



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 03:27 PM JST

PDB ID : 6JLN / pdb_00006jln
Title : XFEL structure of cyanobacterial photosystem II (1F state, dataset2)
Authors : Suga, M.; Shen, J.R.
Deposited on : 2019-03-06
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.5 (274361), CSD as541be (2020)
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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

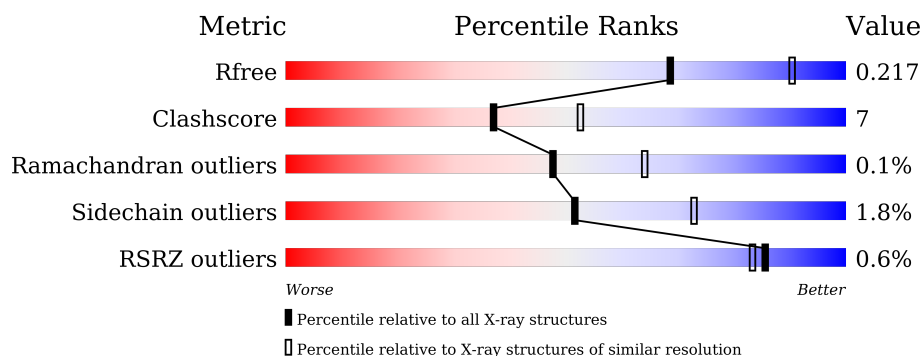
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



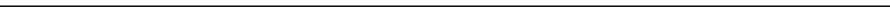
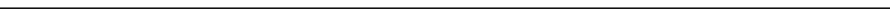
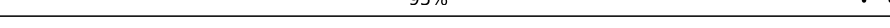
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	344	84% 13% .
1	a	344	84% 13% .
2	B	505	84% 16%
2	b	505	% 86% 14%
3	C	455	86% 13% .
3	c	455	85% 14% .

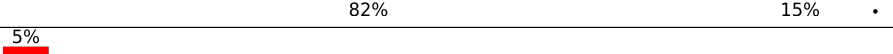
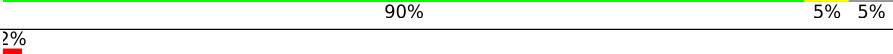
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Mol	Chain	Length	Quality of chain
4	D	342	
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	

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Mol	Chain	Length	Quality of chain
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
40	HEC	V	205	X	-	-	-
40	HEC	v	206	X	-	-	-

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 55631 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	53	0
			3019	1966	498	537	18			
1	a	334	Total	C	N	O	S	0	55	0
			3027	1973	498	538	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	7	0
			3518	2300	587	618	13			
3	c	455	Total	C	N	O	S	0	13	0
			3598	2356	599	629	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	S	0	0	0
			287	191	46	50				
18	x	38	Total	C	N	O	S	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	S	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
			2	2		

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

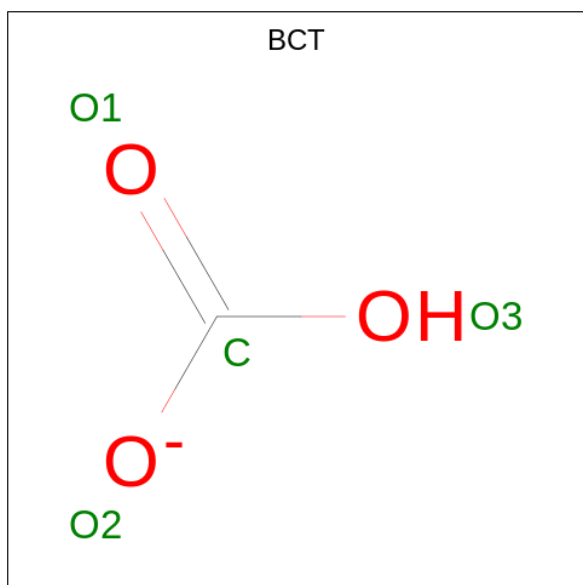
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	2
			4	4		
22	U	1	Total	Cl	0	0
			1	1		

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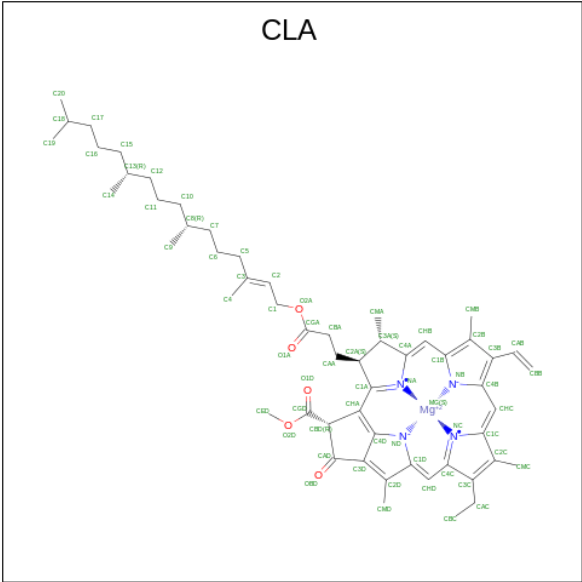
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	a	2	Total	Cl	0	2
			4	4		
22	v	1	Total	Cl	0	0
			1	1		

- Molecule 23 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-).



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

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$).



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

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

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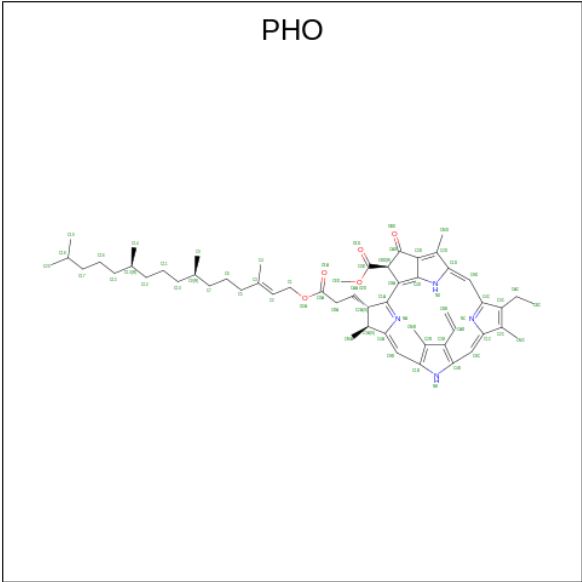
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N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

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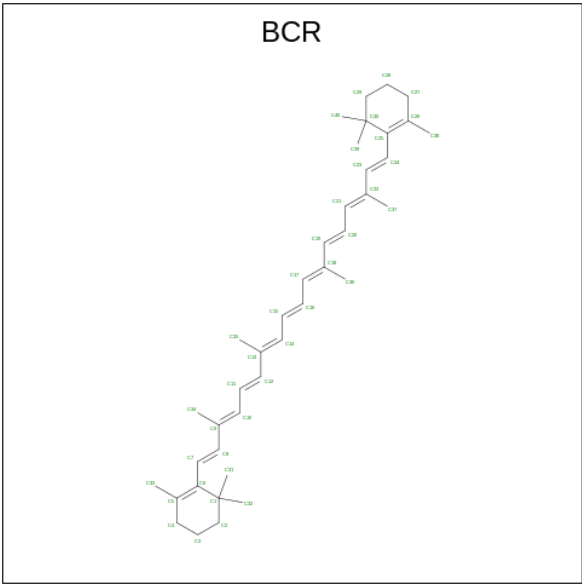
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N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

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



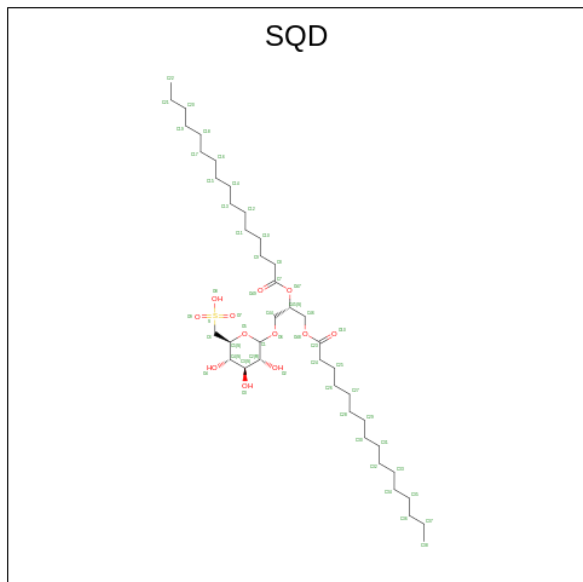
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	D	1	Total	C	N	O	0	1
			128	110	8	10		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	d	1	Total	C	N	O	0	1
			128	110	8	10		

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



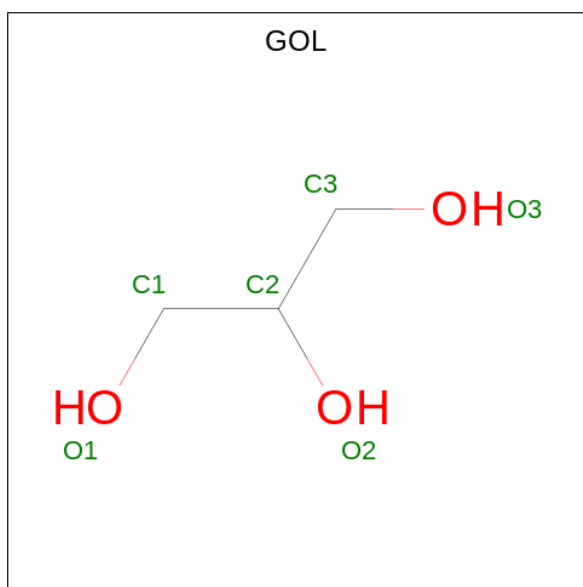
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Y	1	Total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

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



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

- Molecule 28 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



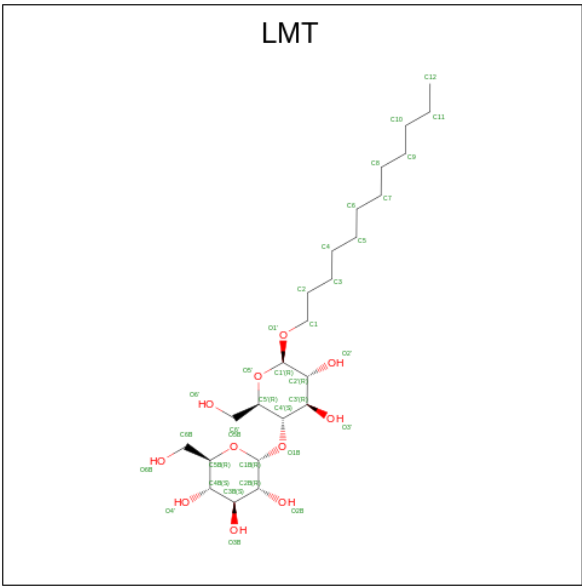
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	C	1	Total	C	O	0	0
			6	3	3		
28	C	1	Total	C	O	0	0
			6	3	3		
28	D	1	Total	C	O	0	0
			6	3	3		
28	F	1	Total	C	O	0	0
			6	3	3		
28	O	1	Total	C	O	0	0
			6	3	3		
28	T	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	T	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	c	1	Total	C	O	0	0
			6	3	3		
28	c	1	Total	C	O	0	0
			6	3	3		
28	o	1	Total	C	O	0	0
			6	3	3		
28	t	1	Total	C	O	0	0
			6	3	3		
28	v	1	Total	C	O	0	0
			6	3	3		
28	v	1	Total	C	O	0	0
			6	3	3		
28	v	1	Total	C	O	0	0
			6	3	3		
28	v	1	Total	C	O	0	0
			6	3	3		

- Molecule 29 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



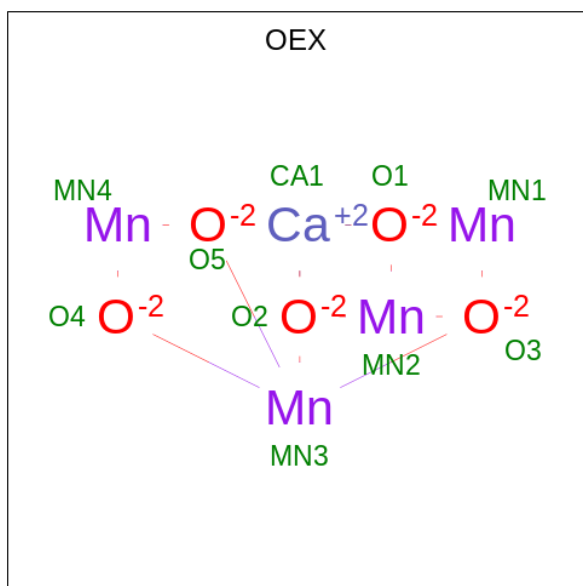
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			35	24	11		
29	C	1	Total	C	O	0	0
			35	24	11		
29	D	1	Total	C	O	0	0
			35	24	11		
29	E	1	Total	C	O	0	0
			35	24	11		
29	M	1	Total	C	O	0	0
			35	24	11		
29	M	1	Total	C	O	0	0
			35	24	11		
29	T	1	Total	C	O	0	0
			25	19	6		
29	a	1	Total	C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

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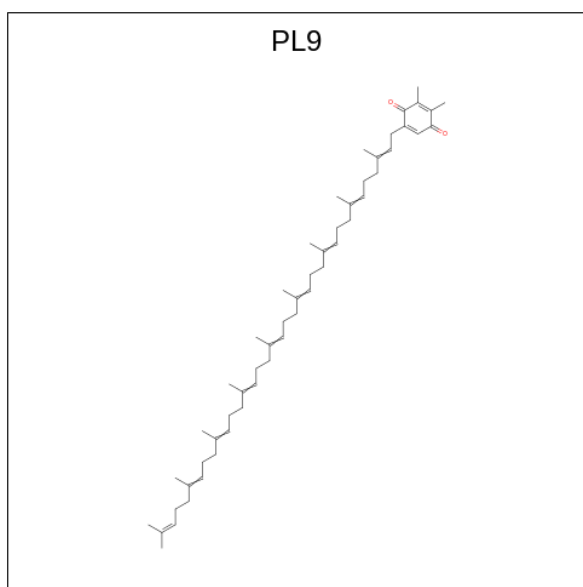
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	t	1	Total	C	O	0	0
			25	19	6		

- Molecule 30 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



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

- Molecule 31 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
31	A	1	Total	C	O	0	1
			110	106	4		
31	D	1	Total	C	O	0	1
			110	106	4		
31	a	1	Total	C	O	0	1
			110	106	4		
31	d	1	Total	C	O	0	1
			110	106	4		

- Molecule 32 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

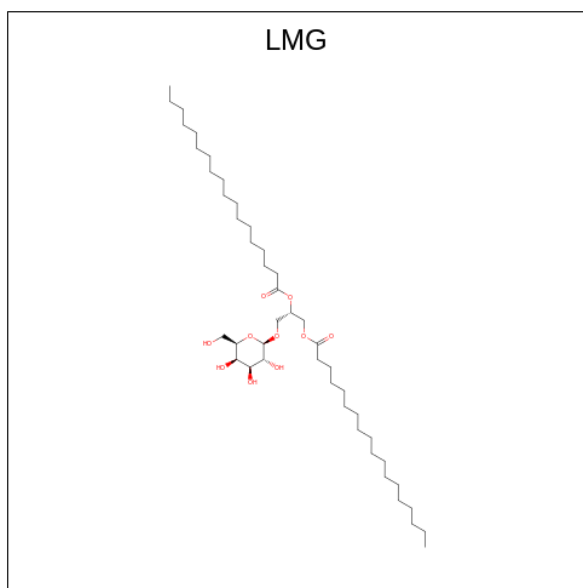
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			28	23	5		
32	B	1	Total	C	O	0	0
			33	28	5		
32	C	1	Total	C	O	0	0
			34	29	5		
32	D	2	Total	C	O	0	0
			57	51	6		
32	I	1	Total	C	O	0	0
			40	35	5		
32	J	1	Total	C		0	0
			10	10			
32	M	1	Total	C		0	0
			10	10			
32	X	1	Total	C	O	0	0
		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

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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	A	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	D	1	Total	C	O	0	0
			51	41	10		

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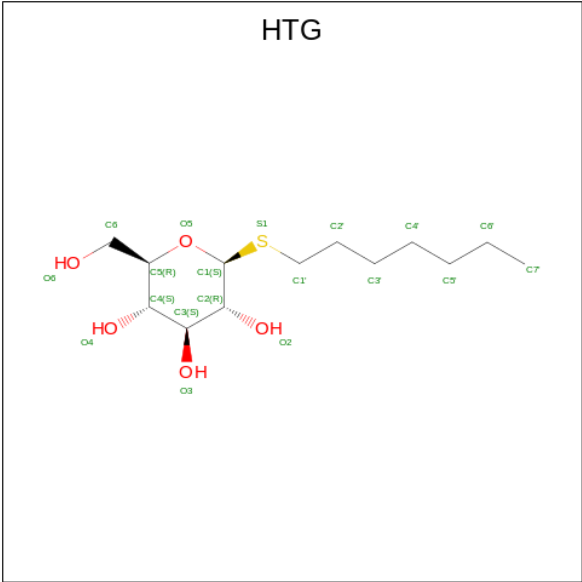
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	M	1	Total	C	O	0	0
			51	41	10		
33	Z	1	Total	C	O	0	0
			37	27	10		
33	a	1	Total	C	O	0	0
			51	41	10		
33	b	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	d	1	Total	C	O	0	0
			51	41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

- Molecule 34 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C₁₃H₂₆O₅S).



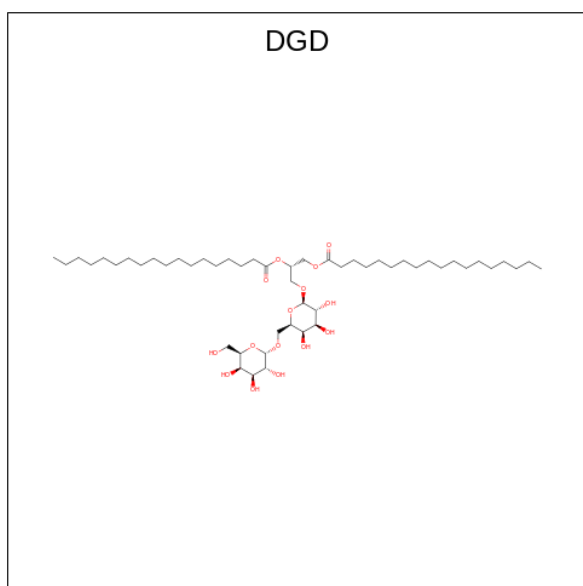
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19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

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

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



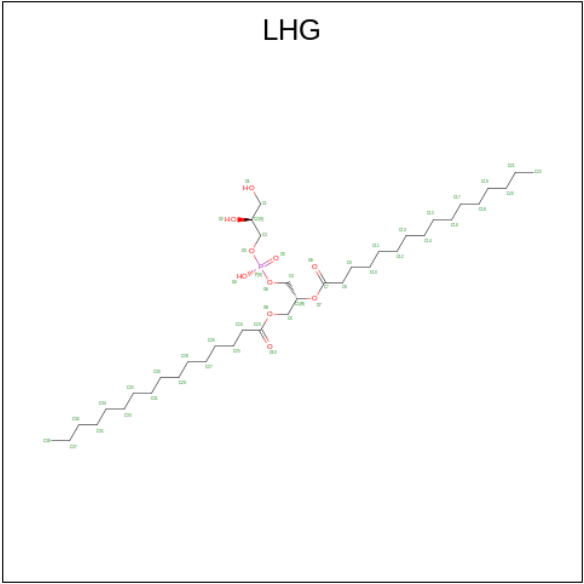
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	C	1	Total	C	O		0	0
			62	47	15			
36	C	1	Total	C	O		0	0
			62	47	15			
36	C	1	Total	C	O		0	0
			62	47	15			
36	D	1	Total	C	O		0	0
			52	42	10			
36	H	1	Total	C	O		0	0
			62	47	15			
36	c	1	Total	C	O		0	0
			62	47	15			
36	c	1	Total	C	O		0	0
			62	47	15	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

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

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



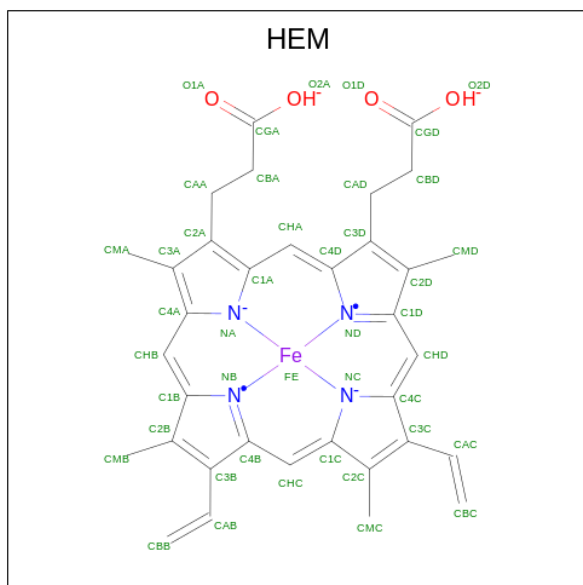
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	E	1	Total	C	O	P	0	0
			42	31	10	1		
37	L	1	Total	C	O	P	0	0
			49	38	10	1		
37	a	1	Total	C	O	P	0	0
			42	31	10	1		
37	b	1	Total	C	O	P	0	0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

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

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

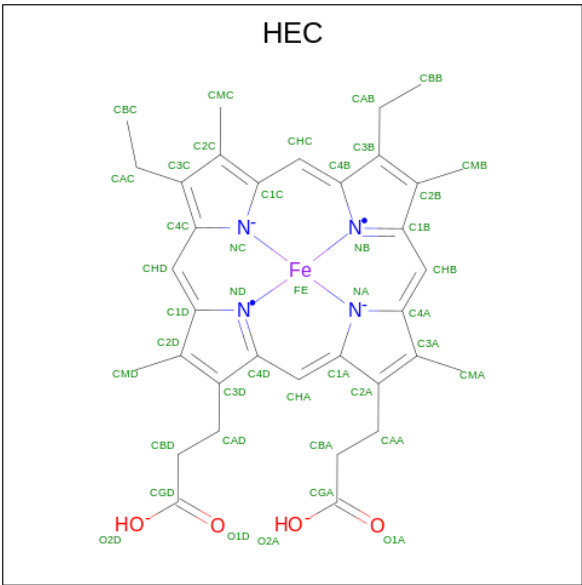


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
38	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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

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

- Molecule 40 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	162	Total	O	0	15
			175	175		
41	B	284	Total	O	0	4
			288	288		
41	C	232	Total	O	0	6
			236	236		
41	D	144	Total	O	0	5
			149	149		
41	E	36	Total	O	0	1
			37	37		
41	F	7	Total	O	0	0
			7	7		
41	H	41	Total	O	0	0
			41	41		
41	I	4	Total	O	0	0
			4	4		
41	J	10	Total	O	0	0
			10	10		
41	K	8	Total	O	0	0
			8	8		

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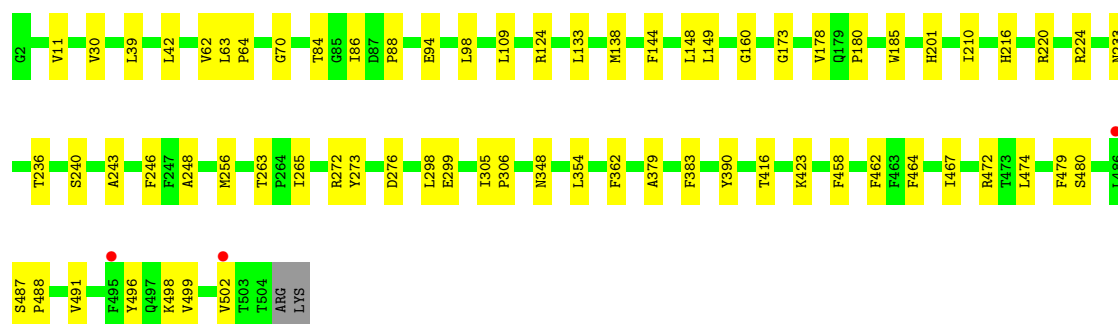
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	L	16	Total 17	O 17	0	1
41	M	23	Total 23	O 23	0	0
41	O	177	Total 179	O 179	0	2
41	T	15	Total 16	O 16	0	1
41	U	83	Total 83	O 83	0	0
41	V	114	Total 116	O 116	0	2
41	Y	4	Total 4	O 4	0	0
41	X	8	Total 8	O 8	0	0
41	Z	1	Total 1	O 1	0	0
41	a	157	Total 168	O 168	0	13
41	b	261	Total 264	O 264	0	3
41	c	200	Total 206	O 206	0	8
41	d	134	Total 137	O 137	0	3
41	e	20	Total 20	O 20	0	0
41	f	6	Total 6	O 6	0	0
41	h	42	Total 42	O 42	0	0
41	i	5	Total 5	O 5	0	0
41	j	7	Total 7	O 7	0	0
41	k	8	Total 8	O 8	0	0
41	l	7	Total 7	O 7	0	0
41	m	15	Total 15	O 15	0	0

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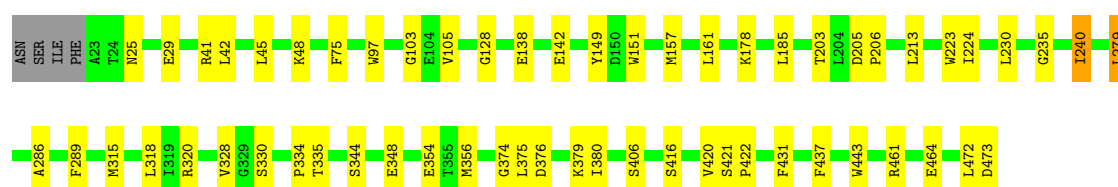
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	o	152	Total 152	O 152	0	0
41	t	14	Total 14	O 14	0	0
41	u	95	Total 95	O 95	0	0
41	v	85	Total 86	O 86	0	1
41	y	2	Total 2	O 2	0	0
41	x	6	Total 6	O 6	0	0



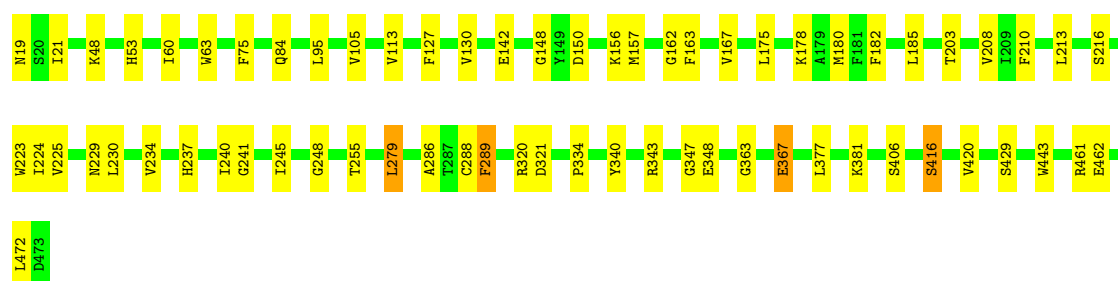
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 86% 13%



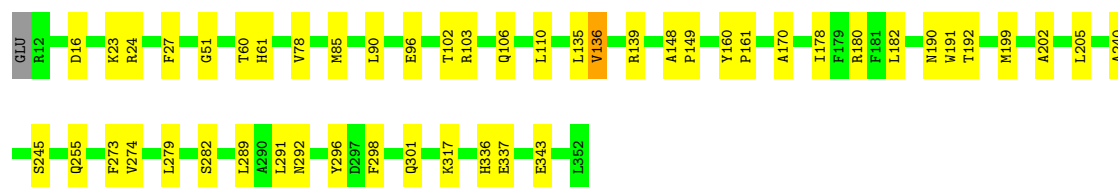
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 85% 14%



• Molecule 4: Photosystem II D2 protein

Chain D: 85% 14%



• Molecule 4: Photosystem II D2 protein

Chain d: 87% 12%





- Molecule 5: Cytochrome b559 subunit alpha

Chain E: 77% 19% .



- Molecule 5: Cytochrome b559 subunit alpha

Chain e: 77% 19% .



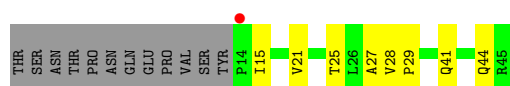
- Molecule 6: Cytochrome b559 subunit beta

Chain F: 61% 16% 23%



- Molecule 6: Cytochrome b559 subunit beta

Chain f: 55% 18% 27%



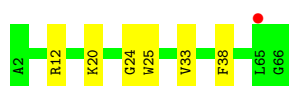
- Molecule 7: Photosystem II reaction center protein H

Chain H: 83% 15% 3%



- Molecule 7: Photosystem II reaction center protein H

Chain h: 91% 9% 2%

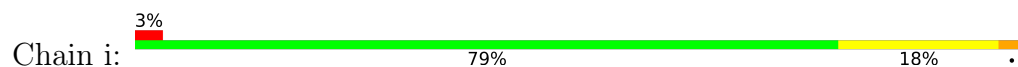


- Molecule 8: Photosystem II reaction center protein I

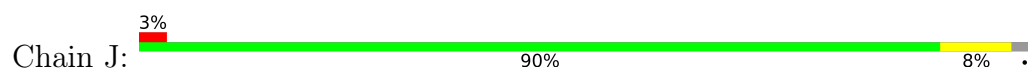
Chain I: 84% 16%



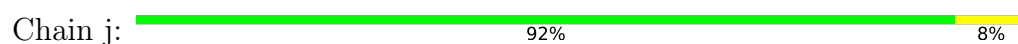
- Molecule 8: Photosystem II reaction center protein I



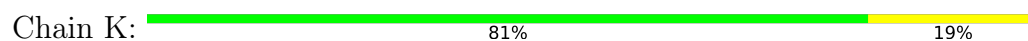
- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



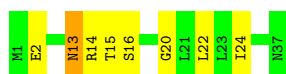
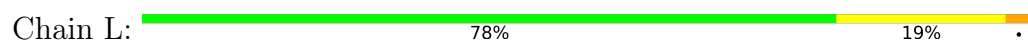
- Molecule 10: Photosystem II reaction center protein K



- 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: 61% 31% 6%



- Molecule 12: Photosystem II reaction center protein M

Chain m: 67% 22% 6% 6%



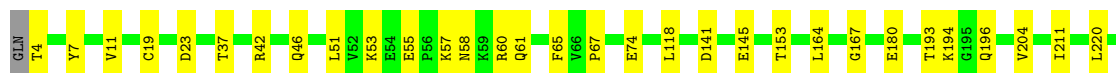
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 84% 16%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 86% 13%



- Molecule 14: Photosystem II reaction center protein T

Chain T: 69% 22% 6%



- Molecule 14: Photosystem II reaction center protein T

Chain t: 3% 78% 16% 6%



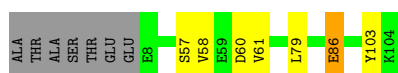
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 81% 12% • 7%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 87% 6% • 7%



- Molecule 16: Cytochrome c-550

Chain V: 93% 7%



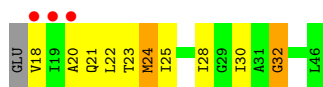
- Molecule 16: Cytochrome c-550

Chain v: 88% 12%



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y: 10% 63% 27% 7% •



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y: 3% 70% 23% • •

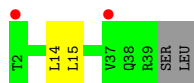
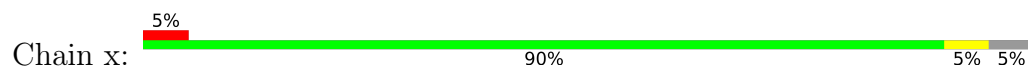


- Molecule 18: Photosystem II reaction center protein X

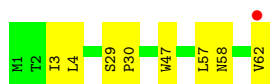
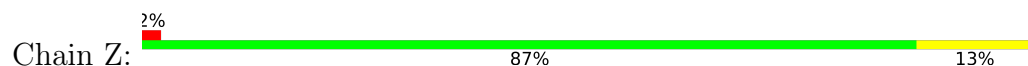
Chain X: 82% 15% •



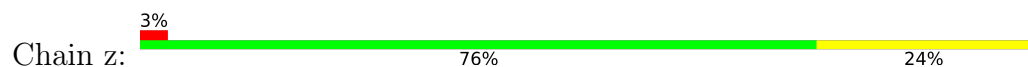
- Molecule 18: Photosystem II reaction center protein X



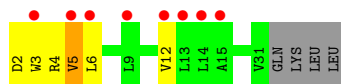
- Molecule 19: Photosystem II reaction center protein Z



- 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 – 2.40 19.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.99-2.40) 99.7 (19.99-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.154 , 0.212 0.161 , 0.217	Depositor DCC
R_{free} test set	17838 reflections (3.31%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.604	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 89.7	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	55631	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% 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: CLA, GOL, UNL, PHO, HEM, LHG, MG, OEX, LMG, CL, BCT, LMT, FME, HTG, BCR, CA, PL9, HEC, FE2, SQD, DGD

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	0/3121	0.81	2/4250 (0.0%)
1	a	0.53	0/3135	0.81	0/4269
2	B	0.52	0/4191	0.83	1/5709 (0.0%)
2	b	0.51	0/4198	0.82	0/5720
3	C	0.47	0/3643	0.81	0/4958
3	c	0.47	0/3731	0.82	2/5076 (0.0%)
4	D	0.55	0/2952	0.81	2/4021 (0.0%)
4	d	0.55	1/2952 (0.0%)	0.83	3/4021 (0.1%)
5	E	0.48	0/693	0.80	0/944
5	e	0.42	0/695	0.83	2/948 (0.2%)
6	F	0.53	0/284	0.85	0/387
6	f	0.50	0/265	0.78	0/360
7	H	0.48	0/535	0.82	0/728
7	h	0.43	0/524	0.79	0/713
8	I	0.46	0/311	0.86	1/419 (0.2%)
8	i	0.49	0/311	0.85	0/419
9	J	0.50	0/278	0.71	0/376
9	j	0.44	0/286	0.78	0/386
10	K	0.45	0/303	0.85	0/416
10	k	0.48	0/303	0.78	0/416
11	L	0.57	0/319	0.73	0/433
11	l	0.49	0/319	0.74	0/433
12	M	0.63	0/270	0.88	0/368
12	m	0.56	0/262	0.98	2/357 (0.6%)
13	O	0.47	0/1958	0.78	0/2654
13	o	0.46	0/1937	0.79	2/2625 (0.1%)
14	T	0.51	0/266	0.77	0/362
14	t	0.60	0/266	0.76	0/362
15	U	0.47	0/785	0.77	0/1064
15	u	0.48	0/785	0.76	0/1064
16	V	0.49	0/1109	0.76	0/1502

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.46	0/1098	0.81	0/1488
17	Y	0.50	0/216	0.90	2/289 (0.7%)
17	y	0.46	0/216	0.80	0/289
18	X	0.44	0/290	0.77	0/392
18	x	0.44	0/284	0.80	0/384
19	Z	0.38	0/490	0.79	0/669
19	z	0.39	0/490	0.83	0/669
20	R	0.37	0/245	0.70	0/338
All	All	0.50	1/44316 (0.0%)	0.81	19/60278 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	274	VAL	CA-C	5.12	1.58	1.52

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	170	ALA	CA-C-N	-7.10	112.68	119.85
4	d	170	ALA	C-N-CA	-7.10	112.68	119.85
1	A	334	ARG	N-CA-C	6.16	119.23	111.84
12	m	17	VAL	CA-C-N	-5.82	112.56	119.84
12	m	17	VAL	C-N-CA	-5.82	112.56	119.84

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	3019	0	2872	32	0
1	a	3027	0	2888	39	0
2	B	4021	0	3898	64	0
2	b	4022	0	3908	53	0
3	C	3518	0	3439	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	c	3598	0	3529	48	0
4	D	2849	0	2741	39	0
4	d	2849	0	2741	33	0
5	E	668	0	658	14	0
5	e	670	0	664	12	0
6	F	275	0	282	5	0
6	f	257	0	269	5	0
7	H	519	0	545	12	0
7	h	511	0	532	9	0
8	I	314	0	328	2	0
8	i	314	0	328	4	0
9	J	272	0	279	3	0
9	j	280	0	291	2	0
10	K	293	0	305	6	0
10	k	293	0	305	10	0
11	L	309	0	327	6	0
11	l	309	0	327	2	0
12	M	274	0	299	12	0
12	m	269	0	288	9	0
13	O	1903	0	1886	23	0
13	o	1891	0	1870	17	0
14	T	264	0	267	6	0
14	t	264	0	267	3	0
15	U	774	0	773	9	0
15	u	774	0	773	4	0
16	V	1085	0	1095	6	0
16	v	1077	0	1082	9	0
17	Y	215	0	246	6	0
17	y	215	0	246	5	0
18	X	287	0	317	5	0
18	x	281	0	312	2	0
19	Z	479	0	516	5	0
19	z	479	0	516	10	0
20	R	239	0	262	4	0
21	A	2	0	0	0	0
21	a	2	0	0	0	0
22	A	4	0	0	0	0
22	U	1	0	0	1	0
22	a	4	0	0	0	0
22	v	1	0	0	0	0
23	A	8	0	0	0	0
23	d	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	A	260	0	288	11	0
24	B	1040	0	1152	48	0
24	C	845	0	936	41	0
24	D	130	0	144	4	0
24	a	195	0	216	12	0
24	b	1040	0	1152	39	0
24	c	845	0	936	42	0
24	d	195	0	216	12	0
25	A	64	0	74	1	0
25	D	128	0	148	3	0
25	a	64	0	74	2	0
25	d	128	0	148	5	0
26	A	40	0	56	1	0
26	B	120	0	168	11	0
26	C	80	0	112	3	0
26	D	40	0	56	2	0
26	H	40	0	56	5	0
26	K	40	0	56	3	0
26	T	40	0	56	6	0
26	Y	40	0	56	6	0
26	a	40	0	56	1	0
26	b	120	0	168	6	0
26	c	80	0	112	6	0
26	d	40	0	56	1	0
26	h	40	0	56	5	0
26	k	40	0	56	1	0
26	t	40	0	56	6	0
26	y	40	0	56	2	0
27	A	108	0	156	4	0
27	B	54	0	78	1	0
27	F	43	0	53	0	0
27	L	54	0	78	2	0
27	a	108	0	156	4	0
27	f	43	0	53	3	0
28	A	6	0	8	0	0
28	B	42	0	56	2	0
28	C	12	0	16	2	0
28	D	6	0	8	2	0
28	F	6	0	8	0	0
28	O	6	0	8	0	0
28	T	12	0	16	4	0
28	V	24	0	32	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	a	18	0	24	3	0
28	b	30	0	40	1	0
28	c	12	0	16	1	0
28	o	6	0	8	0	0
28	t	6	0	8	0	0
28	v	24	0	32	2	0
29	A	35	0	46	3	0
29	C	35	0	46	2	0
29	D	35	0	46	1	0
29	E	35	0	46	1	0
29	M	70	0	92	3	0
29	T	25	0	35	1	0
29	a	70	0	92	1	0
29	b	25	0	35	0	0
29	e	35	0	46	1	0
29	m	70	0	92	3	0
29	t	25	0	35	0	0
30	A	20	0	0	0	0
30	a	20	0	0	1	0
31	A	110	0	160	8	0
31	D	110	0	160	3	0
31	a	110	0	160	19	0
31	d	110	0	160	0	0
32	A	28	0	0	0	0
32	B	33	0	0	0	0
32	C	34	0	0	0	0
32	D	57	0	0	0	0
32	I	40	0	0	0	0
32	J	10	0	0	0	0
32	M	10	0	0	0	0
32	X	18	0	0	0	0
32	a	30	0	0	0	0
32	b	33	0	0	0	0
32	c	32	0	0	0	0
32	d	71	0	0	0	0
32	i	40	0	0	0	0
32	j	10	0	0	0	0
32	m	10	0	0	0	0
33	A	51	0	72	3	0
33	C	102	0	144	4	0
33	D	51	0	72	1	0
33	M	51	0	72	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	Z	37	0	44	2	0
33	a	51	0	72	5	0
33	b	51	0	72	3	0
33	c	51	0	72	5	0
33	d	51	0	72	4	0
33	k	51	0	72	2	0
33	z	39	0	48	6	0
34	B	1	0	0	0	0
34	C	1	0	0	0	0
34	F	1	0	0	0	0
34	O	1	0	0	0	0
34	b	1	0	0	0	0
34	c	2	0	0	0	0
34	f	1	0	0	0	0
34	o	1	0	0	0	0
35	B	95	0	130	1	0
35	C	38	0	52	1	0
35	D	16	0	17	2	0
35	V	19	0	26	1	0
35	b	95	0	130	5	0
35	c	38	0	52	1	0
35	d	16	0	17	3	0
36	C	186	0	246	6	0
36	D	52	0	71	2	0
36	H	62	0	82	2	0
36	c	186	0	246	8	0
36	e	62	0	82	7	0
36	h	62	0	82	1	0
37	D	147	0	222	12	0
37	E	42	0	57	2	0
37	L	49	0	74	2	0
37	a	42	0	57	4	0
37	b	49	0	74	4	0
37	d	147	0	222	14	0
38	E	43	0	30	2	0
38	f	43	0	30	4	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	V	43	0	30	0	0
40	v	43	0	30	0	0
41	A	175	0	0	2	0
41	B	288	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	C	236	0	0	4	0
41	D	149	0	0	3	0
41	E	37	0	0	0	0
41	F	7	0	0	0	0
41	H	41	0	0	0	0
41	I	4	0	0	0	0
41	J	10	0	0	0	0
41	K	8	0	0	1	0
41	L	17	0	0	1	0
41	M	23	0	0	0	0
41	O	179	0	0	3	0
41	T	16	0	0	1	0
41	U	83	0	0	3	0
41	V	116	0	0	1	0
41	X	8	0	0	0	0
41	Y	4	0	0	0	0
41	Z	1	0	0	0	0
41	a	168	0	0	3	0
41	b	264	0	0	4	0
41	c	206	0	0	3	0
41	d	137	0	0	2	0
41	e	20	0	0	1	0
41	f	6	0	0	0	0
41	h	42	0	0	1	0
41	i	5	0	0	0	0
41	j	7	0	0	0	0
41	k	8	0	0	0	0
41	l	7	0	0	0	0
41	m	15	0	0	0	0
41	o	152	0	0	1	0
41	t	14	0	0	0	0
41	u	95	0	0	1	0
41	v	86	0	0	1	0
41	x	6	0	0	0	0
41	y	2	0	0	0	0
All	All	55631	0	54163	754	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 754 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)
24:C:503:CLA:HBB1	24:C:512:CLA:H41	1.50	0.93
1:A:214[A]:MET:HG2	31:A:417[A]:PL9:H102	1.50	0.92
1:A:214[B]:MET:HG2	31:A:417[B]:PL9:H102	1.54	0.89
4:d:192:THR:HG23	24:d:404:CLA:HBC2	1.59	0.84
24:B:616:CLA:H71	24:B:617:CLA:H192	1.62	0.82

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	384/344 (112%)	377 (98%)	5 (1%)	2 (0%)	24	37
1	a	386/344 (112%)	378 (98%)	7 (2%)	1 (0%)	36	50
2	B	512/505 (101%)	505 (99%)	7 (1%)	0	100	100
2	b	513/505 (102%)	503 (98%)	10 (2%)	0	100	100
3	C	456/455 (100%)	446 (98%)	8 (2%)	2 (0%)	30	43
3	c	466/455 (102%)	450 (97%)	14 (3%)	2 (0%)	30	43
4	D	355/342 (104%)	343 (97%)	12 (3%)	0	100	100
4	d	355/342 (104%)	346 (98%)	9 (2%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
6	F	32/44 (73%)	30 (94%)	2 (6%)	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	64/65 (98%)	58 (91%)	6 (9%)	0	100	100
7	h	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	34 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	J	36/39 (92%)	36 (100%)	0	0	100	100
9	j	37/39 (95%)	34 (92%)	3 (8%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	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%)	241 (97%)	8 (3%)	0	100	100
13	o	246/244 (101%)	235 (96%)	11 (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%)	93 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
16	V	136/137 (99%)	130 (96%)	6 (4%)	0	100	100
16	v	135/137 (98%)	130 (96%)	5 (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%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	57 (95%)	1 (2%)	2 (3%)	3	2
20	R	28/34 (82%)	28 (100%)	0	0	100	100
All	All	5419/5384 (101%)	5272 (97%)	138 (2%)	9 (0%)	48	58

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
1	a	259	ILE

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	314/279 (112%)	313 (100%)	1 (0%)	86	93
2	B	412/403 (102%)	408 (99%)	4 (1%)	68	84
2	b	413/403 (102%)	407 (98%)	6 (2%)	57	77
3	C	357/356 (100%)	351 (98%)	6 (2%)	53	74
3	c	367/356 (103%)	357 (97%)	10 (3%)	39	62
4	D	290/277 (105%)	288 (99%)	2 (1%)	76	88
4	d	290/277 (105%)	287 (99%)	3 (1%)	68	84
5	E	74/73 (101%)	74 (100%)	0	100	100
5	e	74/73 (101%)	72 (97%)	2 (3%)	39	62
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	26/38 (68%)	24 (92%)	2 (8%)	12	20
7	H	55/54 (102%)	54 (98%)	1 (2%)	51	73
7	h	54/54 (100%)	54 (100%)	0	100	100
8	I	34/34 (100%)	33 (97%)	1 (3%)	37	60
8	i	34/34 (100%)	33 (97%)	1 (3%)	37	60
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	27/27 (100%)	26 (96%)	1 (4%)	30	51
10	K	30/30 (100%)	29 (97%)	1 (3%)	33	55
10	k	30/30 (100%)	29 (97%)	1 (3%)	33	55
11	L	36/35 (103%)	34 (94%)	2 (6%)	19	33
11	l	36/35 (103%)	35 (97%)	1 (3%)	38	60
12	M	31/32 (97%)	30 (97%)	1 (3%)	34	56
12	m	30/32 (94%)	29 (97%)	1 (3%)	33	55
13	O	214/207 (103%)	209 (98%)	5 (2%)	44	66
13	o	211/207 (102%)	204 (97%)	7 (3%)	33	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	T	27/28 (96%)	25 (93%)	2 (7%)	13	22
14	t	27/28 (96%)	25 (93%)	2 (7%)	13	22
15	U	84/89 (94%)	82 (98%)	2 (2%)	43	65
15	u	84/89 (94%)	82 (98%)	2 (2%)	43	65
16	V	119/117 (102%)	118 (99%)	1 (1%)	73	86
16	v	118/117 (101%)	114 (97%)	4 (3%)	32	54
17	Y	22/23 (96%)	19 (86%)	3 (14%)	3	5
17	y	22/23 (96%)	19 (86%)	3 (14%)	3	5
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%)	50 (96%)	2 (4%)	29	49
19	z	52/52 (100%)	50 (96%)	2 (4%)	29	49
20	R	25/29 (86%)	23 (92%)	2 (8%)	11	19
All	All	4500/4403 (102%)	4416 (98%)	84 (2%)	51	71

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	f	15	ILE
14	t	25[A]	GLU
8	i	36	ASP
13	o	23	ASP
16	v	2	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
4	d	83	ASN
15	u	81	HIS
4	d	186	GLN
13	o	124	ASN
16	v	118	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
14	FME	t	1	14	8,9,10	0.79	0	7,9,11	2.10	3 (42%)
14	FME	T	1	14	8,9,10	0.70	0	7,9,11	1.32	1 (14%)
8	FME	i	1	8	8,9,10	0.66	0	7,9,11	1.22	1 (14%)
12	FME	m	1	12	8,9,10	0.61	0	7,9,11	1.37	1 (14%)
8	FME	I	1	8	8,9,10	0.75	0	7,9,11	1.44	2 (28%)
12	FME	M	1	12	8,9,10	0.70	0	7,9,11	1.36	2 (28%)

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

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

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	C-CA-N	3.25	115.61	109.73
14	t	1	FME	CA-N-CN	-2.77	118.57	122.82
8	I	1	FME	CA-N-CN	-2.50	118.97	122.82
14	T	1	FME	O-C-CA	-2.41	118.45	124.78
14	t	1	FME	O-C-CA	-2.37	118.57	124.78

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 267 ligands modelled in this entry, 25 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	$\# Z > 2$
24	CLA	B	606	2	69,73,73	2.07	20 (28%)	83,113,113	2.85	27 (32%)
26	BCR	h	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.33	8 (14%)
28	GOL	T	102	-	5,5,5	0.40	0	5,5,5	0.29	0
24	CLA	B	616	2	69,73,73	2.05	18 (26%)	83,113,113	2.77	28 (33%)
36	DGD	C	518	-	63,63,67	0.90	2 (3%)	77,77,81	0.98	4 (5%)
24	CLA	B	610	2	69,73,73	2.02	19 (27%)	83,113,113	2.79	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	C	506	3	69,73,73	2.02	19 (27%)	83,113,113	2.68	30 (36%)
28	GOL	V	202	-	5,5,5	0.33	0	5,5,5	0.36	0
28	GOL	o	301	-	5,5,5	0.41	0	5,5,5	0.34	0
28	GOL	a	421	34	5,5,5	0.33	0	5,5,5	0.43	0
26	BCR	H	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.56	7 (12%)
26	BCR	b	628	-	41,41,41	1.06	1 (2%)	56,56,56	1.42	10 (17%)
28	GOL	a	402	-	5,5,5	0.38	0	5,5,5	0.33	0
31	PL9	a	416[A]	-	55,55,55	0.63	2 (3%)	68,69,69	1.91	20 (29%)
28	GOL	B	628	-	5,5,5	0.34	0	5,5,5	0.39	0
31	PL9	A	417[A]	-	55,55,55	0.64	2 (3%)	68,69,69	1.77	22 (32%)
24	CLA	a	410	41	69,73,73	2.02	20 (28%)	83,113,113	2.86	31 (37%)
24	CLA	C	505	3	69,73,73	2.03	20 (28%)	83,113,113	2.72	28 (33%)
28	GOL	c	501	-	5,5,5	0.40	0	5,5,5	0.23	0
28	GOL	T	101	-	5,5,5	0.39	0	5,5,5	0.28	0
27	SQD	B	621	-	53,54,54	1.01	3 (5%)	62,65,65	1.41	5 (8%)
24	CLA	c	517	3	69,73,73	2.06	20 (28%)	83,113,113	2.82	30 (36%)
24	CLA	b	622	2	69,73,73	2.06	20 (28%)	83,113,113	2.76	30 (36%)
33	LMG	d	415	39	51,51,55	0.94	2 (3%)	59,59,63	1.12	7 (11%)
23	BCT	A	404[B]	21	2,3,3	0.66	0	2,3,3	1.00	0
26	BCR	d	406	-	41,41,41	1.08	1 (2%)	56,56,56	1.66	15 (26%)
29	LMT	T	104	-	25,25,36	0.55	1 (4%)	30,30,47	1.06	2 (6%)
28	GOL	V	204	-	5,5,5	0.35	0	5,5,5	0.28	0
24	CLA	a	409	1	69,73,73	2.06	20 (28%)	83,113,113	2.84	31 (37%)
24	CLA	b	613	2	69,73,73	2.01	20 (28%)	83,113,113	2.77	27 (32%)
25	PHO	d	402[B]	-	58,69,69	2.76	14 (24%)	56,99,99	2.93	15 (26%)
26	BCR	k	102	-	41,41,41	1.05	1 (2%)	56,56,56	1.52	11 (19%)
30	OEX	A	415[A]	3,41,1	0,14,14	-	-	-	-	-
24	CLA	C	510	3	69,73,73	2.09	20 (28%)	83,113,113	2.71	32 (38%)
24	CLA	C	512	3	69,73,73	2.06	20 (28%)	83,113,113	2.80	29 (34%)
33	LMG	C	520	-	51,51,55	0.95	2 (3%)	59,59,63	1.12	3 (5%)
24	CLA	B	613	2	69,73,73	1.94	17 (24%)	83,113,113	2.83	29 (34%)
33	LMG	D	415	39	51,51,55	0.89	2 (3%)	59,59,63	0.96	3 (5%)
24	CLA	c	507	3	69,73,73	2.05	20 (28%)	83,113,113	2.79	29 (34%)
35	HTG	c	524	-	19,19,19	1.02	2 (10%)	23,24,24	1.50	2 (8%)
24	CLA	b	611	2	69,73,73	2.07	21 (30%)	83,113,113	2.94	32 (38%)
36	DGD	e	101	-	63,63,67	0.95	3 (4%)	77,77,81	1.28	7 (9%)
28	GOL	A	412	-	5,5,5	0.40	0	5,5,5	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	OEX	A	416[B]	3,41,1	0,14,14	-	-	-		
35	HTG	d	413	-	16,16,19	1.23	2 (12%)	20,21,24	1.81	2 (10%)
37	LHG	D	410	-	48,48,48	0.93	2 (4%)	51,54,54	0.73	2 (3%)
28	GOL	v	201	-	5,5,5	0.33	0	5,5,5	0.32	0
38	HEM	E	103	6,5	50,50,50	1.50	5 (10%)	66,82,82	1.85	15 (22%)
26	BCR	c	518	-	41,41,41	1.04	1 (2%)	56,56,56	1.60	11 (19%)
24	CLA	b	610	41	69,73,73	2.10	19 (27%)	83,113,113	2.80	30 (36%)
37	LHG	a	420	-	41,41,48	1.03	2 (4%)	44,47,54	0.93	2 (4%)
25	PHO	D	401[B]	-	58,69,69	2.82	15 (25%)	56,99,99	2.74	14 (25%)
33	LMG	A	419	-	51,51,55	0.92	2 (3%)	59,59,63	1.08	3 (5%)
28	GOL	C	525	-	5,5,5	0.42	0	5,5,5	0.41	0
24	CLA	b	625	2	69,73,73	2.06	19 (27%)	83,113,113	2.78	31 (37%)
24	CLA	C	509	3	69,73,73	2.08	20 (28%)	83,113,113	2.81	31 (37%)
26	BCR	K	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.56	13 (23%)
28	GOL	v	203	-	5,5,5	0.33	0	5,5,5	0.47	0
24	CLA	A	406	41	69,73,73	2.05	21 (30%)	83,113,113	2.96	30 (36%)
35	HTG	C	522	-	19,19,19	1.03	2 (10%)	23,24,24	1.67	1 (4%)
35	HTG	b	602	-	19,19,19	0.95	1 (5%)	23,24,24	1.07	2 (8%)
24	CLA	B	604	2	69,73,73	2.06	20 (28%)	83,113,113	2.80	29 (34%)
24	CLA	b	619	41	69,73,73	2.06	21 (30%)	83,113,113	2.85	32 (38%)
29	LMT	m	103	-	36,36,36	0.51	0	47,47,47	1.06	4 (8%)
37	LHG	d	410	-	48,48,48	0.91	2 (4%)	51,54,54	1.07	3 (5%)
28	GOL	C	524	-	5,5,5	0.36	0	5,5,5	0.75	0
24	CLA	D	404	4	69,73,73	1.96	20 (28%)	83,113,113	2.90	30 (36%)
28	GOL	b	605	-	5,5,5	0.38	0	5,5,5	0.32	0
24	CLA	B	615	2	69,73,73	2.03	19 (27%)	83,113,113	2.90	32 (38%)
31	PL9	d	407[B]	-	55,55,55	0.66	1 (1%)	68,69,69	1.64	17 (25%)
30	OEX	a	418[B]	3,41,1	0,14,14	-	-	-		
26	BCR	B	620	-	41,41,41	1.01	1 (2%)	56,56,56	1.59	12 (21%)
31	PL9	D	407[A]	-	55,55,55	0.66	1 (1%)	68,69,69	1.74	20 (29%)
26	BCR	y	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.57	10 (17%)
24	CLA	d	404	4	69,73,73	2.00	20 (28%)	83,113,113	2.81	30 (36%)
28	GOL	D	402	-	5,5,5	0.42	0	5,5,5	0.29	0
24	CLA	c	508	41	69,73,73	2.01	20 (28%)	83,113,113	2.83	31 (37%)
35	HTG	B	622	-	19,19,19	1.10	1 (5%)	23,24,24	1.35	1 (4%)
38	HEM	f	101	6,5	50,50,50	1.52	6 (12%)	66,82,82	1.72	13 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	b	615	2	69,73,73	2.04	19 (27%)	83,113,113	2.81	29 (34%)
29	LMT	D	403	-	36,36,36	0.43	0	47,47,47	1.00	1 (2%)
27	SQD	F	101	-	42,43,54	1.17	3 (7%)	51,54,65	1.69	11 (21%)
29	LMT	a	404	-	36,36,36	0.47	1 (2%)	47,47,47	1.16	3 (6%)
28	GOL	F	103	34	5,5,5	0.36	0	5,5,5	0.24	0
33	LMG	a	415	-	51,51,55	0.91	2 (3%)	59,59,63	1.18	5 (8%)
37	LHG	E	101	-	41,41,48	1.04	2 (4%)	44,47,54	1.15	4 (9%)
24	CLA	b	624	2	69,73,73	2.05	20 (28%)	83,113,113	2.75	25 (30%)
28	GOL	B	625	-	5,5,5	0.40	0	5,5,5	0.15	0
26	BCR	a	413	-	41,41,41	1.03	1 (2%)	56,56,56	1.48	9 (16%)
27	SQD	L	102	-	53,54,54	1.05	3 (5%)	62,65,65	1.59	12 (19%)
24	CLA	b	621	2	69,73,73	2.04	20 (28%)	83,113,113	2.87	29 (34%)
24	CLA	A	409	1	69,73,73	2.07	20 (28%)	83,113,113	2.77	31 (37%)
24	CLA	A	405	1	69,73,73	2.11	20 (28%)	83,113,113	2.82	30 (36%)
40	HEC	v	206	16	50,50,50	1.70	10 (20%)	68,82,82	1.87	18 (26%)
24	CLA	C	507	41	69,73,73	2.04	19 (27%)	83,113,113	2.72	27 (32%)
26	BCR	c	526	-	41,41,41	1.05	1 (2%)	56,56,56	1.57	9 (16%)
37	LHG	d	408	-	48,48,48	0.90	3 (6%)	51,54,54	1.06	5 (9%)
31	PL9	a	416[B]	-	55,55,55	0.64	2 (3%)	68,69,69	1.84	19 (27%)
24	CLA	b	612	2	69,73,73	2.00	20 (28%)	83,113,113	2.86	30 (36%)
31	PL9	A	417[B]	-	55,55,55	0.64	2 (3%)	68,69,69	1.80	22 (32%)
35	HTG	b	632	-	19,19,19	1.19	2 (10%)	23,24,24	1.68	3 (13%)
24	CLA	a	412	1	69,73,73	2.02	19 (27%)	83,113,113	2.87	31 (37%)
24	CLA	B	607	2	69,73,73	2.03	20 (28%)	83,113,113	2.91	31 (37%)
24	CLA	C	503	3	69,73,73	2.09	20 (28%)	83,113,113	2.87	28 (33%)
36	DGD	H	102	-	63,63,67	0.90	2 (3%)	77,77,81	1.03	5 (6%)
36	DGD	c	519	-	63,63,67	0.83	2 (3%)	77,77,81	1.04	6 (7%)
27	SQD	a	414	-	53,54,54	0.95	3 (5%)	62,65,65	1.57	11 (17%)
24	CLA	B	609	2	69,73,73	2.04	21 (30%)	83,113,113	2.74	29 (34%)
24	CLA	B	614	2	69,73,73	2.06	19 (27%)	83,113,113	2.75	29 (34%)
35	HTG	b	608	-	19,19,19	1.05	2 (10%)	23,24,24	1.11	3 (13%)
26	BCR	Y	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.76	11 (19%)
24	CLA	C	511	3	69,73,73	2.09	20 (28%)	83,113,113	2.79	30 (36%)
24	CLA	c	509	3	69,73,73	2.04	20 (28%)	83,113,113	2.73	28 (33%)
29	LMT	a	419	-	36,36,36	0.43	0	47,47,47	0.78	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	DGD	c	520	-	63,63,67	0.88	3 (4%)	77,77,81	1.03	6 (7%)
26	BCR	T	103	-	41,41,41	1.01	1 (2%)	56,56,56	1.77	14 (25%)
24	CLA	A	407	41	69,73,73	2.02	20 (28%)	83,113,113	2.90	33 (39%)
25	PHO	a	411	-	58,69,69	2.83	15 (25%)	56,99,99	2.69	16 (28%)
28	GOL	b	606	-	5,5,5	0.38	0	5,5,5	0.22	0
24	CLA	c	506	3	69,73,73	2.05	21 (30%)	83,113,113	2.71	25 (30%)
25	PHO	d	402[A]	-	58,69,69	2.77	14 (24%)	56,99,99	2.94	13 (23%)
24	CLA	d	403	41	69,73,73	2.01	20 (28%)	83,113,113	2.89	31 (37%)
26	BCR	A	410	-	41,41,41	1.07	1 (2%)	56,56,56	1.15	3 (5%)
36	DGD	C	516	-	63,63,67	0.86	2 (3%)	77,77,81	1.09	6 (7%)
24	CLA	b	618	2	69,73,73	2.05	19 (27%)	83,113,113	2.83	31 (37%)
29	LMT	b	630	-	25,25,36	0.50	0	30,30,47	0.66	0
28	GOL	b	603	-	5,5,5	0.40	0	5,5,5	0.37	0
27	SQD	a	405	-	53,54,54	1.08	3 (5%)	62,65,65	1.19	4 (6%)
27	SQD	A	413	-	53,54,54	1.02	3 (5%)	62,65,65	1.15	6 (9%)
33	LMG	C	519	-	51,51,55	0.95	2 (3%)	59,59,63	1.02	5 (8%)
24	CLA	C	501	3	69,73,73	2.06	20 (28%)	83,113,113	2.82	29 (34%)
28	GOL	B	626	-	5,5,5	0.33	0	5,5,5	0.37	0
36	DGD	D	408	-	52,52,67	1.03	3 (5%)	60,60,81	1.19	5 (8%)
35	HTG	V	206	-	19,19,19	1.02	2 (10%)	23,24,24	1.44	4 (17%)
24	CLA	C	508	3	69,73,73	2.08	20 (28%)	83,113,113	2.80	32 (38%)
28	GOL	v	202	-	5,5,5	0.36	0	5,5,5	0.32	0
35	HTG	D	414	-	16,16,19	1.07	2 (12%)	20,21,24	1.32	1 (5%)
35	HTG	B	624	-	19,19,19	1.05	2 (10%)	23,24,24	2.06	4 (17%)
24	CLA	b	617	2	69,73,73	2.06	20 (28%)	83,113,113	2.76	32 (38%)
24	CLA	b	620	2	69,73,73	1.95	19 (27%)	83,113,113	2.70	31 (37%)
28	GOL	t	103	-	5,5,5	0.41	0	5,5,5	0.23	0
24	CLA	c	511	41	69,73,73	2.02	20 (28%)	83,113,113	2.80	29 (34%)
25	PHO	D	401[A]	-	58,69,69	2.80	15 (25%)	56,99,99	2.79	13 (23%)
23	BCT	d	401[A]	21	2,3,3	0.65	0	2,3,3	0.80	0
24	CLA	B	603	2	69,73,73	2.06	20 (28%)	83,113,113	2.86	31 (37%)
27	SQD	f	102	-	42,43,54	1.19	3 (7%)	51,54,65	1.45	7 (13%)
29	LMT	m	102	-	36,36,36	0.46	0	47,47,47	0.87	0
35	HTG	b	607	-	19,19,19	1.00	1 (5%)	23,24,24	1.39	4 (17%)
28	GOL	v	204	-	5,5,5	0.37	0	5,5,5	0.24	0
28	GOL	a	401	-	5,5,5	0.39	0	5,5,5	0.24	0
37	LHG	D	411	-	48,48,48	0.99	2 (4%)	51,54,54	1.12	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PL9	D	407[B]	-	55,55,55	0.63	1 (1%)	68,69,69	1.81	22 (32%)
24	CLA	B	612	2	69,73,73	2.00	20 (28%)	83,113,113	2.81	32 (38%)
24	CLA	c	516	3	69,73,73	2.08	20 (28%)	83,113,113	2.91	31 (37%)
29	LMT	M	102	-	36,36,36	0.42	0	47,47,47	0.87	1 (2%)
26	BCR	D	406	-	41,41,41	1.05	1 (2%)	56,56,56	1.76	13 (23%)
24	CLA	C	502	3	69,73,73	2.06	20 (28%)	83,113,113	2.76	29 (34%)
24	CLA	c	510	3	69,73,73	2.05	19 (27%)	83,113,113	2.74	28 (33%)
28	GOL	B	627	-	5,5,5	0.36	0	5,5,5	0.51	0
28	GOL	V	201	-	5,5,5	0.37	0	5,5,5	0.31	0
35	HTG	B	623	-	19,19,19	0.85	1 (5%)	23,24,24	1.48	1 (4%)
26	BCR	B	618	-	41,41,41	1.05	1 (2%)	56,56,56	1.37	8 (14%)
36	DGD	c	521	-	63,63,67	0.86	2 (3%)	77,77,81	1.02	3 (3%)
26	BCR	C	514	-	41,41,41	1.06	1 (2%)	56,56,56	1.42	8 (14%)
28	GOL	B	634	-	5,5,5	0.45	0	5,5,5	0.45	0
24	CLA	B	608	41	69,73,73	2.07	20 (28%)	83,113,113	2.74	29 (34%)
24	CLA	B	605	2	69,73,73	1.96	20 (28%)	83,113,113	2.78	30 (36%)
29	LMT	C	521	-	36,36,36	0.49	0	47,47,47	1.11	3 (6%)
24	CLA	c	512	3	69,73,73	2.03	20 (28%)	83,113,113	2.74	29 (34%)
28	GOL	b	601	-	5,5,5	0.38	0	5,5,5	0.44	0
36	DGD	h	102	-	63,63,67	0.90	3 (4%)	77,77,81	0.96	3 (3%)
26	BCR	b	626	-	41,41,41	1.01	1 (2%)	56,56,56	1.59	11 (19%)
35	HTG	B	631	-	19,19,19	1.03	2 (10%)	23,24,24	1.36	2 (8%)
33	LMG	M	101	-	51,51,55	0.93	2 (3%)	59,59,63	0.97	3 (5%)
29	LMT	t	101	-	25,25,36	0.52	0	30,30,47	0.76	1 (3%)
23	BCT	A	404[A]	21	2,3,3	0.59	0	2,3,3	1.28	0
24	CLA	b	616	41	69,73,73	2.04	18 (26%)	83,113,113	2.76	29 (34%)
28	GOL	V	203	-	5,5,5	0.42	0	5,5,5	0.24	0
29	LMT	A	414	-	36,36,36	0.57	1 (2%)	47,47,47	1.27	4 (8%)
24	CLA	c	514	3	69,73,73	2.07	20 (28%)	83,113,113	2.77	30 (36%)
33	LMG	Z	101	-	37,37,55	0.98	3 (8%)	45,45,63	1.36	7 (15%)
24	CLA	C	513	3	69,73,73	2.06	21 (30%)	83,113,113	2.78	29 (34%)
28	GOL	c	502	-	5,5,5	0.39	0	5,5,5	0.37	0
35	HTG	C	523	-	19,19,19	0.97	1 (5%)	23,24,24	1.74	4 (17%)
37	LHG	b	634	-	48,48,48	0.93	2 (4%)	51,54,54	0.96	2 (3%)
24	CLA	c	515	3	69,73,73	2.00	20 (28%)	83,113,113	2.82	29 (34%)
33	LMG	c	522	-	51,51,55	0.95	2 (3%)	59,59,63	1.17	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	C	515	-	41,41,41	1.04	1 (2%)	56,56,56	1.53	10 (17%)
37	LHG	L	101	-	48,48,48	0.92	2 (4%)	51,54,54	1.10	5 (9%)
37	LHG	d	409	-	48,48,48	0.88	2 (4%)	51,54,54	1.01	5 (9%)
24	CLA	B	602	41	69,73,73	2.11	22 (31%)	83,113,113	2.81	29 (34%)
33	LMG	b	629	-	51,51,55	0.91	3 (5%)	59,59,63	1.07	5 (8%)
29	LMT	M	104	-	36,36,36	0.54	1 (2%)	47,47,47	1.14	5 (10%)
24	CLA	B	611	41	69,73,73	2.13	20 (28%)	83,113,113	2.90	34 (40%)
28	GOL	B	630	-	5,5,5	0.37	0	5,5,5	0.28	0
24	CLA	b	623	2	69,73,73	2.02	20 (28%)	83,113,113	2.86	30 (36%)
27	SQD	A	411	-	53,54,54	0.98	3 (5%)	62,65,65	1.53	11 (17%)
29	LMT	E	102	-	36,36,36	0.49	0	47,47,47	0.94	1 (2%)
24	CLA	b	614	2	69,73,73	2.01	21 (30%)	83,113,113	2.91	30 (36%)
33	LMG	k	101	-	51,51,55	0.89	2 (3%)	59,59,63	1.08	5 (8%)
24	CLA	d	405	4	69,73,73	2.04	19 (27%)	83,113,113	2.81	30 (36%)
28	GOL	b	604	-	5,5,5	0.33	0	5,5,5	0.26	0
24	CLA	c	513	3	69,73,73	2.09	20 (28%)	83,113,113	2.75	30 (36%)
35	HTG	b	631	-	19,19,19	0.80	1 (5%)	23,24,24	1.35	1 (4%)
25	PHO	A	408	-	58,69,69	2.75	13 (22%)	56,99,99	2.87	18 (32%)
26	BCR	B	619	-	41,41,41	1.01	1 (2%)	56,56,56	1.37	9 (16%)
24	CLA	D	405	4	69,73,73	2.03	20 (28%)	83,113,113	2.82	31 (37%)
24	CLA	B	617	2	69,73,73	2.04	19 (27%)	83,113,113	2.77	28 (33%)
24	CLA	C	504	41	69,73,73	2.07	20 (28%)	83,113,113	2.88	27 (32%)
26	BCR	b	627	-	41,41,41	1.00	1 (2%)	56,56,56	1.40	7 (12%)
40	HEC	V	205	16	50,50,50	1.73	11 (22%)	68,82,82	1.81	20 (29%)
29	LMT	e	102	-	36,36,36	0.49	0	47,47,47	0.84	1 (2%)
35	HTG	c	523	-	19,19,19	0.99	2 (10%)	23,24,24	1.46	2 (8%)
28	GOL	O	301	-	5,5,5	0.36	0	5,5,5	0.36	0
35	HTG	B	632	-	19,19,19	1.05	2 (10%)	23,24,24	1.43	2 (8%)
37	LHG	D	409	-	48,48,48	0.86	2 (4%)	51,54,54	1.00	3 (5%)
26	BCR	t	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.70	15 (26%)
36	DGD	C	517	-	63,63,67	0.88	2 (3%)	77,77,81	1.05	9 (11%)
24	CLA	c	505	3	69,73,73	2.03	20 (28%)	83,113,113	2.78	29 (34%)
31	PL9	d	407[A]	-	55,55,55	0.69	2 (3%)	68,69,69	1.54	15 (22%)
30	OEX	a	417[A]	3,41,1	0,14,14	-	-	-	-	-
33	LMG	z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.13	4 (8%)
23	BCT	d	401[B]	21	2,3,3	0.66	0	2,3,3	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	GOL	B	629	-	5,5,5	0.44	0	5,5,5	0.30	0

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
24	CLA	B	606	2	-	7/39/115/115	-
26	BCR	h	101	-	-	1/29/63/63	0/2/2/2
28	GOL	T	102	-	-	2/4/4/4	-
24	CLA	B	616	2	-	9/39/115/115	-
36	DGD	C	518	-	-	12/51/91/95	0/2/2/2
24	CLA	B	610	2	-	6/39/115/115	-
24	CLA	C	506	3	-	12/39/115/115	-
28	GOL	V	202	-	-	2/4/4/4	-
28	GOL	o	301	-	-	2/4/4/4	-
28	GOL	a	421	34	-	2/4/4/4	-
26	BCR	H	101	-	-	6/29/63/63	0/2/2/2
26	BCR	b	628	-	-	2/29/63/63	0/2/2/2
28	GOL	a	402	-	-	2/4/4/4	-
31	PL9	a	416[A]	-	-	18/53/73/73	0/1/1/1
28	GOL	B	628	-	-	2/4/4/4	-
31	PL9	A	417[A]	-	-	14/53/73/73	0/1/1/1
24	CLA	a	410	41	-	10/39/115/115	-
24	CLA	C	505	3	-	8/39/115/115	-
28	GOL	c	501	-	-	0/4/4/4	-
28	GOL	T	101	-	-	0/4/4/4	-
27	SQD	B	621	-	-	20/49/69/69	0/1/1/1
24	CLA	c	517	3	-	5/39/115/115	-
24	CLA	b	622	2	-	11/39/115/115	-
33	LMG	d	415	39	-	10/46/66/70	0/1/1/1
26	BCR	d	406	-	-	4/29/63/63	0/2/2/2
29	LMT	T	104	-	-	9/17/37/61	0/1/1/2
28	GOL	V	204	-	-	4/4/4/4	-
24	CLA	a	409	1	-	6/39/115/115	-
24	CLA	b	613	2	-	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PHO	d	402[B]	-	-	2/37/103/103	0/5/6/6
26	BCR	k	102	-	-	1/29/63/63	0/2/2/2
24	CLA	C	510	3	-	11/39/115/115	-
24	CLA	C	512	3	-	8/39/115/115	-
33	LMG	C	520	-	-	13/46/66/70	0/1/1/1
24	CLA	B	613	2	-	3/39/115/115	-
33	LMG	D	415	39	-	8/46/66/70	0/1/1/1
24	CLA	c	507	3	-	6/39/115/115	-
35	HTG	c	524	-	-	2/10/30/30	0/1/1/1
24	CLA	b	611	2	-	6/39/115/115	-
36	DGD	e	101	-	-	26/51/91/95	0/2/2/2
28	GOL	A	412	-	-	1/4/4/4	-
37	LHG	D	410	-	-	6/53/53/53	-
35	HTG	d	413	-	-	1/7/27/30	0/1/1/1
28	GOL	v	201	-	-	1/4/4/4	-
38	HEM	E	103	6,5	-	6/14/54/54	-
26	BCR	c	518	-	-	4/29/63/63	0/2/2/2
24	CLA	b	610	41	-	15/39/115/115	-
37	LHG	a	420	-	-	18/46/46/53	-
25	PHO	D	401[B]	-	-	0/37/103/103	0/5/6/6
33	LMG	A	419	-	-	19/46/66/70	0/1/1/1
28	GOL	C	525	-	-	2/4/4/4	-
24	CLA	b	625	2	-	13/39/115/115	-
24	CLA	C	509	3	-	14/39/115/115	-
26	BCR	K	101	-	-	2/29/63/63	0/2/2/2
28	GOL	v	203	-	-	2/4/4/4	-
24	CLA	A	406	41	-	5/39/115/115	-
35	HTG	C	522	-	-	1/10/30/30	0/1/1/1
35	HTG	b	602	-	-	3/10/30/30	0/1/1/1
24	CLA	B	604	2	-	7/39/115/115	-
24	CLA	b	619	41	-	7/39/115/115	-
29	LMT	m	103	-	-	8/21/61/61	0/2/2/2
37	LHG	d	410	-	-	16/53/53/53	-
28	GOL	C	524	-	-	1/4/4/4	-
24	CLA	D	404	4	-	2/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	b	605	-	-	2/4/4/4	-
24	CLA	B	615	2	-	19/39/115/115	-
31	PL9	d	407[B]	-	-	8/53/73/73	0/1/1/1
38	HEM	f	101	6,5	-	10/14/54/54	-
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
31	PL9	D	407[A]	-	-	7/53/73/73	0/1/1/1
26	BCR	y	101	-	-	2/29/63/63	0/2/2/2
24	CLA	d	404	4	-	5/39/115/115	-
28	GOL	D	402	-	-	4/4/4/4	-
24	CLA	c	508	41	-	11/39/115/115	-
35	HTG	B	622	-	-	2/10/30/30	0/1/1/1
24	CLA	b	615	2	-	13/39/115/115	-
29	LMT	D	403	-	-	10/21/61/61	0/2/2/2
27	SQD	F	101	-	-	14/38/58/69	0/1/1/1
29	LMT	a	404	-	-	7/21/61/61	0/2/2/2
28	GOL	F	103	34	-	1/4/4/4	-
33	LMG	a	415	-	-	17/46/66/70	0/1/1/1
37	LHG	E	101	-	-	23/46/46/53	-
24	CLA	b	624	2	-	5/39/115/115	-
28	GOL	B	625	-	-	0/4/4/4	-
26	BCR	a	413	-	-	0/29/63/63	0/2/2/2
27	SQD	L	102	-	-	20/49/69/69	0/1/1/1
24	CLA	b	621	2	-	1/39/115/115	-
24	CLA	A	409	1	-	12/39/115/115	-
24	CLA	A	405	1	-	4/39/115/115	-
40	HEC	v	206	16	1/1/3/7	2/14/54/54	-
24	CLA	C	507	41	-	6/39/115/115	-
26	BCR	c	526	-	-	1/29/63/63	0/2/2/2
37	LHG	d	408	-	-	13/53/53/53	-
31	PL9	a	416[B]	-	-	15/53/73/73	0/1/1/1
24	CLA	b	612	2	-	10/39/115/115	-
31	PL9	A	417[B]	-	-	10/53/73/73	0/1/1/1
35	HTG	b	632	-	-	4/10/30/30	0/1/1/1
24	CLA	a	412	1	-	12/39/115/115	-
24	CLA	B	607	2	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	503	3	-	4/39/115/115	-
36	DGD	H	102	-	-	10/51/91/95	0/2/2/2
36	DGD	c	519	-	-	15/51/91/95	0/2/2/2
27	SQD	a	414	-	-	15/49/69/69	0/1/1/1
24	CLA	B	609	2	-	0/39/115/115	-
24	CLA	B	614	2	-	8/39/115/115	-
35	HTG	b	608	-	-	0/10/30/30	0/1/1/1
26	BCR	Y	101	-	-	6/29/63/63	0/2/2/2
24	CLA	C	511	3	-	2/39/115/115	-
24	CLA	c	509	3	-	3/39/115/115	-
29	LMT	a	419	-	-	4/21/61/61	0/2/2/2
36	DGD	c	520	-	-	18/51/91/95	0/2/2/2
26	BCR	T	103	-	-	2/29/63/63	0/2/2/2
24	CLA	A	407	41	-	7/39/115/115	-
25	PHO	a	411	-	-	5/37/103/103	0/5/6/6
28	GOL	b	606	-	-	2/4/4/4	-
24	CLA	c	506	3	-	6/39/115/115	-
25	PHO	d	402[A]	-	-	0/37/103/103	0/5/6/6
24	CLA	d	403	41	-	8/39/115/115	-
26	BCR	A	410	-	-	0/29/63/63	0/2/2/2
36	DGD	C	516	-	-	14/51/91/95	0/2/2/2
24	CLA	b	618	2	-	3/39/115/115	-
29	LMT	b	630	-	-	4/17/37/61	0/1/1/2
28	GOL	b	603	-	-	0/4/4/4	-
27	SQD	a	405	-	-	12/49/69/69	0/1/1/1
27	SQD	A	413	-	-	17/49/69/69	0/1/1/1
33	LMG	C	519	-	-	8/46/66/70	0/1/1/1
24	CLA	C	501	3	-	12/39/115/115	-
28	GOL	B	626	-	-	2/4/4/4	-
36	DGD	D	408	-	-	21/47/67/95	0/1/1/2
35	HTG	V	206	-	-	4/10/30/30	0/1/1/1
24	CLA	C	508	3	-	7/39/115/115	-
28	GOL	v	202	-	-	2/4/4/4	-
35	HTG	D	414	-	-	0/7/27/30	0/1/1/1
35	HTG	B	624	-	-	4/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	617	2	-	2/39/115/115	-
24	CLA	b	620	2	-	7/39/115/115	-
28	GOL	t	103	-	-	0/4/4/4	-
24	CLA	c	511	41	-	4/39/115/115	-
25	PHO	D	401[A]	-	-	0/37/103/103	0/5/6/6
24	CLA	B	603	2	-	3/39/115/115	-
27	SQD	f	102	-	-	15/38/58/69	0/1/1/1
29	LMT	m	102	-	-	10/21/61/61	0/2/2/2
35	HTG	b	607	-	-	3/10/30/30	0/1/1/1
28	GOL	v	204	-	-	2/4/4/4	-
28	GOL	a	401	-	-	2/4/4/4	-
37	LHG	D	411	-	-	12/53/53/53	-
31	PL9	D	407[B]	-	-	9/53/73/73	0/1/1/1
24	CLA	B	612	2	-	1/39/115/115	-
24	CLA	c	516	3	-	10/39/115/115	-
29	LMT	M	102	-	-	10/21/61/61	0/2/2/2
26	BCR	D	406	-	-	6/29/63/63	0/2/2/2
24	CLA	C	502	3	-	7/39/115/115	-
24	CLA	c	510	3	-	13/39/115/115	-
28	GOL	B	627	-	-	2/4/4/4	-
28	GOL	V	201	-	-	2/4/4/4	-
35	HTG	B	623	-	-	6/10/30/30	0/1/1/1
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
36	DGD	c	521	-	-	14/51/91/95	0/2/2/2
26	BCR	C	514	-	-	1/29/63/63	0/2/2/2
28	GOL	B	634	-	-	0/4/4/4	-
24	CLA	B	608	41	-	7/39/115/115	-
24	CLA	B	605	2	-	5/39/115/115	-
29	LMT	C	521	-	-	9/21/61/61	0/2/2/2
24	CLA	c	512	3	-	4/39/115/115	-
28	GOL	b	601	-	-	0/4/4/4	-
36	DGD	h	102	-	-	10/51/91/95	0/2/2/2
26	BCR	b	626	-	-	3/29/63/63	0/2/2/2
35	HTG	B	631	-	-	1/10/30/30	0/1/1/1
33	LMG	M	101	-	-	12/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMT	t	101	-	-	7/17/37/61	0/1/1/2
24	CLA	b	616	41	-	3/39/115/115	-
28	GOL	V	203	-	-	0/4/4/4	-
29	LMT	A	414	-	-	6/21/61/61	0/2/2/2
24	CLA	c	514	3	-	8/39/115/115	-
33	LMG	Z	101	-	-	14/31/51/70	0/1/1/1
24	CLA	C	513	3	-	7/39/115/115	-
28	GOL	c	502	-	-	2/4/4/4	-
35	HTG	C	523	-	-	3/10/30/30	0/1/1/1
37	LHG	b	634	-	-	15/53/53/53	-
24	CLA	c	515	3	-	6/39/115/115	-
33	LMG	c	522	-	-	7/46/66/70	0/1/1/1
26	BCR	C	515	-	-	6/29/63/63	0/2/2/2
37	LHG	L	101	-	-	13/53/53/53	-
37	LHG	d	409	-	-	10/53/53/53	-
24	CLA	B	602	41	-	15/39/115/115	-
33	LMG	b	629	-	-	11/46/66/70	0/1/1/1
29	LMT	M	104	-	-	10/21/61/61	0/2/2/2
24	CLA	B	611	41	-	4/39/115/115	-
28	GOL	B	630	-	-	0/4/4/4	-
24	CLA	b	623	2	-	21/39/115/115	-
27	SQD	A	411	-	-	12/49/69/69	0/1/1/1
29	LMT	E	102	-	-	4/21/61/61	0/2/2/2
24	CLA	b	614	2	-	7/39/115/115	-
33	LMG	k	101	-	-	14/46/66/70	0/1/1/1
24	CLA	d	405	4	-	8/39/115/115	-
28	GOL	b	604	-	-	2/4/4/4	-
24	CLA	c	513	3	-	15/39/115/115	-
35	HTG	b	631	-	-	2/10/30/30	0/1/1/1
25	PHO	A	408	-	-	3/37/103/103	0/5/6/6
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
24	CLA	D	405	4	-	6/39/115/115	-
24	CLA	B	617	2	-	8/39/115/115	-
24	CLA	C	504	41	-	8/39/115/115	-
26	BCR	b	627	-	-	1/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	HEC	V	205	16	1/1/3/7	6/14/54/54	-
29	LMT	e	102	-	-	10/21/61/61	0/2/2/2
35	HTG	c	523	-	-	3/10/30/30	0/1/1/1
28	GOL	O	301	-	-	3/4/4/4	-
35	HTG	B	632	-	-	0/10/30/30	0/1/1/1
37	LHG	D	409	-	-	14/53/53/53	-
26	BCR	t	102	-	-	7/29/63/63	0/2/2/2
36	DGD	C	517	-	-	20/51/91/95	0/2/2/2
24	CLA	c	505	3	-	5/39/115/115	-
31	PL9	d	407[A]	-	-	5/53/73/73	0/1/1/1
33	LMG	z	101	-	-	12/34/54/70	0/1/1/1
28	GOL	B	629	-	-	4/4/4/4	-

The worst 5 of 1668 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	411	PHO	C1B-C2B	9.30	1.49	1.39
25	D	401[B]	PHO	C1B-C2B	9.27	1.49	1.39
25	d	402[A]	PHO	C1B-C2B	9.22	1.49	1.39
25	d	402[B]	PHO	C1B-C2B	9.08	1.49	1.39
25	D	401[A]	PHO	C1D-C2D	8.96	1.49	1.39

The worst 5 of 2897 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	402[B]	PHO	C2D-C1D-ND	12.09	117.87	109.53
25	D	401[B]	PHO	C2D-C1D-ND	11.73	117.63	109.53
25	D	401[A]	PHO	C2D-C1D-ND	11.51	117.47	109.53
25	d	402[A]	PHO	C2D-C1D-ND	11.34	117.36	109.53
25	A	408	PHO	C2D-C1D-ND	11.33	117.35	109.53

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
40	V	205	HEC	NA
40	v	206	HEC	NA

5 of 1474 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	607	CLA	C2B-C3B-CAB-CBB
24	B	607	CLA	C4B-C3B-CAB-CBB
24	B	607	CLA	CHA-CBD-CGD-O1D
24	B	607	CLA	CHA-CBD-CGD-O2D
24	B	615	CLA	CAD-CBD-CGD-O1D

There are no ring outliers.

174 monomers are involved in 417 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	606	CLA	6	0
26	h	101	BCR	5	0
28	T	102	GOL	3	0
24	B	616	CLA	4	0
36	C	518	DGD	1	0
24	B	610	CLA	4	0
24	C	506	CLA	6	0
28	a	421	GOL	1	0
26	H	101	BCR	5	0
26	b	628	BCR	3	0
28	a	402	GOL	1	0
31	a	416[A]	PL9	8	0
31	A	417[A]	PL9	5	0
24	a	410	CLA	4	0
24	C	505	CLA	5	0
28	T	101	GOL	1	0
27	B	621	SQD	1	0
24	c	517	CLA	6	0
24	b	622	CLA	7	0
33	d	415	LMG	4	0
26	d	406	BCR	1	0
29	T	104	LMT	1	0
24	a	409	CLA	6	0
24	b	613	CLA	5	0
25	d	402[B]	PHO	3	0
26	k	102	BCR	1	0
24	C	510	CLA	6	0
24	C	512	CLA	4	0
33	C	520	LMG	2	0
24	B	613	CLA	4	0
33	D	415	LMG	1	0
24	c	507	CLA	4	0
24	b	611	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	e	101	DGD	7	0
35	d	413	HTG	3	0
37	D	410	LHG	2	0
28	v	201	GOL	1	0
38	E	103	HEM	2	0
26	c	518	BCR	2	0
24	b	610	CLA	2	0
37	a	420	LHG	4	0
25	D	401[B]	PHO	1	0
33	A	419	LMG	3	0
24	b	625	CLA	4	0
24	C	509	CLA	5	0
26	K	101	BCR	3	0
24	A	406	CLA	1	0
35	C	522	HTG	1	0
35	b	602	HTG	2	0
24	B	604	CLA	1	0
24	b	619	CLA	1	0
29	m	103	LMT	2	0
37	d	410	LHG	8	0
28	C	524	GOL	2	0
24	D	404	CLA	3	0
24	B	615	CLA	8	0
30	a	418[B]	OEX	1	0
26	B	620	BCR	4	0
26	y	101	BCR	2	0
24	d	404	CLA	4	0
28	D	402	GOL	2	0
24	c	508	CLA	1	0
38	f	101	HEM	4	0
29	D	403	LMT	1	0
29	a	404	LMT	1	0
33	a	415	LMG	5	0
37	E	101	LHG	2	0
24	b	624	CLA	6	0
26	a	413	BCR	1	0
27	L	102	SQD	2	0
24	b	621	CLA	1	0
24	A	409	CLA	2	0
24	A	405	CLA	4	0
24	C	507	CLA	4	0
26	c	526	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	d	408	LHG	5	0
31	a	416[B]	PL9	11	0
24	b	612	CLA	3	0
31	A	417[B]	PL9	3	0
35	b	632	HTG	1	0
24	a	412	CLA	2	0
24	B	607	CLA	7	0
24	C	503	CLA	4	0
36	H	102	DGD	2	0
36	c	519	DGD	3	0
27	a	414	SQD	2	0
24	B	609	CLA	1	0
24	B	614	CLA	4	0
35	b	608	HTG	1	0
26	Y	101	BCR	6	0
24	C	511	CLA	2	0
24	c	509	CLA	5	0
36	c	520	DGD	3	0
26	T	103	BCR	6	0
24	A	407	CLA	5	0
25	a	411	PHO	2	0
24	c	506	CLA	3	0
25	d	402[A]	PHO	2	0
24	d	403	CLA	4	0
26	A	410	BCR	1	0
36	C	516	DGD	2	0
24	b	618	CLA	4	0
28	b	603	GOL	1	0
27	a	405	SQD	2	0
27	A	413	SQD	1	0
33	C	519	LMG	2	0
24	C	501	CLA	3	0
36	D	408	DGD	2	0
35	V	206	HTG	1	0
24	C	508	CLA	4	0
28	v	202	GOL	1	0
35	D	414	HTG	2	0
35	B	624	HTG	1	0
24	b	617	CLA	1	0
24	b	620	CLA	2	0
24	c	511	CLA	3	0
25	D	401[A]	PHO	2	0

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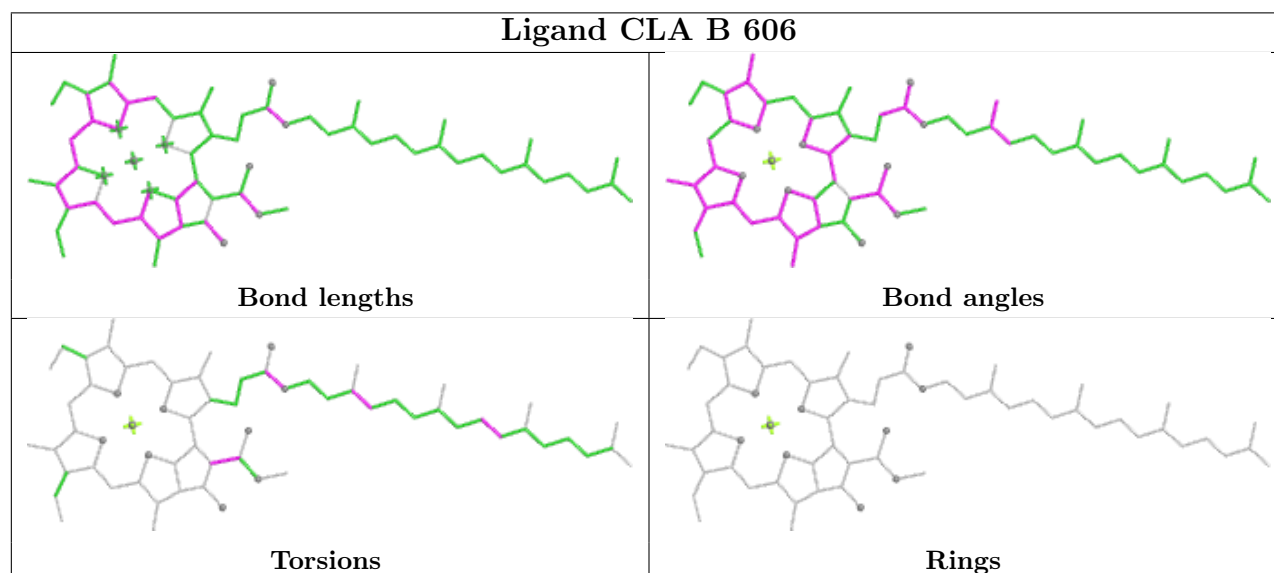
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24	B	603	CLA	2	0
27	f	102	SQD	3	0
29	m	102	LMT	1	0
35	b	607	HTG	1	0
28	a	401	GOL	1	0
37	D	411	LHG	7	0
31	D	407[B]	PL9	3	0
24	c	516	CLA	4	0
29	M	102	LMT	3	0
26	D	406	BCR	2	0
24	C	502	CLA	3	0
24	c	510	CLA	2	0
26	B	618	BCR	2	0
36	c	521	DGD	3	0
26	C	514	BCR	1	0
24	B	608	CLA	3	0
24	B	605	CLA	3	0
29	C	521	LMT	2	0
24	c	512	CLA	10	0
36	h	102	DGD	1	0
26	b	626	BCR	2	0
33	M	101	LMG	3	0
29	A	414	LMT	3	0
24	c	514	CLA	4	0
33	Z	101	LMG	2	0
24	C	513	CLA	5	0
28	c	502	GOL	1	0
37	b	634	LHG	4	0
24	c	515	CLA	2	0
33	c	522	LMG	5	0
26	C	515	BCR	2	0
37	L	101	LHG	2	0
37	d	409	LHG	1	0
24	B	602	CLA	2	0
33	b	629	LMG	3	0
24	B	611	CLA	3	0
24	b	623	CLA	3	0
27	A	411	SQD	3	0
29	E	102	LMT	1	0
24	b	614	CLA	5	0
33	k	101	LMG	2	0
24	d	405	CLA	4	0

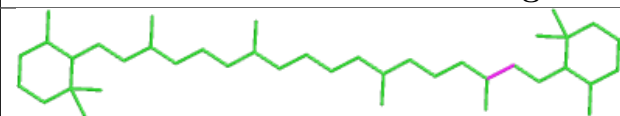
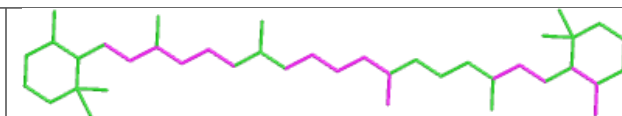
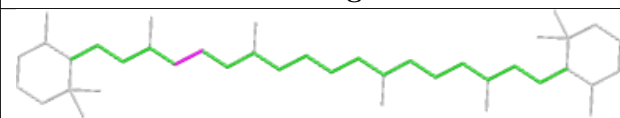
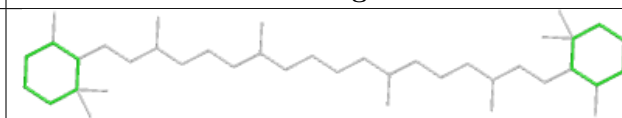
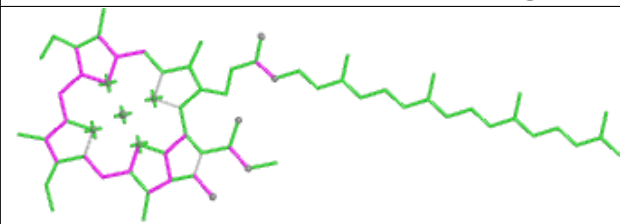
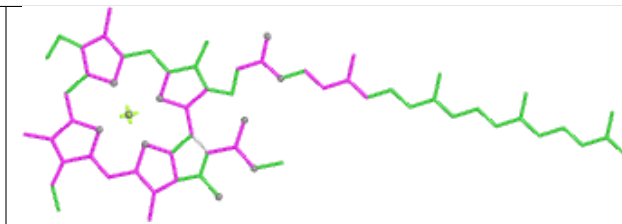
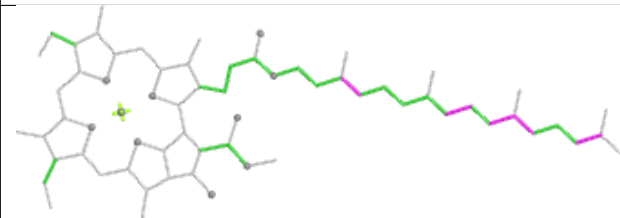
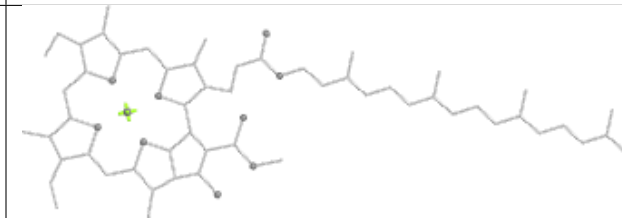
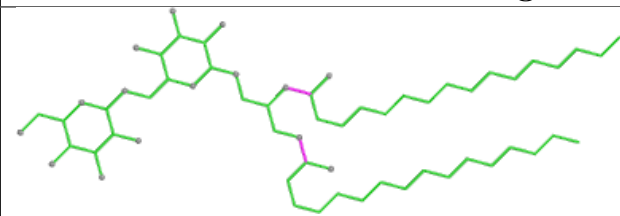
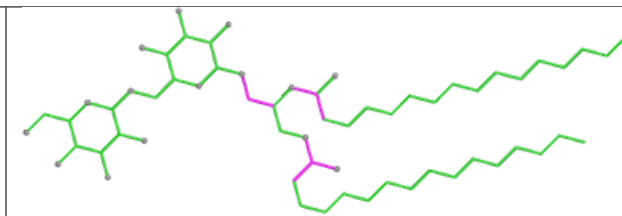
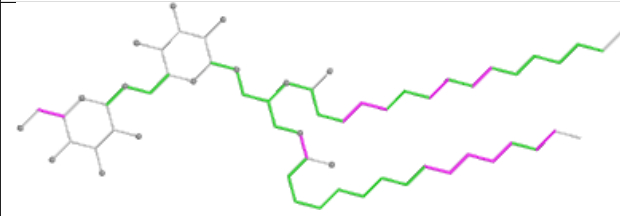
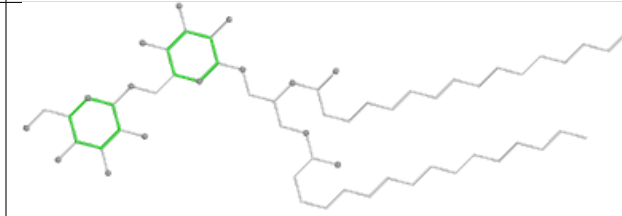
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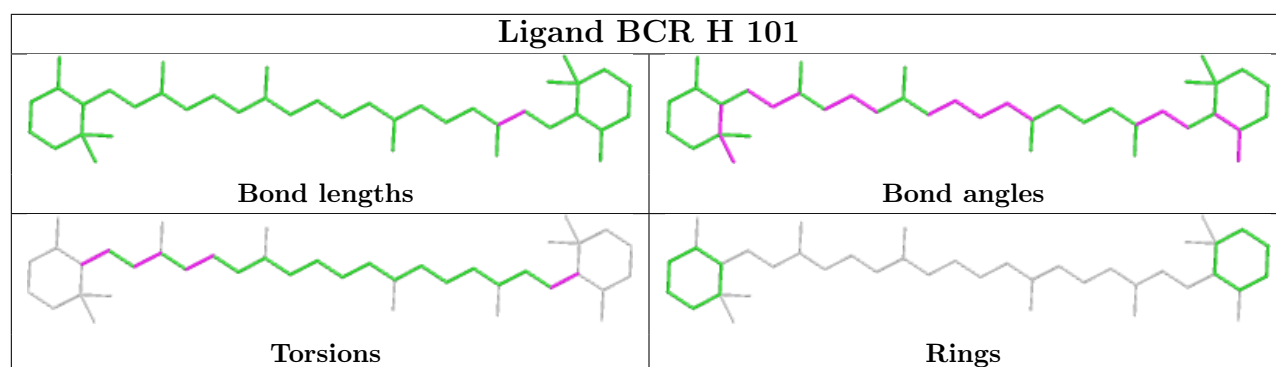
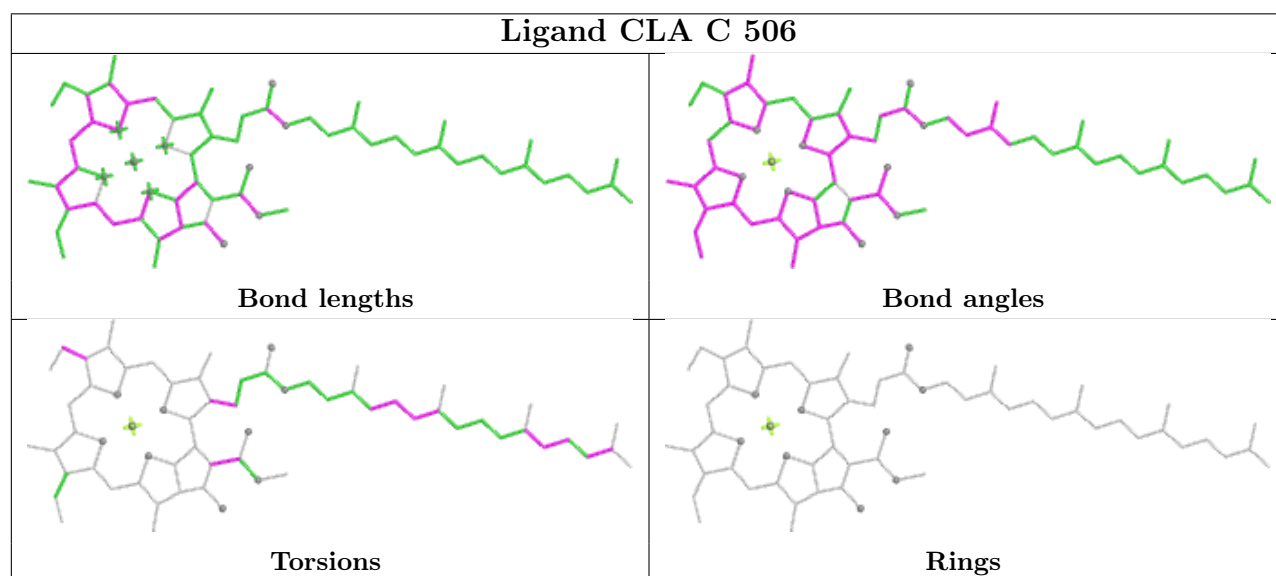
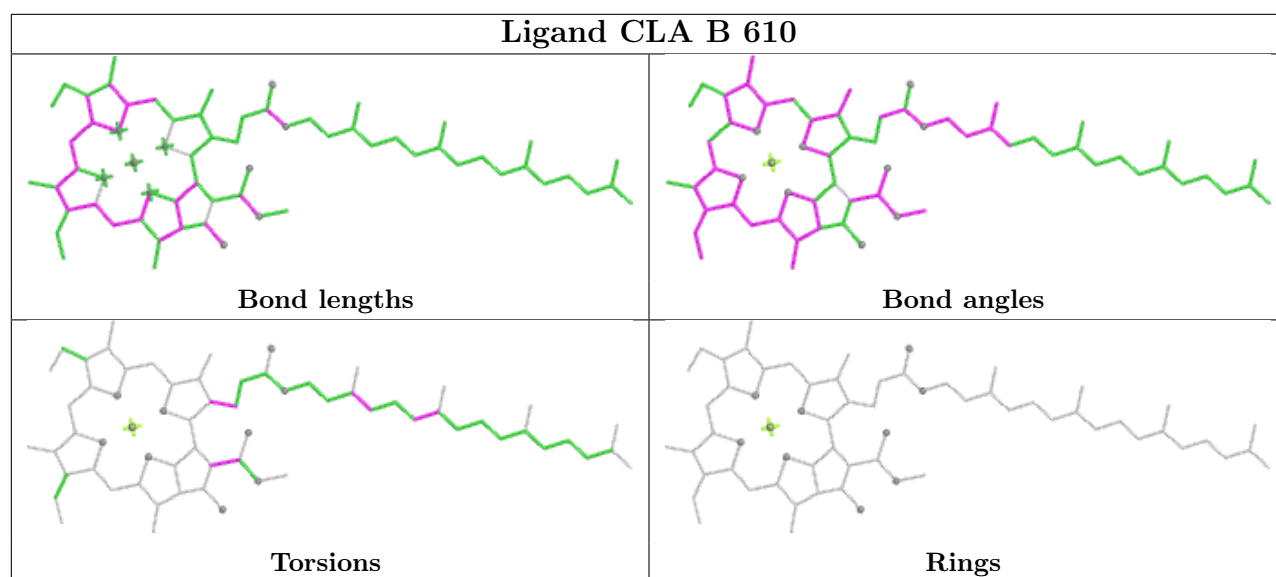
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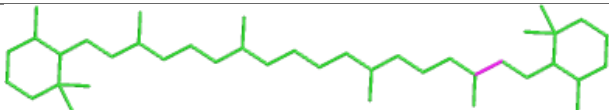
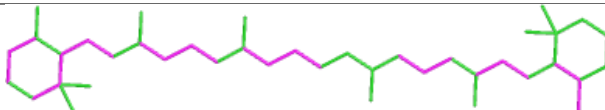
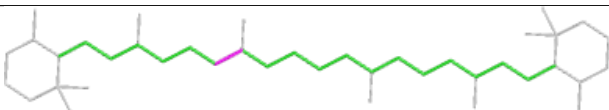
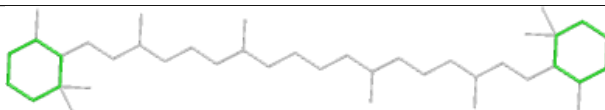
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	c	513	CLA	1	0
35	b	631	HTG	1	0
25	A	408	PHO	1	0
26	B	619	BCR	5	0
24	D	405	CLA	1	0
24	B	617	CLA	6	0
26	b	627	BCR	1	0
29	e	102	LMT	1	0
35	c	523	HTG	1	0
37	D	409	LHG	3	0
26	t	102	BCR	6	0
36	C	517	DGD	3	0
24	c	505	CLA	5	0
33	z	101	LMG	6	0
28	B	629	GOL	2	0

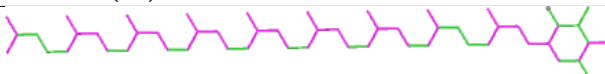
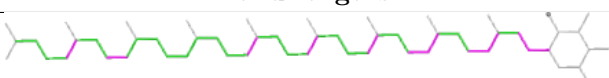
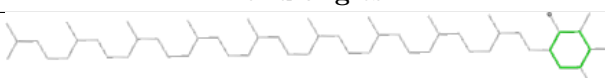
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

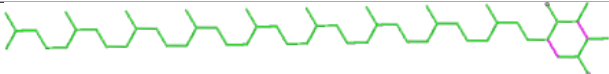
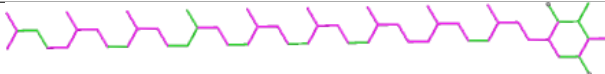
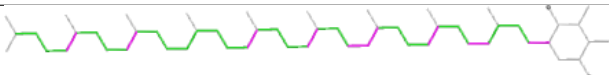


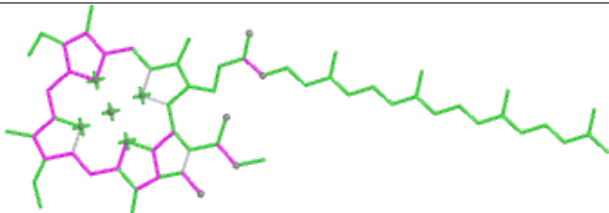
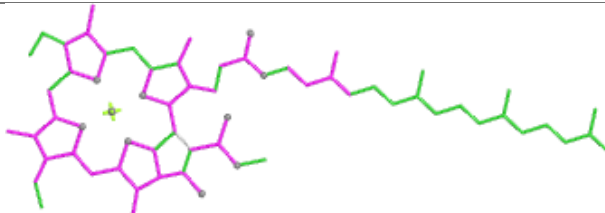
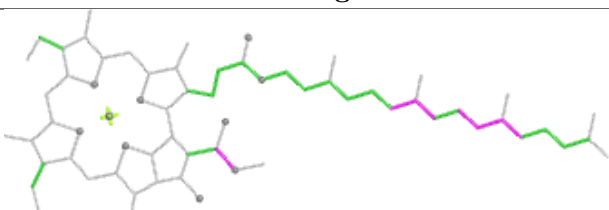
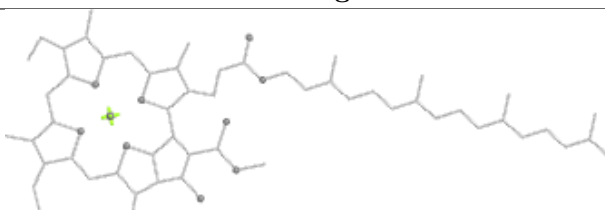
Ligand BCR h 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 616	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand DGD C 518	
 Bond lengths	 Bond angles
 Torsions	 Rings

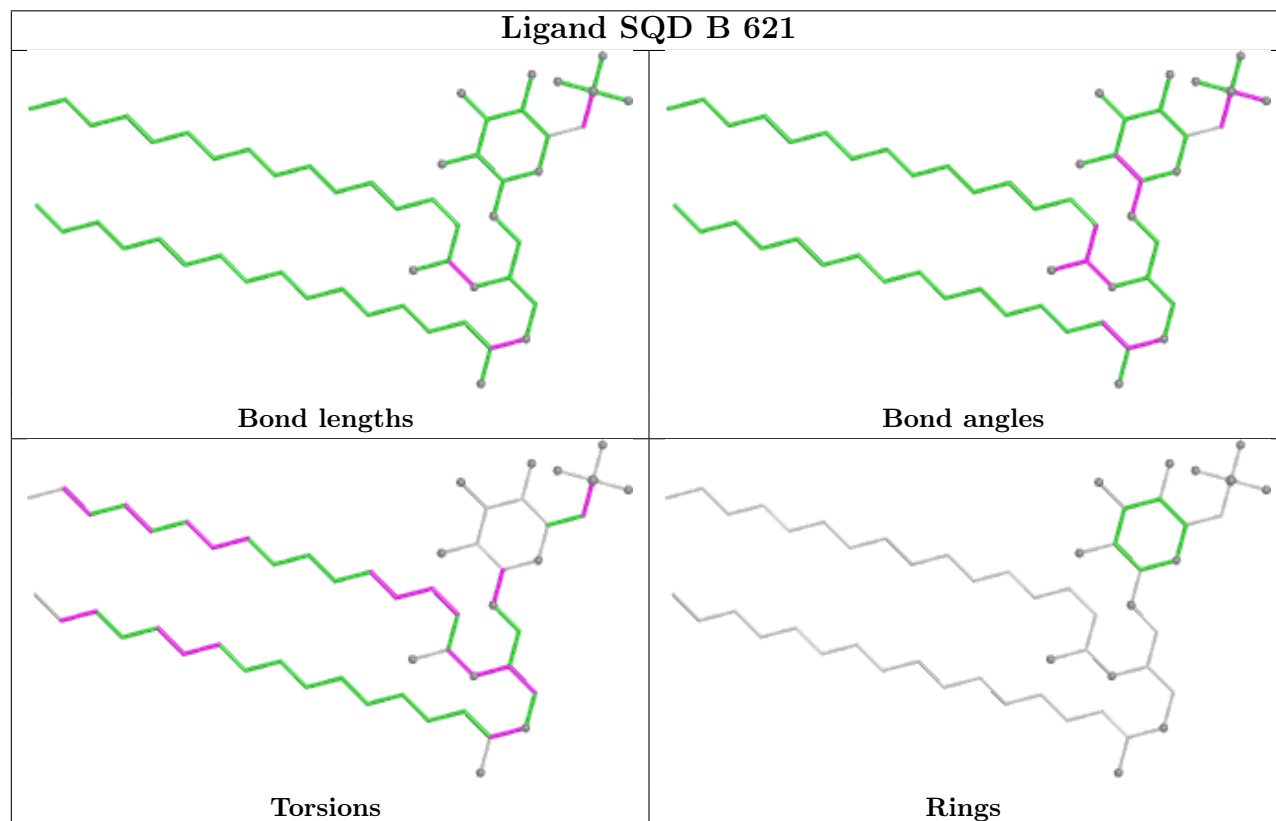
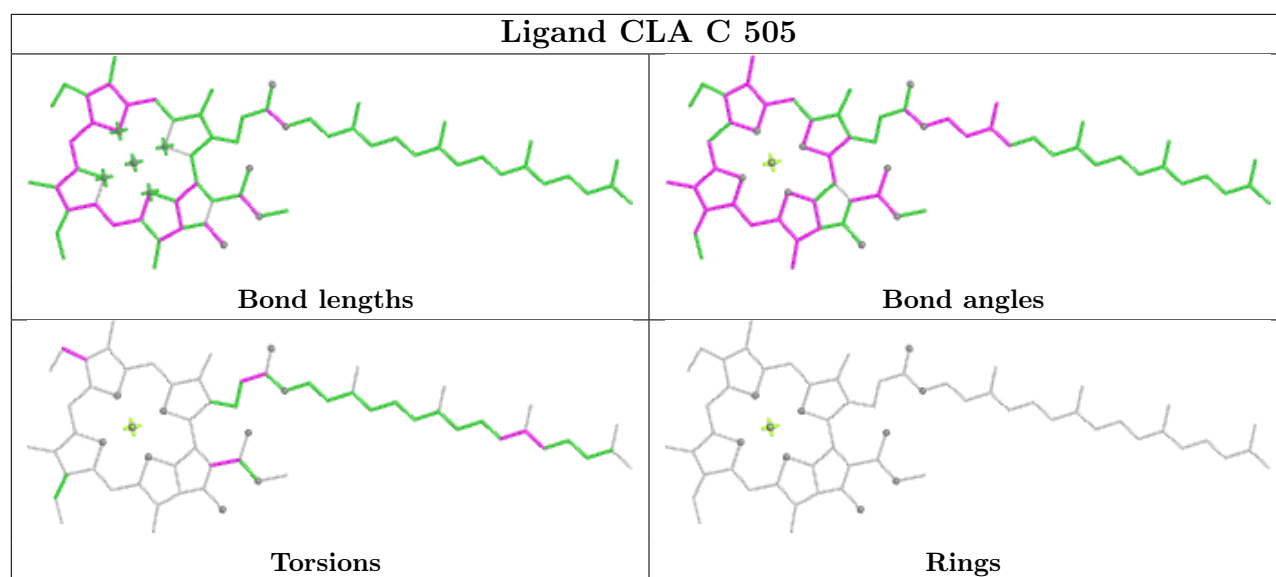


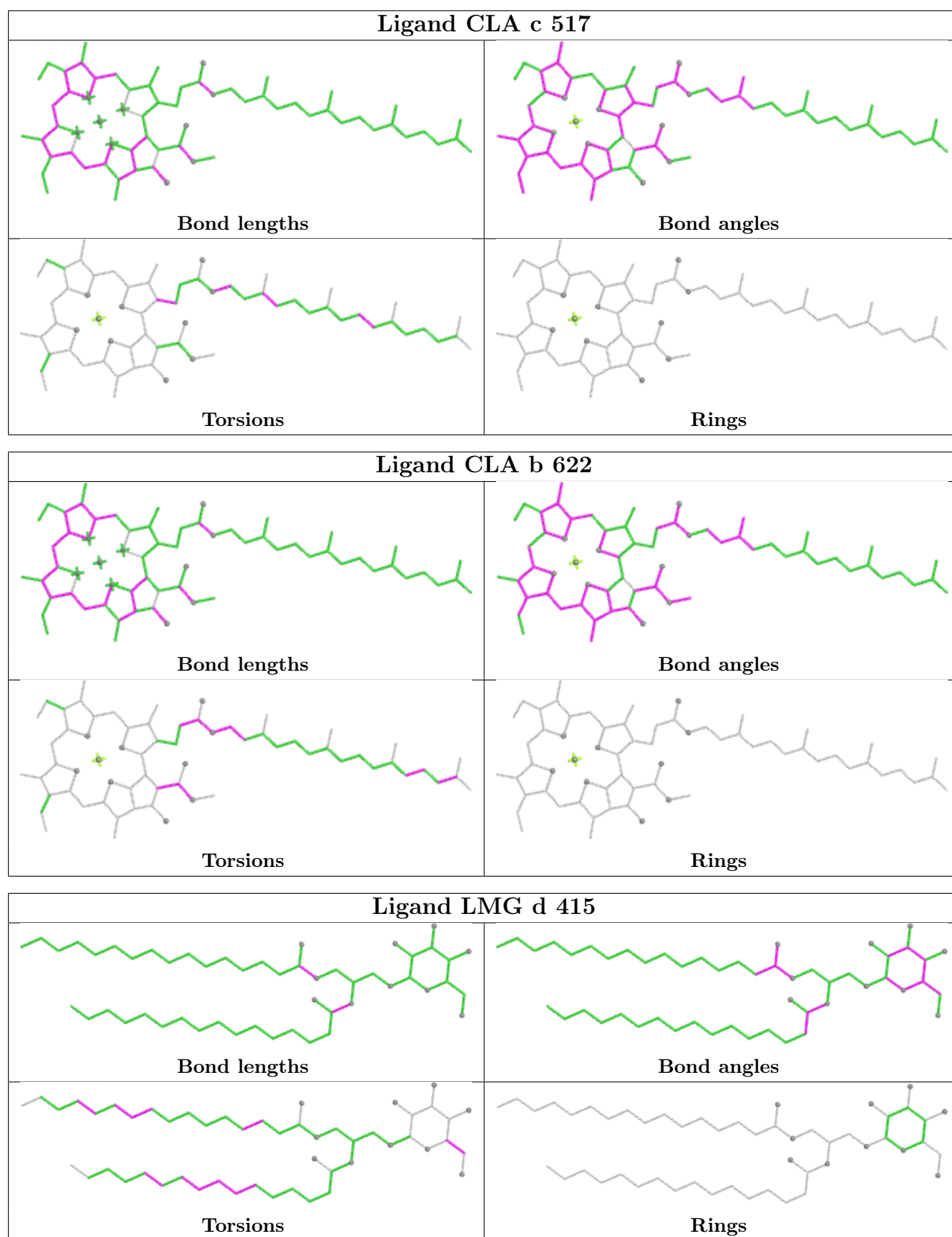
Ligand BCR b 628	
	
Bond lengths	Bond angles
	
Torsions	Rings

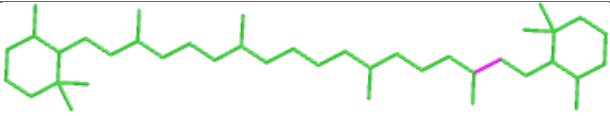
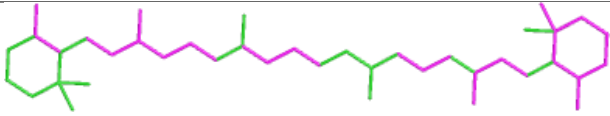
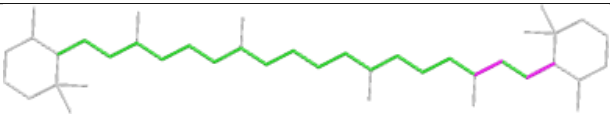
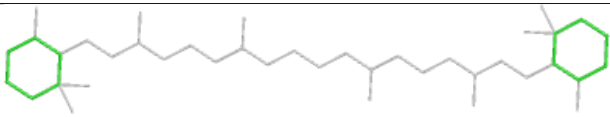
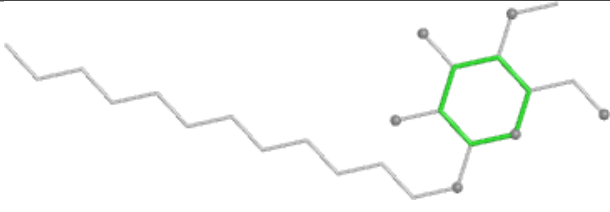
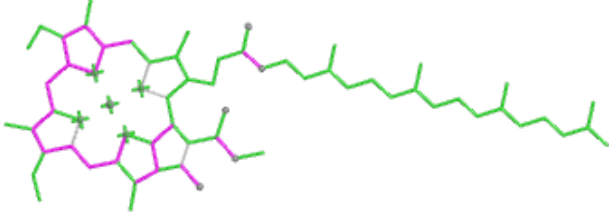
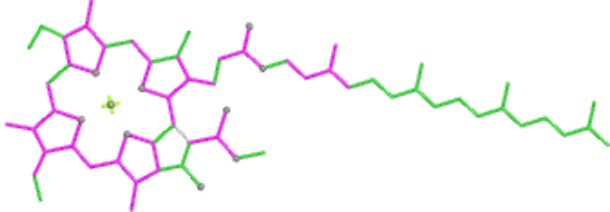
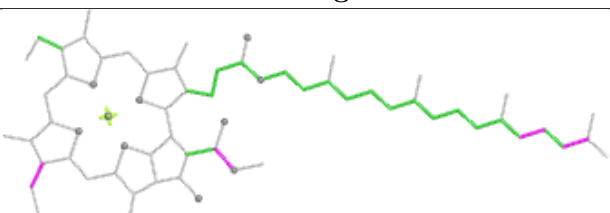
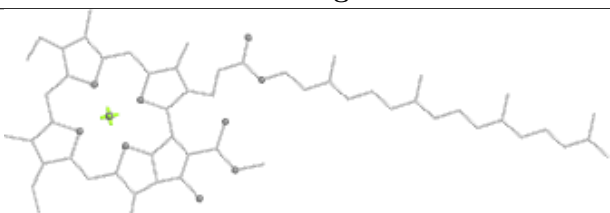
Ligand PL9 a 416 (A)	
	
Bond lengths	Bond angles
	
Torsions	Rings

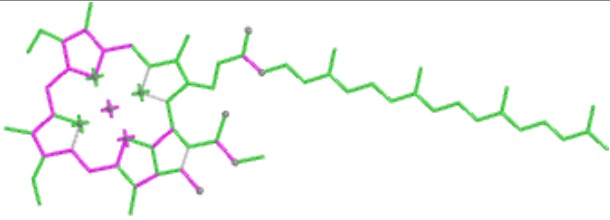
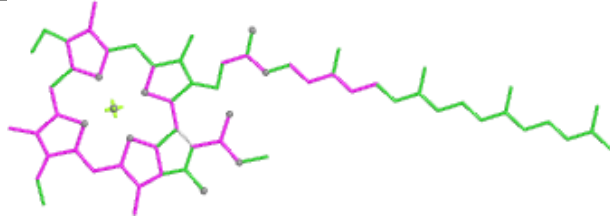
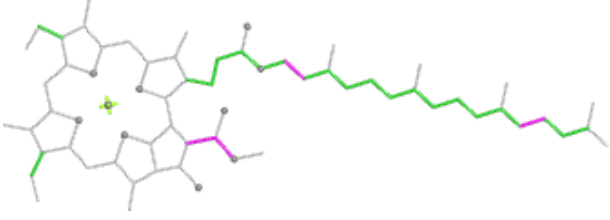
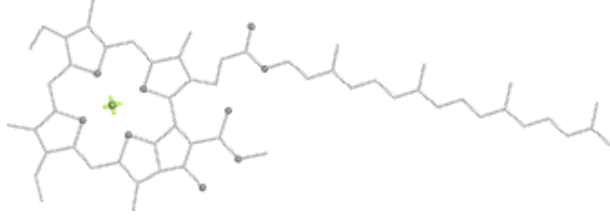
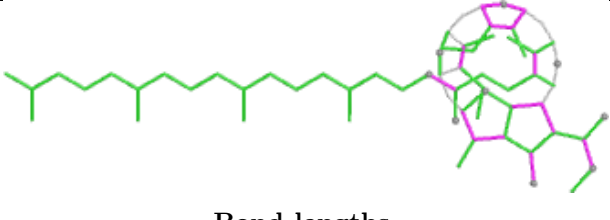
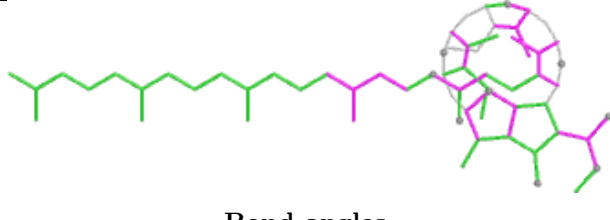
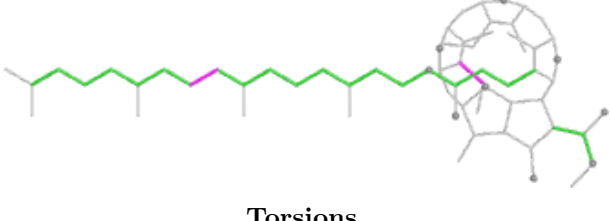
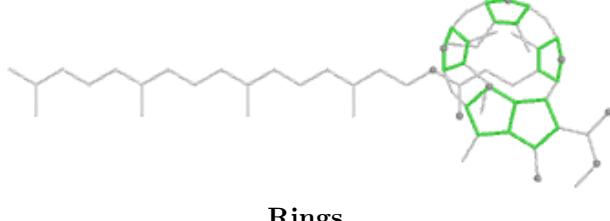
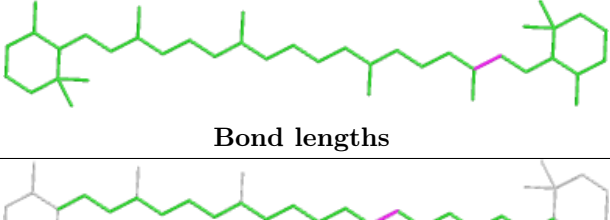
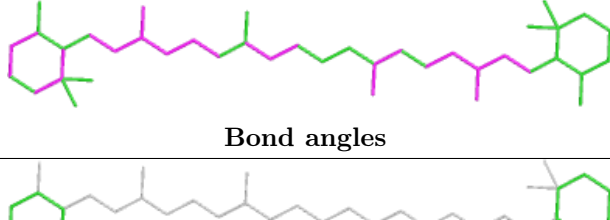
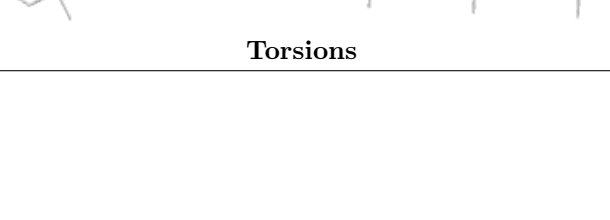
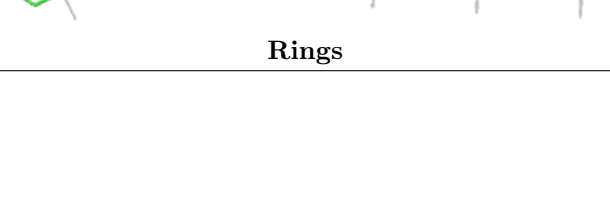
Ligand PL9 A 417 (A)	
	
Bond lengths	Bond angles
	
Torsions	Rings

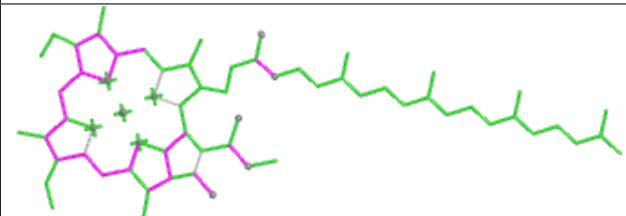
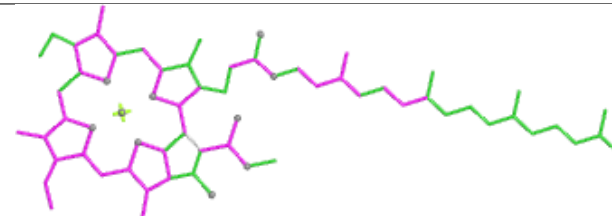
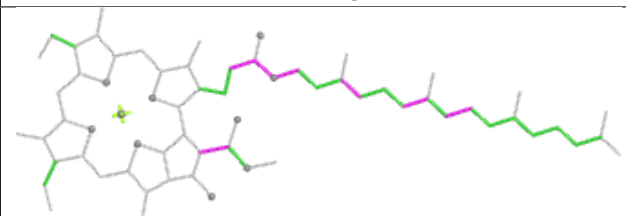
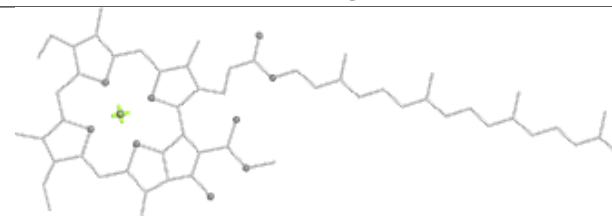
Ligand CLA a 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

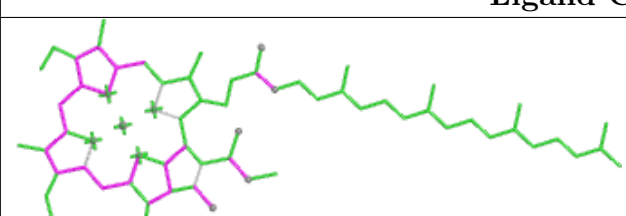
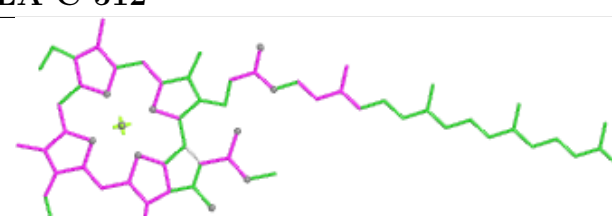
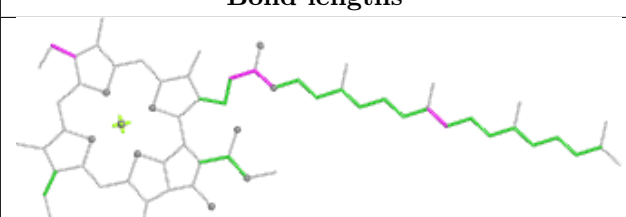
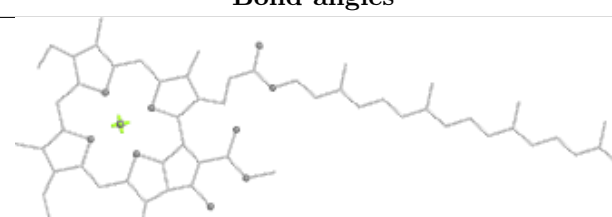


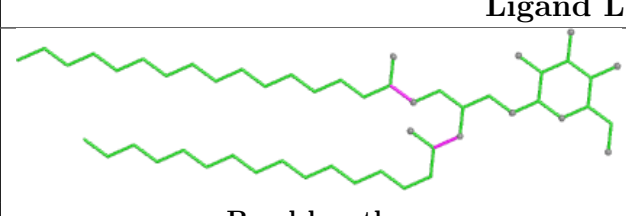
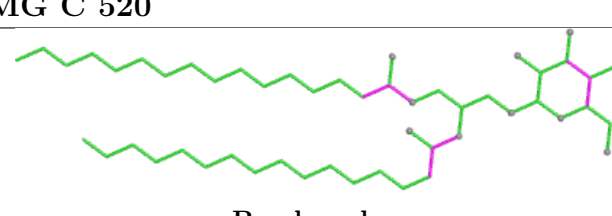
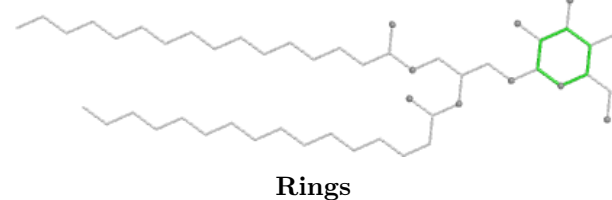


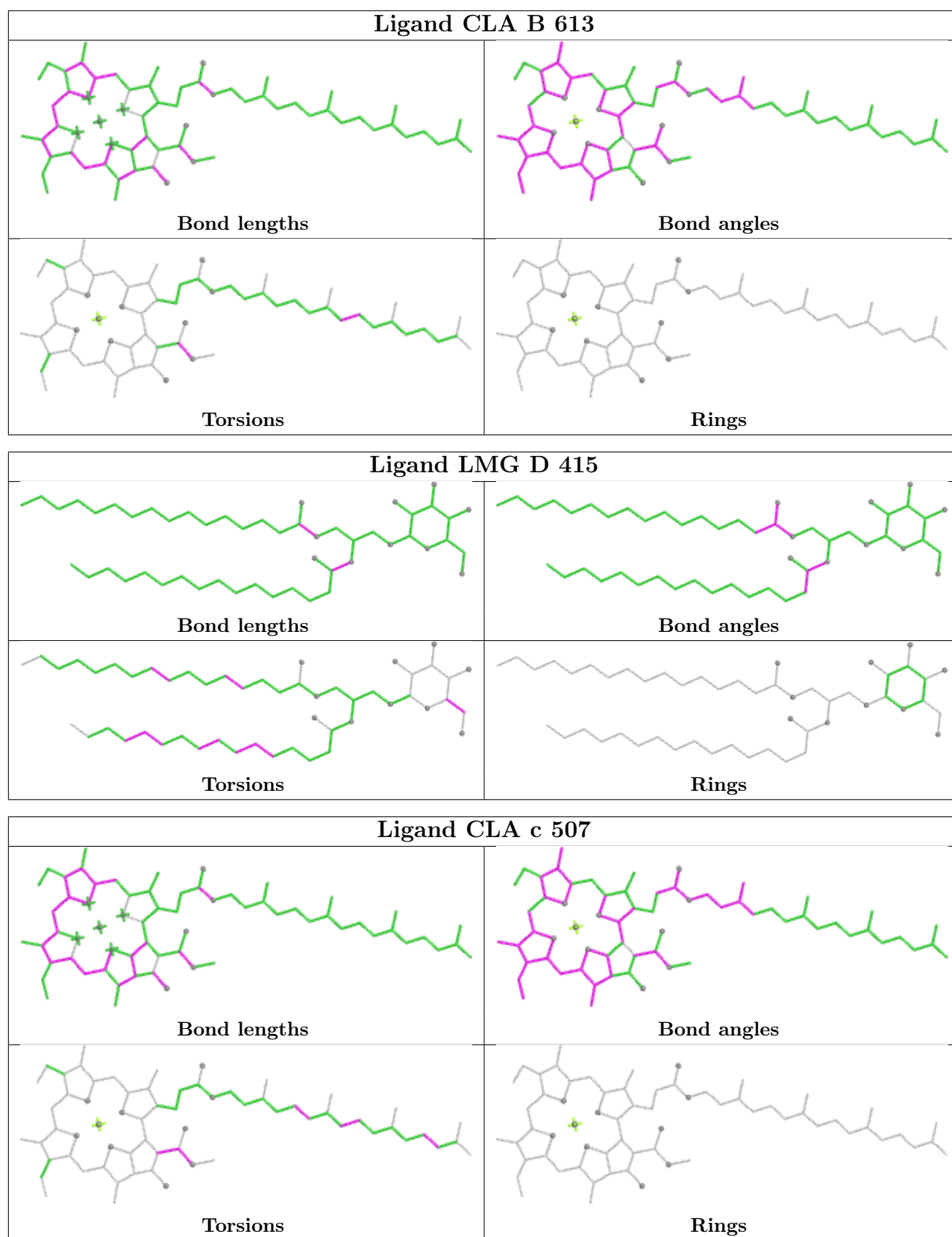
Ligand BCR d 406	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMT T 104	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA a 409	
 Bond lengths	 Bond angles
 Torsions	 Rings

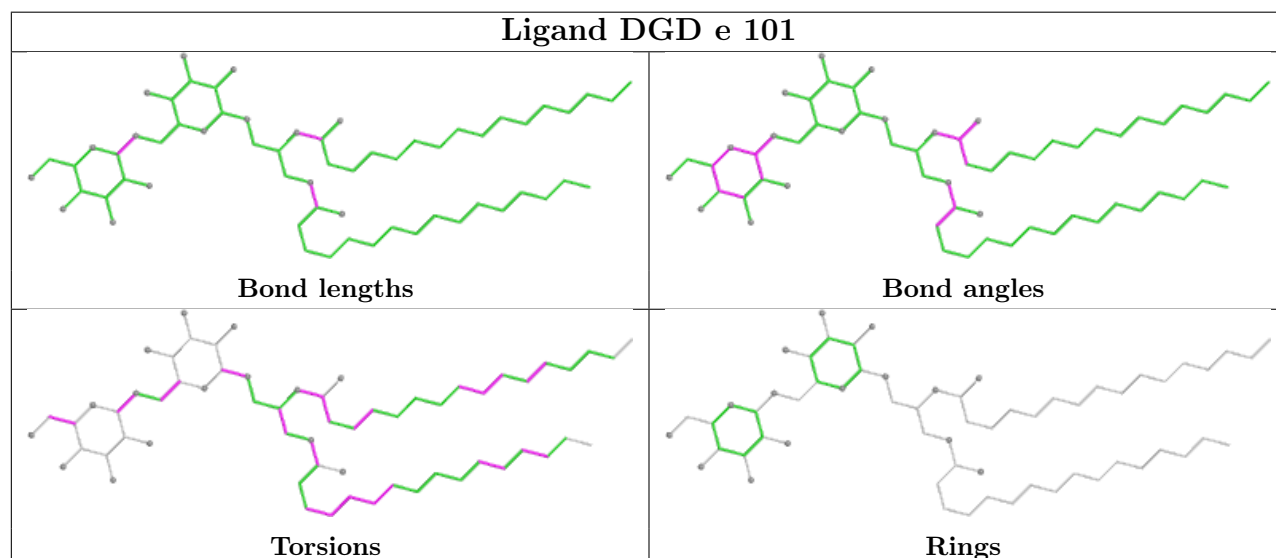
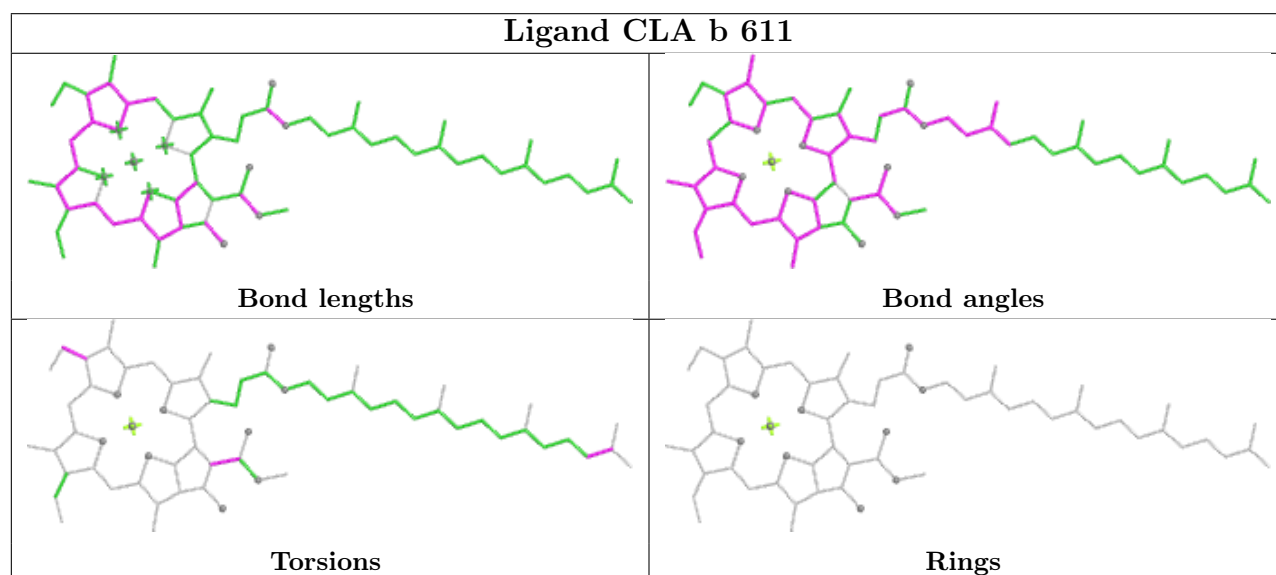
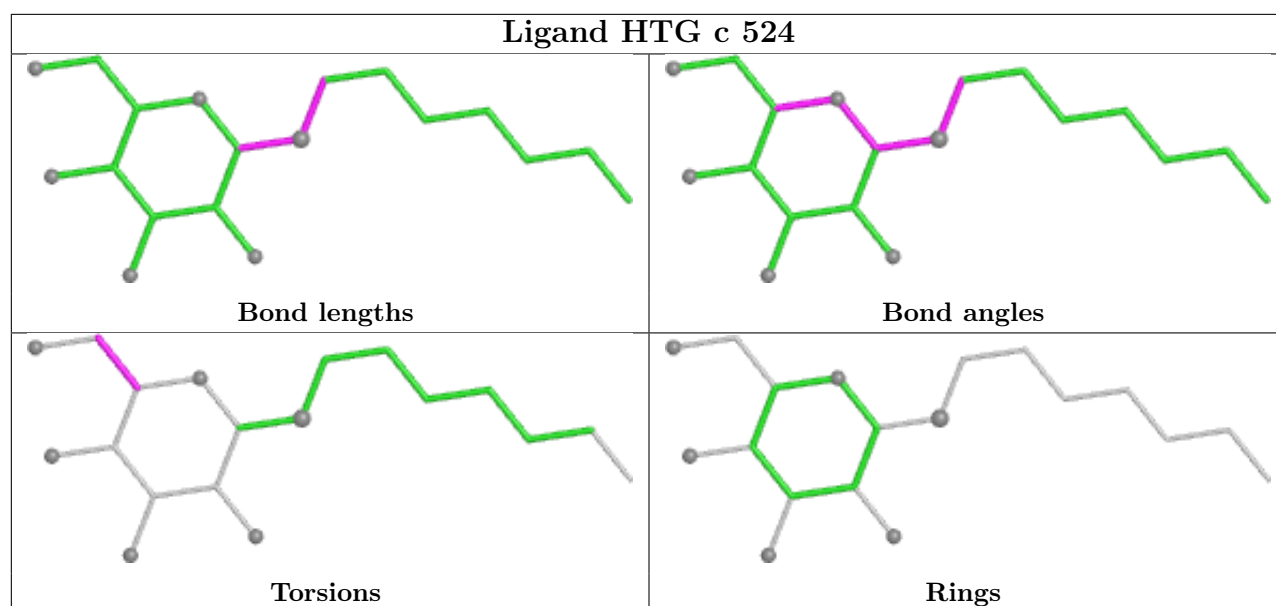
Ligand CLA b 613	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PHO d 402 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR k 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

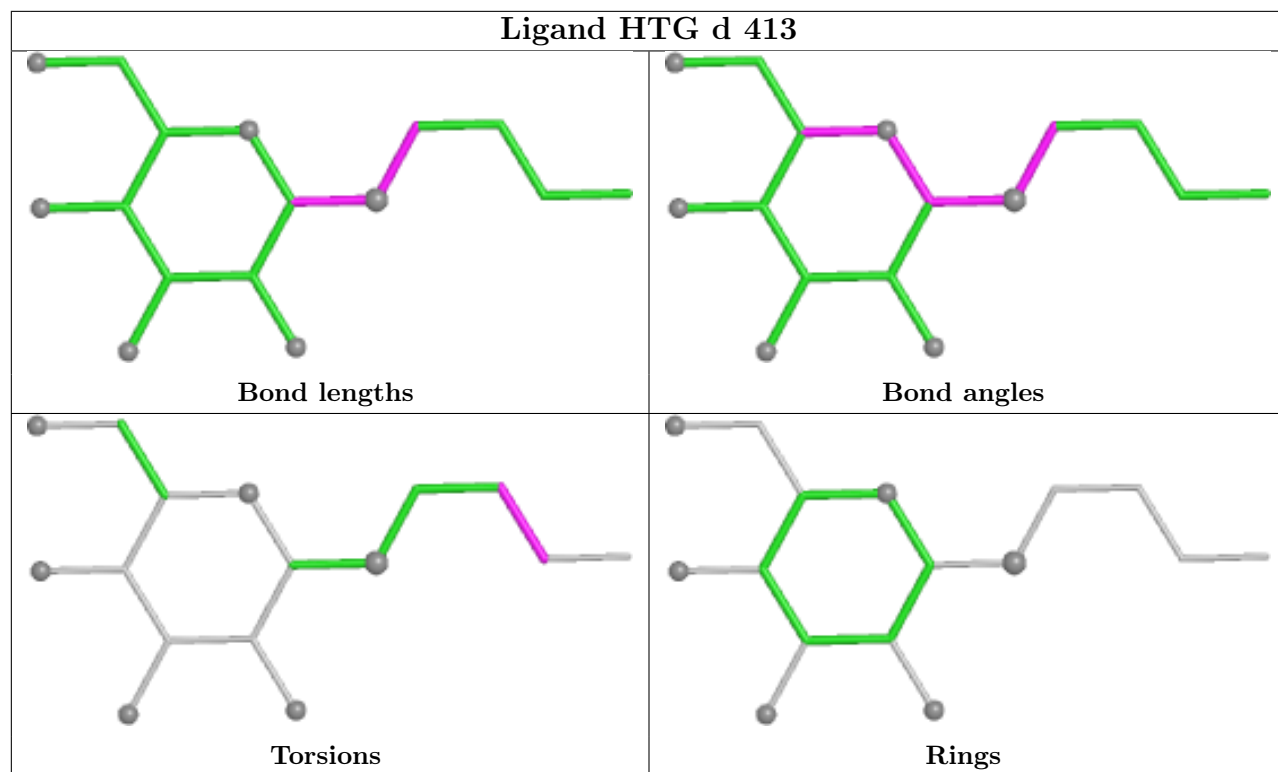
Ligand CLA C 510	
	
Bond lengths	Bond angles
	
Torsions	Rings

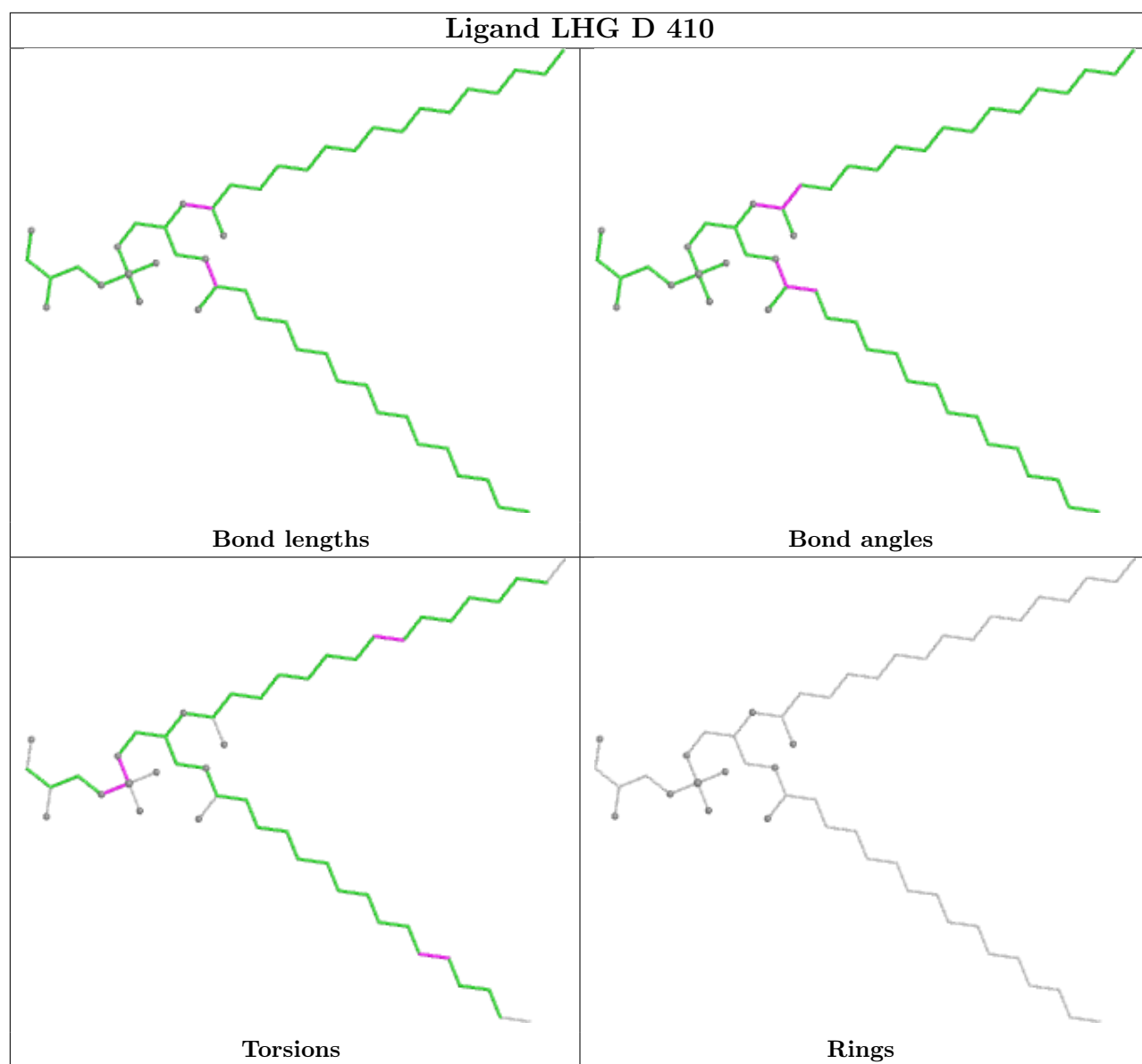
Ligand CLA C 512	
	
Bond lengths	Bond angles
	
Torsions	Rings

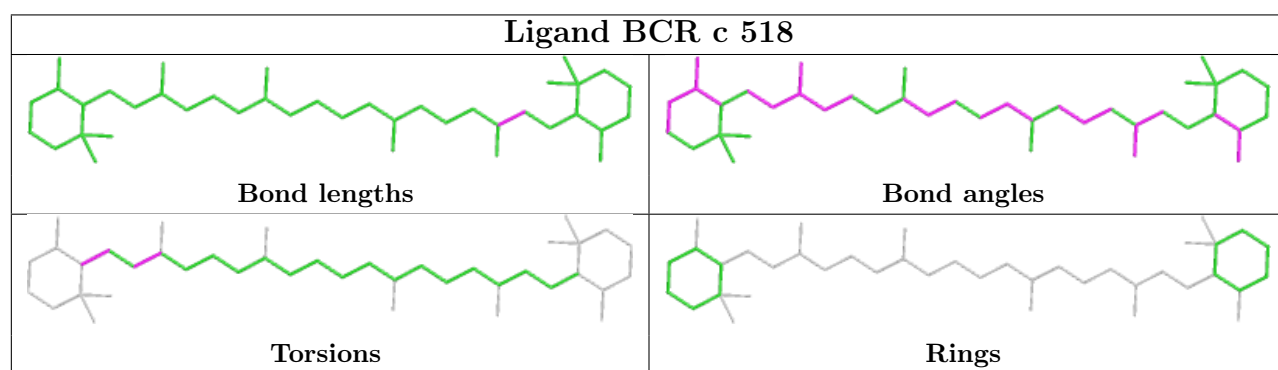
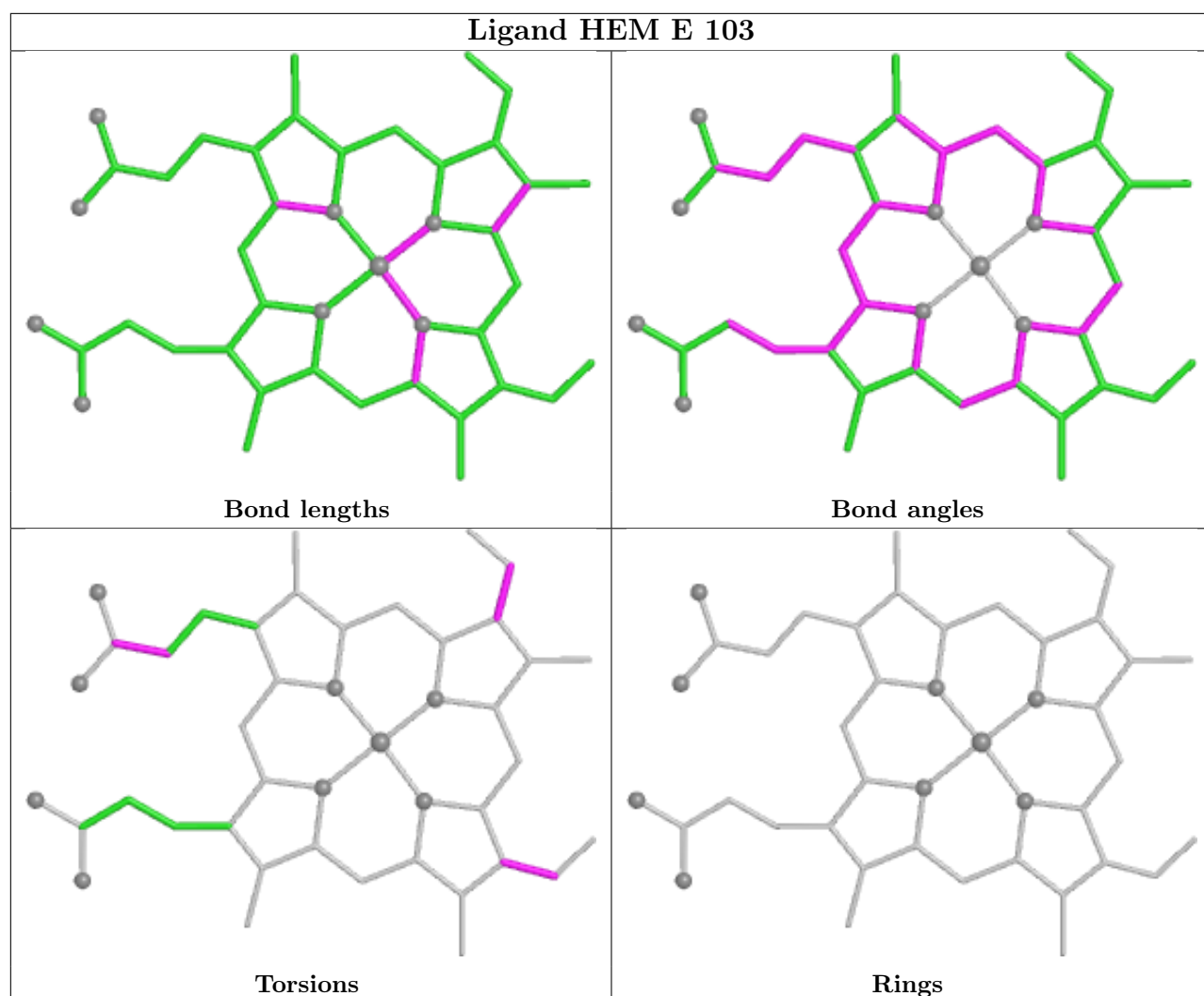
Ligand LMG C 520	
	
Bond lengths	Bond angles
	
Torsions	Rings



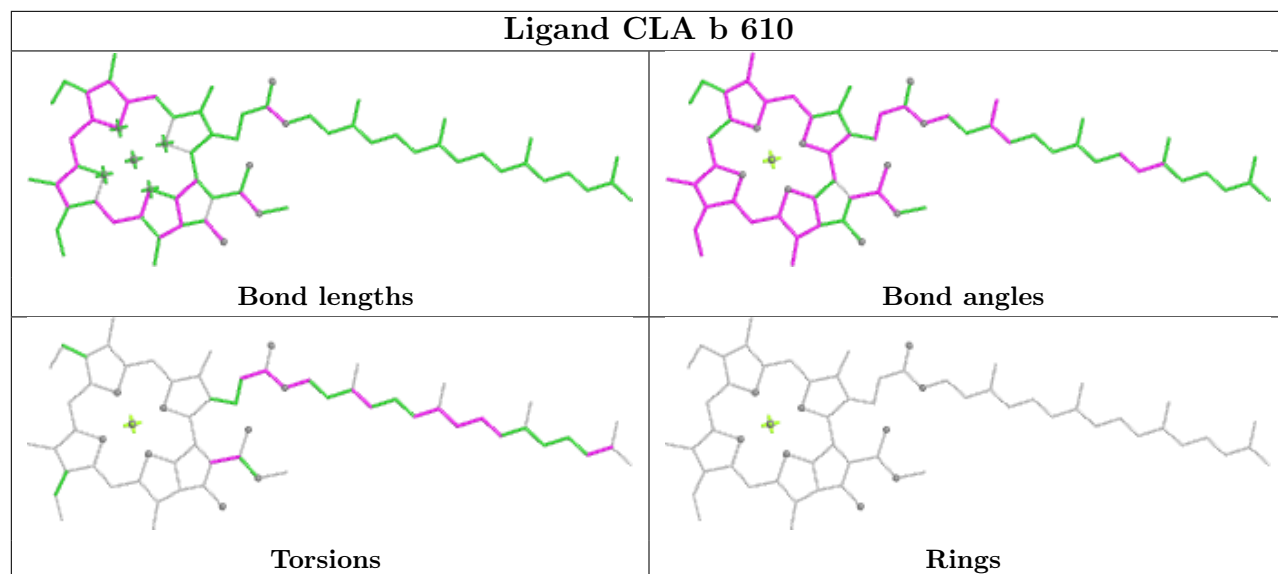




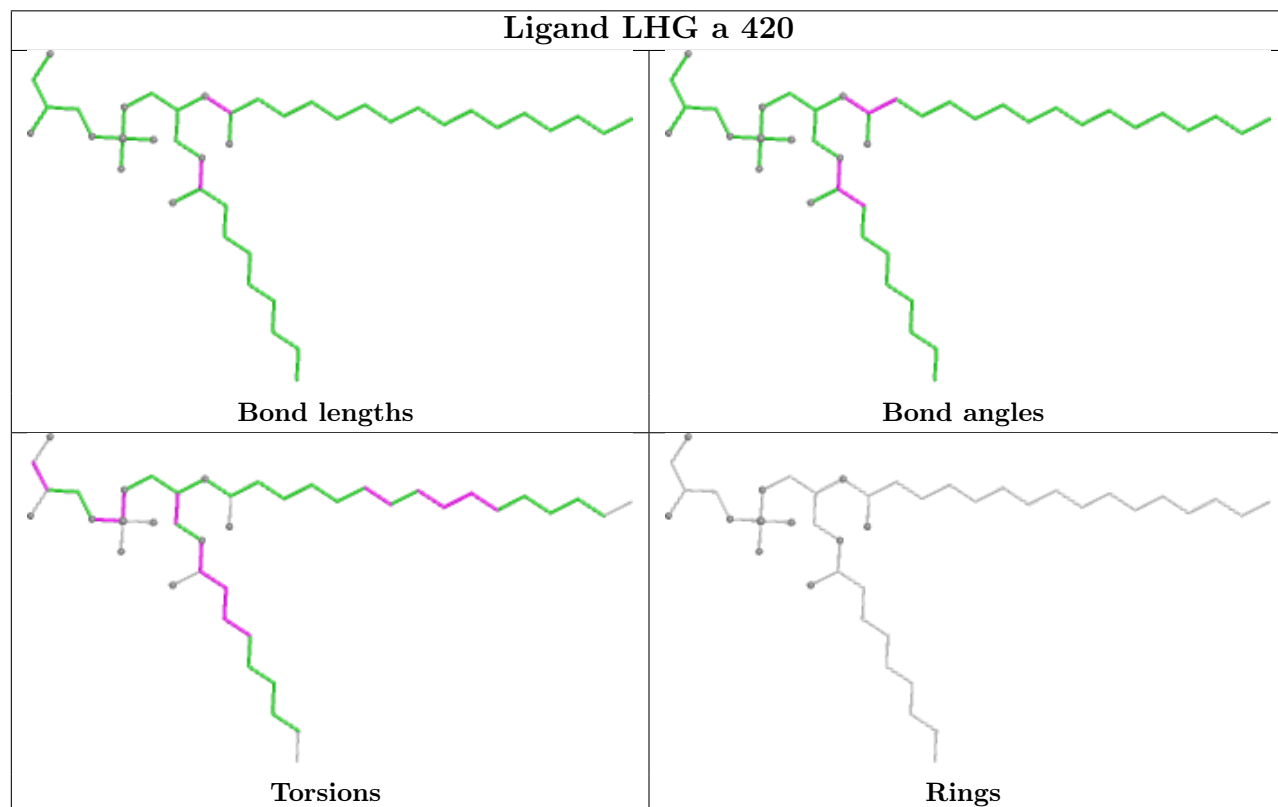


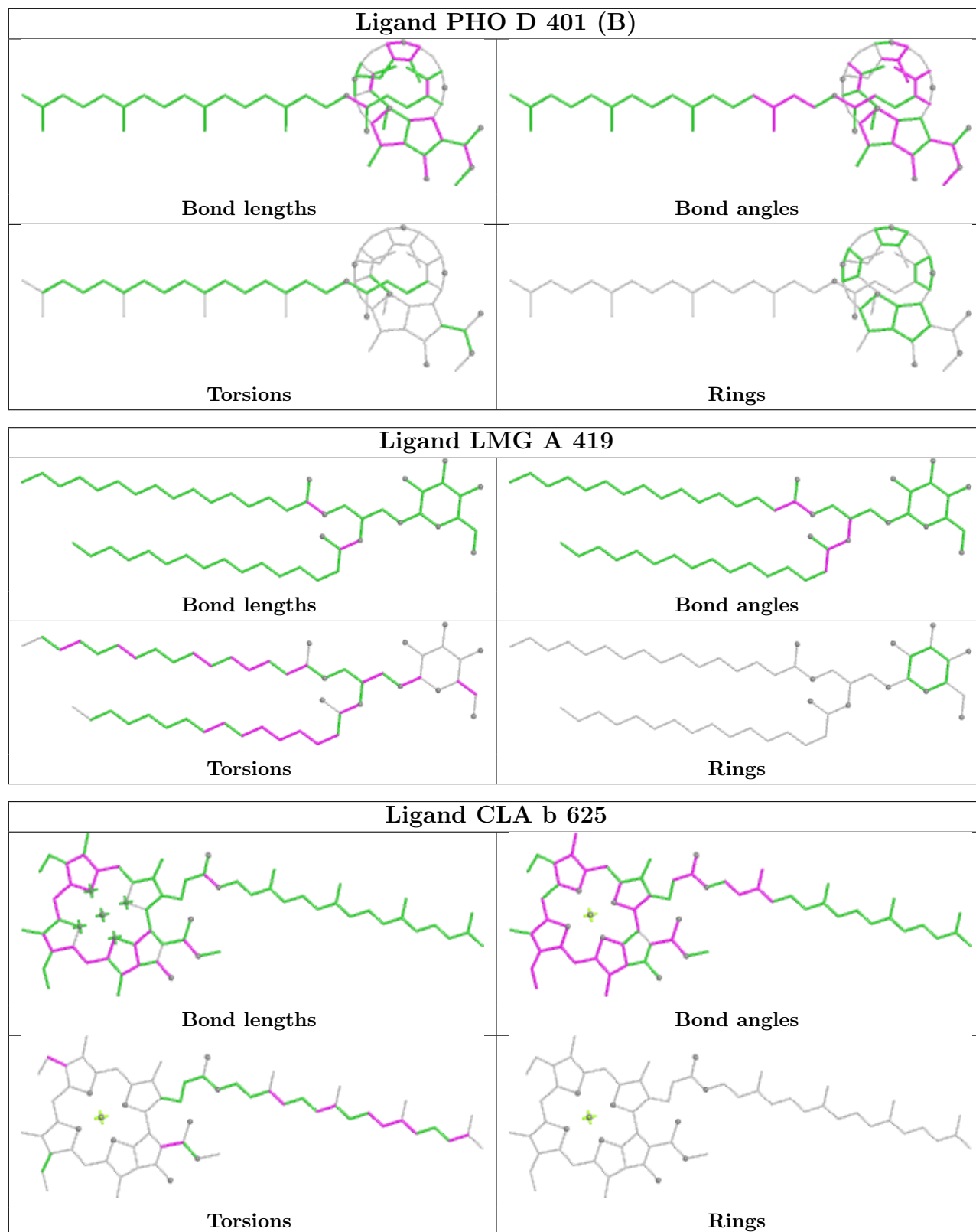


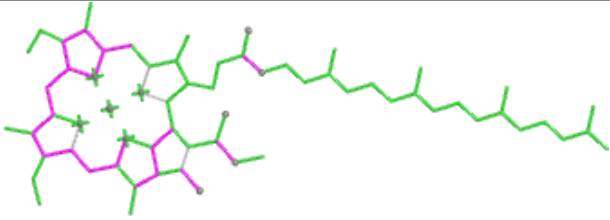
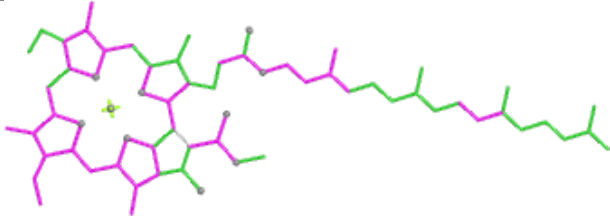
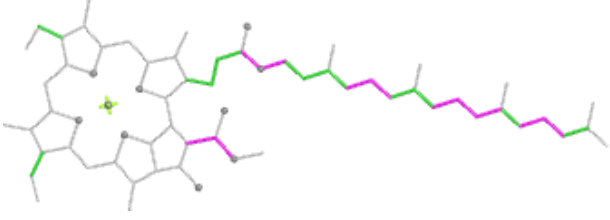
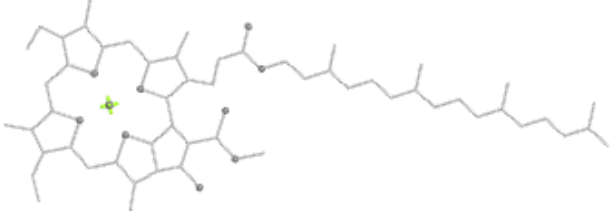
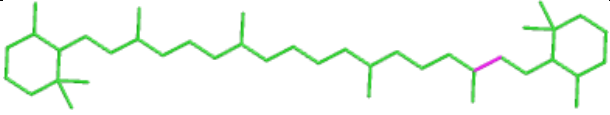
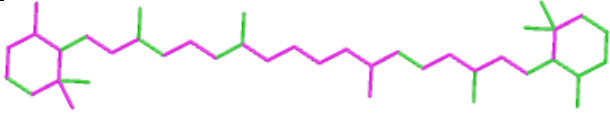
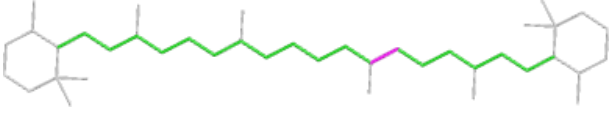
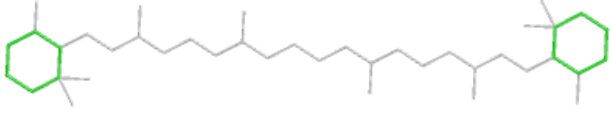
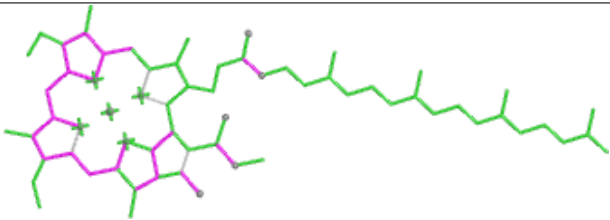
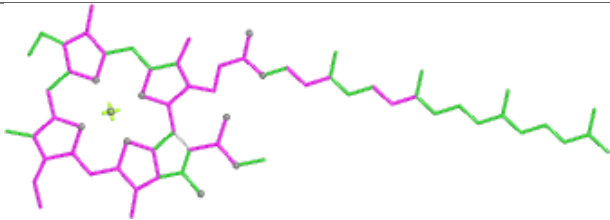
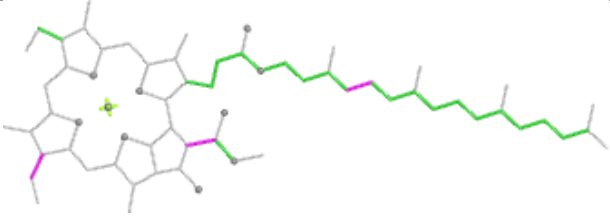
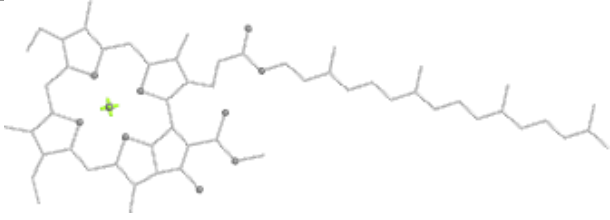
Ligand CLA b 610

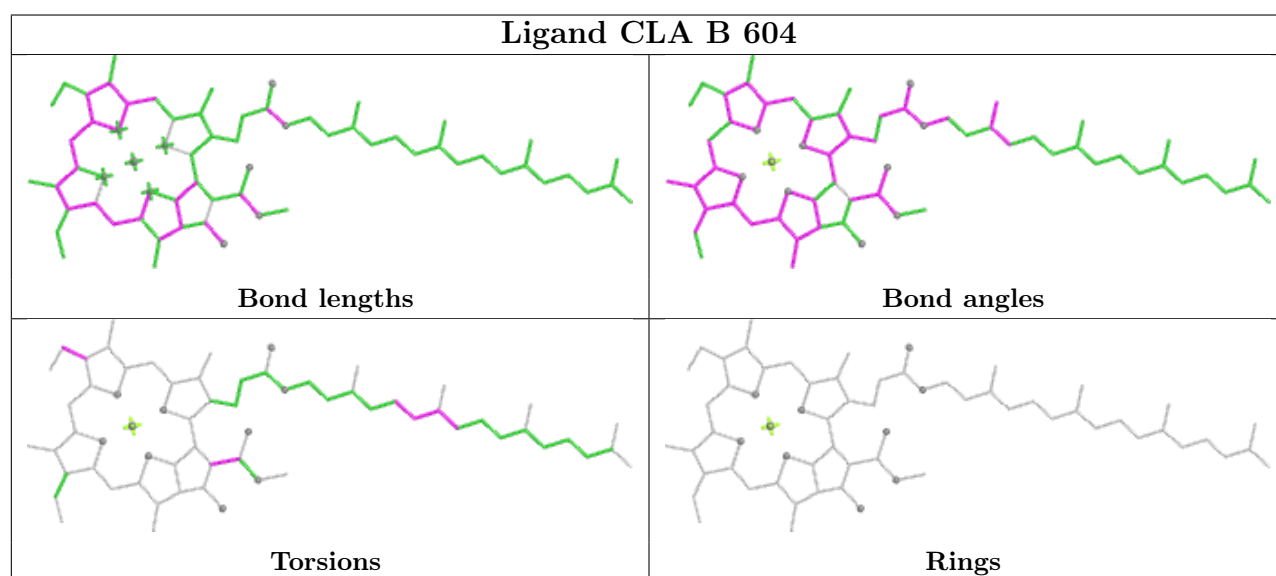
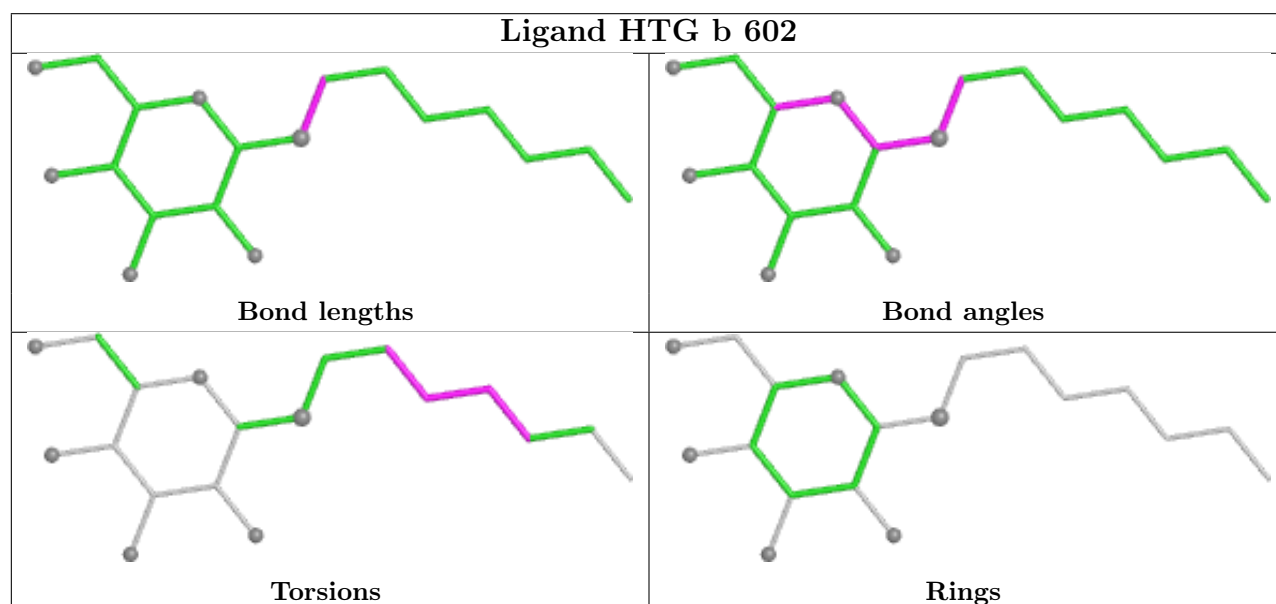
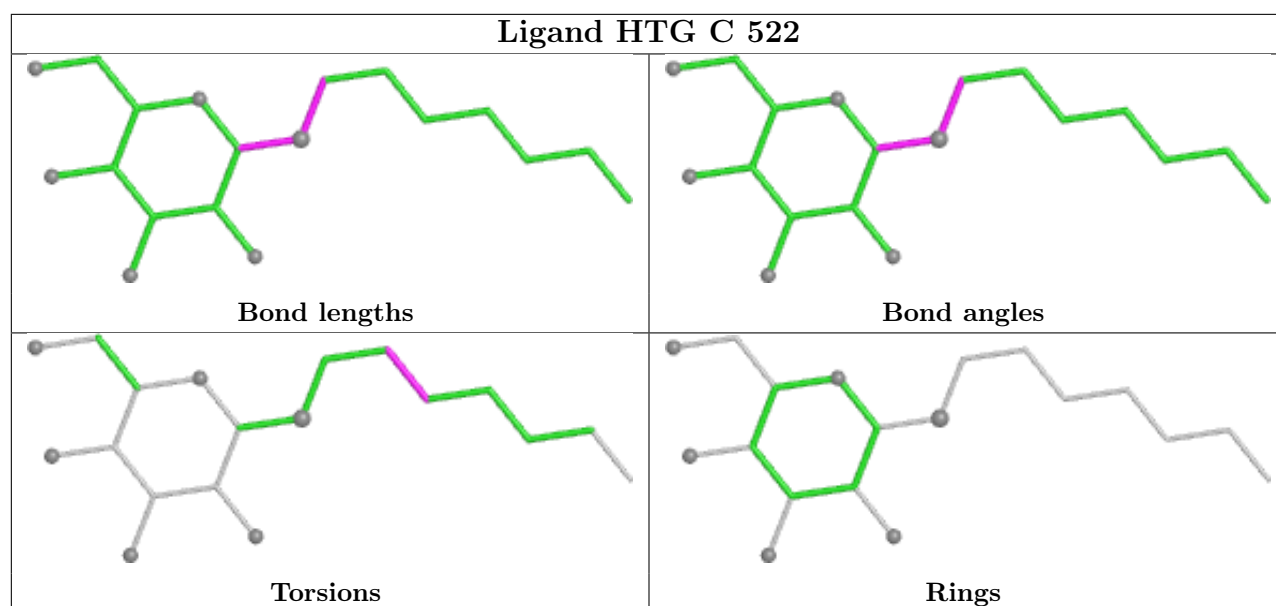


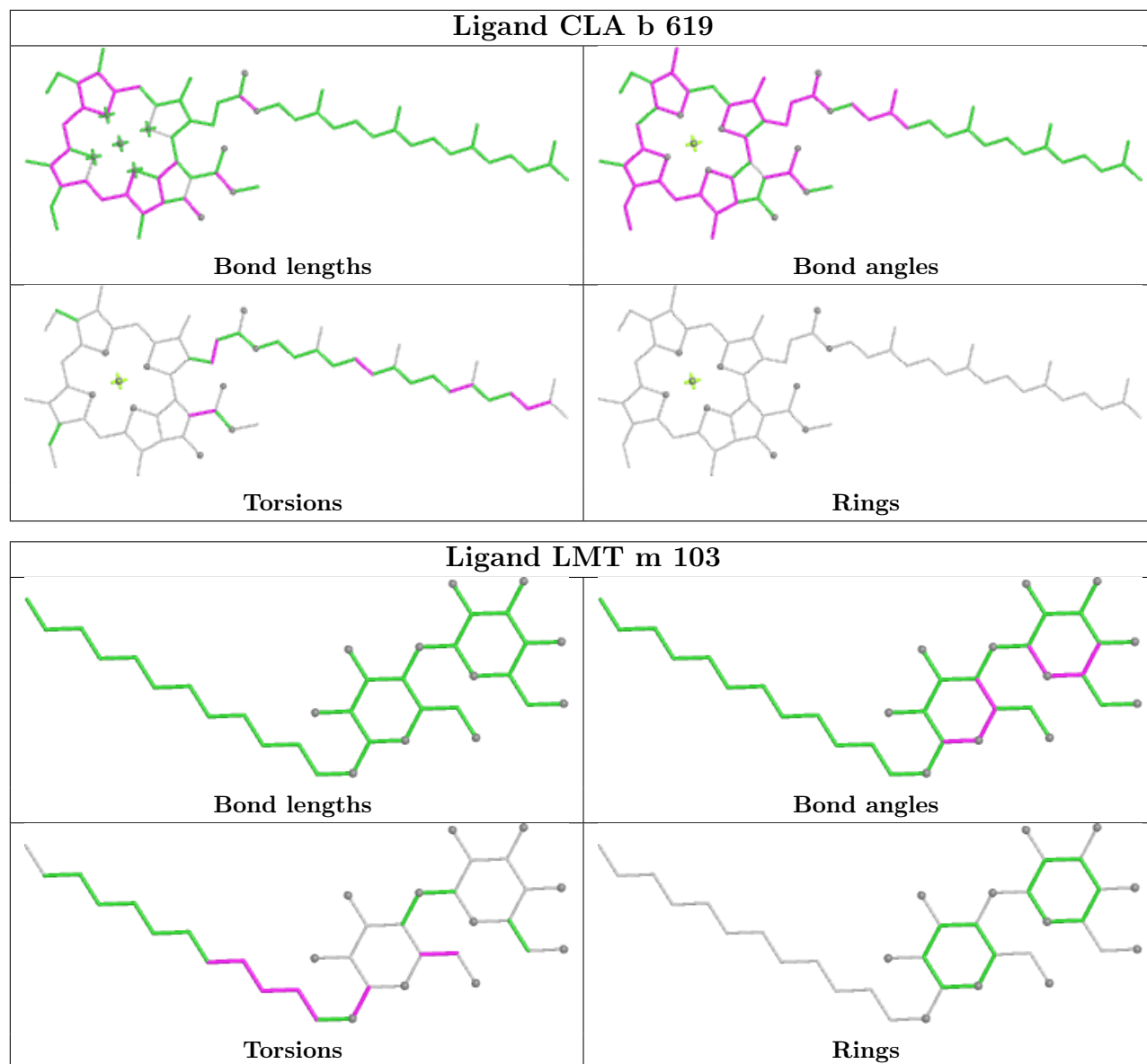
Ligand LHG a 420

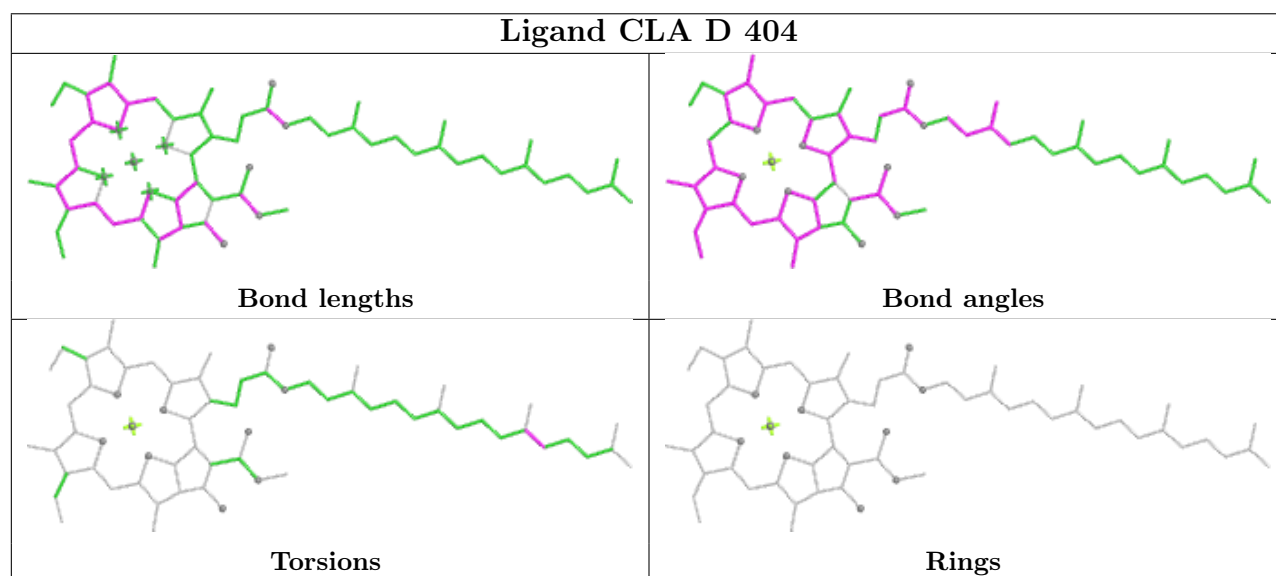
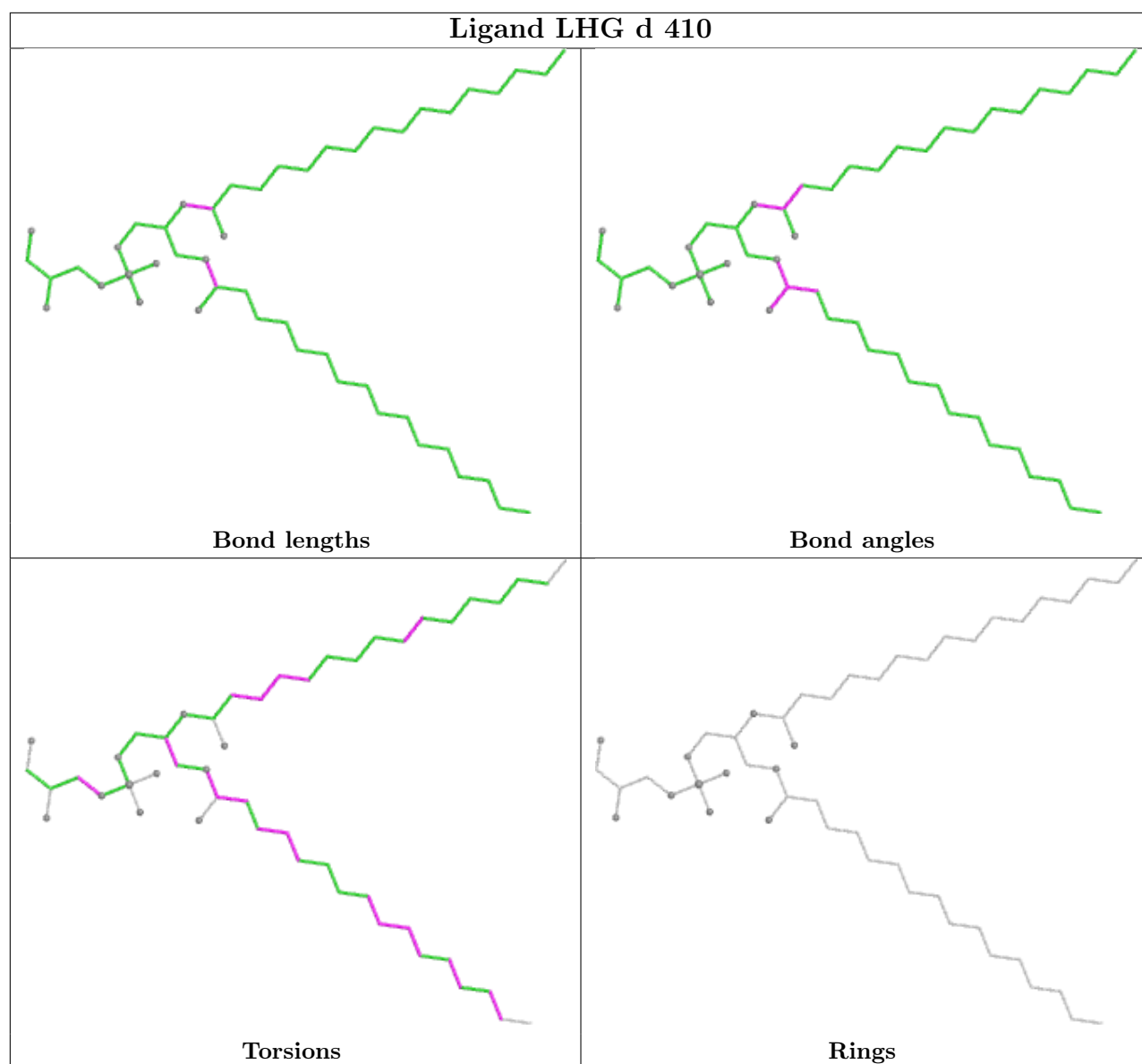


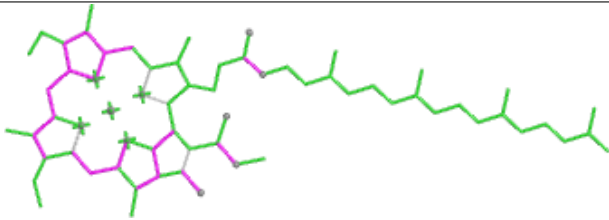
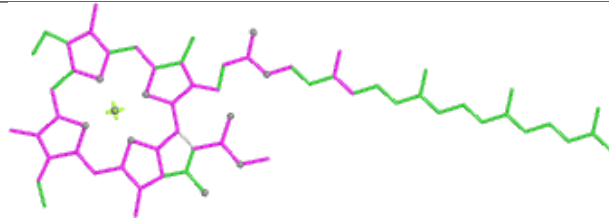
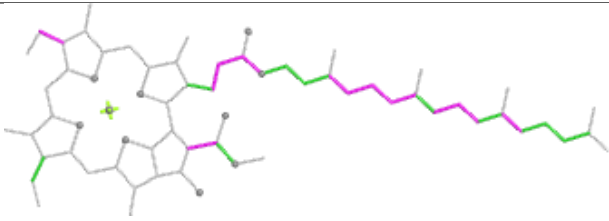
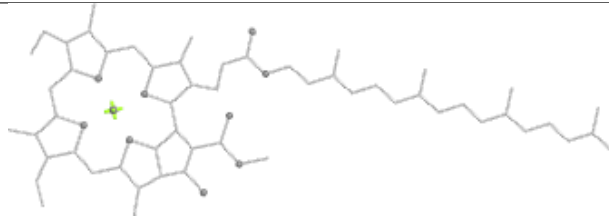


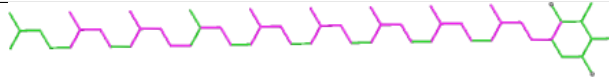
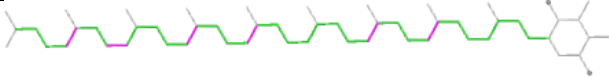
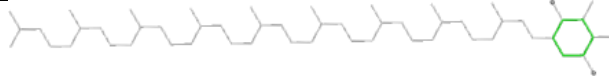
Ligand CLA C 509	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR K 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA A 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

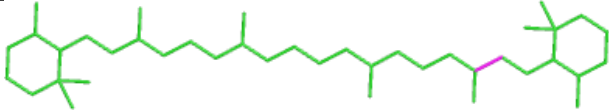
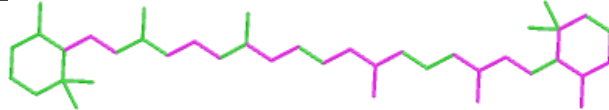
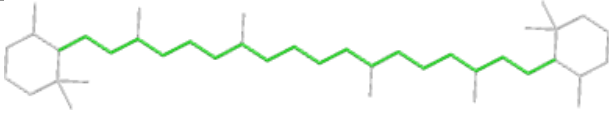
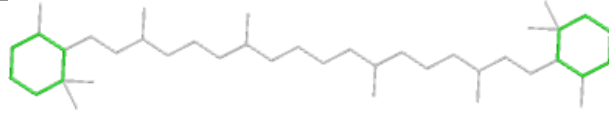


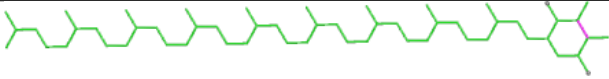
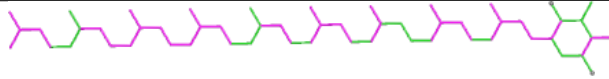
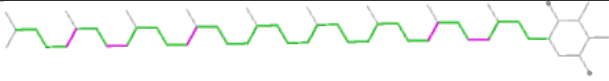
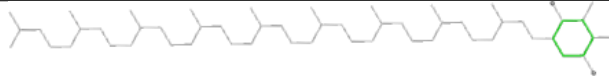


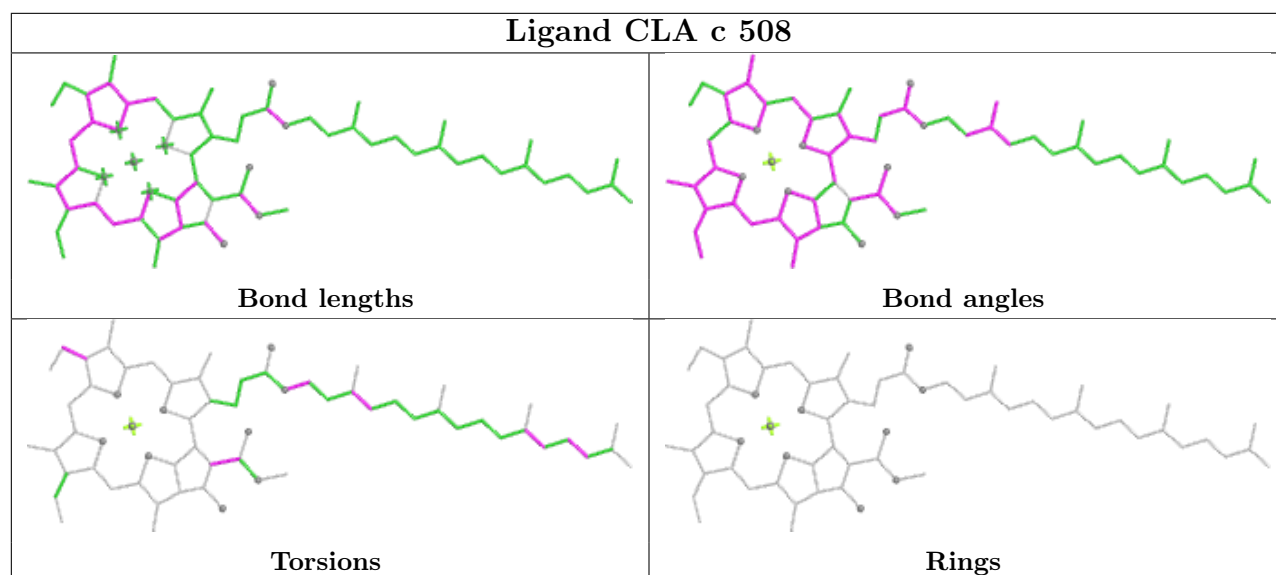
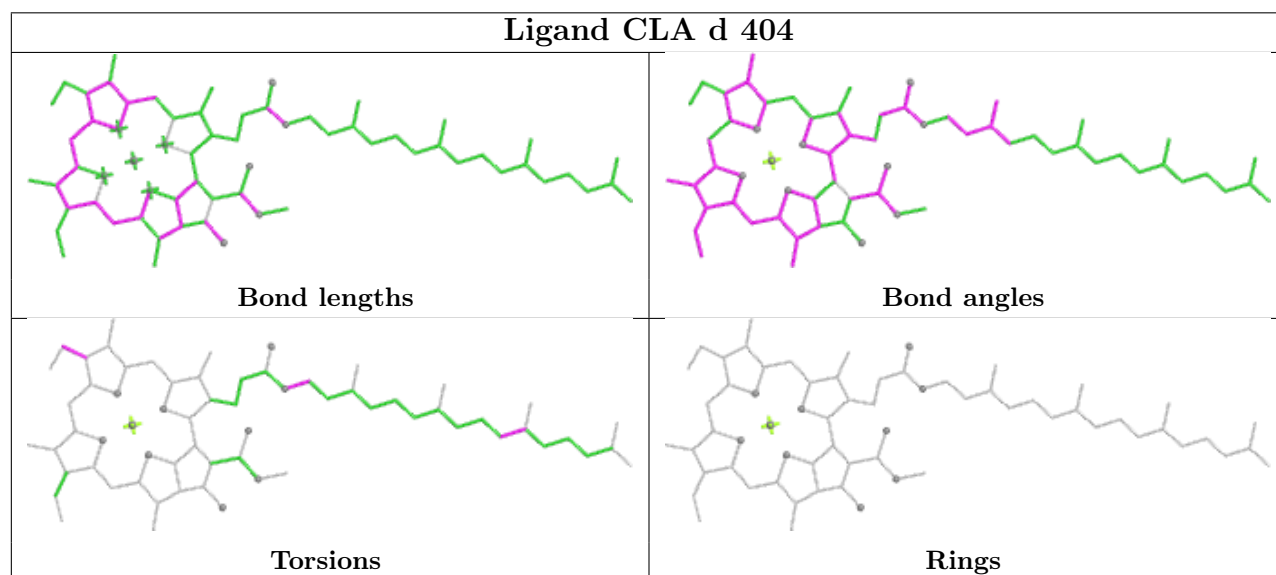
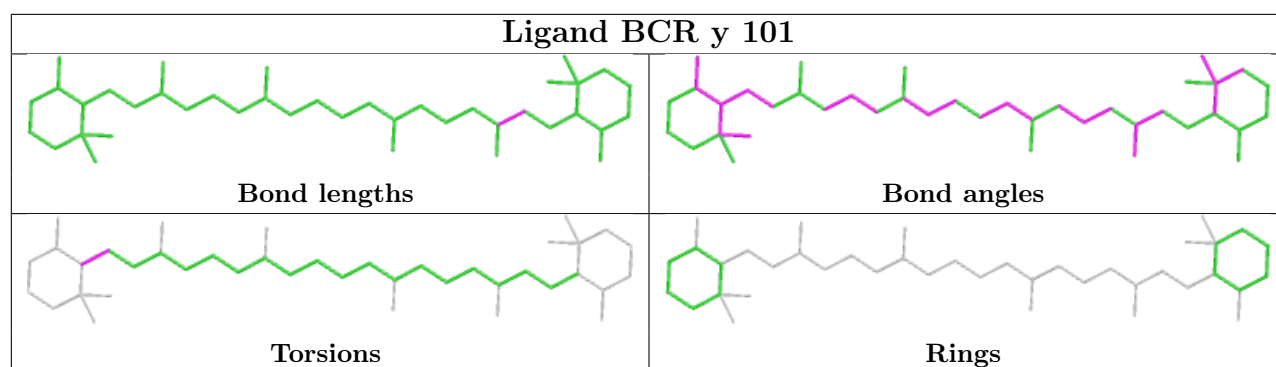


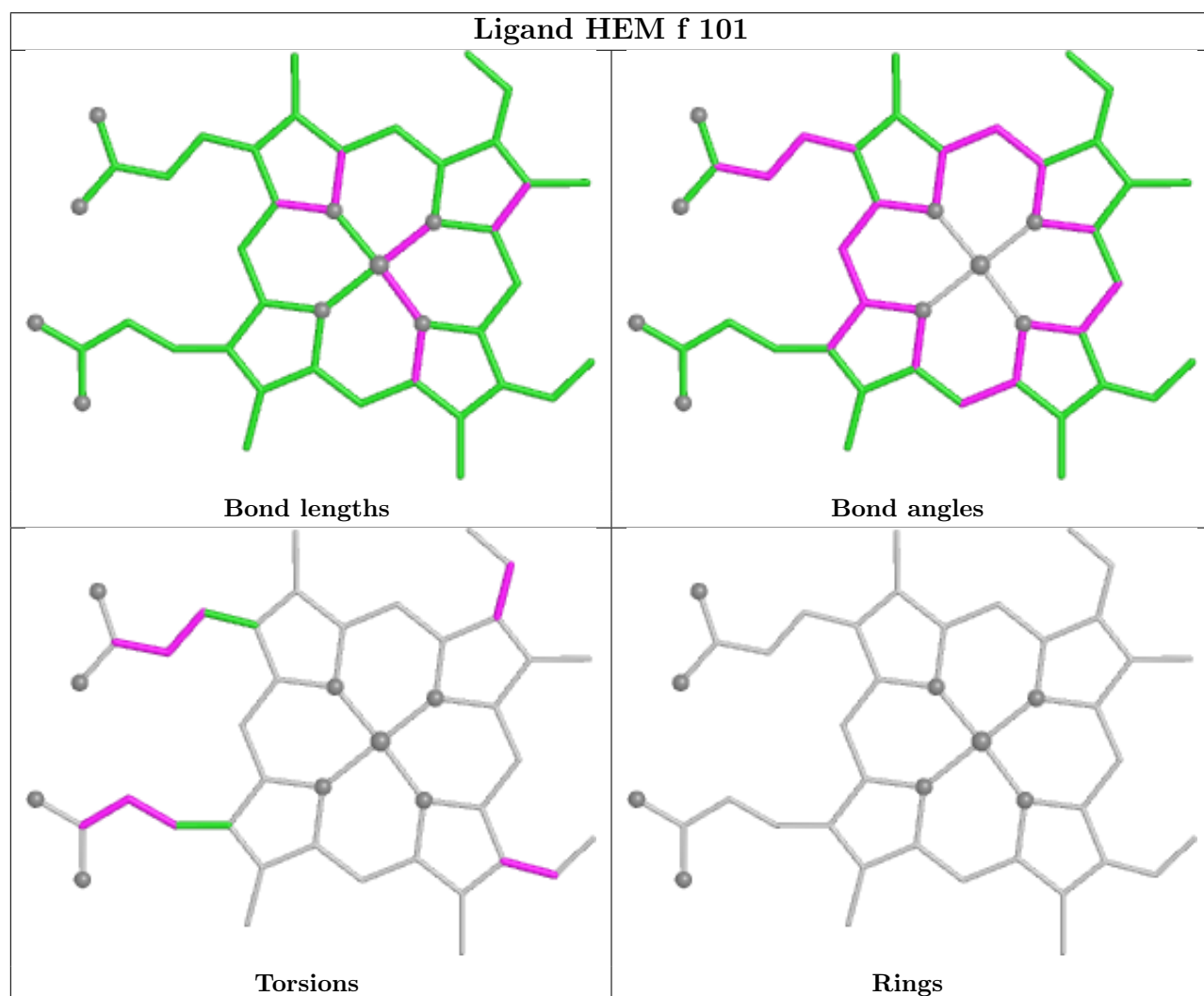
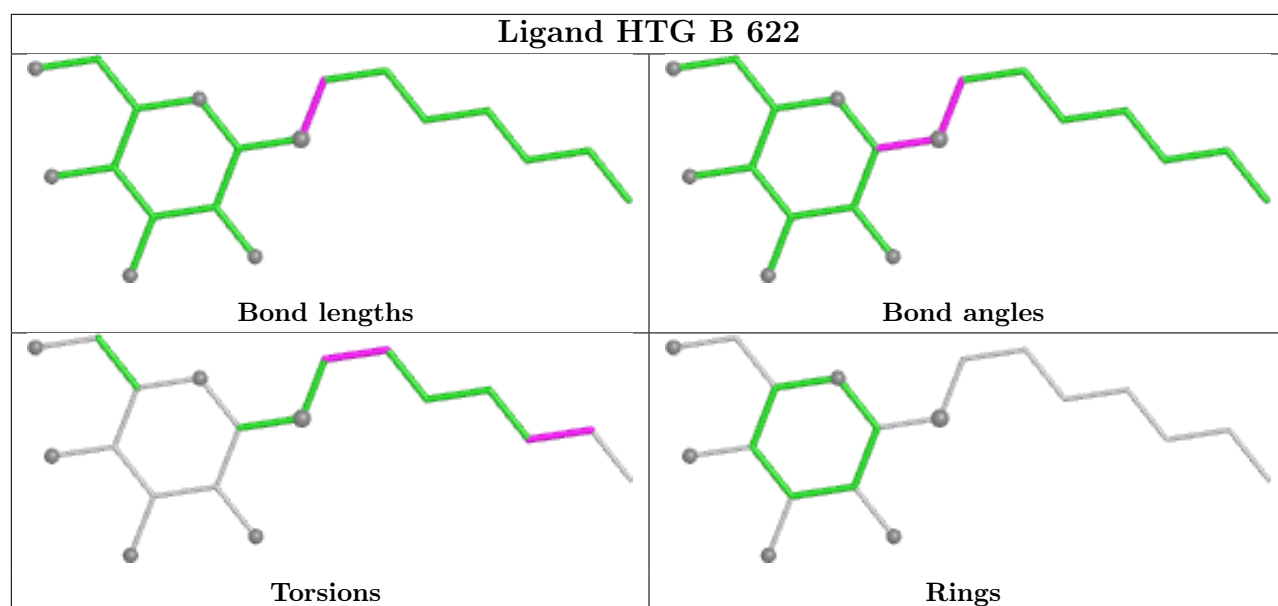
Ligand CLA B 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

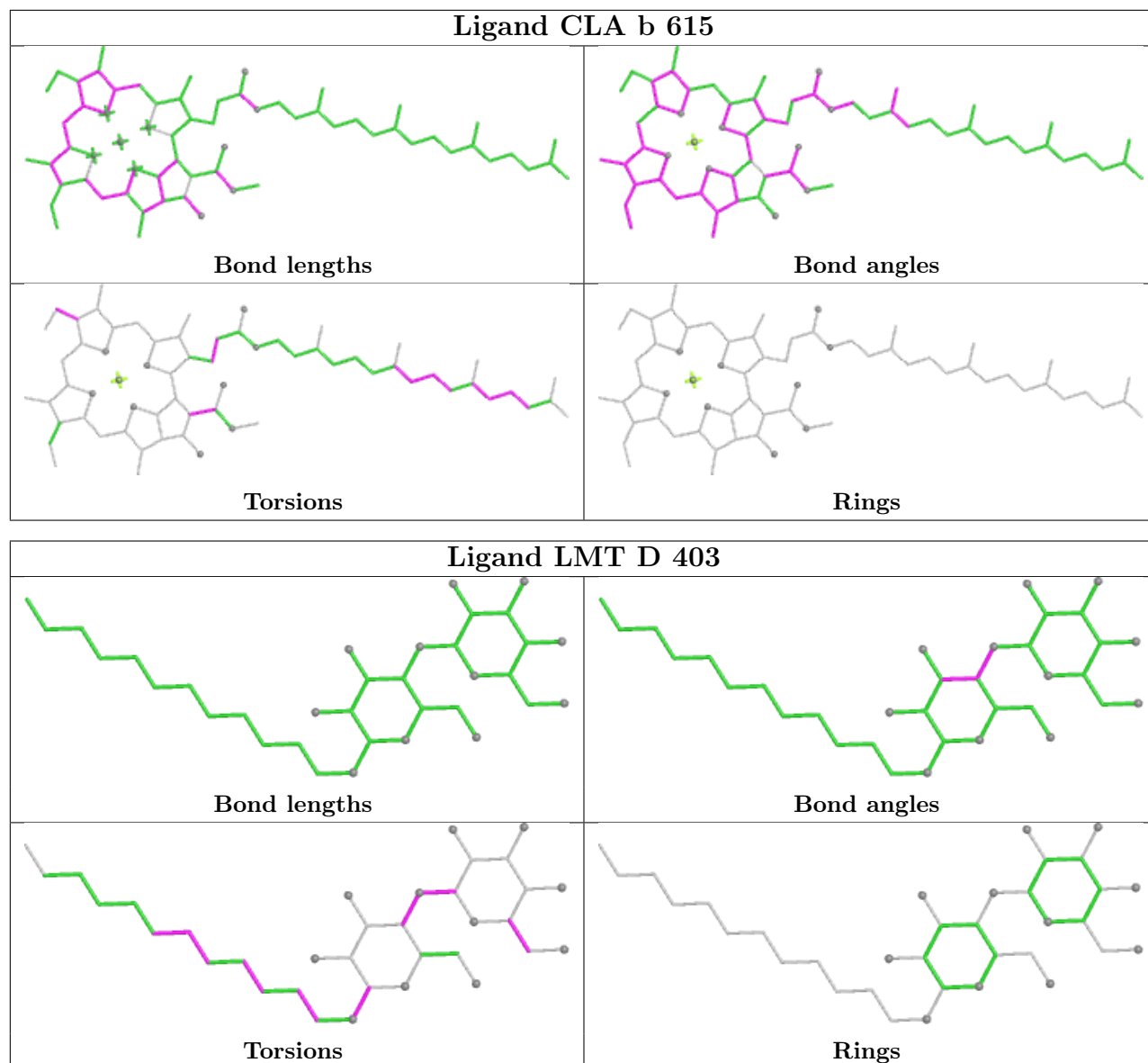
Ligand PL9 d 407 (B)	
	
Bond lengths	Bond angles
	
Torsions	Rings

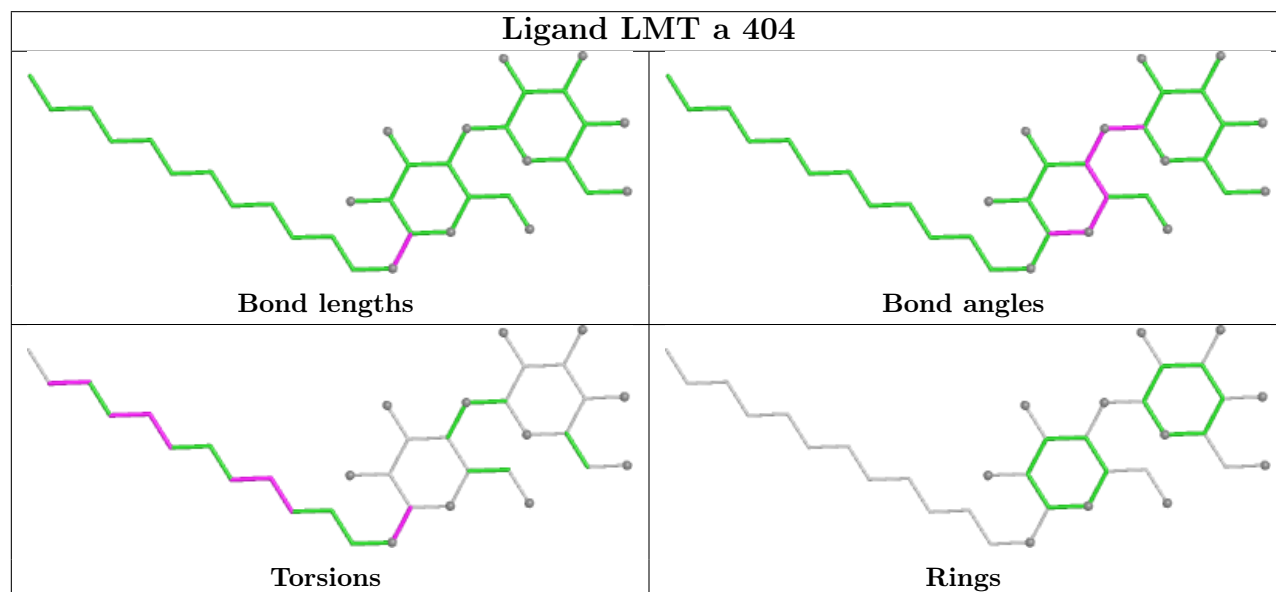
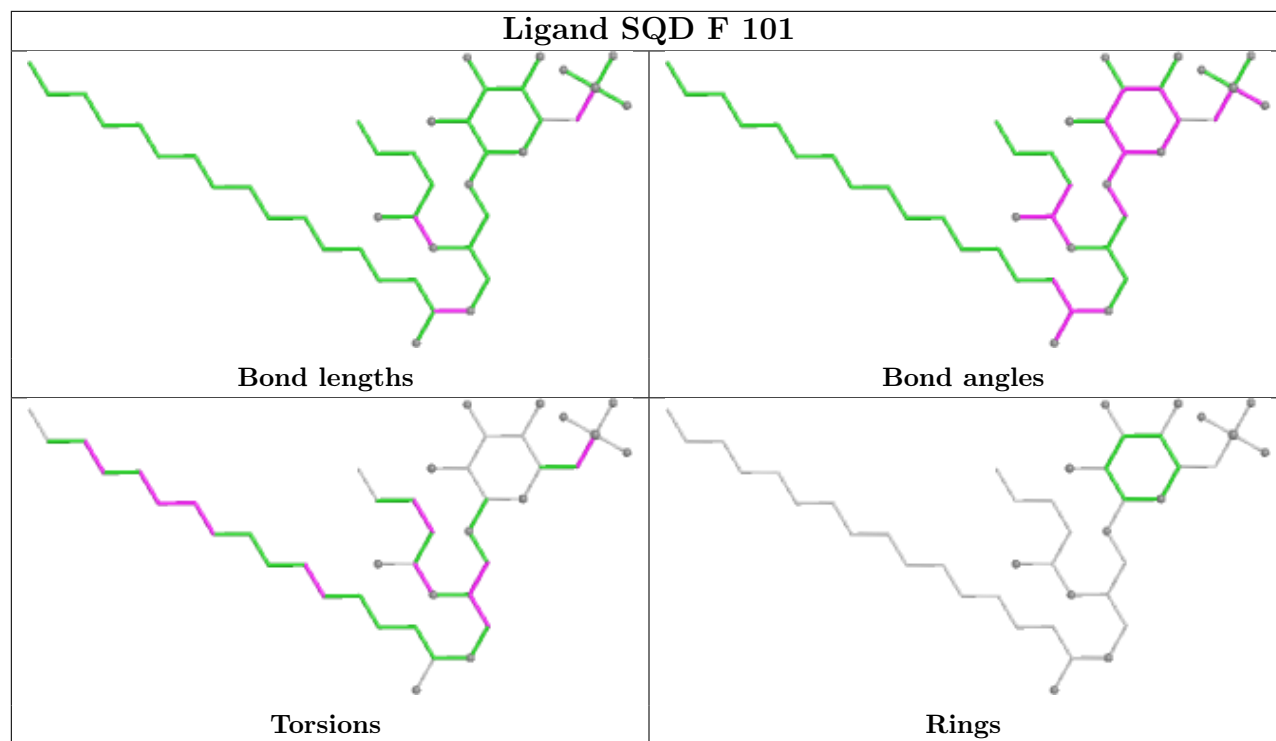
Ligand BCR B 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

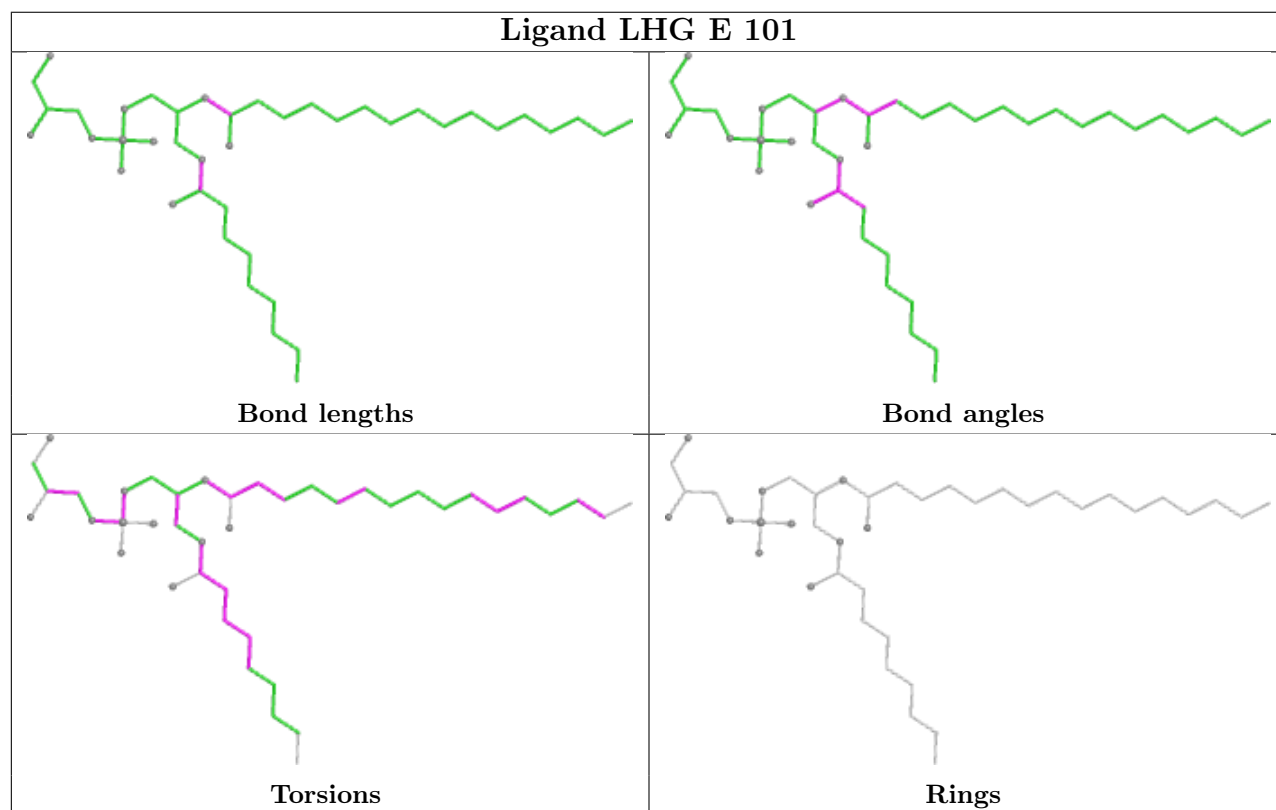
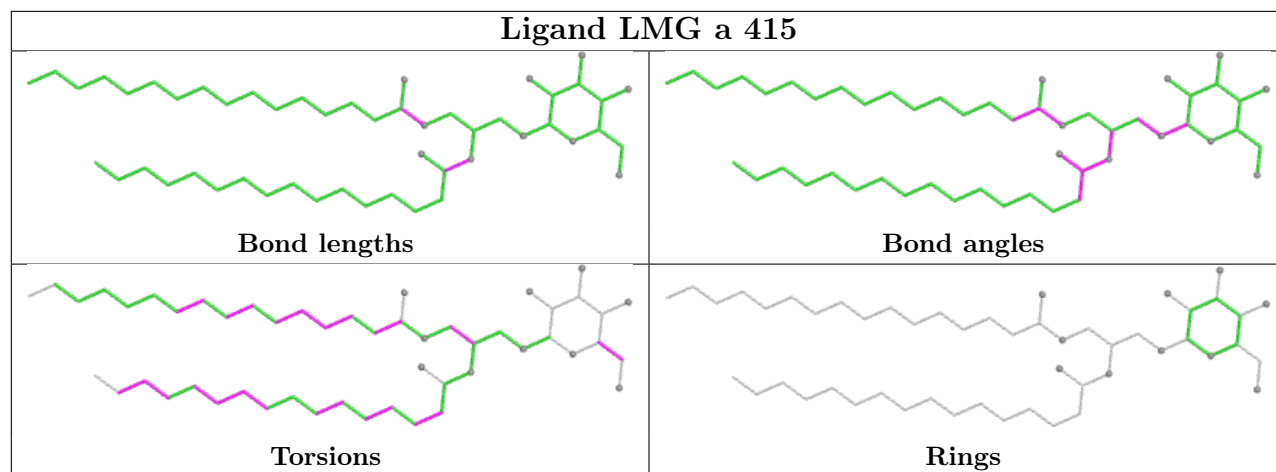
Ligand PL9 D 407 (A)	
	
Bond lengths	Bond angles
	
Torsions	Rings

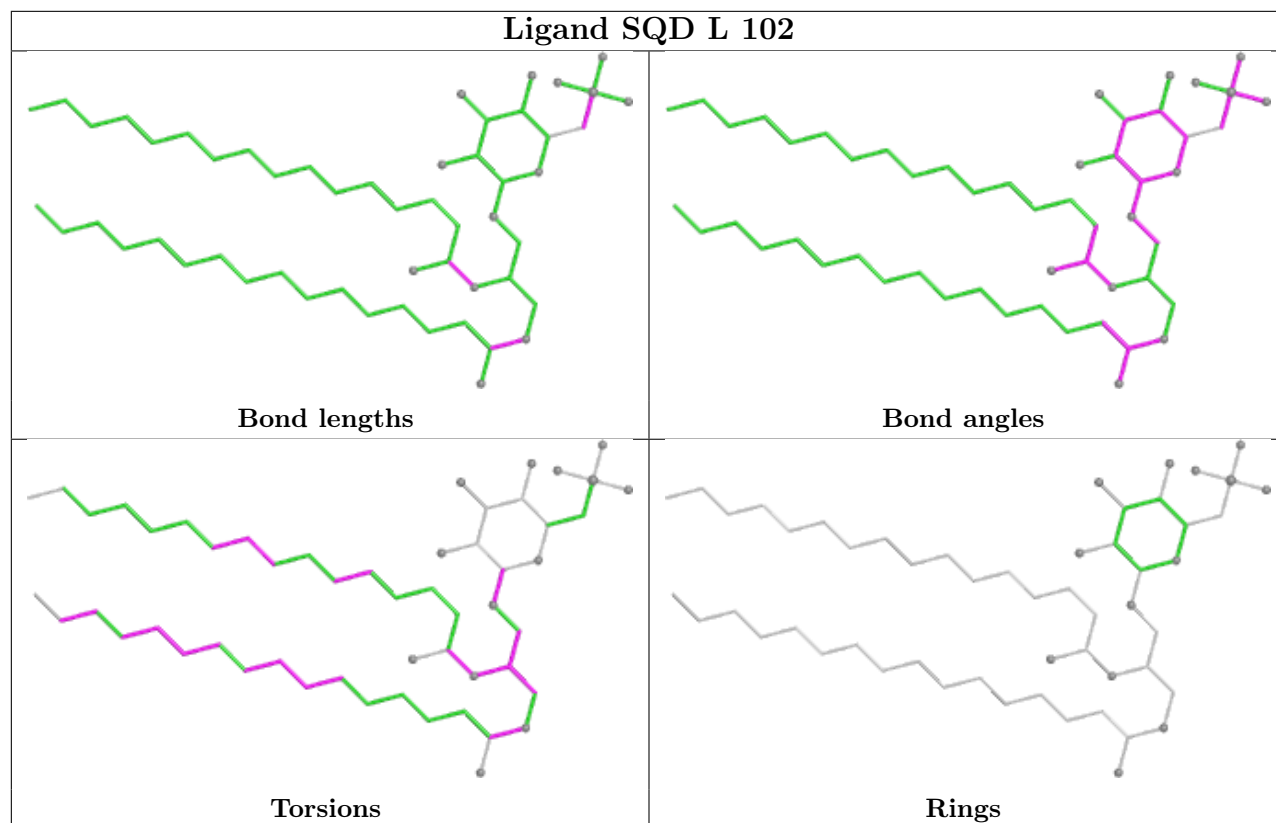
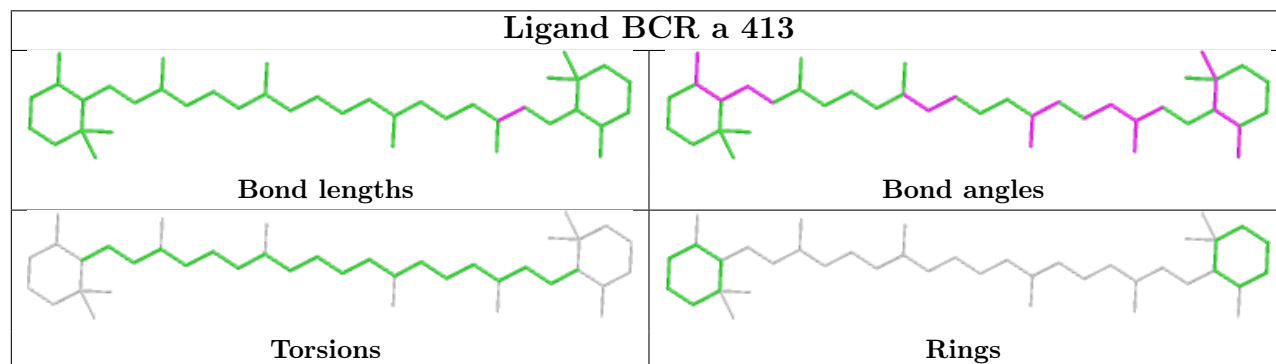
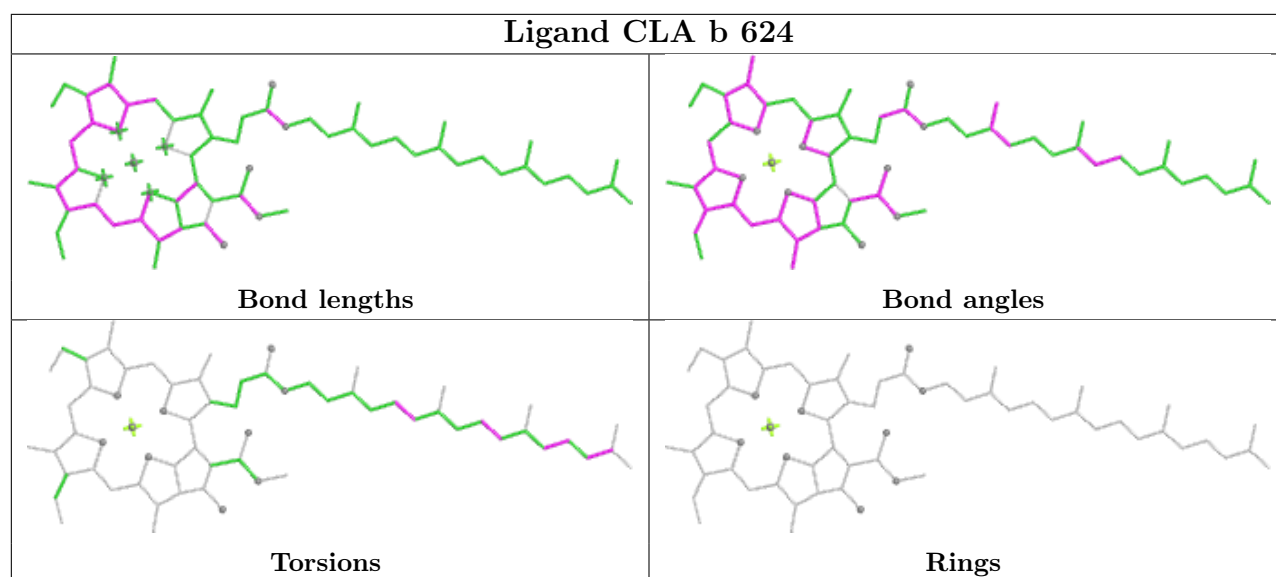


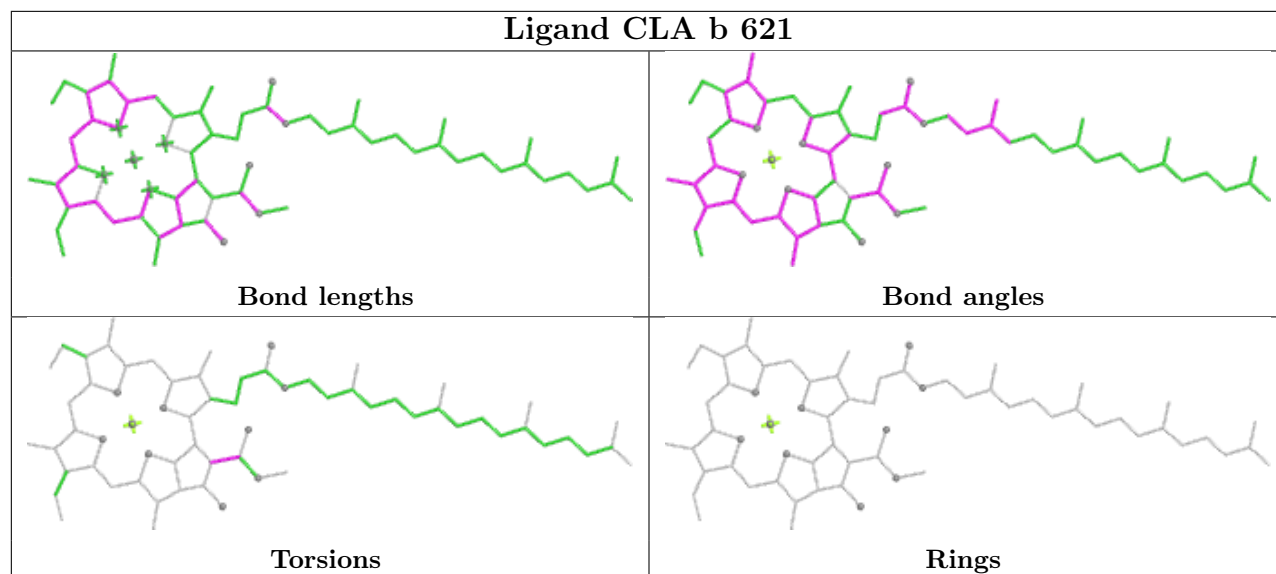
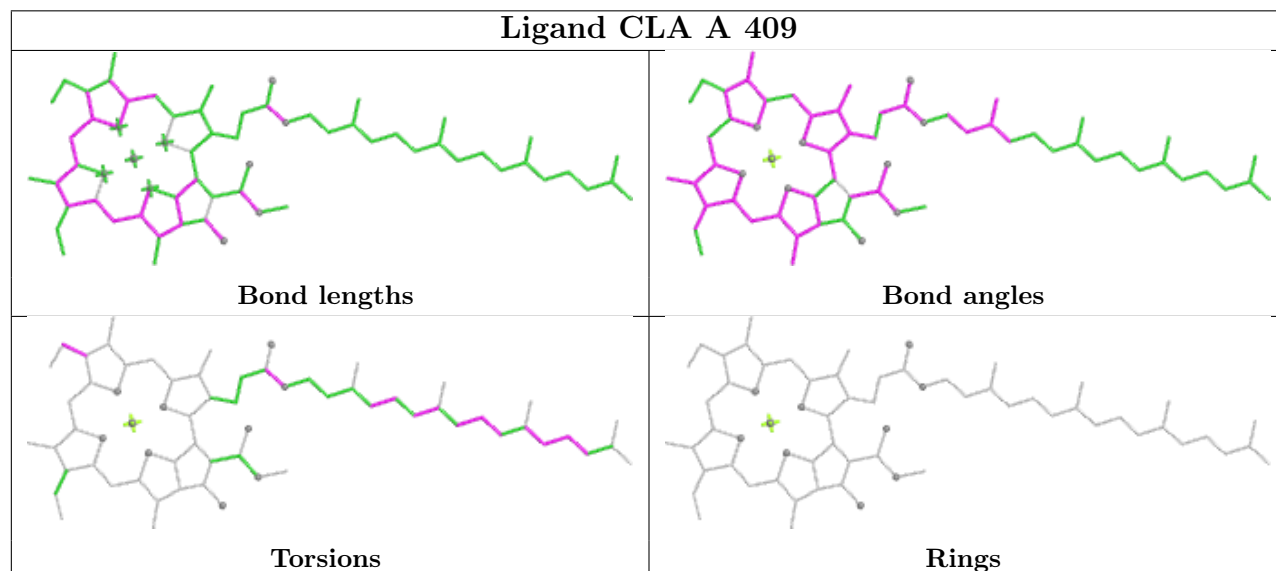
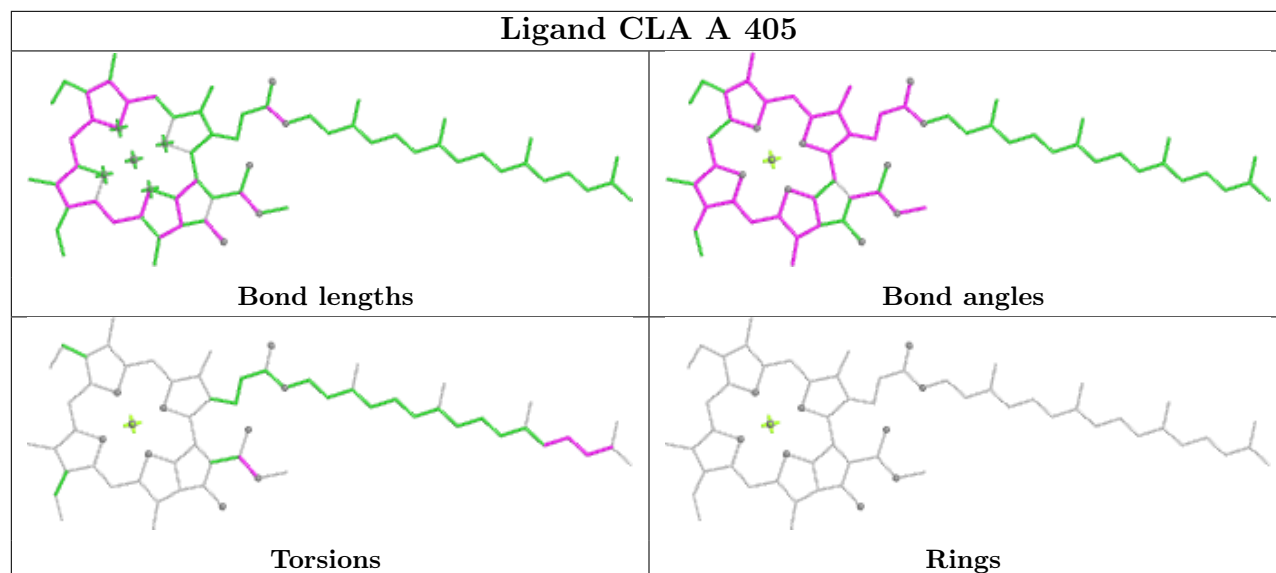




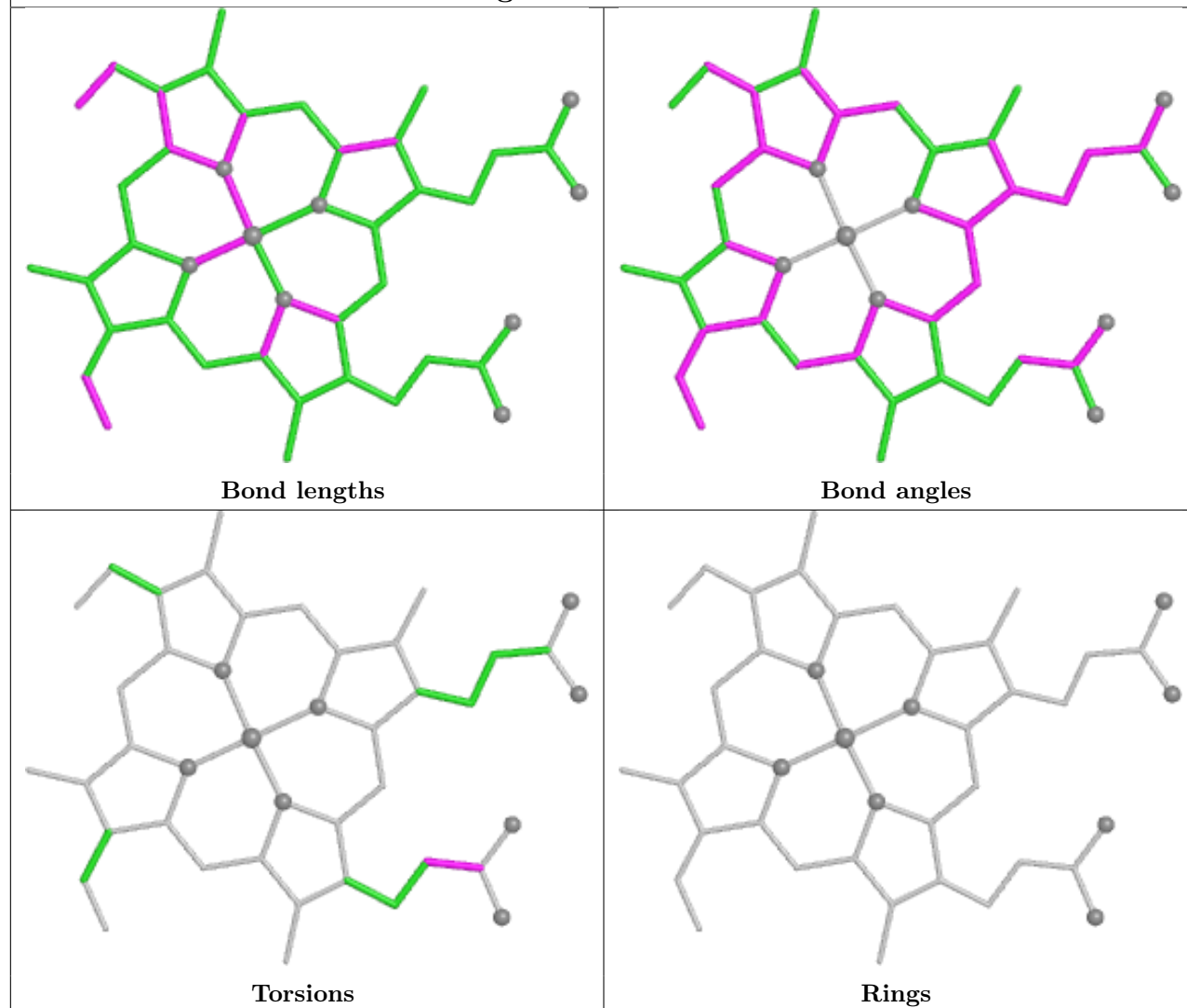




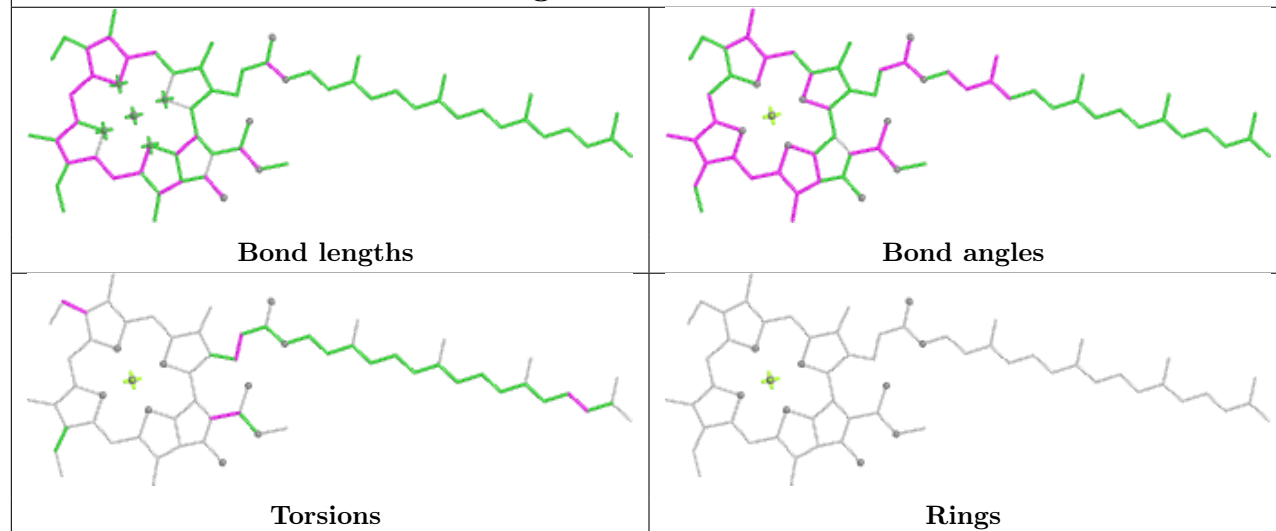


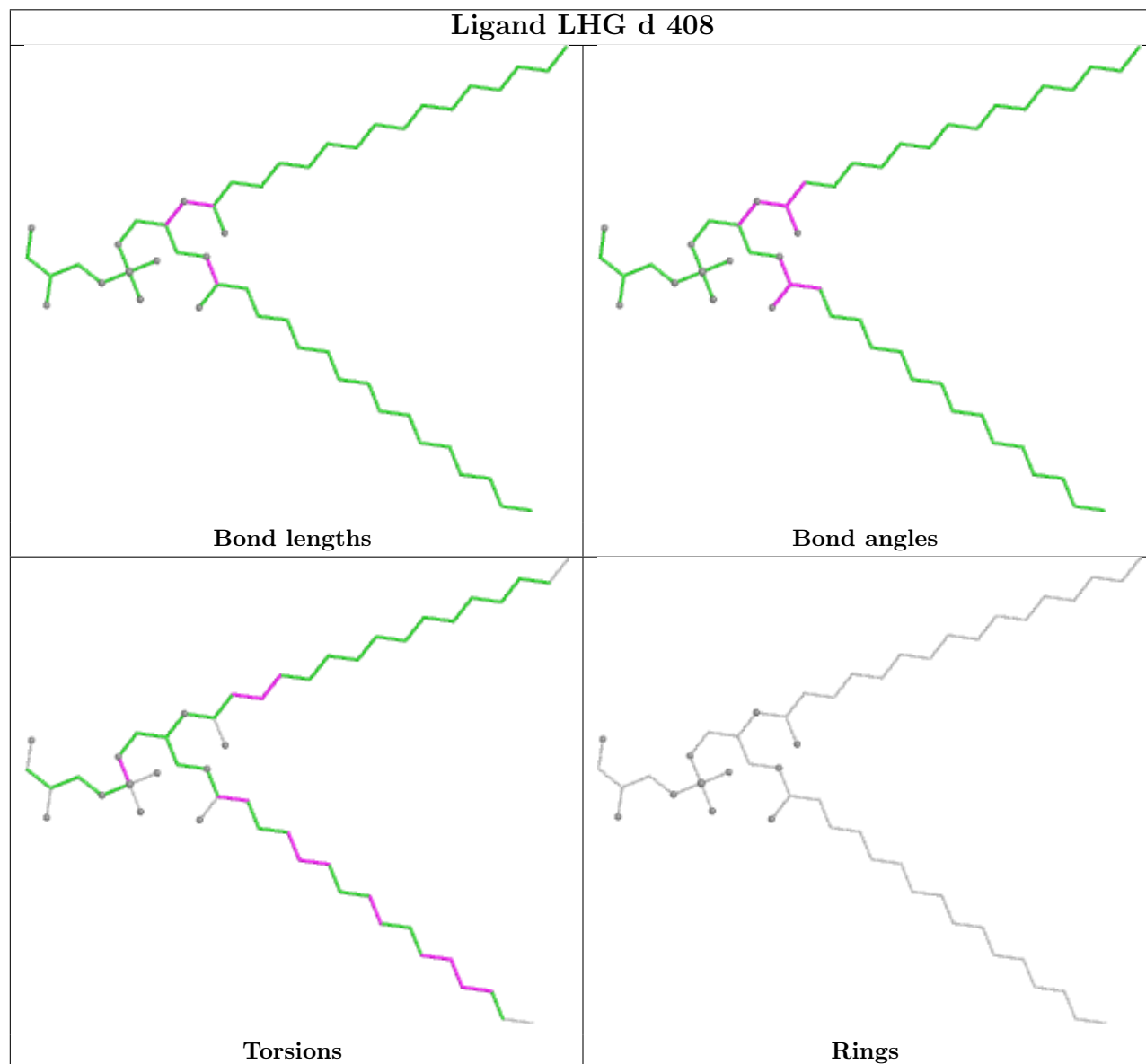
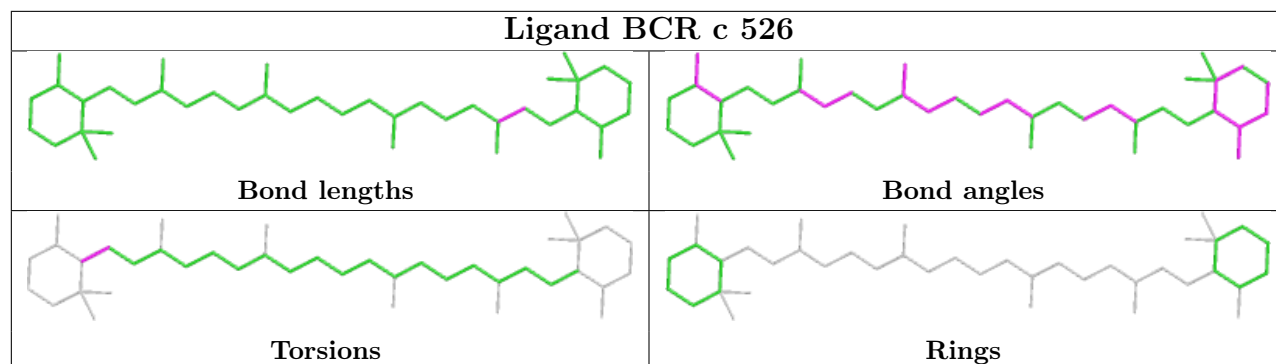
Ligand CLA b 621**Ligand CLA A 409****Ligand CLA A 405**

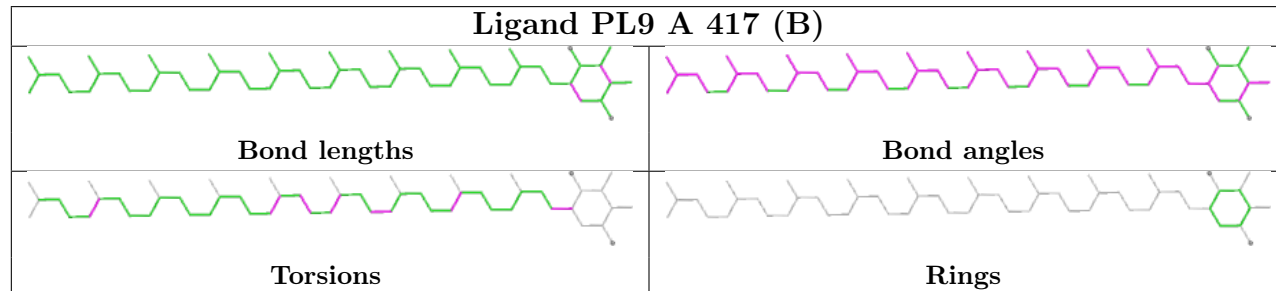
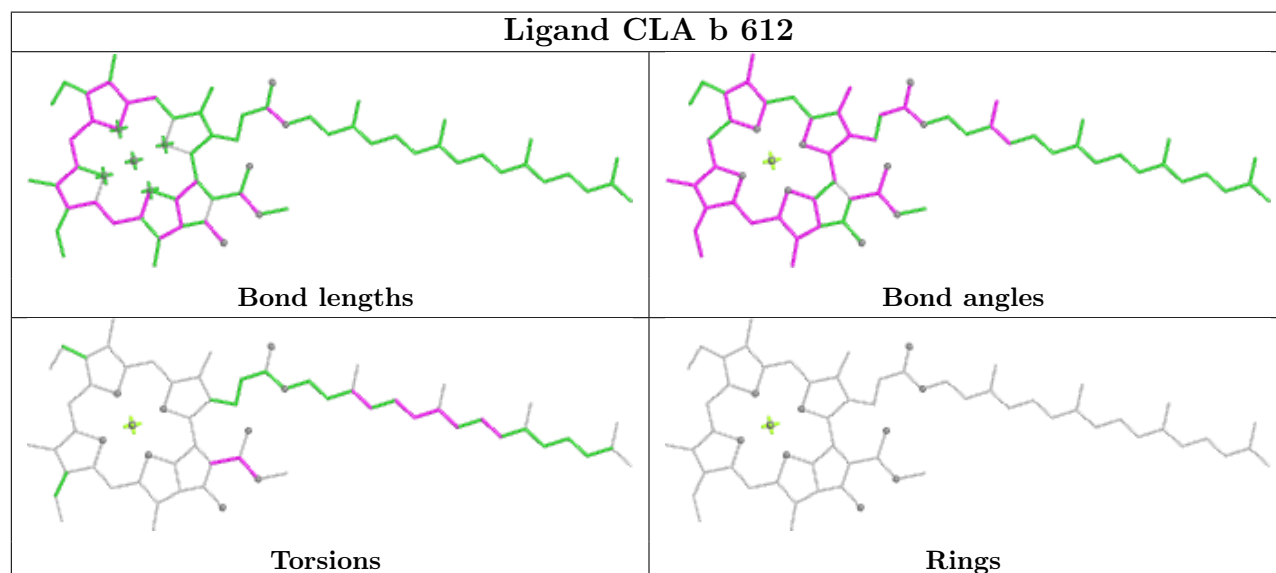
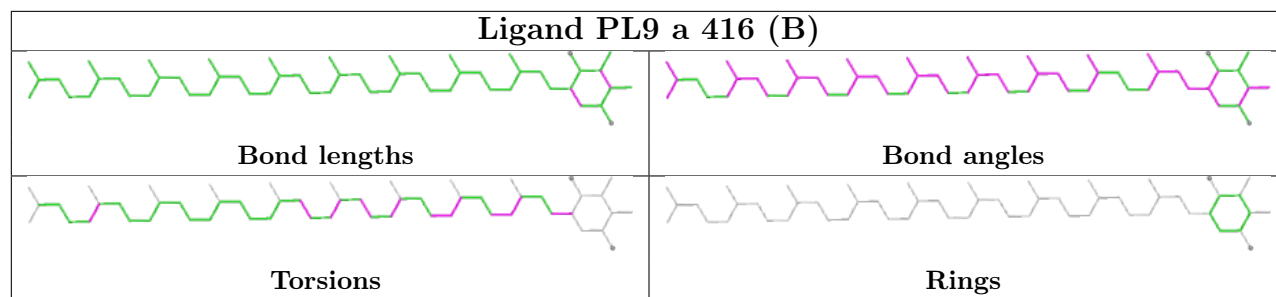
Ligand HEC v 206

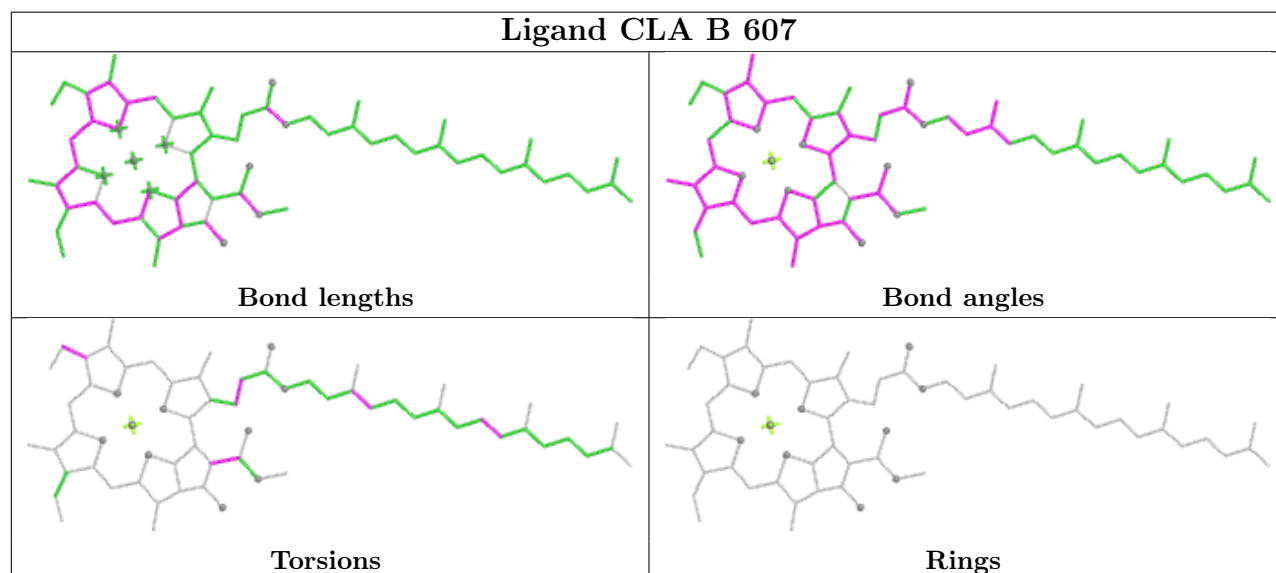
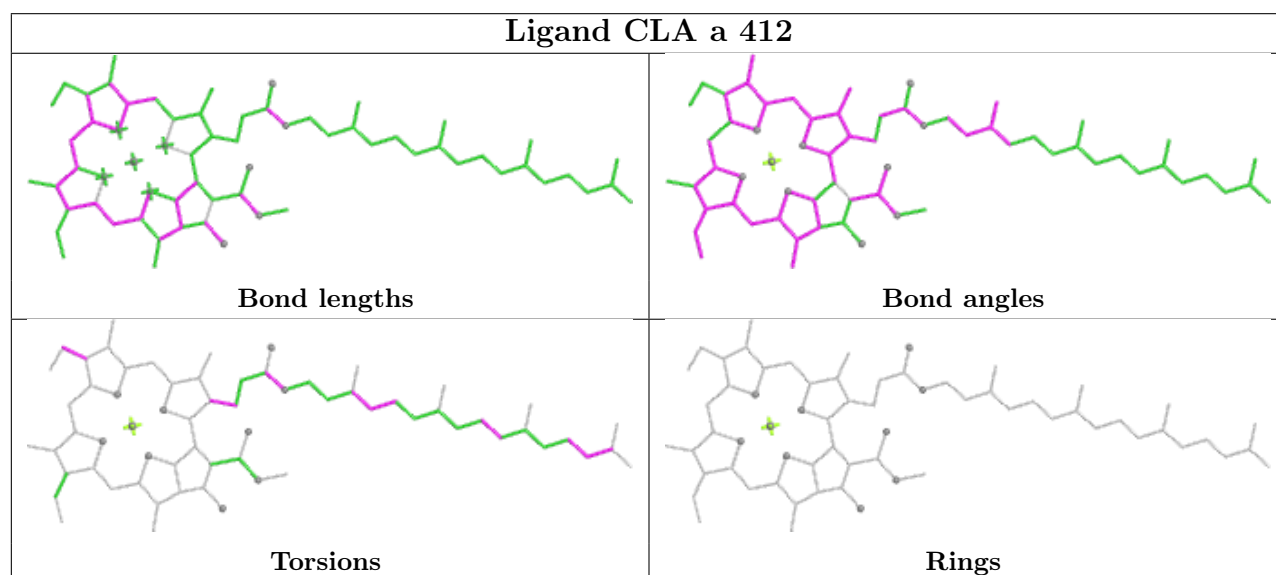
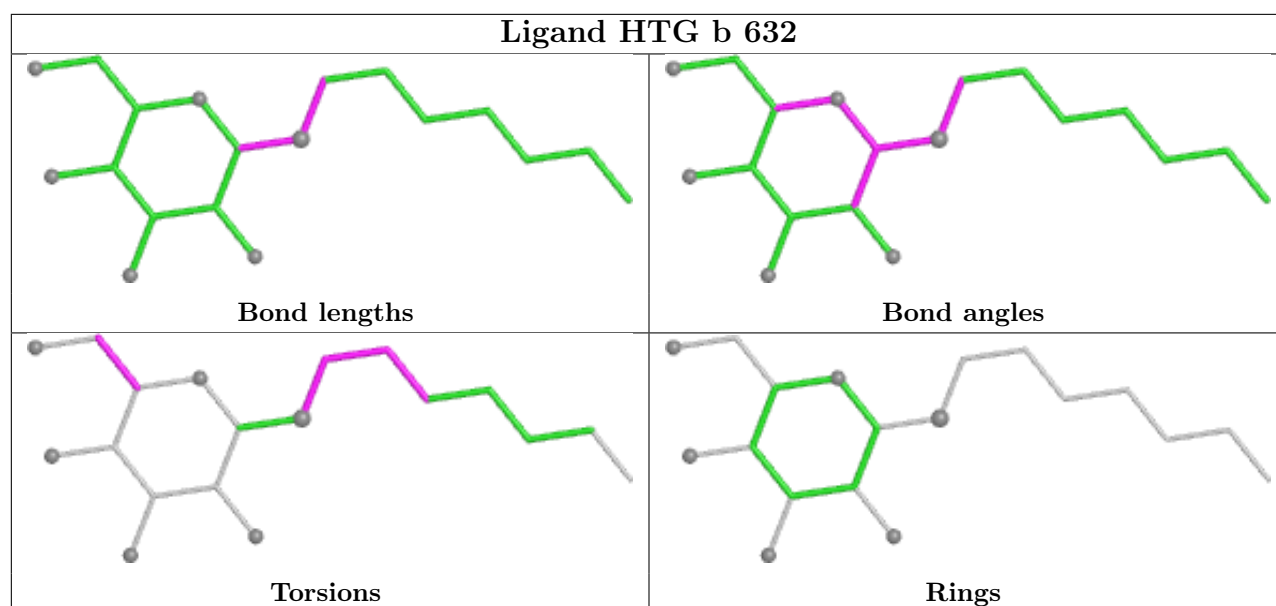


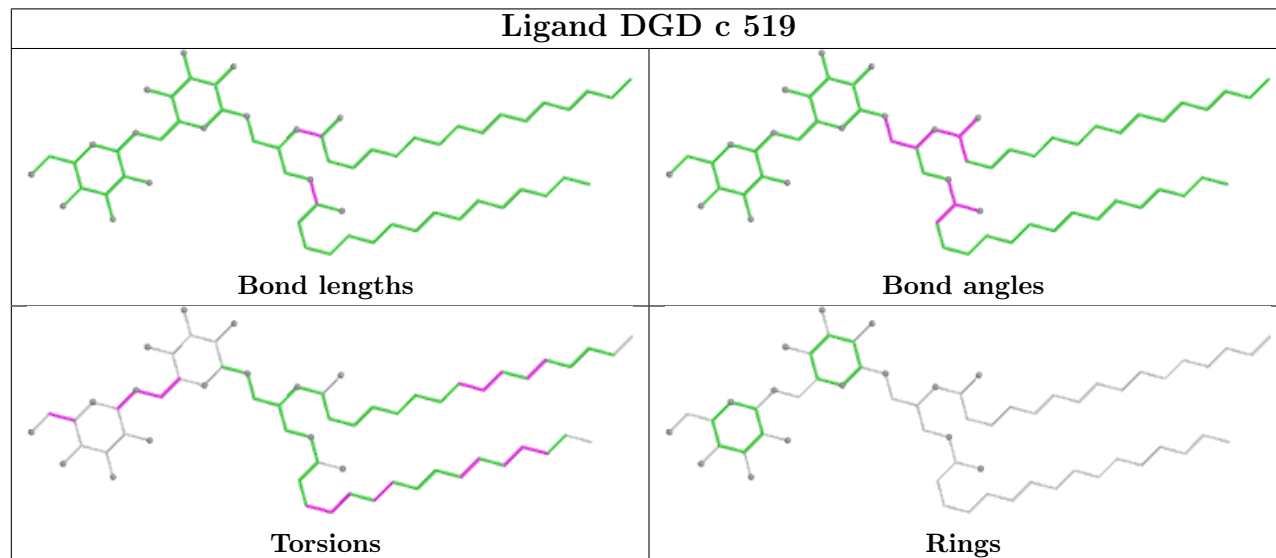
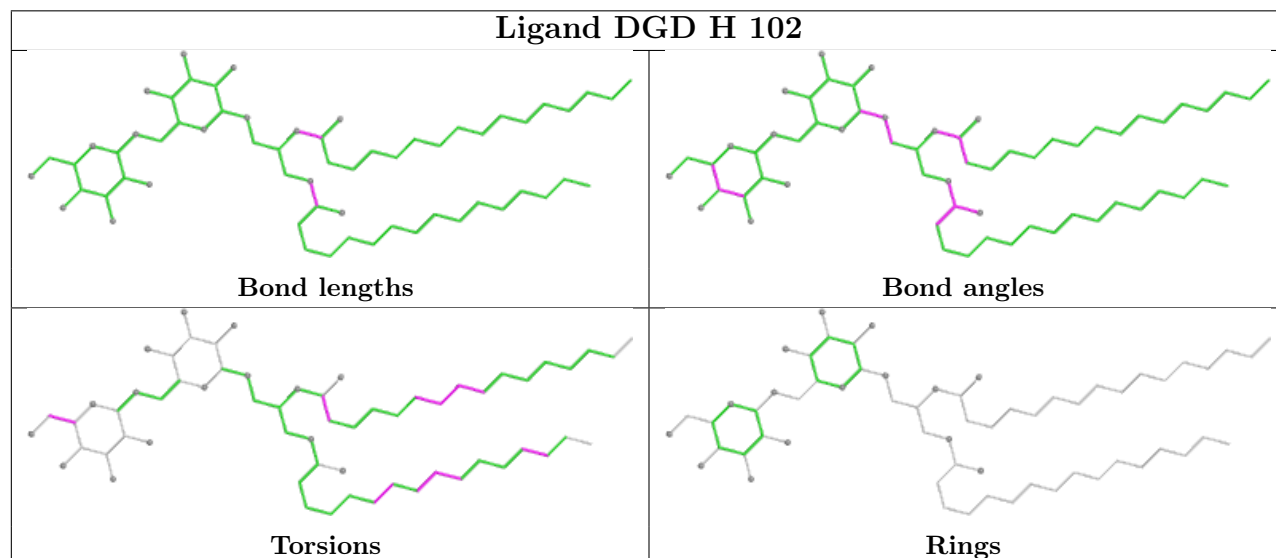
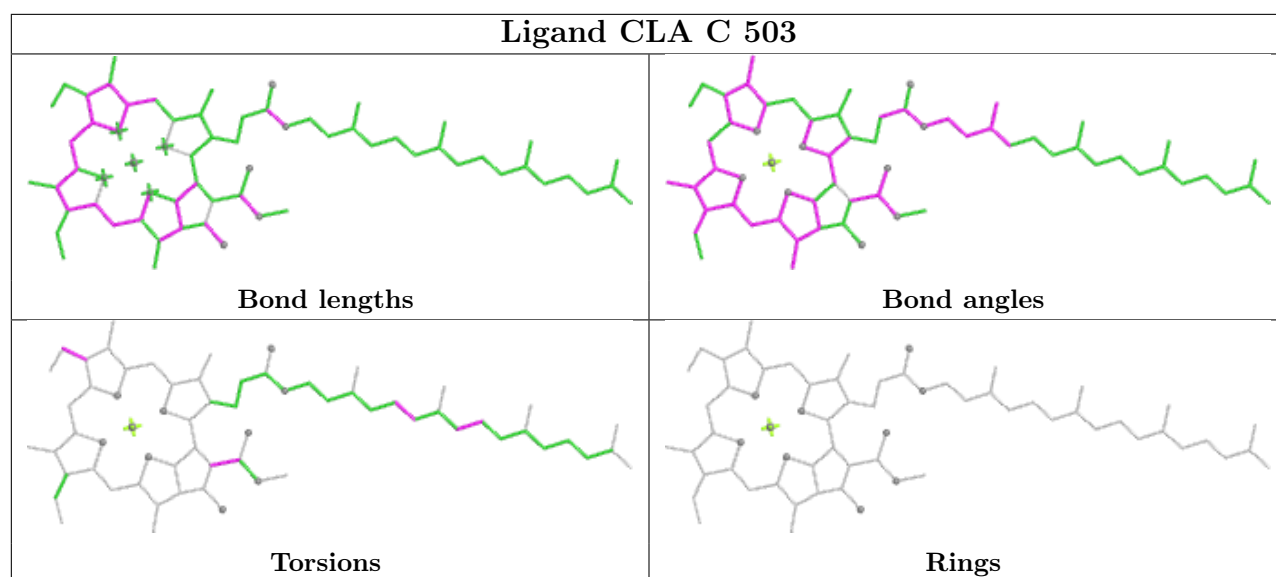
Ligand CLA C 507

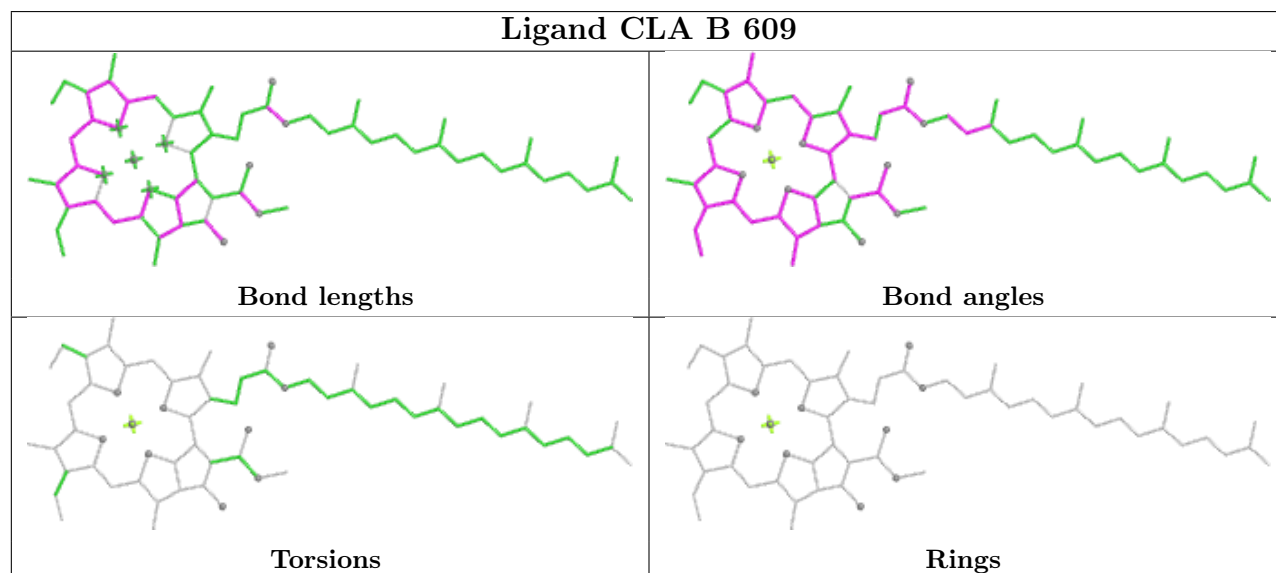
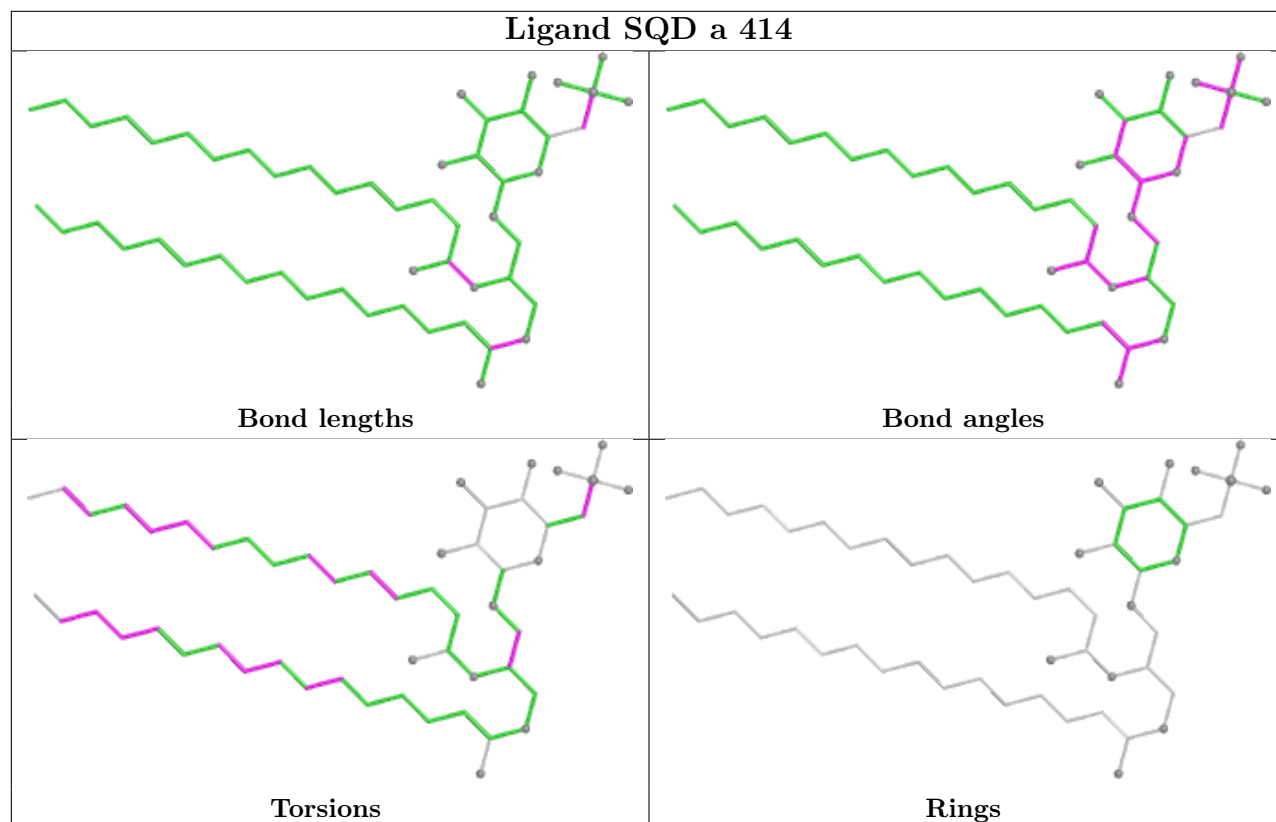


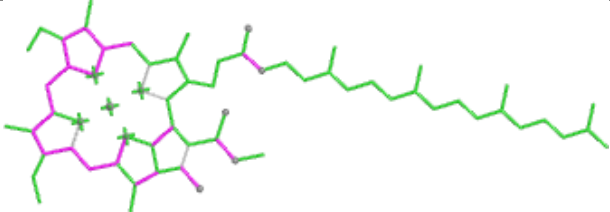
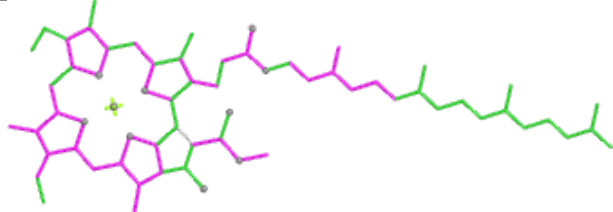
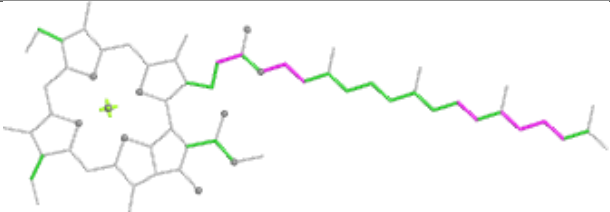
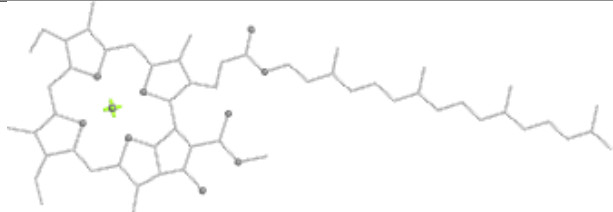
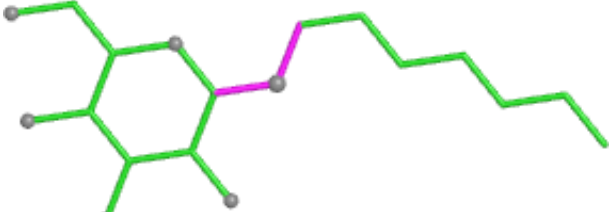
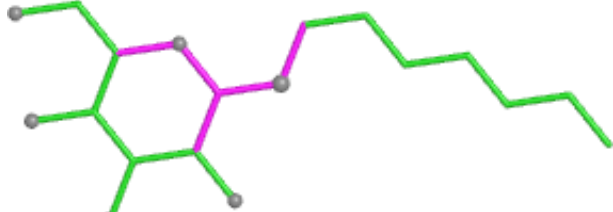
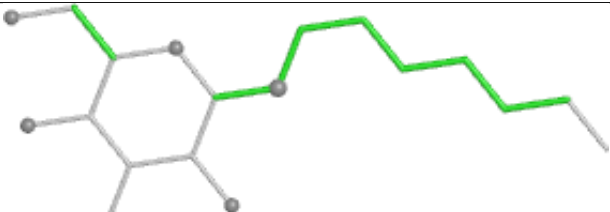
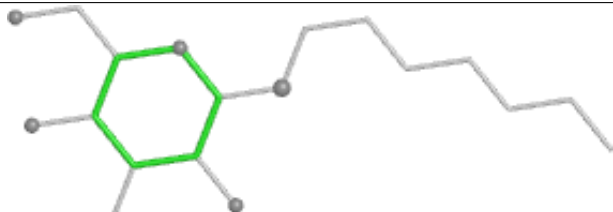
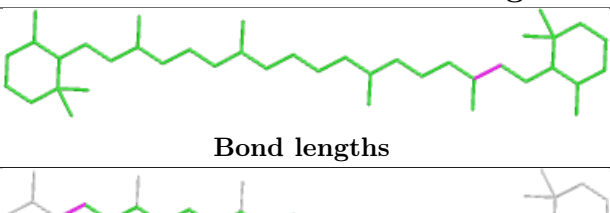
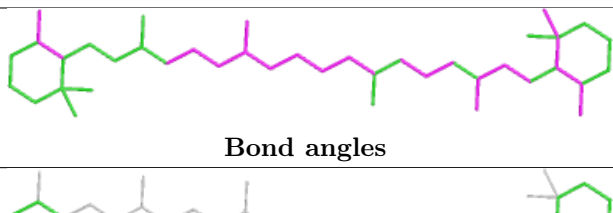
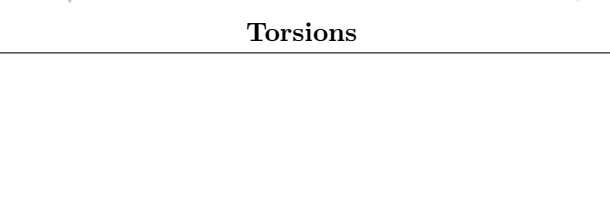
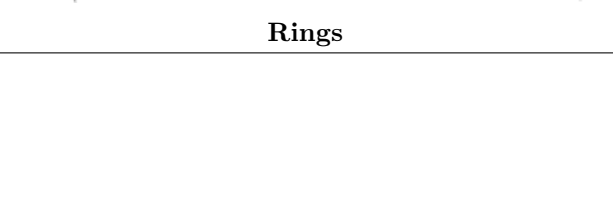


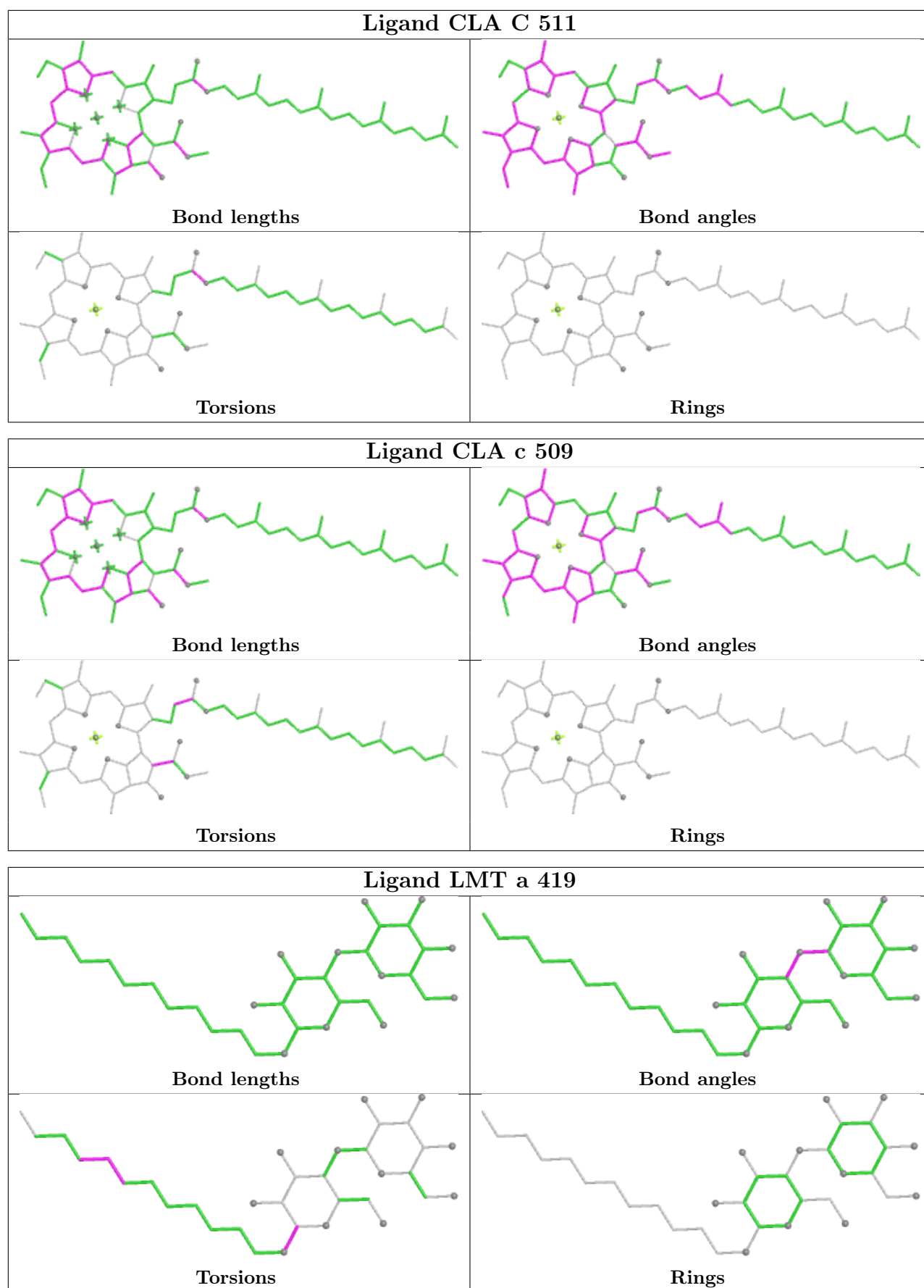


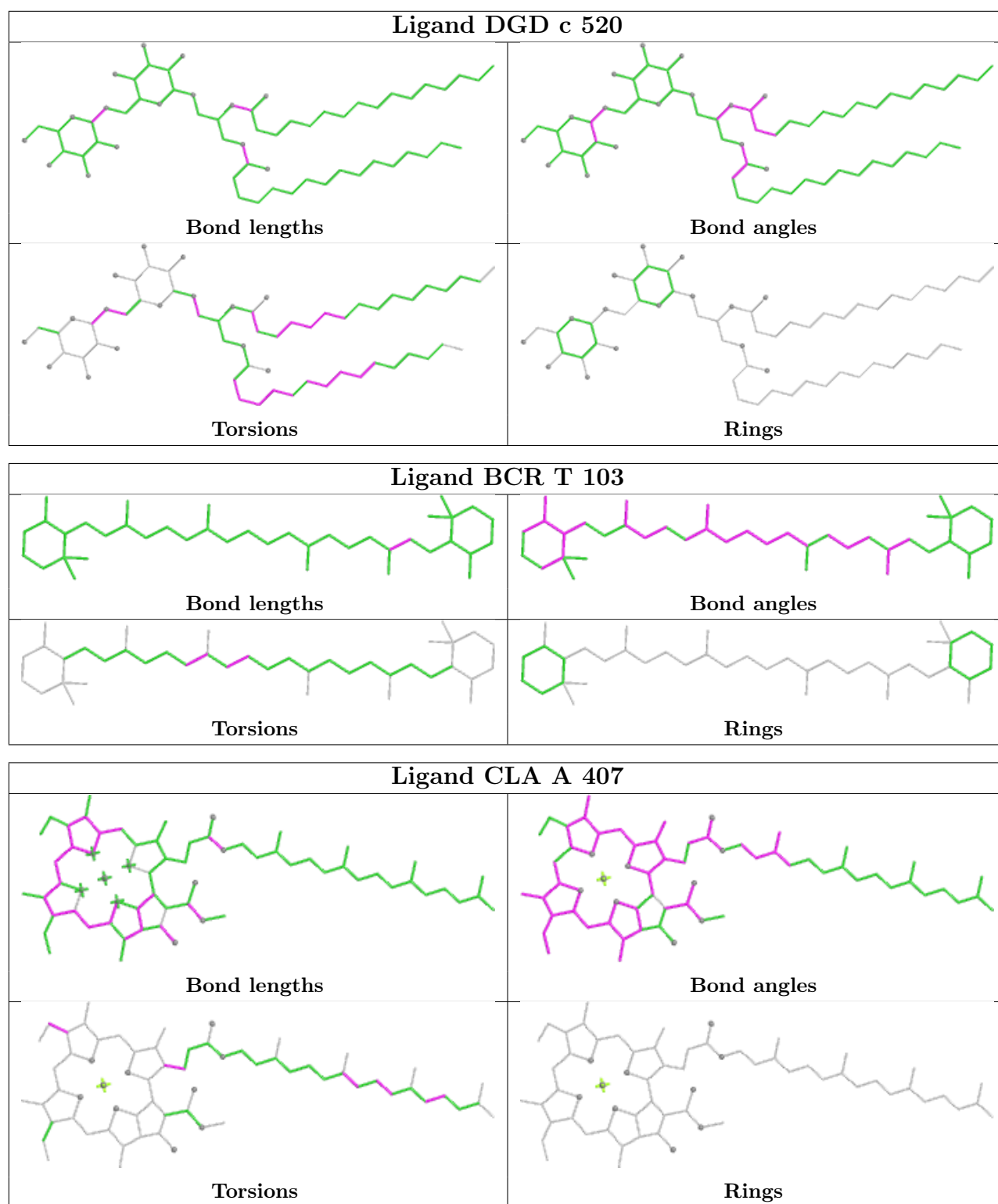


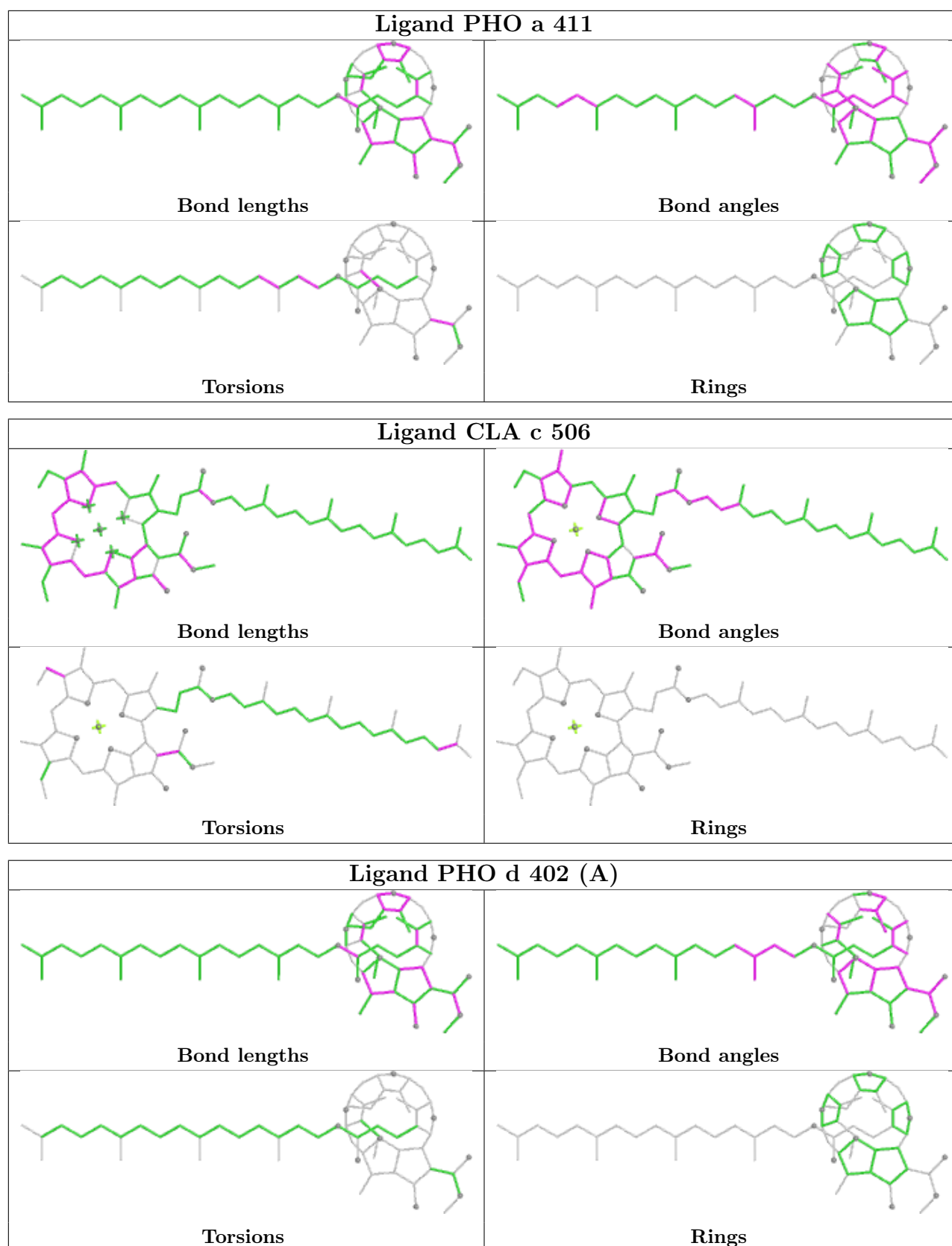


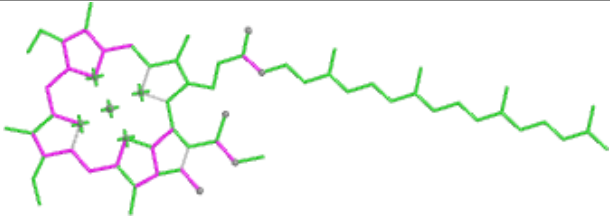
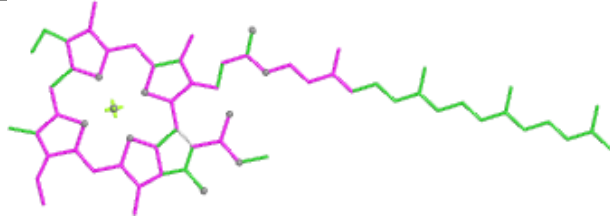
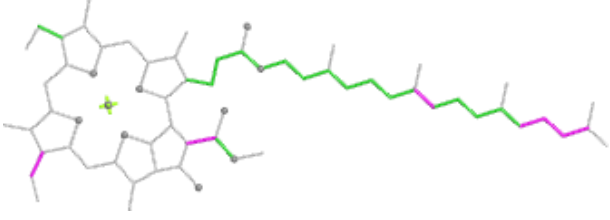
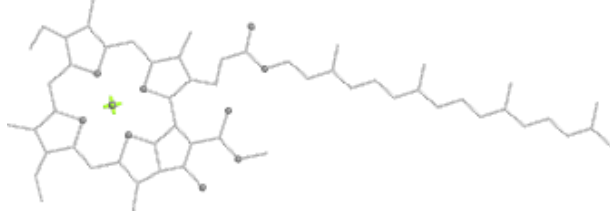
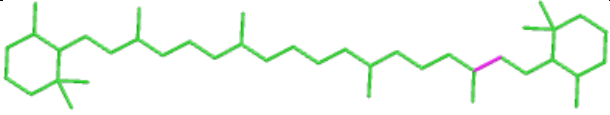
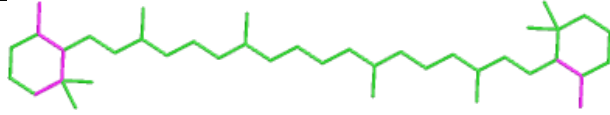
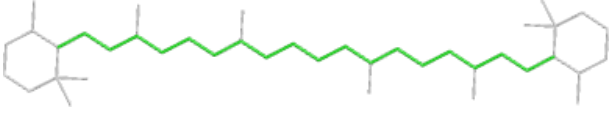
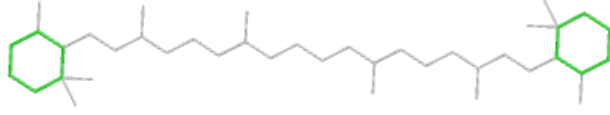
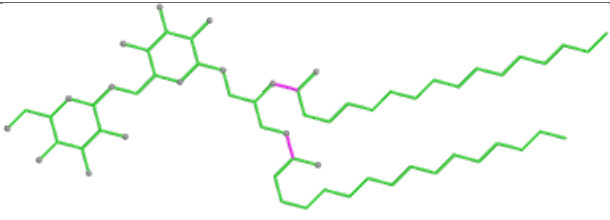
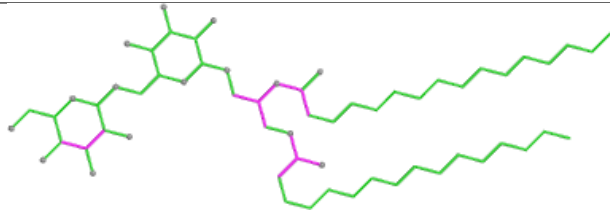
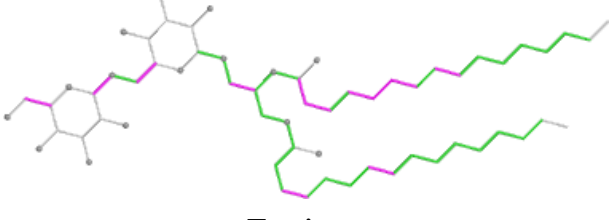
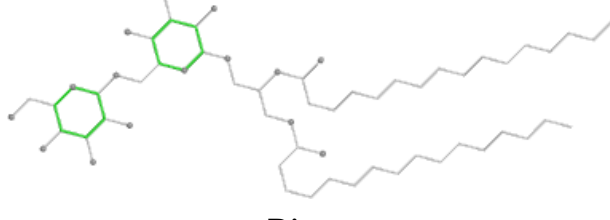


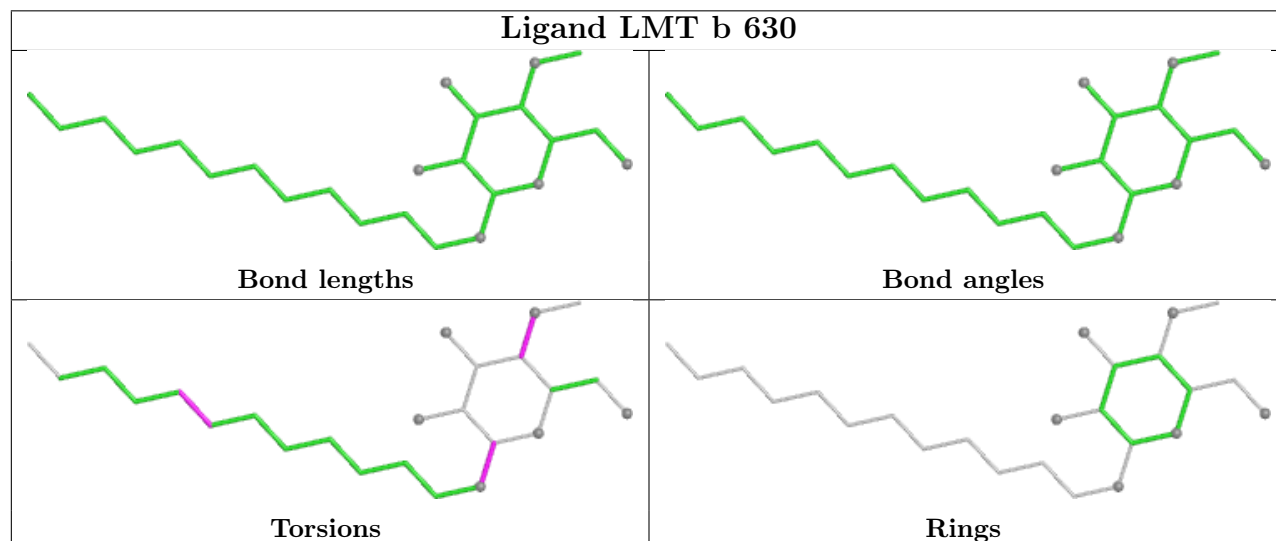
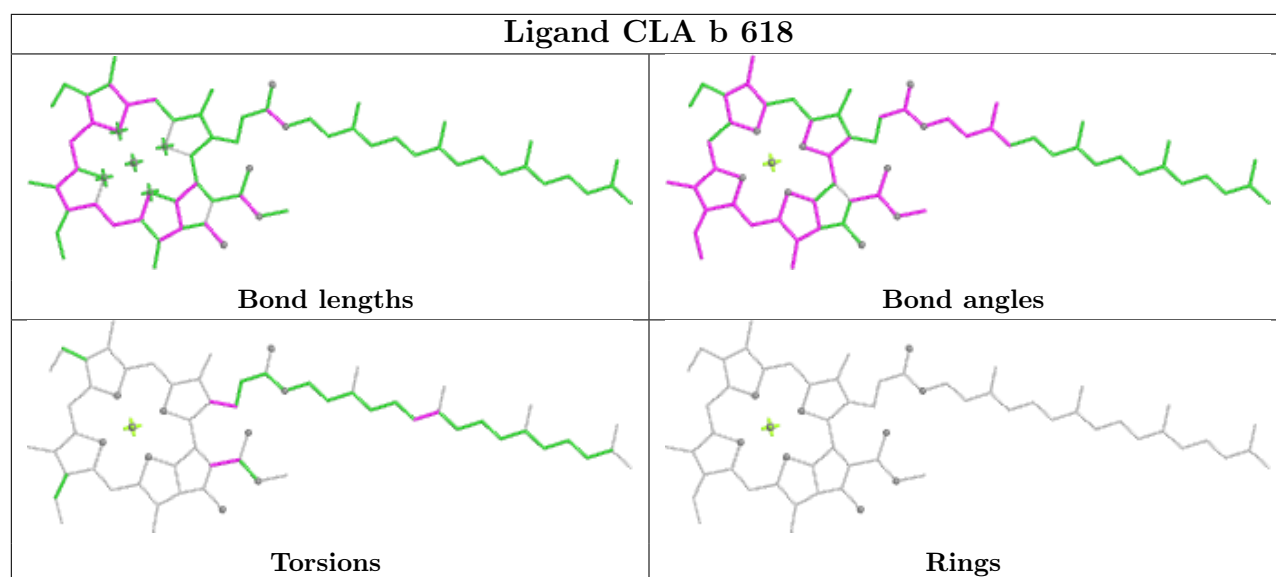
Ligand CLA B 614	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand HTG b 608	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR Y 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

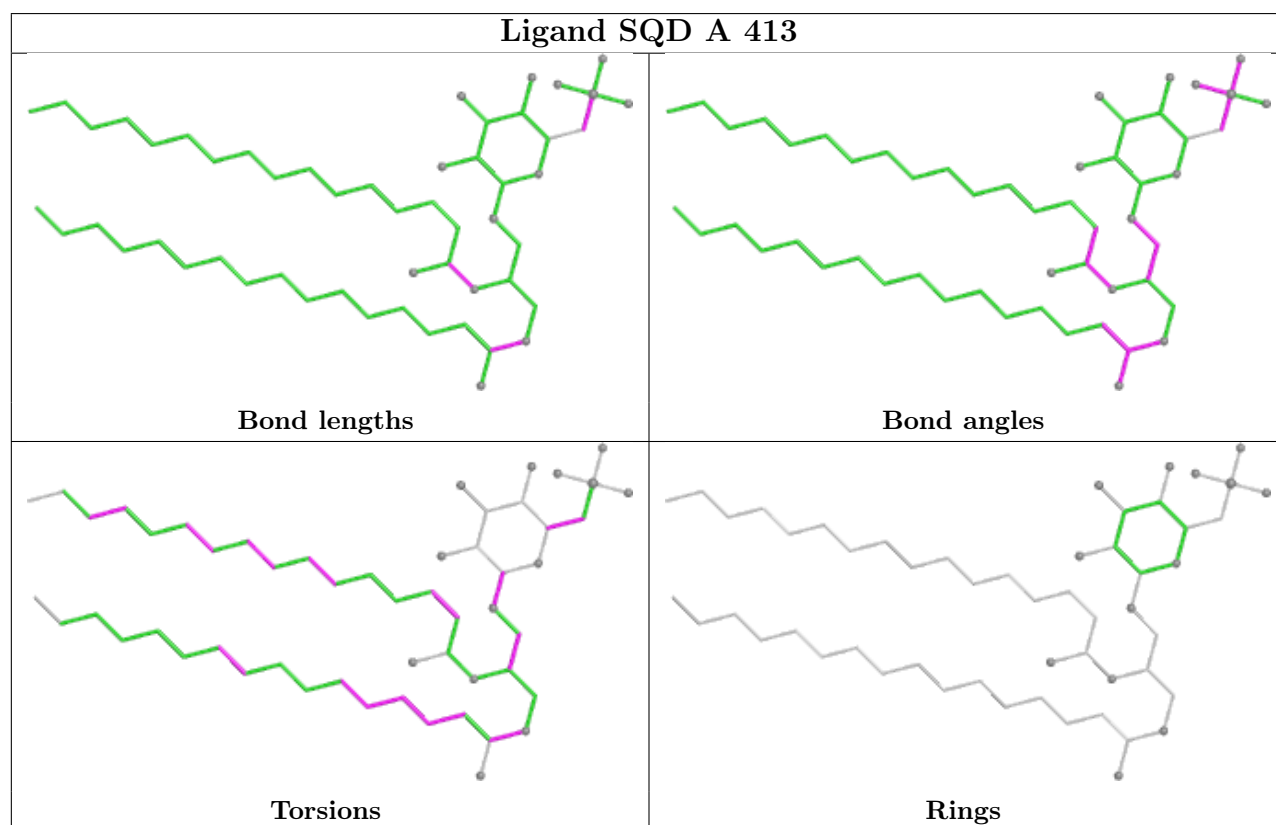
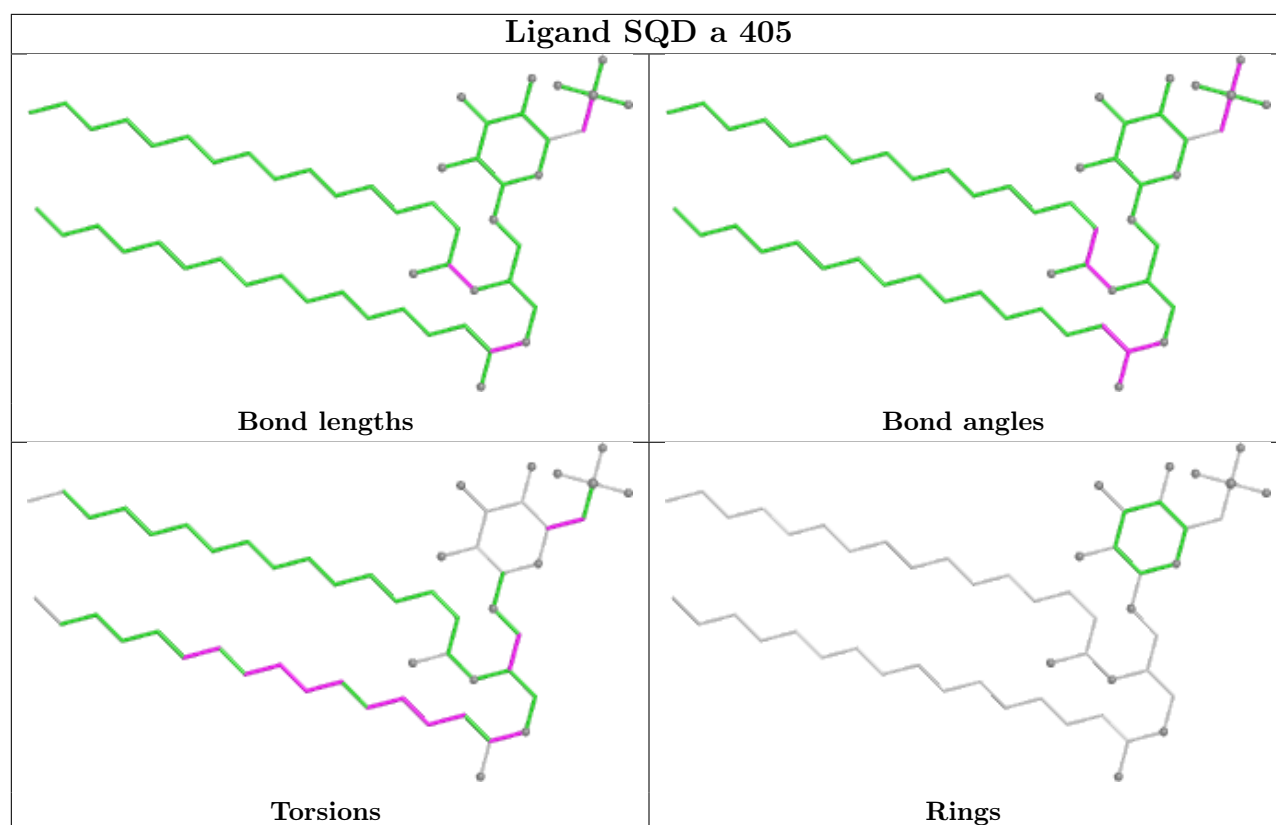


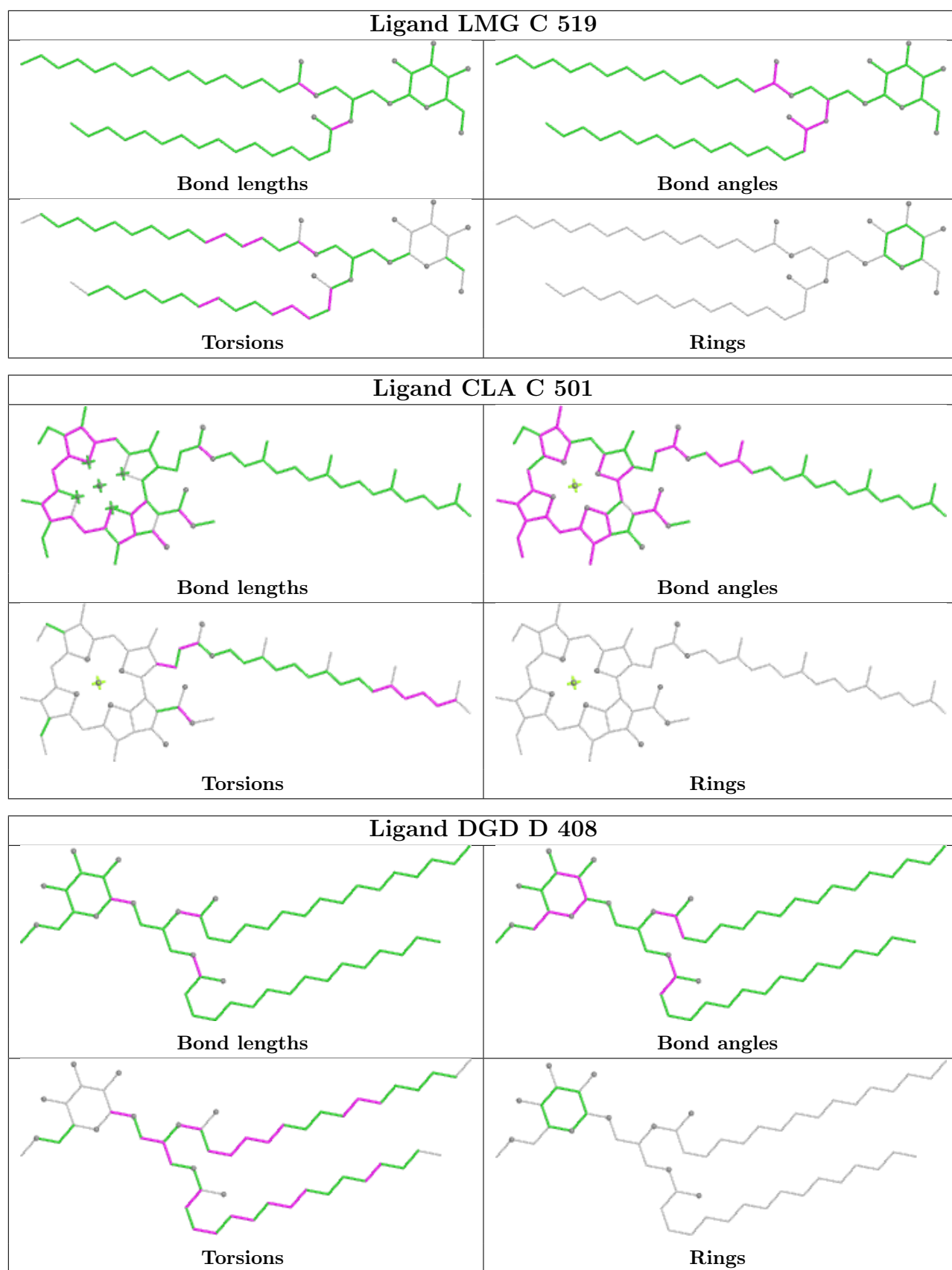


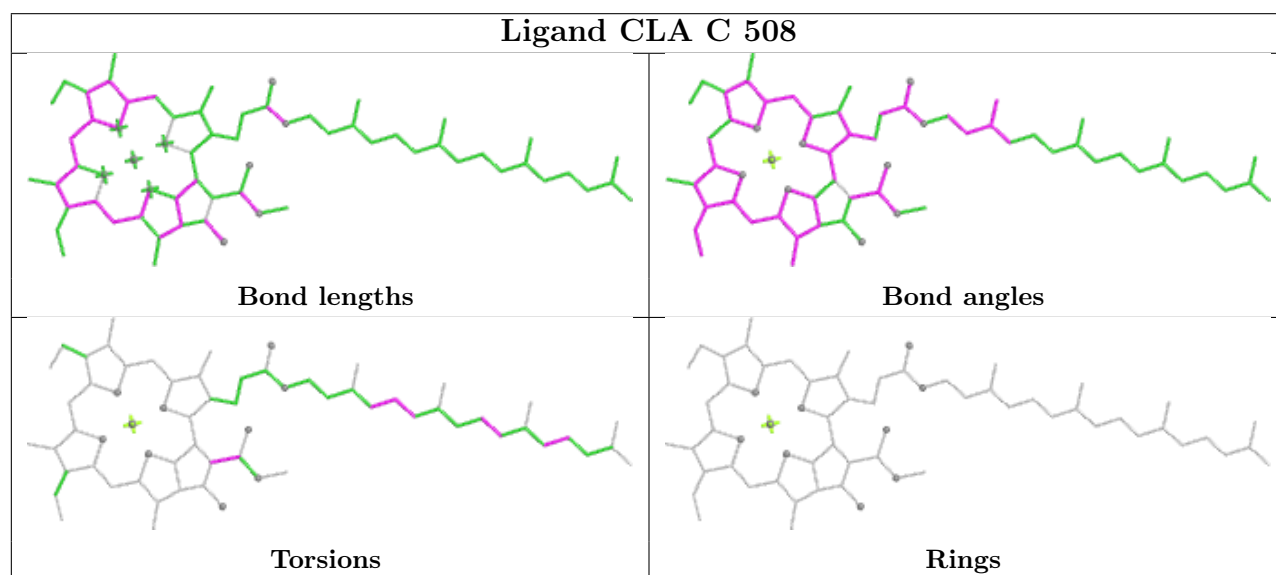
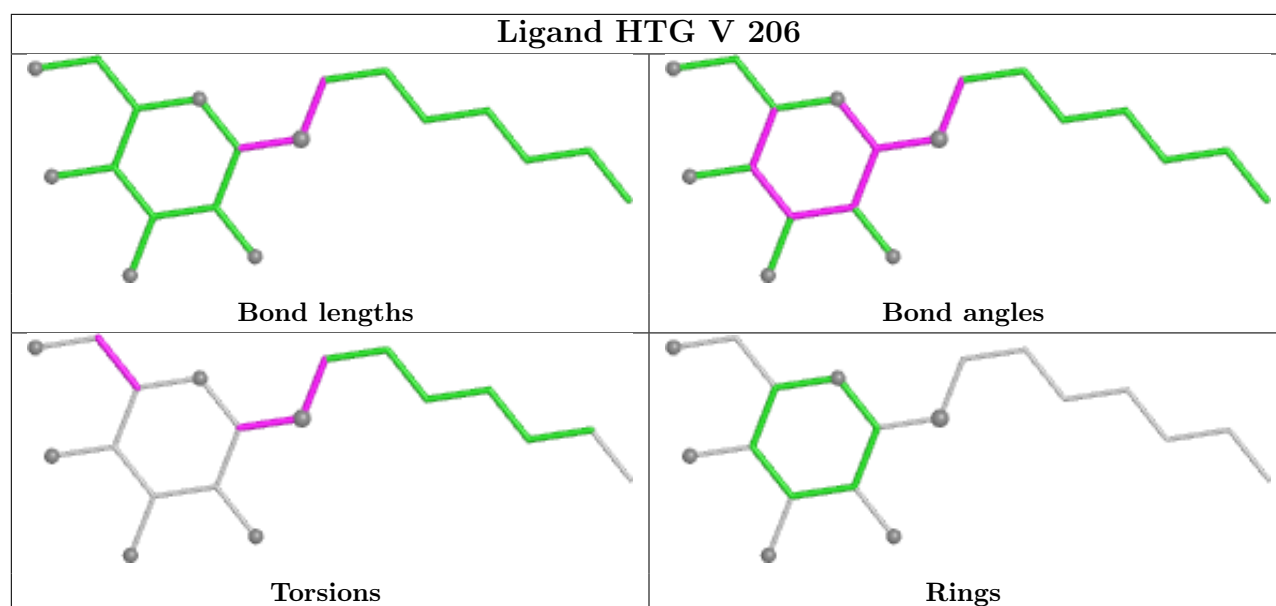


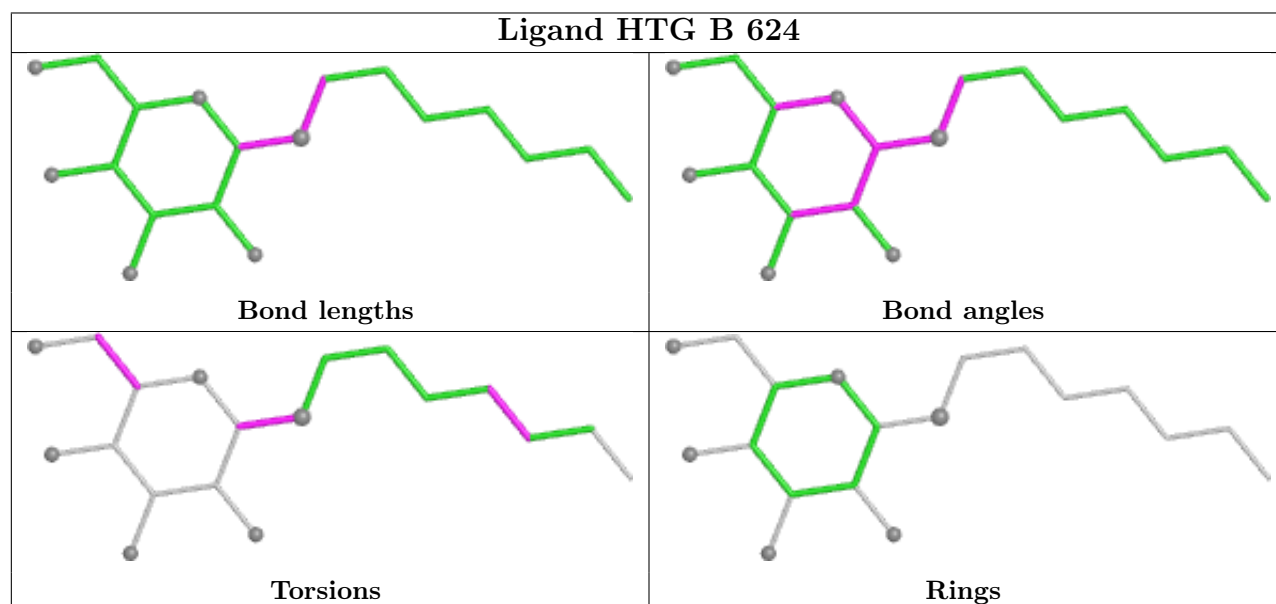
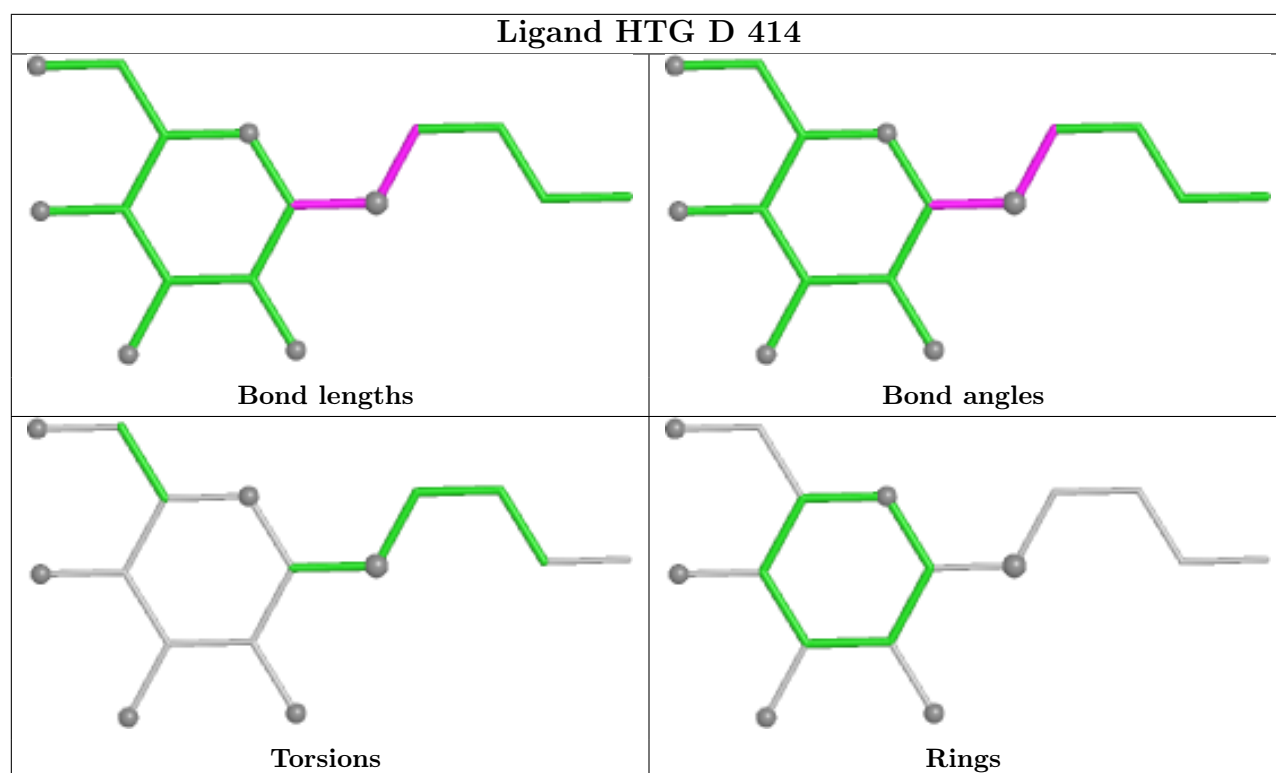
Ligand CLA d 403	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR A 410	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand DGD C 516	
 Bond lengths	 Bond angles
 Torsions	 Rings

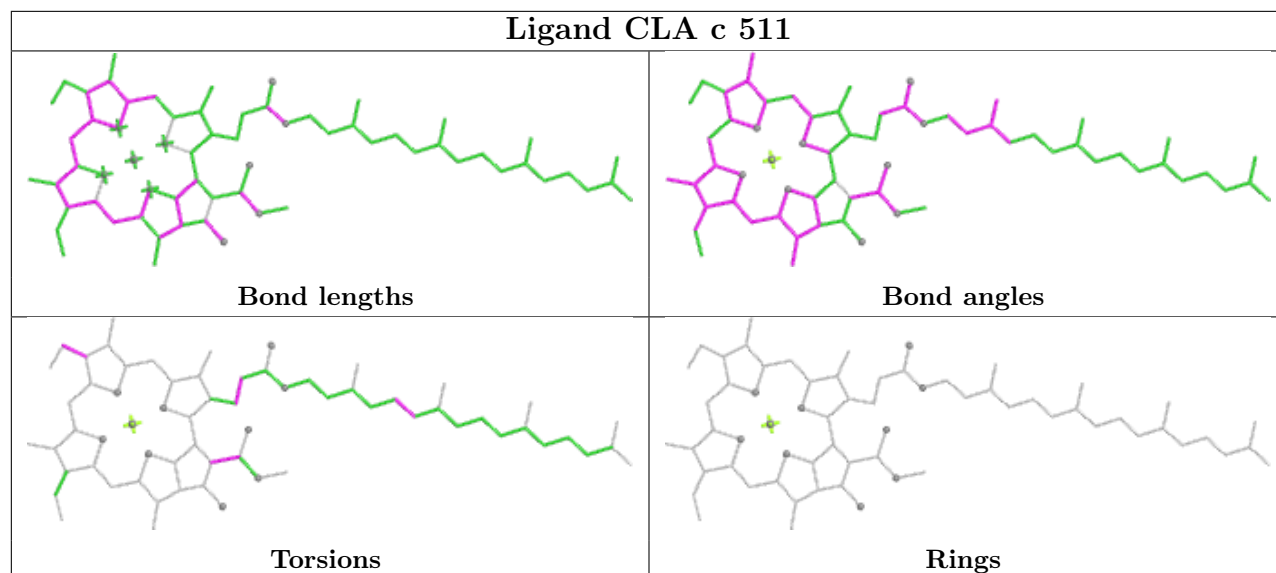
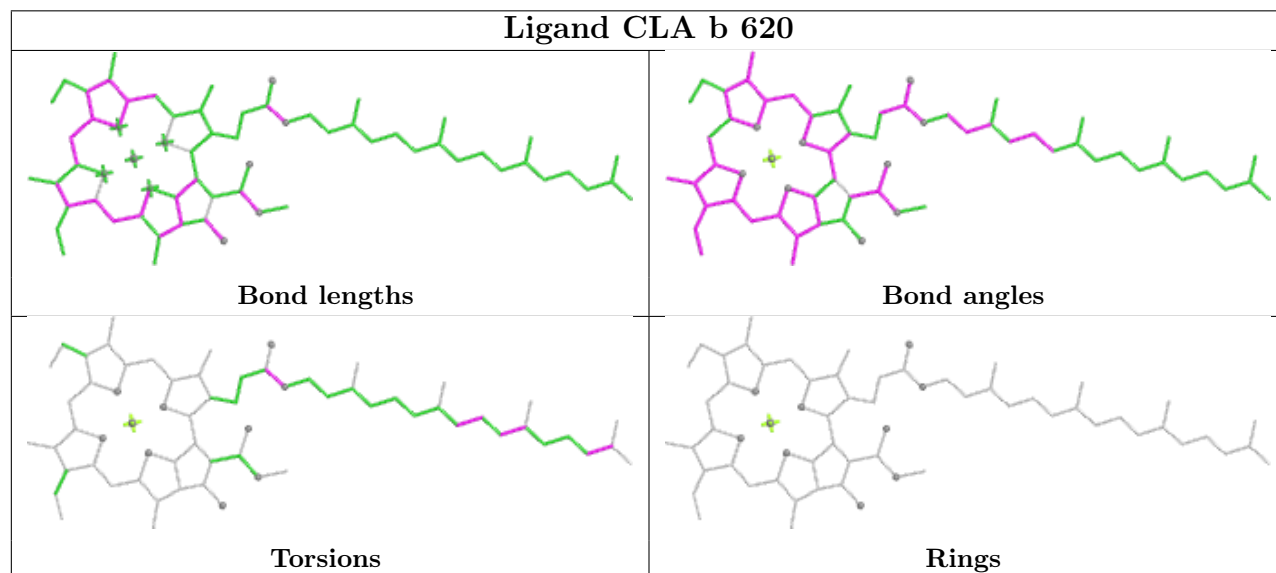
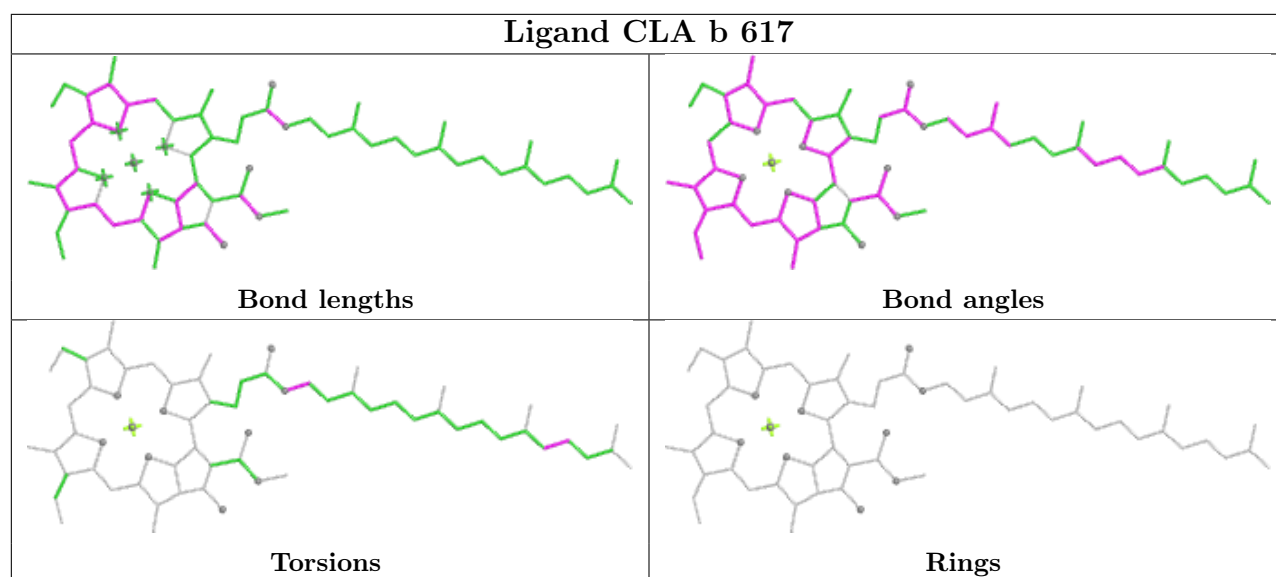


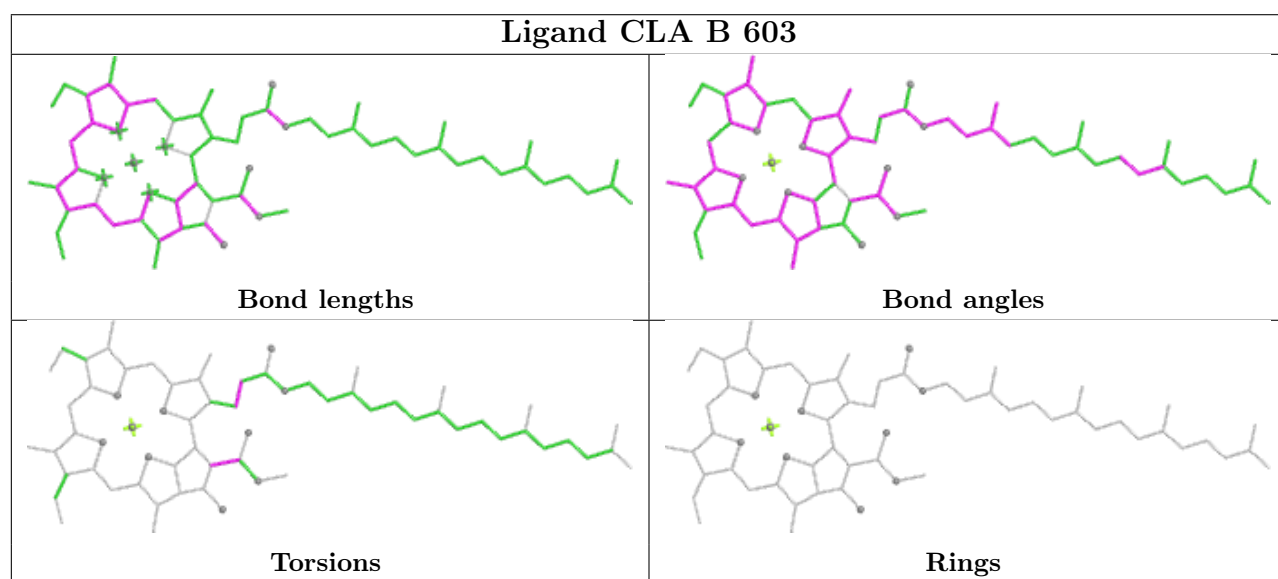
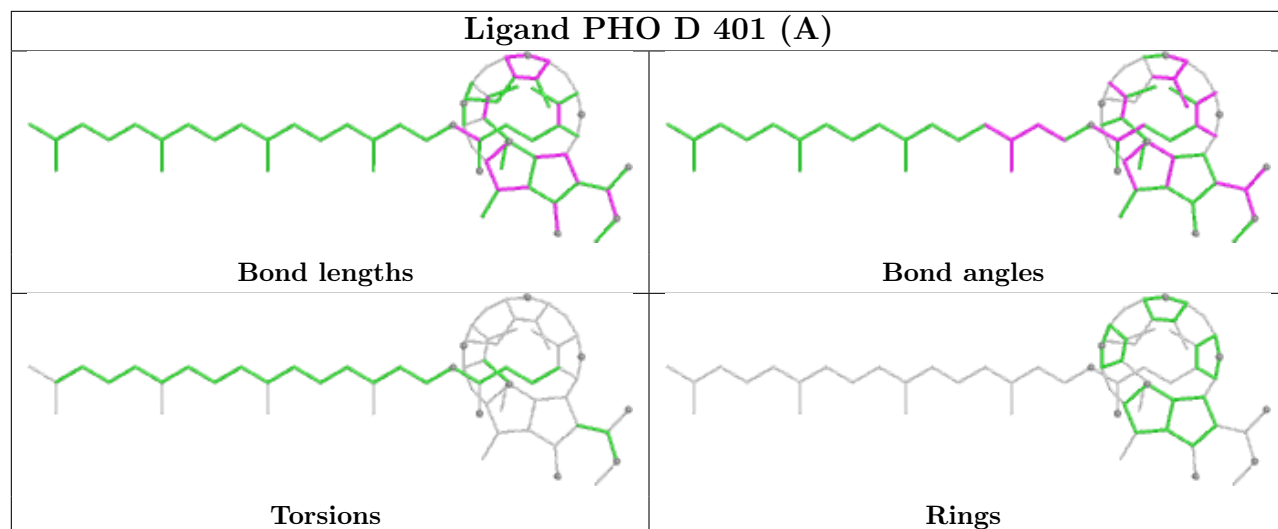


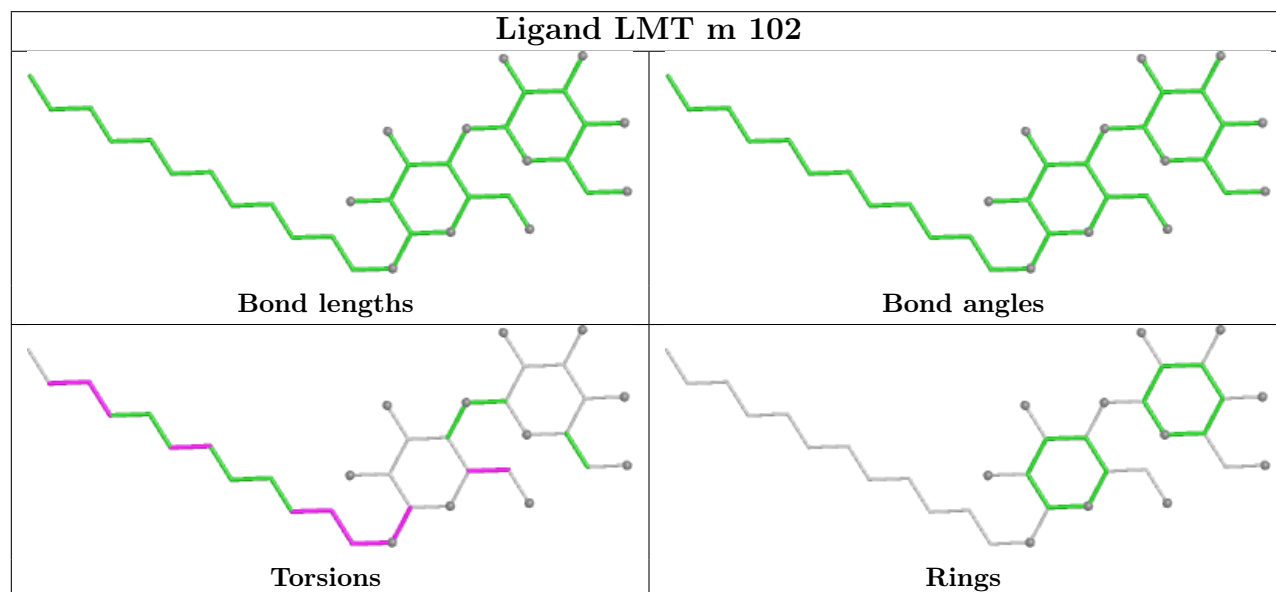
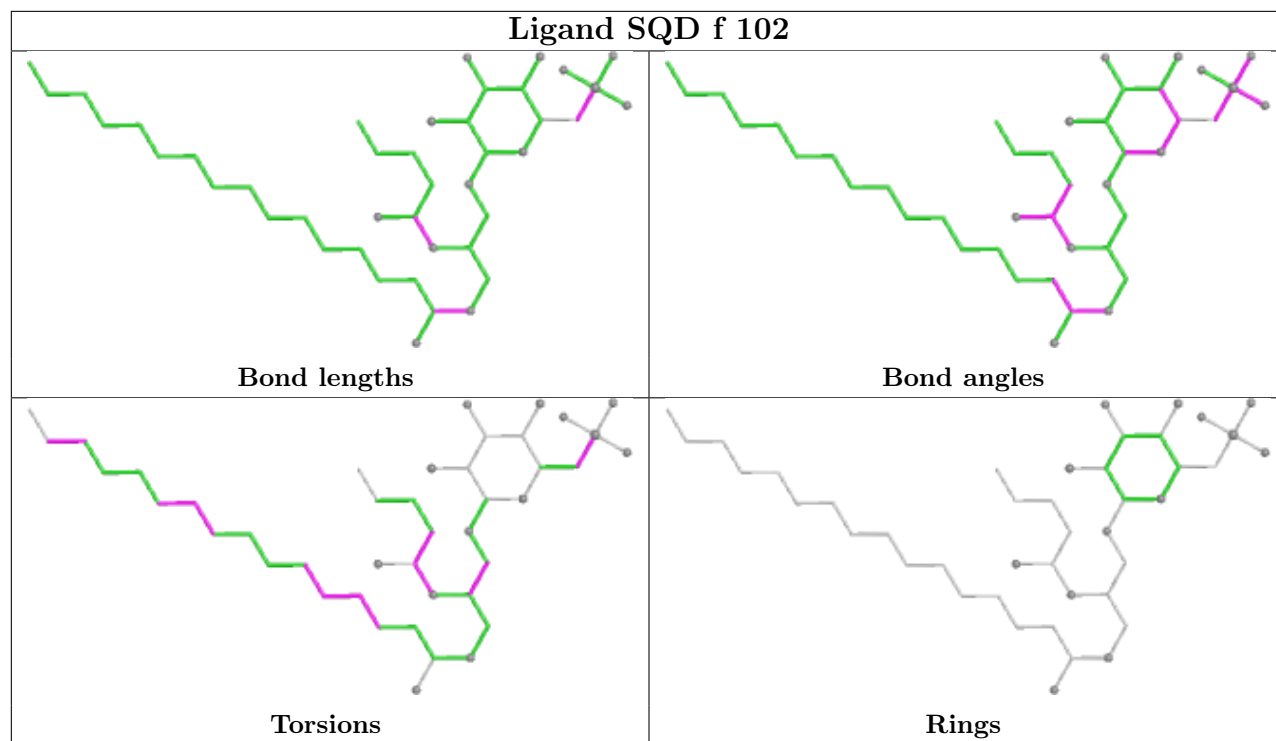


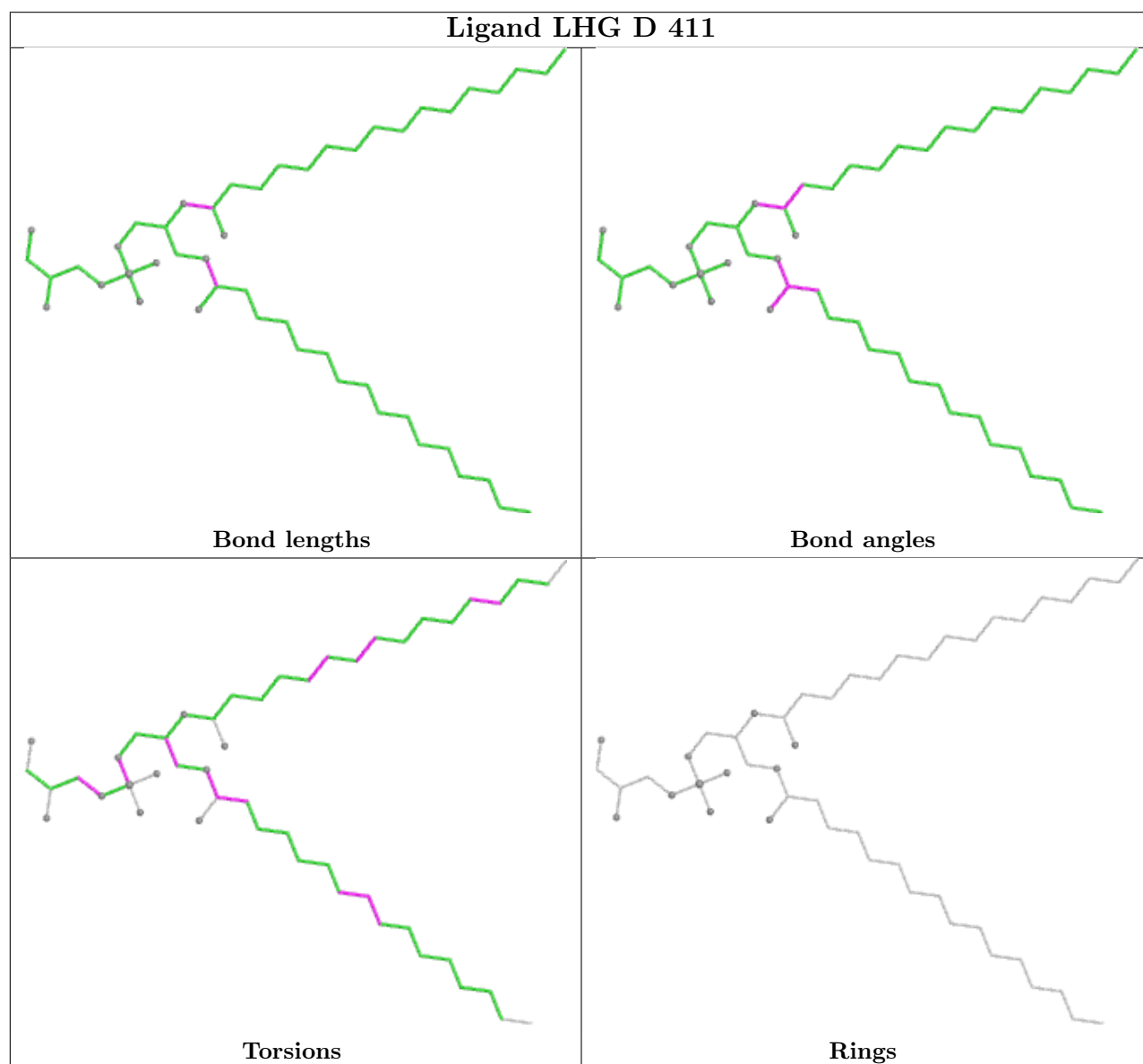
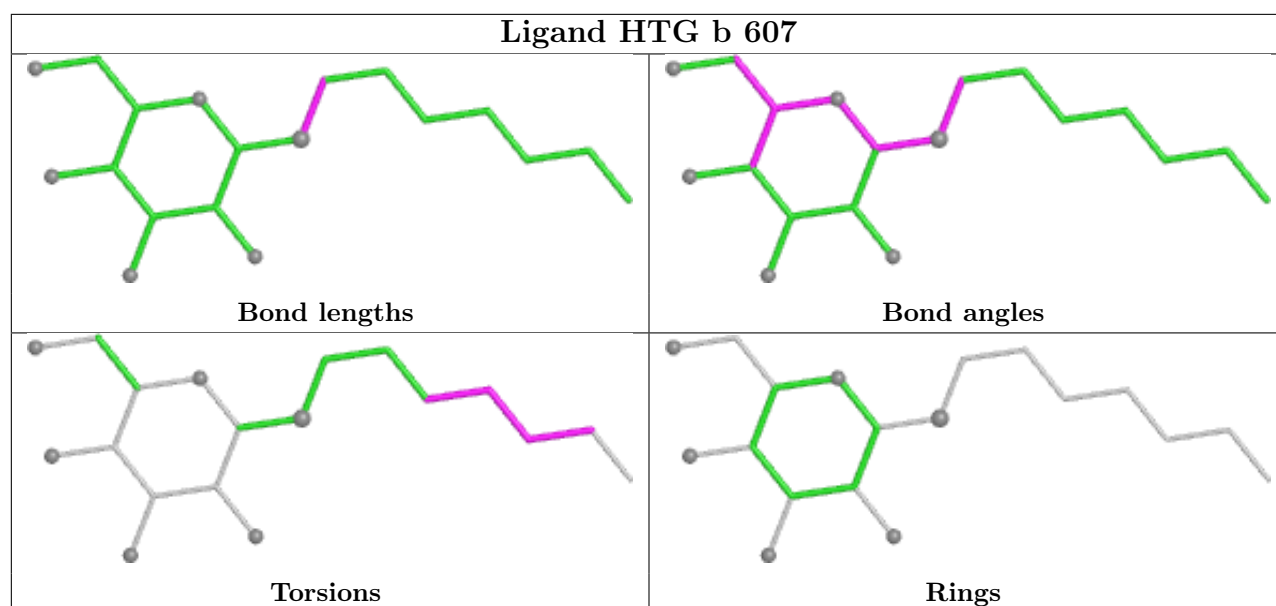


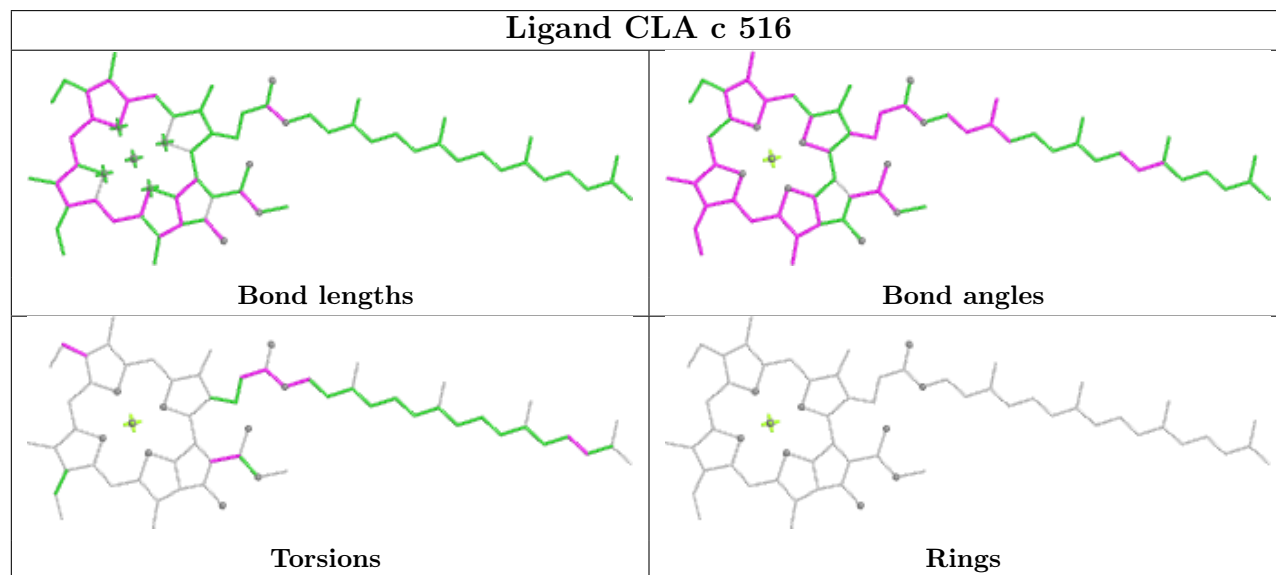
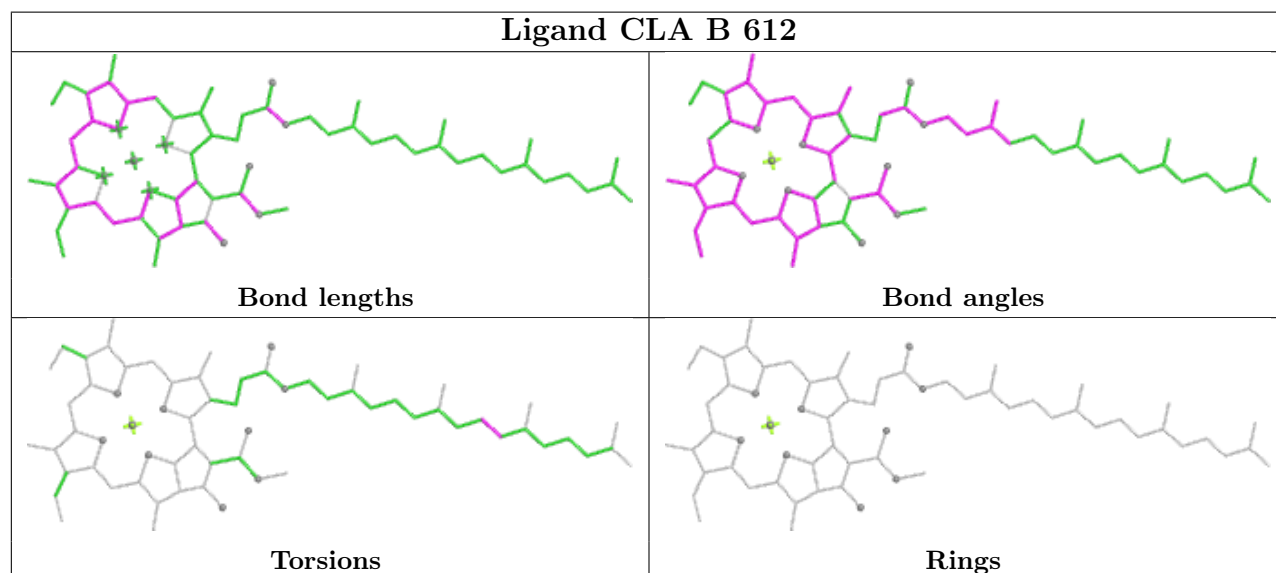
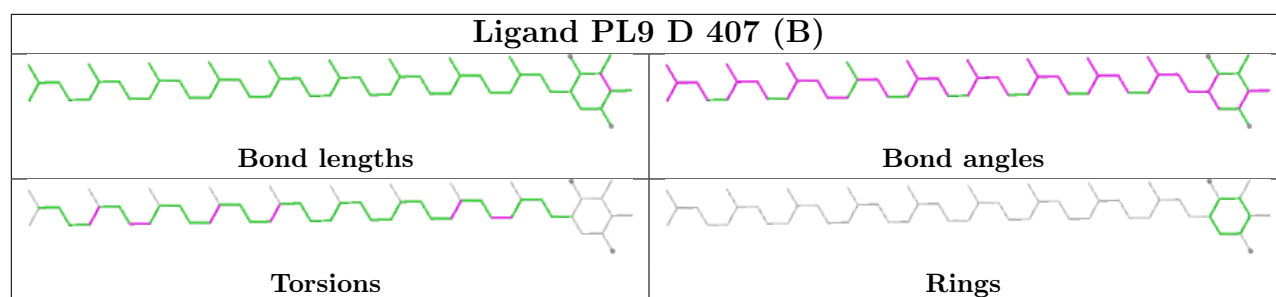


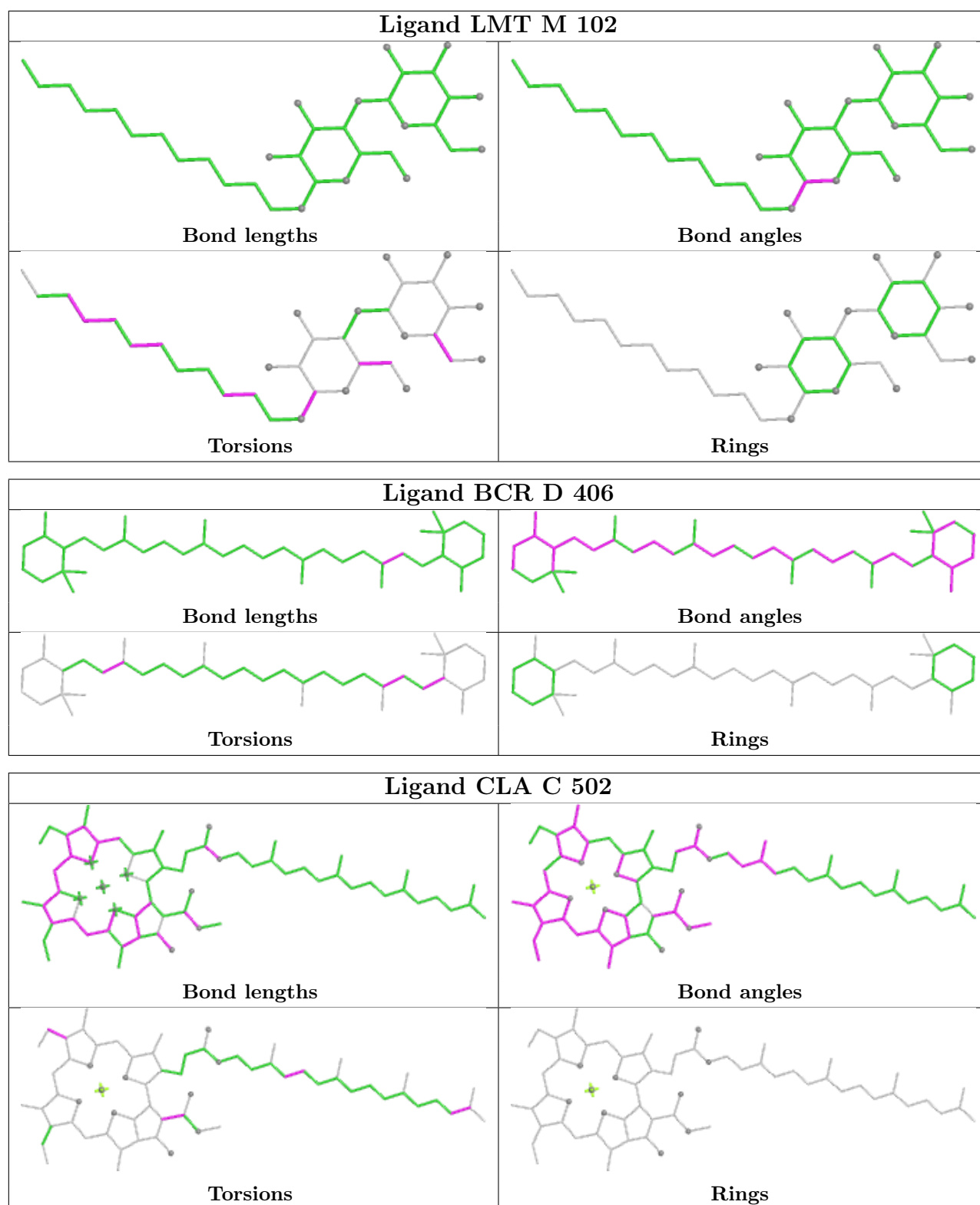


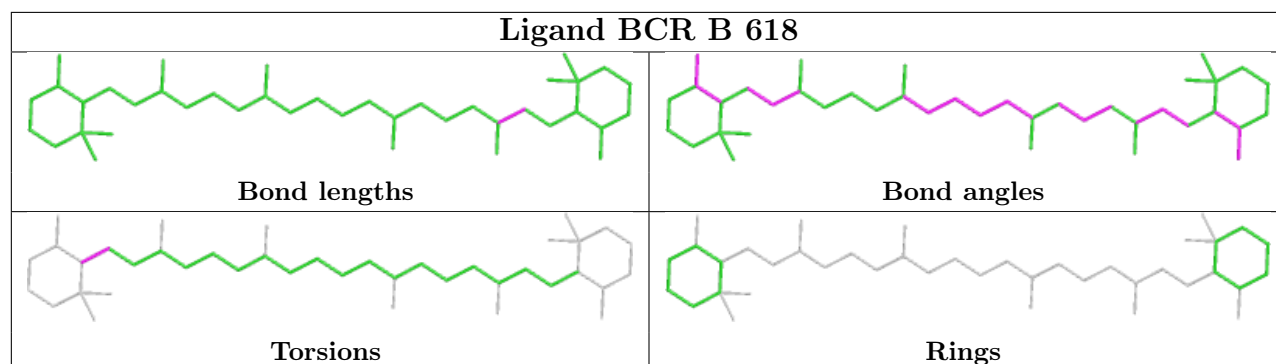
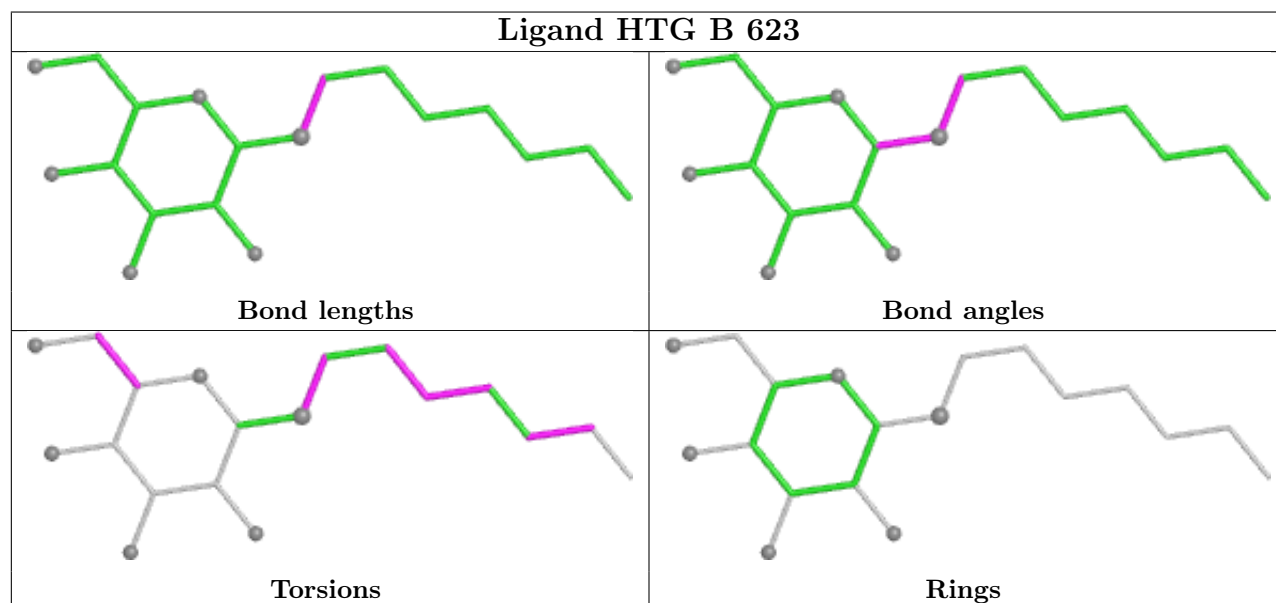
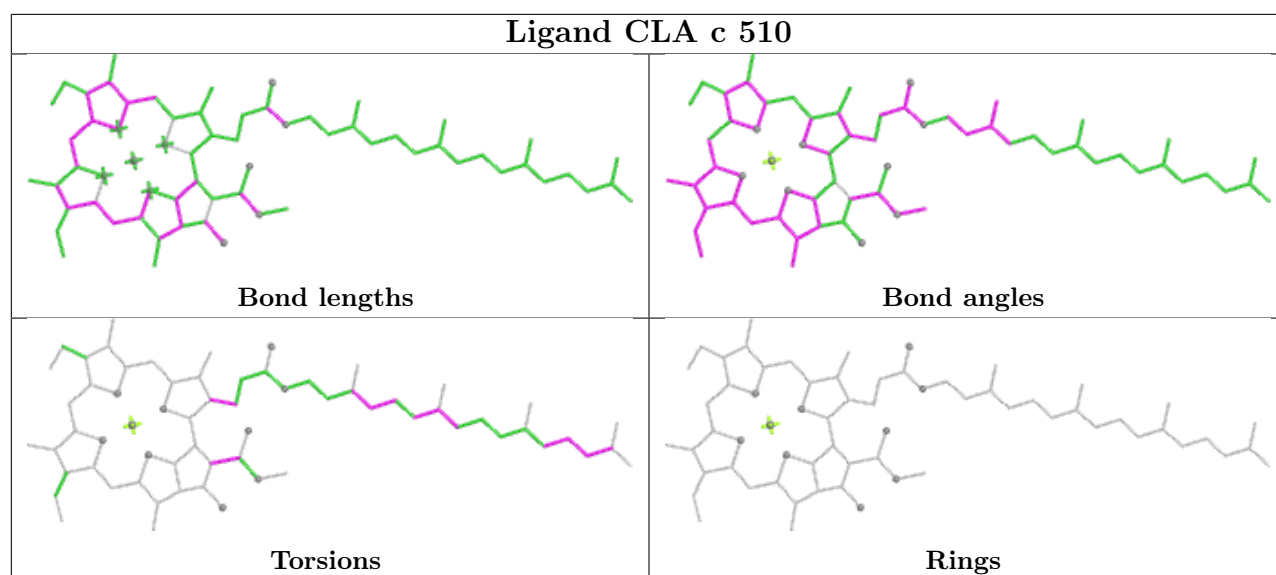


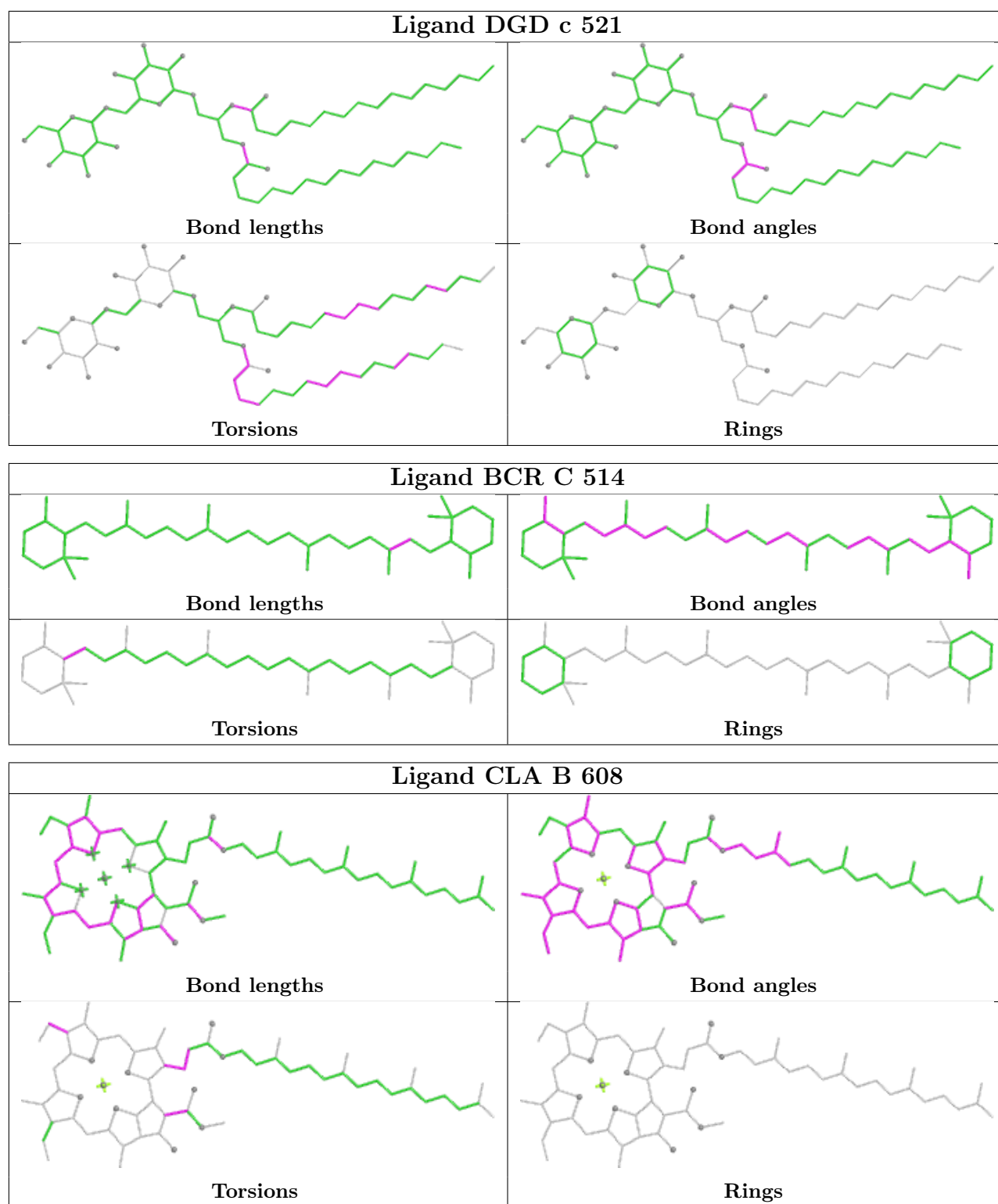


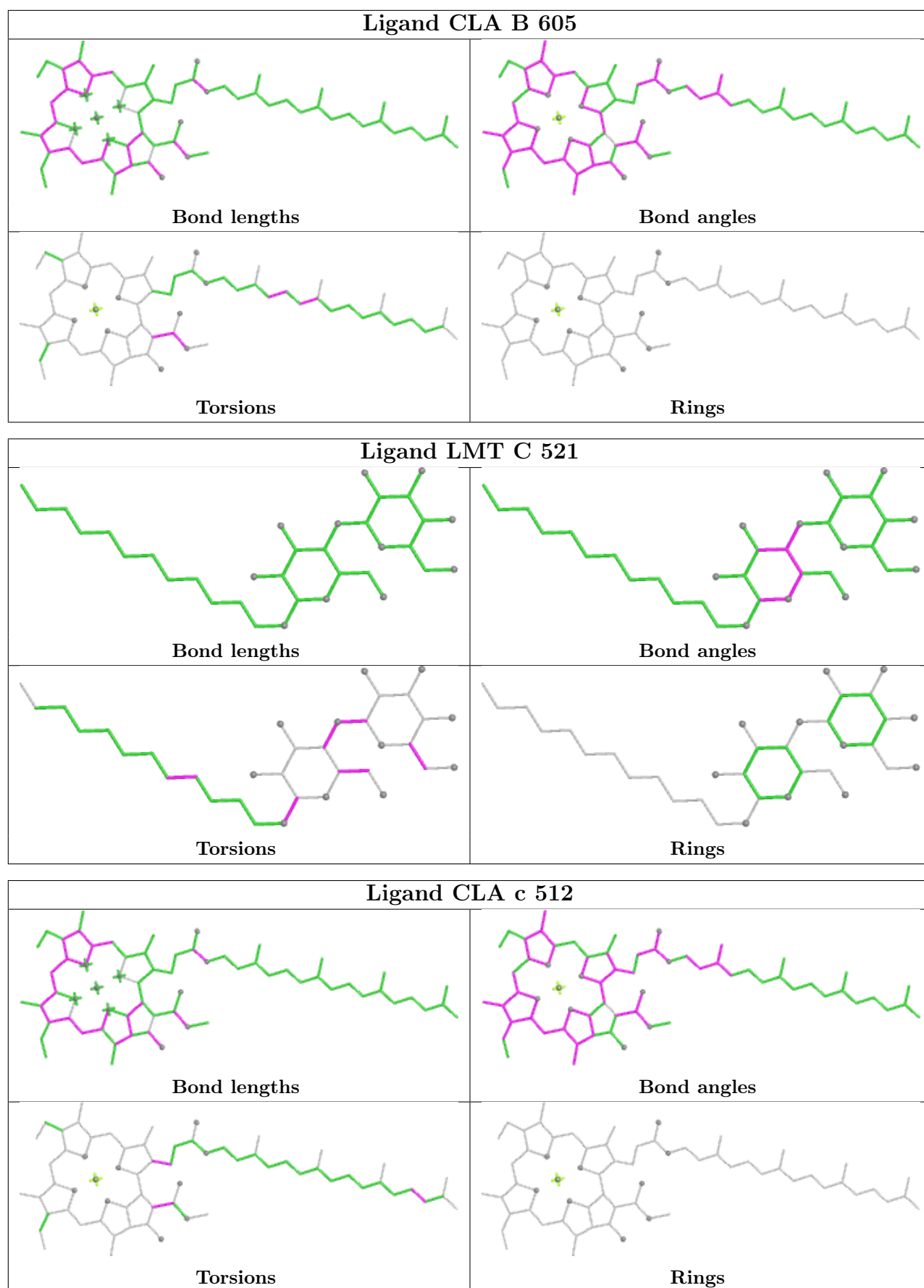


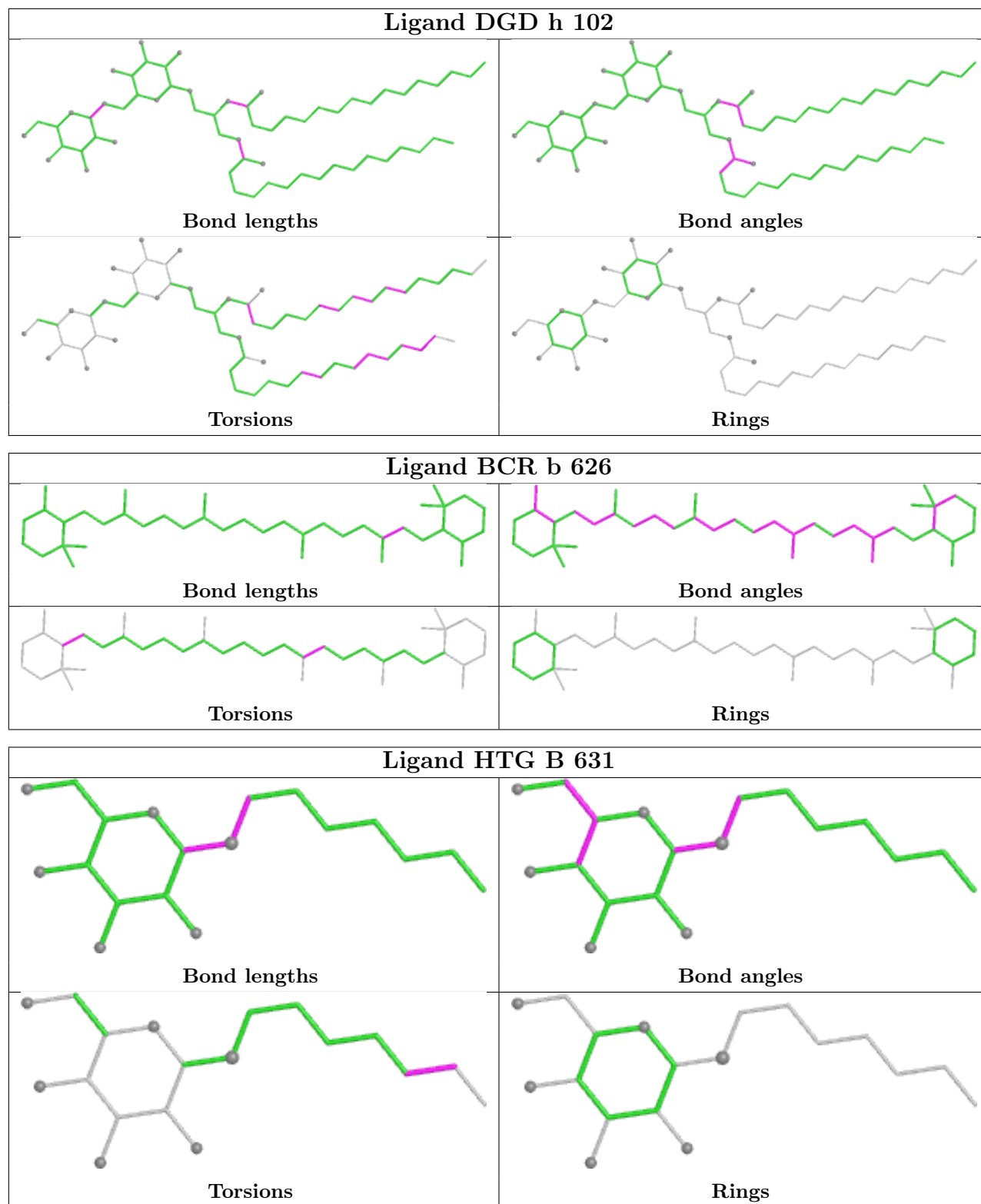


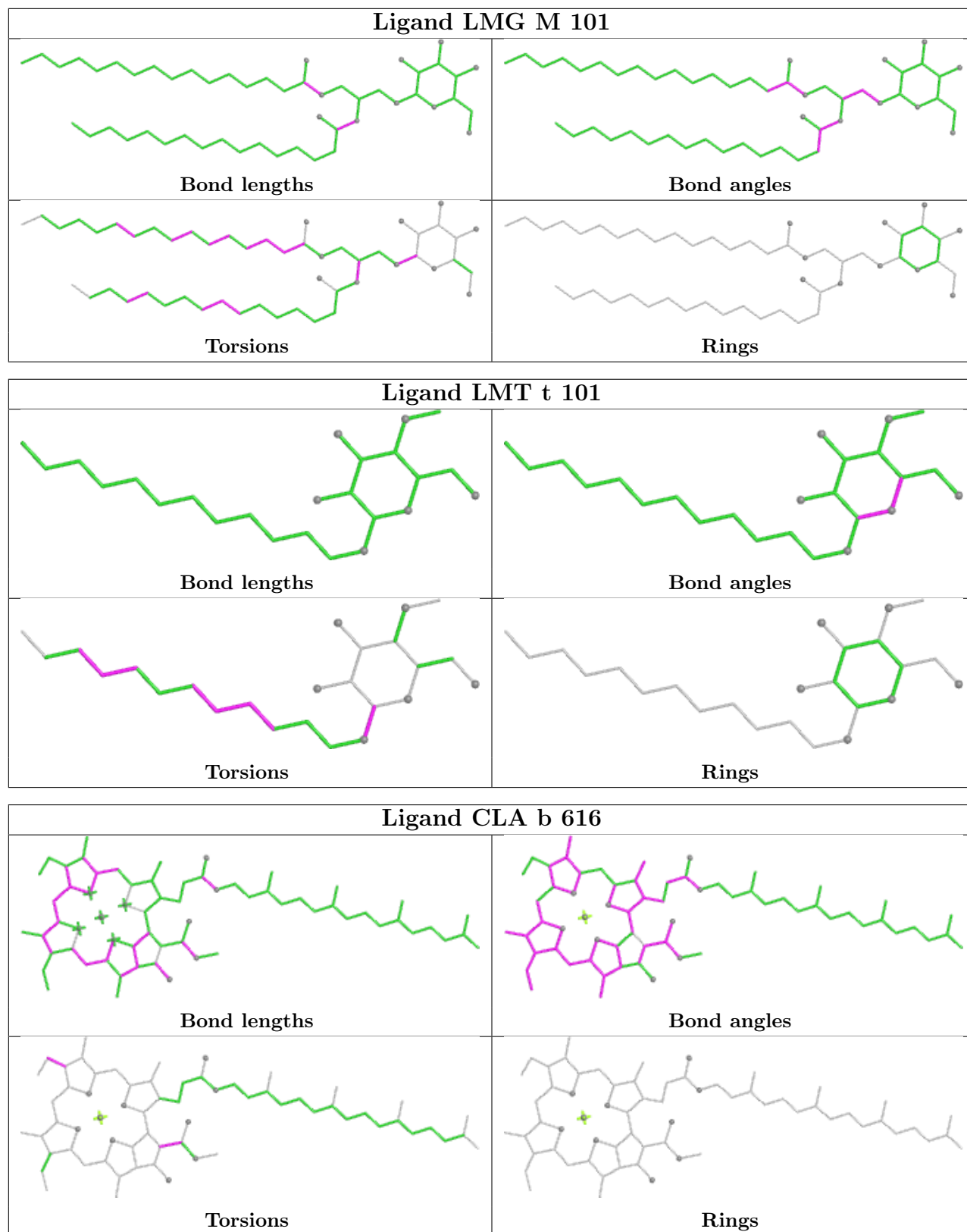


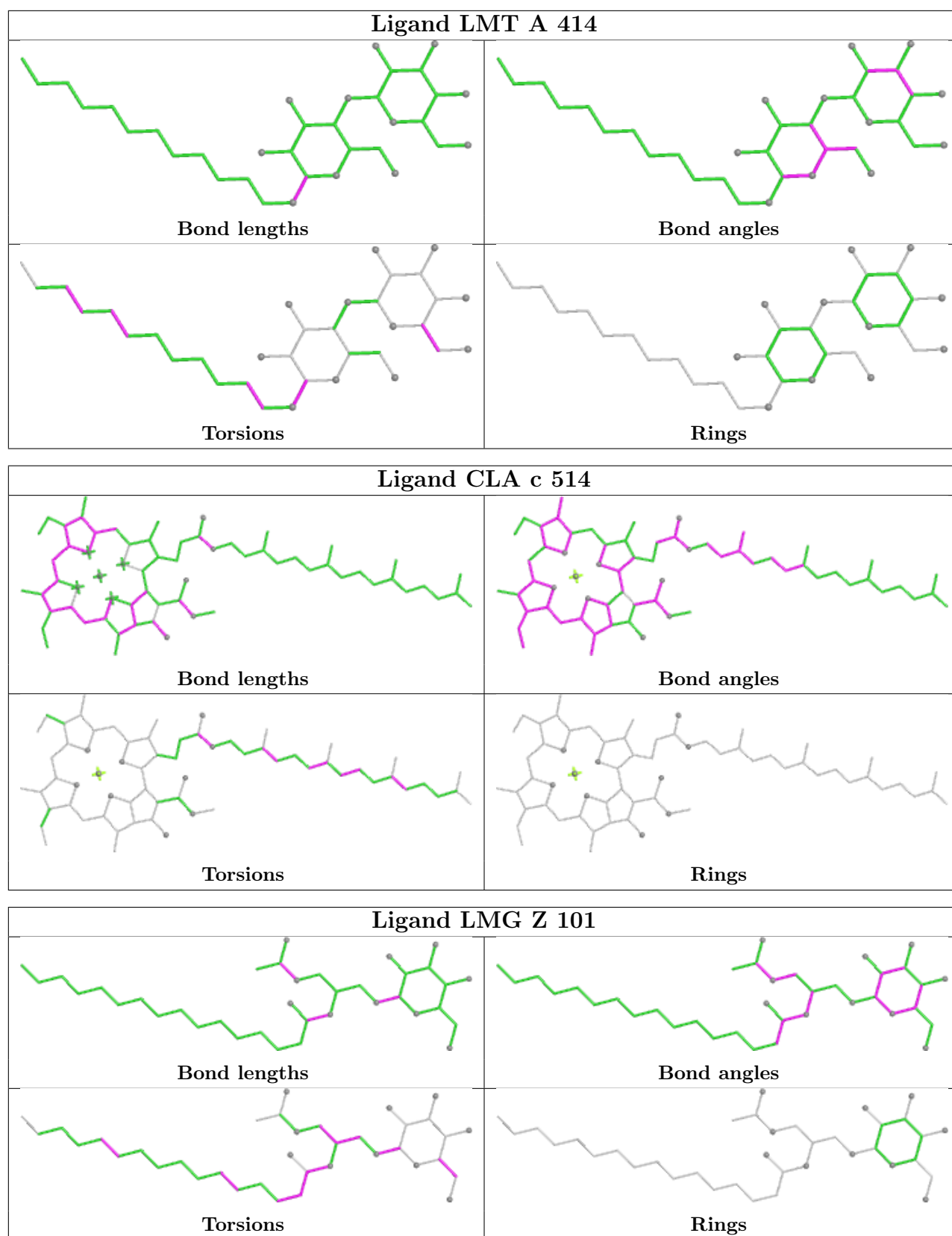


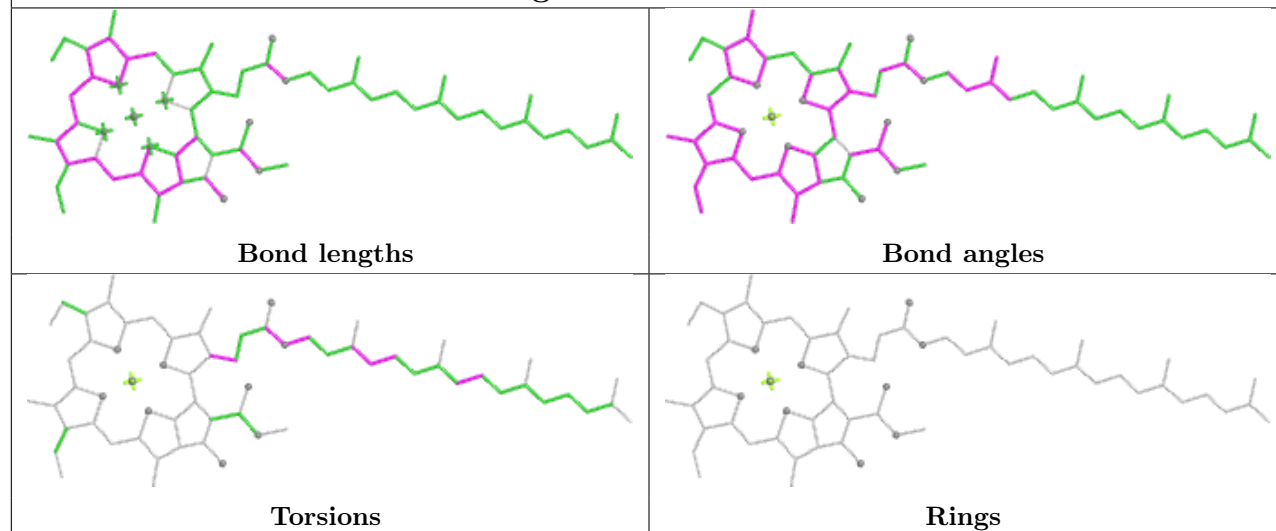
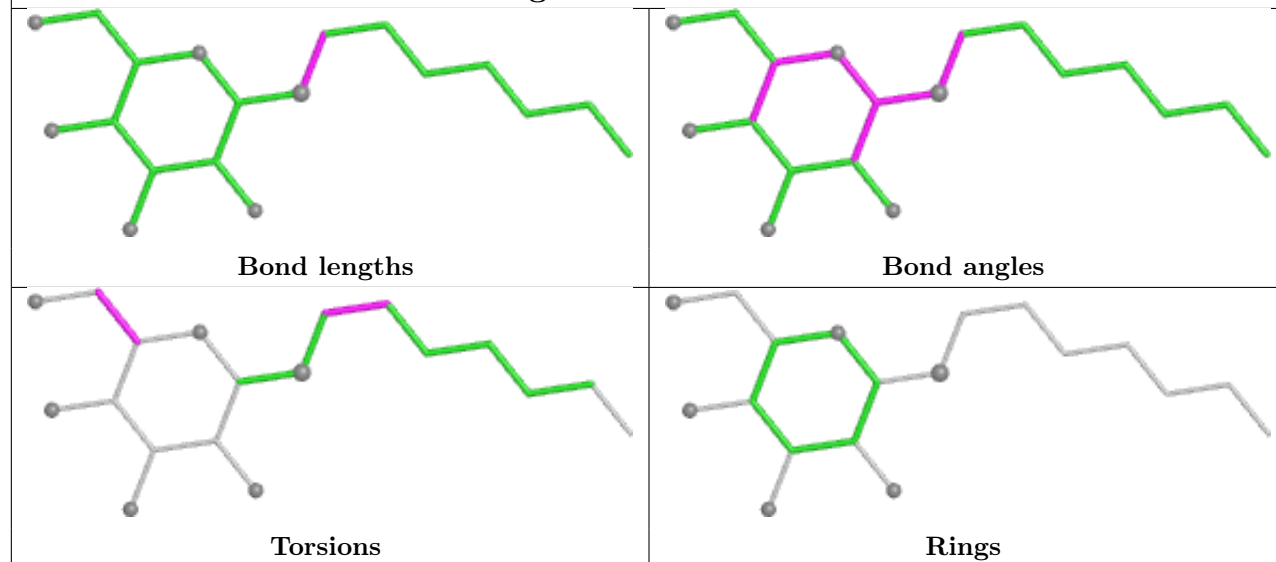


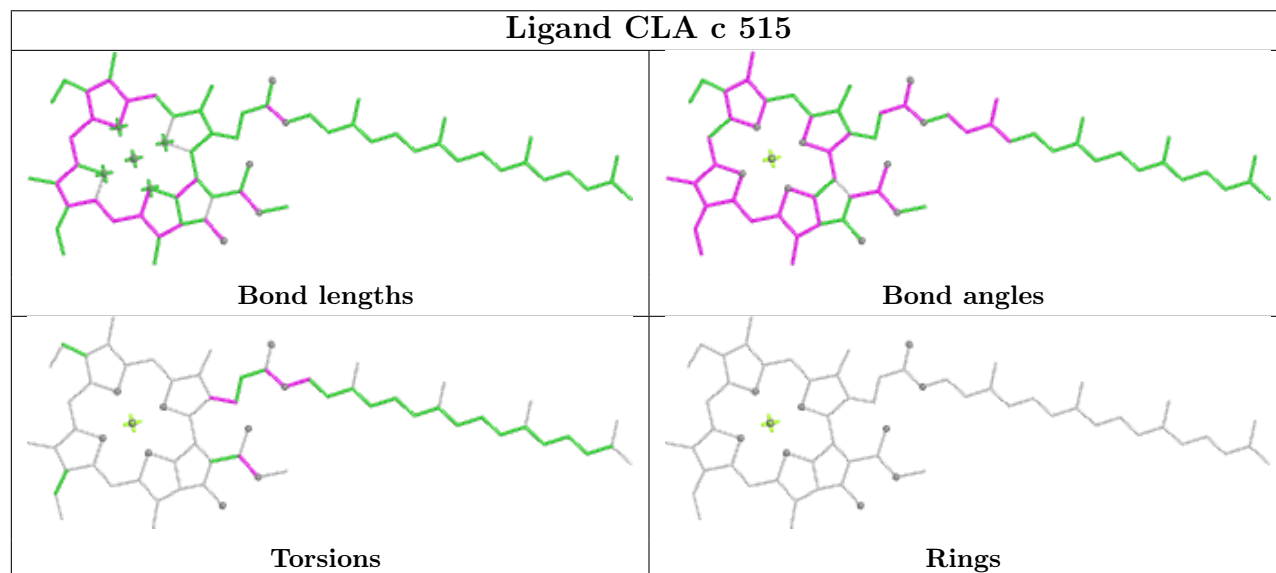
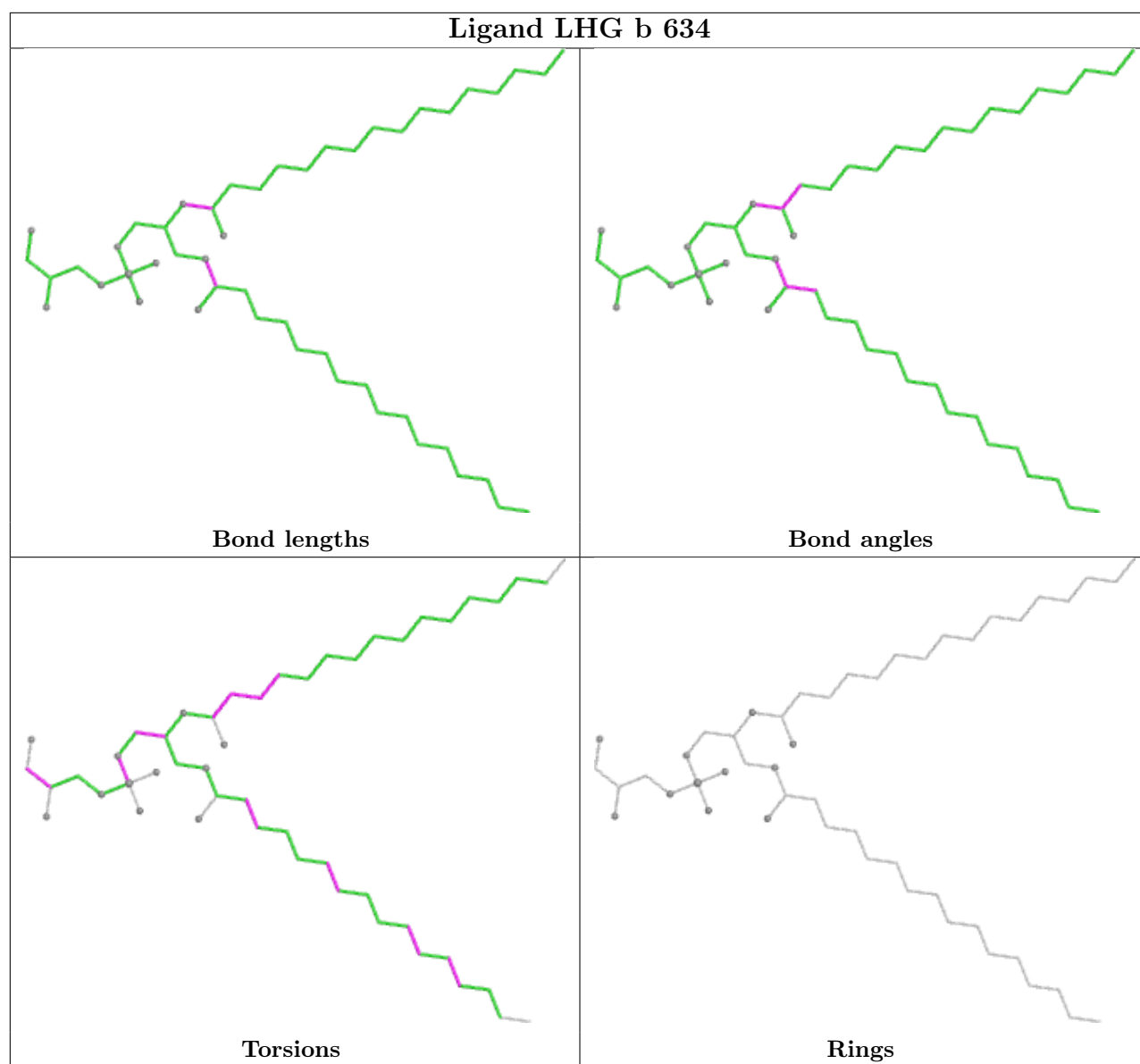


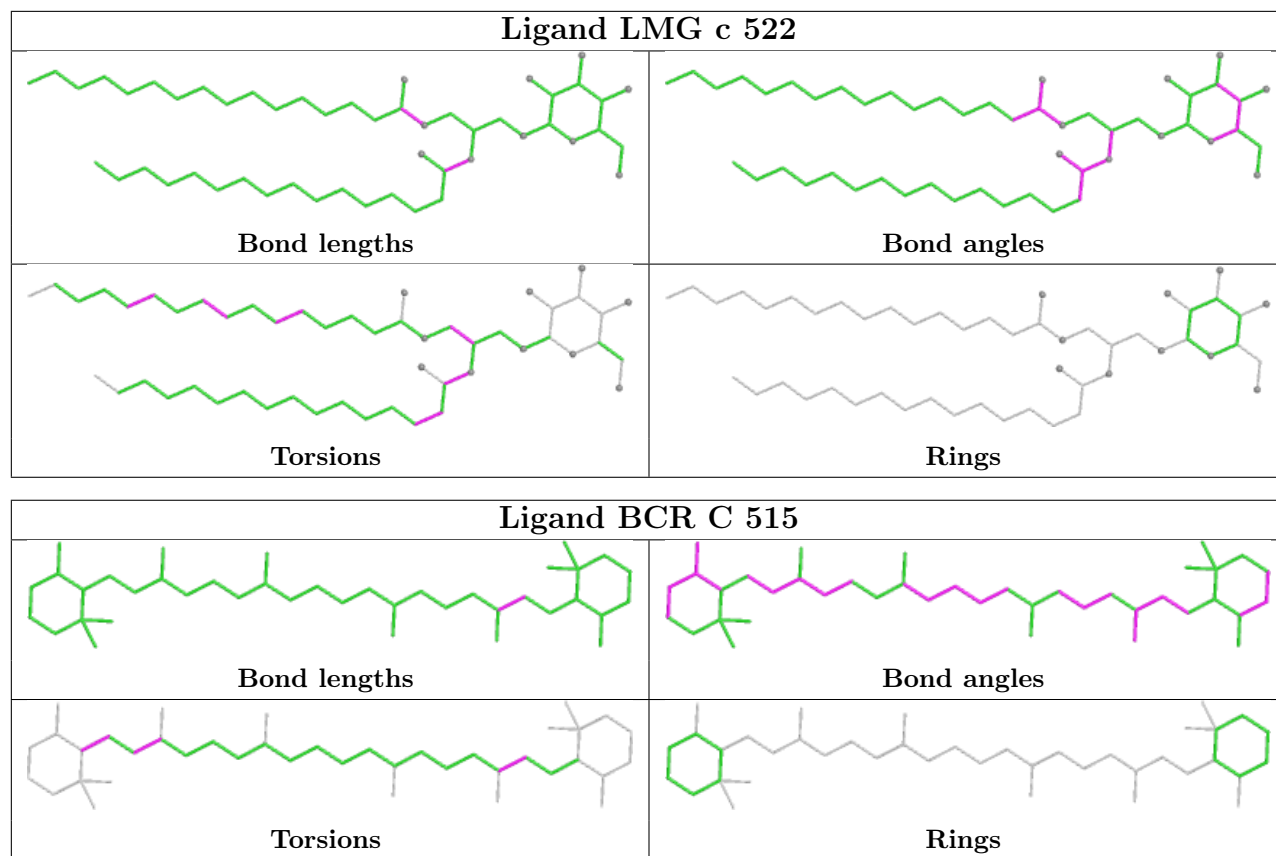


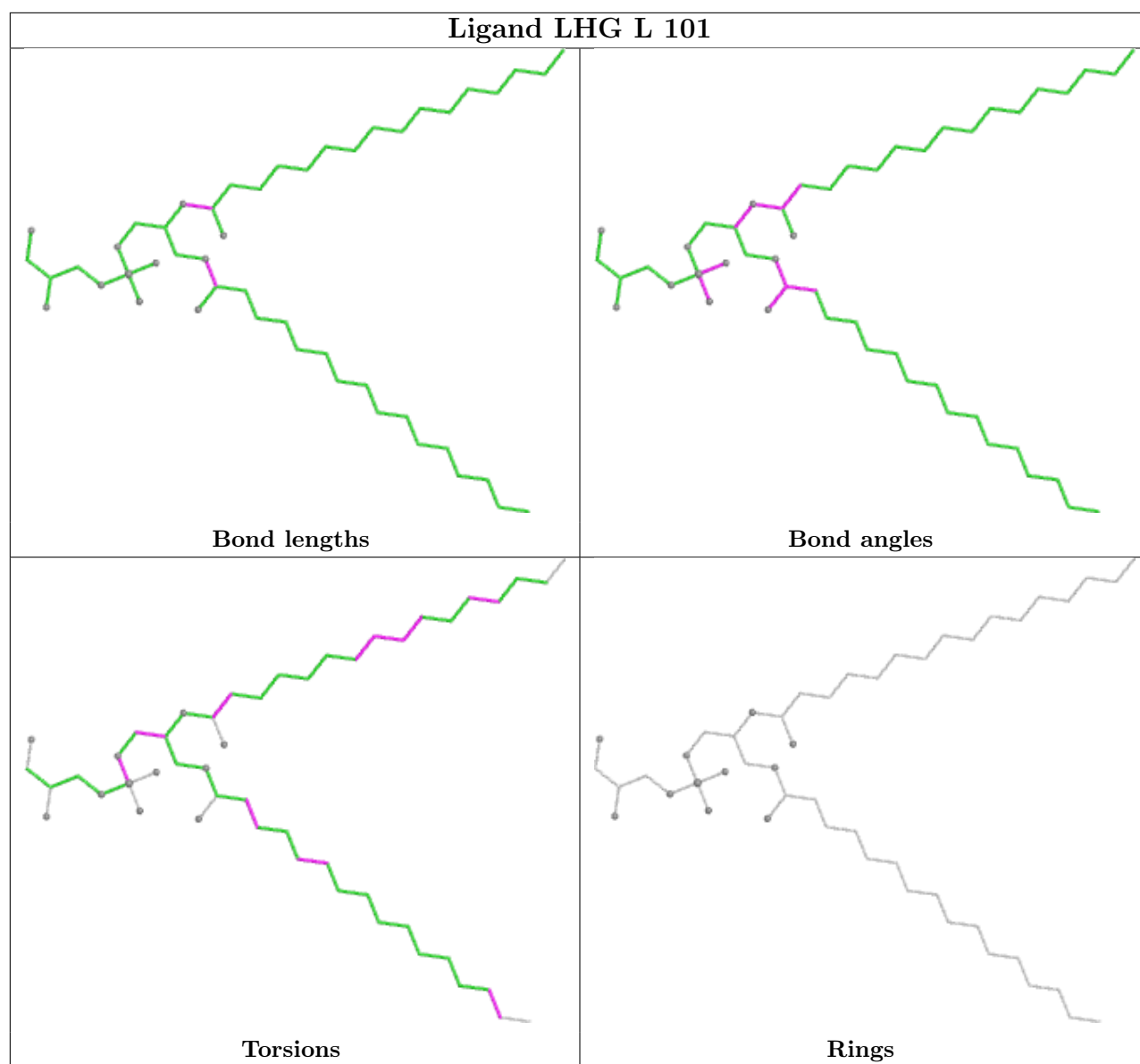


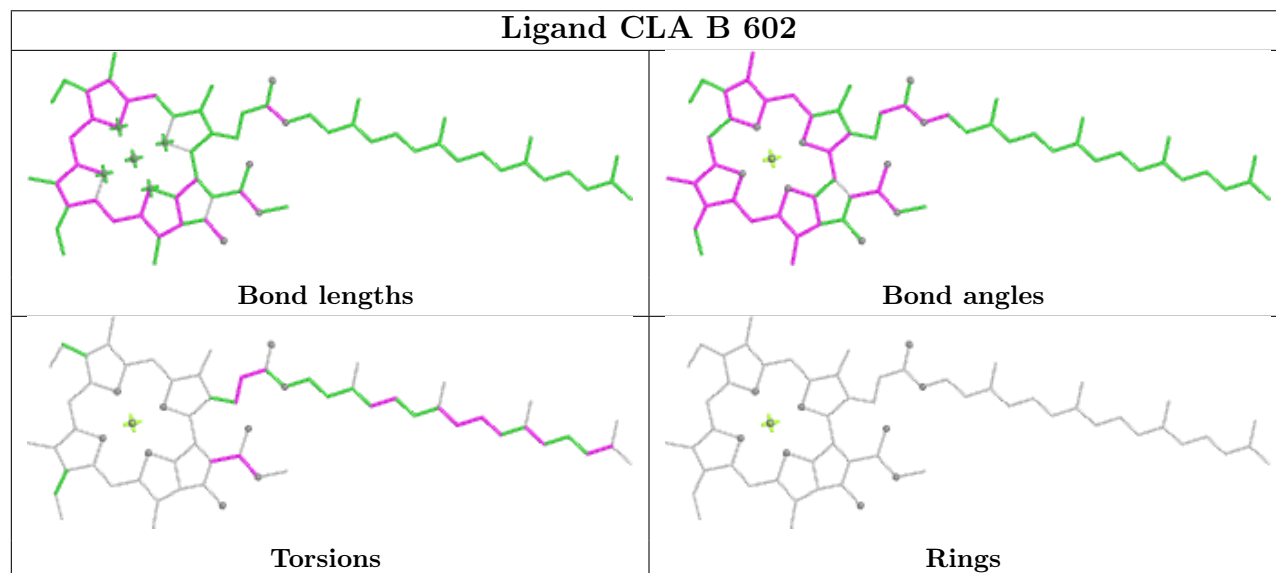
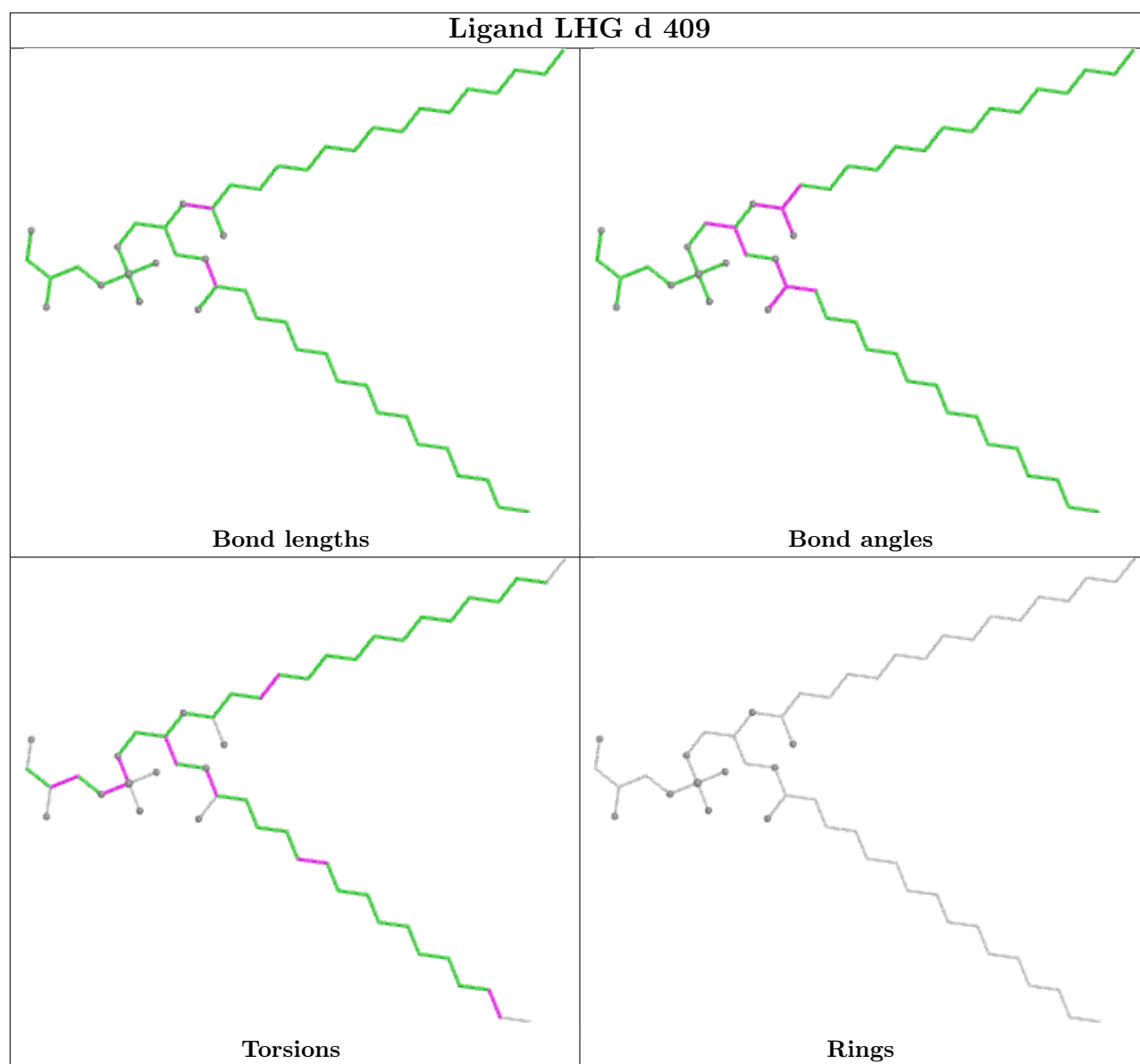


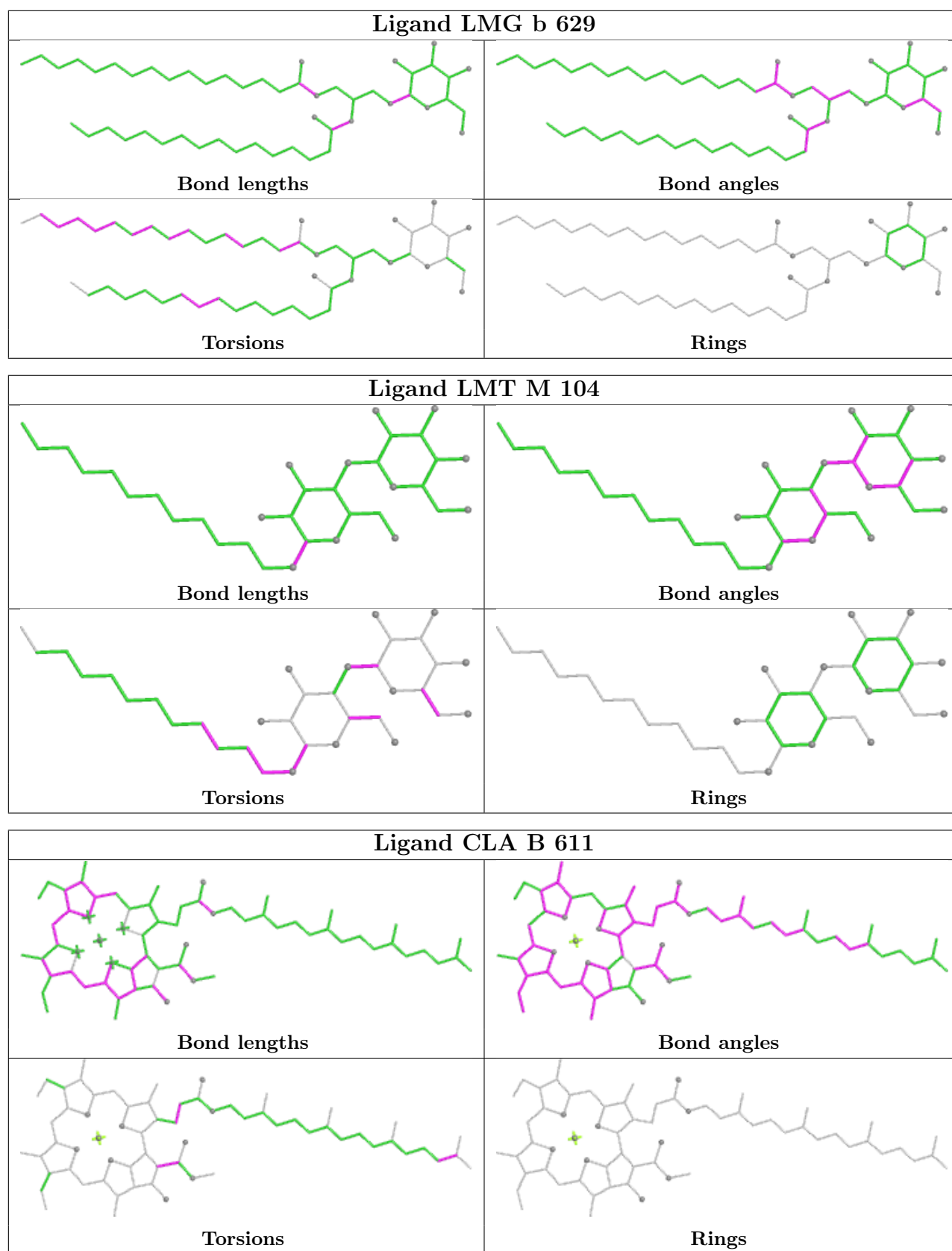
Ligand CLA C 513**Ligand HTG C 523**



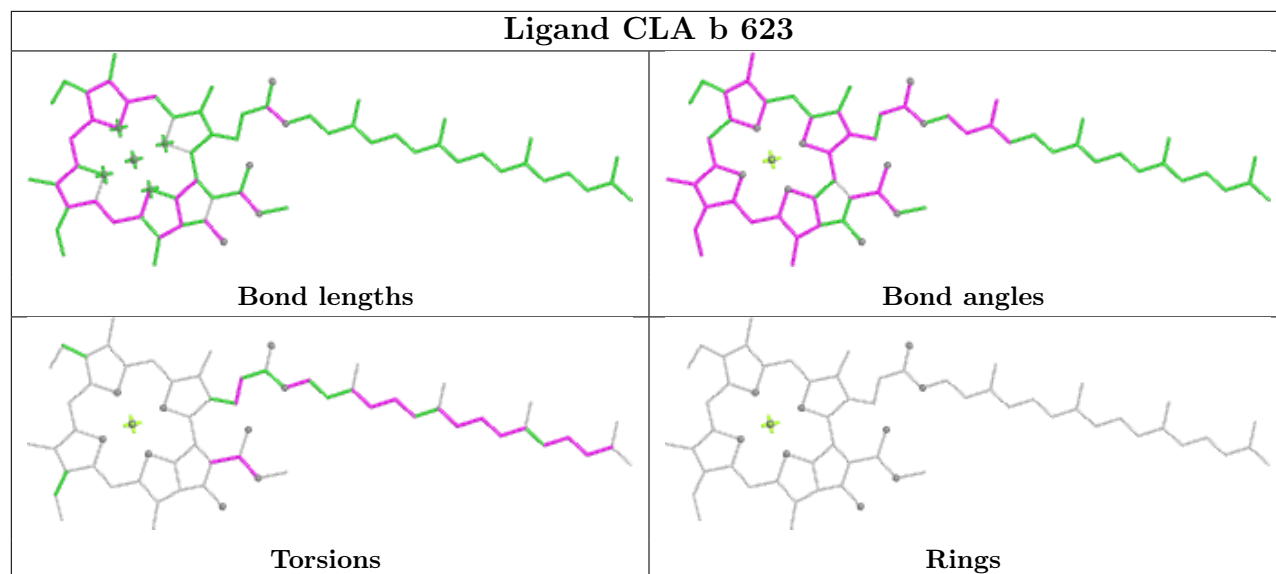




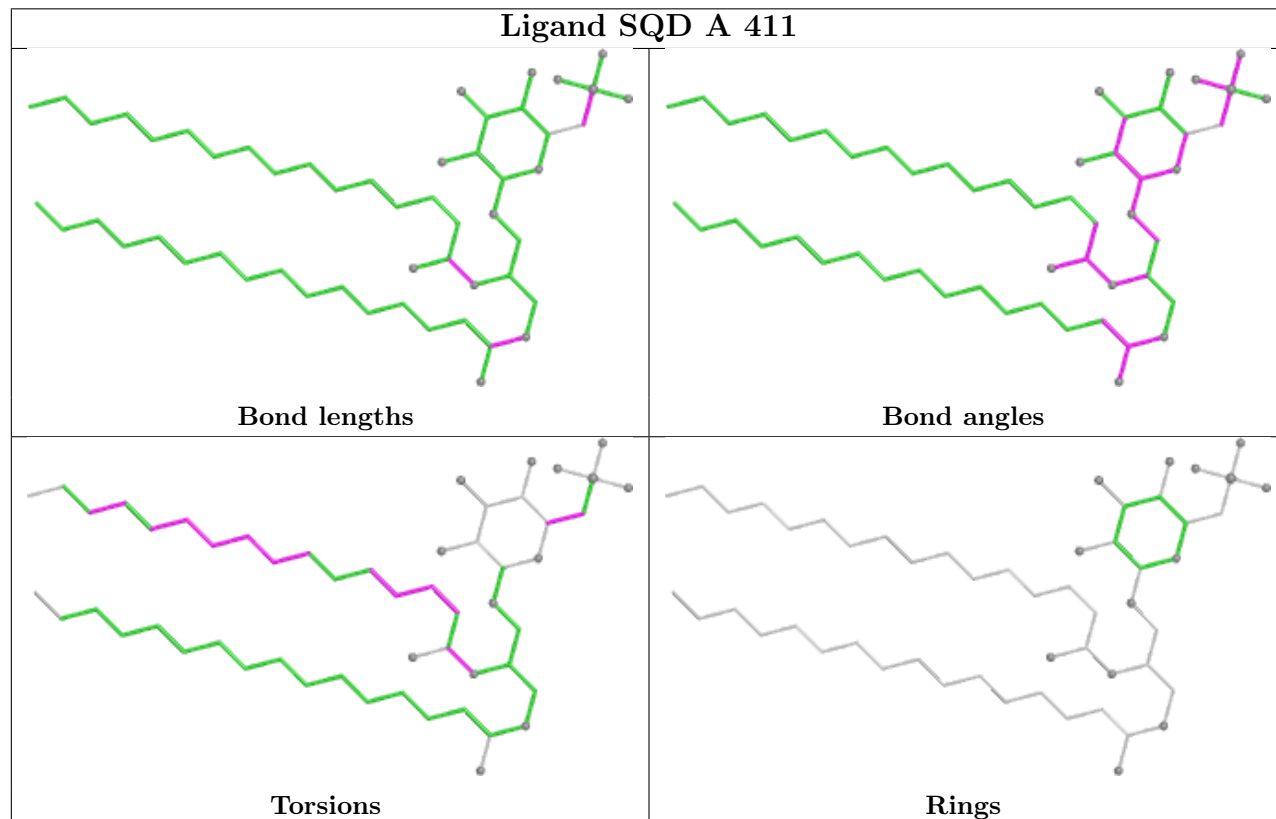


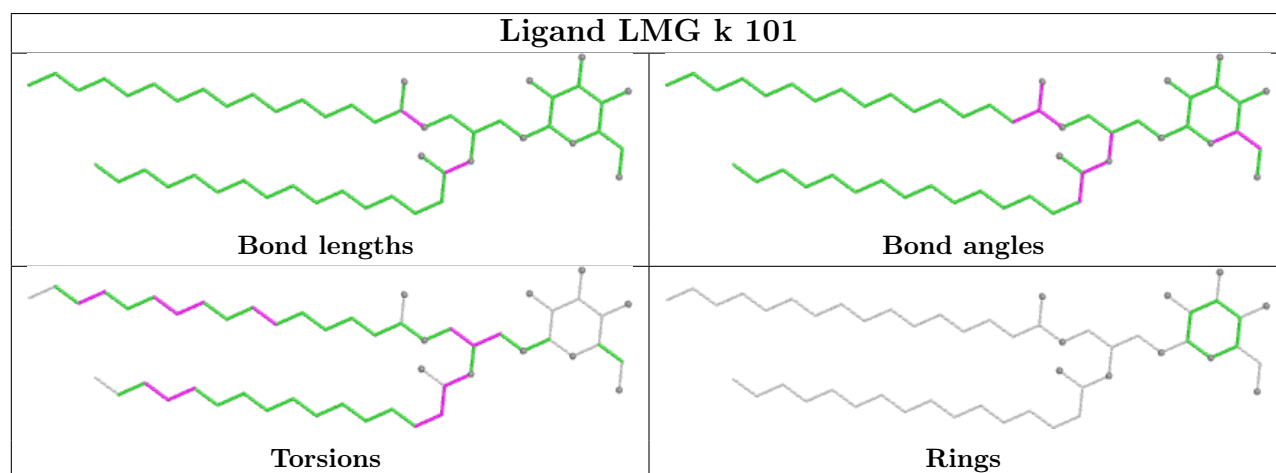
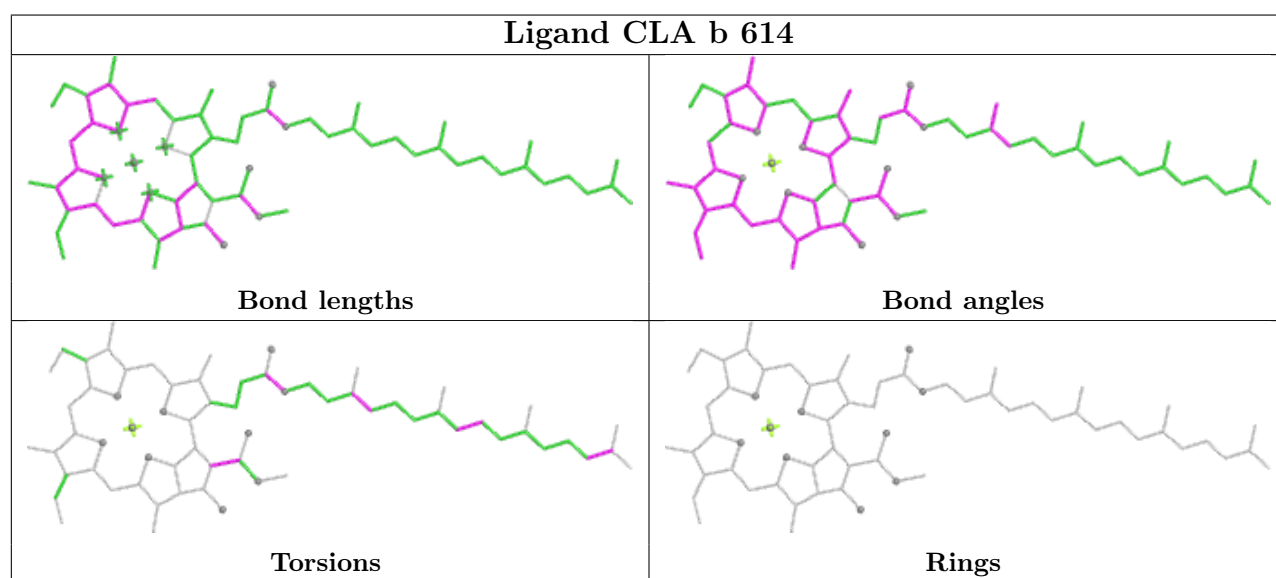
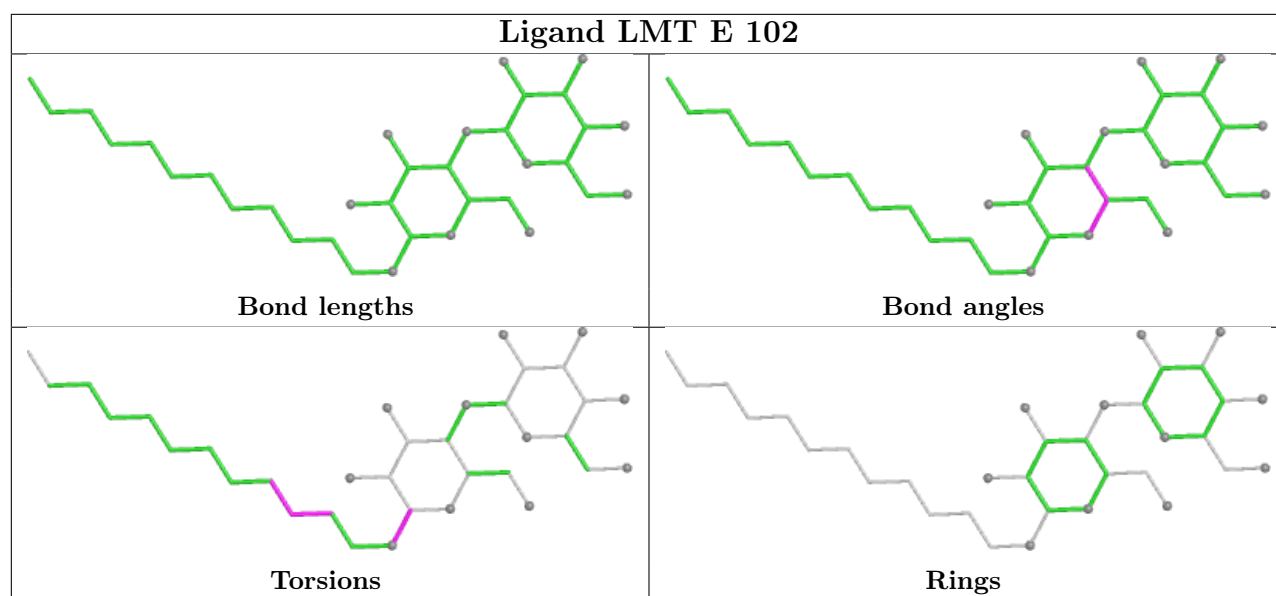


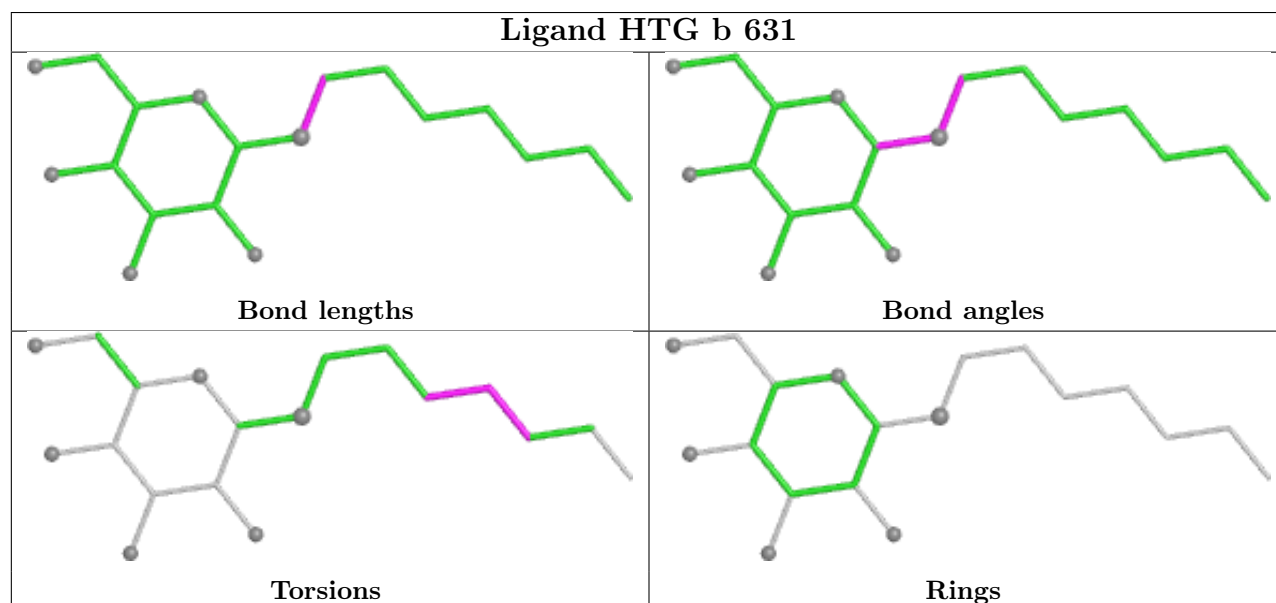
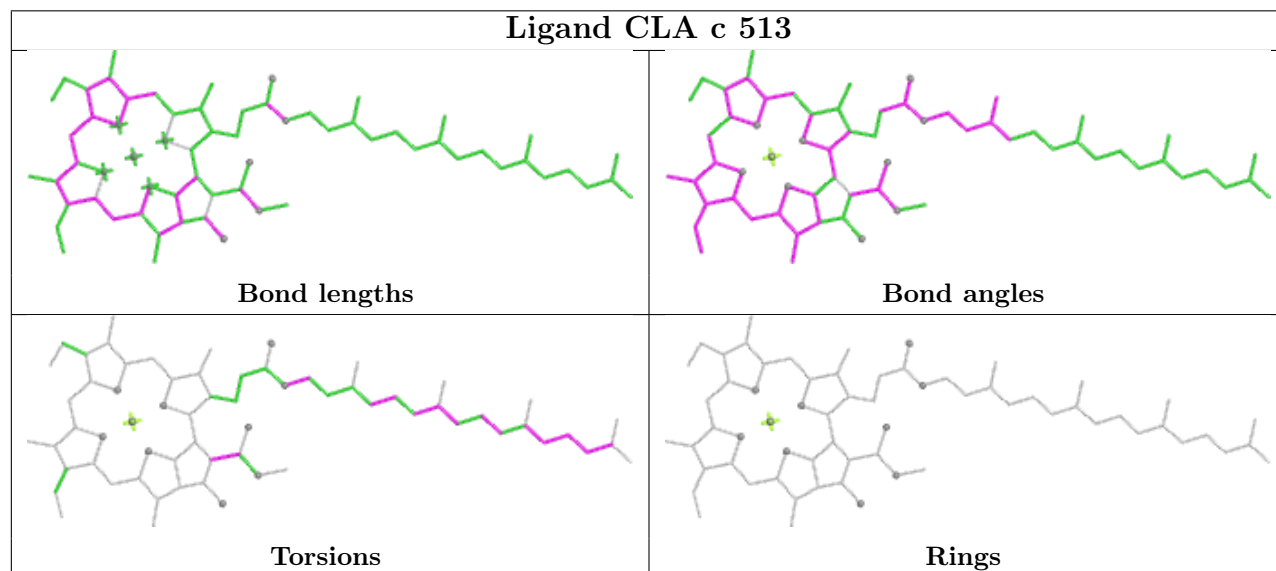
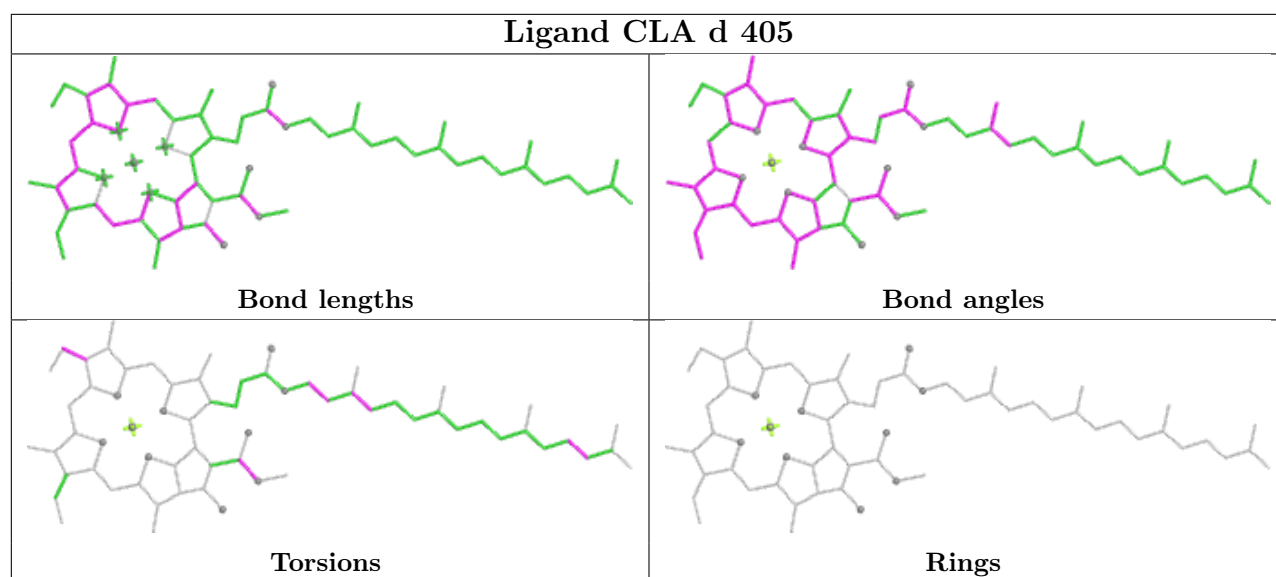
Ligand CLA b 623

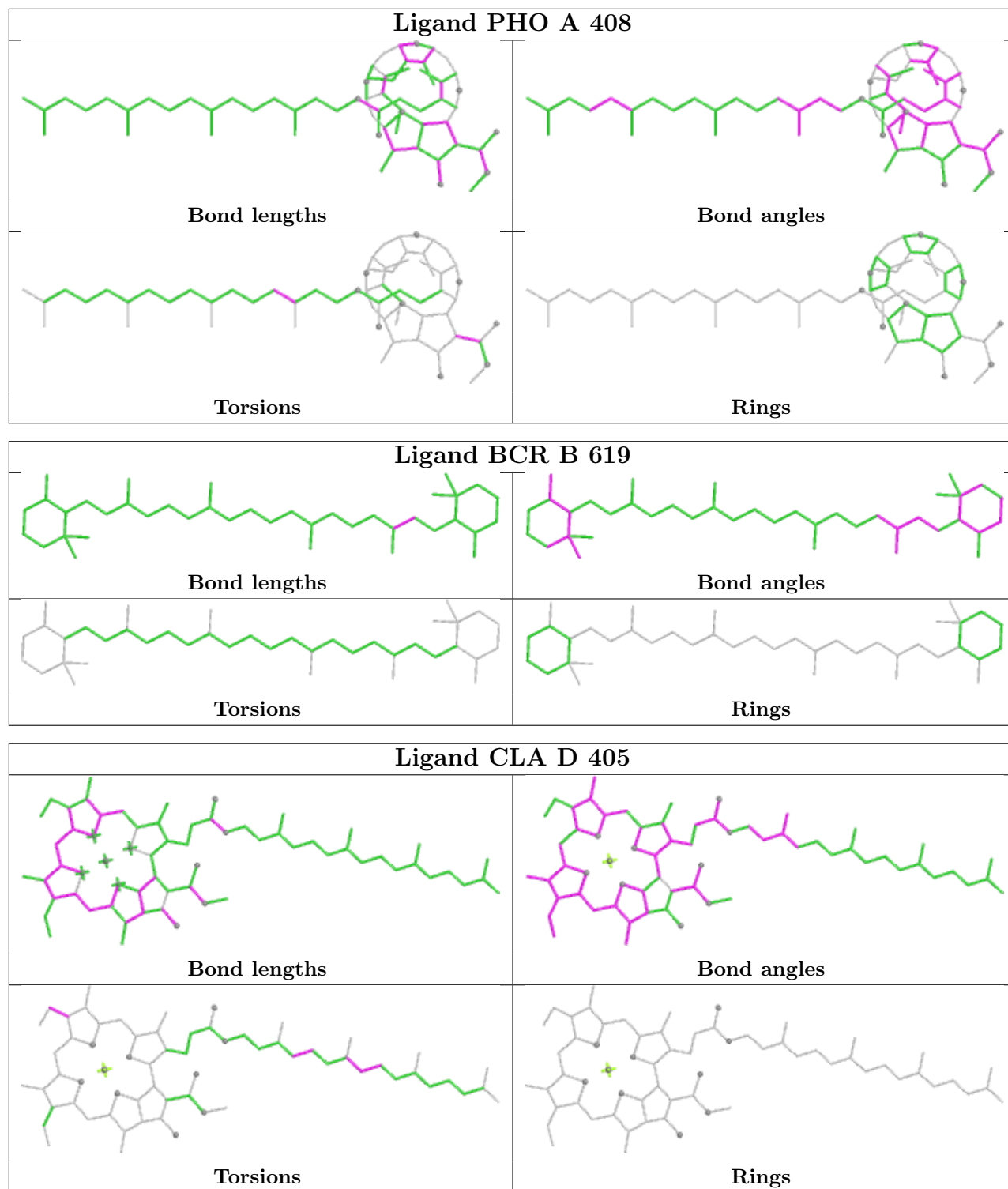


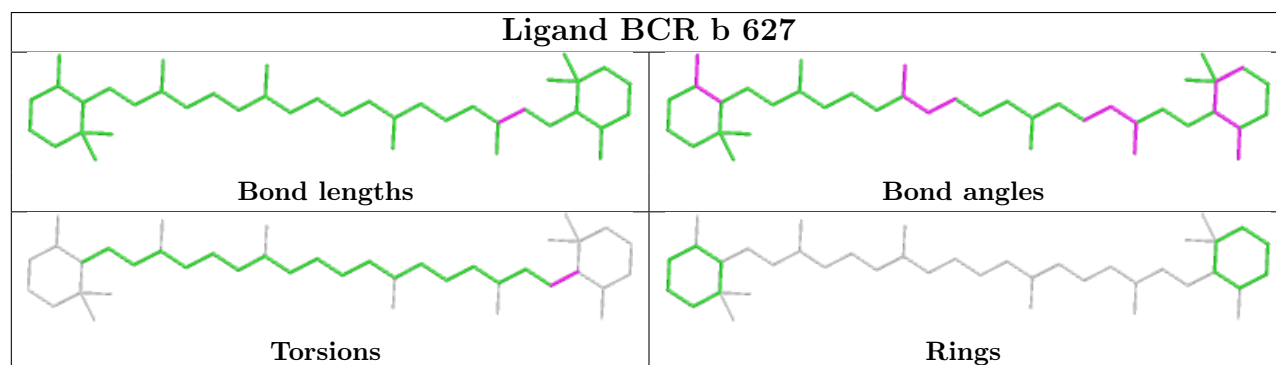
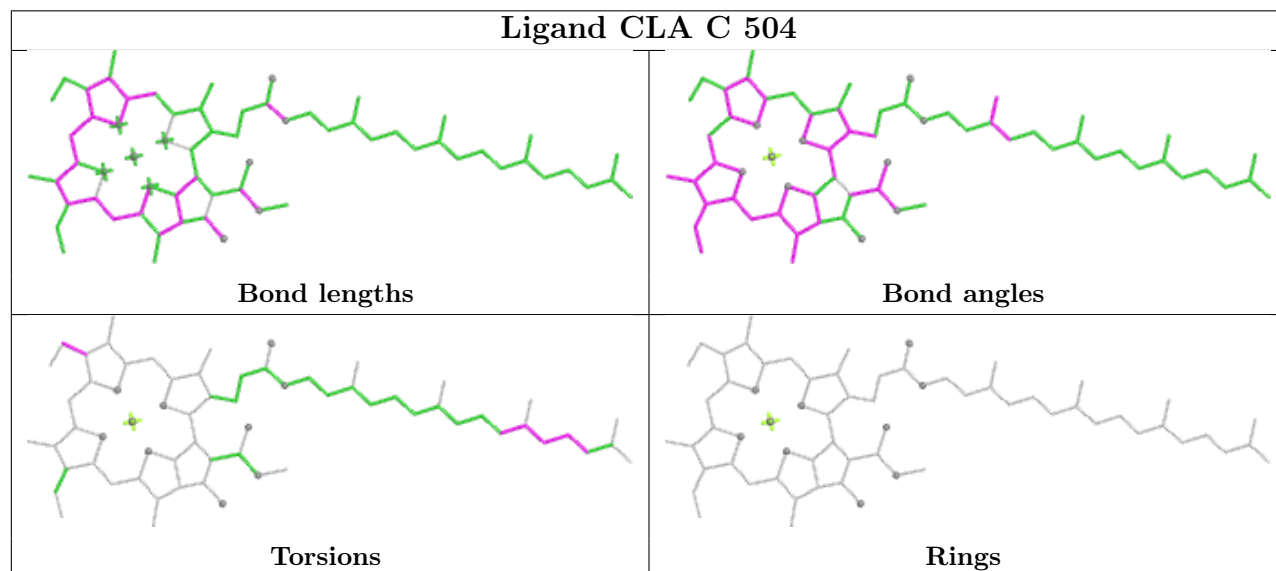
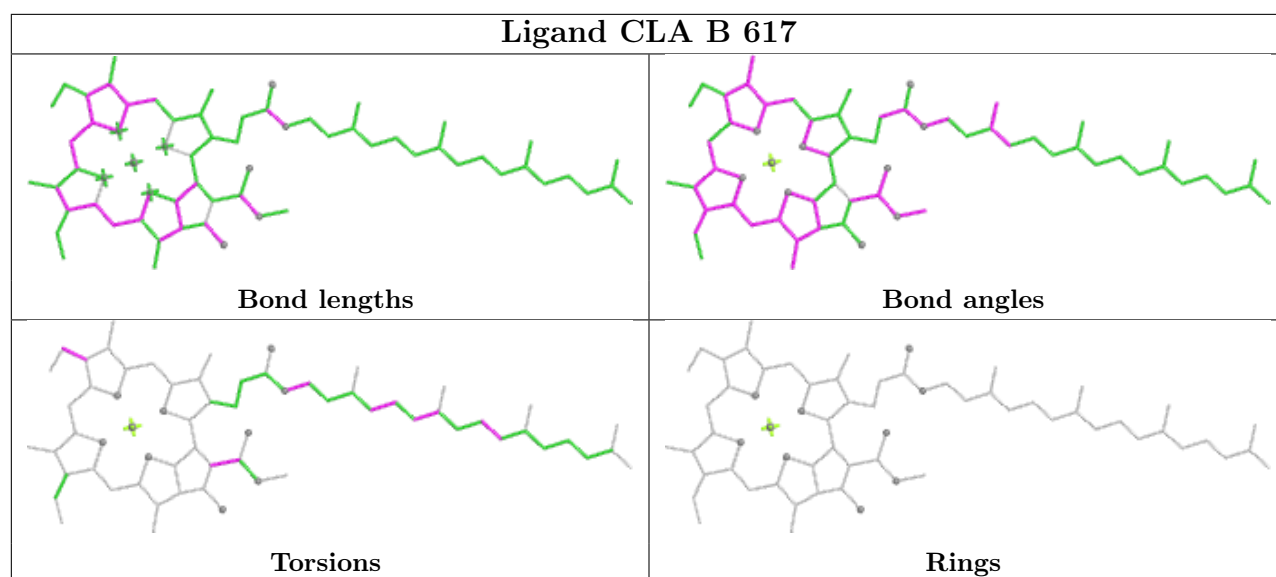
Ligand SQD A 411



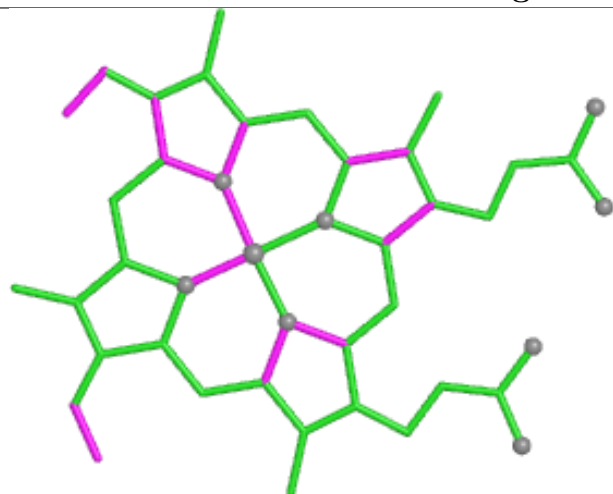




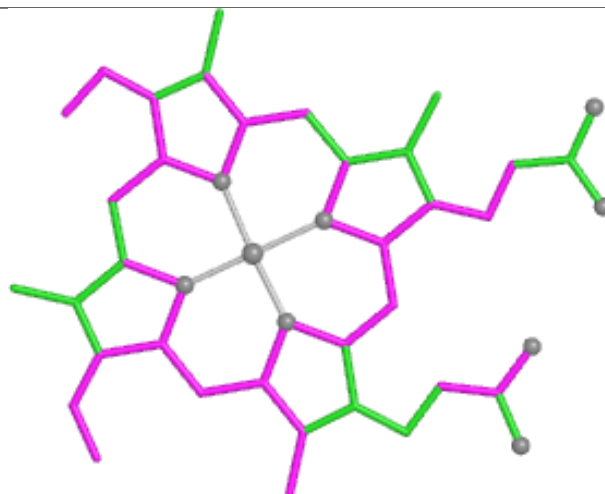




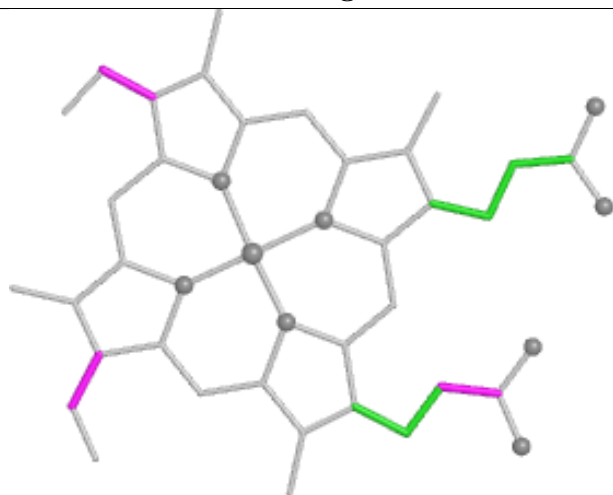
Ligand HEC V 205



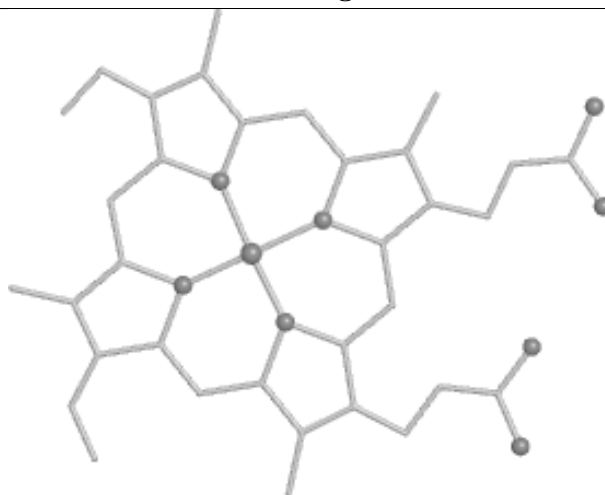
Bond lengths



Bond angles

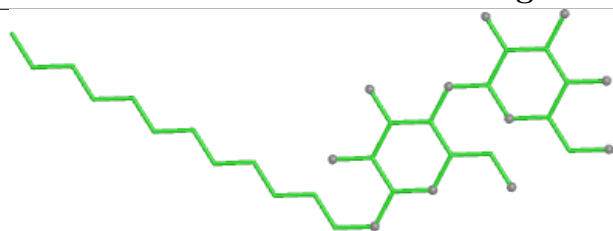


Torsions

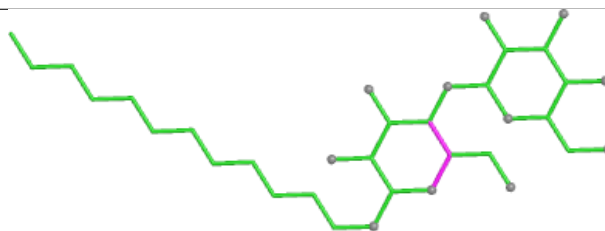


Rings

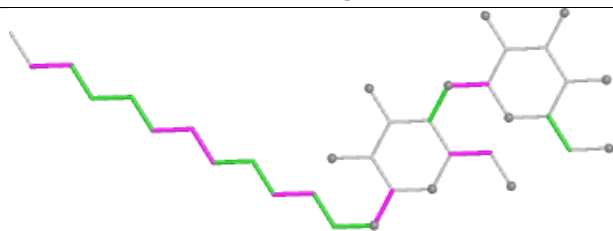
Ligand LMT e 102



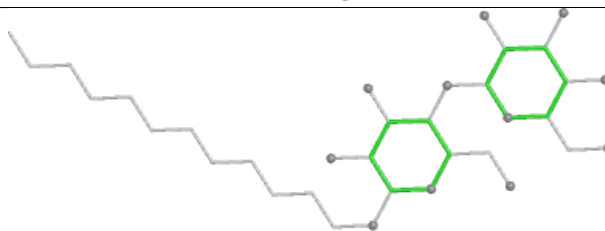
Bond lengths



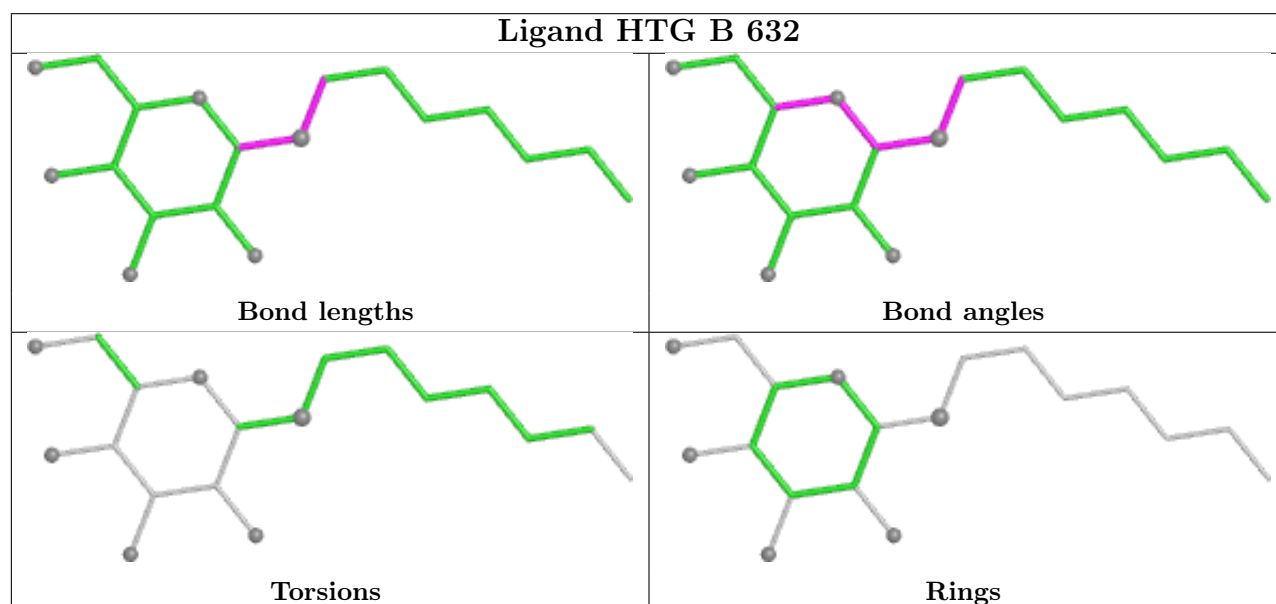
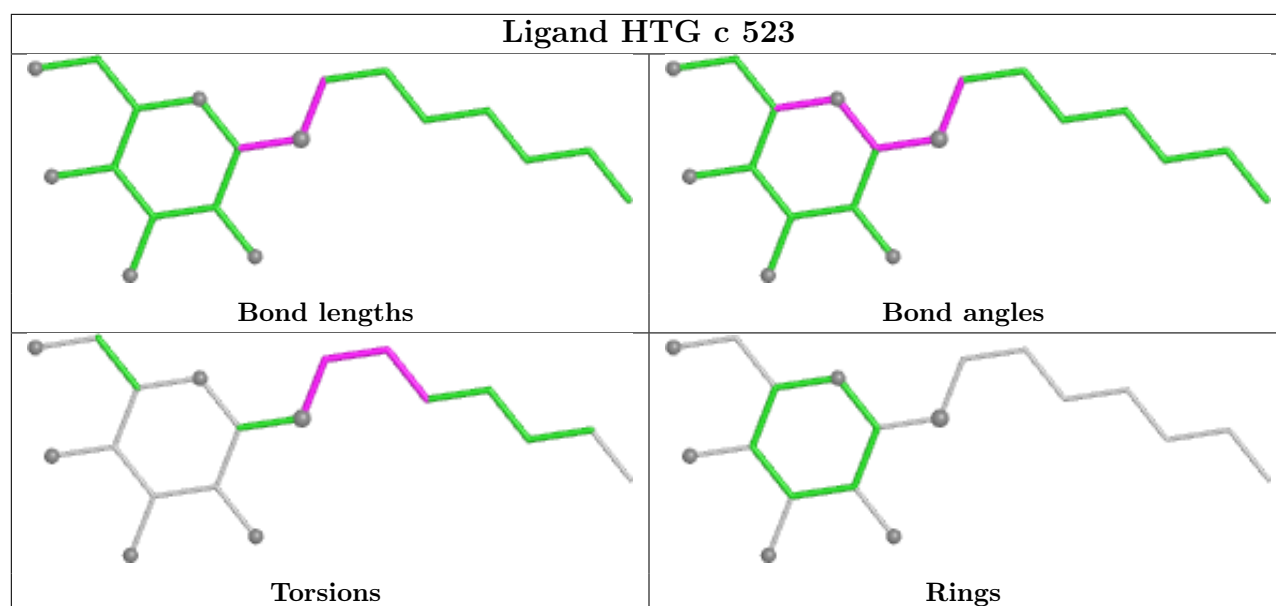
Bond angles

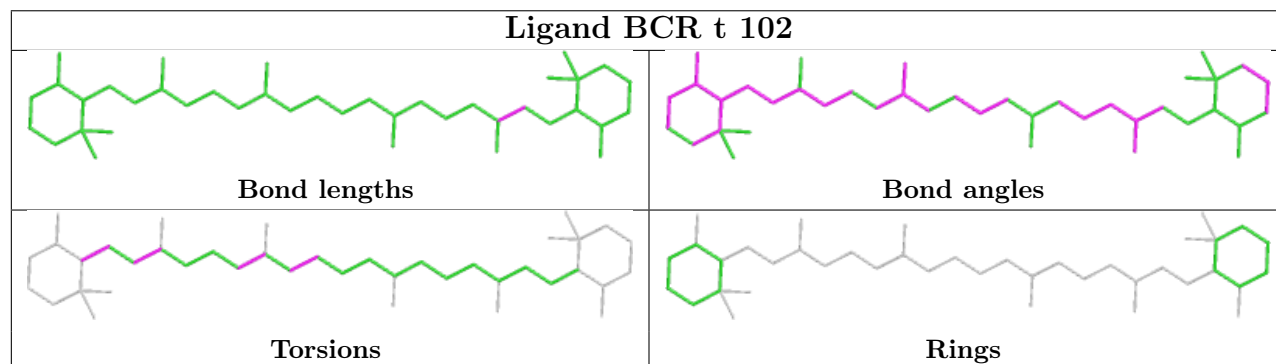
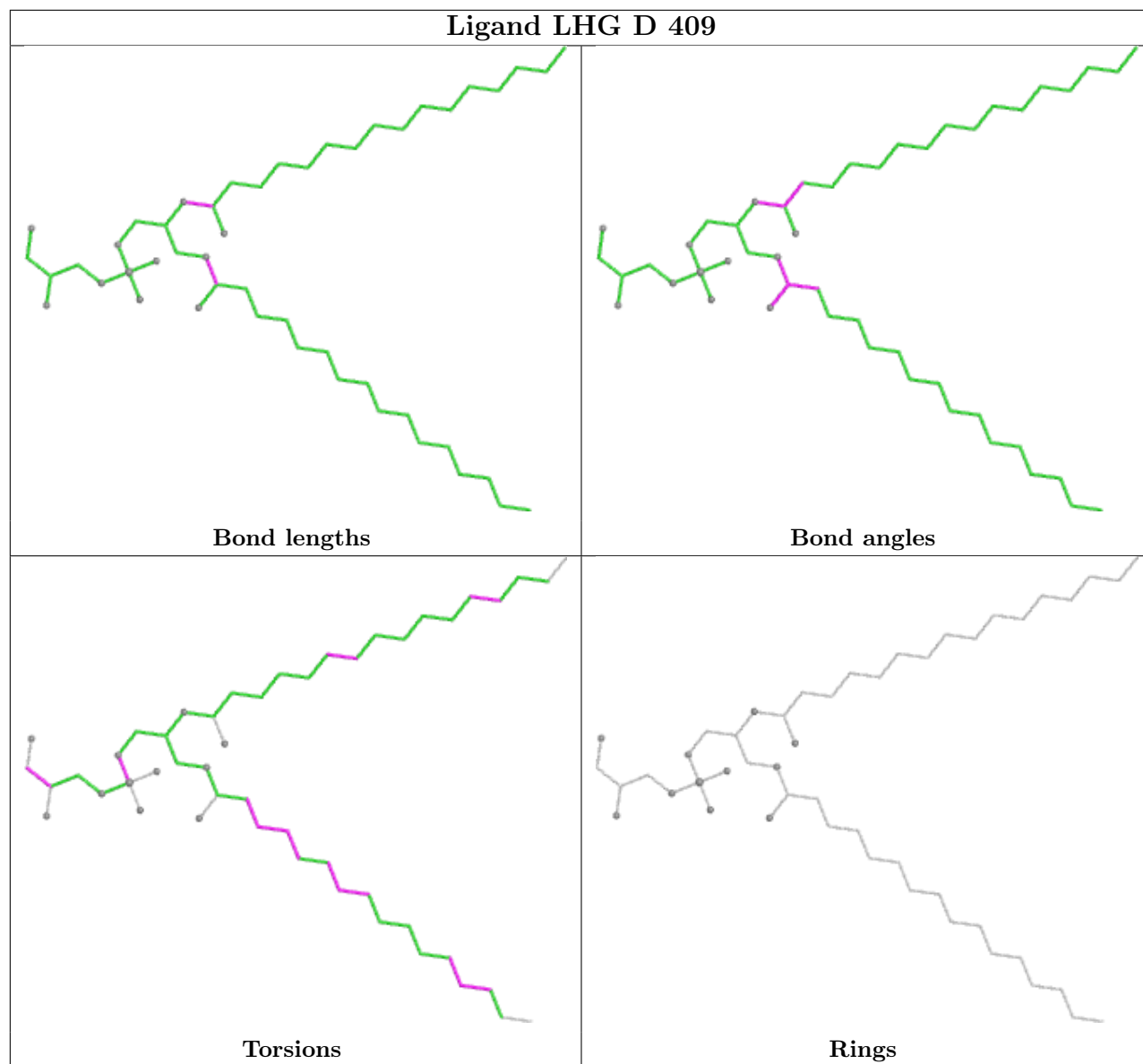


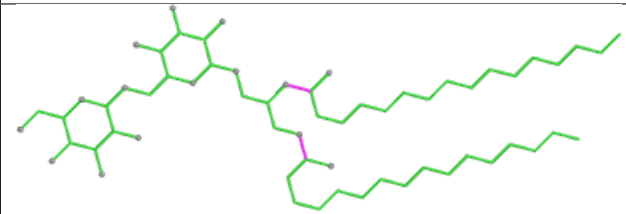
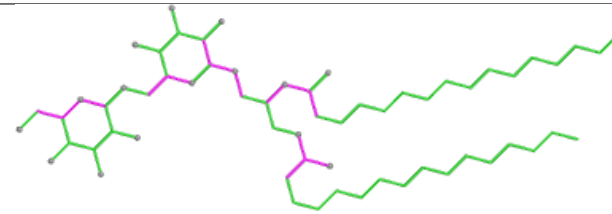
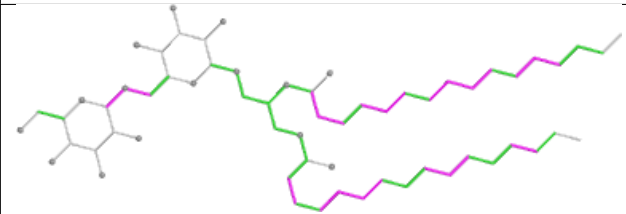
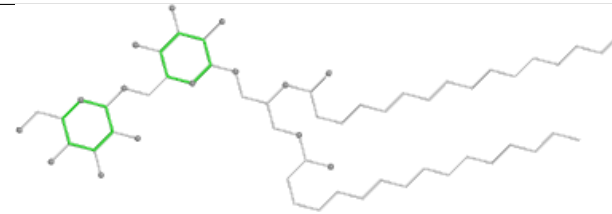
Torsions

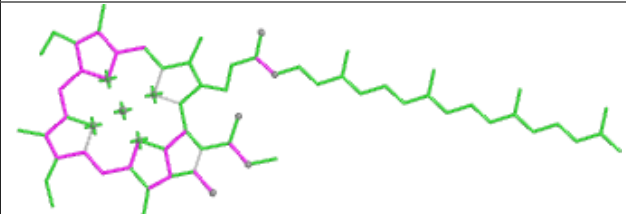
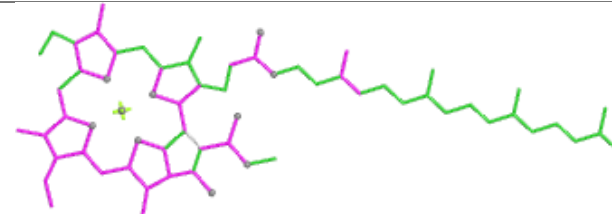
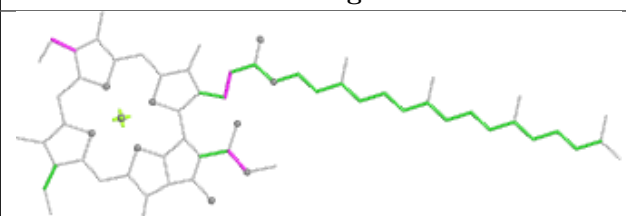
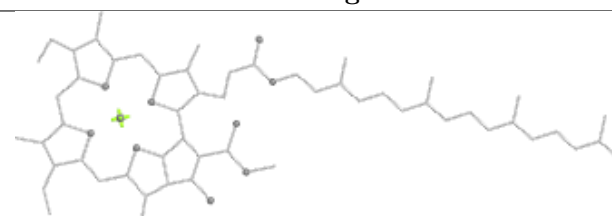


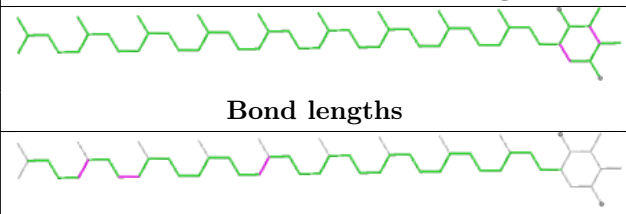
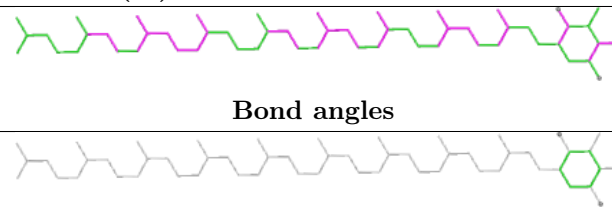
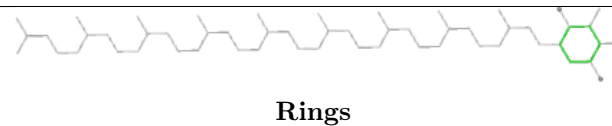
Rings

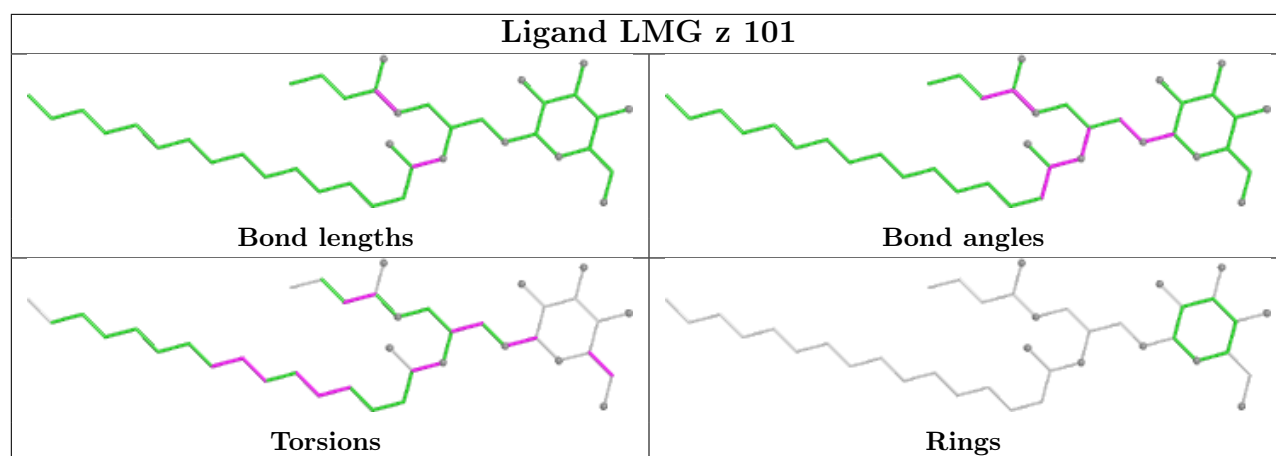




Ligand DGD C 517	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.53	0 100 100	21, 47, 72, 117	53 (15%)
1	a	334/344 (97%)	-0.52	1 (0%) 90 88	22, 48, 80, 156	55 (16%)
2	B	504/505 (99%)	-0.47	1 (0%) 91 89	31, 54, 93, 141	10 (1%)
2	b	503/505 (99%)	-0.44	3 (0%) 85 83	31, 54, 96, 194	12 (2%)
3	C	451/455 (99%)	-0.45	0 100 100	21, 62, 87, 140	7 (1%)
3	c	455/455 (100%)	-0.43	0 100 100	23, 65, 87, 139	13 (2%)
4	D	341/342 (99%)	-0.60	0 100 100	24, 50, 76, 139	16 (4%)
4	d	341/342 (99%)	-0.55	0 100 100	24, 51, 74, 122	16 (4%)
5	E	81/84 (96%)	-0.10	0 100 100	40, 78, 113, 169	2 (2%)
5	e	81/84 (96%)	-0.06	2 (2%) 58 54	42, 78, 131, 187	2 (2%)
6	F	34/44 (77%)	-0.18	0 100 100	59, 70, 111, 118	0
6	f	32/44 (72%)	-0.22	1 (3%) 51 47	57, 69, 132, 154	0
7	H	65/65 (100%)	-0.30	2 (3%) 51 47	40, 65, 86, 160	1 (1%)
7	h	65/65 (100%)	-0.46	1 (1%) 72 68	54, 67, 85, 172	0
8	I	37/38 (97%)	-0.06	0 100 100	53, 67, 127, 178	0
8	i	37/38 (97%)	-0.23	1 (2%) 56 52	49, 64, 131, 156	0
9	J	38/39 (97%)	-0.04	1 (2%) 57 53	58, 76, 160, 184	0
9	j	39/39 (100%)	-0.11	0 100 100	59, 71, 147, 178	0
10	K	37/37 (100%)	-0.28	0 100 100	65, 77, 94, 113	0
10	k	37/37 (100%)	-0.35	0 100 100	65, 76, 98, 113	0
11	L	37/37 (100%)	-0.60	0 100 100	25, 44, 98, 137	1 (2%)
11	l	37/37 (100%)	-0.48	0 100 100	28, 46, 98, 140	1 (2%)
12	M	33/36 (91%)	-0.53	0 100 100	27, 46, 80, 122	1 (3%)
12	m	33/36 (91%)	-0.61	0 100 100	39, 48, 87, 122	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.52	0 100 100	31, 59, 100, 159	8 (3%)
13	o	243/244 (99%)	-0.44	0 100 100	34, 63, 115, 176	5 (2%)
14	T	29/32 (90%)	-0.67	0 100 100	36, 45, 78, 136	1 (3%)
14	t	29/32 (90%)	-0.54	1 (3%) 48 44	36, 45, 71, 137	1 (3%)
15	U	97/104 (93%)	-0.59	0 100 100	46, 59, 89, 121	0
15	u	97/104 (93%)	-0.57	0 100 100	47, 61, 81, 129	0
16	V	137/137 (100%)	-0.58	0 100 100	25, 59, 83, 119	2 (1%)
16	v	137/137 (100%)	-0.49	0 100 100	26, 69, 98, 139	1 (0%)
17	Y	29/30 (96%)	0.71	3 (10%) 12 9	81, 91, 187, 209	0
17	y	29/30 (96%)	0.27	1 (3%) 48 44	82, 96, 146, 162	0
18	X	39/40 (97%)	-0.04	0 100 100	62, 73, 120, 151	0
18	x	38/40 (95%)	0.17	2 (5%) 32 28	63, 72, 133, 157	0
19	Z	62/62 (100%)	0.05	1 (1%) 70 66	78, 93, 132, 152	0
19	z	62/62 (100%)	0.23	2 (3%) 50 46	83, 97, 151, 188	0
20	R	18/34 (52%)	1.84	8 (44%) 0 0	96, 143, 171, 174	0
All	All	5275/5384 (97%)	-0.42	31 (0%) 85 83	21, 58, 106, 209	208 (3%)

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	R	15	ALA	3.9
17	Y	20	ALA	3.6
7	H	65	LEU	3.4
7	h	65	LEU	3.1
5	e	4	THR	3.0

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	0.92	0.08	33,45,52,103	0
14	FME	T	1	10/11	0.93	0.08	40,51,58,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	FME	m	1	10/11	0.95	0.09	37,59,100,111	0
8	FME	I	1	10/11	0.95	0.07	36,59,66,70	0
12	FME	M	1	10/11	0.97	0.07	38,56,95,98	0
8	FME	i	1	10/11	0.97	0.07	45,62,71,72	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
36	DGD	e	101	62/66	0.68	0.17	89,127,190,192	0
36	DGD	D	408	52/66	0.70	0.15	75,107,156,165	0
32	UNL	m	101	10/-	0.70	0.18	64,66,90,92	0
29	LMT	E	102	35/35	0.73	0.17	116,153,169,172	0
27	SQD	f	102	43/54	0.73	0.16	109,123,162,167	0
32	UNL	J	101	10/-	0.75	0.17	61,84,93,93	0
29	LMT	C	521	35/35	0.75	0.14	96,134,162,166	0
32	UNL	a	403	30/-	0.76	0.14	77,96,125,131	0
29	LMT	b	630	25/35	0.76	0.16	80,112,160,160	0
37	LHG	a	420	42/49	0.76	0.11	75,138,182,183	0
32	UNL	C	527	34/-	0.77	0.14	92,125,135,139	0
32	UNL	j	101	10/-	0.77	0.15	76,91,98,99	0
32	UNL	A	418	28/-	0.77	0.14	65,94,113,117	0
34	CA	f	103	1/1	0.78	0.07	124,124,124,124	0
37	LHG	E	101	42/49	0.78	0.12	73,119,141,142	0
32	UNL	i	101	40/-	0.78	0.14	54,88,139,142	0
29	LMT	a	419	35/35	0.79	0.13	104,129,159,162	0
29	LMT	e	102	35/35	0.79	0.14	86,143,166,167	0
35	HTG	D	414	16/19	0.79	0.12	81,137,154,157	0
35	HTG	V	206	19/19	0.79	0.14	62,103,129,237	0
29	LMT	A	414	35/35	0.80	0.13	59,96,114,123	0
32	UNL	d	412	36/-	0.80	0.13	69,89,135,139	0
29	LMT	M	104	35/35	0.81	0.13	56,102,155,159	0
35	HTG	d	413	16/19	0.81	0.12	72,110,117,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	LMT	D	403	35/35	0.81	0.12	75,127,151,153	0
32	UNL	D	413	40/-	0.81	0.12	63,88,132,140	0
35	HTG	B	632	19/19	0.81	0.11	55,118,140,210	0
32	UNL	I	101	40/-	0.81	0.14	60,95,150,153	0
33	LMG	C	520	51/55	0.82	0.12	67,122,137,143	0
32	UNL	B	633	33/-	0.82	0.14	62,87,128,133	0
35	HTG	b	608	19/19	0.82	0.11	55,112,147,160	0
28	GOL	V	201	6/6	0.82	0.16	81,91,96,100	0
35	HTG	c	524	19/19	0.83	0.11	90,122,133,164	0
32	UNL	M	103	10/-	0.83	0.10	48,53,74,76	0
29	LMT	a	404	35/35	0.83	0.12	42,99,122,150	0
32	UNL	c	525	32/-	0.83	0.13	85,102,136,143	0
27	SQD	F	101	43/54	0.83	0.12	80,119,134,139	0
33	LMG	Z	101	37/55	0.83	0.14	72,131,146,147	0
28	GOL	A	412	6/6	0.84	0.12	76,86,88,92	0
33	LMG	z	101	39/55	0.84	0.13	77,125,148,160	0
34	CA	b	609	1/1	0.84	0.09	134,134,134,134	0
32	UNL	b	633	33/-	0.84	0.14	58,97,147,148	0
35	HTG	B	624	19/19	0.84	0.11	78,133,147,176	0
28	GOL	a	402	6/6	0.84	0.13	93,97,103,103	0
35	HTG	C	523	19/19	0.84	0.12	78,117,141,143	0
28	GOL	O	301	6/6	0.84	0.10	74,89,90,93	0
33	LMG	c	522	51/55	0.85	0.12	59,111,124,132	0
27	SQD	L	102	54/54	0.85	0.11	54,82,126,138	0
29	LMT	t	101	25/35	0.85	0.13	52,86,147,149	0
31	PL9	a	416[A]	55/55	0.85	0.16	87,114,123,124	55
31	PL9	a	416[B]	55/55	0.85	0.16	87,114,123,124	55
35	HTG	c	523	19/19	0.85	0.11	91,114,126,129	0
31	PL9	A	417[B]	55/55	0.86	0.15	84,104,120,121	55
35	HTG	b	631	19/19	0.86	0.14	67,83,98,102	0
35	HTG	b	632	19/19	0.86	0.12	77,138,158,165	0
27	SQD	a	405	54/54	0.86	0.10	40,83,122,127	0
35	HTG	B	623	19/19	0.86	0.13	60,79,91,92	0
27	SQD	A	413	54/54	0.86	0.10	56,81,130,137	0
29	LMT	T	104	25/35	0.86	0.14	43,83,140,150	0
29	LMT	m	103	35/35	0.86	0.10	46,103,128,129	0
27	SQD	B	621	54/54	0.86	0.12	56,82,141,145	0
31	PL9	A	417[A]	55/55	0.86	0.15	85,104,120,121	55
28	GOL	T	101	6/6	0.87	0.19	70,88,93,93	0
28	GOL	v	202	6/6	0.87	0.12	83,96,98,100	0
28	GOL	B	627	6/6	0.87	0.12	71,86,88,88	0
29	LMT	m	102	35/35	0.88	0.11	56,93,121,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	CA	F	102	1/1	0.88	0.10	119,119,119,119	0
22	CL	A	403[A]	1/1	0.88	0.12	47,47,47,47	1
22	CL	A	403[B]	1/1	0.88	0.12	45,45,45,45	1
33	LMG	A	419	51/55	0.88	0.10	57,90,109,115	0
33	LMG	C	519	51/55	0.88	0.10	62,99,117,120	0
28	GOL	C	524	6/6	0.88	0.15	86,89,104,108	0
28	GOL	b	605	6/6	0.88	0.15	66,82,107,110	0
22	CL	v	205	1/1	0.88	0.09	128,128,128,128	0
33	LMG	k	101	51/55	0.88	0.11	62,94,123,126	0
24	CLA	C	513	65/65	0.89	0.10	61,87,117,123	0
28	GOL	T	102	6/6	0.89	0.12	104,114,118,118	0
28	GOL	c	502	6/6	0.89	0.16	85,111,119,127	0
28	GOL	t	103	6/6	0.89	0.17	60,88,99,102	0
35	HTG	C	522	19/19	0.89	0.10	91,102,119,121	0
28	GOL	B	629	6/6	0.89	0.13	55,69,74,78	0
28	GOL	b	606	6/6	0.90	0.10	70,91,98,100	0
24	CLA	C	506	65/65	0.90	0.10	52,75,116,119	0
32	UNL	d	411	17/-	0.90	0.11	57,77,101,101	0
28	GOL	a	421	6/6	0.90	0.10	88,100,106,106	0
32	UNL	d	414	18/-	0.90	0.13	76,84,116,118	0
24	CLA	B	602	65/65	0.90	0.10	57,74,114,132	0
28	GOL	v	203	6/6	0.90	0.12	96,105,112,124	0
34	CA	B	601	1/1	0.91	0.06	135,135,135,135	0
29	LMT	M	102	35/35	0.91	0.10	46,102,124,132	0
28	GOL	b	601	6/6	0.91	0.10	55,59,64,68	0
22	CL	U	201	1/1	0.91	0.12	117,117,117,117	0
24	CLA	b	610	65/65	0.91	0.10	57,79,127,133	0
24	CLA	c	517	65/65	0.91	0.09	76,94,106,111	0
35	HTG	B	631	19/19	0.91	0.10	52,105,123,128	0
33	LMG	a	415	51/55	0.91	0.09	61,90,100,101	0
28	GOL	o	301	6/6	0.91	0.10	84,90,97,98	0
37	LHG	D	411	49/49	0.91	0.10	51,71,118,127	0
27	SQD	A	411	54/54	0.91	0.10	52,94,103,105	0
32	UNL	X	101	18/-	0.91	0.10	70,77,101,105	0
26	BCR	d	406	40/40	0.92	0.08	48,61,83,91	0
23	BCT	A	404[A]	4/4	0.92	0.11	72,74,78,88	4
36	DGD	C	517	62/66	0.92	0.09	55,71,102,113	0
33	LMG	d	415	51/55	0.92	0.09	53,70,112,122	0
24	CLA	C	504	65/65	0.92	0.09	45,67,93,102	0
23	BCT	A	404[B]	4/4	0.92	0.11	71,72,78,90	4
33	LMG	D	415	51/55	0.92	0.10	51,73,119,129	0
26	BCR	C	514	40/40	0.92	0.09	58,81,93,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	UNL	D	412	17/-	0.93	0.09	46,71,89,96	0
26	BCR	c	526	40/40	0.93	0.09	72,87,94,96	0
24	CLA	B	615	65/65	0.93	0.09	34,46,97,100	0
28	GOL	B	626	6/6	0.93	0.10	56,67,87,100	0
26	BCR	y	101	40/40	0.93	0.08	58,70,81,83	0
35	HTG	b	602	19/19	0.93	0.08	46,64,75,77	0
33	LMG	b	629	51/55	0.93	0.08	40,57,76,83	0
28	GOL	B	628	6/6	0.93	0.11	56,69,75,78	0
23	BCT	d	401[B]	4/4	0.93	0.12	85,85,88,93	4
28	GOL	B	630	6/6	0.93	0.11	59,95,102,108	0
28	GOL	B	634	6/6	0.93	0.08	56,58,65,66	0
24	CLA	c	510	65/65	0.93	0.08	52,74,96,102	0
23	BCT	d	401[A]	4/4	0.93	0.12	86,88,90,94	4
24	CLA	C	512	65/65	0.93	0.08	62,81,95,102	0
26	BCR	D	406	40/40	0.93	0.09	52,65,99,107	0
26	BCR	K	101	40/40	0.93	0.09	58,71,80,87	0
28	GOL	V	203	6/6	0.93	0.09	68,76,82,85	0
27	SQD	a	414	54/54	0.93	0.09	54,87,114,116	0
24	CLA	B	607	65/65	0.94	0.08	40,54,94,98	0
31	PL9	d	407[A]	55/55	0.94	0.07	31,46,53,59	55
31	PL9	d	407[B]	55/55	0.94	0.07	31,45,55,63	55
24	CLA	d	405	65/65	0.94	0.08	49,64,115,122	0
25	PHO	d	402[A]	64/64	0.94	0.07	39,50,56,59	64
25	PHO	d	402[B]	64/64	0.94	0.07	40,50,56,60	64
26	BCR	A	410	40/40	0.94	0.07	37,48,57,65	0
26	BCR	B	620	40/40	0.94	0.07	39,53,64,79	0
35	HTG	B	622	19/19	0.94	0.09	53,65,88,92	0
24	CLA	A	409	65/65	0.94	0.09	40,58,123,132	0
24	CLA	a	412	65/65	0.94	0.10	40,59,116,123	0
26	BCR	H	101	40/40	0.94	0.08	45,64,78,85	0
24	CLA	C	508	65/65	0.94	0.08	46,66,133,146	0
26	BCR	Y	101	40/40	0.94	0.08	62,72,92,98	0
26	BCR	b	627	40/40	0.94	0.07	37,52,68,78	0
28	GOL	D	402	6/6	0.94	0.13	55,64,73,77	0
24	CLA	b	615	65/65	0.94	0.08	41,54,100,112	0
24	CLA	b	625	65/65	0.94	0.08	40,61,106,112	0
35	HTG	b	607	19/19	0.94	0.07	52,88,101,103	0
26	BCR	h	101	40/40	0.94	0.07	46,66,76,77	0
24	CLA	c	507	65/65	0.94	0.08	50,62,75,87	0
28	GOL	V	202	6/6	0.94	0.09	54,65,76,78	0
24	CLA	C	510	65/65	0.94	0.07	55,71,84,92	0
28	GOL	V	204	6/6	0.94	0.10	90,103,105,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	c	511	65/65	0.94	0.09	53,68,79,83	0
36	DGD	C	516	62/66	0.94	0.08	40,58,89,91	0
24	CLA	c	512	65/65	0.94	0.08	44,59,125,141	0
24	CLA	c	516	65/65	0.94	0.08	63,79,91,99	0
36	DGD	c	519	62/66	0.94	0.08	41,62,97,101	0
36	DGD	c	520	62/66	0.94	0.08	47,65,115,133	0
36	DGD	c	521	62/66	0.94	0.08	51,62,87,100	0
33	LMG	M	101	51/55	0.94	0.08	41,61,83,89	0
36	DGD	h	102	62/66	0.94	0.07	44,60,79,85	0
37	LHG	D	409	49/49	0.94	0.08	39,56,65,72	0
31	PL9	D	407[A]	55/55	0.94	0.08	34,45,52,64	55
31	PL9	D	407[B]	55/55	0.94	0.08	34,45,53,67	55
28	GOL	b	603	6/6	0.94	0.10	60,73,78,87	0
37	LHG	d	410	49/49	0.94	0.10	42,65,113,119	0
26	BCR	T	103	40/40	0.95	0.06	32,51,66,72	0
24	CLA	b	624	65/65	0.95	0.07	42,56,74,78	0
24	CLA	B	609	65/65	0.95	0.07	42,53,62,66	0
26	BCR	b	628	40/40	0.95	0.07	41,59,69,72	0
26	BCR	c	518	40/40	0.95	0.07	49,63,73,78	0
28	GOL	a	401	6/6	0.95	0.10	55,63,75,82	0
24	CLA	c	505	65/65	0.95	0.08	50,67,75,77	0
24	CLA	c	506	65/65	0.95	0.07	47,61,79,88	0
24	CLA	C	507	65/65	0.95	0.08	51,71,84,91	0
26	BCR	k	102	40/40	0.95	0.08	54,75,85,87	0
28	GOL	b	604	6/6	0.95	0.09	62,73,80,84	0
26	BCR	t	102	40/40	0.95	0.07	36,53,75,77	0
24	CLA	c	508	65/65	0.95	0.07	49,62,85,99	0
24	CLA	c	509	65/65	0.95	0.07	43,56,75,78	0
24	CLA	B	614	65/65	0.95	0.07	31,45,67,82	0
24	CLA	C	509	65/65	0.95	0.09	49,72,86,92	0
24	CLA	A	407	65/65	0.95	0.07	33,47,101,110	0
24	CLA	c	513	65/65	0.95	0.09	53,68,85,94	0
28	GOL	v	204	6/6	0.95	0.10	59,64,71,78	0
24	CLA	c	515	65/65	0.95	0.08	51,73,89,101	0
24	CLA	C	511	65/65	0.95	0.08	56,74,89,101	0
24	CLA	B	617	65/65	0.95	0.11	45,62,136,139	0
24	CLA	C	502	65/65	0.95	0.07	45,66,73,81	0
28	GOL	B	625	6/6	0.95	0.08	55,65,74,83	0
36	DGD	C	518	62/66	0.95	0.07	45,63,82,96	0
24	CLA	D	405	65/65	0.95	0.08	47,62,111,116	0
36	DGD	H	102	62/66	0.95	0.08	41,58,95,103	0
24	CLA	a	410	65/65	0.95	0.07	38,51,113,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	C	503	65/65	0.95	0.07	50,62,77,82	0
26	BCR	B	619	40/40	0.95	0.06	37,51,64,71	0
24	CLA	B	608	65/65	0.95	0.07	32,45,58,70	0
24	CLA	C	505	65/65	0.95	0.07	48,60,75,91	0
26	BCR	C	515	40/40	0.95	0.07	47,63,75,80	0
24	CLA	b	618	65/65	0.95	0.07	45,57,67,77	0
28	GOL	F	103	6/6	0.95	0.07	88,95,100,104	0
24	CLA	b	620	65/65	0.95	0.07	35,49,59,65	0
37	LHG	d	408	49/49	0.95	0.07	44,60,70,72	0
24	CLA	b	623	65/65	0.95	0.07	31,47,93,106	0
39	MG	j	102	1/1	0.95	0.06	70,70,70,70	0
25	PHO	A	408	64/64	0.96	0.06	28,44,52,61	0
25	PHO	D	401[A]	64/64	0.96	0.07	41,51,60,63	64
25	PHO	D	401[B]	64/64	0.96	0.07	40,50,59,64	64
24	CLA	b	622	65/65	0.96	0.06	36,49,62,68	0
24	CLA	B	611	65/65	0.96	0.08	42,56,67,71	0
24	CLA	B	612	65/65	0.96	0.06	35,46,54,63	0
26	BCR	B	618	40/40	0.96	0.05	36,49,59,62	0
24	CLA	B	613	65/65	0.96	0.07	32,47,57,60	0
24	CLA	A	405	65/65	0.96	0.06	32,41,52,62	0
24	CLA	B	603	65/65	0.96	0.06	40,53,62,66	0
24	CLA	B	616	65/65	0.96	0.06	40,56,68,77	0
28	GOL	c	501	6/6	0.96	0.07	47,52,56,58	0
24	CLA	b	611	65/65	0.96	0.07	41,57,65,73	0
24	CLA	b	612	65/65	0.96	0.06	45,55,63,71	0
24	CLA	b	613	65/65	0.96	0.07	32,48,75,84	0
24	CLA	b	614	65/65	0.96	0.07	36,46,60,70	0
24	CLA	B	605	65/65	0.96	0.06	31,45,75,79	0
26	BCR	a	413	40/40	0.96	0.06	34,47,58,61	0
26	BCR	b	626	40/40	0.96	0.05	36,49,59,64	0
24	CLA	b	616	65/65	0.96	0.06	31,42,54,62	0
28	GOL	C	525	6/6	0.96	0.08	52,54,59,60	0
37	LHG	D	410	49/49	0.96	0.07	34,49,75,92	0
24	CLA	c	514	65/65	0.96	0.07	47,64,74,80	0
24	CLA	b	617	65/65	0.96	0.06	43,57,64,73	0
24	CLA	C	501	65/65	0.96	0.07	50,62,87,97	0
37	LHG	b	634	49/49	0.96	0.07	39,54,68,82	0
24	CLA	B	610	65/65	0.96	0.07	38,58,67,75	0
37	LHG	d	409	49/49	0.96	0.07	35,51,69,90	0
24	CLA	d	403	65/65	0.96	0.05	35,44,53,57	0
24	CLA	b	621	65/65	0.96	0.07	35,50,59,63	0
24	CLA	A	406	65/65	0.97	0.05	31,42,51,53	0

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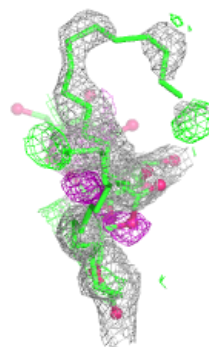
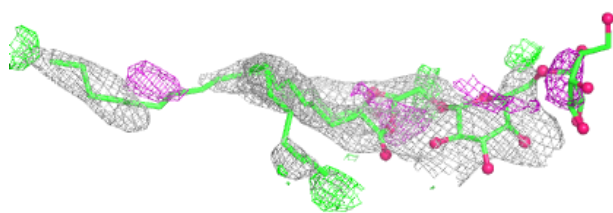
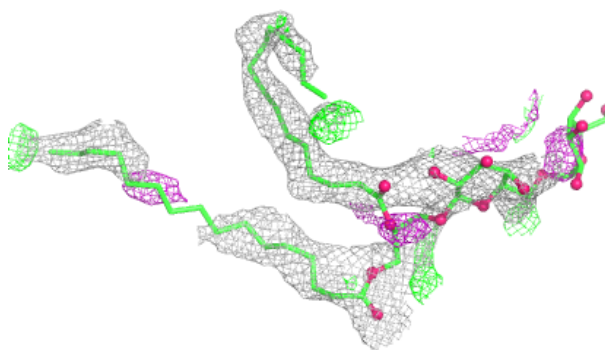
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	b	619	65/65	0.97	0.07	41,58,66,77	0
28	GOL	v	201	6/6	0.97	0.08	74,84,87,96	0
37	LHG	L	101	49/49	0.97	0.06	39,52,64,67	0
25	PHO	a	411	64/64	0.97	0.05	38,45,54,63	0
24	CLA	B	606	65/65	0.97	0.06	36,47,58,61	0
24	CLA	D	404	65/65	0.97	0.06	30,42,61,69	0
24	CLA	d	404	65/65	0.97	0.06	32,45,58,73	0
24	CLA	B	604	65/65	0.97	0.07	43,55,63,68	0
38	HEM	E	103	43/43	0.97	0.08	63,82,103,115	0
38	HEM	f	101	43/43	0.97	0.09	66,90,130,144	0
39	MG	J	102	1/1	0.97	0.05	71,71,71,71	0
24	CLA	a	409	65/65	0.97	0.06	34,44,56,71	0
34	CA	o	302	1/1	0.98	0.03	97,97,97,97	0
22	CL	a	408[B]	1/1	0.98	0.04	49,49,49,49	1
34	CA	O	302	1/1	0.98	0.03	100,100,100,100	0
22	CL	a	408[A]	1/1	0.98	0.04	49,49,49,49	1
34	CA	c	503	1/1	0.98	0.09	77,77,77,77	0
34	CA	C	526	1/1	0.98	0.06	87,87,87,87	0
40	HEC	V	205	43/43	0.98	0.06	44,53,65,67	0
40	HEC	v	206	43/43	0.98	0.06	51,65,74,75	0
21	FE2	A	401[B]	1/1	0.99	0.03	65,65,65,65	1
21	FE2	a	406[A]	1/1	0.99	0.02	62,62,62,62	1
22	CL	a	407[A]	1/1	0.99	0.07	43,43,43,43	1
22	CL	a	407[B]	1/1	0.99	0.07	45,45,45,45	1
21	FE2	a	406[B]	1/1	0.99	0.02	62,62,62,62	1
22	CL	A	402[A]	1/1	0.99	0.04	41,41,41,41	1
34	CA	c	504	1/1	0.99	0.03	84,84,84,84	0
30	OEX	A	415[A]	10/10	0.99	0.03	47,57,59,70	10
30	OEX	A	416[B]	10/10	0.99	0.03	43,52,60,68	10
30	OEX	a	417[A]	10/10	0.99	0.04	47,51,57,61	10
30	OEX	a	418[B]	10/10	0.99	0.04	47,51,57,60	10
22	CL	A	402[B]	1/1	0.99	0.04	41,41,41,41	1
21	FE2	A	401[A]	1/1	0.99	0.03	66,66,66,66	1

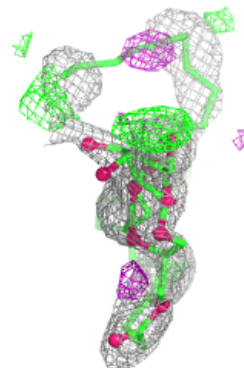
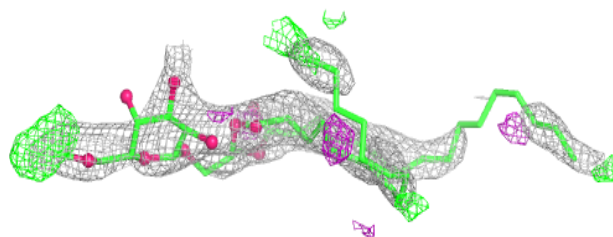
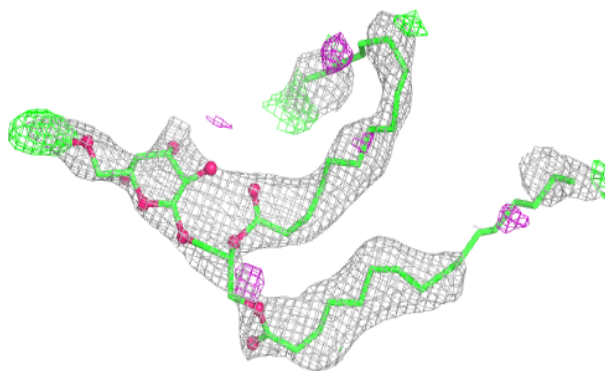
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DGD 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)

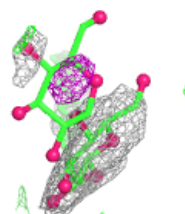
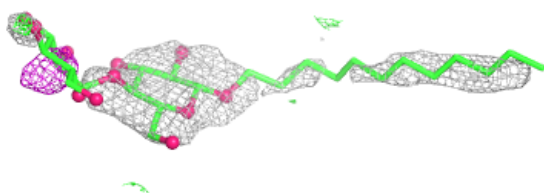
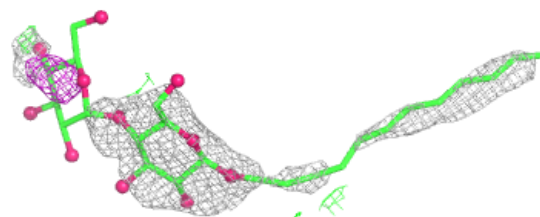
**Electron density around DGD D 408:**

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

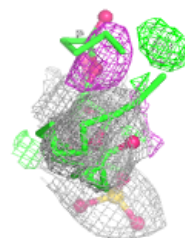
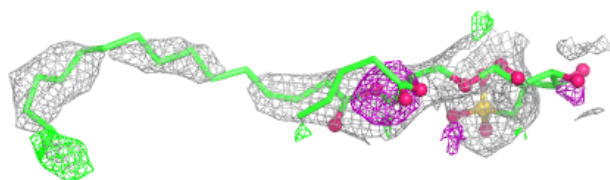
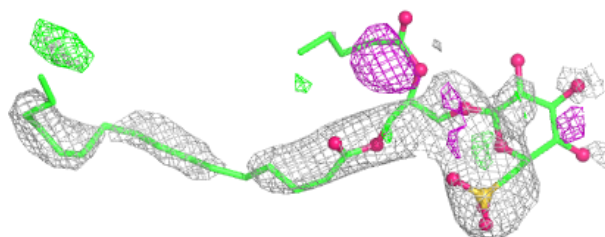


Electron density around LMT E 102:

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

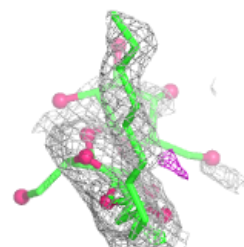
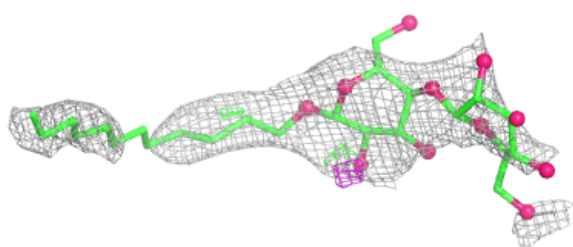
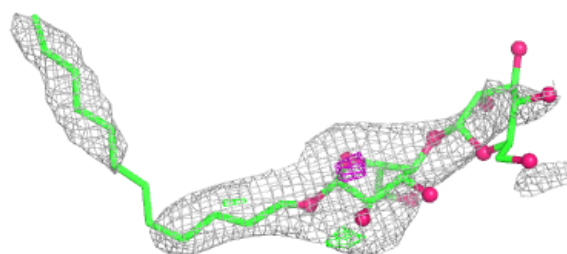
**Electron density around SQD f 102:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

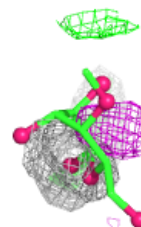
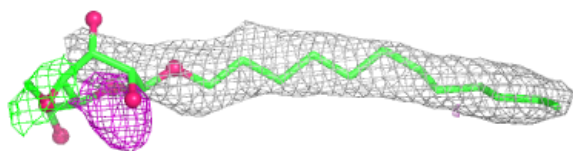
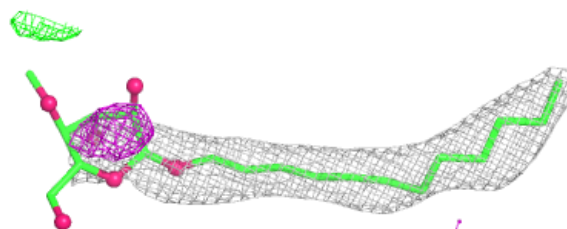


Electron density around LMT C 521:

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

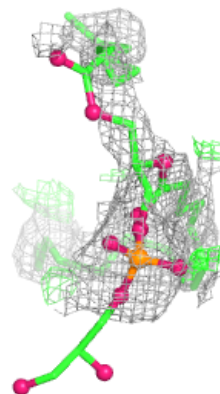
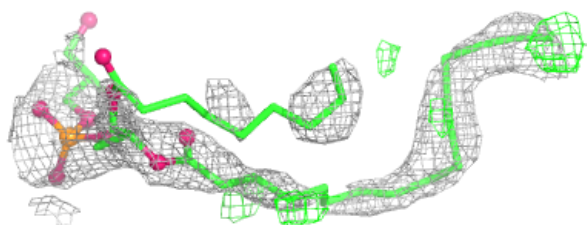
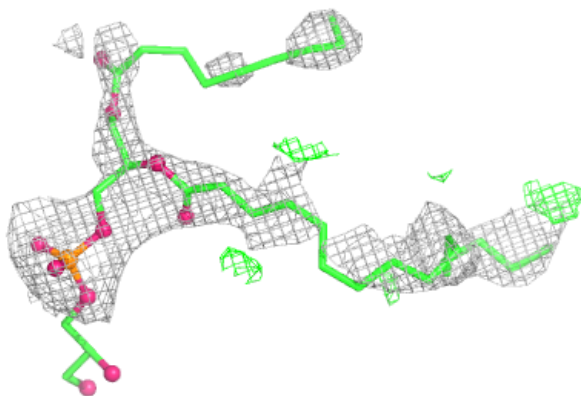
**Electron density around LMT b 630:**

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



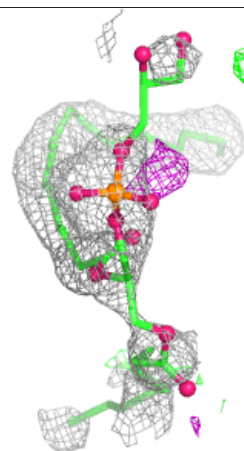
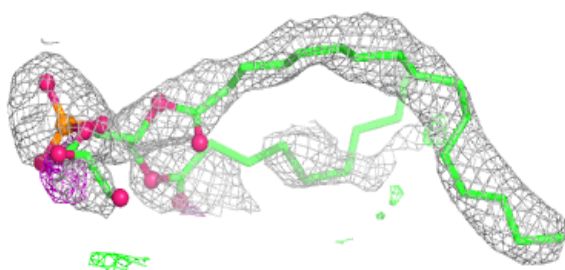
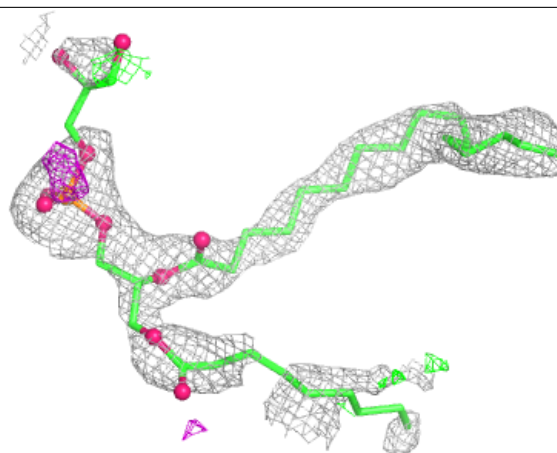
Electron density around LHG a 420:

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



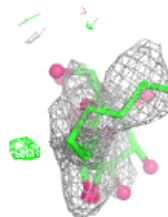
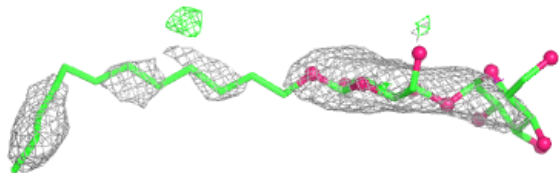
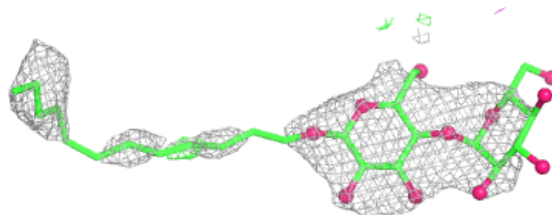
Electron density around LHG E 101:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

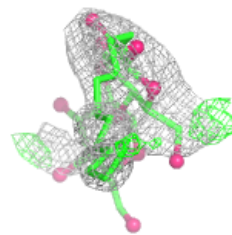
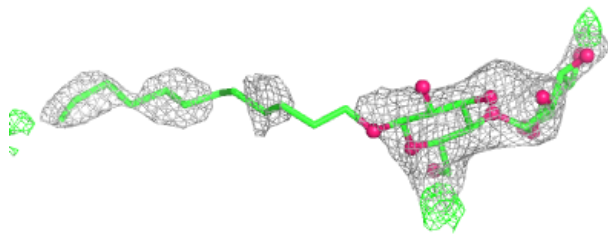
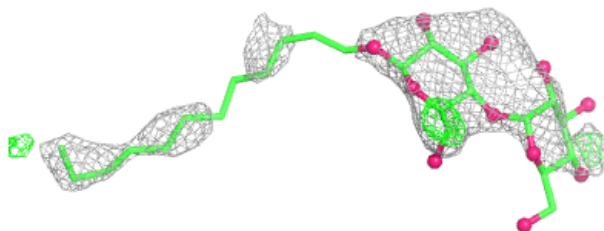


Electron density around LMT a 419:

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

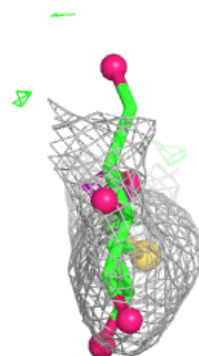
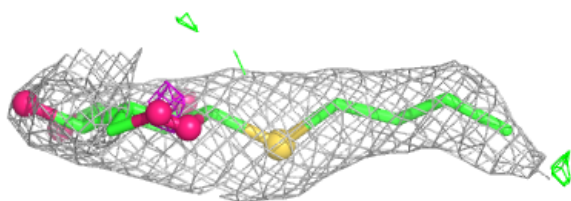
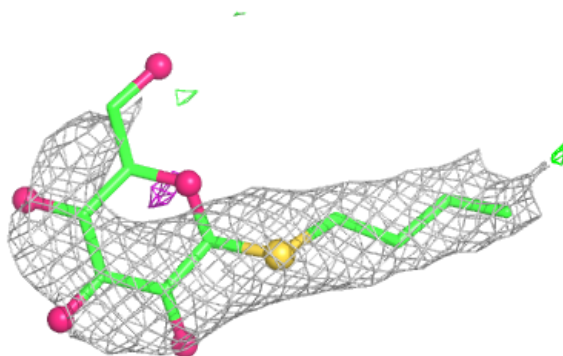
**Electron density around LMT e 102:**

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

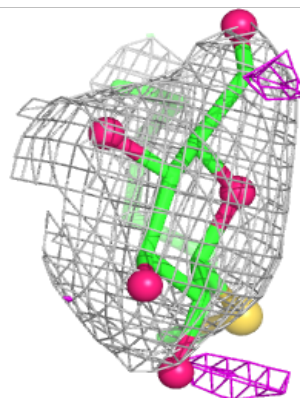
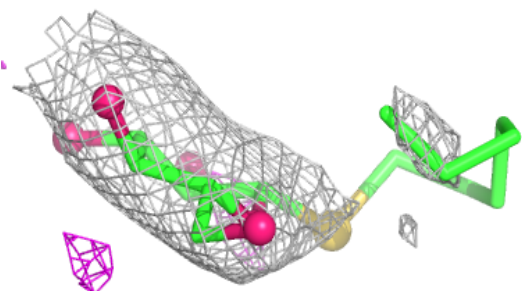
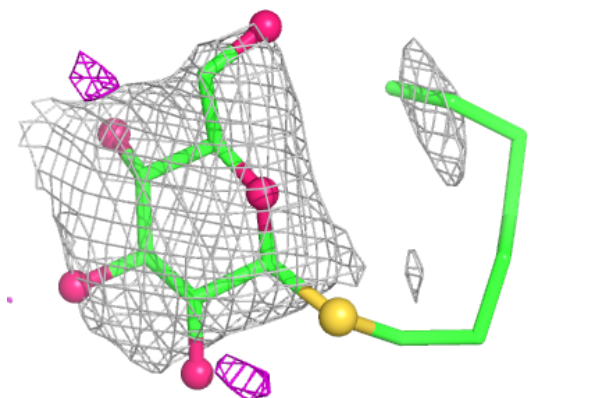


Electron density around HTG D 414:

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

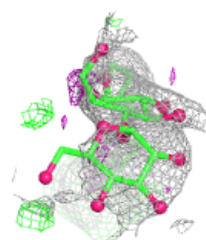
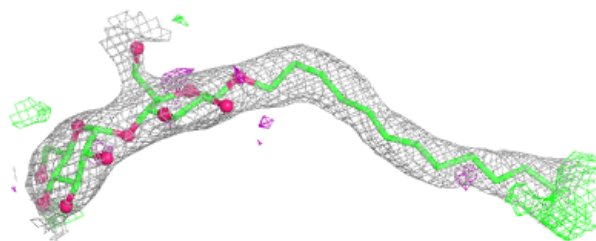
**Electron density around HTG V 206:**

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

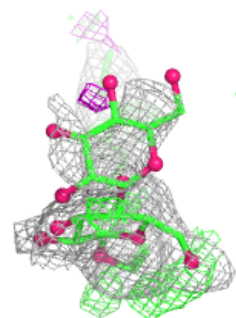
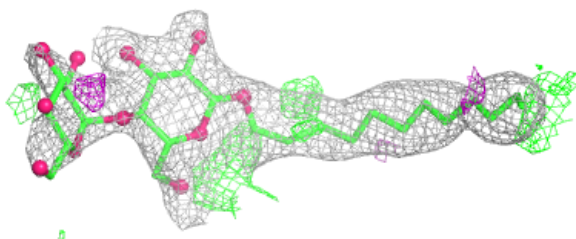
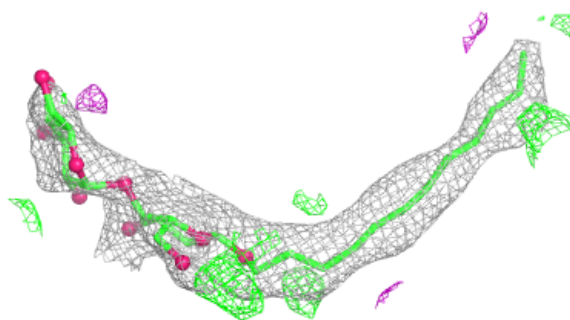


Electron density around LMT A 414:

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

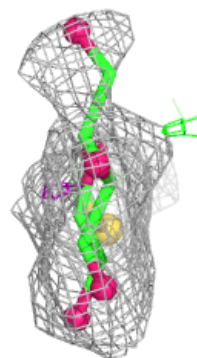
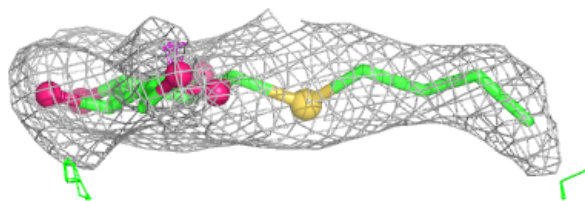
**Electron density around LMT M 104:**

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

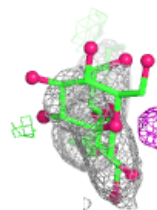
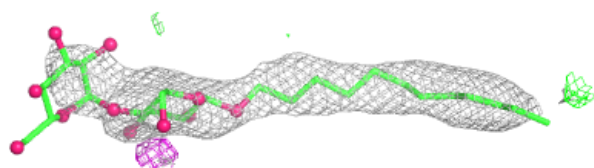
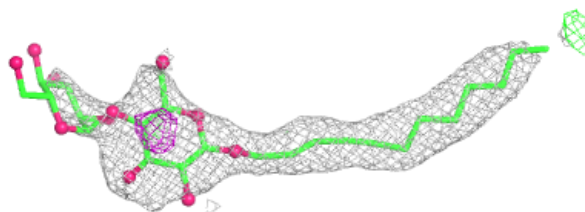


Electron density around HTG d 413:

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

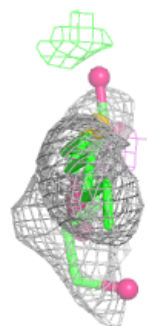
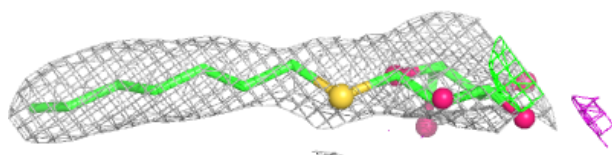
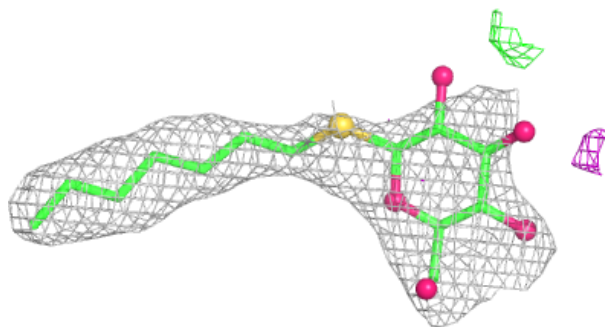
**Electron density around LMT D 403:**

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

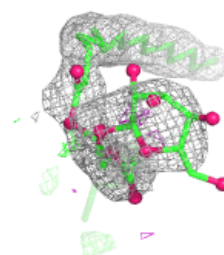
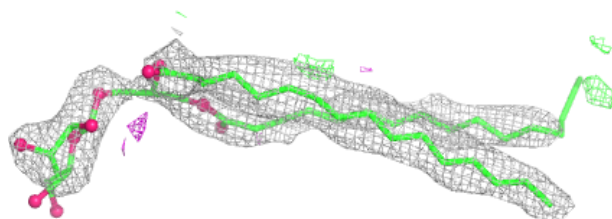
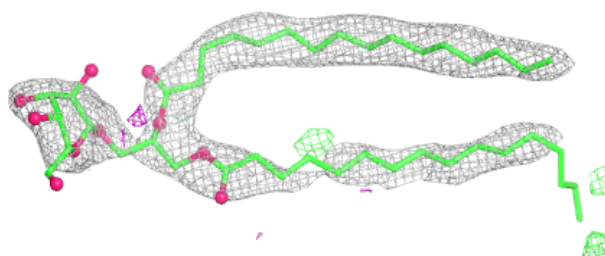


Electron density around HTG B 632:

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

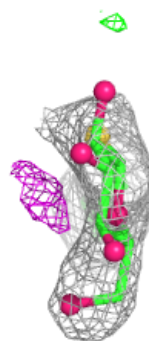
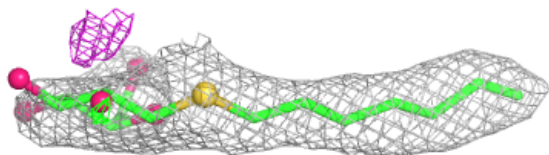
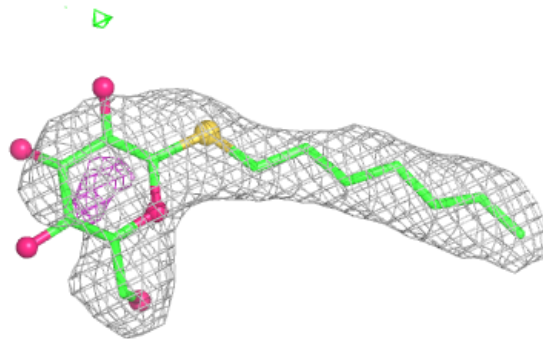
**Electron density around LMG C 520:**

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

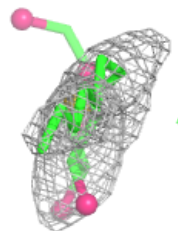
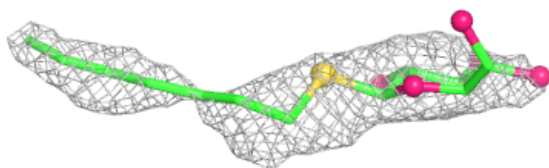
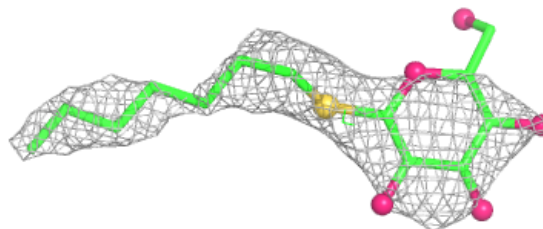


Electron density around HTG b 608:

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

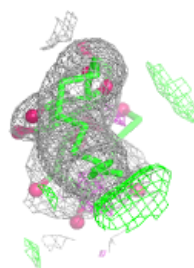
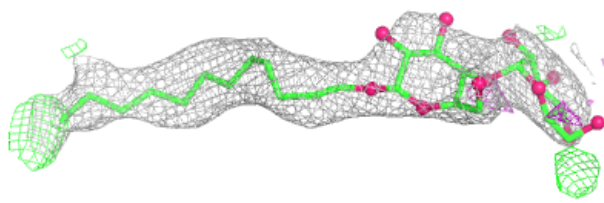
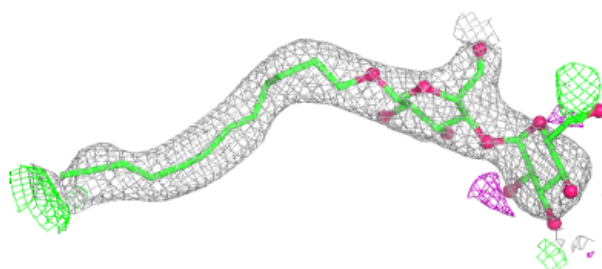
**Electron density around HTG c 524:**

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

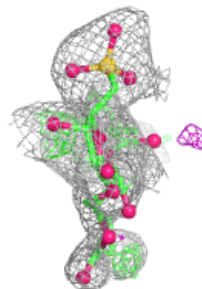
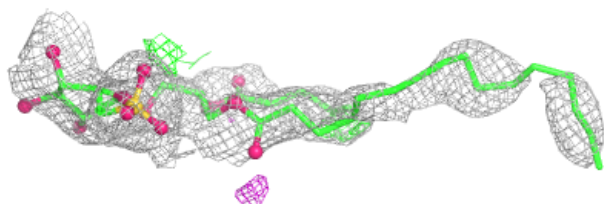
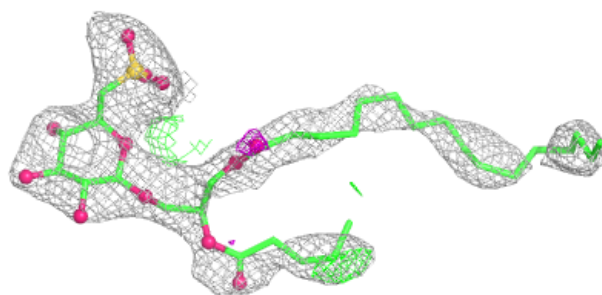


Electron density around LMT a 404:

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

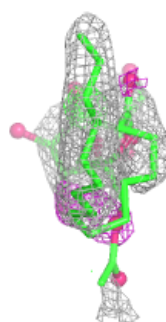
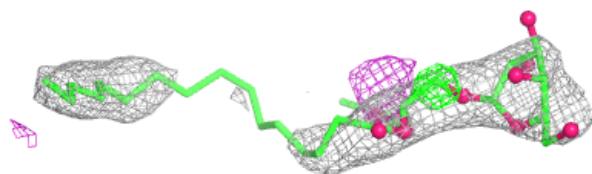
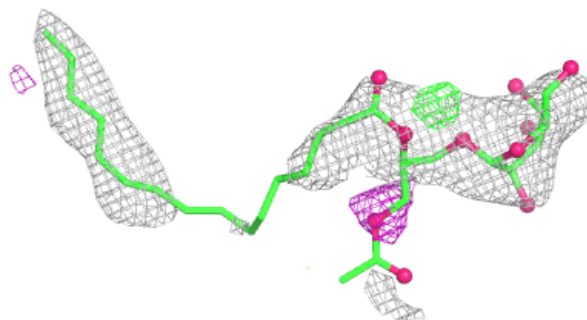
**Electron density around SQD F 101:**

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

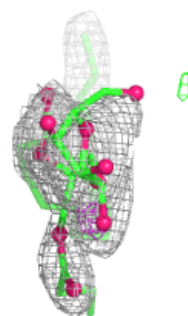
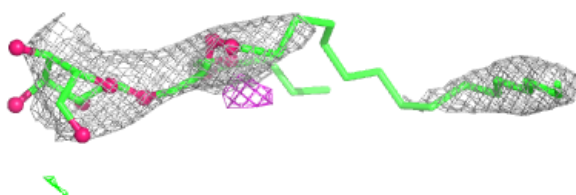
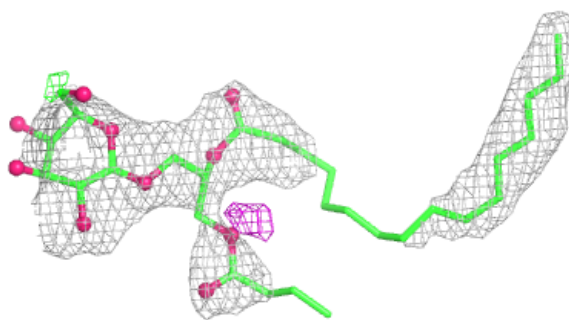


Electron density around LMG Z 101:

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

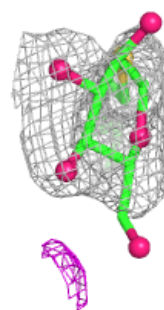
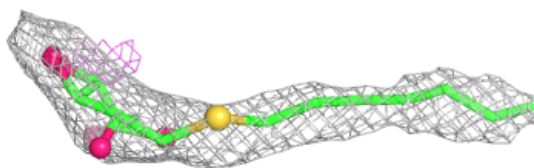
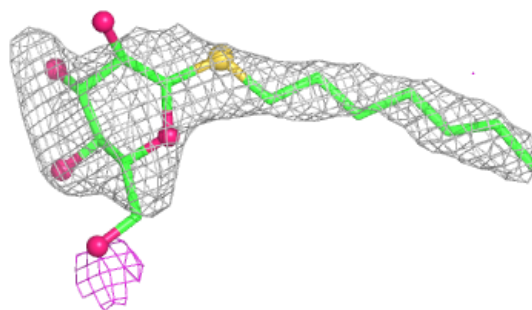
**Electron density around LMG z 101:**

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

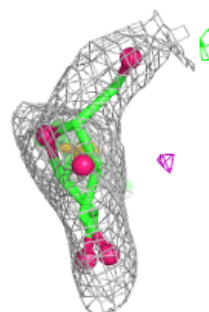
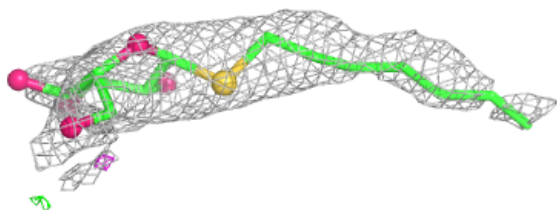
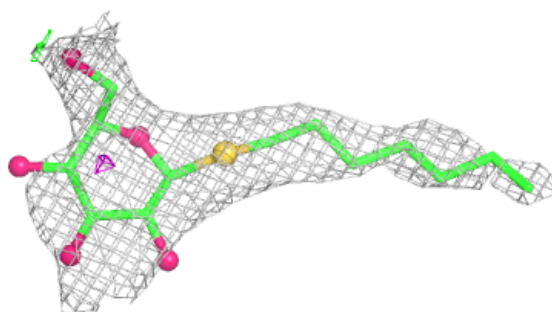


Electron density around HTG B 624:

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

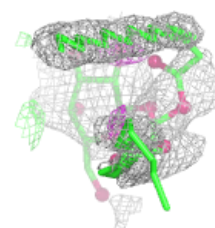
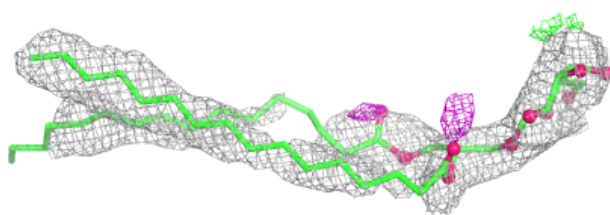
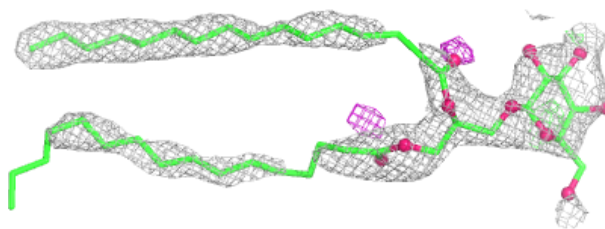
**Electron density around HTG C 523:**

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

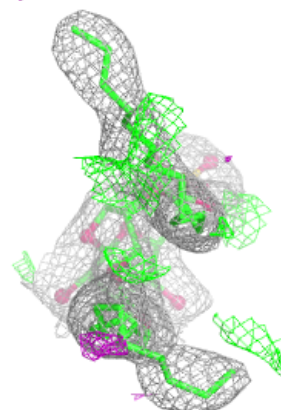
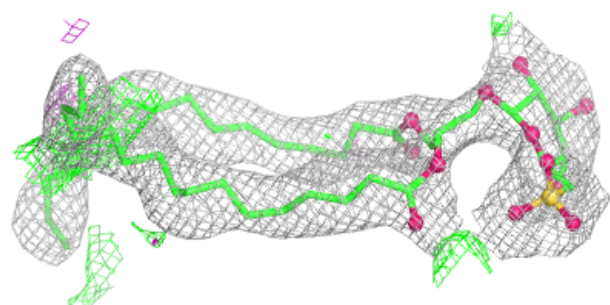
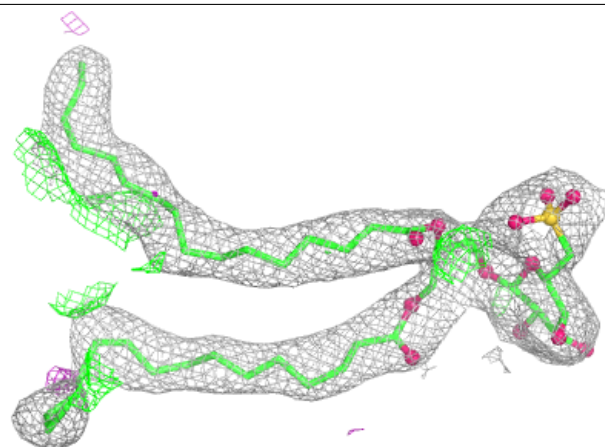


Electron density around LMG c 522:

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

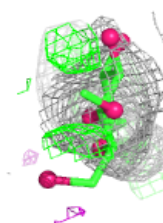
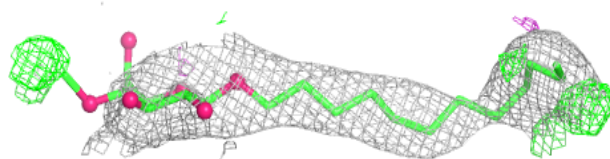
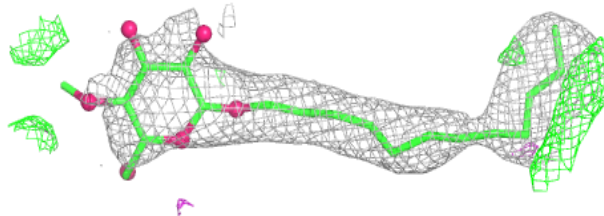
**Electron density around SQD L 102:**

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

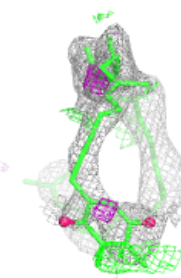
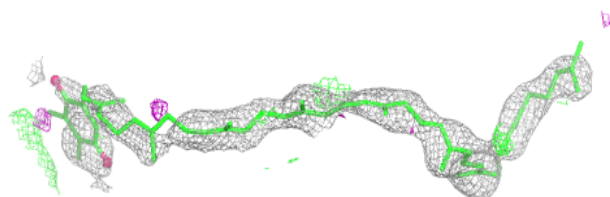
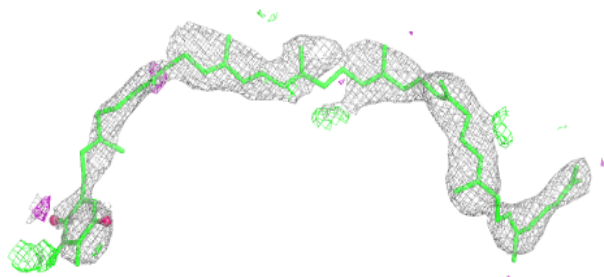


Electron density around LMT t 101:

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

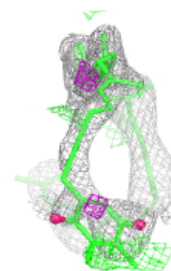
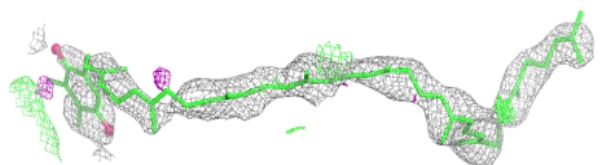
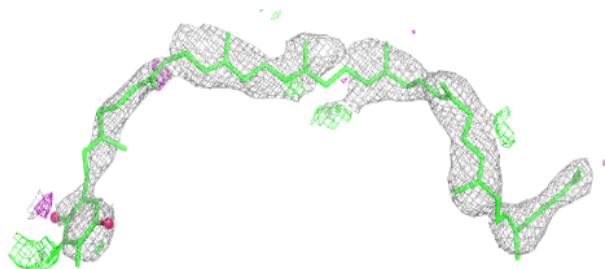
**Electron density around PL9 a 416 (A):**

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

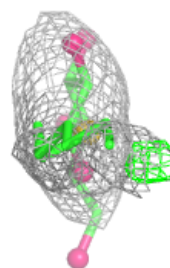
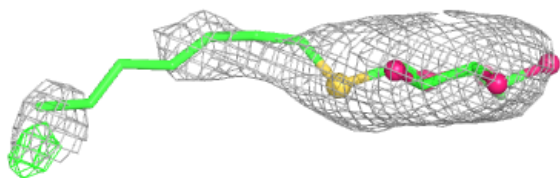
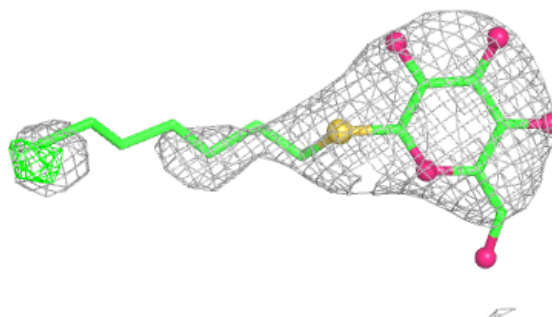


Electron density around PL9 a 416 (B):

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

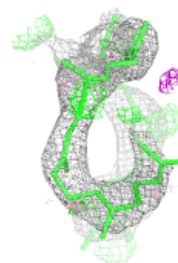
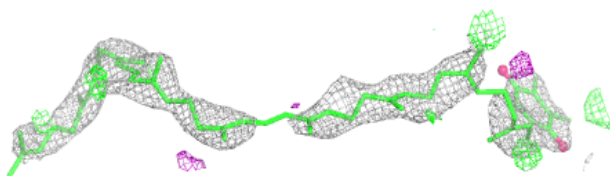
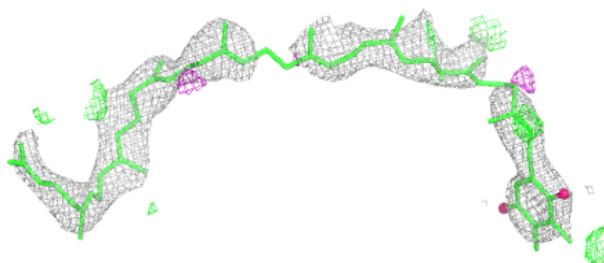
**Electron density around HTG c 523:**

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

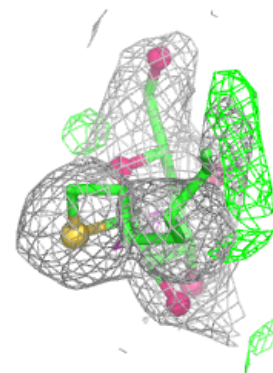
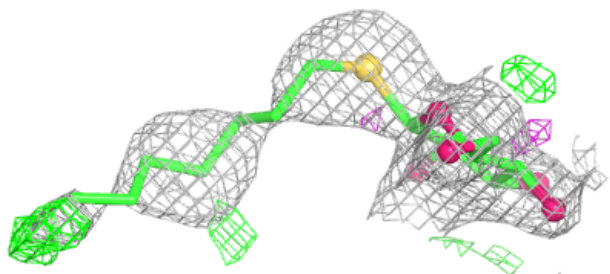
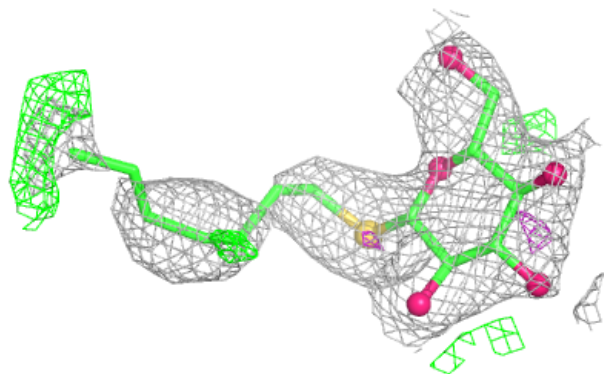


Electron density around PL9 A 417 (B):

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

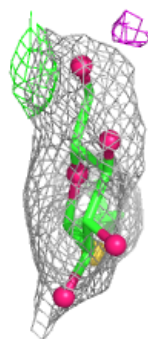
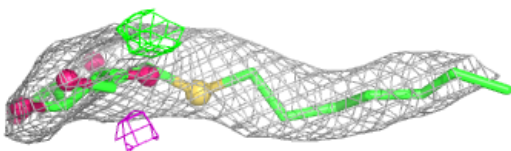
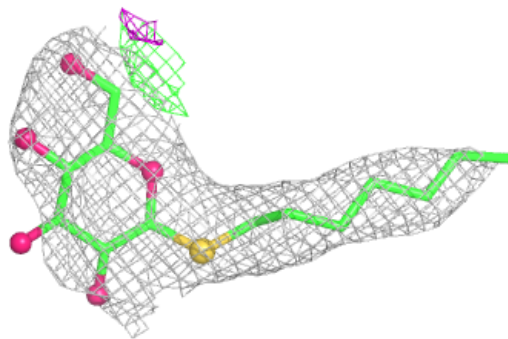
**Electron density around HTG b 631:**

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

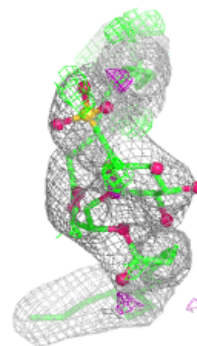
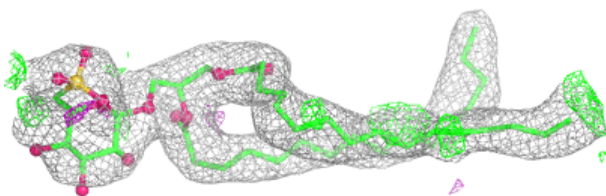
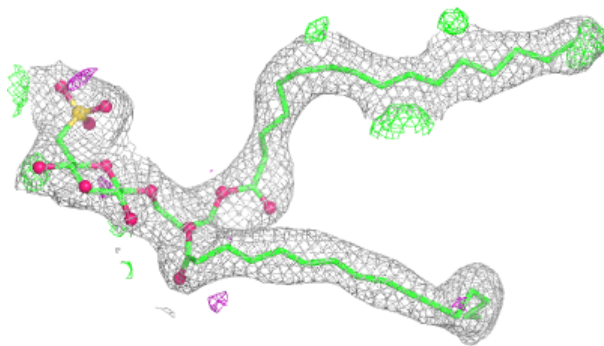


Electron density around HTG b 632:

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

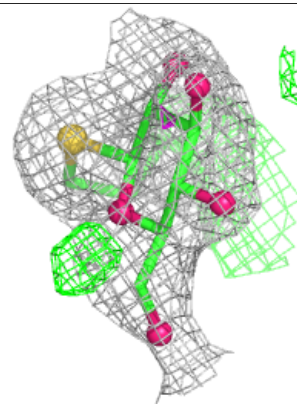
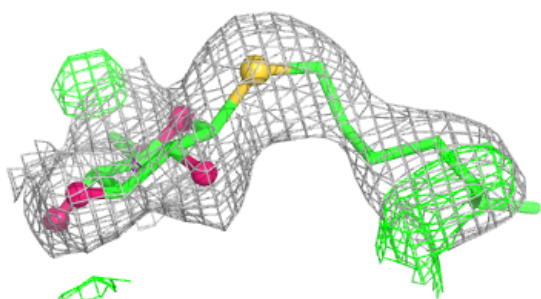
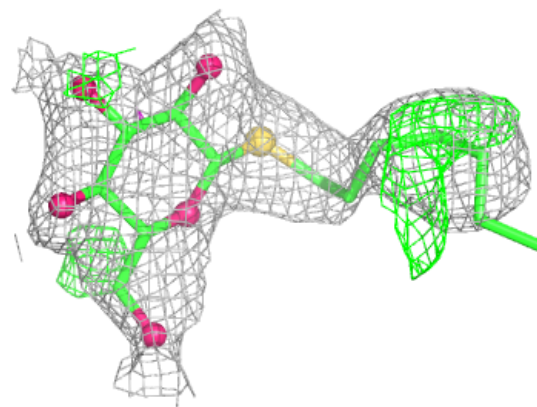
**Electron density around SQD a 405:**

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

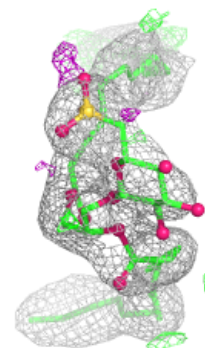
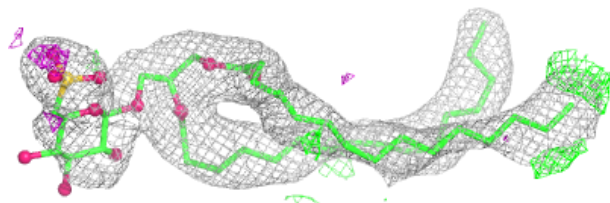
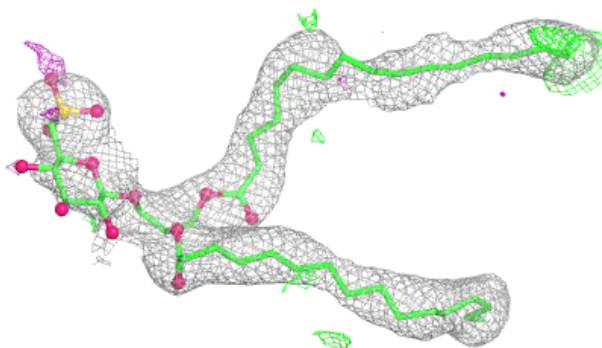


Electron density around HTG B 623:

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

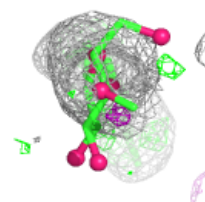
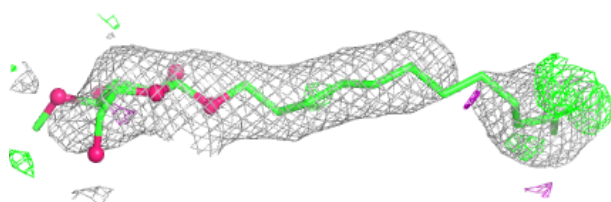
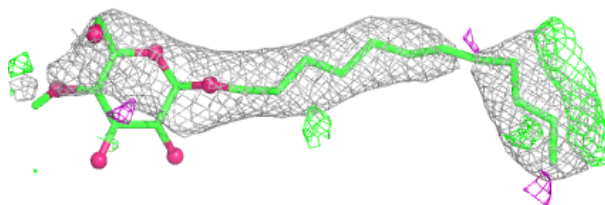
**Electron density around SQD A 413:**

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

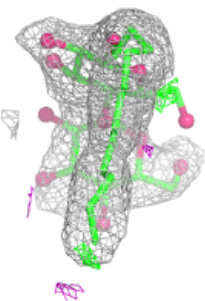
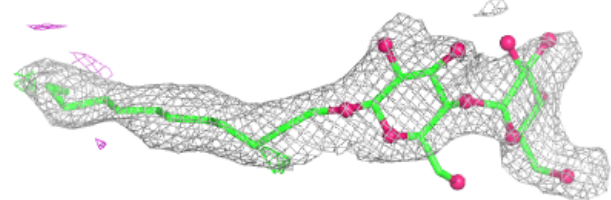
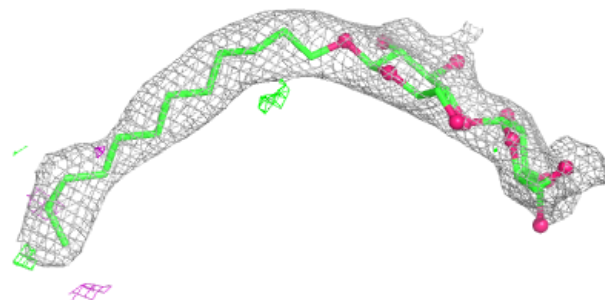


Electron density around LMT T 104:

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

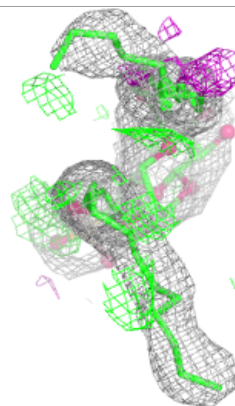
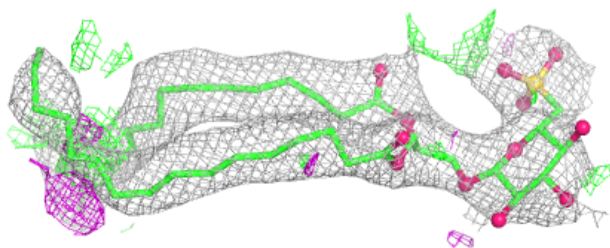
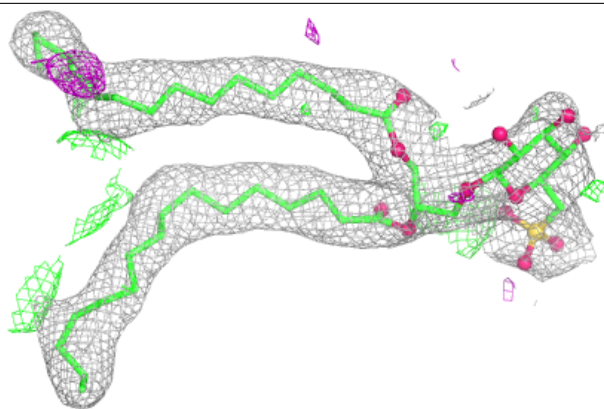
**Electron density around LMT m 103:**

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

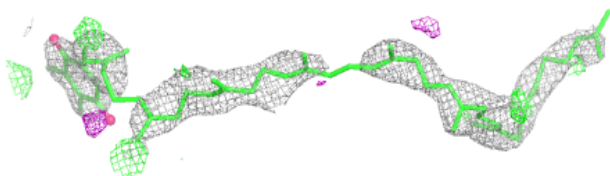
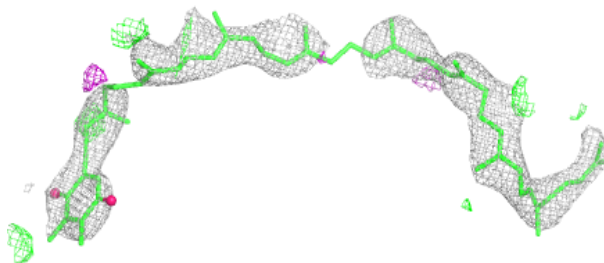


Electron density around SQD B 621:

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

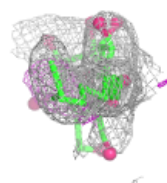
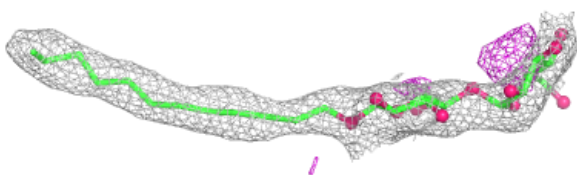
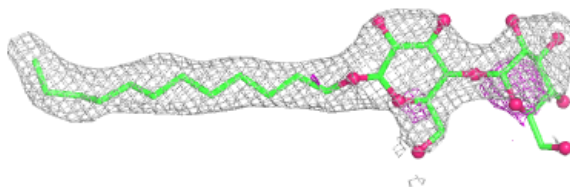
**Electron density around PL9 A 417 (A):**

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

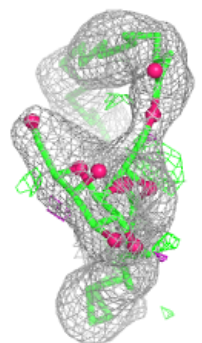
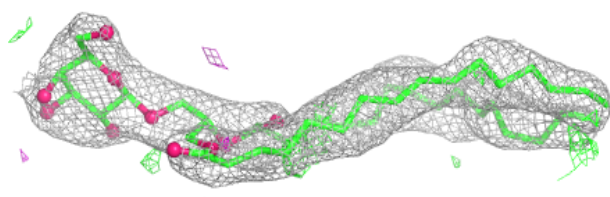
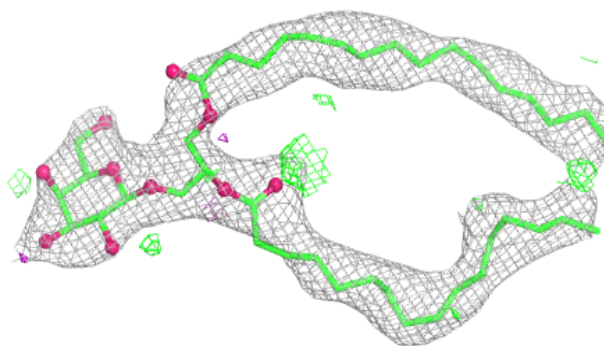


Electron density around LMT m 102:

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

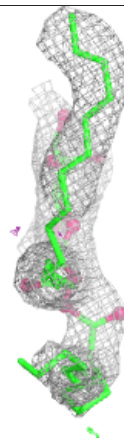
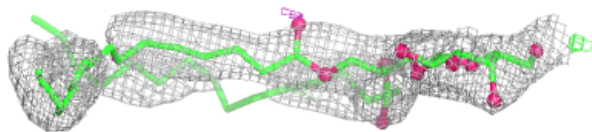
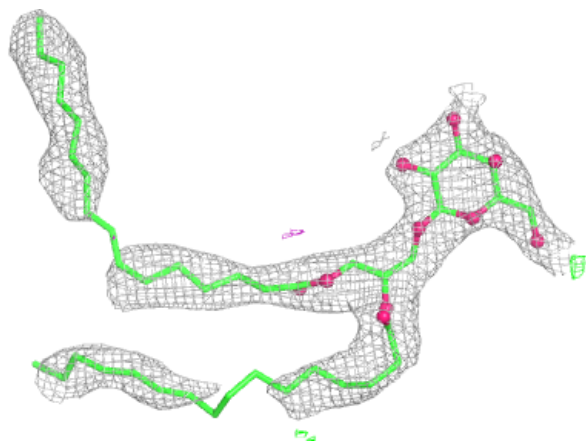
**Electron density around LMG A 419:**

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



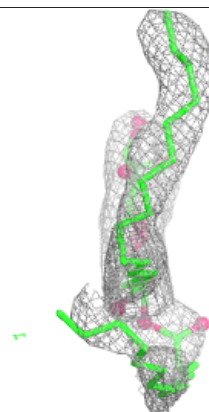
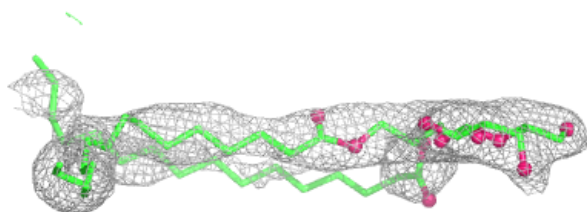
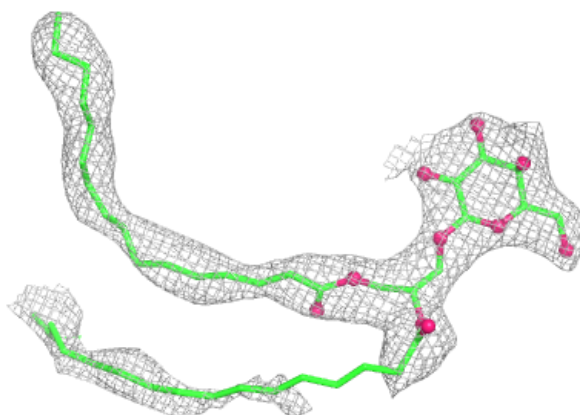
Electron density around LMG C 519:

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

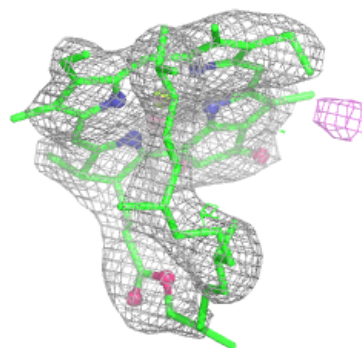
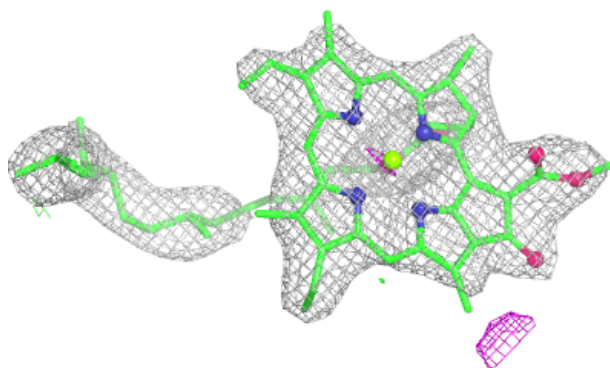
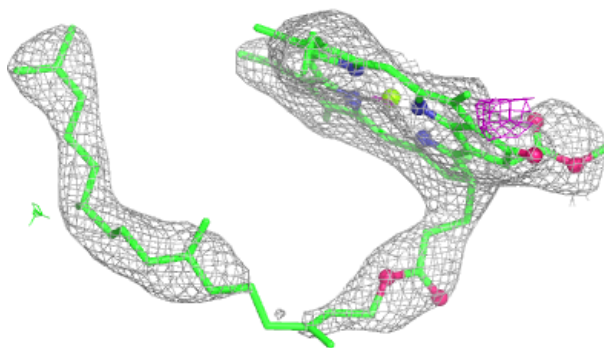


Electron density around LMG k 101:

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

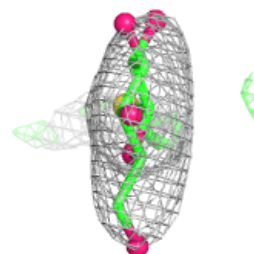
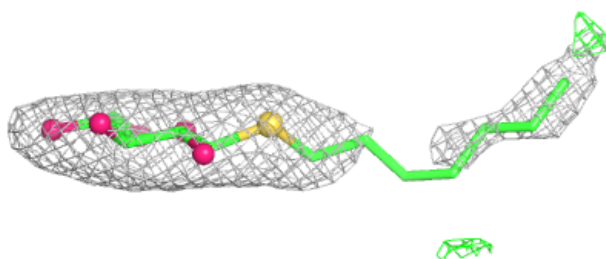
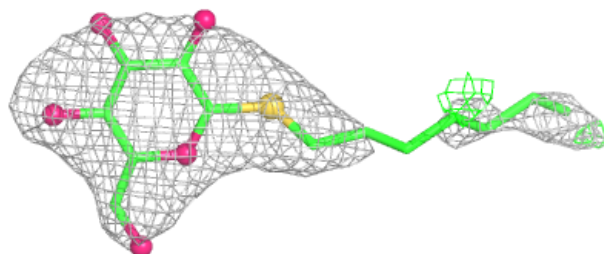
**Electron density around CLA C 513:**

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

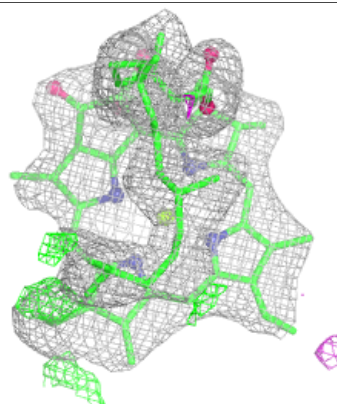
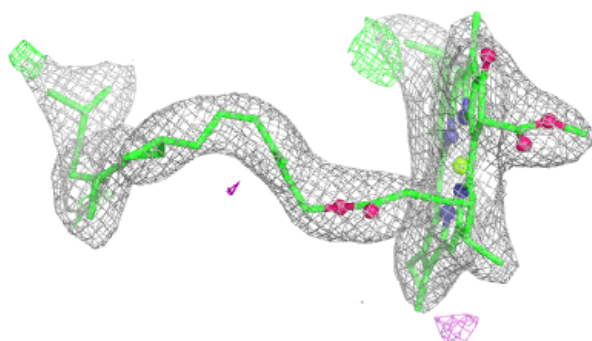
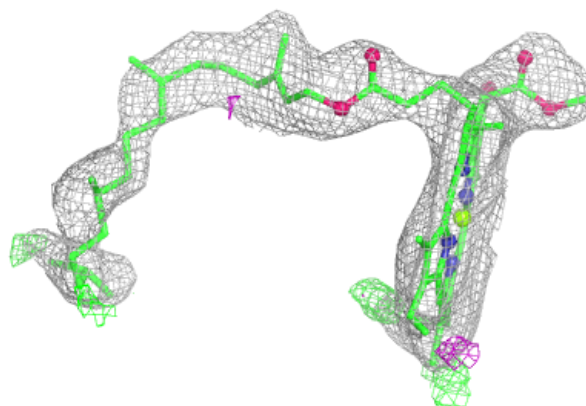


Electron density around HTG C 522:

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

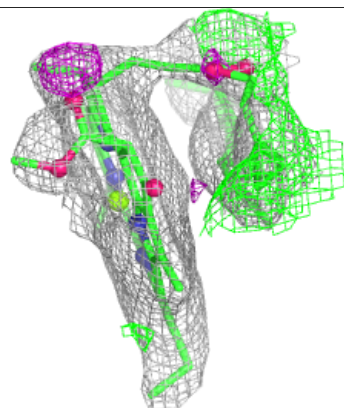
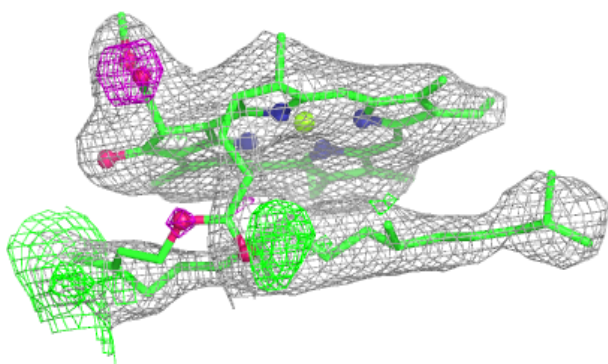
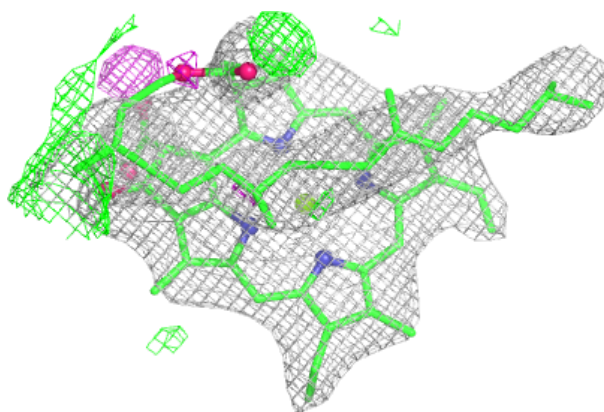
**Electron density around CLA C 506:**

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

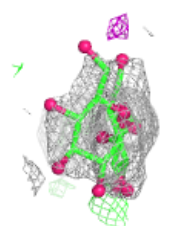
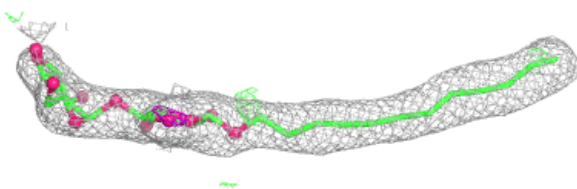
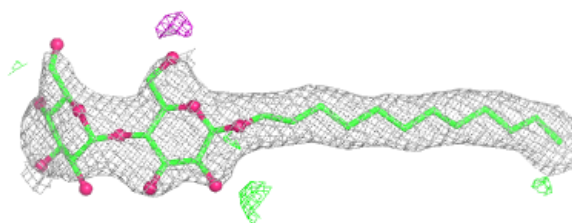


Electron density around CLA B 602:

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

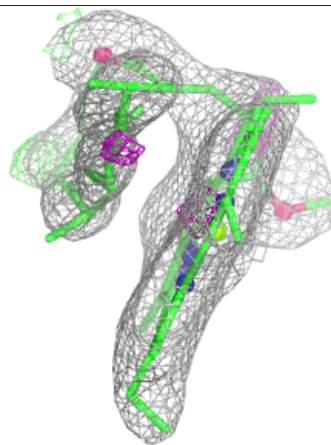
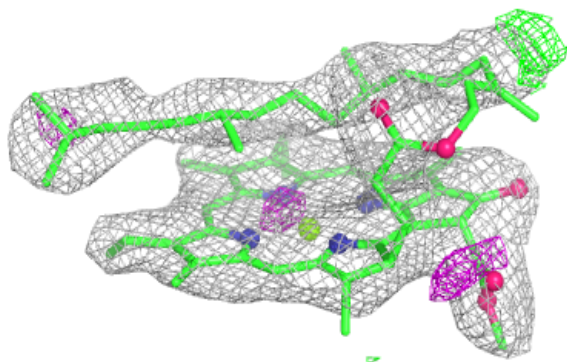
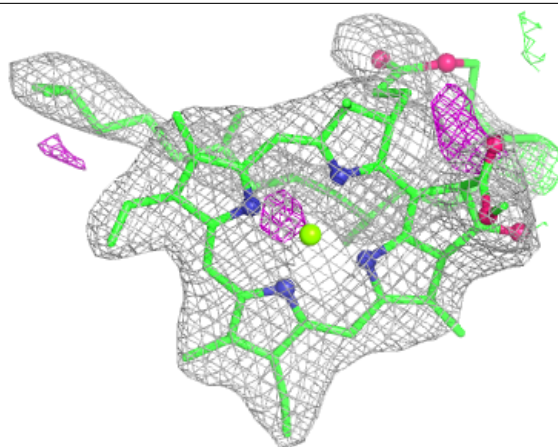
**Electron density around LMT M 102:**

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



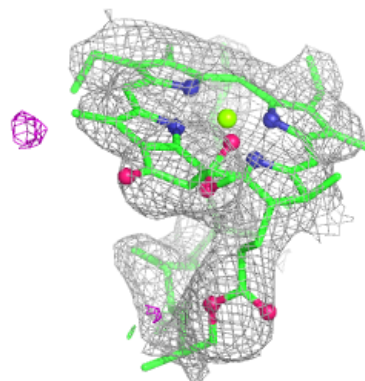
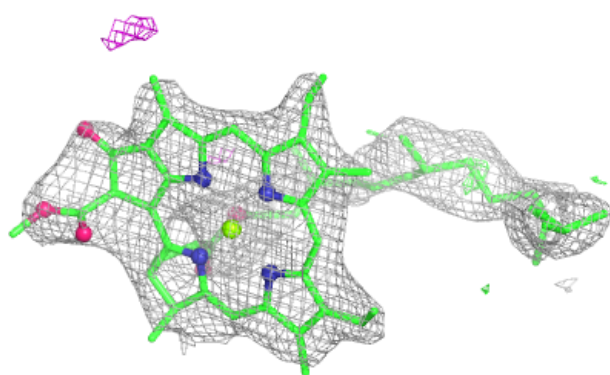
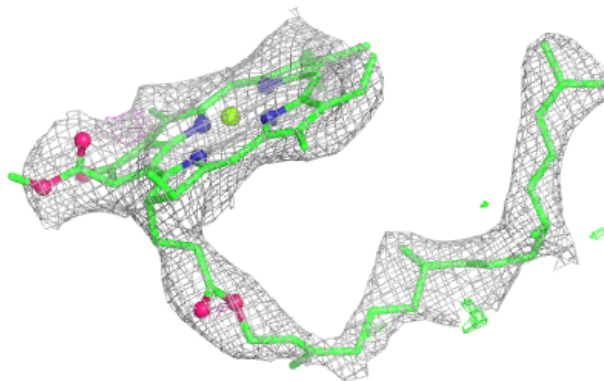
Electron density around CLA b 610:

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

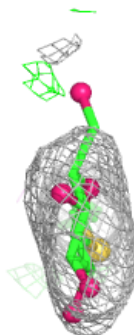
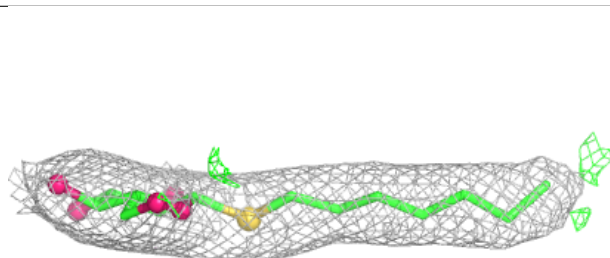
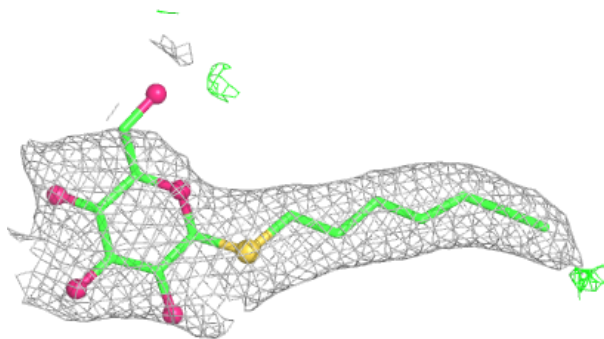


Electron density around CLA c 517:

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

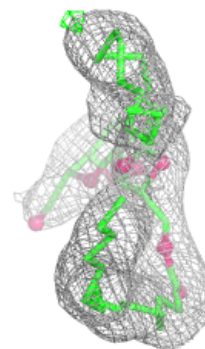
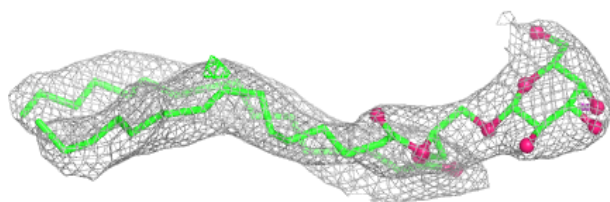
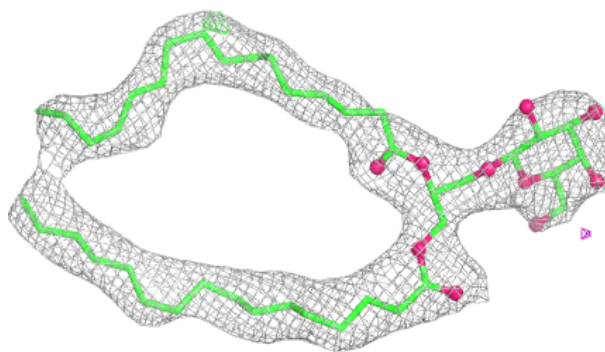
**Electron density around HTG B 631:**

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

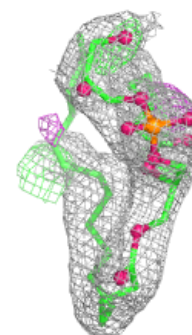
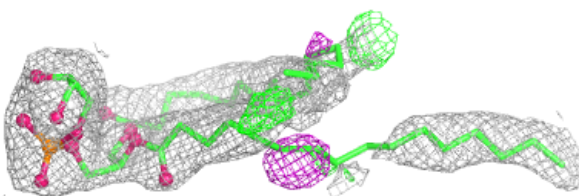
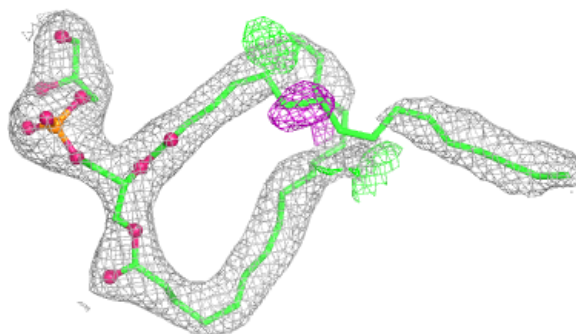


Electron density around LMG a 415:

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

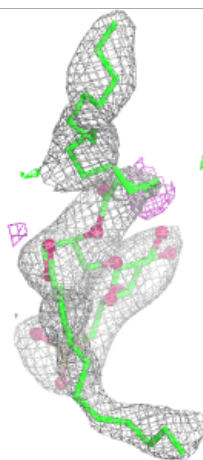
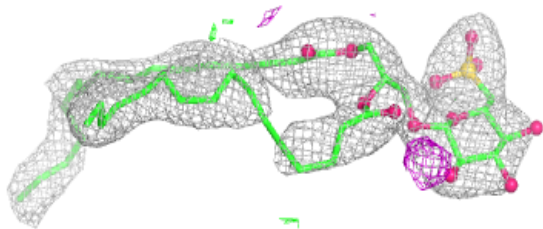
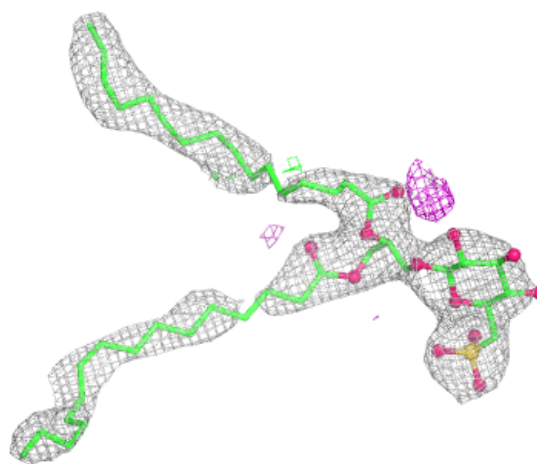
**Electron density around LHG D 411:**

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



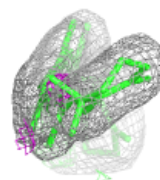
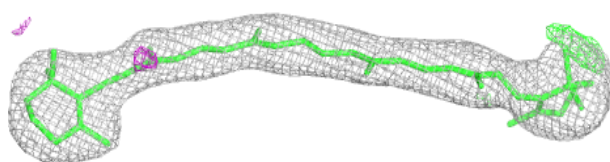
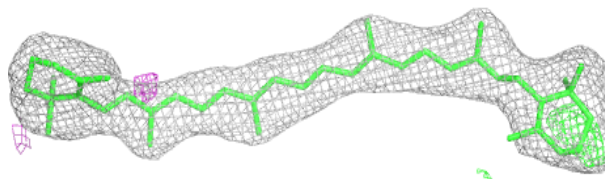
Electron density around SQD A 411:

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

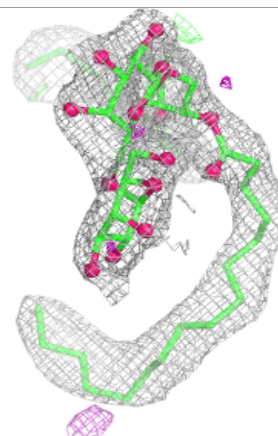
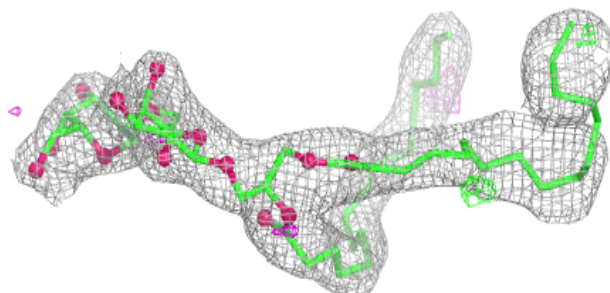
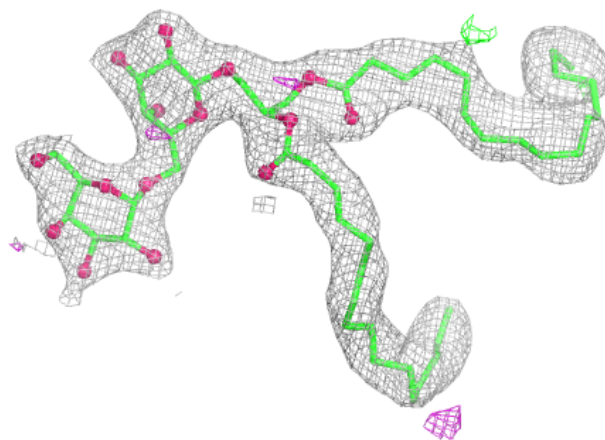


Electron density around BCR d 406:

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

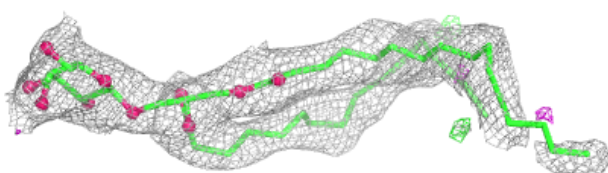
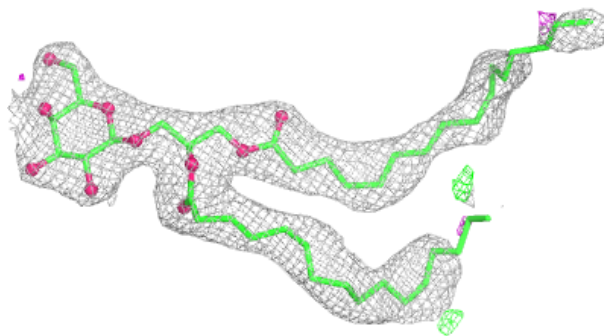
**Electron density around DGD C 517:**

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

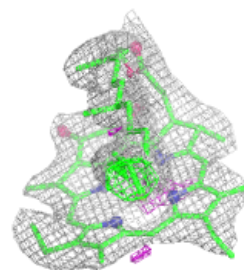
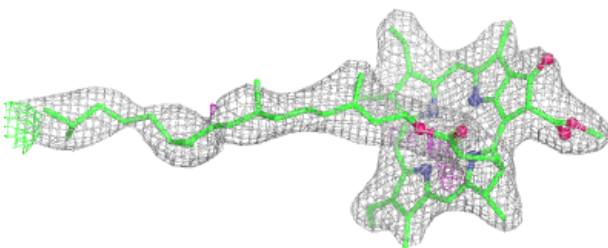
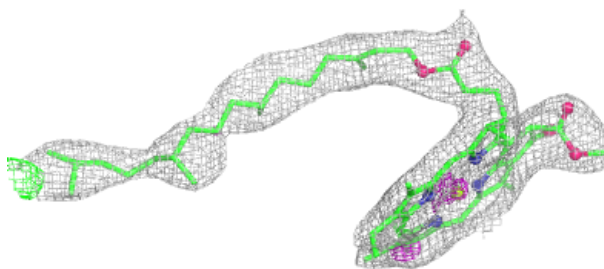


Electron density around LMG d 415:

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

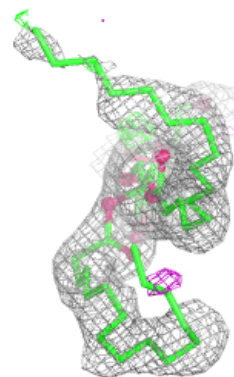
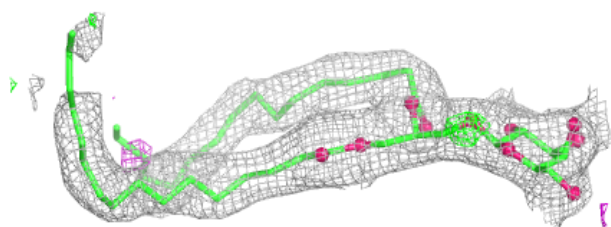
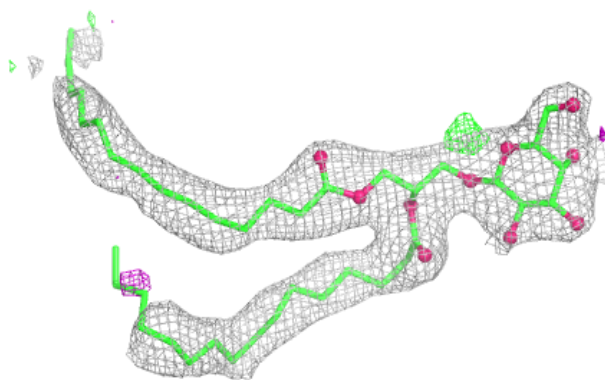
**Electron density around CLA C 504:**

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

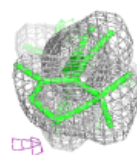
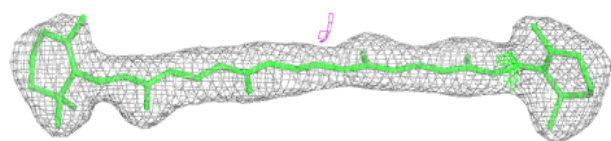
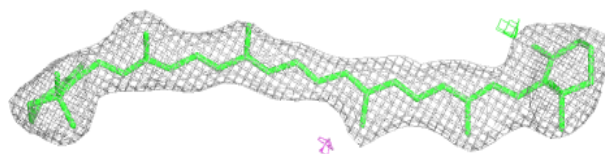


Electron density around LMG D 415:

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

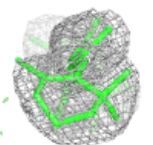
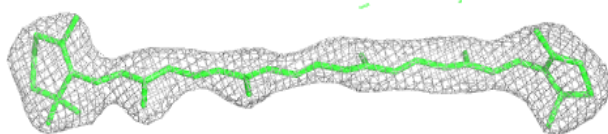
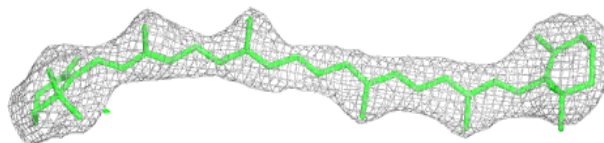
**Electron density around BCR C 514:**

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

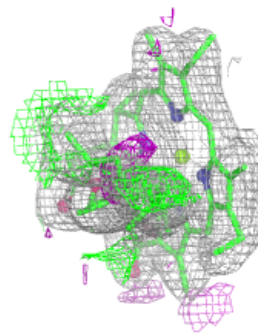
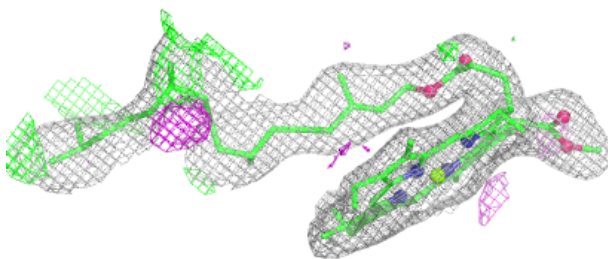
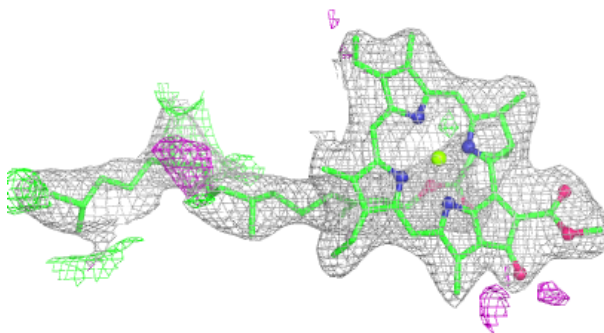


Electron density around BCR c 526:

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

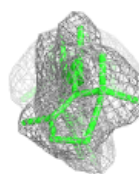
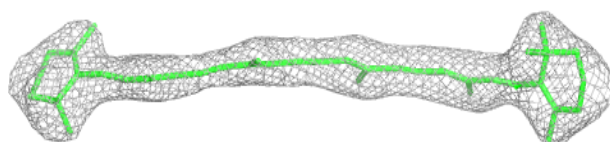
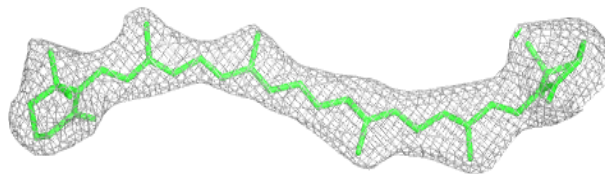
**Electron density around CLA B 615:**

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

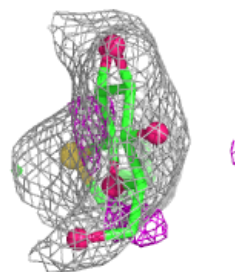
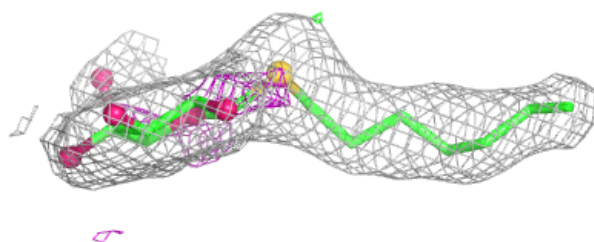
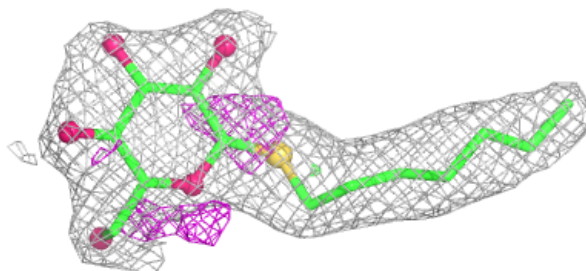


Electron density around BCR y 101:

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

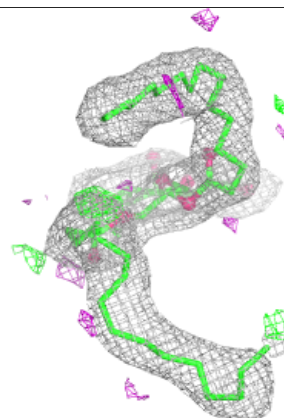
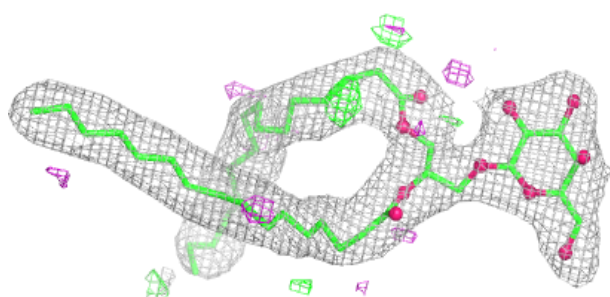
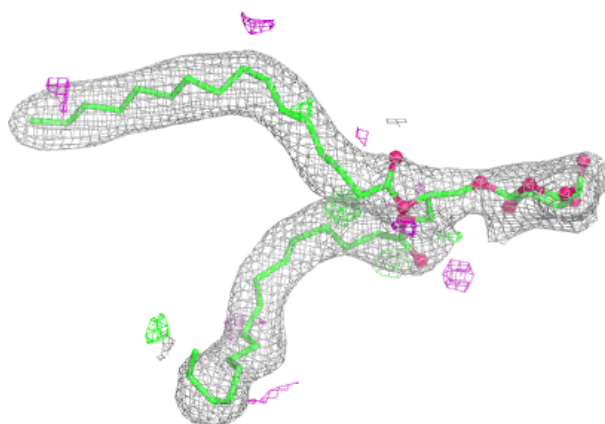
**Electron density around HTG b 602:**

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

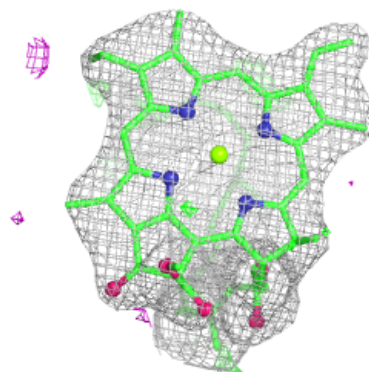
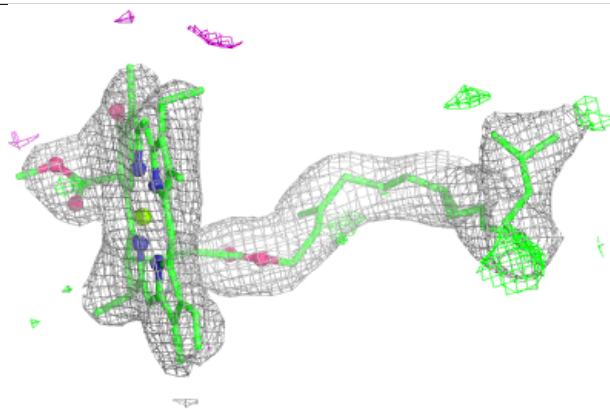
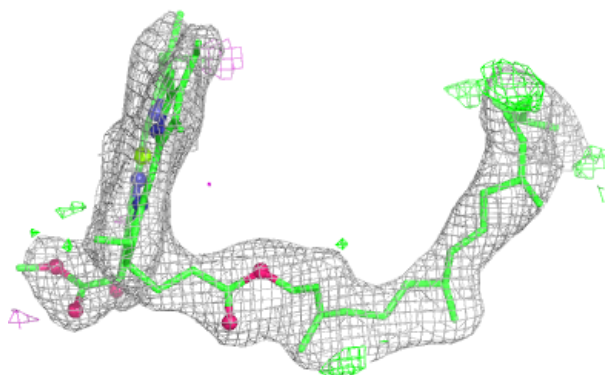


Electron density around LMG b 629:

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

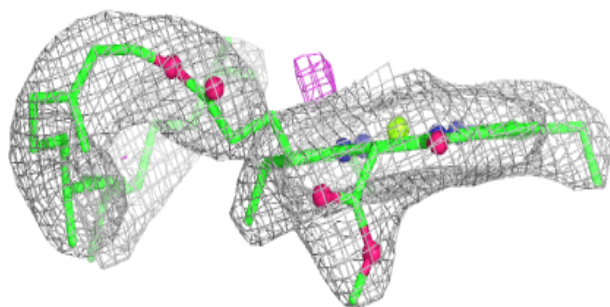
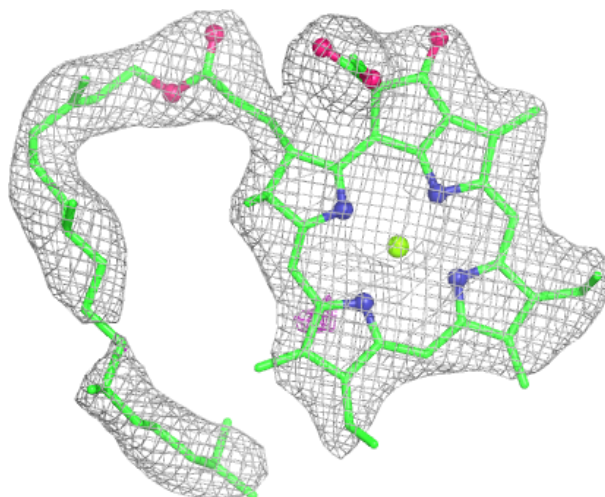
**Electron density around CLA c 510:**

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



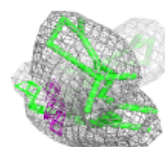
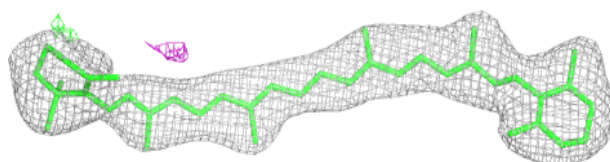
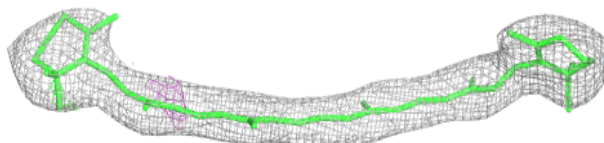
Electron density around CLA C 512:

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

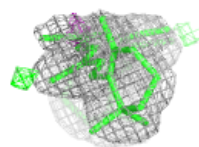
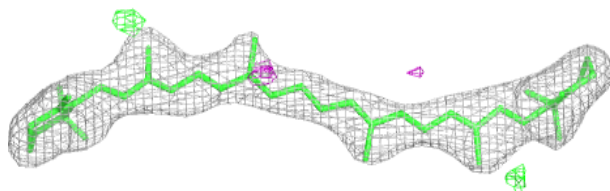
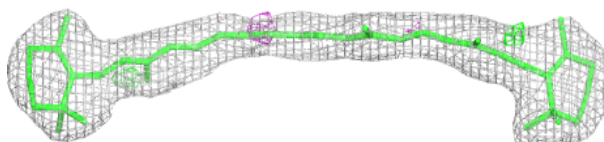


Electron density around BCR D 406:

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

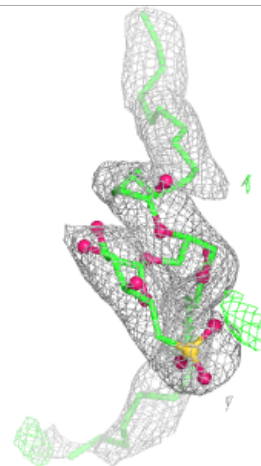
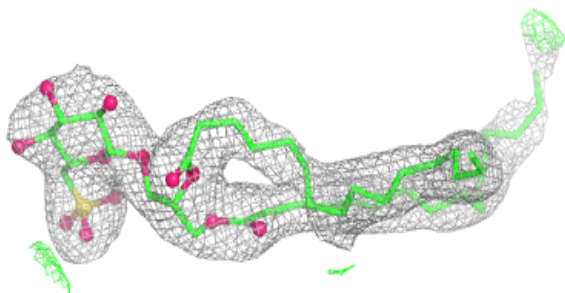
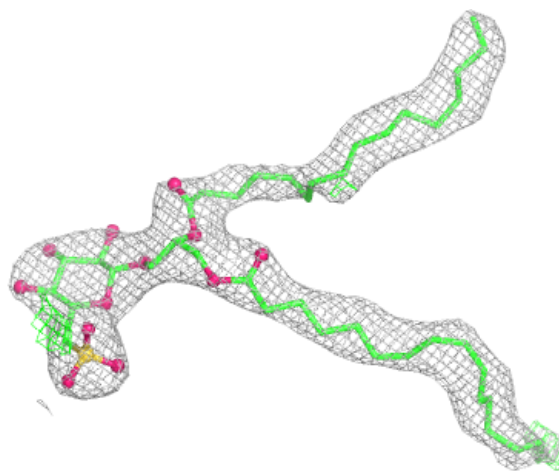
**Electron density around BCR K 101:**

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



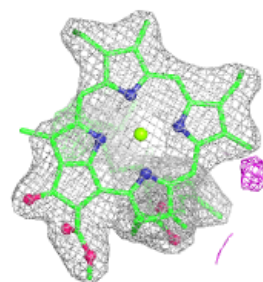
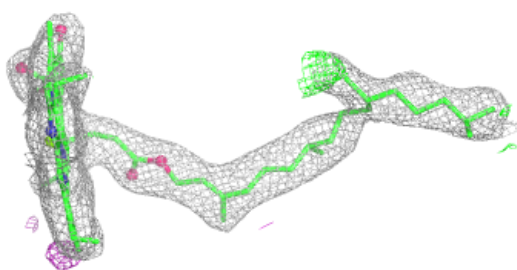
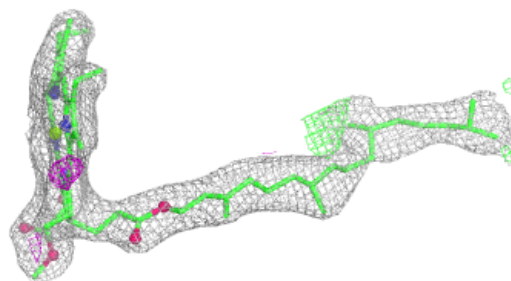
Electron density around SQD a 414:

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

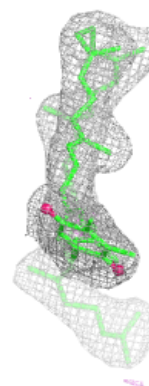
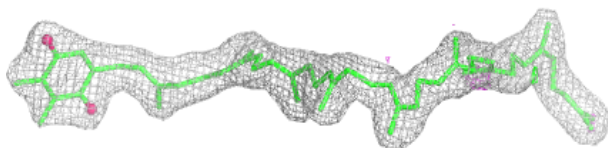
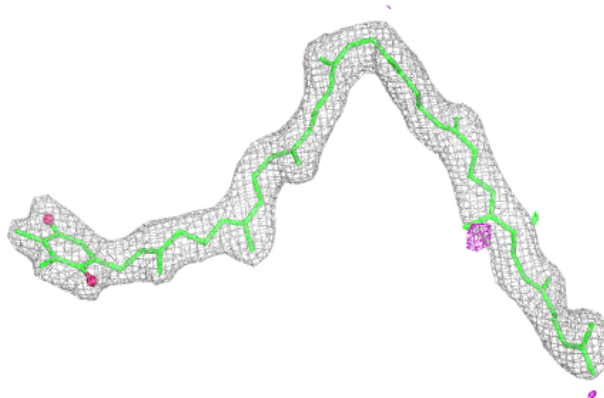


Electron density around CLA B 607:

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

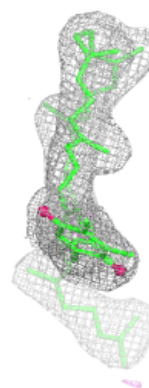
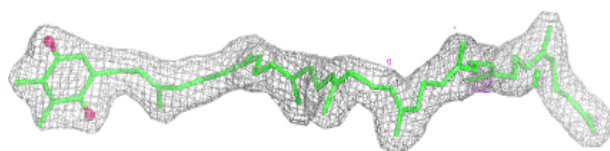
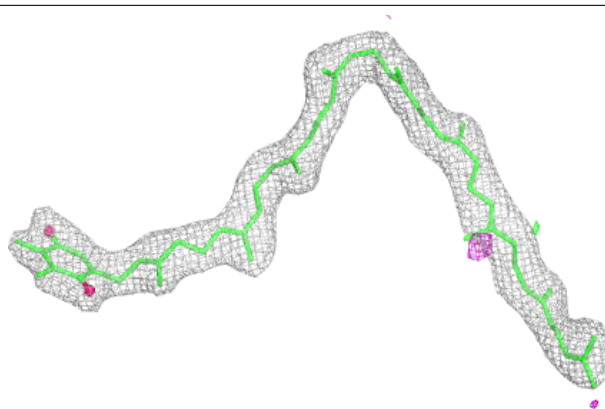
**Electron density around PL9 d 407 (A):**

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

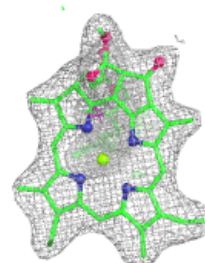
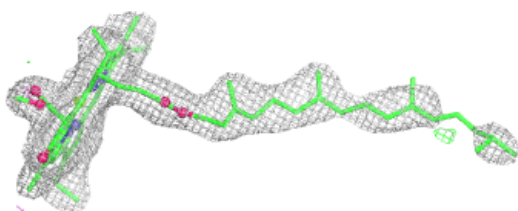
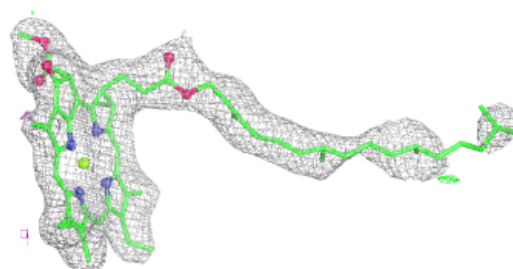


Electron density around PL9 d 407 (B):

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

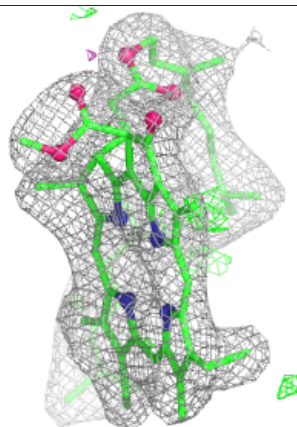
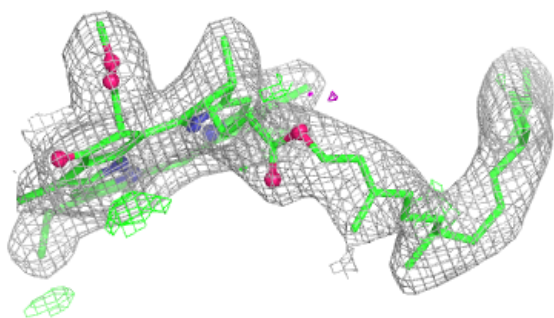
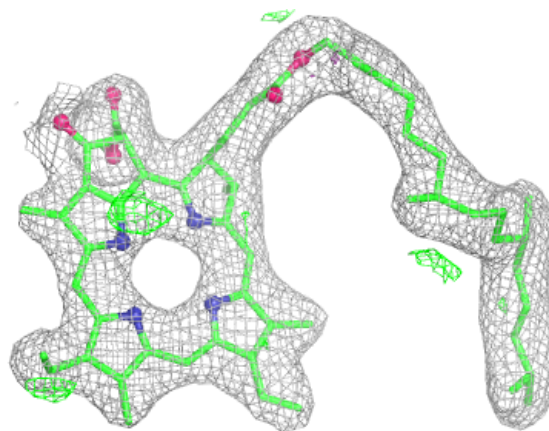
**Electron density around CLA d 405:**

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



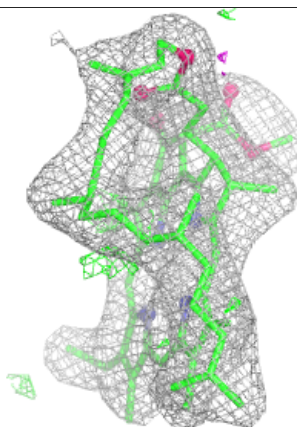
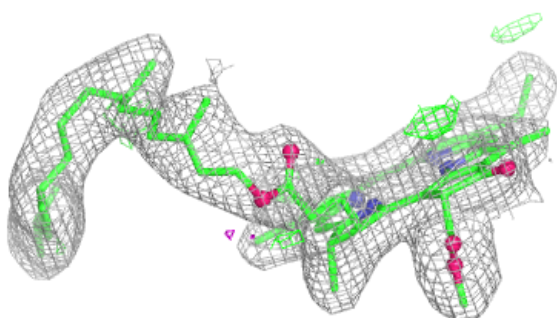
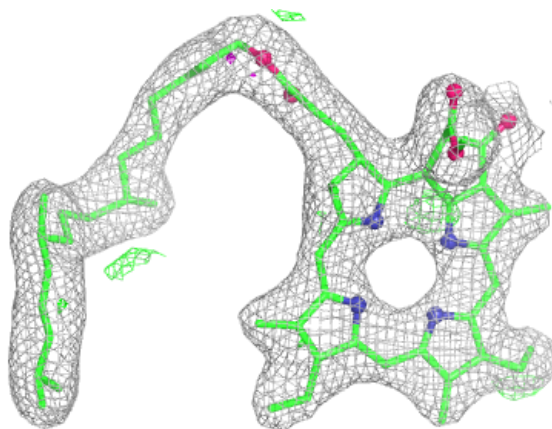
Electron density around PHO d 402 (A):

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

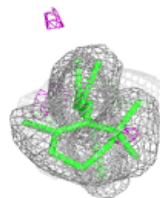
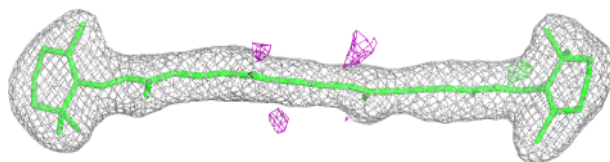
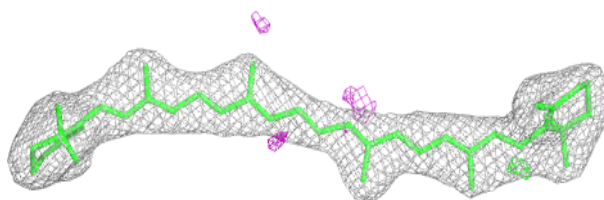


Electron density around PHO d 402 (B):

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

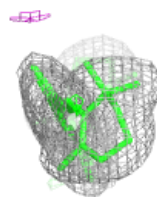
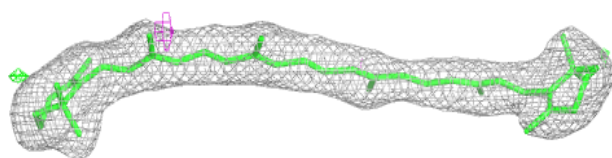
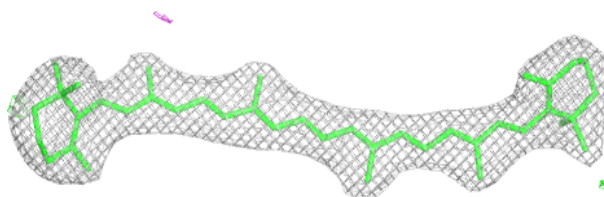
**Electron density around BCR A 410:**

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

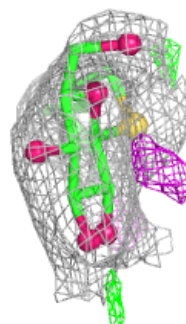
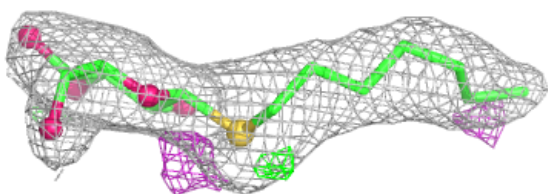
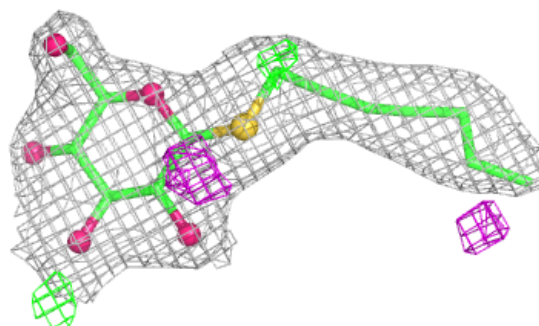


Electron density around BCR B 620:

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

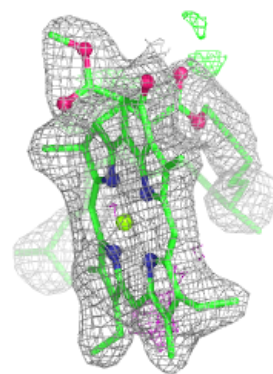
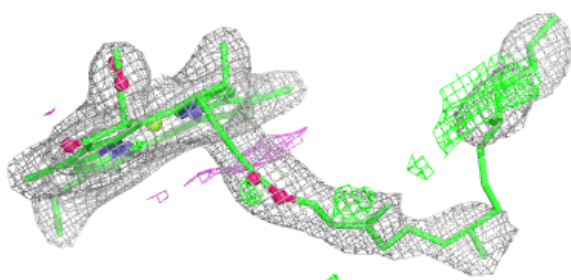
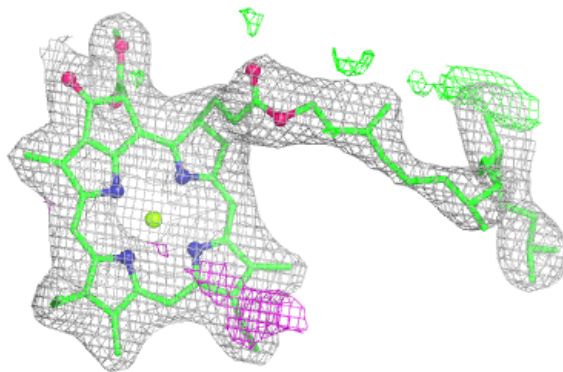
**Electron density around HTG B 622:**

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

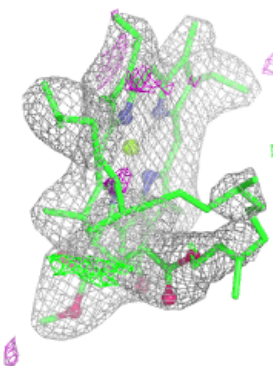
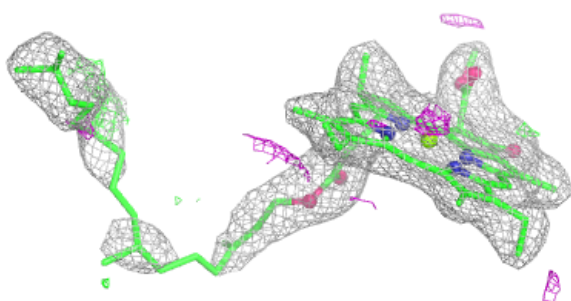
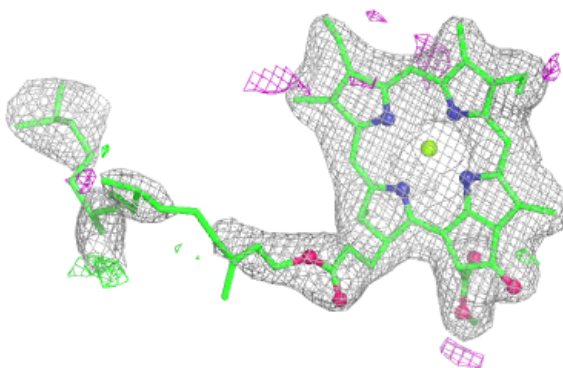


Electron density around CLA A 409:

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

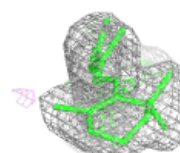
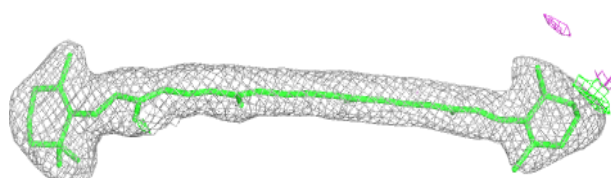
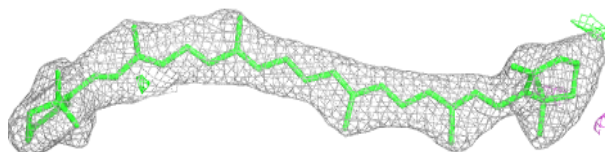
**Electron density around CLA a 412:**

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

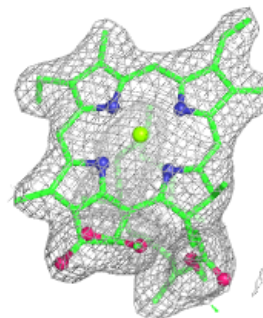
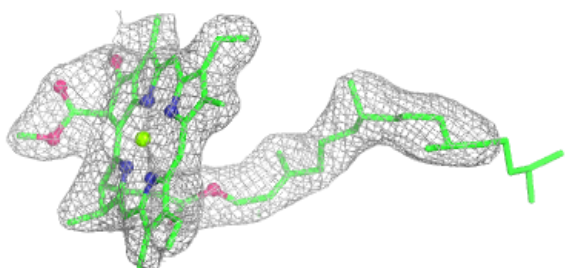
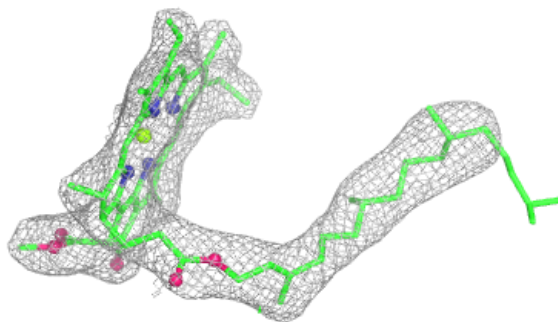


Electron density around BCR H 101:

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

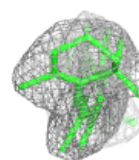
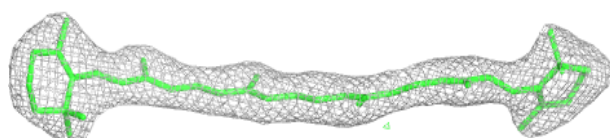
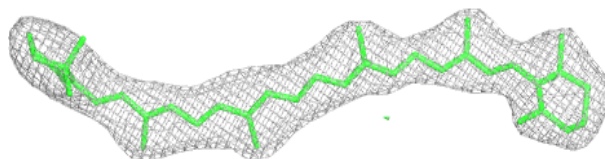
**Electron density around CLA C 508:**

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

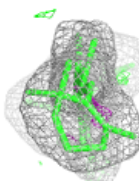
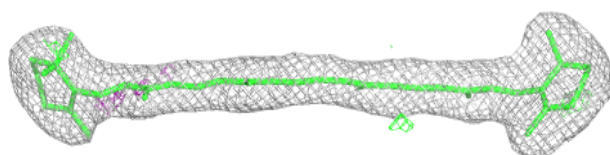
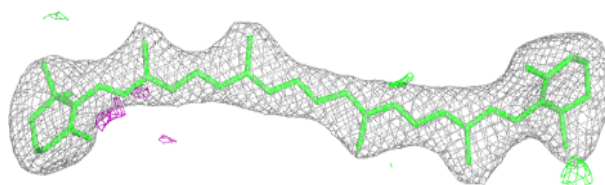


Electron density around BCR Y 101:

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

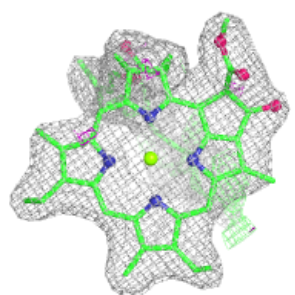
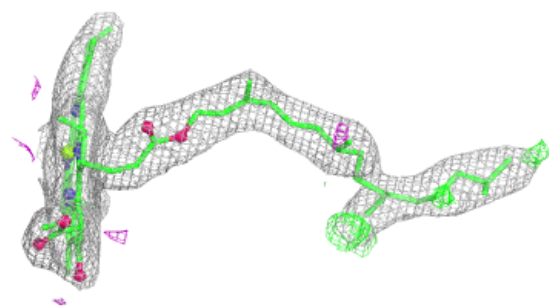
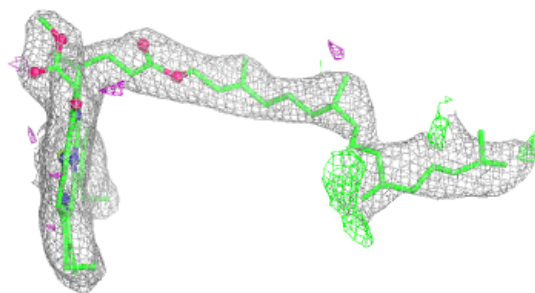
**Electron density around BCR b 627:**

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



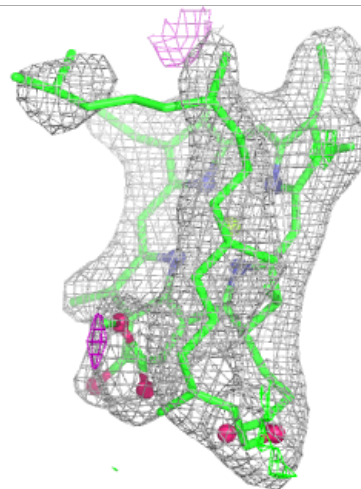
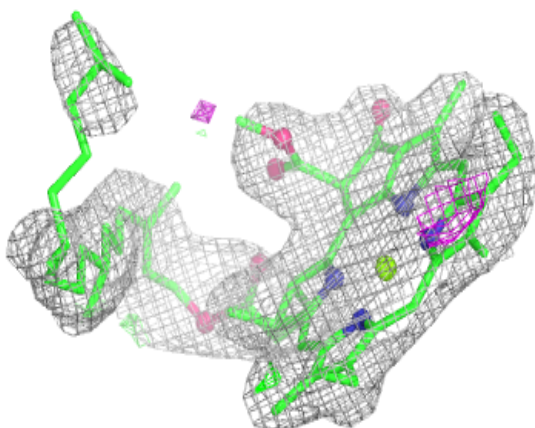
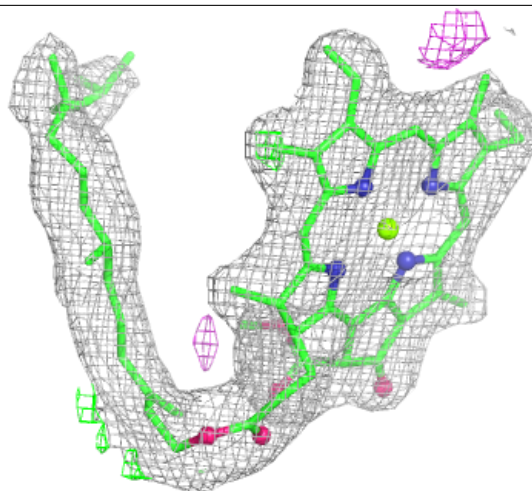
Electron density around CLA b 615:

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



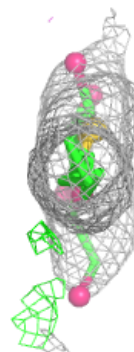
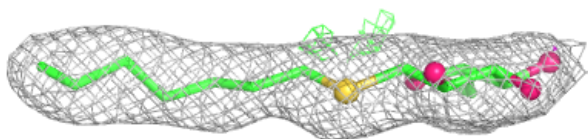
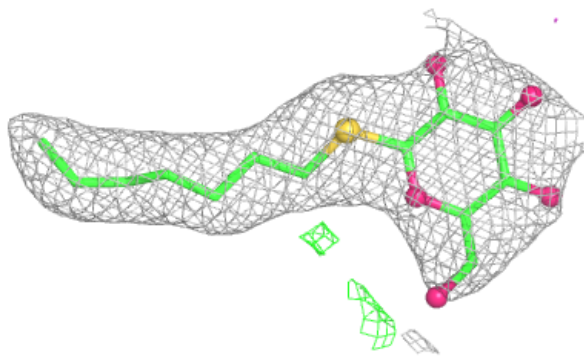
Electron density around CLA b 625:

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

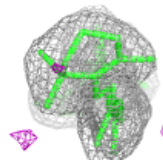
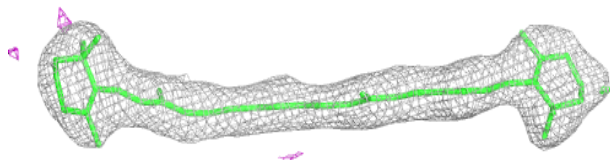
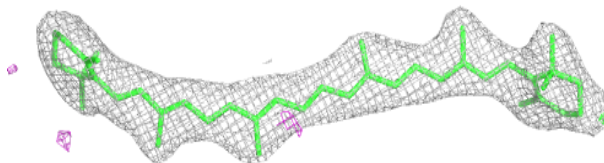


Electron density around HTG b 607:

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

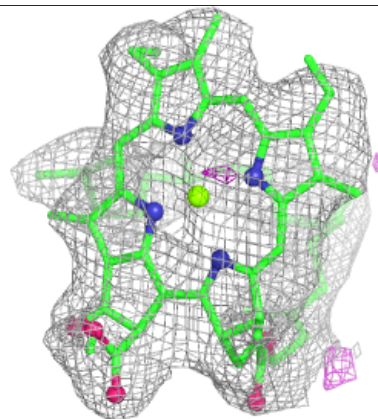
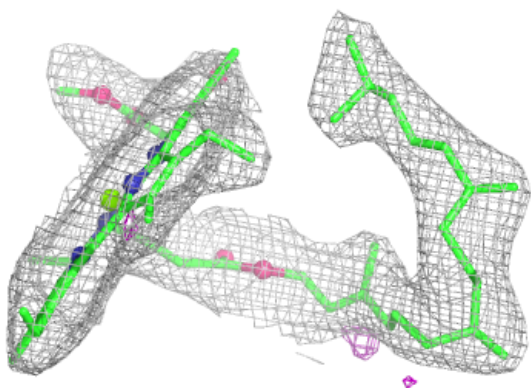
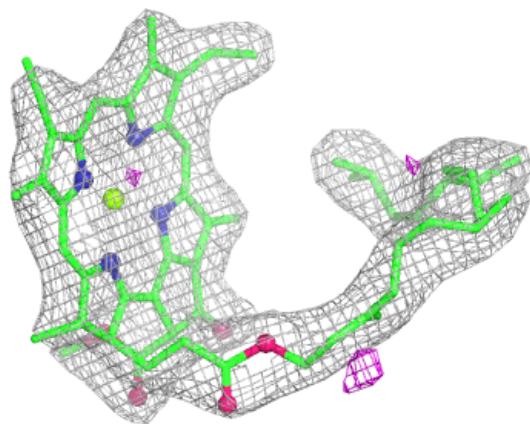
**Electron density around BCR h 101:**

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



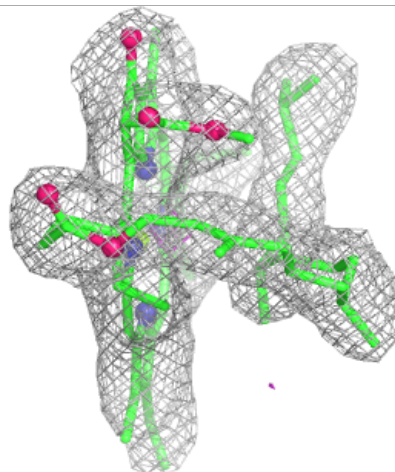
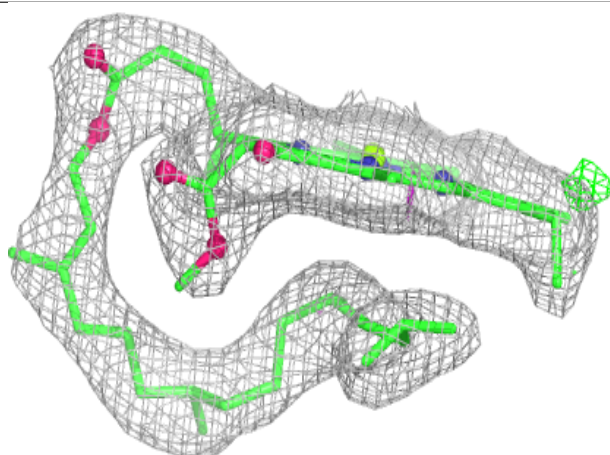
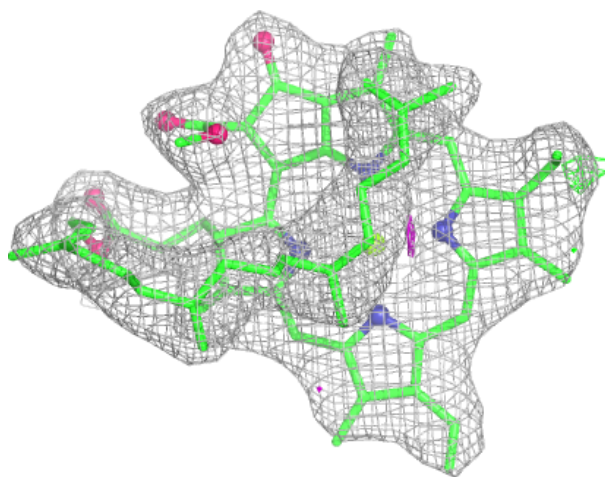
Electron density around CLA c 507:

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



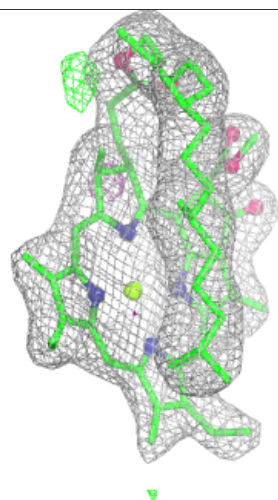
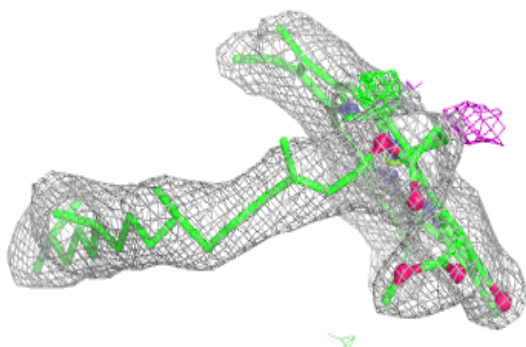
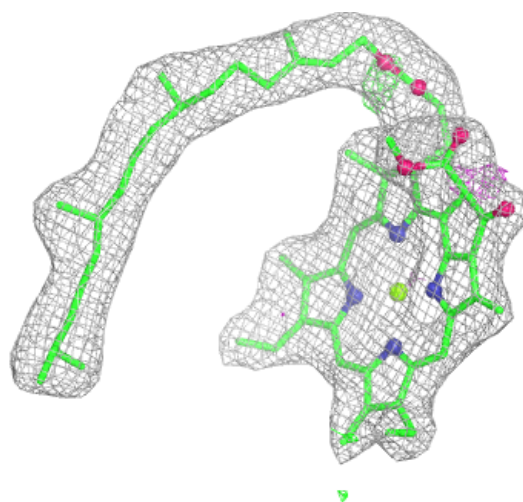
Electron density around CLA C 510:

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



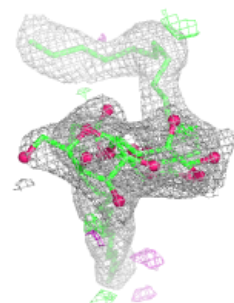
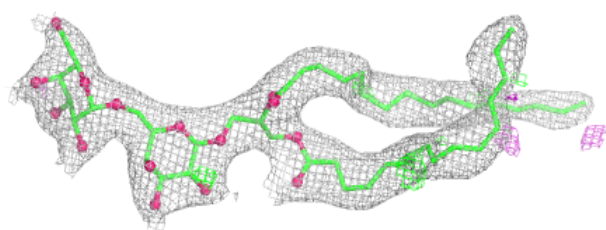
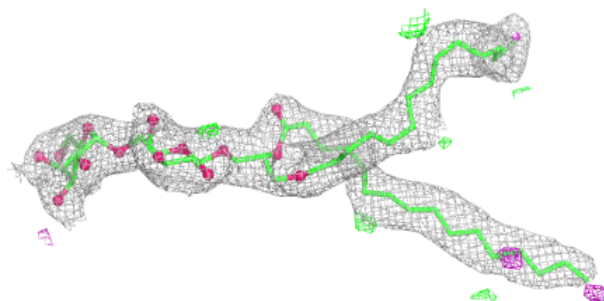
Electron density around CLA c 511:

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

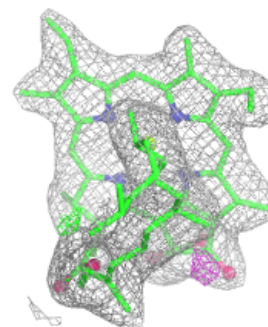
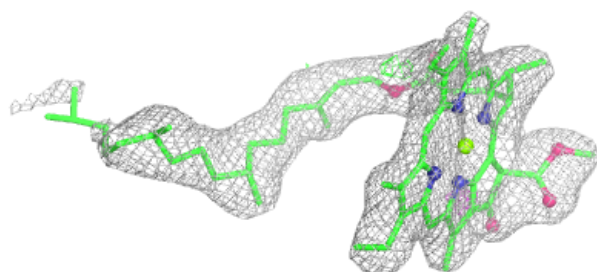
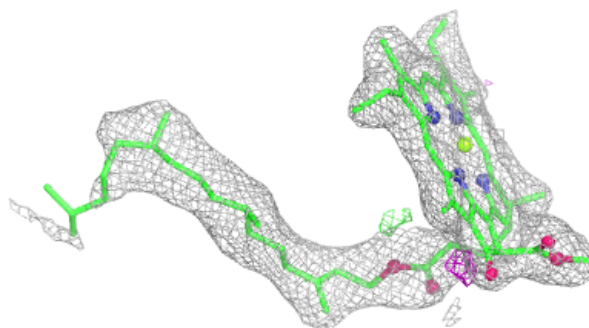


Electron density around DGD C 516:

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

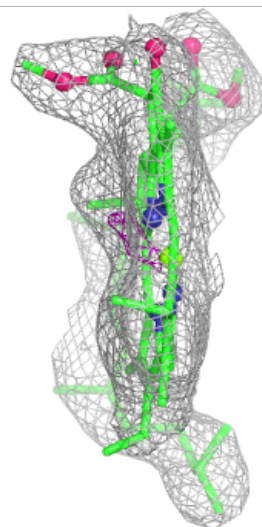
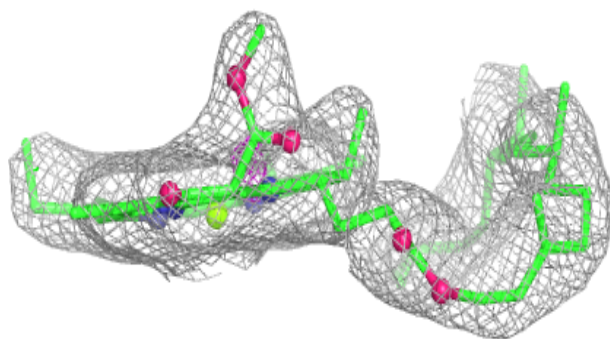
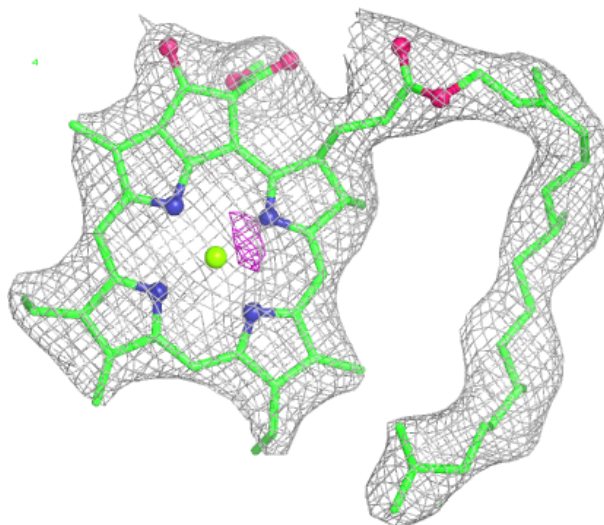
**Electron density around CLA c 512:**

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



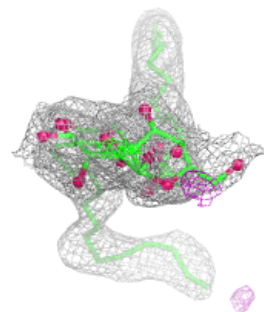
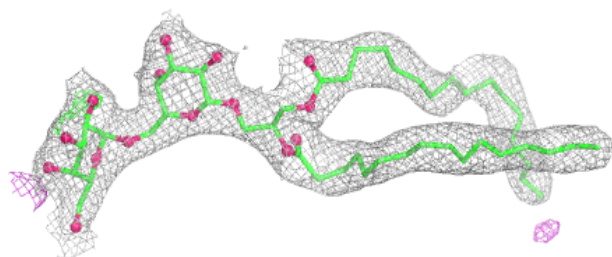
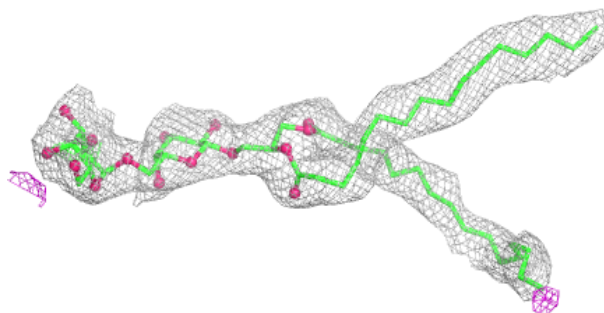
Electron density around CLA c 516:

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

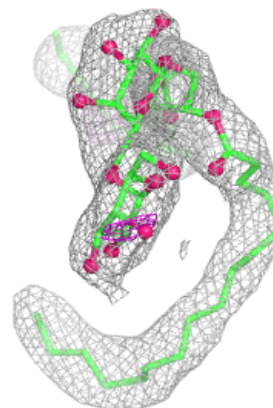
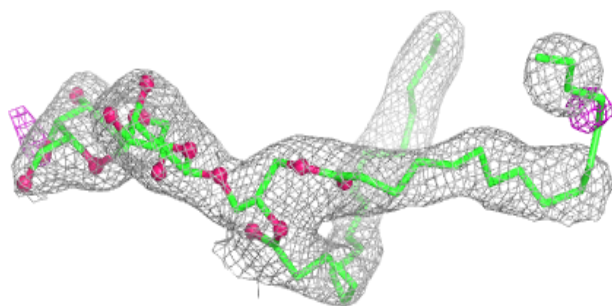
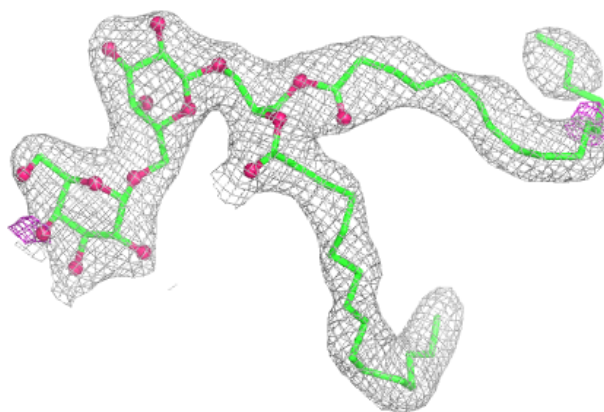


Electron density around DGD c 519:

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

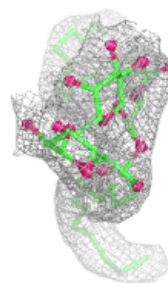
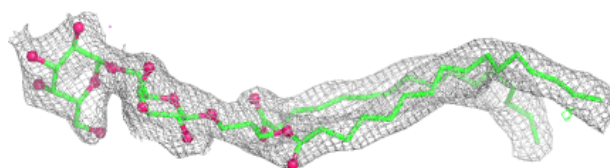
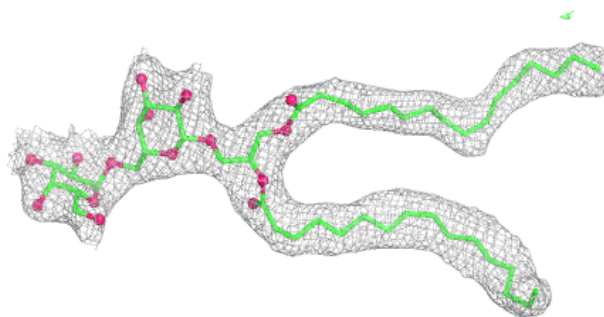
**Electron density around DGD c 520:**

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

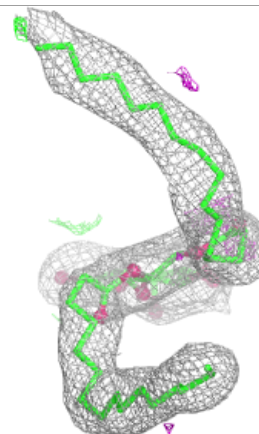
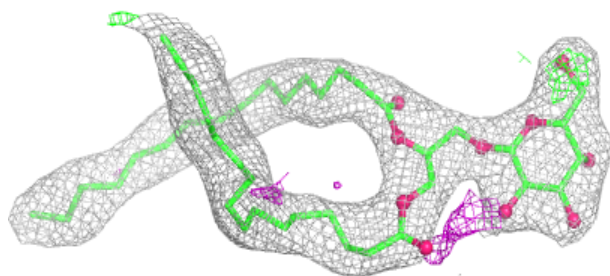
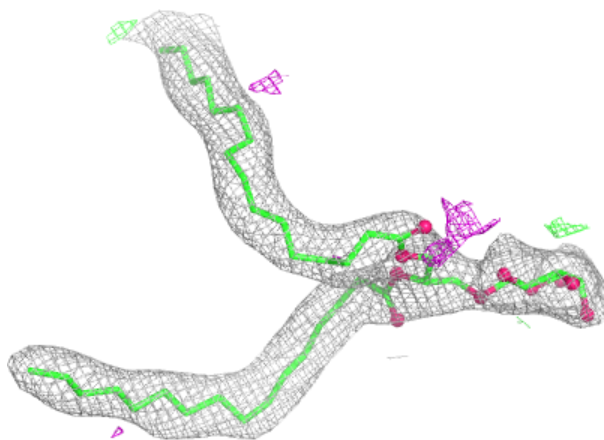


Electron density around DGD c 521:

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

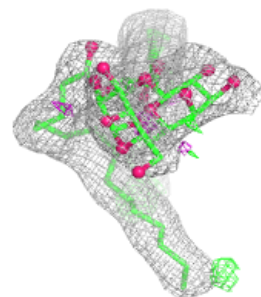
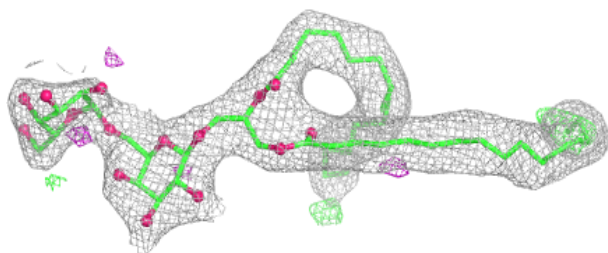
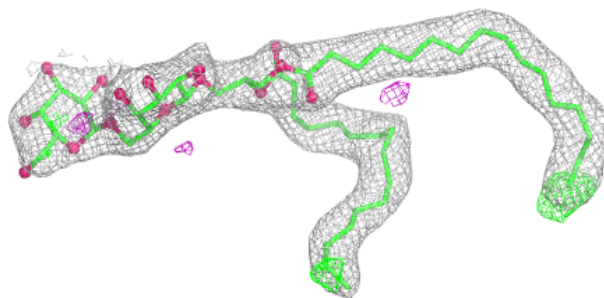
**Electron density around LMG M 101:**

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

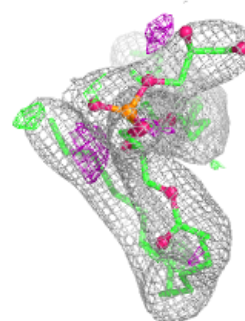
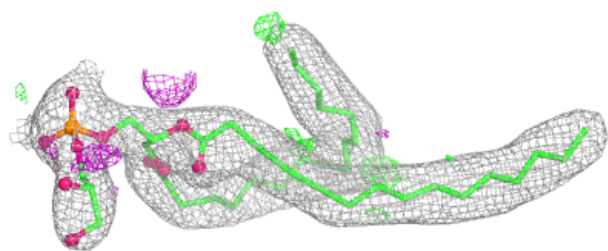
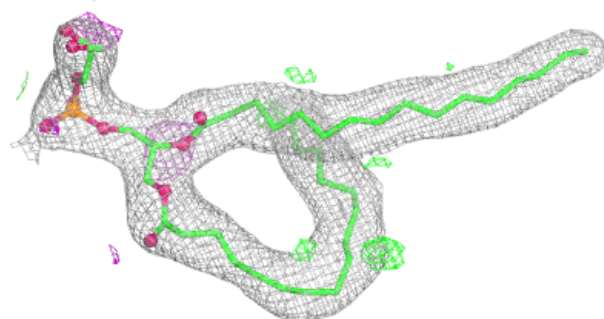


Electron density around DGD h 102:

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

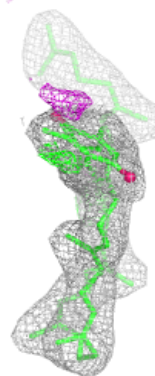
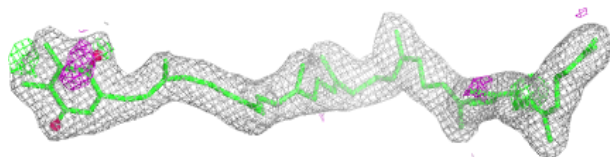
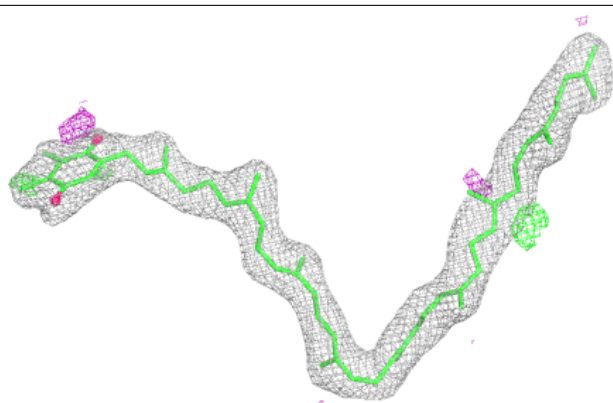
**Electron density around LHG D 409:**

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

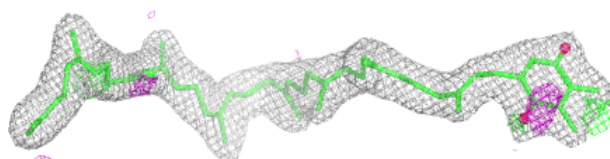
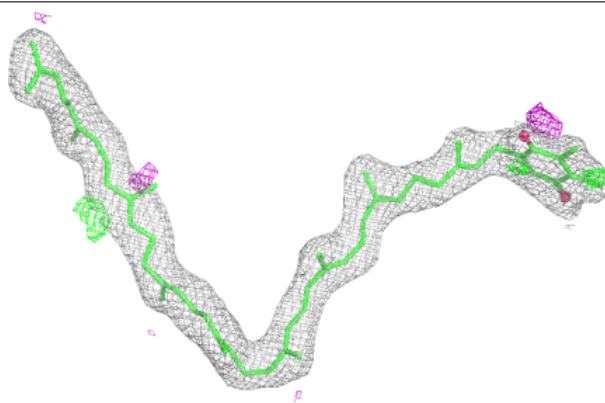


Electron density around PL9 D 407 (A):

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

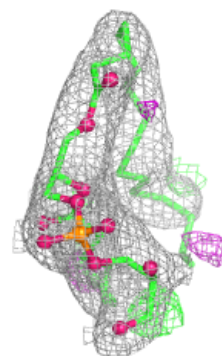
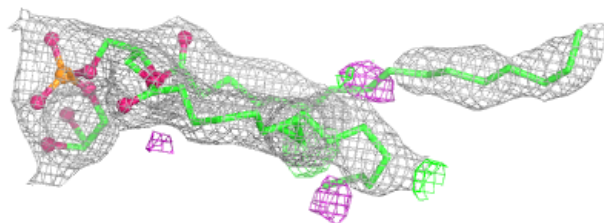
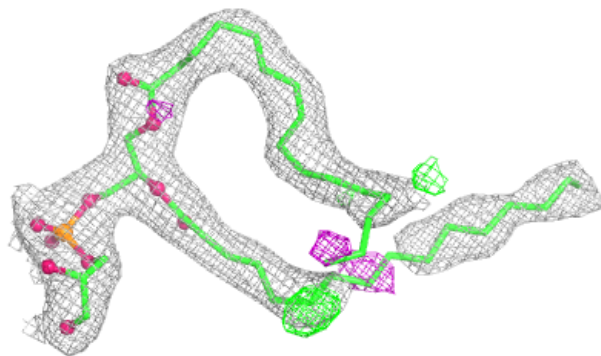
**Electron density around PL9 D 407 (B):**

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

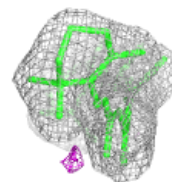
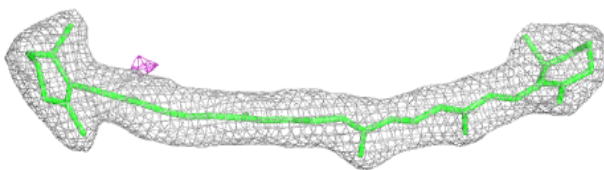
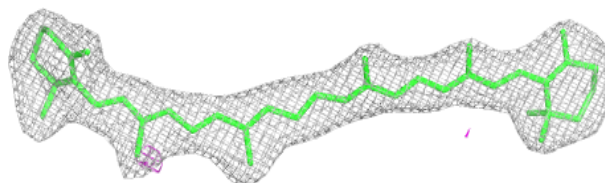


Electron density around LHG d 410:

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

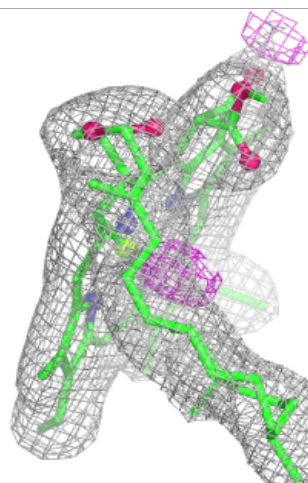
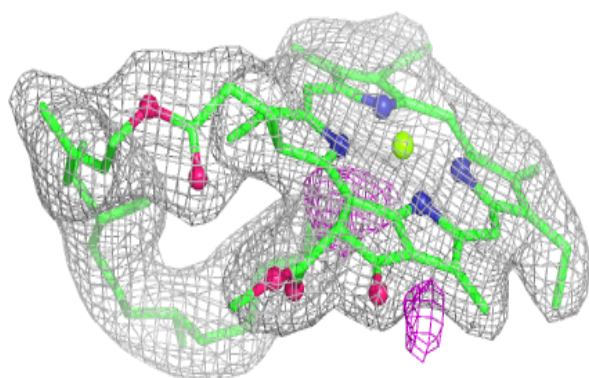
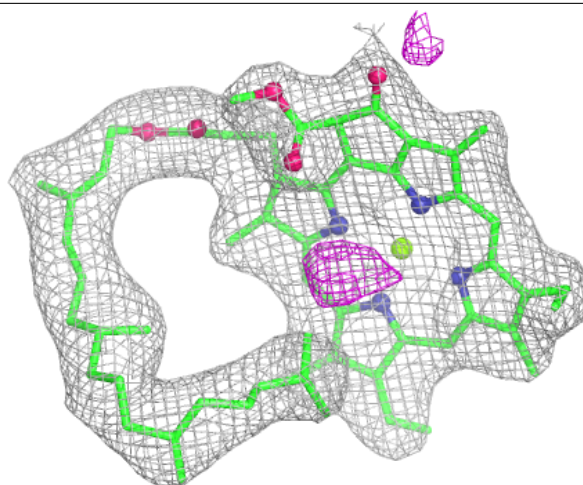
**Electron density around BCR T 103:**

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



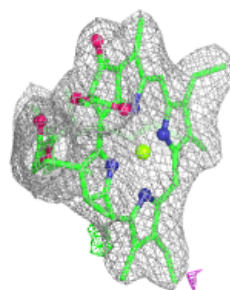
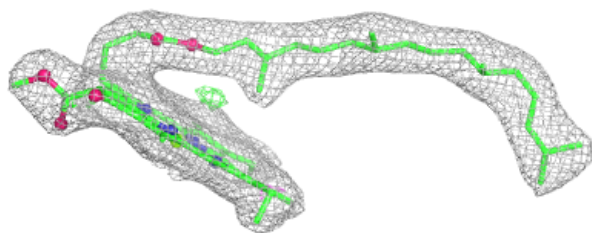
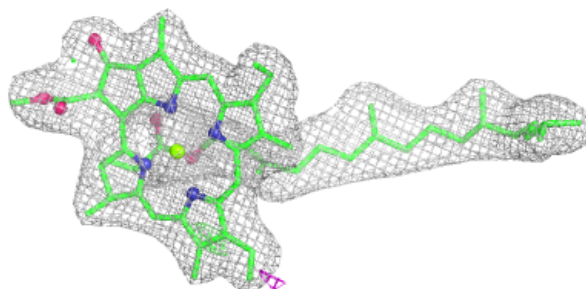
Electron density around CLA b 624:

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

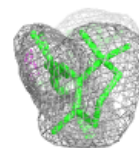
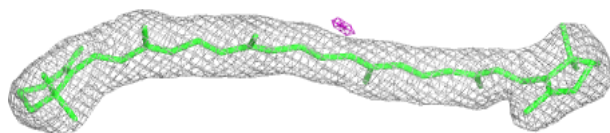
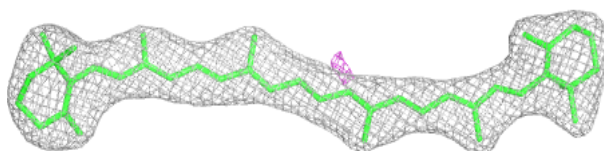


Electron density around CLA B 609:

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

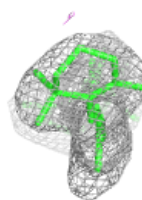
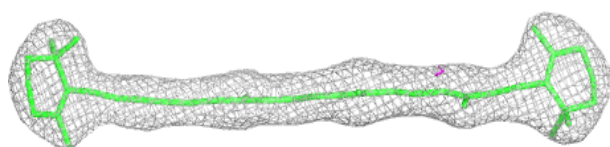
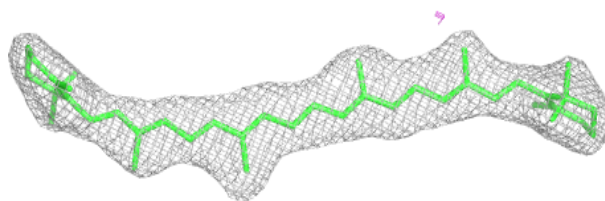
**Electron density around BCR b 628:**

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

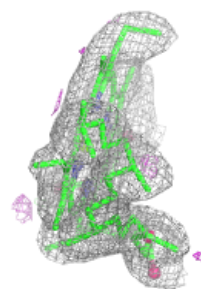
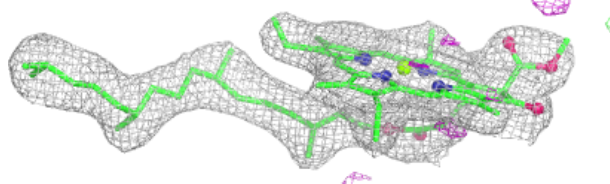
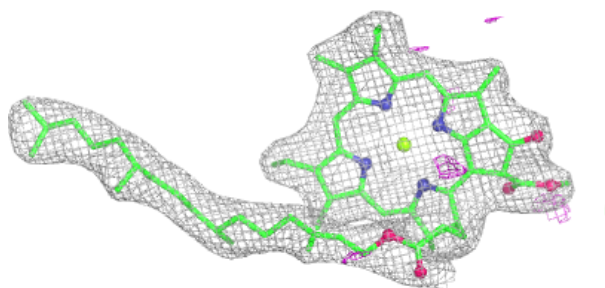


Electron density around BCR c 518:

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

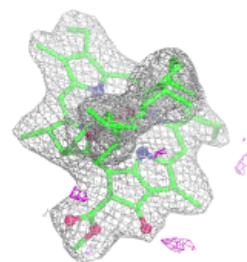
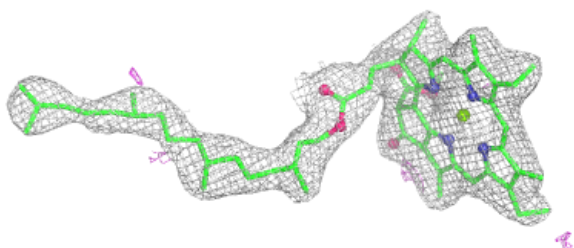
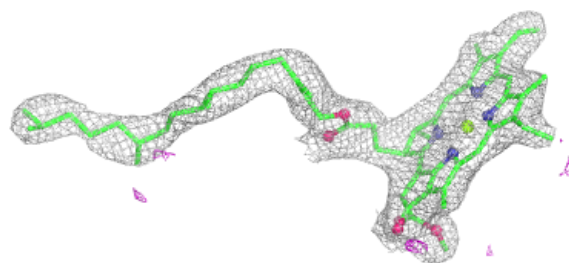
**Electron density around CLA c 505:**

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



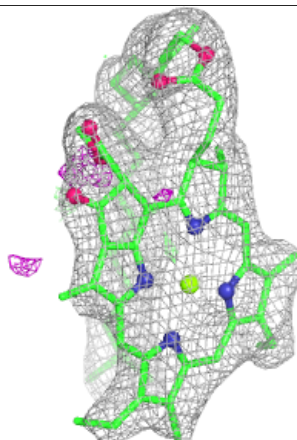
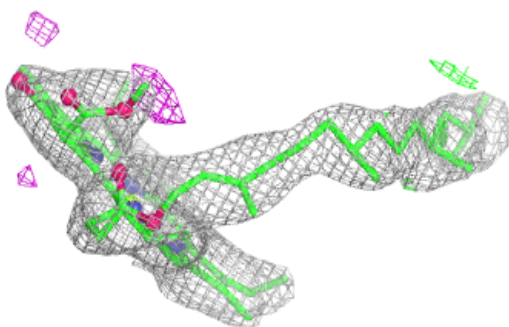
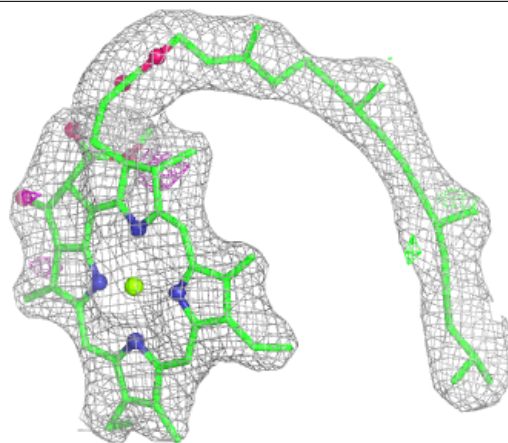
Electron density around CLA c 506:

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

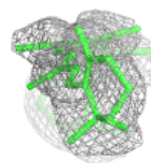
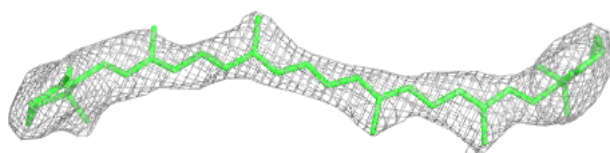
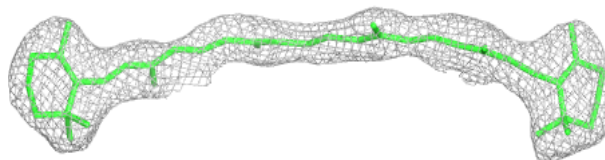


Electron density around CLA C 507:

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

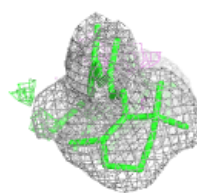
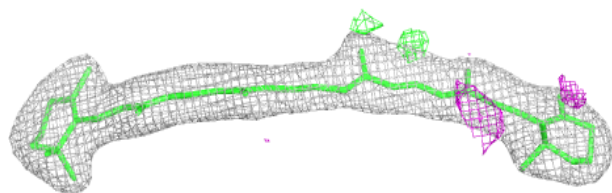
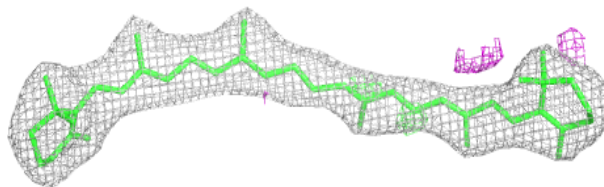
**Electron density around BCR k 102:**

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

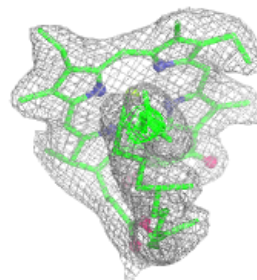
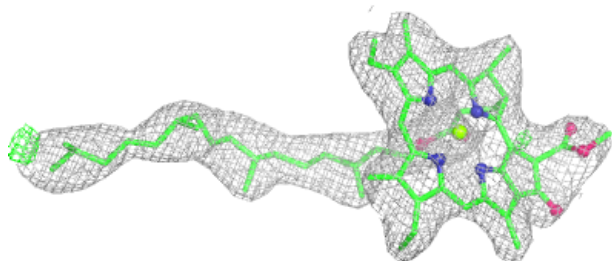
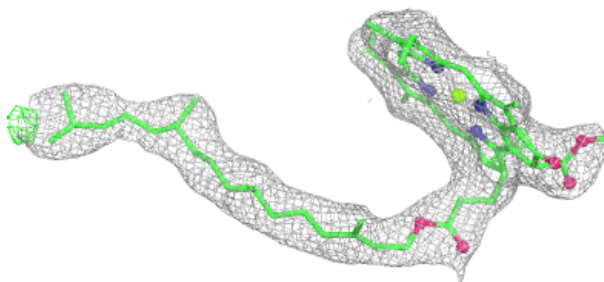


Electron density around BCR t 102:

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

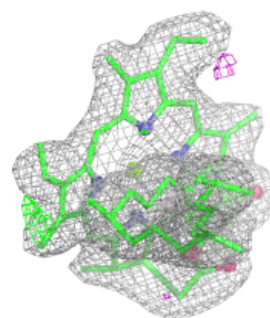
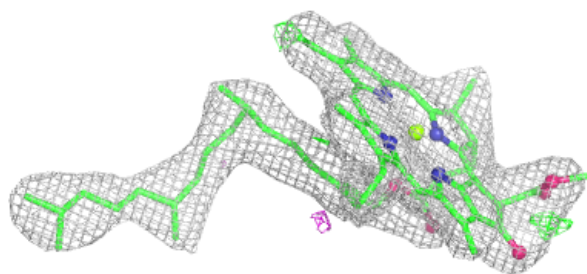
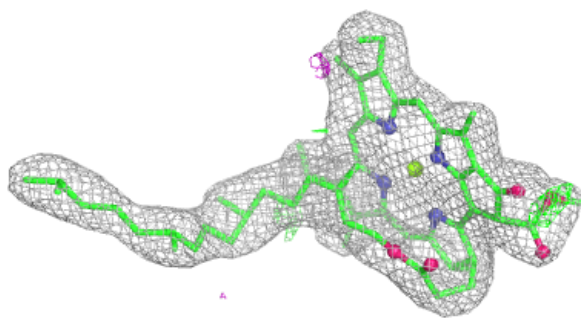
**Electron density around CLA c 508:**

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



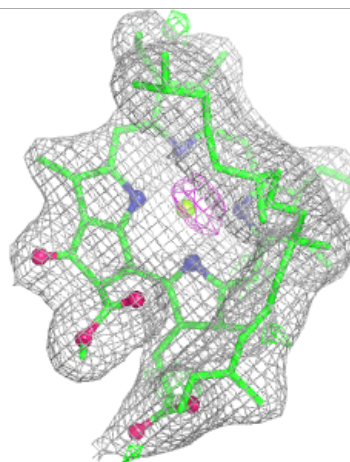
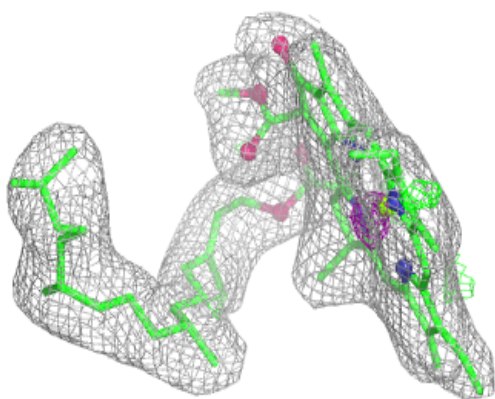
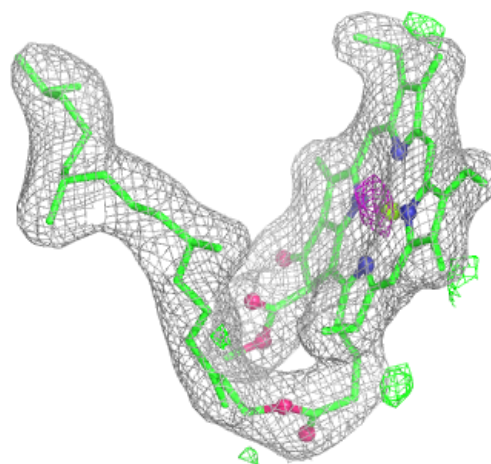
Electron density around CLA c 509:

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



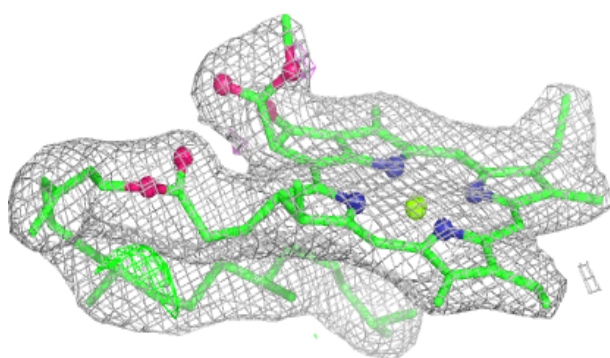
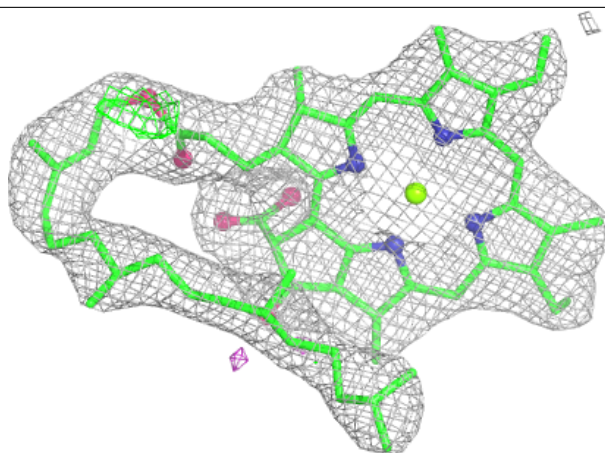
Electron density around CLA B 614:

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



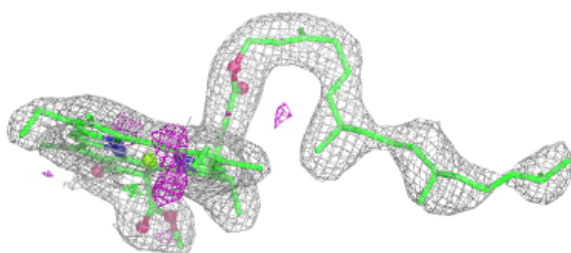
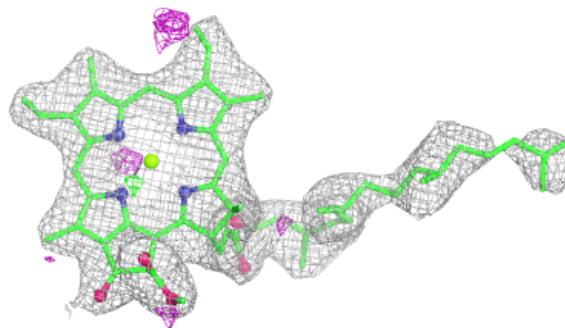
Electron density around CLA C 509:

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



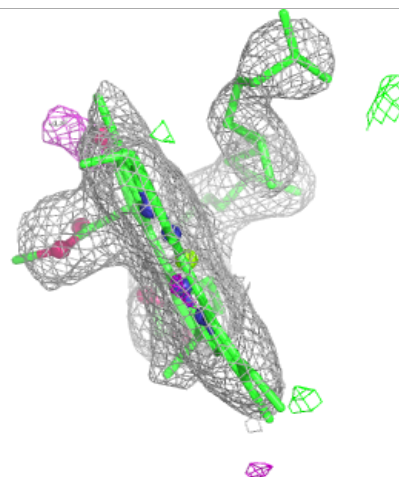
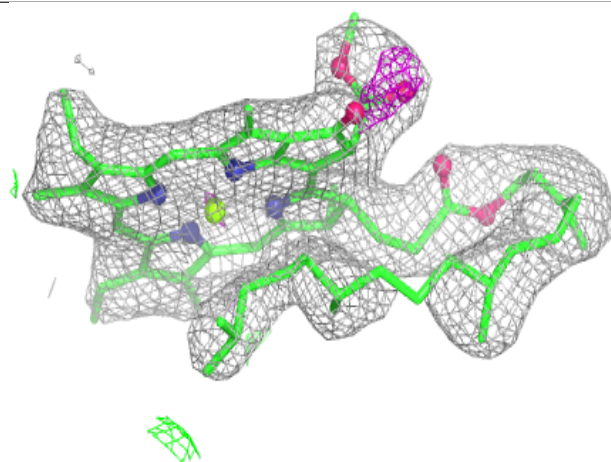
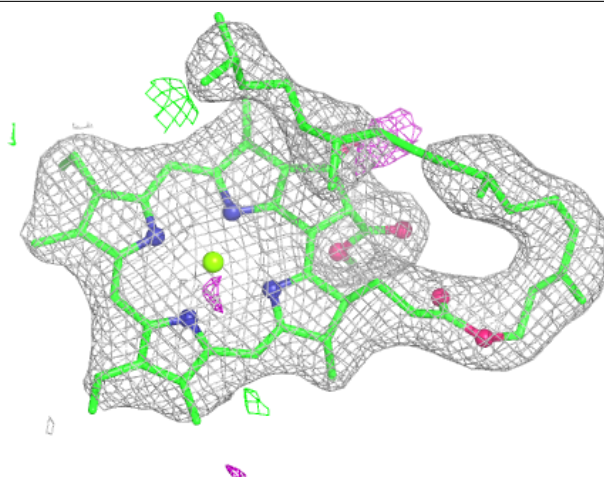
Electron density around CLA A 407:

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



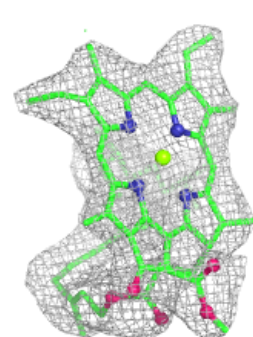
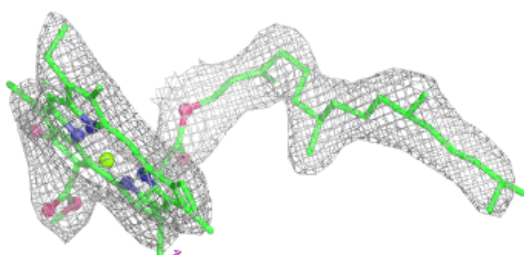
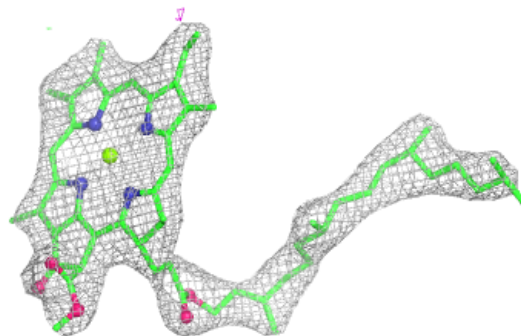
Electron density around CLA c 513:

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

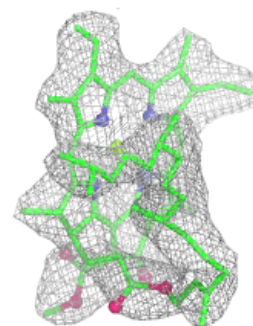
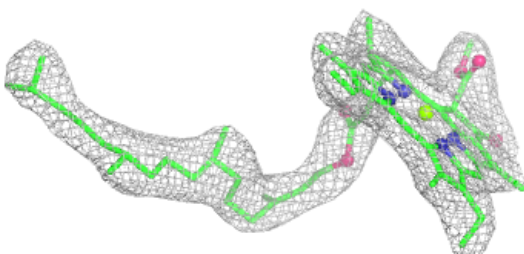
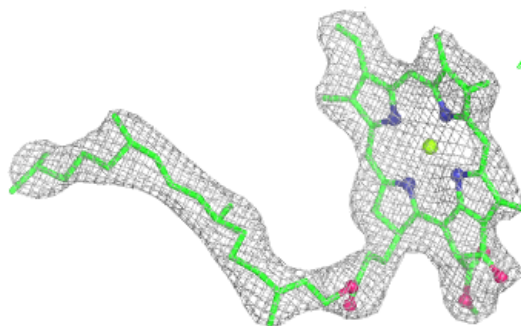


Electron density around CLA c 515:

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

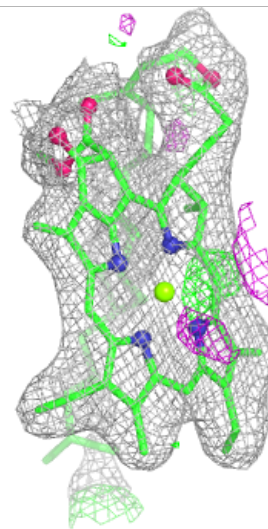
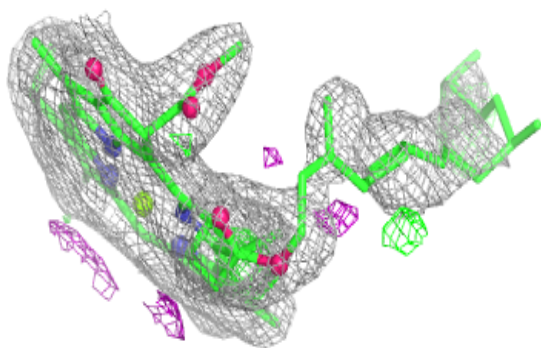
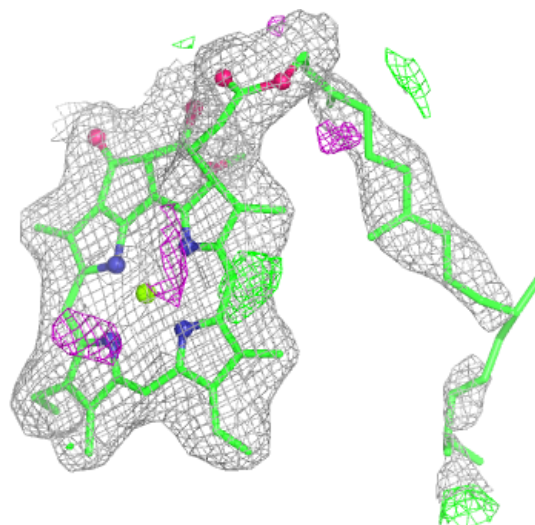
**Electron density around CLA C 511:**

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



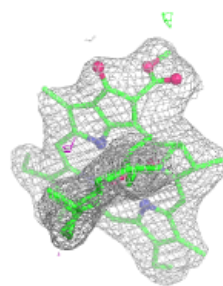
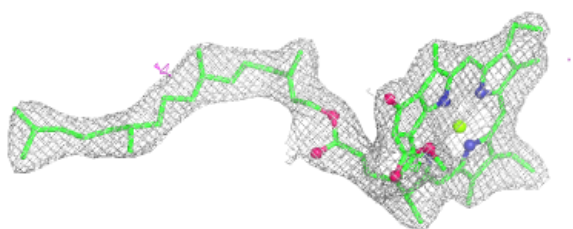
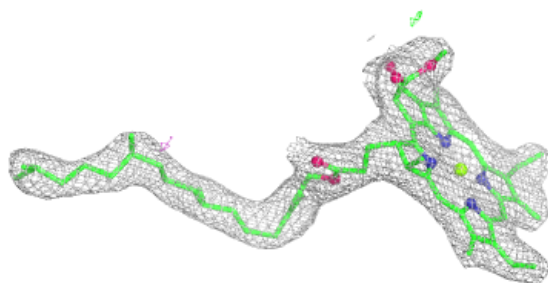
Electron density around CLA B 617:

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

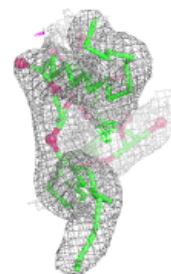
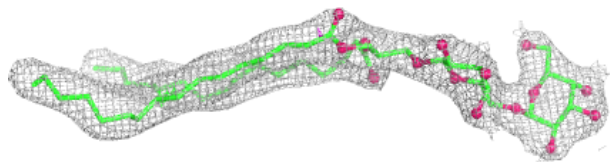


Electron density around CLA C 502:

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

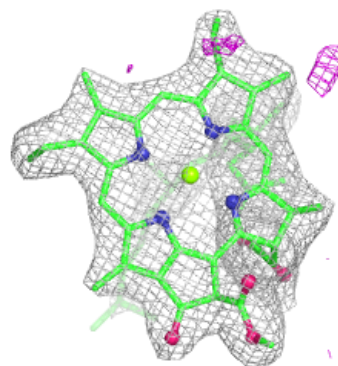
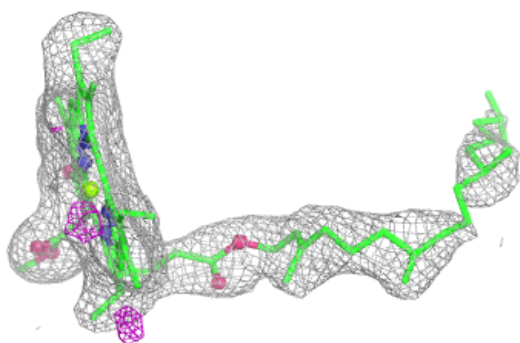
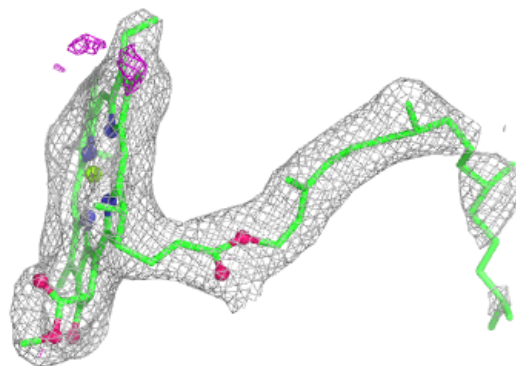
**Electron density around DGD C 518:**

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

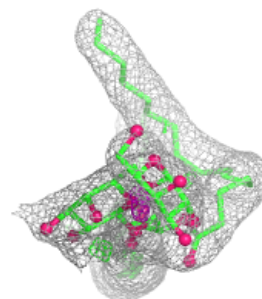
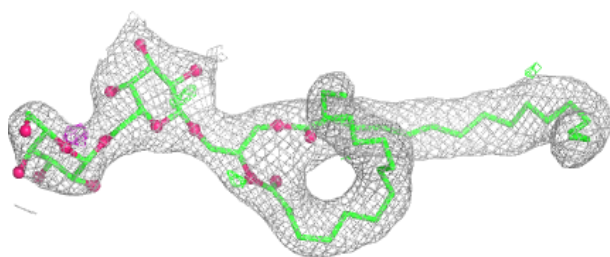
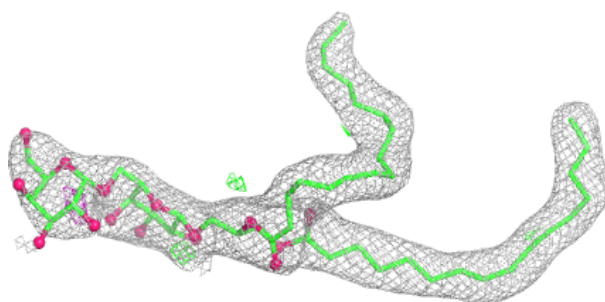


Electron density around CLA D 405:

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

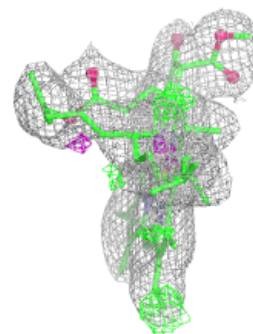
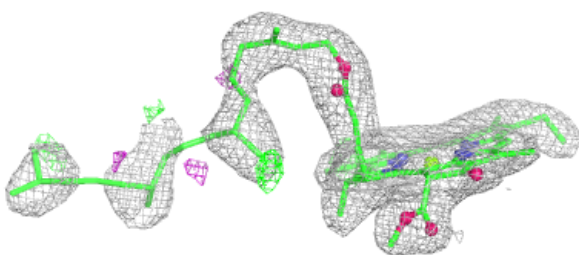
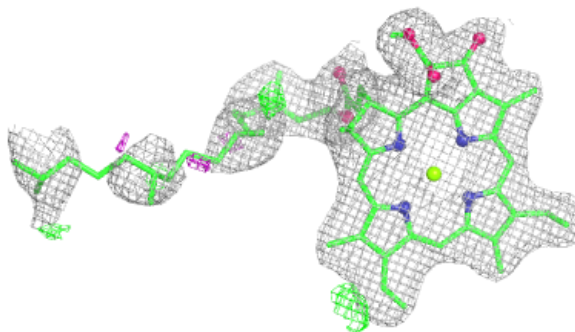
**Electron density around DGD H 102:**

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



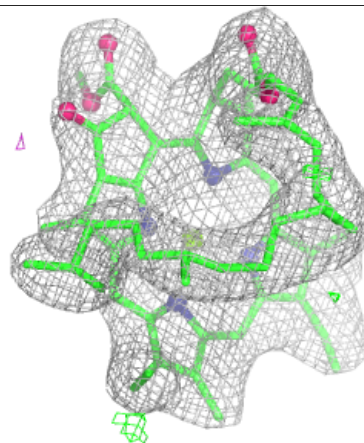
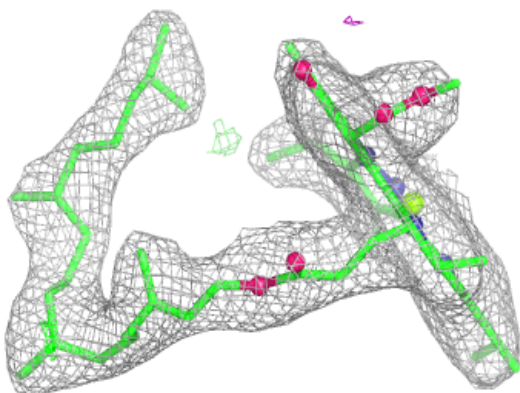
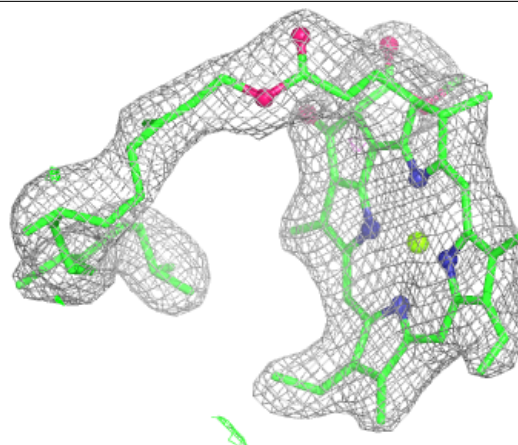
Electron density around CLA a 410:

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

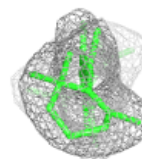
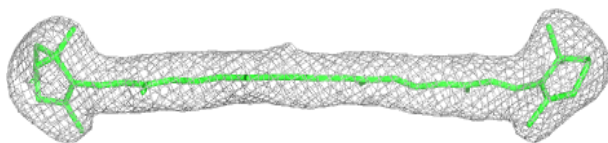
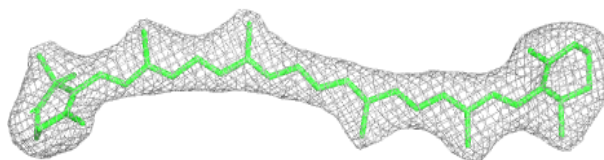


Electron density around CLA C 503:

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

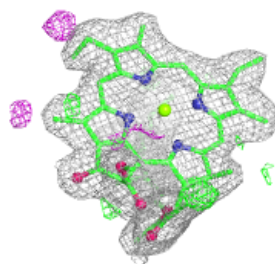
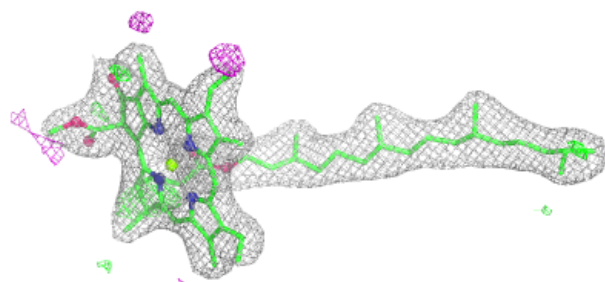
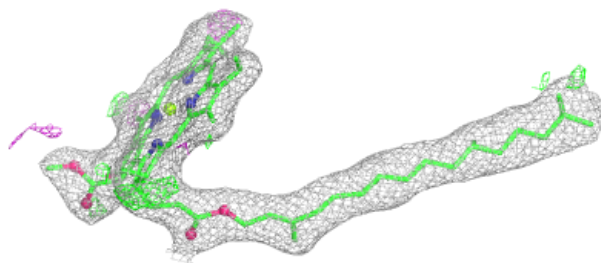
**Electron density around BCR B 619:**

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

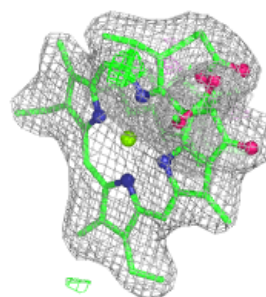
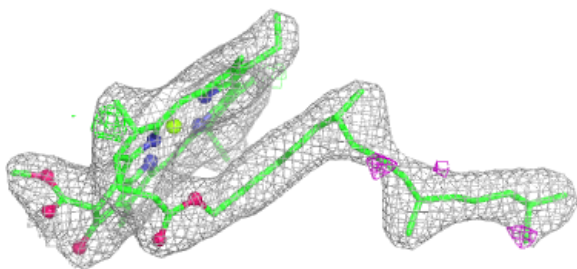
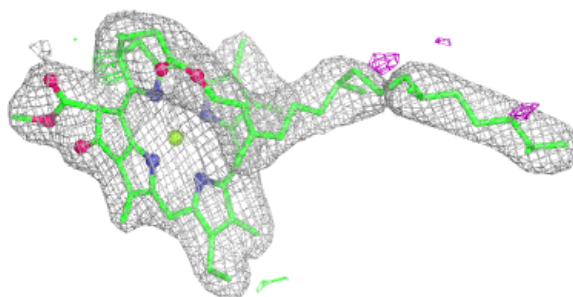


Electron density around CLA B 608:

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

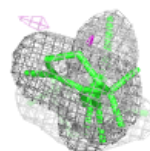
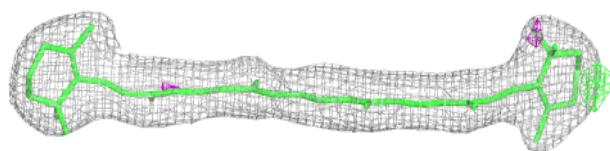
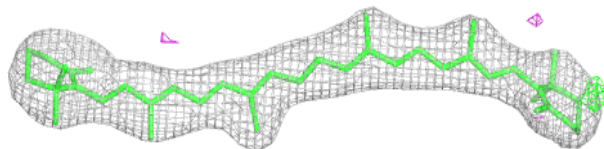
**Electron density around CLA C 505:**

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

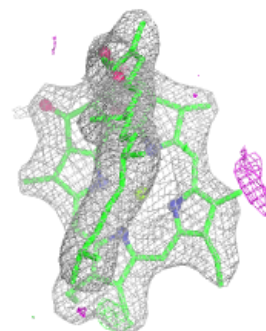
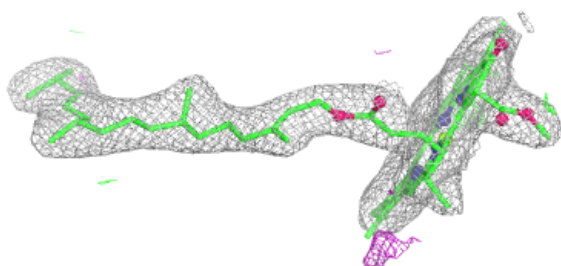
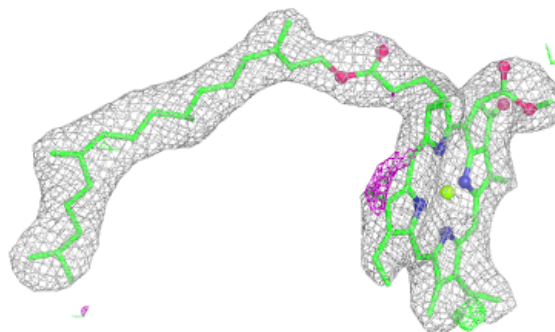


Electron density around BCR C 515:

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

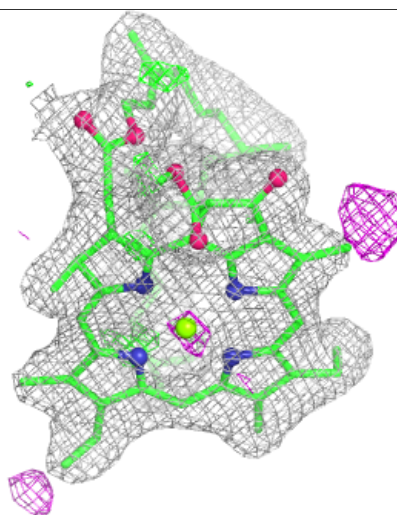
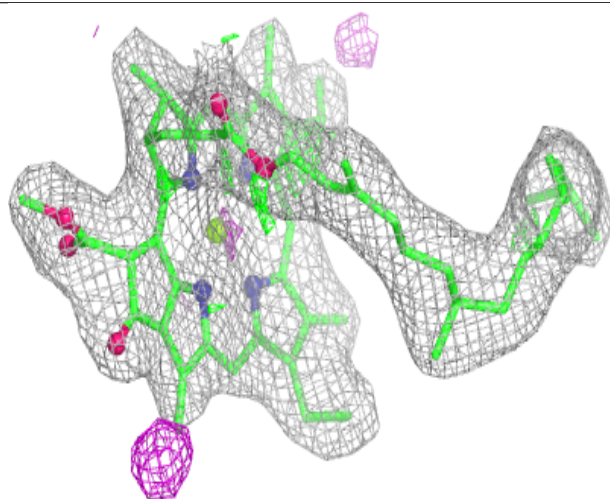
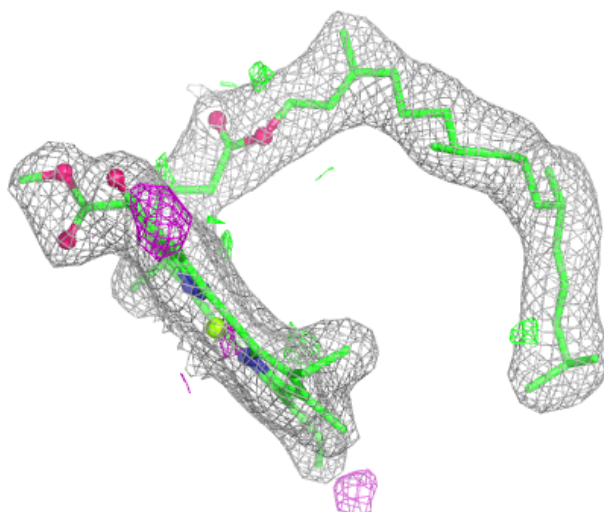
**Electron density around CLA b 618:**

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



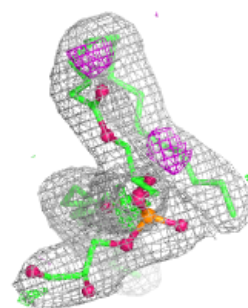
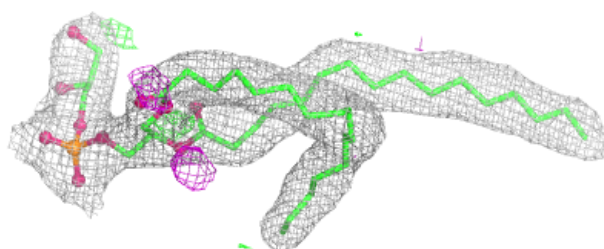
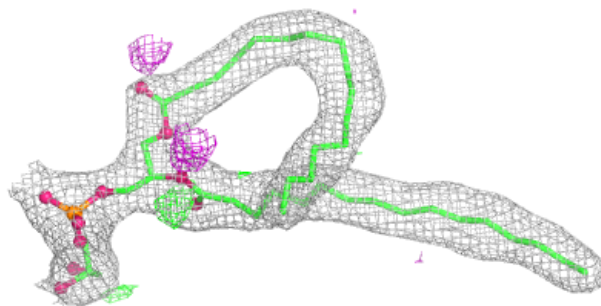
Electron density around CLA b 620:

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

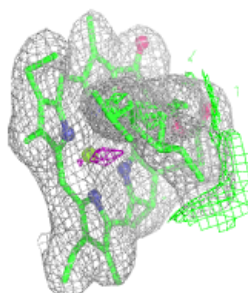
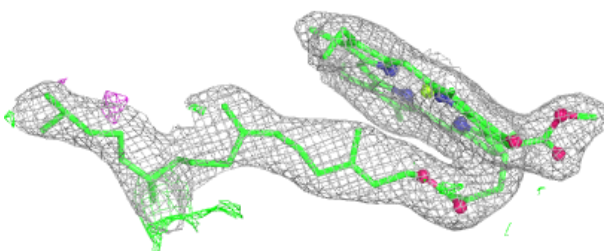
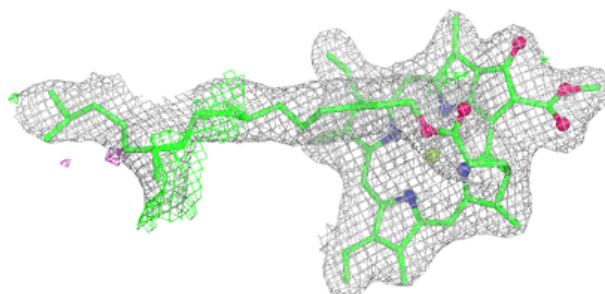


Electron density around LHG d 408:

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

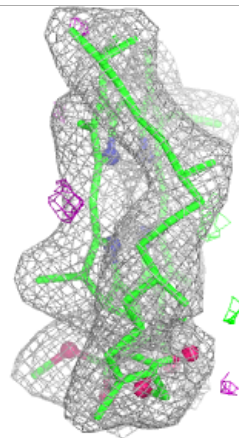
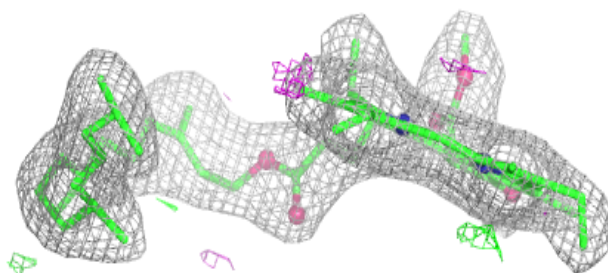
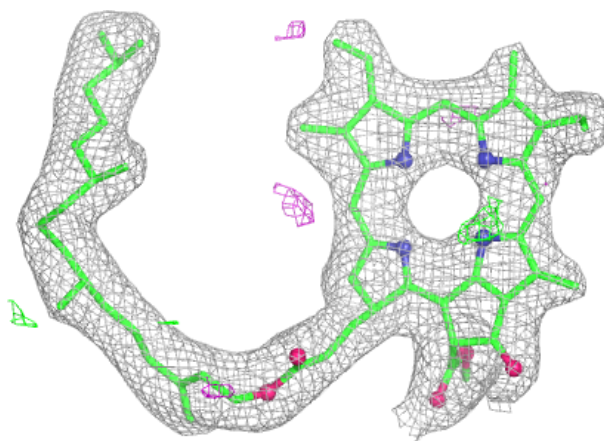
**Electron density around CLA b 623:**

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



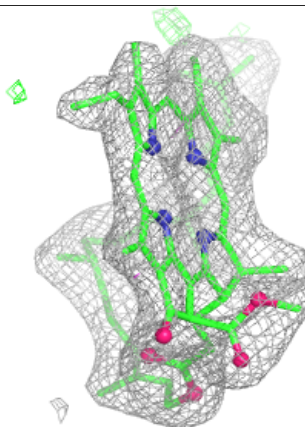
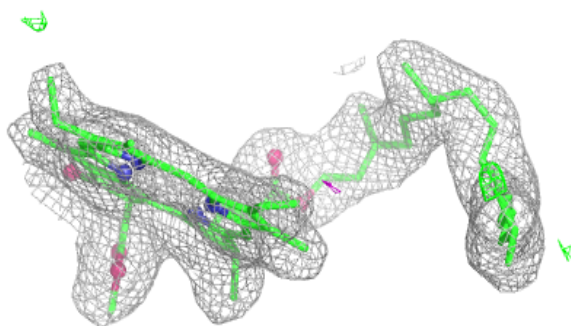
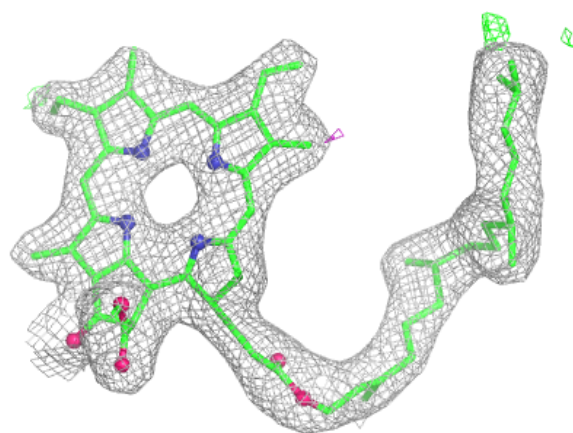
Electron density around PHO A 408:

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



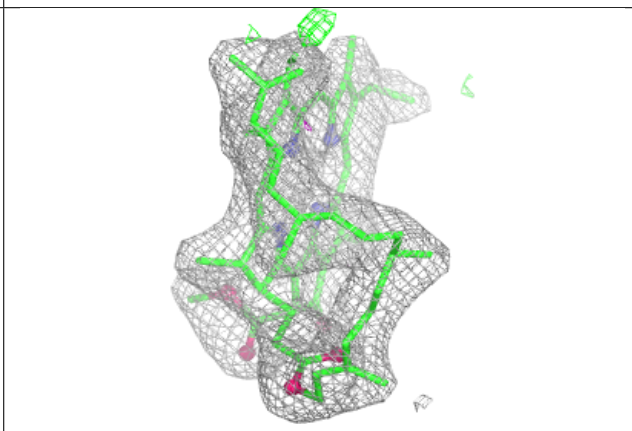
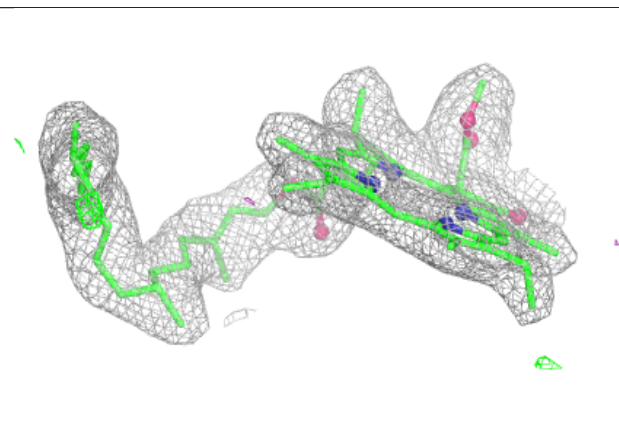
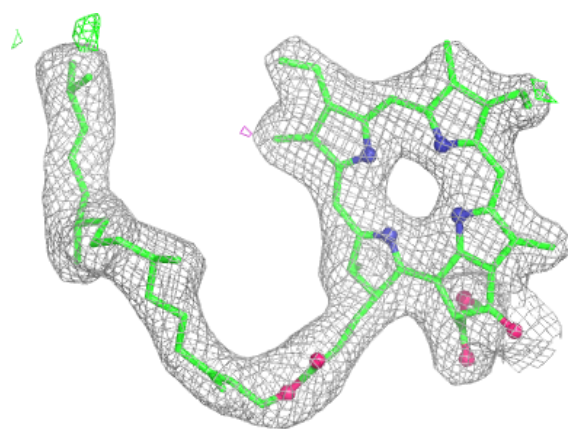
Electron density around PHO D 401 (A):

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



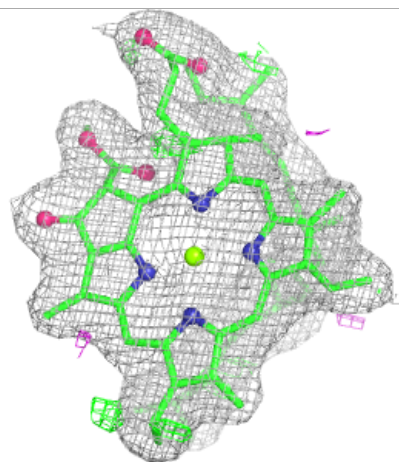
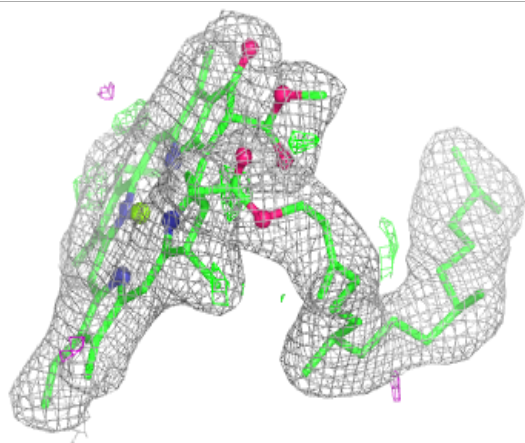
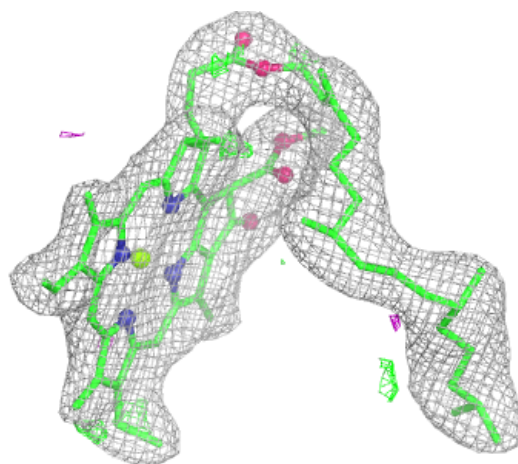
Electron density around PHO D 401 (B):

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



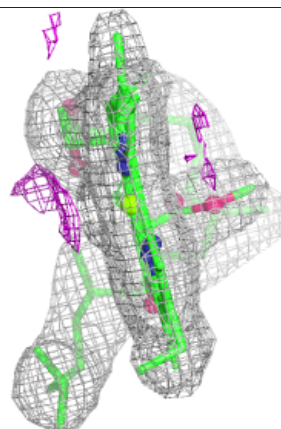
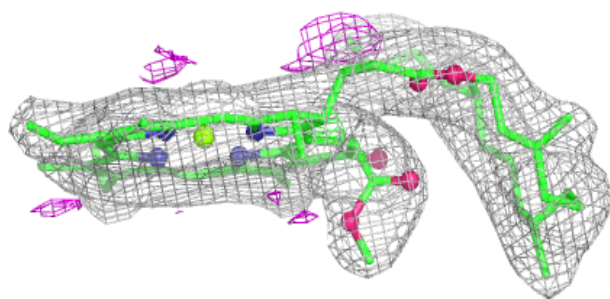
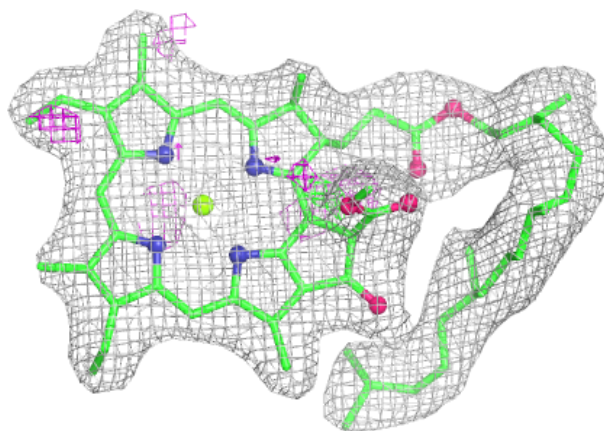
Electron density around CLA b 622:

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



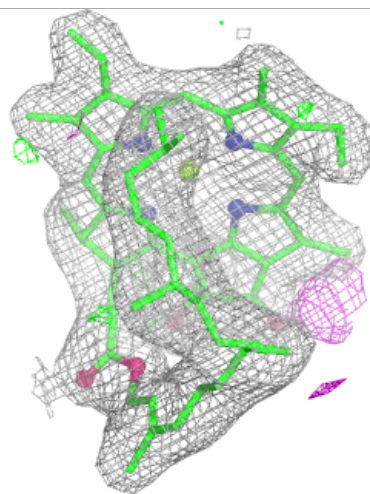
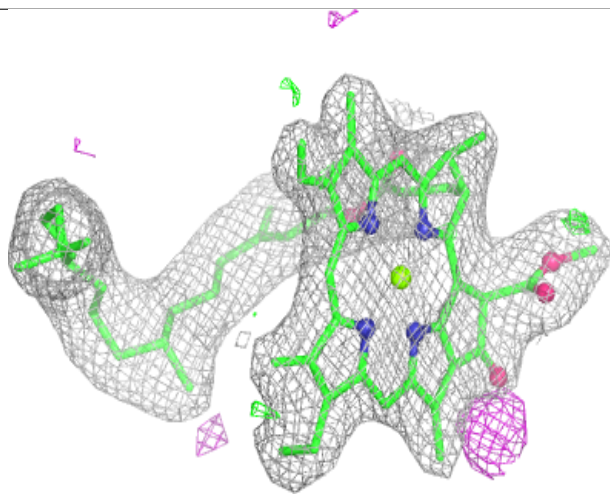
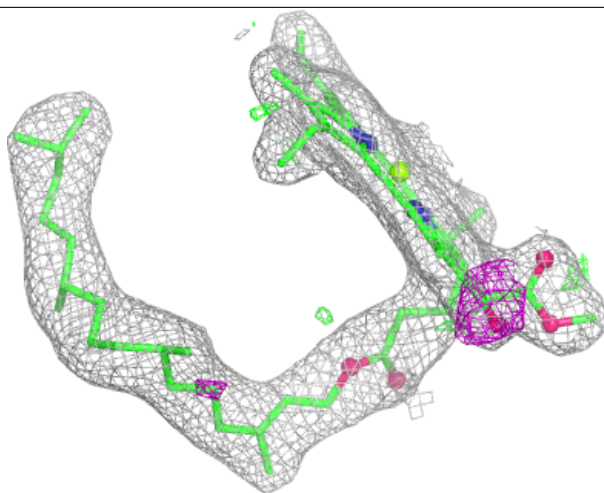
Electron density around CLA B 611:

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



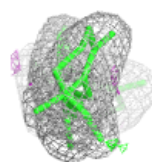
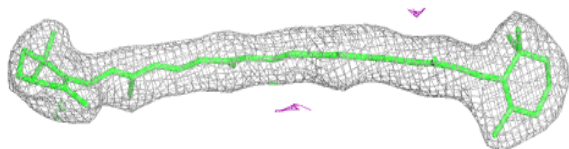
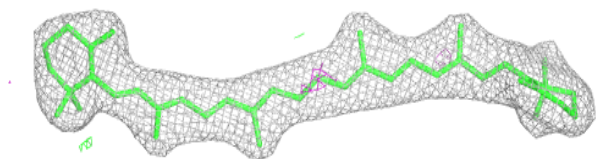
Electron density around CLA B 612:

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

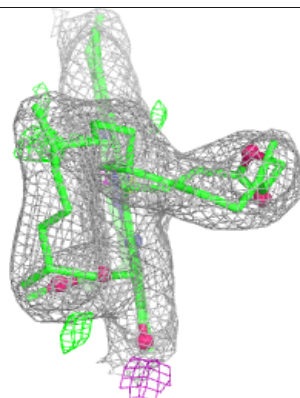
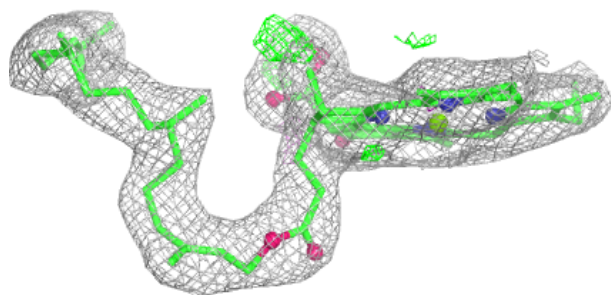
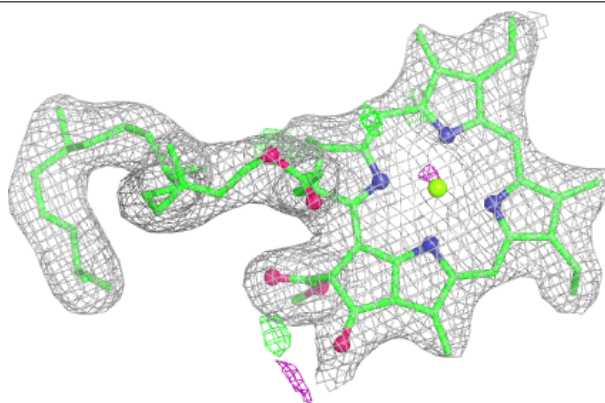


Electron density around BCR B 618:

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

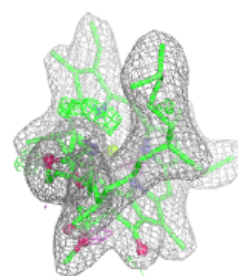
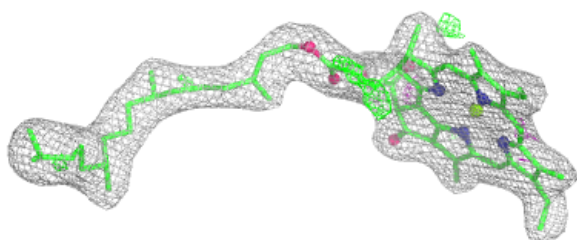
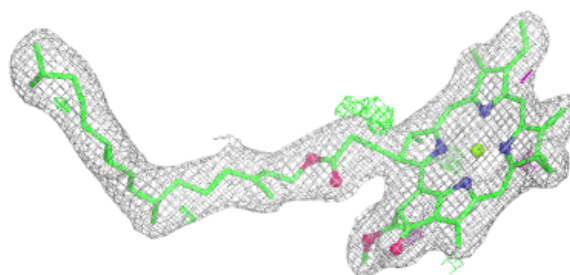
**Electron density around CLA B 613:**

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

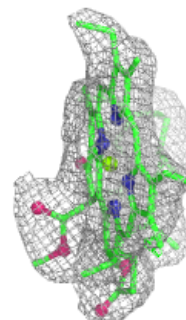
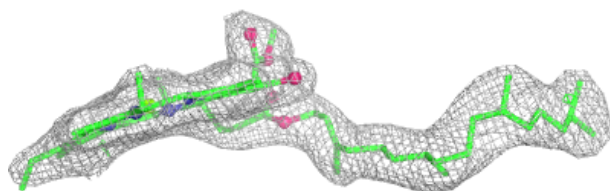
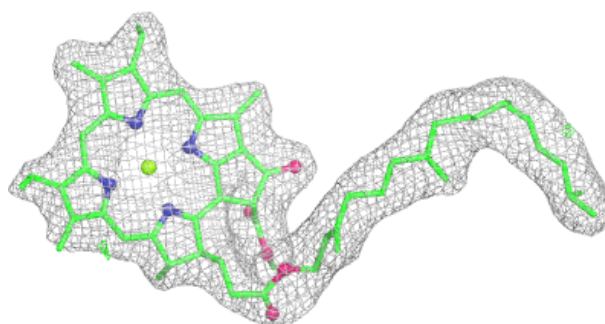


Electron density around CLA A 405:

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

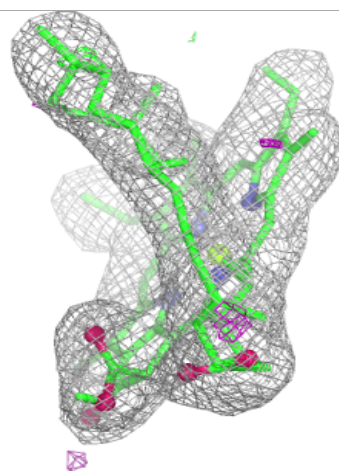
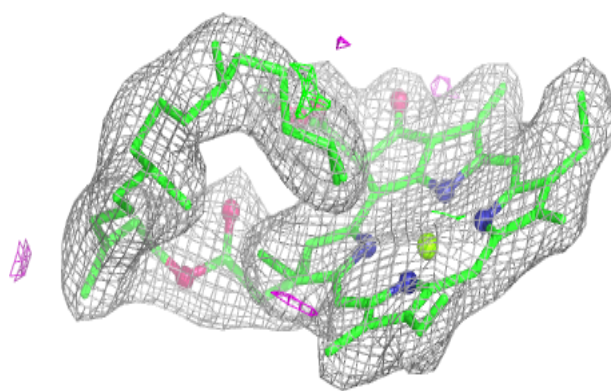
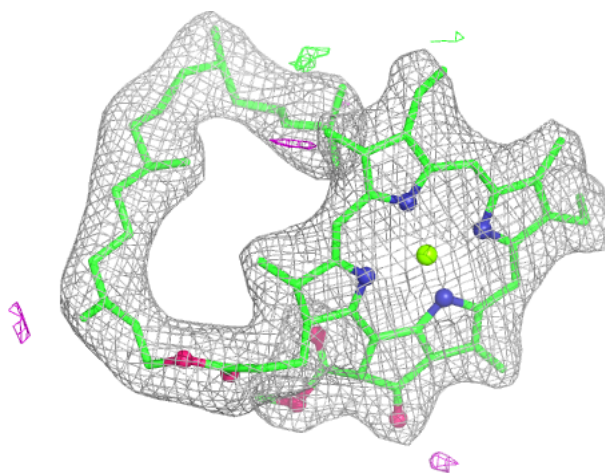
**Electron density around CLA B 603:**

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



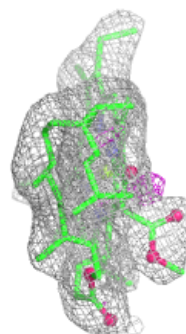
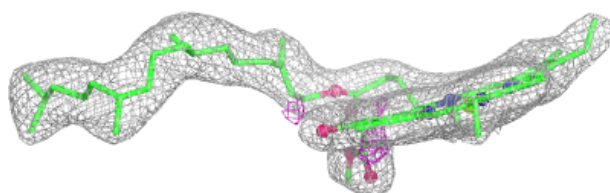
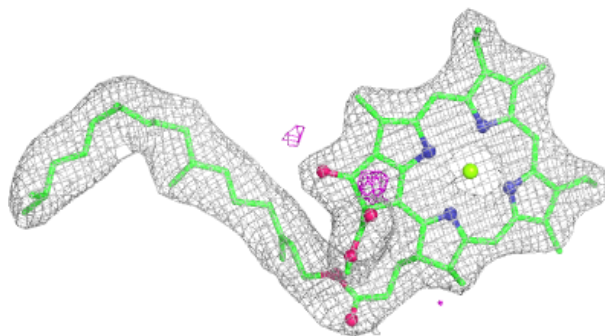
Electron density around CLA B 616:

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

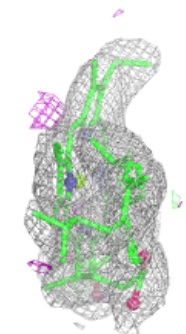
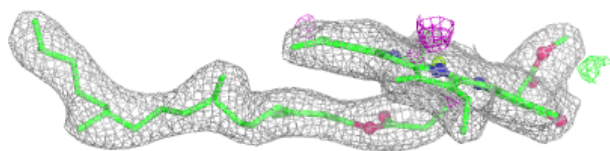
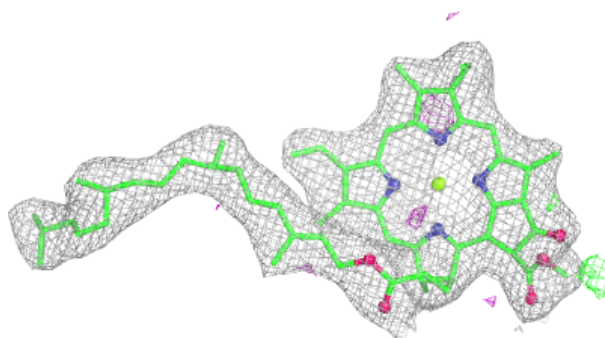


Electron density around CLA b 611:

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

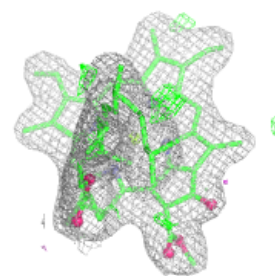
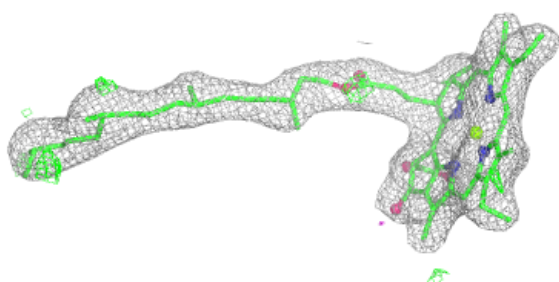
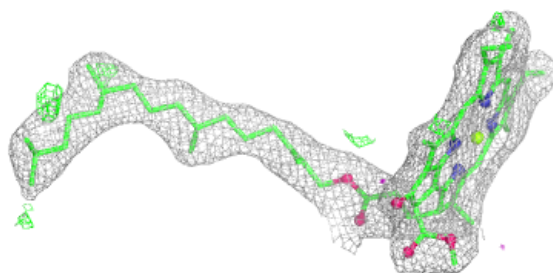
**Electron density around CLA b 612:**

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

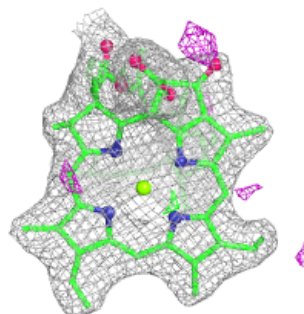
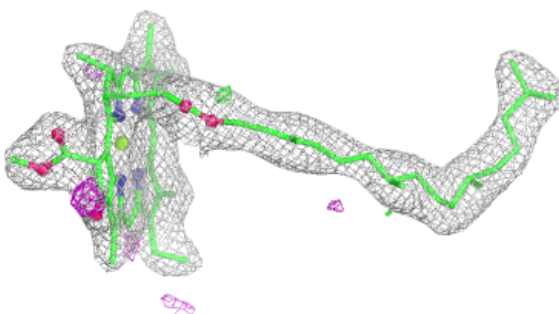
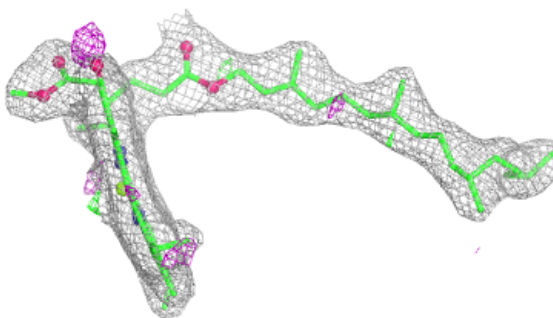


Electron density around CLA b 613:

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

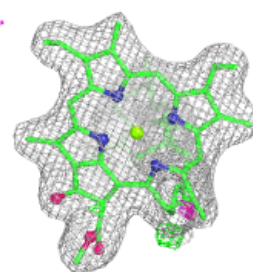
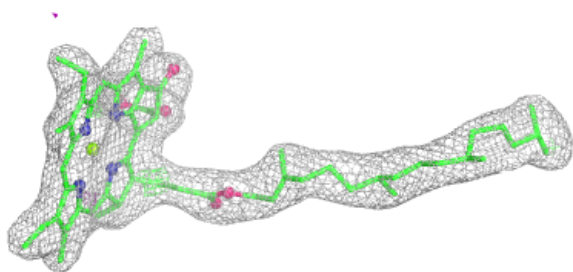
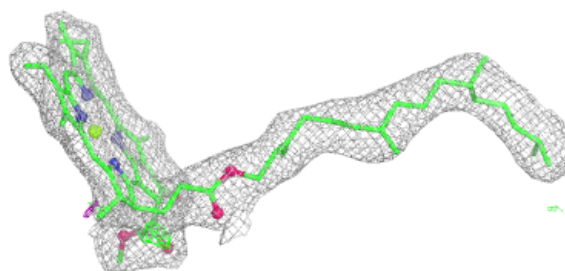
**Electron density around CLA b 614:**

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

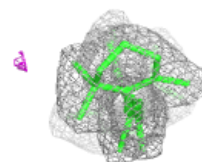
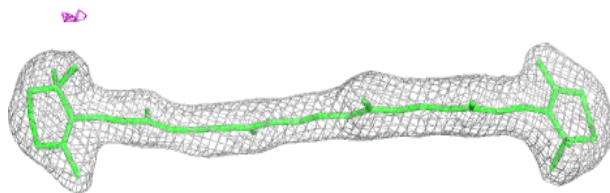
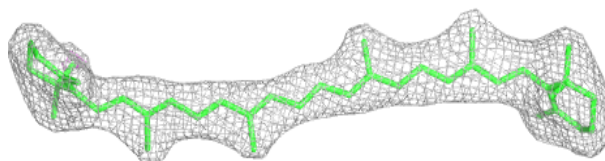


Electron density around CLA B 605:

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

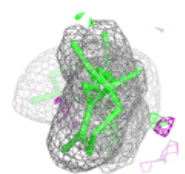
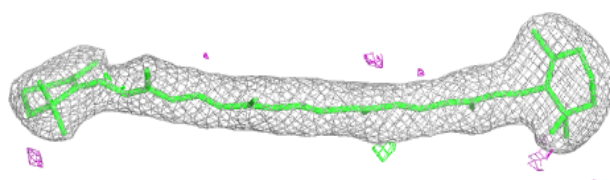
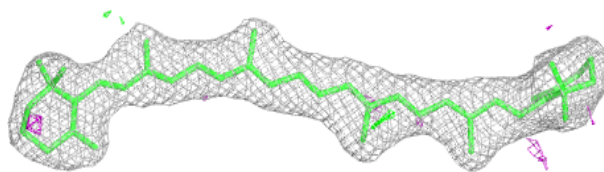
**Electron density around BCR a 413:**

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

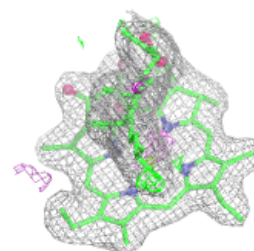
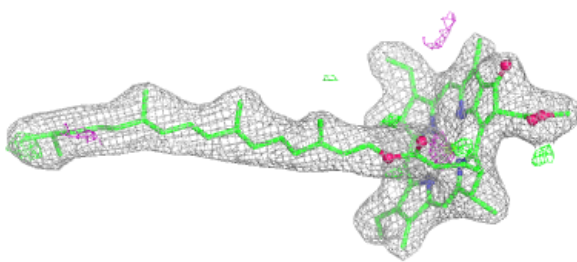
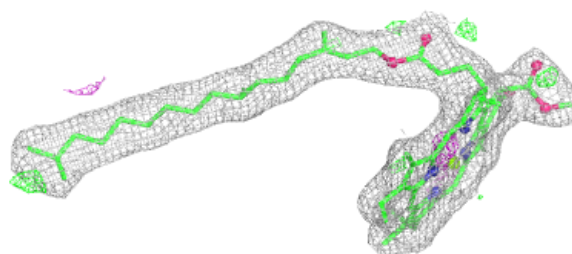


Electron density around BCR b 626:

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

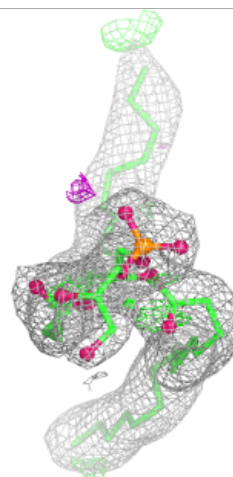
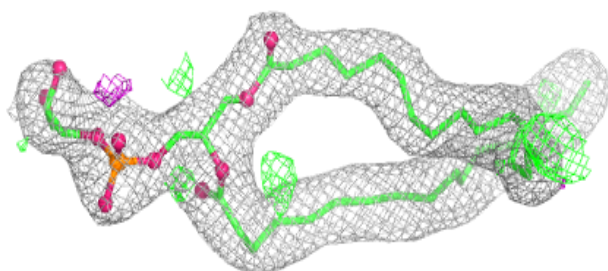
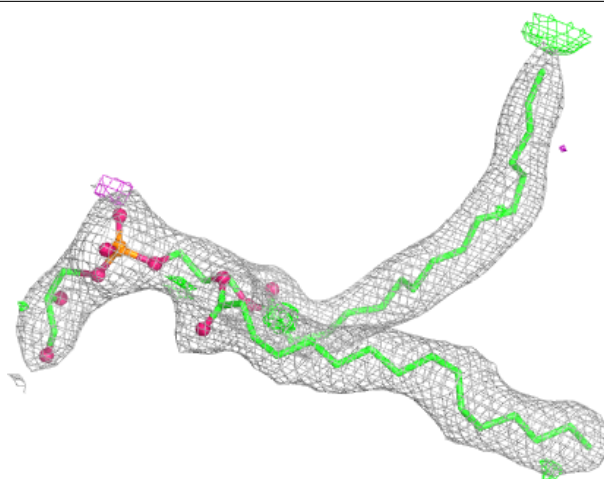
**Electron density around CLA b 616:**

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



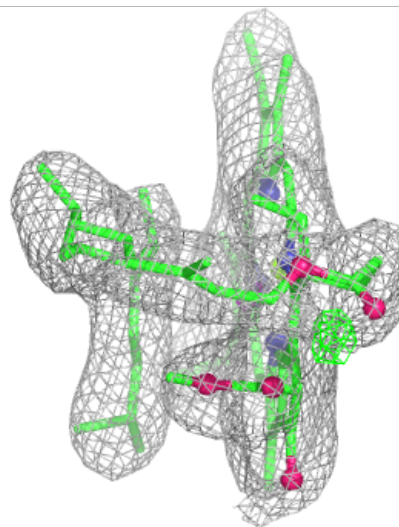
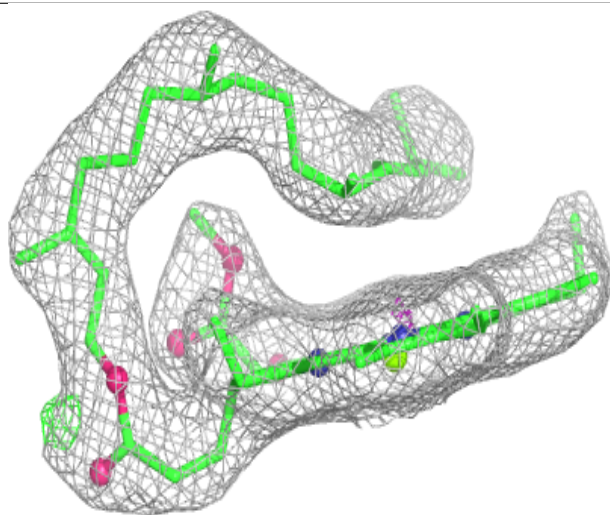
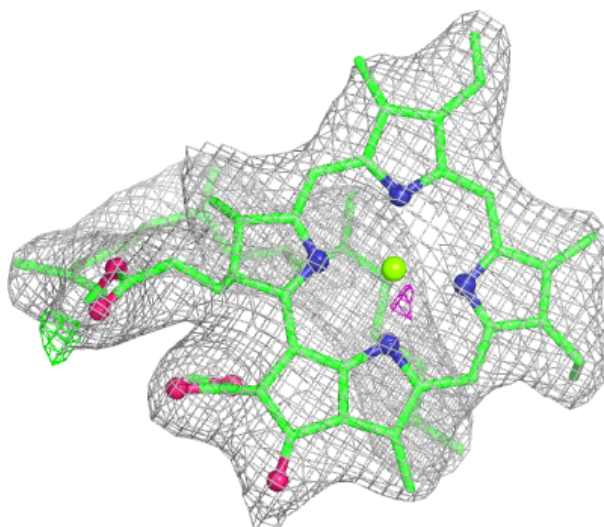
Electron density around LHG D 410:

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



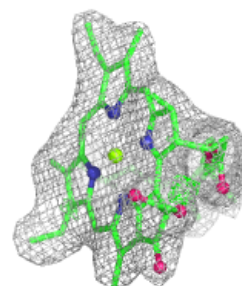
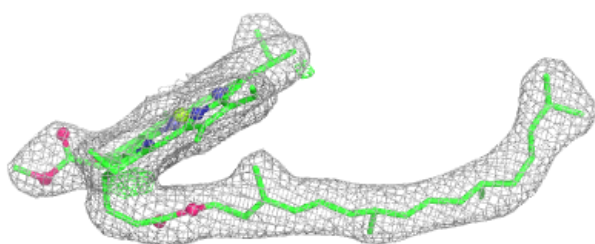
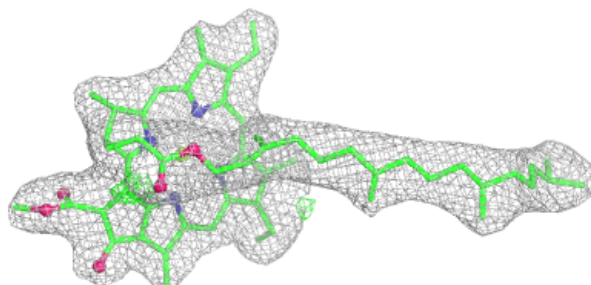
Electron density around CLA c 514:

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

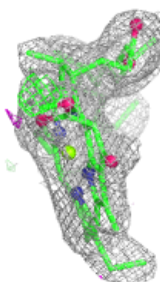
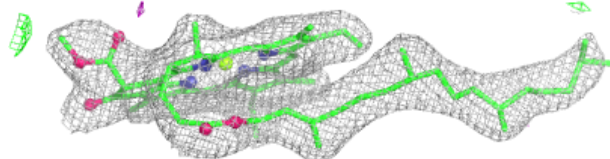
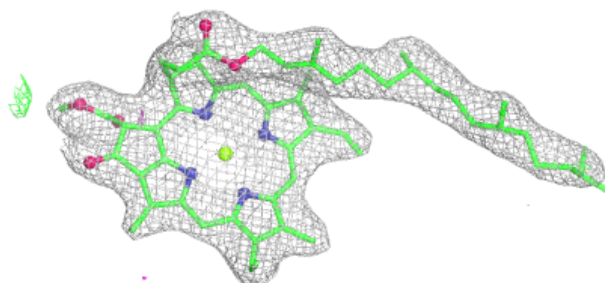


Electron density around CLA b 617:

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

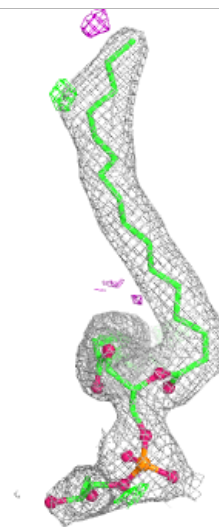
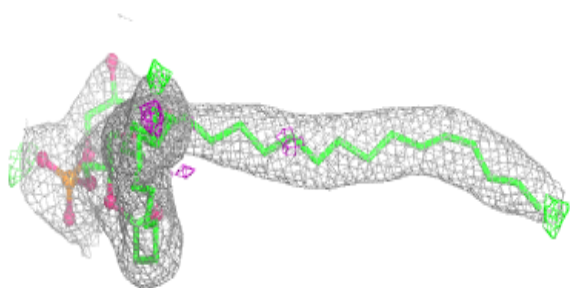
**Electron density around CLA C 501:**

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



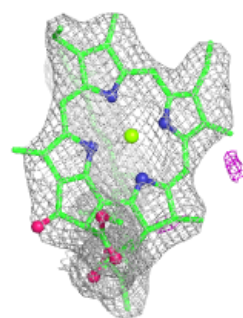
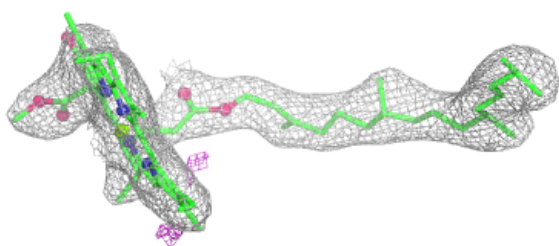
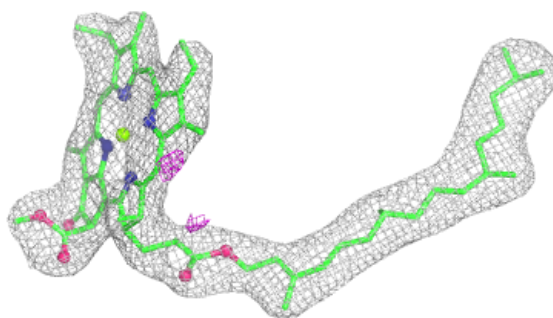
Electron density around LHG b 634:

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



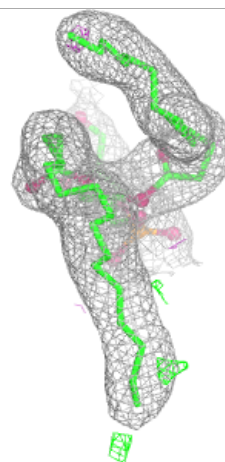
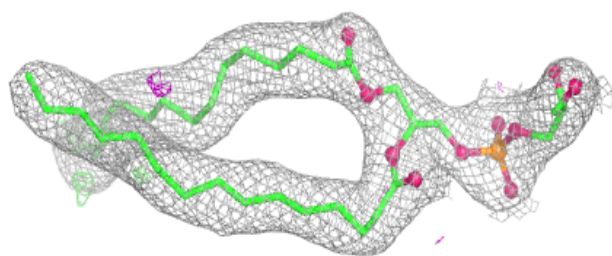
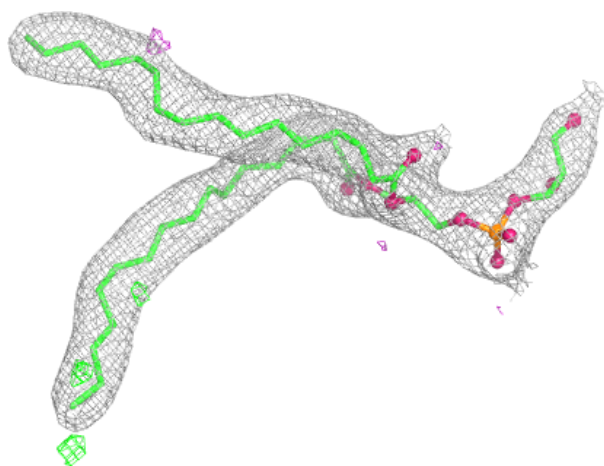
Electron density around CLA B 610:

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



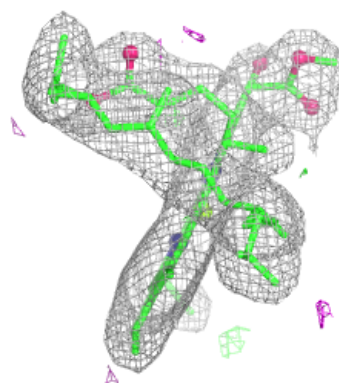
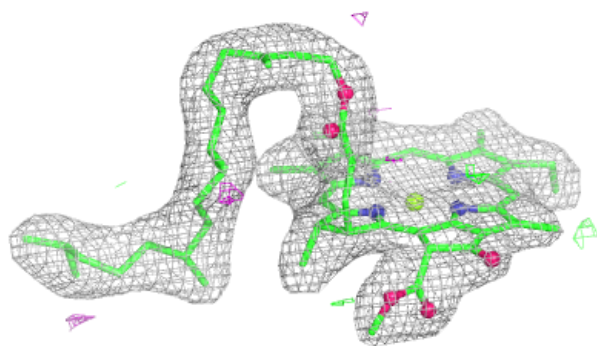
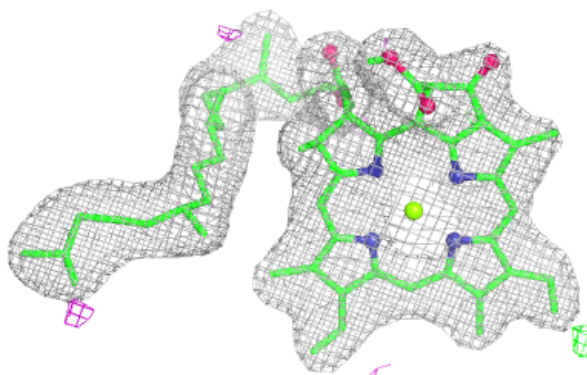
Electron density around LHG d 409:

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

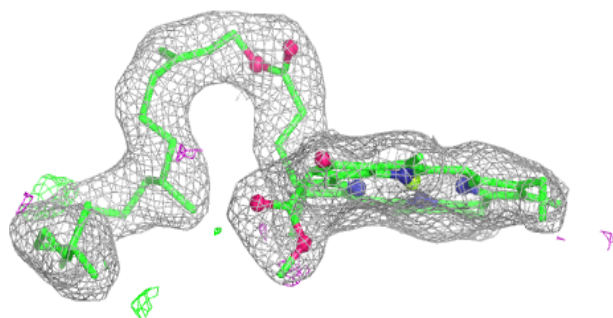
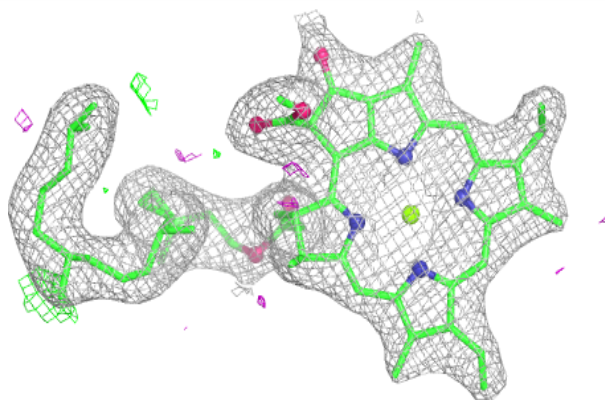


Electron density around CLA d 403:

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

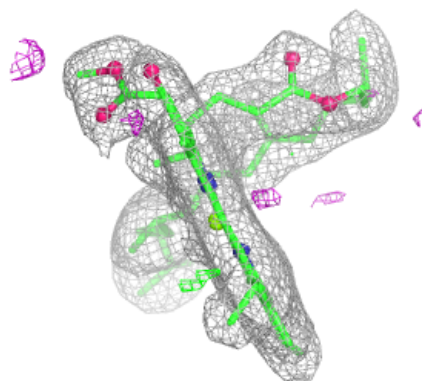
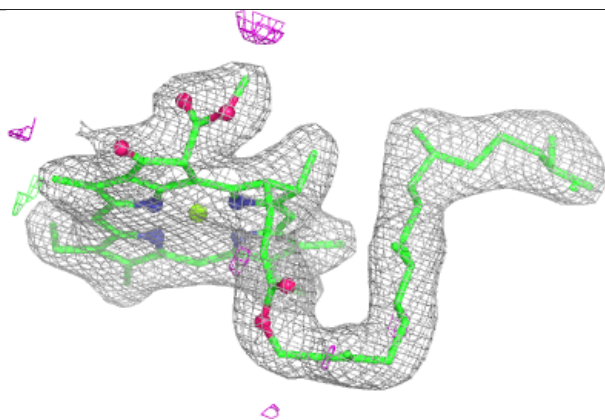
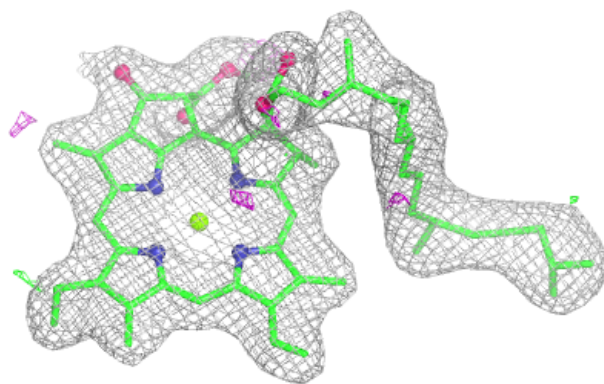
**Electron density around CLA b 621:**

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



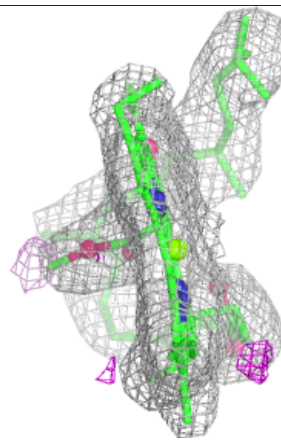
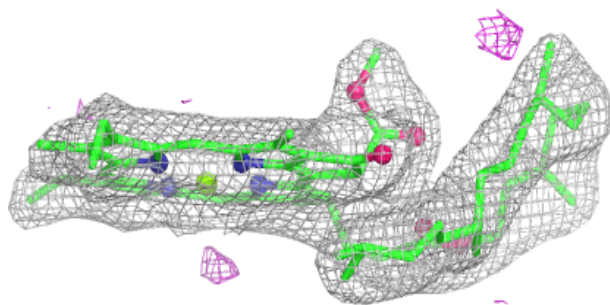
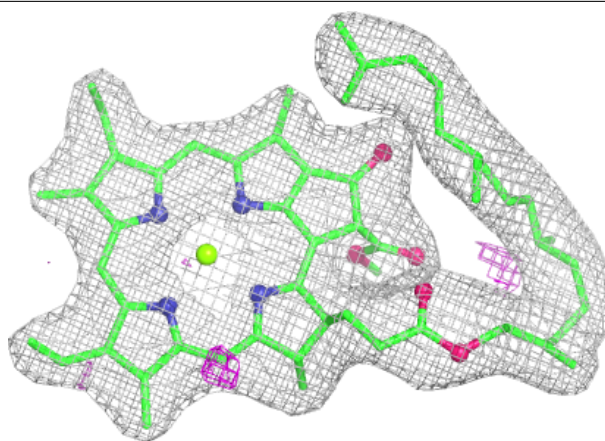
Electron density around CLA A 406:

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



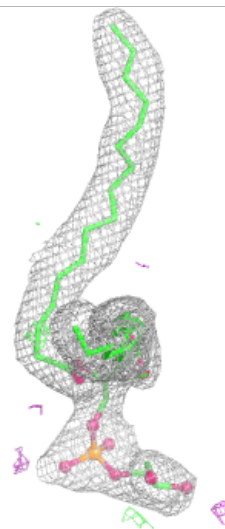
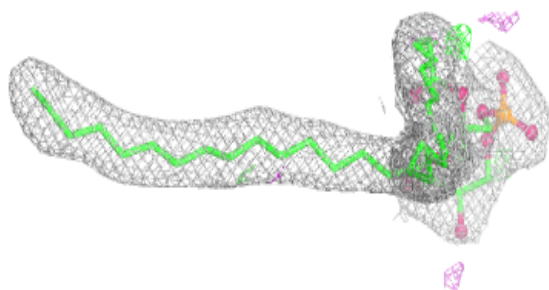
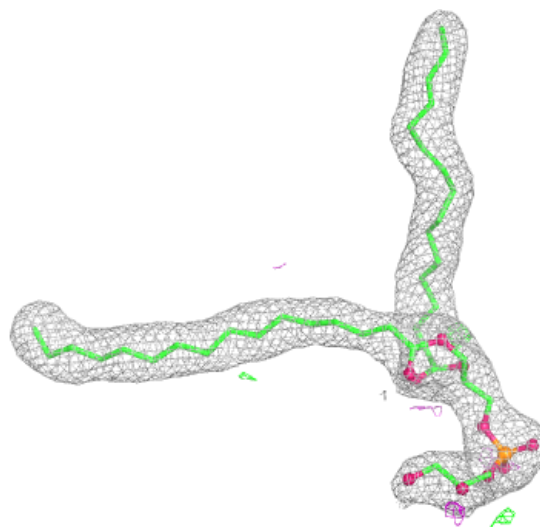
Electron density around CLA b 619:

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



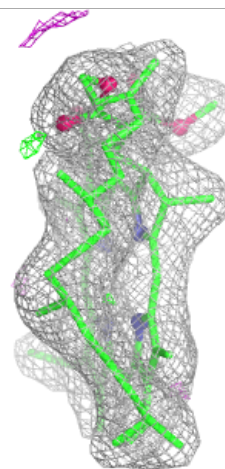
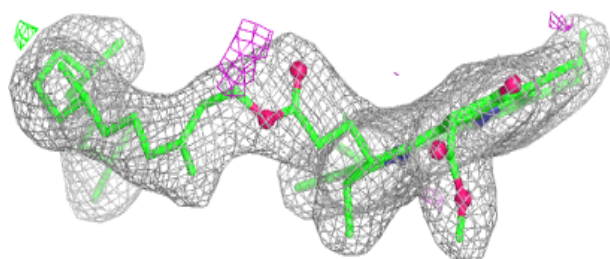
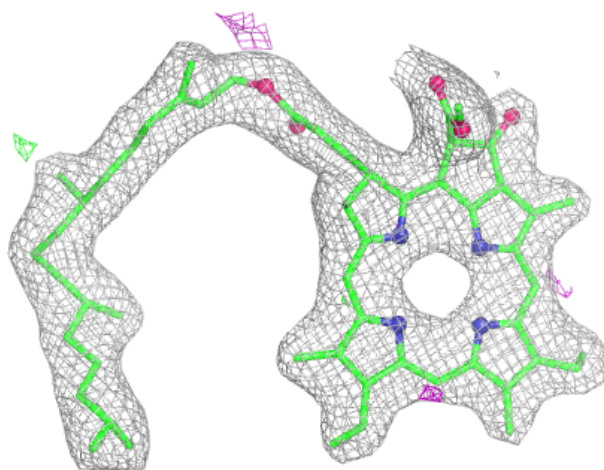
Electron density around LHG L 101:

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



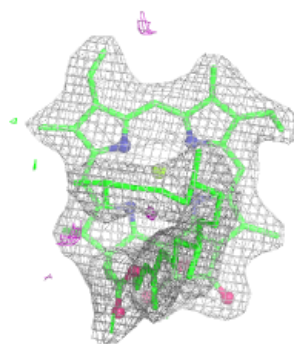
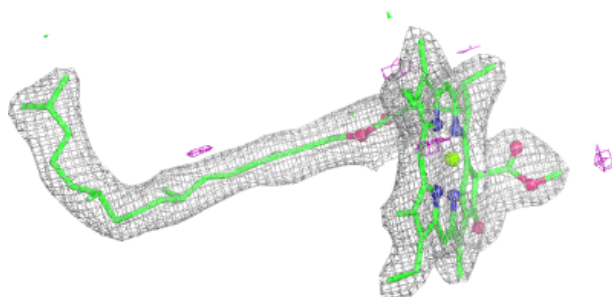
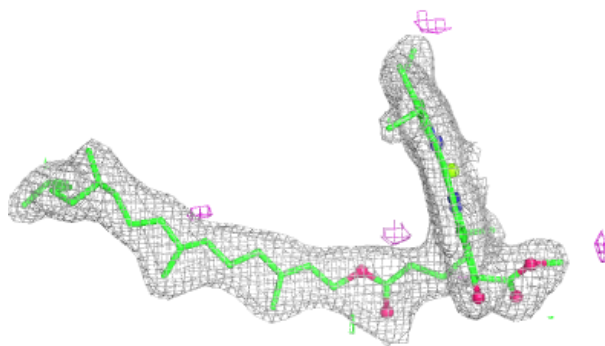
Electron density around PHO a 411:

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

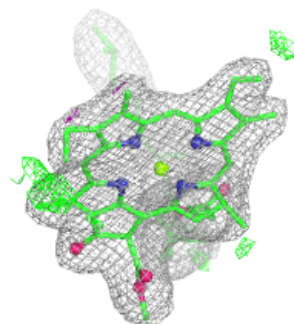
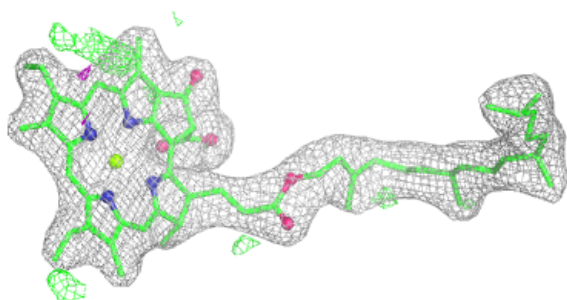
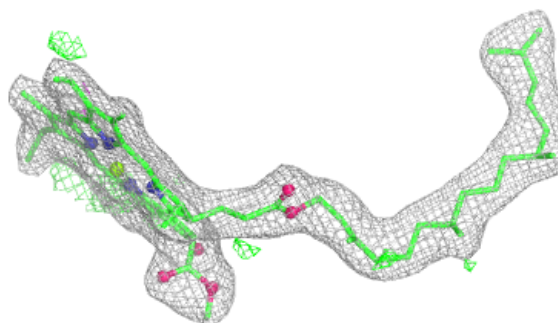


Electron density around CLA B 606:

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

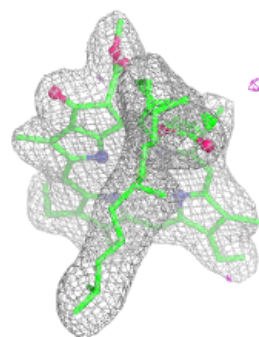
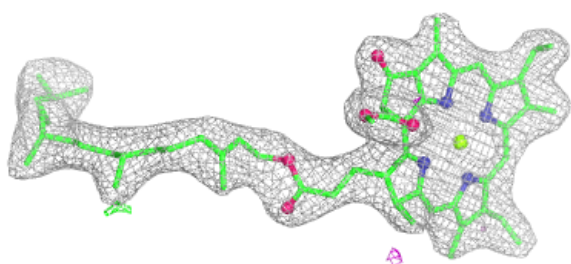
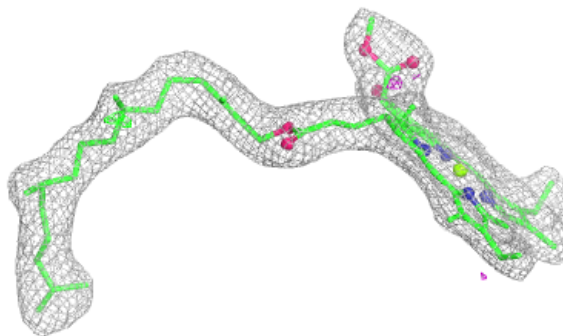
**Electron density around CLA D 404:**

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

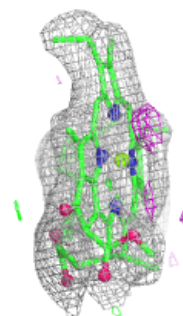
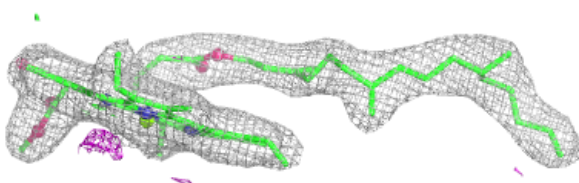
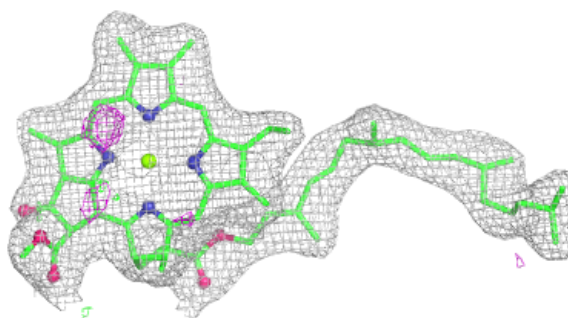


Electron density around CLA d 404:

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

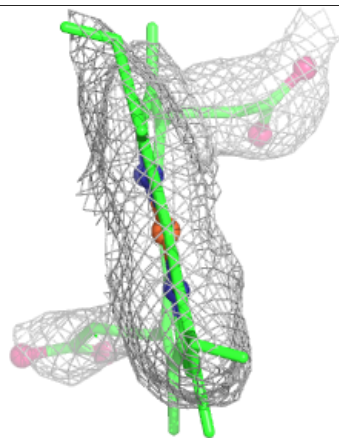
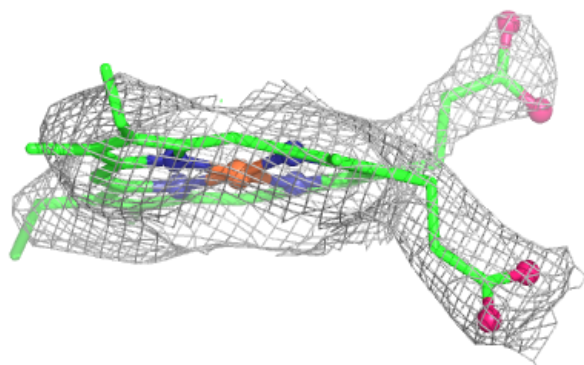
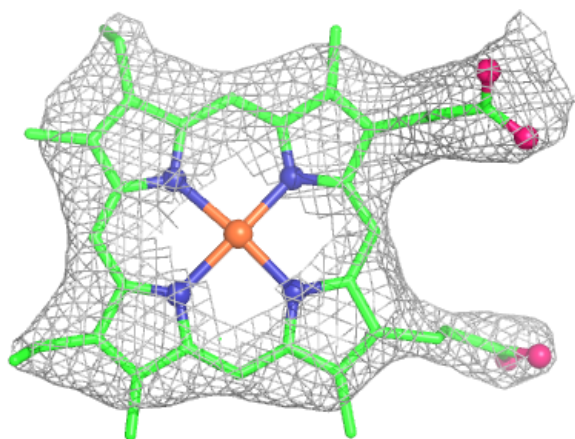
**Electron density around CLA B 604:**

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



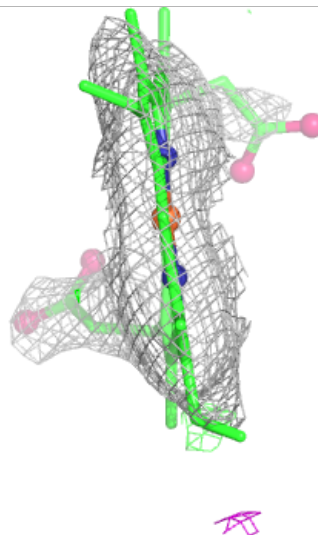
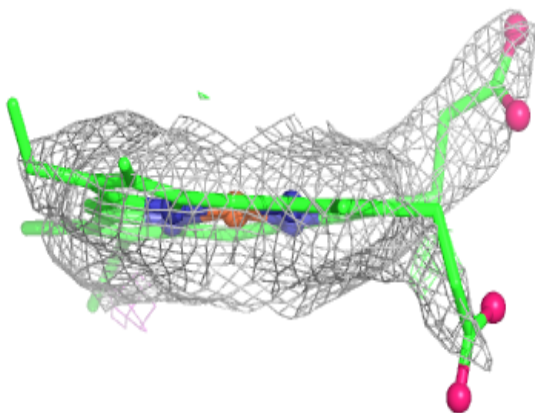
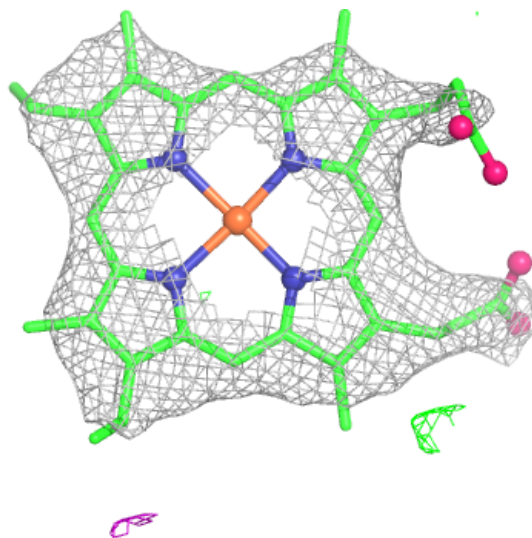
Electron density around HEM E 103:

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



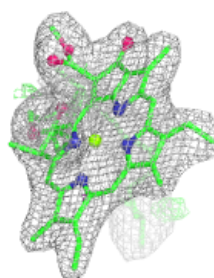
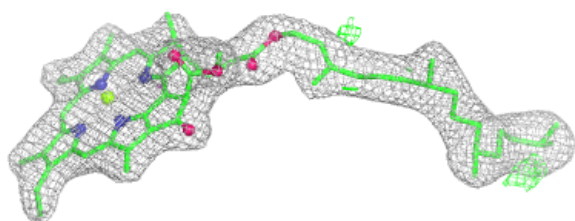
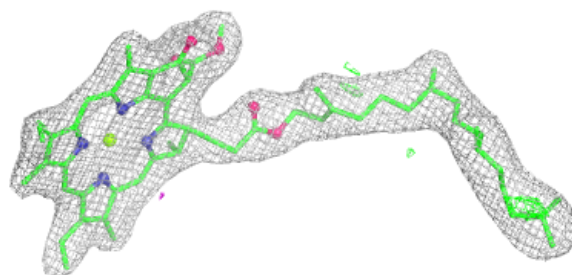
Electron density around HEM f 101:

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



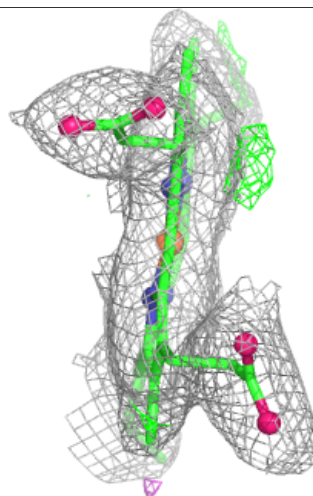
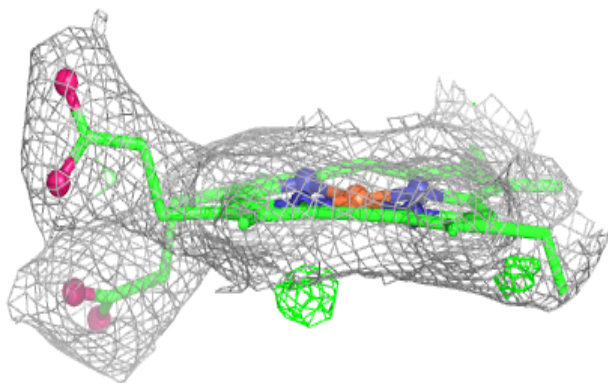
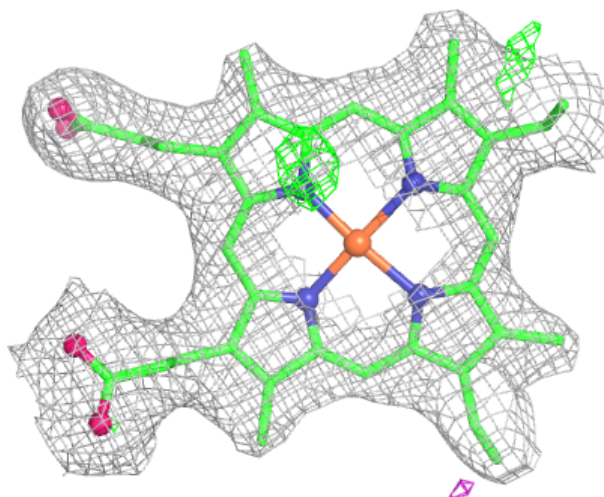
Electron density around CLA a 409:

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



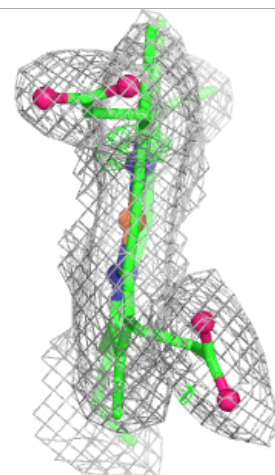
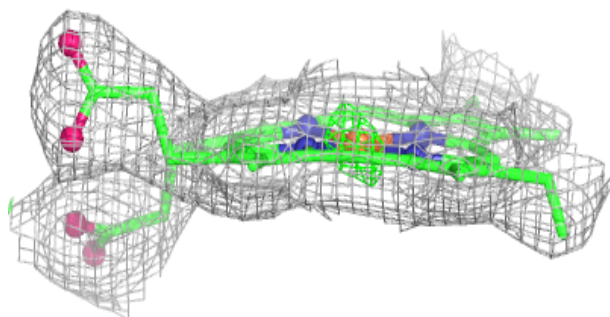
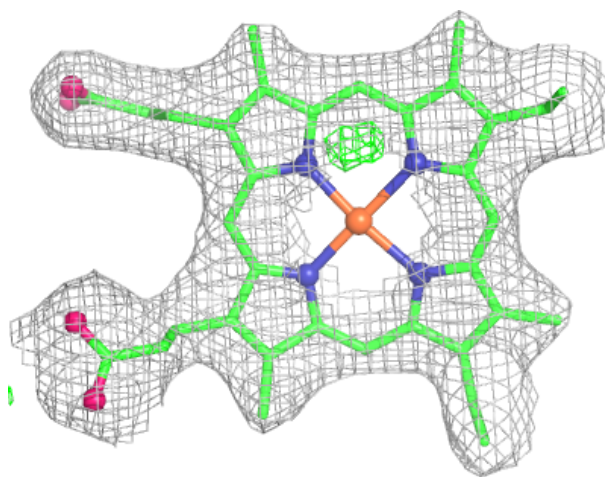
Electron density around HEC V 205:

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



Electron density around 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.