



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 02:39 PM JST

PDB ID : 6JLM / pdb_00006jlm
Title : XFEL structure of cyanobacterial photosystem II (dark state, dataset2)
Authors : Suga, M.; Shen, J.R.
Deposited on : 2019-03-06
Resolution : 2.35 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

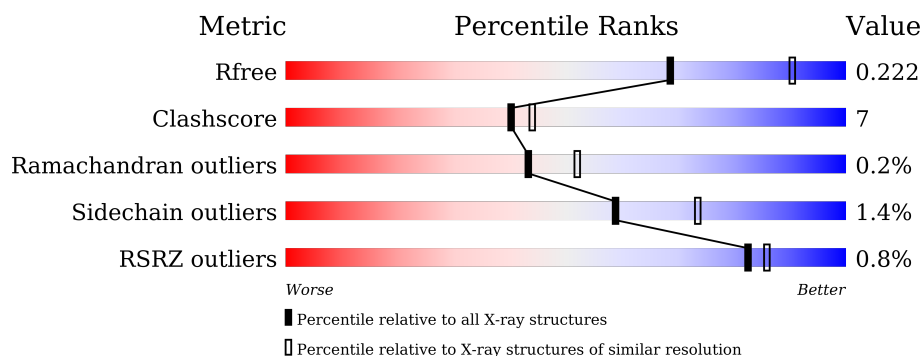
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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% 12% .
1	a	344	86% 11% .
2	B	505	86% 13%
2	b	505	% 88% 12%
3	C	455	89% 10% ..
3	c	455	87% 12% .

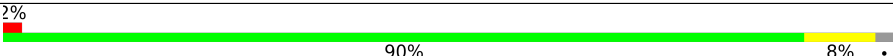
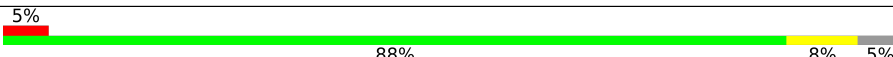
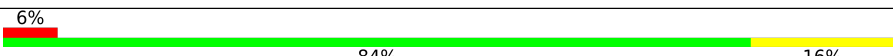
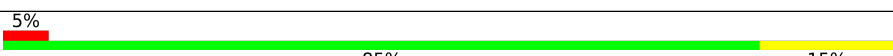
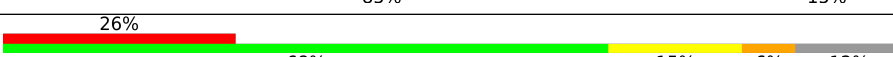
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Mol	Chain	Length	Quality of chain
4	D	342	
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	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	202	X	-	-	-
40	HEC	v	202	X	-	-	-

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 54101 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	3	0
			2634	1728	432	459	15			
1	a	334	Total	C	N	O	S	0	6	0
			2645	1737	432	461	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	See sequence details	UNP P51765
a	279	PRO	ARG	See sequence details	UNP P51765

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	10	0
			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	4	0
			3501	2291	584	613	13			
3	c	455	Total	C	N	O	S	0	6	0
			3544	2323	589	619	13			

There are 8 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	See sequence details	UNP D0VWR7
C	22	PHE	-	See sequence details	UNP D0VWR7
c	19	ASN	-	See sequence details	UNP D0VWR7
c	20	SER	-	See sequence details	UNP D0VWR7
c	21	ILE	-	See sequence details	UNP D0VWR7
c	22	PHE	-	See sequence details	UNP D0VWR7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	1	0
			2720	1802	444	462	12			
4	d	341	Total	C	N	O	S	0	1	0
			2720	1802	444	462	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	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	1	0
			1072	680	180	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	30	Total	C	N	O		98	0	0
			239	163	41	35				

- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

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

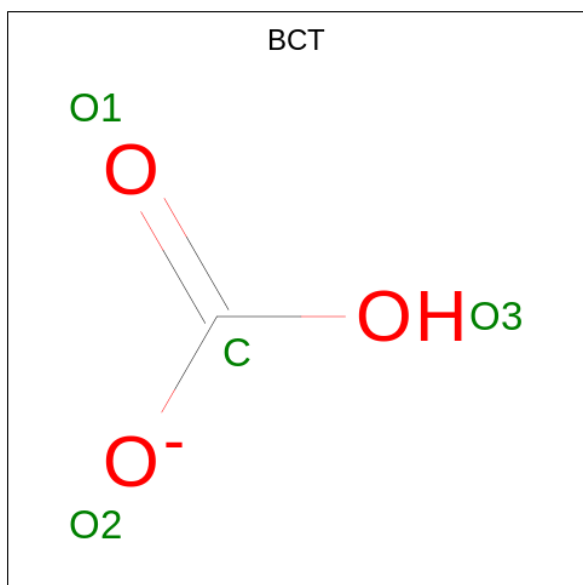
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		
22	U	1	Total	Cl	0	0
			1	1		

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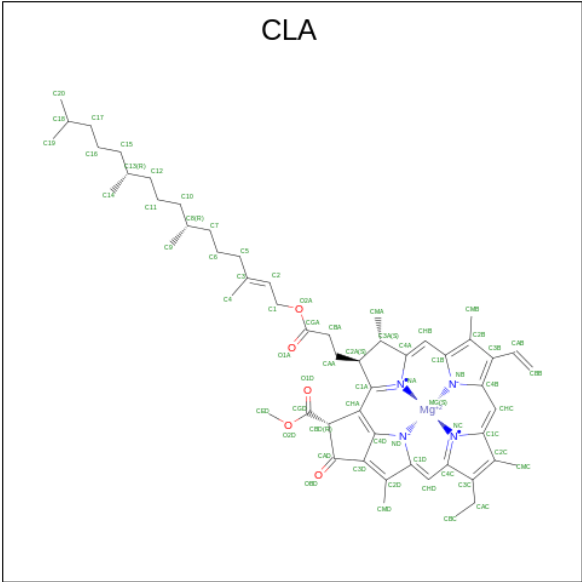
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	a	2	Total	Cl	0	0
			2	2		
22	v	1	Total	Cl	0	0
			1	1		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	0
			4	1	3		
23	d	1	Total	C	O	0	0
			4	1	3		

- 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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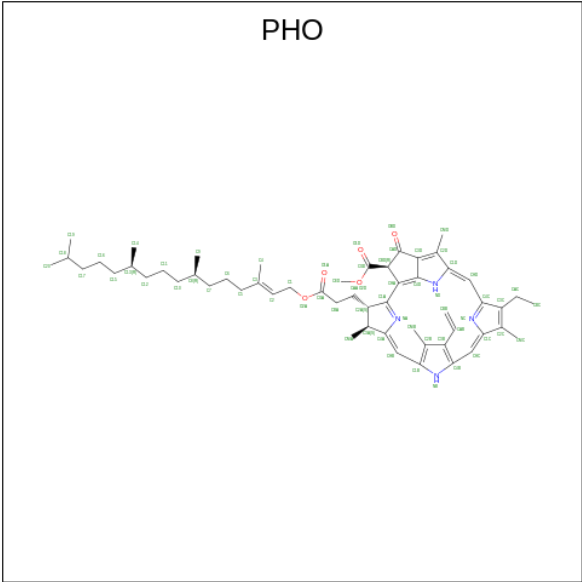
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 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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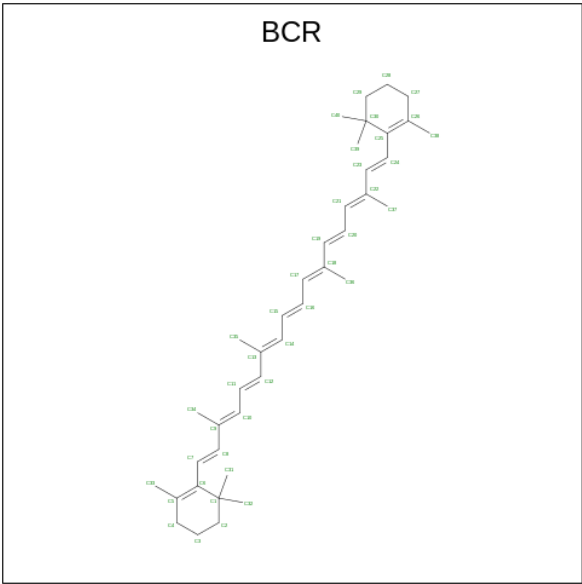
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 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	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: $C_{55}H_{74}N_4O_5$).



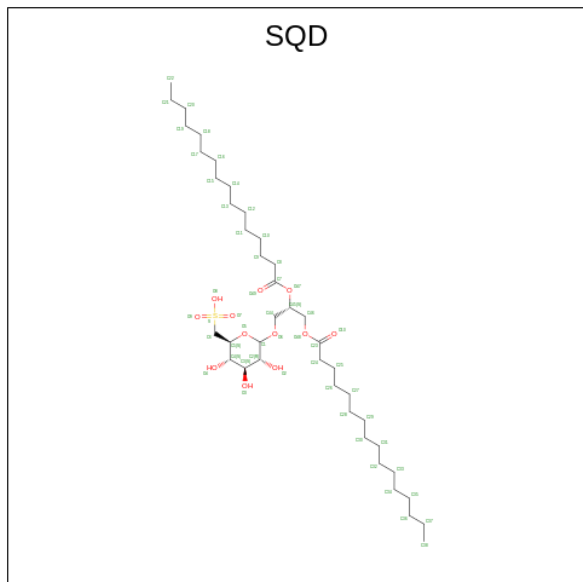
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	D	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



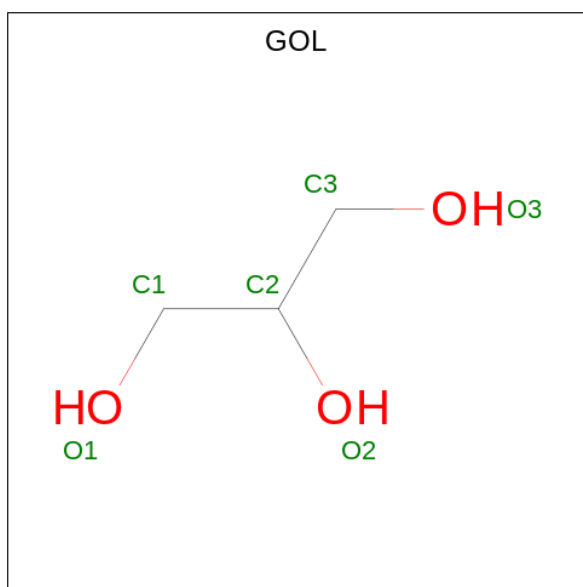
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Y	1	Total 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: $C_3H_8O_3$).



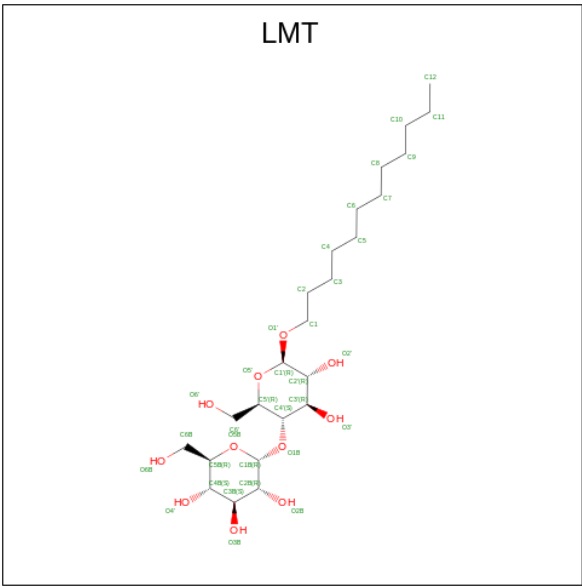
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			6	3	3		
28	A	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	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	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	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	c	1	Total	C	O	0	0
			6	3	3		
28	l	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).



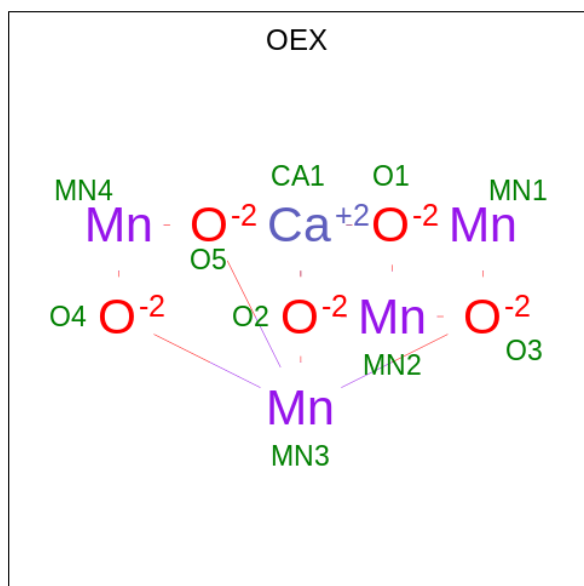
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			35	24	11		
29	C	1	Total	C	O	0	0
			35	24	11		
29	D	1	Total	C	O	0	0
			35	24	11		
29	F	1	Total	C	O	0	0
			35	24	11		
29	M	1	Total	C	O	0	0
			35	24	11		
29	M	1	Total	C	O	0	0
			35	24	11		
29	a	1	Total	C	O	0	0
			35	24	11		
29	a	1	Total	C	O	0	0
			35	24	11		
29	b	1	Total	C	O	0	0
			25	19	6		
29	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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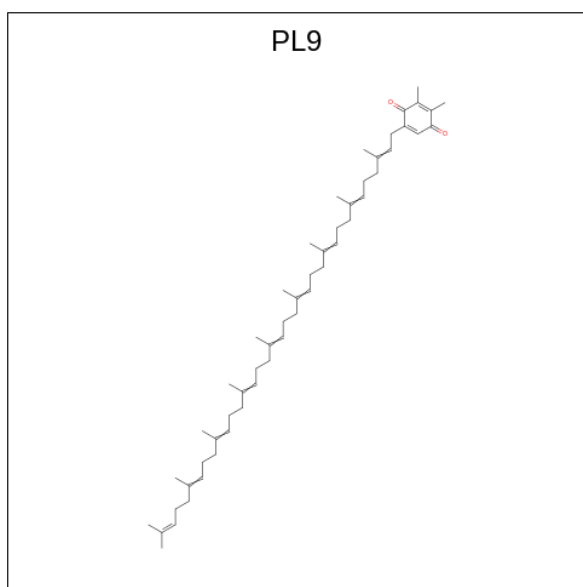
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	t	1	Total	C	O	0	0
			25	19	6		

- 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	0
			10	1	4	5		
30	a	1	Total	Ca	Mn	O	0	0
			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	0
			55	53	2		
31	D	1	Total	C	O	0	0
			55	53	2		
31	a	1	Total	C	O	0	0
			55	53	2		
31	d	1	Total	C	O	0	0
			55	53	2		

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

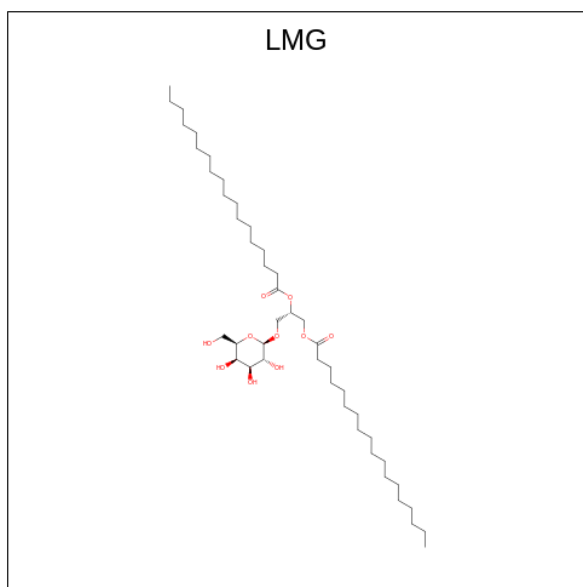
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			28	23	5		
32	B	1	Total	C	O	0	0
			33	28	5		
32	C	1	Total	C	O	0	0
			34	29	5		
32	D	2	Total	C	O	0	0
			57	51	6		
32	I	1	Total	C	O	0	0
			40	35	5		
32	J	1	Total	C		0	0
			10	10			
32	M	1	Total	C		0	0
			10	10			
32	X	1	Total	C	O	0	0
			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	2	Total	C	O	0	0
			53	47	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		

- 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	B	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		

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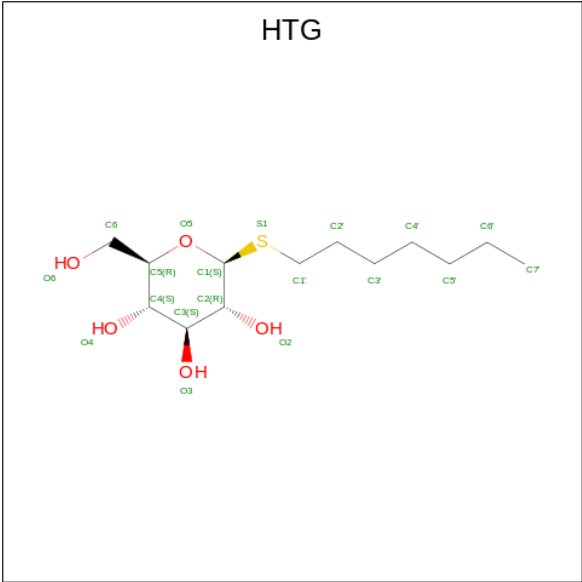
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	J	1	Total C O 51 41 10	0	0
33	Y	1	Total C O 51 41 10	0	0
33	Z	1	Total C O 37 27 10	0	0
33	a	1	Total C O 51 41 10	0	0
33	b	1	Total C O 51 41 10	0	0
33	c	1	Total C O 51 41 10	0	0
33	c	1	Total C O 51 41 10	0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

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

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

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



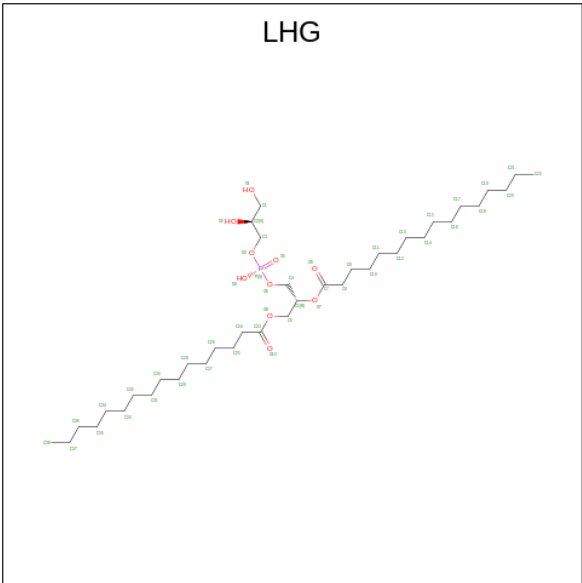
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	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 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



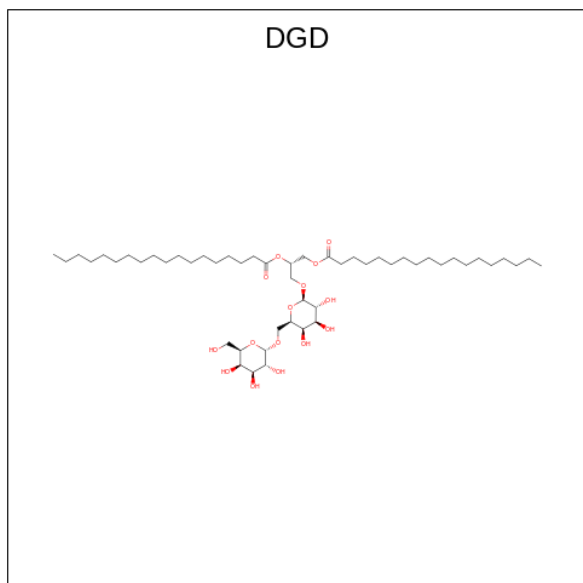
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	B	1	Total	C	O	P	0	0
			49	38	10	1		
36	D	1	Total	C	O	P	0	0
			49	38	10	1		
36	D	1	Total	C	O	P	0	0
			49	38	10	1		
36	E	1	Total	C	O	P	0	0
			42	31	10	1		
36	L	1	Total	C	O	P	0	0
			49	38	10	1		
36	a	1	Total	C	O	P	0	0
			42	31	10	1		
36	b	1	Total	C	O	P	0	0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

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

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



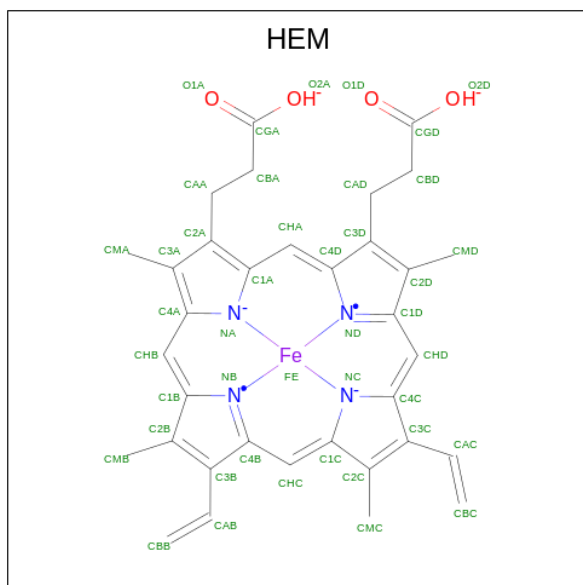
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	C	1	Total	C	O	0	0
			62	47	15		
37	C	1	Total	C	O	0	0
			62	47	15		
37	C	1	Total	C	O	0	0
			62	47	15		
37	D	1	Total	C	O	0	0
			52	42	10		
37	H	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total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

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

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

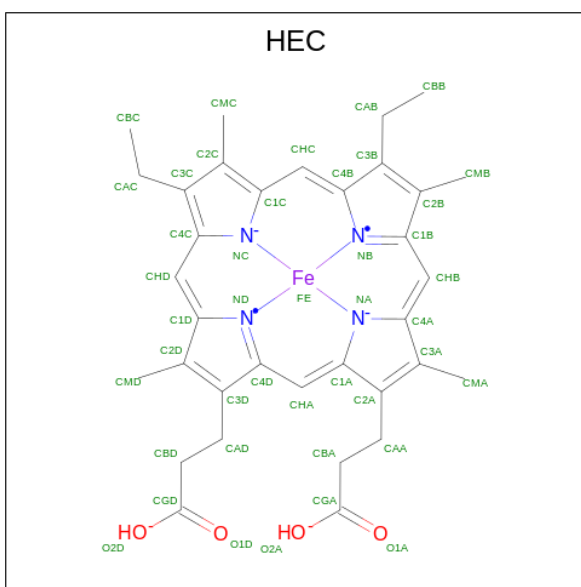


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
38	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
38	f	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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

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

- Molecule 40 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$).



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	164	Total O 167 167	0	3
41	B	295	Total O 299 299	0	4
41	C	232	Total O 234 234	0	2
41	D	140	Total O 144 144	0	4
41	E	30	Total O 31 31	0	1
41	F	10	Total O 10 10	0	0
41	H	48	Total O 48 48	0	0
41	I	6	Total O 6 6	0	0
41	J	12	Total O 12 12	0	0
41	K	7	Total O 7 7	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	L	14	Total 15	O 15	0	1
41	M	13	Total 13	O 13	0	0
41	O	179	Total 181	O 181	0	2
41	T	16	Total 17	O 17	0	1
41	U	80	Total 80	O 80	0	0
41	V	114	Total 116	O 116	0	2
41	Y	4	Total 4	O 4	0	0
41	X	9	Total 9	O 9	0	0
41	Z	1	Total 1	O 1	0	0
41	a	158	Total 159	O 159	0	1
41	b	262	Total 265	O 265	0	3
41	c	207	Total 210	O 210	0	3
41	d	129	Total 132	O 132	0	3
41	e	19	Total 19	O 19	0	0
41	f	6	Total 6	O 6	0	0
41	h	40	Total 40	O 40	0	0
41	i	4	Total 4	O 4	0	0
41	j	6	Total 6	O 6	0	0
41	k	7	Total 7	O 7	0	0
41	l	10	Total 10	O 10	0	0
41	m	15	Total 15	O 15	0	0

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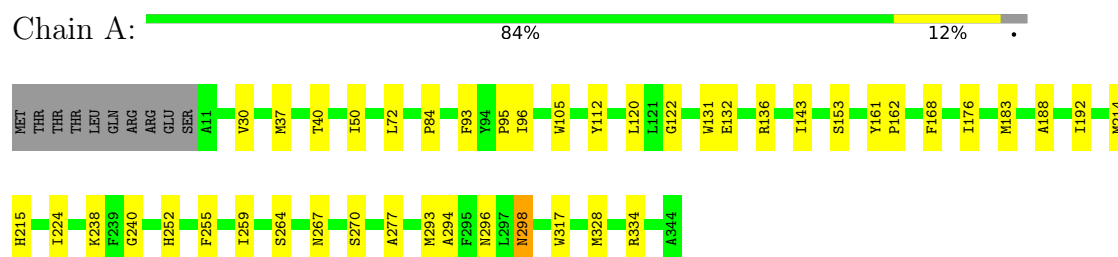
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	o	155	Total 155	O 155	0	0
41	t	11	Total 11	O 11	0	0
41	u	97	Total 97	O 97	0	0
41	v	77	Total 78	O 78	0	1
41	y	2	Total 2	O 2	0	0
41	x	6	Total 6	O 6	0	0

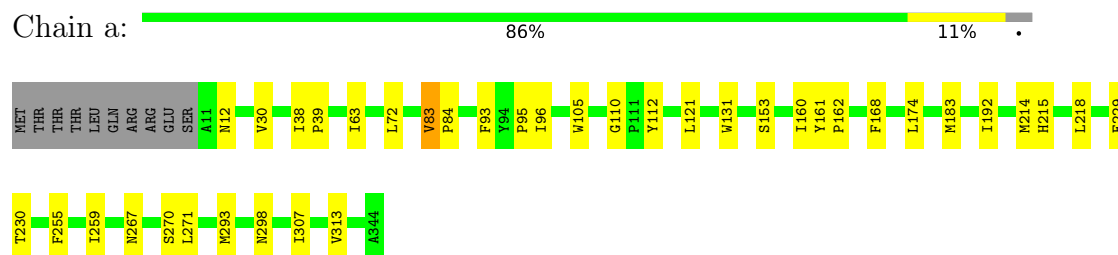
3 Residue-property plots

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

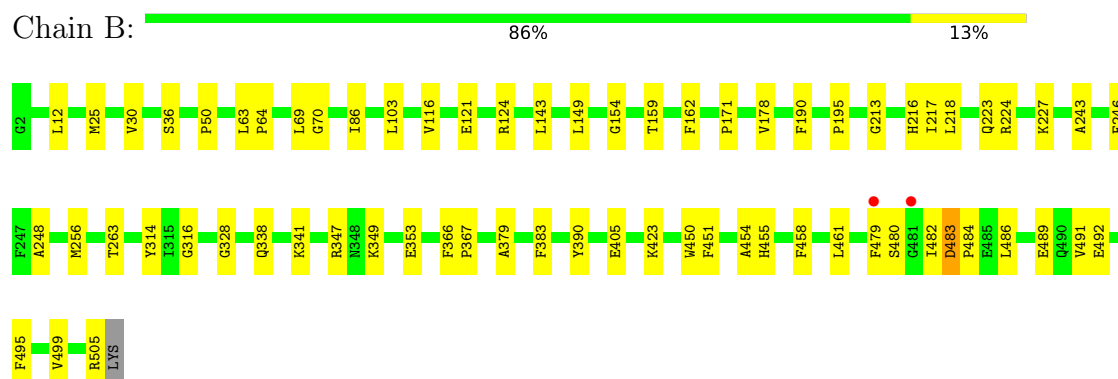
- Molecule 1: Photosystem II protein D1



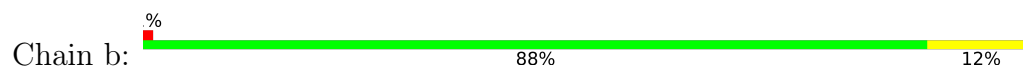
- Molecule 1: Photosystem II protein D1

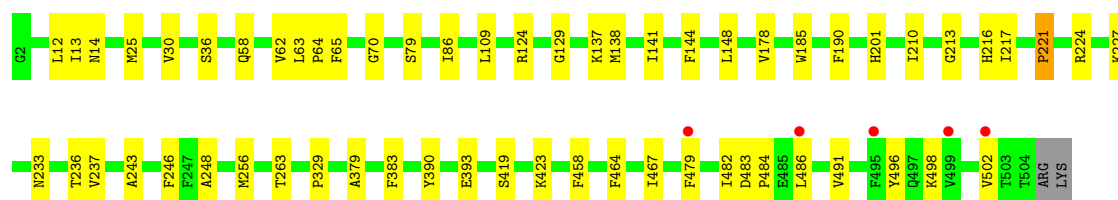


- Molecule 2: Photosystem II CP47 reaction center protein



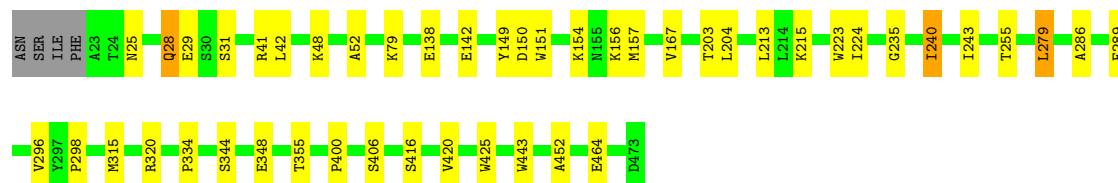
- Molecule 2: Photosystem II CP47 reaction center protein





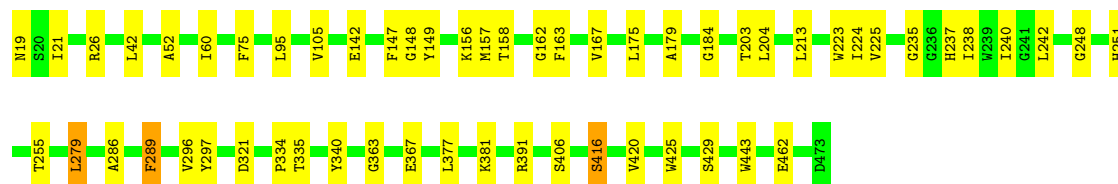
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 89% 10% ..



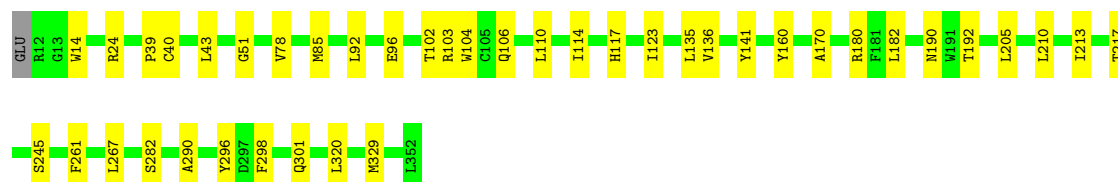
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 87% 12% .



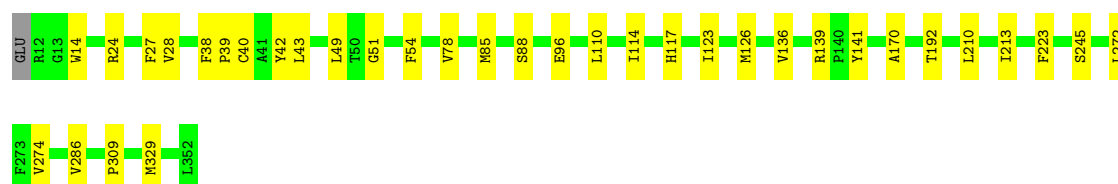
• Molecule 4: Photosystem II D2 protein

Chain D: 88% 12%

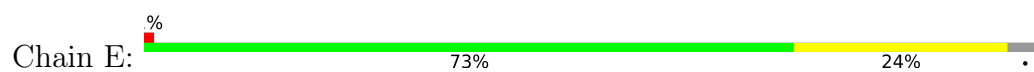


• Molecule 4: Photosystem II D2 protein

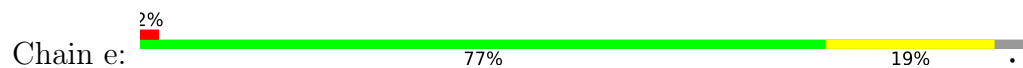
Chain d: 89% 10%



• Molecule 5: Cytochrome b559 subunit alpha



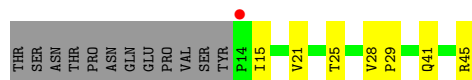
- Molecule 5: Cytochrome b559 subunit alpha



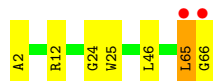
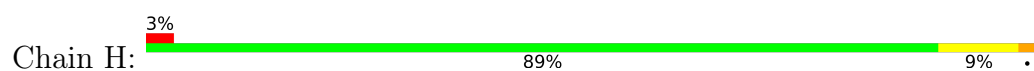
- Molecule 6: Cytochrome b559 subunit beta



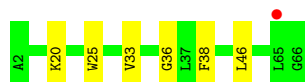
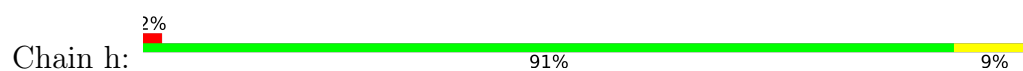
- Molecule 6: Cytochrome b559 subunit beta



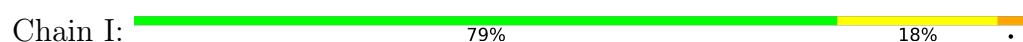
- Molecule 7: Photosystem II reaction center protein H



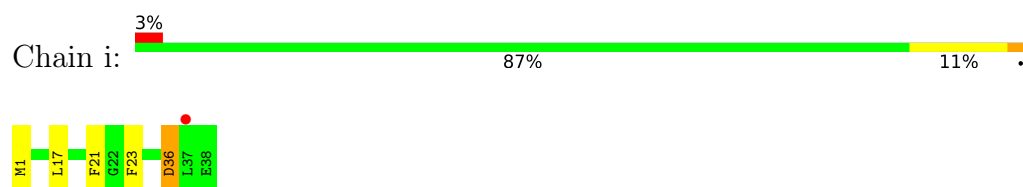
- Molecule 7: Photosystem II reaction center protein H



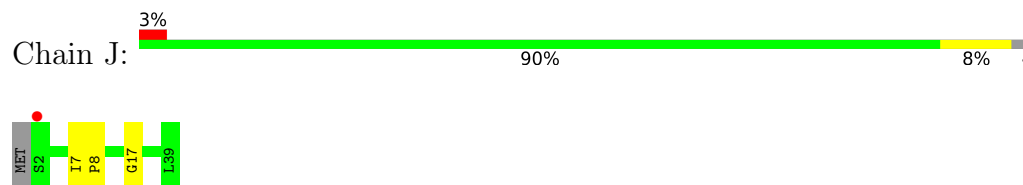
- Molecule 8: Photosystem II reaction center protein I



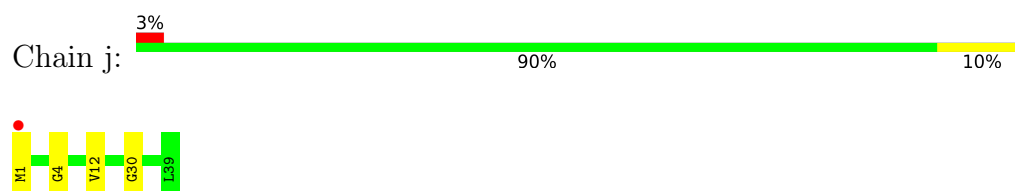
- Molecule 8: Photosystem II reaction center protein I



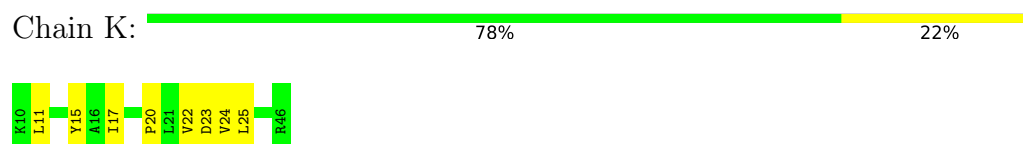
- Molecule 9: Photosystem II reaction center protein J



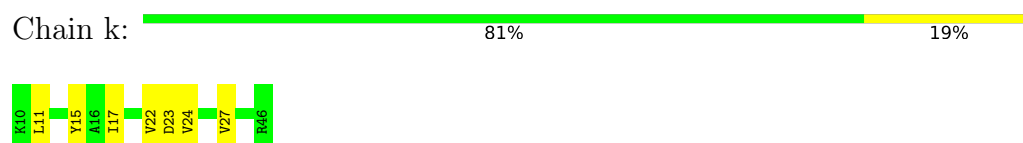
- Molecule 9: Photosystem II reaction center protein J



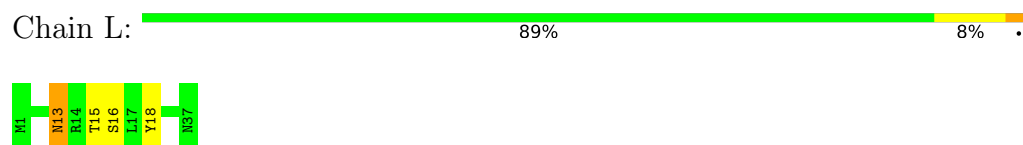
- Molecule 10: Photosystem II reaction center protein K



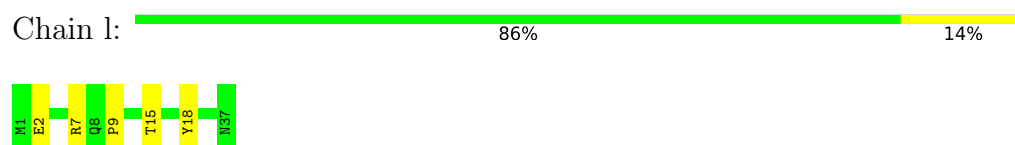
- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



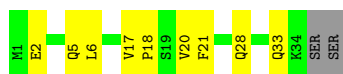
- Molecule 12: Photosystem II reaction center protein M

Chain M:  64% 25% 6% 6%



- Molecule 12: Photosystem II reaction center protein M

Chain m:  69% 25% 6%



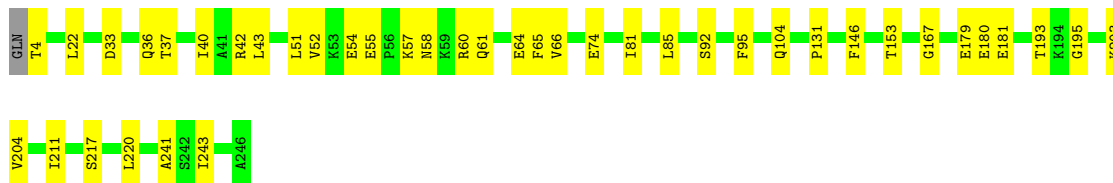
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  86% 13%



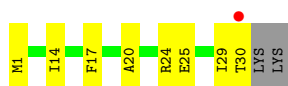
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  83% 17%



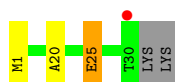
- Molecule 14: Photosystem II reaction center protein T

Chain T:  3% 69% 25% 6%



- Molecule 14: Photosystem II reaction center protein T

Chain t:  3% 84% 6% 6%

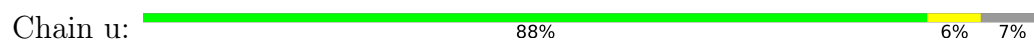


- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  81% 12% 7%



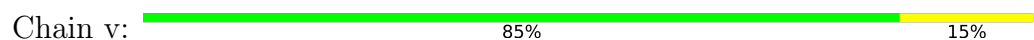
- Molecule 15: Photosystem II 12 kDa extrinsic protein



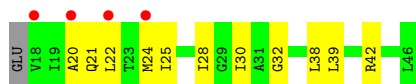
- Molecule 16: Cytochrome c-550



- Molecule 16: Cytochrome c-550



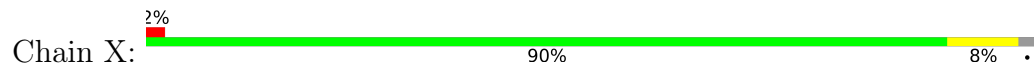
- Molecule 17: Photosystem II reaction center protein Ycf12



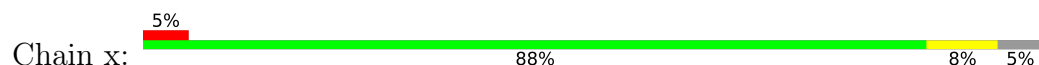
- Molecule 17: Photosystem II reaction center protein Ycf12

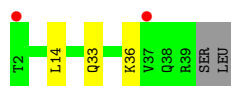


- Molecule 18: Photosystem II reaction center protein X

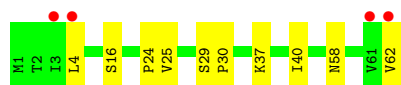
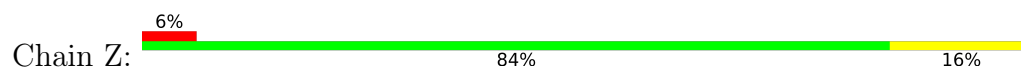


- Molecule 18: Photosystem II reaction center protein X

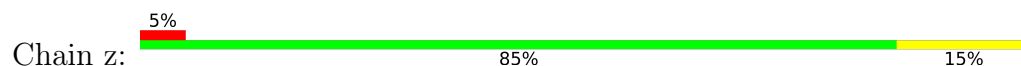




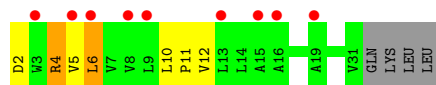
- Molecule 19: Photosystem II reaction center protein Z



- 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 – 2.35 19.99 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.35) 99.8 (19.99-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.153 , 0.209 0.172 , 0.222	Depositor DCC
R_{free} test set	17809 reflections (3.30%)	wwPDB-VP
Wilson B-factor (Å ²)	47.2	Xtriage
Anisotropy	0.577	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 95.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	54101	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.59	0/2728	0.87	1/3719 (0.0%)
1	a	0.59	0/2748	0.88	2/3746 (0.1%)
2	B	0.54	0/4191	0.84	4/5709 (0.1%)
2	b	0.54	0/4198	0.83	2/5720 (0.0%)
3	C	0.50	0/3626	0.82	0/4936
3	c	0.49	0/3676	0.81	0/5004
4	D	0.58	0/2818	0.84	2/3840 (0.1%)
4	d	0.57	1/2818 (0.0%)	0.84	4/3840 (0.1%)
5	E	0.51	0/693	0.81	0/944
5	e	0.47	0/695	0.87	0/948
6	F	0.59	0/284	0.83	0/387
6	f	0.55	0/265	0.80	0/360
7	H	0.47	0/535	0.87	0/728
7	h	0.47	0/524	0.79	0/713
8	I	0.47	0/311	0.76	0/419
8	i	0.52	0/311	0.76	0/419
9	J	0.47	0/278	0.77	0/376
9	j	0.44	0/286	0.77	0/386
10	K	0.48	0/303	0.85	0/416
10	k	0.55	0/303	0.83	0/416
11	L	0.53	0/319	0.77	0/433
11	l	0.53	0/319	0.71	0/433
12	M	0.68	0/270	1.15	3/368 (0.8%)
12	m	0.65	0/262	1.02	2/357 (0.6%)
13	O	0.47	0/1958	0.80	2/2654 (0.1%)
13	o	0.47	0/1937	0.84	4/2625 (0.2%)
14	T	0.54	0/266	0.77	0/362
14	t	0.59	0/266	0.74	0/362
15	U	0.50	0/785	0.76	0/1064
15	u	0.48	0/785	0.77	0/1064
16	V	0.50	0/1096	0.83	0/1487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.49	0/1085	0.85	1/1473 (0.1%)
17	Y	0.51	0/216	0.89	0/289
17	y	0.46	0/216	0.78	0/289
18	X	0.45	0/290	0.79	0/392
18	x	0.45	0/284	0.73	0/384
19	Z	0.42	0/490	0.81	0/669
19	z	0.43	0/490	0.86	0/669
20	R	0.35	0/245	0.69	0/338
All	All	0.53	1/43170 (0.0%)	0.83	27/58738 (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	5.03	1.58	1.52

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	170	ALA	CA-C-N	-7.52	112.24	119.76
4	d	170	ALA	C-N-CA	-7.52	112.24	119.76
4	D	170	ALA	CA-C-N	-6.39	113.37	119.76
4	D	170	ALA	C-N-CA	-6.39	113.37	119.76
16	v	105	ARG	N-CA-C	6.12	118.46	111.11

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	2634	0	2546	33	0
1	a	2645	0	2567	27	0
2	B	4021	0	3898	56	0
2	b	4022	0	3908	49	0
3	C	3501	0	3428	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	c	3544	0	3479	33	0
4	D	2720	0	2626	29	0
4	d	2720	0	2626	27	0
5	E	668	0	658	13	0
5	e	670	0	664	13	0
6	F	275	0	282	5	0
6	f	257	0	269	5	0
7	H	519	0	545	10	0
7	h	511	0	532	8	0
8	I	314	0	328	5	0
8	i	314	0	328	2	0
9	J	272	0	279	3	0
9	j	280	0	291	3	0
10	K	293	0	305	7	0
10	k	293	0	305	6	0
11	L	309	0	327	3	0
11	l	309	0	327	5	0
12	M	274	0	299	8	0
12	m	269	0	288	7	0
13	O	1903	0	1886	18	0
13	o	1891	0	1870	24	0
14	T	264	0	267	6	0
14	t	264	0	267	2	0
15	U	774	0	773	6	1
15	u	774	0	773	4	0
16	V	1072	0	1086	6	0
16	v	1064	0	1073	11	0
17	Y	215	0	246	9	0
17	y	215	0	246	6	0
18	X	287	0	317	3	0
18	x	281	0	312	2	0
19	Z	479	0	516	8	0
19	z	479	0	516	10	0
20	R	239	0	262	5	0
21	A	1	0	0	0	0
21	d	1	0	0	0	0
22	A	2	0	0	0	0
22	U	1	0	0	1	0
22	a	2	0	0	0	0
22	v	1	0	0	0	0
23	A	4	0	0	0	0
23	d	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	A	260	0	288	12	0
24	B	1040	0	1152	42	0
24	C	845	0	936	38	0
24	D	130	0	144	5	0
24	a	195	0	216	7	0
24	b	1040	0	1152	42	0
24	c	845	0	936	44	0
24	d	195	0	216	11	0
25	A	64	0	74	2	0
25	D	64	0	74	3	0
25	a	64	0	74	3	0
25	d	64	0	74	3	0
26	A	40	0	56	1	0
26	B	120	0	168	10	0
26	C	80	0	112	9	0
26	D	40	0	56	1	0
26	H	40	0	56	4	0
26	K	40	0	56	2	0
26	T	40	0	56	4	0
26	Y	40	0	56	6	0
26	a	40	0	56	0	0
26	b	120	0	168	5	0
26	c	80	0	112	8	0
26	d	40	0	56	4	0
26	h	40	0	56	5	0
26	k	40	0	56	1	0
26	t	40	0	56	5	0
26	y	40	0	56	1	0
27	A	108	0	156	7	0
27	B	54	0	78	3	0
27	F	43	0	53	3	0
27	L	54	0	78	4	0
27	a	108	0	156	5	0
27	f	43	0	53	2	1
28	A	12	0	16	0	0
28	B	42	0	56	1	0
28	C	12	0	16	1	0
28	D	6	0	8	1	0
28	O	6	0	8	0	0
28	T	12	0	16	4	0
28	V	30	0	39	1	0
28	a	18	0	23	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	b	30	0	40	2	0
28	c	18	0	24	0	0
28	l	6	0	8	1	0
28	v	18	0	24	1	0
29	A	35	0	46	3	0
29	C	35	0	46	1	0
29	D	35	0	46	1	0
29	F	35	0	46	0	0
29	M	70	0	92	4	0
29	a	70	0	92	2	0
29	b	50	0	70	2	0
29	e	35	0	46	1	0
29	m	70	0	92	5	0
29	t	25	0	35	0	0
30	A	10	0	0	0	0
30	a	10	0	0	0	0
31	A	55	0	80	7	0
31	D	55	0	80	0	0
31	a	55	0	80	11	0
31	d	55	0	80	1	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	53	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
33	A	51	0	72	6	0
33	B	51	0	72	3	0
33	C	51	0	72	2	0
33	J	51	0	72	0	0
33	Y	51	0	72	2	0
33	Z	37	0	44	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	a	51	0	72	2	0
33	b	51	0	72	4	0
33	c	102	0	144	6	0
33	d	51	0	72	3	0
33	z	39	0	48	5	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	0	0
35	C	38	0	52	0	0
35	D	16	0	17	3	0
35	V	19	0	26	2	0
35	b	95	0	130	3	0
35	c	38	0	52	1	0
35	d	16	0	17	2	0
36	B	49	0	74	3	0
36	D	98	0	148	8	0
36	E	42	0	57	1	0
36	L	49	0	74	0	0
36	a	42	0	57	6	0
36	b	49	0	74	5	0
36	d	147	0	222	10	0
37	C	186	0	246	7	0
37	D	52	0	71	4	0
37	H	62	0	82	1	0
37	c	186	0	246	9	0
37	e	62	0	82	5	0
37	h	62	0	82	2	0
38	F	43	0	30	3	0
38	f	43	0	30	0	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	V	43	0	30	0	0
40	v	43	0	30	0	0
41	A	167	0	0	3	0
41	B	299	0	0	3	0
41	C	234	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	D	144	0	0	1	0
41	E	31	0	0	1	0
41	F	10	0	0	0	0
41	H	48	0	0	0	0
41	I	6	0	0	1	0
41	J	12	0	0	0	0
41	K	7	0	0	1	0
41	L	15	0	0	0	0
41	M	13	0	0	1	0
41	O	181	0	0	4	0
41	T	17	0	0	1	0
41	U	80	0	0	1	0
41	V	116	0	0	1	0
41	X	9	0	0	0	0
41	Y	4	0	0	0	0
41	Z	1	0	0	0	0
41	a	159	0	0	1	0
41	b	265	0	0	1	0
41	c	210	0	0	0	0
41	d	132	0	0	3	0
41	e	19	0	0	0	0
41	f	6	0	0	1	0
41	h	40	0	0	1	0
41	i	4	0	0	0	0
41	j	6	0	0	0	0
41	k	7	0	0	0	0
41	l	10	0	0	1	0
41	m	15	0	0	2	0
41	o	155	0	0	4	0
41	t	11	0	0	0	0
41	u	97	0	0	1	0
41	v	78	0	0	1	0
41	x	6	0	0	0	0
41	y	2	0	0	0	0
All	All	54101	0	52737	685	1

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 685 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:MET:HG2	31:A:417:PL9:H102	1.42	0.99
24:B:616:CLA:H71	24:B:617:CLA:H192	1.51	0.90
24:c:904:CLA:HBB1	24:c:913:CLA:H41	1.58	0.84
24:c:914:CLA:HHC	24:c:914:CLA:HBB1	1.65	0.78
33:a:411:LMG:H221	37:c:916:DGD:HA81	1.66	0.77

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:69:GLU:OE1	27:f:102:SQD:O3[2_554]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/344 (97%)	328 (98%)	5 (2%)	2 (1%)	21	24
1	a	338/344 (98%)	331 (98%)	5 (2%)	2 (1%)	21	24
2	B	512/505 (101%)	506 (99%)	6 (1%)	0	100	100
2	b	513/505 (102%)	504 (98%)	9 (2%)	0	100	100
3	C	453/455 (100%)	442 (98%)	9 (2%)	2 (0%)	30	34
3	c	459/455 (101%)	448 (98%)	9 (2%)	2 (0%)	30	34
4	D	340/342 (99%)	331 (97%)	9 (3%)	0	100	100
4	d	340/342 (99%)	331 (97%)	9 (3%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
6	F	32/44 (73%)	31 (97%)	1 (3%)	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	64/65 (98%)	58 (91%)	6 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	h	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
8	I	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	4	2
8	i	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	33 (89%)	4 (11%)	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%)	32 (97%)	1 (3%)	0	100	100
12	m	32/36 (89%)	32 (100%)	0	0	100	100
13	O	249/244 (102%)	242 (97%)	6 (2%)	1 (0%)	30	34
13	o	246/244 (101%)	240 (98%)	6 (2%)	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%)	132 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	129 (96%)	6 (4%)	0	100	100
17	Y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
17	y	27/30 (90%)	24 (89%)	3 (11%)	0	100	100
18	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
18	x	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
20	R	28/34 (82%)	27 (96%)	1 (4%)	0	100	100
All	All	5282/5384 (98%)	5151 (98%)	121 (2%)	10 (0%)	43	52

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER

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Mol	Chain	Res	Type
3	c	416[A]	SER
3	c	416[B]	SER
8	I	34	ARG

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	272/279 (98%)	272 (100%)	0	100	100
1	a	275/279 (99%)	274 (100%)	1 (0%)	84	91
2	B	412/403 (102%)	408 (99%)	4 (1%)	68	81
2	b	413/403 (102%)	412 (100%)	1 (0%)	87	94
3	C	356/356 (100%)	347 (98%)	9 (2%)	42	55
3	c	362/356 (102%)	350 (97%)	12 (3%)	33	44
4	D	277/277 (100%)	276 (100%)	1 (0%)	84	91
4	d	277/277 (100%)	276 (100%)	1 (0%)	84	91
5	E	74/73 (101%)	72 (97%)	2 (3%)	39	52
5	e	74/73 (101%)	74 (100%)	0	100	100
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	26/38 (68%)	25 (96%)	1 (4%)	29	39
7	H	55/54 (102%)	54 (98%)	1 (2%)	51	66
7	h	54/54 (100%)	54 (100%)	0	100	100
8	I	34/34 (100%)	34 (100%)	0	100	100
8	i	34/34 (100%)	32 (94%)	2 (6%)	18	22
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	27/27 (100%)	26 (96%)	1 (4%)	30	40
10	K	30/30 (100%)	29 (97%)	1 (3%)	33	44
10	k	30/30 (100%)	29 (97%)	1 (3%)	33	44
11	L	36/35 (103%)	34 (94%)	2 (6%)	19	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	l	36/35 (103%)	35 (97%)	1 (3%)	38	51
12	M	31/32 (97%)	30 (97%)	1 (3%)	34	46
12	m	30/32 (94%)	29 (97%)	1 (3%)	33	44
13	O	214/207 (103%)	211 (99%)	3 (1%)	59	73
13	o	211/207 (102%)	207 (98%)	4 (2%)	50	65
14	T	27/28 (96%)	27 (100%)	0	100	100
14	t	27/28 (96%)	25 (93%)	2 (7%)	13	14
15	U	84/89 (94%)	82 (98%)	2 (2%)	43	57
15	u	84/89 (94%)	84 (100%)	0	100	100
16	V	118/117 (101%)	116 (98%)	2 (2%)	53	68
16	v	117/117 (100%)	115 (98%)	2 (2%)	53	68
17	Y	22/23 (96%)	20 (91%)	2 (9%)	9	9
17	y	22/23 (96%)	20 (91%)	2 (9%)	9	9
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%)	51 (98%)	1 (2%)	50	65
19	z	52/52 (100%)	51 (98%)	1 (2%)	50	65
20	R	25/29 (86%)	23 (92%)	2 (8%)	11	12
All	All	4387/4403 (100%)	4321 (98%)	66 (2%)	59	72

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	o	217[A]	SER
14	t	25[A]	GLU
19	z	34	ASP
15	U	59	GLU
13	O	69	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
13	o	124	ASN
19	z	58	ASN
13	o	130	GLN

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Mol	Chain	Res	Type
15	u	81	HIS
19	Z	58	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	FME	t	1	14	8,9,10	0.80	0	7,9,11	2.51	5 (71%)
12	FME	M	1	12	8,9,10	0.64	0	7,9,11	1.16	1 (14%)
8	FME	I	1	8	8,9,10	0.75	0	7,9,11	1.26	1 (14%)
14	FME	T	1	14	8,9,10	0.69	0	7,9,11	1.44	1 (14%)
12	FME	m	1	12	8,9,10	0.67	0	7,9,11	1.08	0
8	FME	i	1	8	8,9,10	0.66	0	7,9,11	1.23	1 (14%)

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	-	3/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
14	FME	T	1	14	-	3/7/9/11	-
12	FME	m	1	12	-	2/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	CA-N-CN	-4.15	116.44	122.82
14	t	1	FME	C-CA-N	3.05	115.23	109.73
14	T	1	FME	O-C-CA	-2.50	118.21	124.78
14	t	1	FME	O-C-CA	-2.47	118.31	124.78
14	t	1	FME	CE-SD-CG	-2.19	92.88	100.40

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 251 ligands modelled in this entry, 19 are monoatomic and 18 are unknown - leaving 214 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
26	BCR	c	927	-	41,41,41	1.02	1 (2%)	56,56,56	1.59	11 (19%)
28	GOL	T	101	-	5,5,5	0.38	0	5,5,5	0.22	0
35	HTG	b	601	-	19,19,19	1.03	1 (5%)	23,24,24	1.28	1 (4%)
29	LMT	a	417	-	36,36,36	0.42	0	47,47,47	0.79	1 (2%)
24	CLA	B	614	2	69,73,73	2.08	19 (27%)	83,113,113	2.78	33 (39%)
29	LMT	M	103	-	36,36,36	0.59	1 (2%)	47,47,47	1.08	4 (8%)
35	HTG	c	921	-	19,19,19	1.00	2 (10%)	23,24,24	1.56	1 (4%)
28	GOL	v	204	-	5,5,5	0.36	0	5,5,5	0.34	0
28	GOL	b	632	-	5,5,5	0.38	0	5,5,5	0.33	0
24	CLA	b	619	2	69,73,73	2.04	20 (28%)	83,113,113	2.89	33 (39%)
24	CLA	C	505	3	69,73,73	1.98	20 (28%)	83,113,113	2.69	29 (34%)
24	CLA	B	612	2	69,73,73	1.97	20 (28%)	83,113,113	2.93	33 (39%)
36	LHG	L	101	-	48,48,48	0.95	3 (6%)	51,54,54	1.13	5 (9%)
24	CLA	b	618	2	69,73,73	2.03	20 (28%)	83,113,113	2.75	30 (36%)
24	CLA	c	905	41	69,73,73	2.03	19 (27%)	83,113,113	2.85	32 (38%)
28	GOL	a	412	-	5,5,5	0.39	0	5,5,5	0.53	0
28	GOL	a	413	-	5,5,5	0.41	0	5,5,5	0.26	0
28	GOL	T	103	-	5,5,5	0.40	0	5,5,5	0.30	0
28	GOL	B	636	-	5,5,5	0.41	0	5,5,5	0.47	0
26	BCR	B	619	-	41,41,41	1.03	1 (2%)	56,56,56	1.48	9 (16%)
27	SQD	B	621	-	53,54,54	1.03	3 (5%)	62,65,65	1.44	8 (12%)
24	CLA	C	511	3	69,73,73	2.07	20 (28%)	83,113,113	2.75	29 (34%)
24	CLA	c	914	3	69,73,73	2.06	20 (28%)	83,113,113	2.88	29 (34%)
28	GOL	V	201	34	5,5,5	0.34	0	5,5,5	0.26	0
35	HTG	B	623	-	19,19,19	1.20	1 (5%)	23,24,24	1.28	1 (4%)
24	CLA	a	406	41	69,73,73	2.03	19 (27%)	83,113,113	2.90	30 (36%)
33	LMG	a	411	-	51,51,55	0.91	2 (3%)	59,59,63	1.16	5 (8%)
37	DGD	C	517	-	63,63,67	0.88	3 (4%)	77,77,81	1.07	7 (9%)
36	LHG	B	635	-	48,48,48	0.91	2 (4%)	51,54,54	1.11	5 (9%)
28	GOL	V	206	-	5,5,5	0.43	0	5,5,5	0.32	0
24	CLA	c	907	3	69,73,73	2.00	20 (28%)	83,113,113	2.77	30 (36%)
24	CLA	c	906	3	69,73,73	2.01	19 (27%)	83,113,113	2.68	29 (34%)
28	GOL	D	402	-	5,5,5	0.43	0	5,5,5	0.35	0
23	BCT	d	402	21	2,3,3	0.67	0	2,3,3	0.71	0
24	CLA	C	510	3	69,73,73	2.09	20 (28%)	83,113,113	2.76	29 (34%)
35	HTG	C	521	-	19,19,19	1.02	2 (10%)	23,24,24	1.76	3 (13%)
24	CLA	b	615	41	69,73,73	2.06	21 (30%)	83,113,113	2.74	32 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	C	507	41	69,73,73	2.04	20 (28%)	83,113,113	2.78	29 (34%)
29	LMT	C	520	-	36,36,36	0.48	0	47,47,47	1.17	4 (8%)
26	BCR	k	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.46	14 (25%)
25	PHO	A	408	-	58,69,69	2.70	14 (24%)	56,99,99	2.70	12 (21%)
24	CLA	C	506	3	69,73,73	2.05	20 (28%)	83,113,113	2.75	29 (34%)
30	OEX	a	416	41,1,3	0,14,14	-	-	-	-	-
38	HEM	F	102	6,5	50,50,50	1.56	6 (12%)	66,82,82	1.85	15 (22%)
35	HTG	B	625	-	19,19,19	1.05	2 (10%)	23,24,24	1.64	2 (8%)
24	CLA	b	606	41	69,73,73	2.09	19 (27%)	83,113,113	2.82	26 (31%)
26	BCR	K	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.47	12 (21%)
37	DGD	e	101	-	63,63,67	0.93	2 (3%)	77,77,81	1.24	7 (9%)
29	LMT	e	102	-	36,36,36	0.48	0	47,47,47	0.86	1 (2%)
28	GOL	V	205	-	5,5,5	0.37	0	5,5,5	0.57	0
24	CLA	C	501	3	69,73,73	2.07	20 (28%)	83,113,113	2.83	30 (36%)
33	LMG	Y	101	-	51,51,55	0.95	2 (3%)	59,59,63	1.00	4 (6%)
24	CLA	C	503	3	69,73,73	2.09	20 (28%)	83,113,113	2.82	27 (32%)
28	GOL	V	204	-	5,5,5	0.38	0	5,5,5	0.37	0
31	PL9	a	415	-	55,55,55	0.64	2 (3%)	68,69,69	1.88	21 (30%)
29	LMT	m	102	-	36,36,36	0.46	0	47,47,47	0.85	1 (2%)
26	BCR	T	102	-	41,41,41	1.03	1 (2%)	56,56,56	1.85	17 (30%)
26	BCR	D	406	-	41,41,41	1.06	1 (2%)	56,56,56	1.74	10 (17%)
26	BCR	c	915	-	41,41,41	1.02	1 (2%)	56,56,56	1.40	10 (17%)
35	HTG	D	413	-	16,16,19	1.07	2 (12%)	20,21,24	1.52	1 (5%)
36	LHG	d	411	-	48,48,48	0.94	2 (4%)	51,54,54	1.08	3 (5%)
36	LHG	D	409	-	48,48,48	0.89	2 (4%)	51,54,54	0.89	3 (5%)
35	HTG	b	627	-	19,19,19	0.81	1 (5%)	23,24,24	1.54	3 (13%)
26	BCR	h	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.37	8 (14%)
27	SQD	a	402	-	53,54,54	1.07	3 (5%)	62,65,65	1.19	6 (9%)
24	CLA	B	603	2	69,73,73	2.02	21 (30%)	83,113,113	2.94	31 (37%)
24	CLA	c	911	3	69,73,73	2.05	20 (28%)	83,113,113	2.77	30 (36%)
26	BCR	C	514	-	41,41,41	1.08	1 (2%)	56,56,56	1.52	9 (16%)
37	DGD	c	918	-	63,63,67	0.90	2 (3%)	77,77,81	1.04	5 (6%)
27	SQD	f	102	-	42,43,54	1.20	3 (7%)	51,54,65	1.45	6 (11%)
28	GOL	B	629	-	5,5,5	0.35	0	5,5,5	0.31	0
26	BCR	t	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.68	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PL9	d	408	-	55,55,55	0.67	2 (3%)	68,69,69	1.69	16 (23%)
35	HTG	b	604	-	19,19,19	0.99	2 (10%)	23,24,24	1.11	1 (4%)
29	LMT	b	602	-	25,25,36	0.57	1 (4%)	30,30,47	1.12	2 (6%)
33	LMG	Z	101	-	37,37,55	0.97	2 (5%)	45,45,63	1.39	6 (13%)
24	CLA	D	405	4	69,73,73	2.02	20 (28%)	83,113,113	2.82	29 (34%)
36	LHG	b	635	-	48,48,48	0.96	2 (4%)	51,54,54	1.12	3 (5%)
28	GOL	b	630	-	5,5,5	0.40	0	5,5,5	0.14	0
24	CLA	B	604	2	69,73,73	2.06	19 (27%)	83,113,113	2.88	28 (33%)
37	DGD	C	518	-	63,63,67	0.86	2 (3%)	77,77,81	0.96	5 (6%)
35	HTG	b	603	-	19,19,19	1.00	2 (10%)	23,24,24	1.55	4 (17%)
37	DGD	C	516	-	63,63,67	0.87	2 (3%)	77,77,81	1.12	6 (7%)
33	LMG	J	101	39	51,51,55	0.90	2 (3%)	59,59,63	0.97	3 (5%)
24	CLA	B	615	2	69,73,73	2.05	20 (28%)	83,113,113	2.87	31 (37%)
36	LHG	a	418	-	41,41,48	1.04	2 (4%)	44,47,54	0.95	2 (4%)
27	SQD	A	411	-	53,54,54	0.98	3 (5%)	62,65,65	1.57	11 (17%)
24	CLA	d	406	4	69,73,73	2.08	20 (28%)	83,113,113	2.85	30 (36%)
24	CLA	b	611	2	69,73,73	2.03	20 (28%)	83,113,113	2.86	28 (33%)
26	BCR	B	620	-	41,41,41	1.02	1 (2%)	56,56,56	1.48	10 (17%)
28	GOL	B	630	-	5,5,5	0.39	0	5,5,5	0.21	0
28	GOL	c	924	-	5,5,5	0.37	0	5,5,5	0.61	0
24	CLA	c	902	3	69,73,73	2.04	19 (27%)	83,113,113	2.79	30 (36%)
28	GOL	b	631	-	5,5,5	0.32	0	5,5,5	0.26	0
24	CLA	B	608	41	69,73,73	2.01	20 (28%)	83,113,113	2.72	29 (34%)
27	SQD	A	414	-	53,54,54	1.03	3 (5%)	62,65,65	1.12	6 (9%)
27	SQD	a	410	-	53,54,54	0.98	3 (5%)	62,65,65	1.64	11 (17%)
24	CLA	B	617	2	69,73,73	2.01	19 (27%)	83,113,113	2.85	29 (34%)
37	DGD	c	916	-	63,63,67	0.84	2 (3%)	77,77,81	1.07	7 (9%)
24	CLA	B	602	41	69,73,73	2.06	21 (30%)	83,113,113	2.85	27 (32%)
24	CLA	C	513	3	69,73,73	2.05	19 (27%)	83,113,113	2.84	30 (36%)
31	PL9	A	417	-	55,55,55	0.66	2 (3%)	68,69,69	1.80	23 (33%)
36	LHG	d	409	-	48,48,48	0.92	3 (6%)	51,54,54	1.11	6 (11%)
25	PHO	d	403	-	58,69,69	2.78	12 (20%)	56,99,99	2.91	17 (30%)
24	CLA	b	617	2	69,73,73	2.00	20 (28%)	83,113,113	2.81	33 (39%)
29	LMT	F	101	-	36,36,36	0.46	0	47,47,47	0.90	1 (2%)
28	GOL	C	524	-	5,5,5	0.41	0	5,5,5	0.57	0
24	CLA	c	903	3	69,73,73	2.07	20 (28%)	83,113,113	2.78	27 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	LHG	D	410	-	48,48,48	0.97	2 (4%)	51,54,54	1.20	4 (7%)
24	CLA	B	611	41	69,73,73	2.07	19 (27%)	83,113,113	2.90	32 (38%)
24	CLA	b	612	41	69,73,73	2.05	18 (26%)	83,113,113	2.74	29 (34%)
26	BCR	B	618	-	41,41,41	1.00	1 (2%)	56,56,56	1.40	9 (16%)
24	CLA	d	404	41	69,73,73	2.05	19 (27%)	83,113,113	2.83	32 (38%)
24	CLA	b	610	2	69,73,73	2.01	20 (28%)	83,113,113	2.94	27 (32%)
35	HTG	d	414	-	16,16,19	1.14	2 (12%)	20,21,24	1.76	1 (5%)
26	BCR	H	101	-	41,41,41	1.09	1 (2%)	56,56,56	1.41	9 (16%)
24	CLA	c	912	3	69,73,73	1.98	20 (28%)	83,113,113	2.79	27 (32%)
30	OEX	A	416	41,1,3	0,14,14	-	-	-	-	-
27	SQD	L	102	-	53,54,54	1.04	3 (5%)	62,65,65	1.55	11 (17%)
24	CLA	B	610	2	69,73,73	2.03	19 (27%)	83,113,113	2.74	28 (33%)
24	CLA	B	616	2	69,73,73	2.05	19 (27%)	83,113,113	2.77	28 (33%)
35	HTG	c	922	-	19,19,19	1.00	2 (10%)	23,24,24	1.45	3 (13%)
33	LMG	A	419	-	51,51,55	0.96	2 (3%)	59,59,63	1.12	4 (6%)
37	DGD	c	917	-	63,63,67	0.90	2 (3%)	77,77,81	1.02	6 (7%)
28	GOL	A	412	-	5,5,5	0.39	0	5,5,5	0.29	0
24	CLA	b	607	2	69,73,73	2.06	21 (30%)	83,113,113	2.93	32 (38%)
24	CLA	b	616	2	69,73,73	1.96	20 (28%)	83,113,113	2.81	31 (37%)
28	GOL	B	627	-	5,5,5	0.36	0	5,5,5	0.49	0
29	LMT	D	403	-	36,36,36	0.47	0	47,47,47	1.04	3 (6%)
37	DGD	H	102	-	63,63,67	0.87	2 (3%)	77,77,81	1.02	6 (7%)
24	CLA	a	405	1	69,73,73	2.00	20 (28%)	83,113,113	2.82	31 (37%)
26	BCR	b	622	-	41,41,41	1.01	1 (2%)	56,56,56	1.53	9 (16%)
28	GOL	b	629	-	5,5,5	0.38	0	5,5,5	0.49	0
33	LMG	c	920	-	51,51,55	0.95	2 (3%)	59,59,63	1.30	7 (11%)
28	GOL	C	523	-	5,5,5	0.37	0	5,5,5	0.88	0
24	CLA	c	913	3	69,73,73	2.05	19 (27%)	83,113,113	2.95	31 (37%)
37	DGD	D	408	-	52,52,67	1.04	3 (5%)	60,60,81	1.17	5 (8%)
29	LMT	b	626	-	25,25,36	0.47	0	30,30,47	0.58	0
24	CLA	C	508	3	69,73,73	2.08	20 (28%)	83,113,113	2.80	29 (34%)
28	GOL	O	302	-	5,5,5	0.33	0	5,5,5	0.39	0
35	HTG	B	632	-	19,19,19	0.96	2 (10%)	23,24,24	1.37	2 (8%)
28	GOL	B	626	-	5,5,5	0.41	0	5,5,5	0.34	0
35	HTG	C	522	-	19,19,19	1.00	1 (5%)	23,24,24	1.71	4 (17%)
24	CLA	B	607	2	69,73,73	2.06	19 (27%)	83,113,113	2.93	31 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	b	614	2	69,73,73	2.04	18 (26%)	83,113,113	2.86	29 (34%)
35	HTG	b	628	-	19,19,19	1.21	2 (10%)	23,24,24	1.69	3 (13%)
24	CLA	a	408	1	69,73,73	2.03	19 (27%)	83,113,113	2.91	31 (37%)
24	CLA	b	609	2	69,73,73	2.06	21 (30%)	83,113,113	2.69	26 (31%)
40	HEC	v	202	16	50,50,50	1.66	9 (18%)	68,82,82	1.77	17 (25%)
24	CLA	C	502	3	69,73,73	2.06	20 (28%)	83,113,113	2.75	29 (34%)
35	HTG	V	203	-	19,19,19	1.02	2 (10%)	23,24,24	1.31	3 (13%)
33	LMG	C	519	-	51,51,55	0.96	2 (3%)	59,59,63	1.25	8 (13%)
26	BCR	A	410	-	41,41,41	1.11	1 (2%)	56,56,56	1.11	4 (7%)
33	LMG	c	919	-	51,51,55	0.88	2 (3%)	59,59,63	1.18	4 (6%)
24	CLA	B	606	2	69,73,73	2.03	18 (26%)	83,113,113	2.88	29 (34%)
29	LMT	a	401	-	36,36,36	0.51	1 (2%)	47,47,47	1.15	3 (6%)
25	PHO	D	401	-	58,69,69	2.81	14 (24%)	56,99,99	2.80	15 (26%)
36	LHG	E	101	-	41,41,48	1.02	2 (4%)	44,47,54	1.11	4 (9%)
24	CLA	b	608	2	69,73,73	2.02	20 (28%)	83,113,113	2.83	29 (34%)
24	CLA	c	904	3	69,73,73	2.04	19 (27%)	83,113,113	2.82	27 (32%)
26	BCR	b	624	-	41,41,41	1.09	2 (4%)	56,56,56	1.21	4 (7%)
24	CLA	A	409	1	69,73,73	2.10	19 (27%)	83,113,113	2.75	32 (38%)
28	GOL	A	413	-	5,5,5	0.38	0	5,5,5	0.22	0
28	GOL	v	203	-	5,5,5	0.35	0	5,5,5	0.27	0
24	CLA	D	404	4	69,73,73	1.97	20 (28%)	83,113,113	2.93	33 (39%)
27	SQD	F	103	-	42,43,54	1.17	3 (7%)	51,54,65	1.58	9 (17%)
24	CLA	A	406	41	69,73,73	2.04	20 (28%)	83,113,113	2.96	32 (38%)
24	CLA	c	909	3	69,73,73	2.03	20 (28%)	83,113,113	2.81	29 (34%)
29	LMT	A	415	-	36,36,36	0.67	1 (2%)	47,47,47	1.43	5 (10%)
28	GOL	v	205	-	5,5,5	0.33	0	5,5,5	0.47	0
40	HEC	V	202	16	50,50,50	1.69	10 (20%)	68,82,82	1.81	19 (27%)
29	LMT	m	103	-	36,36,36	0.49	0	47,47,47	1.08	3 (6%)
26	BCR	y	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.48	9 (16%)
26	BCR	Y	102	-	41,41,41	1.07	1 (2%)	56,56,56	1.67	11 (19%)
24	CLA	B	605	2	69,73,73	1.97	20 (28%)	83,113,113	2.81	31 (37%)
24	CLA	B	613	2	69,73,73	1.98	18 (26%)	83,113,113	2.78	28 (33%)
28	GOL	B	631	-	5,5,5	0.33	0	5,5,5	0.43	0
29	LMT	t	101	-	25,25,36	0.50	0	30,30,47	0.77	1 (3%)
24	CLA	b	620	2	69,73,73	2.04	20 (28%)	83,113,113	2.77	32 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	C	515	-	41,41,41	1.02	1 (2%)	56,56,56	1.53	10 (17%)
35	HTG	B	633	-	19,19,19	1.04	2 (10%)	23,24,24	1.39	2 (8%)
35	HTG	B	624	-	19,19,19	0.82	1 (5%)	23,24,24	1.74	4 (17%)
37	DGD	h	102	-	63,63,67	0.91	3 (4%)	77,77,81	1.02	4 (5%)
24	CLA	B	609	2	69,73,73	2.06	20 (28%)	83,113,113	2.70	28 (33%)
28	GOL	B	628	-	5,5,5	0.38	0	5,5,5	0.47	0
28	GOL	a	419	34	5,5,5	0.31	0	5,5,5	0.40	0
33	LMG	B	622	-	51,51,55	0.94	2 (3%)	59,59,63	1.02	3 (5%)
33	LMG	d	415	39	51,51,55	0.94	2 (3%)	59,59,63	1.01	3 (5%)
28	GOL	b	633	-	5,5,5	0.37	0	5,5,5	0.41	0
28	GOL	c	928	-	5,5,5	0.41	0	5,5,5	0.25	0
25	PHO	a	407	-	58,69,69	2.74	14 (24%)	56,99,99	2.89	18 (32%)
24	CLA	C	512	3	69,73,73	2.07	20 (28%)	83,113,113	2.81	30 (36%)
23	BCT	A	404	21	2,3,3	0.65	0	2,3,3	1.14	0
24	CLA	C	504	41	69,73,73	2.06	20 (28%)	83,113,113	2.82	28 (33%)
26	BCR	d	407	-	41,41,41	1.06	1 (2%)	56,56,56	1.66	15 (26%)
31	PL9	D	407	-	55,55,55	0.64	2 (3%)	68,69,69	1.89	22 (32%)
33	LMG	b	625	-	51,51,55	0.89	2 (3%)	59,59,63	1.11	5 (8%)
38	HEM	f	101	6,5	50,50,50	1.53	8 (16%)	66,82,82	1.77	13 (19%)
29	LMT	M	101	-	36,36,36	0.46	0	47,47,47	0.92	0
28	GOL	c	923	-	5,5,5	0.37	0	5,5,5	0.22	0
24	CLA	b	621	2	69,73,73	2.04	19 (27%)	83,113,113	2.82	32 (38%)
24	CLA	A	405	1	69,73,73	2.04	20 (28%)	83,113,113	2.81	31 (37%)
24	CLA	C	509	3	69,73,73	2.10	20 (28%)	83,113,113	2.78	30 (36%)
24	CLA	d	405	4	69,73,73	1.96	20 (28%)	83,113,113	2.88	29 (34%)
28	GOL	V	207	-	5,5,5	0.34	0	5,5,5	0.30	0
36	LHG	d	410	-	48,48,48	0.87	2 (4%)	51,54,54	1.03	4 (7%)
24	CLA	c	910	3	69,73,73	2.12	20 (28%)	83,113,113	2.80	29 (34%)
26	BCR	a	409	-	41,41,41	1.05	1 (2%)	56,56,56	1.28	2 (3%)
24	CLA	b	613	2	69,73,73	2.09	20 (28%)	83,113,113	2.72	31 (37%)
24	CLA	A	407	41	69,73,73	2.05	19 (27%)	83,113,113	2.83	31 (37%)
26	BCR	b	623	-	41,41,41	1.02	1 (2%)	56,56,56	1.29	7 (12%)
33	LMG	z	101	-	39,39,55	1.10	2 (5%)	47,47,63	1.10	4 (8%)
28	GOL	l	101	-	5,5,5	0.47	0	5,5,5	0.24	0
24	CLA	c	908	41	69,73,73	2.01	20 (28%)	83,113,113	2.74	28 (33%)

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
26	BCR	c	927	-	-	0/29/63/63	0/2/2/2
28	GOL	T	101	-	-	0/4/4/4	-
35	HTG	b	601	-	-	3/10/30/30	0/1/1/1
29	LMT	a	417	-	-	4/21/61/61	0/2/2/2
24	CLA	B	614	2	-	8/39/115/115	-
29	LMT	M	103	-	-	11/21/61/61	0/2/2/2
35	HTG	c	921	-	-	4/10/30/30	0/1/1/1
28	GOL	v	204	-	-	2/4/4/4	-
28	GOL	b	632	-	-	2/4/4/4	-
24	CLA	b	619	2	-	20/39/115/115	-
24	CLA	C	505	3	-	6/39/115/115	-
24	CLA	B	612	2	-	1/39/115/115	-
36	LHG	L	101	-	-	16/53/53/53	-
24	CLA	b	618	2	-	3/39/115/115	-
24	CLA	c	905	41	-	6/39/115/115	-
28	GOL	a	412	-	-	4/4/4/4	-
28	GOL	a	413	-	-	2/4/4/4	-
28	GOL	T	103	-	-	2/4/4/4	-
28	GOL	B	636	-	-	2/4/4/4	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
27	SQD	B	621	-	-	20/49/69/69	0/1/1/1
24	CLA	C	511	3	-	4/39/115/115	-
24	CLA	c	914	3	-	5/39/115/115	-
28	GOL	V	201	34	-	2/4/4/4	-
35	HTG	B	623	-	-	3/10/30/30	0/1/1/1
24	CLA	a	406	41	-	11/39/115/115	-
33	LMG	a	411	-	-	14/46/66/70	0/1/1/1
37	DGD	C	517	-	-	19/51/91/95	0/2/2/2
36	LHG	B	635	-	-	13/53/53/53	-
28	GOL	V	206	-	-	2/4/4/4	-
24	CLA	c	907	3	-	13/39/115/115	-
24	CLA	c	906	3	-	8/39/115/115	-
28	GOL	D	402	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	510	3	-	8/39/115/115	-
35	HTG	C	521	-	-	0/10/30/30	0/1/1/1
24	CLA	b	615	41	-	5/39/115/115	-
24	CLA	C	507	41	-	5/39/115/115	-
29	LMT	C	520	-	-	6/21/61/61	0/2/2/2
26	BCR	k	101	-	-	0/29/63/63	0/2/2/2
25	PHO	A	408	-	-	2/37/103/103	0/5/6/6
24	CLA	C	506	3	-	6/39/115/115	-
38	HEM	F	102	6,5	-	6/14/54/54	-
35	HTG	B	625	-	-	5/10/30/30	0/1/1/1
24	CLA	b	606	41	-	16/39/115/115	-
26	BCR	K	101	-	-	0/29/63/63	0/2/2/2
37	DGD	e	101	-	-	26/51/91/95	0/2/2/2
29	LMT	e	102	-	-	9/21/61/61	0/2/2/2
28	GOL	V	205	-	-	0/4/4/4	-
24	CLA	C	501	3	-	7/39/115/115	-
33	LMG	Y	101	-	-	10/46/66/70	0/1/1/1
24	CLA	C	503	3	-	2/39/115/115	-
28	GOL	V	204	-	-	2/4/4/4	-
31	PL9	a	415	-	-	15/53/73/73	0/1/1/1
29	LMT	m	102	-	-	6/21/61/61	0/2/2/2
26	BCR	T	102	-	-	1/29/63/63	0/2/2/2
26	BCR	D	406	-	-	8/29/63/63	0/2/2/2
26	BCR	c	915	-	-	4/29/63/63	0/2/2/2
35	HTG	D	413	-	-	0/7/27/30	0/1/1/1
36	LHG	d	411	-	-	12/53/53/53	-
36	LHG	D	409	-	-	11/53/53/53	-
35	HTG	b	627	-	-	2/10/30/30	0/1/1/1
26	BCR	h	101	-	-	2/29/63/63	0/2/2/2
27	SQD	a	402	-	-	10/49/69/69	0/1/1/1
24	CLA	B	603	2	-	5/39/115/115	-
24	CLA	c	911	3	-	7/39/115/115	-
26	BCR	C	514	-	-	1/29/63/63	0/2/2/2
37	DGD	c	918	-	-	13/51/91/95	0/2/2/2
27	SQD	f	102	-	-	15/38/58/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	B	629	-	-	3/4/4/4	-
26	BCR	t	102	-	-	5/29/63/63	0/2/2/2
31	PL9	d	408	-	-	3/53/73/73	0/1/1/1
35	HTG	b	604	-	-	1/10/30/30	0/1/1/1
29	LMT	b	602	-	-	7/17/37/61	0/1/1/2
33	LMG	Z	101	-	-	13/31/51/70	0/1/1/1
24	CLA	D	405	4	-	6/39/115/115	-
36	LHG	b	635	-	-	20/53/53/53	-
28	GOL	b	630	-	-	0/4/4/4	-
24	CLA	B	604	2	-	6/39/115/115	-
37	DGD	C	518	-	-	10/51/91/95	0/2/2/2
35	HTG	b	603	-	-	1/10/30/30	0/1/1/1
37	DGD	C	516	-	-	16/51/91/95	0/2/2/2
33	LMG	J	101	39	-	11/46/66/70	0/1/1/1
24	CLA	B	615	2	-	18/39/115/115	-
36	LHG	a	418	-	-	15/46/46/53	-
27	SQD	A	411	-	-	11/49/69/69	0/1/1/1
24	CLA	d	406	4	-	8/39/115/115	-
24	CLA	b	611	2	-	14/39/115/115	-
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
28	GOL	B	630	-	-	4/4/4/4	-
28	GOL	c	924	-	-	2/4/4/4	-
24	CLA	c	902	3	-	7/39/115/115	-
28	GOL	b	631	-	-	4/4/4/4	-
24	CLA	B	608	41	-	6/39/115/115	-
27	SQD	A	414	-	-	13/49/69/69	0/1/1/1
27	SQD	a	410	-	-	14/49/69/69	0/1/1/1
24	CLA	B	617	2	-	8/39/115/115	-
37	DGD	c	916	-	-	12/51/91/95	0/2/2/2
24	CLA	B	602	41	-	15/39/115/115	-
24	CLA	C	513	3	-	8/39/115/115	-
31	PL9	A	417	-	-	13/53/73/73	0/1/1/1
36	LHG	d	409	-	-	18/53/53/53	-
25	PHO	d	403	-	-	3/37/103/103	0/5/6/6
24	CLA	b	617	2	-	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMT	F	101	-	-	6/21/61/61	0/2/2/2
28	GOL	C	524	-	-	2/4/4/4	-
24	CLA	c	903	3	-	7/39/115/115	-
36	LHG	D	410	-	-	18/53/53/53	-
24	CLA	B	611	41	-	4/39/115/115	-
24	CLA	b	612	41	-	3/39/115/115	-
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
24	CLA	d	404	41	-	6/39/115/115	-
24	CLA	b	610	2	-	4/39/115/115	-
35	HTG	d	414	-	-	0/7/27/30	0/1/1/1
26	BCR	H	101	-	-	2/29/63/63	0/2/2/2
24	CLA	c	912	3	-	6/39/115/115	-
27	SQD	L	102	-	-	22/49/69/69	0/1/1/1
24	CLA	B	610	2	-	5/39/115/115	-
24	CLA	B	616	2	-	13/39/115/115	-
35	HTG	c	922	-	-	0/10/30/30	0/1/1/1
33	LMG	A	419	-	-	21/46/66/70	0/1/1/1
37	DGD	c	917	-	-	18/51/91/95	0/2/2/2
28	GOL	A	412	-	-	0/4/4/4	-
24	CLA	b	607	2	-	7/39/115/115	-
24	CLA	b	616	2	-	3/39/115/115	-
28	GOL	B	627	-	-	2/4/4/4	-
29	LMT	D	403	-	-	10/21/61/61	0/2/2/2
37	DGD	H	102	-	-	9/51/91/95	0/2/2/2
24	CLA	a	405	1	-	4/39/115/115	-
26	BCR	b	622	-	-	2/29/63/63	0/2/2/2
28	GOL	b	629	-	-	0/4/4/4	-
33	LMG	c	920	-	-	5/46/66/70	0/1/1/1
28	GOL	C	523	-	-	2/4/4/4	-
24	CLA	c	913	3	-	14/39/115/115	-
37	DGD	D	408	-	-	18/47/67/95	0/1/1/2
29	LMT	b	626	-	-	5/17/37/61	0/1/1/2
24	CLA	C	508	3	-	5/39/115/115	-
28	GOL	O	302	-	-	0/4/4/4	-
35	HTG	B	632	-	-	0/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	B	626	-	-	2/4/4/4	-
35	HTG	C	522	-	-	3/10/30/30	0/1/1/1
24	CLA	B	607	2	-	7/39/115/115	-
24	CLA	b	614	2	-	3/39/115/115	-
35	HTG	b	628	-	-	4/10/30/30	0/1/1/1
24	CLA	a	408	1	-	10/39/115/115	-
24	CLA	b	609	2	-	3/39/115/115	-
40	HEC	v	202	16	1/1/3/7	2/14/54/54	-
24	CLA	C	502	3	-	10/39/115/115	-
35	HTG	V	203	-	-	5/10/30/30	0/1/1/1
33	LMG	C	519	-	-	10/46/66/70	0/1/1/1
26	BCR	A	410	-	-	4/29/63/63	0/2/2/2
33	LMG	c	919	-	-	12/46/66/70	0/1/1/1
24	CLA	B	606	2	-	6/39/115/115	-
29	LMT	a	401	-	-	7/21/61/61	0/2/2/2
25	PHO	D	401	-	-	3/37/103/103	0/5/6/6
36	LHG	E	101	-	-	19/46/46/53	-
24	CLA	b	608	2	-	5/39/115/115	-
24	CLA	c	904	3	-	8/39/115/115	-
26	BCR	b	624	-	-	0/29/63/63	0/2/2/2
24	CLA	A	409	1	-	12/39/115/115	-
28	GOL	A	413	-	-	2/4/4/4	-
28	GOL	v	203	-	-	2/4/4/4	-
24	CLA	D	404	4	-	2/39/115/115	-
27	SQD	F	103	-	-	15/38/58/69	0/1/1/1
24	CLA	A	406	41	-	4/39/115/115	-
24	CLA	c	909	3	-	7/39/115/115	-
29	LMT	A	415	-	-	5/21/61/61	0/2/2/2
28	GOL	v	205	-	-	2/4/4/4	-
40	HEC	V	202	16	1/1/3/7	6/14/54/54	-
29	LMT	m	103	-	-	8/21/61/61	0/2/2/2
26	BCR	y	101	-	-	4/29/63/63	0/2/2/2
26	BCR	Y	102	-	-	4/29/63/63	0/2/2/2
24	CLA	B	605	2	-	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	613	2	-	5/39/115/115	-
28	GOL	B	631	-	-	1/4/4/4	-
29	LMT	t	101	-	-	7/17/37/61	0/1/1/2
24	CLA	b	620	2	-	9/39/115/115	-
26	BCR	C	515	-	-	4/29/63/63	0/2/2/2
35	HTG	B	633	-	-	0/10/30/30	0/1/1/1
35	HTG	B	624	-	-	4/10/30/30	0/1/1/1
37	DGD	h	102	-	-	9/51/91/95	0/2/2/2
24	CLA	B	609	2	-	1/39/115/115	-
28	GOL	B	628	-	-	2/4/4/4	-
28	GOL	a	419	34	-	3/4/4/4	-
33	LMG	B	622	-	-	8/46/66/70	0/1/1/1
33	LMG	d	415	39	-	10/46/66/70	0/1/1/1
28	GOL	b	633	-	-	2/4/4/4	-
28	GOL	c	928	-	-	2/4/4/4	-
25	PHO	a	407	-	-	4/37/103/103	0/5/6/6
24	CLA	C	512	3	-	9/39/115/115	-
24	CLA	C	504	41	-	7/39/115/115	-
26	BCR	d	407	-	-	4/29/63/63	0/2/2/2
31	PL9	D	407	-	-	9/53/73/73	0/1/1/1
33	LMG	b	625	-	-	8/46/66/70	0/1/1/1
38	HEM	f	101	6,5	-	10/14/54/54	-
29	LMT	M	101	-	-	6/21/61/61	0/2/2/2
28	GOL	c	923	-	-	0/4/4/4	-
24	CLA	b	621	2	-	9/39/115/115	-
24	CLA	A	405	1	-	4/39/115/115	-
24	CLA	C	509	3	-	14/39/115/115	-
24	CLA	d	405	4	-	7/39/115/115	-
28	GOL	V	207	-	-	4/4/4/4	-
36	LHG	d	410	-	-	9/53/53/53	-
24	CLA	c	910	3	-	15/39/115/115	-
26	BCR	a	409	-	-	2/29/63/63	0/2/2/2
24	CLA	b	613	2	-	1/39/115/115	-
24	CLA	A	407	41	-	8/39/115/115	-
26	BCR	b	623	-	-	1/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	z	101	-	-	11/34/54/70	0/1/1/1
28	GOL	l	101	-	-	0/4/4/4	-
24	CLA	c	908	41	-	6/39/115/115	-

The worst 5 of 1621 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	403	PHO	C1B-C2B	9.34	1.49	1.39
25	a	407	PHO	C1B-C2B	8.98	1.49	1.39
25	D	401	PHO	C1B-C2B	8.94	1.49	1.39
25	D	401	PHO	C1D-C2D	8.68	1.49	1.39
25	A	408	PHO	C1B-C2B	8.33	1.48	1.39

The worst 5 of 2792 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	407	PHO	C2D-C1D-ND	11.94	117.77	109.53
25	d	403	PHO	C2D-C1D-ND	11.93	117.76	109.53
25	D	401	PHO	C2D-C1D-ND	11.53	117.49	109.53
25	A	408	PHO	C2D-C1D-ND	11.16	117.23	109.53
24	c	914	CLA	C1D-ND-C4D	-10.25	99.05	106.33

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
40	V	202	HEC	NA
40	v	202	HEC	NA

5 of 1380 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	406	CLA	CHA-CBD-CGD-O1D
24	A	406	CLA	CHA-CBD-CGD-O2D
24	B	602	CLA	CHA-CBD-CGD-O1D
24	B	602	CLA	CHA-CBD-CGD-O2D
24	B	602	CLA	C11-C10-C8-C9

There are no ring outliers.

162 monomers are involved in 391 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	c	927	BCR	5	0
28	T	101	GOL	2	0
35	b	601	HTG	1	0
24	B	614	CLA	1	0
29	M	103	LMT	1	0
35	c	921	HTG	1	0
24	b	619	CLA	1	0
24	C	505	CLA	7	0
24	b	618	CLA	3	0
24	c	905	CLA	2	0
28	a	413	GOL	1	0
28	T	103	GOL	2	0
26	B	619	BCR	3	0
27	B	621	SQD	3	0
24	C	511	CLA	4	0
24	c	914	CLA	8	0
24	a	406	CLA	2	0
33	a	411	LMG	2	0
37	C	517	DGD	3	0
36	B	635	LHG	3	0
24	c	907	CLA	2	0
24	c	906	CLA	8	0
28	D	402	GOL	1	0
24	C	510	CLA	3	0
24	b	615	CLA	2	0
24	C	507	CLA	5	0
29	C	520	LMT	1	0
26	k	101	BCR	1	0
25	A	408	PHO	2	0
24	C	506	CLA	3	0
38	F	102	HEM	3	0
24	b	606	CLA	3	0
26	K	101	BCR	2	0
37	e	101	DGD	5	0
29	e	102	LMT	1	0
24	C	501	CLA	3	0
33	Y	101	LMG	2	0
24	C	503	CLA	2	0
31	a	415	PL9	11	0
29	m	102	LMT	3	0
26	T	102	BCR	4	0
26	D	406	BCR	1	0
26	c	915	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	D	413	HTG	3	0
36	d	411	LHG	4	0
36	D	409	LHG	2	0
35	b	627	HTG	1	0
26	h	101	BCR	5	0
24	B	603	CLA	3	0
24	c	911	CLA	3	0
26	C	514	BCR	7	0
37	c	918	DGD	1	0
27	f	102	SQD	2	1
26	t	102	BCR	5	0
31	d	408	PL9	1	0
33	Z	101	LMG	3	0
24	D	405	CLA	2	0
36	b	635	LHG	5	0
24	B	604	CLA	2	0
37	C	516	DGD	4	0
24	B	615	CLA	6	0
36	a	418	LHG	6	0
27	A	411	SQD	6	0
24	d	406	CLA	3	0
24	b	611	CLA	2	0
26	B	620	BCR	5	0
28	B	630	GOL	1	0
24	c	902	CLA	4	0
28	b	631	GOL	1	0
24	B	608	CLA	3	0
27	A	414	SQD	1	0
27	a	410	SQD	5	0
24	B	617	CLA	5	0
37	c	916	DGD	5	0
24	B	602	CLA	4	0
24	C	513	CLA	6	0
31	A	417	PL9	7	0
36	d	409	LHG	5	0
25	d	403	PHO	3	0
24	b	617	CLA	2	0
24	c	903	CLA	2	0
36	D	410	LHG	6	0
24	B	611	CLA	2	0
24	b	612	CLA	2	0
26	B	618	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	d	404	CLA	3	0
24	b	610	CLA	6	0
35	d	414	HTG	2	0
26	H	101	BCR	4	0
24	c	912	CLA	3	0
27	L	102	SQD	4	0
24	B	610	CLA	3	0
24	B	616	CLA	4	0
33	A	419	LMG	6	0
37	c	917	DGD	3	0
24	b	607	CLA	5	0
24	b	616	CLA	4	0
29	D	403	LMT	1	0
37	H	102	DGD	1	0
24	a	405	CLA	5	0
26	b	622	BCR	2	0
33	c	920	LMG	4	0
28	C	523	GOL	1	0
24	c	913	CLA	3	0
37	D	408	DGD	4	0
29	b	626	LMT	2	0
24	C	508	CLA	2	0
24	B	607	CLA	4	0
24	b	614	CLA	3	0
35	b	628	HTG	1	0
24	b	609	CLA	5	0
24	C	502	CLA	2	0
35	V	203	HTG	2	0
33	C	519	LMG	2	0
26	A	410	BCR	1	0
33	c	919	LMG	2	0
24	B	606	CLA	4	0
29	a	401	LMT	2	0
25	D	401	PHO	3	0
36	E	101	LHG	1	0
24	b	608	CLA	2	0
24	c	904	CLA	5	0
26	b	624	BCR	1	0
24	A	409	CLA	1	0
28	v	203	GOL	1	0
24	D	404	CLA	3	0
27	F	103	SQD	3	0

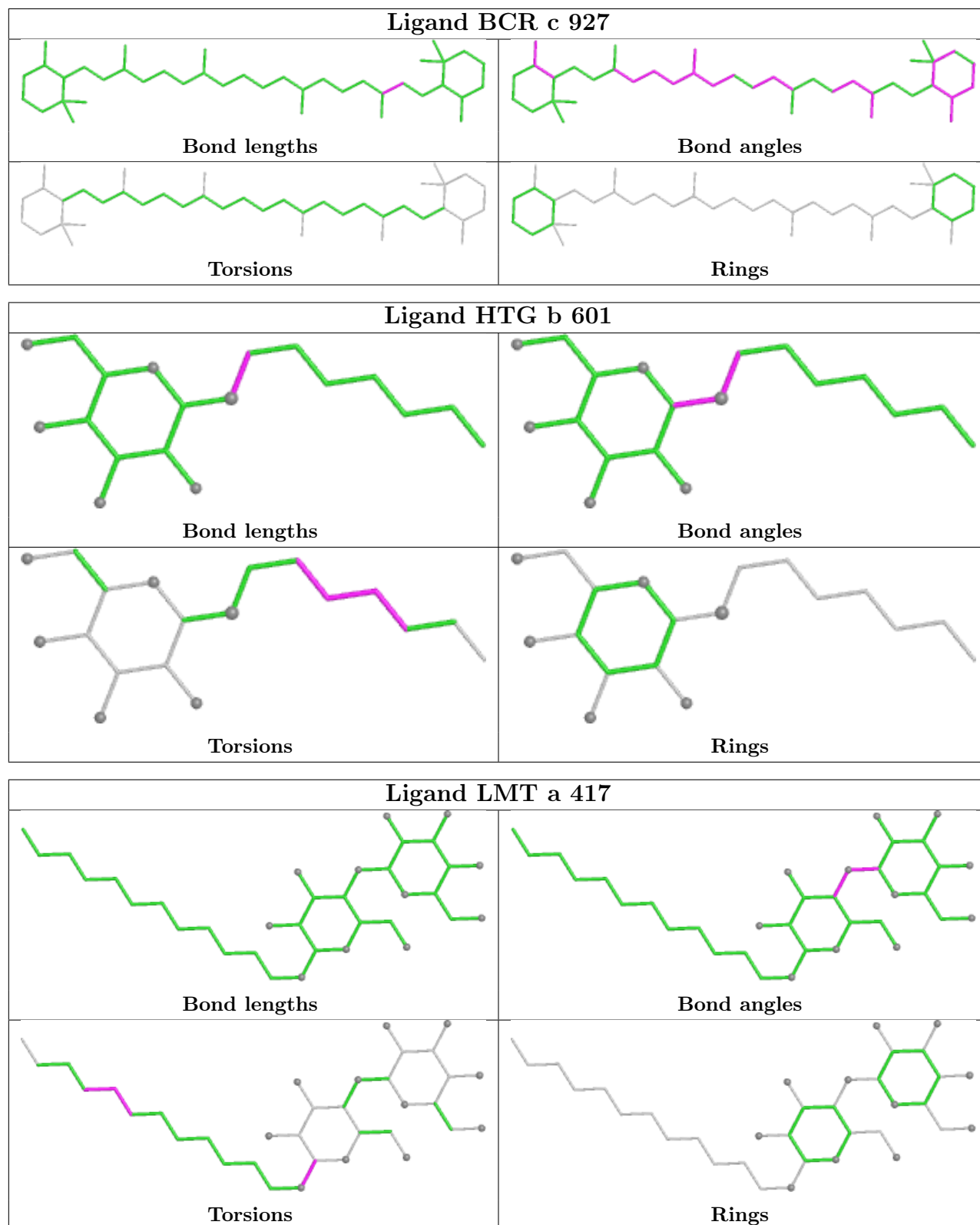
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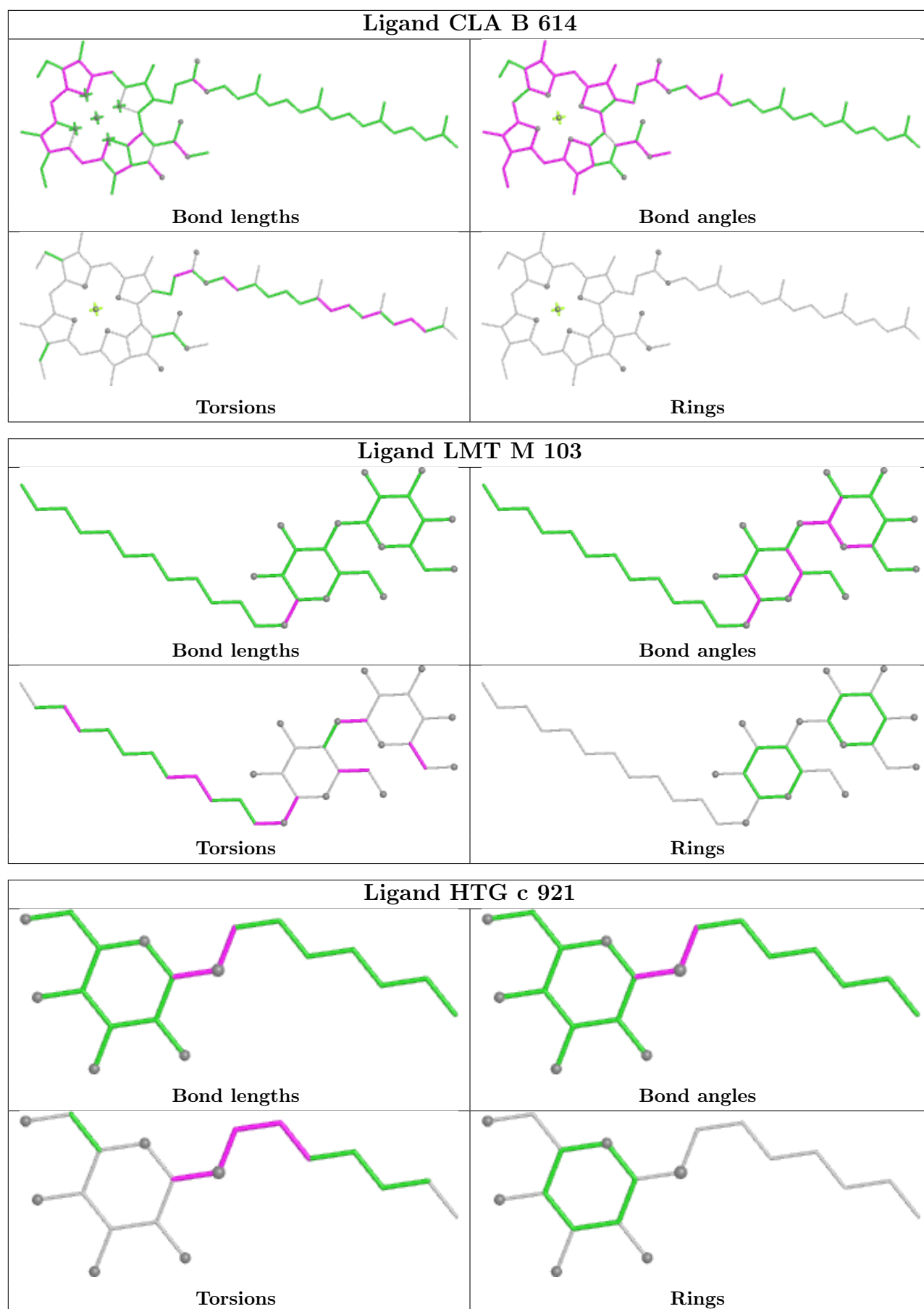
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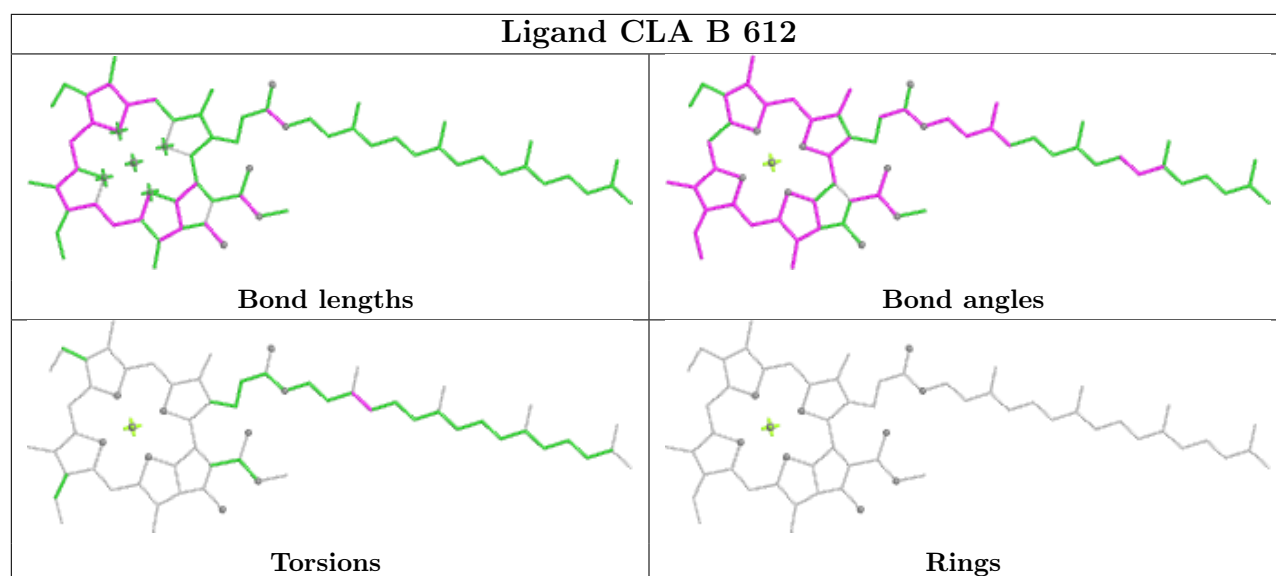
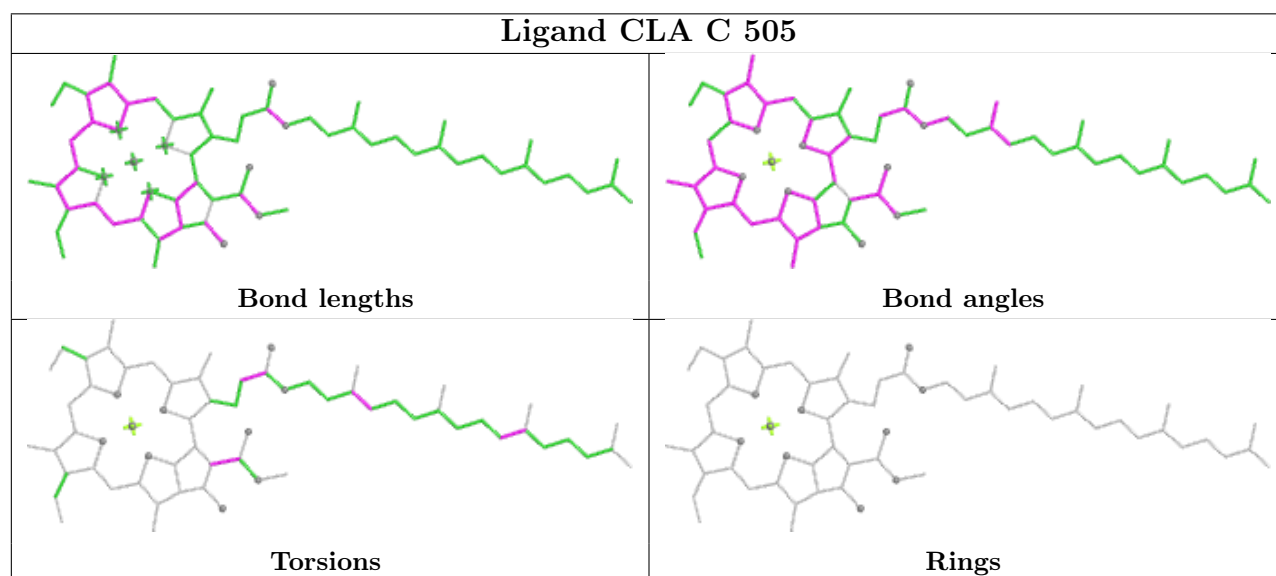
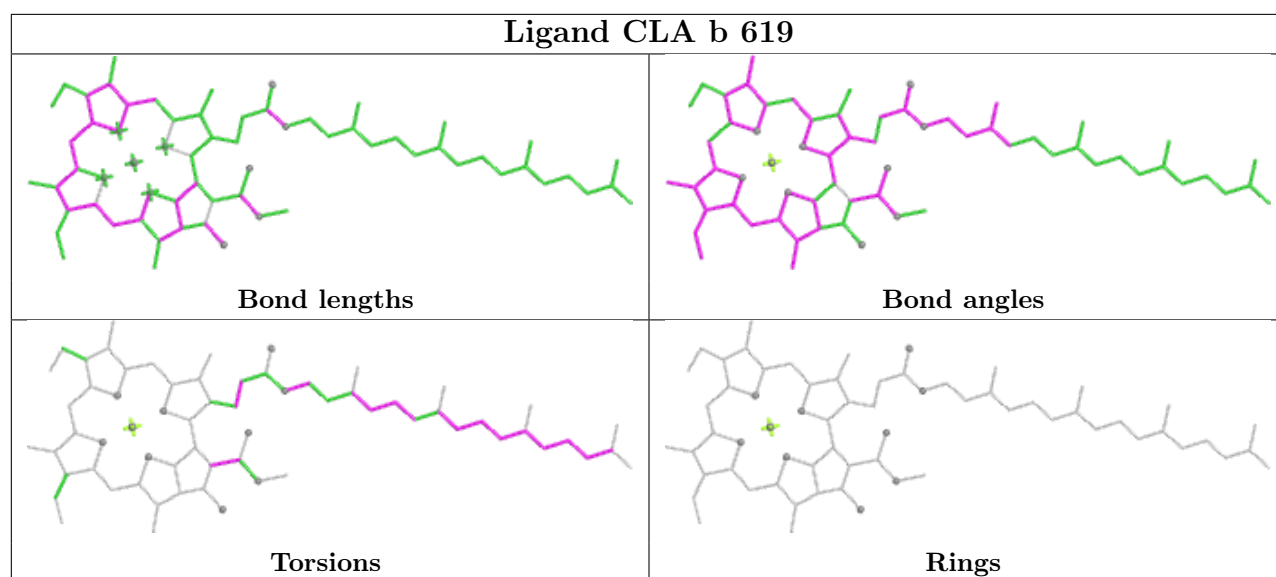
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	406	CLA	4	0
24	c	909	CLA	9	0
29	A	415	LMT	3	0
29	m	103	LMT	2	0
26	y	101	BCR	1	0
26	Y	102	BCR	6	0
24	B	605	CLA	4	0
24	B	613	CLA	2	0
24	b	620	CLA	4	0
26	C	515	BCR	2	0
37	h	102	DGD	2	0
24	B	609	CLA	1	0
28	a	419	GOL	1	0
33	B	622	LMG	3	0
33	d	415	LMG	3	0
28	b	633	GOL	1	0
25	a	407	PHO	3	0
24	C	512	CLA	5	0
24	C	504	CLA	1	0
26	d	407	BCR	4	0
33	b	625	LMG	4	0
29	M	101	LMT	3	0
24	b	621	CLA	3	0
24	A	405	CLA	7	0
24	C	509	CLA	4	0
24	d	405	CLA	5	0
28	V	207	GOL	1	0
36	d	410	LHG	1	0
24	c	910	CLA	2	0
24	b	613	CLA	1	0
24	A	407	CLA	2	0
26	b	623	BCR	2	0
33	z	101	LMG	5	0
28	l	101	GOL	1	0
24	c	908	CLA	2	0

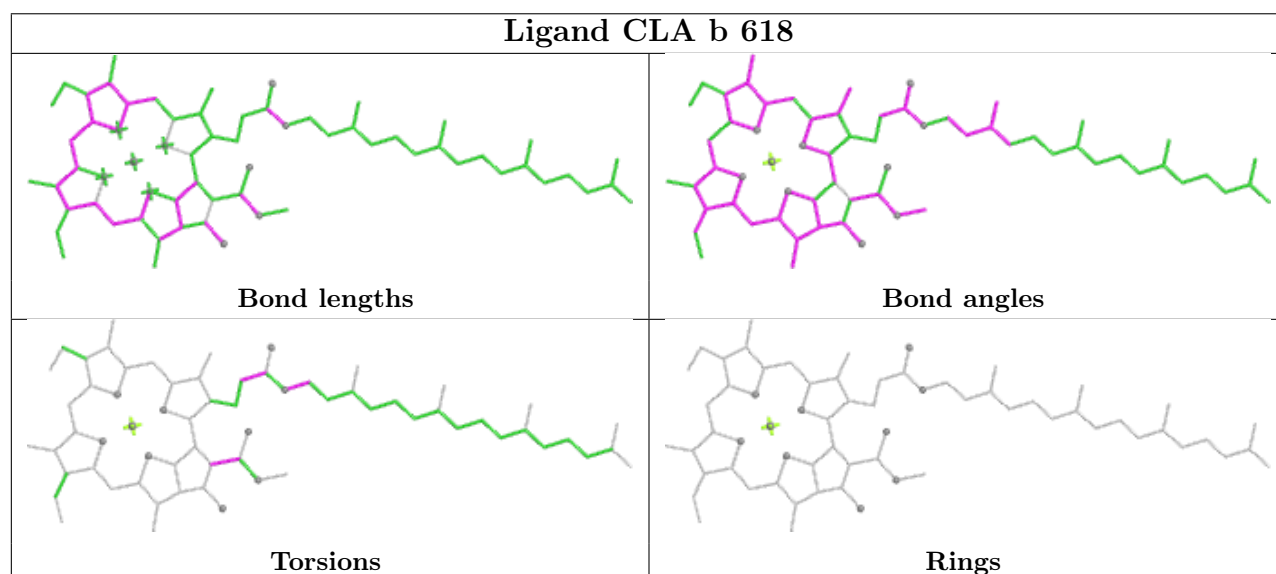
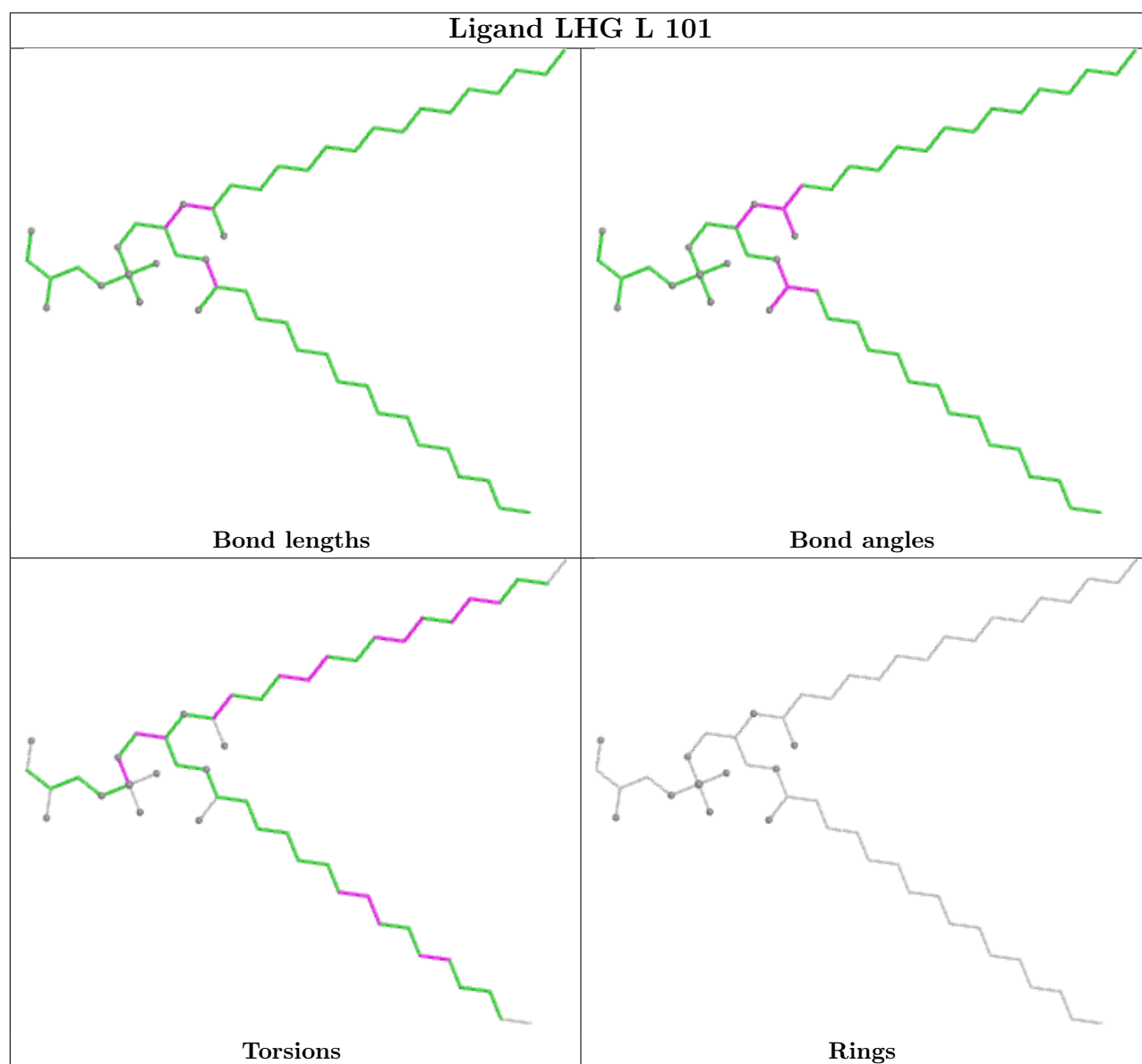
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

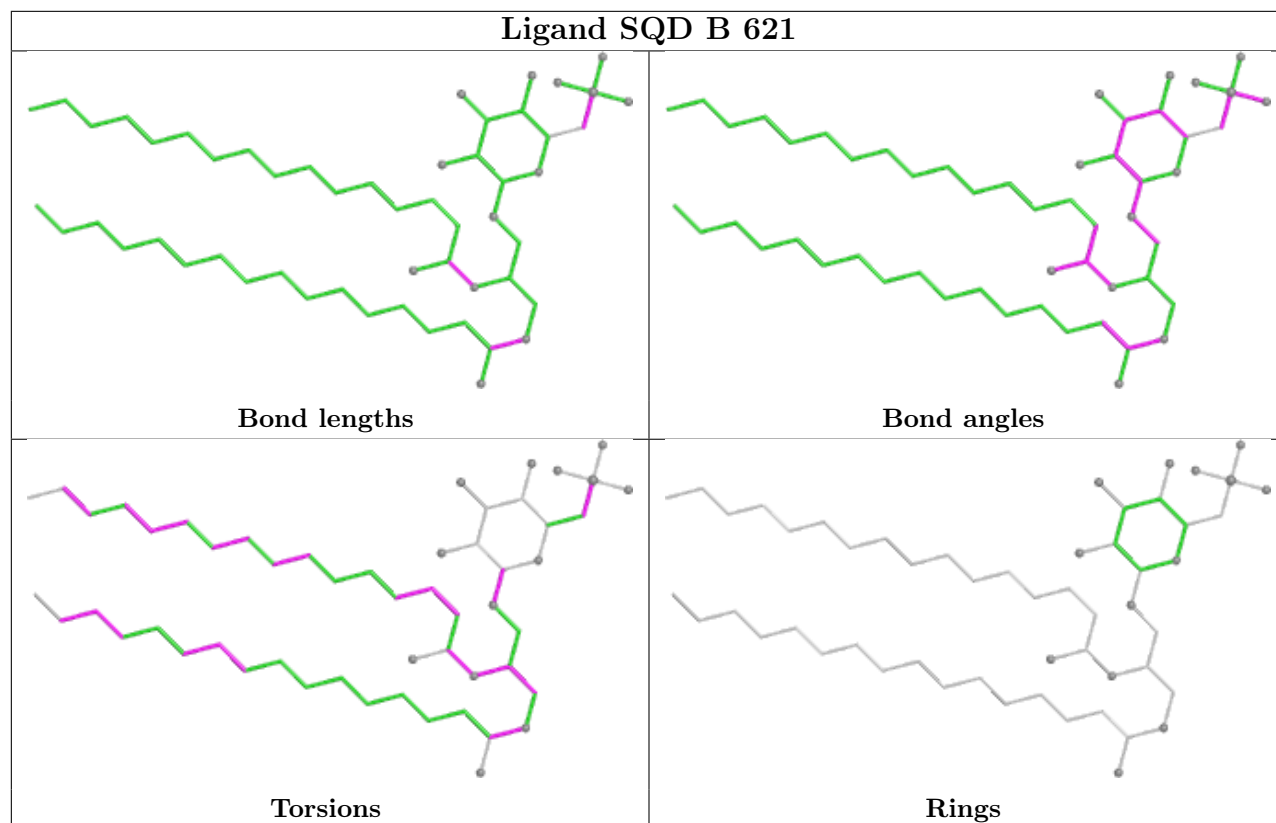
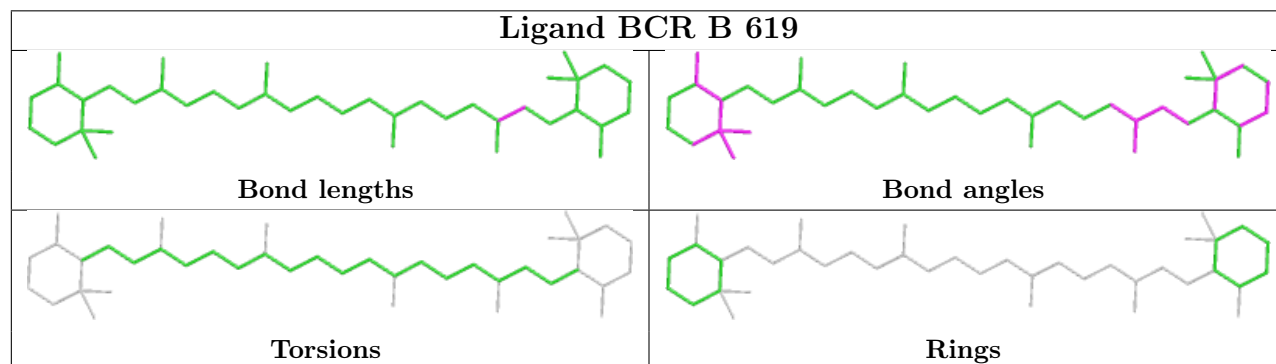
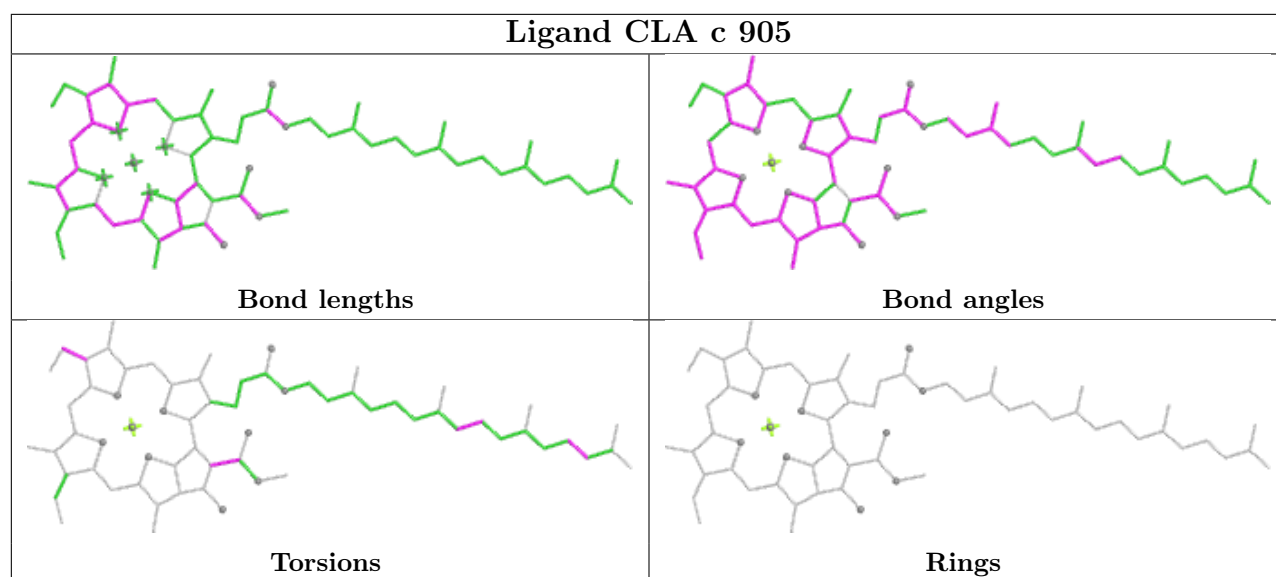
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

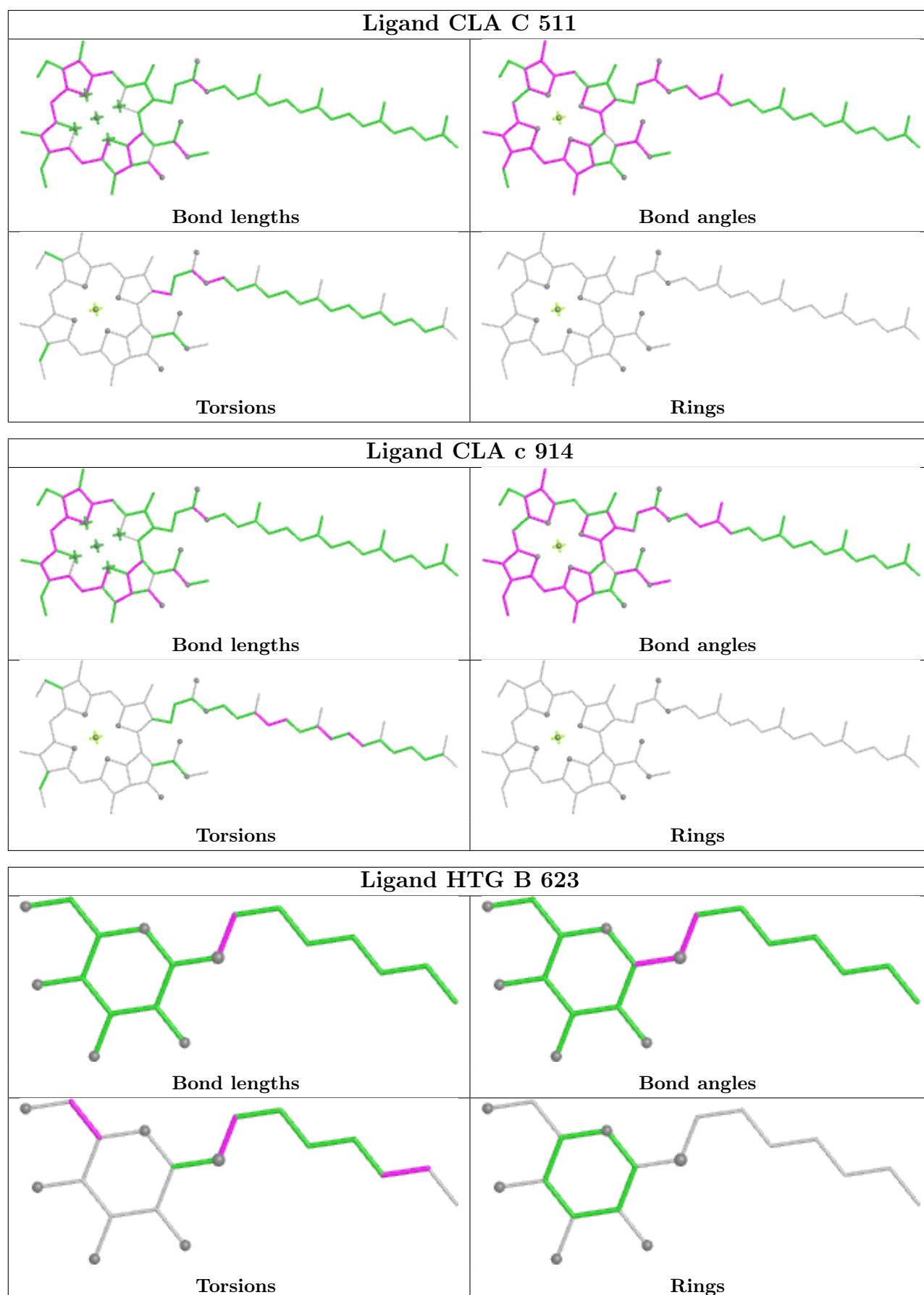


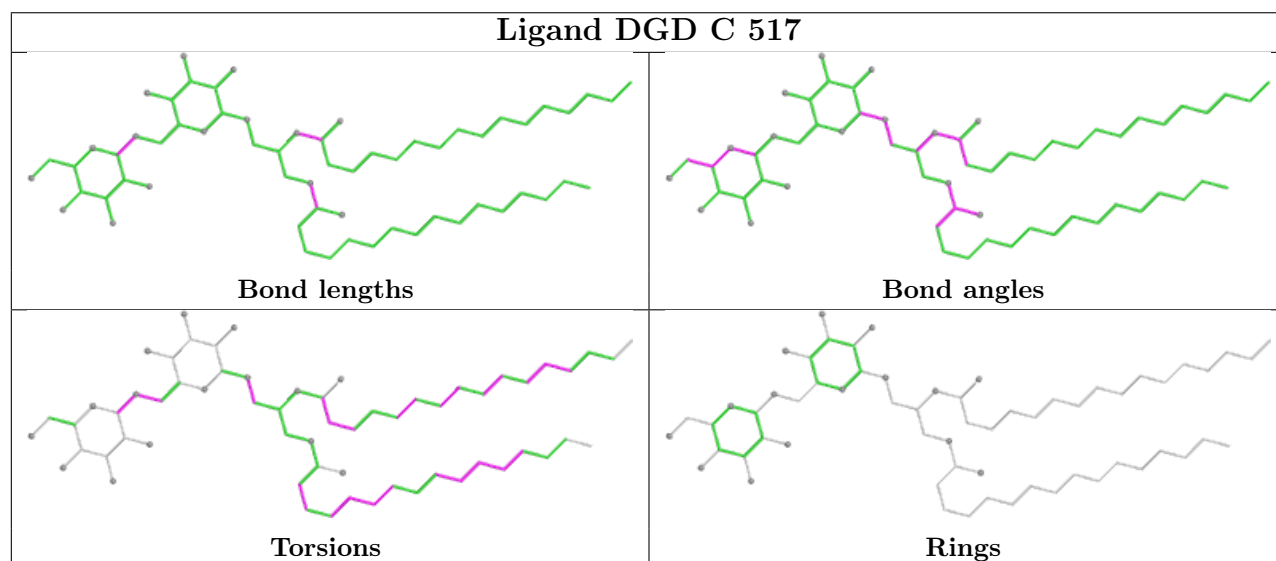
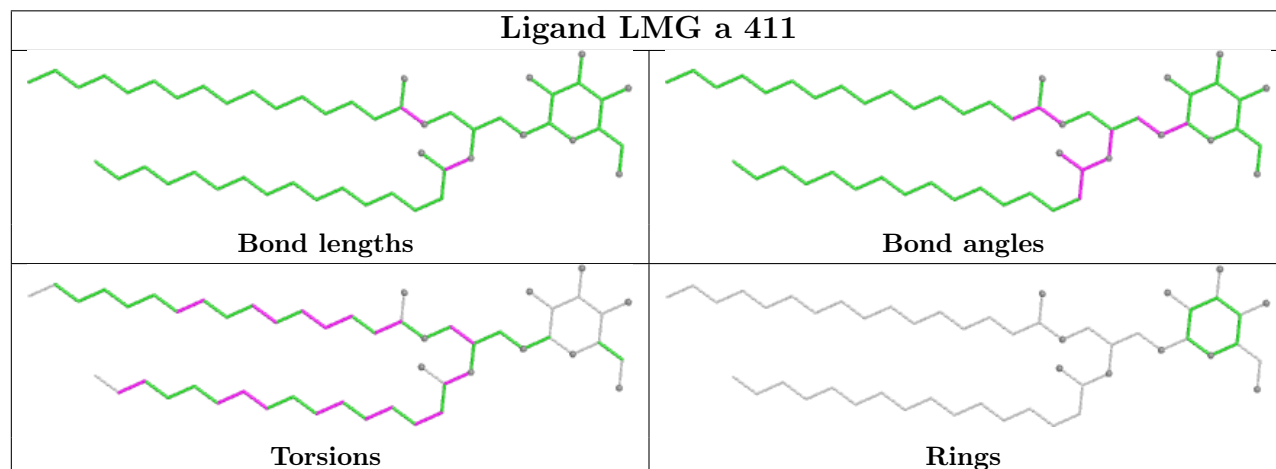
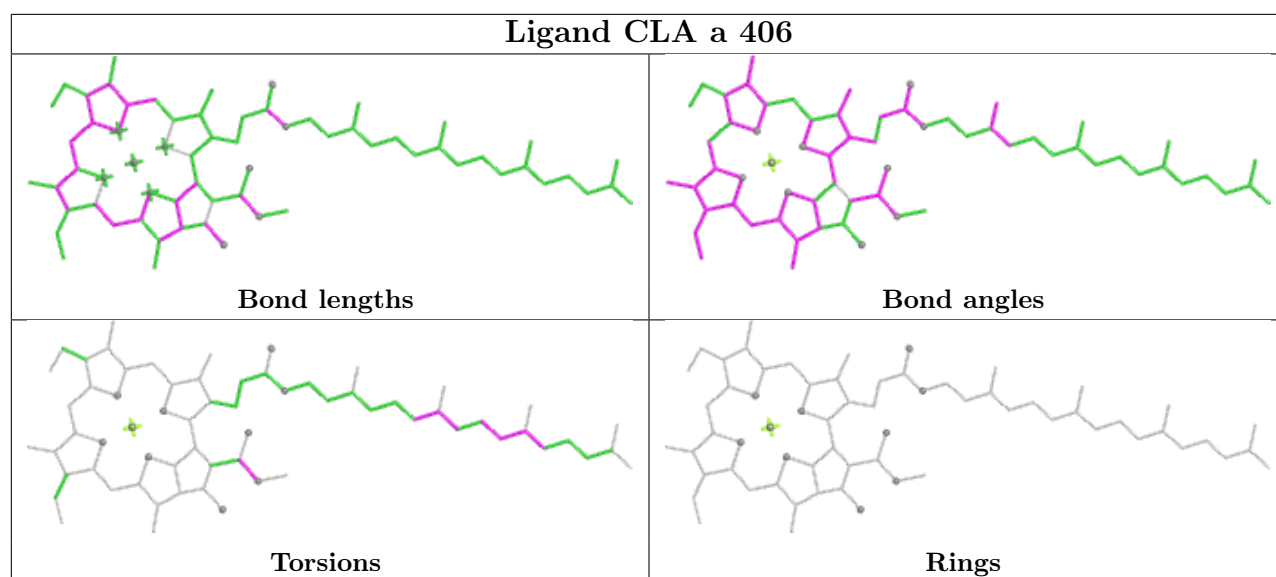


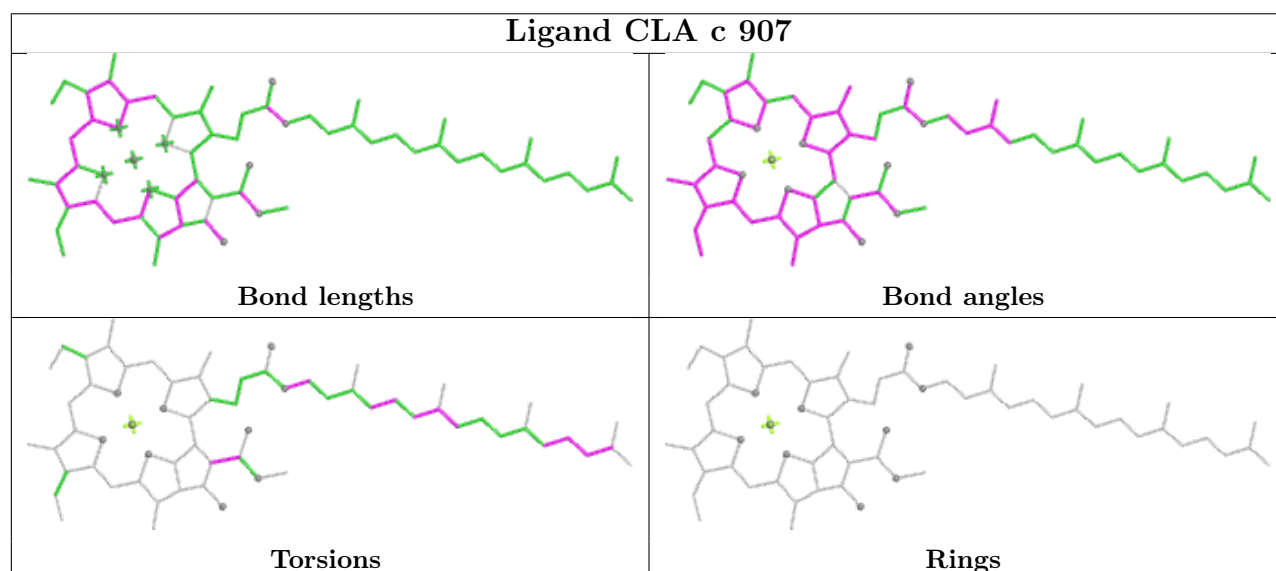
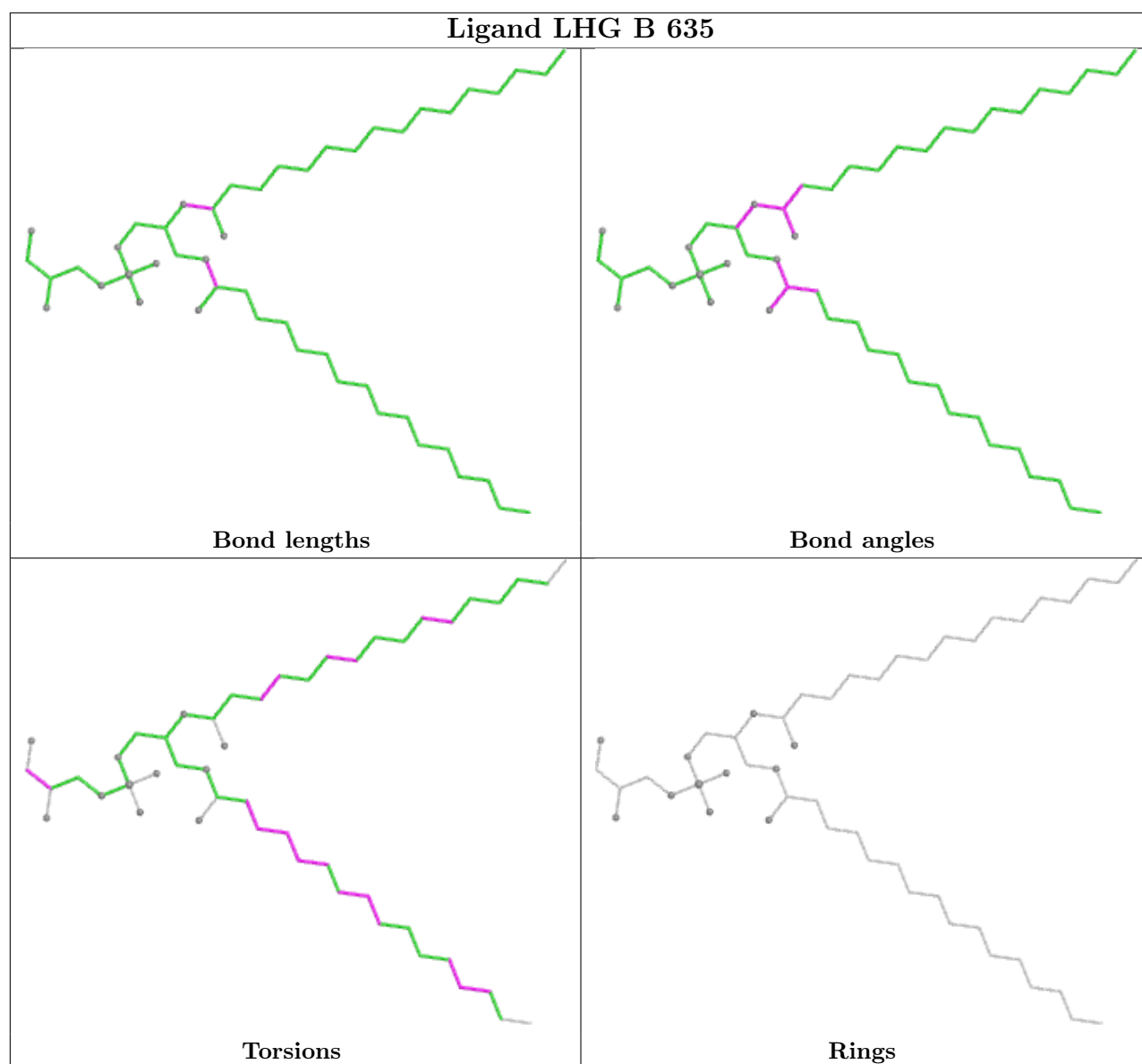


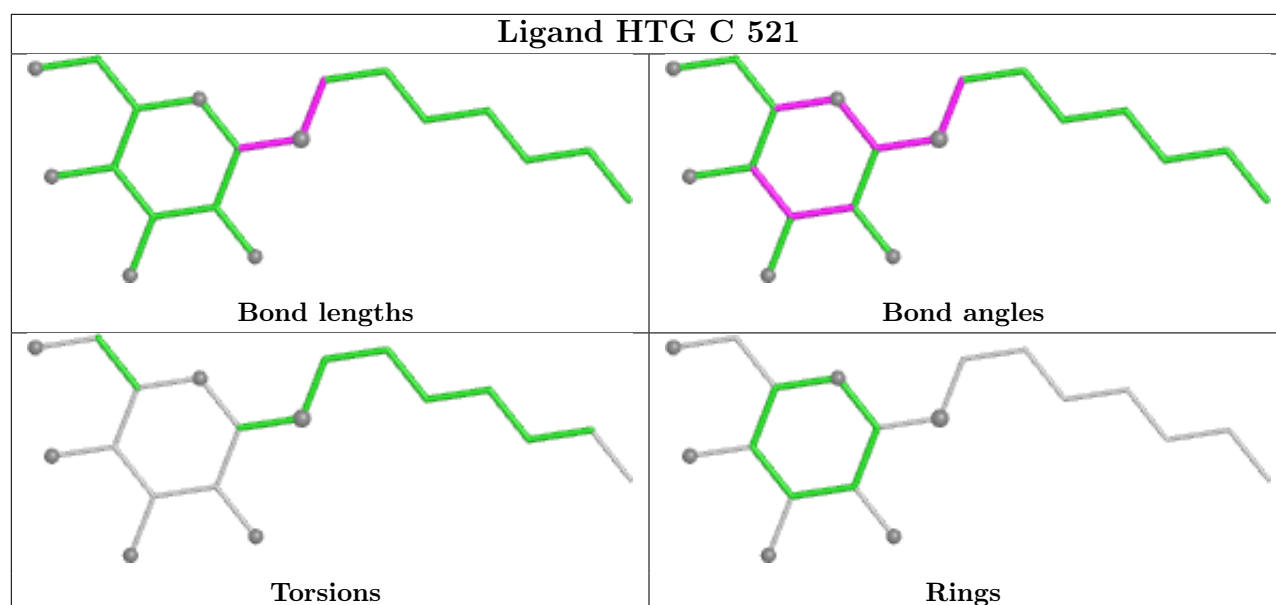
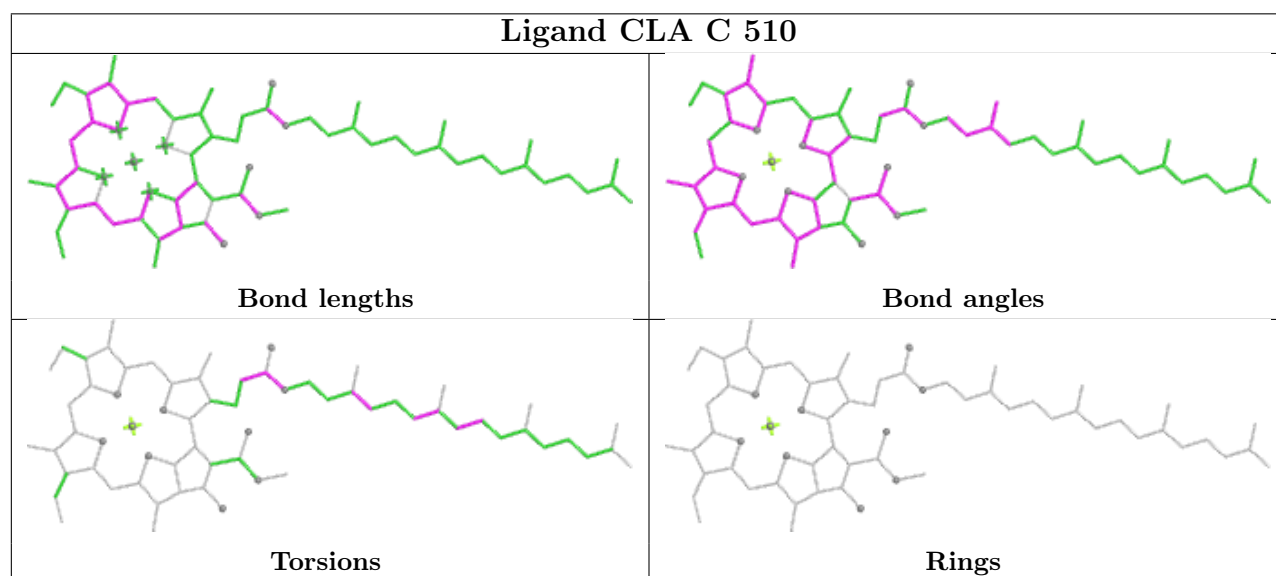
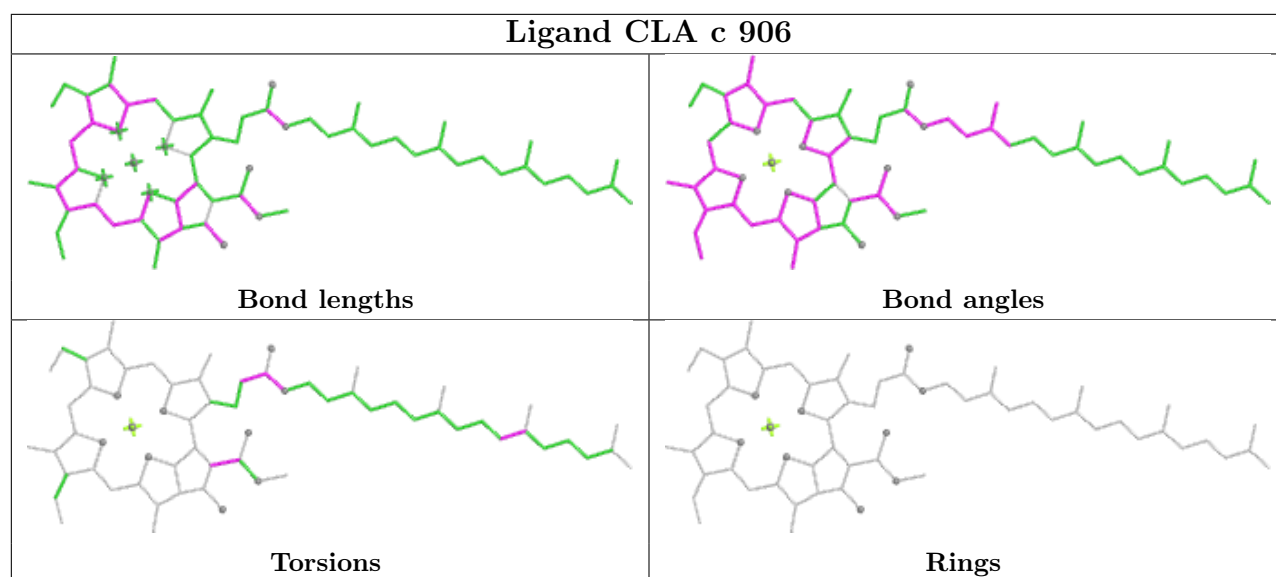


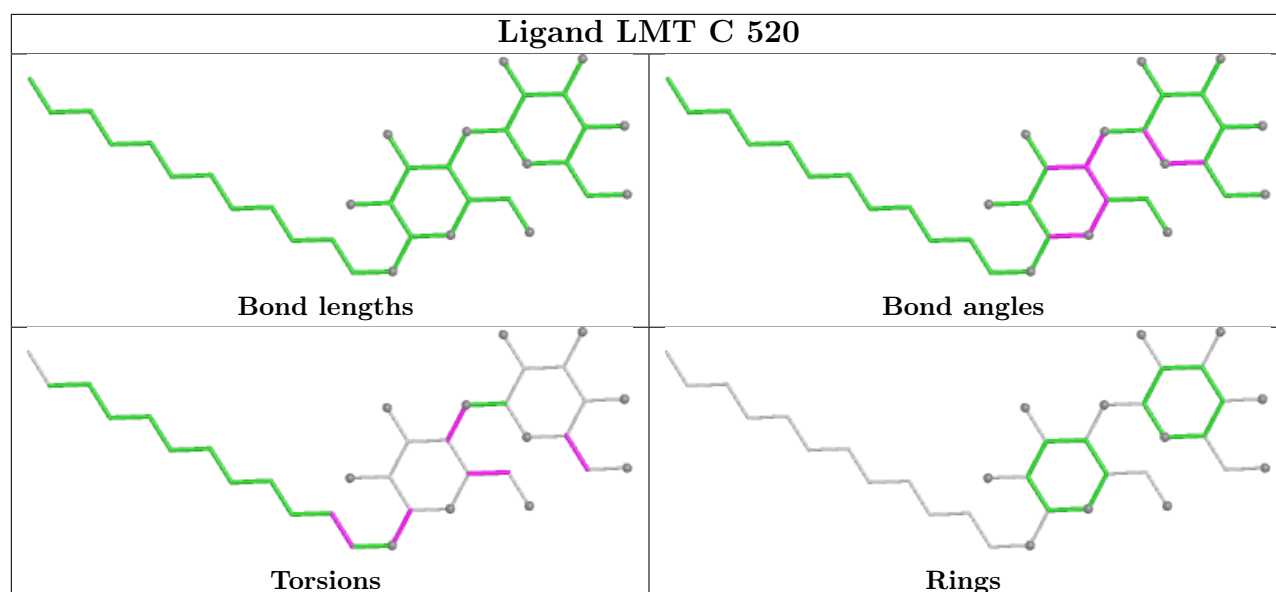
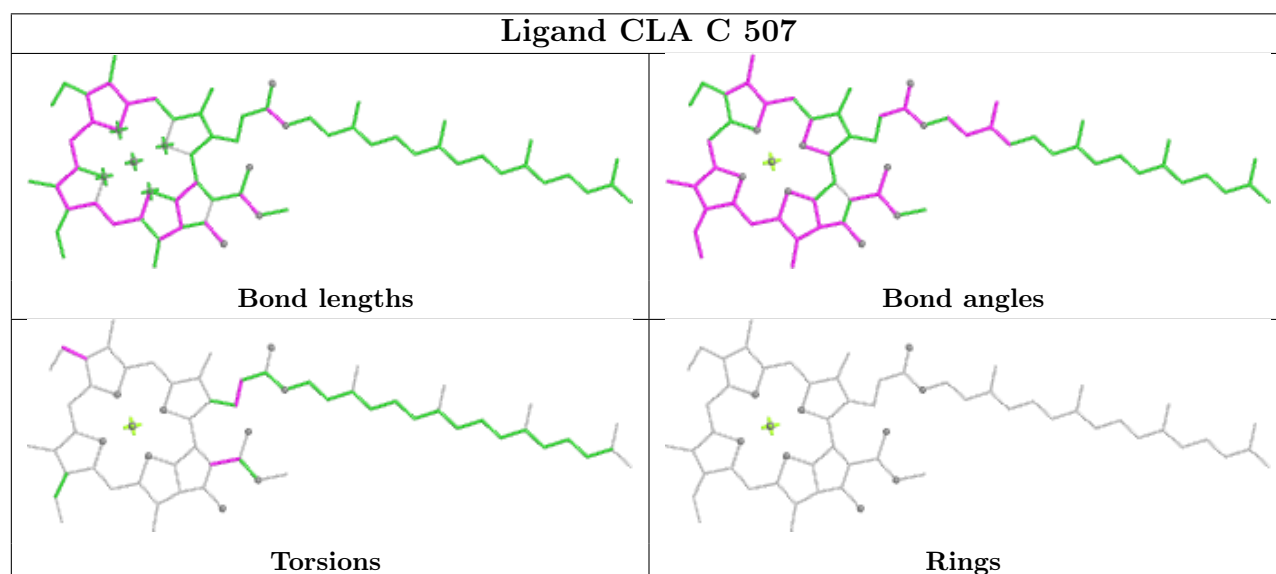
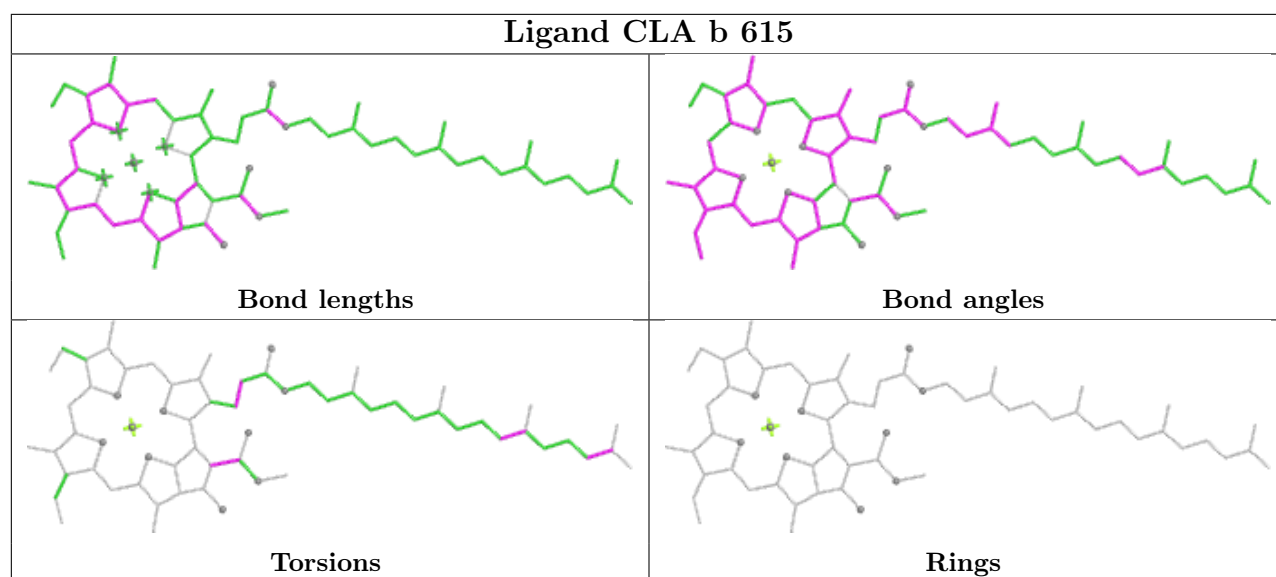


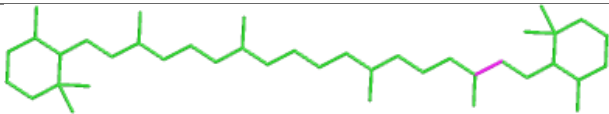
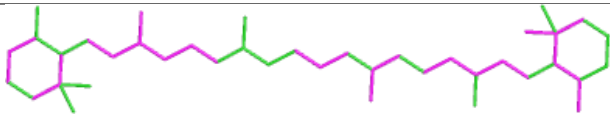
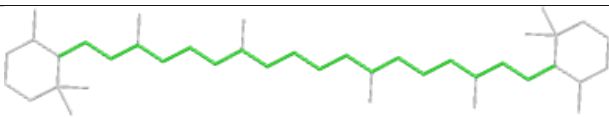
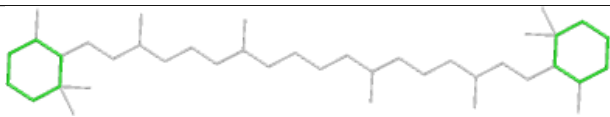


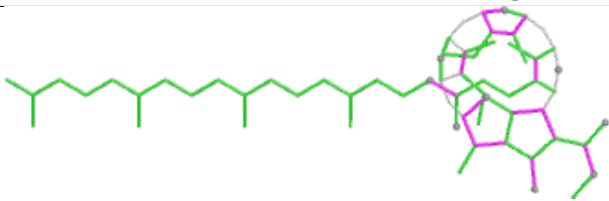
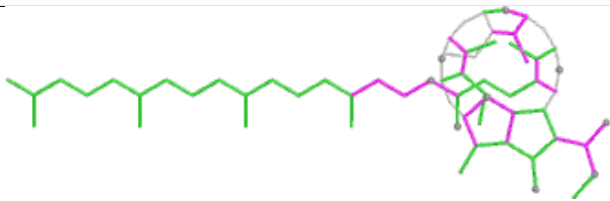
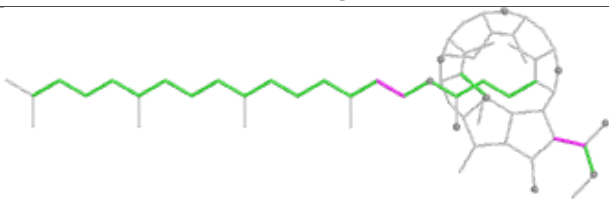
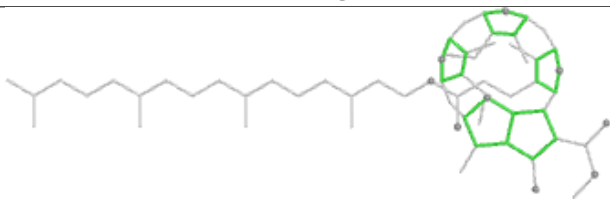


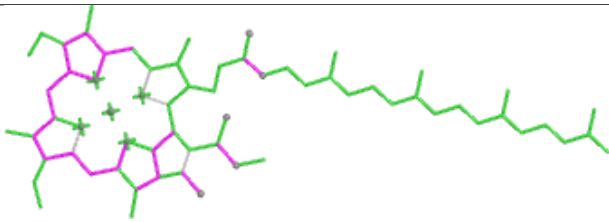
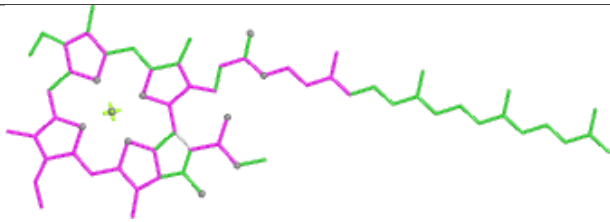
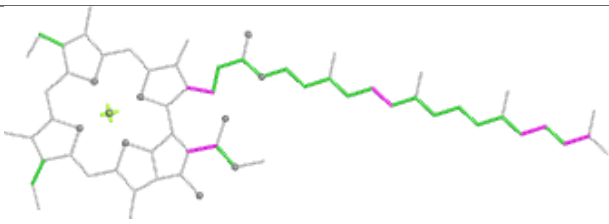
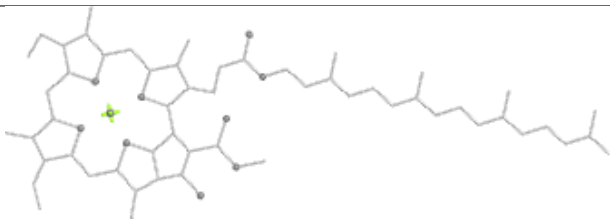


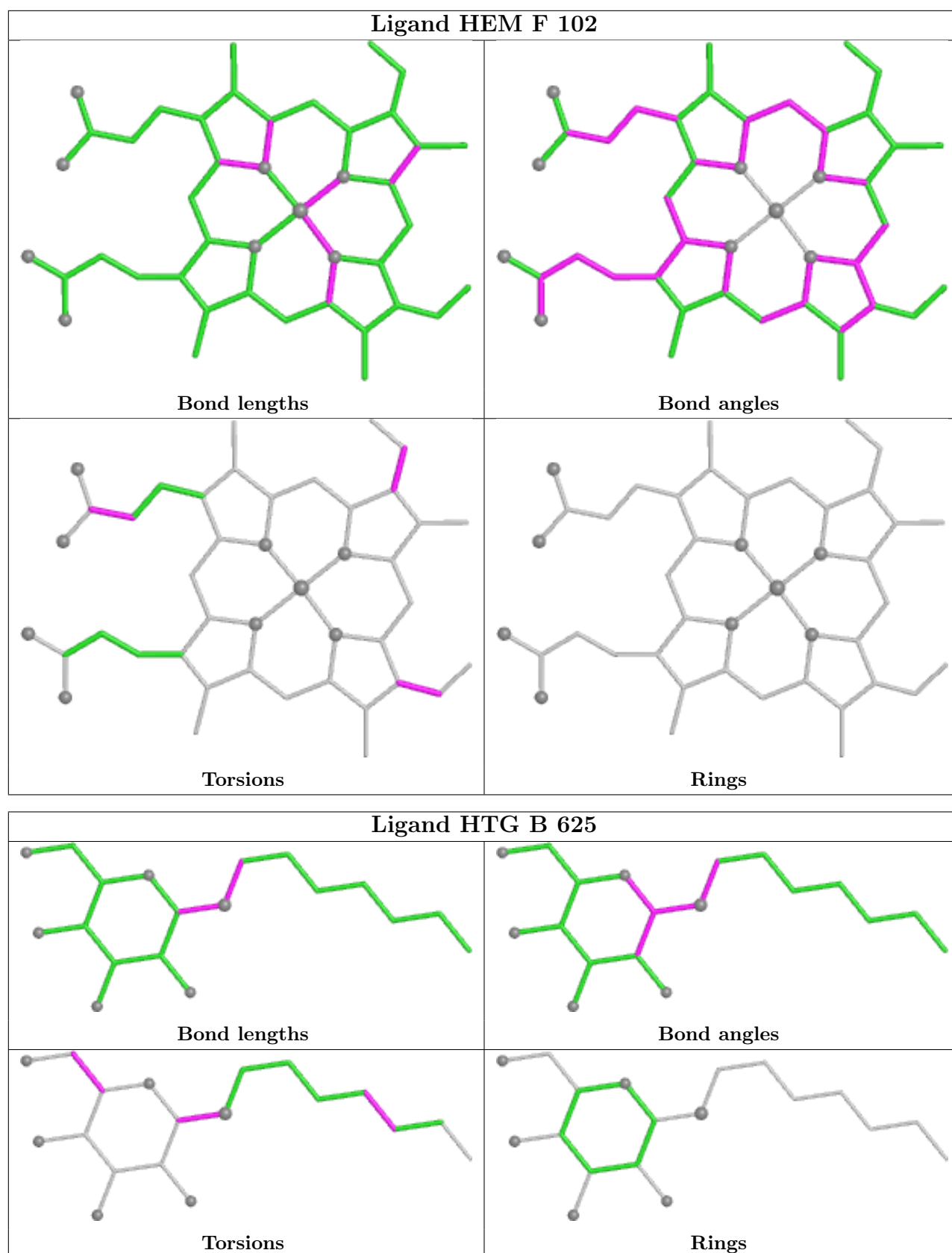


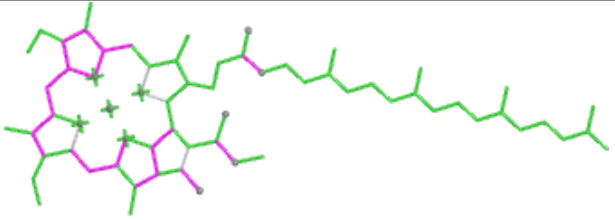
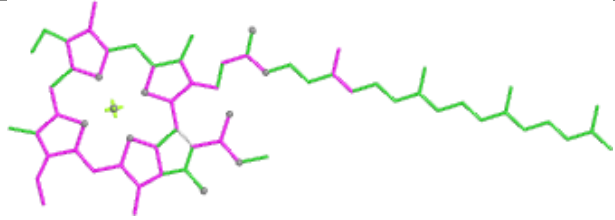
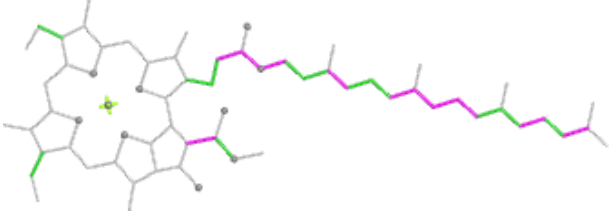
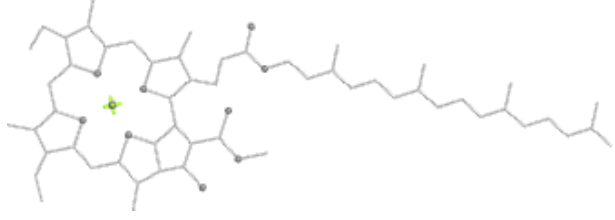
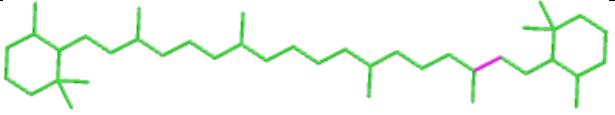
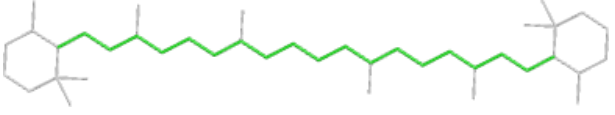
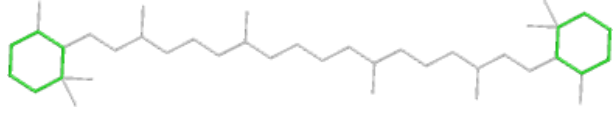
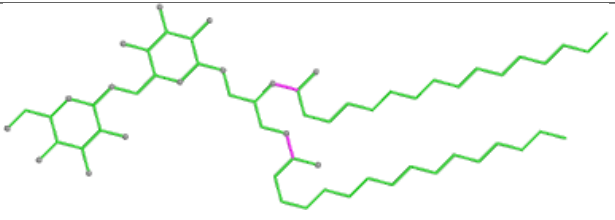
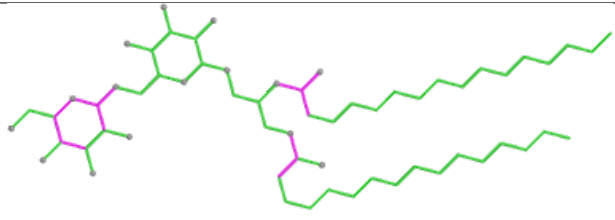
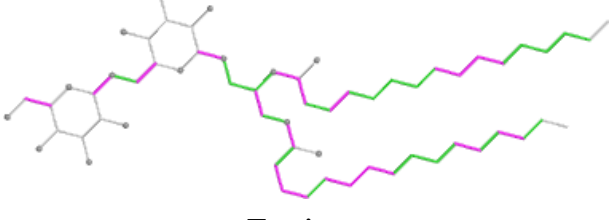
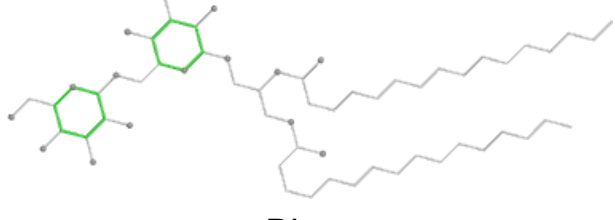


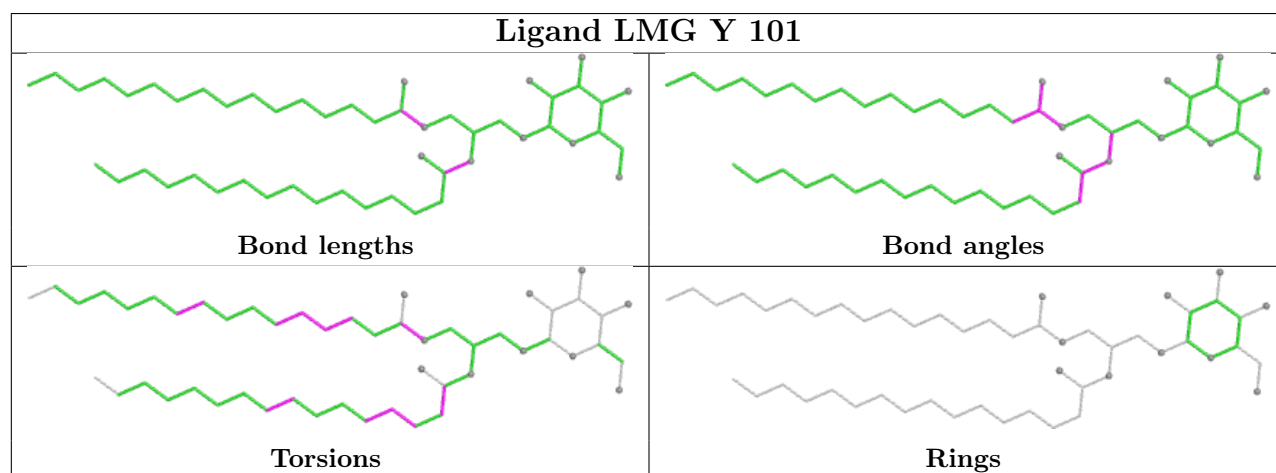
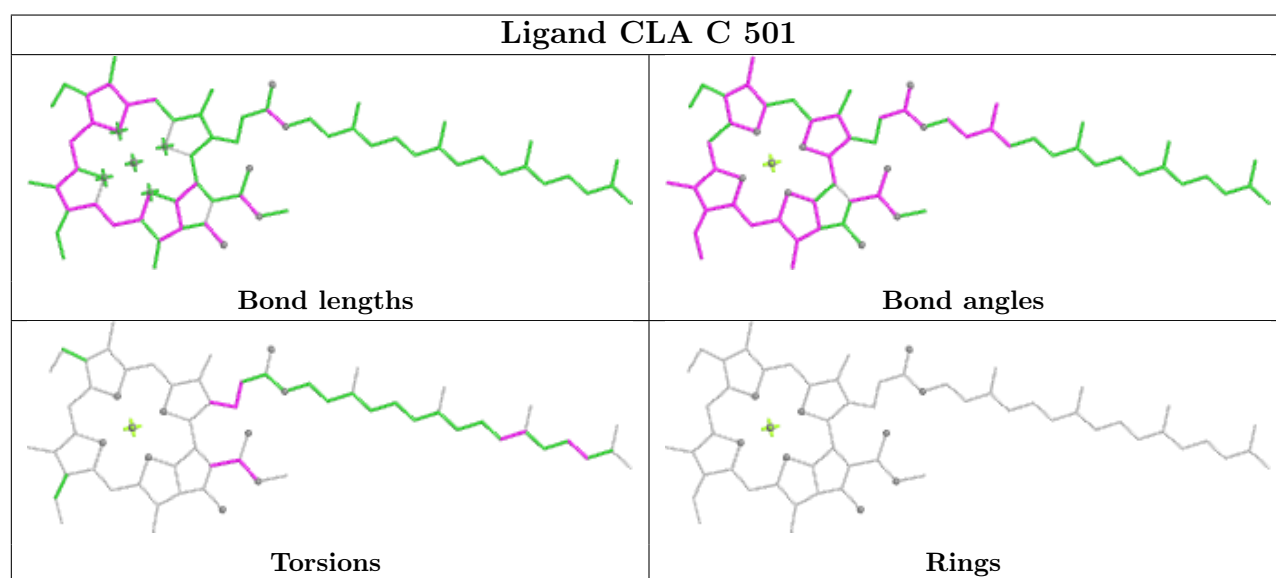
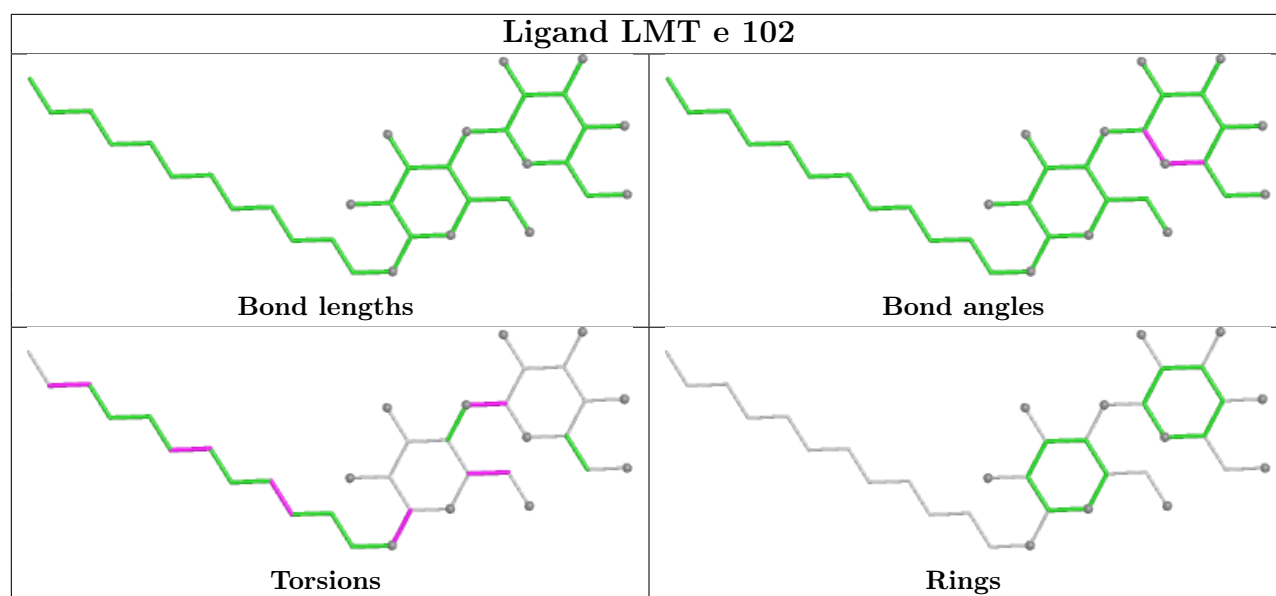
Ligand BCR k 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

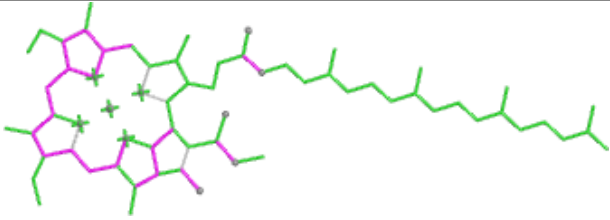
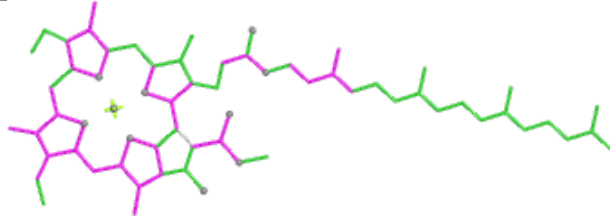
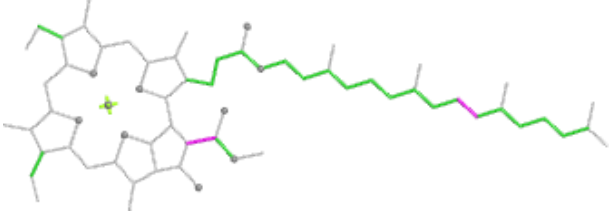
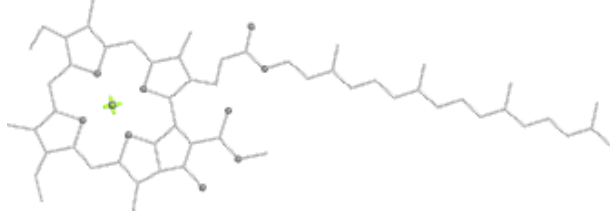
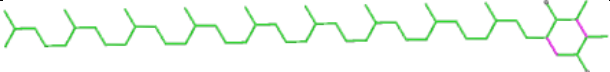
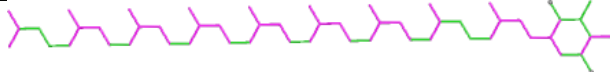
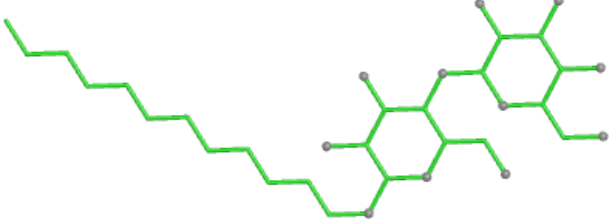
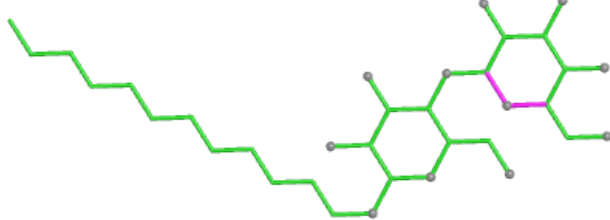
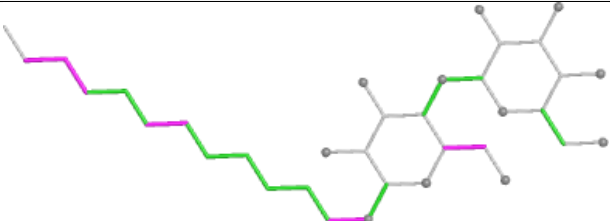
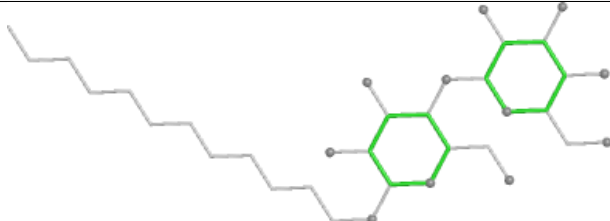
Ligand PHO A 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

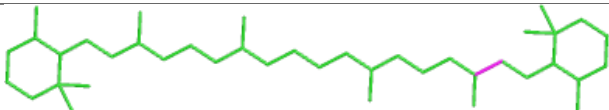
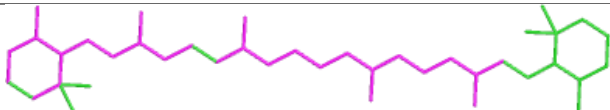
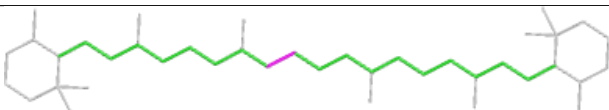
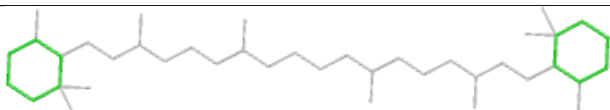
Ligand CLA C 506	
	
Bond lengths	Bond angles
	
Torsions	Rings

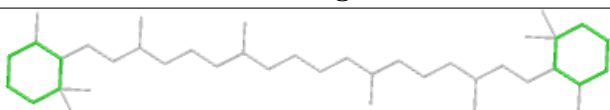


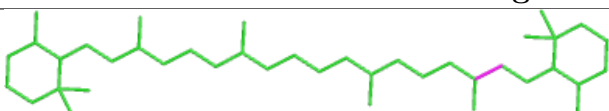
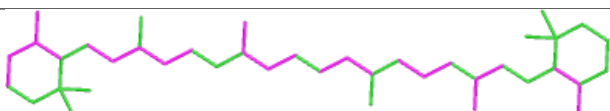
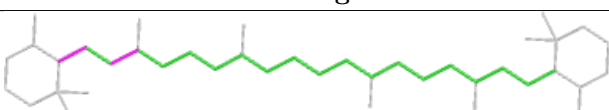
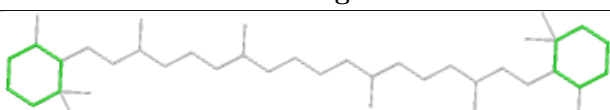
Ligand CLA b 606	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR K 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand DGD e 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

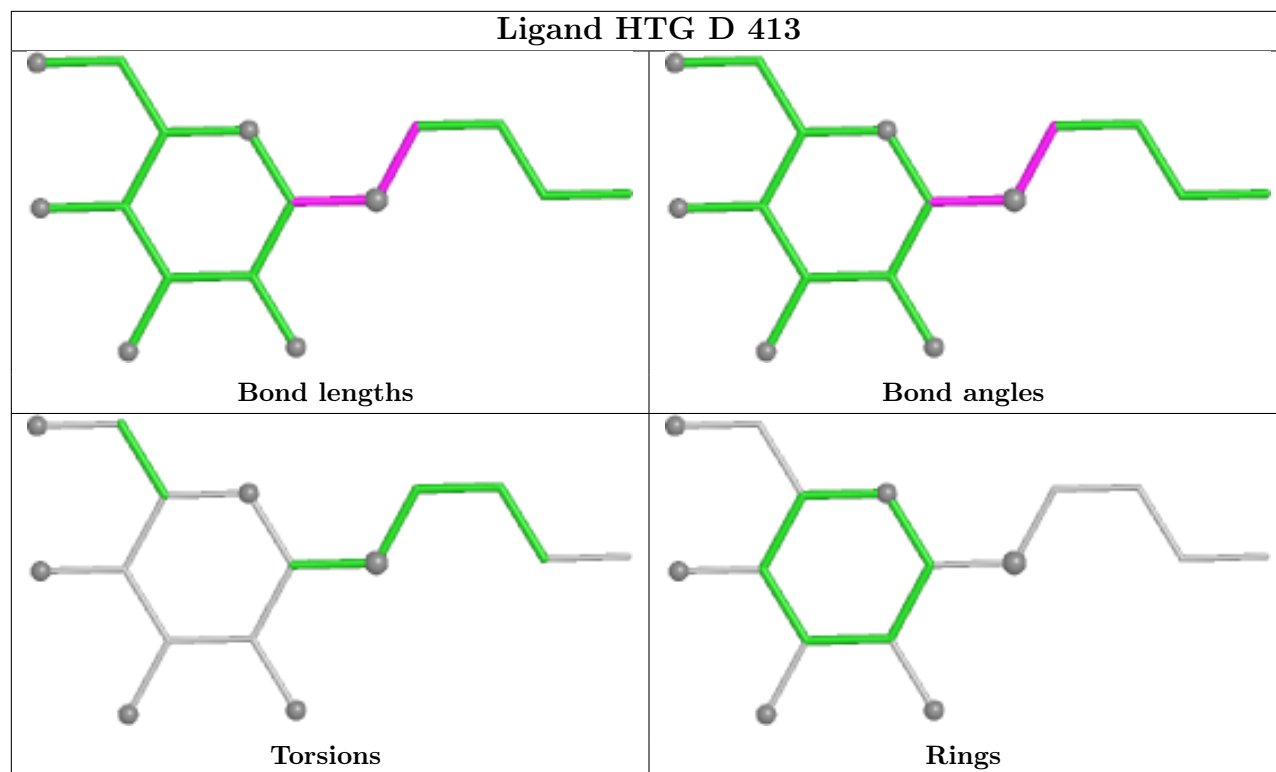


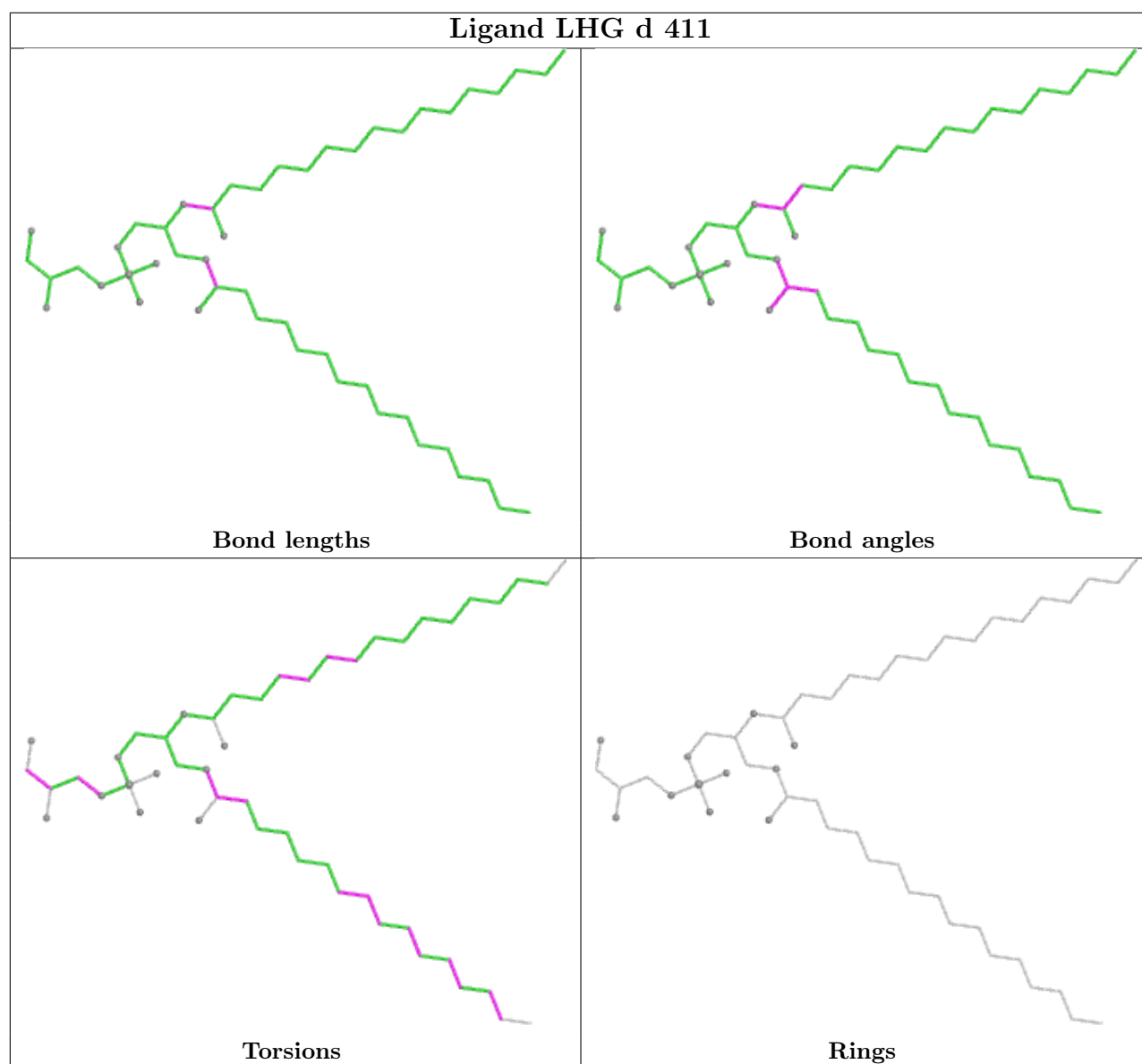
Ligand CLA C 503	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 a 415	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMT m 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

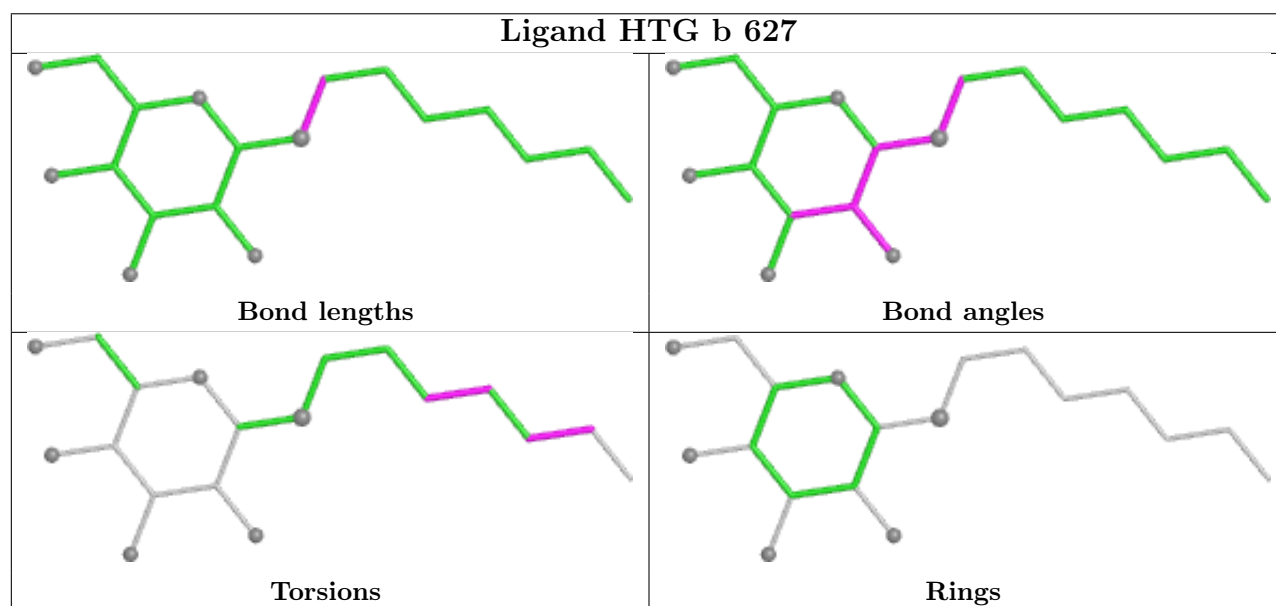
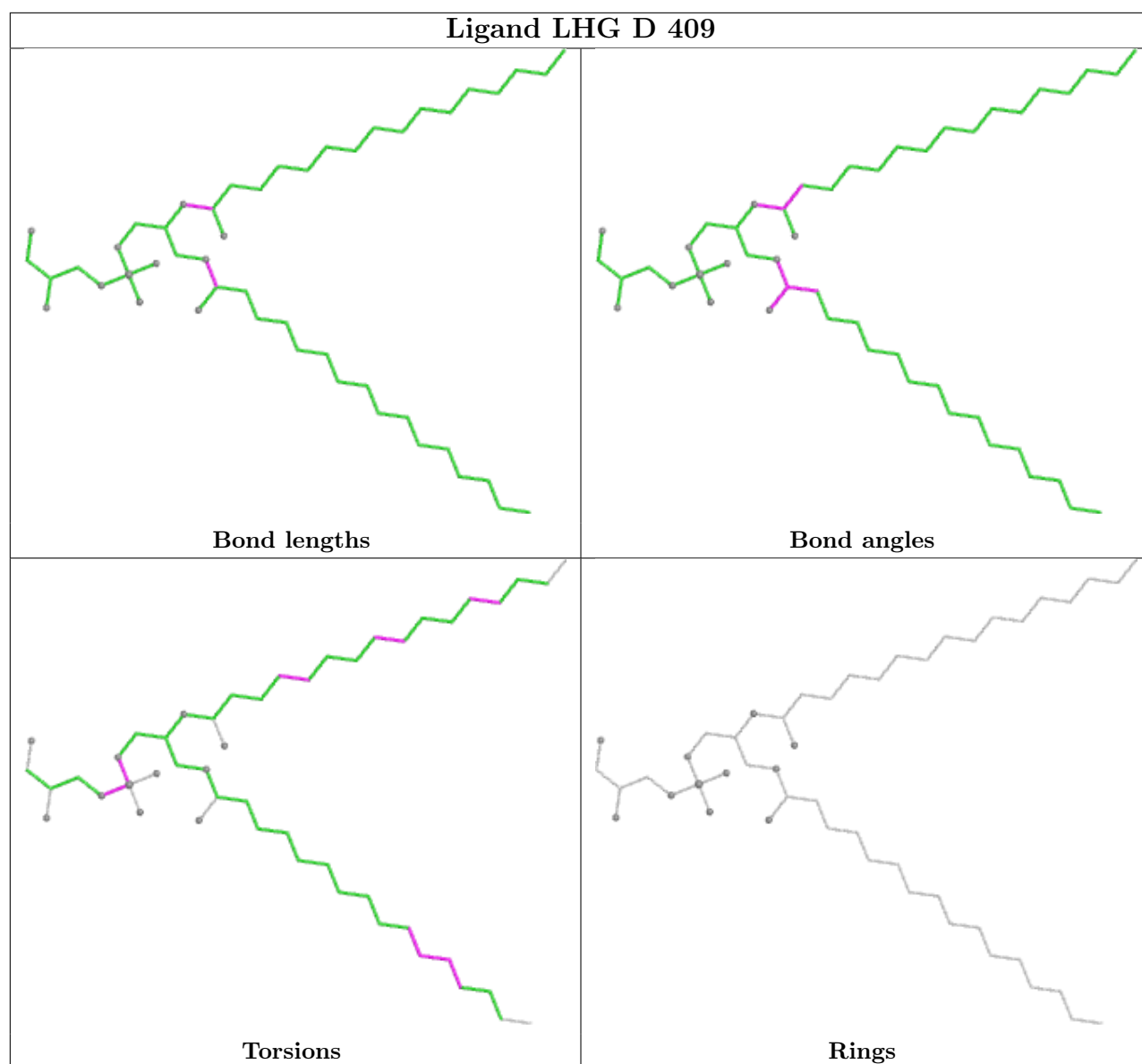
Ligand BCR T 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

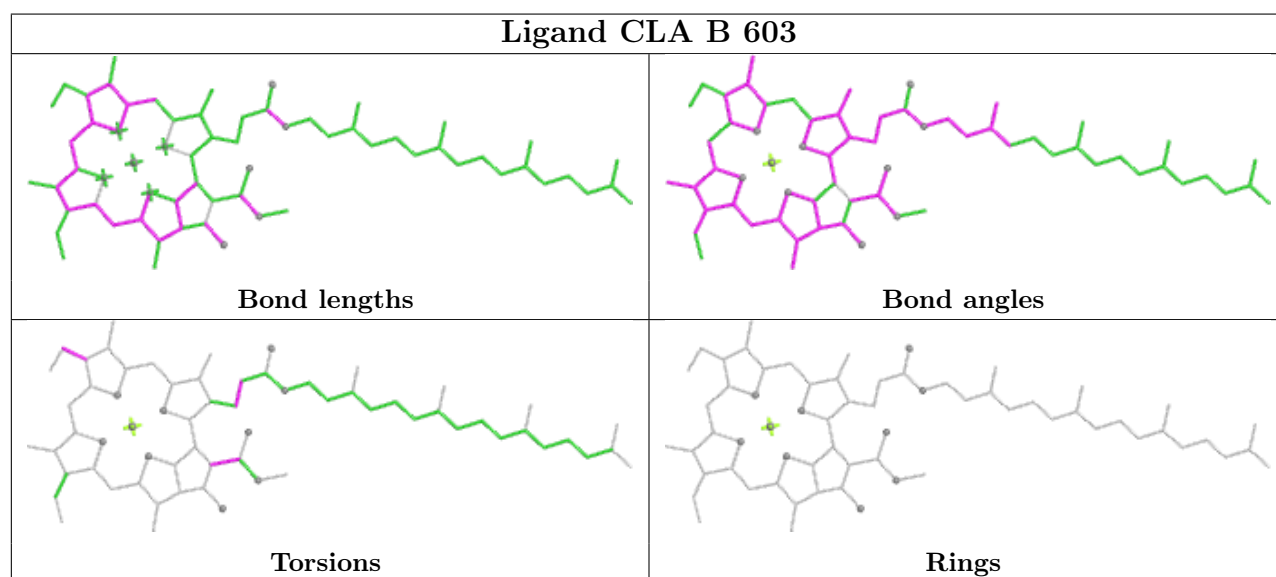
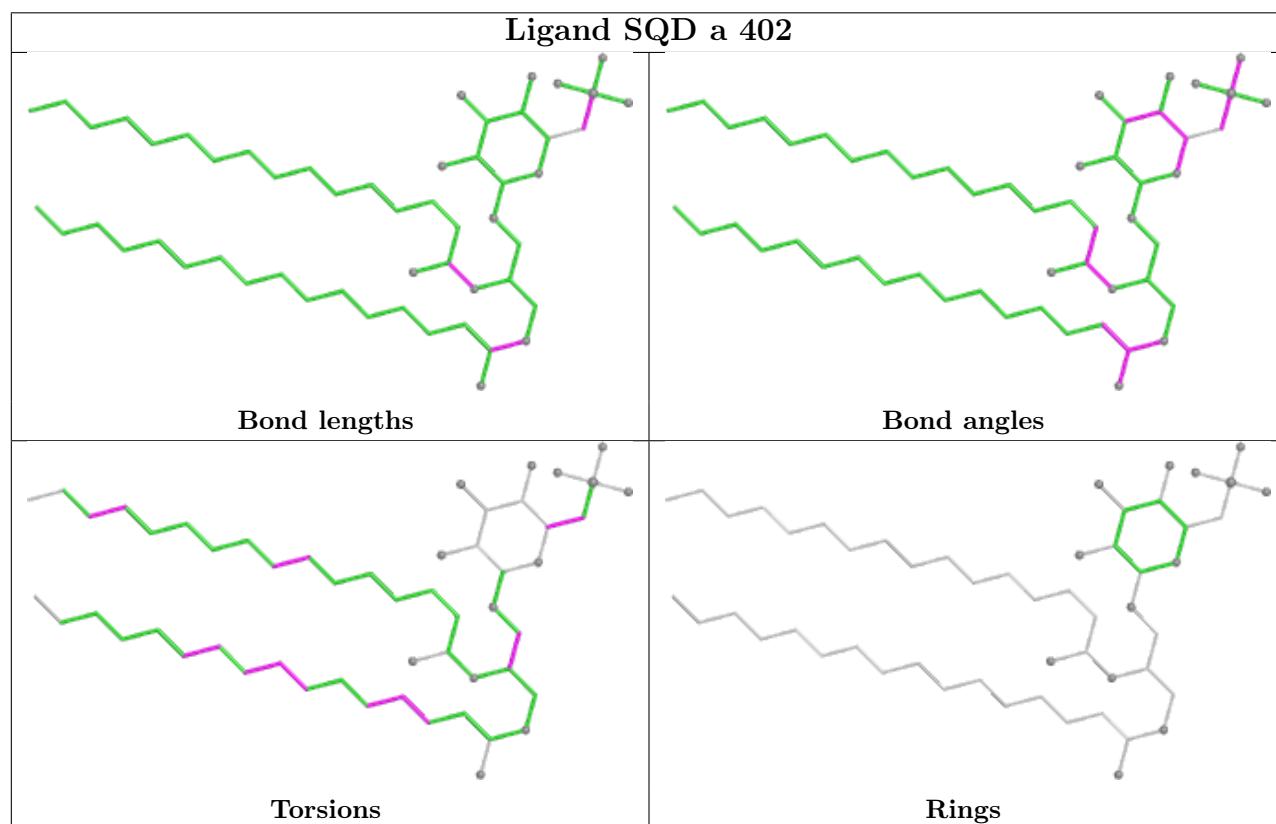
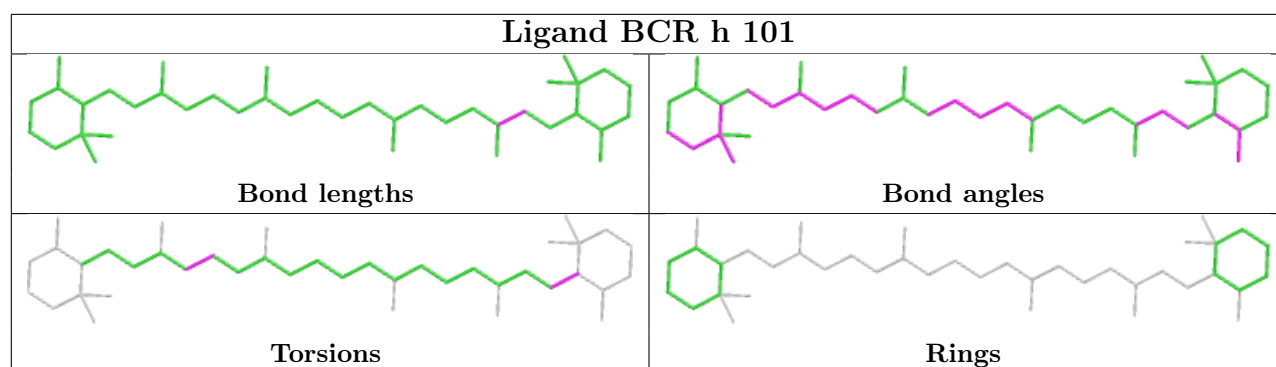
Ligand BCR D 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

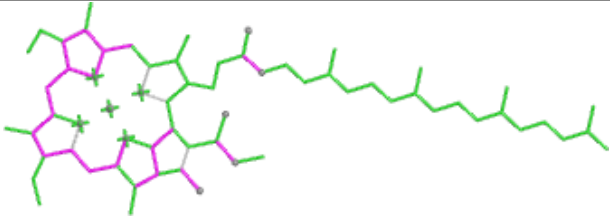
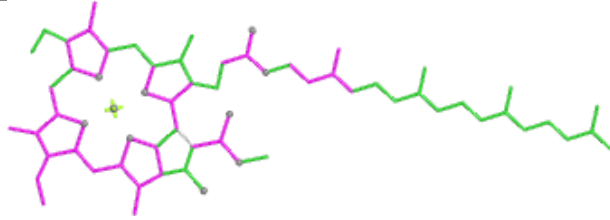
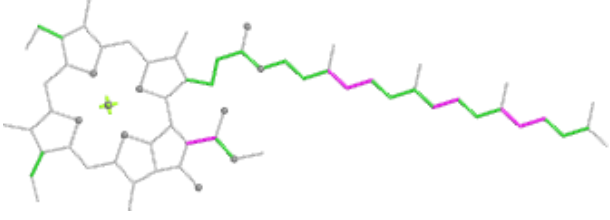
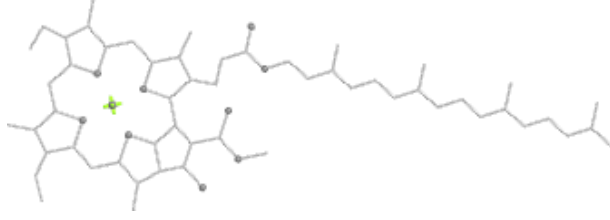
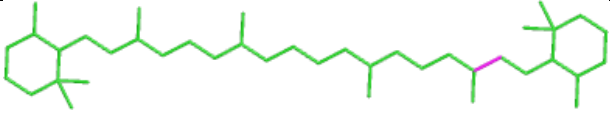
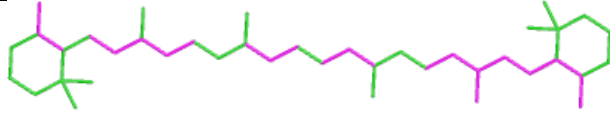
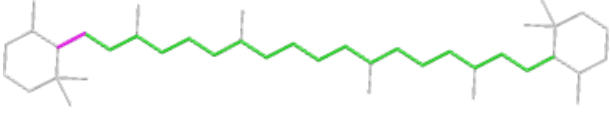
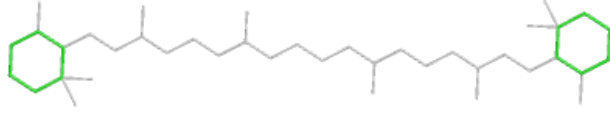
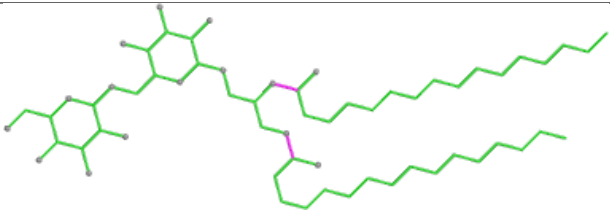
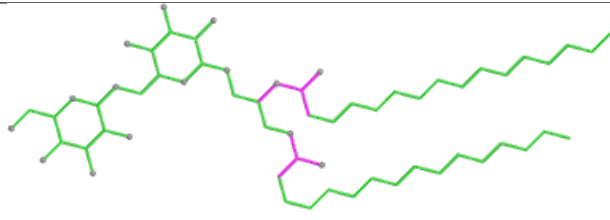
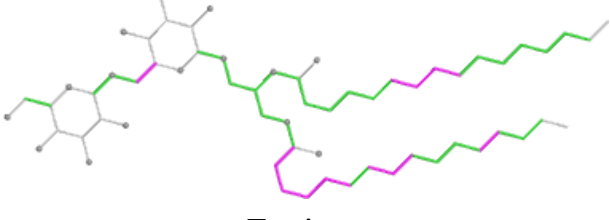
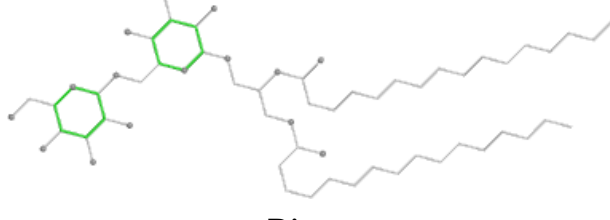
Ligand BCR c 915	
	
Bond lengths	Bond angles
	
Torsions	Rings

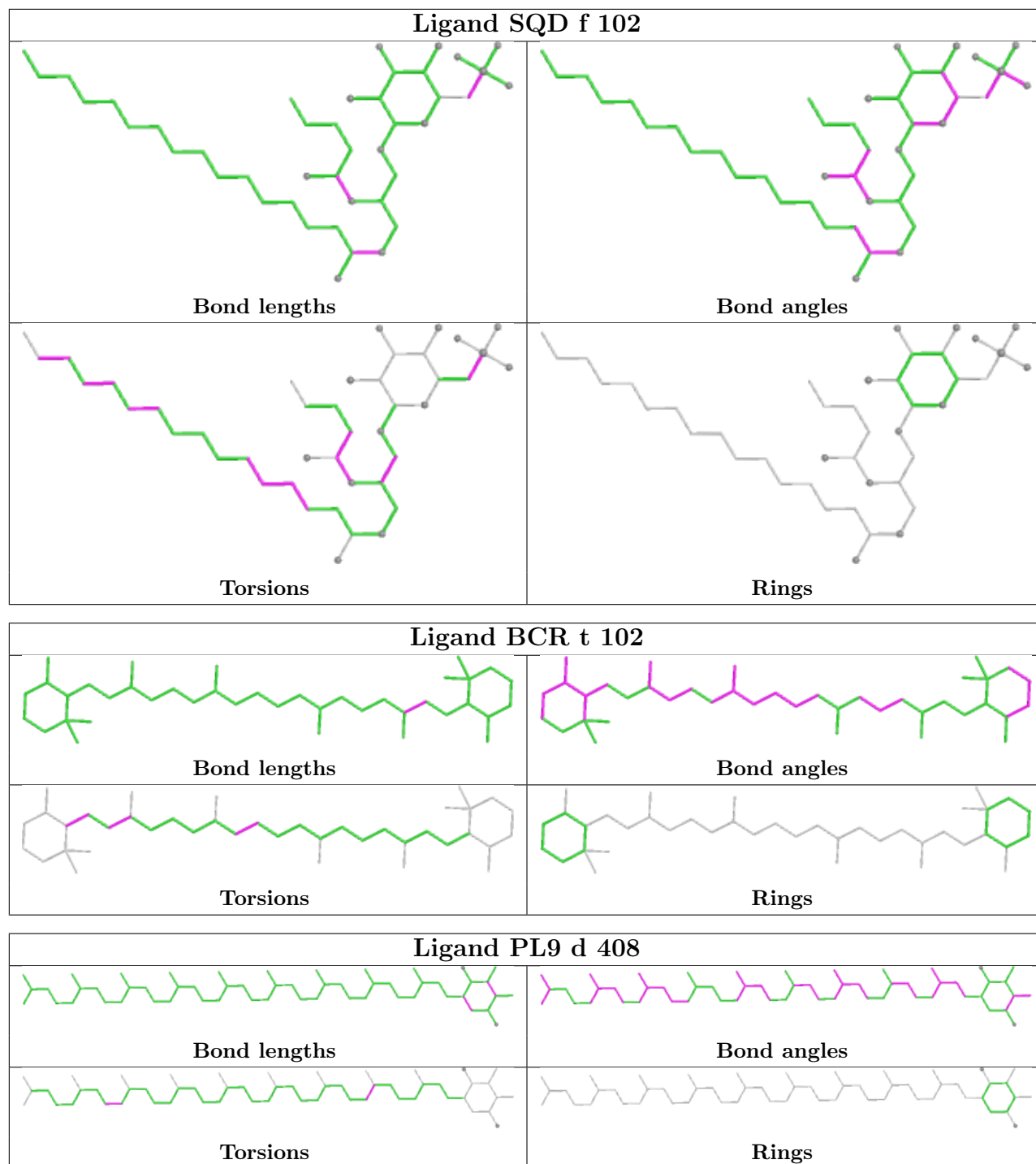


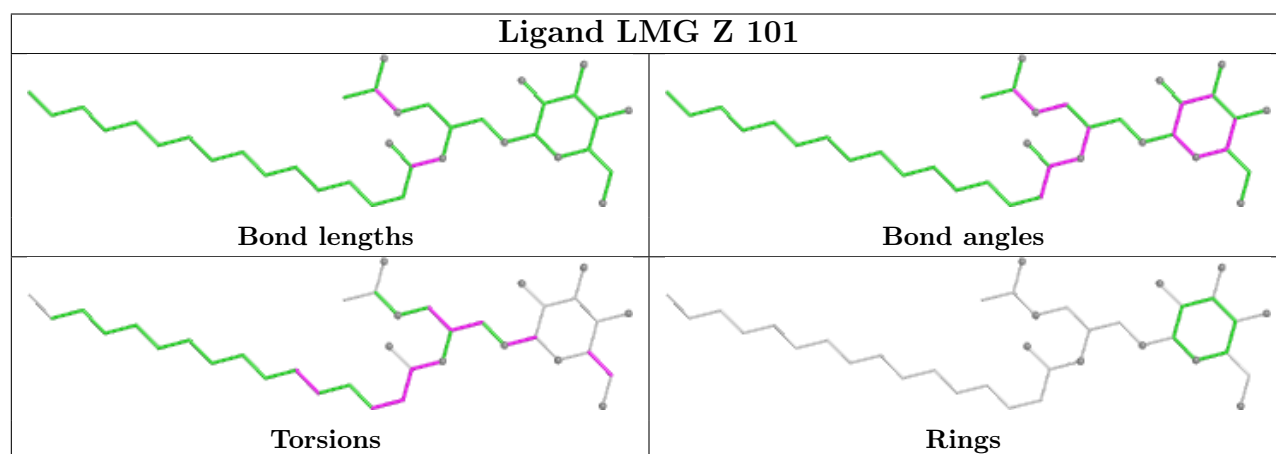
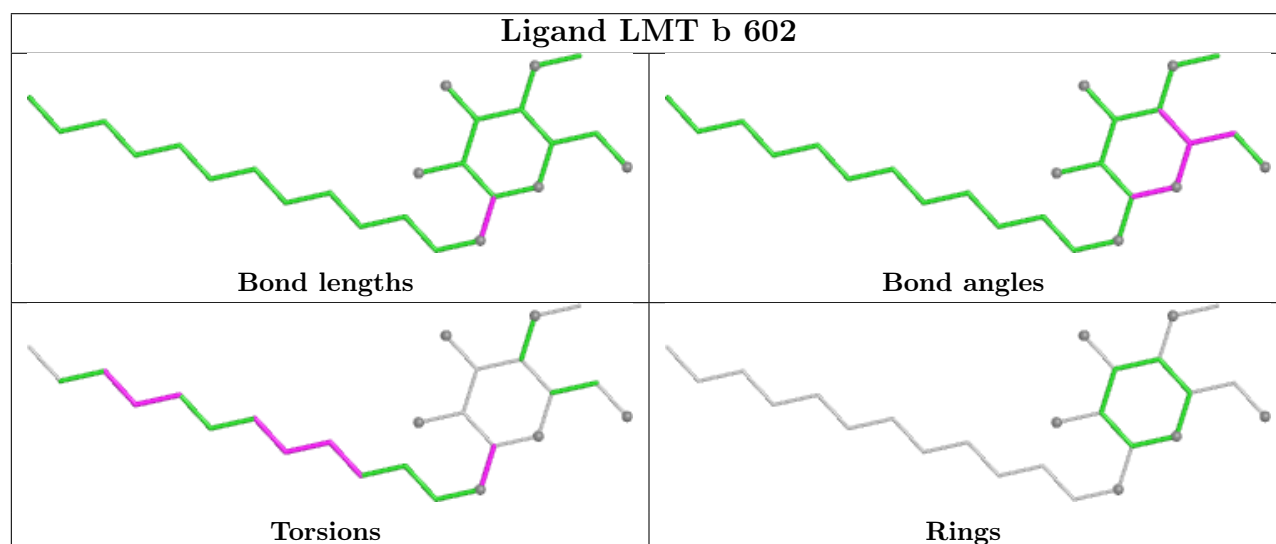
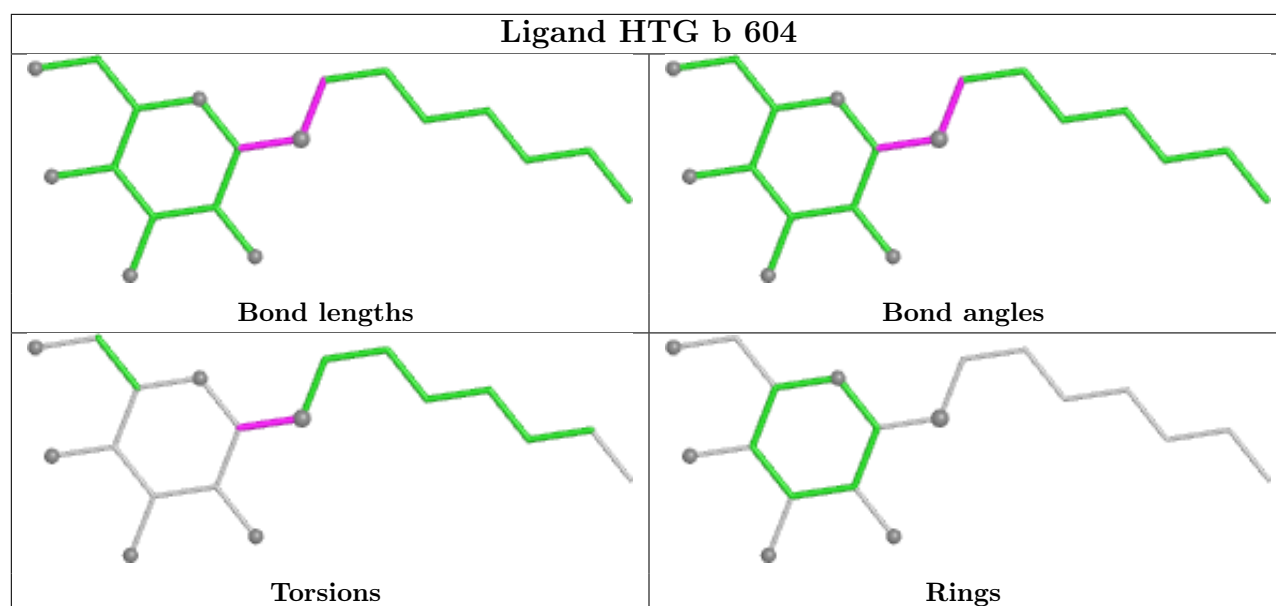


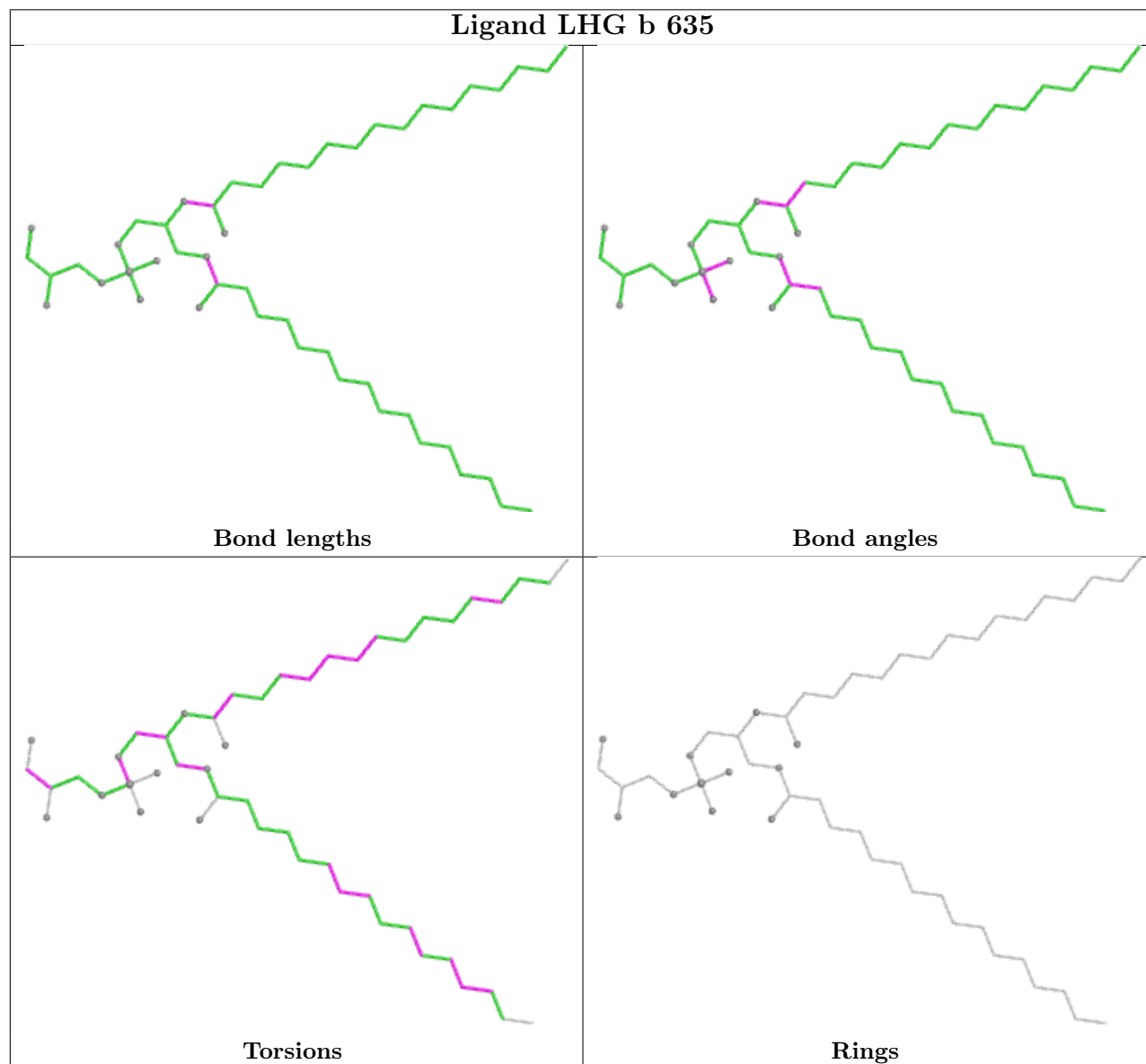
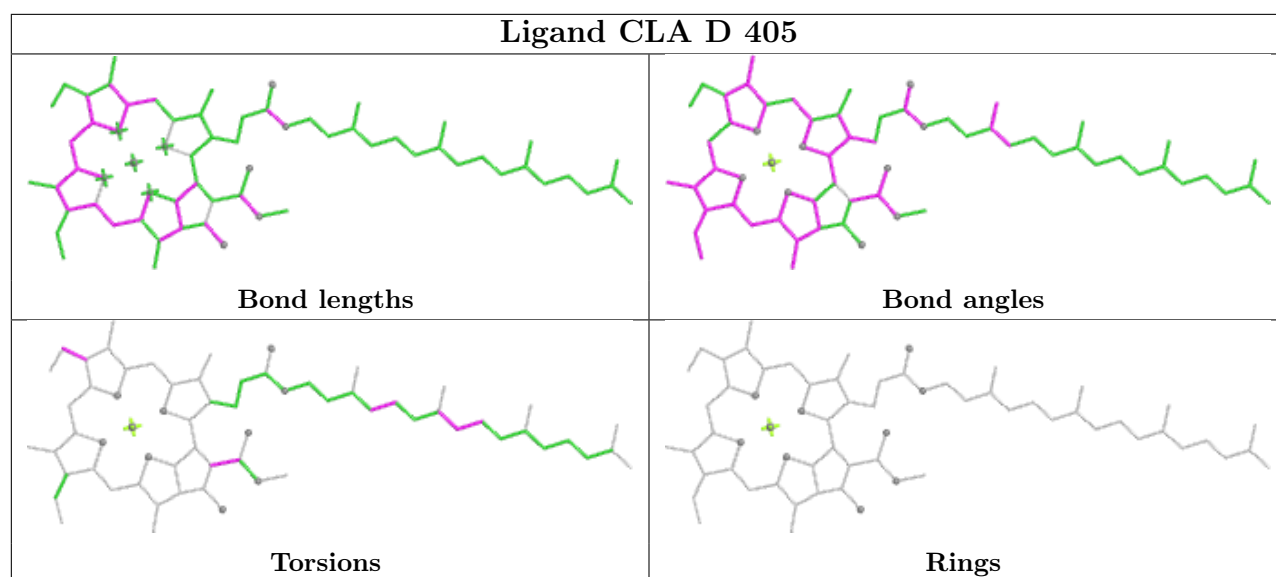


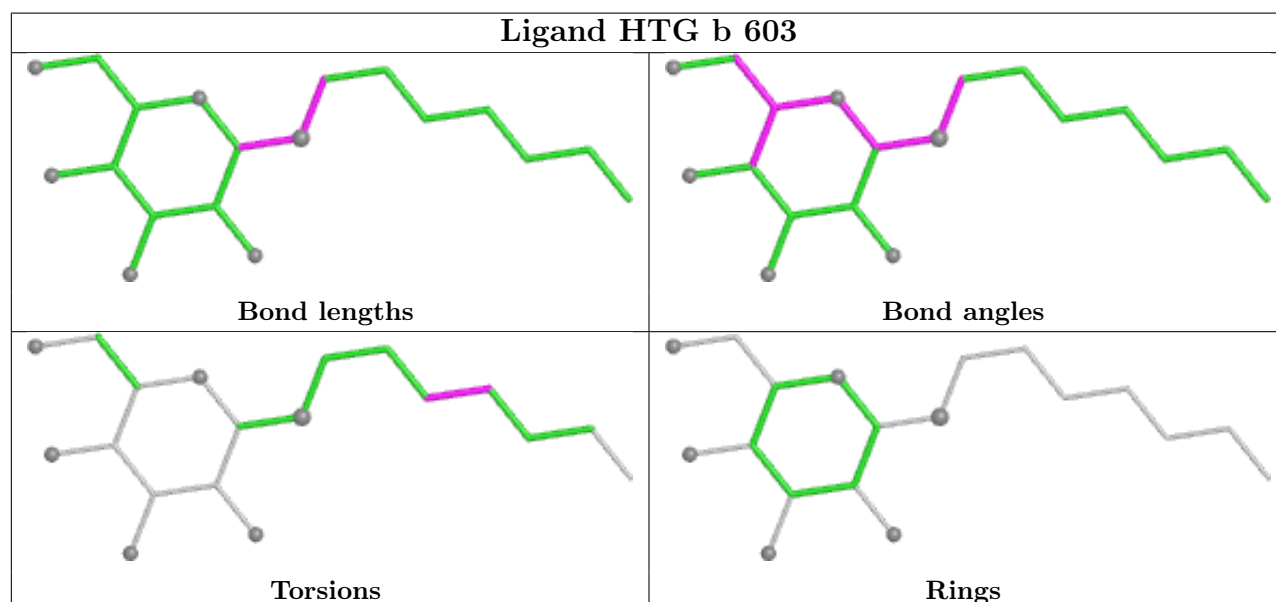
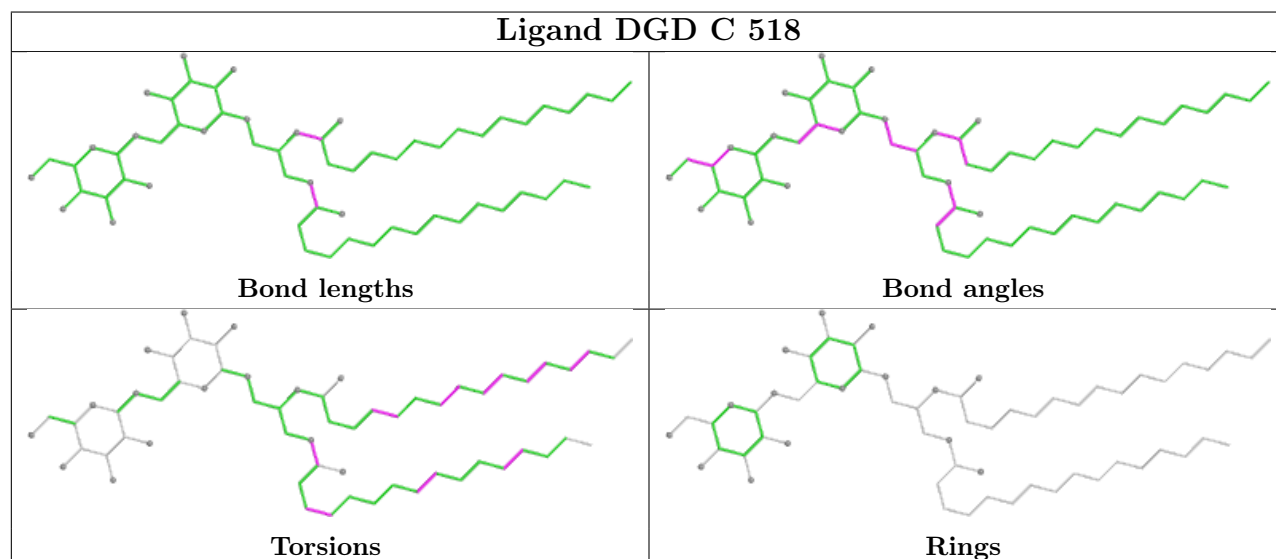
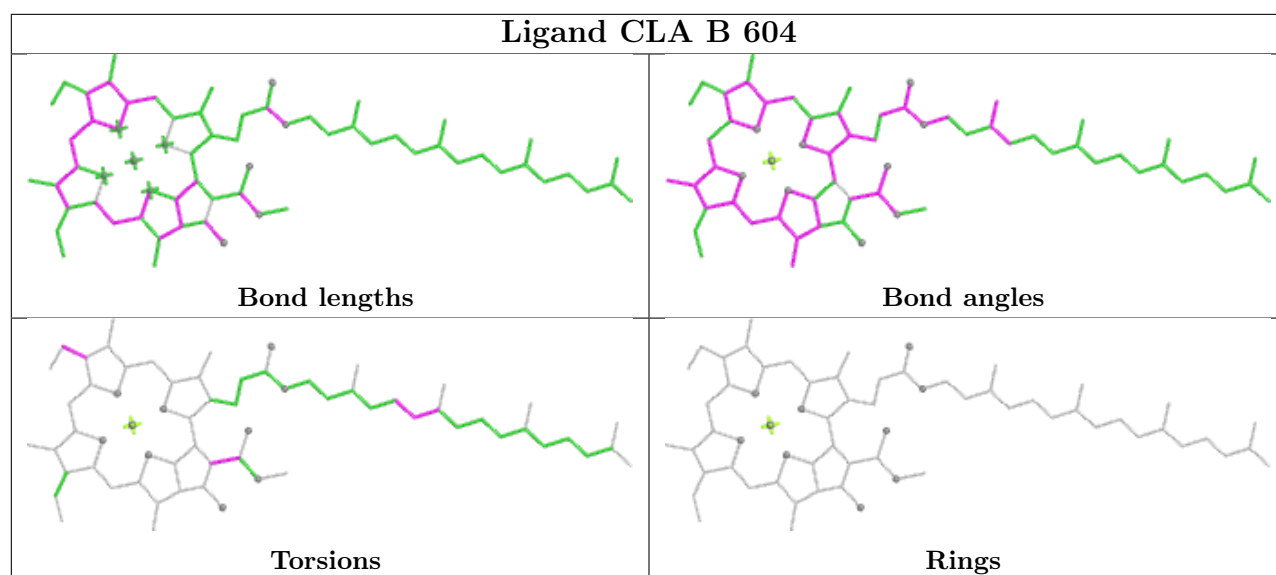


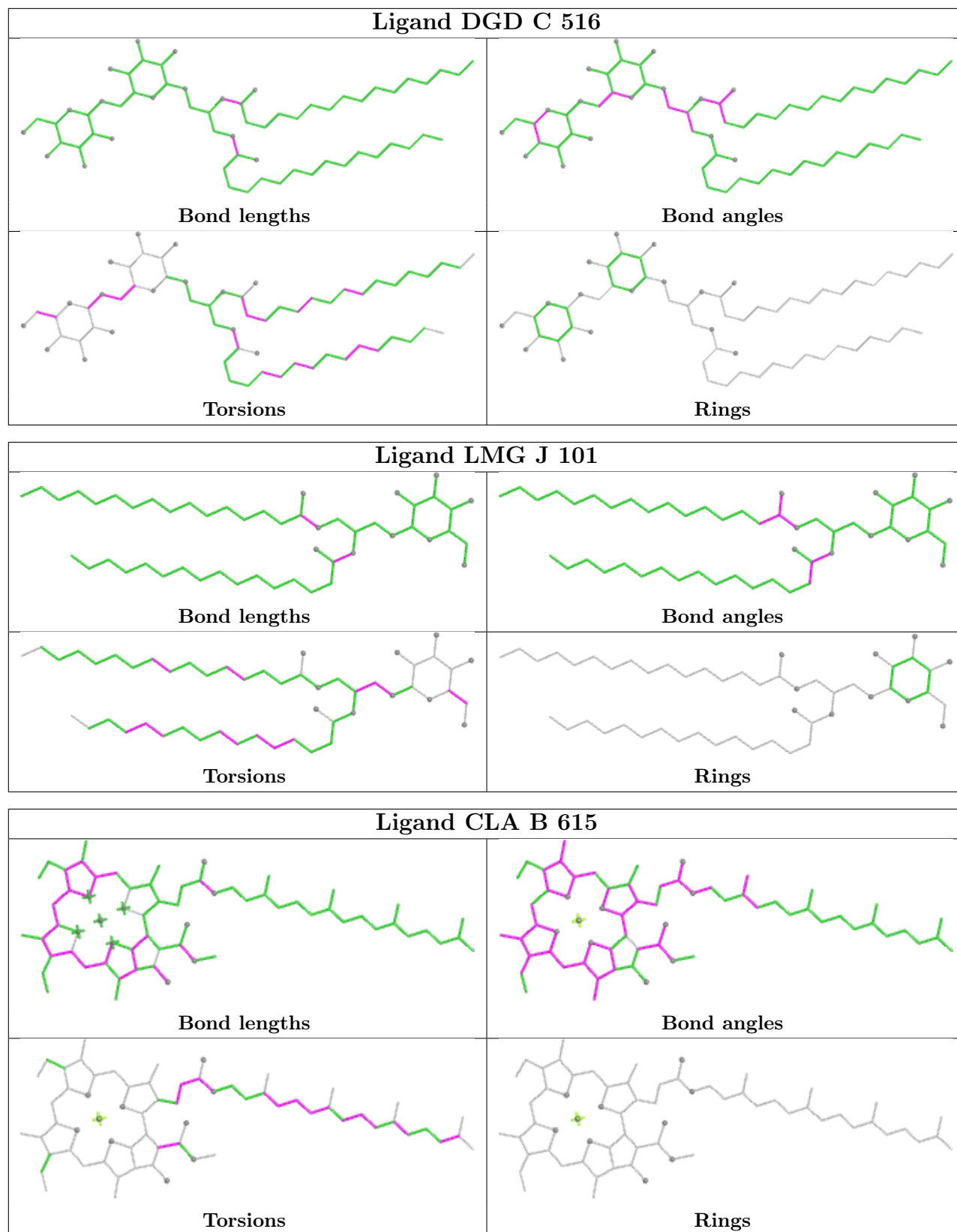
Ligand CLA c 911	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR C 514	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand DGD c 918	
 Bond lengths	 Bond angles
 Torsions	 Rings

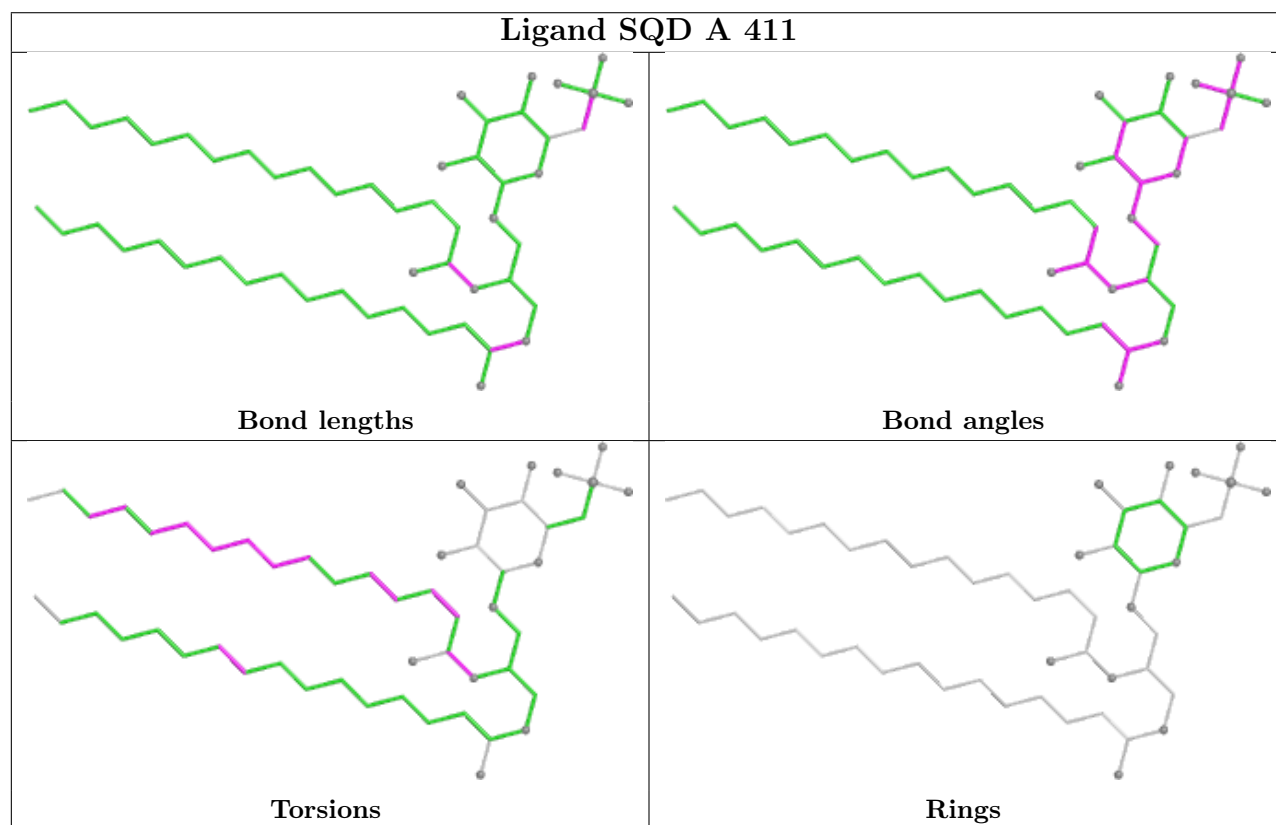
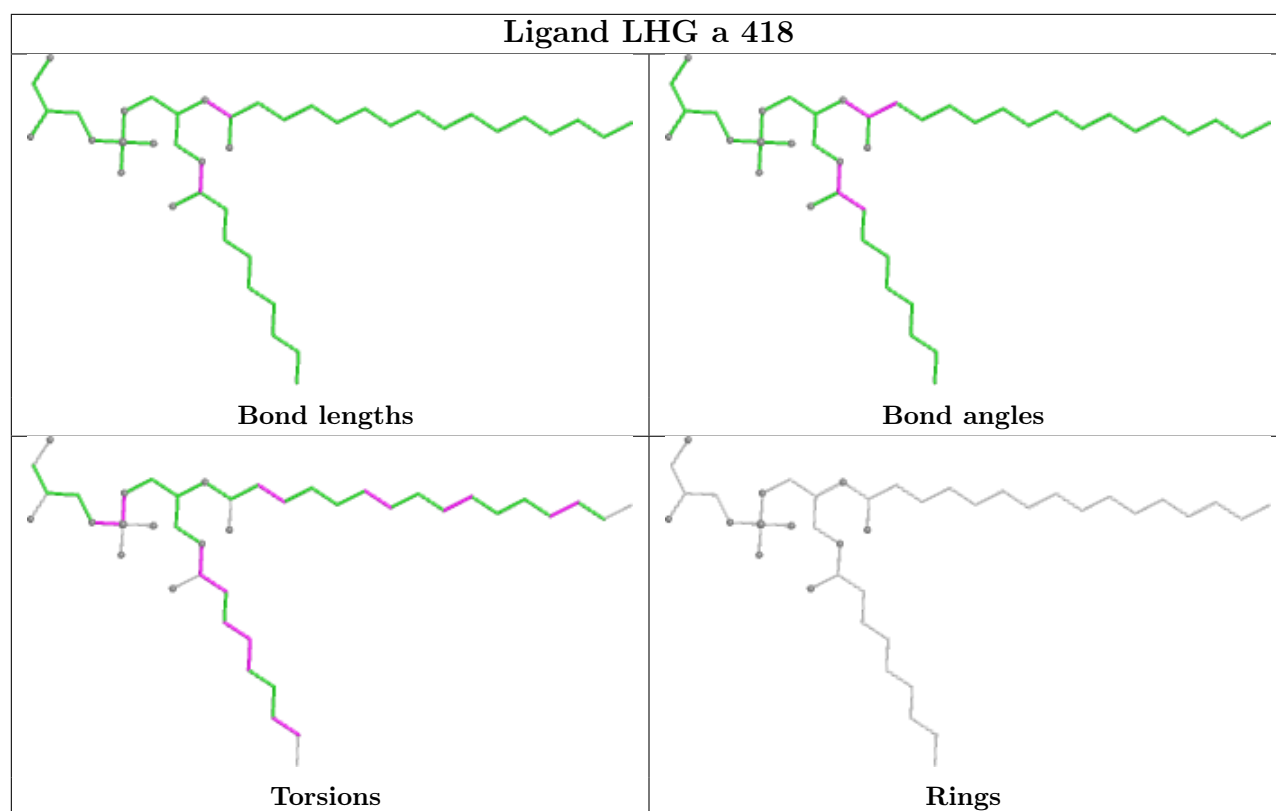


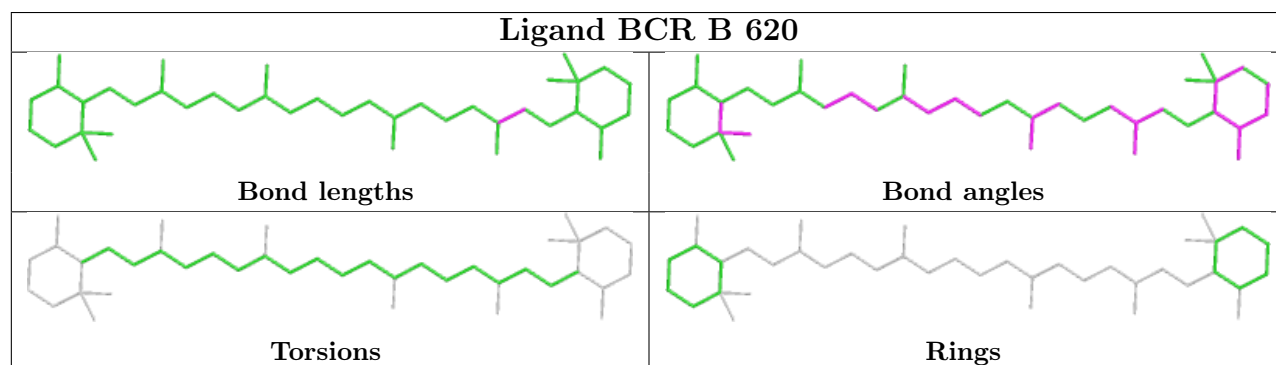
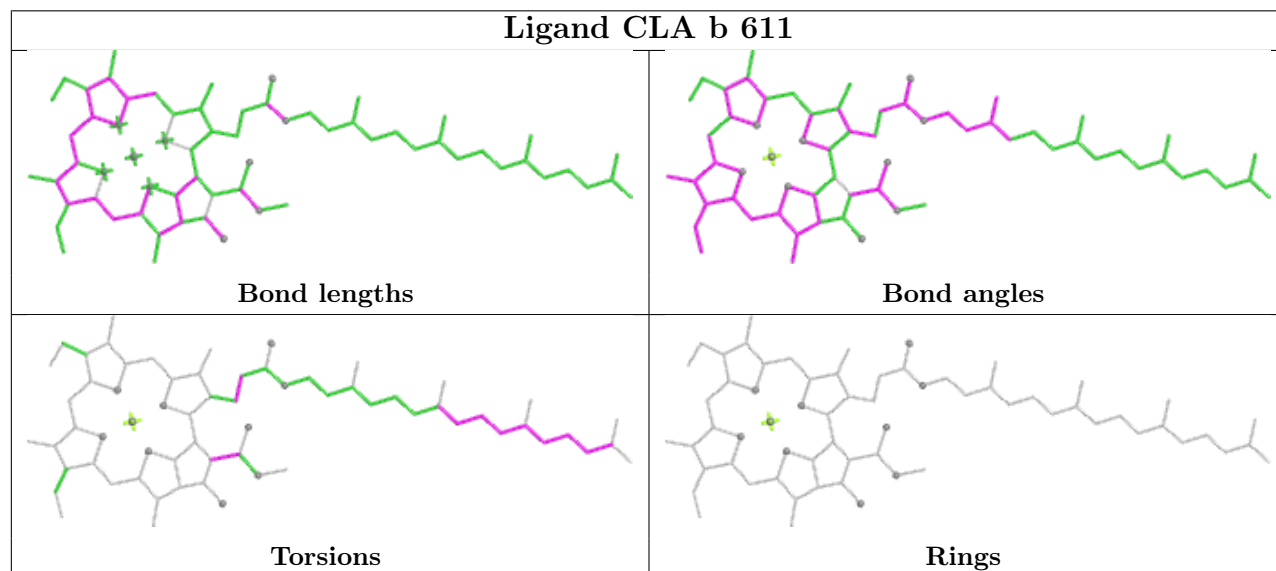
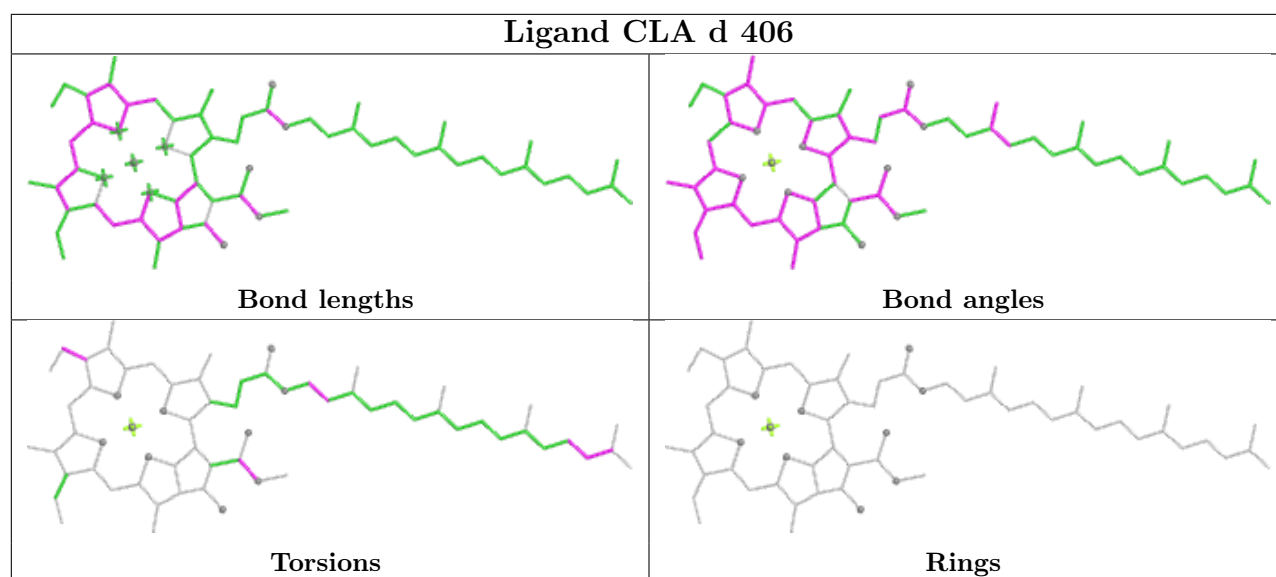


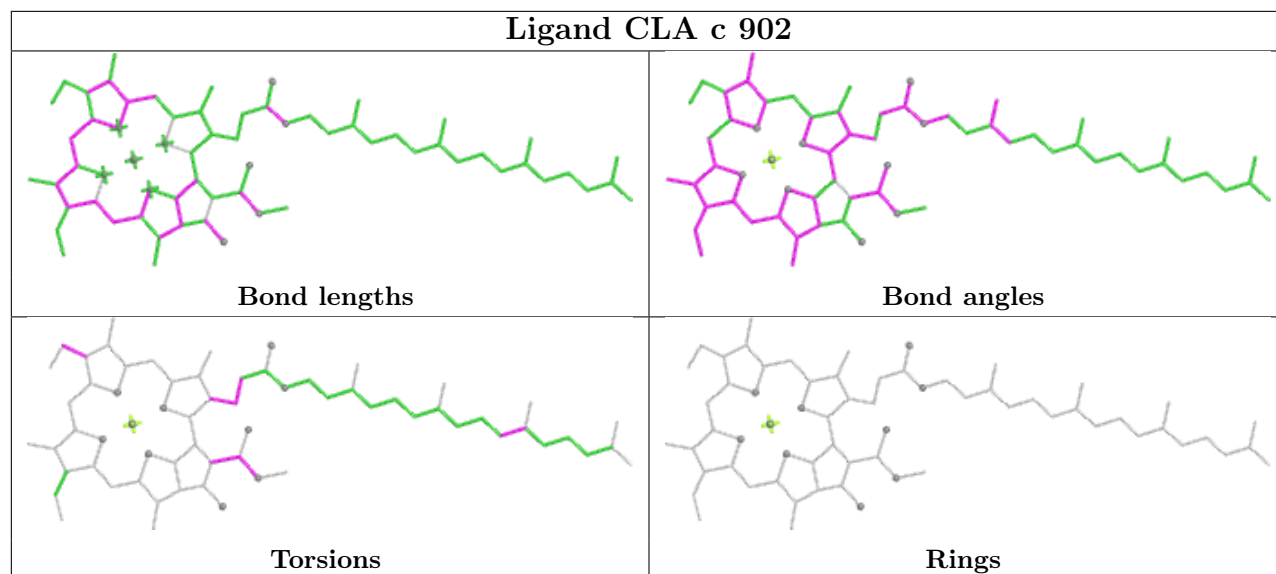
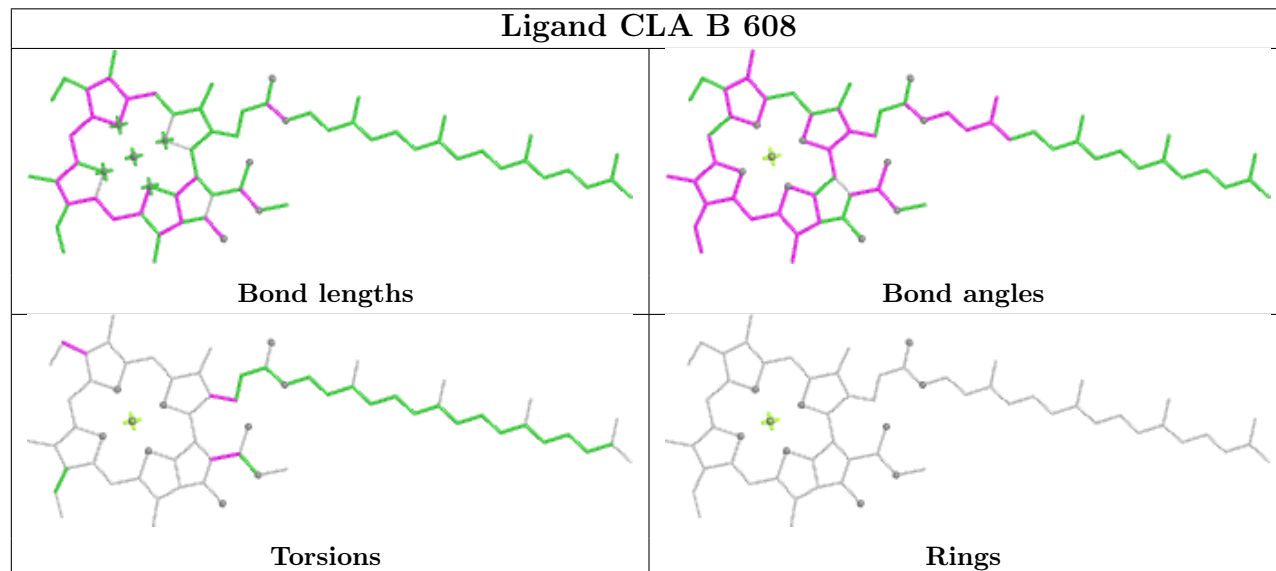


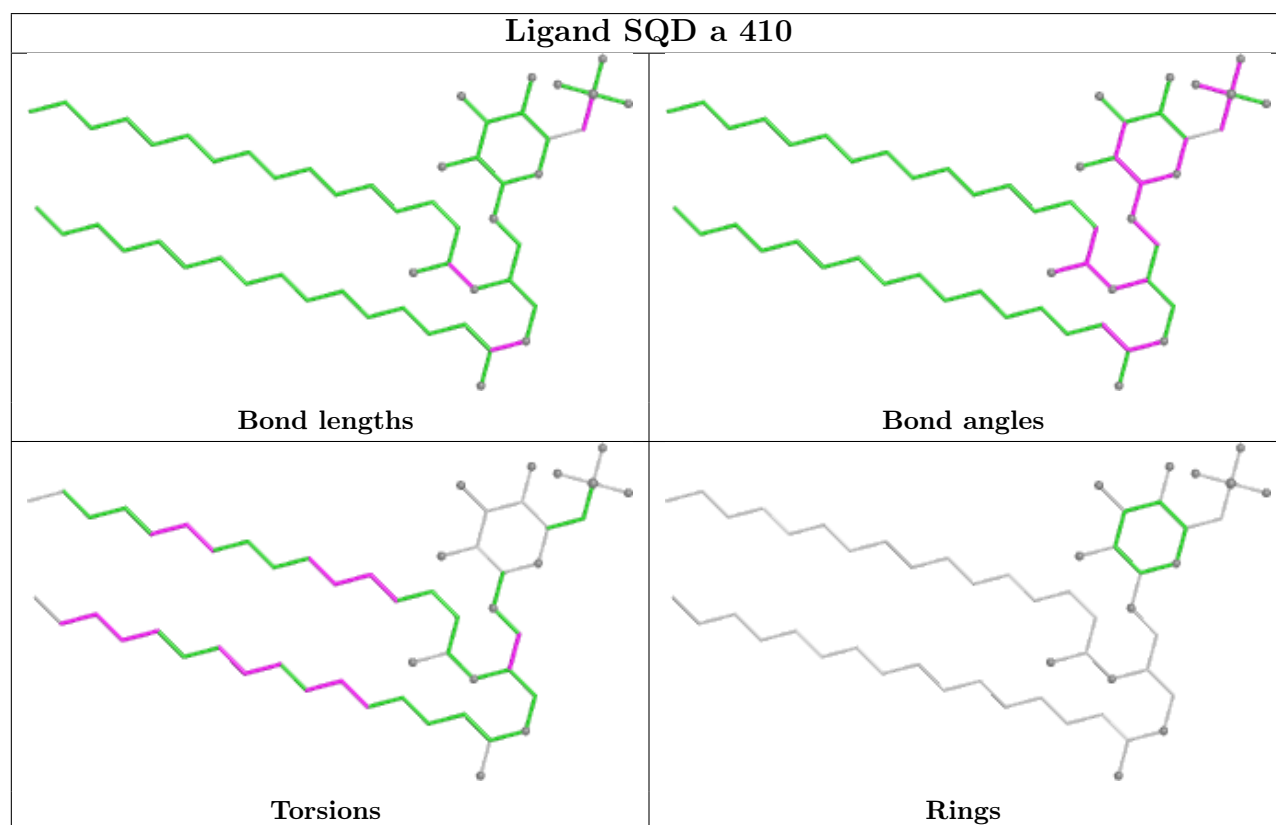
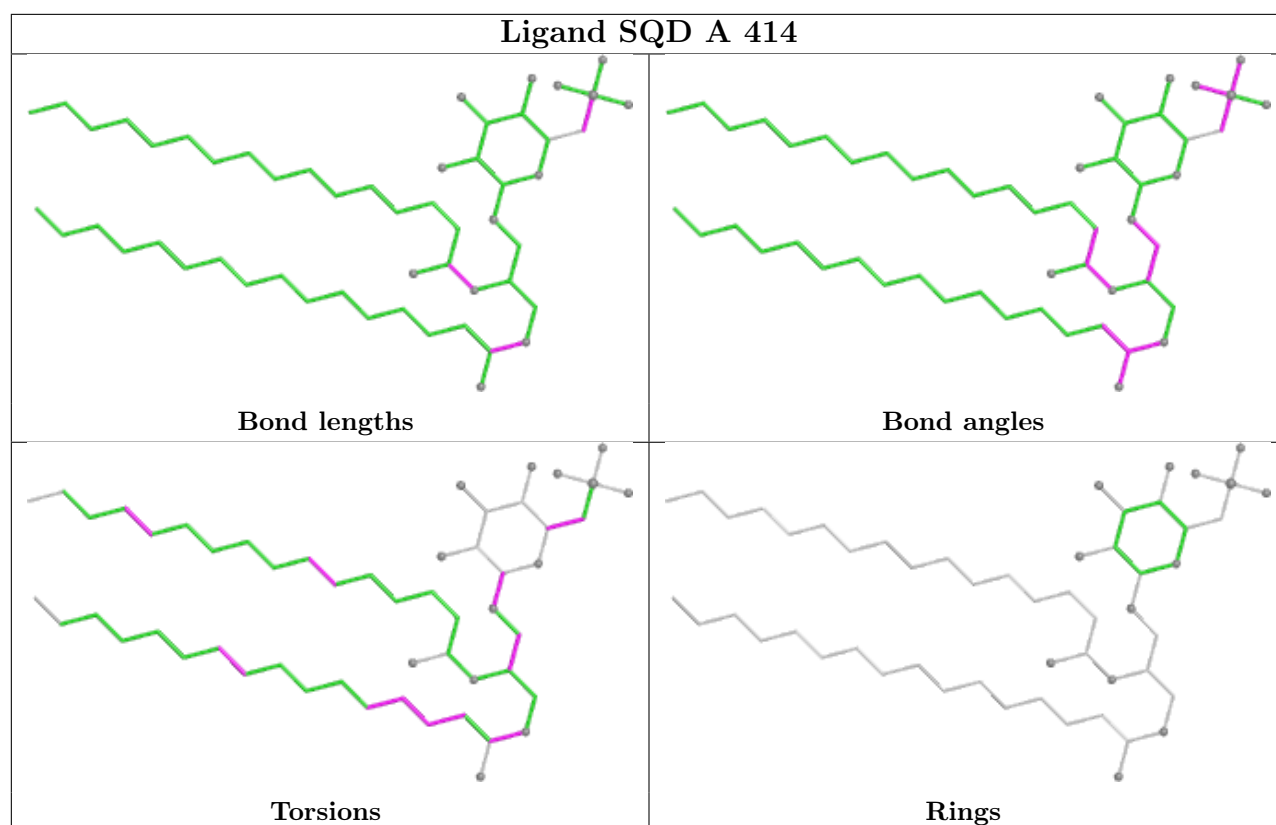




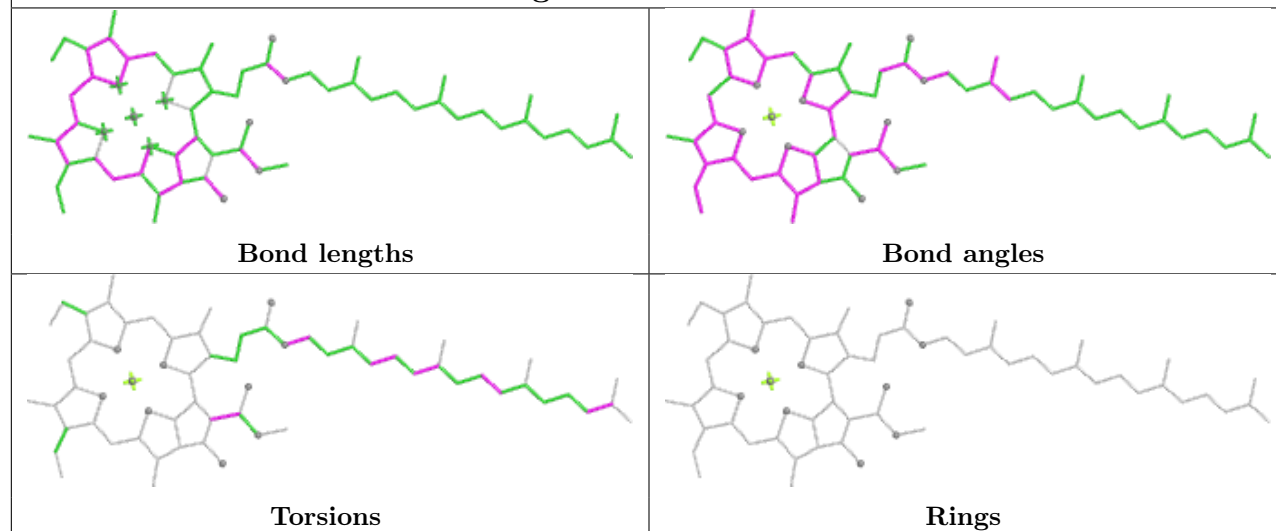




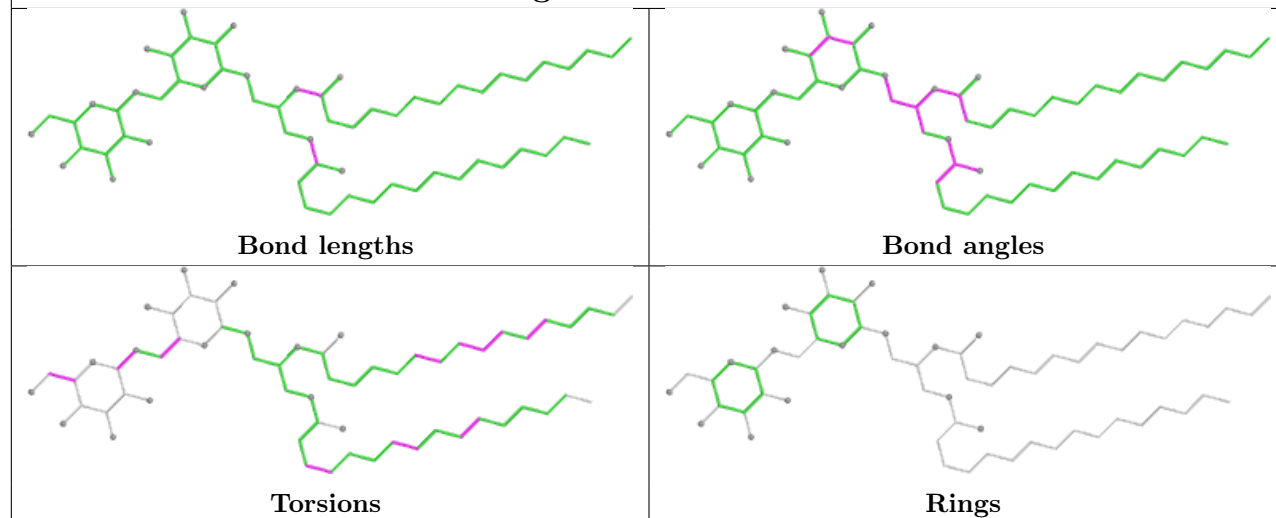
Ligand CLA c 902**Ligand CLA B 608**



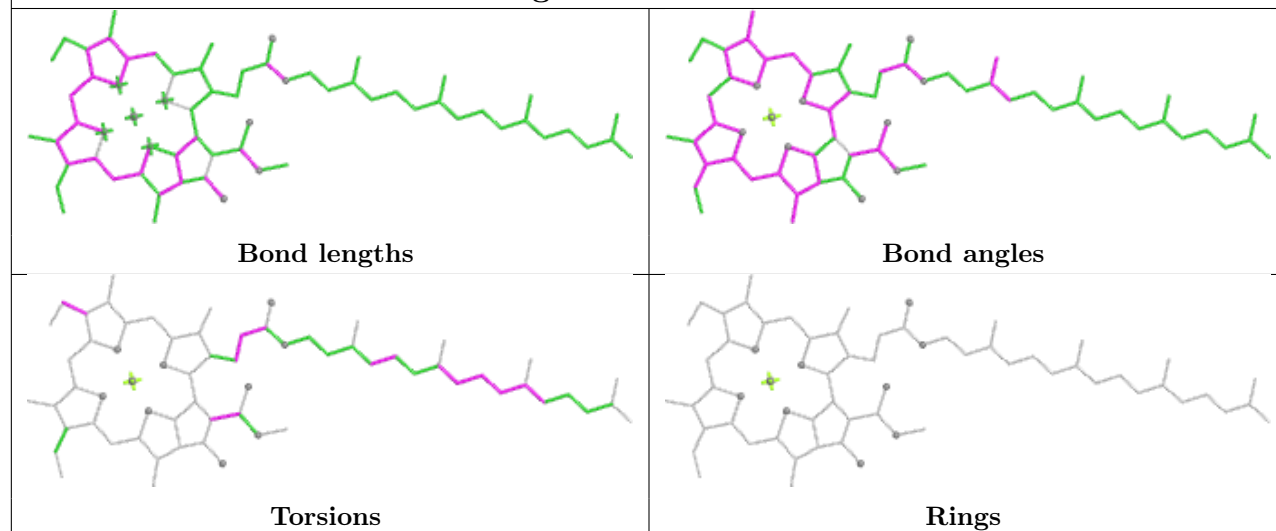
Ligand CLA B 617

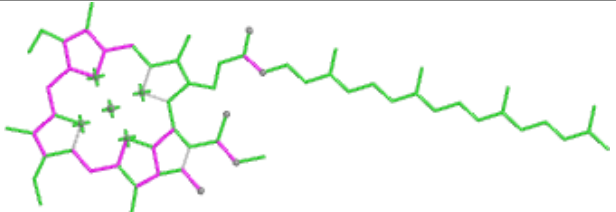
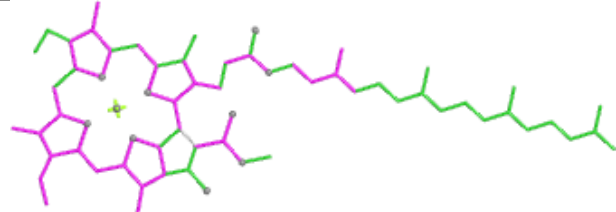
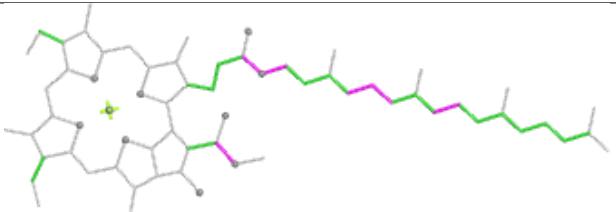
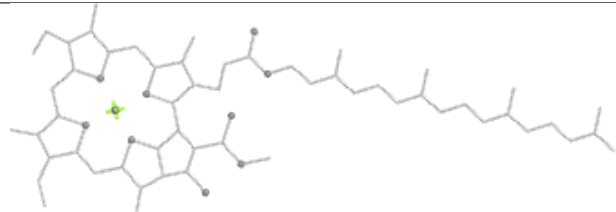


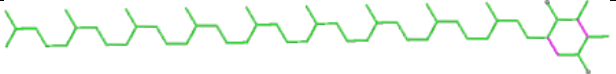
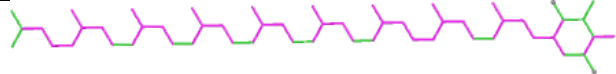
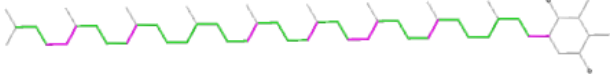
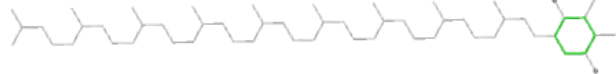
Ligand DGD c 916

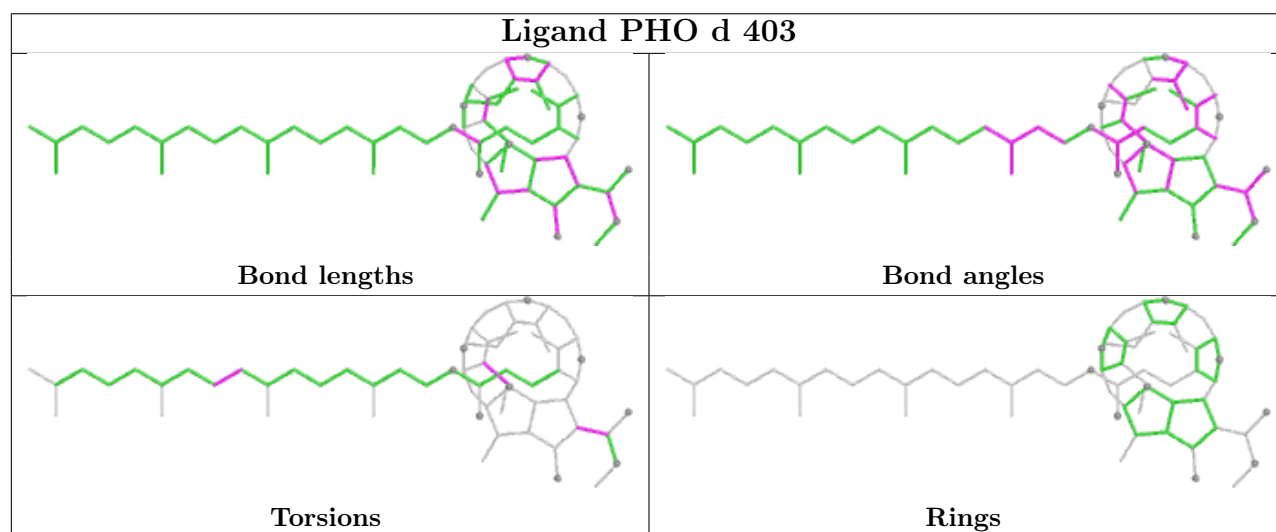
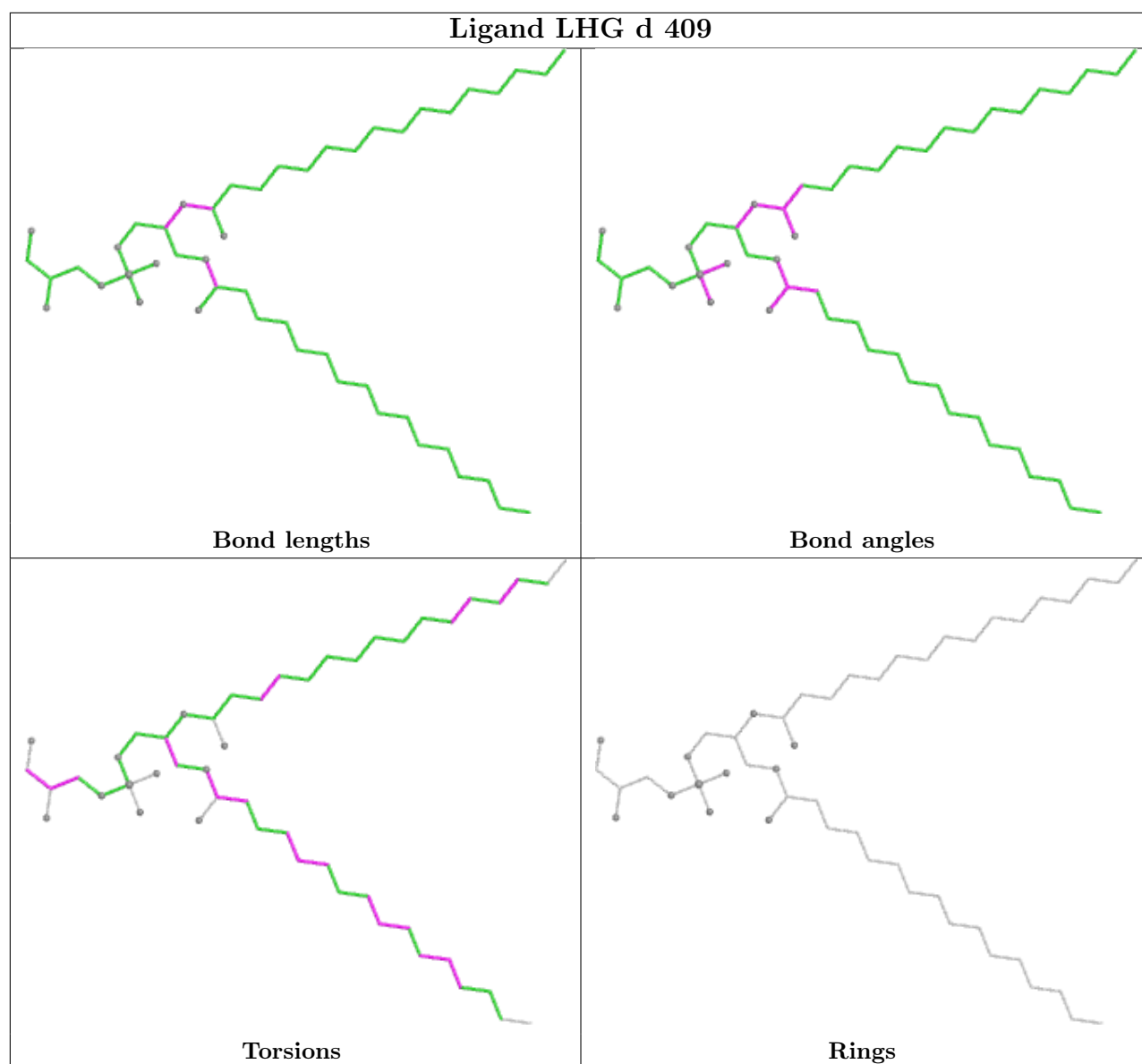


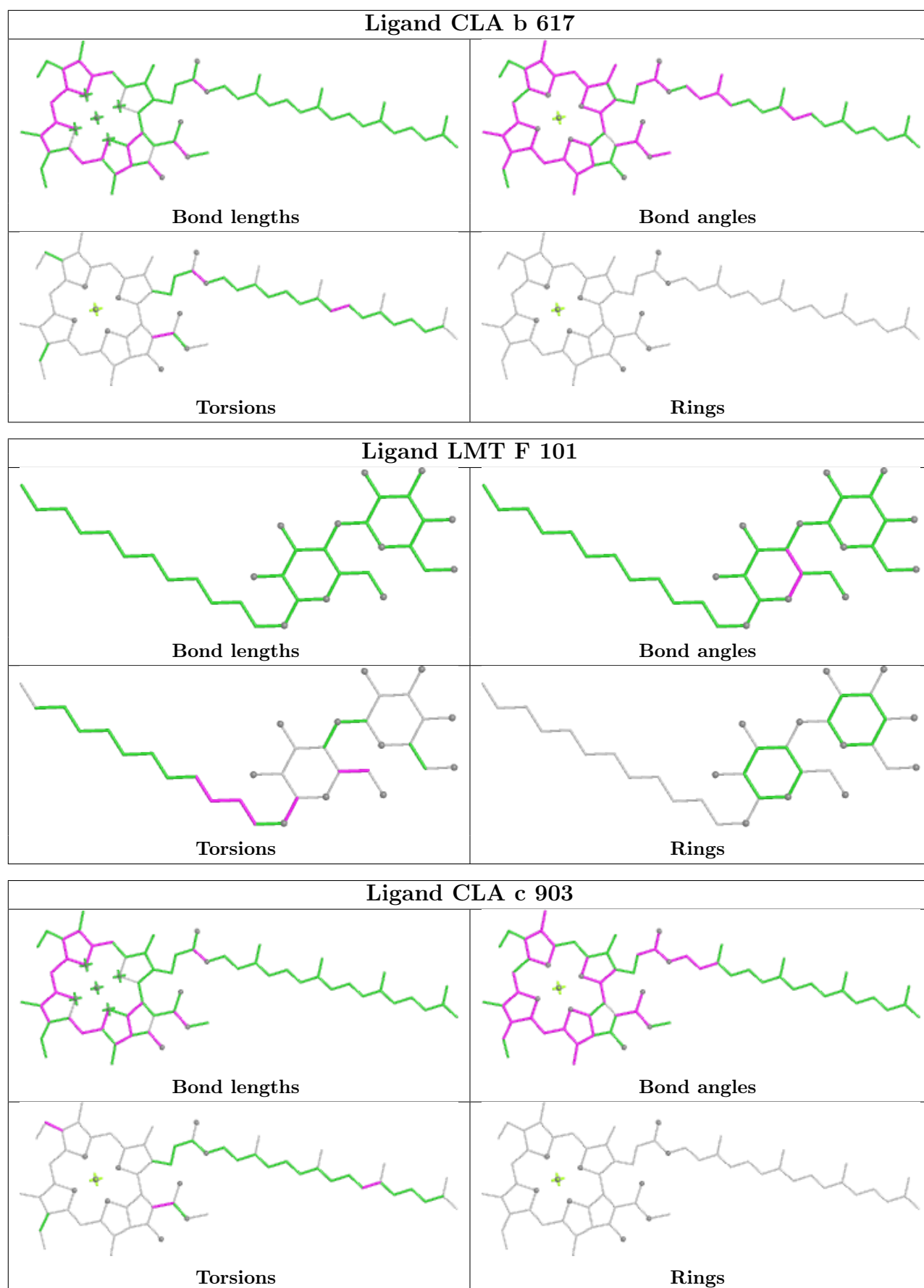
Ligand CLA B 602

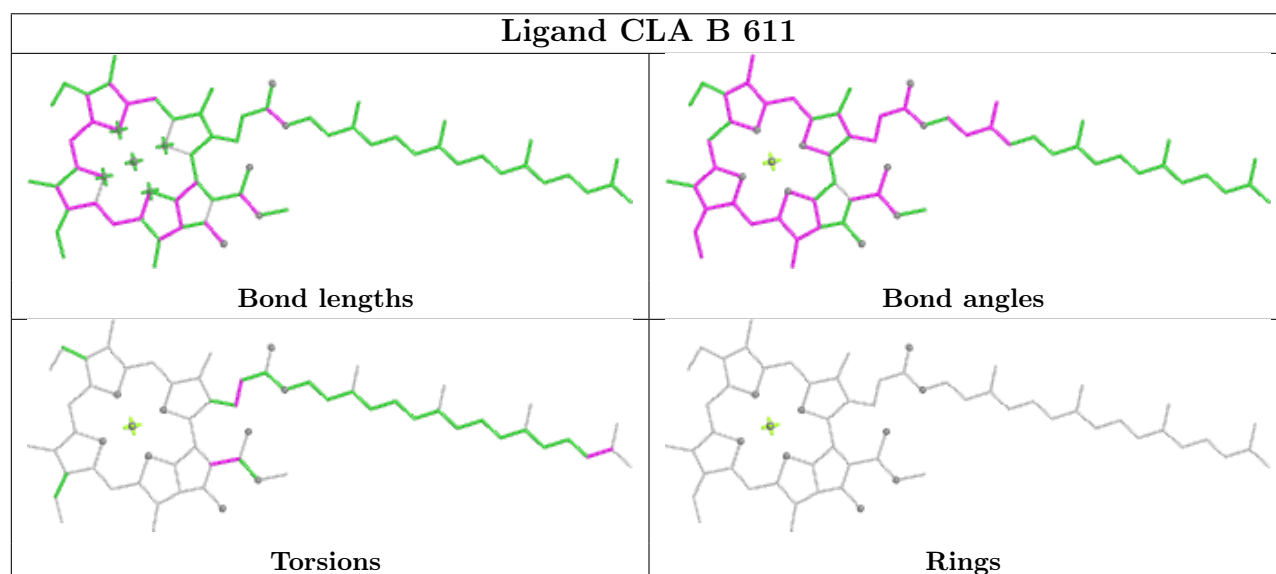
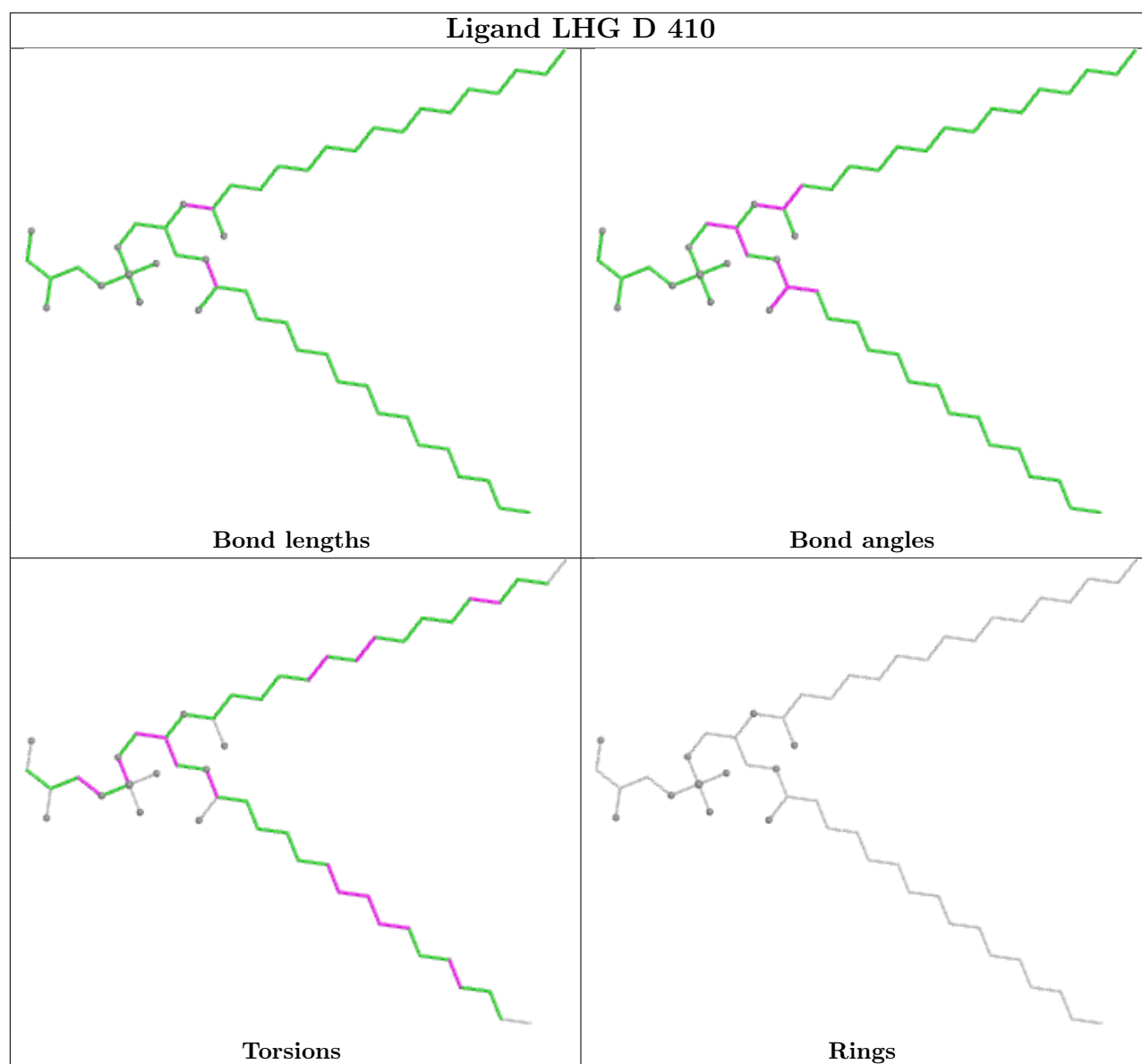


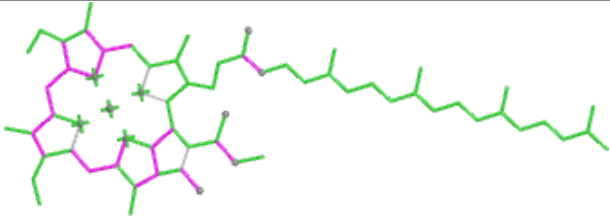
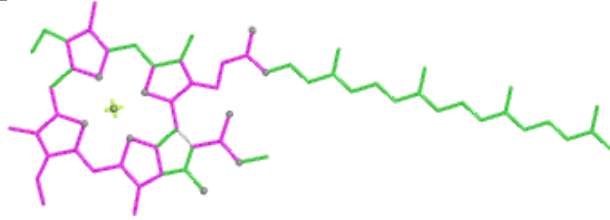
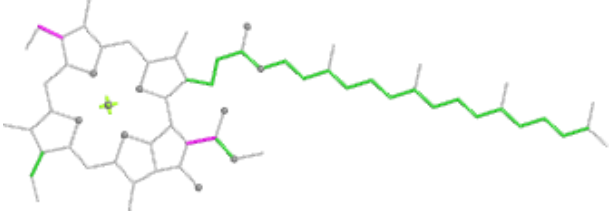
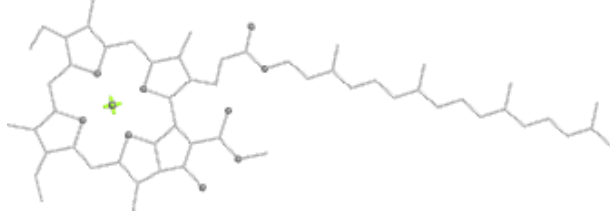
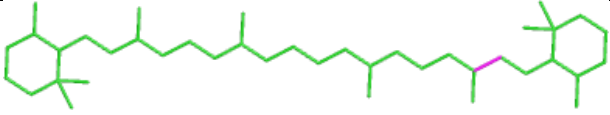
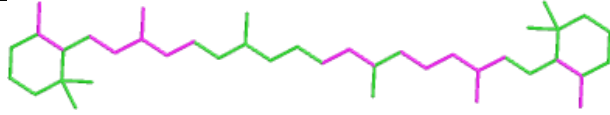
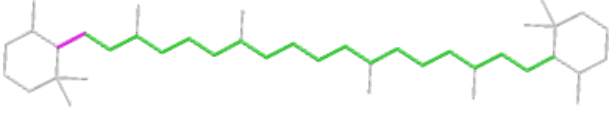
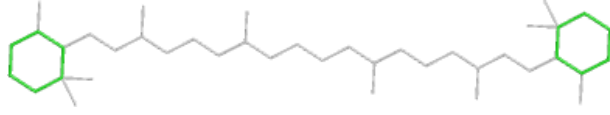
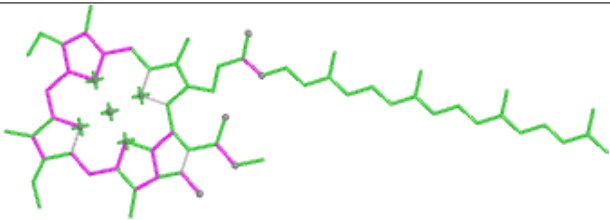
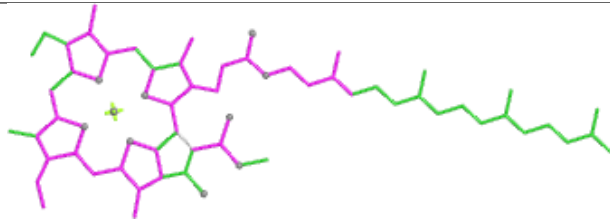
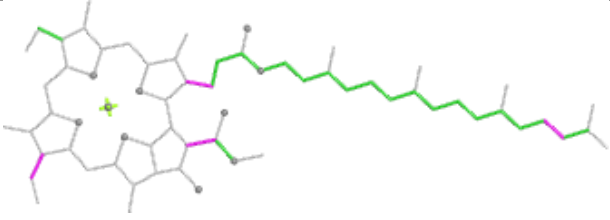
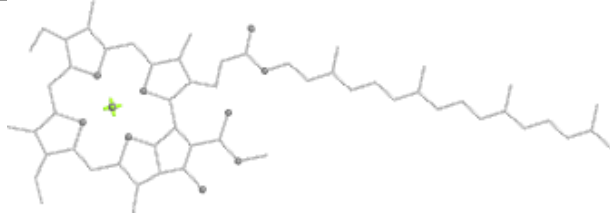
Ligand CLA C 513	
	
Bond lengths	Bond angles
	
Torsions	Rings

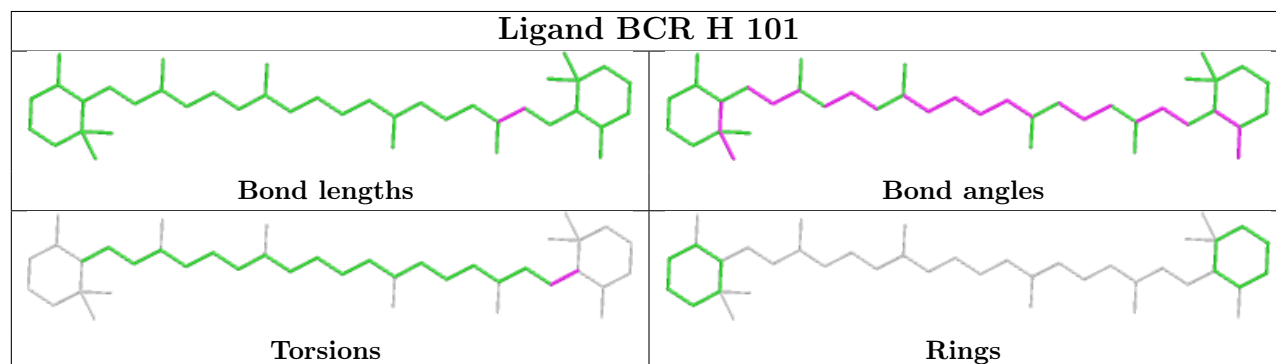
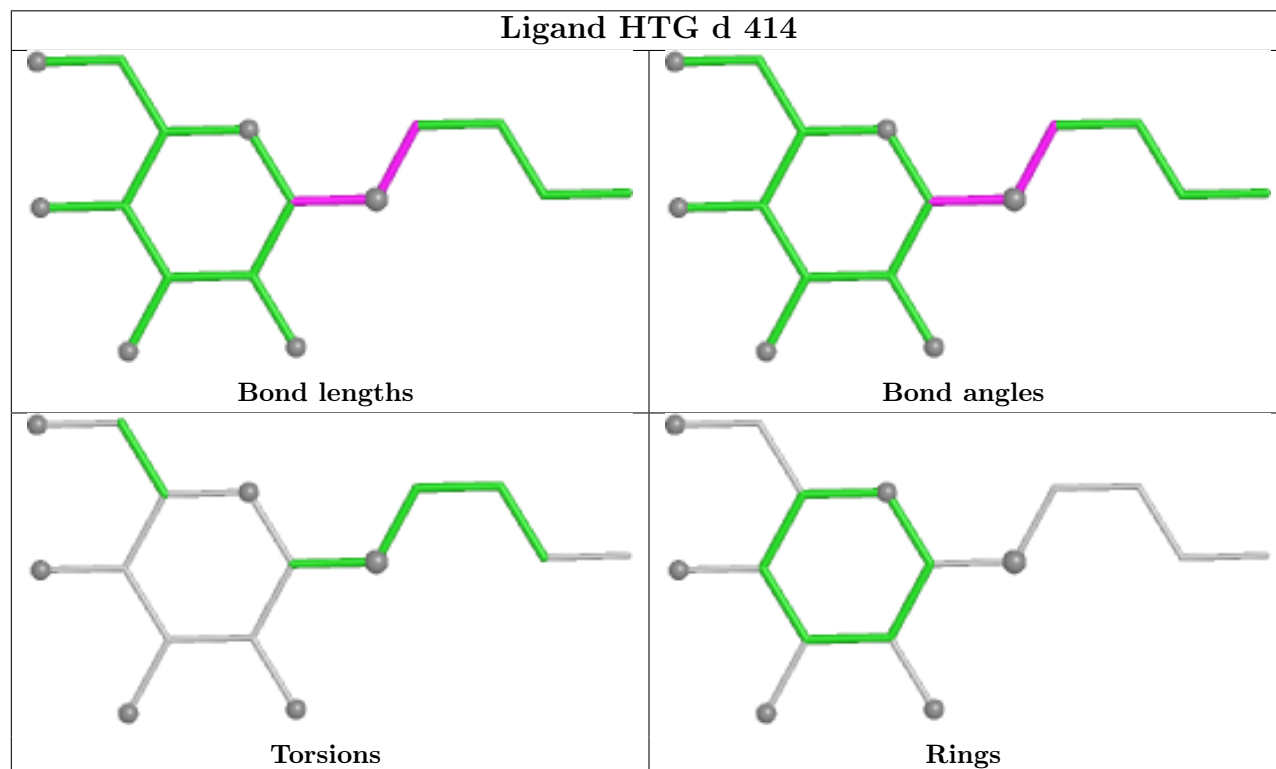
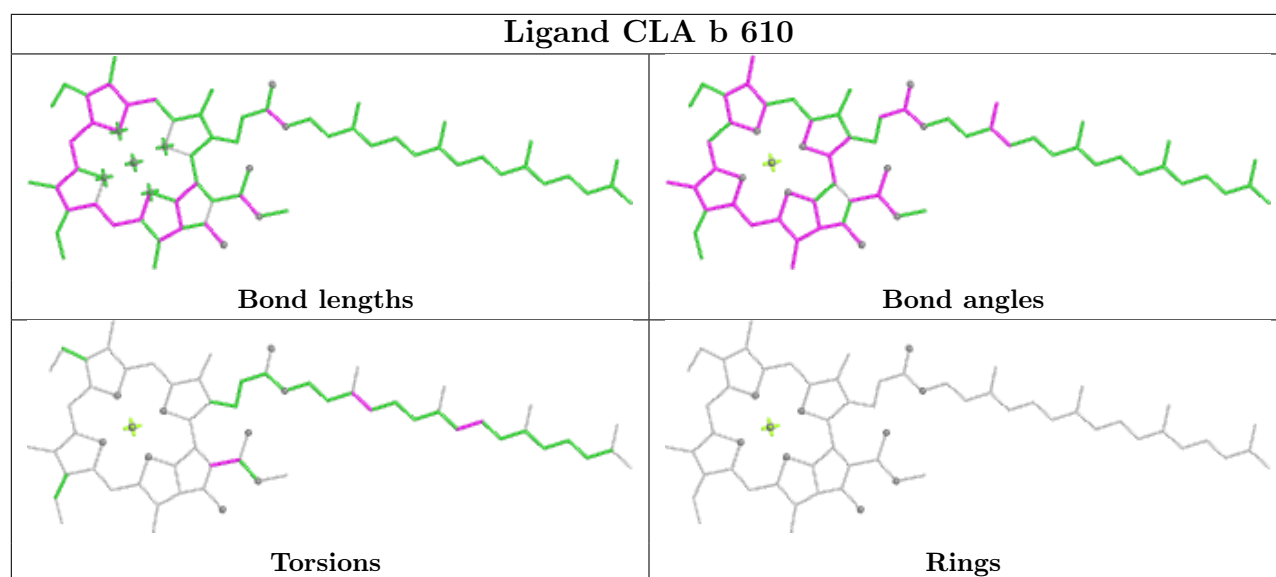
Ligand PL9 A 417	
	
Bond lengths	Bond angles
	
Torsions	Rings



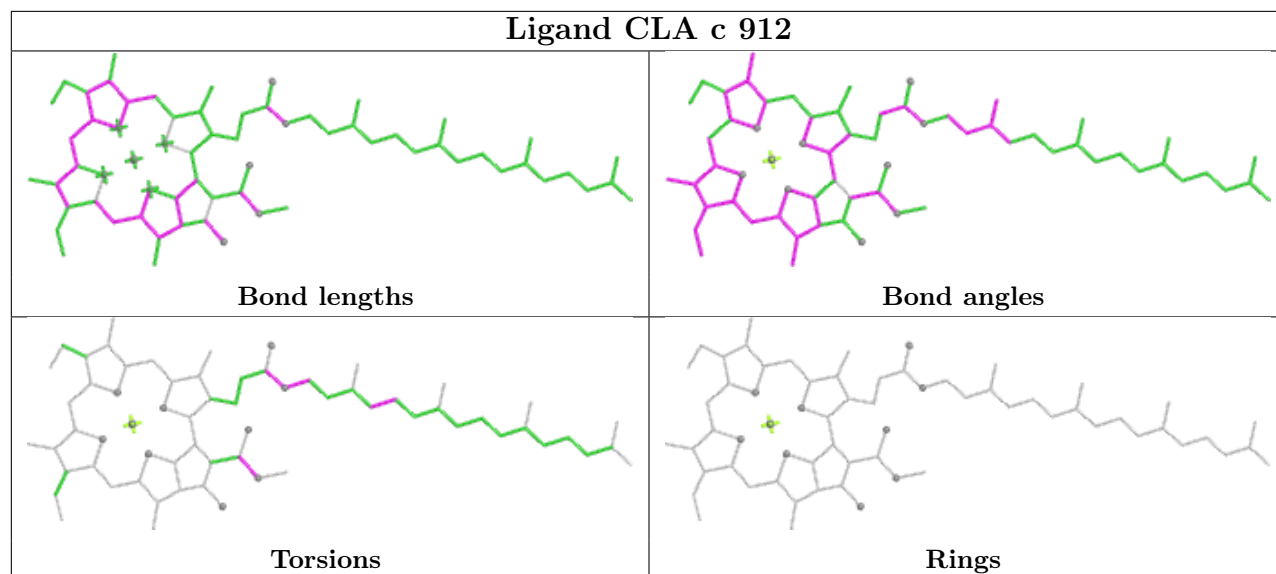




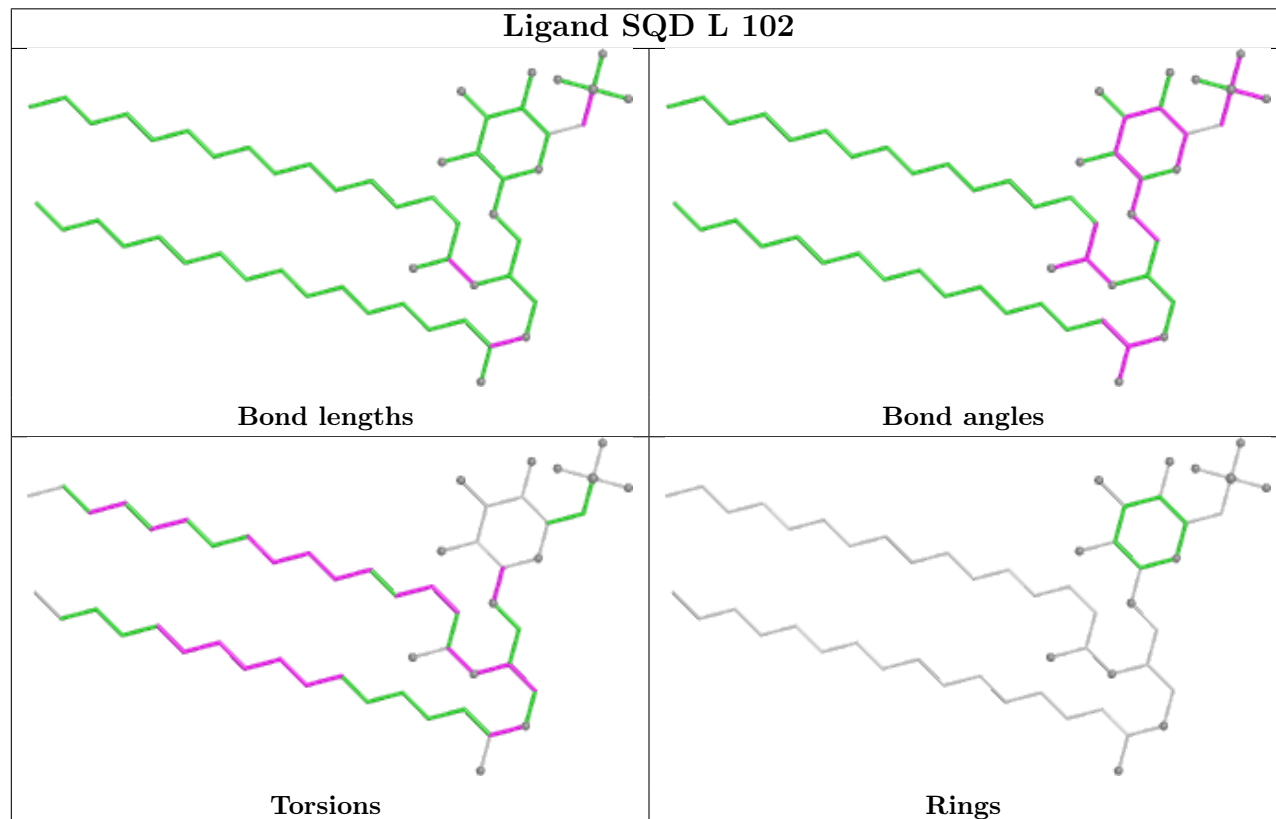
Ligand CLA b 612	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 618	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA d 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

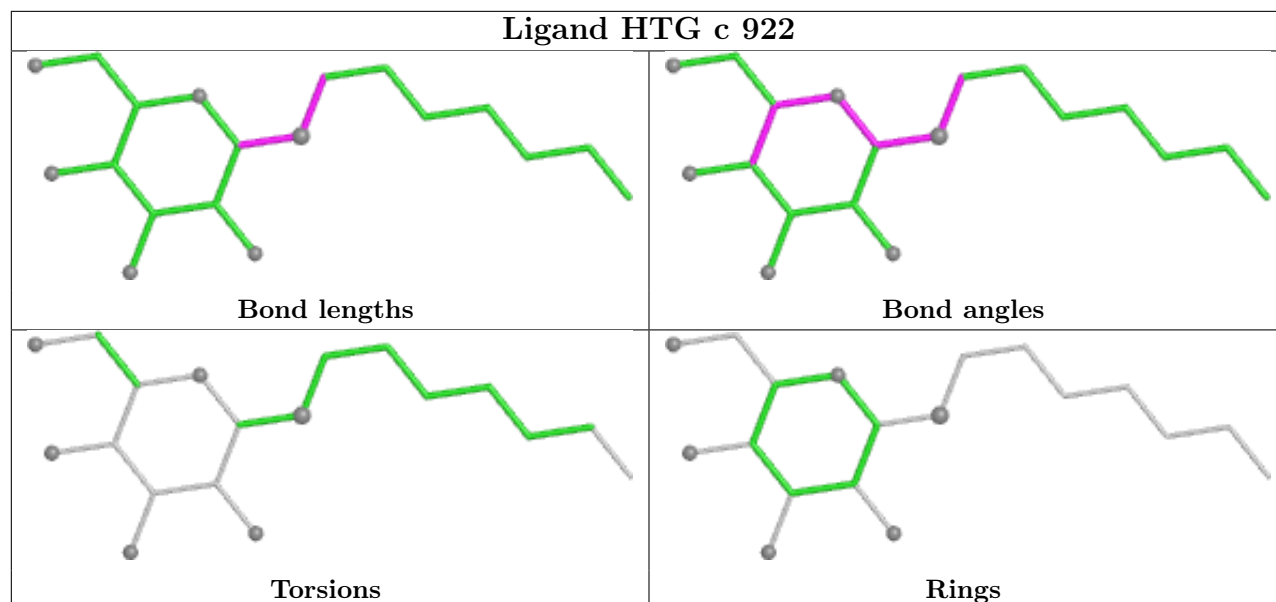
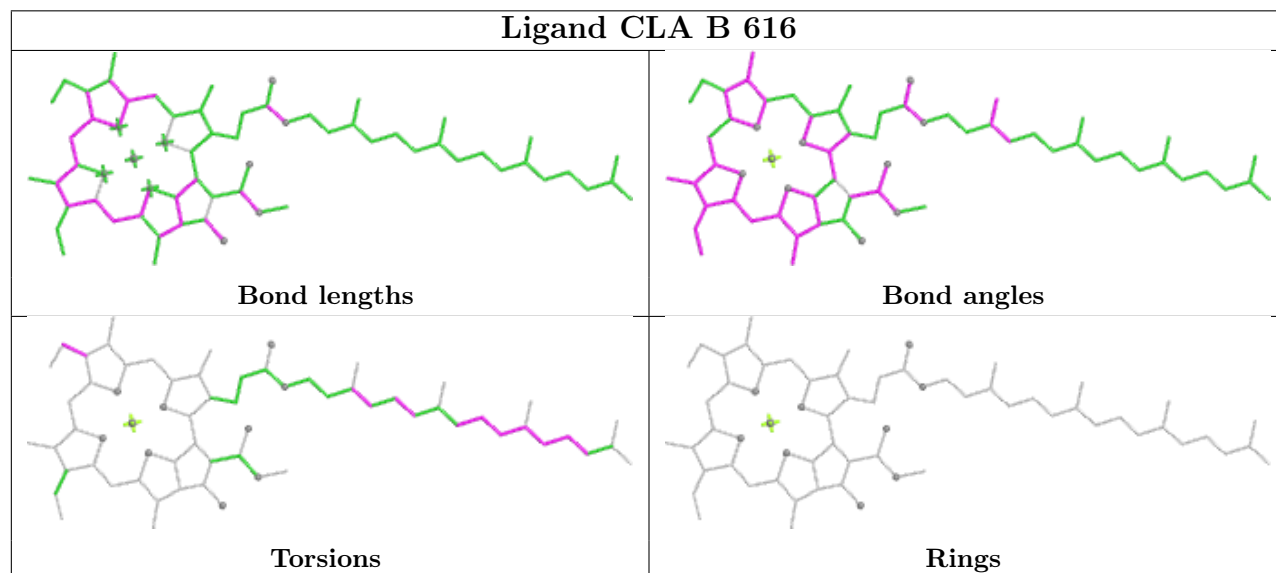
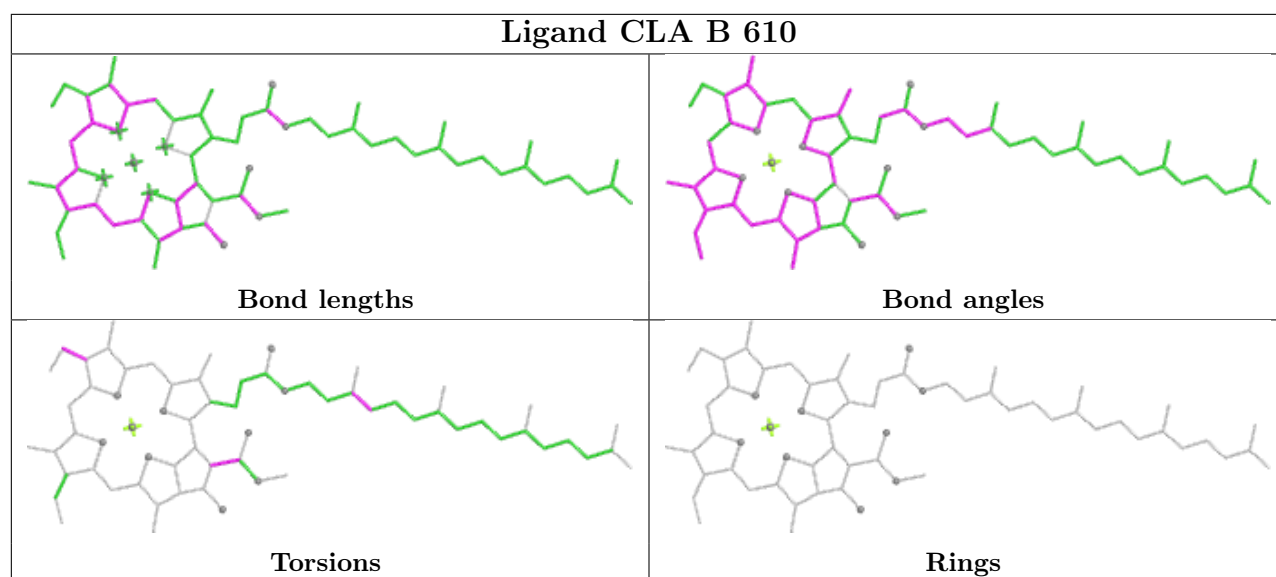


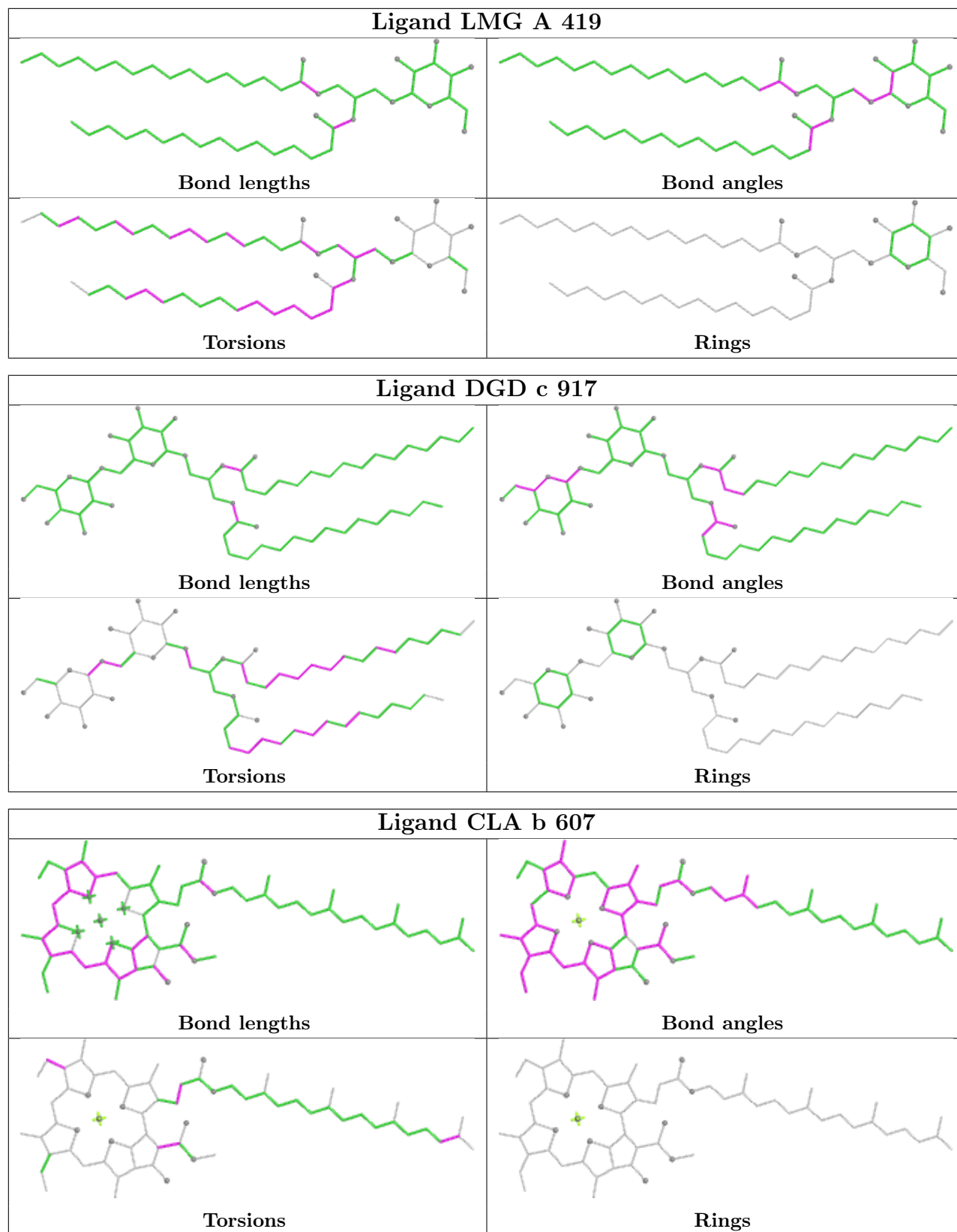
Ligand CLA c 912

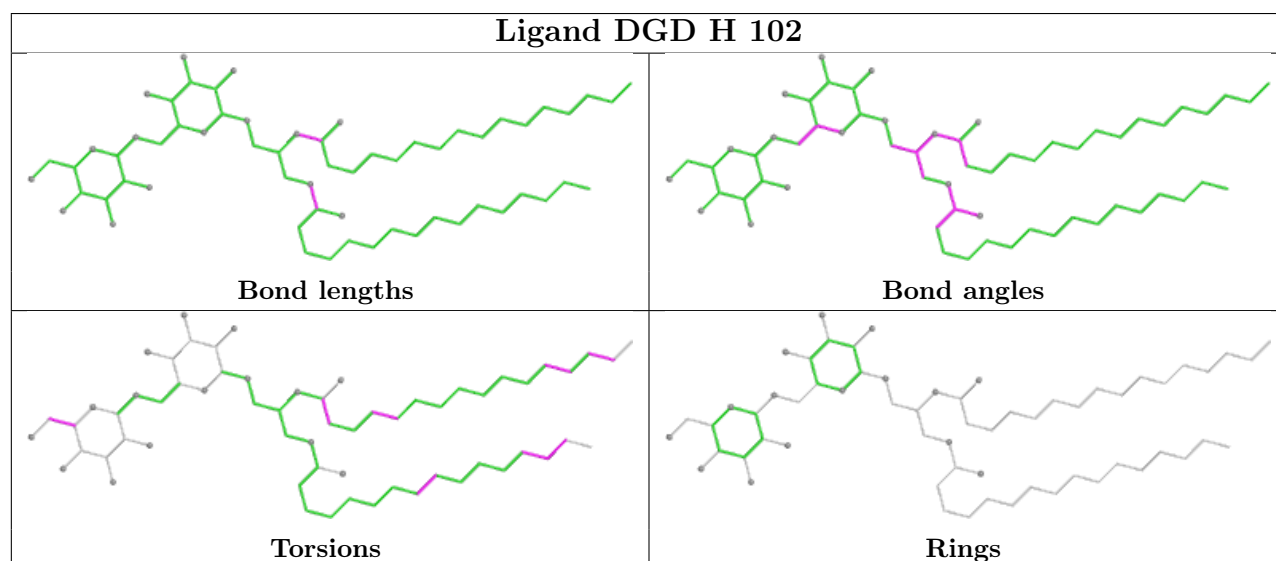
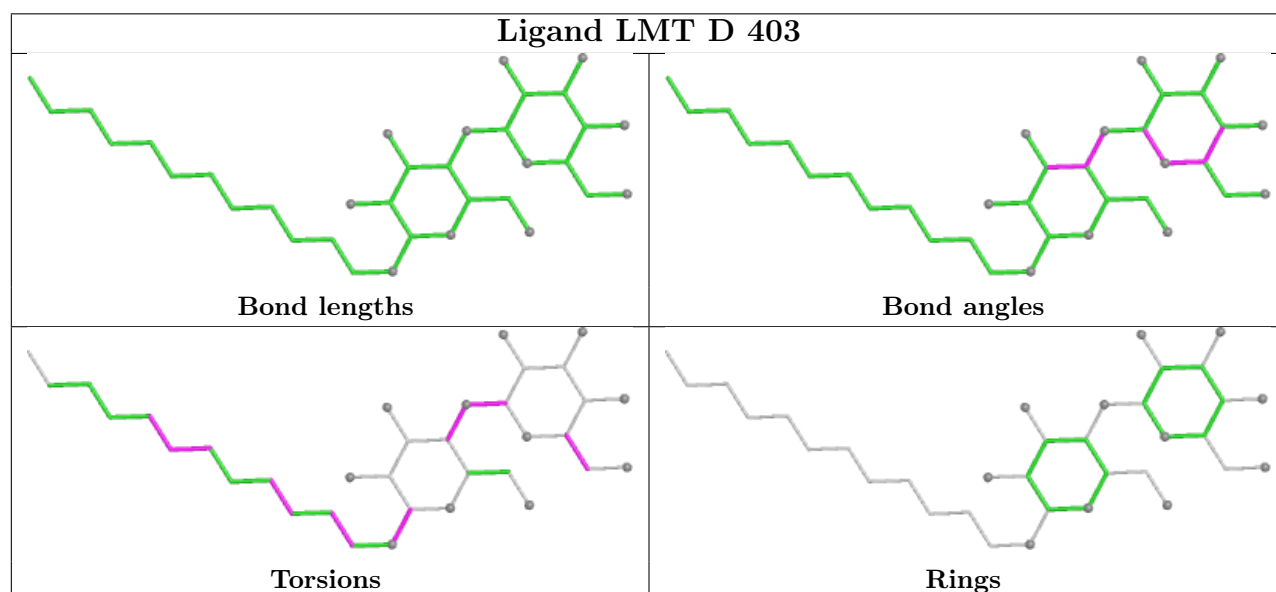
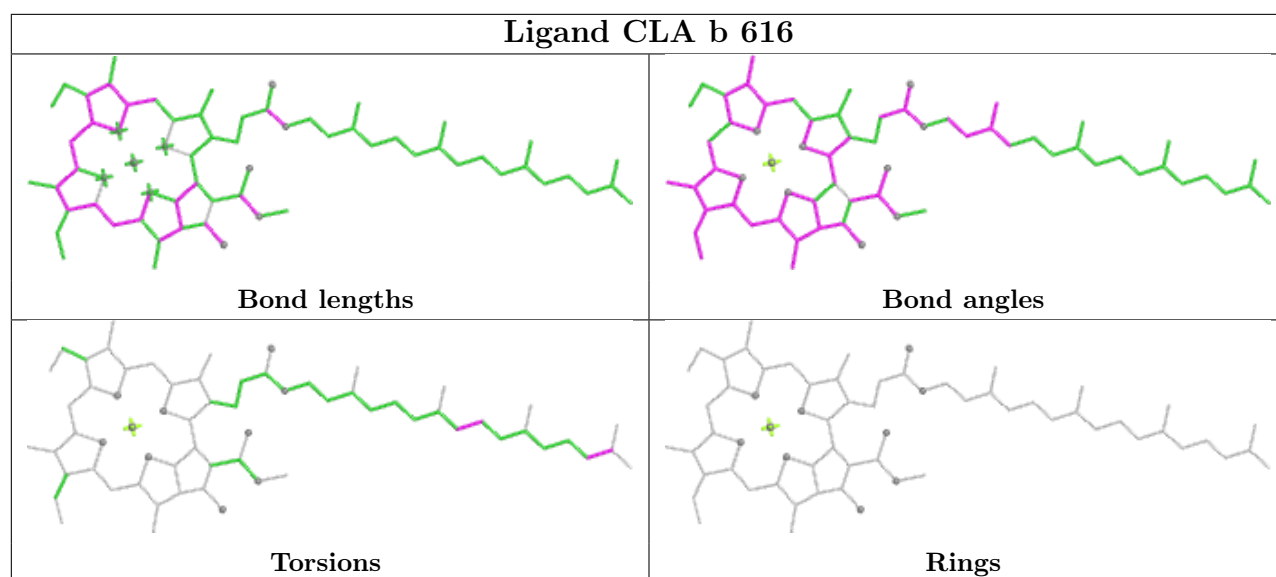


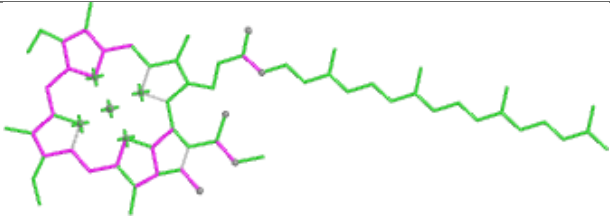
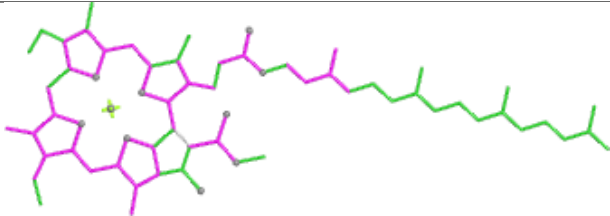
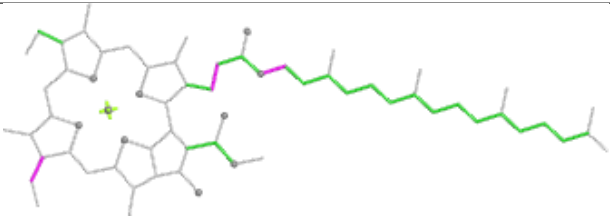
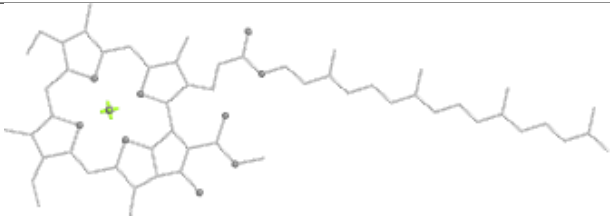
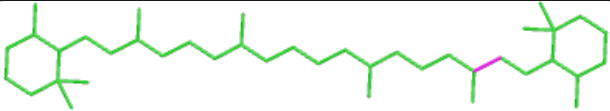
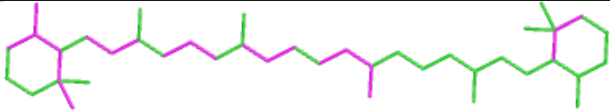
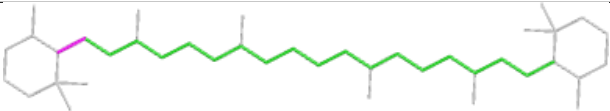
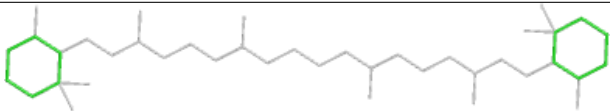
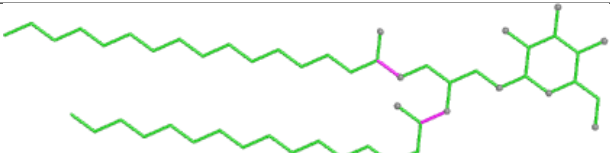
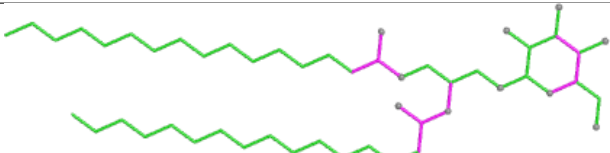
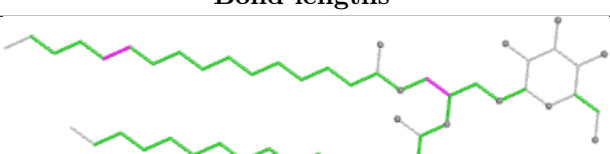
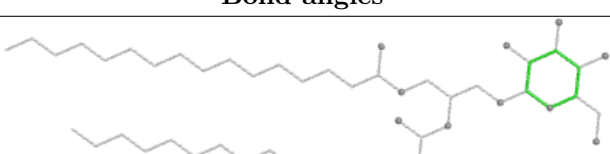
Ligand SQD L 102

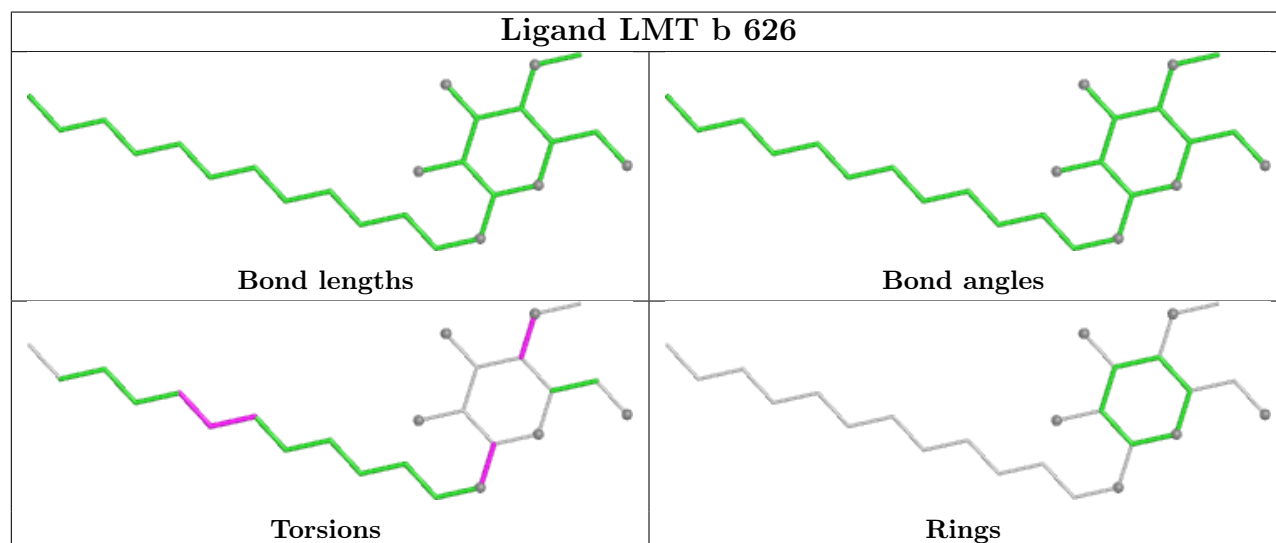
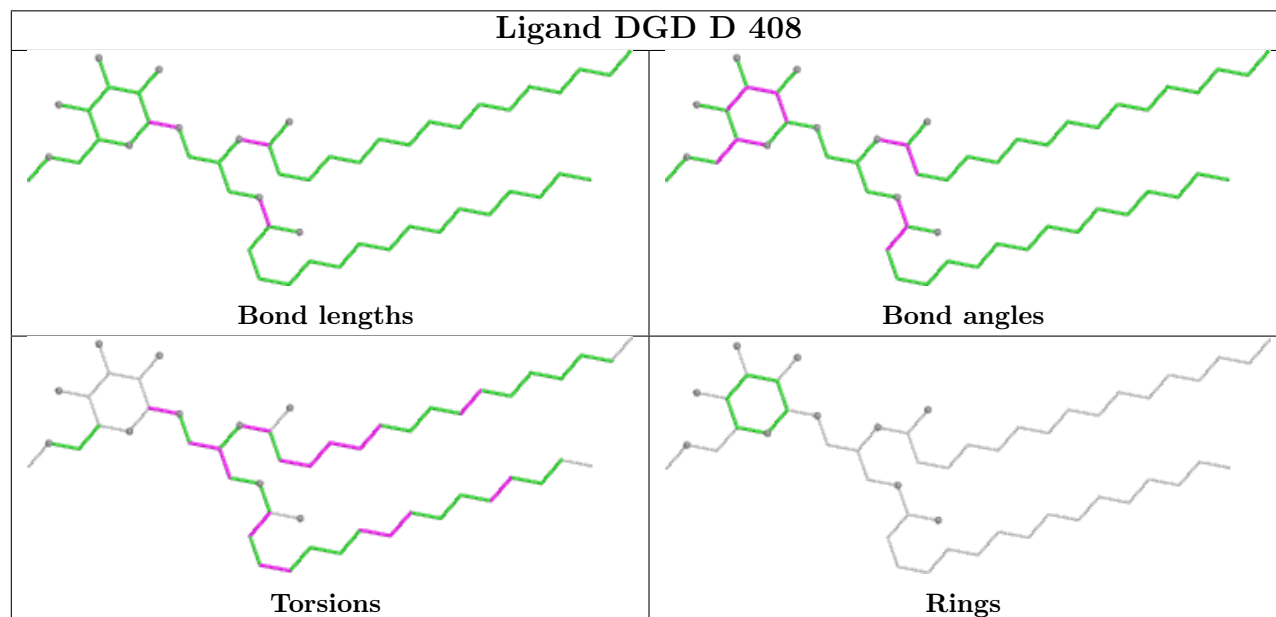
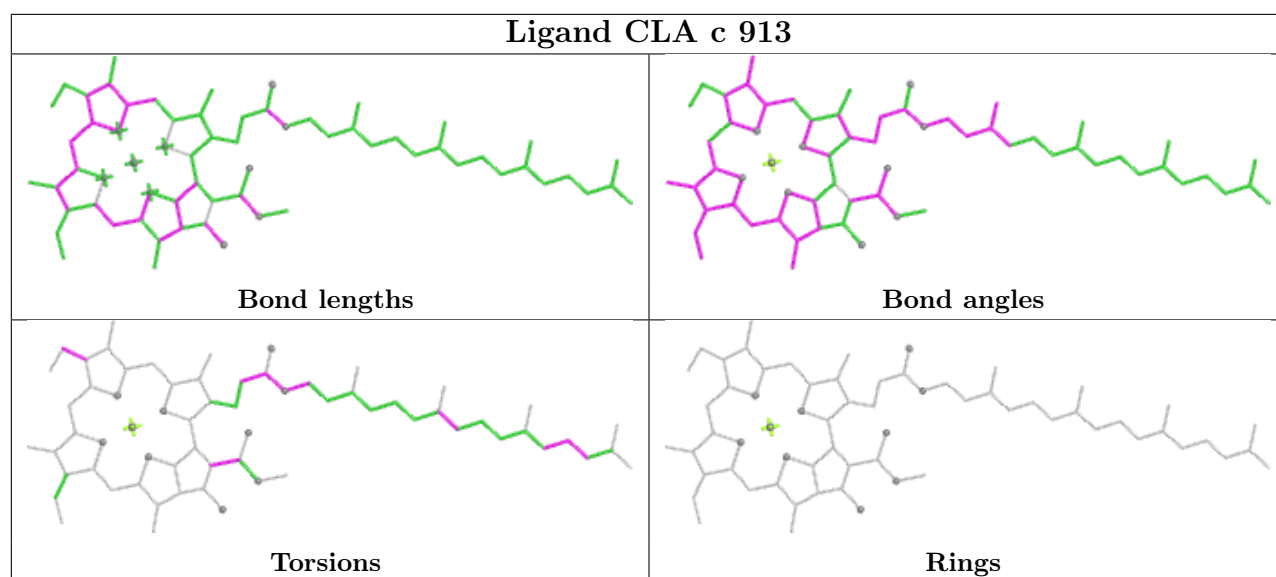


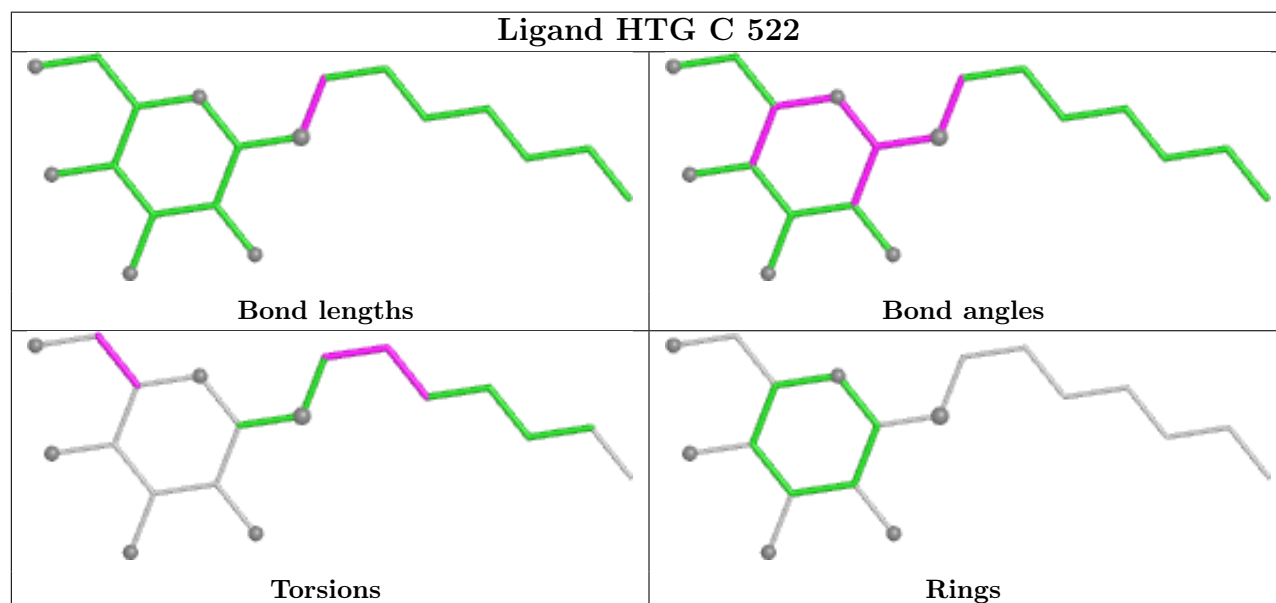
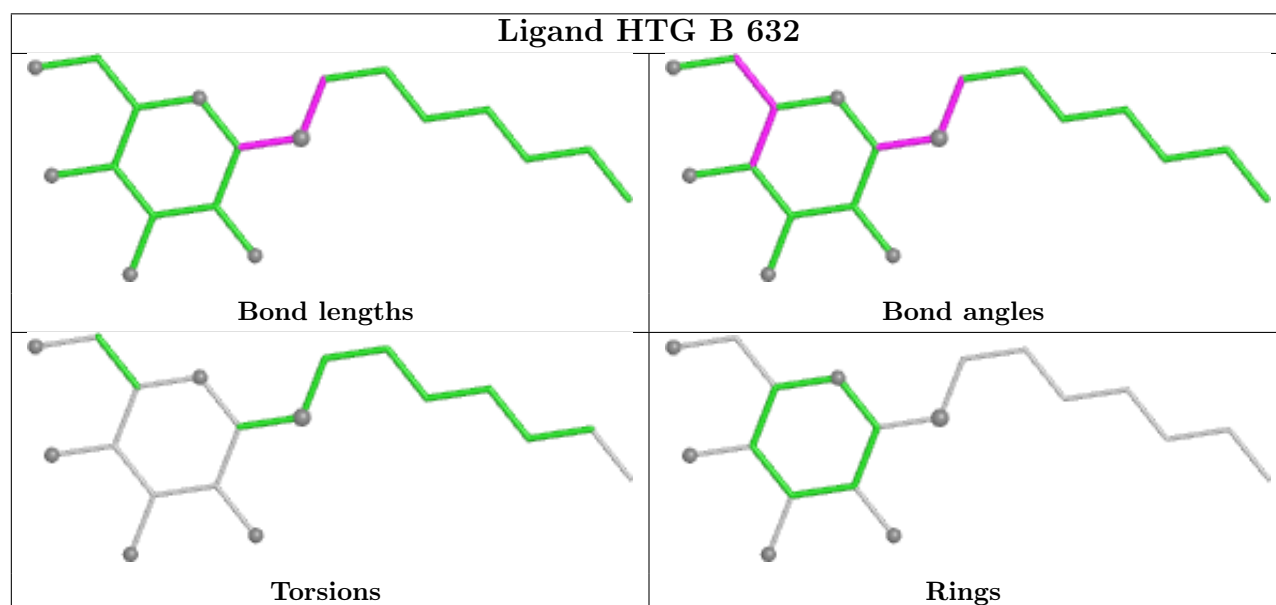
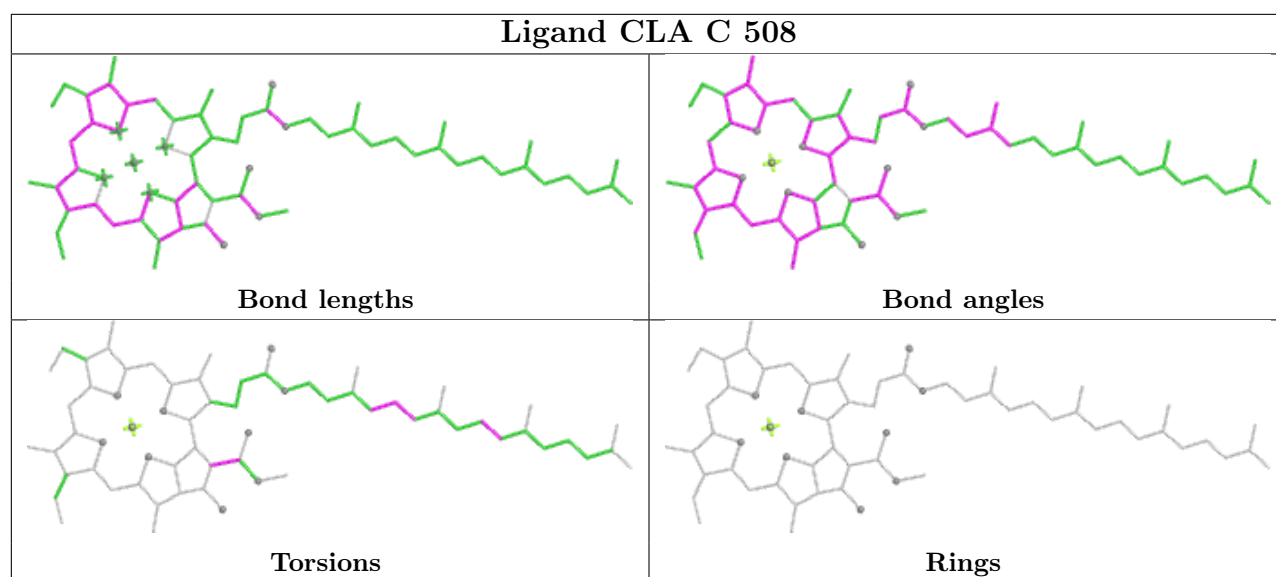


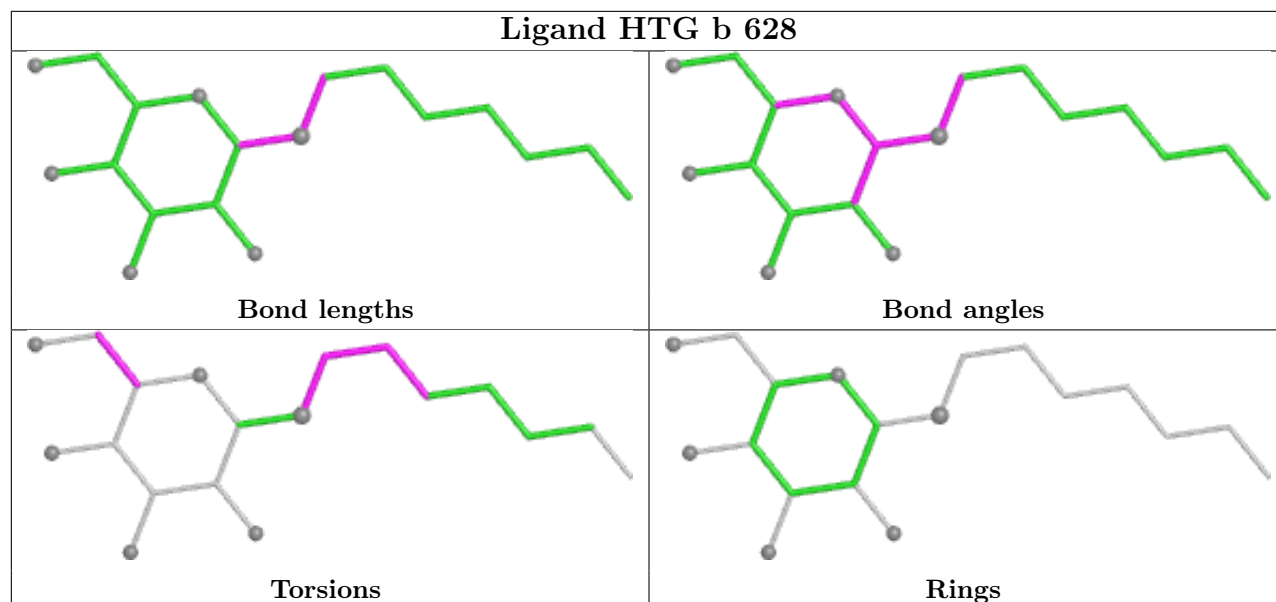
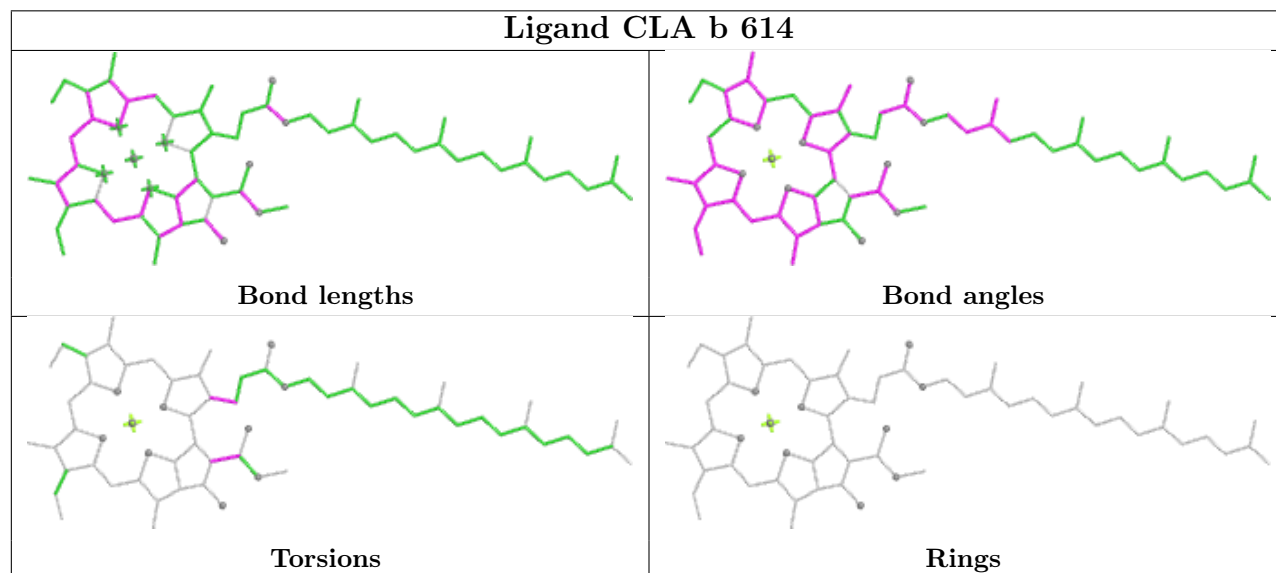
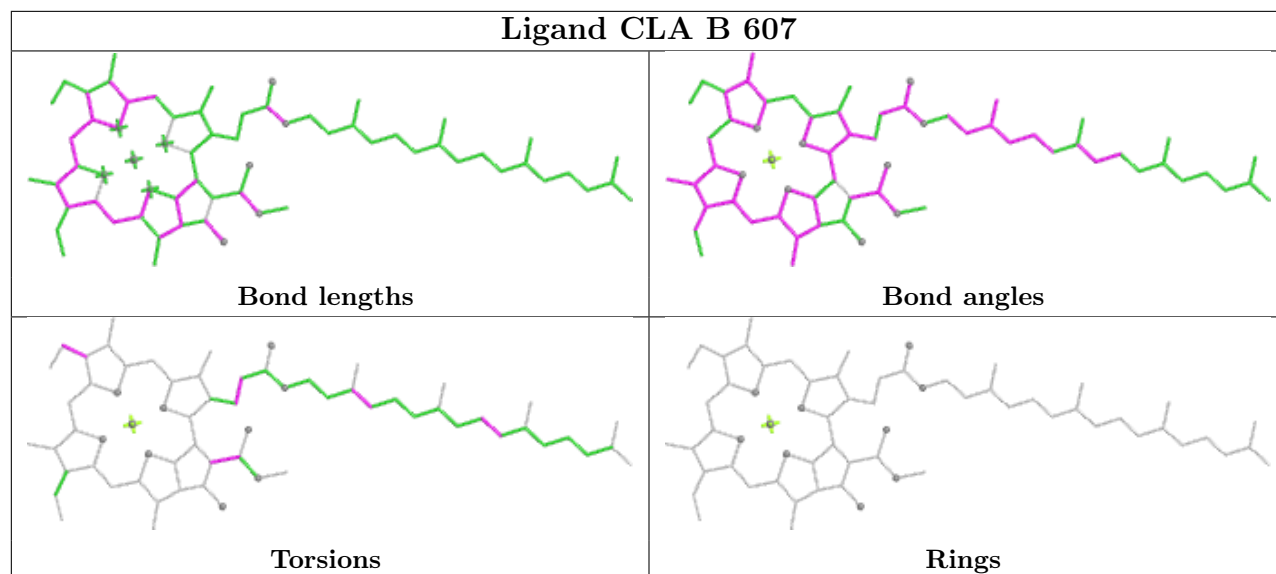


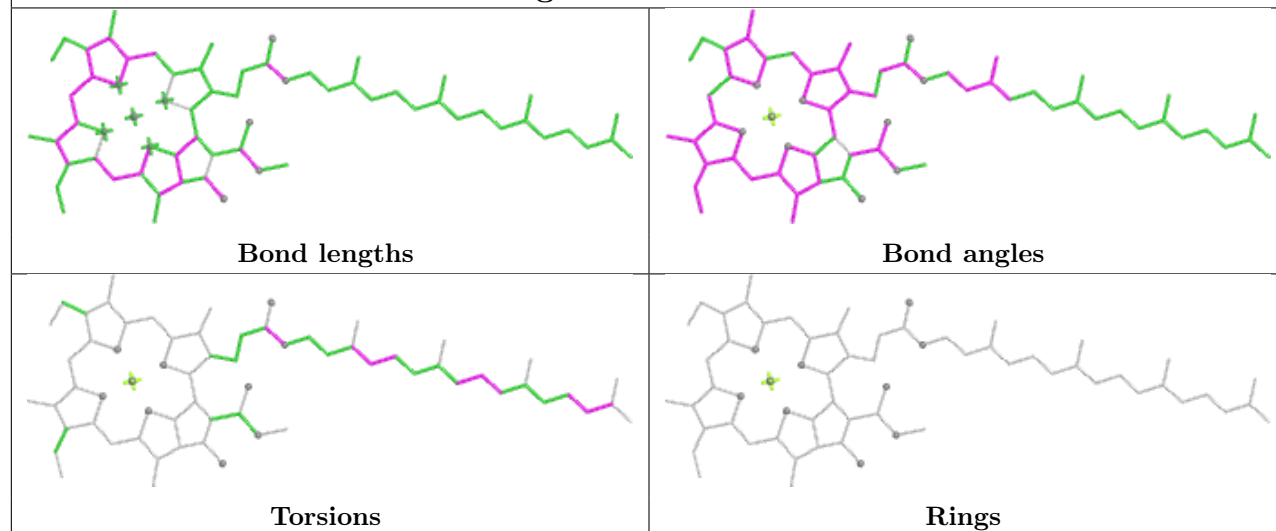
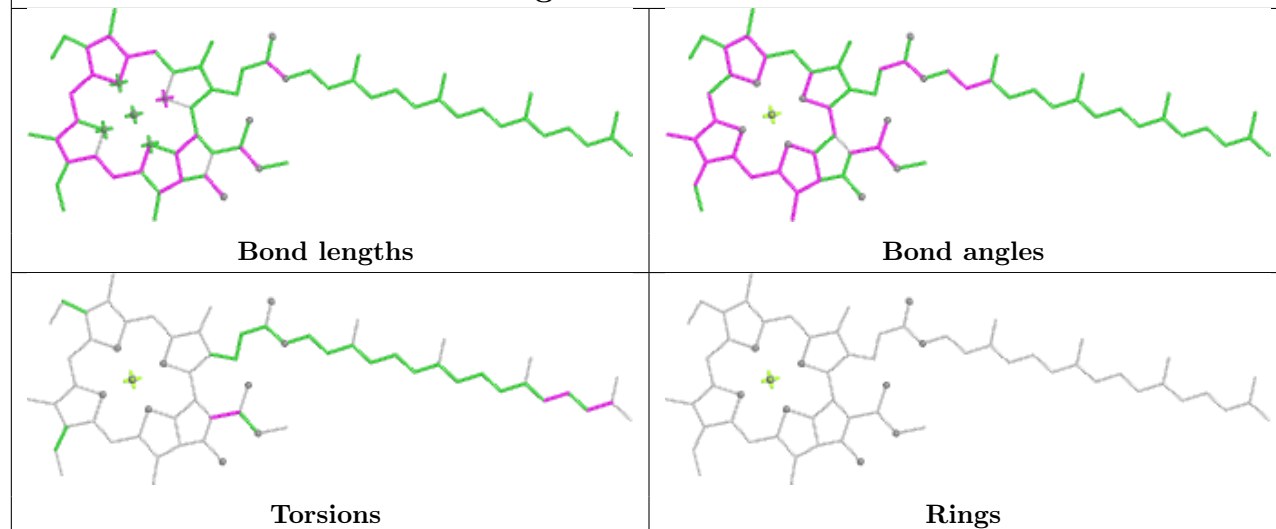


Ligand CLA a 405	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b 622	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG c 920	
 Bond lengths	 Bond angles
 Torsions	 Rings

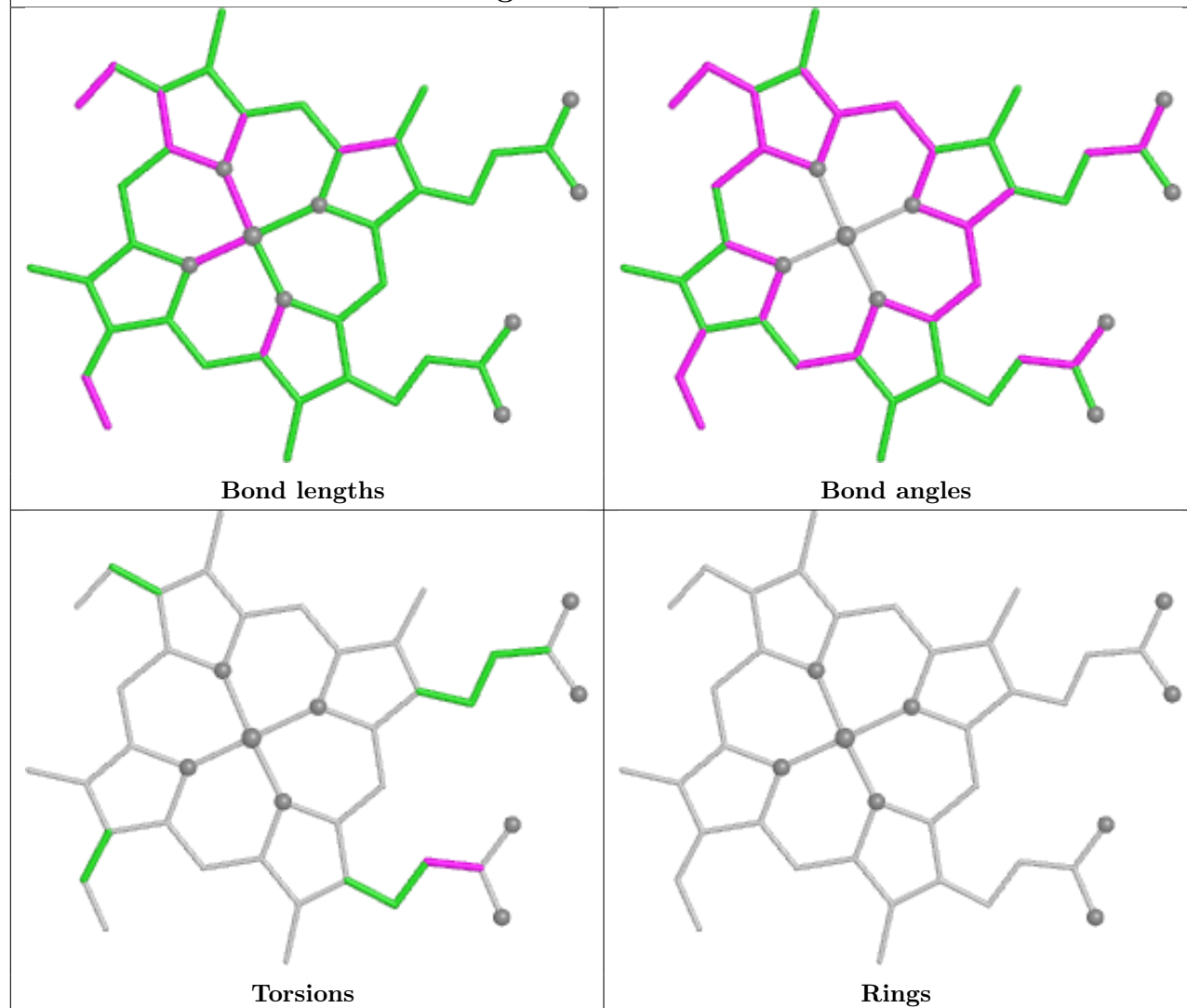




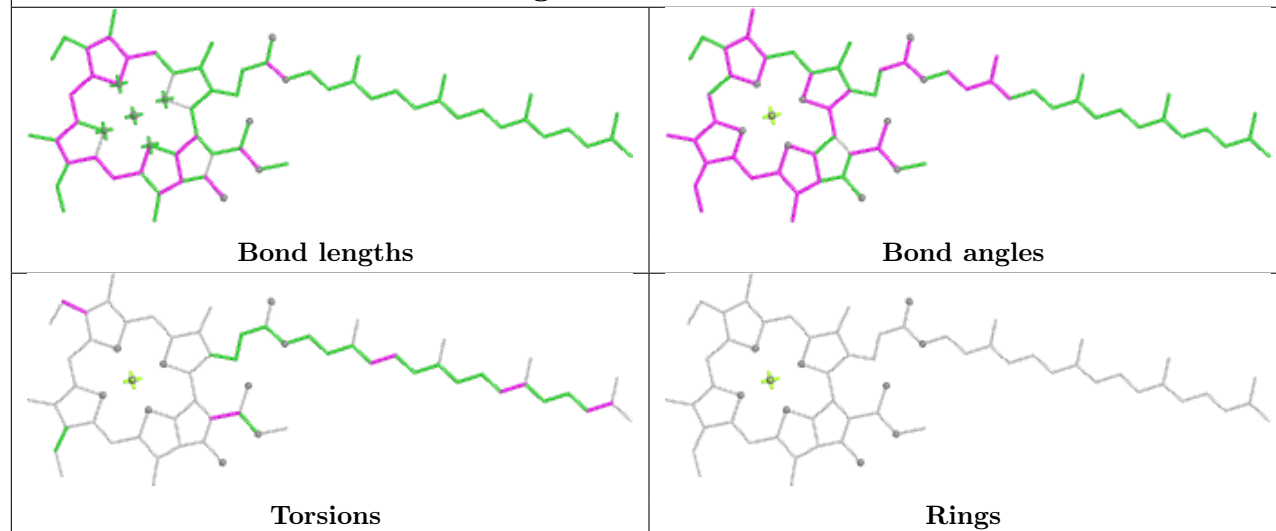


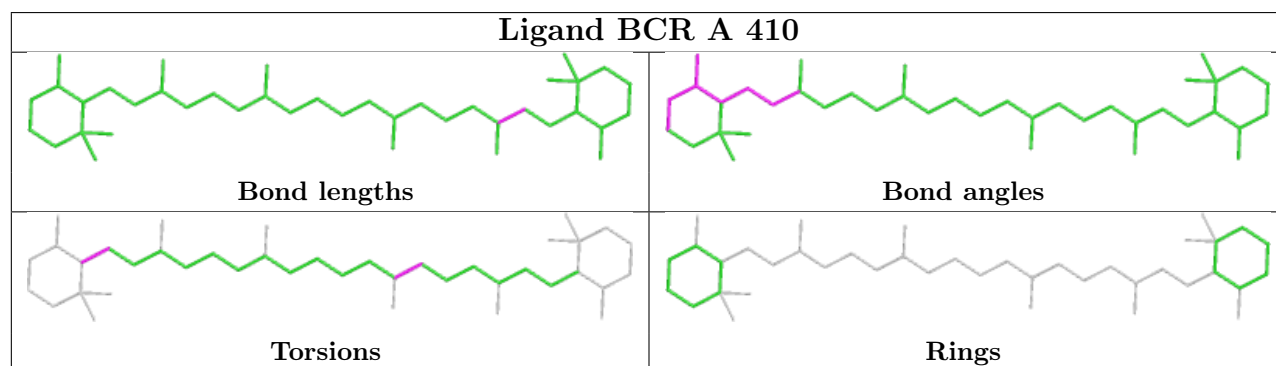
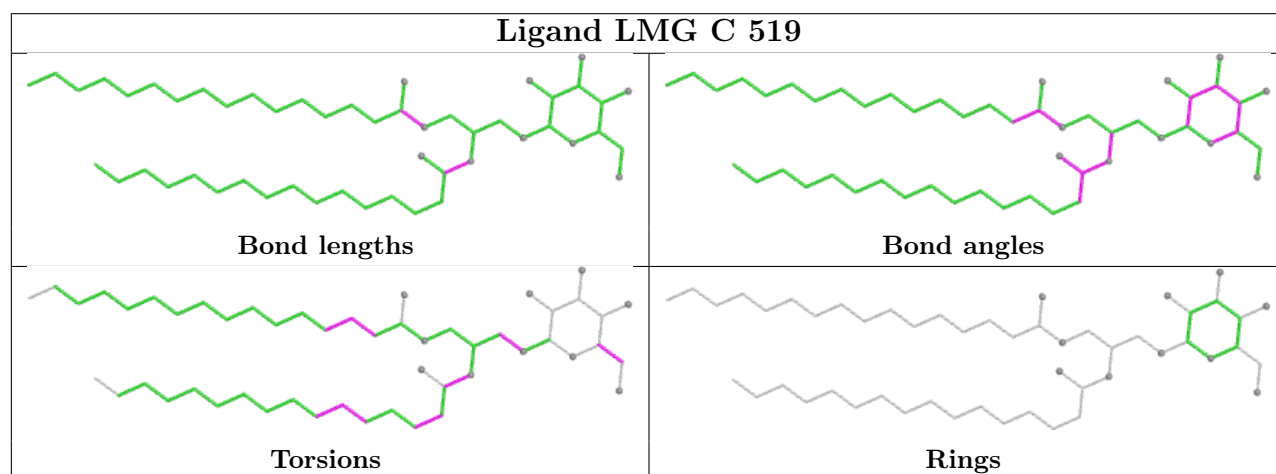
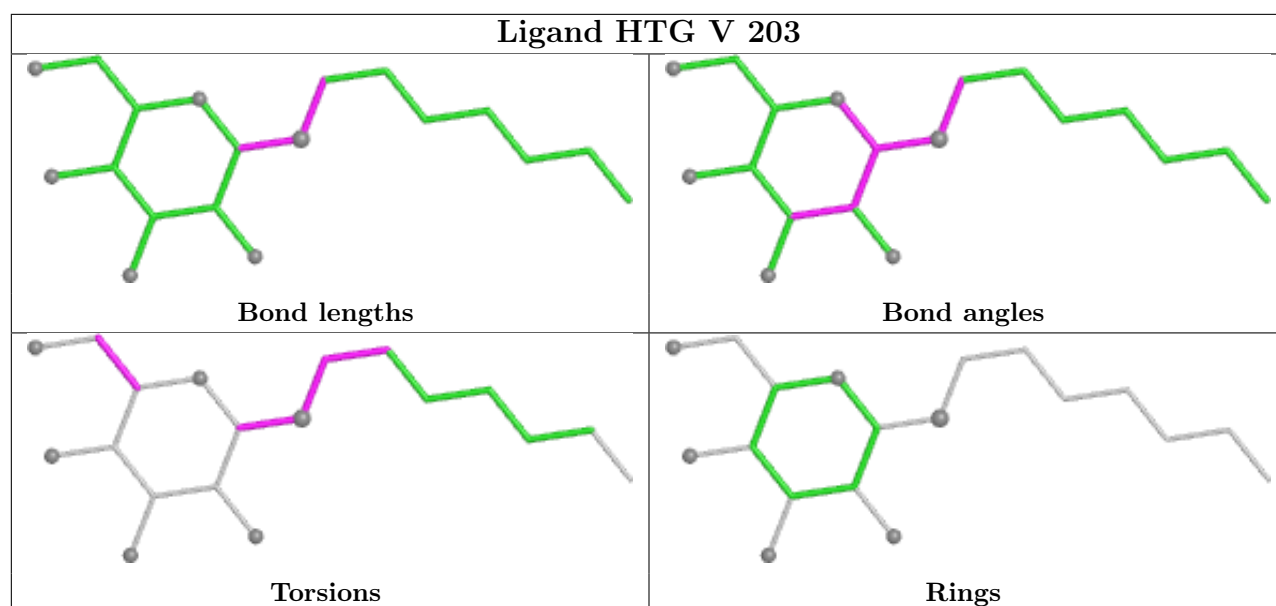
Ligand CLA a 408**Ligand CLA b 609**

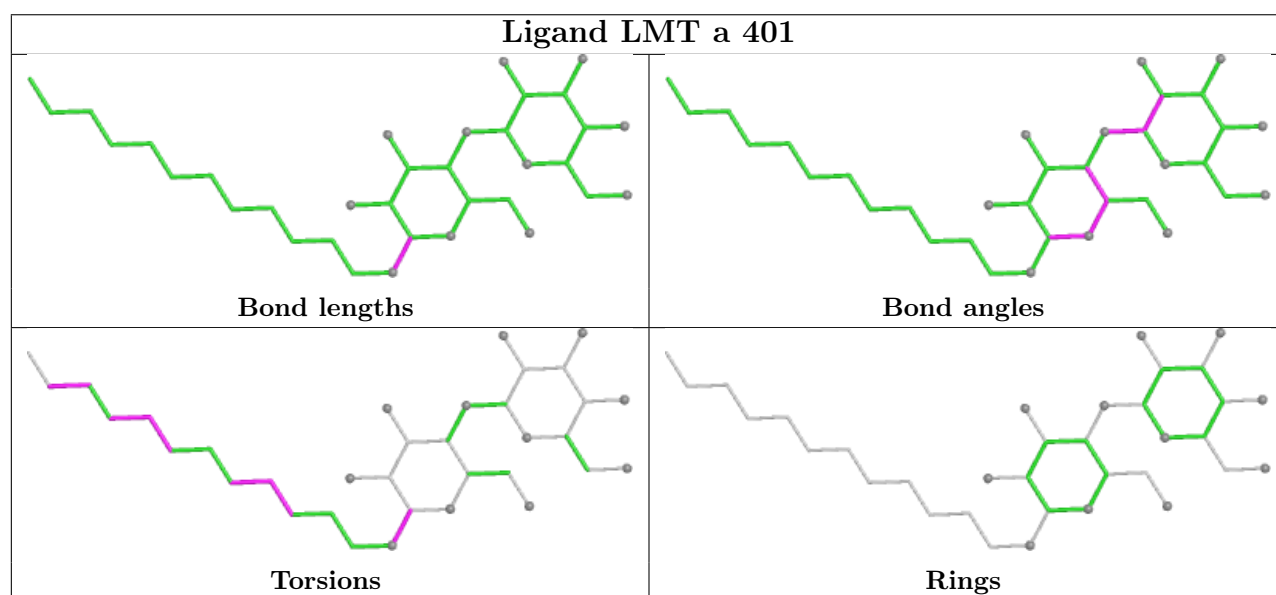
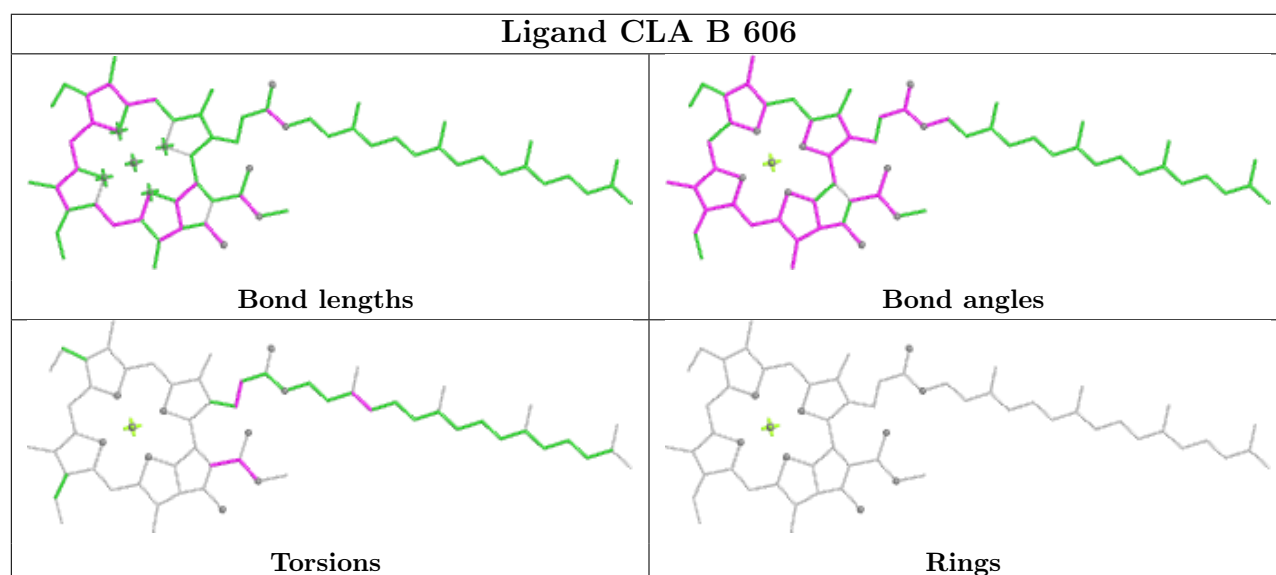
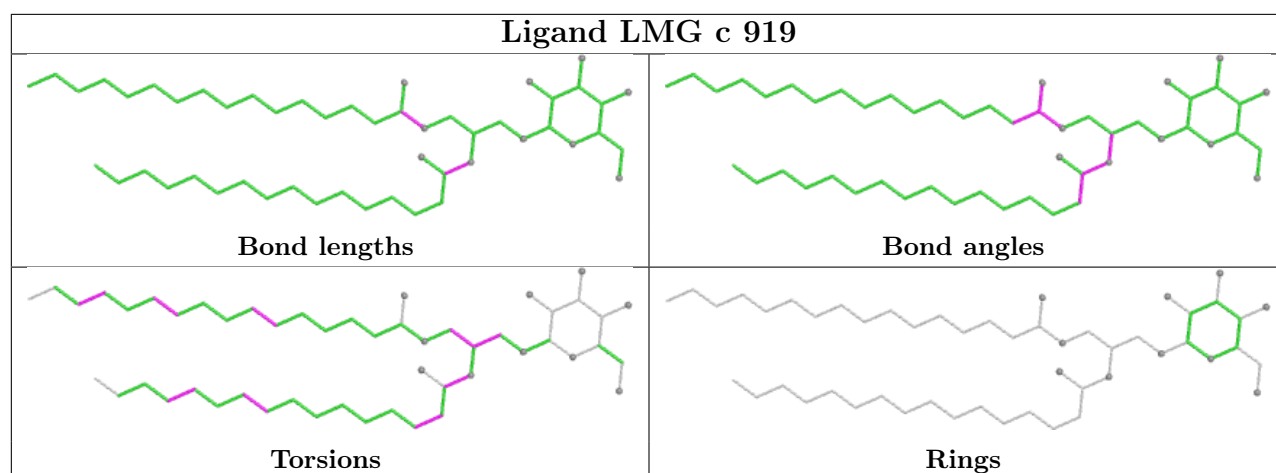
Ligand HEC v 202

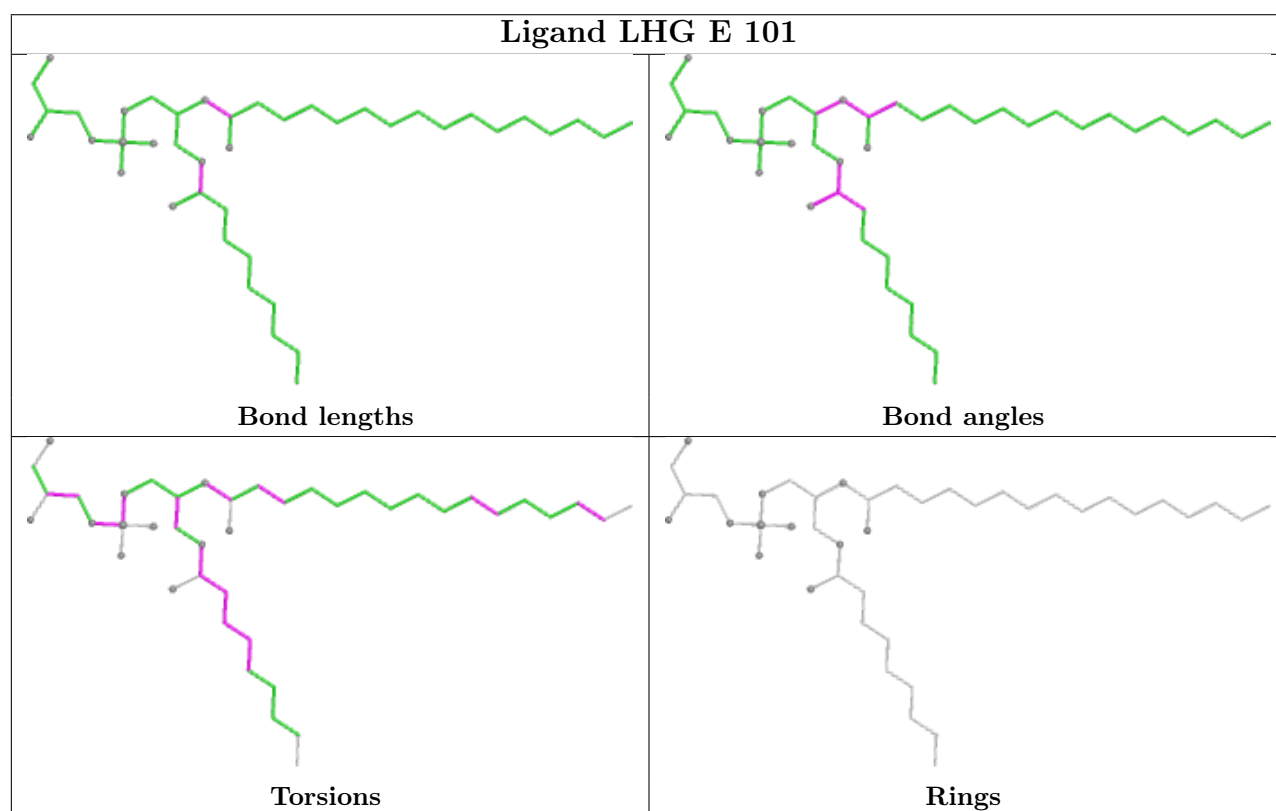
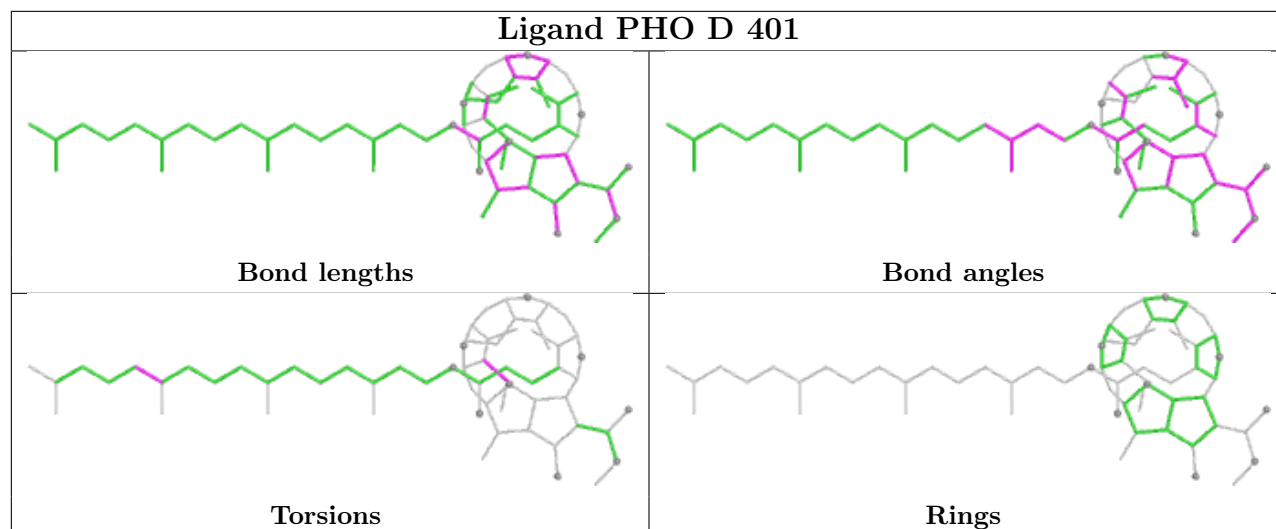


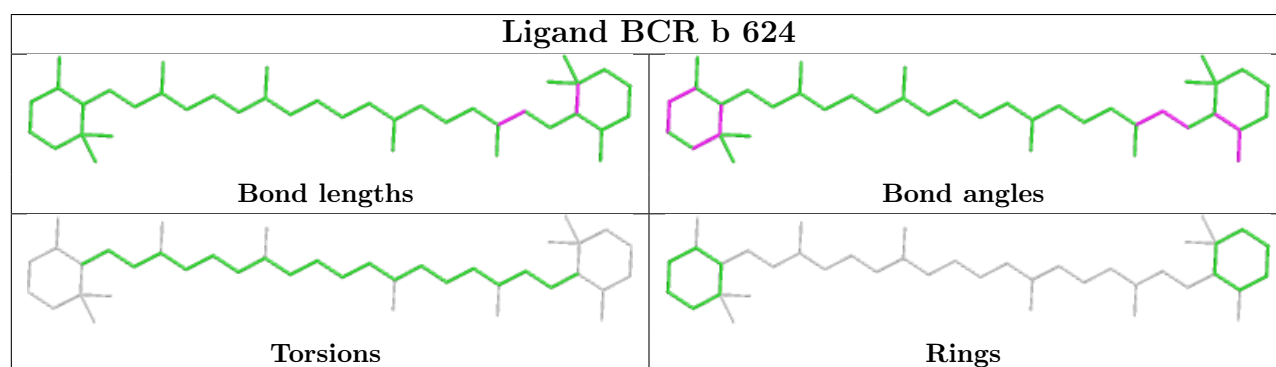
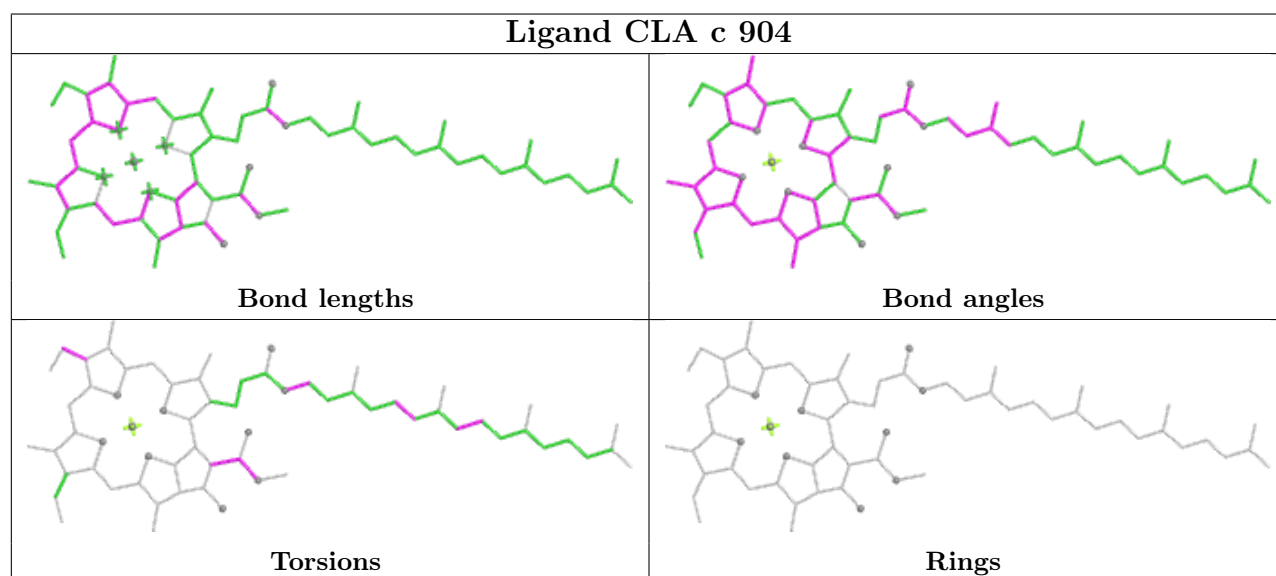
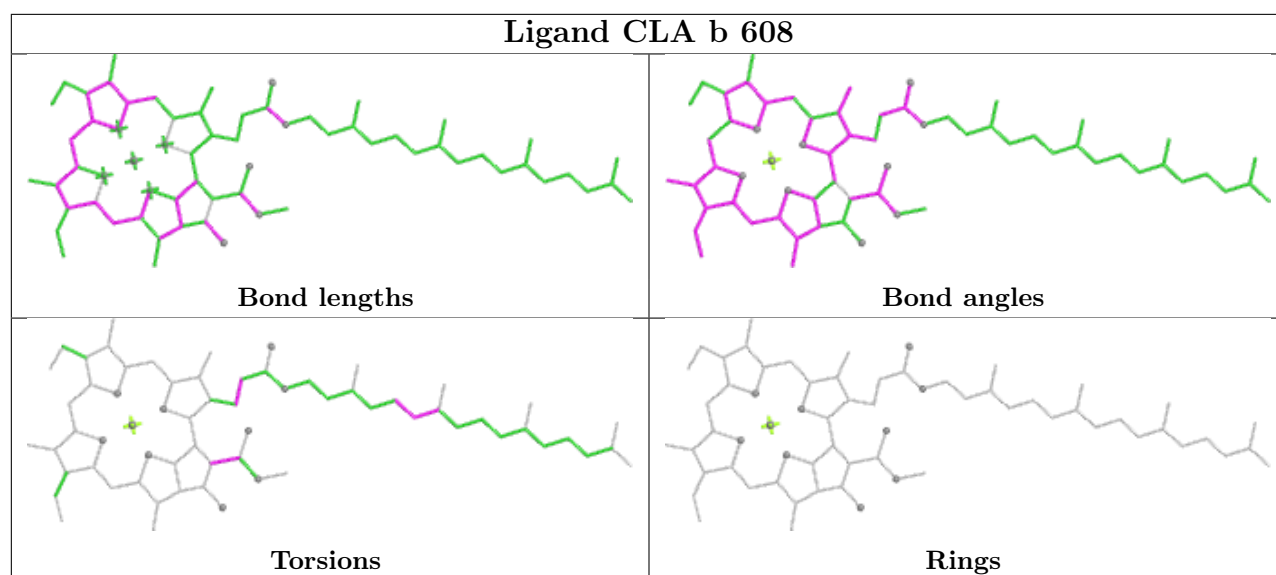
Ligand CLA C 502



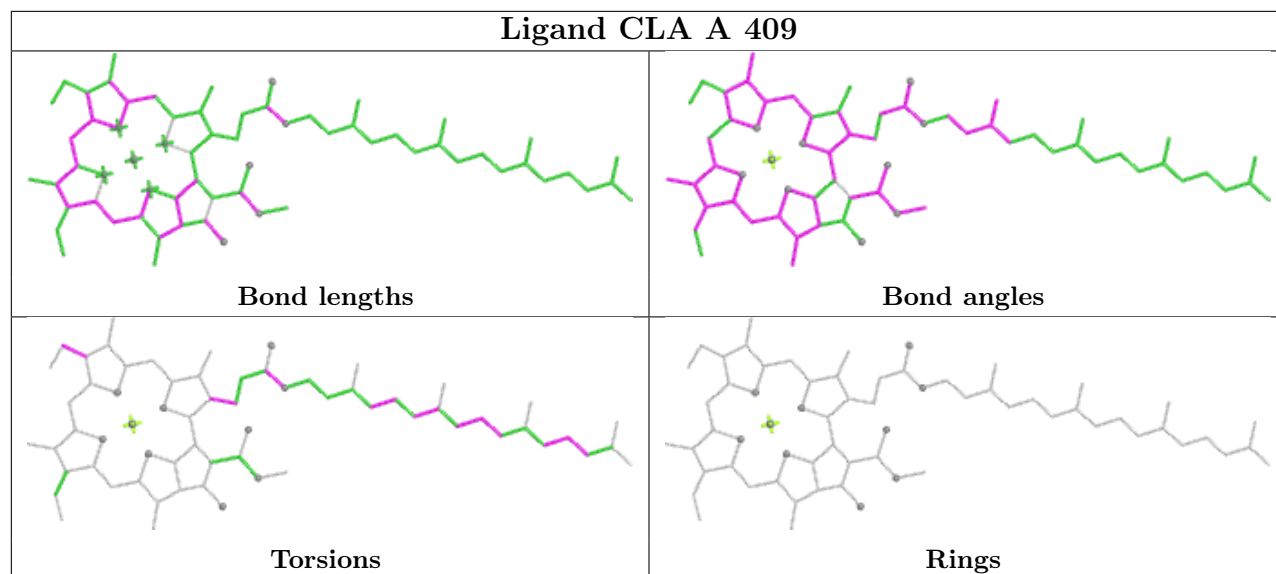




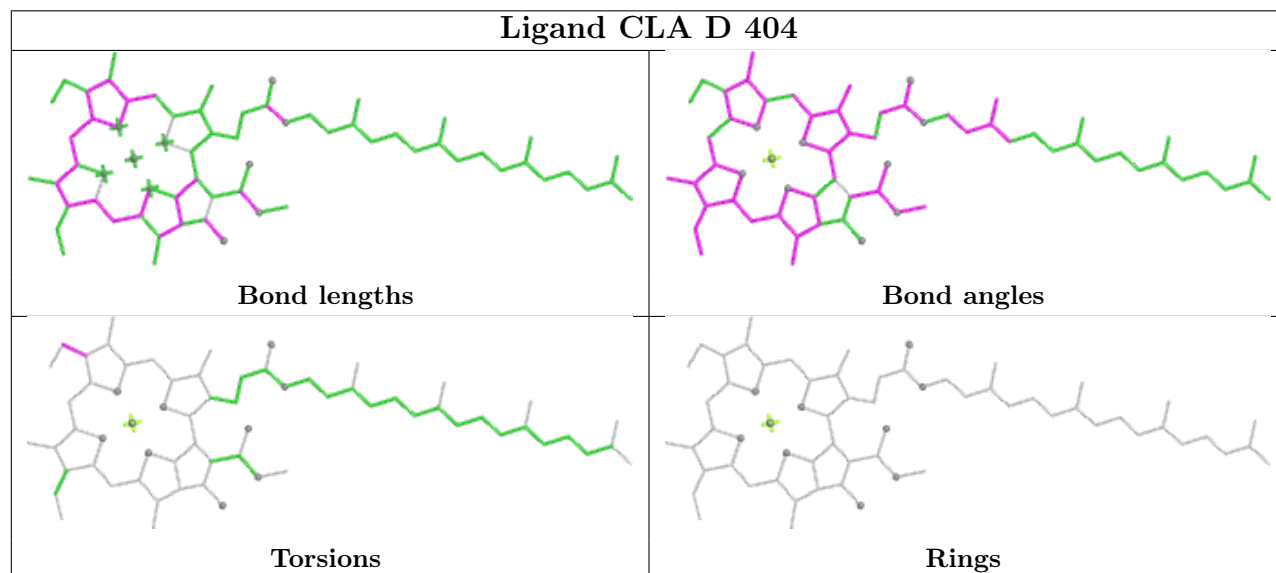


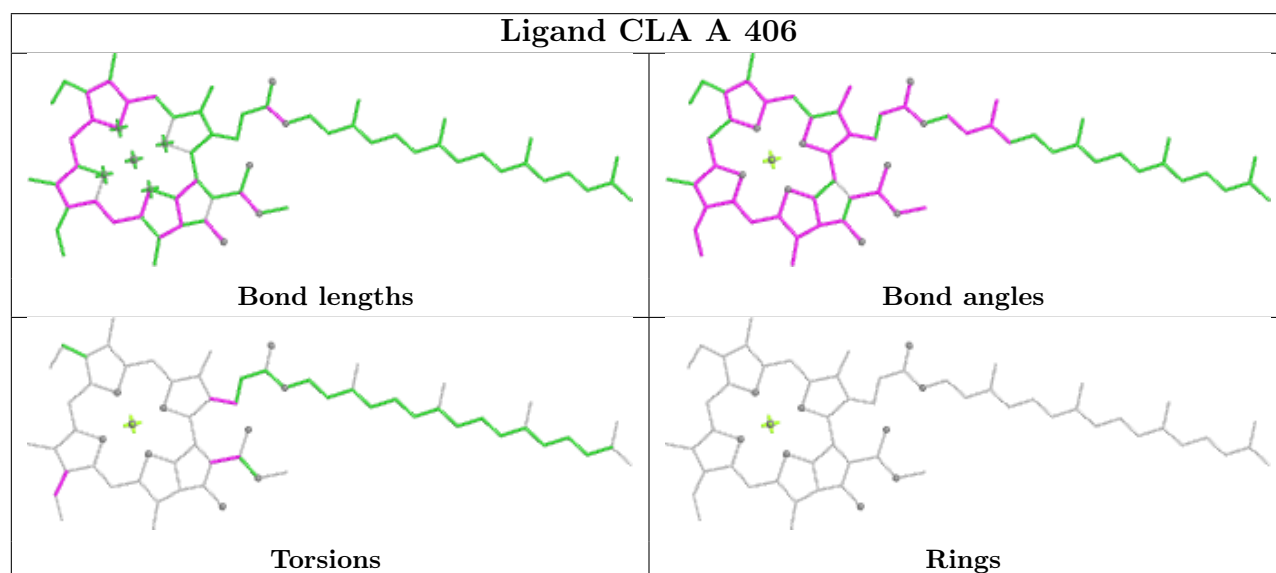
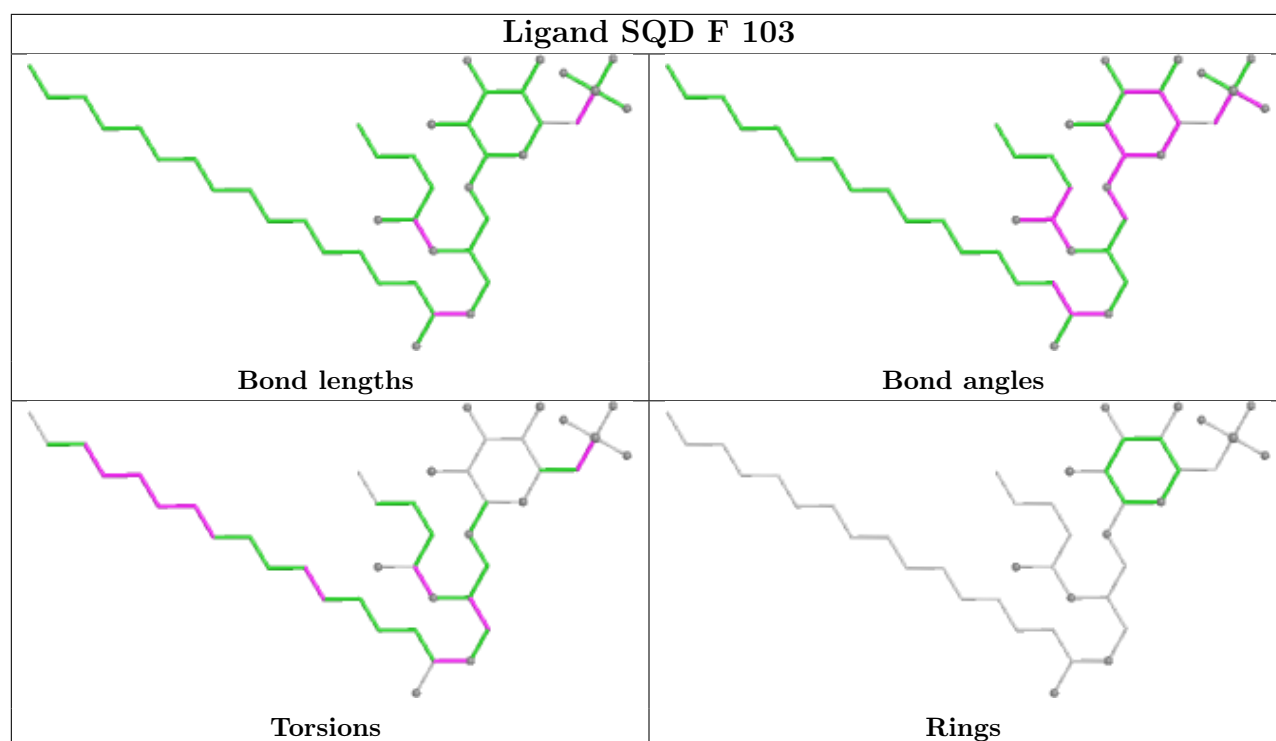


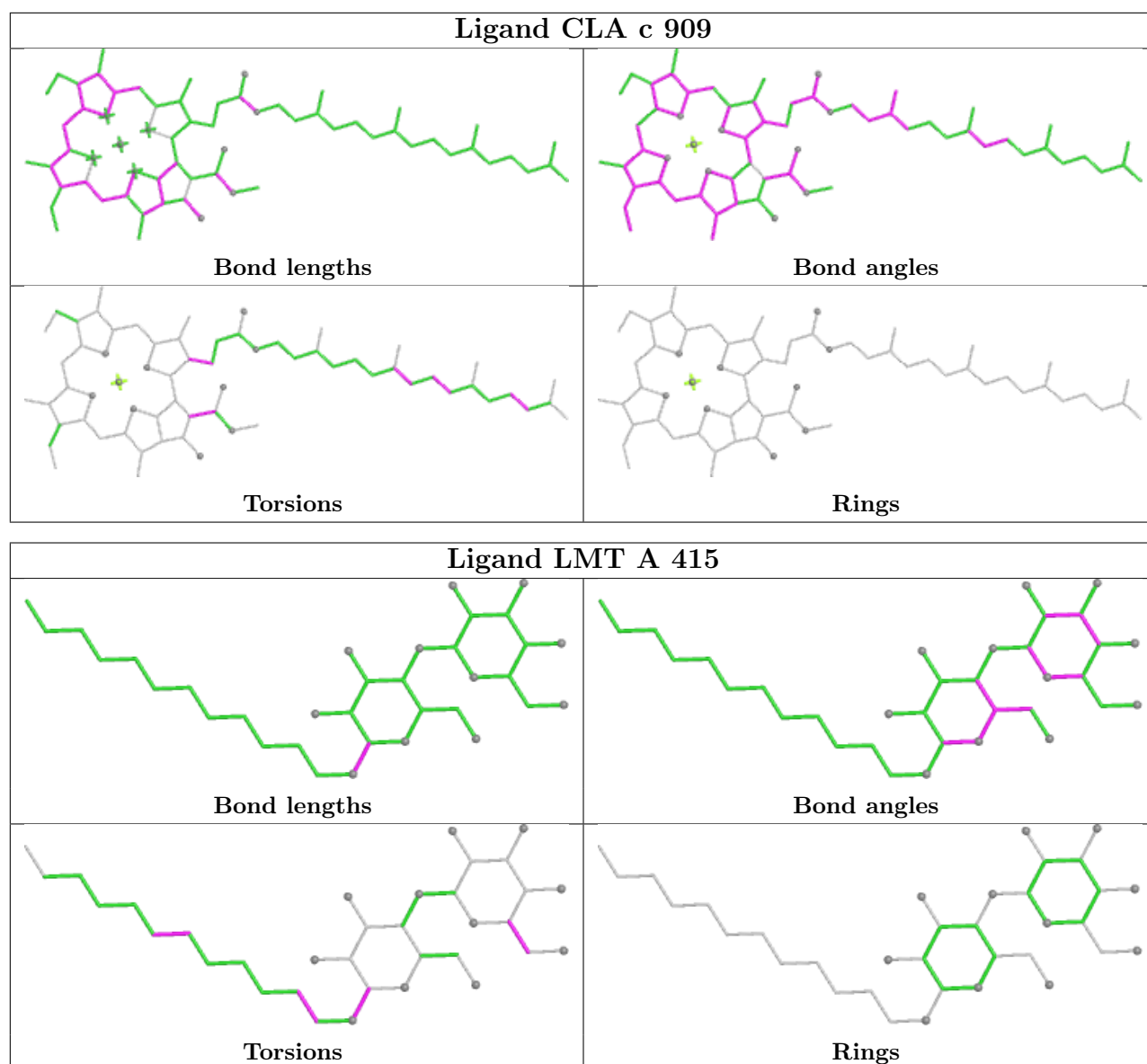
Ligand CLA A 409



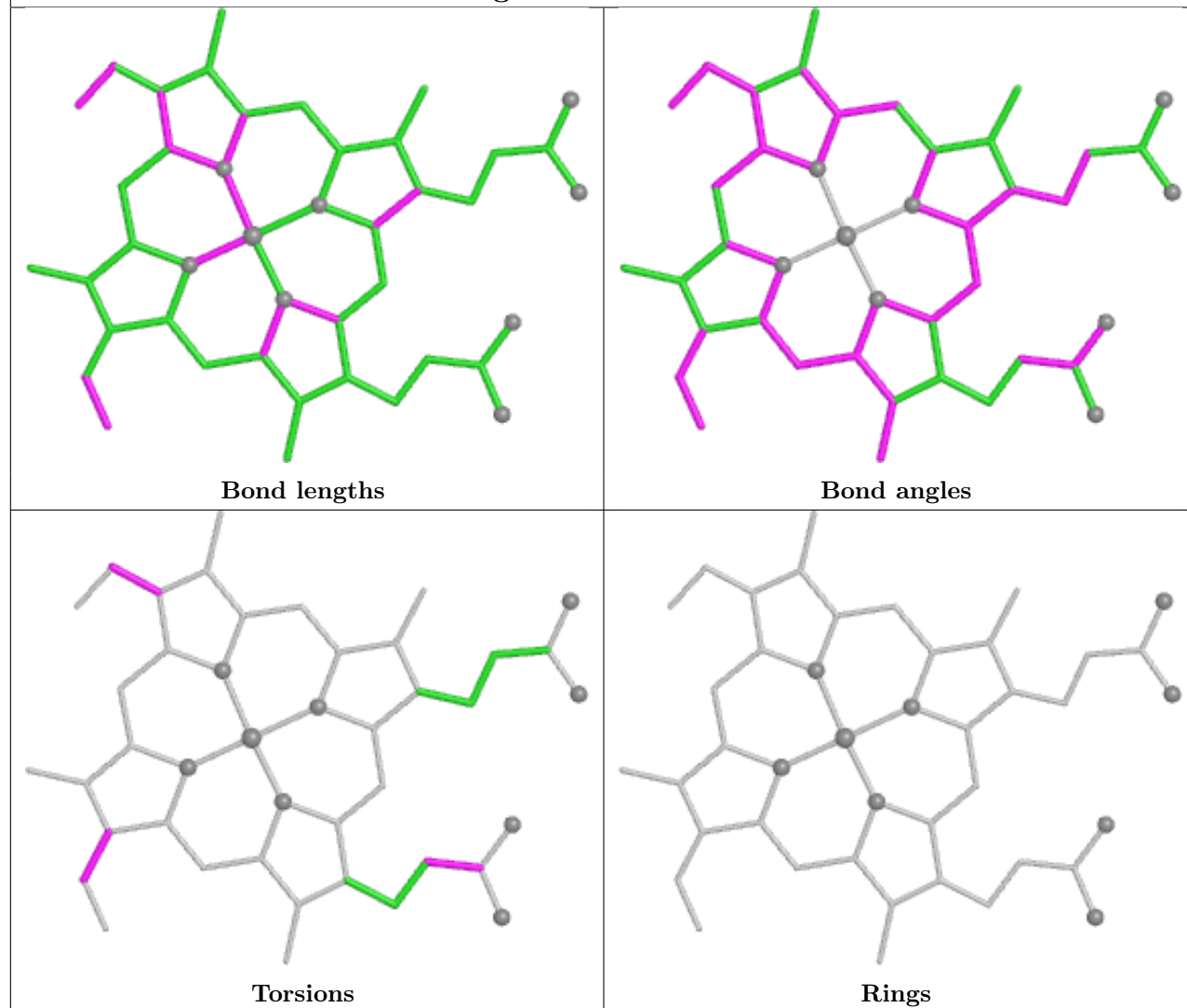
Ligand CLA D 404



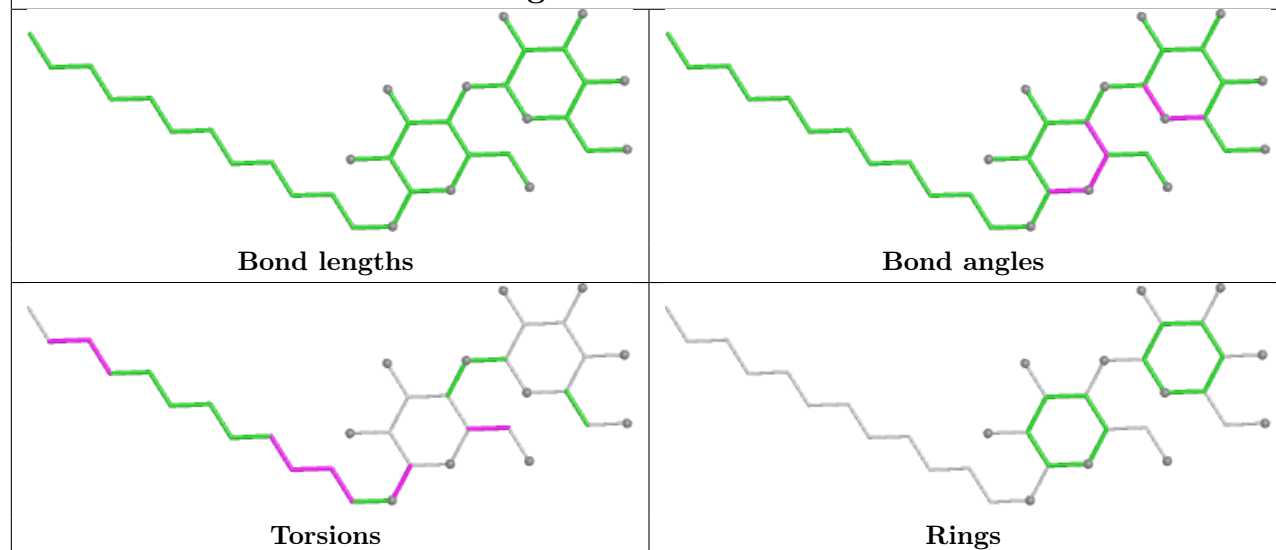


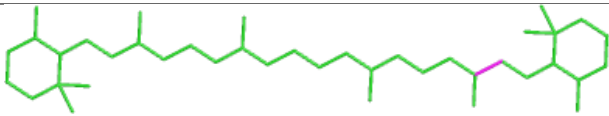
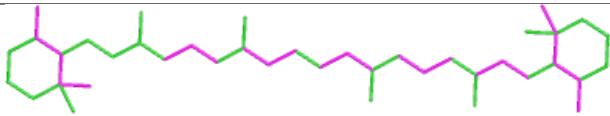
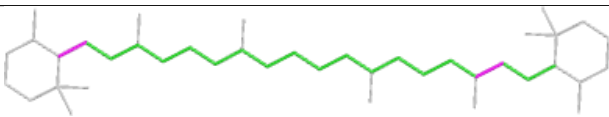
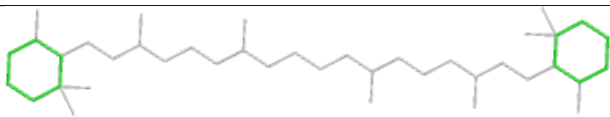


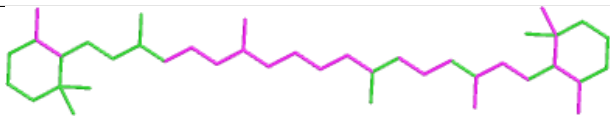
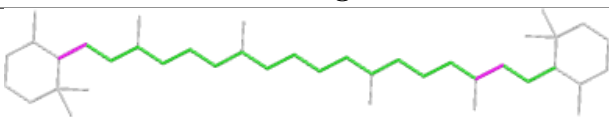
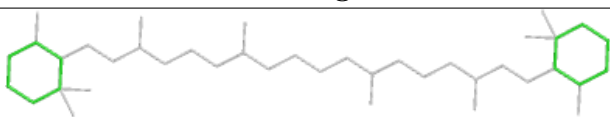
Ligand HEC V 202

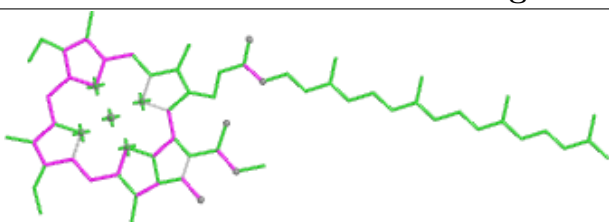
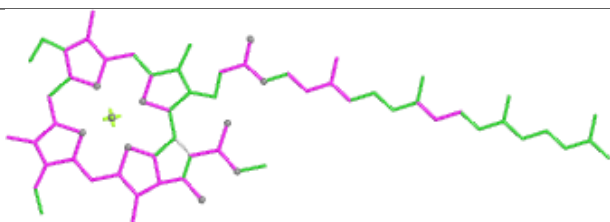
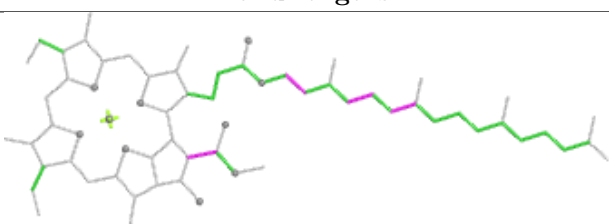
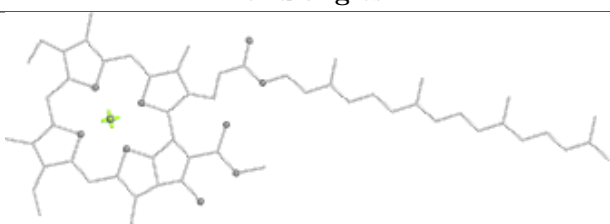


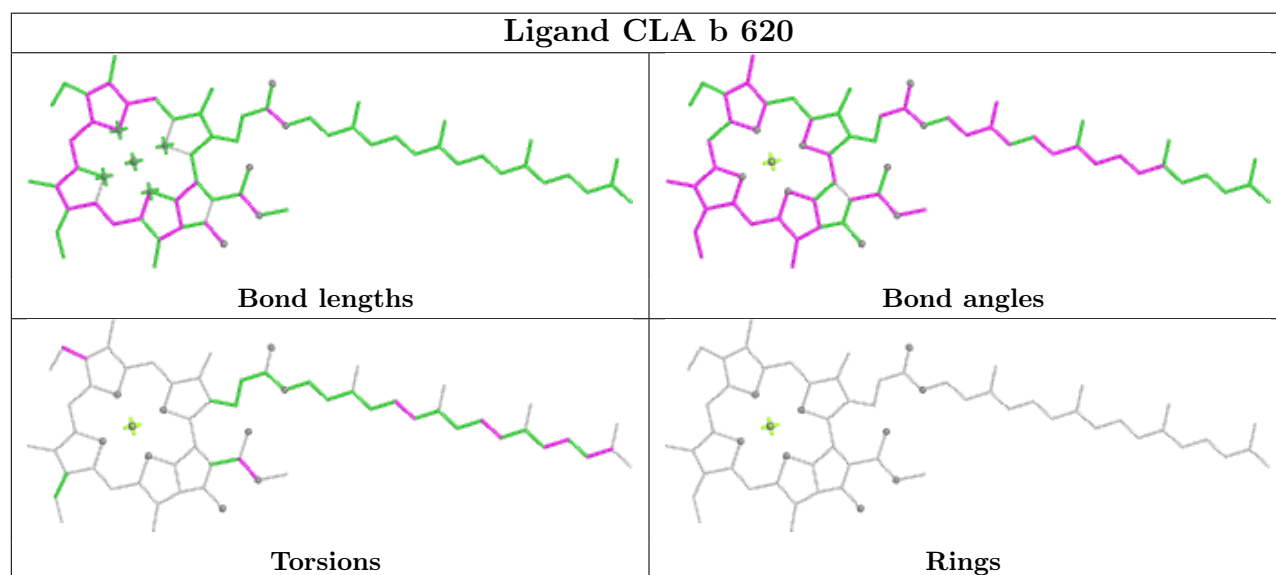
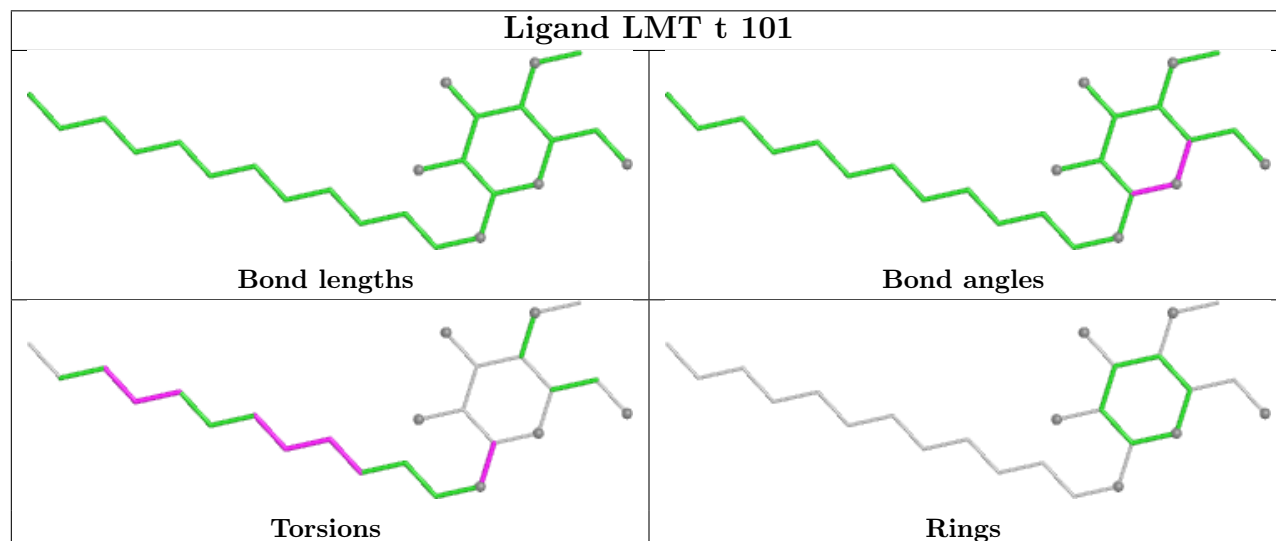
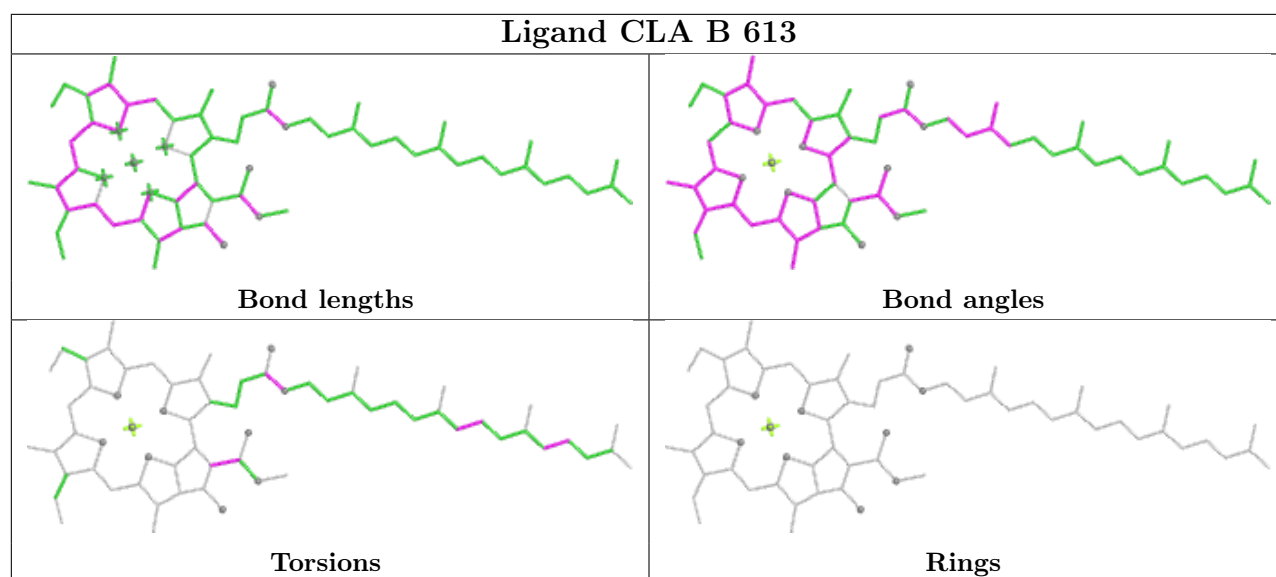
Ligand LMT m 103

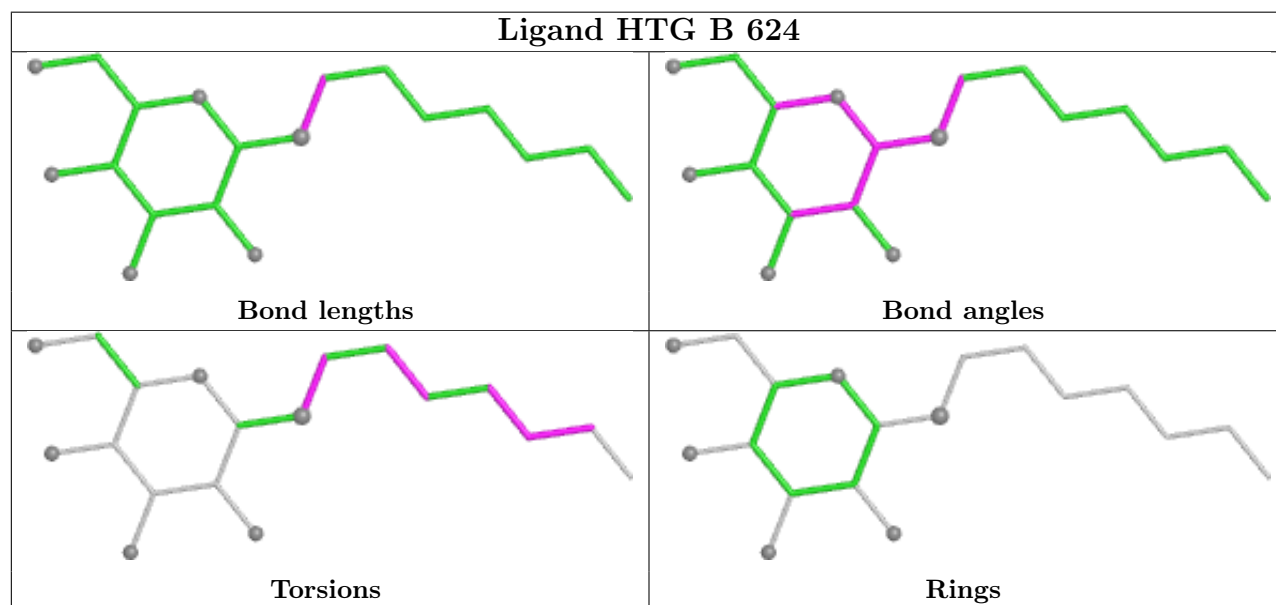
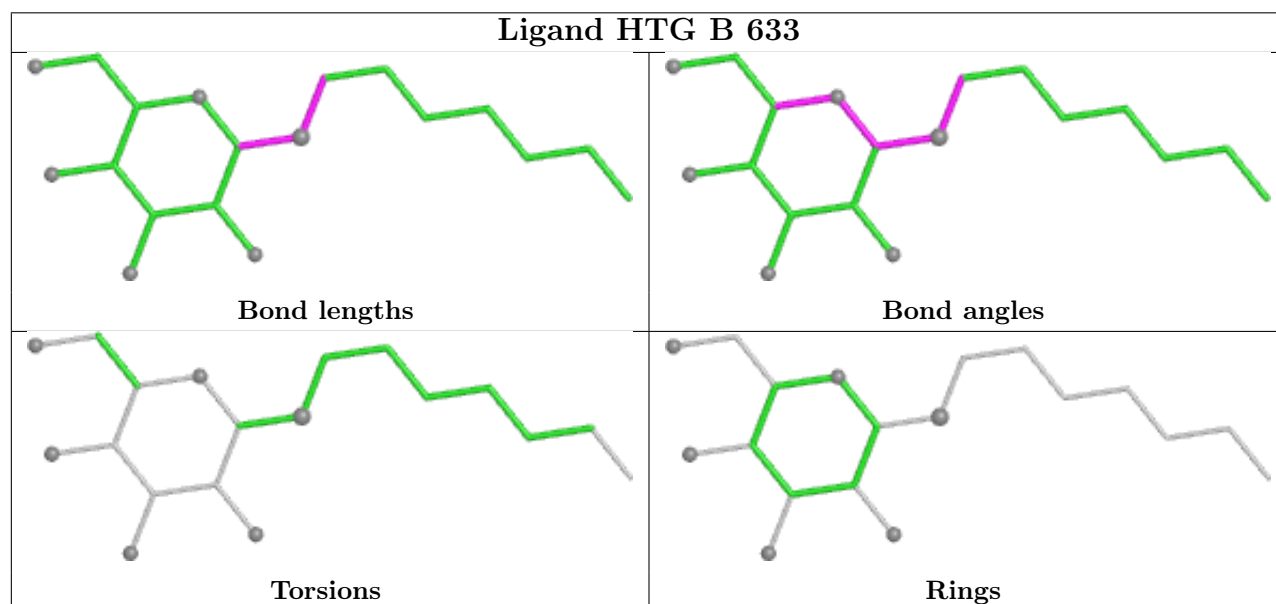
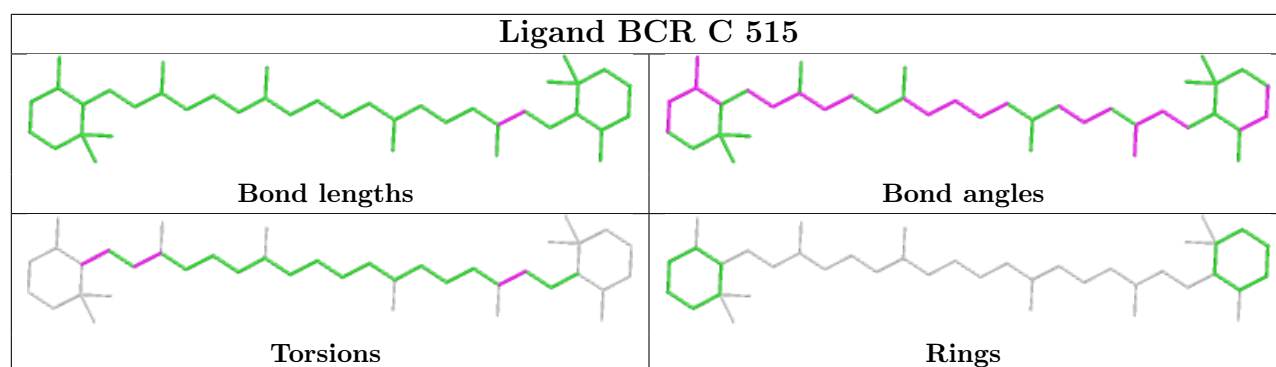


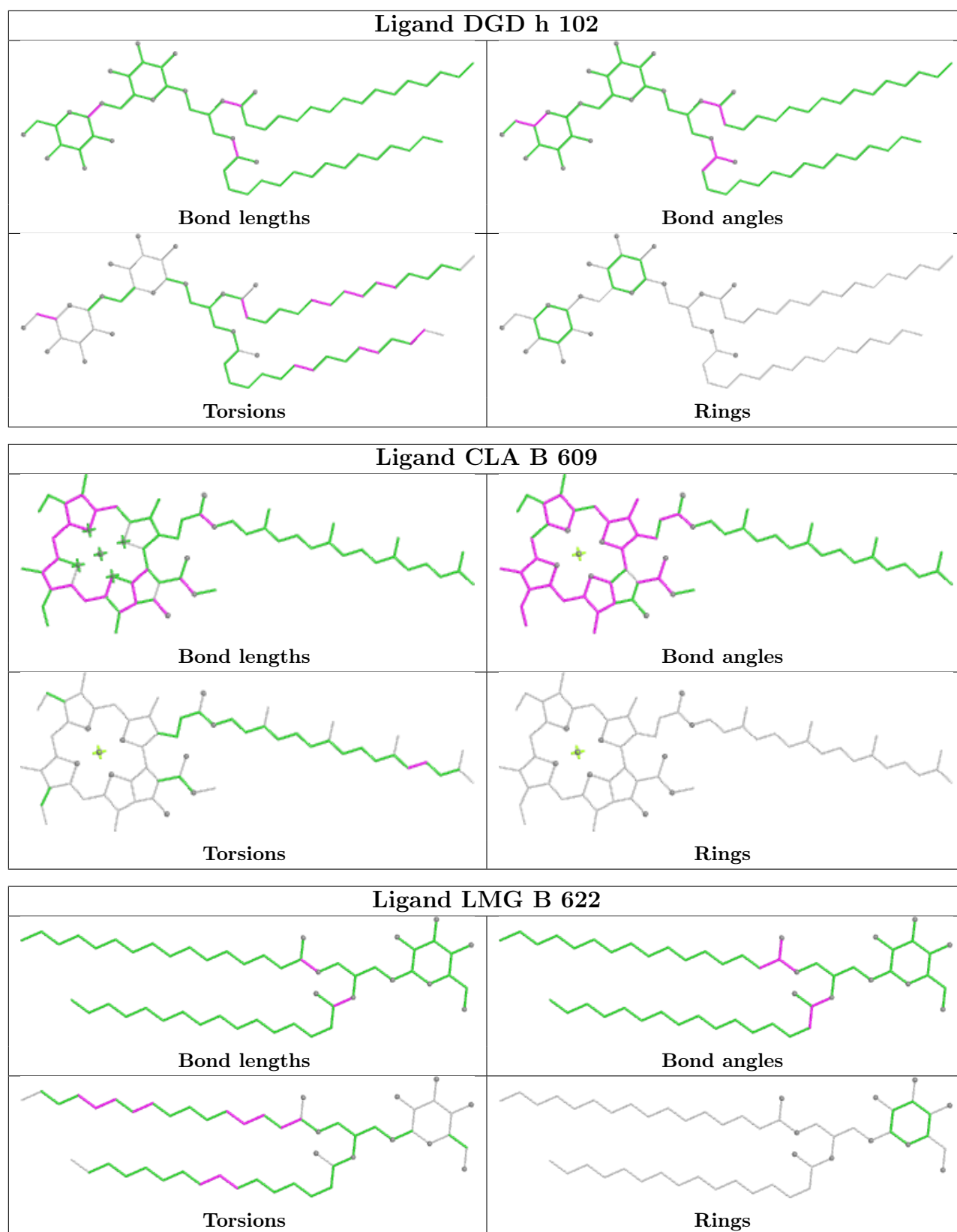
Ligand BCR y 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

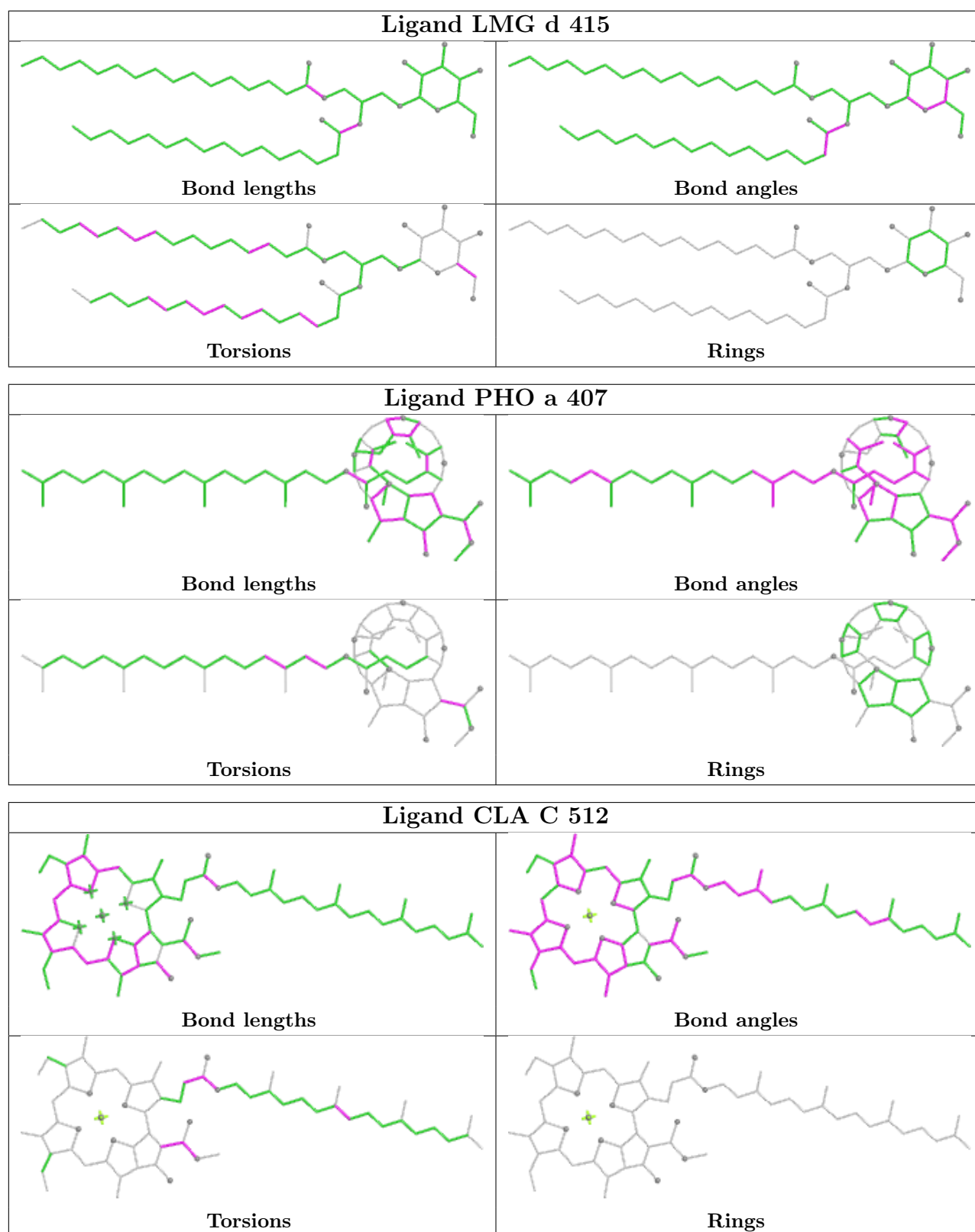
Ligand BCR Y 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

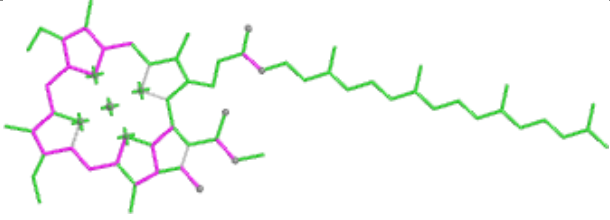
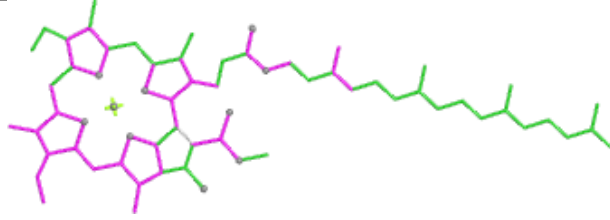
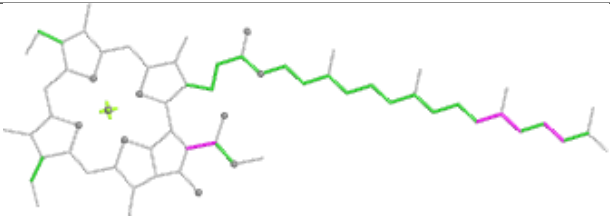
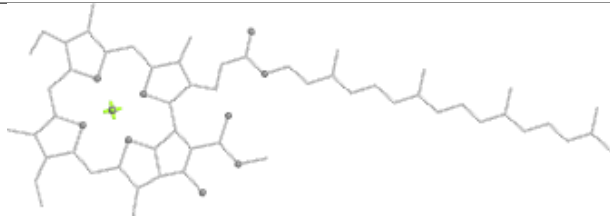
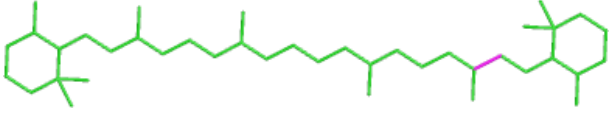
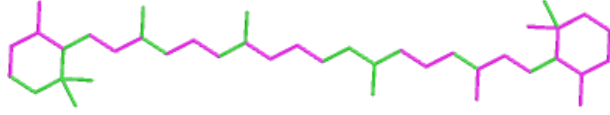
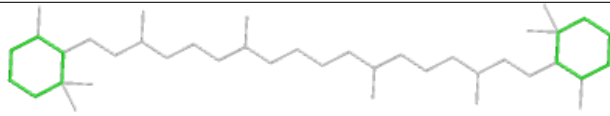
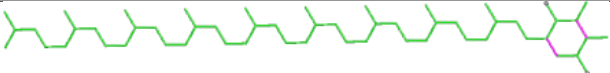
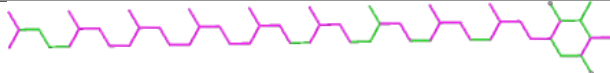
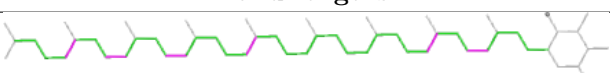
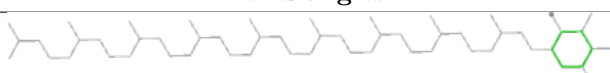
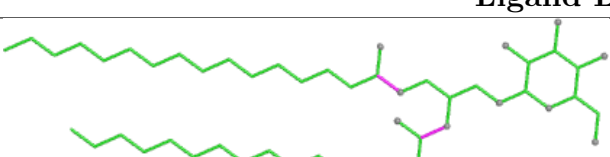
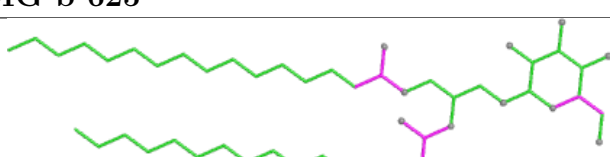
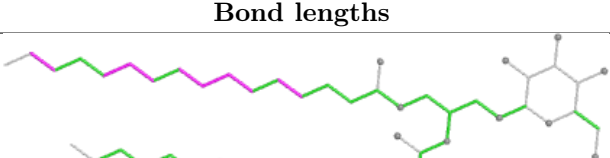
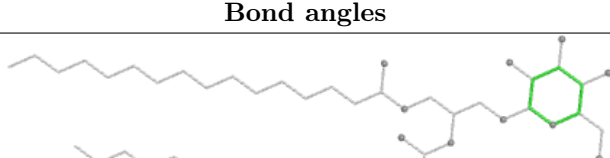
Ligand CLA B 605	
	
Bond lengths	Bond angles
	
Torsions	Rings



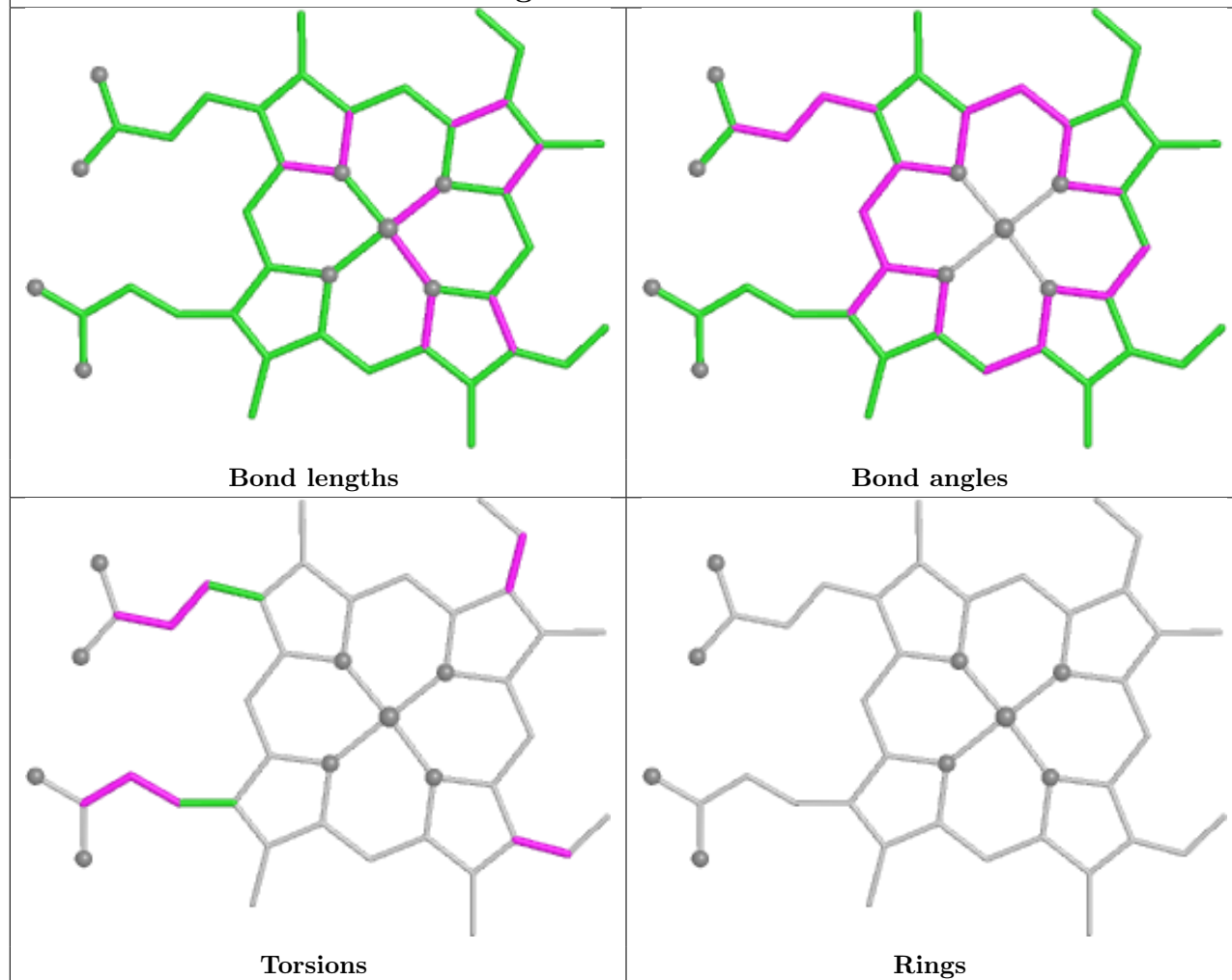




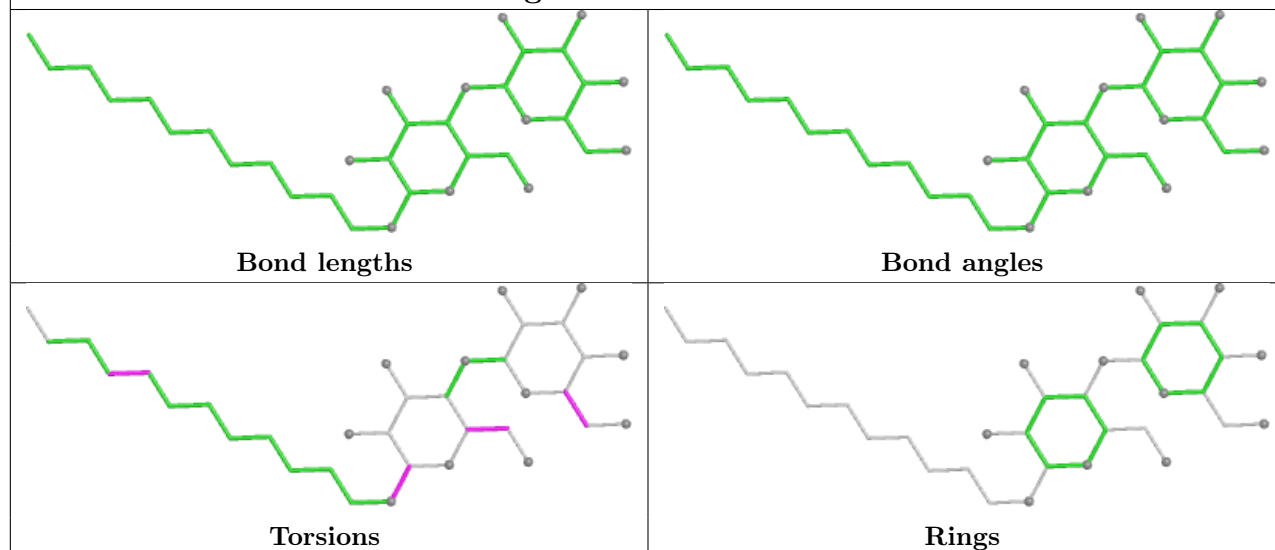


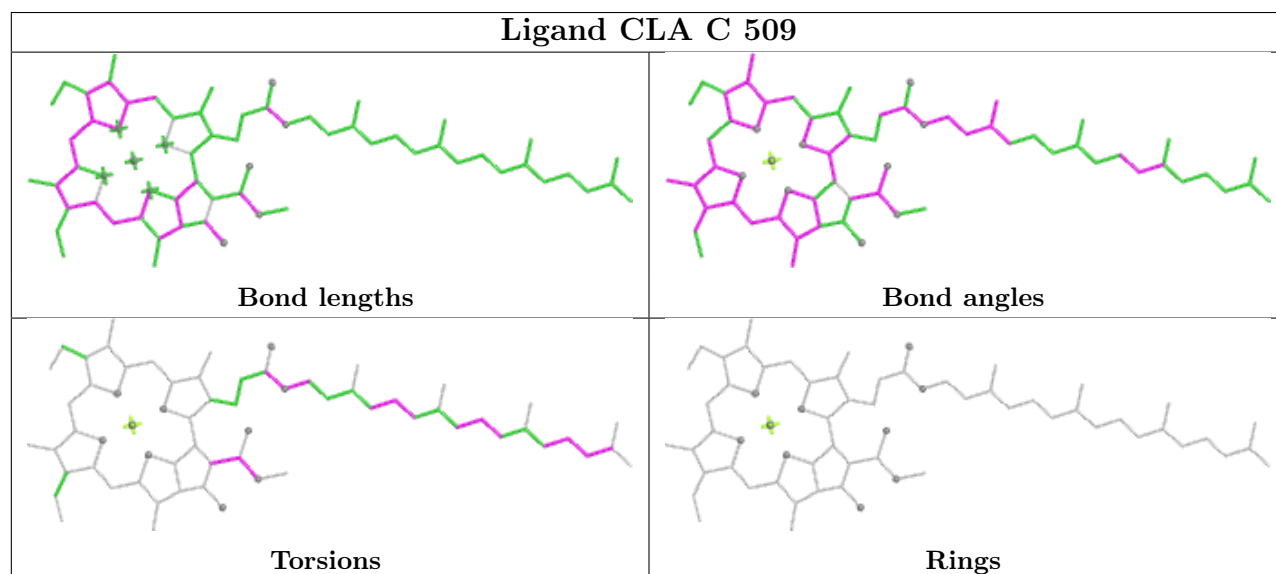
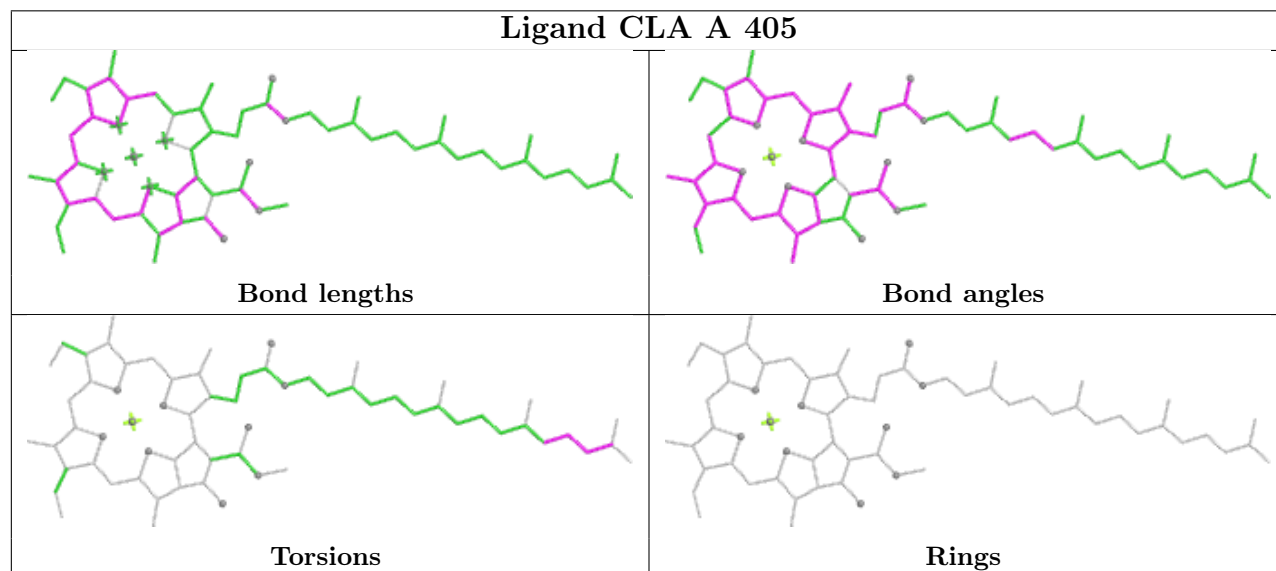
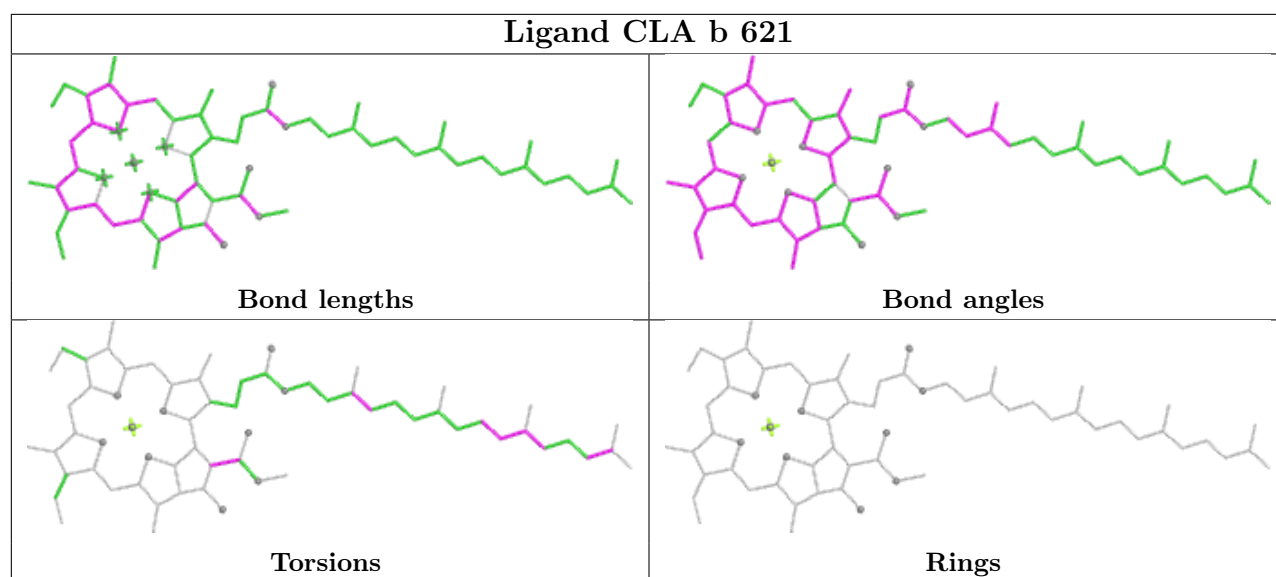
Ligand CLA C 504	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR d 407	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 D 407	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG b 625	
 Bond lengths	 Bond angles
 Torsions	 Rings

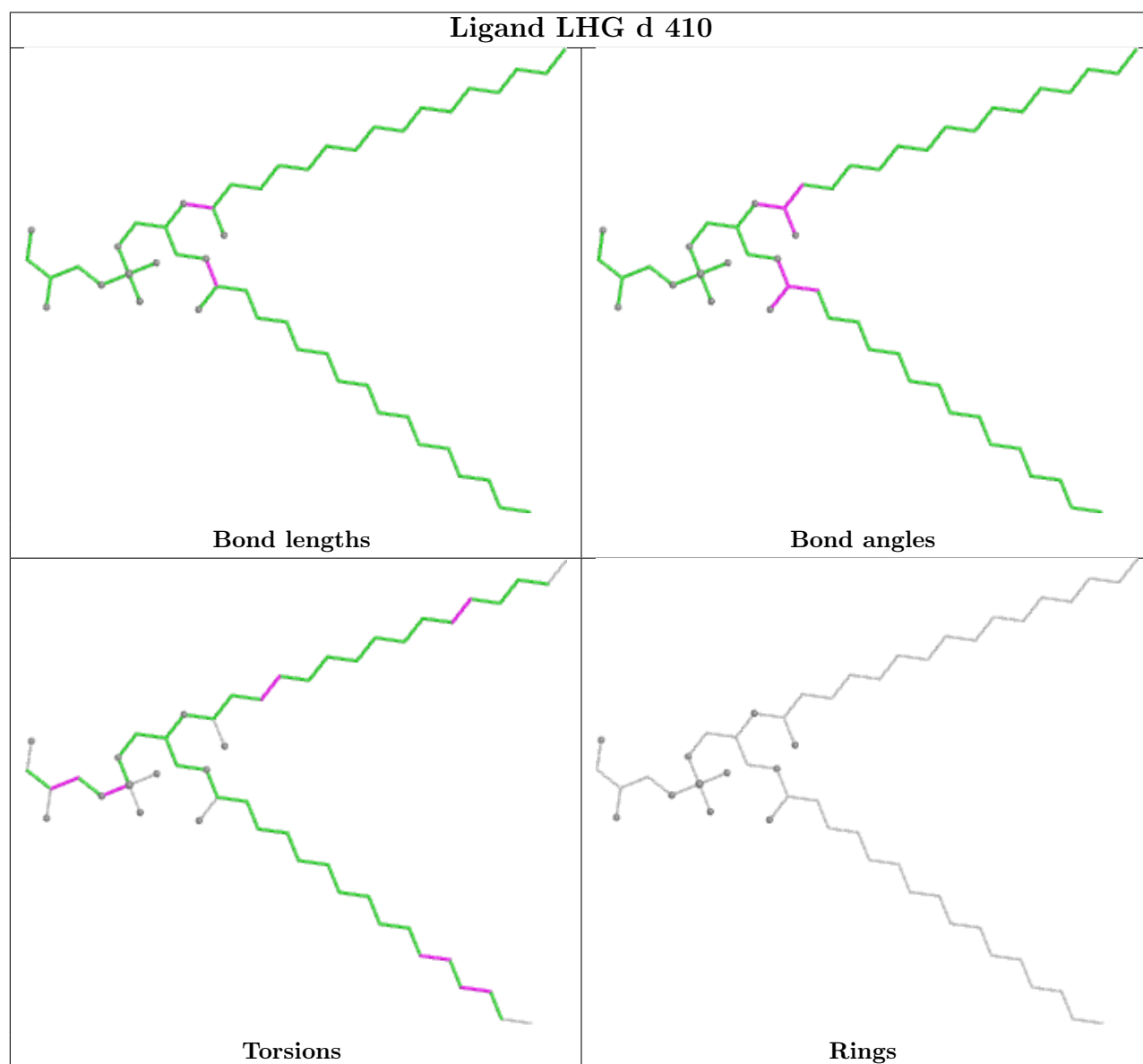
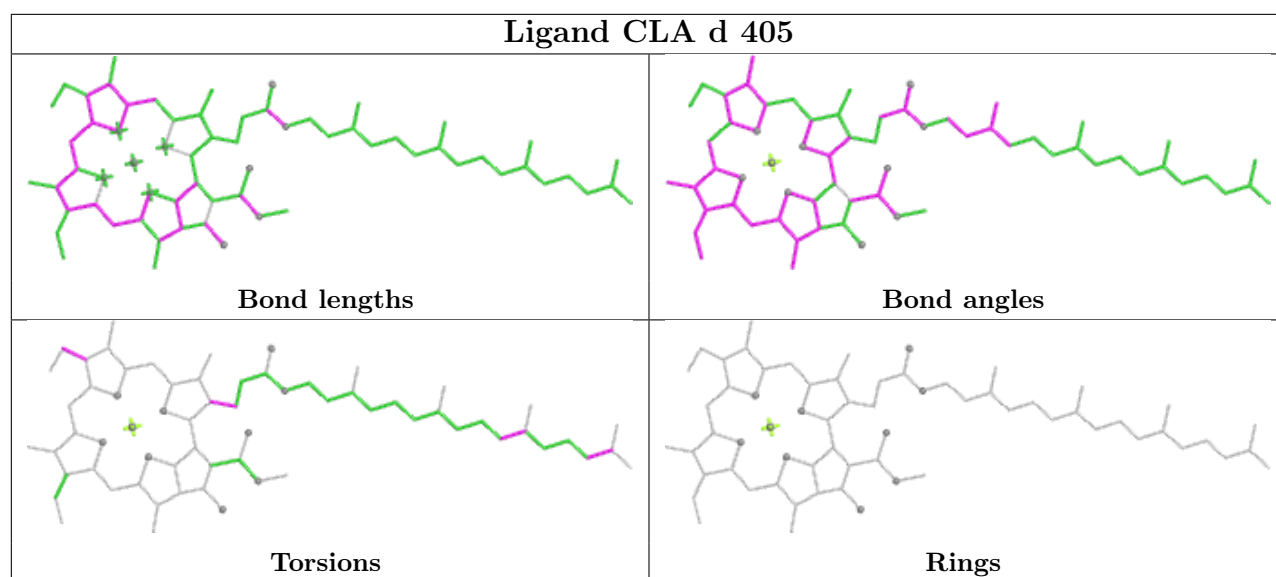
Ligand HEM f 101

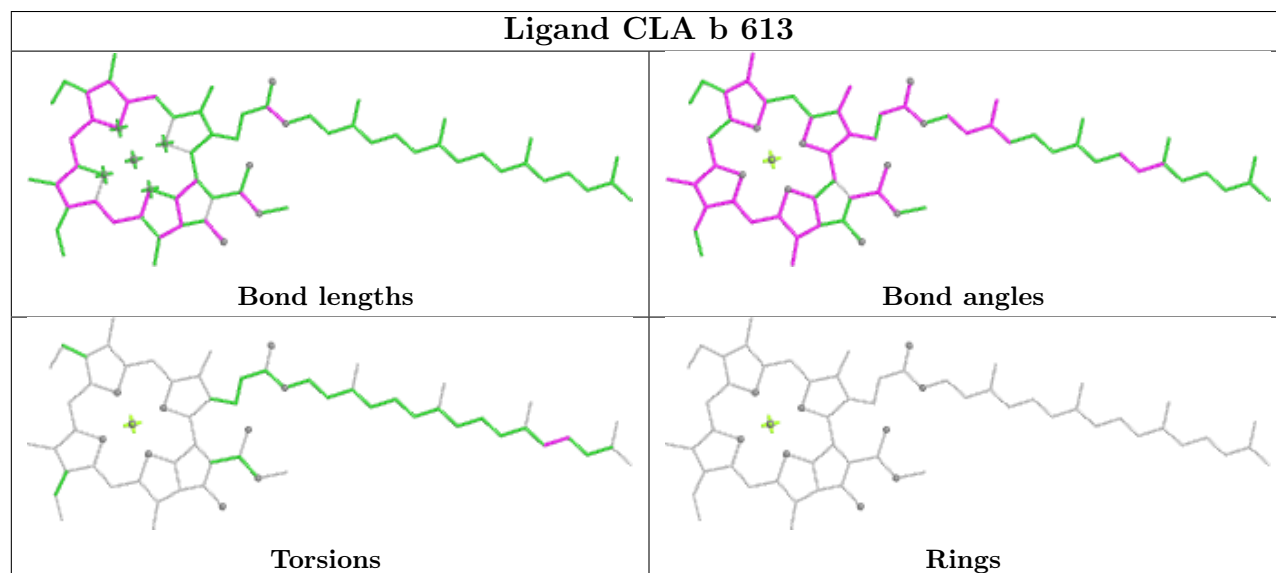
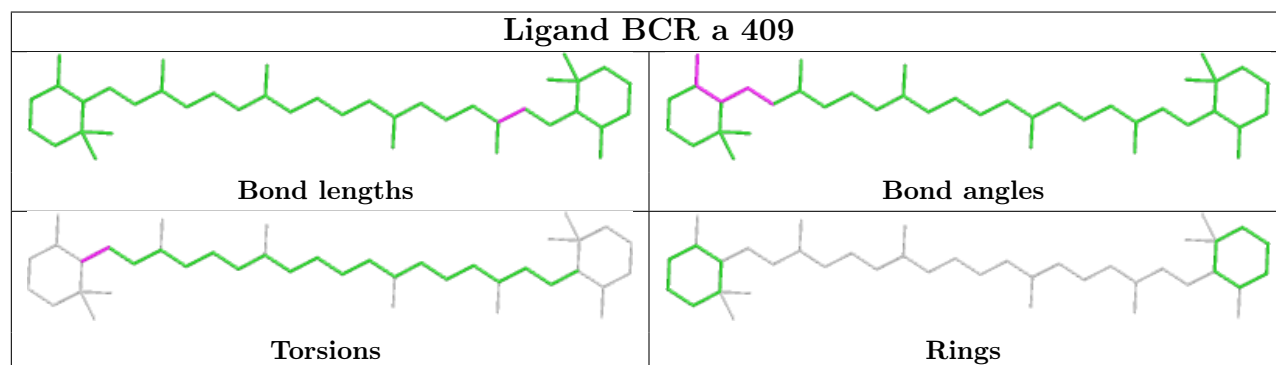
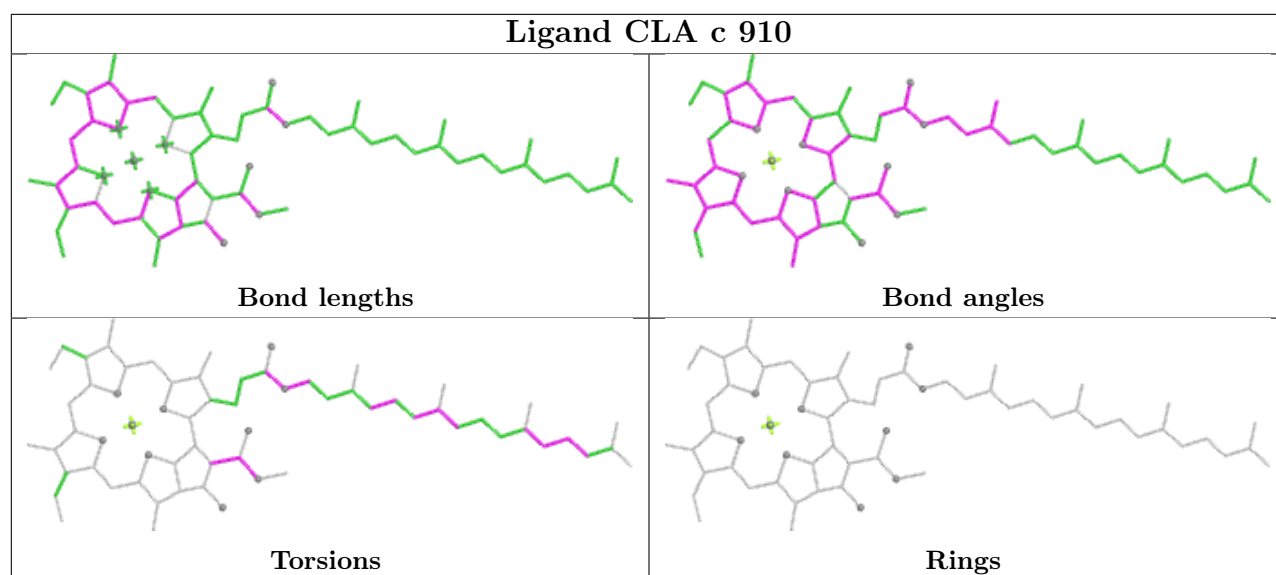


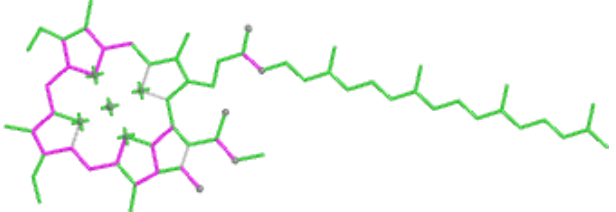
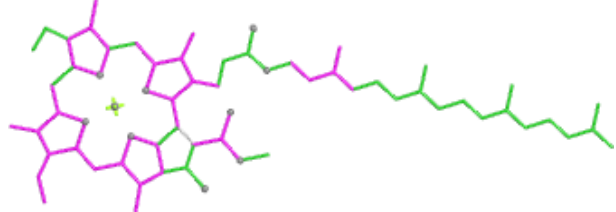
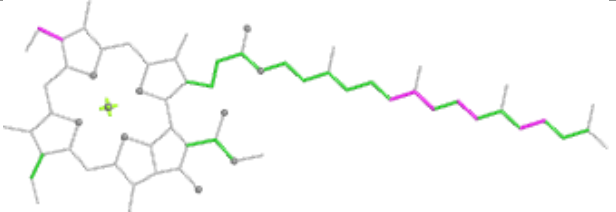
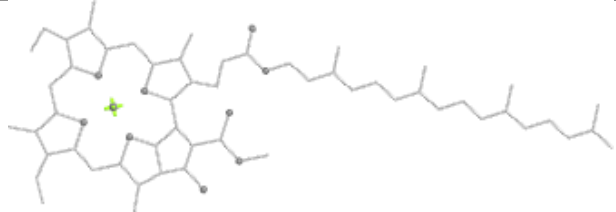
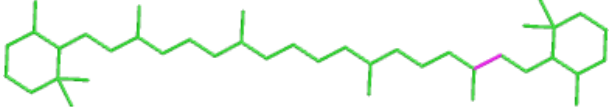
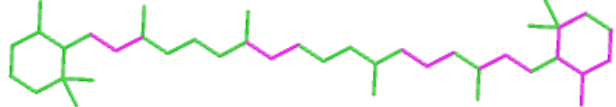
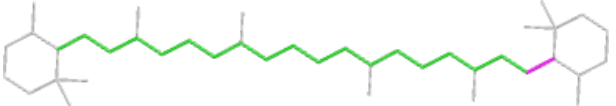
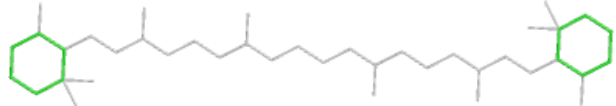
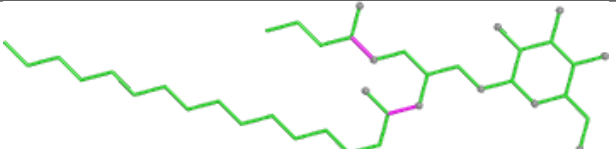
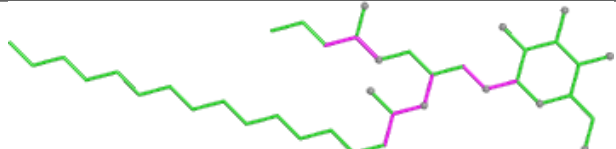
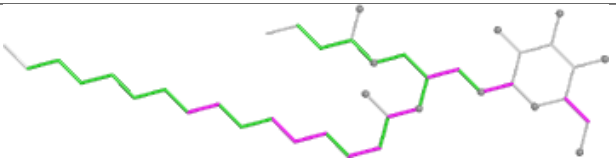
Ligand LMT M 101

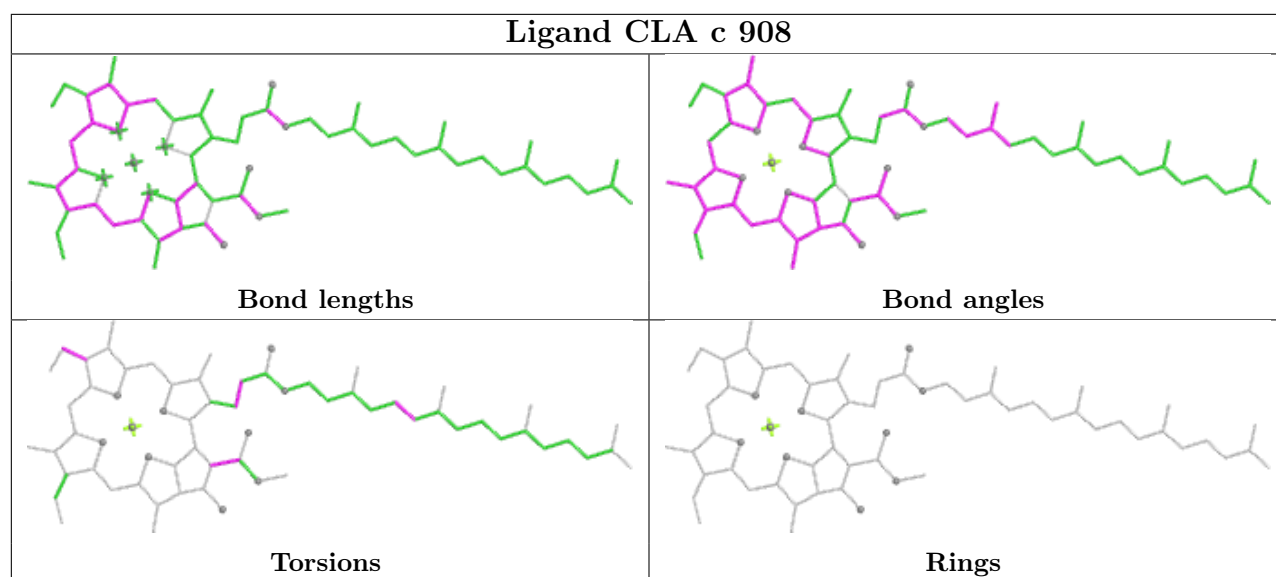








Ligand CLA A 407	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b 623	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG z 101	
 Bond lengths	 Bond angles
 Torsions	 Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.55	0 100 100	30, 43, 75, 139	3 (0%)
1	a	334/344 (97%)	-0.57	0 100 100	24, 44, 84, 146	6 (1%)
2	B	504/505 (99%)	-0.48	2 (0%) 88 91	24, 48, 86, 137	10 (1%)
2	b	503/505 (99%)	-0.44	5 (0%) 79 83	27, 48, 91, 193	12 (2%)
3	C	451/455 (99%)	-0.40	0 100 100	35, 56, 82, 134	4 (0%)
3	c	455/455 (100%)	-0.41	0 100 100	26, 58, 83, 118	6 (1%)
4	D	341/342 (99%)	-0.60	0 100 100	25, 45, 70, 129	1 (0%)
4	d	341/342 (99%)	-0.62	0 100 100	26, 45, 69, 115	1 (0%)
5	E	81/84 (96%)	0.01	1 (1%) 76 81	36, 71, 116, 150	2 (2%)
5	e	81/84 (96%)	0.03	2 (2%) 58 64	38, 71, 125, 201	2 (2%)
6	F	34/44 (77%)	-0.13	0 100 100	51, 62, 103, 104	0
6	f	32/44 (72%)	-0.16	1 (3%) 51 58	50, 62, 118, 148	0
7	H	65/65 (100%)	-0.28	2 (3%) 51 58	39, 57, 83, 145	1 (1%)
7	h	65/65 (100%)	-0.41	1 (1%) 72 77	47, 60, 83, 167	0
8	I	37/38 (97%)	-0.10	0 100 100	45, 58, 123, 187	0
8	i	37/38 (97%)	-0.15	1 (2%) 56 63	44, 57, 116, 159	0
9	J	38/39 (97%)	0.01	1 (2%) 57 63	52, 68, 151, 185	0
9	j	39/39 (100%)	0.00	1 (2%) 57 63	52, 68, 140, 190	0
10	K	37/37 (100%)	-0.20	0 100 100	60, 68, 88, 112	0
10	k	37/37 (100%)	-0.27	0 100 100	59, 67, 88, 112	0
11	L	37/37 (100%)	-0.61	0 100 100	22, 39, 101, 132	1 (2%)
11	l	37/37 (100%)	-0.49	0 100 100	23, 40, 105, 130	1 (2%)
12	M	33/36 (91%)	-0.48	0 100 100	24, 41, 75, 126	1 (3%)
12	m	33/36 (91%)	-0.52	0 100 100	35, 42, 78, 126	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.47	0 100 100	29, 54, 102, 146	8 (3%)
13	o	243/244 (99%)	-0.42	0 100 100	28, 55, 112, 179	5 (2%)
14	T	29/32 (90%)	-0.68	1 (3%) 48 55	31, 39, 70, 142	1 (3%)
14	t	29/32 (90%)	-0.60	1 (3%) 48 55	32, 39, 68, 141	1 (3%)
15	U	97/104 (93%)	-0.54	0 100 100	39, 51, 82, 128	0
15	u	97/104 (93%)	-0.53	0 100 100	42, 52, 76, 126	0
16	V	137/137 (100%)	-0.47	0 100 100	27, 54, 88, 123	1 (0%)
16	v	137/137 (100%)	-0.46	0 100 100	43, 58, 89, 121	0
17	Y	29/30 (96%)	0.86	4 (13%) 6 7	73, 85, 162, 203	0
17	y	29/30 (96%)	0.56	1 (3%) 48 55	75, 85, 164, 202	0
18	X	39/40 (97%)	0.13	1 (2%) 57 63	52, 67, 135, 143	0
18	x	38/40 (95%)	0.31	2 (5%) 32 37	55, 67, 130, 140	0
19	Z	62/62 (100%)	0.41	4 (6%) 25 28	75, 89, 144, 191	0
19	z	62/62 (100%)	0.43	3 (4%) 35 41	75, 90, 144, 188	0
20	R	18/34 (52%)	1.99	9 (50%) 0 0	102, 135, 170, 172	0
All	All	5275/5384 (97%)	-0.40	43 (0%) 82 86	22, 52, 103, 203	67 (1%)

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	Y	20	ALA	4.0
19	Z	61	VAL	3.9
18	x	37	VAL	3.8
7	H	65	LEU	3.6
20	R	15	ALA	3.5

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	t	1	10/11	0.94	0.07	26,36,47,88	0
12	FME	m	1	10/11	0.95	0.08	31,50,100,103	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	0.96	0.08	30,50,87,93	0
14	FME	T	1	10/11	0.96	0.07	30,49,67,82	0
8	FME	I	1	10/11	0.97	0.06	28,49,62,64	0
8	FME	i	1	10/11	0.97	0.06	43,60,73,75	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
37	DGD	e	101	62/66	0.69	0.16	72,118,208,212	0
37	DGD	D	408	52/66	0.72	0.14	58,108,151,171	0
29	LMT	F	101	35/35	0.73	0.17	102,149,179,184	0
36	LHG	a	418	42/49	0.75	0.12	69,131,187,193	0
28	GOL	V	204	6/6	0.75	0.18	75,90,97,100	0
28	GOL	O	302	6/6	0.75	0.11	68,79,84,89	0
29	LMT	e	102	35/35	0.76	0.14	83,129,164,170	0
32	UNL	m	101	10/-	0.77	0.15	58,66,81,81	0
35	HTG	V	203	19/19	0.77	0.13	73,95,125,231	0
29	LMT	b	626	25/35	0.77	0.14	71,102,168,175	0
29	LMT	C	520	35/35	0.77	0.14	88,135,162,175	0
32	UNL	j	101	10/-	0.77	0.15	56,83,95,98	0
27	SQD	f	102	43/54	0.78	0.14	97,116,175,182	0
29	LMT	a	417	35/35	0.78	0.14	95,123,147,148	0
35	HTG	d	414	16/19	0.79	0.12	68,115,134,134	0
32	UNL	C	526	34/-	0.79	0.13	76,120,132,136	0
32	UNL	J	102	10/-	0.79	0.18	50,85,104,107	0
32	UNL	M	102	10/-	0.79	0.11	50,55,74,86	0
35	HTG	B	633	19/19	0.80	0.11	53,103,141,160	0
32	UNL	a	414	30/-	0.80	0.12	64,85,117,134	0
29	LMT	A	415	35/35	0.81	0.12	41,84,115,119	0
33	LMG	Z	101	37/55	0.81	0.15	55,121,146,154	0
32	UNL	i	101	40/-	0.82	0.12	48,77,140,147	0
36	LHG	E	101	42/49	0.82	0.11	59,115,138,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	LMG	z	101	39/55	0.82	0.14	65,124,153,161	0
32	UNL	D	412	40/-	0.82	0.12	51,88,141,144	0
29	LMT	M	103	35/35	0.82	0.12	47,99,150,158	0
33	LMG	c	920	51/55	0.83	0.12	50,111,142,145	0
28	GOL	a	413	6/6	0.83	0.12	73,83,95,97	0
35	HTG	B	625	19/19	0.83	0.12	75,132,140,190	0
29	LMT	D	403	35/35	0.83	0.12	58,132,172,179	0
35	HTG	D	413	16/19	0.83	0.14	76,142,160,166	0
28	GOL	c	924	6/6	0.83	0.17	81,87,97,102	0
32	UNL	A	418	28/-	0.83	0.12	59,88,108,111	0
27	SQD	F	103	43/54	0.83	0.13	77,120,145,149	0
29	LMT	a	401	35/35	0.83	0.12	52,87,118,142	0
33	LMG	C	519	51/55	0.83	0.12	53,121,145,151	0
32	UNL	I	101	40/-	0.83	0.14	42,88,155,156	0
31	PL9	A	417	55/55	0.84	0.13	61,98,125,131	0
34	CA	f	103	1/1	0.84	0.08	126,126,126,126	0
35	HTG	b	604	19/19	0.84	0.11	51,112,150,150	0
35	HTG	C	522	19/19	0.84	0.11	81,112,138,140	0
35	HTG	c	922	19/19	0.85	0.10	73,114,134,192	0
32	UNL	c	925	32/-	0.85	0.12	66,101,138,147	0
32	UNL	d	413	36/-	0.85	0.11	60,85,140,142	0
35	HTG	b	627	19/19	0.86	0.12	55,73,94,109	0
35	HTG	b	628	19/19	0.86	0.12	72,130,158,159	0
35	HTG	c	921	19/19	0.86	0.09	93,101,107,111	0
28	GOL	l	101	6/6	0.86	0.17	48,92,98,103	0
32	UNL	b	634	33/-	0.86	0.13	47,86,155,158	0
29	LMT	m	103	35/35	0.86	0.11	42,109,140,144	0
22	CL	U	201	1/1	0.86	0.12	117,117,117,117	0
27	SQD	B	621	54/54	0.86	0.11	53,88,137,156	0
32	UNL	B	634	33/-	0.86	0.12	54,73,126,134	0
28	GOL	C	523	6/6	0.87	0.15	74,80,89,92	0
29	LMT	t	101	25/35	0.87	0.12	43,92,140,150	0
29	LMT	b	602	25/35	0.87	0.13	41,91,134,149	0
31	PL9	a	415	55/55	0.87	0.13	65,110,127,130	0
27	SQD	L	102	54/54	0.87	0.10	48,79,126,149	0
35	HTG	B	624	19/19	0.87	0.12	50,73,82,92	0
28	GOL	A	413	6/6	0.87	0.10	61,79,84,86	0
27	SQD	A	414	54/54	0.88	0.10	49,75,134,141	0
22	CL	v	201	1/1	0.88	0.09	124,124,124,124	0
28	GOL	B	630	6/6	0.88	0.13	51,59,70,81	0
34	CA	b	605	1/1	0.88	0.06	124,124,124,124	0
28	GOL	b	633	6/6	0.88	0.10	68,74,80,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
27	SQD	a	402	54/54	0.88	0.09	45,75,125,133	0
33	LMG	Y	101	51/55	0.88	0.10	60,93,118,127	0
29	LMT	m	102	35/35	0.89	0.11	42,90,122,128	0
34	CA	B	601	1/1	0.89	0.06	138,138,138,138	0
33	LMG	A	419	51/55	0.89	0.10	54,88,107,128	0
29	LMT	M	101	35/35	0.89	0.10	45,93,118,133	0
28	GOL	T	101	6/6	0.90	0.14	60,77,82,83	0
28	GOL	T	103	6/6	0.90	0.11	103,108,112,114	0
28	GOL	c	928	6/6	0.90	0.11	75,83,90,98	0
24	CLA	C	513	65/65	0.90	0.09	53,84,113,119	0
28	GOL	v	203	6/6	0.90	0.11	72,88,91,94	0
33	LMG	a	411	51/55	0.90	0.10	51,84,96,105	0
35	HTG	C	521	19/19	0.90	0.10	70,99,121,123	0
33	LMG	c	919	51/55	0.90	0.10	51,89,123,128	0
28	GOL	v	204	6/6	0.90	0.11	84,87,94,112	0
28	GOL	B	636	6/6	0.90	0.10	49,56,64,65	0
24	CLA	b	606	65/65	0.91	0.10	39,67,123,145	0
24	CLA	c	914	65/65	0.91	0.09	68,84,105,115	0
35	HTG	B	632	19/19	0.91	0.09	48,84,110,115	0
26	BCR	d	407	40/40	0.91	0.08	39,54,85,88	0
32	UNL	X	101	18/-	0.91	0.10	53,73,112,114	0
32	UNL	x	101	18/-	0.91	0.11	51,71,116,116	0
28	GOL	b	632	6/6	0.91	0.14	77,78,102,105	0
24	CLA	C	506	65/65	0.91	0.08	41,70,114,128	0
24	CLA	B	602	65/65	0.91	0.10	43,67,119,143	0
26	BCR	C	514	40/40	0.92	0.08	50,72,86,87	0
32	UNL	d	412	17/-	0.92	0.09	47,62,95,102	0
36	LHG	D	410	49/49	0.92	0.10	47,67,121,138	0
28	GOL	a	419	6/6	0.92	0.09	73,85,94,95	0
24	CLA	C	512	65/65	0.92	0.08	49,76,99,106	0
27	SQD	A	411	54/54	0.92	0.09	43,87,114,116	0
28	GOL	A	412	6/6	0.92	0.09	49,55,57,69	0
27	SQD	a	410	54/54	0.93	0.09	51,81,110,114	0
35	HTG	b	603	19/19	0.93	0.08	47,75,92,93	0
32	UNL	D	411	17/-	0.93	0.09	40,71,92,94	0
26	BCR	y	101	40/40	0.93	0.07	47,63,74,82	0
24	CLA	c	913	65/65	0.93	0.08	47,74,93,99	0
24	CLA	B	615	65/65	0.93	0.08	26,43,97,103	0
28	GOL	B	628	6/6	0.93	0.10	62,80,83,84	0
24	CLA	C	504	65/65	0.93	0.08	36,57,79,95	0
33	LMG	J	101	51/55	0.93	0.10	44,65,120,137	0
28	GOL	B	631	6/6	0.93	0.14	40,78,87,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	BCR	D	406	40/40	0.93	0.07	39,58,89,104	0
26	BCR	c	927	40/40	0.93	0.09	54,77,91,100	0
23	BCT	d	402	4/4	0.93	0.12	70,72,76,97	0
28	GOL	b	629	6/6	0.94	0.10	57,62,67,81	0
24	CLA	c	907	65/65	0.94	0.07	44,65,104,111	0
28	GOL	B	626	6/6	0.94	0.09	44,53,66,87	0
26	BCR	k	101	40/40	0.94	0.08	51,64,75,80	0
28	GOL	B	629	6/6	0.94	0.12	56,60,69,95	0
24	CLA	c	908	65/65	0.94	0.08	45,63,74,84	0
31	PL9	D	407	55/55	0.94	0.07	29,42,52,60	0
24	CLA	c	909	65/65	0.94	0.07	38,54,125,137	0
24	CLA	B	607	65/65	0.94	0.08	31,52,95,99	0
33	LMG	B	622	51/55	0.94	0.07	38,53,78,91	0
35	HTG	b	601	19/19	0.94	0.08	42,57,82,87	0
24	CLA	b	611	65/65	0.94	0.07	37,51,97,108	0
28	GOL	D	402	6/6	0.94	0.13	52,57,83,90	0
24	CLA	b	619	65/65	0.94	0.07	25,43,86,108	0
24	CLA	b	621	65/65	0.94	0.08	33,53,103,118	0
26	BCR	H	101	40/40	0.94	0.07	33,57,78,85	0
33	LMG	b	625	51/55	0.94	0.08	40,54,73,98	0
26	BCR	K	101	40/40	0.94	0.08	43,63,79,82	0
36	LHG	B	635	49/49	0.94	0.07	30,52,68,77	0
28	GOL	V	207	6/6	0.94	0.09	81,86,89,98	0
33	LMG	d	415	51/55	0.94	0.08	38,61,112,126	0
26	BCR	Y	102	40/40	0.94	0.08	51,71,90,107	0
36	LHG	d	411	49/49	0.94	0.09	37,53,112,120	0
37	DGD	C	517	62/66	0.94	0.08	48,65,94,116	0
24	CLA	c	904	65/65	0.94	0.07	41,60,73,84	0
37	DGD	c	917	62/66	0.94	0.08	35,60,112,137	0
34	CA	F	104	1/1	0.94	0.06	107,107,107,107	0
24	CLA	b	616	65/65	0.95	0.06	29,41,54,66	0
28	GOL	V	201	6/6	0.95	0.10	88,99,104,109	0
24	CLA	B	614	65/65	0.95	0.06	29,41,64,93	0
28	GOL	V	205	6/6	0.95	0.08	45,51,58,72	0
28	GOL	V	206	6/6	0.95	0.13	52,60,67,71	0
26	BCR	h	101	40/40	0.95	0.07	36,60,79,81	0
35	HTG	B	623	19/19	0.95	0.08	38,56,78,93	0
24	CLA	C	507	65/65	0.95	0.08	41,66,77,86	0
26	BCR	t	102	40/40	0.95	0.06	33,46,62,64	0
24	CLA	c	902	65/65	0.95	0.07	44,60,72,81	0
24	CLA	C	508	65/65	0.95	0.07	35,61,138,148	0
24	CLA	c	905	65/65	0.95	0.06	31,57,74,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	C	509	65/65	0.95	0.08	53,65,82,93	0
24	CLA	C	510	65/65	0.95	0.07	40,60,77,92	0
24	CLA	C	511	65/65	0.95	0.08	48,67,85,109	0
24	CLA	c	910	65/65	0.95	0.08	43,58,77,81	0
23	BCT	A	404	4/4	0.95	0.10	59,62,74,108	0
28	GOL	v	205	6/6	0.95	0.09	48,59,69,78	0
24	CLA	B	617	65/65	0.95	0.10	34,54,130,139	0
24	CLA	d	406	65/65	0.95	0.08	40,54,106,124	0
25	PHO	d	403	64/64	0.95	0.06	27,44,54,62	0
26	BCR	A	410	40/40	0.95	0.06	32,42,54,54	0
28	GOL	B	627	6/6	0.95	0.10	54,64,88,102	0
26	BCR	B	620	40/40	0.95	0.06	36,52,64,67	0
24	CLA	D	405	65/65	0.95	0.08	39,55,106,121	0
24	CLA	a	408	65/65	0.95	0.09	32,53,122,130	0
24	CLA	A	409	65/65	0.95	0.08	33,50,116,132	0
24	CLA	C	505	65/65	0.95	0.08	41,54,71,89	0
37	DGD	C	516	62/66	0.95	0.08	32,50,88,97	0
26	BCR	T	102	40/40	0.95	0.06	29,46,64,65	0
37	DGD	C	518	62/66	0.95	0.07	39,58,92,100	0
24	CLA	b	614	65/65	0.95	0.07	39,51,61,72	0
37	DGD	c	916	62/66	0.95	0.07	38,56,100,114	0
26	BCR	b	623	40/40	0.95	0.06	29,46,66,68	0
37	DGD	c	918	62/66	0.95	0.07	41,56,90,110	0
26	BCR	c	915	40/40	0.95	0.06	32,56,67,75	0
24	CLA	b	617	65/65	0.96	0.06	25,42,53,65	0
24	CLA	b	618	65/65	0.96	0.06	24,44,60,67	0
24	CLA	A	405	65/65	0.96	0.06	24,37,51,66	0
26	BCR	a	409	40/40	0.96	0.05	28,43,54,59	0
26	BCR	b	622	40/40	0.96	0.05	32,44,56,60	0
31	PL9	d	408	55/55	0.96	0.06	22,39,53,73	0
24	CLA	b	620	65/65	0.96	0.06	36,50,64,69	0
26	BCR	b	624	40/40	0.96	0.06	39,50,61,65	0
24	CLA	B	616	65/65	0.96	0.06	37,50,65,77	0
24	CLA	B	603	65/65	0.96	0.06	38,50,57,66	0
24	CLA	c	903	65/65	0.96	0.07	39,52,76,80	0
24	CLA	C	501	65/65	0.96	0.06	39,57,85,91	0
24	CLA	C	502	65/65	0.96	0.06	42,56,69,85	0
28	GOL	b	630	6/6	0.96	0.08	50,82,94,95	0
28	GOL	b	631	6/6	0.96	0.09	58,70,81,100	0
24	CLA	c	906	65/65	0.96	0.06	36,51,70,76	0
24	CLA	C	503	65/65	0.96	0.07	36,59,72,85	0
24	CLA	a	406	65/65	0.96	0.07	31,44,118,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	B	605	65/65	0.96	0.06	28,41,72,78	0
24	CLA	A	407	65/65	0.96	0.06	28,43,106,119	0
24	CLA	c	911	65/65	0.96	0.06	43,55,69,81	0
24	CLA	c	912	65/65	0.96	0.07	43,63,83,99	0
24	CLA	b	607	65/65	0.96	0.06	30,50,60,63	0
24	CLA	b	608	65/65	0.96	0.06	38,48,58,66	0
24	CLA	b	610	65/65	0.96	0.06	31,43,53,61	0
36	LHG	L	101	49/49	0.96	0.06	36,47,56,62	0
25	PHO	A	408	64/64	0.96	0.06	26,39,46,54	0
36	LHG	b	635	49/49	0.96	0.06	30,48,61,64	0
36	LHG	d	409	49/49	0.96	0.06	40,52,66,70	0
25	PHO	D	401	64/64	0.96	0.06	31,46,58,60	0
24	CLA	B	610	65/65	0.96	0.06	36,52,65,82	0
24	CLA	b	612	65/65	0.96	0.06	27,38,48,58	0
26	BCR	B	619	40/40	0.96	0.05	31,42,60,66	0
24	CLA	b	613	65/65	0.96	0.05	36,49,59,62	0
37	DGD	H	102	62/66	0.96	0.07	31,51,88,102	0
24	CLA	B	612	65/65	0.96	0.06	24,40,56,63	0
26	BCR	C	515	40/40	0.96	0.06	38,55,68,78	0
24	CLA	b	615	65/65	0.96	0.07	35,47,61,67	0
22	CL	A	403	1/1	0.96	0.09	38,38,38,38	0
37	DGD	h	102	62/66	0.96	0.07	34,52,71,82	0
39	MG	J	103	1/1	0.96	0.05	54,54,54,54	0
34	CA	c	926	1/1	0.97	0.06	77,77,77,77	0
36	LHG	D	409	49/49	0.97	0.06	31,46,67,79	0
24	CLA	a	405	65/65	0.97	0.06	24,38,53,67	0
24	CLA	B	611	65/65	0.97	0.06	31,50,62,66	0
28	GOL	a	412	6/6	0.97	0.09	54,61,67,72	0
24	CLA	d	404	65/65	0.97	0.05	29,39,48,56	0
24	CLA	d	405	65/65	0.97	0.05	24,40,55,69	0
24	CLA	B	606	65/65	0.97	0.05	28,40,55,57	0
36	LHG	d	410	49/49	0.97	0.06	29,44,63,98	0
24	CLA	B	613	65/65	0.97	0.06	26,42,50,53	0
24	CLA	B	604	65/65	0.97	0.06	35,48,60,63	0
28	GOL	C	524	6/6	0.97	0.07	39,44,53,61	0
25	PHO	a	407	64/64	0.97	0.05	28,40,48,54	0
28	GOL	c	923	6/6	0.97	0.06	41,51,54,57	0
24	CLA	B	608	65/65	0.97	0.05	25,41,51,61	0
24	CLA	b	609	65/65	0.97	0.06	27,42,74,77	0
26	BCR	B	618	40/40	0.97	0.04	29,40,51,54	0
24	CLA	B	609	65/65	0.97	0.06	32,46,59,67	0
34	CA	C	525	1/1	0.97	0.07	79,79,79,79	0

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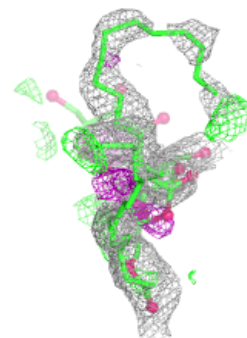
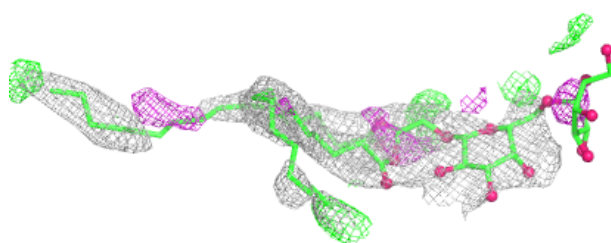
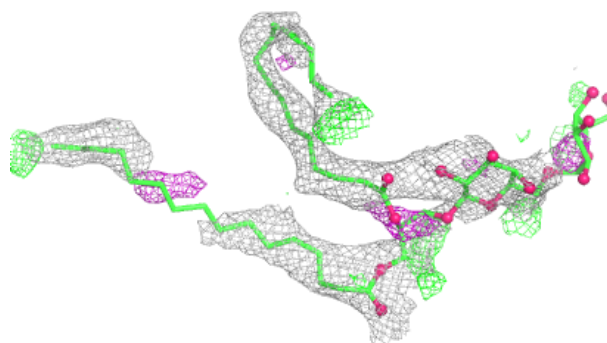
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	D	404	65/65	0.97	0.06	24,37,58,69	0
38	HEM	f	101	43/43	0.97	0.09	51,85,128,152	0
24	CLA	A	406	65/65	0.97	0.05	23,36,45,55	0
39	MG	j	102	1/1	0.97	0.08	61,61,61,61	0
34	CA	o	301	1/1	0.98	0.03	97,97,97,97	0
22	CL	a	403	1/1	0.98	0.06	37,37,37,37	0
38	HEM	F	102	43/43	0.98	0.07	53,74,105,111	0
40	HEC	V	202	43/43	0.98	0.06	31,45,54,59	0
40	HEC	v	202	43/43	0.98	0.06	46,58,65,70	0
21	FE2	d	401	1/1	0.99	0.06	55,55,55,55	0
34	CA	c	901	1/1	0.99	0.02	74,74,74,74	0
22	CL	A	402	1/1	0.99	0.03	35,35,35,35	0
22	CL	a	404	1/1	0.99	0.02	42,42,42,42	0
30	OEX	A	416	10/10	0.99	0.03	39,45,61,77	0
30	OEX	a	416	10/10	0.99	0.04	35,45,63,74	0
21	FE2	A	401	1/1	0.99	0.02	56,56,56,56	0
34	CA	O	301	1/1	0.99	0.03	89,89,89,89	0

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

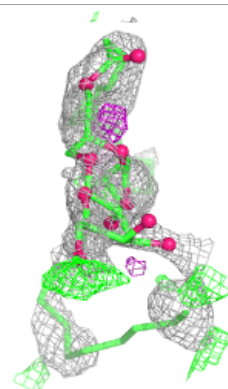
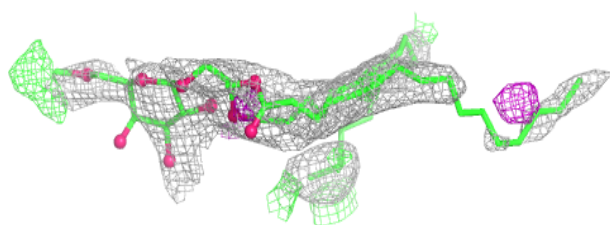
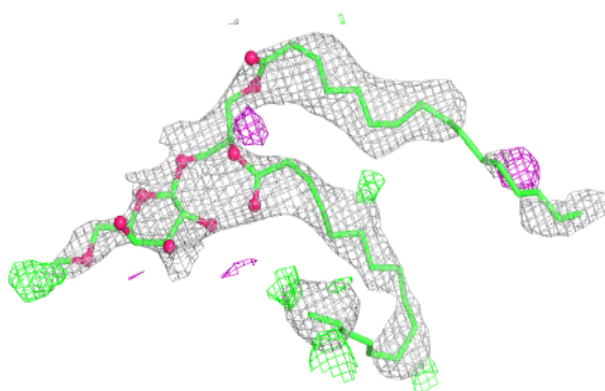
Electron density around DGD e 101:

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

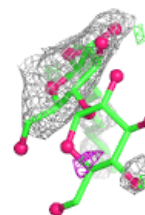
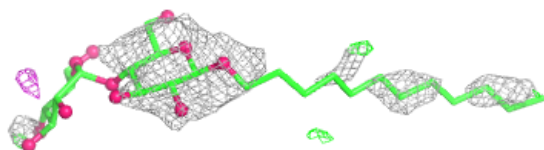
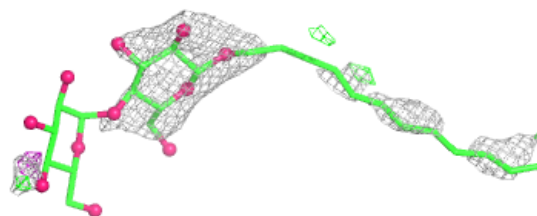


Electron density around DGD D 408:

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

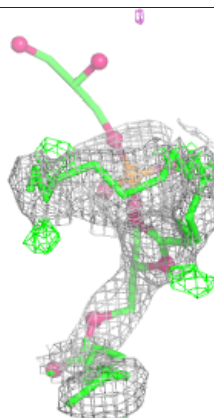
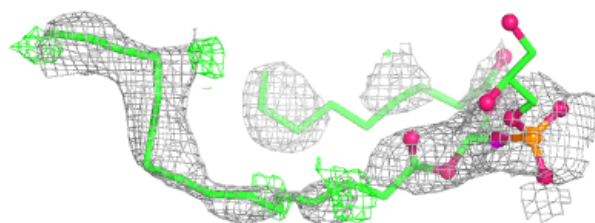
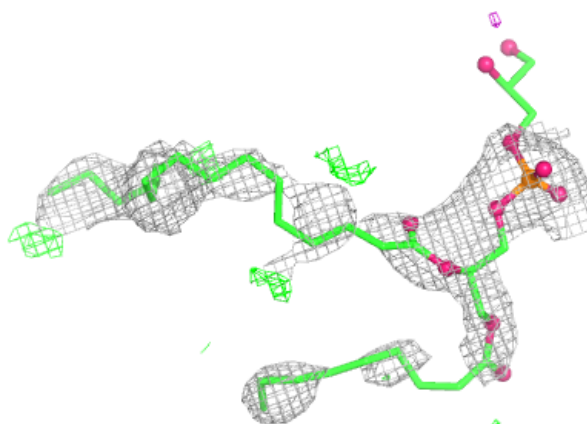
**Electron density around LMT F 101:**

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

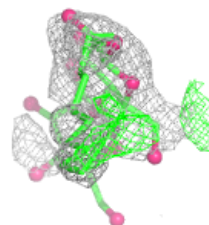
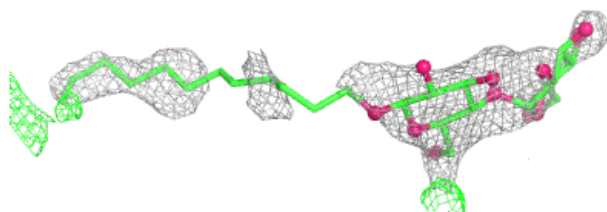
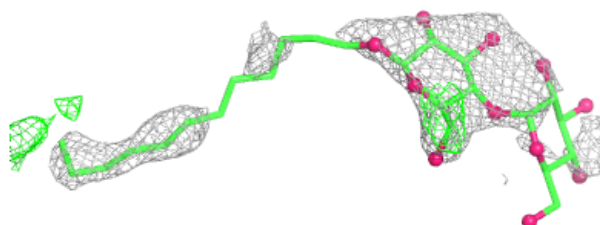


Electron density around LHG a 418:

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

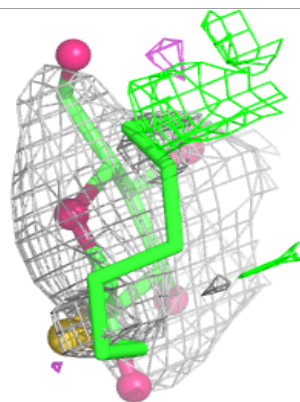
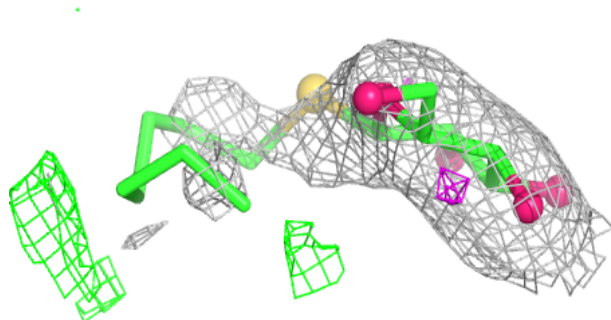
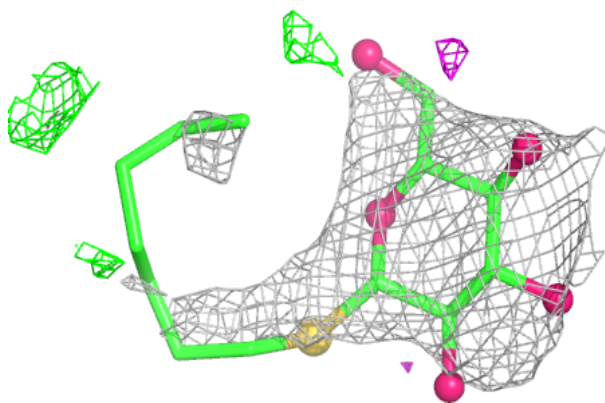
**Electron density around LMT e 102:**

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

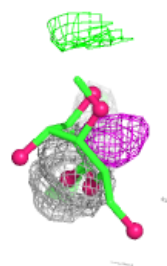
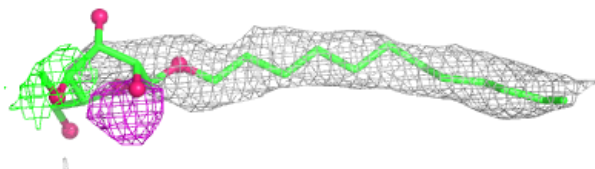
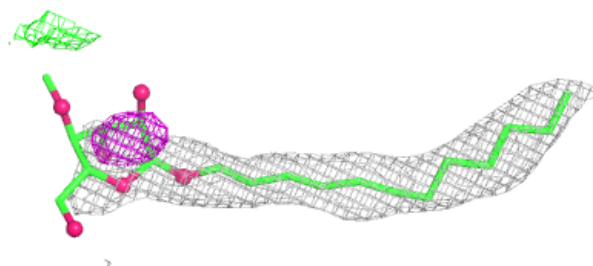


Electron density around HTG V 203:

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

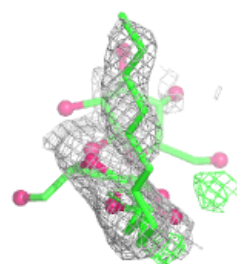
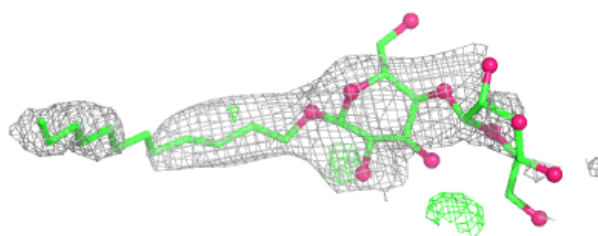
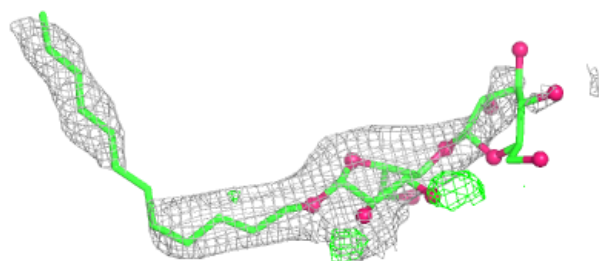
**Electron density around LMT b 626:**

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

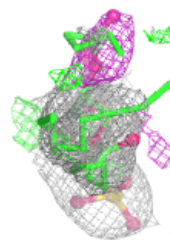
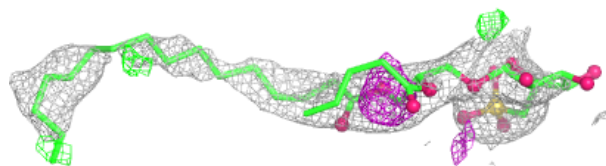
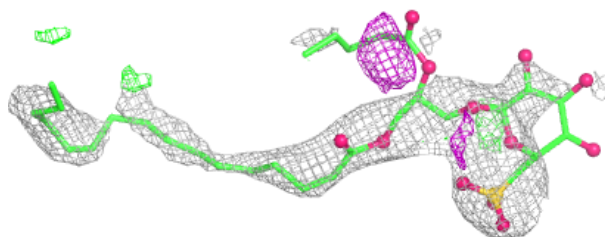


Electron density around LMT C 520:

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

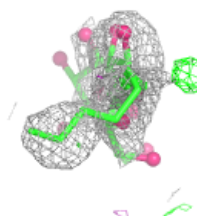
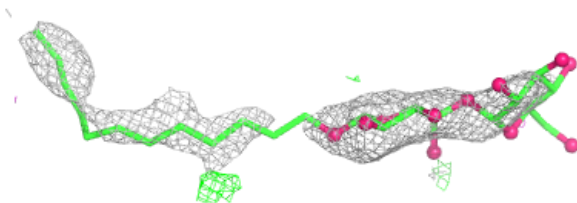
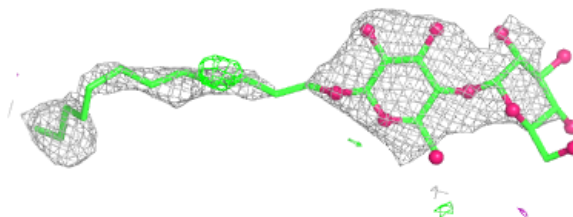
**Electron density around SQD f 102:**

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

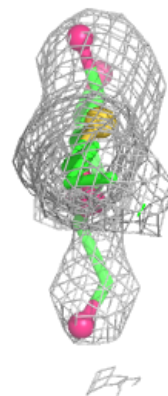
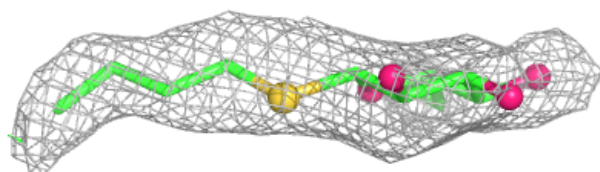
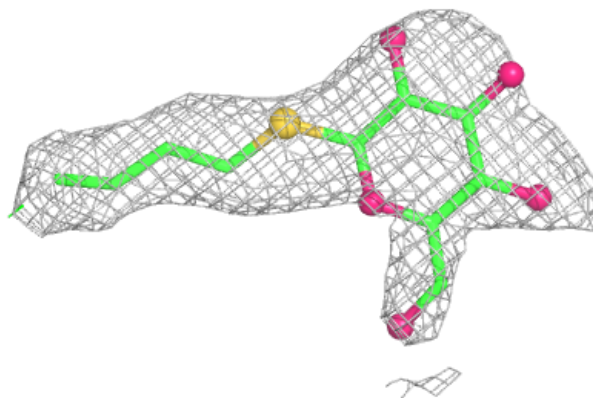


Electron density around LMT a 417:

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

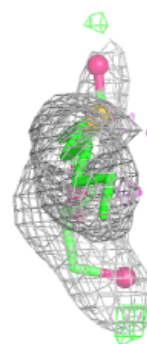
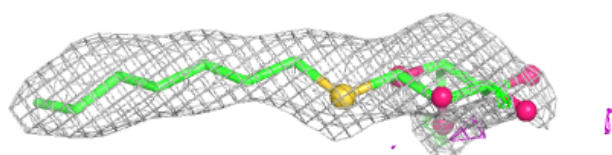
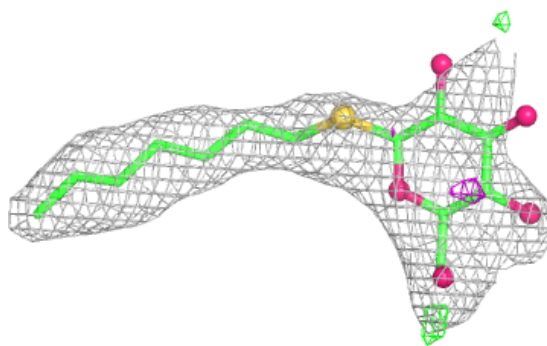
**Electron density around HTG d 414:**

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

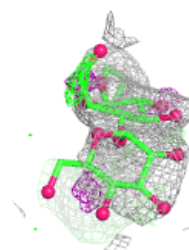
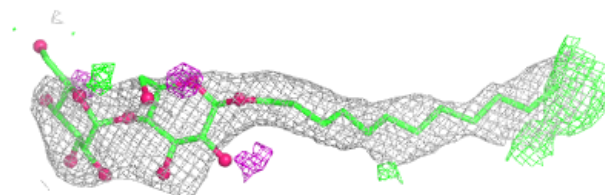
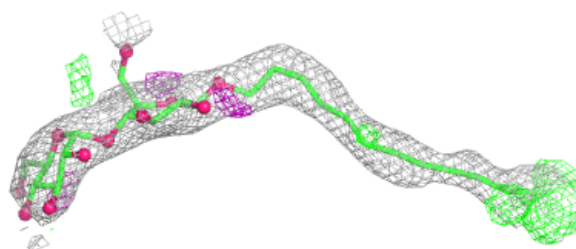


Electron density around HTG B 633:

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

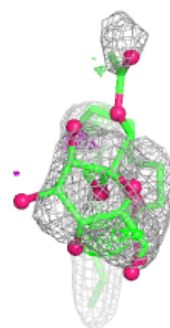
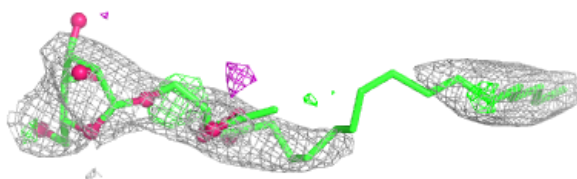
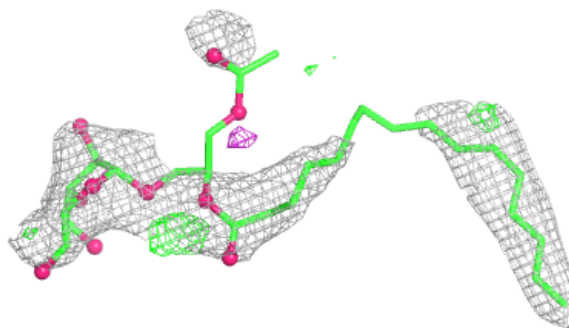
**Electron density around LMT A 415:**

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



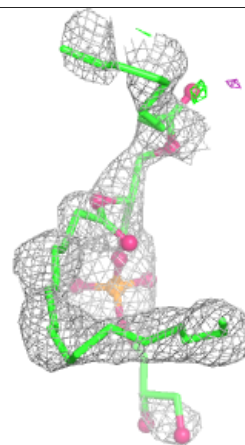
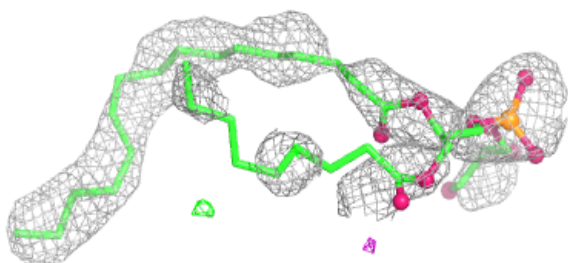
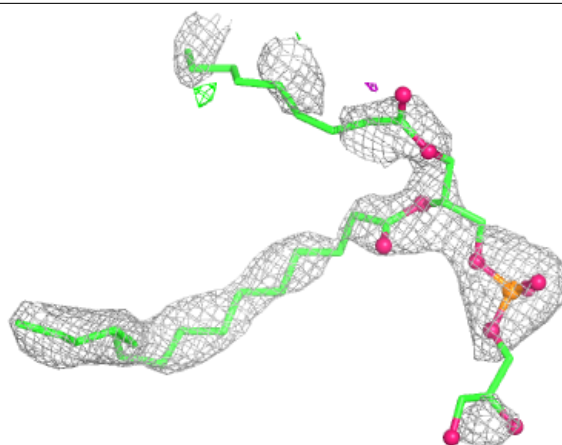
Electron density around LMG Z 101:

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



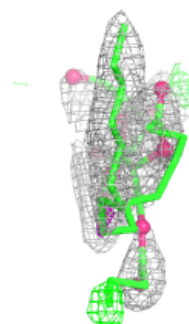
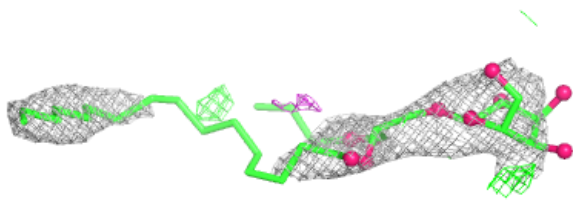
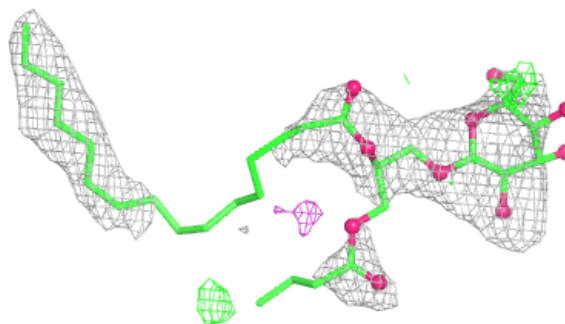
Electron density around LHG E 101:

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

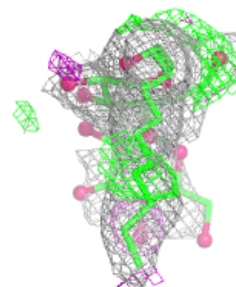
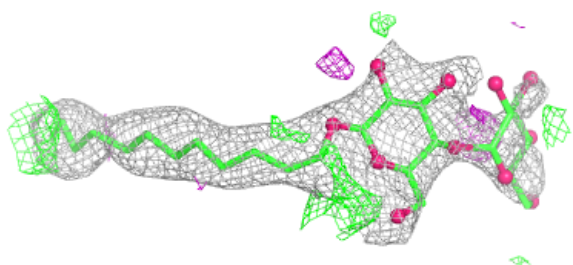
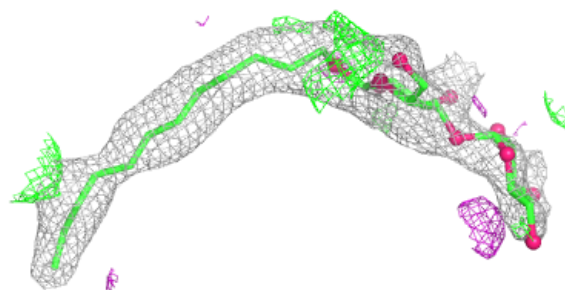


Electron density around LMG z 101:

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

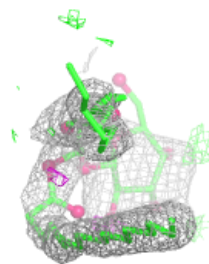
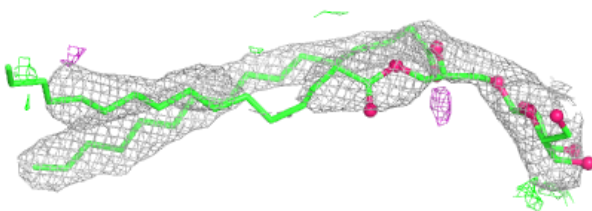
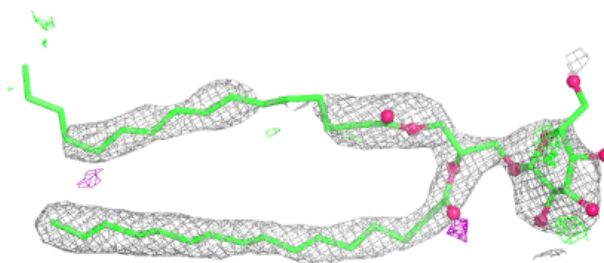
**Electron density around LMT M 103:**

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

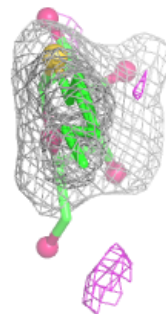
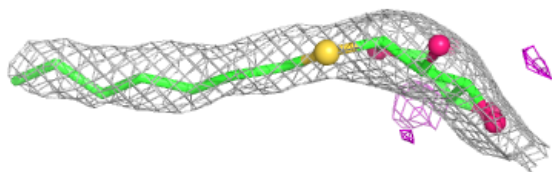
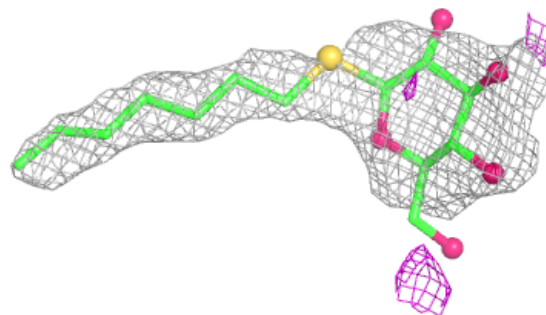


Electron density around LMG c 920:

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

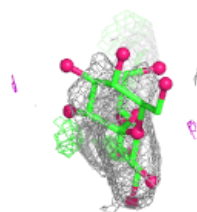
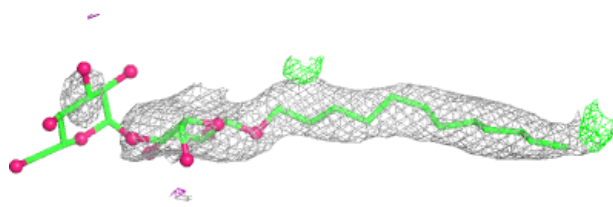
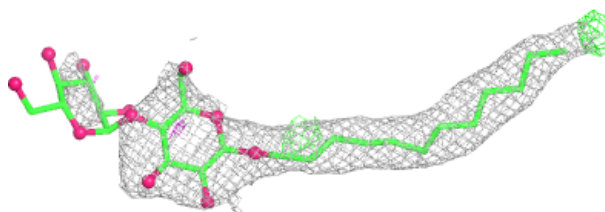
**Electron density around HTG B 625:**

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

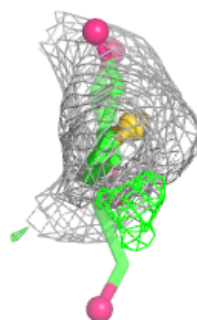
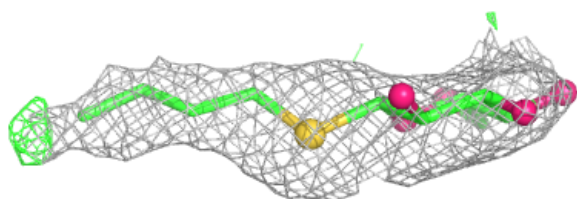
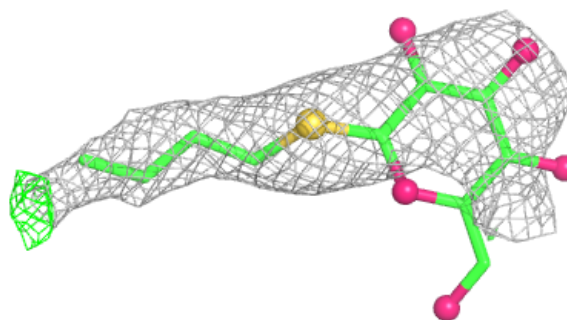


Electron density around LMT D 403:

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

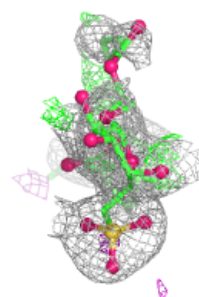
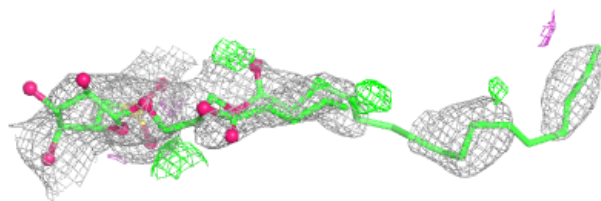
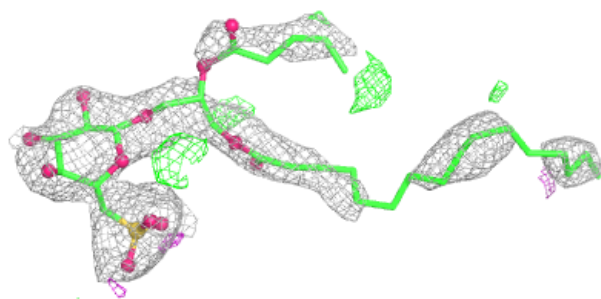
**Electron density around HTG D 413:**

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

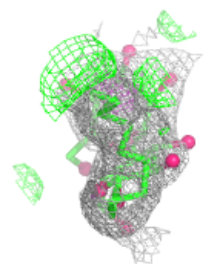
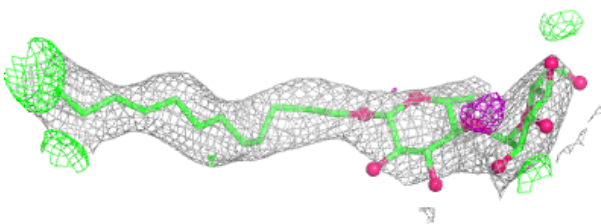
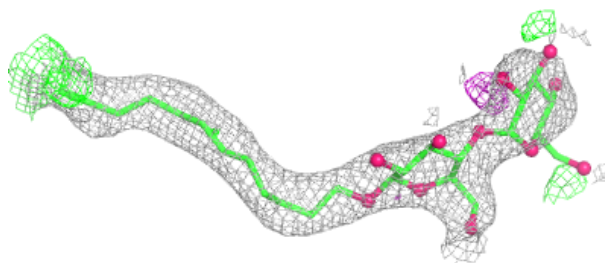


Electron density around SQD F 103:

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

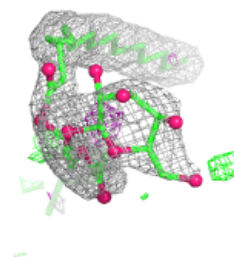
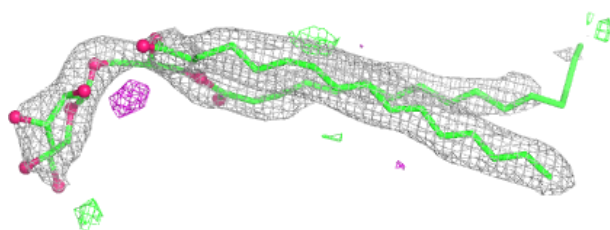
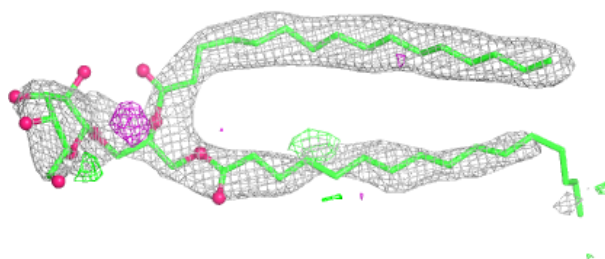
**Electron density around LMT a 401:**

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

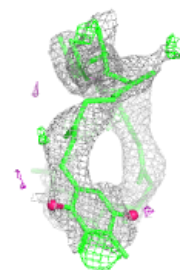
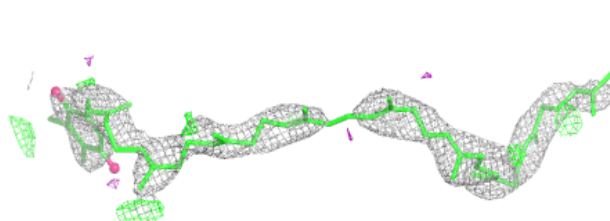
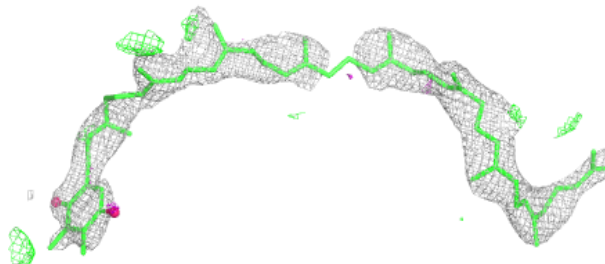


Electron density around LMG C 519:

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

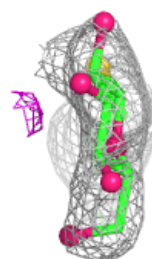
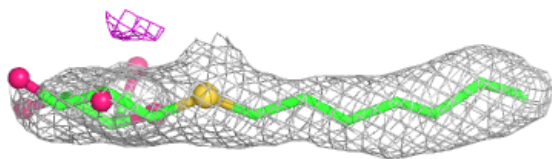
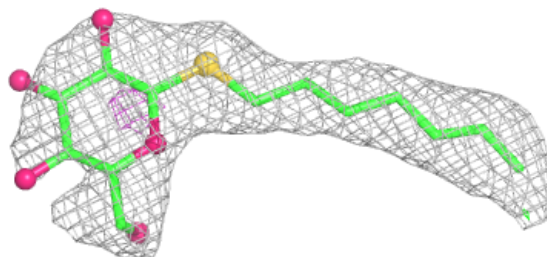
**Electron density around PL9 A 417:**

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

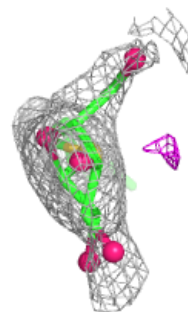
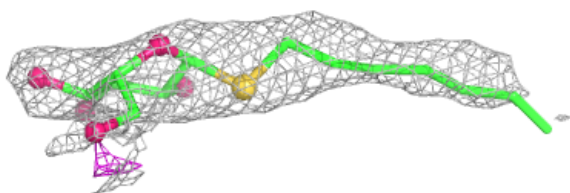
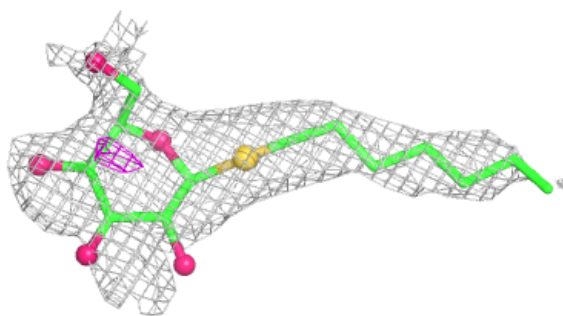


Electron density around HTG b 604:

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

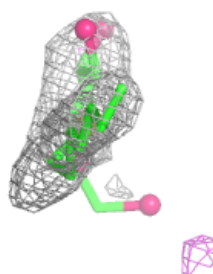
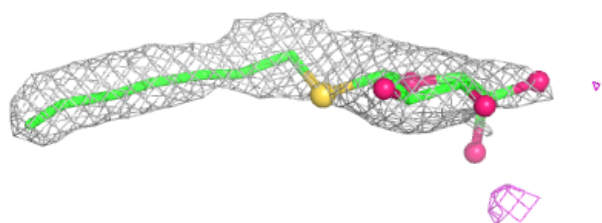
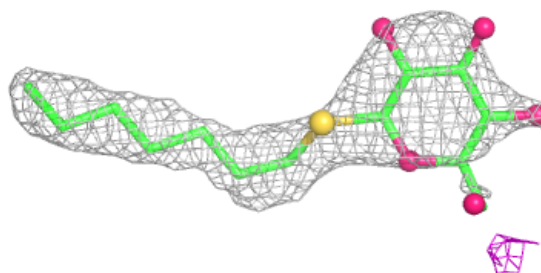
**Electron density around HTG C 522:**

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

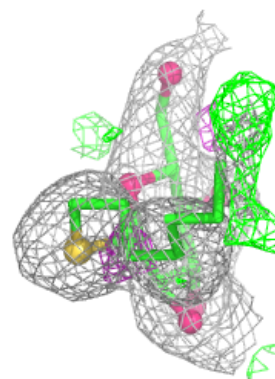
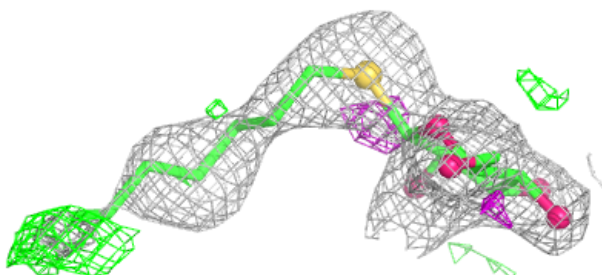
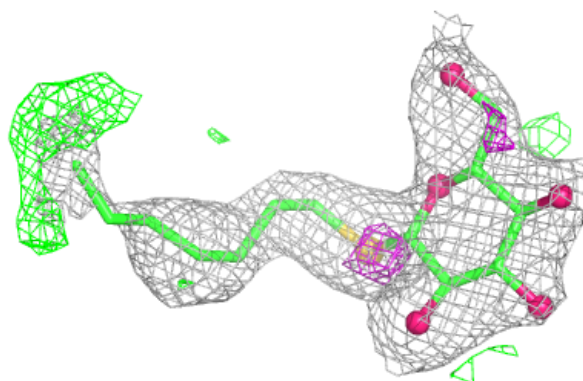


Electron density around HTG c 922:

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

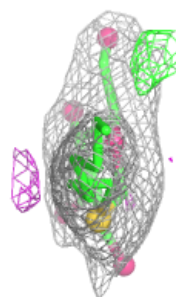
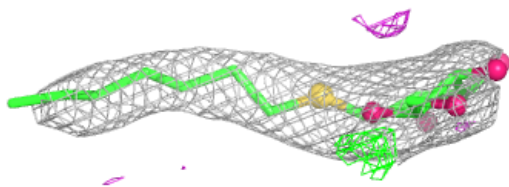
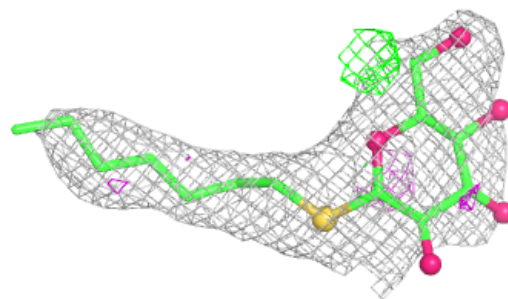
**Electron density around HTG b 627:**

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

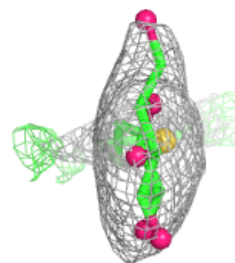
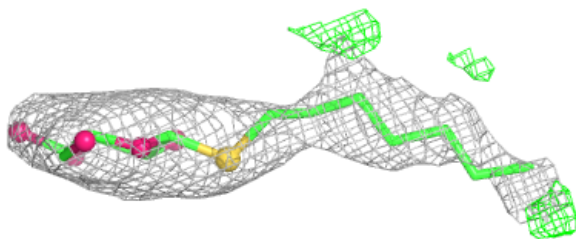
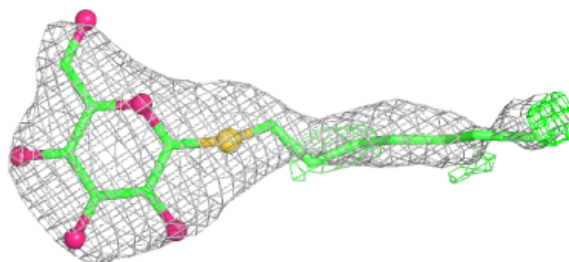


Electron density around HTG b 628:

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

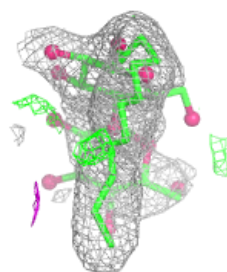
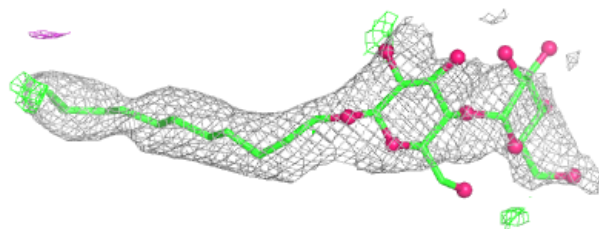
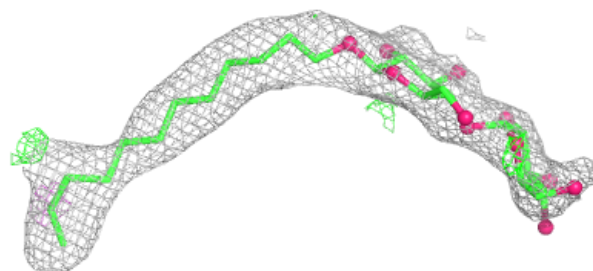
**Electron density around HTG c 921:**

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

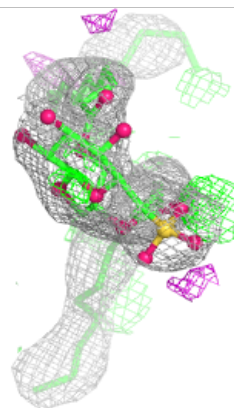
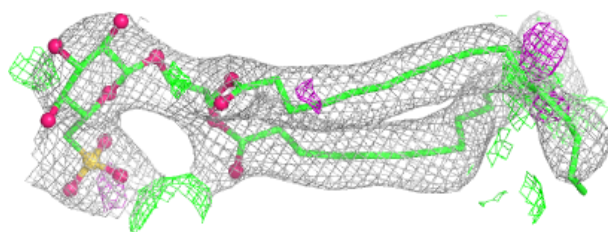
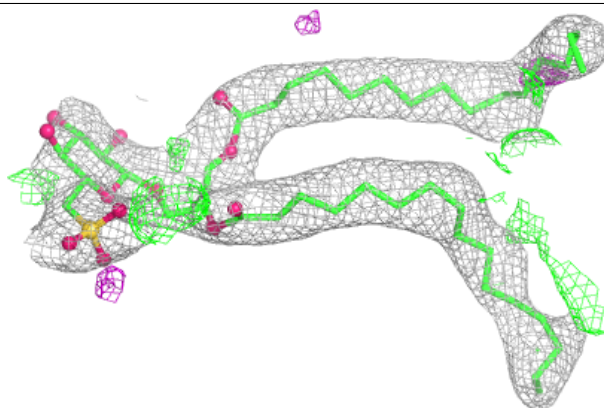


Electron density around LMT m 103:

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

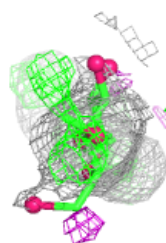
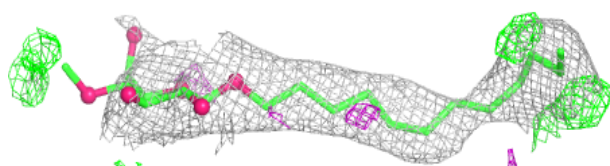
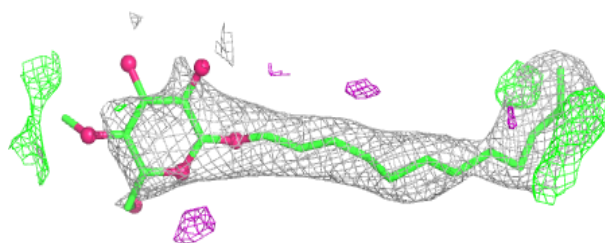
**Electron density around SQD B 621:**

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

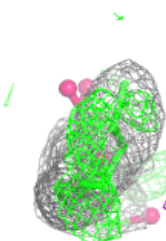
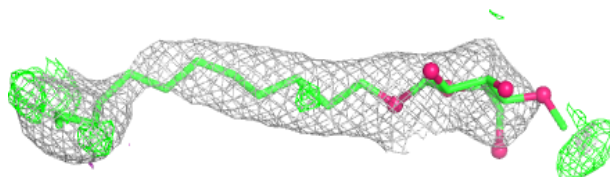
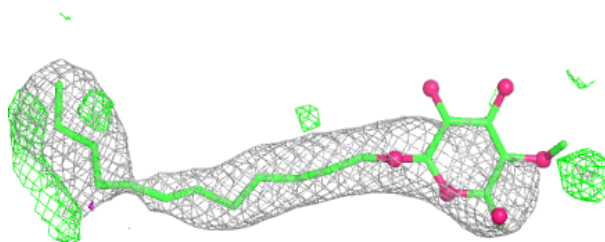


Electron density around LMT t 101:

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

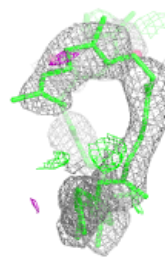
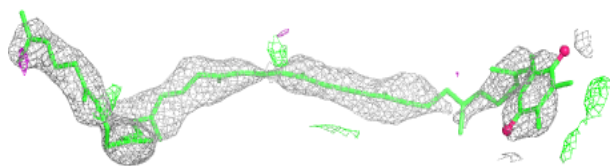
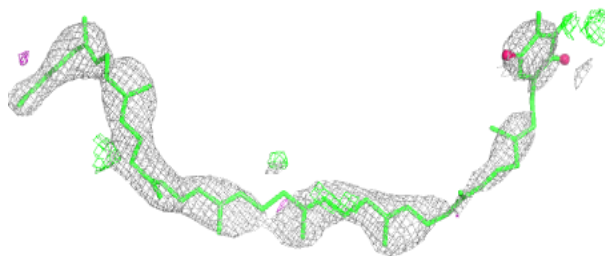
**Electron density around LMT b 602:**

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



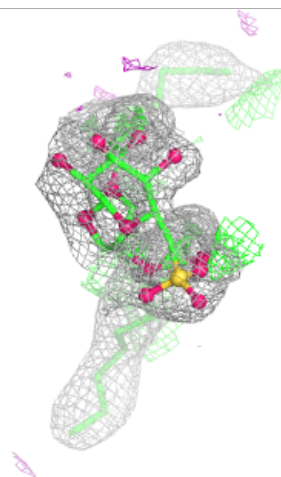
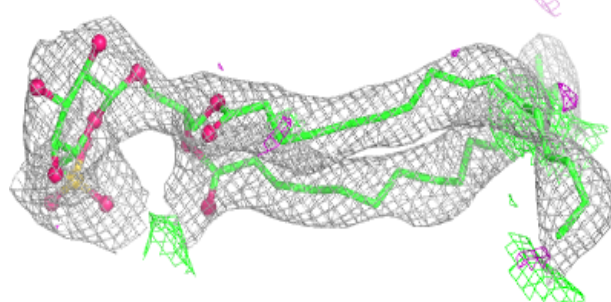
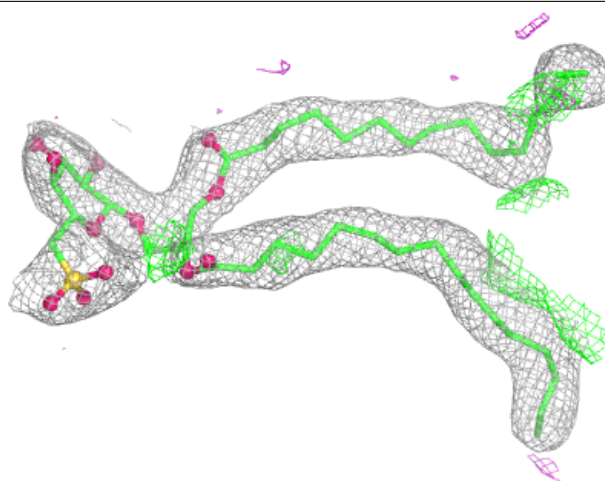
Electron density around PL9 a 415:

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



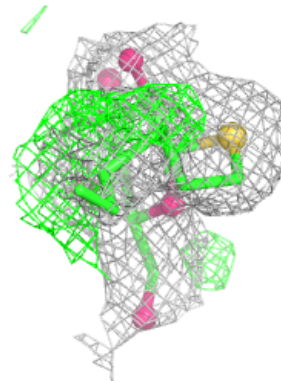
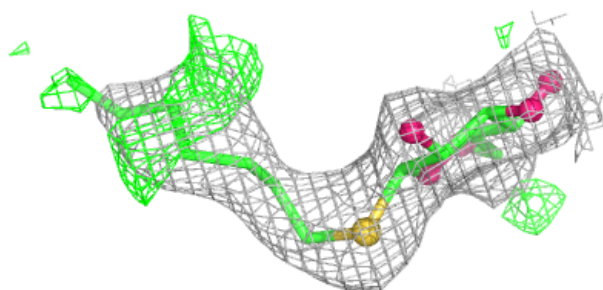
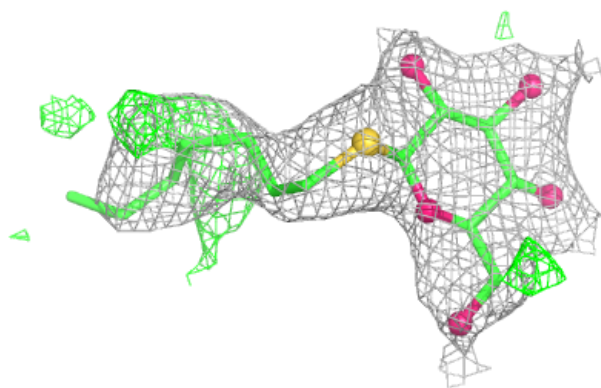
Electron density around SQD L 102:

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

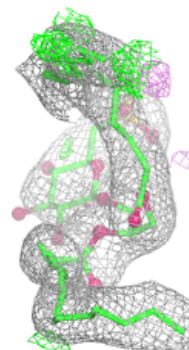
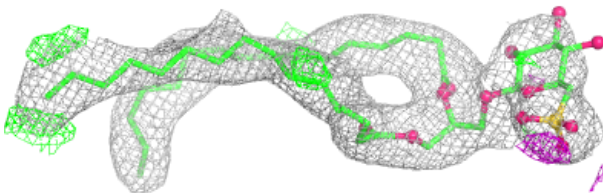
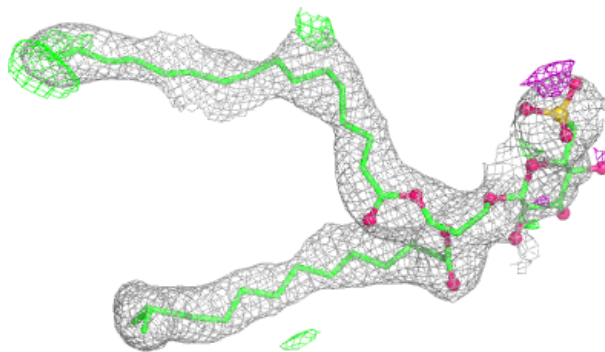


Electron density around HTG B 624:

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

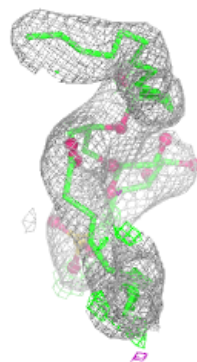
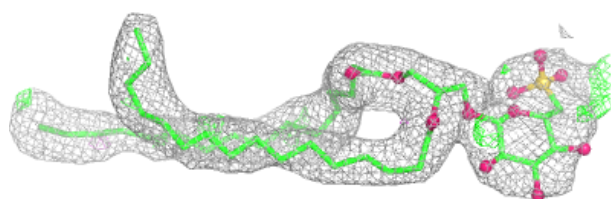
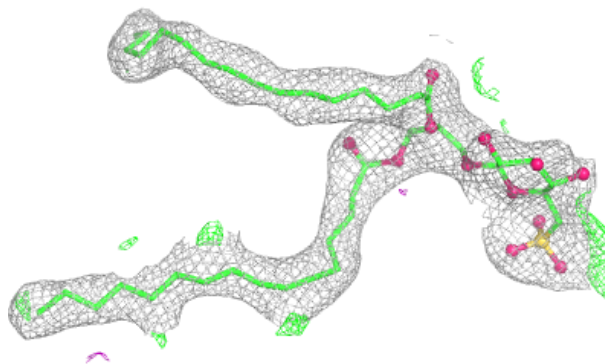
**Electron density around SQD A 414:**

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

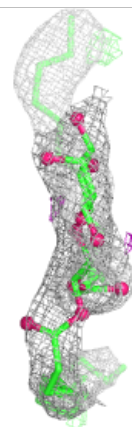
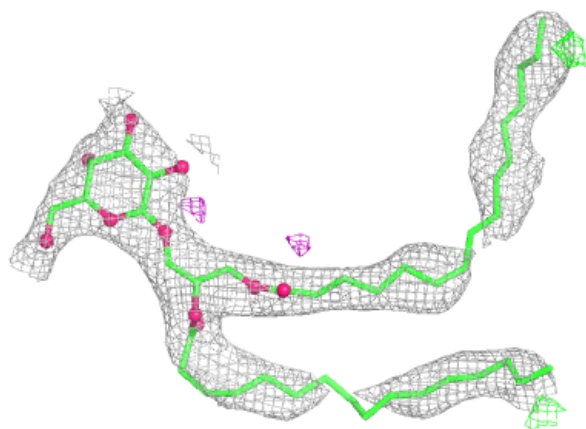


Electron density around SQD a 402:

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

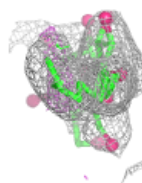
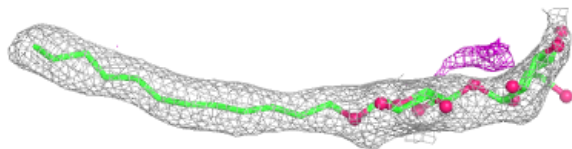
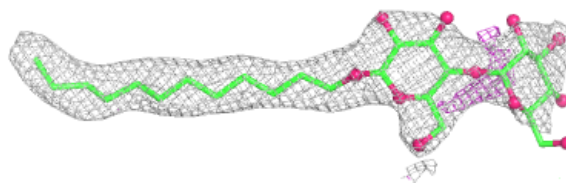
**Electron density around LMG Y 101:**

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

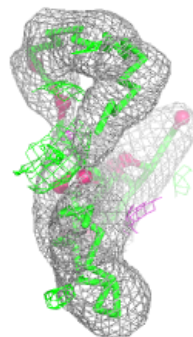
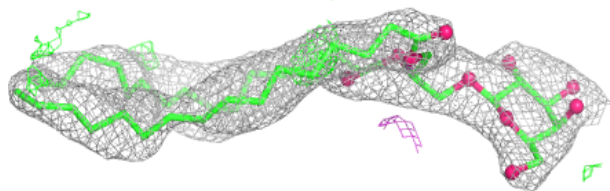
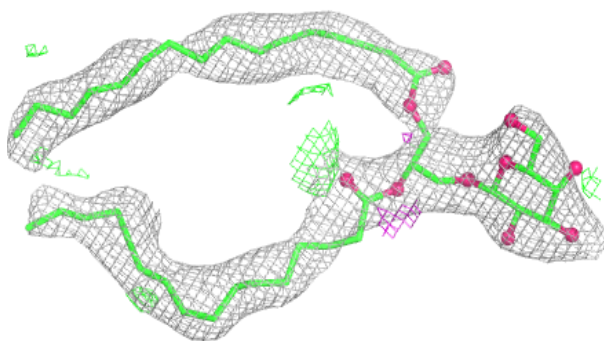


Electron density around LMT m 102:

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

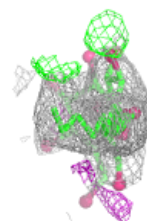
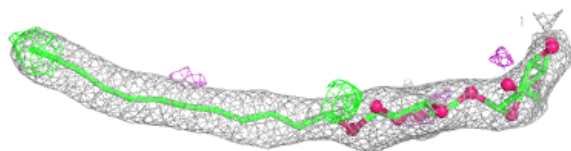
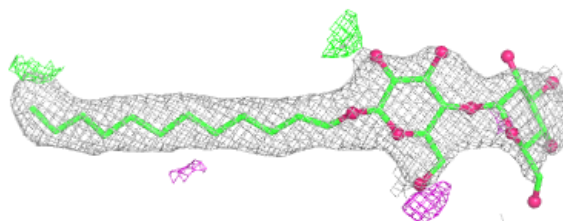
**Electron density around LMG A 419:**

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

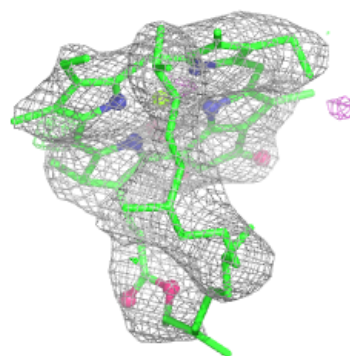
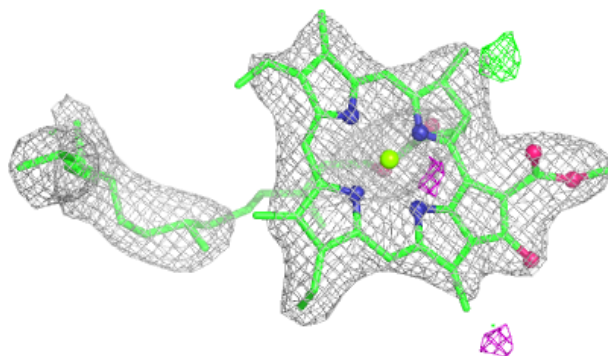
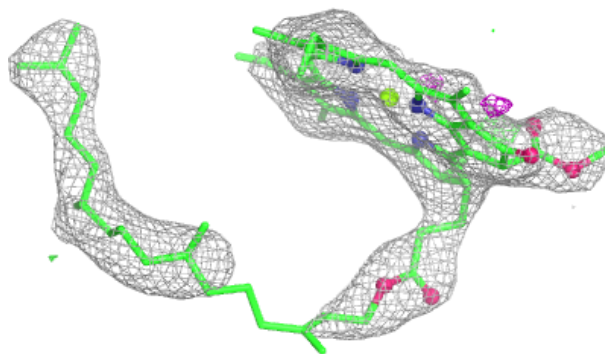


Electron density around LMT M 101:

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

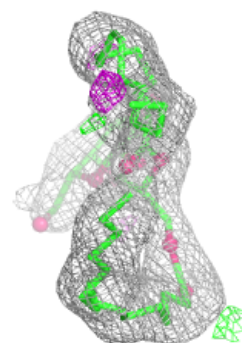
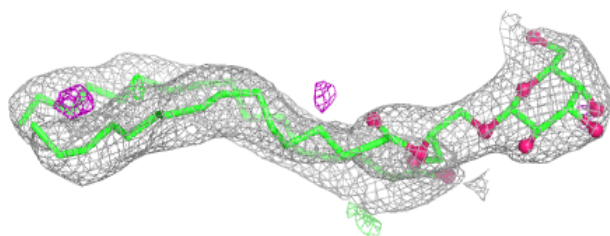
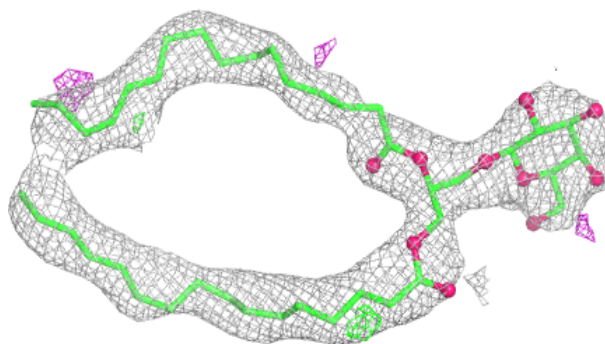
**Electron density around CLA C 513:**

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

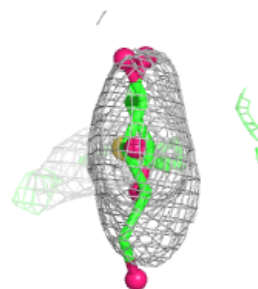
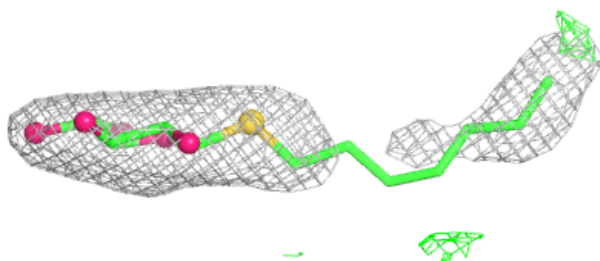
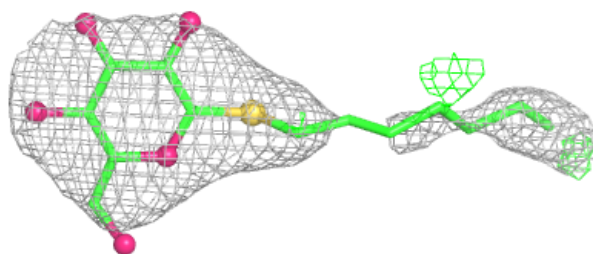


Electron density around LMG a 411:

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

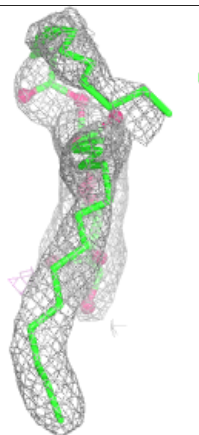
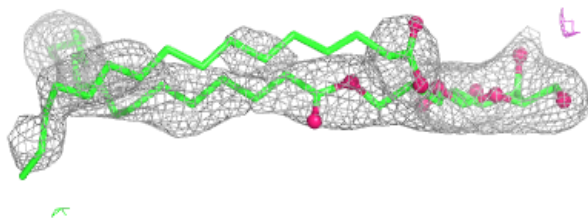
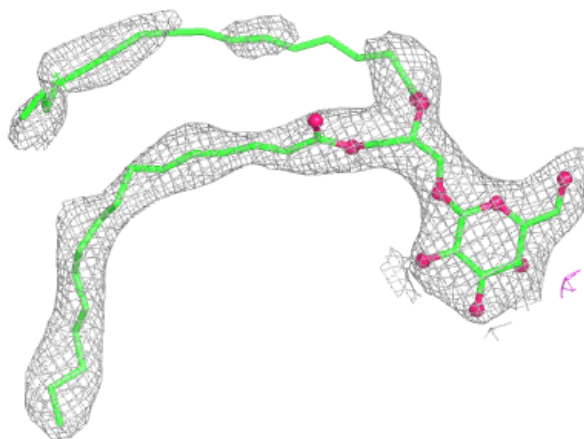
**Electron density around HTG C 521:**

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



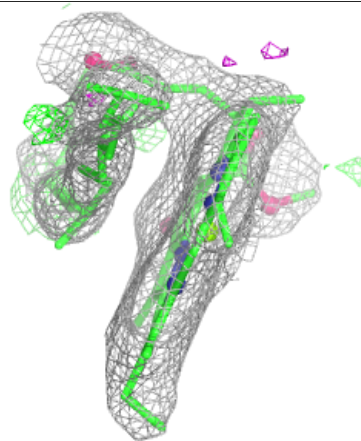
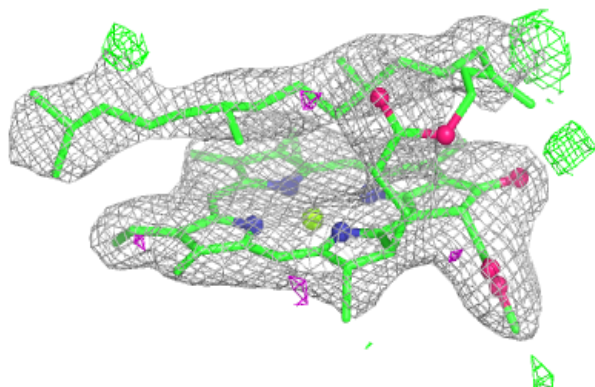
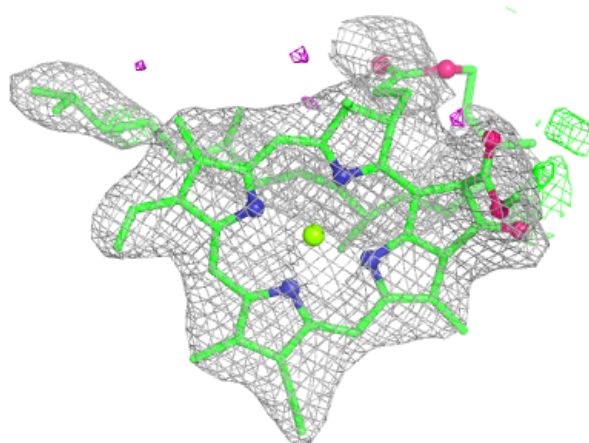
Electron density around LMG c 919:

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

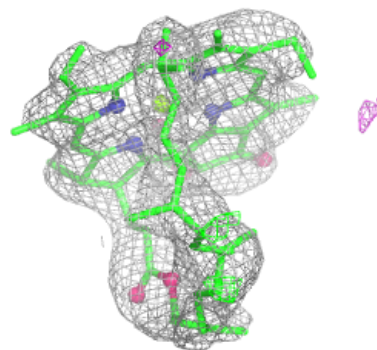
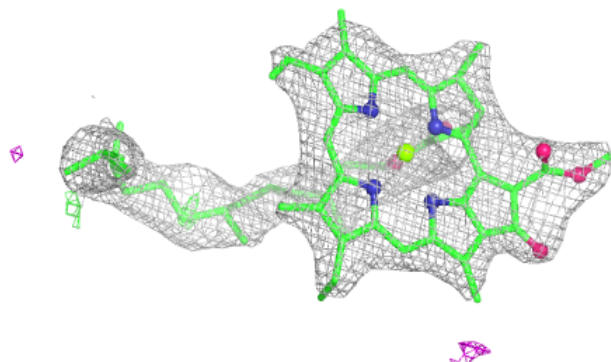
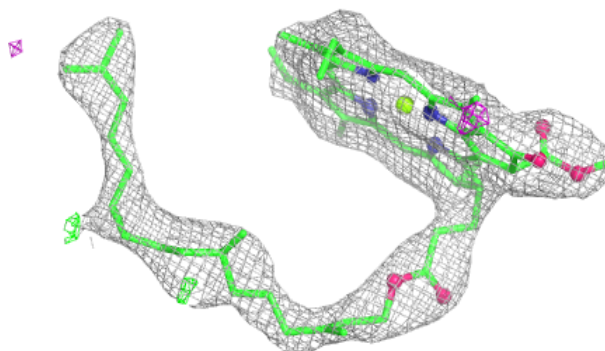


Electron density around CLA b 606:

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

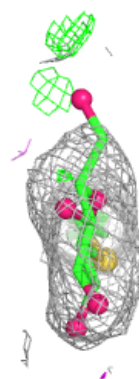
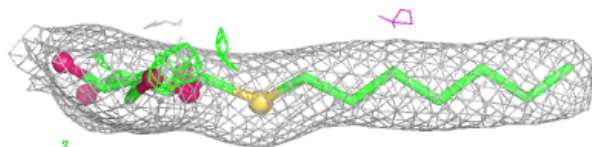
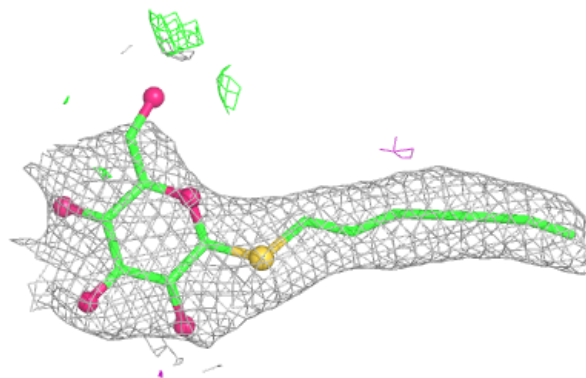
**Electron density around CLA c 914:**

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

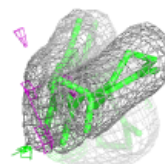
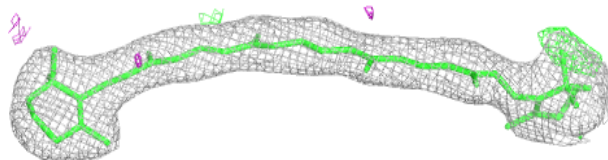
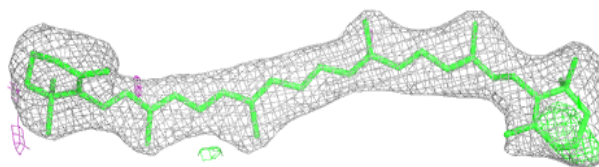


Electron density around HTG B 632:

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

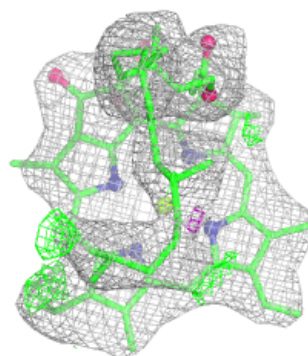
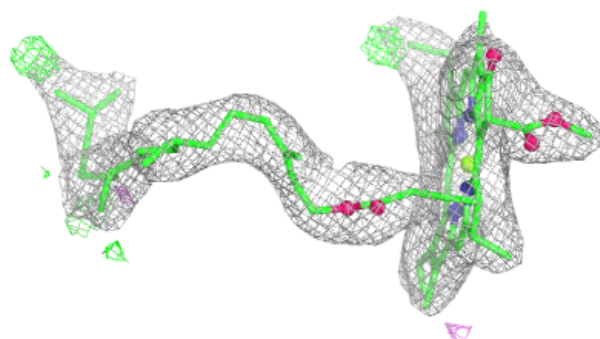
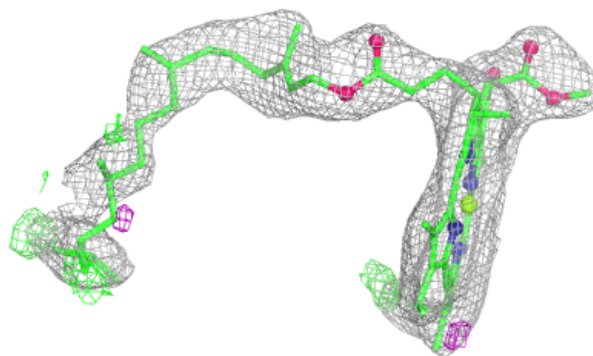
**Electron density around BCR d 407:**

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

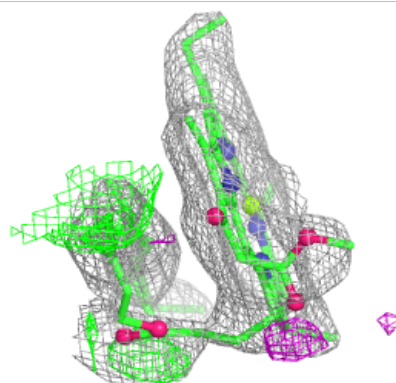
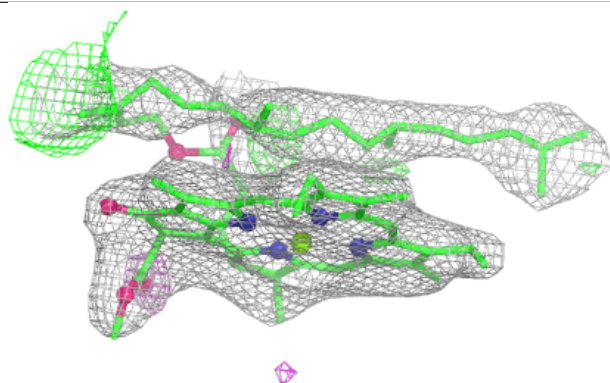
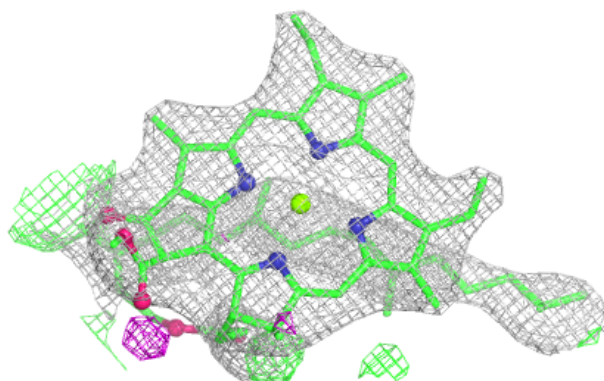


Electron density around CLA C 506:

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

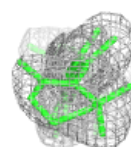
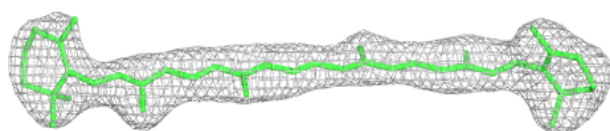
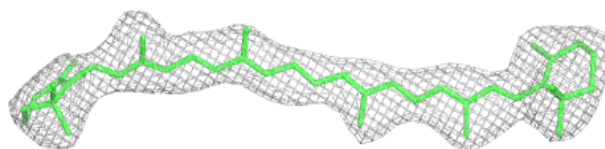
**Electron density around CLA B 602:**

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

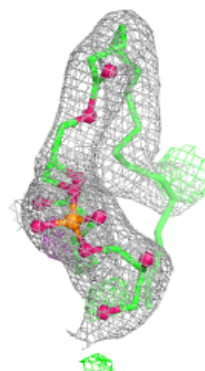
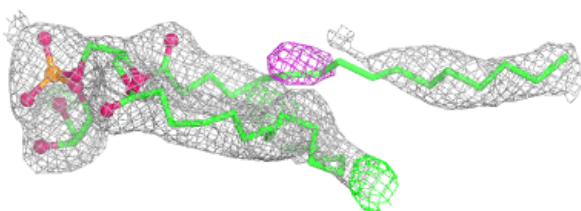
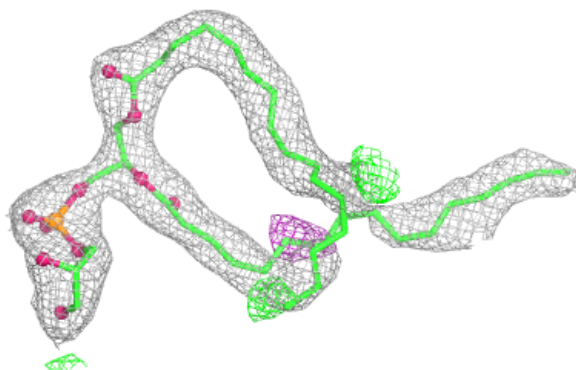


Electron density around BCR C 514:

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

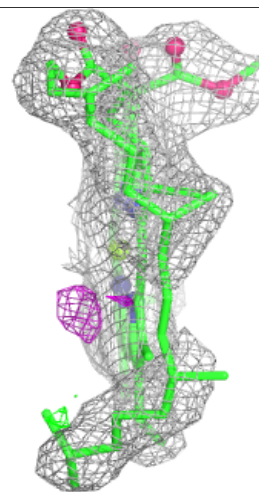
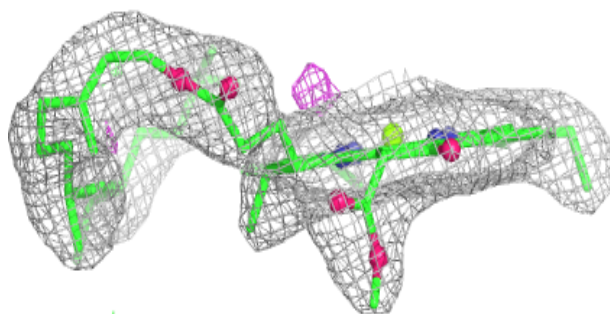
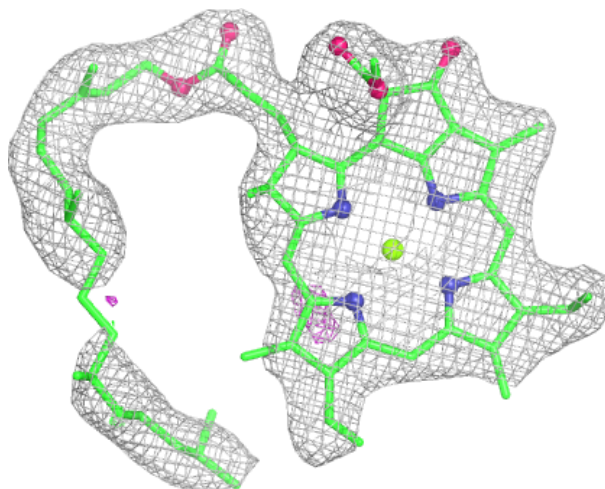
**Electron density around LHG D 410:**

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



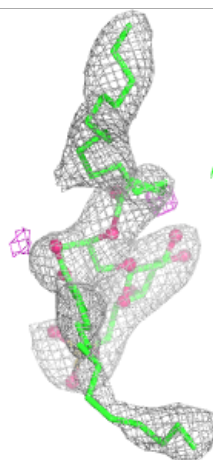
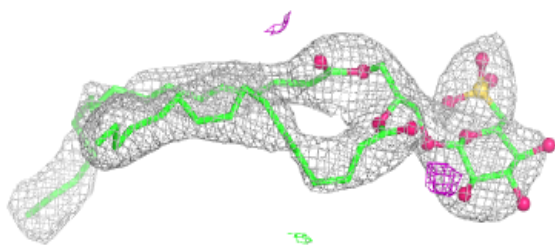
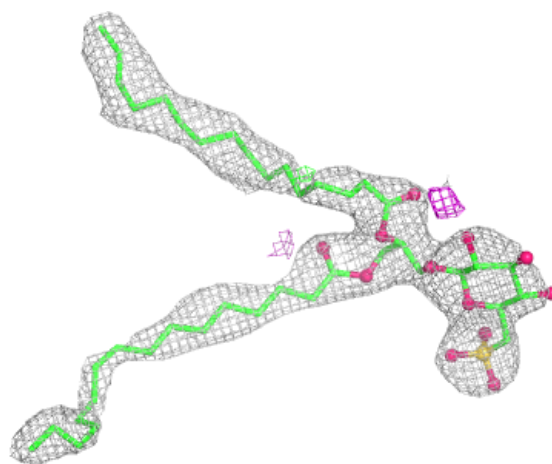
Electron density around CLA C 512:

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



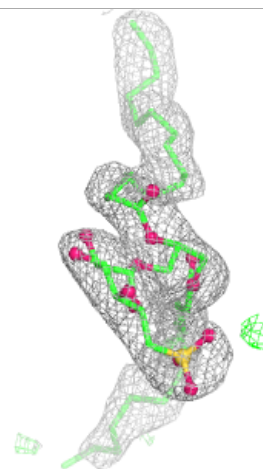
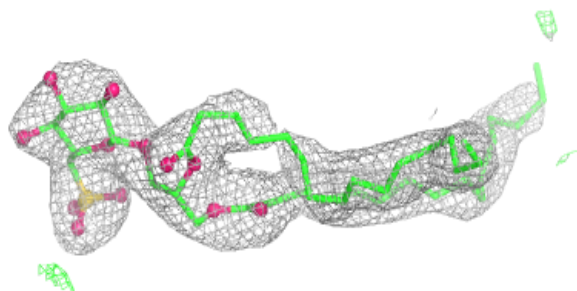
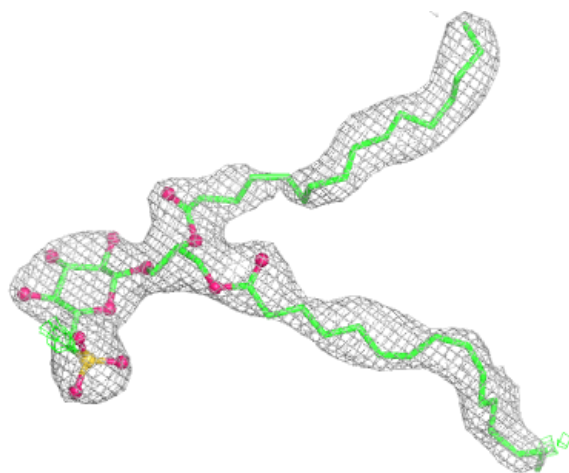
Electron density around SQD A 411:

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



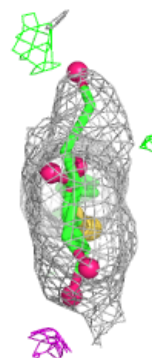
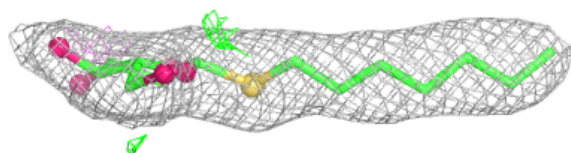
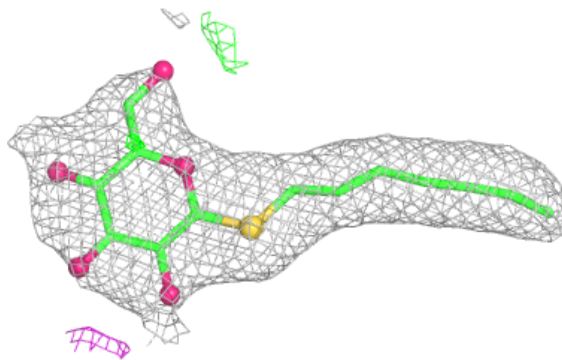
Electron density around SQD a 410:

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

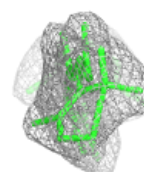
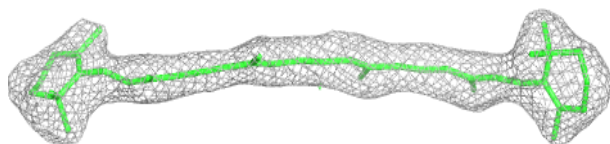
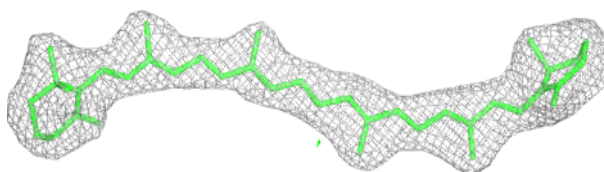


Electron density around HTG b 603:

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

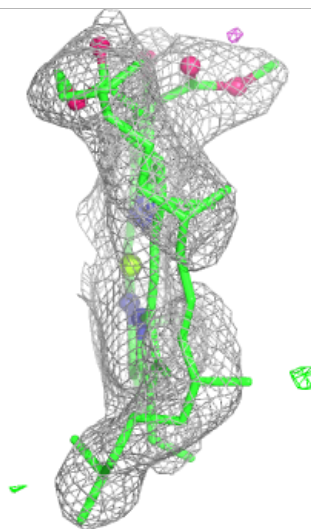
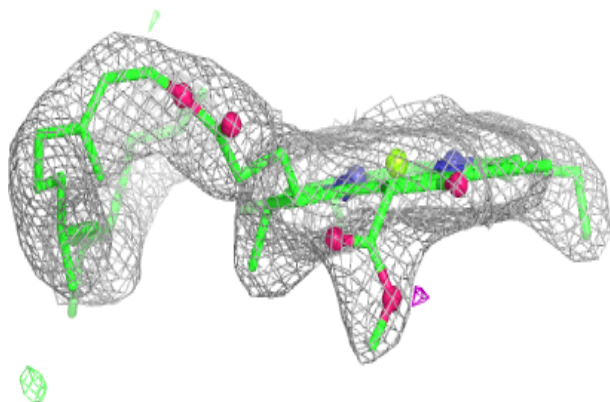
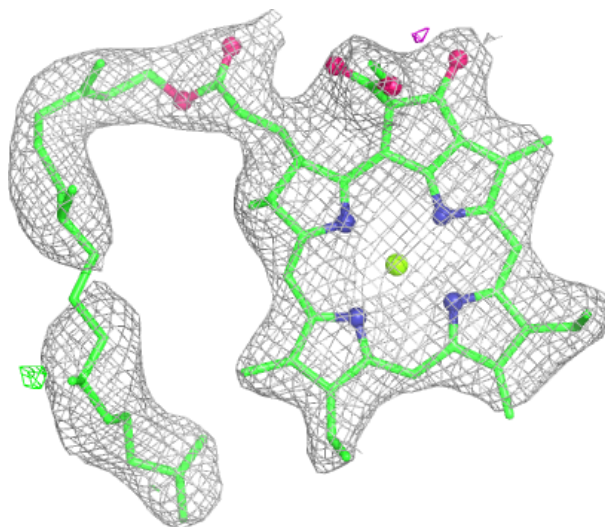
**Electron density around BCR y 101:**

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



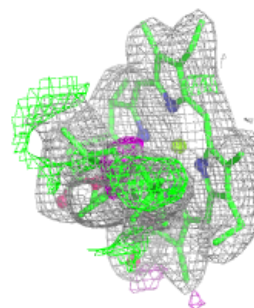
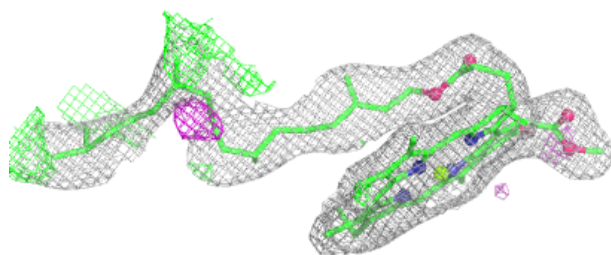
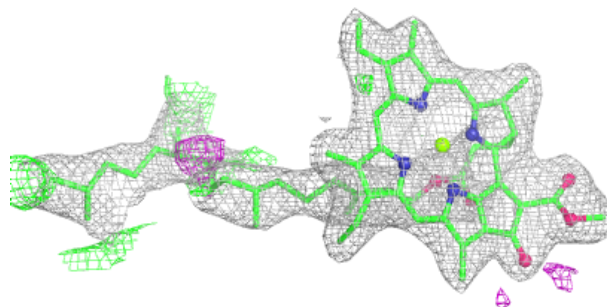
Electron density around CLA c 913:

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

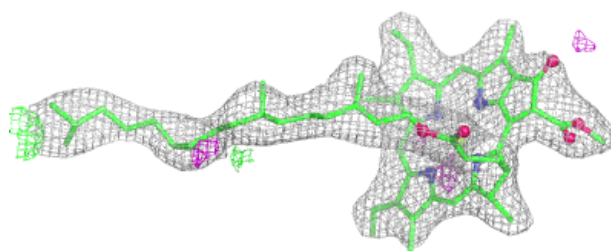
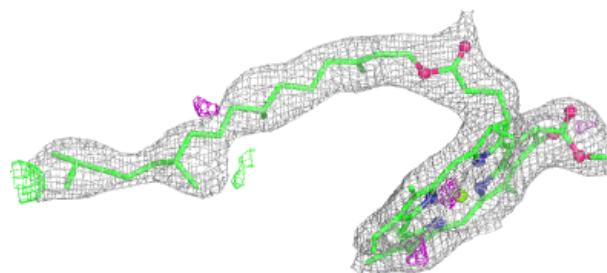


Electron density around CLA B 615:

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

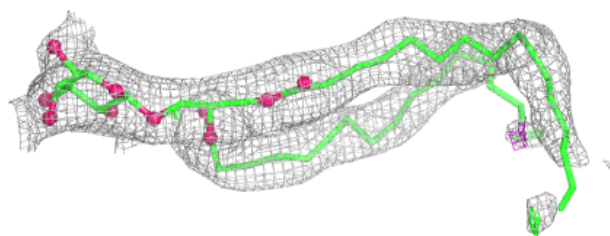
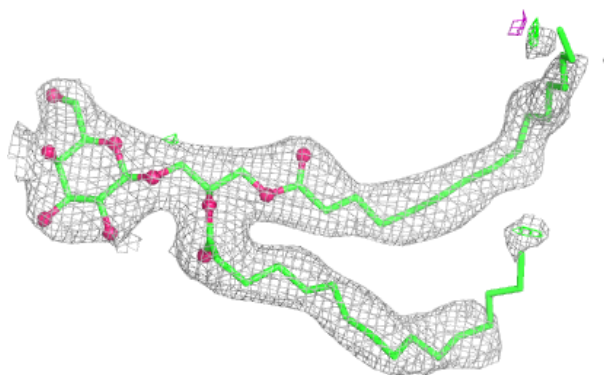
**Electron density around CLA C 504:**

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

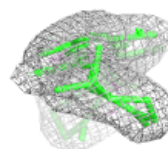
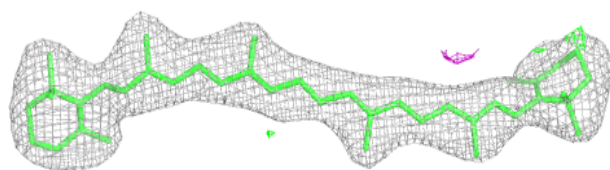
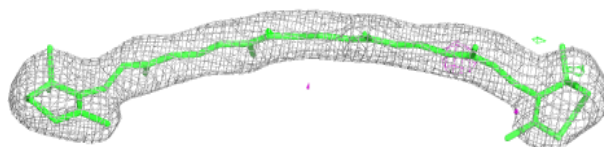


Electron density around LMG J 101:

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

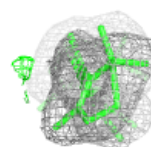
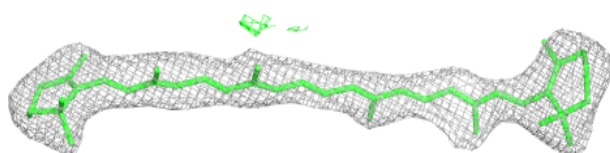
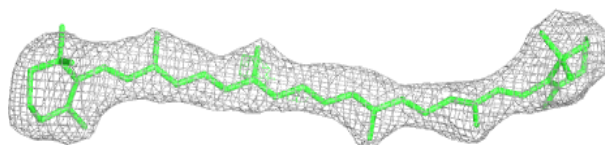
**Electron density around BCR D 406:**

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

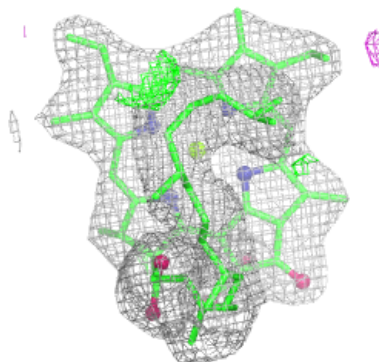
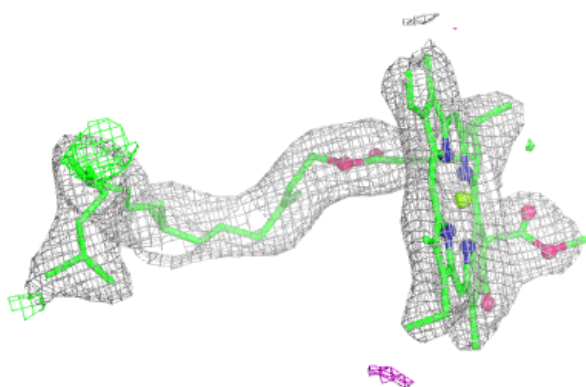
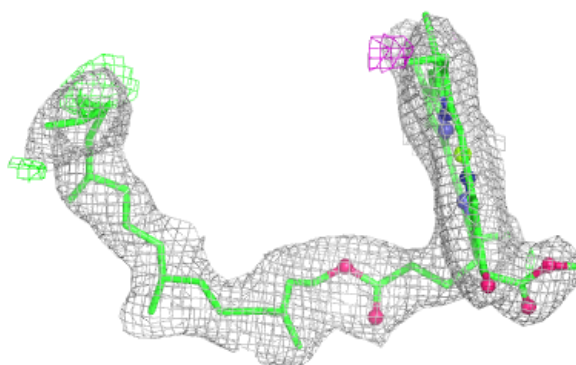


Electron density around BCR c 927:

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

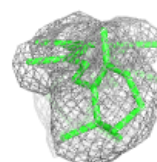
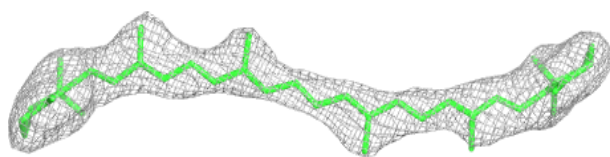
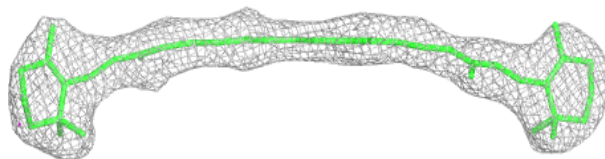
**Electron density around CLA c 907:**

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



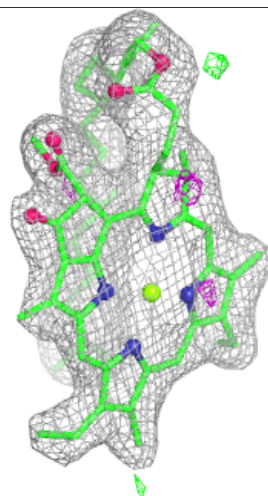
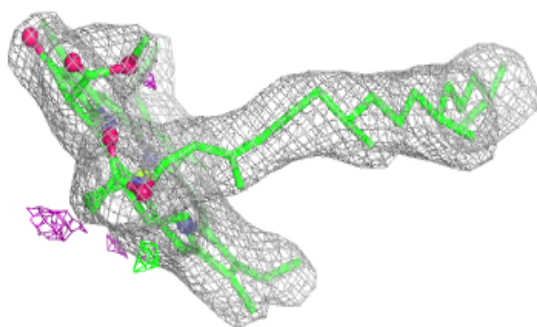
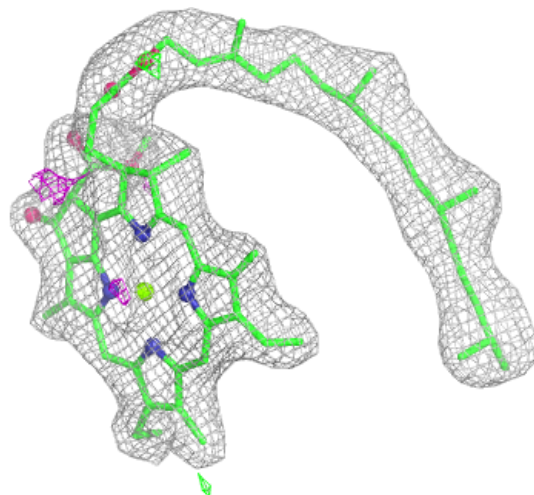
Electron density around BCR k 101:

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



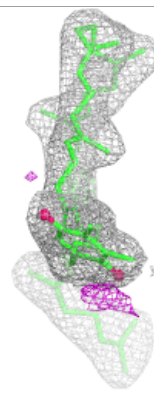
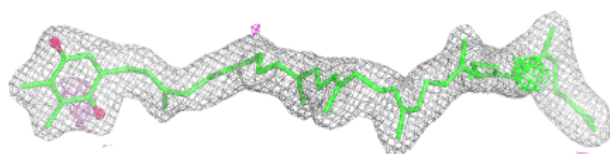
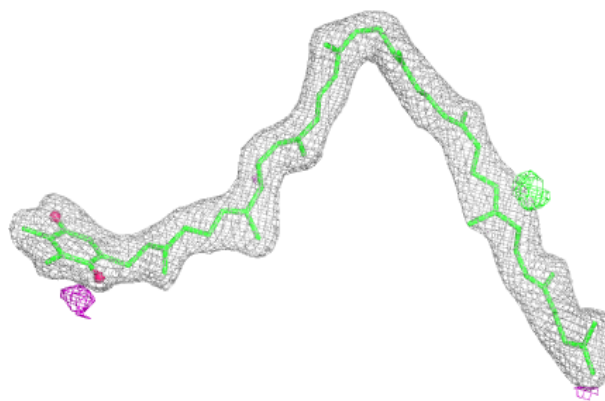
Electron density around CLA c 908:

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

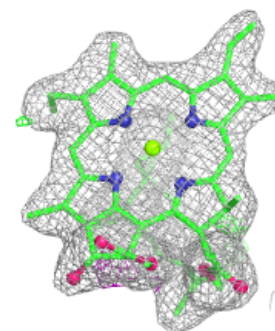
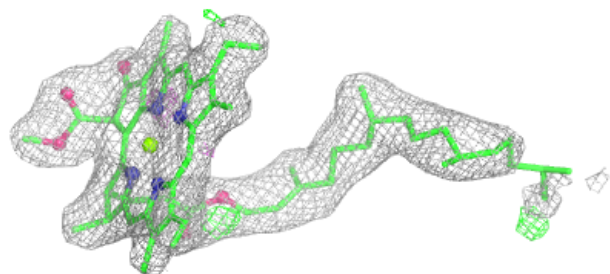
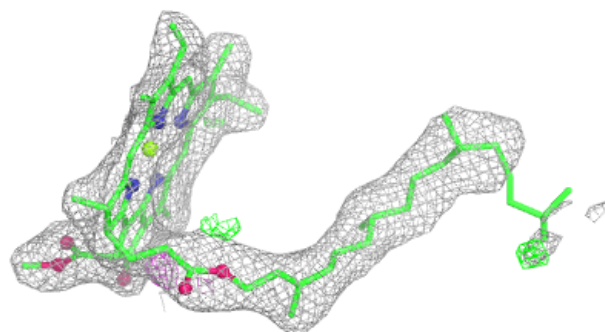


Electron density around PL9 D 407:

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

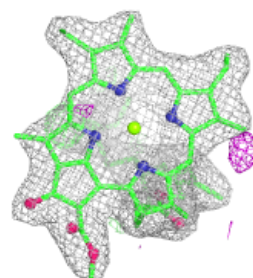
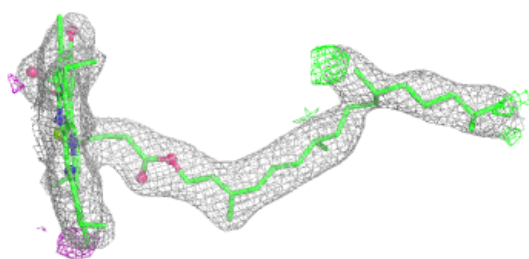
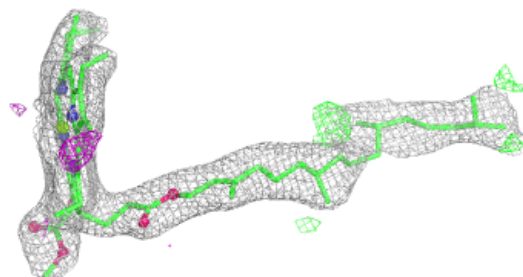
**Electron density around CLA c 909:**

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



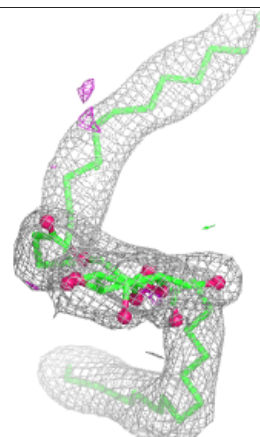
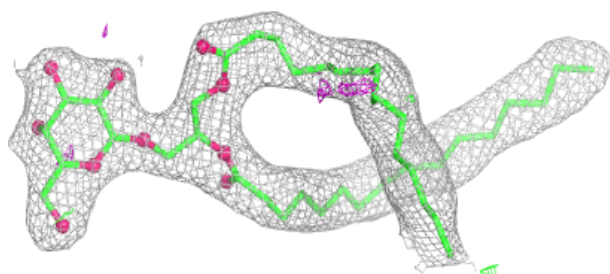
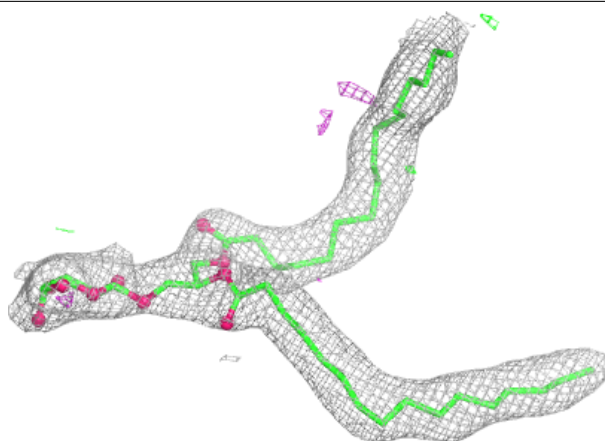
Electron density around CLA B 607:

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



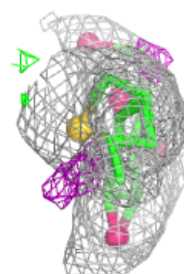
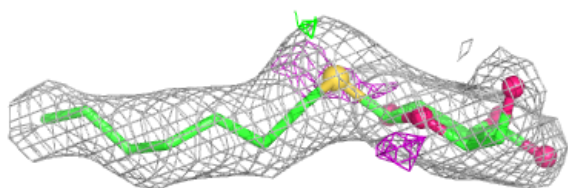
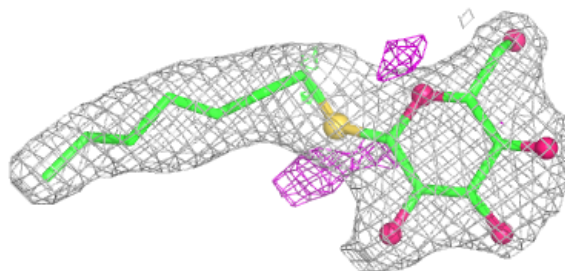
Electron density around LMG B 622:

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

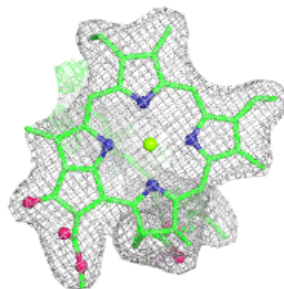
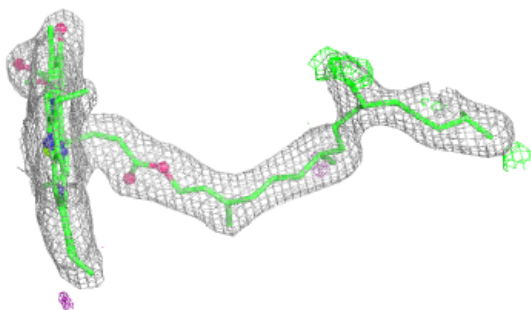
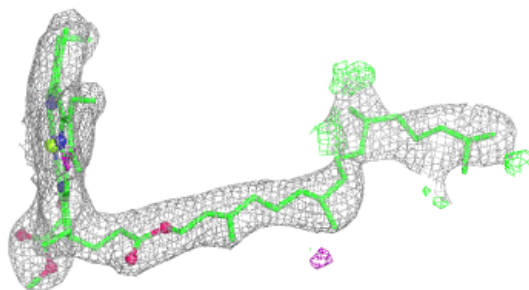


Electron density around HTG b 601:

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

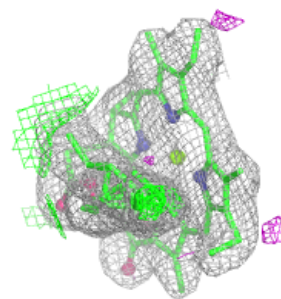
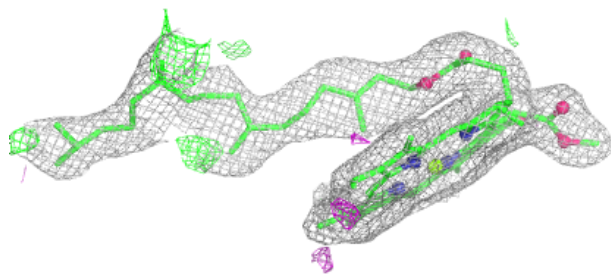
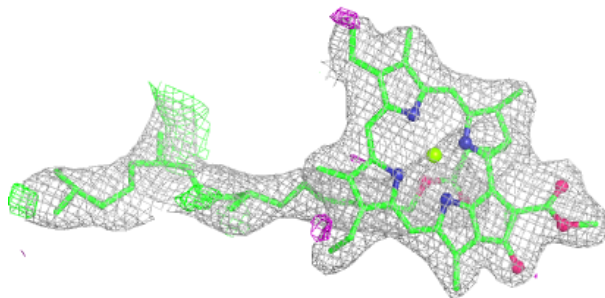
**Electron density around CLA b 611:**

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



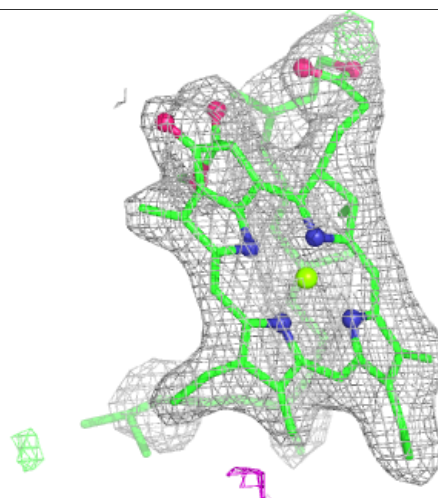
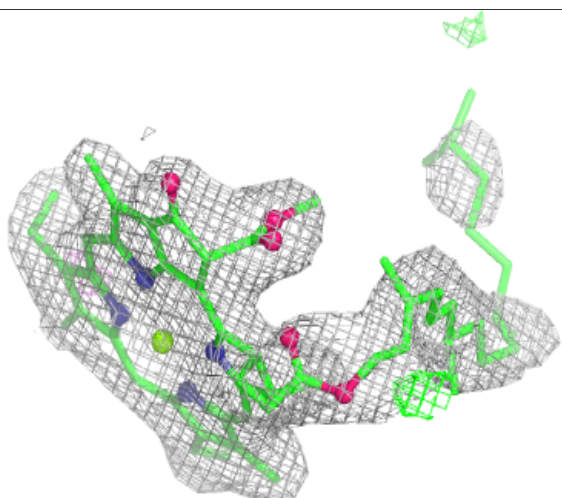
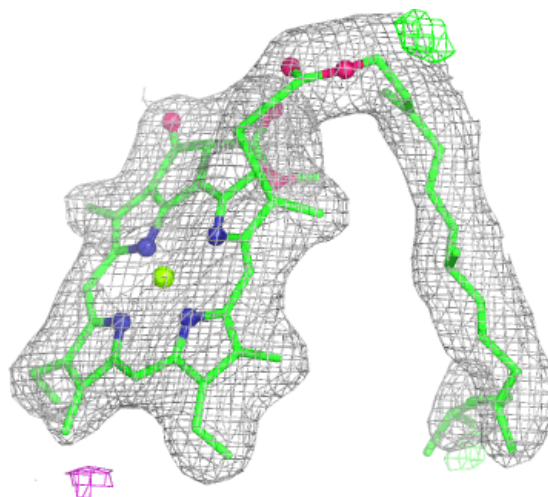
Electron density around CLA b 619:

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



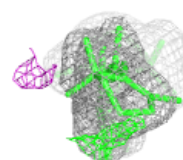
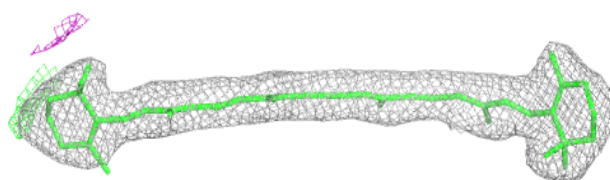
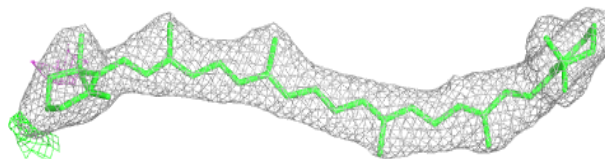
Electron density around CLA b 621:

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

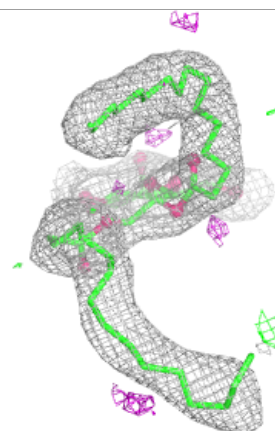
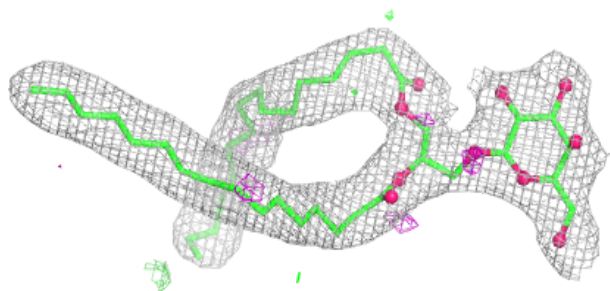
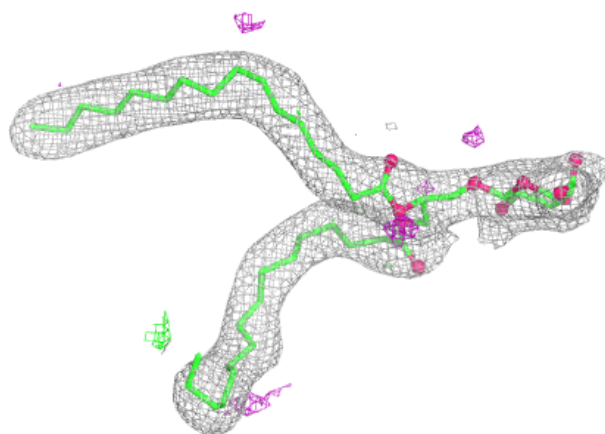


Electron density around BCR H 101:

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

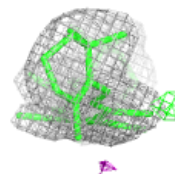
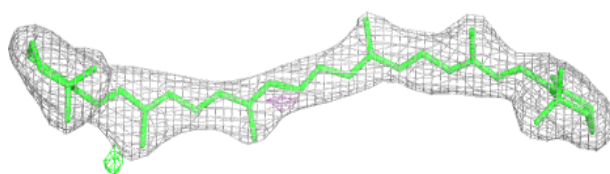
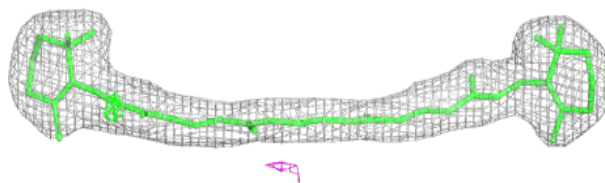
**Electron density around LMG b 625:**

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

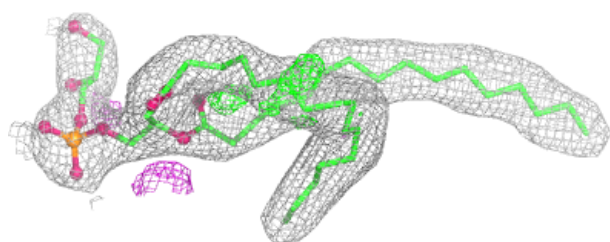
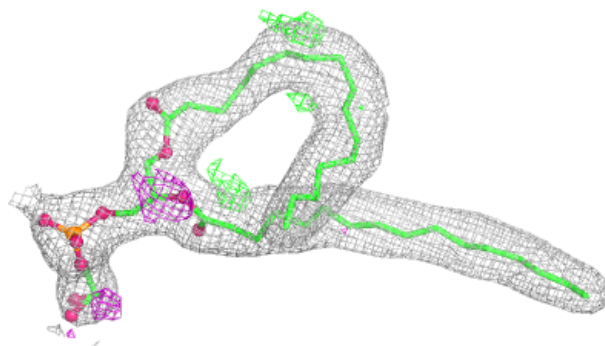


Electron density around BCR K 101:

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

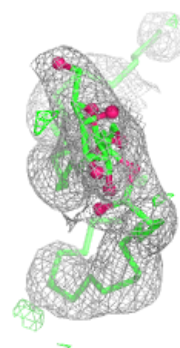
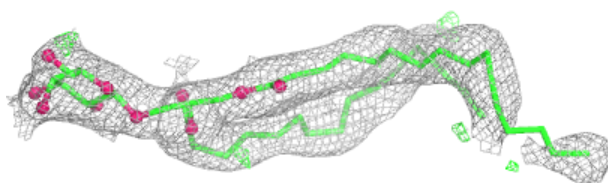
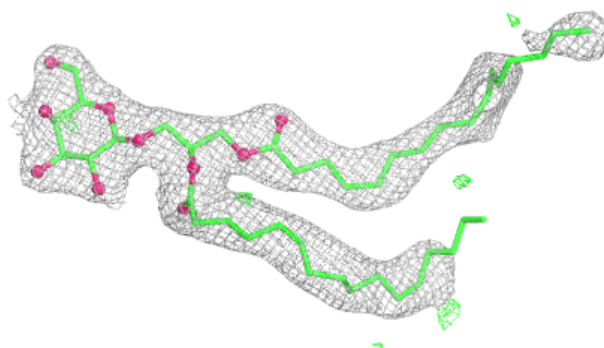
**Electron density around LHG B 635:**

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

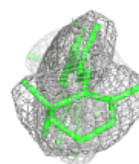
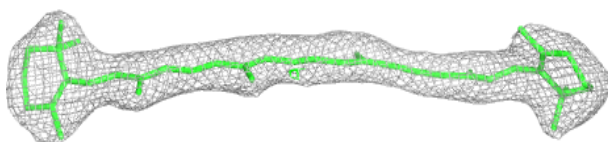
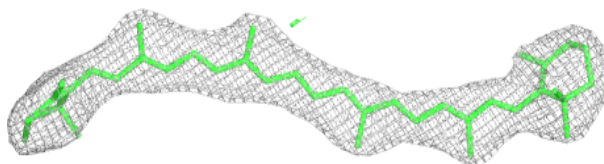


Electron density around LMG d 415:

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

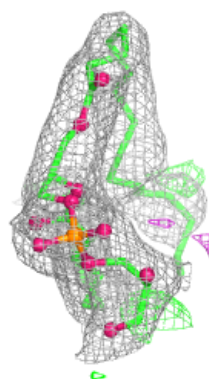
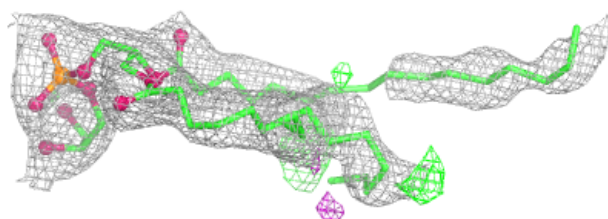
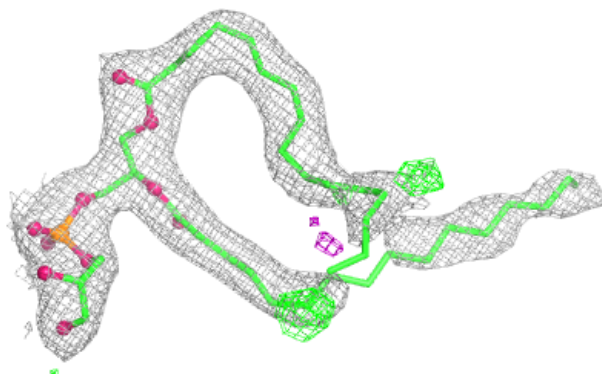
**Electron density around BCR Y 102:**

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

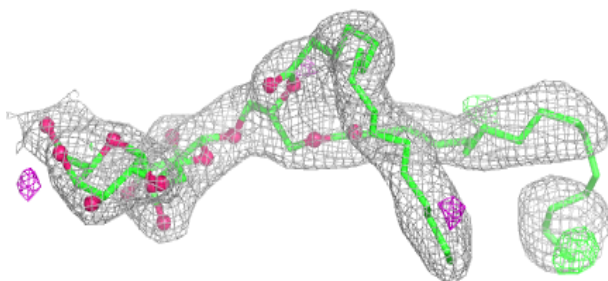
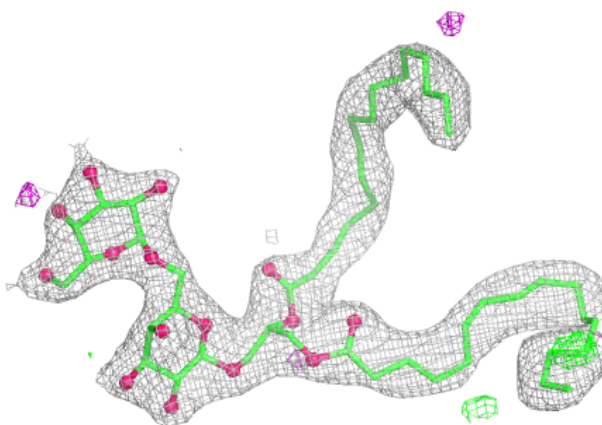


Electron density around LHG d 411:

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

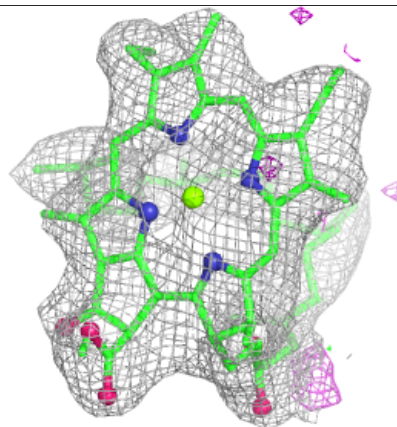
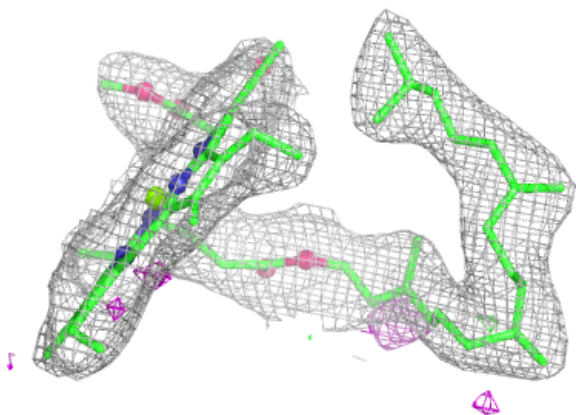
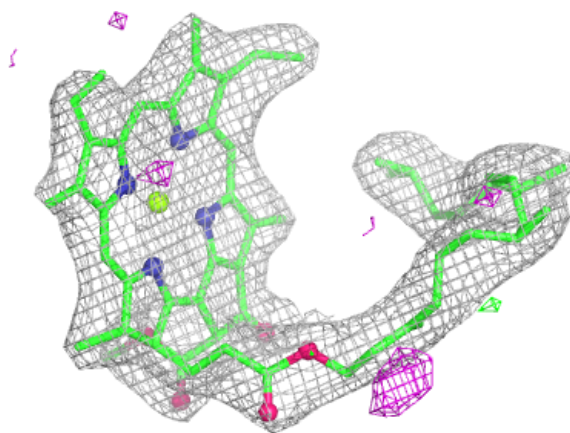
**Electron density around DGD C 517:**

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



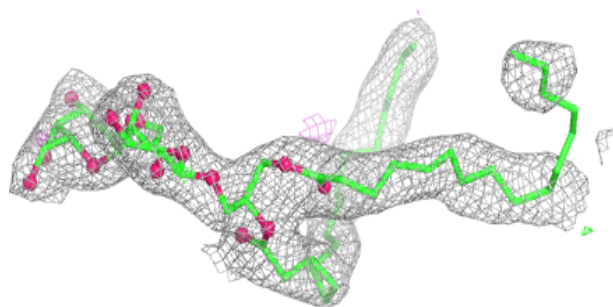
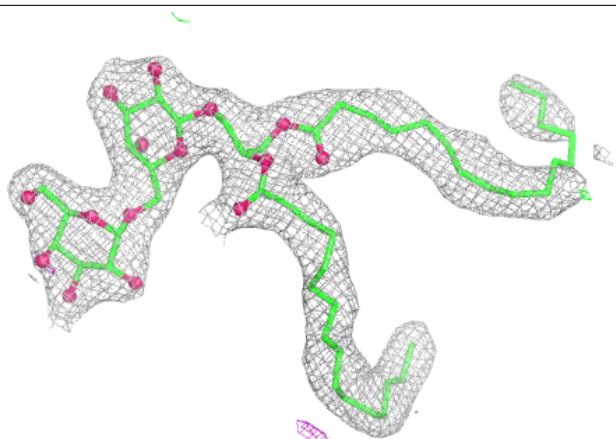
Electron density around CLA c 904:

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



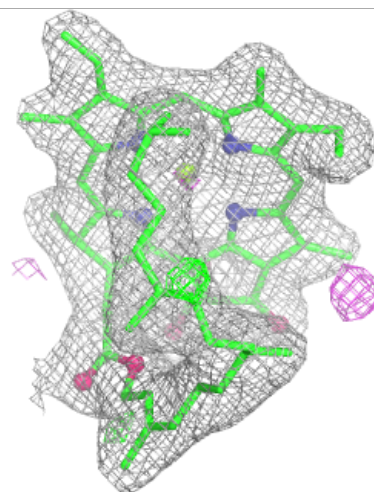
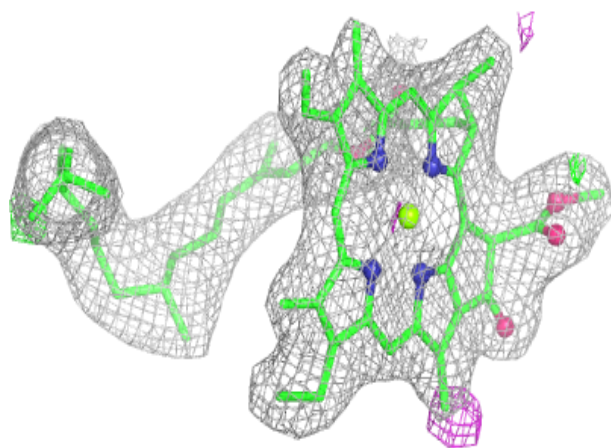
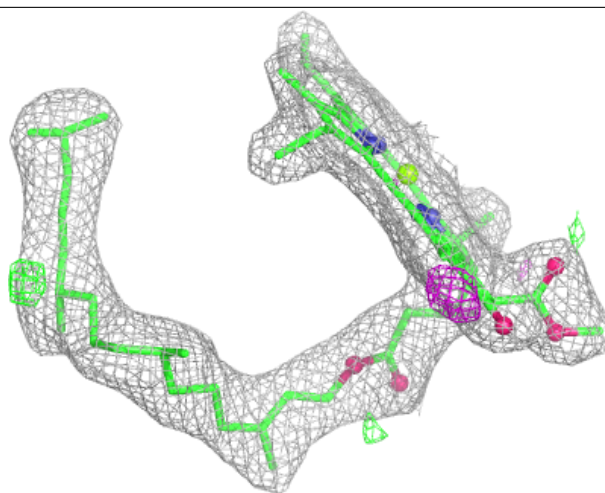
Electron density around DGD c 917:

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



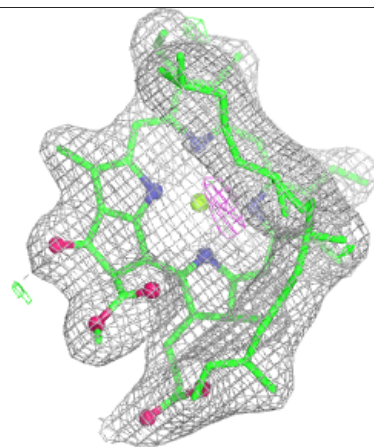
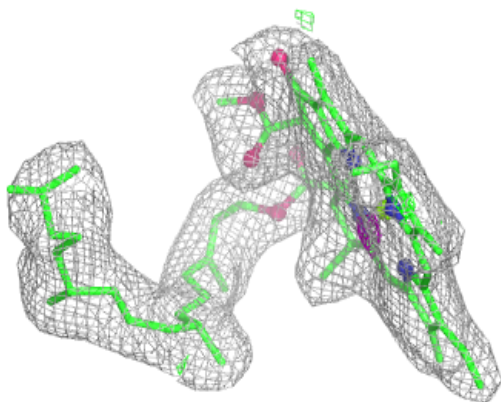
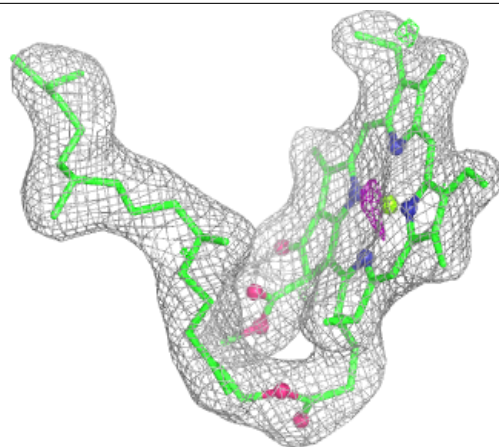
Electron density around CLA b 616:

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

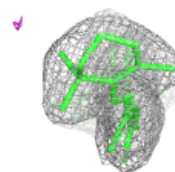
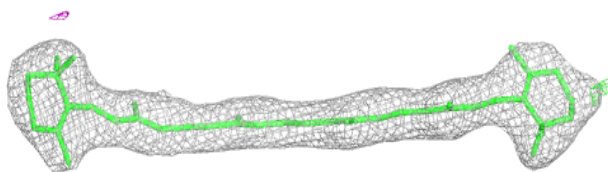
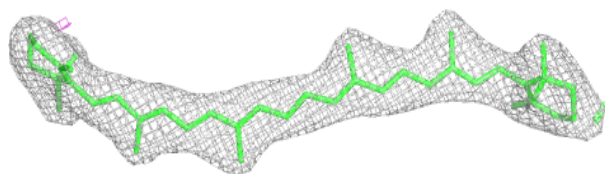


Electron density around CLA B 614:

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

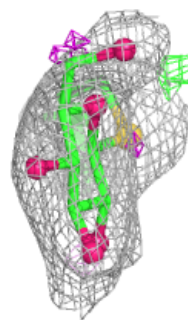
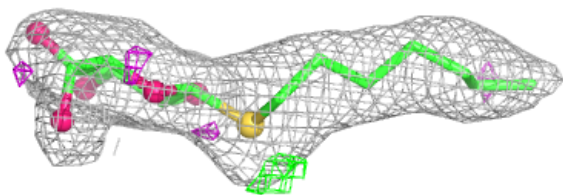
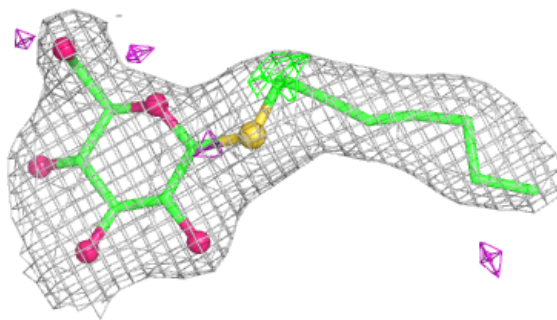
**Electron density around BCR h 101:**

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



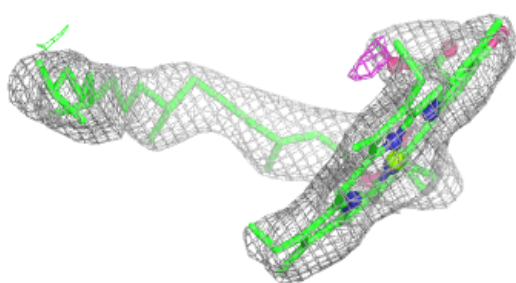
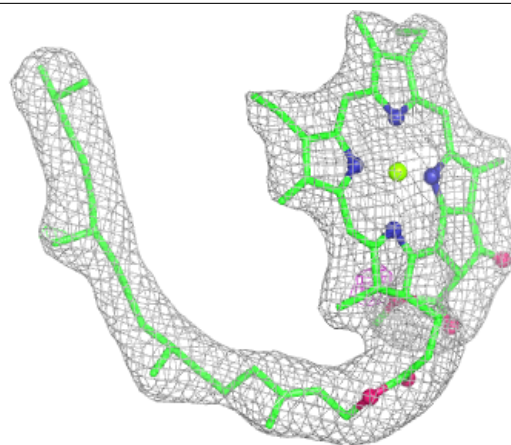
Electron density around HTG B 623:

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

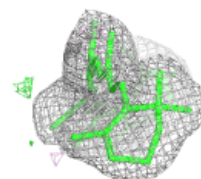
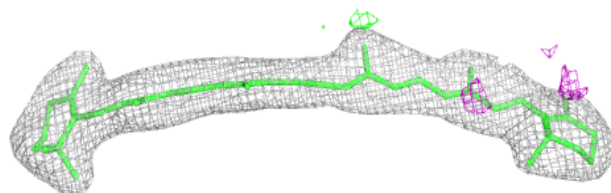
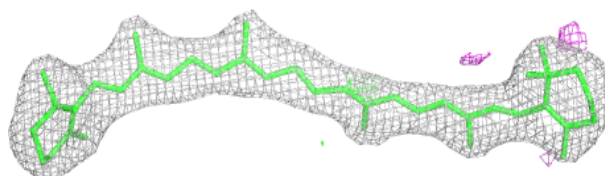


Electron density around CLA C 507:

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

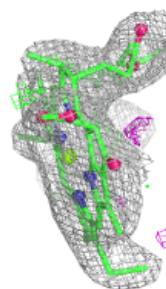
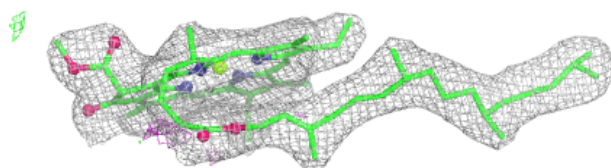
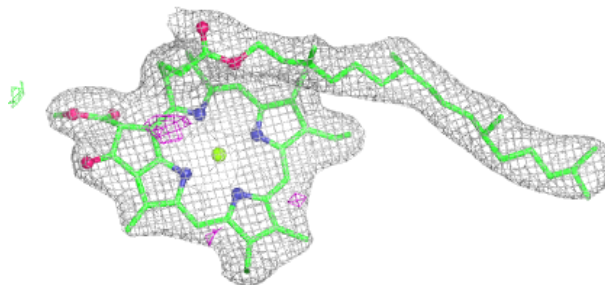
**Electron density around BCR t 102:**

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

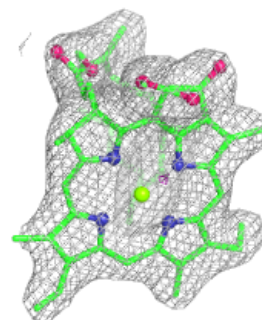
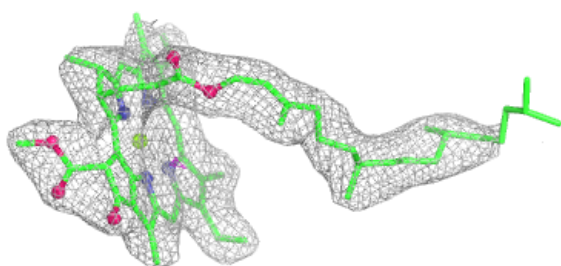
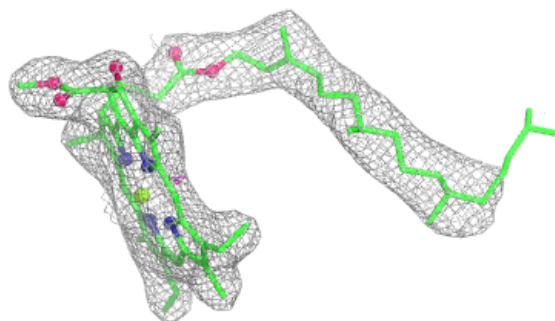


Electron density around CLA c 902:

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

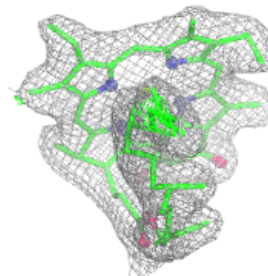
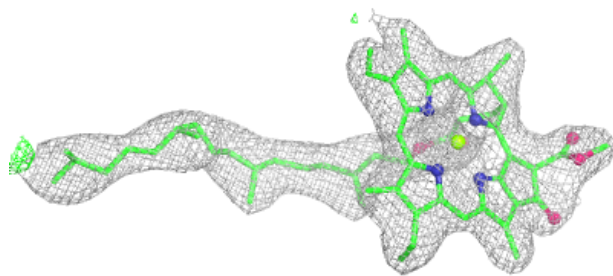
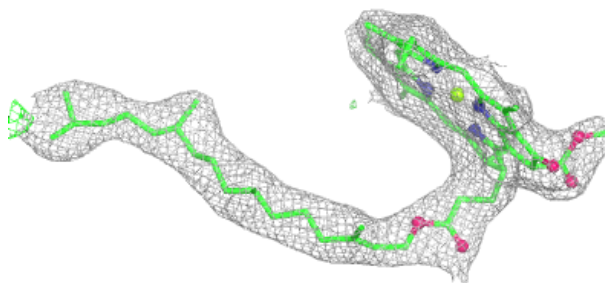
**Electron density around CLA C 508:**

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



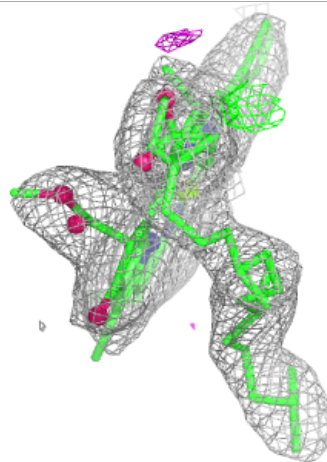
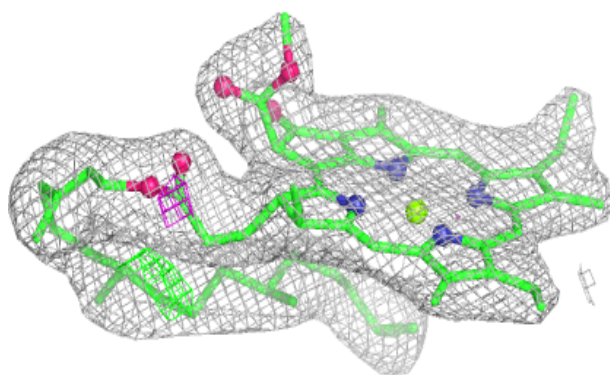
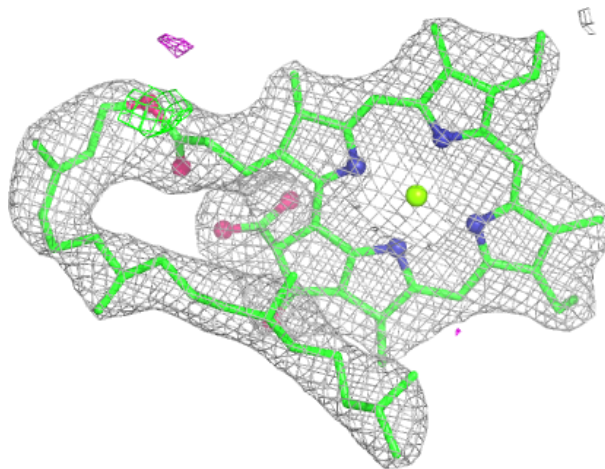
Electron density around CLA c 905:

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



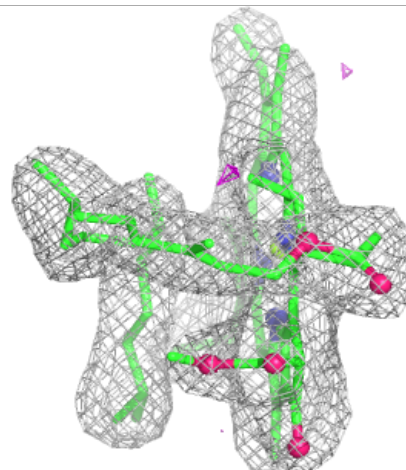
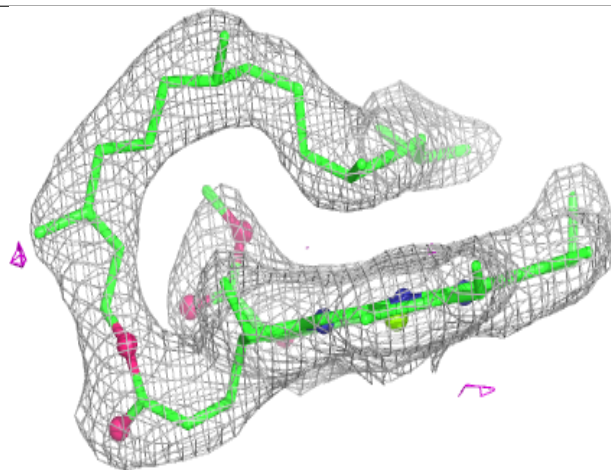
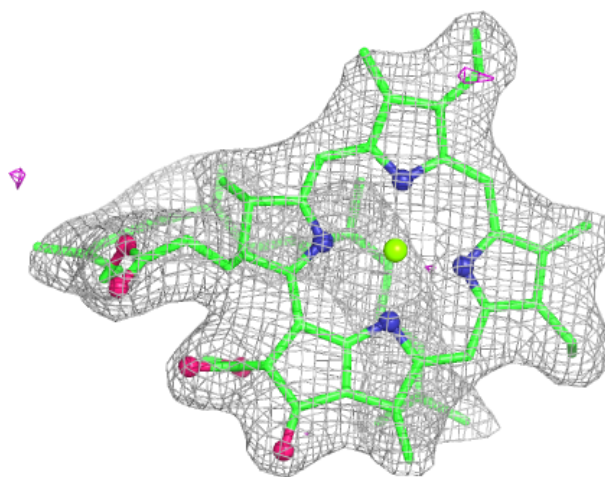
Electron density around CLA C 509:

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



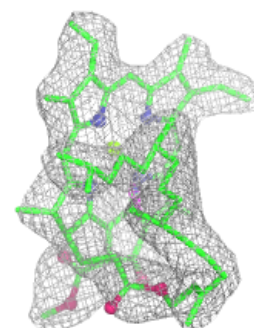
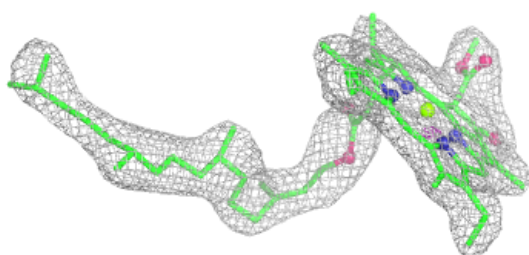
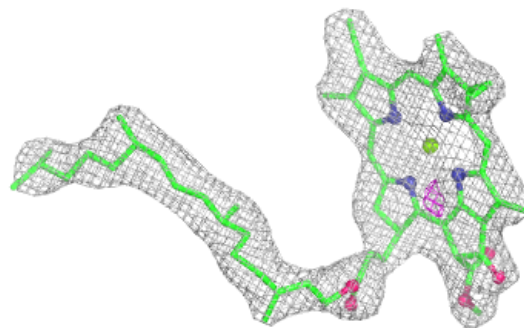
Electron density around CLA C 510:

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



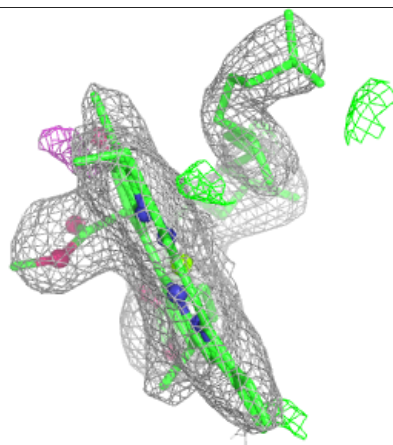
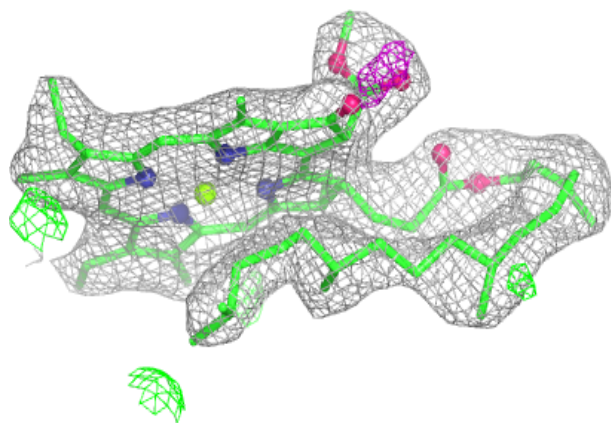
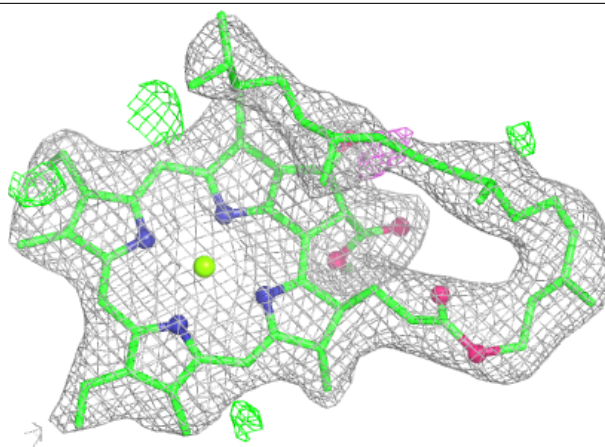
Electron density around CLA C 511:

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



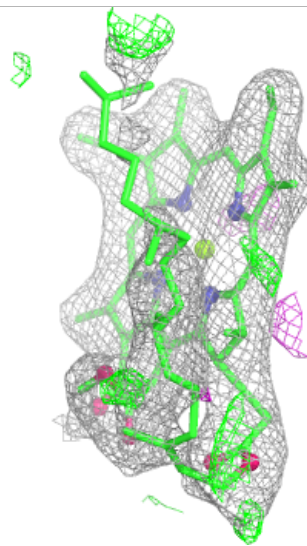
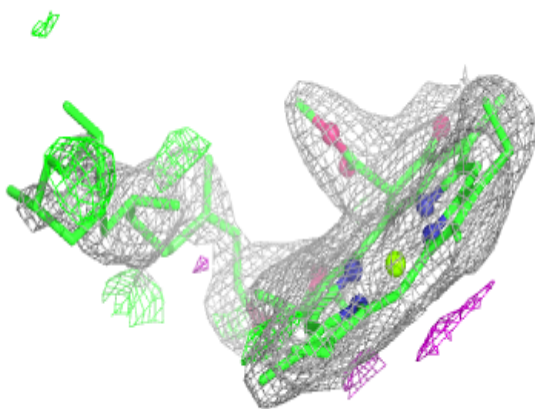
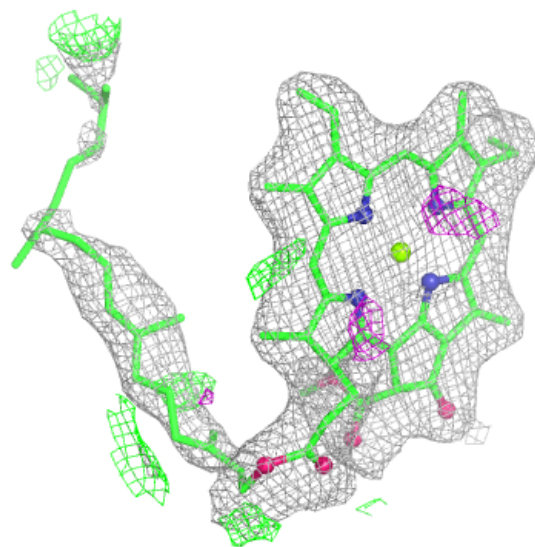
Electron density around CLA c 910:

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



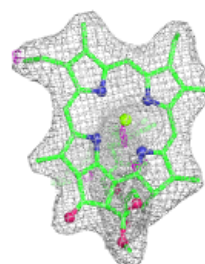
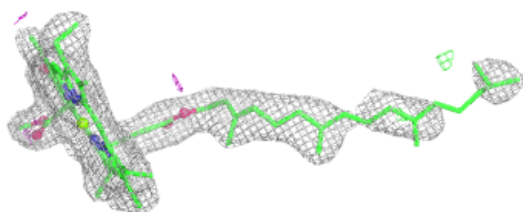
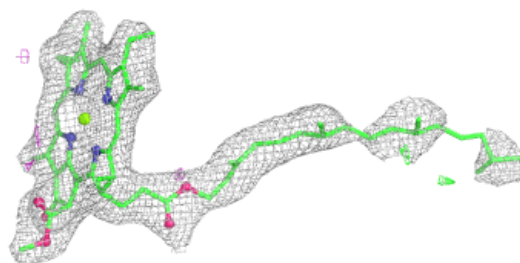
Electron density around CLA B 617:

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



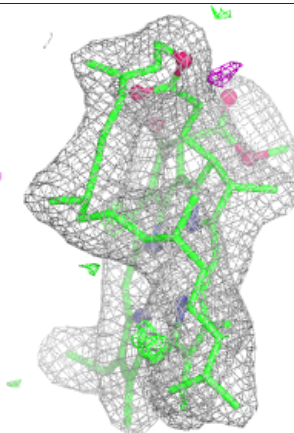
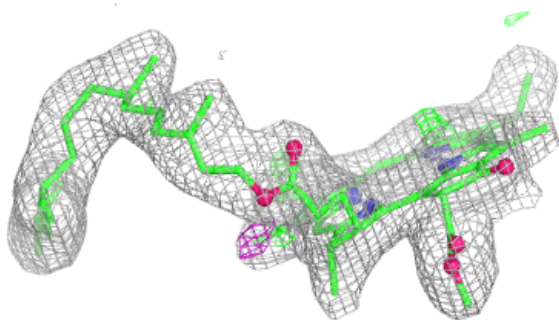
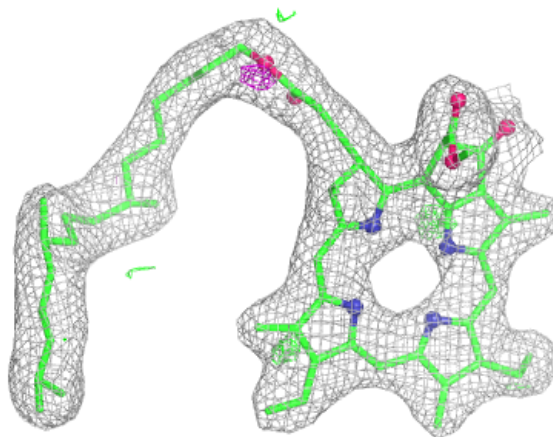
Electron density around CLA d 406:

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

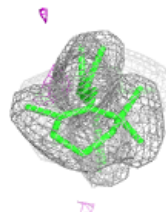
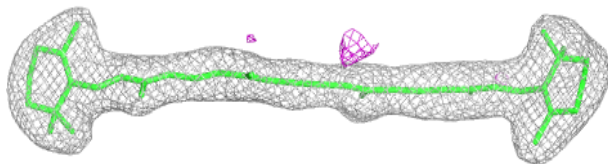
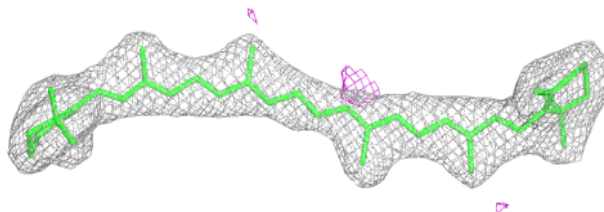


Electron density around PHO d 403:

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

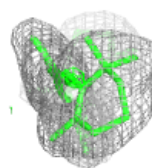
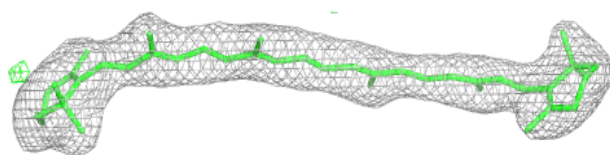
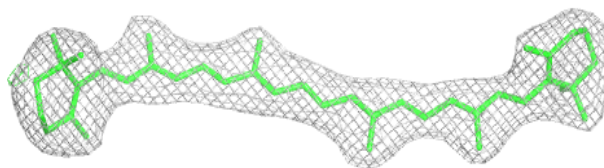
**Electron density around BCR A 410:**

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

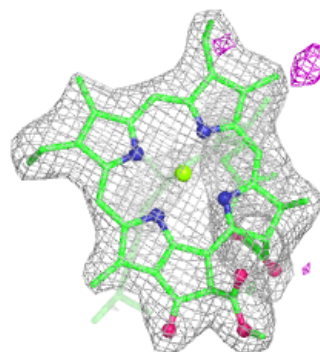
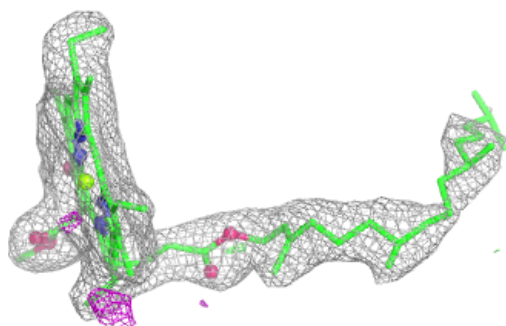
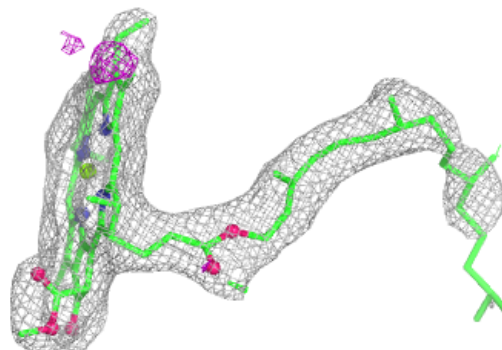


Electron density around BCR B 620:

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

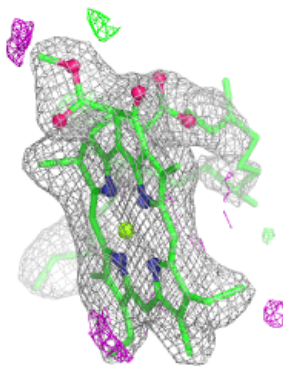
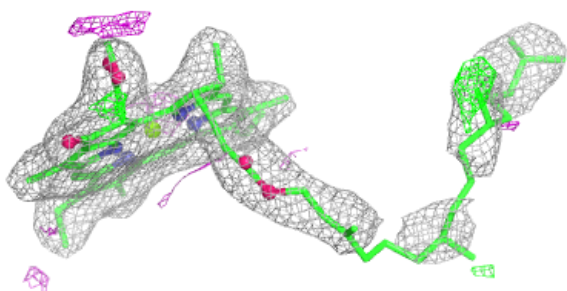
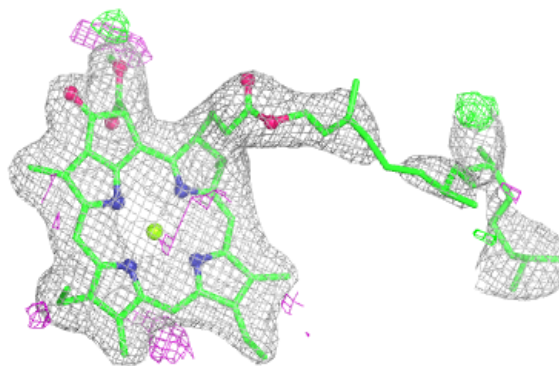
**Electron density around CLA D 405:**

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

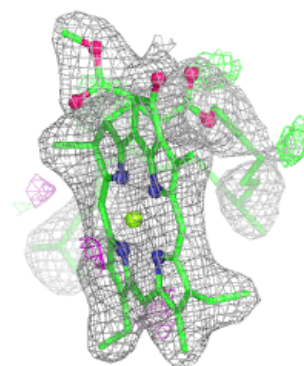
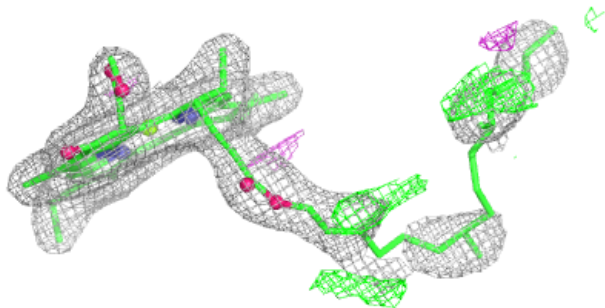
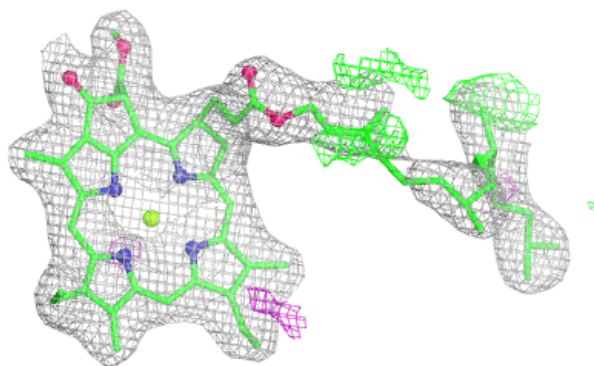


Electron density around CLA a 408:

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

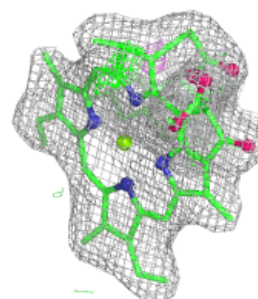
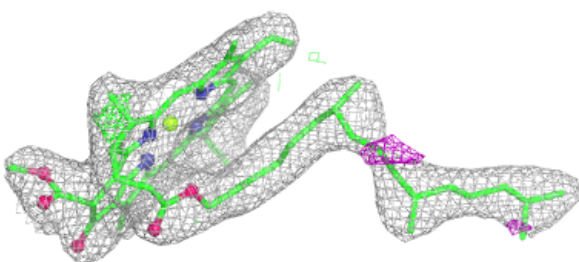
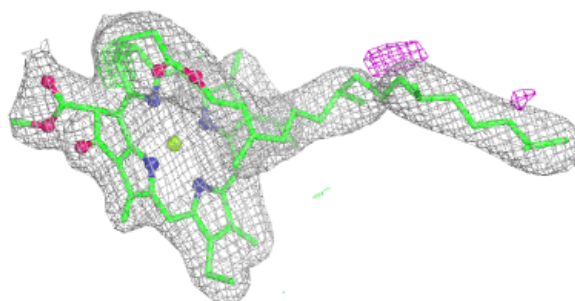
**Electron density around CLA A 409:**

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

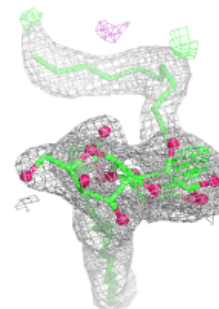
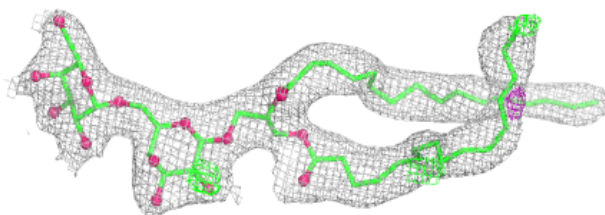
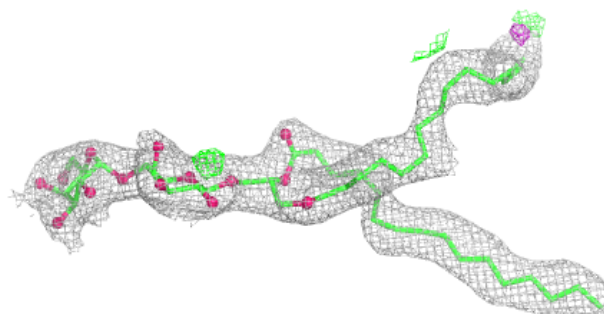


Electron density around CLA C 505:

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

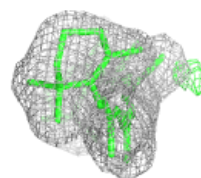
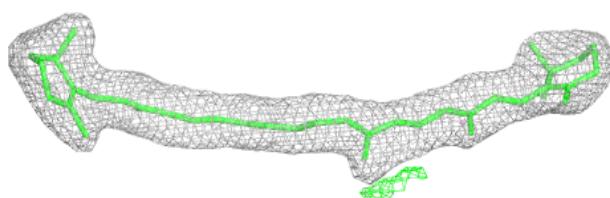
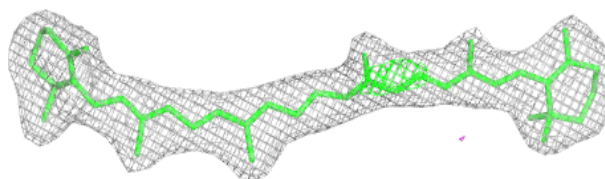
**Electron density around DGD C 516:**

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

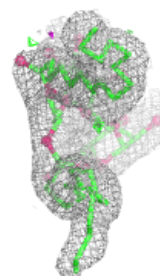
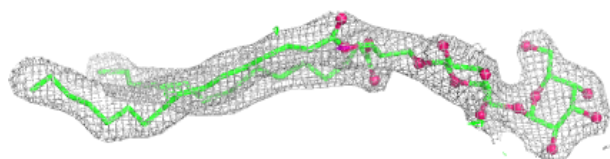
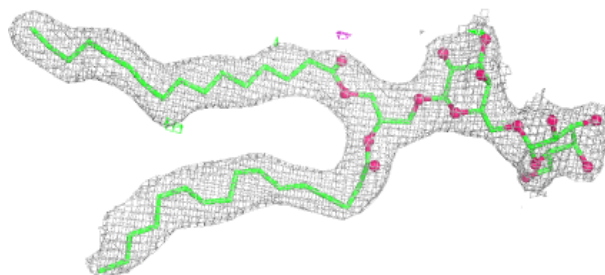


Electron density around BCR T 102:

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

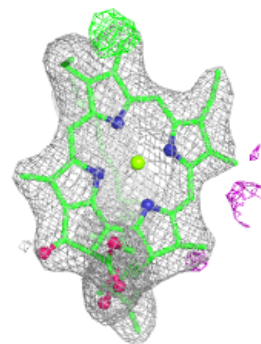
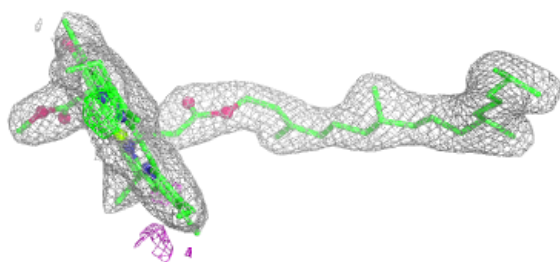
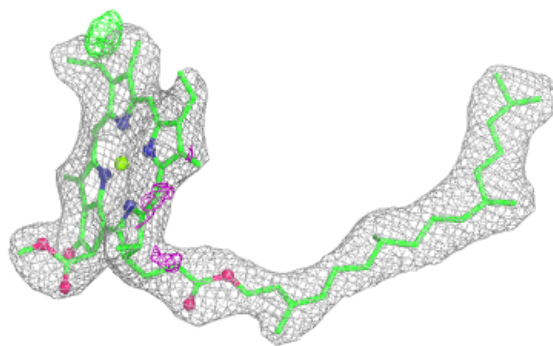
**Electron density around DGD C 518:**

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

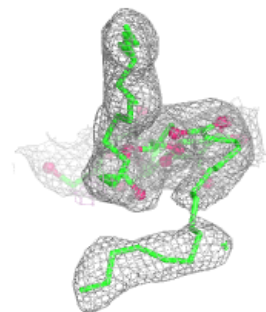
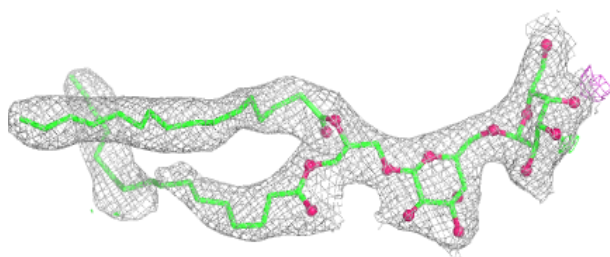
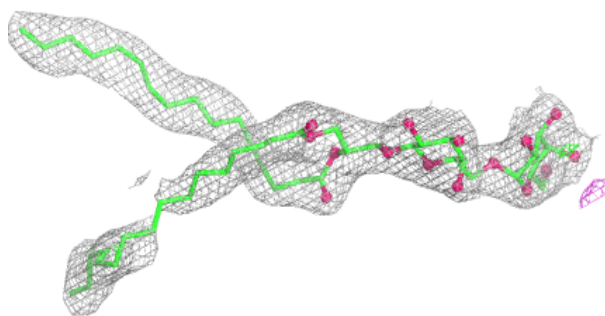


Electron density around CLA b 614:

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

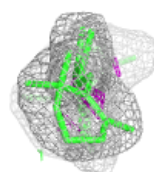
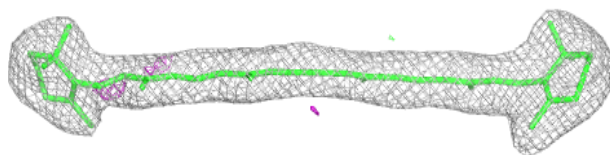
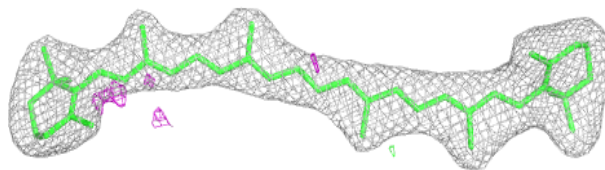
**Electron density around DGD c 916:**

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

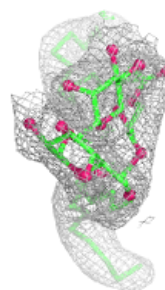
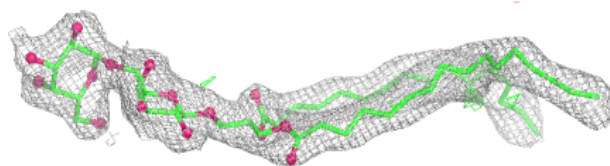
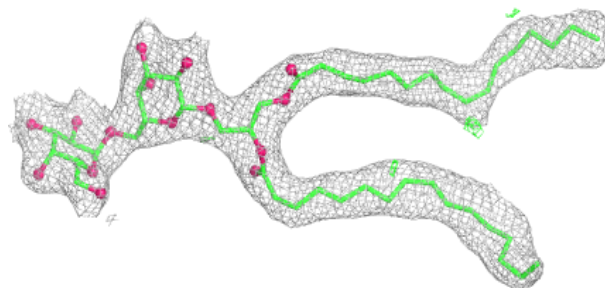


Electron density around BCR b 623:

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

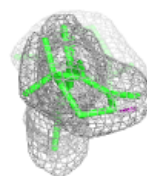
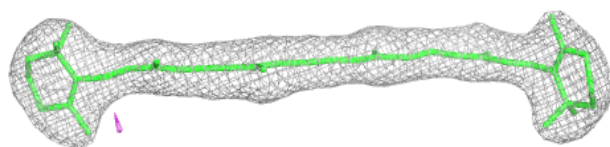
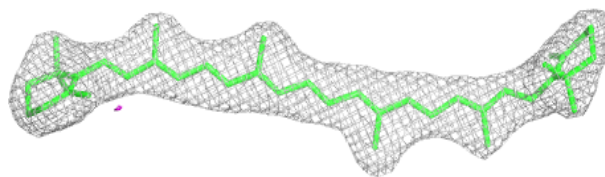
**Electron density around DGD c 918:**

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

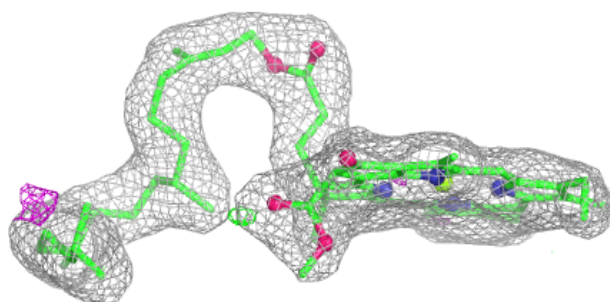
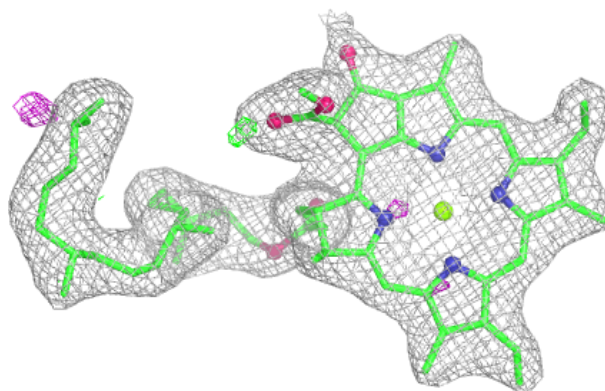


Electron density around BCR c 915:

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

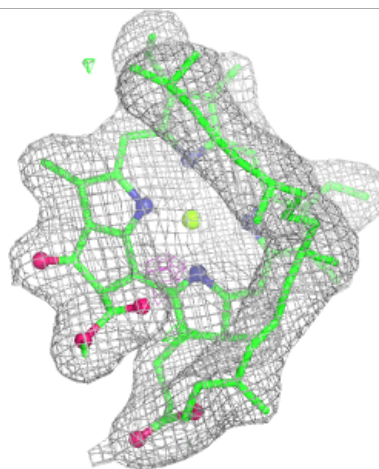
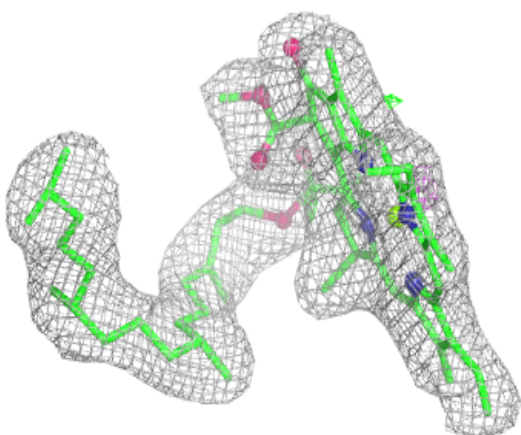
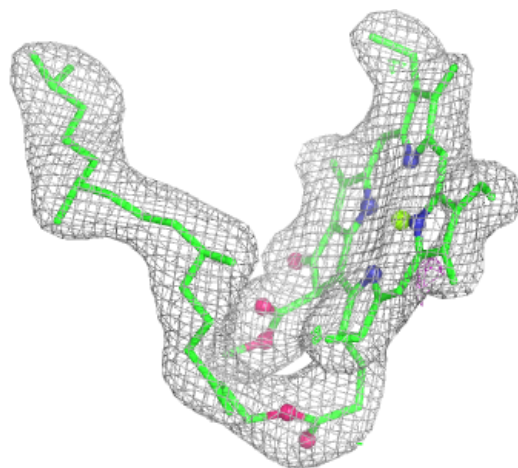
**Electron density around CLA b 617:**

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



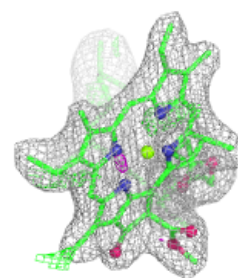
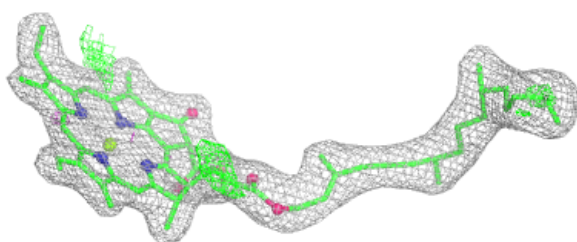
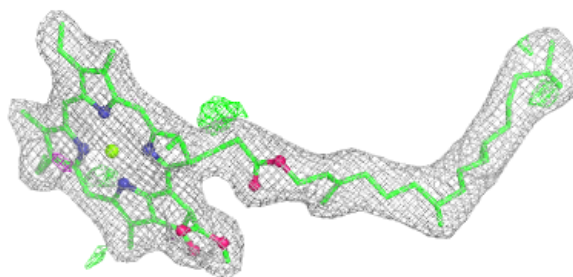
Electron density around CLA b 618:

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

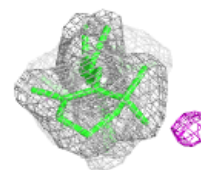
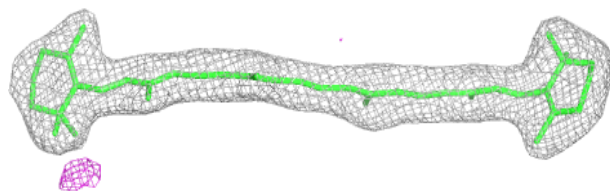
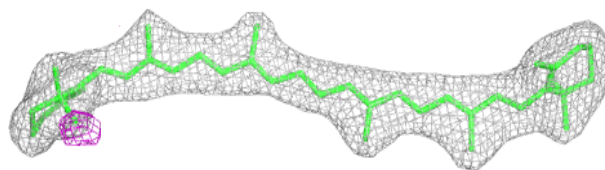


Electron density around CLA A 405:

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

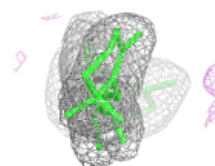
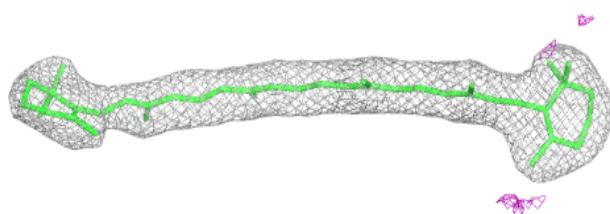
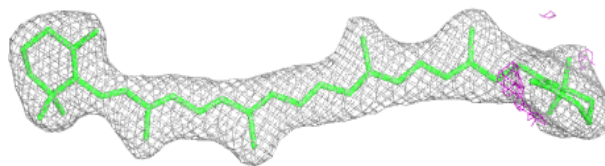
**Electron density around BCR a 409:**

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

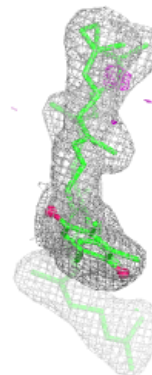
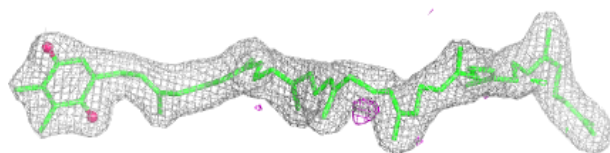
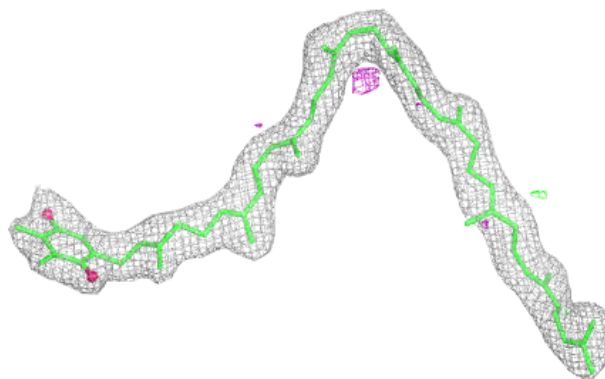


Electron density around BCR b 622:

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

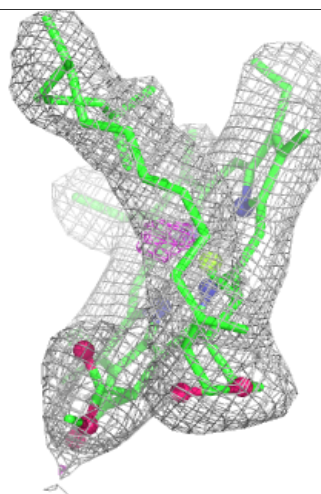
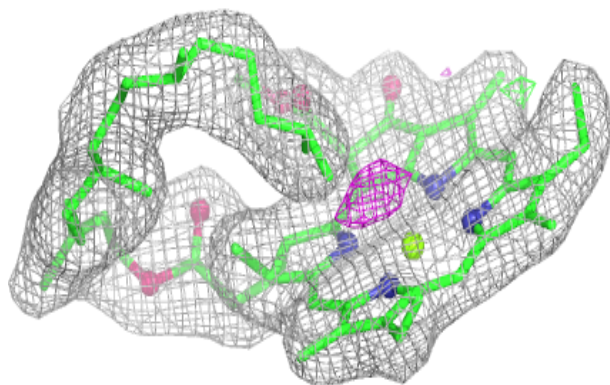
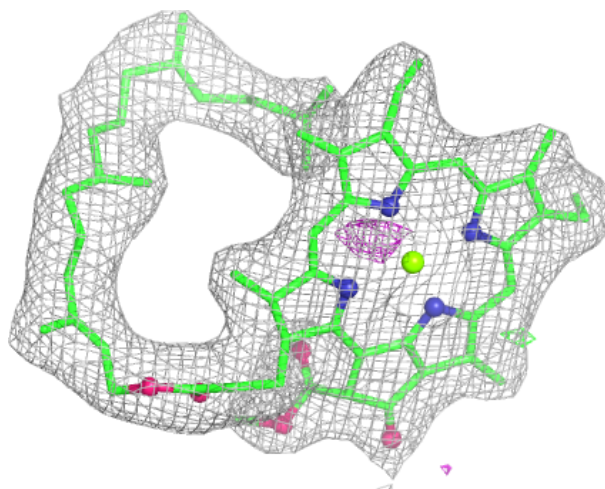
**Electron density around PL9 d 408:**

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



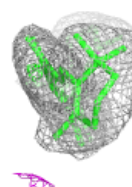
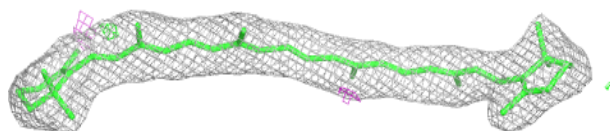
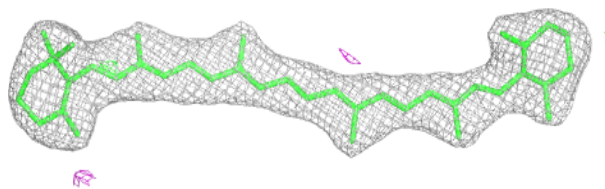
Electron density around CLA b 620:

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



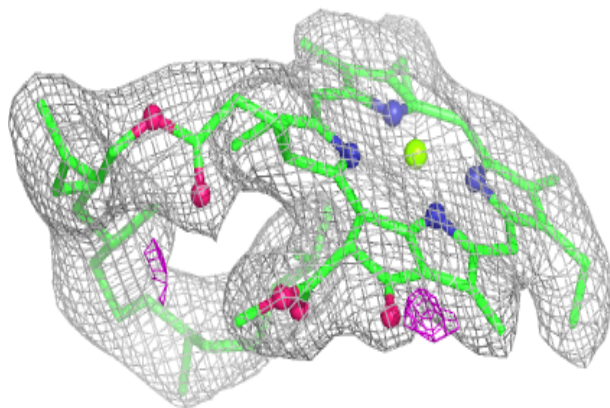
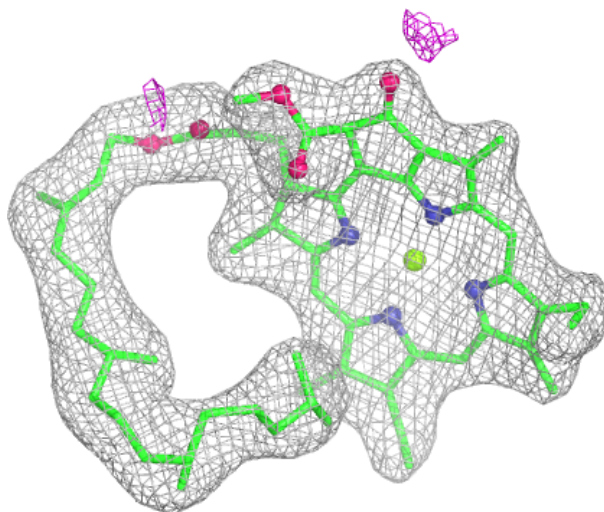
Electron density around BCR b 624:

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



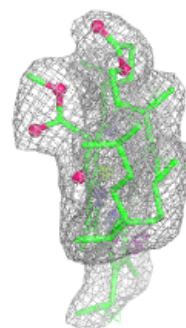
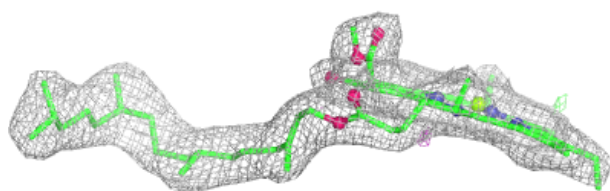
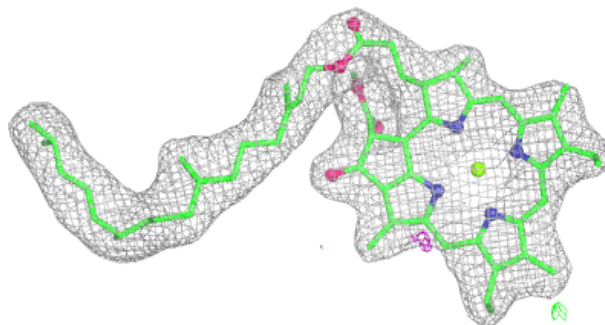
Electron density around CLA B 616:

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

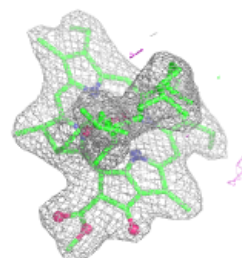
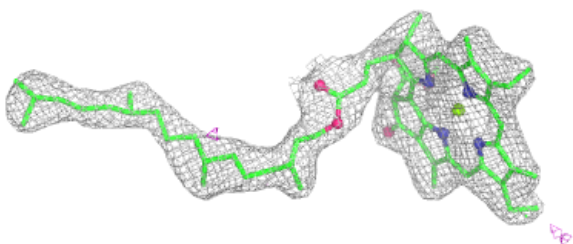
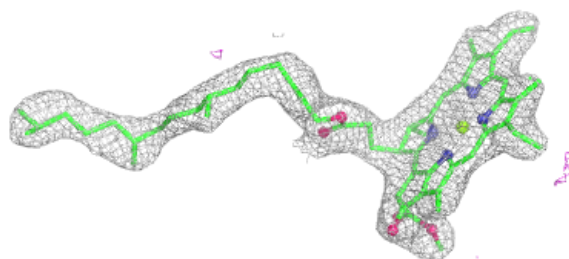


Electron density around CLA B 603:

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

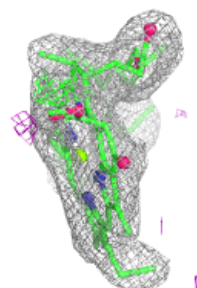
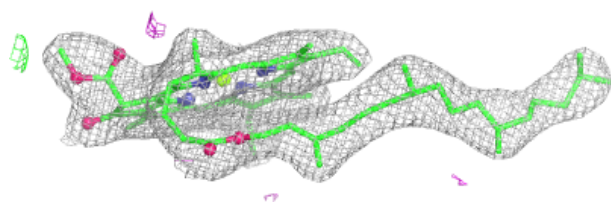
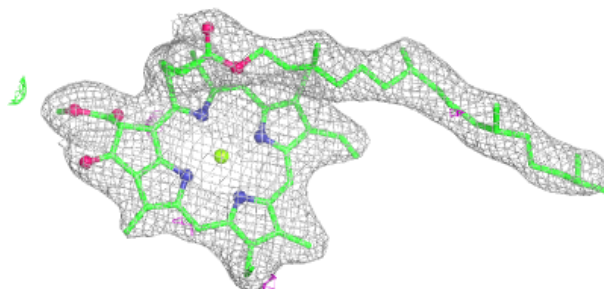
**Electron density around CLA c 903:**

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

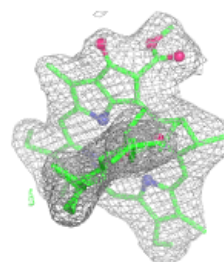
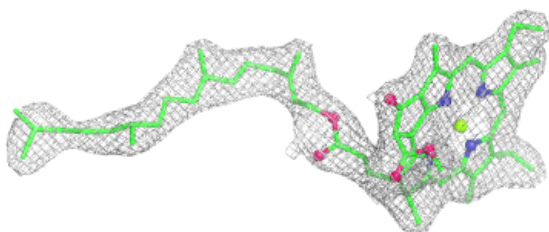
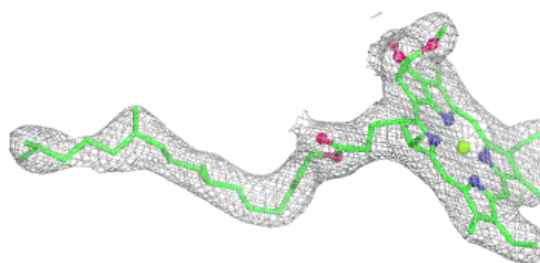


Electron density around CLA C 501:

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

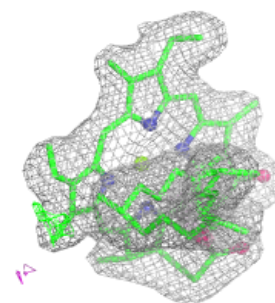
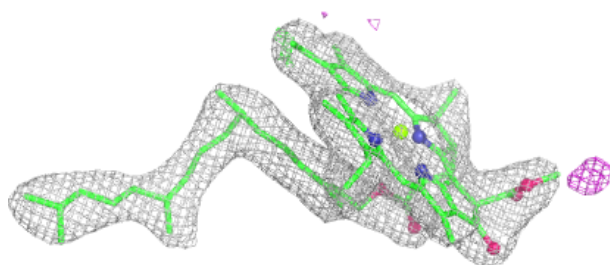
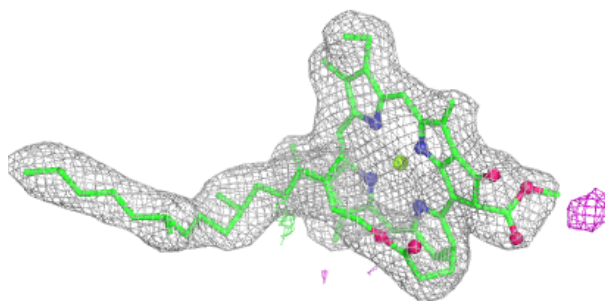
**Electron density around CLA C 502:**

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

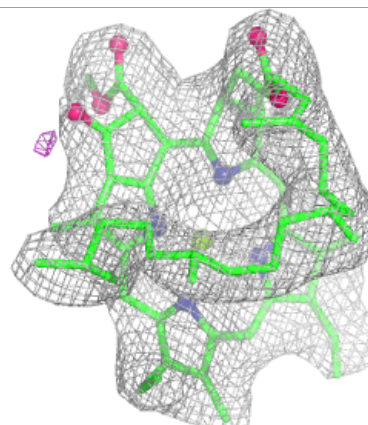
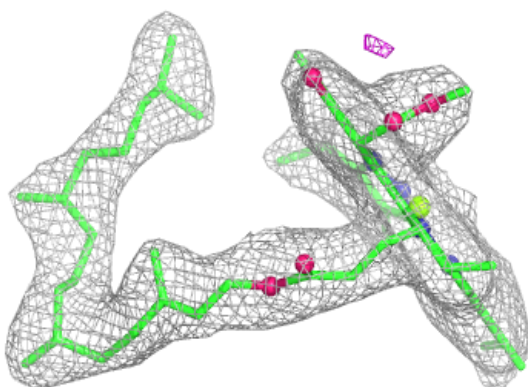
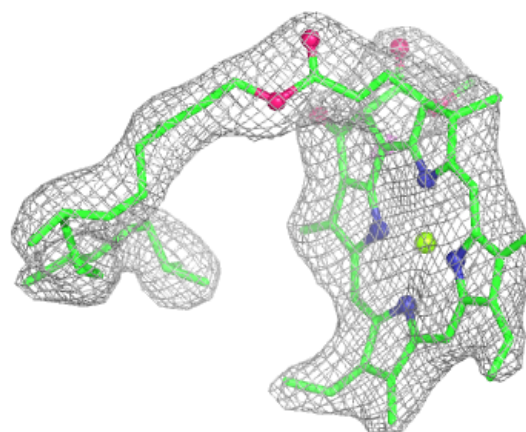


Electron density around CLA c 906:

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

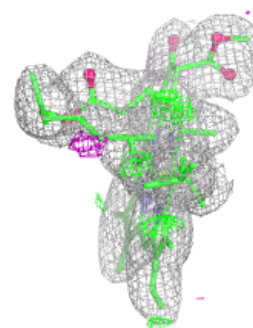
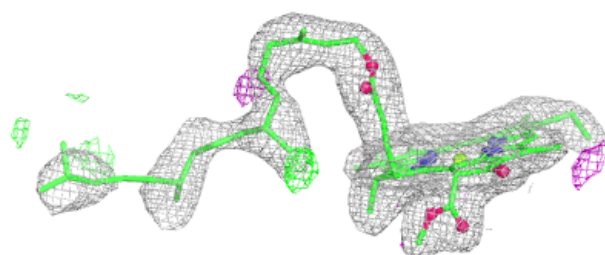
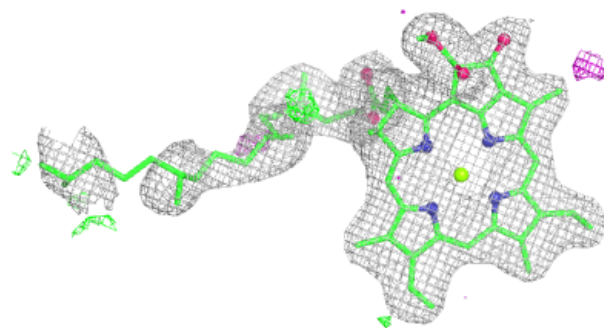
**Electron density around CLA C 503:**

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

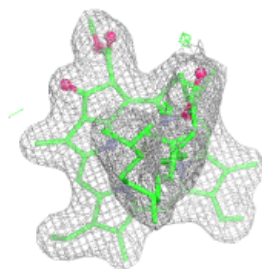
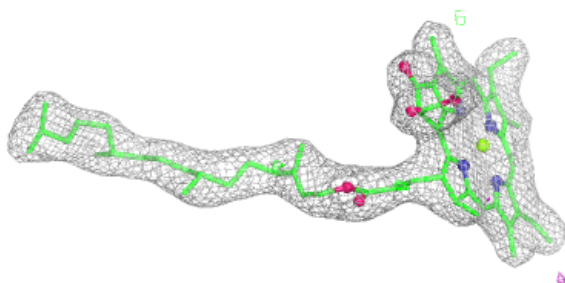
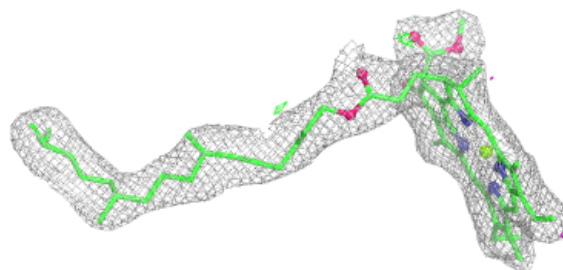


Electron density around CLA a 406:

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

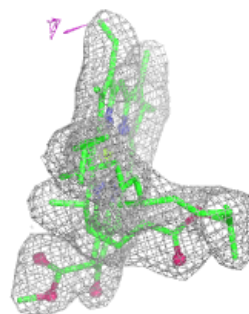
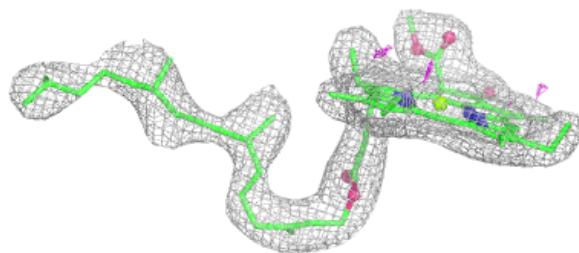
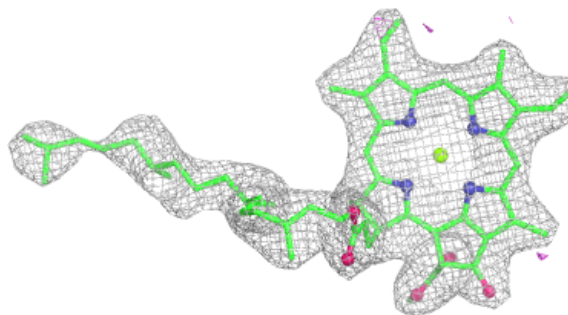
**Electron density around CLA B 605:**

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



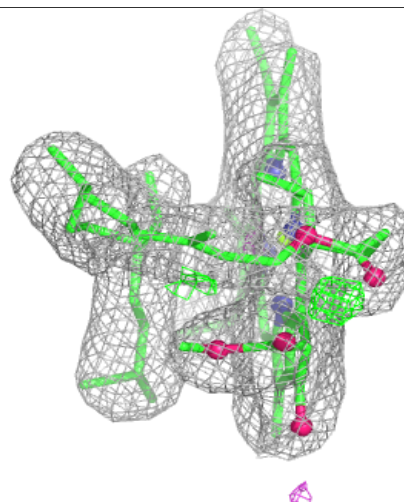
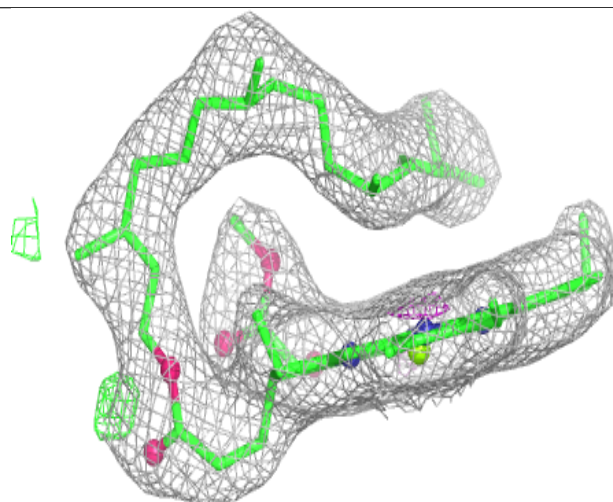
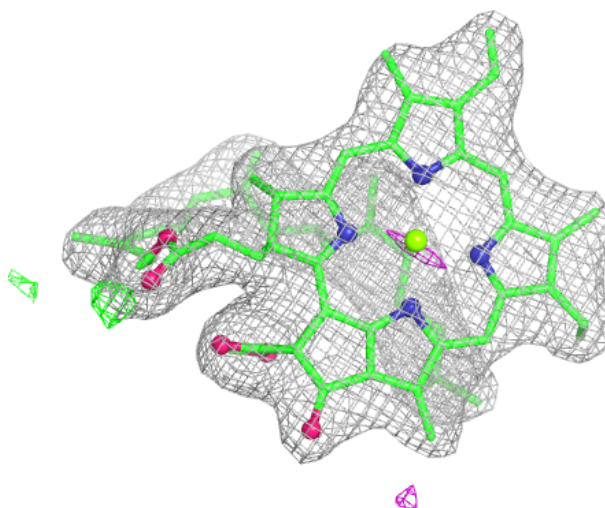
Electron density around CLA A 407:

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



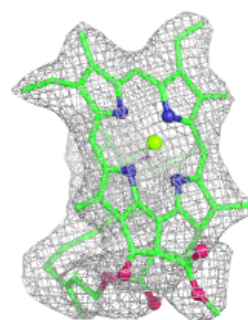
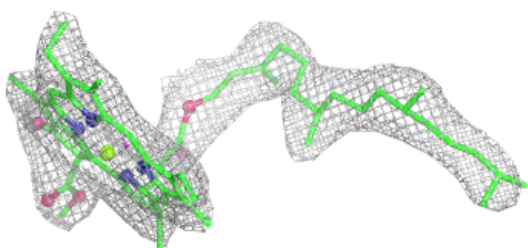
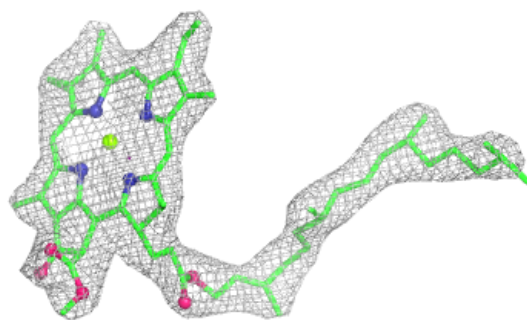
Electron density around CLA c 911:

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

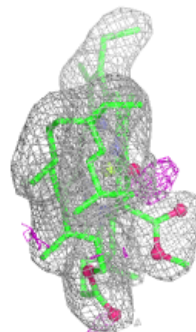
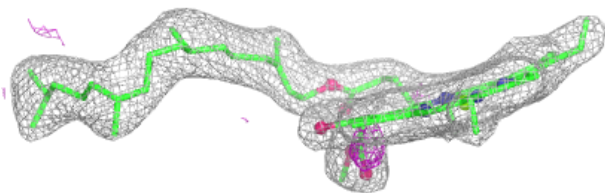
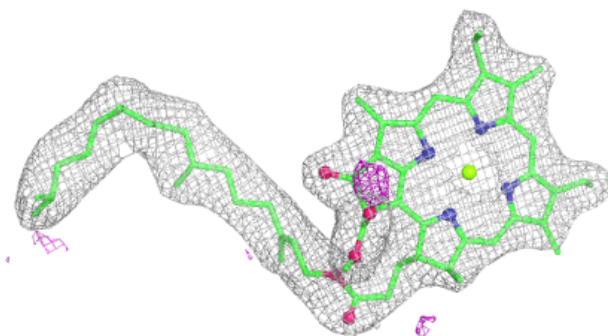


Electron density around CLA c 912:

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

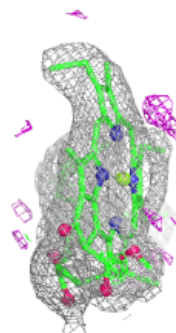
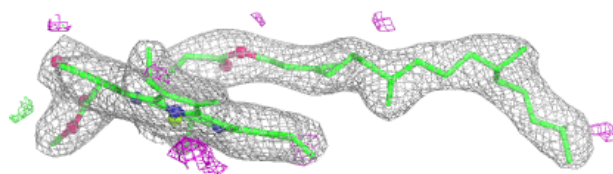
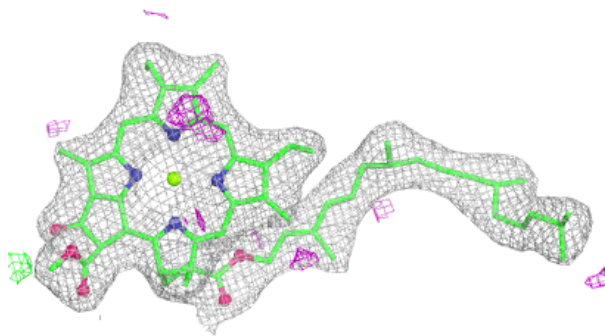
**Electron density around CLA b 607:**

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

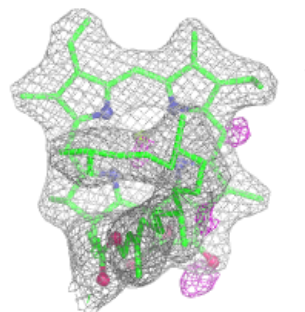
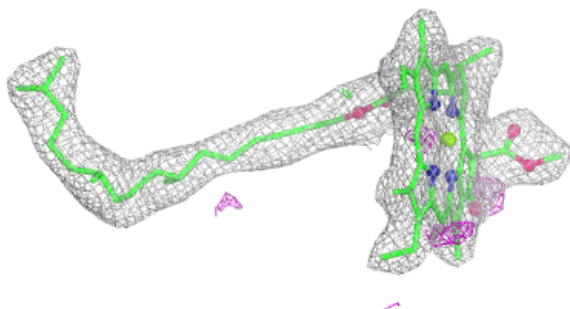
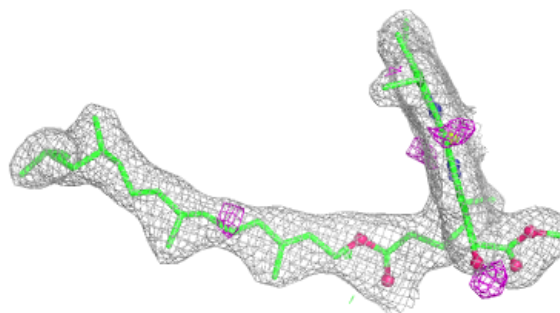


Electron density around CLA b 608:

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

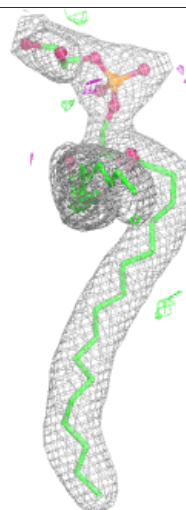
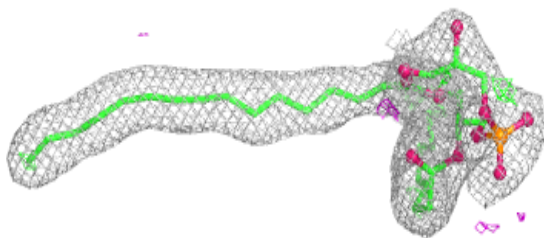
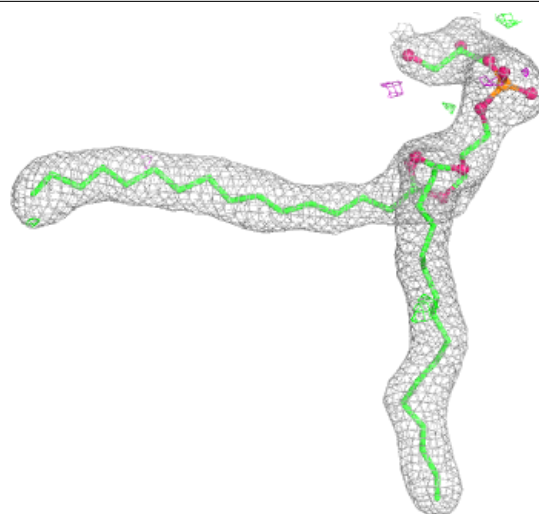
**Electron density around CLA b 610:**

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



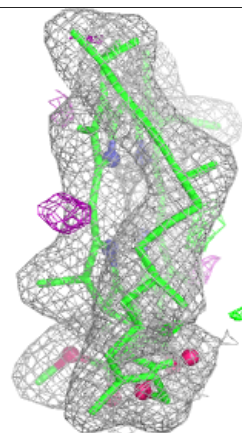
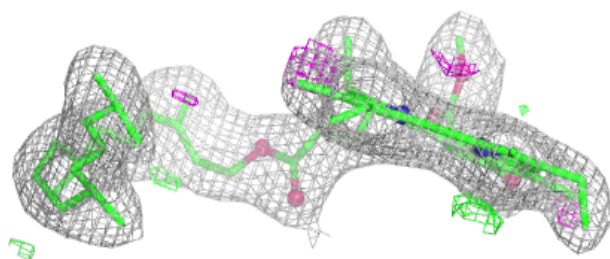
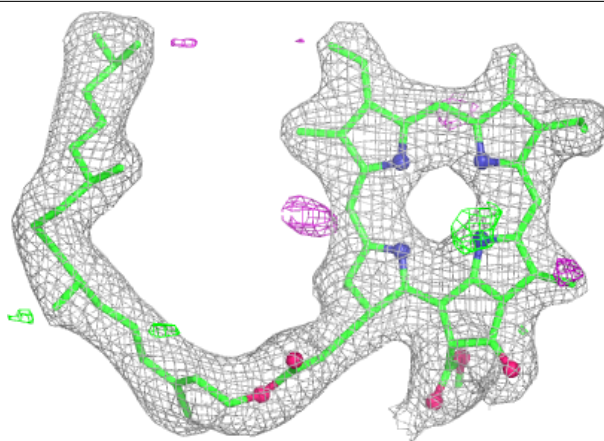
Electron density around LHG L 101:

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



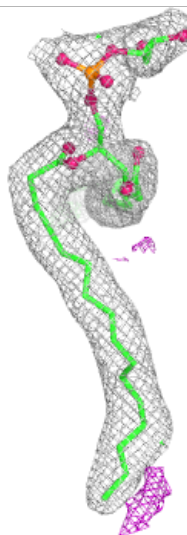
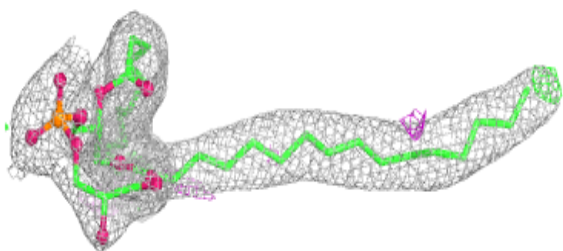
Electron density around PHO A 408:

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



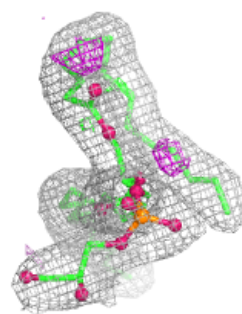
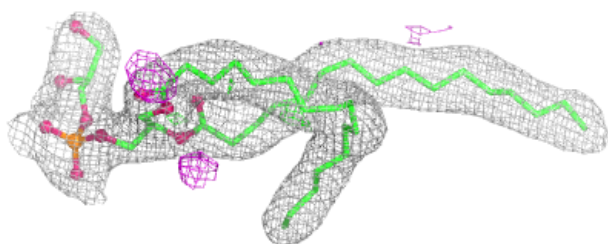
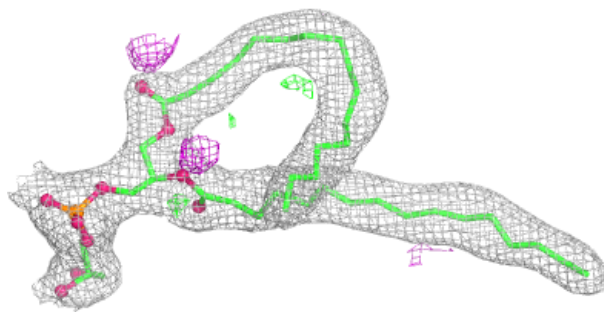
Electron density around LHG b 635:

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

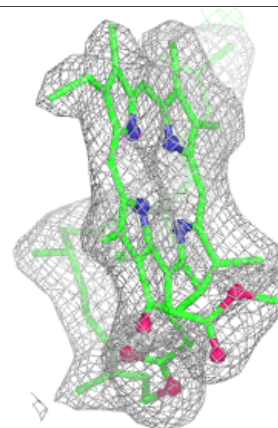
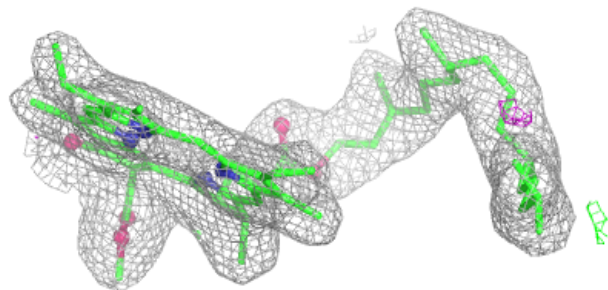
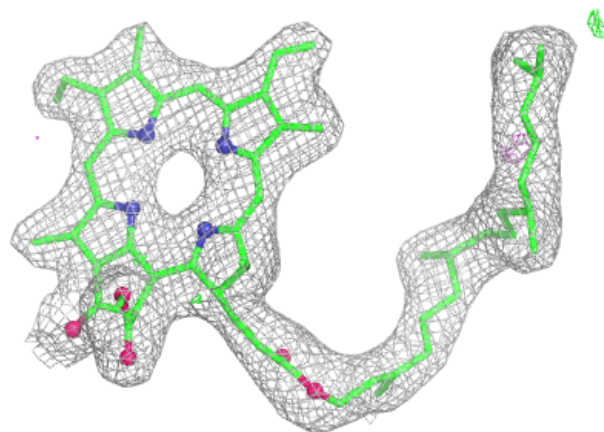


Electron density around LHG d 409:

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

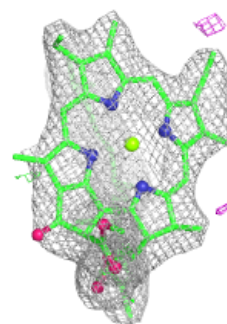
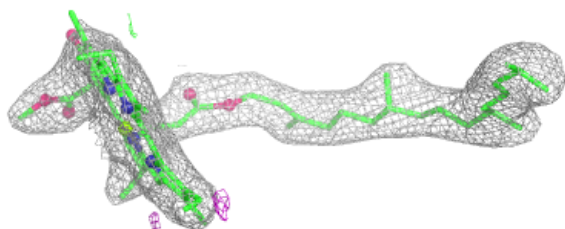
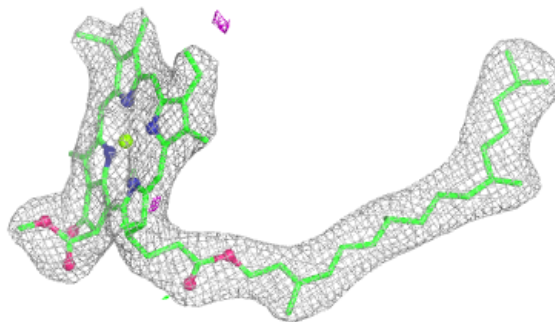
**Electron density around PHO D 401:**

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

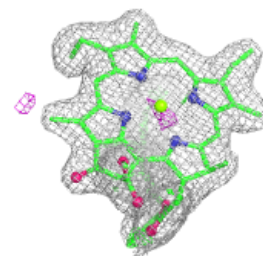
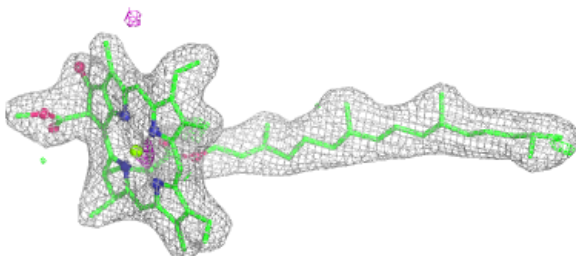
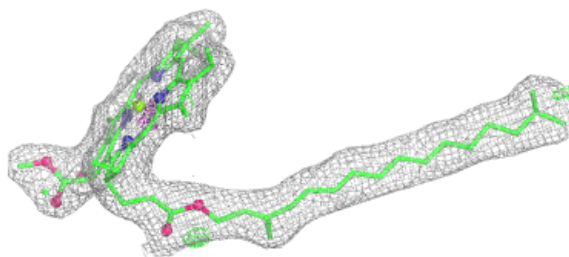


Electron density around CLA B 610:

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

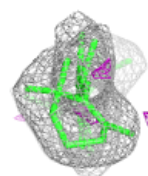
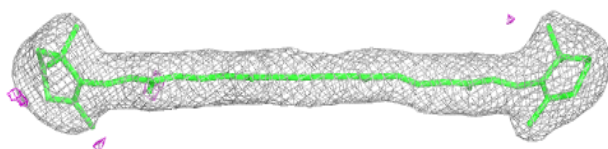
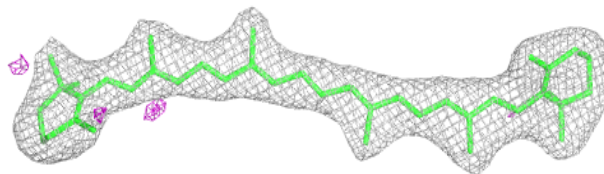
**Electron density around CLA b 612:**

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

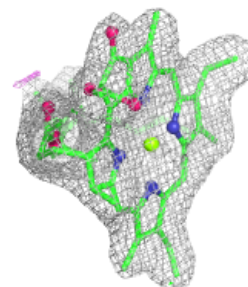
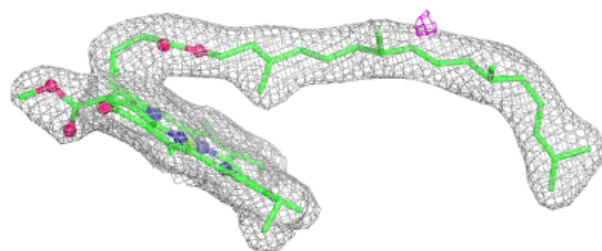
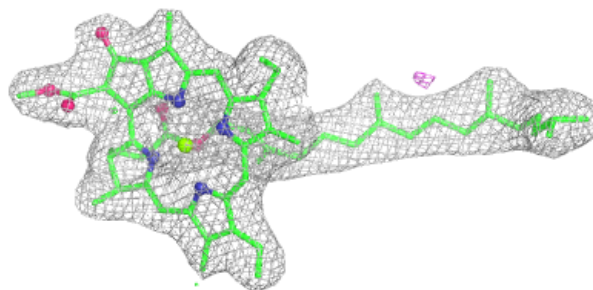


Electron density around BCR B 619:

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

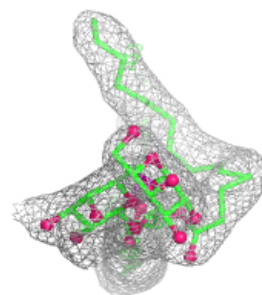
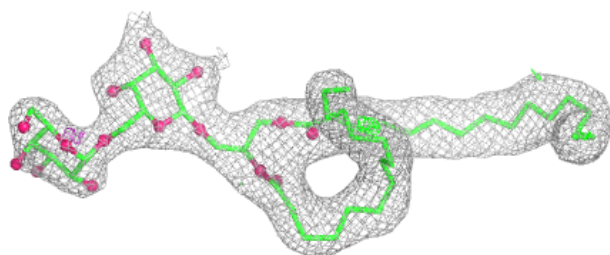
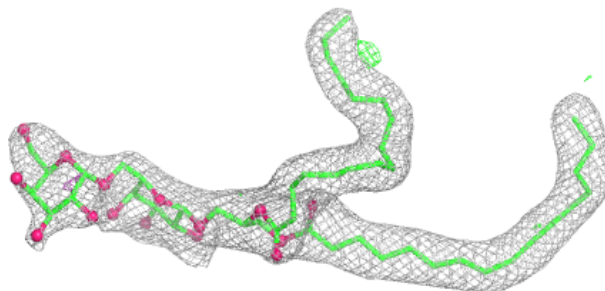
**Electron density around CLA b 613:**

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



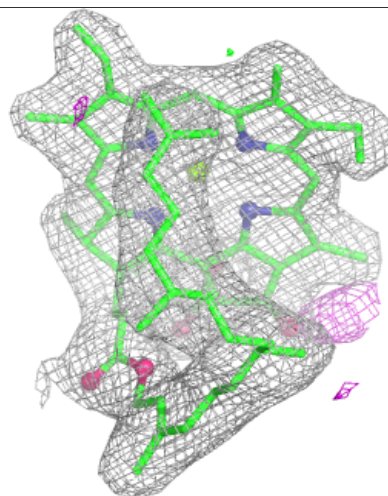
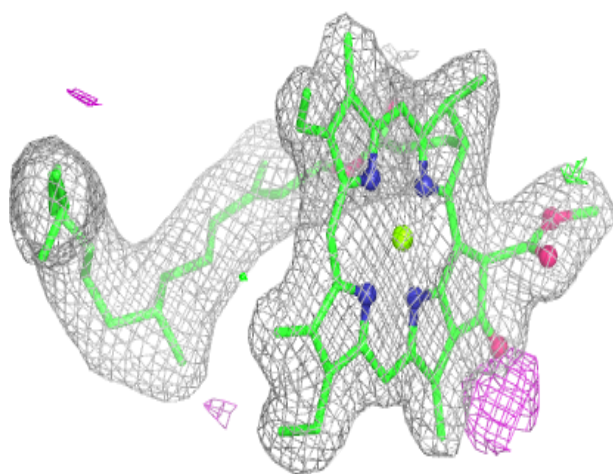
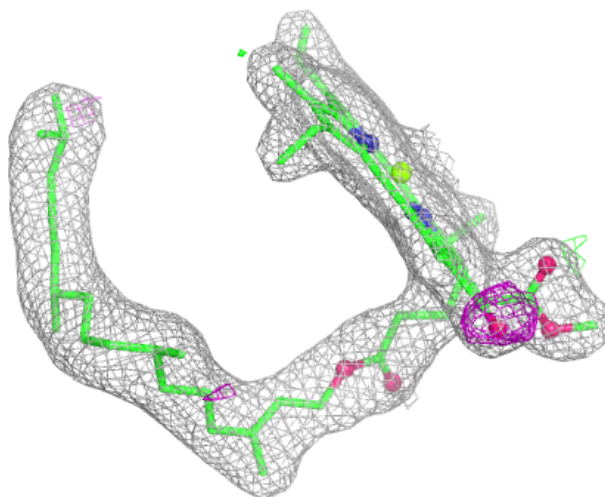
Electron density around DGD H 102:

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



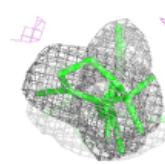
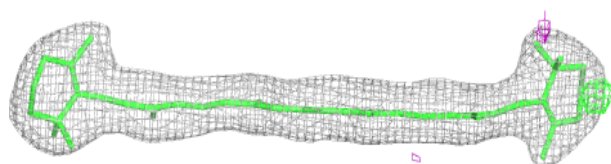
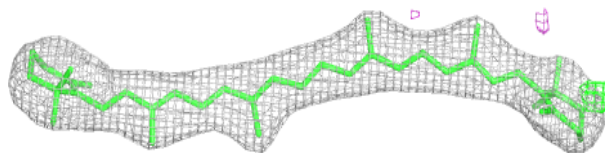
Electron density around CLA B 612:

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

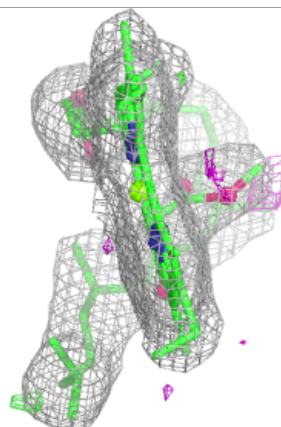
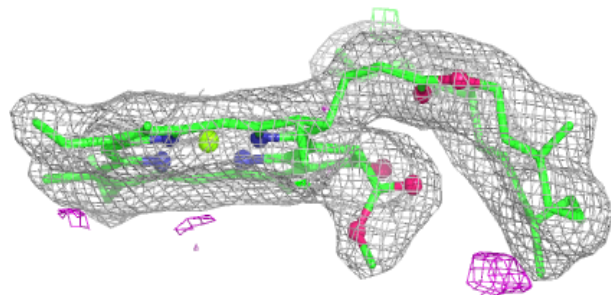
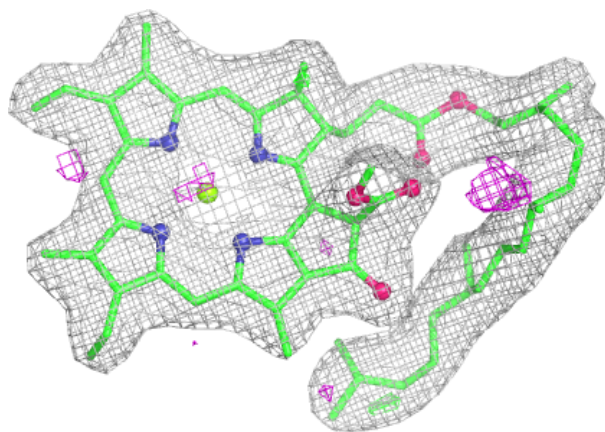


Electron density around BCR C 515:

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

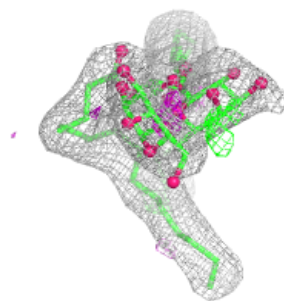
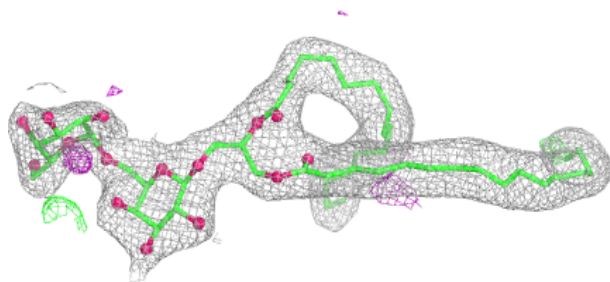
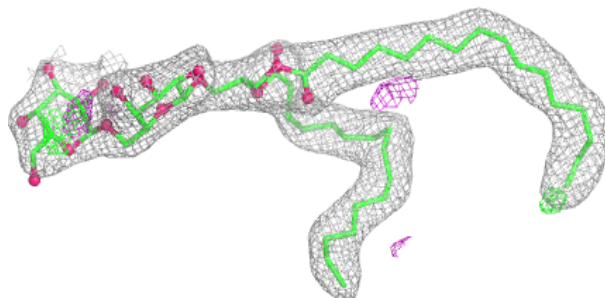
**Electron density around CLA b 615:**

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



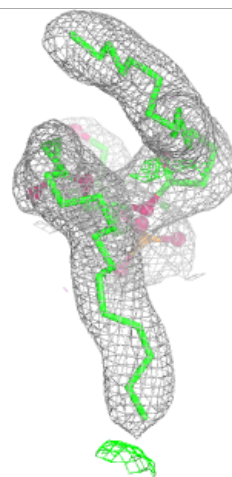
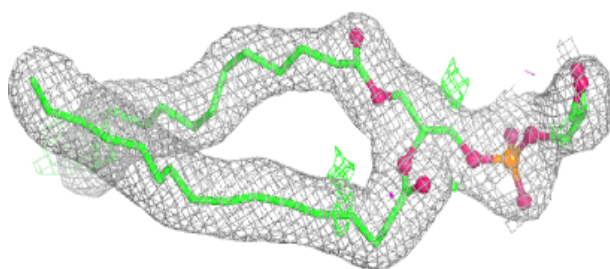
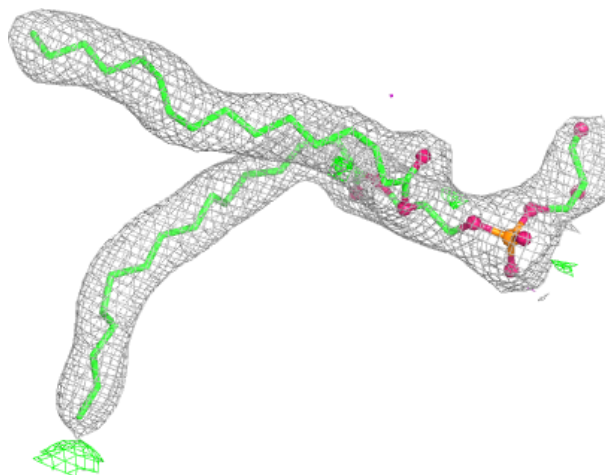
Electron density around DGD h 102:

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



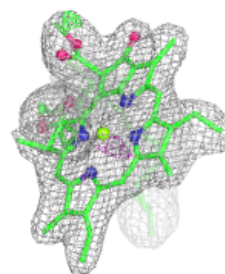
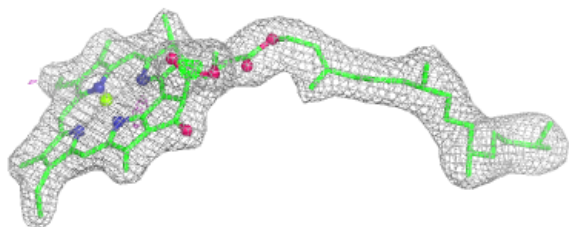
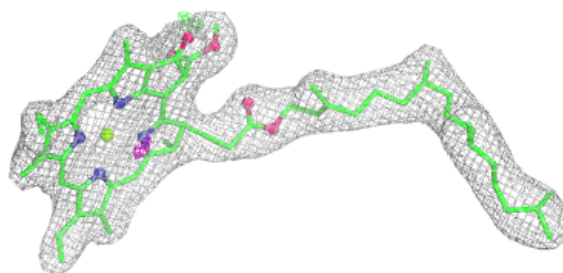
Electron density around LHG D 409:

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



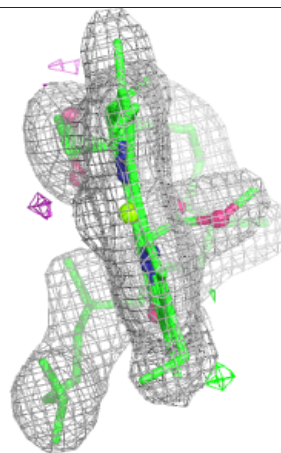
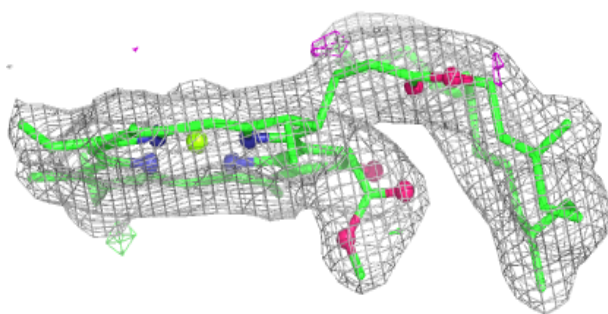
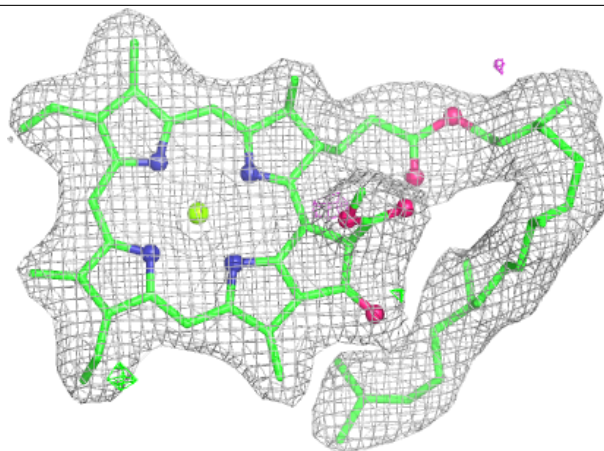
Electron density around CLA a 405:

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



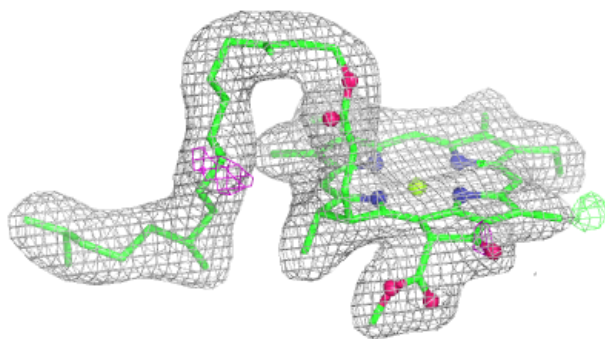
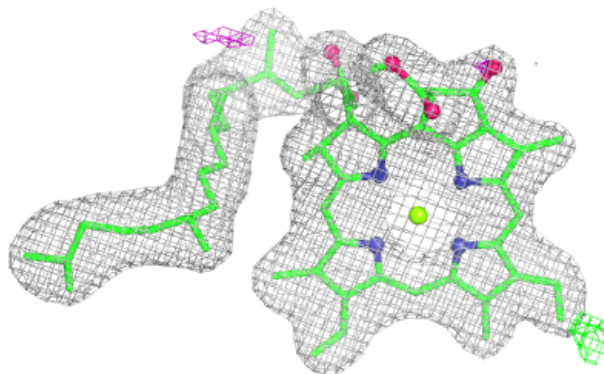
Electron density around CLA B 611:

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

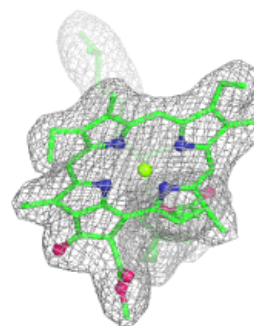
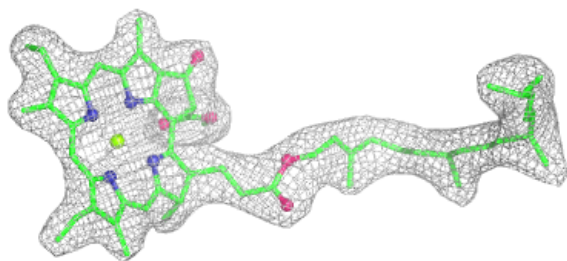
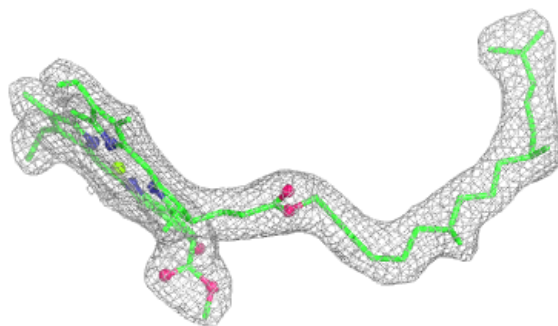


Electron density around CLA d 404:

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

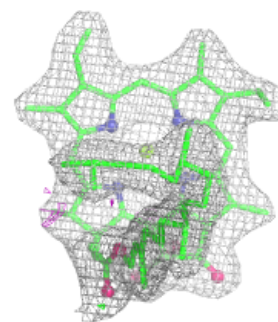
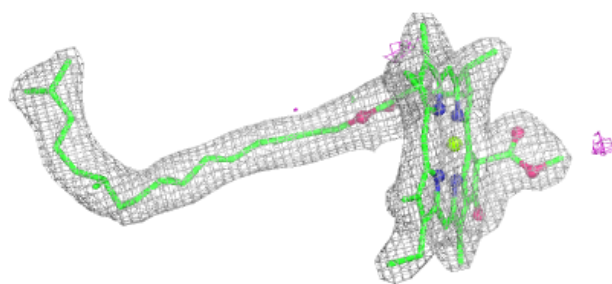
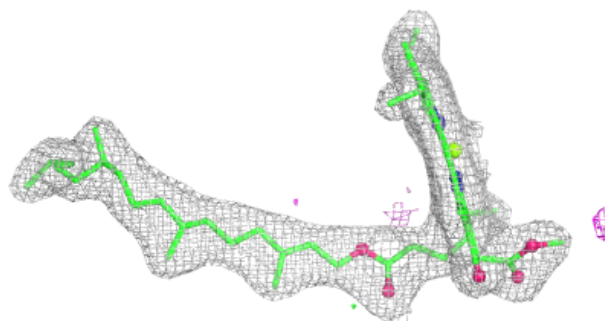
**Electron density around CLA d 405:**

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

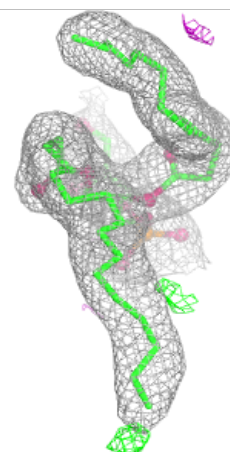
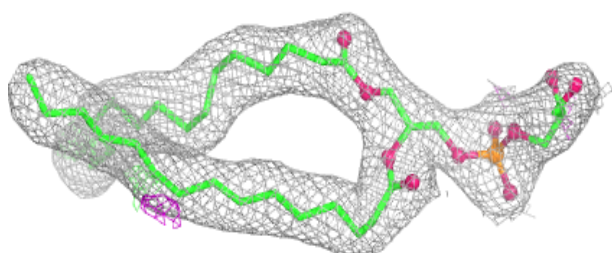
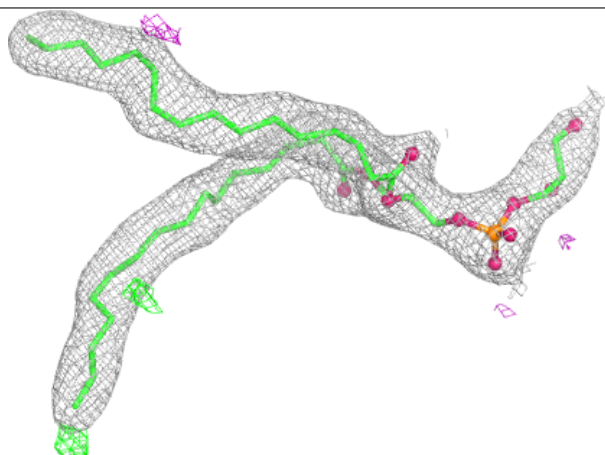


Electron density around CLA B 606:

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

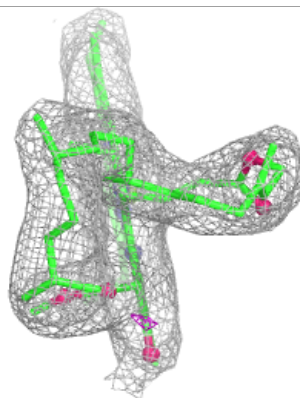
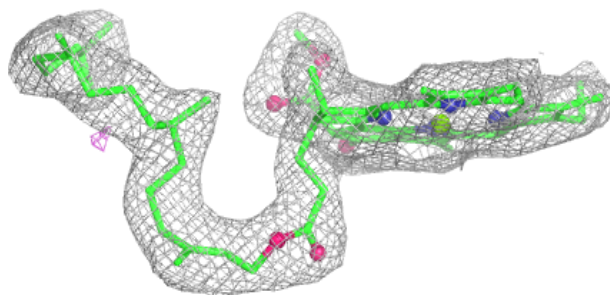
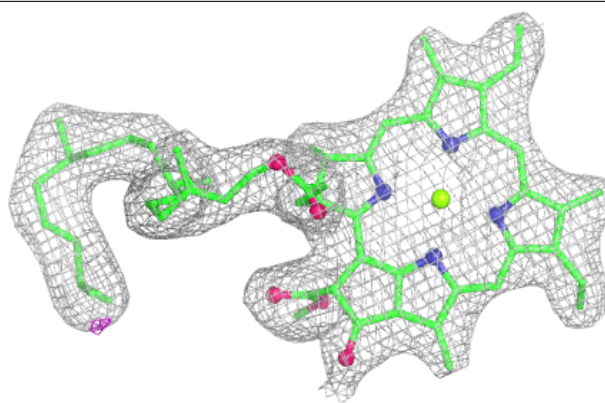
**Electron density around LHG d 410:**

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

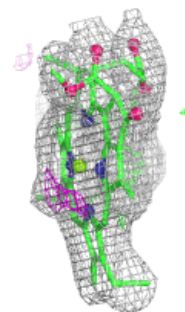
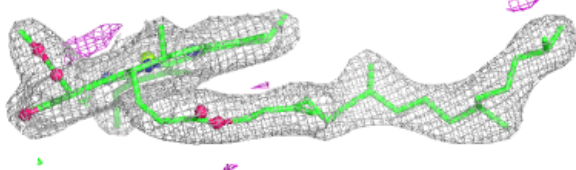
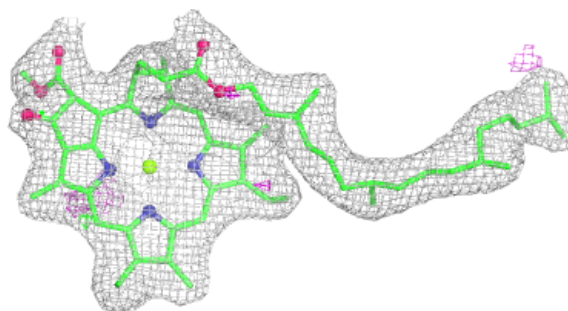


Electron density around CLA B 613:

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

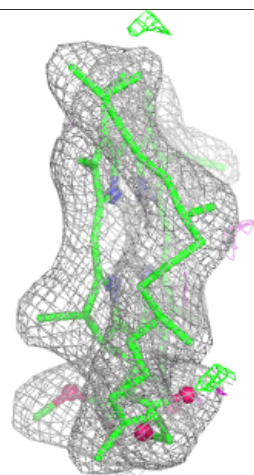
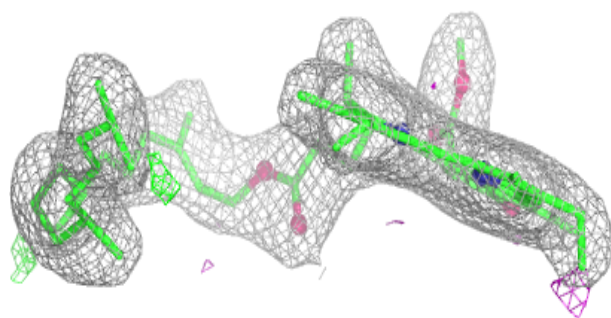
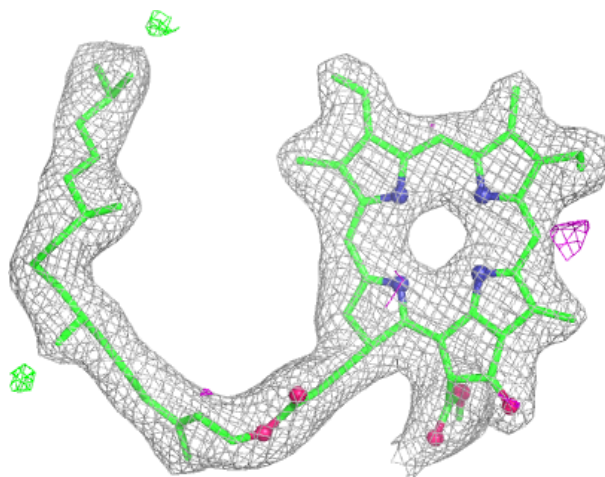
**Electron density around CLA B 604:**

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



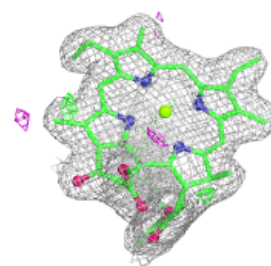
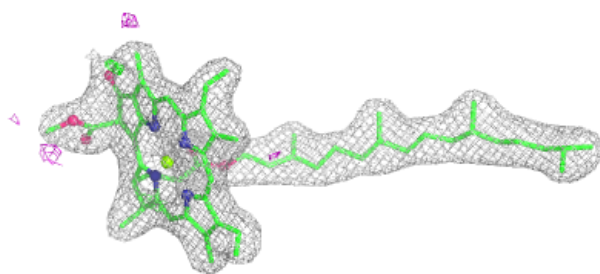
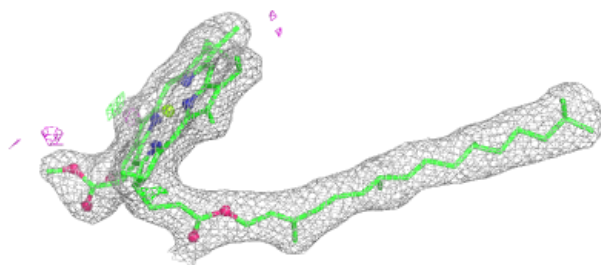
Electron density around PHO a 407:

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

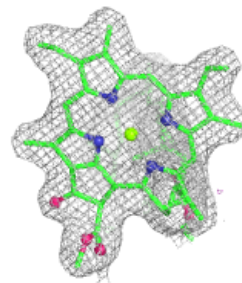
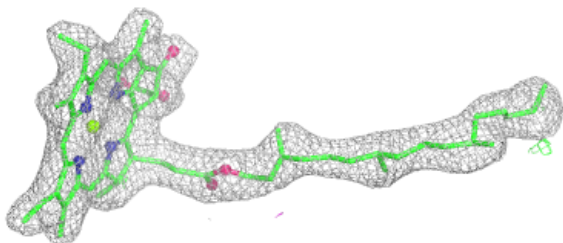
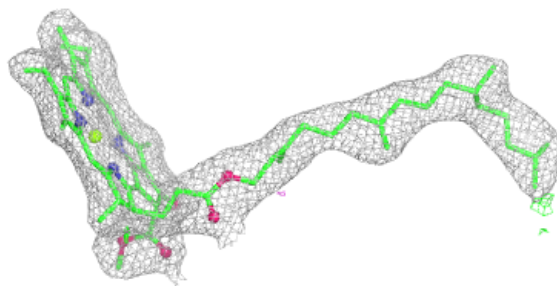


Electron density around CLA B 608:

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

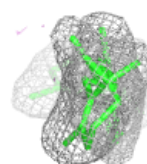
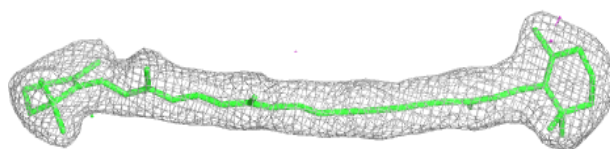
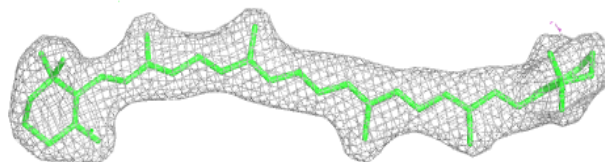
**Electron density around CLA b 609:**

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

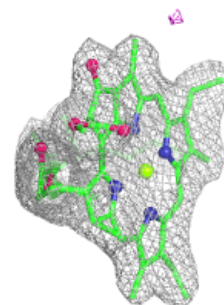
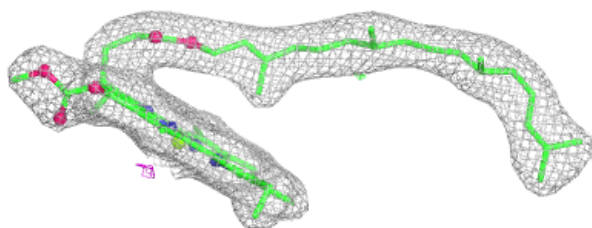
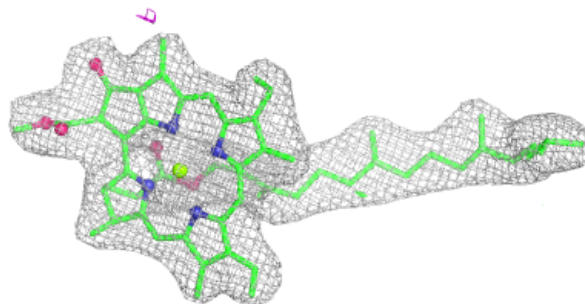


Electron density around BCR B 618:

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

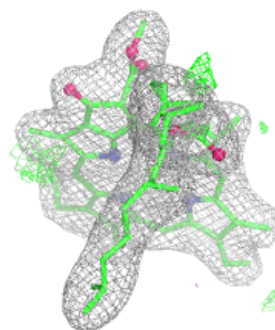
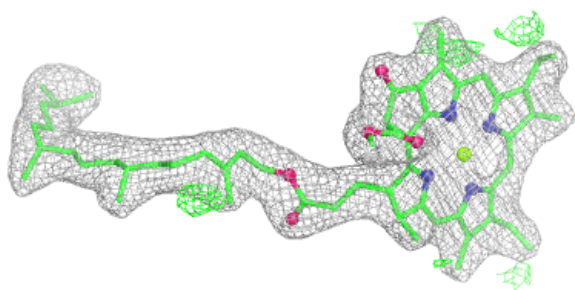
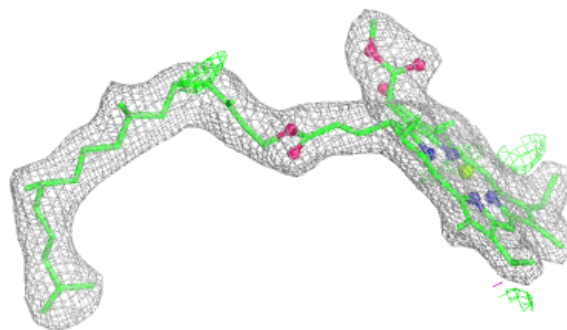
**Electron density around CLA B 609:**

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



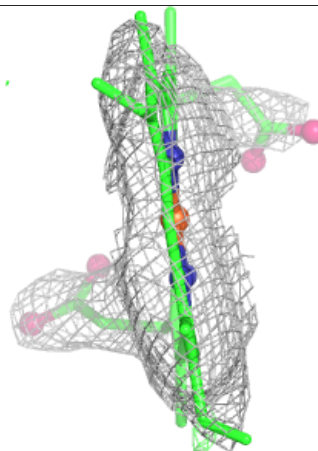
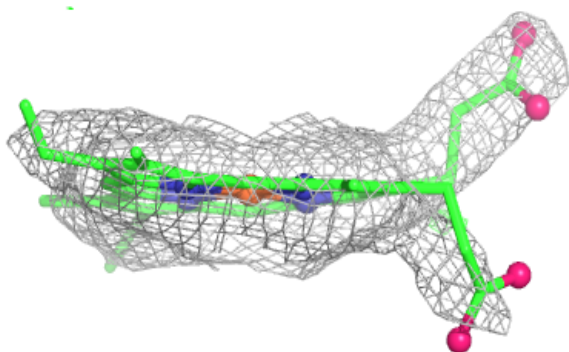
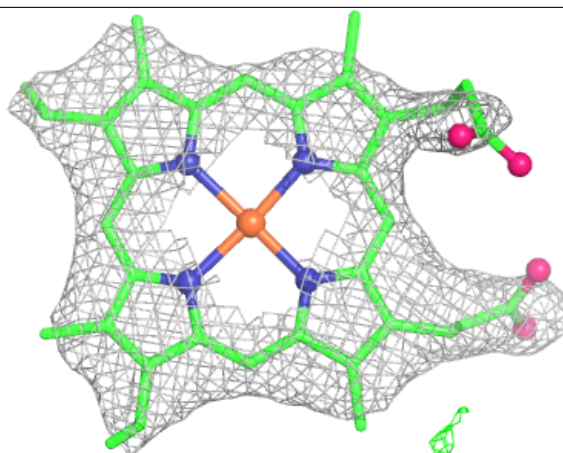
Electron density around CLA D 404:

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



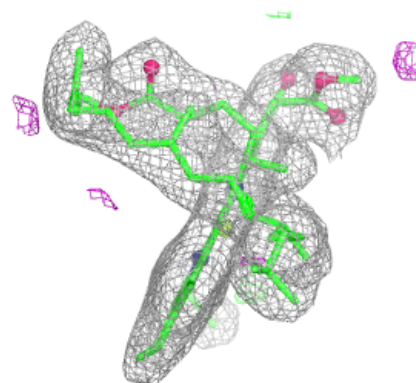
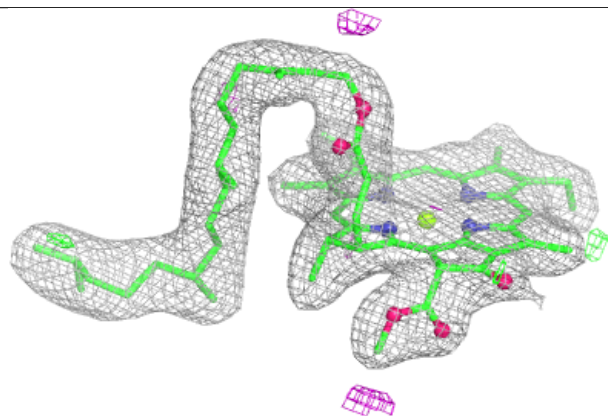
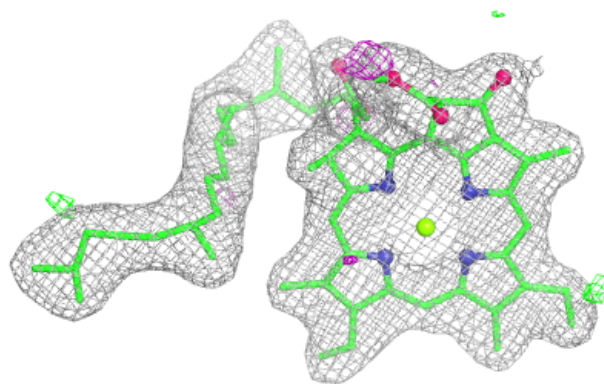
Electron density around HEM f 101:

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



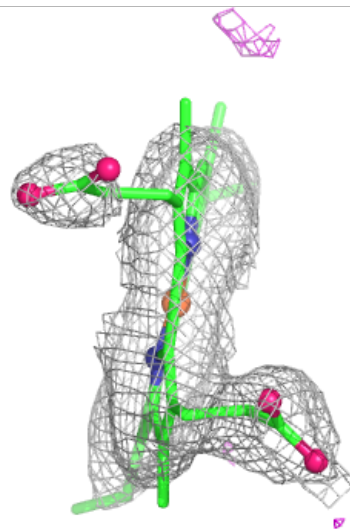
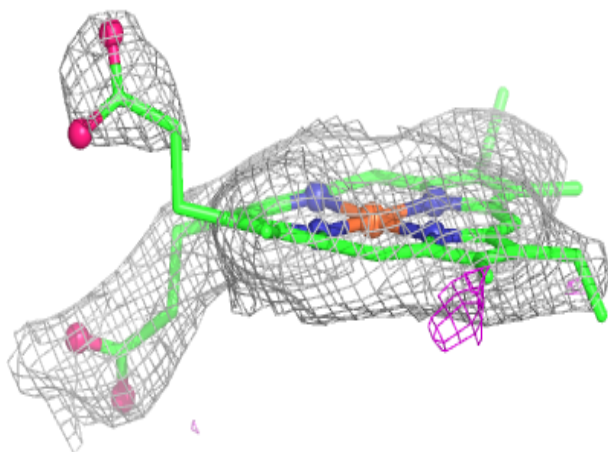
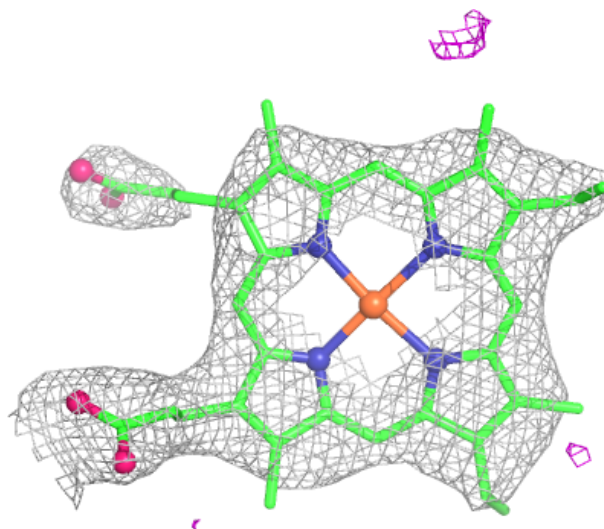
Electron density around CLA A 406:

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



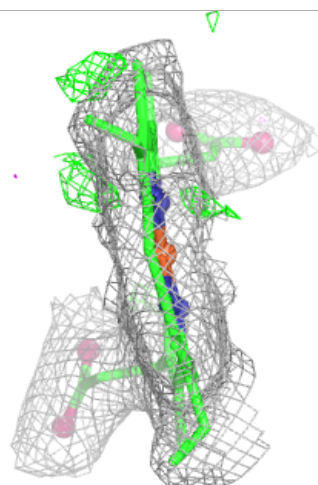
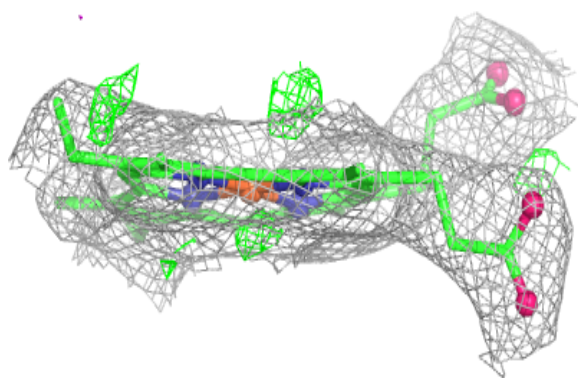
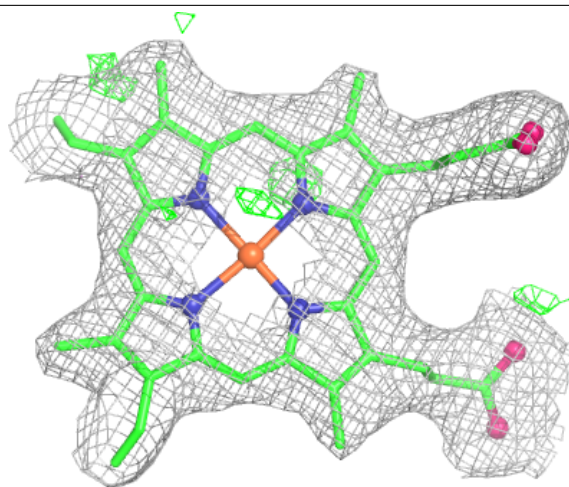
Electron density around HEM F 102:

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



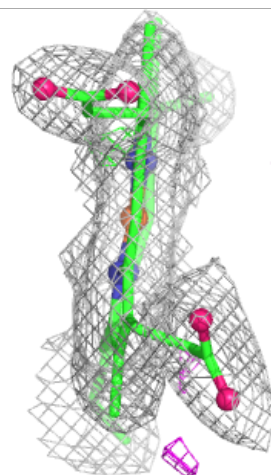
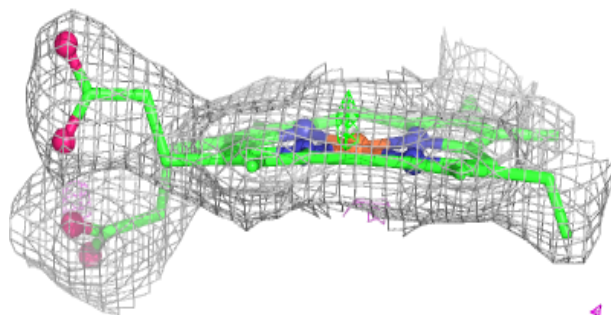
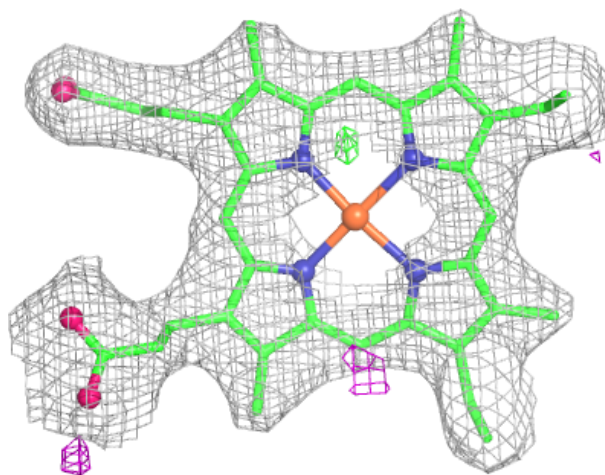
Electron density around HEC V 202:

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



Electron density around HEC v 202:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.