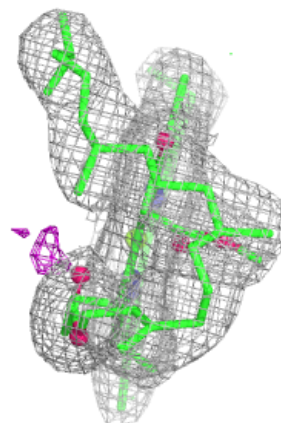
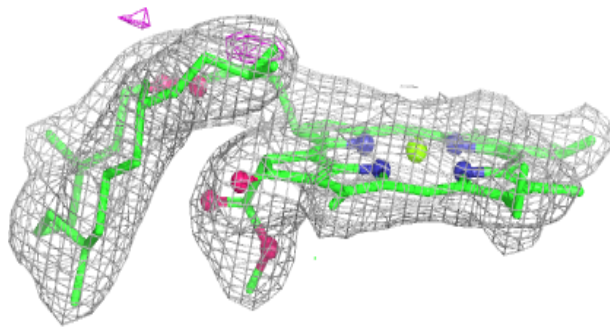
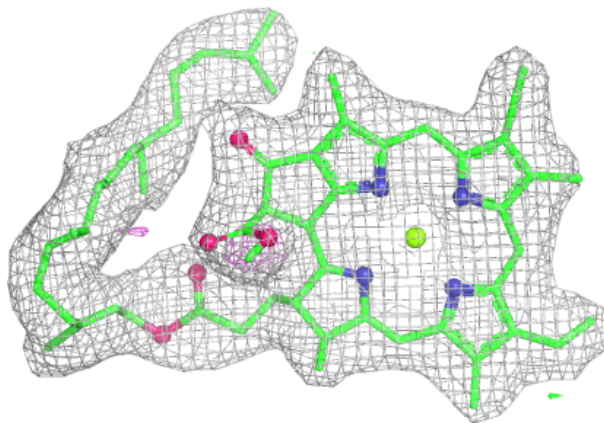
Electron density around BCR B 618:

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



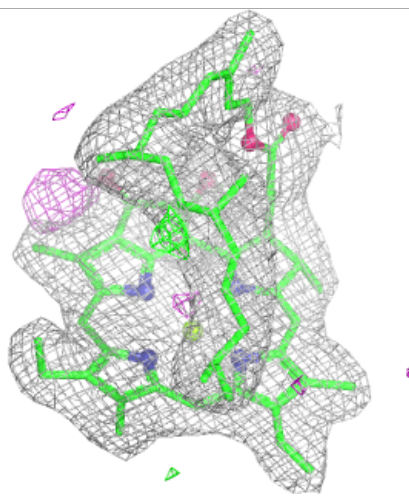
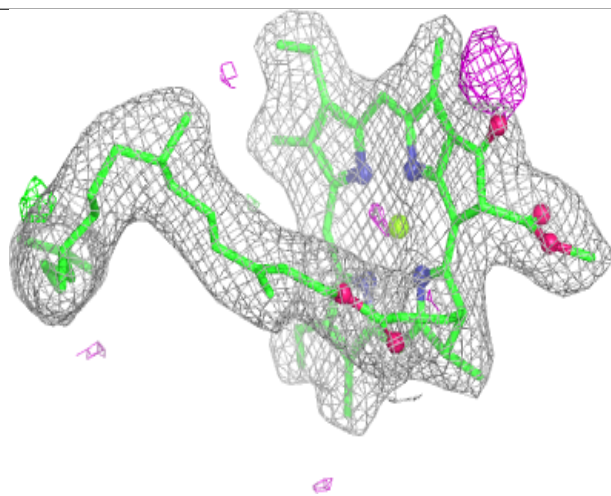
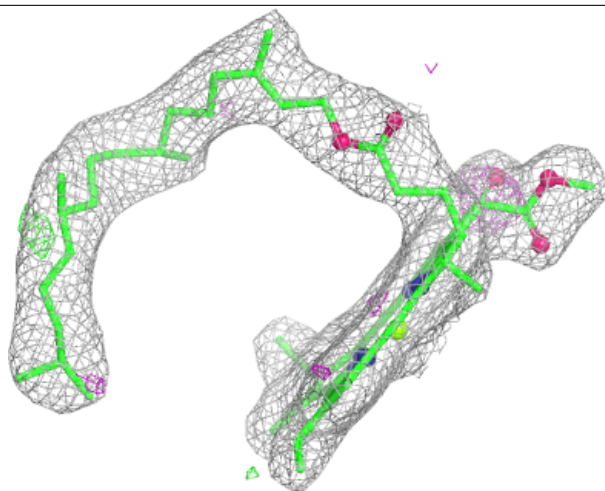
Electron density around CLA B 611:

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



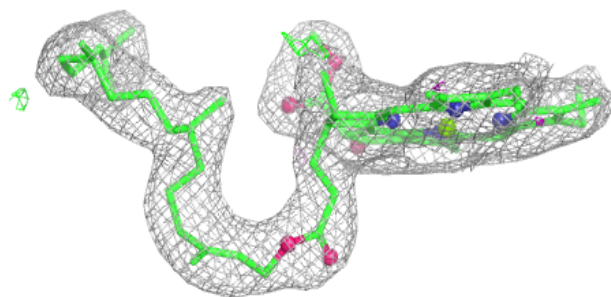
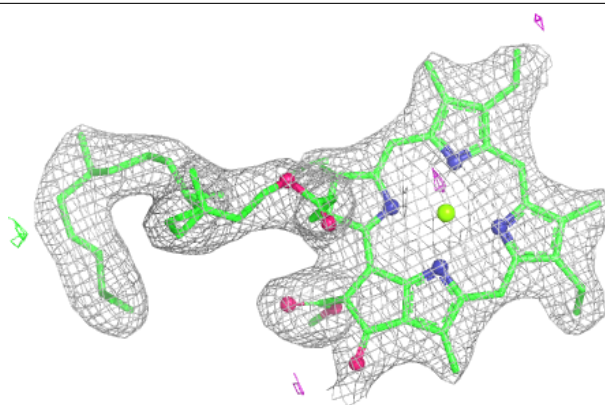
Electron density around CLA B 612:

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

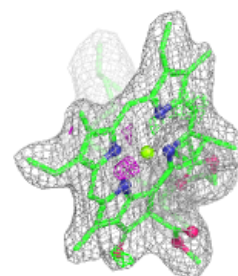
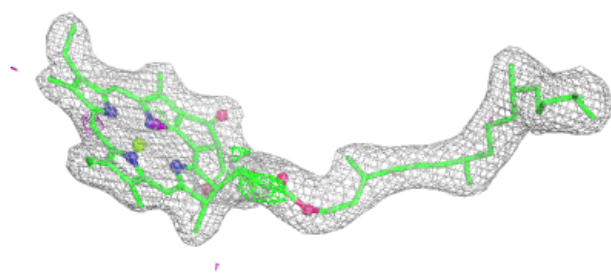
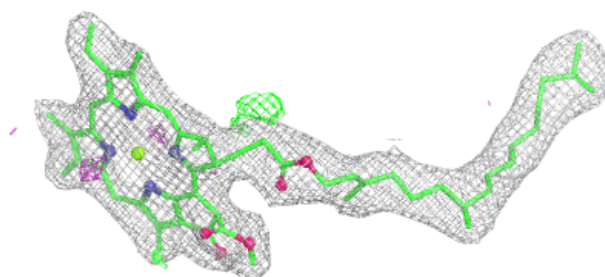


Electron density around CLA B 613:

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

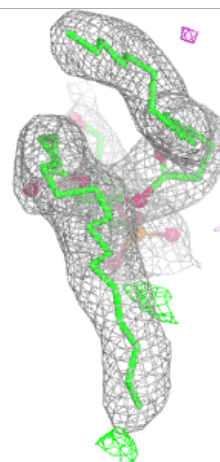
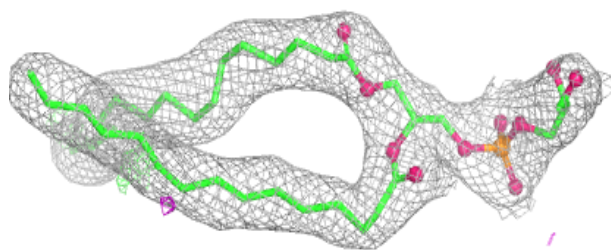
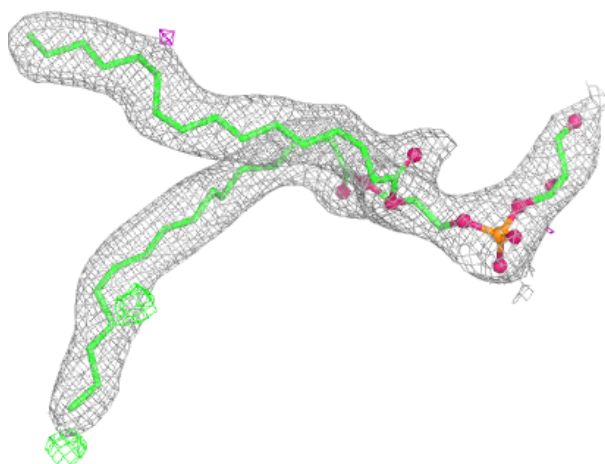
**Electron density around CLA A 404:**

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



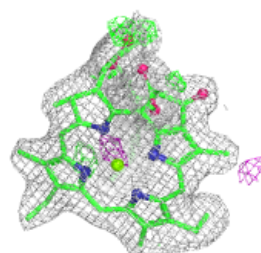
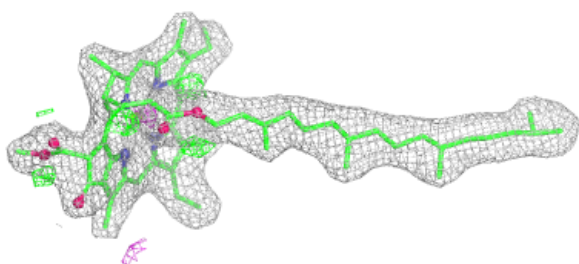
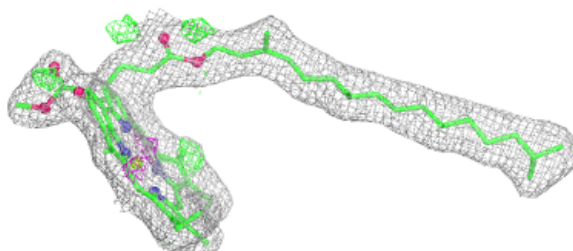
Electron density around LHG d 410:

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

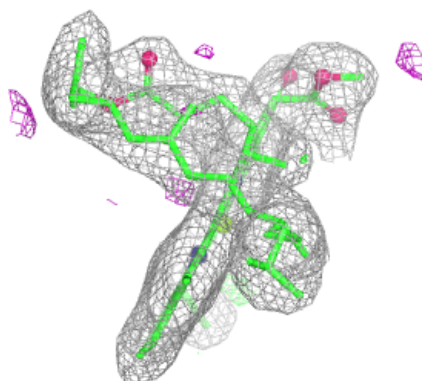
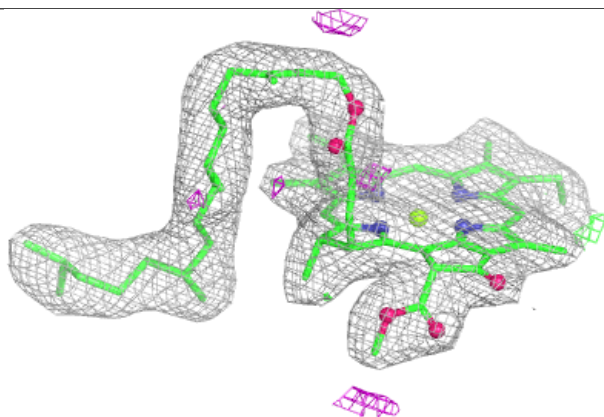
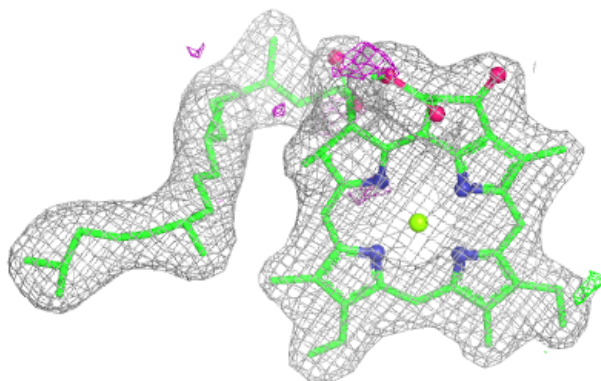


Electron density around CLA b 616:

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

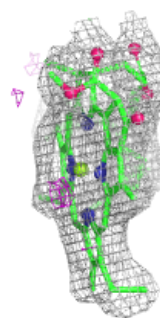
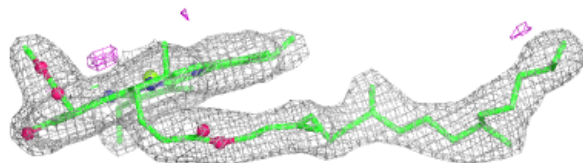
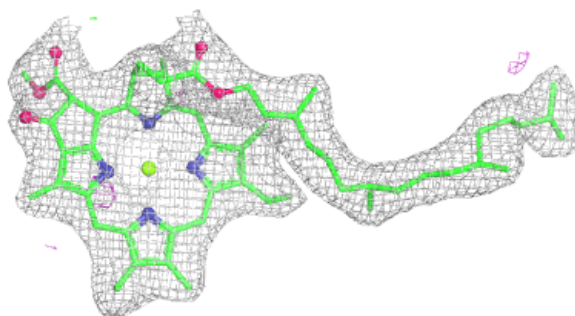
**Electron density around CLA A 405:**

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



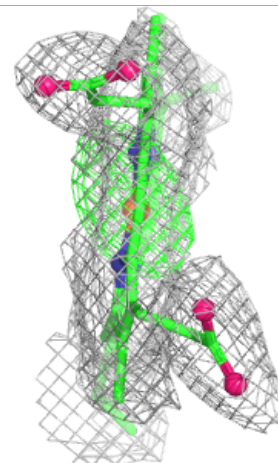
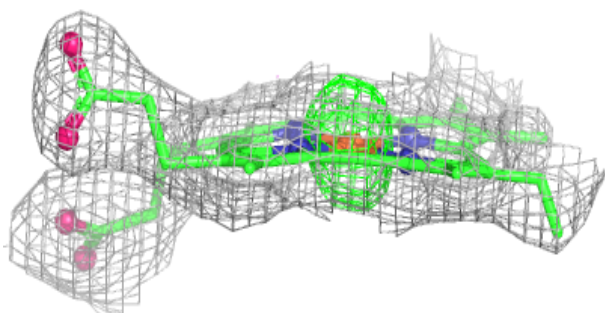
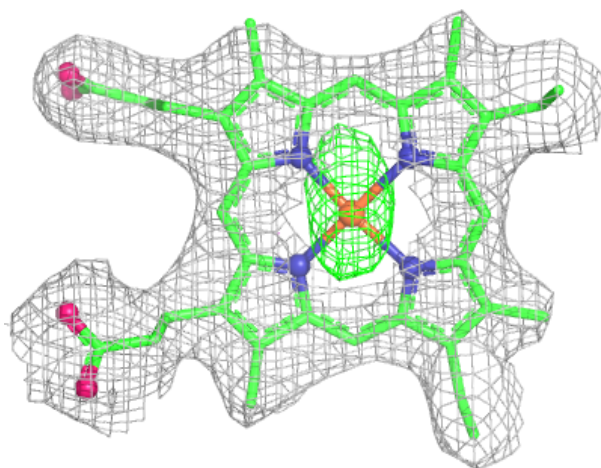
Electron density around CLA B 604:

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



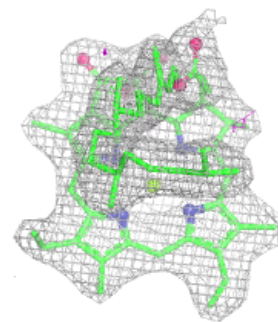
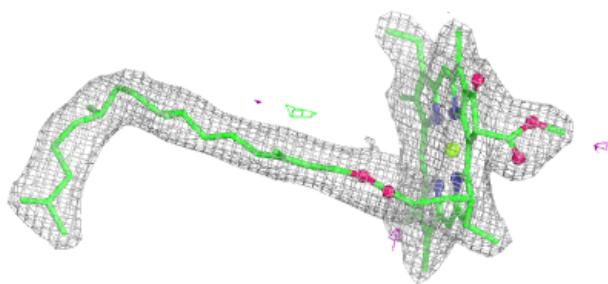
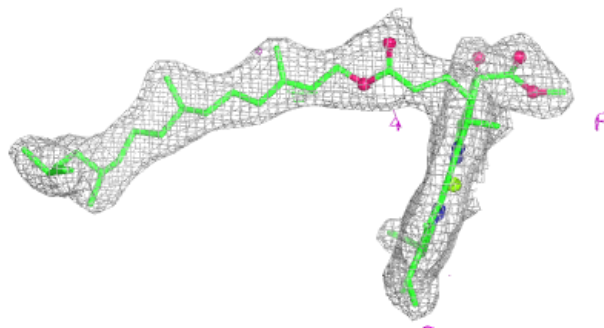
Electron density around HEC v 205:

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



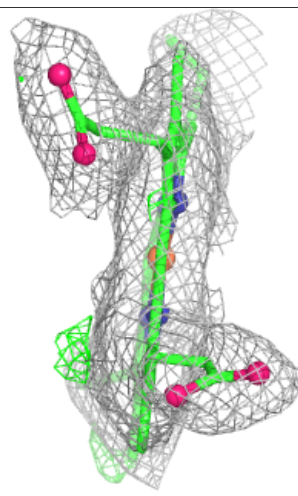
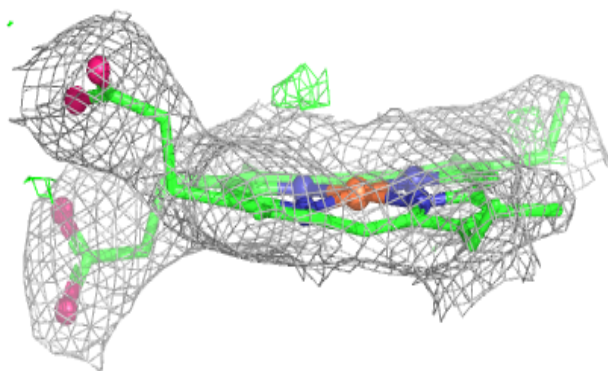
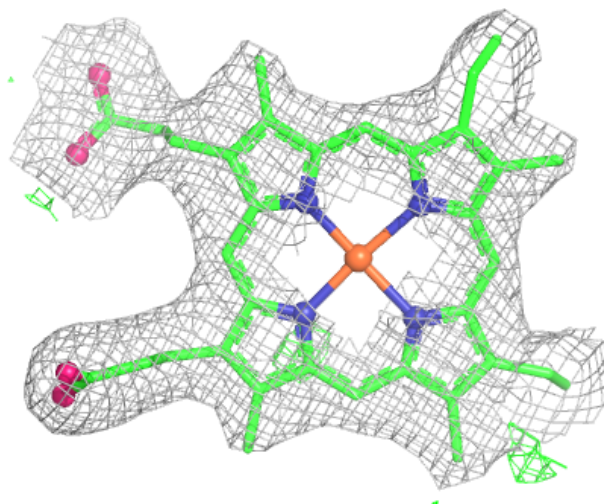
Electron density around CLA B 606:

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



Electron density around HEC V 206:

$2mF_o-DF_c$ (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.