



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 03:28 PM JST

PDB ID : 6JLJ / pdb_00006jlj
Title : XFEL structure of cyanobacterial photosystem II (dark state, dataset1)
Authors : Suga, M.; Shen, J.R.
Deposited on : 2019-03-06
Resolution : 2.15 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>.

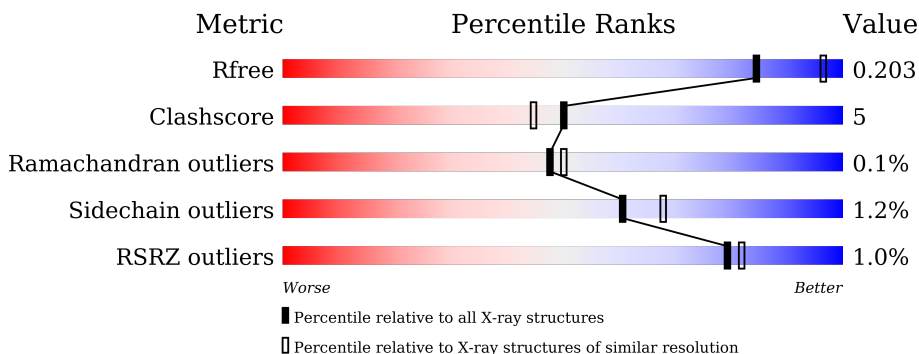
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

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X-RAY DIFFRACTION

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.



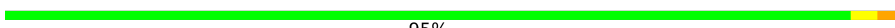
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	89%8%
1	a	344	87%10%
2	B	505	90%10%
2	b	505	90%9%
3	C	455	91%8%
3	c	455	93%7%

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
40	HEC	V	205	X	-	-	-
40	HEC	v	205	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	S	0	0	0
			287	191	46	50				
18	x	38	Total	C	N	O	S	0	0	0
			281	188	45	48				

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

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

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

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

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

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

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

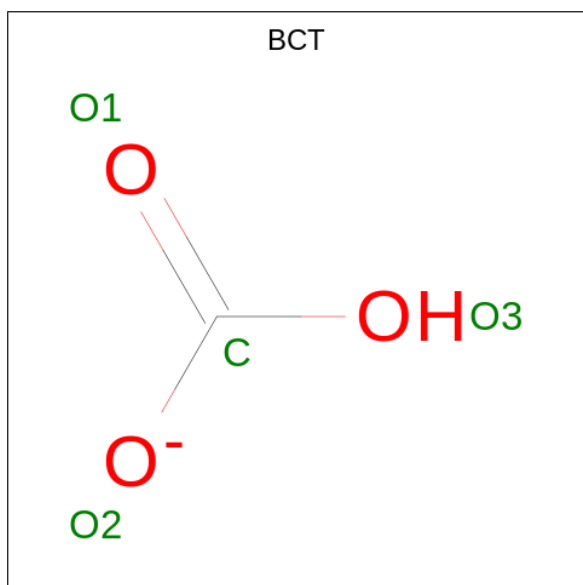
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		
22	U	1	Total	Cl	0	0
			1	1		

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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	a	1	Total	C	O	0	0
			4	1	3		

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



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

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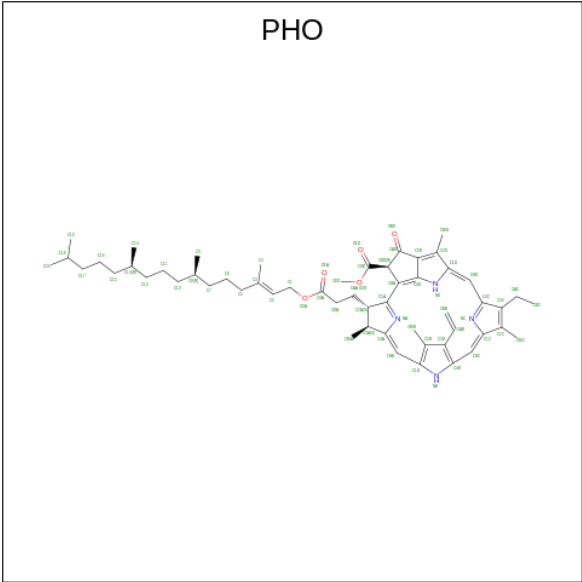
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N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

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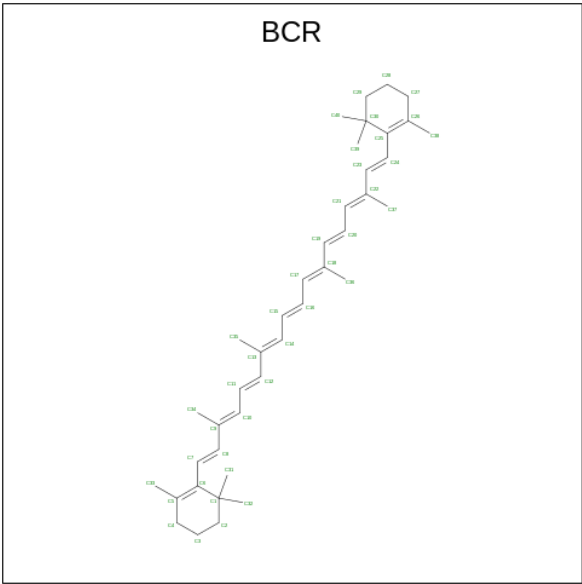
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N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

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



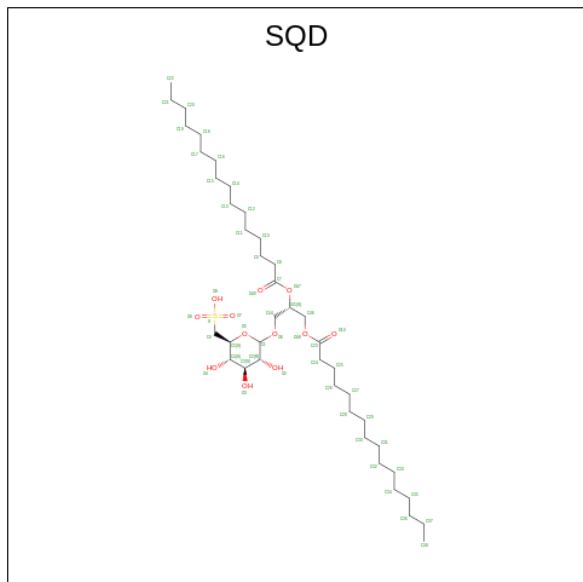
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	D	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	d	1	Total	C	N	O	0	0
			64	55	4	5		

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



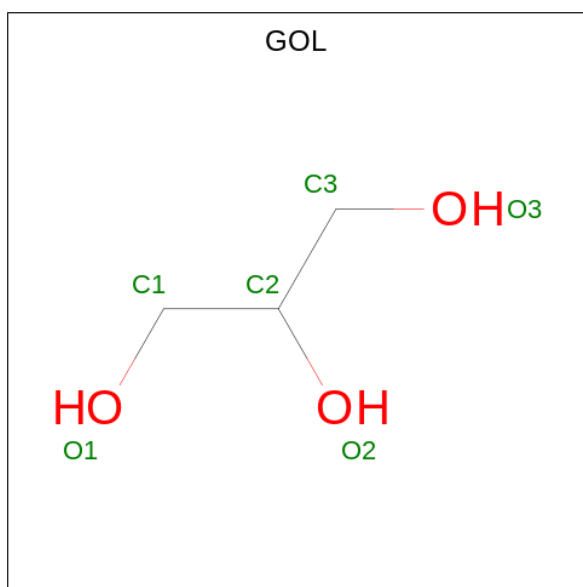
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Y	1	Total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



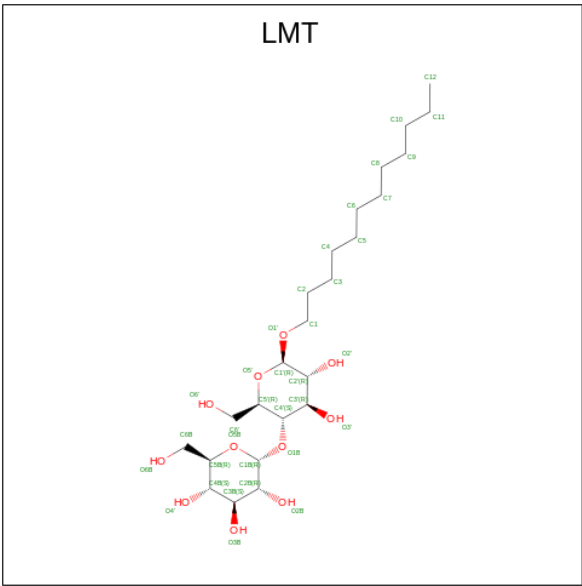
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			6	3	3		
28	A	1	Total	C	O	0	0
			6	3	3		
28	A	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	C	1	Total	C	O	0	0
			6	3	3		
28	C	1	Total	C	O	0	0
			6	3	3		
28	F	1	Total	C	O	0	0
			6	3	3		
28	O	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	T	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	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	f	1	Total	C	O	0	0
			6	3	3		
28	o	1	Total	C	O	0	0
			6	3	3		
28	t	1	Total	C	O	0	0
			6	3	3		
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).



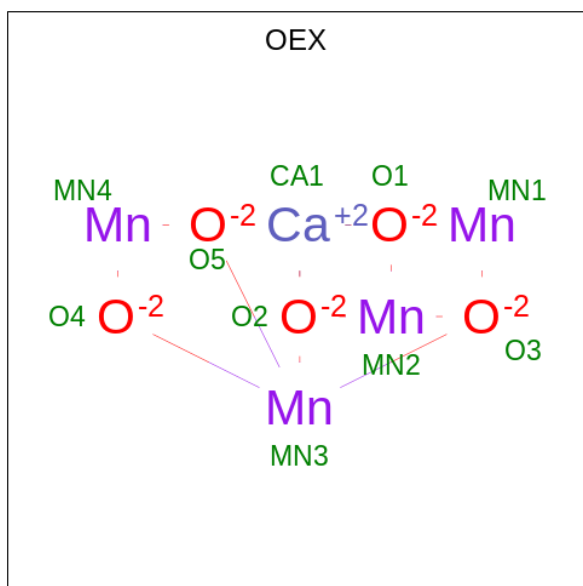
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			35	24	11		
29	B	1	Total	C	O	0	0
			35	24	11		
29	B	1	Total	C	O	0	0
			25	19	6		
29	C	1	Total	C	O	0	0
			35	24	11		
29	F	1	Total	C	O	0	0
			35	24	11		
29	M	1	Total	C	O	0	0
			35	24	11		
29	M	1	Total	C	O	0	0
			35	24	11		
29	M	1	Total	C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

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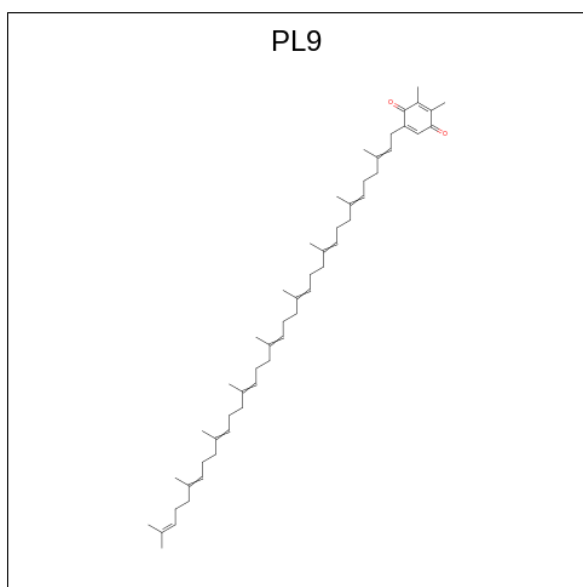
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	m	1	Total	C	O	0	0
			35	24	11		

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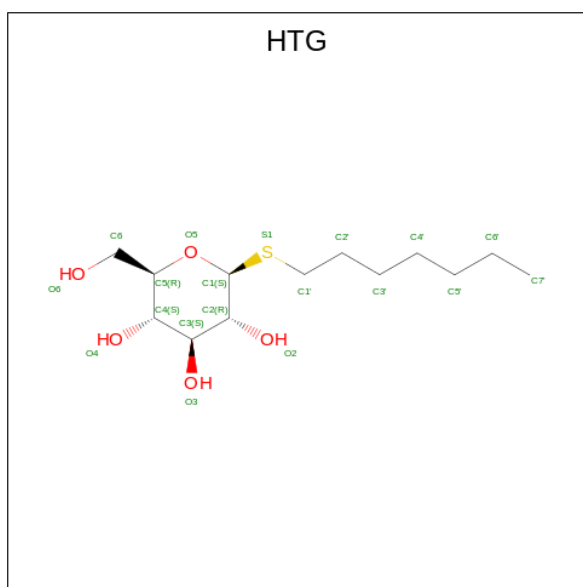
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	a	1	Total C O 30 25 5	0	0
32	b	1	Total C O 33 28 5	0	0
32	c	1	Total C O 32 27 5	0	0
32	d	3	Total C O 71 63 8	0	0
32	i	1	Total C O 40 35 5	0	0
32	j	1	Total C 10 10	0	0
32	m	1	Total C 10 10	0	0

- Molecule 33 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 34 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C₁₃H₂₆O₅S).

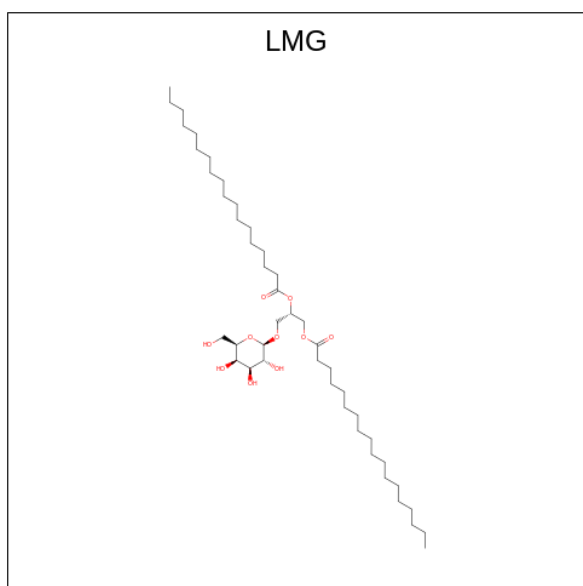
[illegible]

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

- Molecule 35 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



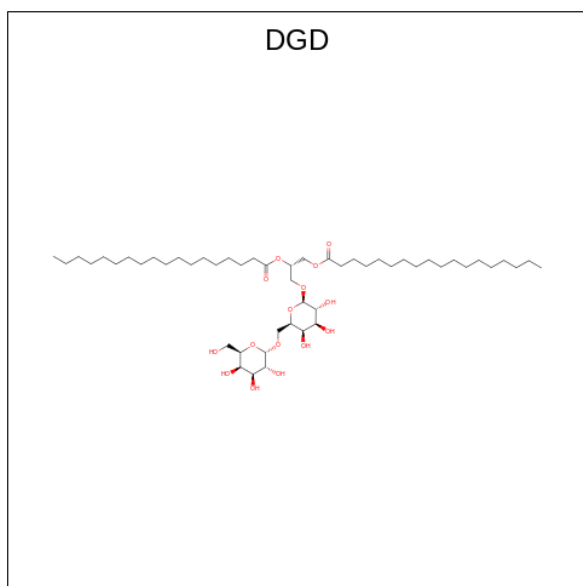
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	C	1	Total	C	O		0	0
			51	41	10			
35	C	1	Total	C	O		0	0
			51	41	10			
35	C	1	Total	C	O		0	0
			51	41	10			
35	J	1	Total	C	O		0	0
			51	41	10			
35	M	1	Total	C	O		0	0
			51	41	10			
35	Z	1	Total	C	O		0	0
			37	27	10			
35	a	1	Total	C	O		0	0
			51	41	10	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

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

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



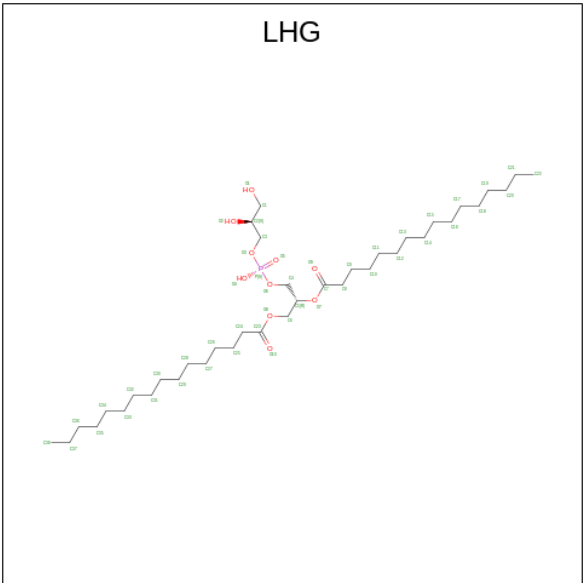
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	C	1	Total	C	O	0	0
			62	47	15		
36	C	1	Total	C	O	0	0
			62	47	15		
36	C	1	Total	C	O	0	0
			62	47	15		
36	D	1	Total	C	O	0	0
			52	42	10		
36	H	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	0
			62	47	15		

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

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



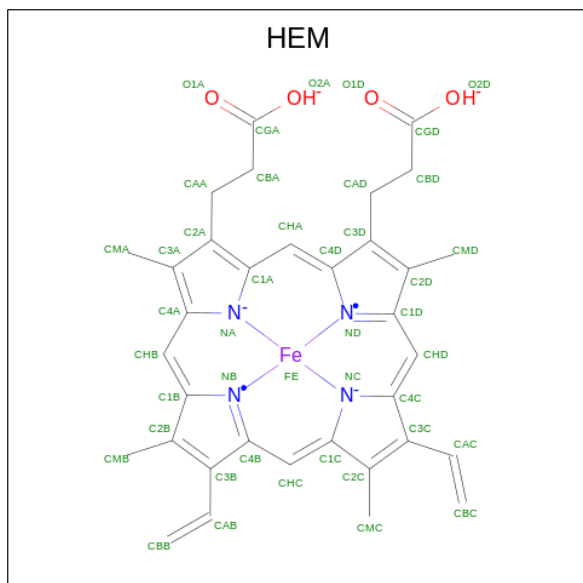
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	E	1	Total	C	O	P	0	0
			42	31	10	1		
37	L	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	e	1	Total	C	O	P	0	0
			42	31	10	1		
37	l	1	Total	C	O	P	0	0
			49	38	10	1		

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

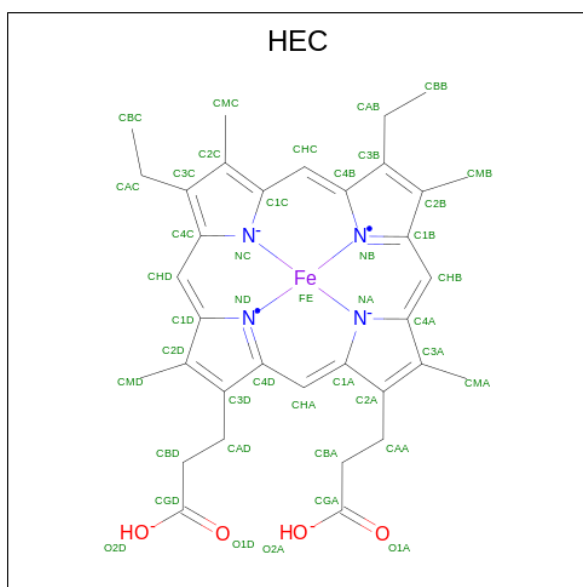


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
38	e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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

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

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



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	A	163	Total O 166 166	0	3
41	B	291	Total O 295 295	0	4
41	C	230	Total O 232 232	0	2
41	D	139	Total O 143 143	0	4
41	E	34	Total O 34 34	0	0
41	F	8	Total O 8 8	0	0
41	H	43	Total O 44 44	0	1
41	I	4	Total O 4 4	0	0
41	J	11	Total O 11 11	0	0
41	K	7	Total O 7 7	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	L	16	Total 17	O 17	0	1
41	M	24	Total 24	O 24	0	0
41	O	177	Total 179	O 179	0	2
41	T	16	Total 17	O 17	0	1
41	U	85	Total 85	O 85	0	0
41	V	115	Total 117	O 117	0	2
41	Y	4	Total 4	O 4	0	0
41	X	8	Total 8	O 8	0	0
41	Z	1	Total 1	O 1	0	0
41	a	158	Total 159	O 159	0	1
41	b	258	Total 261	O 261	0	3
41	c	201	Total 204	O 204	0	3
41	d	128	Total 131	O 131	0	3
41	e	20	Total 20	O 20	0	0
41	f	8	Total 8	O 8	0	0
41	h	42	Total 42	O 42	0	0
41	i	6	Total 6	O 6	0	0
41	j	6	Total 6	O 6	0	0
41	k	7	Total 7	O 7	0	0
41	l	8	Total 8	O 8	0	0
41	m	14	Total 14	O 14	0	0

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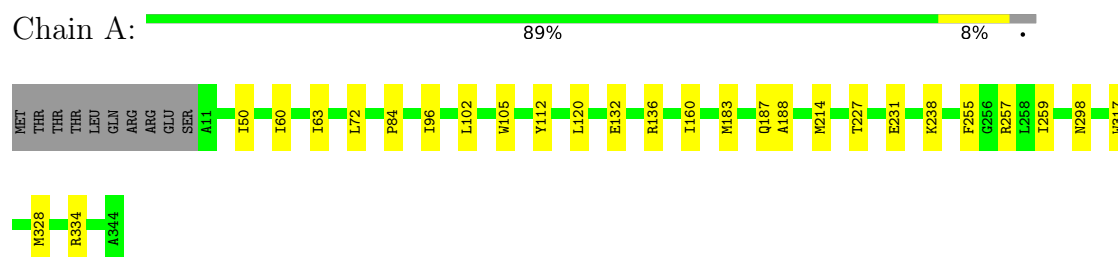
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	o	163	Total 163	O 163	0	0
41	t	9	Total 9	O 9	0	0
41	u	91	Total 91	O 91	0	0
41	v	82	Total 83	O 83	0	1
41	y	2	Total 2	O 2	0	0
41	x	6	Total 6	O 6	0	0

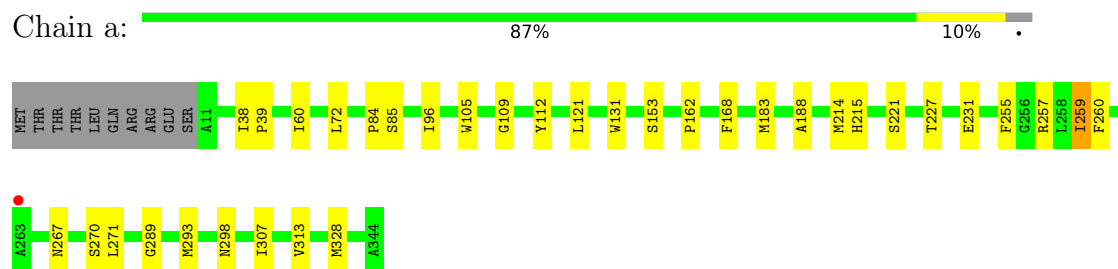
3 Residue-property plots [i](#)

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

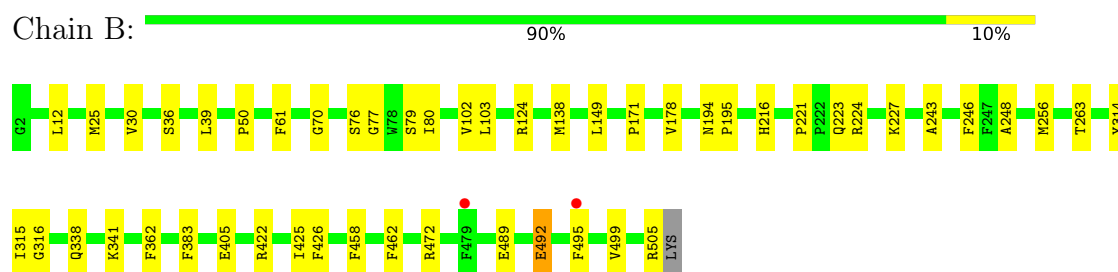
- Molecule 1: Photosystem II protein D1



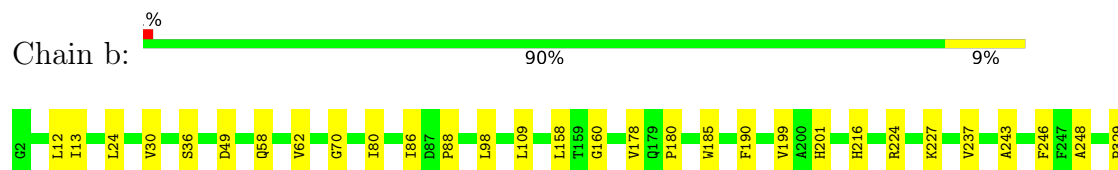
- Molecule 1: Photosystem II protein D1



- Molecule 2: Photosystem II CP47 reaction center protein



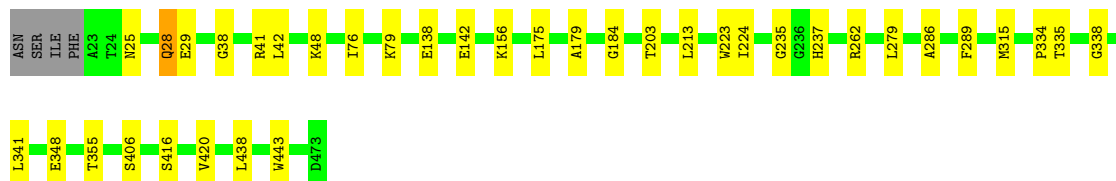
- Molecule 2: Photosystem II CP47 reaction center protein





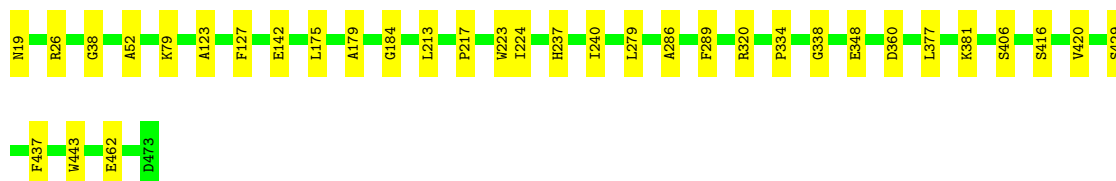
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 91% 8%



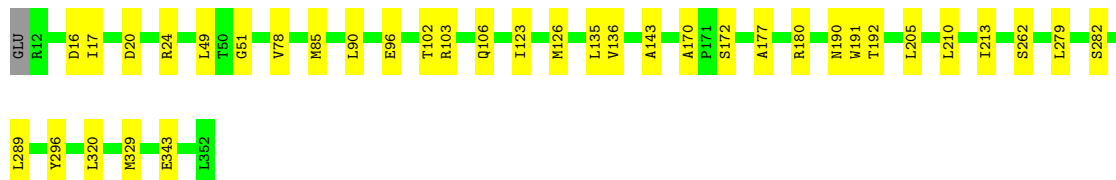
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 93% 7%



- Molecule 4: Photosystem II D2 protein

Chain D: 89% 11%



- Molecule 4: Photosystem II D2 protein

Chain d: 91% 8%

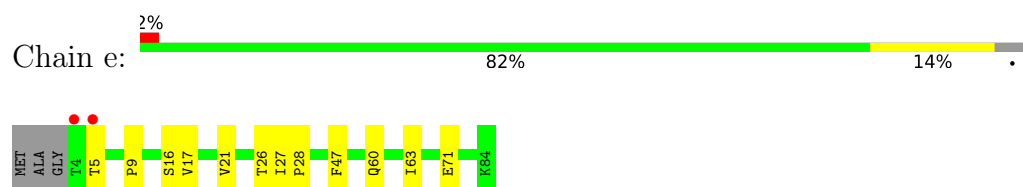


- Molecule 5: Cytochrome b559 subunit alpha

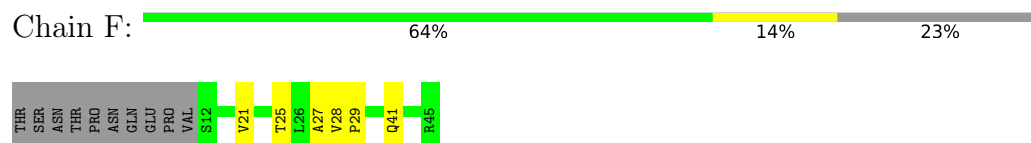
Chain E: 87% 8%



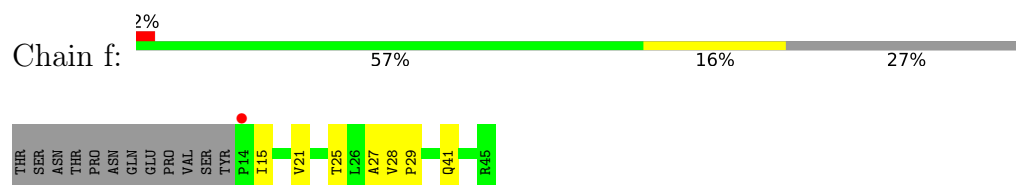
- Molecule 5: Cytochrome b559 subunit alpha



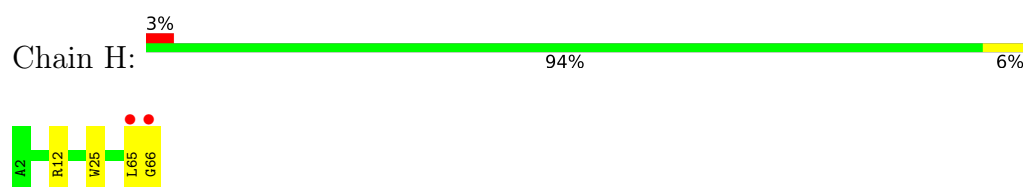
- Molecule 6: Cytochrome b559 subunit beta



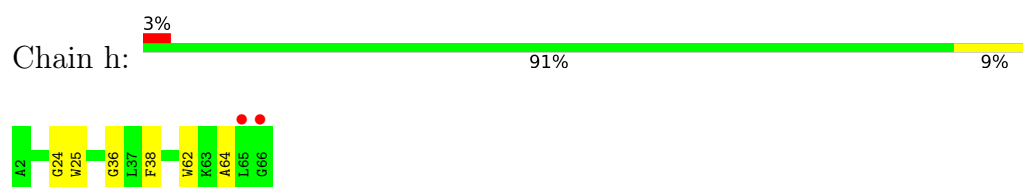
- Molecule 6: Cytochrome b559 subunit beta



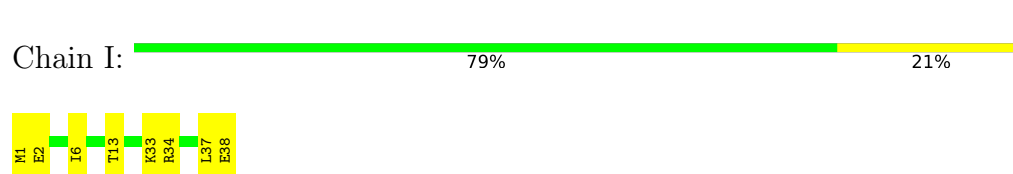
- Molecule 7: Photosystem II reaction center protein H



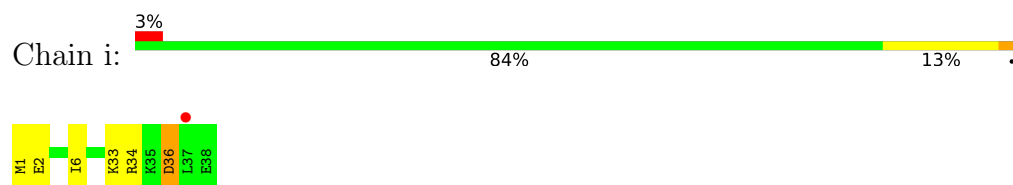
- Molecule 7: Photosystem II reaction center protein H



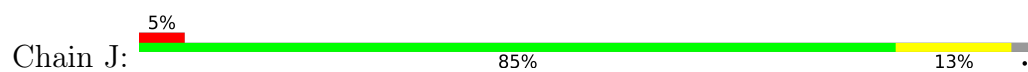
- Molecule 8: Photosystem II reaction center protein I



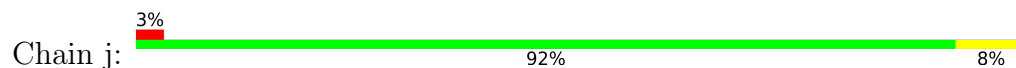
- Molecule 8: Photosystem II reaction center protein I



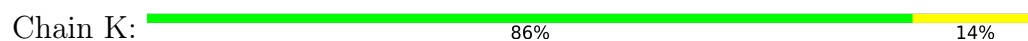
- Molecule 9: Photosystem II reaction center protein J



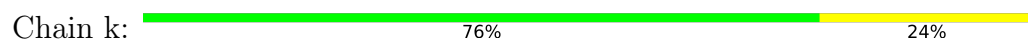
- Molecule 9: Photosystem II reaction center protein J



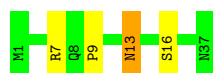
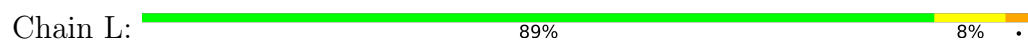
- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K



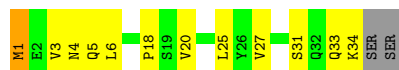
- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M



- Molecule 12: Photosystem II reaction center protein M

Chain m:  72% 22% 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  93% 6%



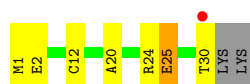
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  87% 11% 2%



- Molecule 14: Photosystem II reaction center protein T

Chain T:  72% 19% 3%



- Molecule 14: Photosystem II reaction center protein T

Chain t:  81% 12% 3%



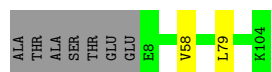
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  86% 8% 7%

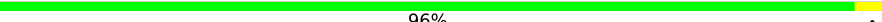


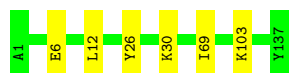
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  91% 7%



- Molecule 16: Cytochrome c-550

Chain V:  96% .



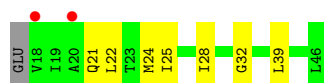
- Molecule 16: Cytochrome c-550

Chain v:  93% 7% .



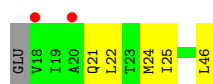
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:  73% 23% .



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:  80% 17% .



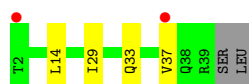
- Molecule 18: Photosystem II reaction center protein X

Chain X:  88% 10% .



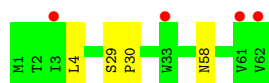
- Molecule 18: Photosystem II reaction center protein X

Chain x:  85% 10% 5% .

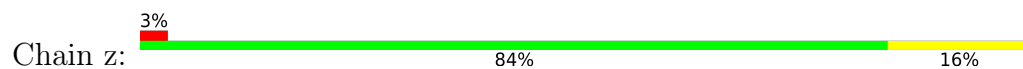


- Molecule 19: Photosystem II reaction center protein Z

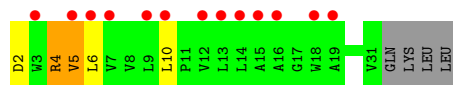
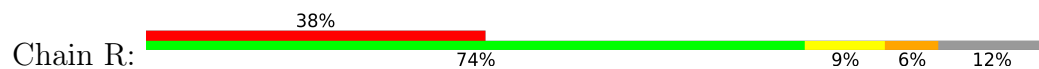
Chain Z:  94% 6% .



- 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	121.97Å 228.72Å 286.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.15 19.99 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.15) 99.8 (19.99-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.152 , 0.198 0.159 , 0.203	Depositor DCC
R_{free} test set	26827 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	35.0	Xtriage
Anisotropy	0.684	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 75.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.97% 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: BCR, DGD, LMG, FME, PHO, SQD, BCT, HTG, FE2, LMT, HEM, LHG, CL, CA, GOL, PL9, UNL, OEX, CLA, MG, HEC

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	0.60	0/2728	0.86	0/3719
1	a	0.61	0/2748	0.84	0/3746
2	B	0.54	0/4191	0.81	1/5709 (0.0%)
2	b	0.53	0/4198	0.80	1/5720 (0.0%)
3	C	0.49	0/3626	0.80	2/4936 (0.0%)
3	c	0.49	0/3676	0.79	0/5004
4	D	0.61	0/2818	0.83	3/3840 (0.1%)
4	d	0.57	0/2818	0.81	0/3840
5	E	0.45	0/693	0.80	1/944 (0.1%)
5	e	0.47	0/695	0.80	0/948
6	F	0.57	0/284	0.79	0/387
6	f	0.53	0/265	0.78	0/360
7	H	0.47	0/535	0.86	0/728
7	h	0.41	0/524	0.84	0/713
8	I	0.43	0/311	0.77	0/419
8	i	0.46	0/311	0.70	0/419
9	J	0.44	0/278	0.77	0/376
9	j	0.42	0/286	0.77	0/386
10	K	0.44	0/303	0.87	0/416
10	k	0.52	0/303	0.78	0/416
11	L	0.55	0/319	0.70	0/433
11	l	0.51	0/319	0.70	0/433
12	M	0.63	0/270	0.87	0/368
12	m	0.62	0/262	0.83	0/357
13	O	0.45	0/1958	0.77	0/2654
13	o	0.46	0/1937	0.81	2/2625 (0.1%)
14	T	0.60	0/266	0.72	0/362
14	t	0.60	0/266	0.71	0/362
15	U	0.48	0/785	0.75	0/1064
15	u	0.49	0/785	0.73	0/1064
16	V	0.51	0/1096	0.79	0/1487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.47	0/1085	0.79	1/1473 (0.1%)
17	Y	0.53	0/216	0.87	0/289
17	y	0.43	0/216	0.78	0/289
18	X	0.40	0/290	0.78	0/392
18	x	0.43	0/284	0.76	0/384
19	Z	0.41	0/490	0.77	0/669
19	z	0.38	0/490	0.83	0/669
20	R	0.36	0/245	0.67	0/338
All	All	0.52	0/43170	0.80	11/58738 (0.0%)

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	170	ALA	CA-C-N	-6.04	113.72	119.76
4	D	170	ALA	C-N-CA	-6.04	113.72	119.76
4	D	262	SER	N-CA-C	-5.93	107.03	114.56
3	C	76	ILE	CA-C-N	5.81	125.67	119.28
3	C	76	ILE	C-N-CA	5.81	125.67	119.28

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	21	0
1	a	2645	0	2567	25	0
2	B	4021	0	3898	38	0
2	b	4022	0	3908	41	0
3	C	3501	0	3428	23	0
3	c	3544	0	3480	26	0
4	D	2720	0	2626	23	0
4	d	2720	0	2626	24	0
5	E	668	0	658	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	e	670	0	664	8	0
6	F	275	0	282	5	0
6	f	257	0	269	4	0
7	H	519	0	545	6	0
7	h	511	0	532	8	0
8	I	314	0	328	5	0
8	i	314	0	328	3	0
9	J	272	0	279	4	0
9	j	280	0	291	2	0
10	K	293	0	305	3	0
10	k	293	0	305	7	0
11	L	309	0	327	5	0
11	l	309	0	327	3	0
12	M	274	0	299	12	0
12	m	269	0	288	8	0
13	O	1903	0	1886	9	0
13	o	1891	0	1870	17	0
14	T	264	0	267	5	0
14	t	264	0	267	2	0
15	U	774	0	773	4	1
15	u	774	0	773	1	0
16	V	1072	0	1086	5	0
16	v	1064	0	1073	8	0
17	Y	215	0	246	5	0
17	y	215	0	246	4	0
18	X	287	0	317	3	0
18	x	281	0	312	3	0
19	Z	479	0	516	3	0
19	z	479	0	516	7	0
20	R	239	0	262	3	0
21	A	1	0	0	0	0
21	a	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	1	0
23	A	4	0	0	0	0
23	a	4	0	0	0	0
24	A	260	0	288	11	0
24	B	1040	0	1152	42	0
24	C	845	0	936	34	0
24	D	130	0	144	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	195	0	216	7	0
24	b	1040	0	1152	29	0
24	c	845	0	936	34	0
24	d	195	0	216	8	0
25	A	64	0	74	3	0
25	D	64	0	74	1	0
25	a	64	0	74	2	0
25	d	64	0	74	2	0
26	A	40	0	56	2	0
26	B	120	0	168	8	0
26	C	80	0	112	11	0
26	D	40	0	56	1	0
26	H	40	0	56	4	0
26	K	40	0	56	3	0
26	T	40	0	56	6	0
26	Y	40	0	56	3	0
26	a	40	0	56	1	0
26	b	120	0	168	8	0
26	c	80	0	112	5	0
26	d	40	0	56	3	0
26	h	40	0	56	4	0
26	k	40	0	56	1	0
26	t	40	0	56	6	0
26	y	40	0	56	2	0
27	A	108	0	156	7	0
27	B	54	0	78	1	0
27	F	43	0	53	1	0
27	L	54	0	78	2	0
27	a	108	0	156	4	0
27	f	43	0	53	2	1
28	A	18	0	24	1	0
28	B	42	0	56	1	0
28	C	12	0	16	0	0
28	F	6	0	8	0	0
28	O	6	0	8	0	0
28	T	12	0	16	3	0
28	V	24	0	32	0	0
28	a	12	0	16	1	0
28	b	30	0	40	1	0
28	c	12	0	16	2	0
28	f	6	0	7	1	0
28	o	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	t	6	0	8	0	0
28	v	18	0	24	1	0
29	A	35	0	46	2	0
29	B	60	0	81	1	0
29	C	35	0	46	2	0
29	F	35	0	46	0	0
29	M	105	0	138	4	0
29	T	25	0	35	0	0
29	a	70	0	92	4	0
29	b	25	0	35	3	0
29	f	35	0	46	1	0
29	m	35	0	46	2	0
30	A	10	0	0	0	0
30	a	10	0	0	0	0
31	A	55	0	80	5	0
31	D	55	0	80	2	0
31	a	55	0	80	6	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	71	0	0	0	0
32	i	40	0	0	0	0
32	j	10	0	0	0	0
32	m	10	0	0	0	0
33	B	1	0	0	0	0
33	C	1	0	0	0	0
33	F	1	0	0	0	0
33	O	1	0	0	0	0
33	b	1	0	0	0	0
33	c	2	0	0	0	0
33	f	1	0	0	0	0
33	o	1	0	0	0	0
34	B	95	0	130	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	C	38	0	52	0	0
34	D	16	0	17	2	0
34	V	19	0	26	2	0
34	b	95	0	130	3	0
34	c	38	0	52	0	0
34	d	16	0	17	3	0
35	C	153	0	216	8	0
35	J	51	0	72	1	0
35	M	51	0	72	2	0
35	Z	37	0	44	1	0
35	a	51	0	72	1	0
35	b	51	0	72	3	0
35	c	102	0	144	4	0
35	j	51	0	72	2	0
35	z	39	0	48	4	0
36	C	186	0	246	5	0
36	D	52	0	71	2	0
36	H	62	0	82	0	0
36	c	186	0	246	4	0
36	e	62	0	82	9	0
36	h	62	0	82	0	0
37	D	147	0	222	9	0
37	E	42	0	57	2	0
37	L	49	0	74	2	0
37	d	147	0	222	9	0
37	e	42	0	57	4	0
37	l	49	0	74	2	0
38	E	43	0	30	3	0
38	e	43	0	30	2	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	166	0	0	1	0
41	B	295	0	0	2	0
41	C	232	0	0	2	0
41	D	143	0	0	1	0
41	E	34	0	0	0	0
41	F	8	0	0	0	0
41	H	44	0	0	0	0
41	I	4	0	0	1	0
41	J	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	K	7	0	0	0	0
41	L	17	0	0	0	0
41	M	24	0	0	0	0
41	O	179	0	0	0	0
41	T	17	0	0	1	0
41	U	85	0	0	2	0
41	V	117	0	0	3	0
41	X	8	0	0	0	0
41	Y	4	0	0	0	0
41	Z	1	0	0	1	0
41	a	159	0	0	2	0
41	b	261	0	0	2	0
41	c	204	0	0	2	0
41	d	131	0	0	1	0
41	e	20	0	0	0	0
41	f	8	0	0	0	0
41	h	42	0	0	0	0
41	i	6	0	0	0	0
41	j	6	0	0	0	0
41	k	7	0	0	1	0
41	l	8	0	0	0	0
41	m	14	0	0	0	0
41	o	163	0	0	2	0
41	t	9	0	0	0	0
41	u	91	0	0	0	0
41	v	83	0	0	1	0
41	x	6	0	0	0	0
41	y	2	0	0	0	0
All	All	54101	0	52739	547	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 5.

The worst 5 of 547 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:418:PL9:H102	1.47	0.95
24:B:616:CLA:H71	24:B:617:CLA:H192	1.52	0.88
24:c:517:CLA:HHC	24:c:517:CLA:HBB1	1.57	0.86
41:B:960:HOH:O	22:U:201:CL:CL	2.30	0.84
4:d:192:THR:HG23	24:d:403:CLA:HBC2	1.67	0.76

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]	2.16	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/344 (97%)	327 (98%)	7 (2%)	1 (0%)	36	34
1	a	338/344 (98%)	332 (98%)	5 (2%)	1 (0%)	36	34
2	B	512/505 (101%)	506 (99%)	6 (1%)	0	100	100
2	b	513/505 (102%)	502 (98%)	11 (2%)	0	100	100
3	C	453/455 (100%)	444 (98%)	7 (2%)	2 (0%)	30	26
3	c	459/455 (101%)	449 (98%)	8 (2%)	2 (0%)	30	26
4	D	340/342 (99%)	333 (98%)	7 (2%)	0	100	100
4	d	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
5	E	81/84 (96%)	81 (100%)	0	0	100	100
5	e	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	64/65 (98%)	60 (94%)	4 (6%)	0	100	100
7	h	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/36 (92%)	33 (100%)	0	0	100	100
12	m	32/36 (89%)	32 (100%)	0	0	100	100
13	O	249/244 (102%)	243 (98%)	6 (2%)	0	100	100
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%)	131 (96%)	5 (4%)	0	100	100
16	v	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
17	Y	27/30 (90%)	27 (100%)	0	0	100	100
17	y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
18	X	37/40 (92%)	37 (100%)	0	0	100	100
18	x	36/40 (90%)	36 (100%)	0	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%)	5166 (98%)	110 (2%)	6 (0%)	48	50

5 of 6 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	272/279 (98%)	272 (100%)	0	100	100
1	a	275/279 (99%)	275 (100%)	0	100	100
2	B	412/403 (102%)	407 (99%)	5 (1%)	63	70
2	b	413/403 (102%)	410 (99%)	3 (1%)	76	82
3	C	356/356 (100%)	350 (98%)	6 (2%)	53	60
3	c	362/356 (102%)	357 (99%)	5 (1%)	59	66
4	D	277/277 (100%)	274 (99%)	3 (1%)	65	72
4	d	277/277 (100%)	274 (99%)	3 (1%)	65	72
5	E	74/73 (101%)	73 (99%)	1 (1%)	59	66
5	e	74/73 (101%)	72 (97%)	2 (3%)	39	41
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	26/38 (68%)	25 (96%)	1 (4%)	29	29
7	H	55/54 (102%)	54 (98%)	1 (2%)	51	58
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%)	33 (97%)	1 (3%)	37	39
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	27/27 (100%)	26 (96%)	1 (4%)	30	30
10	K	30/30 (100%)	29 (97%)	1 (3%)	33	34
10	k	30/30 (100%)	29 (97%)	1 (3%)	33	34
11	L	36/35 (103%)	35 (97%)	1 (3%)	38	40
11	l	36/35 (103%)	35 (97%)	1 (3%)	38	40
12	M	31/32 (97%)	30 (97%)	1 (3%)	34	36
12	m	30/32 (94%)	30 (100%)	0	100	100
13	O	214/207 (103%)	211 (99%)	3 (1%)	59	66
13	o	211/207 (102%)	205 (97%)	6 (3%)	38	40
14	T	27/28 (96%)	25 (93%)	2 (7%)	13	8
14	t	27/28 (96%)	25 (93%)	2 (7%)	13	8
15	U	84/89 (94%)	83 (99%)	1 (1%)	63	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	u	84/89 (94%)	84 (100%)	0	100	100
16	V	118/117 (101%)	118 (100%)	0	100	100
16	v	117/117 (100%)	115 (98%)	2 (2%)	53	60
17	Y	22/23 (96%)	21 (96%)	1 (4%)	24	22
17	y	22/23 (96%)	21 (96%)	1 (4%)	24	22
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	56
19	z	52/52 (100%)	52 (100%)	0	100	100
20	R	25/29 (86%)	23 (92%)	2 (8%)	11	7
All	All	4387/4403 (100%)	4329 (99%)	58 (1%)	61	68

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	R	5	VAL
16	v	2	GLU
3	c	462[A]	GLU
14	t	25[B]	GLU
13	o	37	THR

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

Mol	Chain	Res	Type
4	d	301	GLN
15	u	81	HIS
4	d	332	GLN
13	o	124	ASN
19	z	31	GLN

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	0.85	0	7,9,11	2.25	4 (57%)
8	FME	I	1	8	8,9,10	0.66	0	7,9,11	1.17	1 (14%)
8	FME	i	1	8	8,9,10	0.63	0	7,9,11	1.37	2 (28%)
12	FME	m	1	12	8,9,10	0.68	0	7,9,11	1.53	2 (28%)
14	FME	T	1	14	8,9,10	0.71	0	7,9,11	1.36	1 (14%)
12	FME	M	1	12	8,9,10	0.63	0	7,9,11	1.36	2 (28%)

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

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

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	CA-N-CN	-3.38	117.62	122.82
14	t	1	FME	C-CA-N	2.62	114.47	109.73
12	m	1	FME	CA-N-CN	-2.46	119.03	122.82
8	i	1	FME	CA-N-CN	-2.45	119.05	122.82
14	t	1	FME	O1-CN-N	-2.43	118.87	125.27

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

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$
28	GOL	A	412	-	5,5,5	0.32	0	5,5,5	0.36	0
37	LHG	d	409	-	48,48,48	0.93	2 (4%)	51,54,54	1.05	2 (3%)
24	CLA	B	607	2	69,73,73	2.02	20 (28%)	83,113,113	2.91	30 (36%)
24	CLA	b	614	2	69,73,73	2.04	19 (27%)	83,113,113	2.96	29 (34%)
29	LMT	M	105	-	36,36,36	0.47	0	47,47,47	0.85	0
28	GOL	V	203	-	5,5,5	0.40	0	5,5,5	0.28	0
26	BCR	y	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.57	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LMT	f	103	-	36,36,36	0.48	0	47,47,47	0.94	2 (4%)
30	OEX	A	417	1,41,3	0,14,14	-	-	-		
40	HEC	v	205	16	50,50,50	1.67	10 (20%)	68,82,82	1.80	18 (26%)
24	CLA	C	503	3	69,73,73	2.07	20 (28%)	83,113,113	2.74	29 (34%)
37	LHG	D	407	-	48,48,48	0.87	2 (4%)	51,54,54	1.11	5 (9%)
27	SQD	a	405	-	53,54,54	1.06	3 (5%)	62,65,65	1.24	6 (9%)
37	LHG	E	101	-	41,41,48	1.03	2 (4%)	44,47,54	1.10	3 (6%)
24	CLA	c	515	3	69,73,73	2.02	19 (27%)	83,113,113	2.75	31 (37%)
25	PHO	d	401	-	58,69,69	2.76	14 (24%)	56,99,99	2.93	14 (25%)
24	CLA	d	403	4	69,73,73	2.02	19 (27%)	83,113,113	2.77	29 (34%)
26	BCR	A	410	-	41,41,41	1.00	1 (2%)	56,56,56	1.23	7 (12%)
26	BCR	a	413	-	41,41,41	1.07	1 (2%)	56,56,56	1.14	4 (7%)
27	SQD	B	621	-	53,54,54	1.01	3 (5%)	62,65,65	1.53	9 (14%)
27	SQD	A	415	-	53,54,54	1.05	3 (5%)	62,65,65	1.15	4 (6%)
35	LMG	c	523	-	51,51,55	0.96	2 (3%)	59,59,63	1.22	7 (11%)
24	CLA	B	609	2	69,73,73	2.02	20 (28%)	83,113,113	2.76	32 (38%)
24	CLA	b	611	2	69,73,73	2.07	21 (30%)	83,113,113	2.88	30 (36%)
28	GOL	B	628	-	5,5,5	0.36	0	5,5,5	0.52	0
28	GOL	B	631	-	5,5,5	0.37	0	5,5,5	0.38	0
26	BCR	C	515	-	41,41,41	1.07	1 (2%)	56,56,56	1.57	7 (12%)
24	CLA	C	508	41	69,73,73	2.03	20 (28%)	83,113,113	2.72	28 (33%)
24	CLA	b	624	2	69,73,73	2.02	19 (27%)	83,113,113	2.84	27 (32%)
35	LMG	J	101	39	51,51,55	0.86	2 (3%)	59,59,63	0.99	4 (6%)
24	CLA	C	506	3	69,73,73	1.99	20 (28%)	83,113,113	2.69	28 (33%)
29	LMT	F	102	-	36,36,36	0.46	0	47,47,47	1.01	2 (4%)
35	LMG	b	629	-	51,51,55	0.90	2 (3%)	59,59,63	1.01	3 (5%)
24	CLA	D	402	4	69,73,73	1.96	20 (28%)	83,113,113	2.89	30 (36%)
26	BCR	B	619	-	41,41,41	1.10	1 (2%)	56,56,56	1.38	6 (10%)
24	CLA	C	507	3	69,73,73	2.05	20 (28%)	83,113,113	2.71	29 (34%)
26	BCR	Y	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.53	9 (16%)
28	GOL	B	626	-	5,5,5	0.43	0	5,5,5	0.30	0
24	CLA	a	410	41	69,73,73	2.00	20 (28%)	83,113,113	2.83	30 (36%)
29	LMT	M	102	-	36,36,36	0.40	0	47,47,47	0.90	1 (2%)
37	LHG	e	102	-	41,41,48	1.03	2 (4%)	44,47,54	0.93	2 (4%)
24	CLA	C	510	3	69,73,73	2.11	20 (28%)	83,113,113	2.77	28 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	A	407	41	69,73,73	2.03	19 (27%)	83,113,113	2.89	32 (38%)
24	CLA	A	406	41	69,73,73	2.03	20 (28%)	83,113,113	2.91	32 (38%)
37	LHG	l	101	-	48,48,48	0.93	2 (4%)	51,54,54	0.98	3 (5%)
24	CLA	a	409	1	69,73,73	2.05	20 (28%)	83,113,113	2.82	31 (37%)
24	CLA	c	513	3	69,73,73	2.09	20 (28%)	83,113,113	2.77	29 (34%)
24	CLA	B	604	2	69,73,73	2.08	20 (28%)	83,113,113	2.76	30 (36%)
24	CLA	c	506	3	69,73,73	2.03	21 (30%)	83,113,113	2.75	29 (34%)
36	DGD	C	519	-	63,63,67	0.87	2 (3%)	77,77,81	0.88	2 (2%)
36	DGD	C	517	-	63,63,67	0.89	2 (3%)	77,77,81	1.12	7 (9%)
36	DGD	c	519	-	63,63,67	0.84	2 (3%)	77,77,81	1.12	7 (9%)
29	LMT	T	104	-	25,25,36	0.52	0	30,30,47	0.92	1 (3%)
28	GOL	b	603	-	5,5,5	0.33	0	5,5,5	0.20	0
26	BCR	H	101	-	41,41,41	1.09	1 (2%)	56,56,56	1.44	9 (16%)
28	GOL	o	301	-	5,5,5	0.38	0	5,5,5	0.26	0
24	CLA	B	612	2	69,73,73	2.02	20 (28%)	83,113,113	2.78	27 (32%)
28	GOL	C	525	-	5,5,5	0.38	0	5,5,5	0.73	0
24	CLA	b	625	2	69,73,73	2.02	20 (28%)	83,113,113	2.79	30 (36%)
24	CLA	c	512	3	69,73,73	2.07	20 (28%)	83,113,113	2.75	29 (34%)
35	LMG	c	522	-	51,51,55	0.90	2 (3%)	59,59,63	1.12	4 (6%)
24	CLA	B	611	41	69,73,73	2.08	18 (26%)	83,113,113	2.84	34 (40%)
29	LMT	b	630	-	25,25,36	0.52	0	30,30,47	0.64	0
34	HTG	c	525	-	19,19,19	1.03	2 (10%)	23,24,24	1.49	3 (13%)
35	LMG	j	101	39	51,51,55	0.92	2 (3%)	59,59,63	1.04	3 (5%)
24	CLA	C	514	3	69,73,73	2.05	19 (27%)	83,113,113	2.81	31 (37%)
28	GOL	a	401	-	5,5,5	0.42	0	5,5,5	0.46	0
24	CLA	B	610	2	69,73,73	2.02	18 (26%)	83,113,113	2.76	29 (34%)
37	LHG	L	101	-	48,48,48	0.91	2 (4%)	51,54,54	1.11	5 (9%)
28	GOL	B	630	-	5,5,5	0.40	0	5,5,5	0.36	0
34	HTG	b	631	-	19,19,19	0.79	1 (5%)	23,24,24	1.26	2 (8%)
35	LMG	C	521	-	51,51,55	0.95	2 (3%)	59,59,63	1.18	5 (8%)
28	GOL	B	629	-	5,5,5	0.37	0	5,5,5	0.28	0
35	LMG	C	501	-	51,51,55	0.94	2 (3%)	59,59,63	1.10	4 (6%)
24	CLA	C	511	3	69,73,73	2.07	20 (28%)	83,113,113	2.70	32 (38%)
34	HTG	b	608	-	19,19,19	1.07	2 (10%)	23,24,24	1.27	3 (13%)
35	LMG	a	415	-	51,51,55	0.90	2 (3%)	59,59,63	1.17	5 (8%)
24	CLA	b	619	41	69,73,73	2.05	21 (30%)	83,113,113	2.84	31 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	LHG	d	408	-	48,48,48	0.88	2 (4%)	51,54,54	1.00	4 (7%)
28	GOL	A	413	-	5,5,5	0.46	0	5,5,5	0.46	0
29	LMT	B	622	-	36,36,36	0.43	0	47,47,47	1.06	2 (4%)
26	BCR	B	620	-	41,41,41	1.05	1 (2%)	56,56,56	1.50	10 (17%)
31	PL9	A	418	-	55,55,55	0.66	2 (3%)	68,69,69	1.77	20 (29%)
34	HTG	C	523	-	19,19,19	0.99	2 (10%)	23,24,24	1.58	2 (8%)
26	BCR	C	516	-	41,41,41	1.01	1 (2%)	56,56,56	1.53	13 (23%)
24	CLA	c	508	41	69,73,73	2.04	20 (28%)	83,113,113	2.84	31 (37%)
24	CLA	B	614	2	69,73,73	2.04	19 (27%)	83,113,113	2.76	32 (38%)
24	CLA	C	513	3	69,73,73	2.04	20 (28%)	83,113,113	2.86	30 (36%)
24	CLA	b	622	2	69,73,73	2.04	20 (28%)	83,113,113	2.70	31 (37%)
38	HEM	e	103	6,5	50,50,50	1.52	7 (14%)	66,82,82	1.72	15 (22%)
36	DGD	e	101	-	63,63,67	0.93	2 (3%)	77,77,81	1.21	7 (9%)
24	CLA	C	502	3	69,73,73	2.03	18 (26%)	83,113,113	2.81	30 (36%)
28	GOL	T	102	-	5,5,5	0.40	0	5,5,5	0.30	0
24	CLA	c	509	3	69,73,73	1.99	20 (28%)	83,113,113	2.69	26 (31%)
24	CLA	a	412	1	69,73,73	2.05	19 (27%)	83,113,113	2.84	32 (38%)
35	LMG	M	101	-	51,51,55	0.94	2 (3%)	59,59,63	1.02	3 (5%)
24	CLA	b	623	2	69,73,73	1.99	19 (27%)	83,113,113	2.92	32 (38%)
24	CLA	c	505	3	69,73,73	2.01	20 (28%)	83,113,113	2.79	29 (34%)
28	GOL	v	203	-	5,5,5	0.41	0	5,5,5	0.27	0
24	CLA	C	509	3	69,73,73	2.06	20 (28%)	83,113,113	2.85	29 (34%)
28	GOL	t	102	-	5,5,5	0.45	0	5,5,5	0.12	0
37	LHG	D	409	-	48,48,48	0.96	2 (4%)	51,54,54	1.04	3 (5%)
24	CLA	B	613	2	69,73,73	2.00	19 (27%)	83,113,113	2.90	29 (34%)
26	BCR	k	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.47	11 (19%)
24	CLA	B	603	2	69,73,73	2.06	21 (30%)	83,113,113	2.89	28 (33%)
24	CLA	C	512	3	69,73,73	2.06	20 (28%)	83,113,113	2.80	32 (38%)
34	HTG	b	632	-	19,19,19	1.14	2 (10%)	23,24,24	1.75	3 (13%)
26	BCR	h	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.39	11 (19%)
28	GOL	V	202	-	5,5,5	0.38	0	5,5,5	0.32	0
24	CLA	b	610	41	69,73,73	2.07	20 (28%)	83,113,113	2.81	26 (31%)
26	BCR	d	405	-	41,41,41	1.06	1 (2%)	56,56,56	1.65	13 (23%)
34	HTG	c	524	-	19,19,19	1.04	2 (10%)	23,24,24	1.49	1 (4%)
24	CLA	A	409	1	69,73,73	2.07	20 (28%)	83,113,113	2.79	31 (37%)
28	GOL	f	101	33	5,5,5	0.32	0	5,5,5	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LMT	a	404	-	36,36,36	0.48	1 (2%)	47,47,47	1.10	2 (4%)
36	DGD	c	521	-	63,63,67	0.89	2 (3%)	77,77,81	1.01	4 (5%)
34	HTG	B	623	-	19,19,19	1.07	1 (5%)	23,24,24	1.09	1 (4%)
24	CLA	c	507	3	69,73,73	2.06	19 (27%)	83,113,113	2.77	27 (32%)
34	HTG	D	412	-	16,16,19	1.10	2 (12%)	20,21,24	1.49	1 (5%)
34	HTG	C	524	-	19,19,19	1.01	2 (10%)	23,24,24	1.78	4 (17%)
28	GOL	b	604	-	5,5,5	0.37	0	5,5,5	0.24	0
29	LMT	m	102	-	36,36,36	0.49	0	47,47,47	0.98	2 (4%)
36	DGD	c	520	-	63,63,67	0.88	2 (3%)	77,77,81	0.98	4 (5%)
25	PHO	A	408	-	58,69,69	2.78	15 (25%)	56,99,99	2.81	13 (23%)
24	CLA	c	510	3	69,73,73	2.02	20 (28%)	83,113,113	2.75	30 (36%)
28	GOL	T	101	-	5,5,5	0.43	0	5,5,5	0.17	0
24	CLA	B	602	41	69,73,73	2.07	20 (28%)	83,113,113	2.85	29 (34%)
34	HTG	d	412	-	16,16,19	1.22	2 (12%)	20,21,24	1.80	3 (15%)
29	LMT	M	104	-	36,36,36	0.54	1 (2%)	47,47,47	1.04	4 (8%)
24	CLA	B	616	2	69,73,73	2.01	18 (26%)	83,113,113	2.88	30 (36%)
24	CLA	B	606	2	69,73,73	2.03	18 (26%)	83,113,113	2.92	30 (36%)
24	CLA	c	511	41	69,73,73	2.00	20 (28%)	83,113,113	2.76	27 (32%)
26	BCR	c	527	-	41,41,41	1.03	1 (2%)	56,56,56	1.53	8 (14%)
27	SQD	A	411	-	53,54,54	0.96	3 (5%)	62,65,65	1.52	11 (17%)
38	HEM	E	102	6,5	50,50,50	1.55	6 (12%)	66,82,82	1.84	14 (21%)
36	DGD	C	518	-	63,63,67	0.89	2 (3%)	77,77,81	1.02	5 (6%)
24	CLA	b	620	2	69,73,73	2.00	19 (27%)	83,113,113	2.79	29 (34%)
34	HTG	B	624	-	19,19,19	0.78	1 (5%)	23,24,24	1.56	3 (13%)
36	DGD	H	102	-	63,63,67	0.88	2 (3%)	77,77,81	1.00	6 (7%)
31	PL9	d	406	-	55,55,55	0.71	2 (3%)	68,69,69	1.54	16 (23%)
28	GOL	A	414	-	5,5,5	0.39	0	5,5,5	0.17	0
28	GOL	C	526	-	5,5,5	0.34	0	5,5,5	0.52	0
28	GOL	a	402	-	5,5,5	0.38	0	5,5,5	0.27	0
24	CLA	b	621	2	69,73,73	2.03	21 (30%)	83,113,113	2.79	33 (39%)
24	CLA	c	517	3	69,73,73	2.08	20 (28%)	83,113,113	2.84	32 (38%)
24	CLA	d	404	4	69,73,73	2.03	21 (30%)	83,113,113	2.86	32 (38%)
27	SQD	a	414	-	53,54,54	0.97	3 (5%)	62,65,65	1.59	13 (20%)
28	GOL	V	201	-	5,5,5	0.37	0	5,5,5	0.32	0
34	HTG	b	601	-	19,19,19	0.96	1 (5%)	23,24,24	1.04	1 (4%)
35	LMG	C	520	-	51,51,55	0.95	2 (3%)	59,59,63	0.98	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	d	402	41	69,73,73	2.04	20 (28%)	83,113,113	2.79	32 (38%)
24	CLA	c	516	3	69,73,73	2.04	19 (27%)	83,113,113	2.95	32 (38%)
24	CLA	b	616	41	69,73,73	2.03	19 (27%)	83,113,113	2.80	30 (36%)
34	HTG	B	632	-	19,19,19	1.02	2 (10%)	23,24,24	1.39	3 (13%)
24	CLA	C	505	41	69,73,73	2.05	20 (28%)	83,113,113	2.84	30 (36%)
23	BCT	a	418	21	2,3,3	0.64	0	2,3,3	0.73	0
26	BCR	K	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.43	11 (19%)
34	HTG	V	206	-	19,19,19	1.04	2 (10%)	23,24,24	1.30	3 (13%)
26	BCR	B	618	-	41,41,41	1.02	1 (2%)	56,56,56	1.38	7 (12%)
25	PHO	D	401	-	58,69,69	2.77	12 (20%)	56,99,99	2.67	14 (25%)
34	HTG	B	633	-	19,19,19	1.03	2 (10%)	23,24,24	1.41	1 (4%)
24	CLA	b	615	2	69,73,73	2.01	20 (28%)	83,113,113	2.88	29 (34%)
23	BCT	A	404	21	2,3,3	0.59	0	2,3,3	1.30	0
29	LMT	a	419	-	36,36,36	0.45	0	47,47,47	0.79	1 (2%)
29	LMT	B	635	-	25,25,36	0.55	1 (4%)	30,30,47	0.80	1 (3%)
24	CLA	A	405	1	69,73,73	2.05	20 (28%)	83,113,113	2.73	30 (36%)
26	BCR	b	628	-	41,41,41	1.07	1 (2%)	56,56,56	1.25	7 (12%)
28	GOL	b	602	-	5,5,5	0.41	0	5,5,5	0.44	0
37	LHG	d	407	-	48,48,48	0.88	3 (6%)	51,54,54	1.04	5 (9%)
26	BCR	b	627	-	41,41,41	1.00	1 (2%)	56,56,56	1.38	7 (12%)
28	GOL	c	501	-	5,5,5	0.37	0	5,5,5	0.29	0
36	DGD	h	102	-	63,63,67	0.91	3 (4%)	77,77,81	0.92	4 (5%)
28	GOL	b	606	-	5,5,5	0.37	0	5,5,5	0.28	0
28	GOL	B	627	-	5,5,5	0.30	0	5,5,5	0.45	0
30	OEX	a	417	1,41,3	0,14,14	-	-	-	-	-
24	CLA	B	605	2	69,73,73	1.97	21 (30%)	83,113,113	2.77	32 (38%)
31	PL9	D	405	-	55,55,55	0.65	1 (1%)	68,69,69	1.71	18 (26%)
24	CLA	B	608	41	69,73,73	2.01	20 (28%)	83,113,113	2.71	31 (37%)
40	HEC	V	205	16	50,50,50	1.71	9 (18%)	68,82,82	1.73	20 (29%)
28	GOL	v	201	-	5,5,5	0.35	0	5,5,5	0.21	0
24	CLA	D	403	4	69,73,73	2.05	21 (30%)	83,113,113	2.80	30 (36%)
24	CLA	b	618	2	69,73,73	2.00	18 (26%)	83,113,113	2.78	30 (36%)
26	BCR	D	404	-	41,41,41	1.05	1 (2%)	56,56,56	1.73	14 (25%)
35	LMG	Z	101	-	37,37,55	0.96	2 (5%)	45,45,63	1.38	6 (13%)
37	LHG	D	408	-	48,48,48	0.89	2 (4%)	51,54,54	0.89	4 (7%)
34	HTG	B	625	-	19,19,19	1.04	2 (10%)	23,24,24	1.83	4 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LMT	C	522	-	36,36,36	0.50	0	47,47,47	1.22	3 (6%)
28	GOL	c	502	-	5,5,5	0.40	0	5,5,5	0.48	0
26	BCR	t	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.61	16 (28%)
29	LMT	A	416	-	36,36,36	0.56	1 (2%)	47,47,47	1.28	3 (6%)
31	PL9	a	416	-	55,55,55	0.64	2 (3%)	68,69,69	1.91	18 (26%)
26	BCR	T	103	-	41,41,41	1.08	1 (2%)	56,56,56	1.62	13 (23%)
34	HTG	b	607	-	19,19,19	1.08	2 (10%)	23,24,24	1.32	1 (4%)
27	SQD	L	102	-	53,54,54	1.02	3 (5%)	62,65,65	1.58	10 (16%)
27	SQD	F	103	-	42,43,54	1.15	3 (7%)	51,54,65	1.59	11 (21%)
24	CLA	b	613	2	69,73,73	2.01	20 (28%)	83,113,113	2.72	31 (37%)
26	BCR	b	626	-	41,41,41	1.02	1 (2%)	56,56,56	1.45	8 (14%)
28	GOL	V	204	-	5,5,5	0.35	0	5,5,5	0.29	0
27	SQD	f	102	-	42,43,54	1.19	3 (7%)	51,54,65	1.47	8 (15%)
28	GOL	F	101	33	5,5,5	0.37	0	5,5,5	0.22	0
24	CLA	B	615	2	69,73,73	2.03	20 (28%)	83,113,113	2.86	29 (34%)
28	GOL	O	301	-	5,5,5	0.35	0	5,5,5	0.40	0
36	DGD	D	406	-	52,52,67	1.02	3 (5%)	60,60,81	1.21	5 (8%)
24	CLA	b	617	2	69,73,73	2.10	20 (28%)	83,113,113	2.70	31 (37%)
24	CLA	c	514	3	69,73,73	2.05	20 (28%)	83,113,113	2.81	33 (39%)
26	BCR	c	518	-	41,41,41	1.03	1 (2%)	56,56,56	1.45	8 (14%)
25	PHO	a	411	-	58,69,69	2.77	14 (24%)	56,99,99	2.70	16 (28%)
35	LMG	z	101	-	39,39,55	1.08	2 (5%)	47,47,63	1.11	3 (6%)
28	GOL	B	636	-	5,5,5	0.41	0	5,5,5	0.57	0
24	CLA	B	617	2	69,73,73	2.03	20 (28%)	83,113,113	2.77	29 (34%)
28	GOL	b	605	-	5,5,5	0.37	0	5,5,5	0.30	0
24	CLA	b	612	2	69,73,73	2.03	20 (28%)	83,113,113	2.86	32 (38%)
28	GOL	v	202	-	5,5,5	0.34	0	5,5,5	0.28	0
24	CLA	C	504	3	69,73,73	2.08	19 (27%)	83,113,113	2.77	27 (32%)

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
28	GOL	A	412	-	-	0/4/4/4	-
37	LHG	d	409	-	-	13/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	607	2	-	5/39/115/115	-
24	CLA	b	614	2	-	3/39/115/115	-
29	LMT	M	105	-	-	7/21/61/61	0/2/2/2
28	GOL	V	203	-	-	1/4/4/4	-
26	BCR	y	101	-	-	4/29/63/63	0/2/2/2
29	LMT	f	103	-	-	10/21/61/61	0/2/2/2
40	HEC	v	205	16	1/1/3/7	5/14/54/54	-
24	CLA	C	503	3	-	5/39/115/115	-
37	LHG	D	407	-	-	13/53/53/53	-
27	SQD	a	405	-	-	16/49/69/69	0/1/1/1
37	LHG	E	101	-	-	22/46/46/53	-
24	CLA	c	515	3	-	5/39/115/115	-
25	PHO	d	401	-	-	1/37/103/103	0/5/6/6
24	CLA	d	403	4	-	4/39/115/115	-
26	BCR	A	410	-	-	0/29/63/63	0/2/2/2
26	BCR	a	413	-	-	0/29/63/63	0/2/2/2
27	SQD	B	621	-	-	20/49/69/69	0/1/1/1
27	SQD	A	415	-	-	14/49/69/69	0/1/1/1
35	LMG	c	523	-	-	3/46/66/70	0/1/1/1
24	CLA	B	609	2	-	1/39/115/115	-
24	CLA	b	611	2	-	7/39/115/115	-
28	GOL	B	628	-	-	2/4/4/4	-
28	GOL	B	631	-	-	0/4/4/4	-
26	BCR	C	515	-	-	2/29/63/63	0/2/2/2
24	CLA	C	508	41	-	7/39/115/115	-
24	CLA	b	624	2	-	4/39/115/115	-
35	LMG	J	101	39	-	9/46/66/70	0/1/1/1
24	CLA	C	506	3	-	6/39/115/115	-
29	LMT	F	102	-	-	3/21/61/61	0/2/2/2
35	LMG	b	629	-	-	10/46/66/70	0/1/1/1
24	CLA	D	402	4	-	0/39/115/115	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
24	CLA	C	507	3	-	9/39/115/115	-
26	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
28	GOL	B	626	-	-	2/4/4/4	-
24	CLA	a	410	41	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMT	M	102	-	-	5/21/61/61	0/2/2/2
37	LHG	e	102	-	-	20/46/46/53	-
24	CLA	C	510	3	-	11/39/115/115	-
24	CLA	A	407	41	-	4/39/115/115	-
24	CLA	A	406	41	-	4/39/115/115	-
37	LHG	l	101	-	-	14/53/53/53	-
24	CLA	a	409	1	-	6/39/115/115	-
24	CLA	c	513	3	-	11/39/115/115	-
24	CLA	B	604	2	-	8/39/115/115	-
24	CLA	c	506	3	-	7/39/115/115	-
36	DGD	C	519	-	-	8/51/91/95	0/2/2/2
36	DGD	C	517	-	-	16/51/91/95	0/2/2/2
36	DGD	c	519	-	-	15/51/91/95	0/2/2/2
29	LMT	T	104	-	-	7/17/37/61	0/1/1/2
28	GOL	b	603	-	-	0/4/4/4	-
26	BCR	H	101	-	-	0/29/63/63	0/2/2/2
28	GOL	o	301	-	-	3/4/4/4	-
24	CLA	B	612	2	-	6/39/115/115	-
28	GOL	C	525	-	-	2/4/4/4	-
24	CLA	b	625	2	-	8/39/115/115	-
24	CLA	c	512	3	-	4/39/115/115	-
35	LMG	c	522	-	-	13/46/66/70	0/1/1/1
24	CLA	B	611	41	-	6/39/115/115	-
29	LMT	b	630	-	-	4/17/37/61	0/1/1/2
34	HTG	c	525	-	-	0/10/30/30	0/1/1/1
35	LMG	j	101	39	-	12/46/66/70	0/1/1/1
24	CLA	C	514	3	-	6/39/115/115	-
28	GOL	a	401	-	-	2/4/4/4	-
24	CLA	B	610	2	-	5/39/115/115	-
37	LHG	L	101	-	-	15/53/53/53	-
28	GOL	B	630	-	-	4/4/4/4	-
34	HTG	b	631	-	-	3/10/30/30	0/1/1/1
35	LMG	C	521	-	-	9/46/66/70	0/1/1/1
28	GOL	B	629	-	-	3/4/4/4	-
35	LMG	C	501	-	-	18/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	511	3	-	8/39/115/115	-
34	HTG	b	608	-	-	1/10/30/30	0/1/1/1
35	LMG	a	415	-	-	18/46/66/70	0/1/1/1
24	CLA	b	619	41	-	6/39/115/115	-
37	LHG	d	408	-	-	9/53/53/53	-
28	GOL	A	413	-	-	2/4/4/4	-
29	LMT	B	622	-	-	10/21/61/61	0/2/2/2
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
31	PL9	A	418	-	-	13/53/73/73	0/1/1/1
34	HTG	C	523	-	-	0/10/30/30	0/1/1/1
26	BCR	C	516	-	-	4/29/63/63	0/2/2/2
24	CLA	c	508	41	-	8/39/115/115	-
24	CLA	B	614	2	-	7/39/115/115	-
24	CLA	C	513	3	-	12/39/115/115	-
24	CLA	b	622	2	-	4/39/115/115	-
38	HEM	e	103	6,5	-	10/14/54/54	-
36	DGD	e	101	-	-	26/51/91/95	0/2/2/2
24	CLA	C	502	3	-	5/39/115/115	-
28	GOL	T	102	-	-	2/4/4/4	-
24	CLA	c	509	3	-	4/39/115/115	-
24	CLA	a	412	1	-	9/39/115/115	-
35	LMG	M	101	-	-	7/46/66/70	0/1/1/1
24	CLA	b	623	2	-	20/39/115/115	-
24	CLA	c	505	3	-	5/39/115/115	-
28	GOL	v	203	-	-	2/4/4/4	-
24	CLA	C	509	3	-	5/39/115/115	-
28	GOL	t	102	-	-	0/4/4/4	-
37	LHG	D	409	-	-	14/53/53/53	-
24	CLA	B	613	2	-	1/39/115/115	-
26	BCR	k	101	-	-	1/29/63/63	0/2/2/2
24	CLA	B	603	2	-	7/39/115/115	-
24	CLA	C	512	3	-	3/39/115/115	-
34	HTG	b	632	-	-	5/10/30/30	0/1/1/1
26	BCR	h	101	-	-	1/29/63/63	0/2/2/2
28	GOL	V	202	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	610	41	-	16/39/115/115	-
26	BCR	d	405	-	-	5/29/63/63	0/2/2/2
34	HTG	c	524	-	-	3/10/30/30	0/1/1/1
24	CLA	A	409	1	-	10/39/115/115	-
28	GOL	f	101	33	-	3/4/4/4	-
29	LMT	a	404	-	-	9/21/61/61	0/2/2/2
36	DGD	c	521	-	-	16/51/91/95	0/2/2/2
34	HTG	B	623	-	-	3/10/30/30	0/1/1/1
24	CLA	c	507	3	-	2/39/115/115	-
34	HTG	D	412	-	-	1/7/27/30	0/1/1/1
34	HTG	C	524	-	-	3/10/30/30	0/1/1/1
28	GOL	b	604	-	-	2/4/4/4	-
29	LMT	m	102	-	-	5/21/61/61	0/2/2/2
36	DGD	c	520	-	-	16/51/91/95	0/2/2/2
25	PHO	A	408	-	-	0/37/103/103	0/5/6/6
24	CLA	c	510	3	-	14/39/115/115	-
28	GOL	T	101	-	-	0/4/4/4	-
24	CLA	B	602	41	-	12/39/115/115	-
34	HTG	d	412	-	-	0/7/27/30	0/1/1/1
29	LMT	M	104	-	-	10/21/61/61	0/2/2/2
24	CLA	B	616	2	-	11/39/115/115	-
24	CLA	B	606	2	-	6/39/115/115	-
24	CLA	c	511	41	-	7/39/115/115	-
26	BCR	c	527	-	-	0/29/63/63	0/2/2/2
27	SQD	A	411	-	-	11/49/69/69	0/1/1/1
38	HEM	E	102	6,5	-	9/14/54/54	-
36	DGD	C	518	-	-	18/51/91/95	0/2/2/2
24	CLA	b	620	2	-	3/39/115/115	-
34	HTG	B	624	-	-	5/10/30/30	0/1/1/1
36	DGD	H	102	-	-	13/51/91/95	0/2/2/2
31	PL9	d	406	-	-	3/53/73/73	0/1/1/1
28	GOL	A	414	-	-	2/4/4/4	-
28	GOL	C	526	-	-	0/4/4/4	-
28	GOL	a	402	-	-	2/4/4/4	-
24	CLA	b	621	2	-	2/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	517	3	-	5/39/115/115	-
24	CLA	d	404	4	-	3/39/115/115	-
27	SQD	a	414	-	-	15/49/69/69	0/1/1/1
28	GOL	V	201	-	-	2/4/4/4	-
34	HTG	b	601	-	-	3/10/30/30	0/1/1/1
35	LMG	C	520	-	-	11/46/66/70	0/1/1/1
24	CLA	d	402	41	-	8/39/115/115	-
24	CLA	c	516	3	-	11/39/115/115	-
24	CLA	b	616	41	-	4/39/115/115	-
34	HTG	B	632	-	-	3/10/30/30	0/1/1/1
24	CLA	C	505	41	-	8/39/115/115	-
26	BCR	K	101	-	-	1/29/63/63	0/2/2/2
34	HTG	V	206	-	-	4/10/30/30	0/1/1/1
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
25	PHO	D	401	-	-	5/37/103/103	0/5/6/6
34	HTG	B	633	-	-	0/10/30/30	0/1/1/1
24	CLA	b	615	2	-	11/39/115/115	-
29	LMT	a	419	-	-	5/21/61/61	0/2/2/2
29	LMT	B	635	-	-	7/17/37/61	0/1/1/2
24	CLA	A	405	1	-	4/39/115/115	-
26	BCR	b	628	-	-	2/29/63/63	0/2/2/2
28	GOL	b	602	-	-	4/4/4/4	-
37	LHG	d	407	-	-	12/53/53/53	-
26	BCR	b	627	-	-	2/29/63/63	0/2/2/2
28	GOL	c	501	-	-	0/4/4/4	-
36	DGD	h	102	-	-	10/51/91/95	0/2/2/2
28	GOL	b	606	-	-	3/4/4/4	-
28	GOL	B	627	-	-	2/4/4/4	-
24	CLA	B	605	2	-	6/39/115/115	-
31	PL9	D	405	-	-	8/53/73/73	0/1/1/1
40	HEC	V	205	16	1/1/3/7	4/14/54/54	-
24	CLA	B	608	41	-	4/39/115/115	-
28	GOL	v	201	-	-	2/4/4/4	-
24	CLA	D	403	4	-	5/39/115/115	-
24	CLA	b	618	2	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	D	404	-	-	8/29/63/63	0/2/2/2
35	LMG	Z	101	-	-	14/31/51/70	0/1/1/1
37	LHG	D	408	-	-	11/53/53/53	-
34	HTG	B	625	-	-	5/10/30/30	0/1/1/1
29	LMT	C	522	-	-	10/21/61/61	0/2/2/2
28	GOL	c	502	-	-	0/4/4/4	-
26	BCR	t	101	-	-	3/29/63/63	0/2/2/2
29	LMT	A	416	-	-	5/21/61/61	0/2/2/2
31	PL9	a	416	-	-	15/53/73/73	0/1/1/1
26	BCR	T	103	-	-	2/29/63/63	0/2/2/2
34	HTG	b	607	-	-	2/10/30/30	0/1/1/1
27	SQD	L	102	-	-	20/49/69/69	0/1/1/1
27	SQD	F	103	-	-	16/38/58/69	0/1/1/1
24	CLA	b	613	2	-	3/39/115/115	-
26	BCR	b	626	-	-	2/29/63/63	0/2/2/2
28	GOL	V	204	-	-	0/4/4/4	-
27	SQD	f	102	-	-	15/38/58/69	0/1/1/1
28	GOL	F	101	33	-	2/4/4/4	-
24	CLA	B	615	2	-	14/39/115/115	-
28	GOL	O	301	-	-	2/4/4/4	-
36	DGD	D	406	-	-	21/47/67/95	0/1/1/2
24	CLA	b	617	2	-	3/39/115/115	-
24	CLA	c	514	3	-	9/39/115/115	-
26	BCR	c	518	-	-	2/29/63/63	0/2/2/2
25	PHO	a	411	-	-	5/37/103/103	0/5/6/6
35	LMG	z	101	-	-	13/34/54/70	0/1/1/1
28	GOL	B	636	-	-	0/4/4/4	-
24	CLA	B	617	2	-	6/39/115/115	-
28	GOL	b	605	-	-	2/4/4/4	-
24	CLA	b	612	2	-	5/39/115/115	-
28	GOL	v	202	-	-	3/4/4/4	-
24	CLA	C	504	3	-	1/39/115/115	-

The worst 5 of 1622 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	401	PHO	C1B-C2B	9.25	1.49	1.39
25	D	401	PHO	C1D-C2D	9.21	1.49	1.39
25	d	401	PHO	C1B-C2B	9.14	1.49	1.39
25	a	411	PHO	C1D-C2D	8.92	1.49	1.39
25	A	408	PHO	C1D-C2D	8.78	1.49	1.39

The worst 5 of 2777 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	408	PHO	C2D-C1D-ND	11.95	117.78	109.53
25	d	401	PHO	C2D-C1D-ND	11.26	117.30	109.53
25	a	411	PHO	C2D-C1D-ND	10.82	117.00	109.53
24	a	410	CLA	C1D-ND-C4D	-10.50	98.87	106.33
24	B	606	CLA	C1D-ND-C4D	-10.46	98.90	106.33

All (2) chirality outliers are listed below:

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

5 of 1342 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	606	CLA	C2-C3-C5-C6
24	B	606	CLA	C4-C3-C5-C6

There are no ring outliers.

161 monomers are involved in 342 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	d	409	LHG	6	0
24	B	607	CLA	2	0
24	b	614	CLA	6	0
29	M	105	LMT	1	0
26	y	101	BCR	2	0
29	f	103	LMT	1	0
24	C	503	CLA	2	0
37	D	407	LHG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	a	405	SQD	2	0
37	E	101	LHG	2	0
24	c	515	CLA	3	0
25	d	401	PHO	2	0
24	d	403	CLA	3	0
26	A	410	BCR	2	0
26	a	413	BCR	1	0
27	B	621	SQD	1	0
27	A	415	SQD	1	0
35	c	523	LMG	1	0
24	B	609	CLA	2	0
24	b	611	CLA	3	0
26	C	515	BCR	6	0
24	C	508	CLA	4	0
24	b	624	CLA	5	0
35	J	101	LMG	1	0
24	C	506	CLA	7	0
35	b	629	LMG	3	0
24	D	402	CLA	3	0
26	B	619	BCR	4	0
24	C	507	CLA	2	0
26	Y	101	BCR	3	0
24	a	410	CLA	3	0
29	M	102	LMT	3	0
37	e	102	LHG	4	0
24	C	510	CLA	3	0
24	A	407	CLA	1	0
24	A	406	CLA	4	0
37	l	101	LHG	2	0
24	a	409	CLA	4	0
24	c	513	CLA	1	0
24	B	604	CLA	2	0
24	c	506	CLA	2	0
36	C	517	DGD	4	0
36	c	519	DGD	2	0
26	H	101	BCR	4	0
24	B	612	CLA	3	0
24	b	625	CLA	2	0
24	c	512	CLA	6	0
35	c	522	LMG	3	0
24	B	611	CLA	2	0
29	b	630	LMT	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	j	101	LMG	2	0
24	C	514	CLA	9	0
24	B	610	CLA	3	0
37	L	101	LHG	2	0
28	B	630	GOL	1	0
34	b	631	HTG	1	0
35	C	521	LMG	1	0
35	C	501	LMG	6	0
24	C	511	CLA	1	0
35	a	415	LMG	1	0
24	b	619	CLA	1	0
37	d	408	LHG	1	0
28	A	413	GOL	1	0
29	B	622	LMT	1	0
26	B	620	BCR	3	0
31	A	418	PL9	5	0
26	C	516	BCR	5	0
24	c	508	CLA	1	0
24	B	614	CLA	4	0
24	C	513	CLA	6	0
24	b	622	CLA	2	0
38	e	103	HEM	2	0
36	e	101	DGD	9	0
24	C	502	CLA	1	0
28	T	102	GOL	2	0
24	c	509	CLA	7	0
35	M	101	LMG	2	0
24	b	623	CLA	1	0
24	c	505	CLA	2	0
24	C	509	CLA	2	0
37	D	409	LHG	8	0
24	B	613	CLA	1	0
26	k	101	BCR	1	0
24	B	603	CLA	1	0
24	C	512	CLA	4	0
34	b	632	HTG	1	0
26	h	101	BCR	4	0
24	b	610	CLA	2	0
26	d	405	BCR	3	0
24	A	409	CLA	4	0
28	f	101	GOL	1	0
29	a	404	LMT	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	B	623	HTG	2	0
24	c	507	CLA	3	0
34	D	412	HTG	2	0
28	b	604	GOL	1	0
29	m	102	LMT	2	0
36	c	520	DGD	2	0
25	A	408	PHO	3	0
24	c	510	CLA	2	0
28	T	101	GOL	1	0
24	B	602	CLA	1	0
34	d	412	HTG	3	0
24	B	616	CLA	7	0
24	B	606	CLA	3	0
24	c	511	CLA	4	0
26	c	527	BCR	4	0
27	A	411	SQD	6	0
38	E	102	HEM	3	0
36	C	518	DGD	1	0
24	b	620	CLA	2	0
31	d	406	PL9	1	0
28	a	402	GOL	1	0
24	b	621	CLA	1	0
24	c	517	CLA	6	0
24	d	404	CLA	2	0
27	a	414	SQD	2	0
34	b	601	HTG	1	0
35	C	520	LMG	1	0
24	d	402	CLA	3	0
24	c	516	CLA	2	0
24	b	616	CLA	1	0
26	K	101	BCR	3	0
34	V	206	HTG	2	0
26	B	618	BCR	1	0
25	D	401	PHO	1	0
24	b	615	CLA	1	0
29	a	419	LMT	1	0
24	A	405	CLA	3	0
26	b	628	BCR	3	0
37	d	407	LHG	2	0
26	b	627	BCR	3	0
24	B	605	CLA	3	0
31	D	405	PL9	2	0

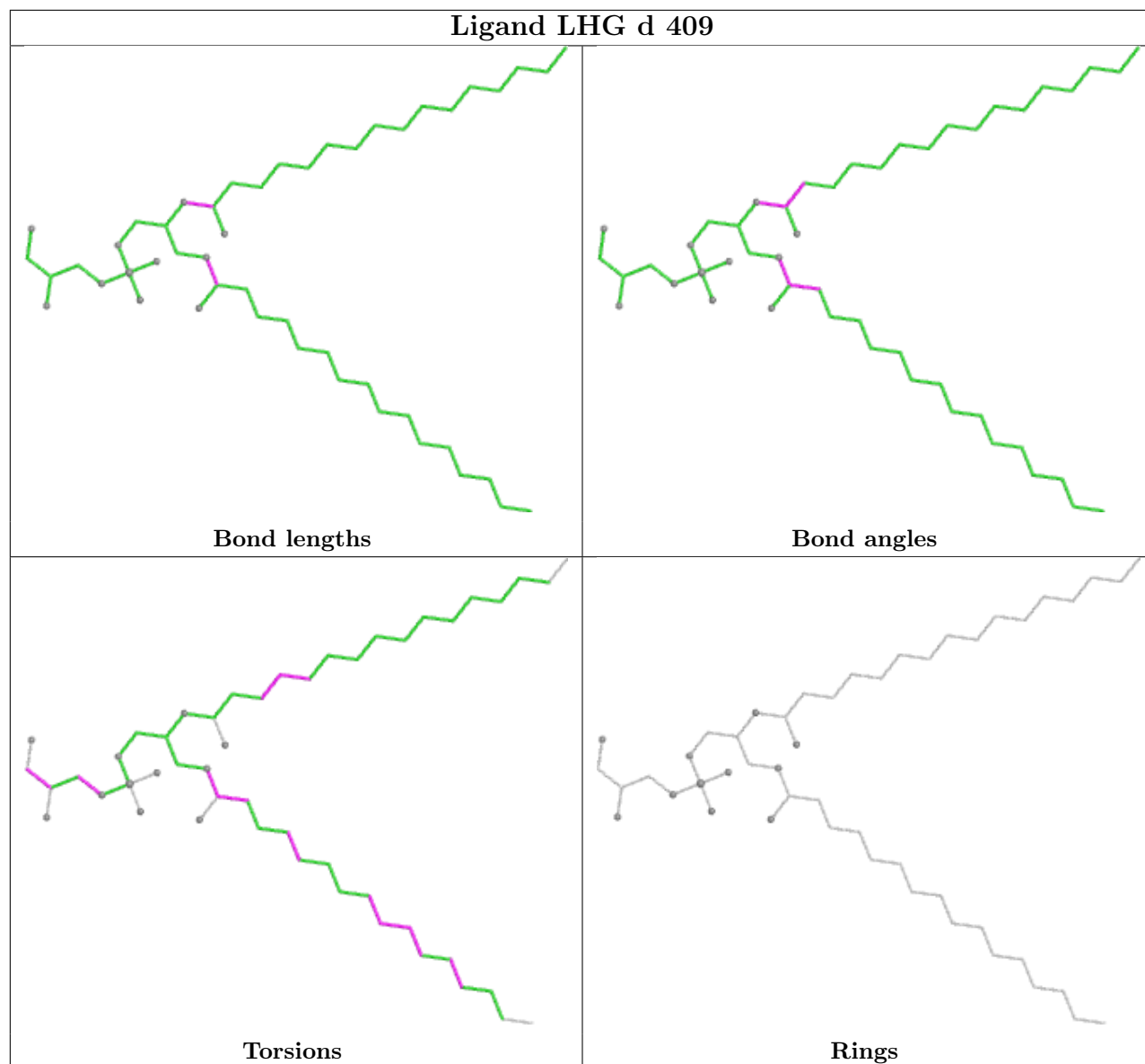
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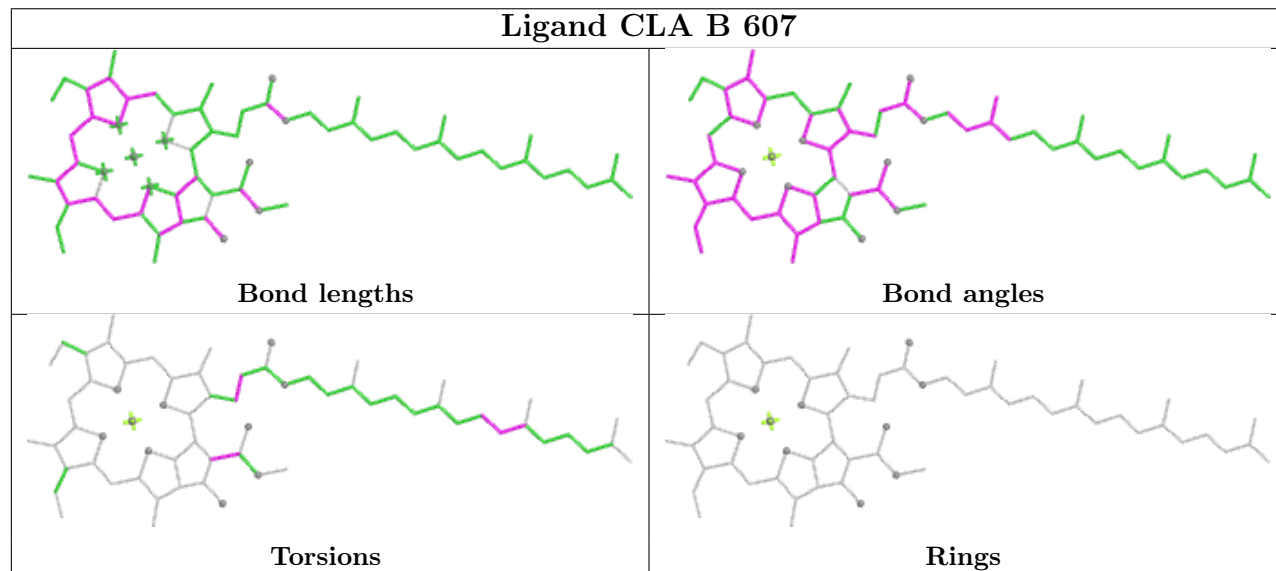
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28	v	201	GOL	1	0
24	D	403	CLA	1	0
24	b	618	CLA	1	0
26	D	404	BCR	1	0
35	Z	101	LMG	1	0
29	C	522	LMT	2	0
28	c	502	GOL	2	0
26	t	101	BCR	6	0
29	A	416	LMT	2	0
31	a	416	PL9	6	0
26	T	103	BCR	6	0
27	L	102	SQD	2	0
27	F	103	SQD	1	0
24	b	613	CLA	2	0
26	b	626	BCR	2	0
27	f	102	SQD	2	1
24	B	615	CLA	4	0
36	D	406	DGD	2	0
24	b	617	CLA	1	0
24	c	514	CLA	2	0
26	c	518	BCR	1	0
25	a	411	PHO	2	0
35	z	101	LMG	4	0
24	B	617	CLA	8	0
24	b	612	CLA	1	0
24	C	504	CLA	3	0

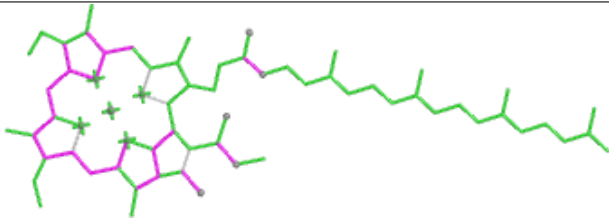
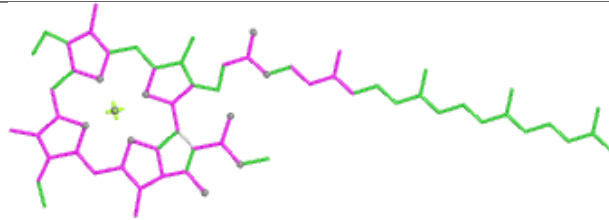
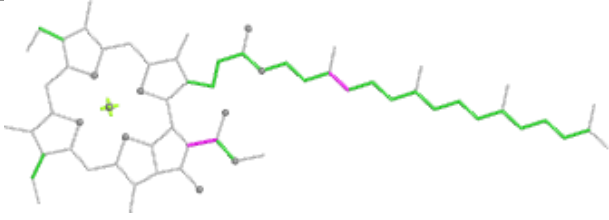
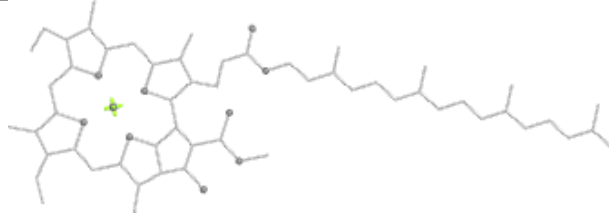
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

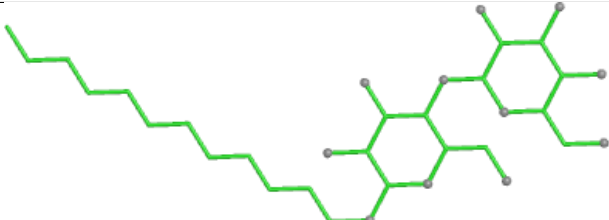
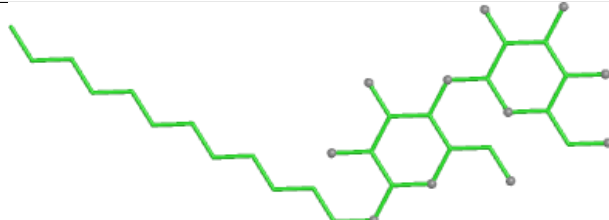
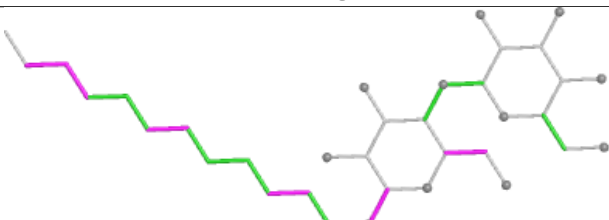
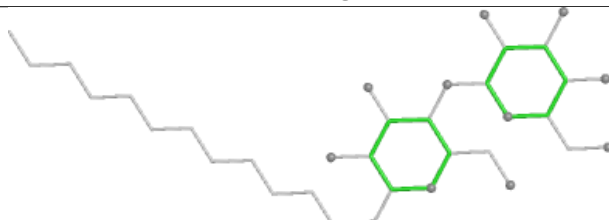
Ligand LHG d 409

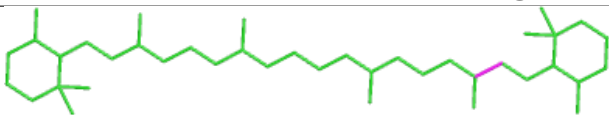
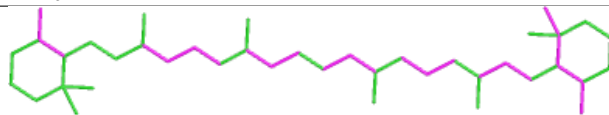
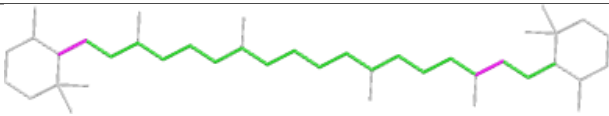
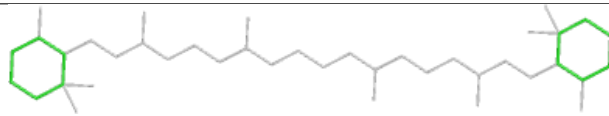


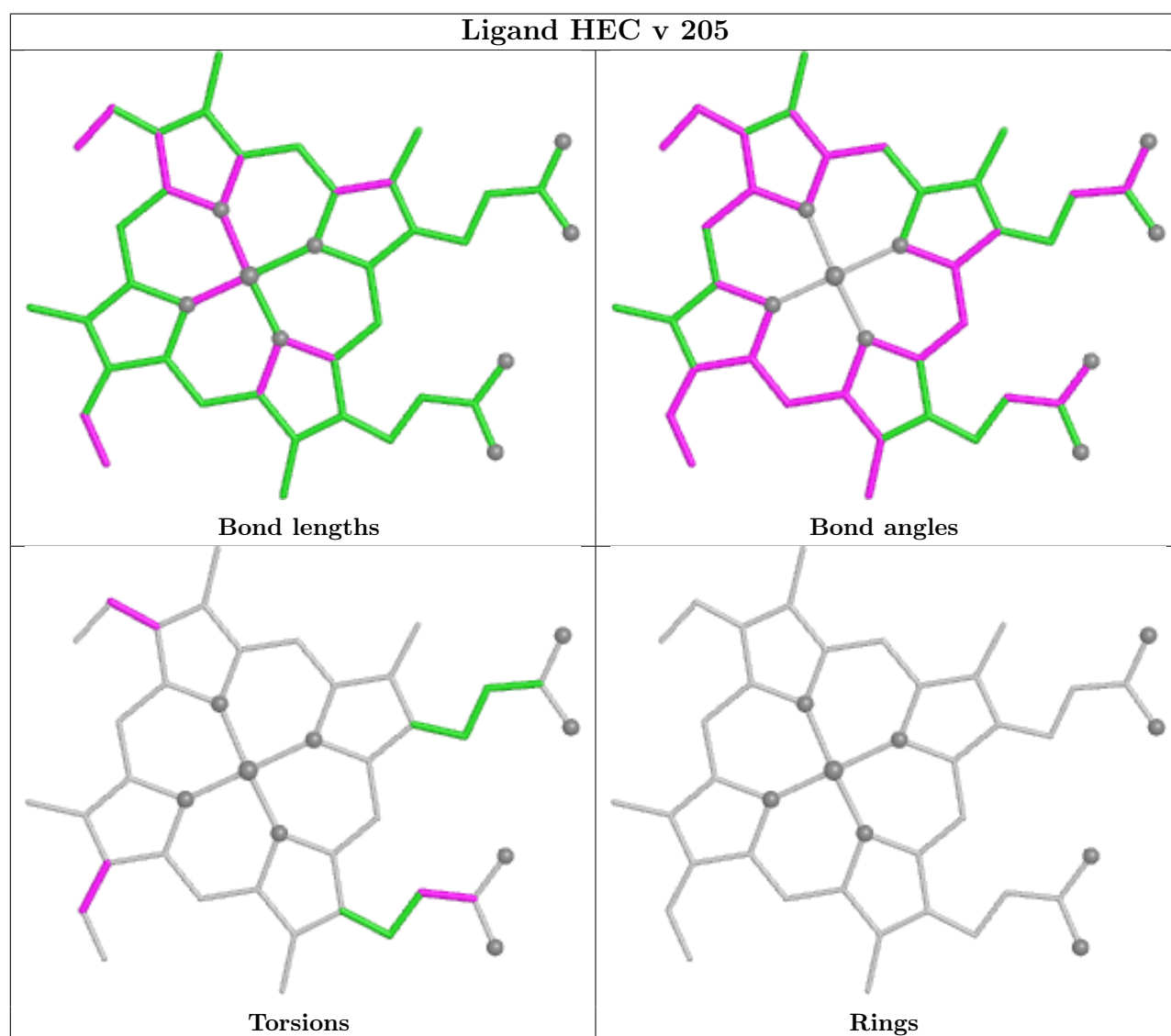
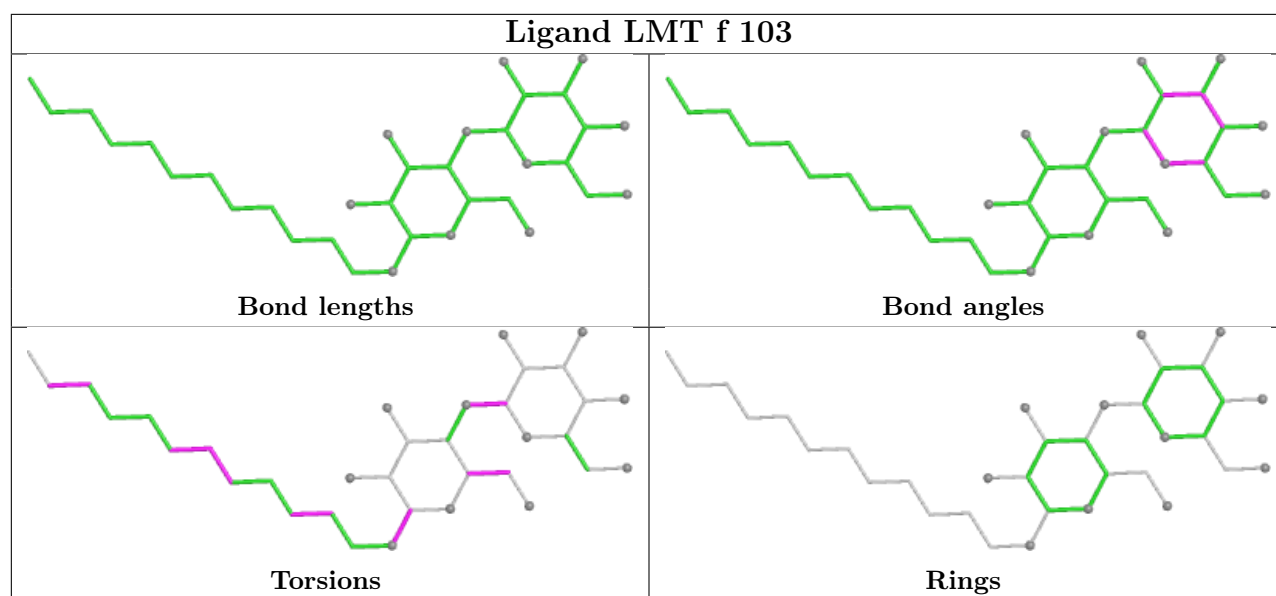
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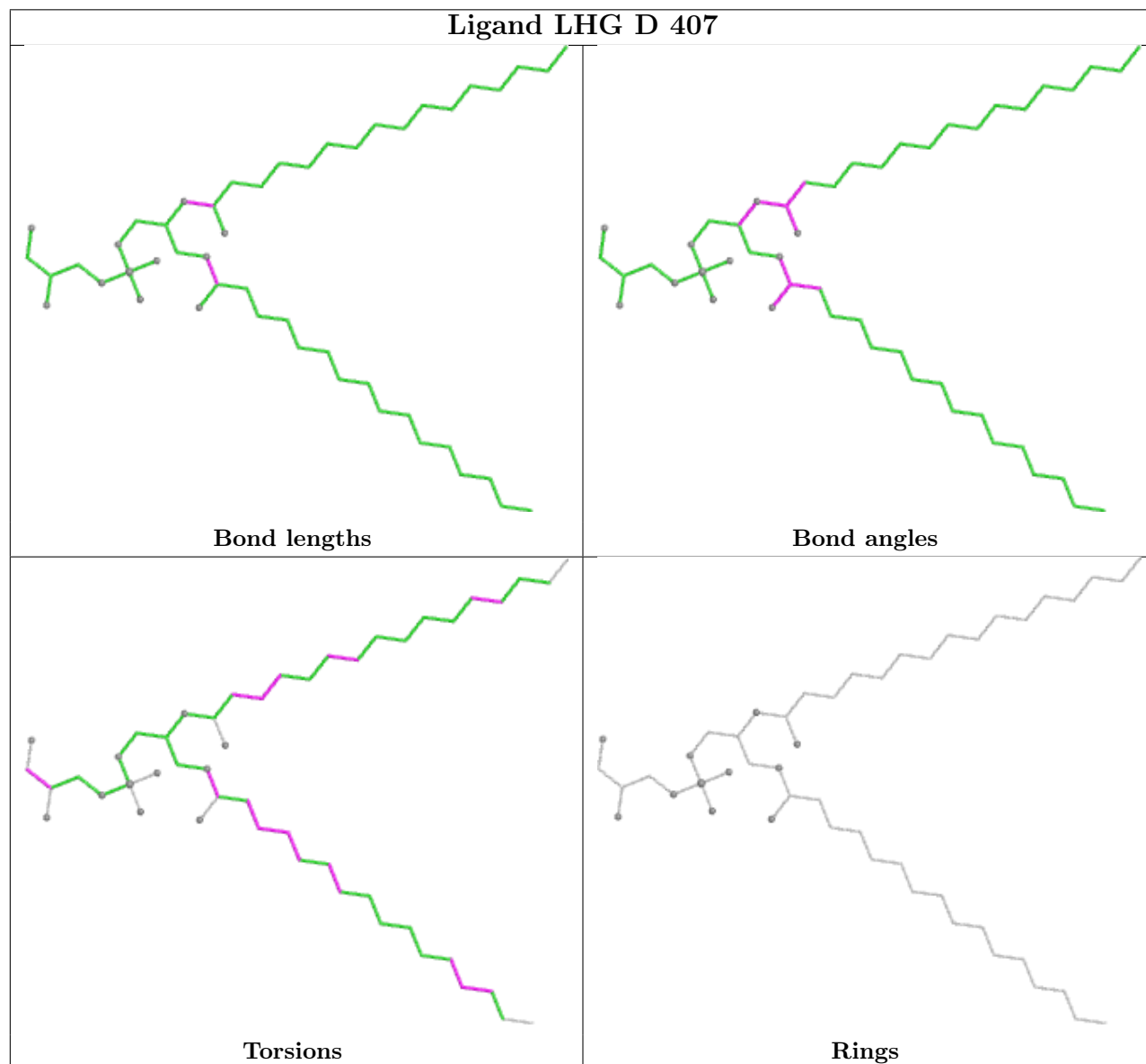
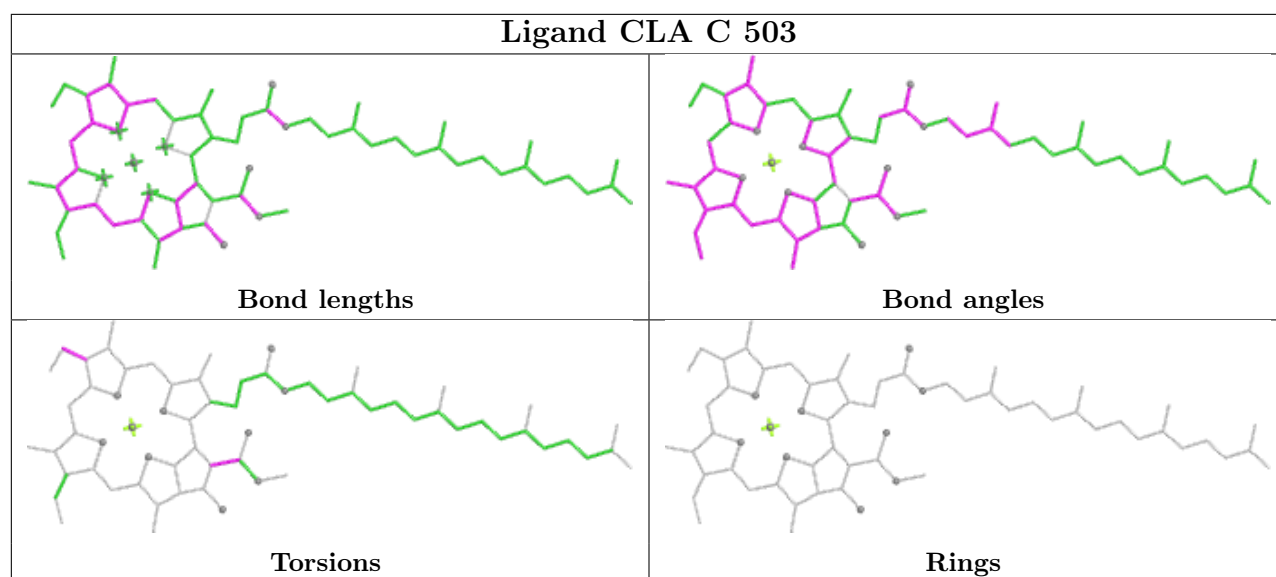


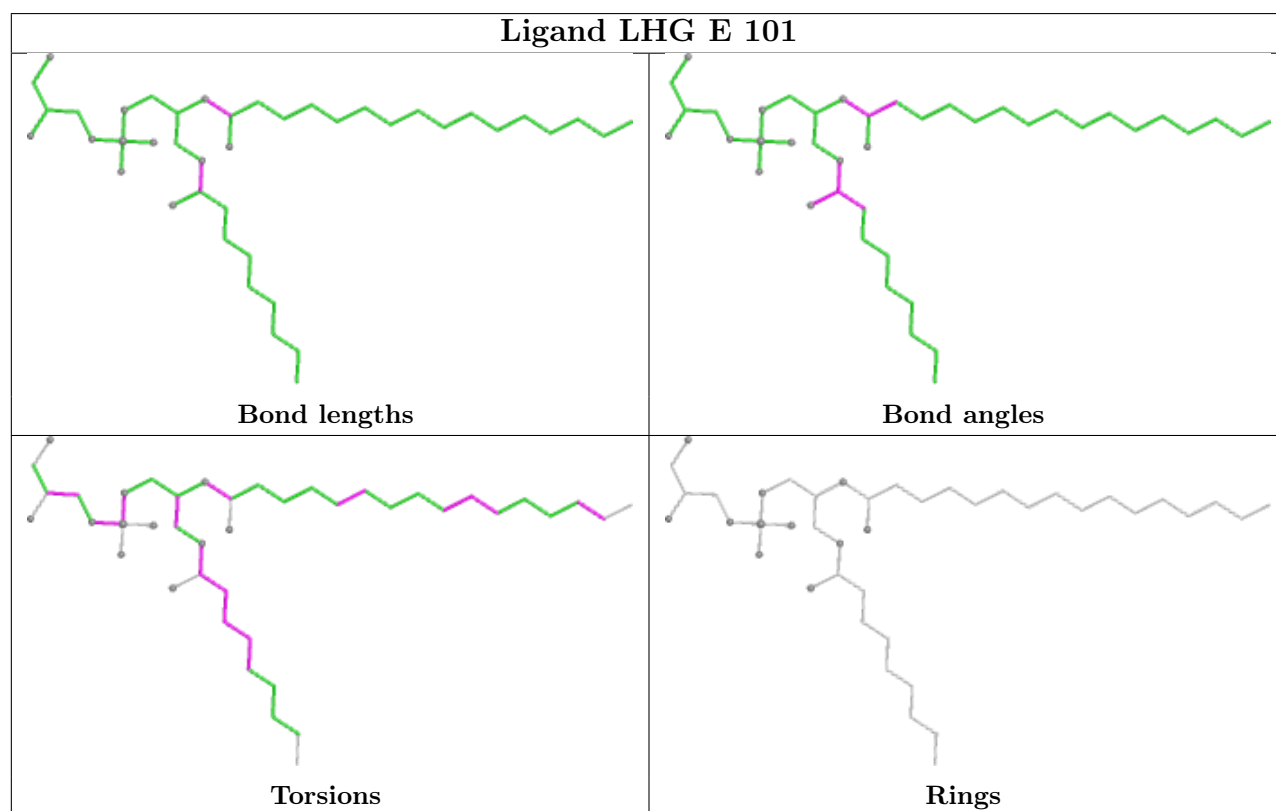
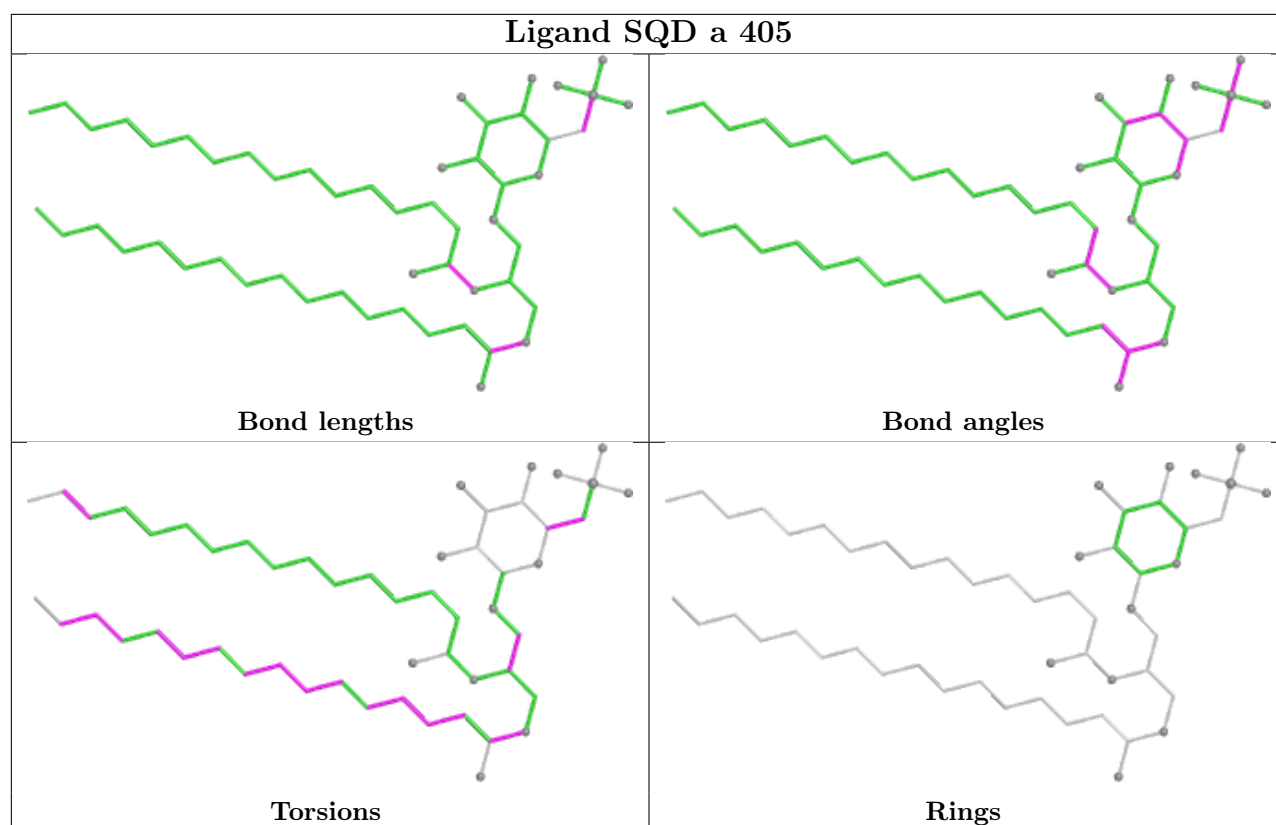
Ligand CLA b 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMT M 105	
	
Bond lengths	Bond angles
	
Torsions	Rings

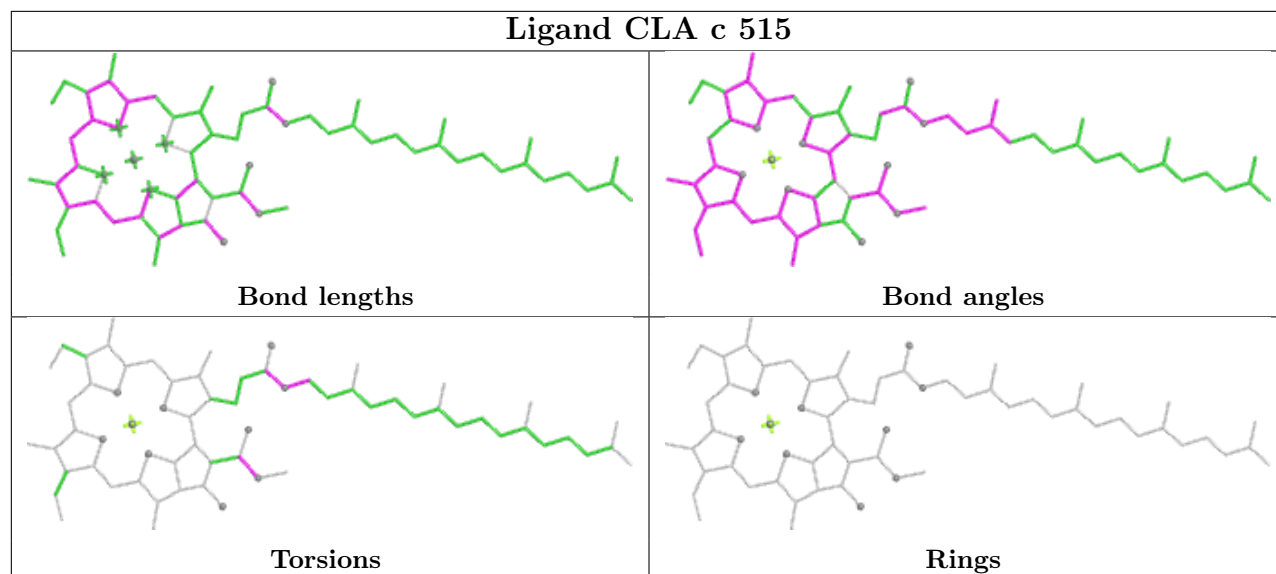
Ligand BCR y 101	
	
Bond lengths	Bond angles
	
Torsions	Rings



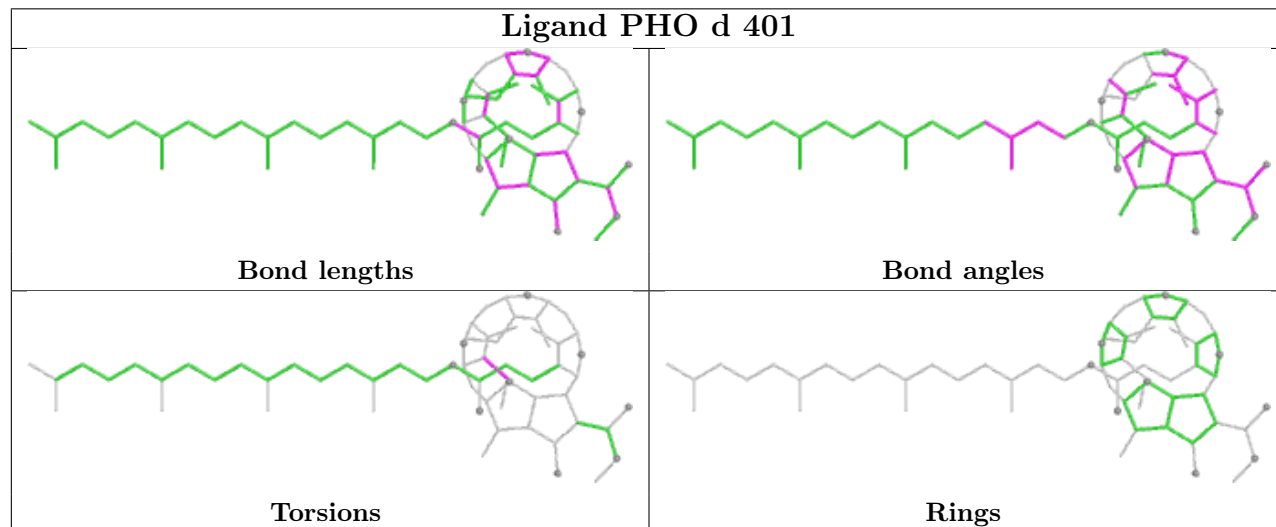




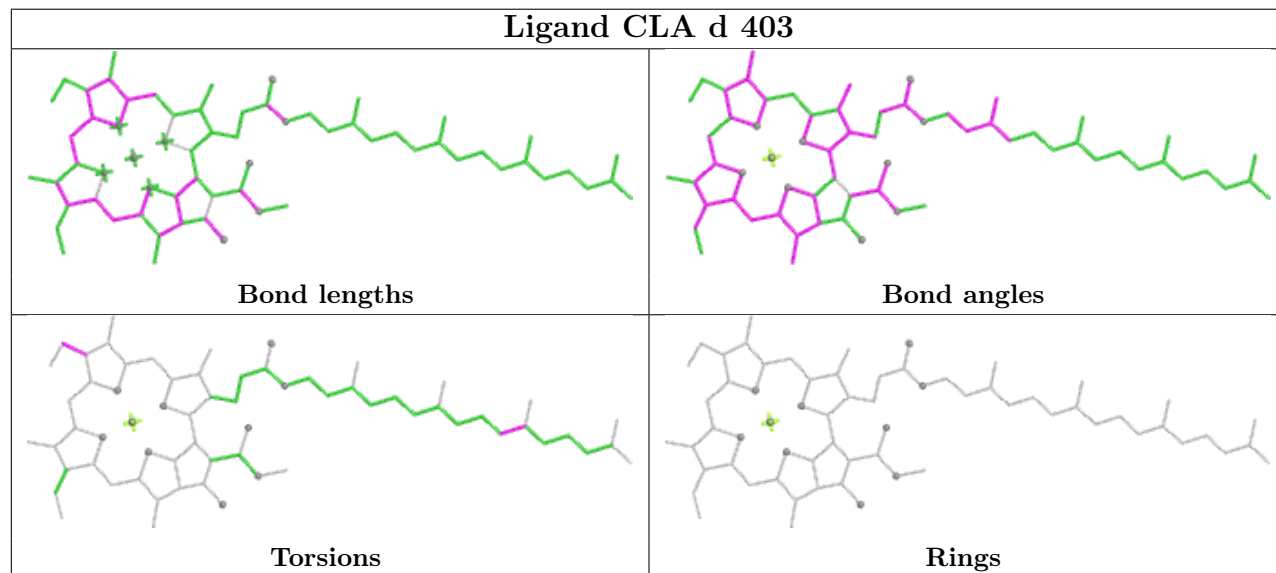
Ligand CLA c 515

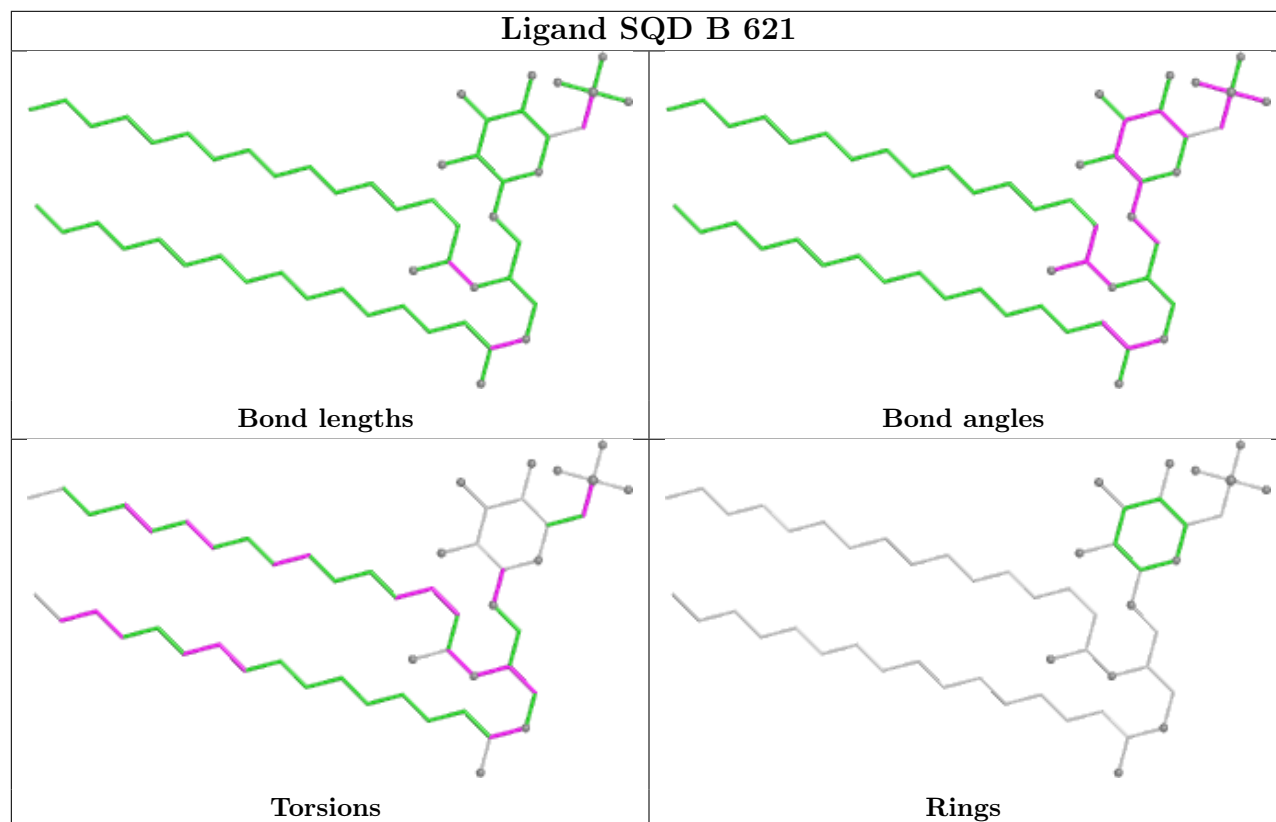
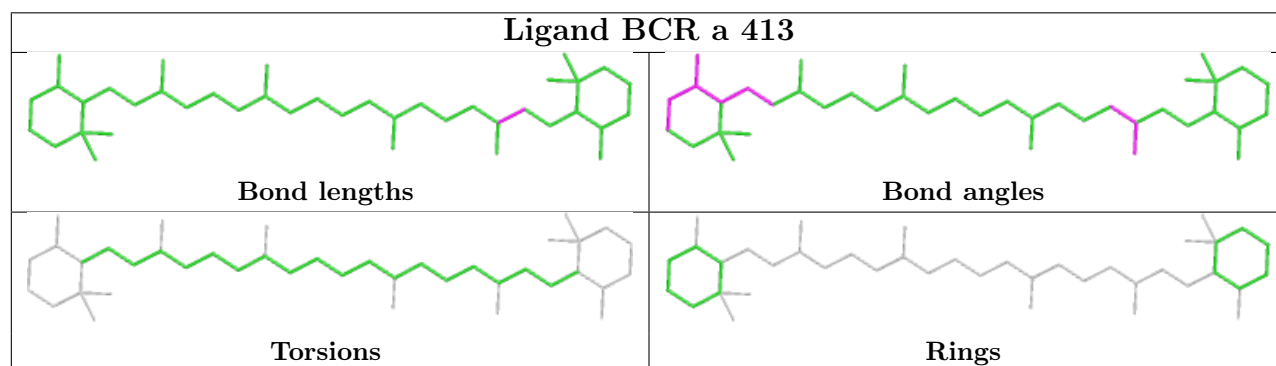
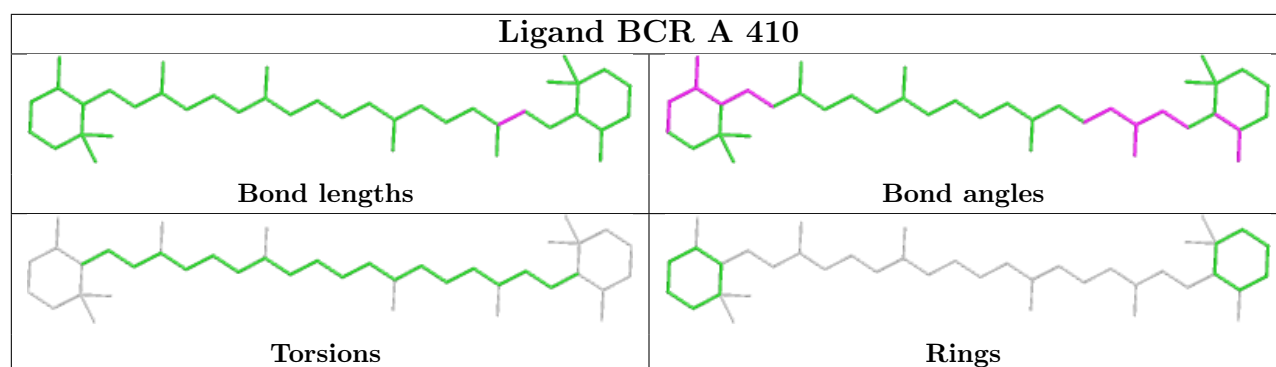


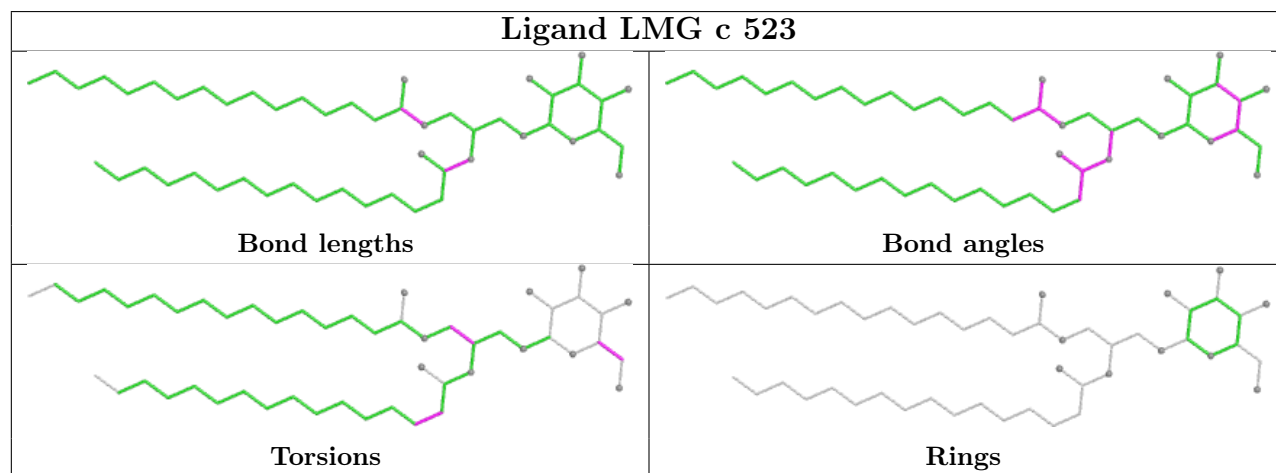
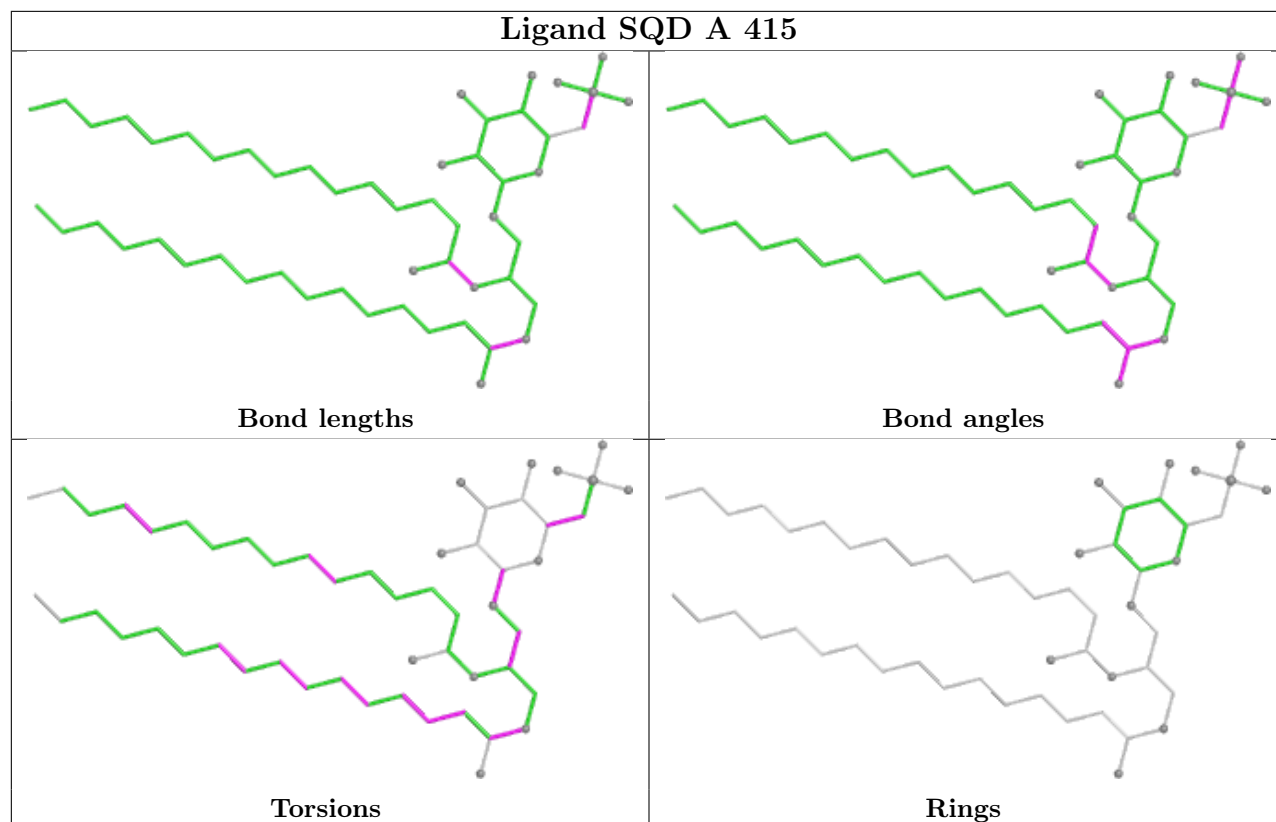
Ligand PHO d 401

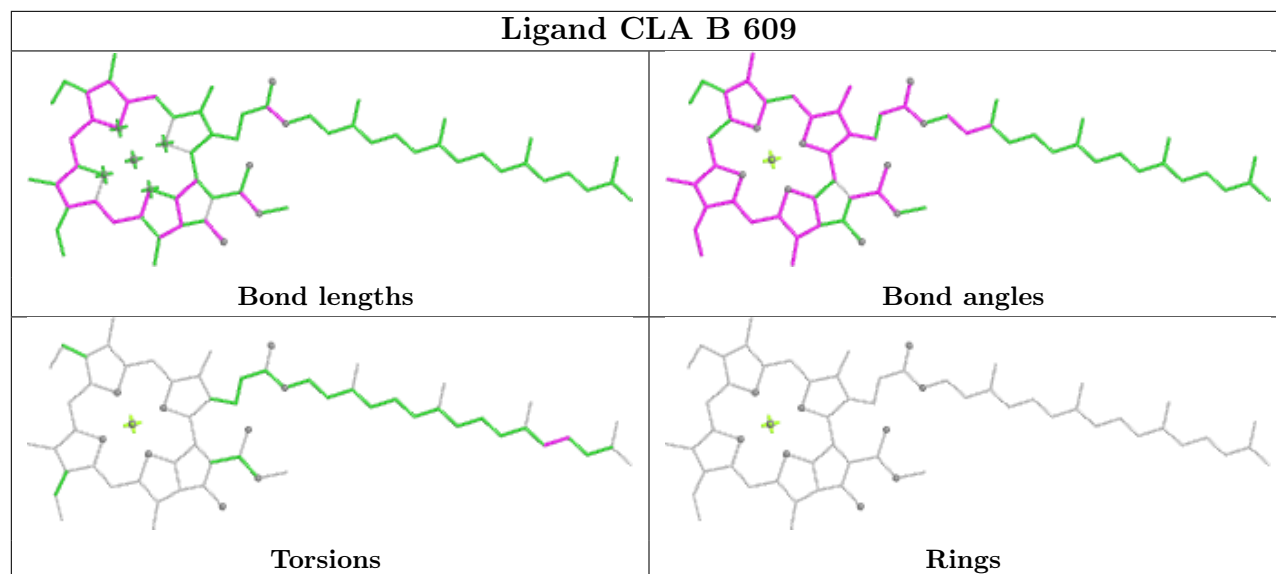
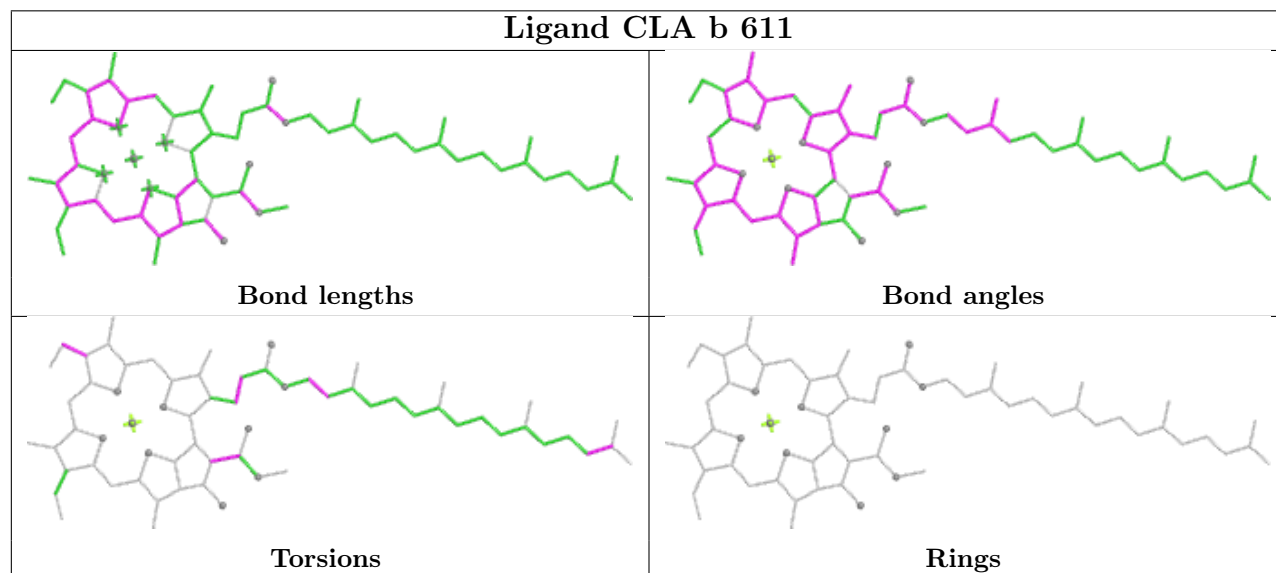
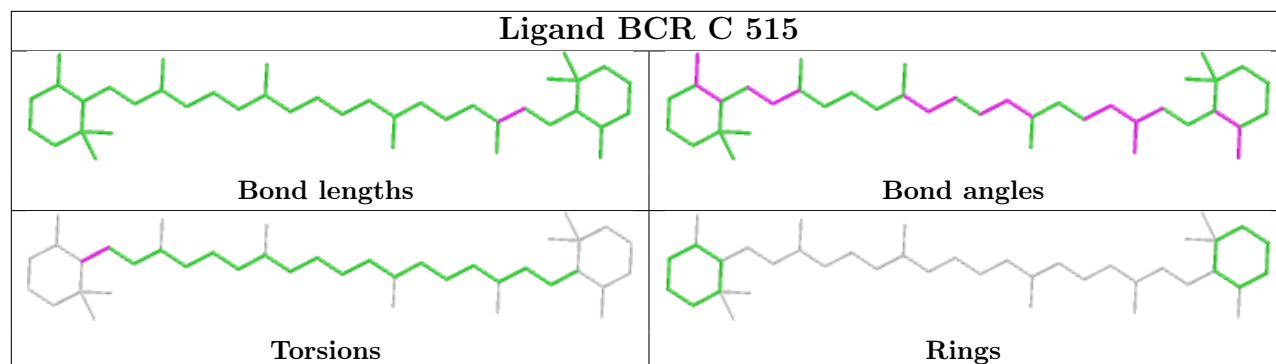


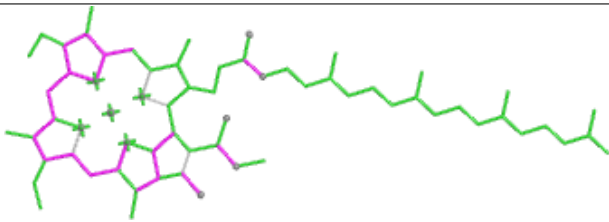
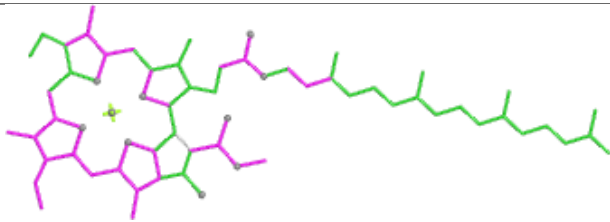
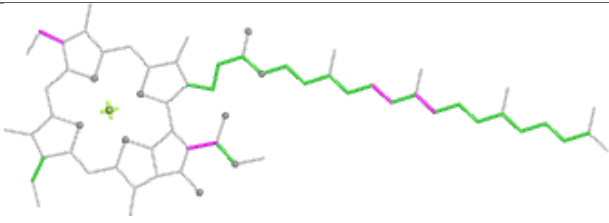
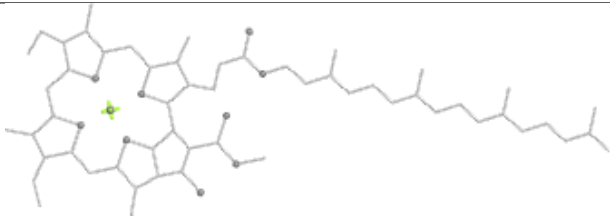
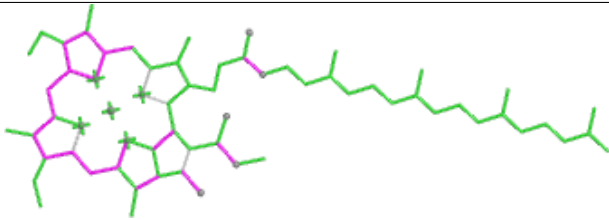
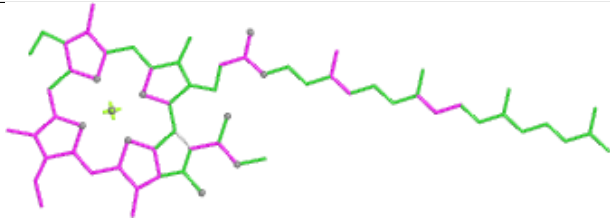
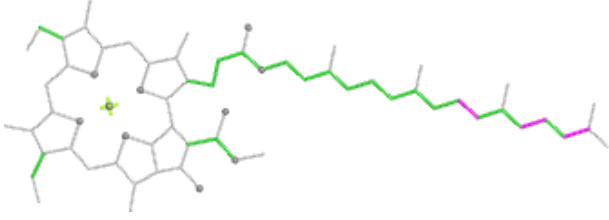
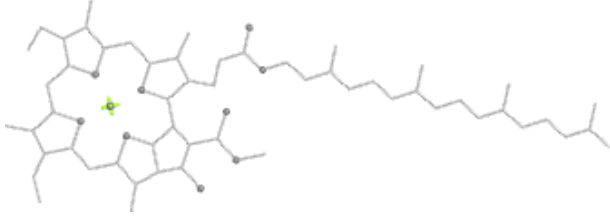
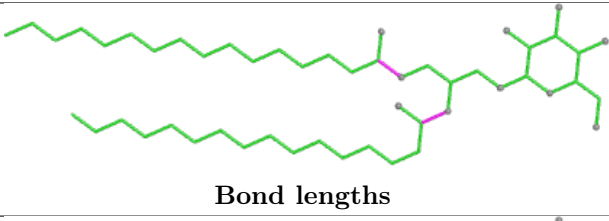
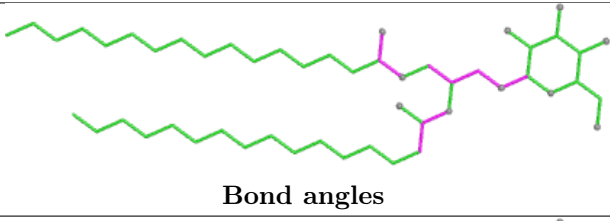
Ligand CLA d 403

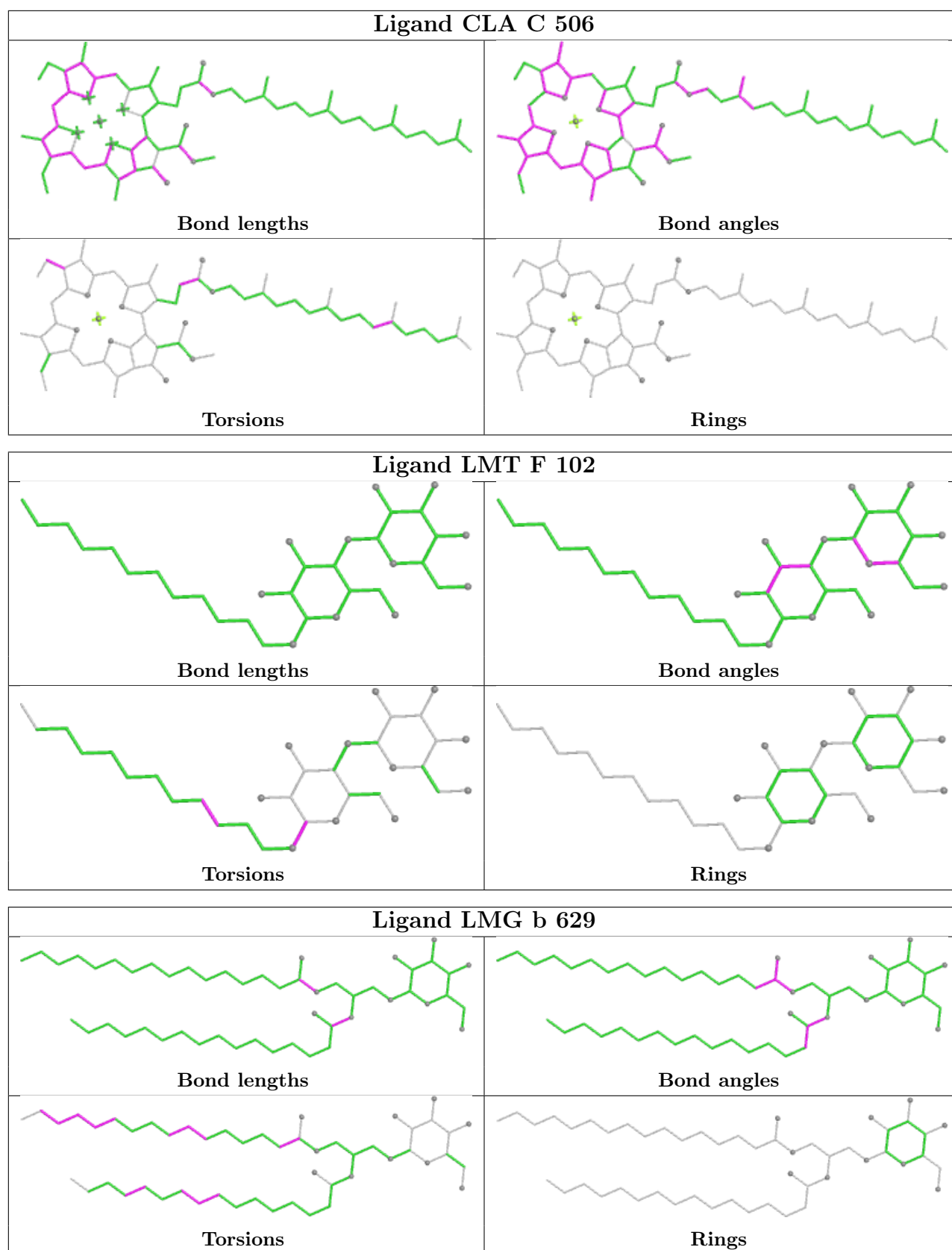


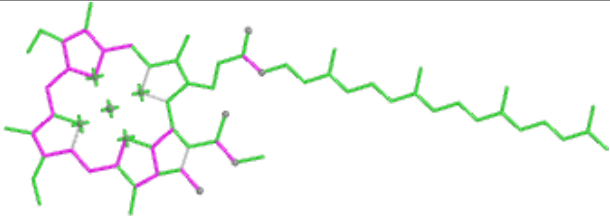
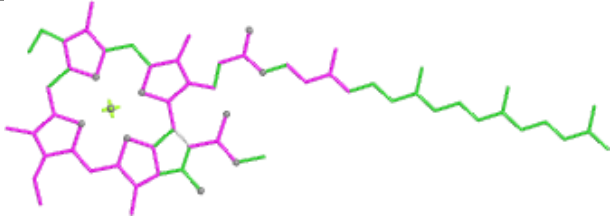
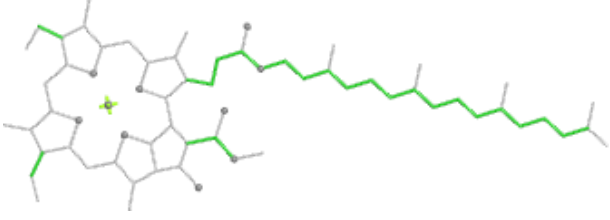
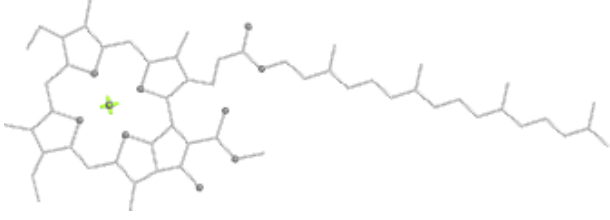
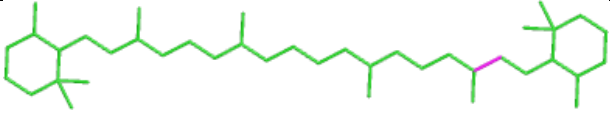
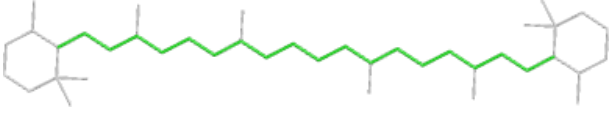
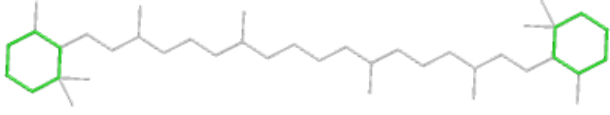
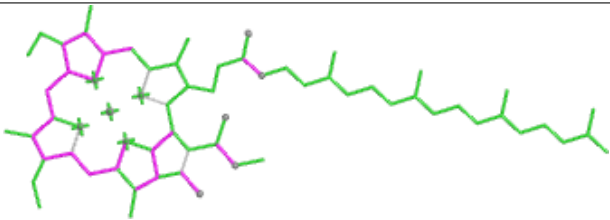
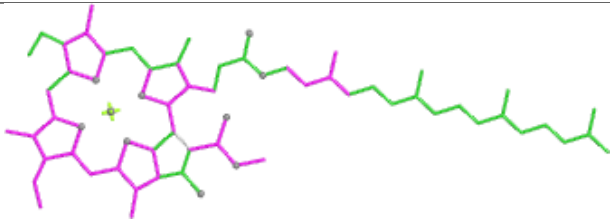
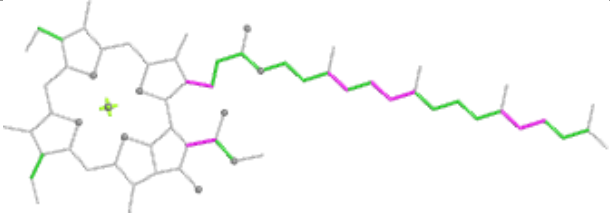
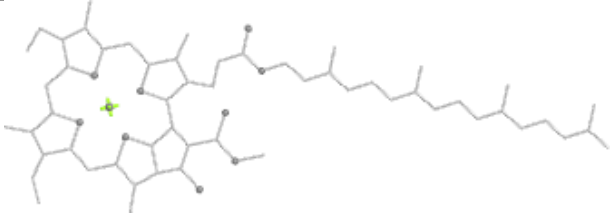


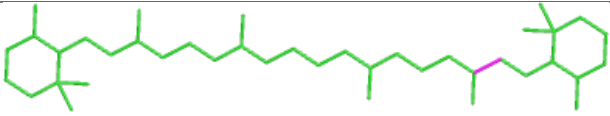
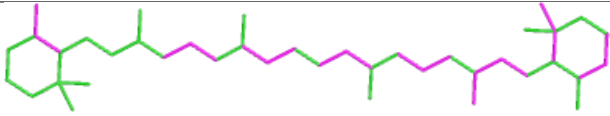
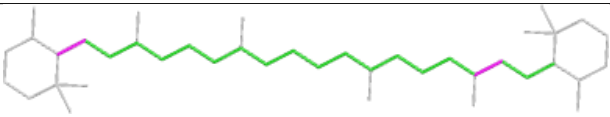
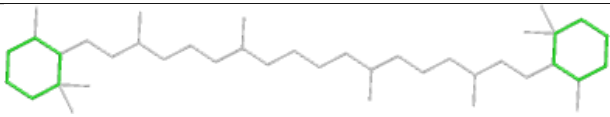
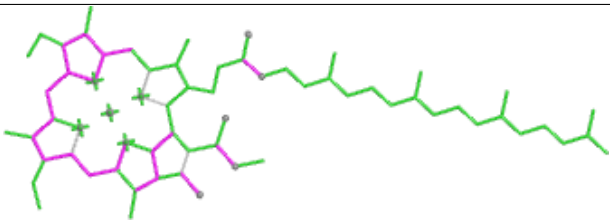
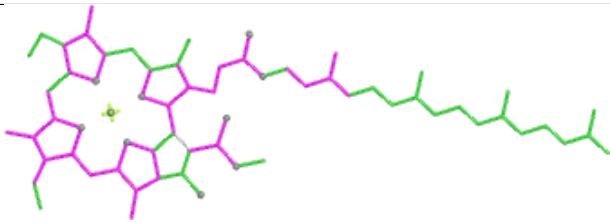
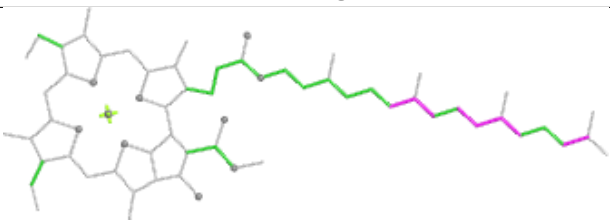
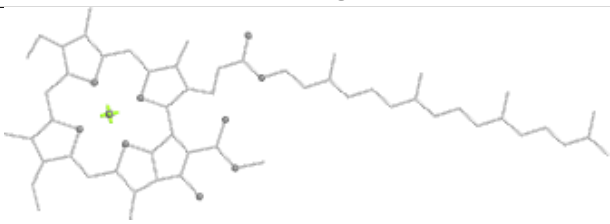
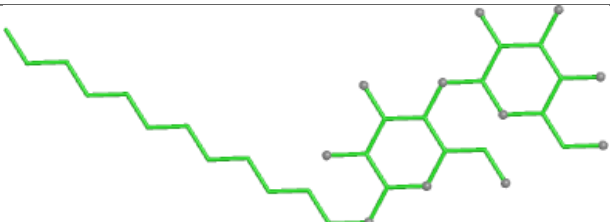
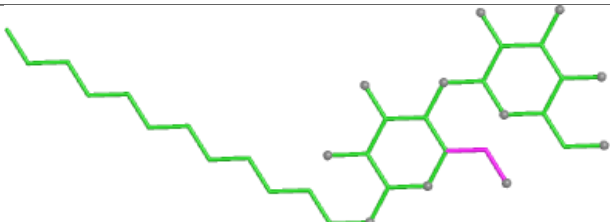
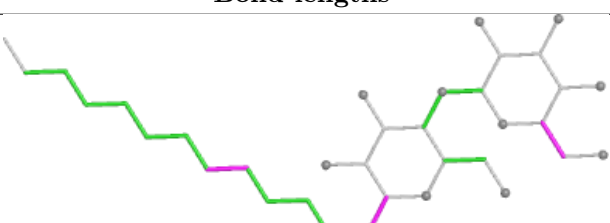
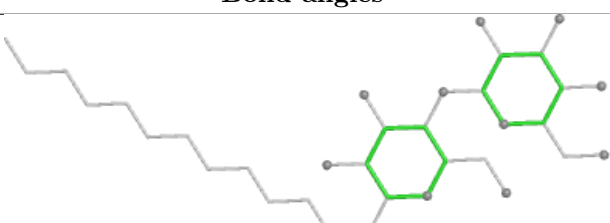


Ligand CLA B 609**Ligand CLA b 611****Ligand BCR C 515**

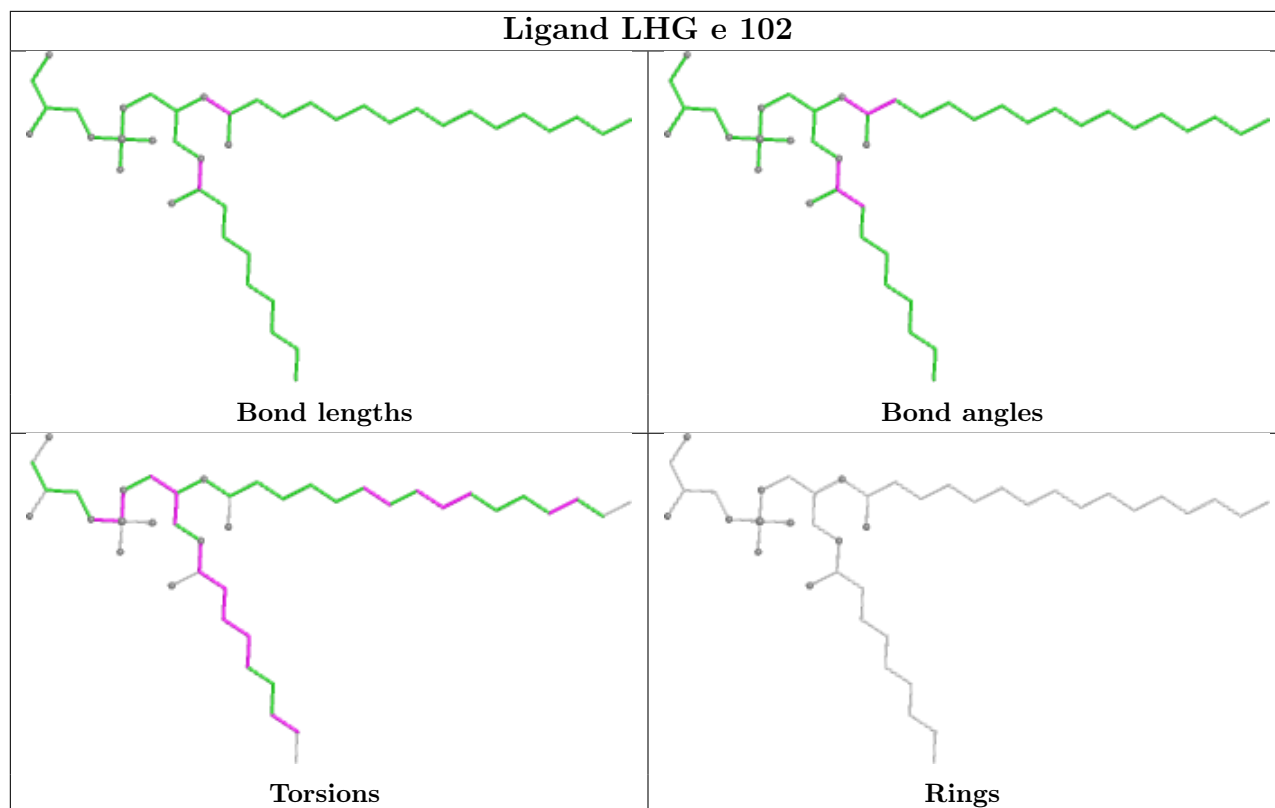
Ligand CLA C 508	
	
Bond lengths	
	Bond angles
	
Torsions	
	Rings
Ligand CLA b 624	
	
Bond lengths	
	Bond angles
	
Torsions	
	Rings
Ligand LMG J 101	
	
Bond lengths	
	Bond angles
	
Torsions	
	Rings



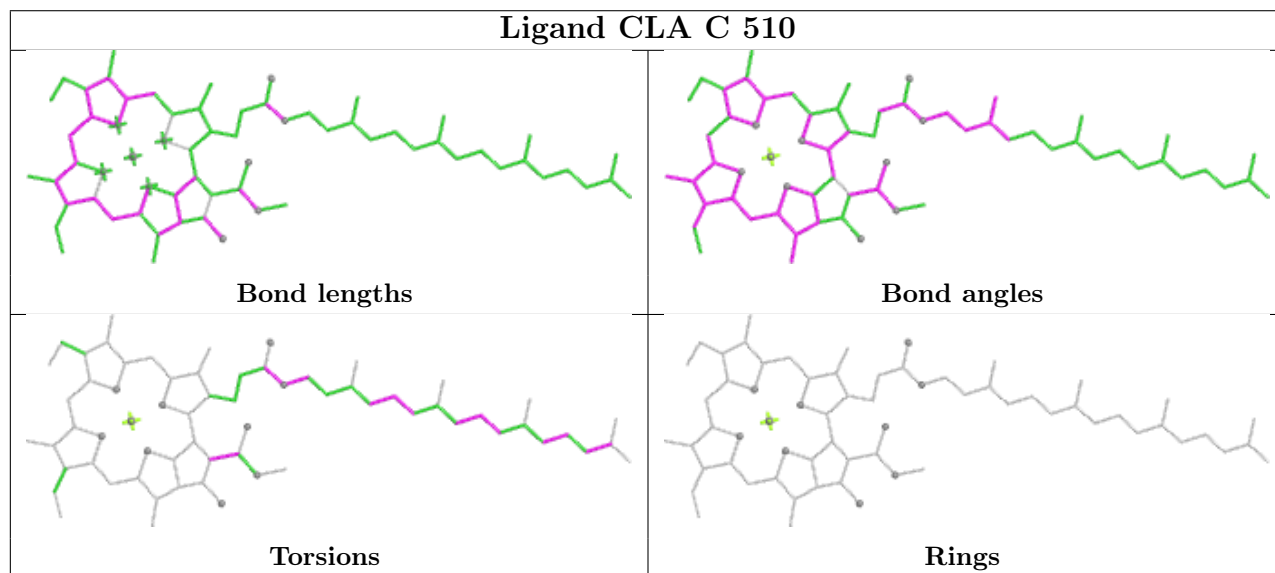
Ligand CLA D 402	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 619	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA C 507	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR Y 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA a 410	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMT M 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

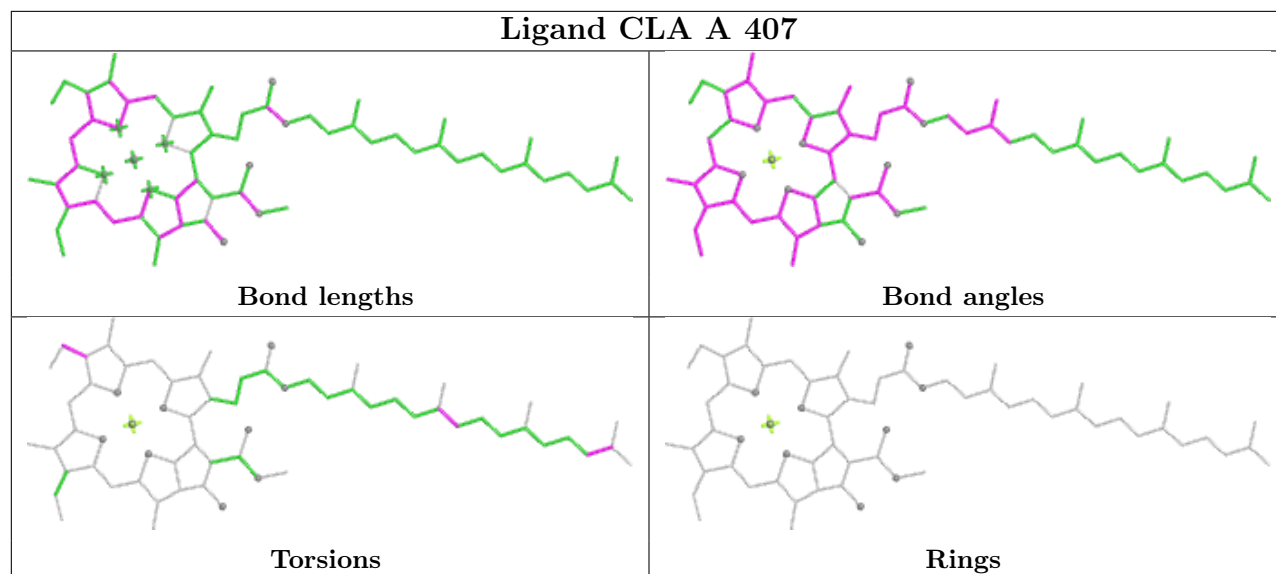
Ligand LHG e 102



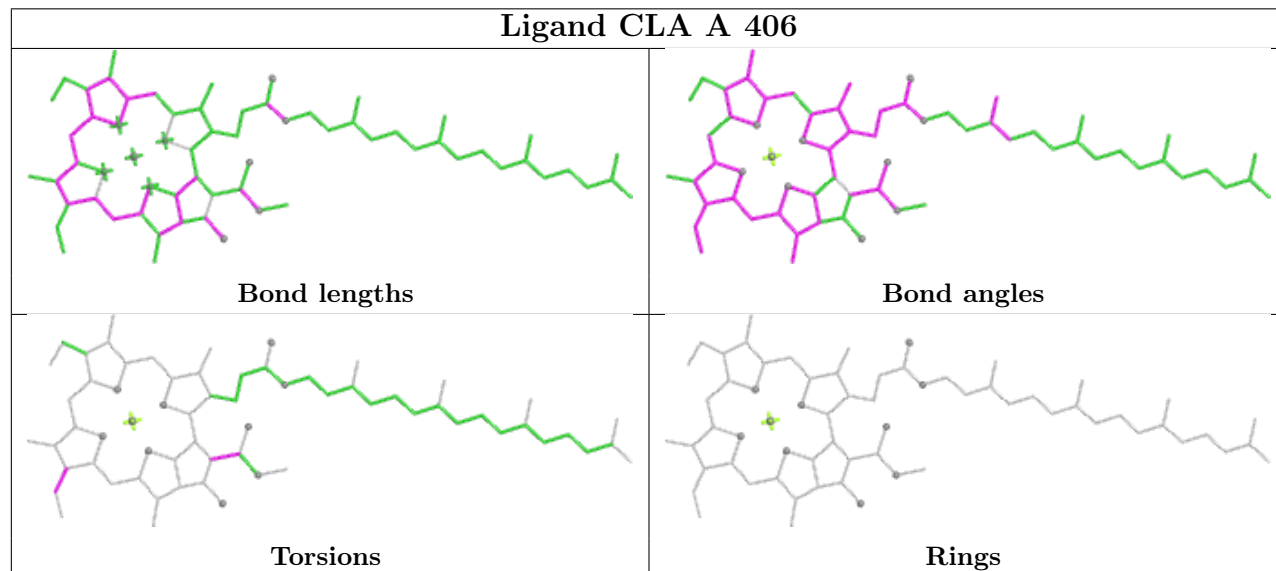
Ligand CLA C 510

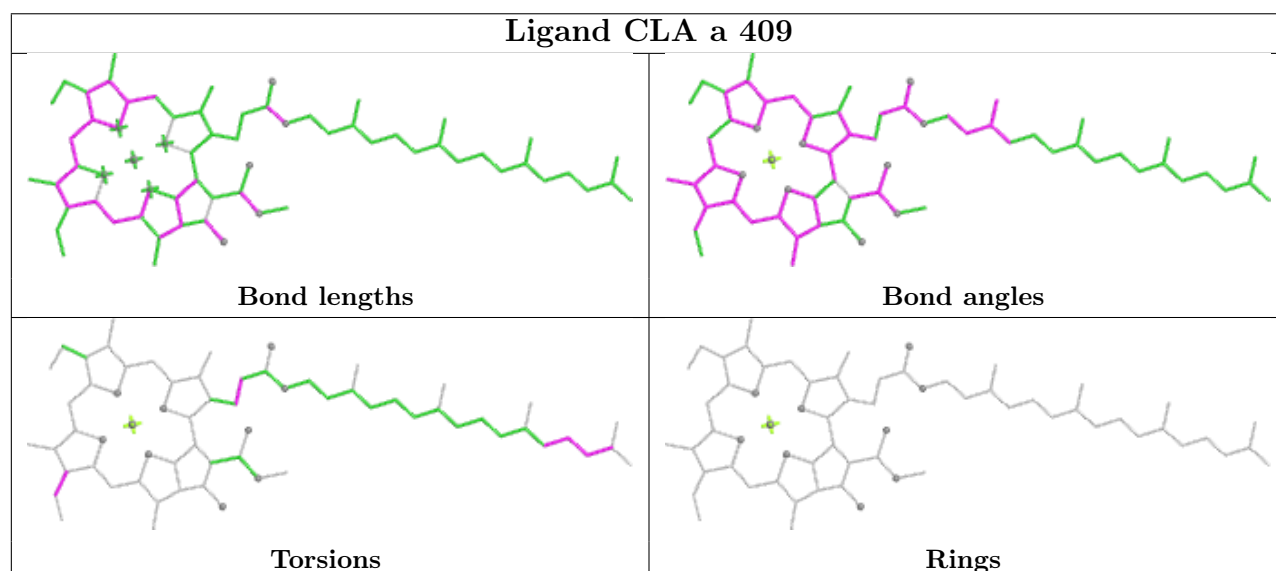
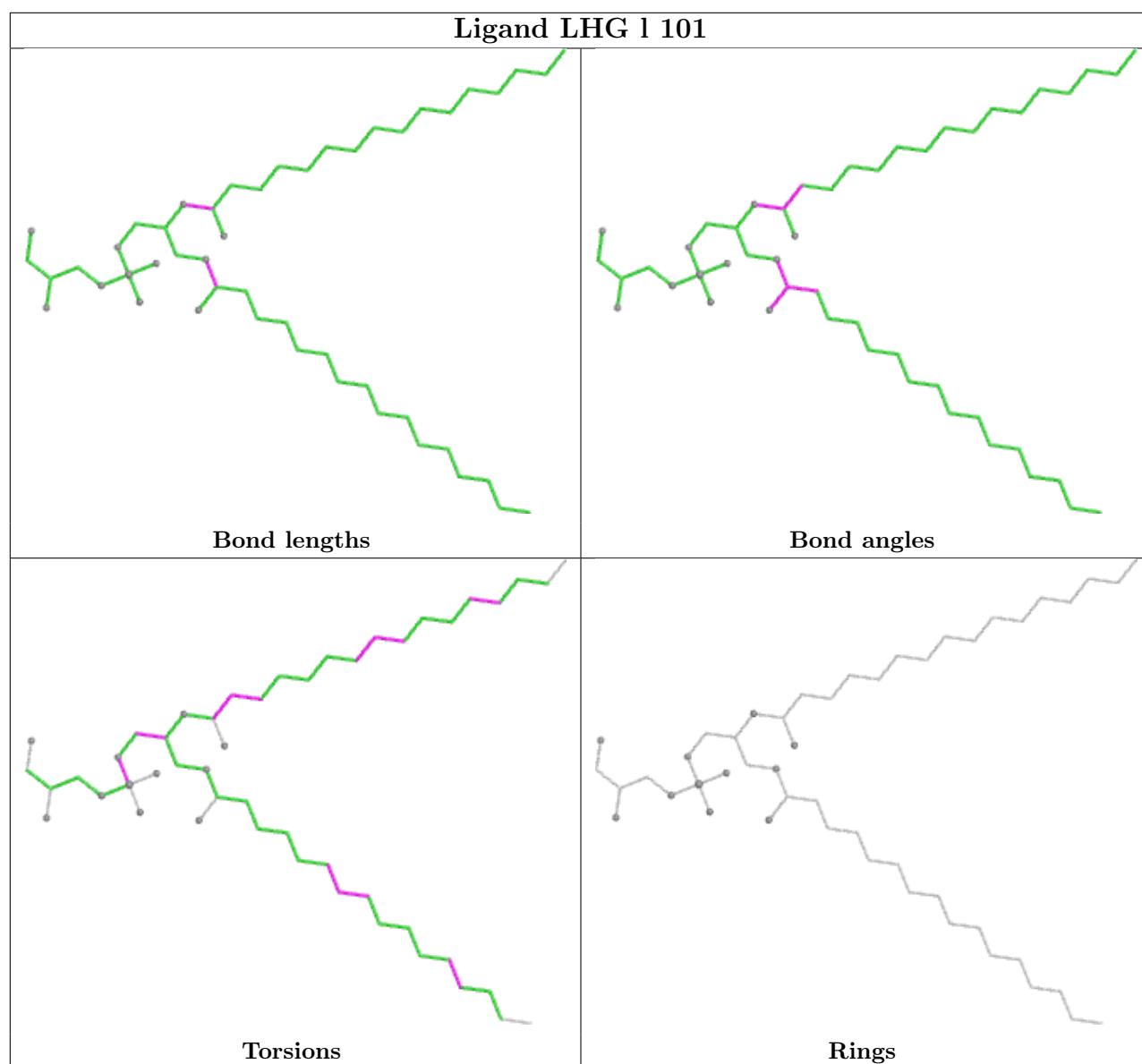


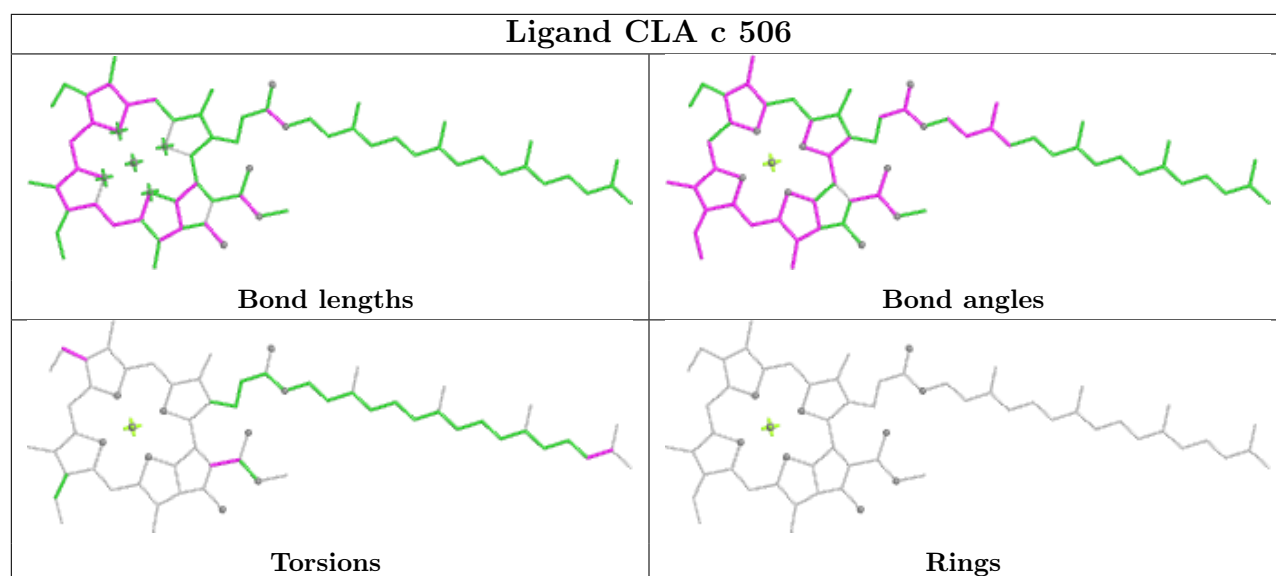
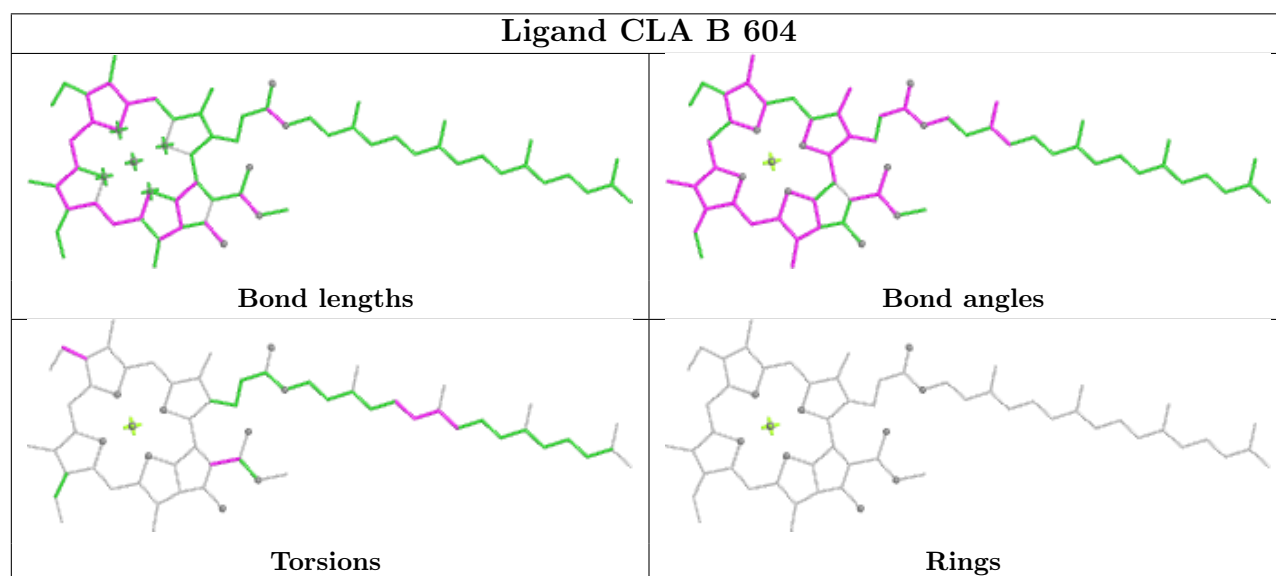
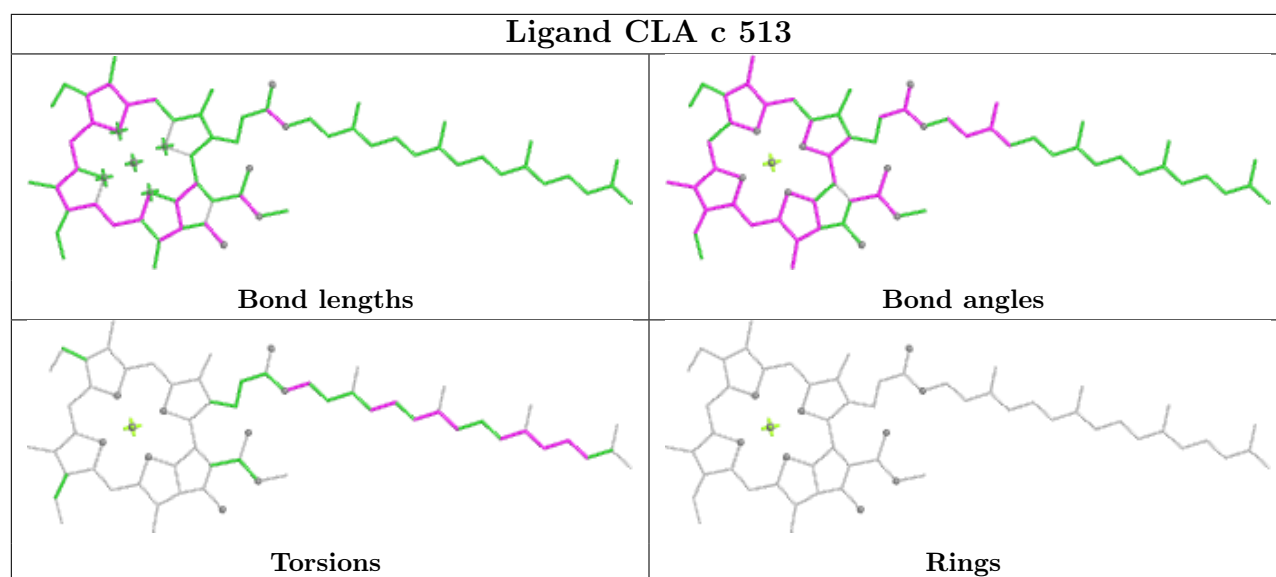
Ligand CLA A 407

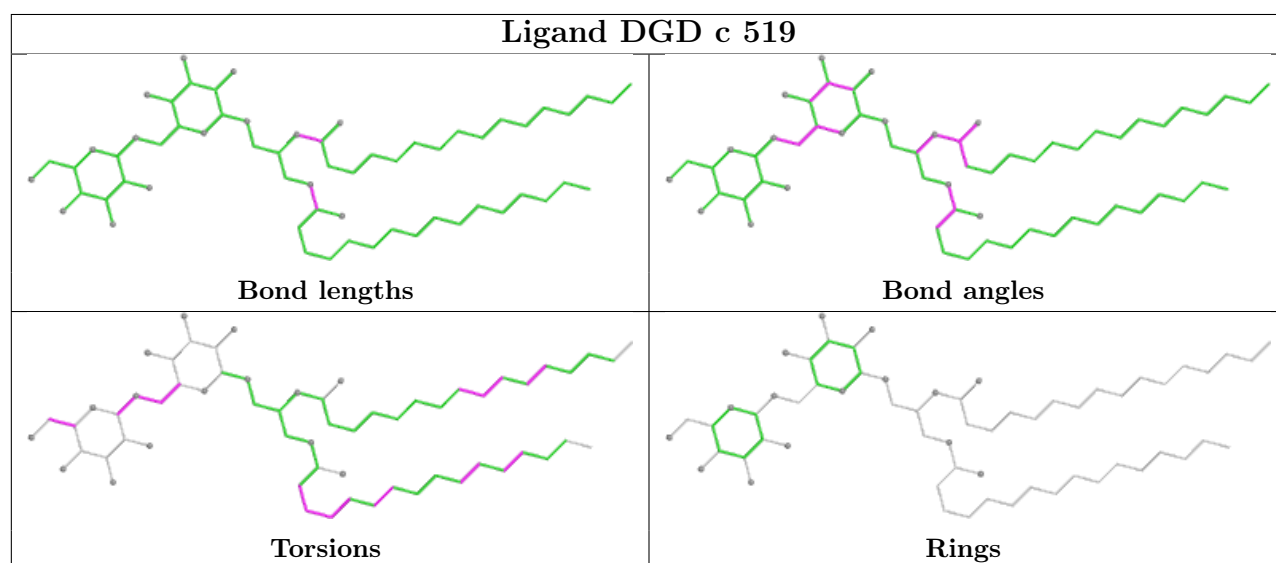
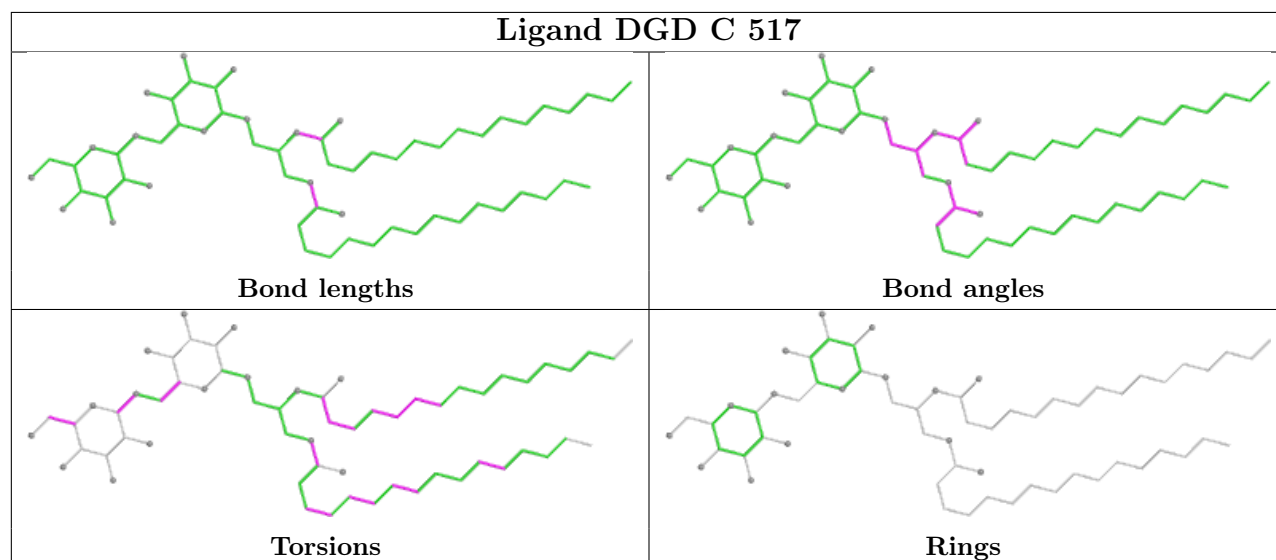
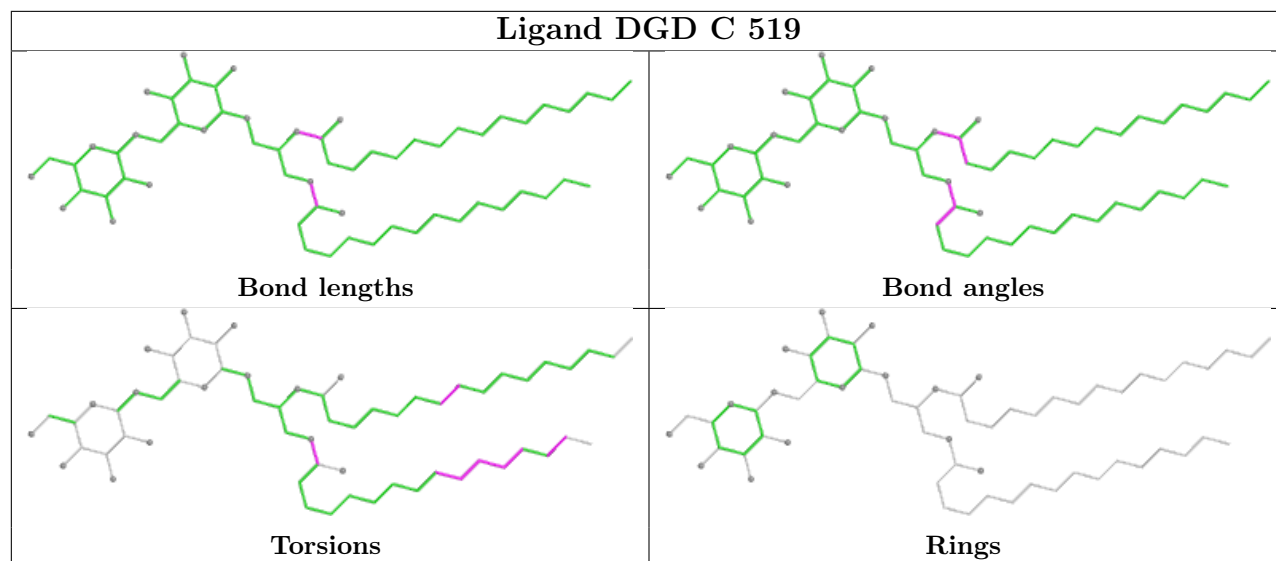


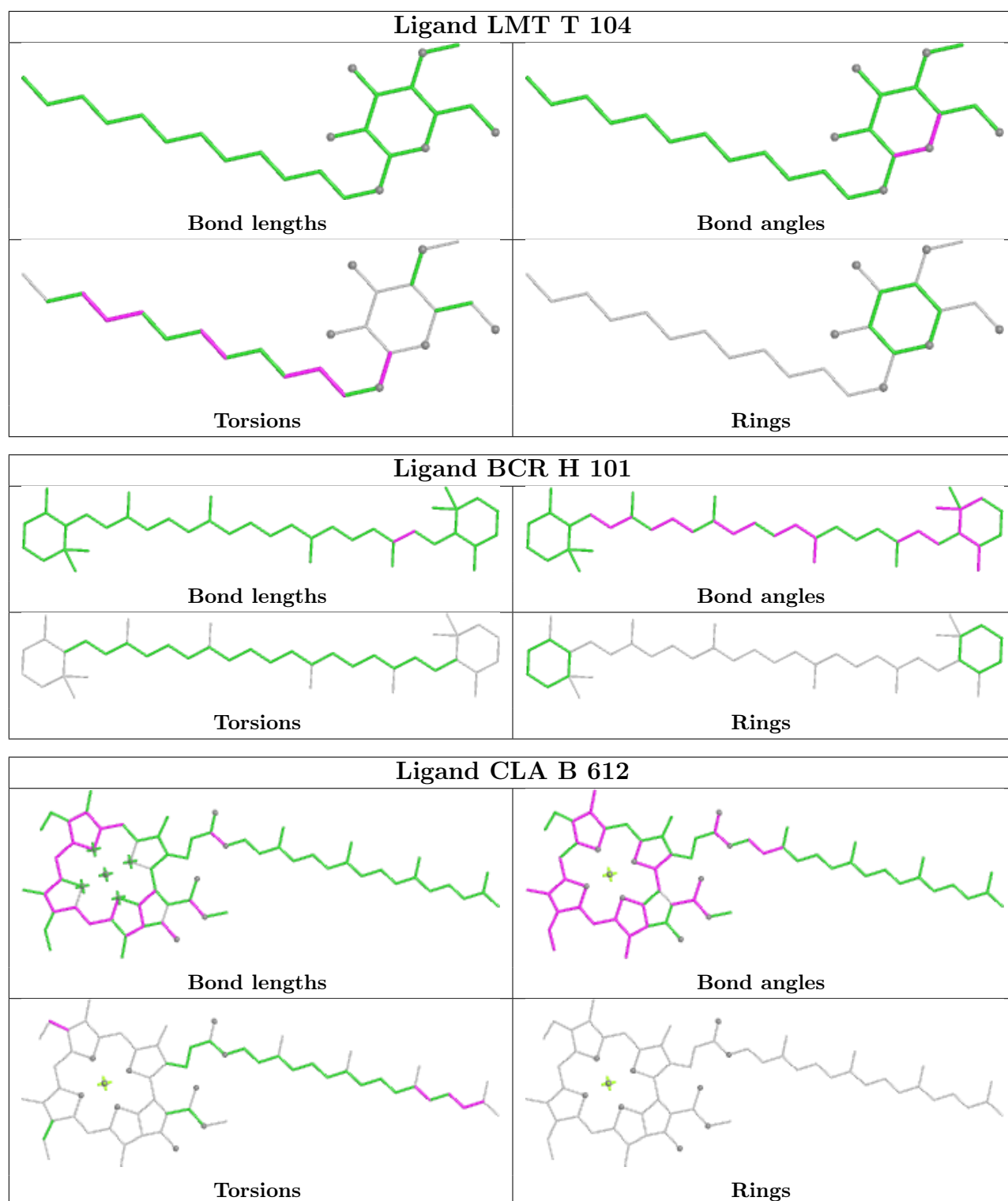
Ligand CLA A 406

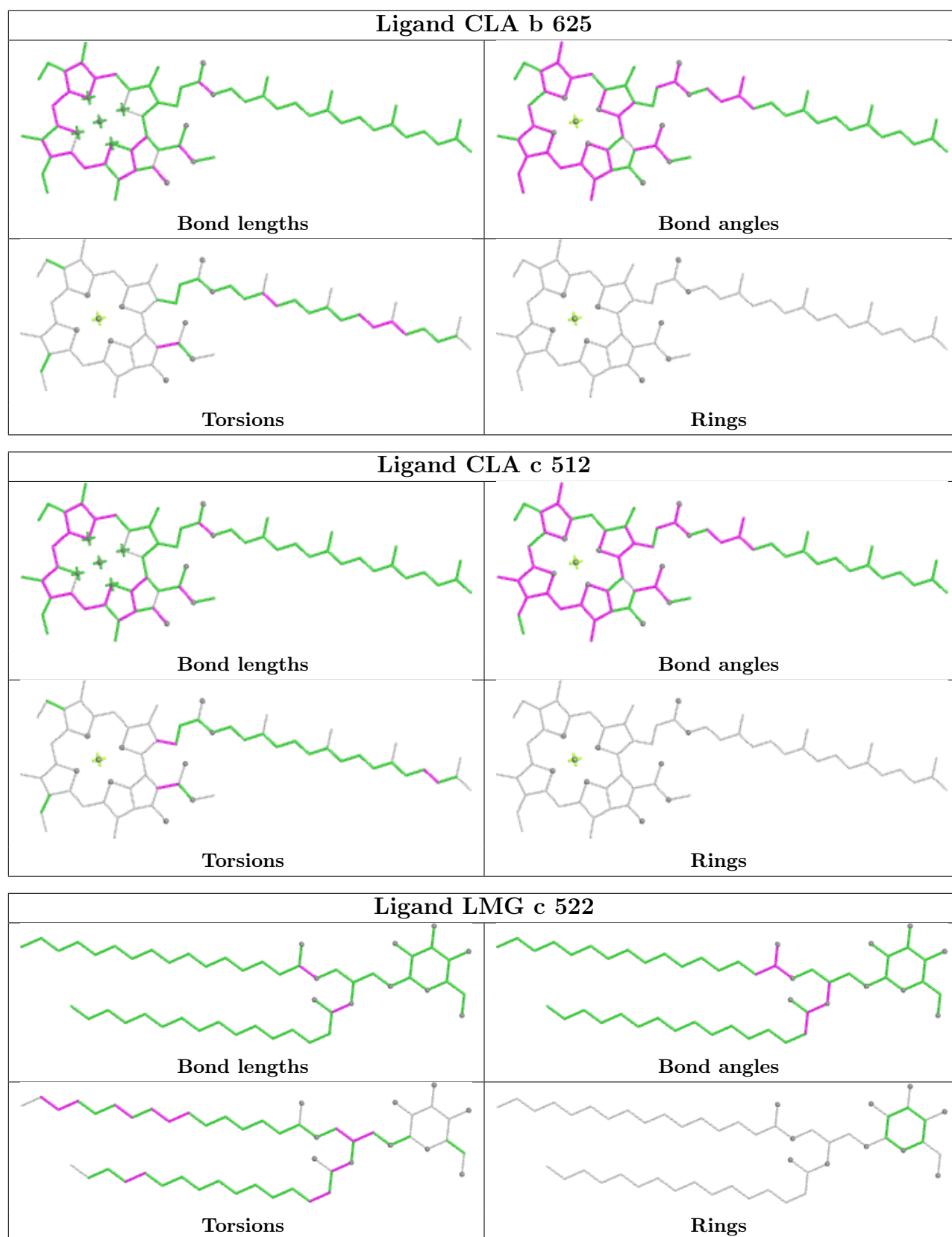


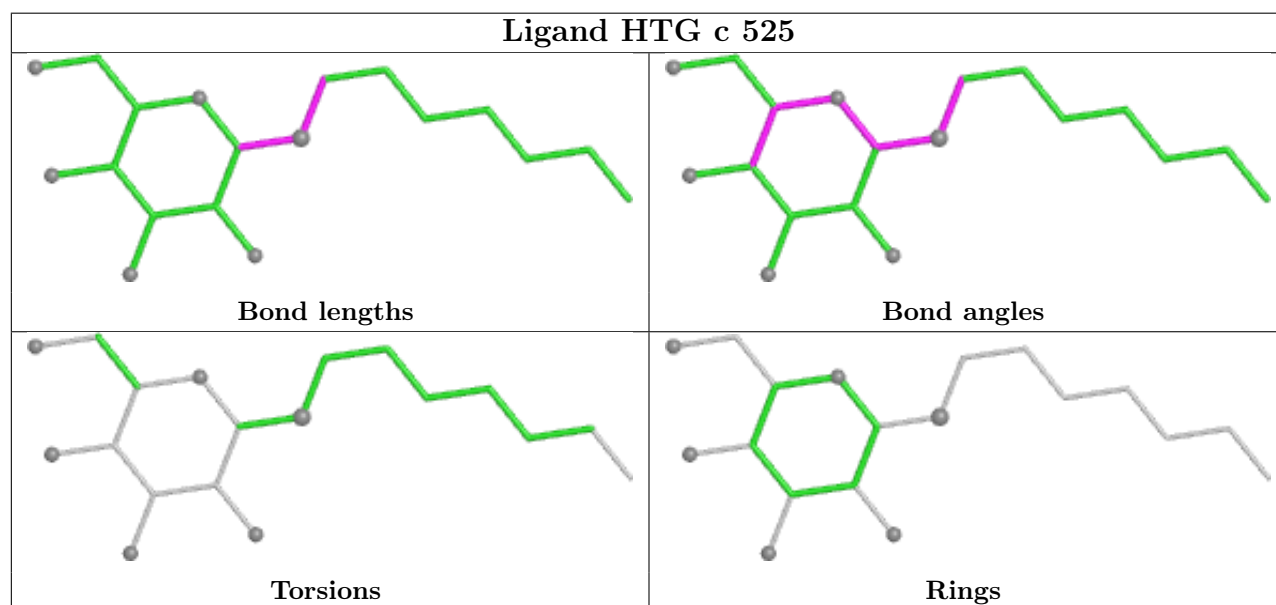
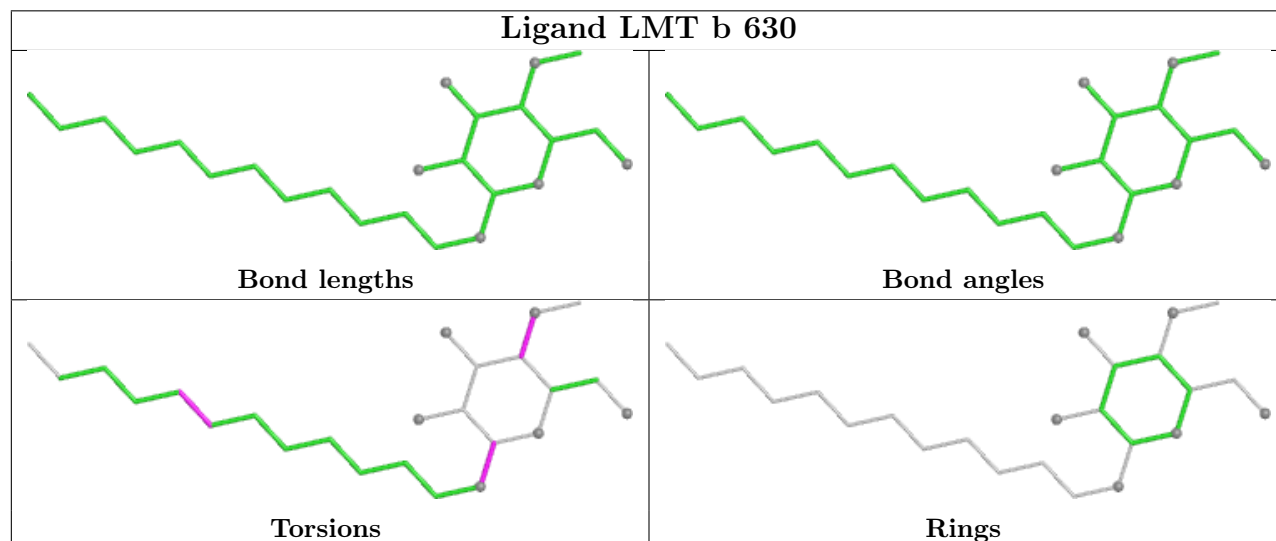
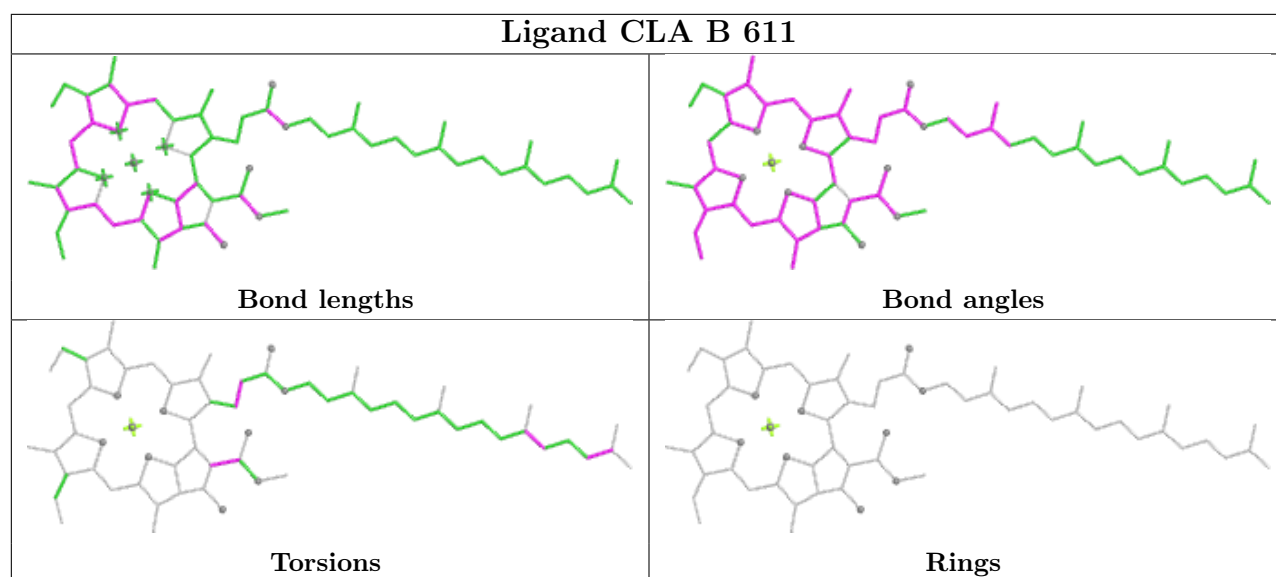


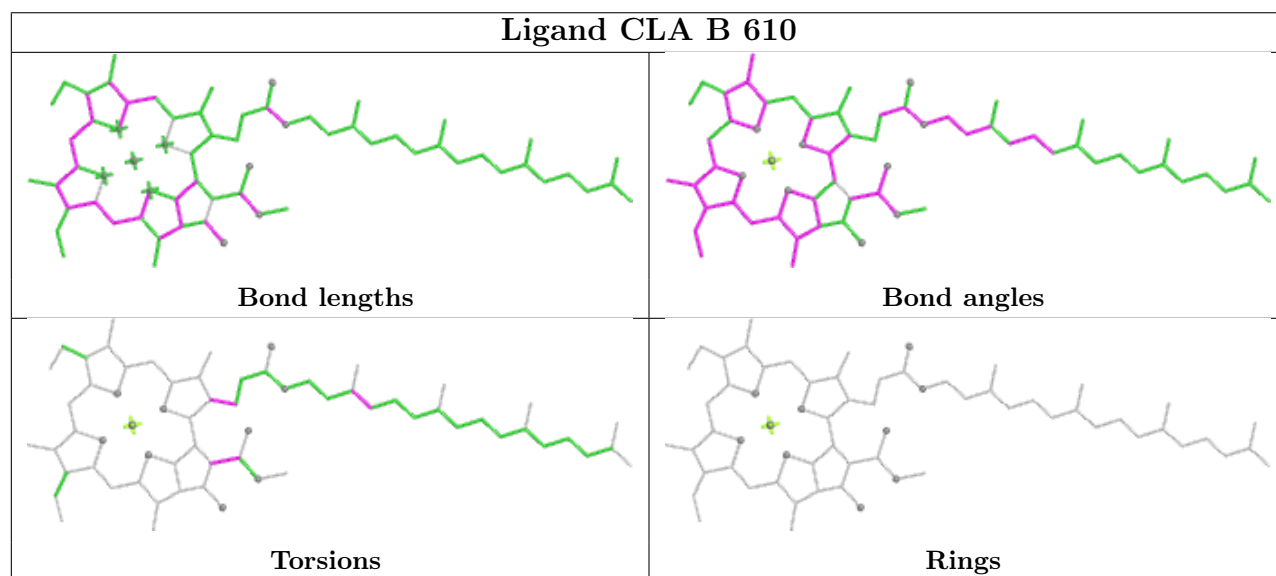
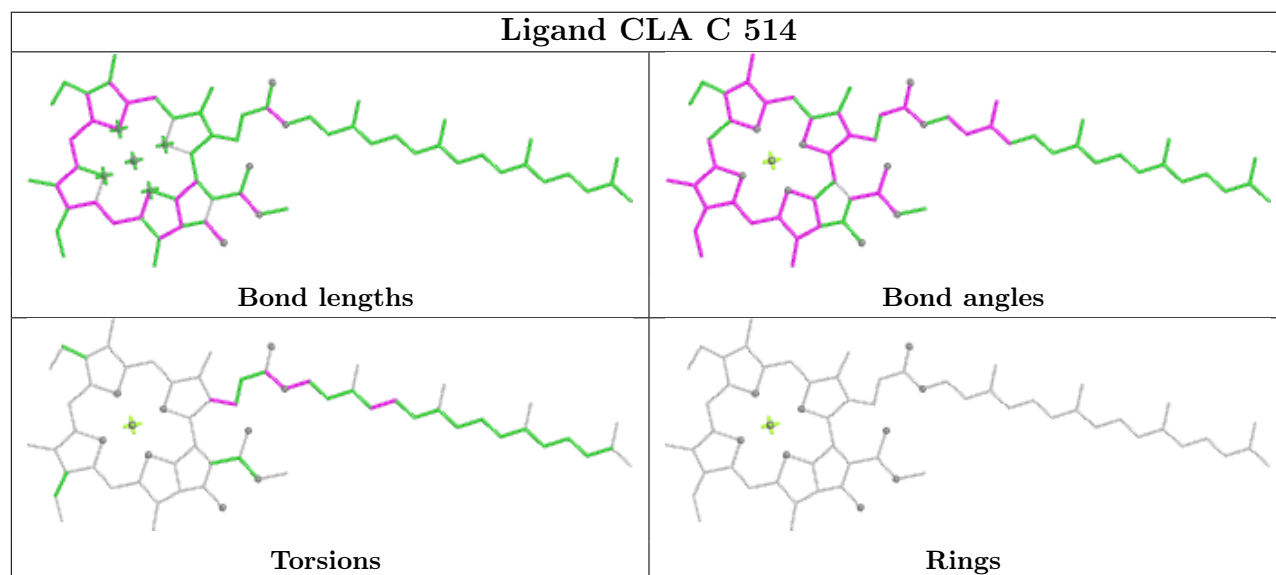
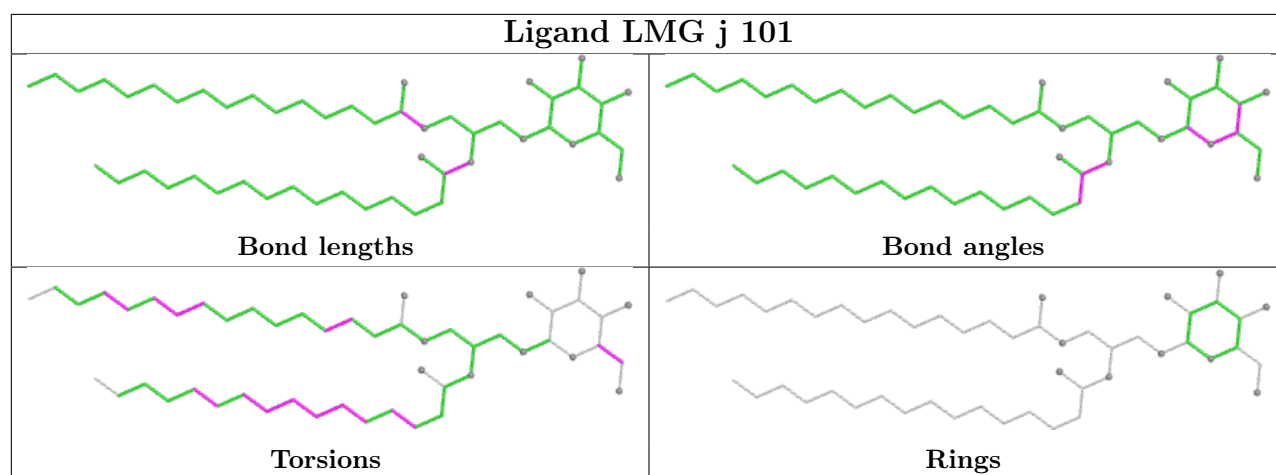




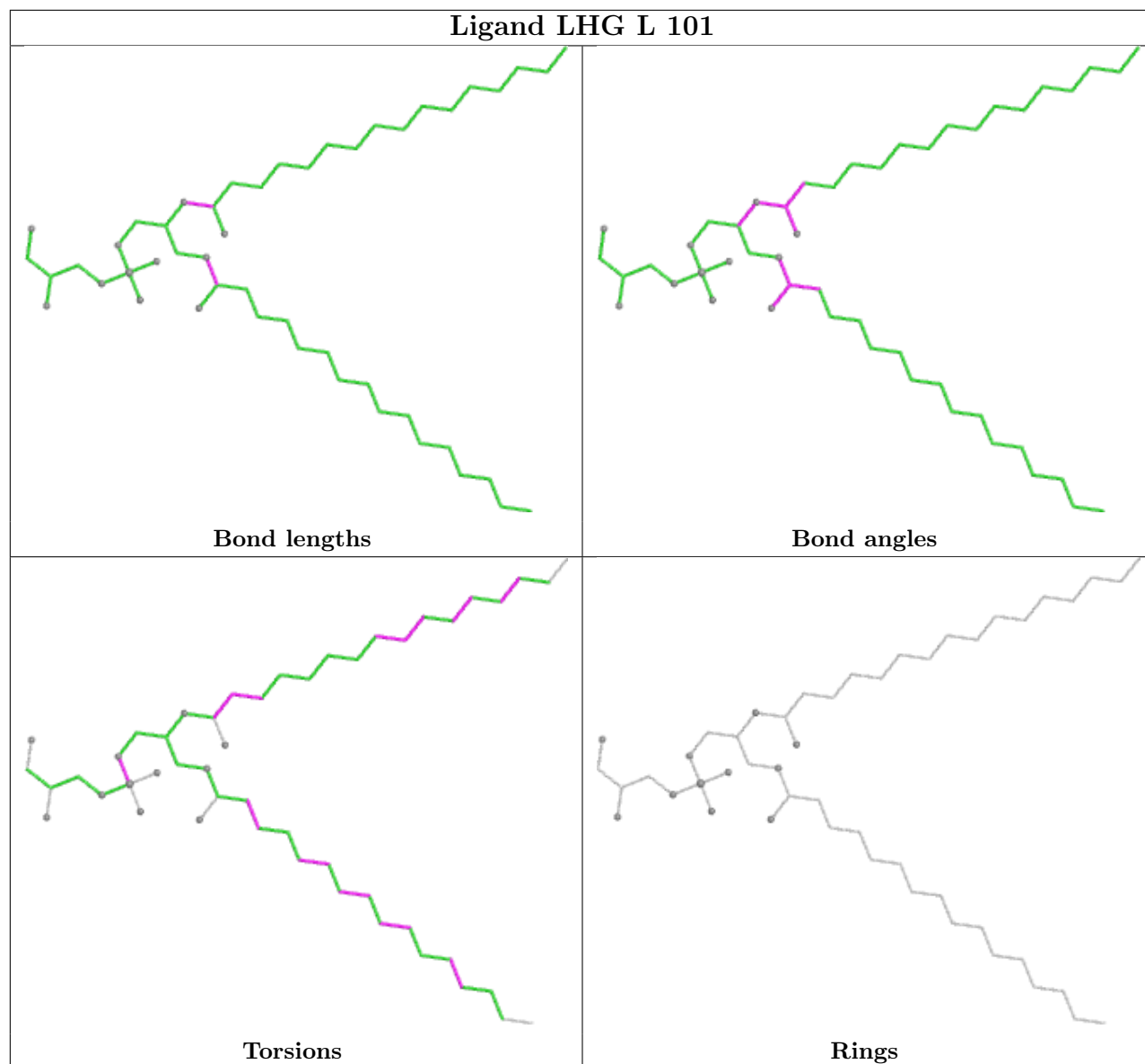




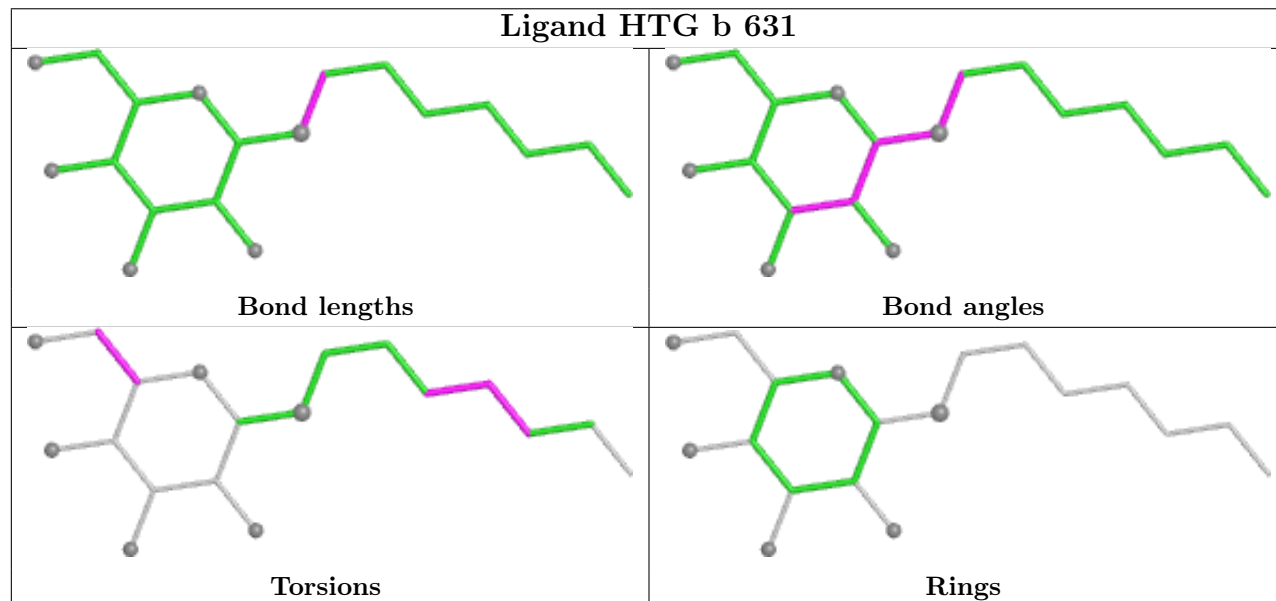


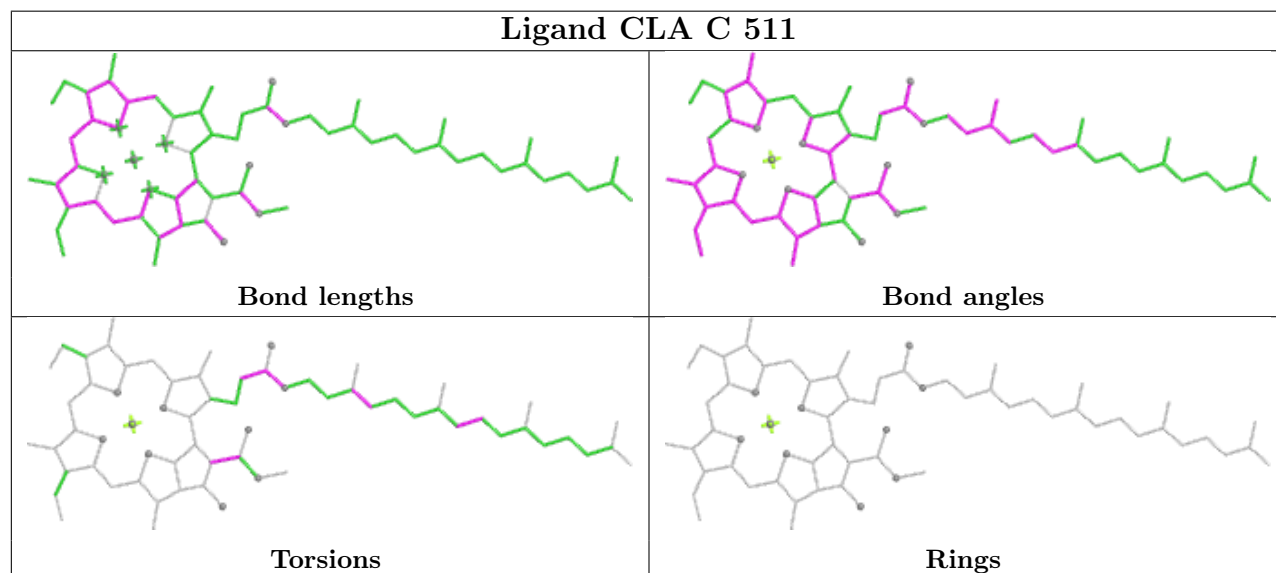
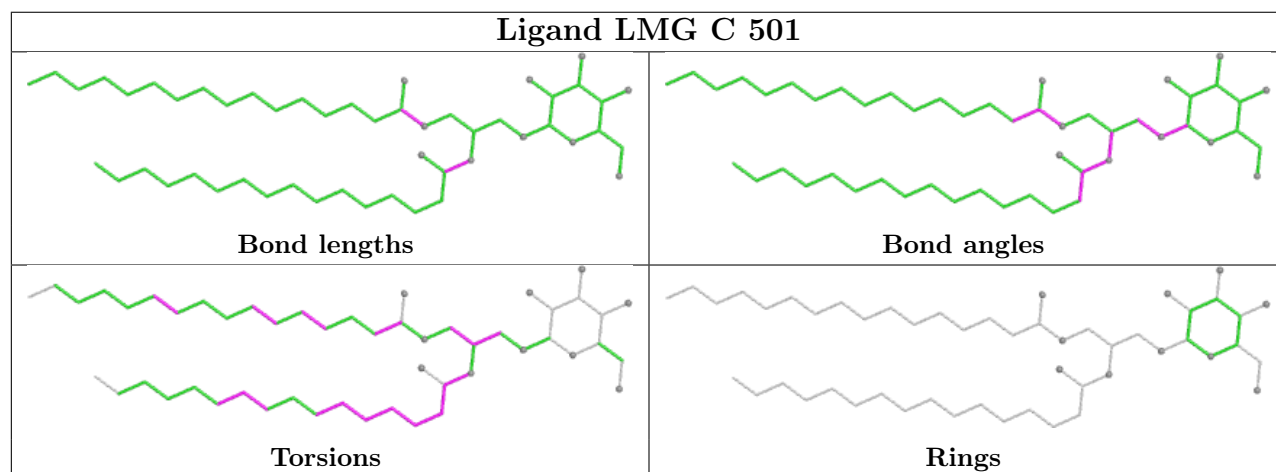
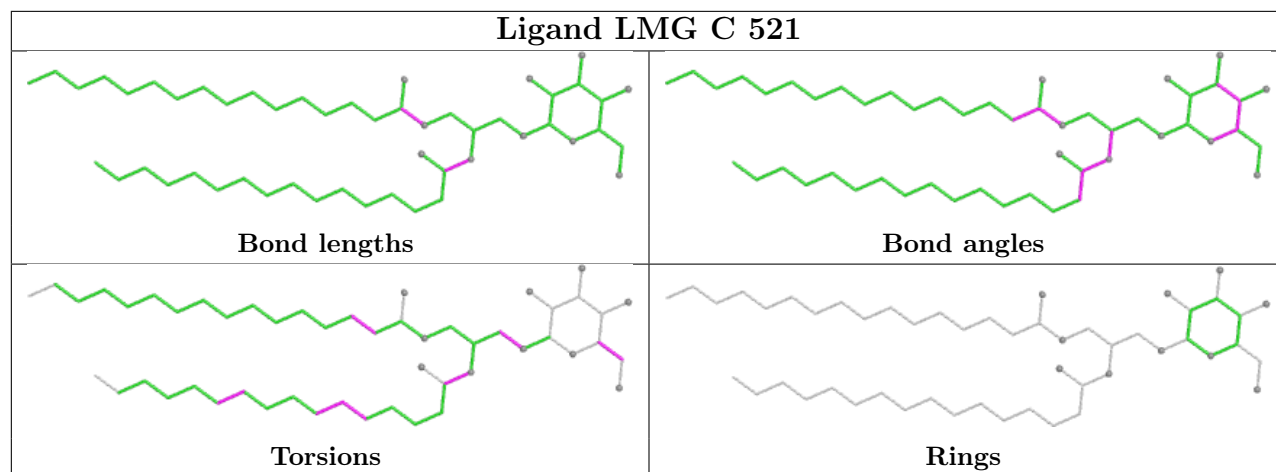


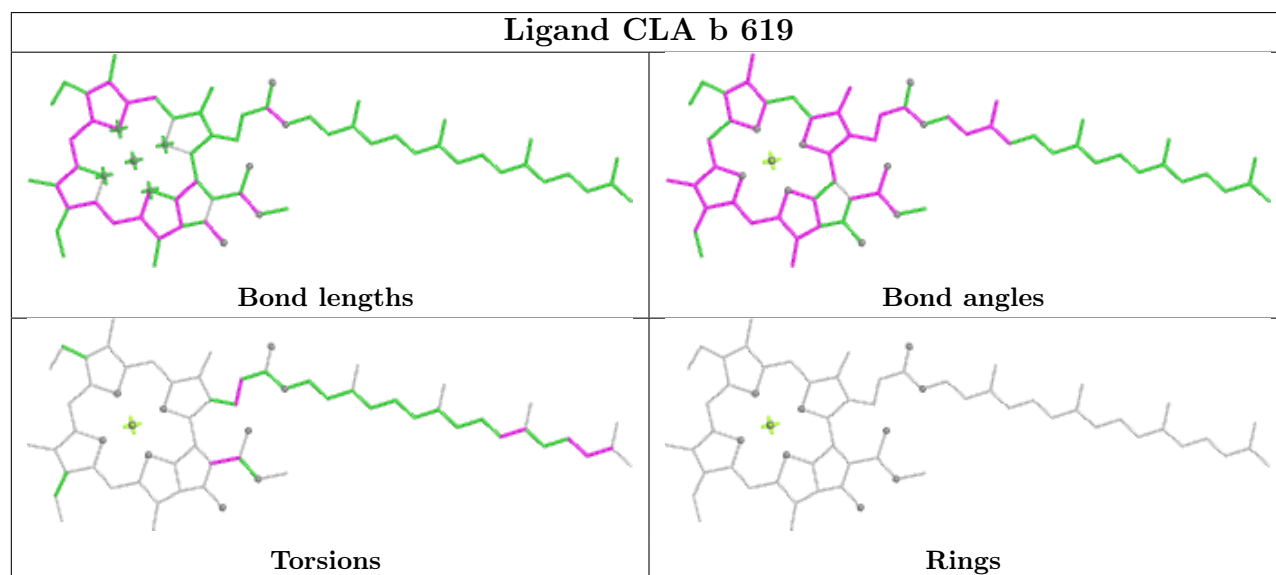
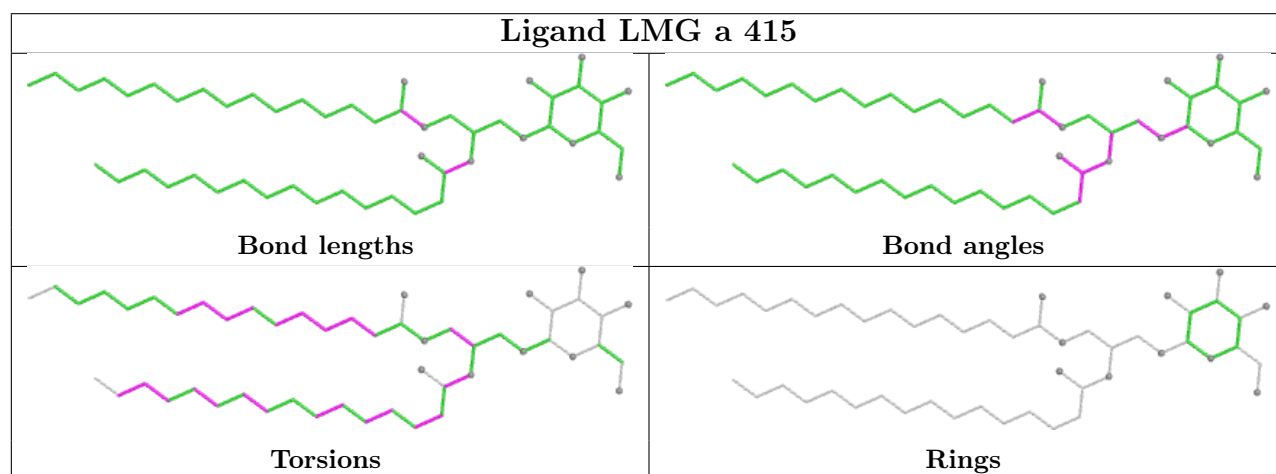
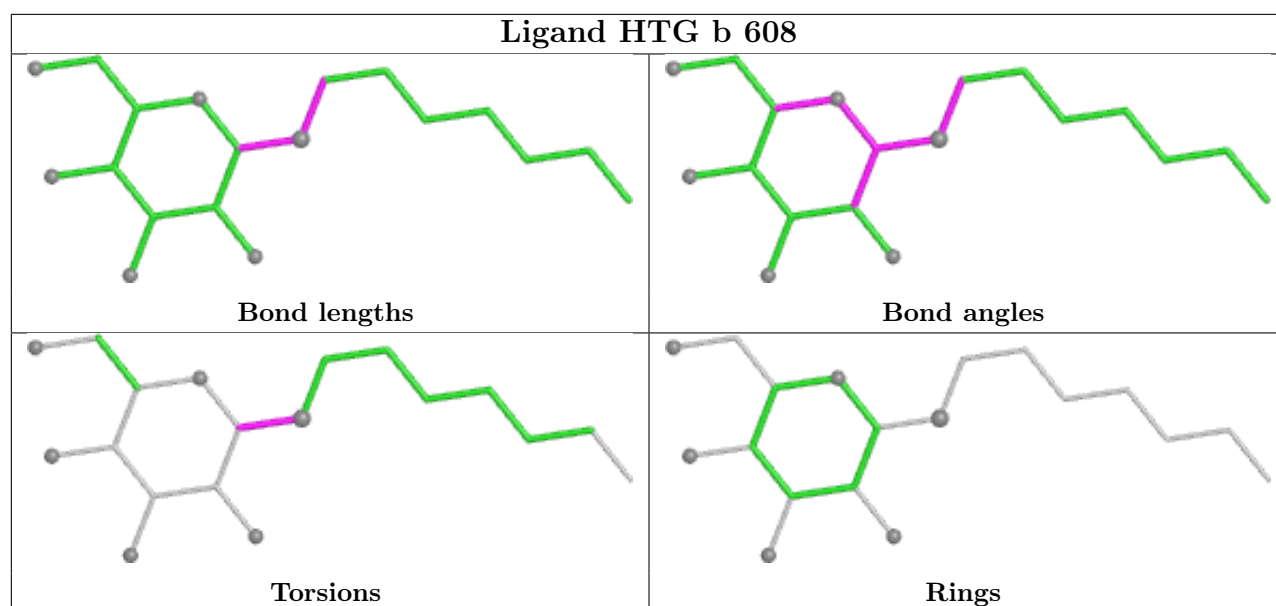
Ligand LHG L 101



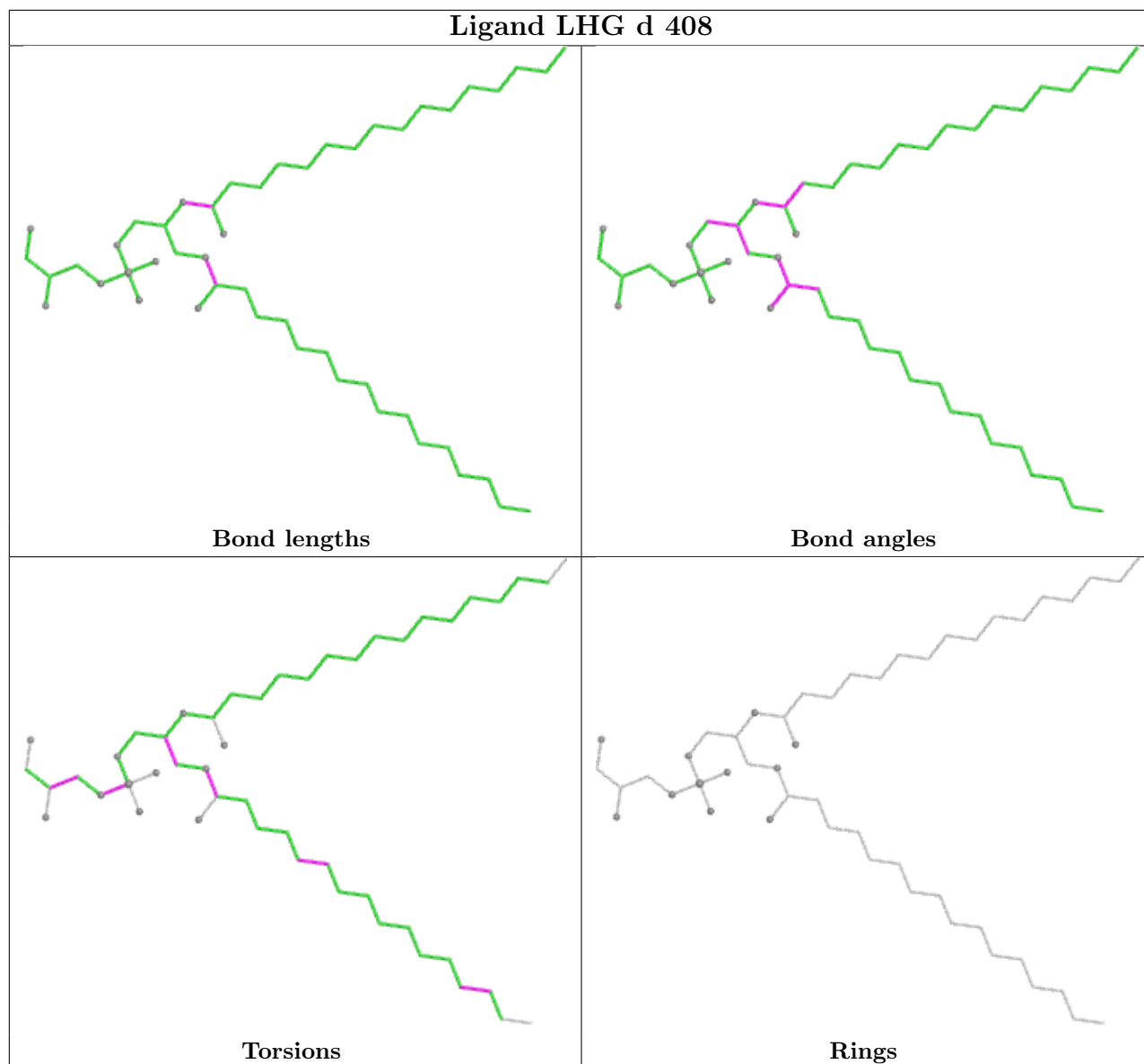
Ligand HTG b 631



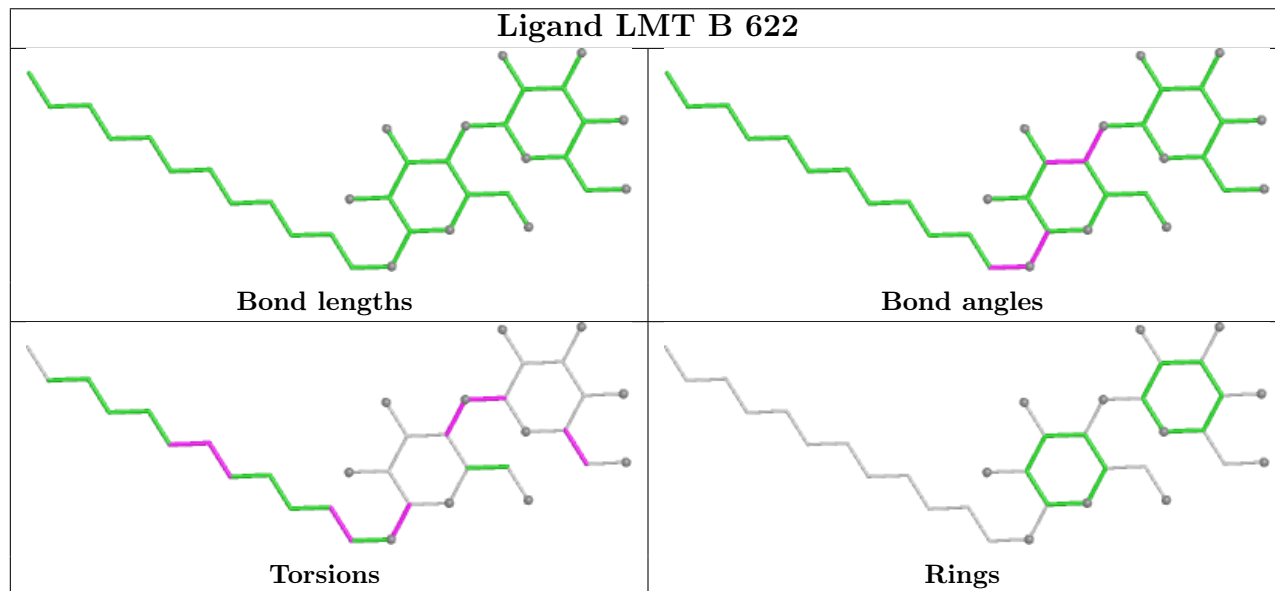


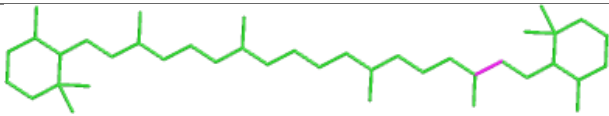
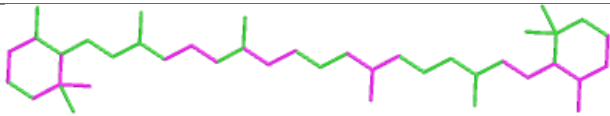
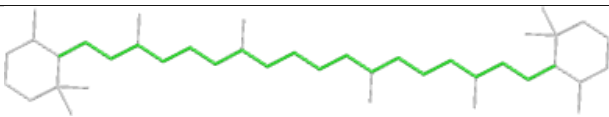
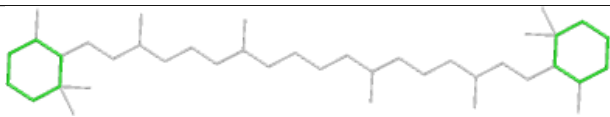


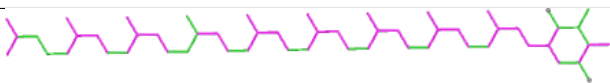
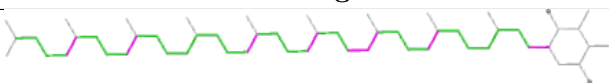
Ligand LHG d 408

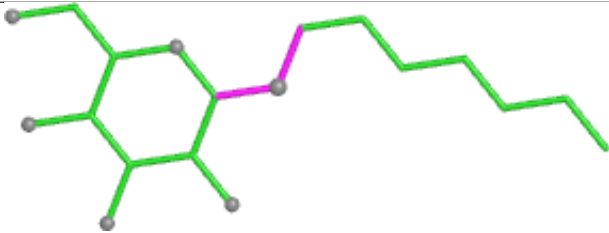
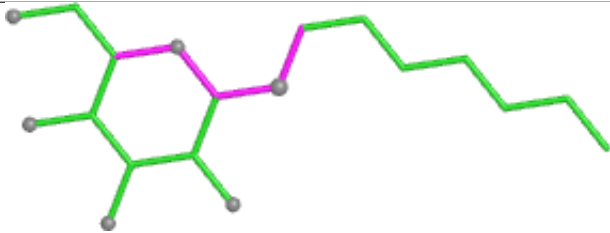
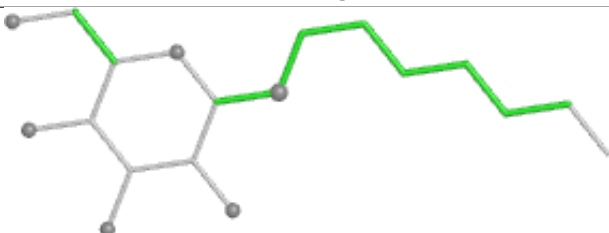
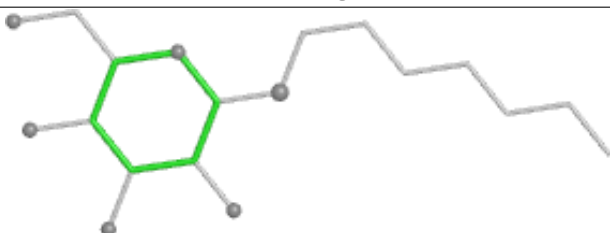


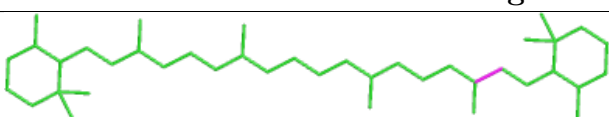
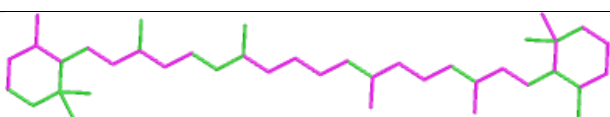
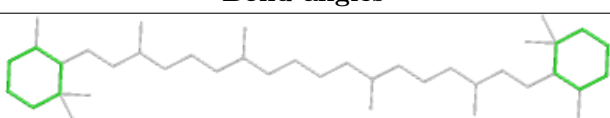
Ligand LMT B 622

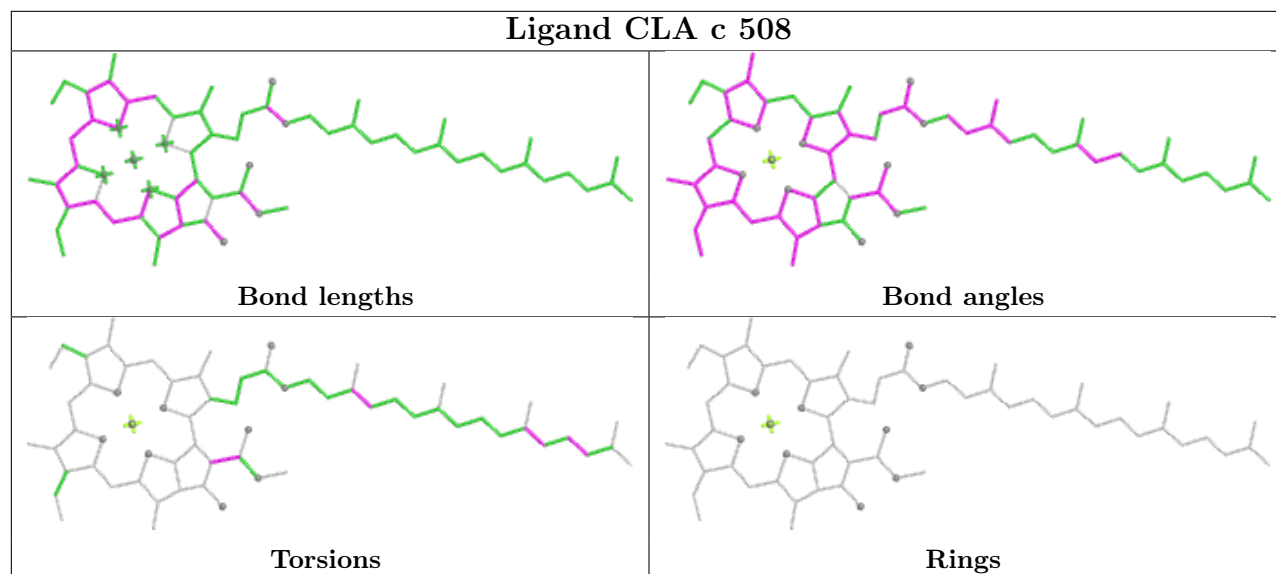
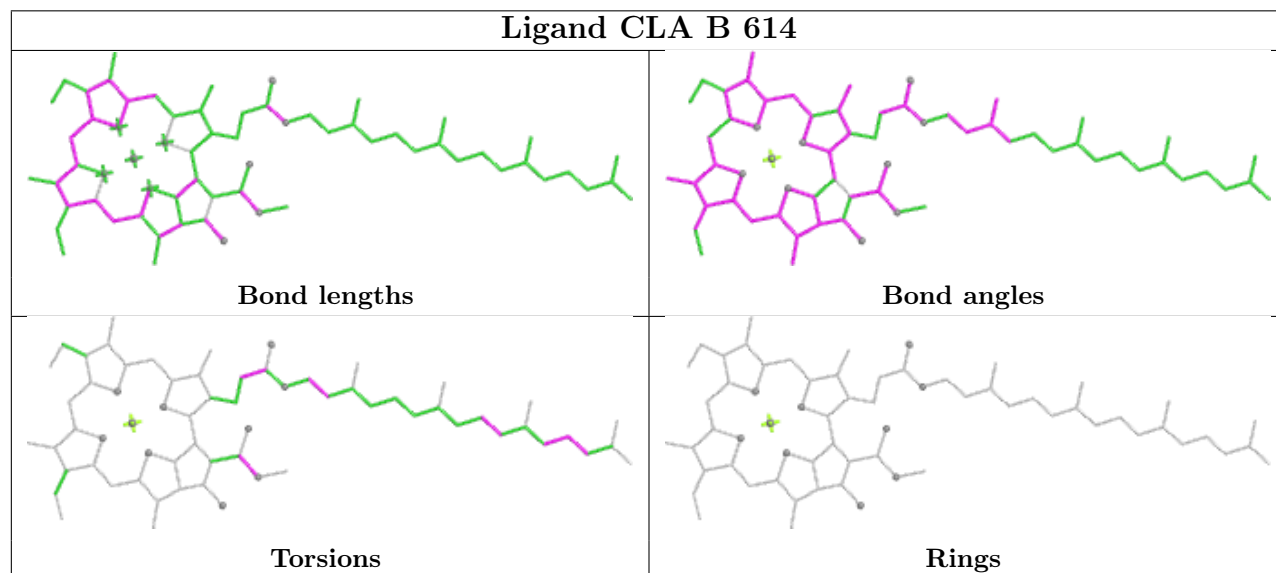
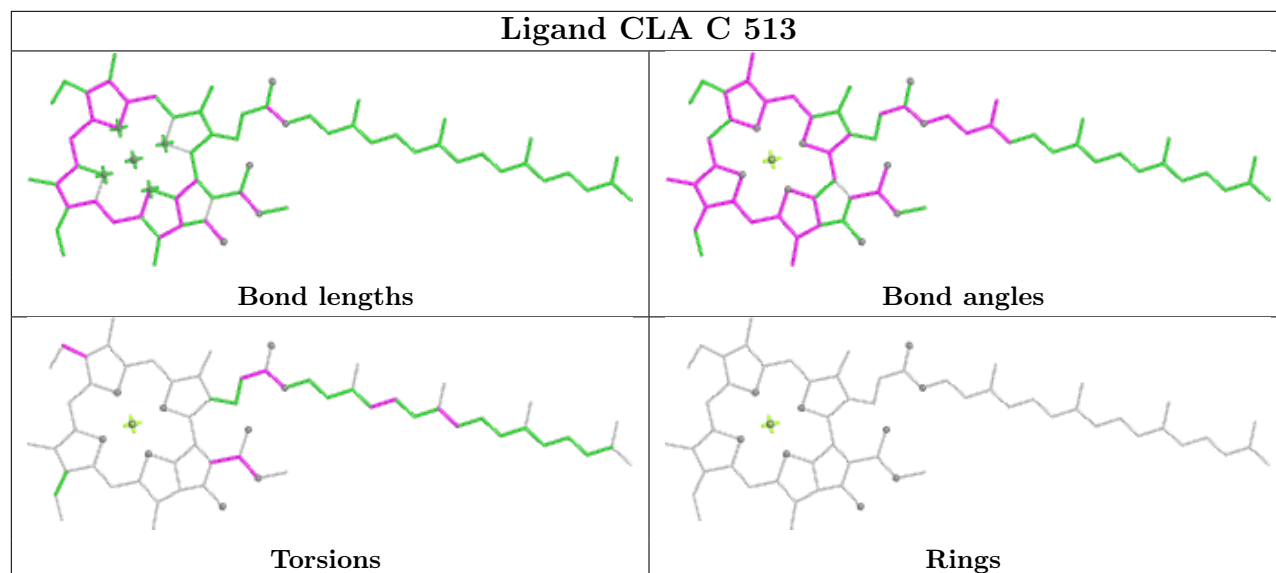


Ligand BCR B 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

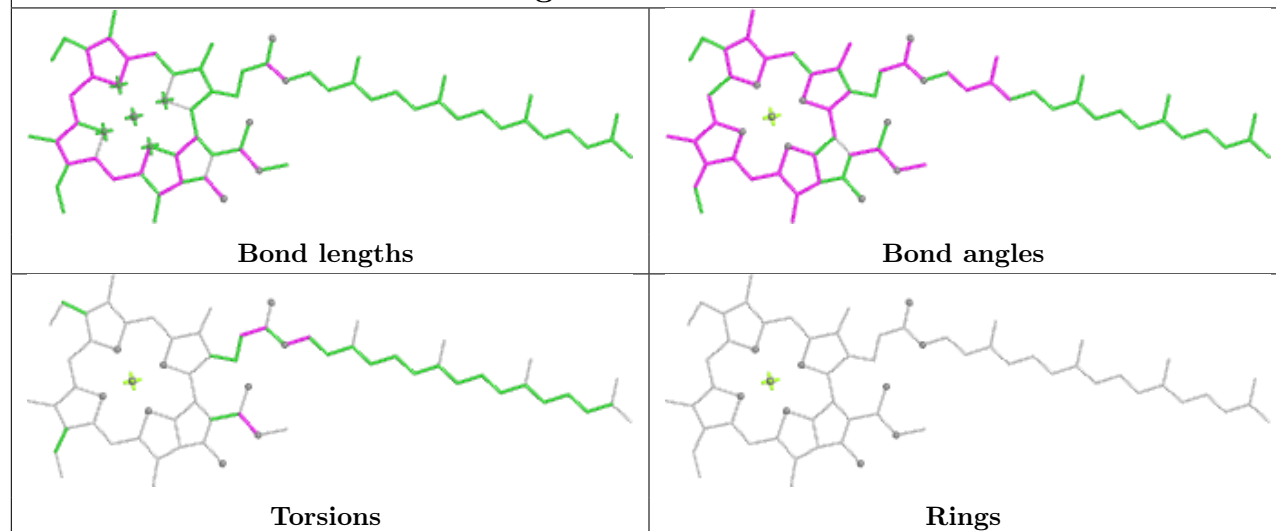
Ligand PL9 A 418	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand HTG C 523	
	
Bond lengths	Bond angles
	
Torsions	Rings

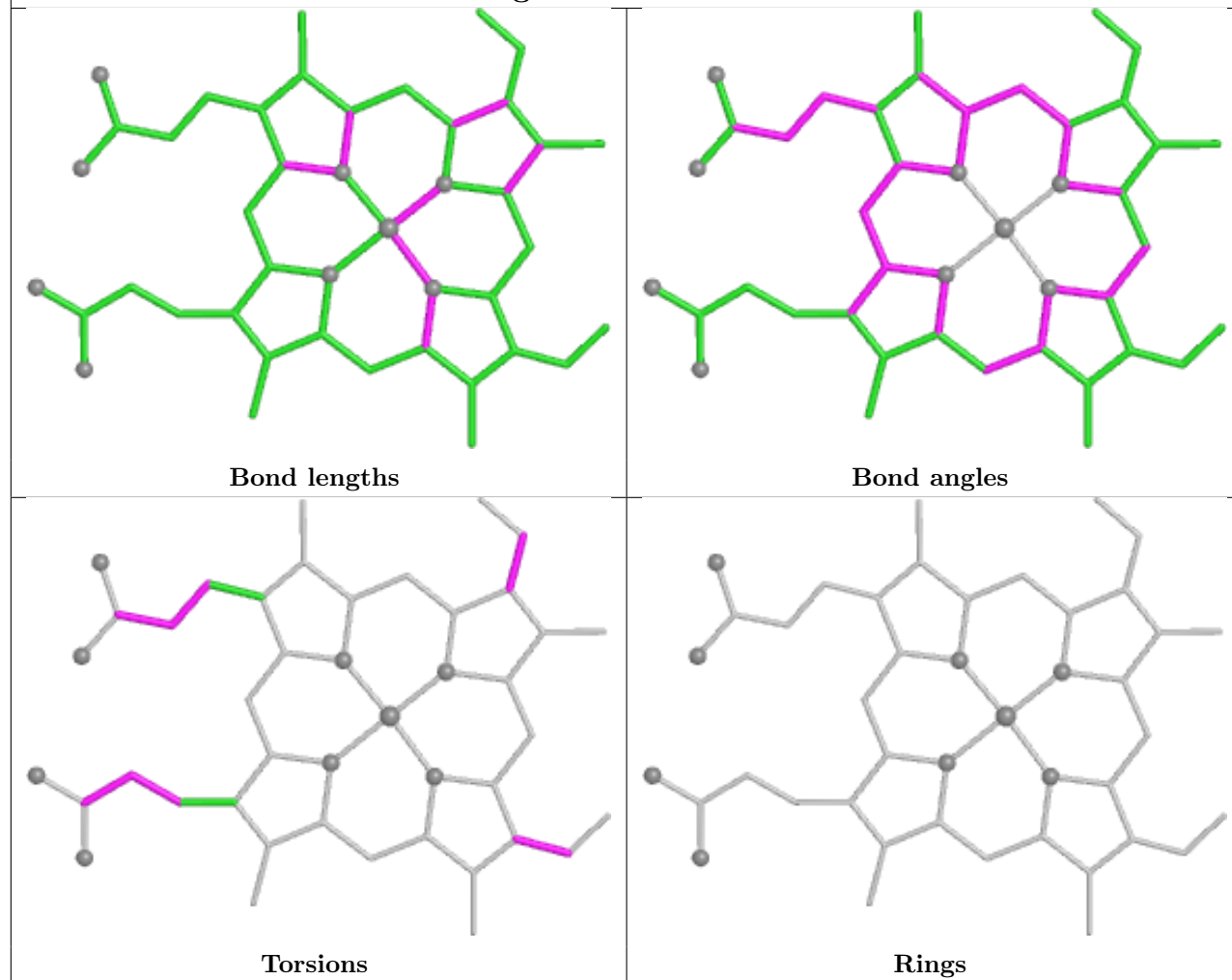
Ligand BCR C 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 508**Ligand CLA B 614****Ligand CLA C 513**

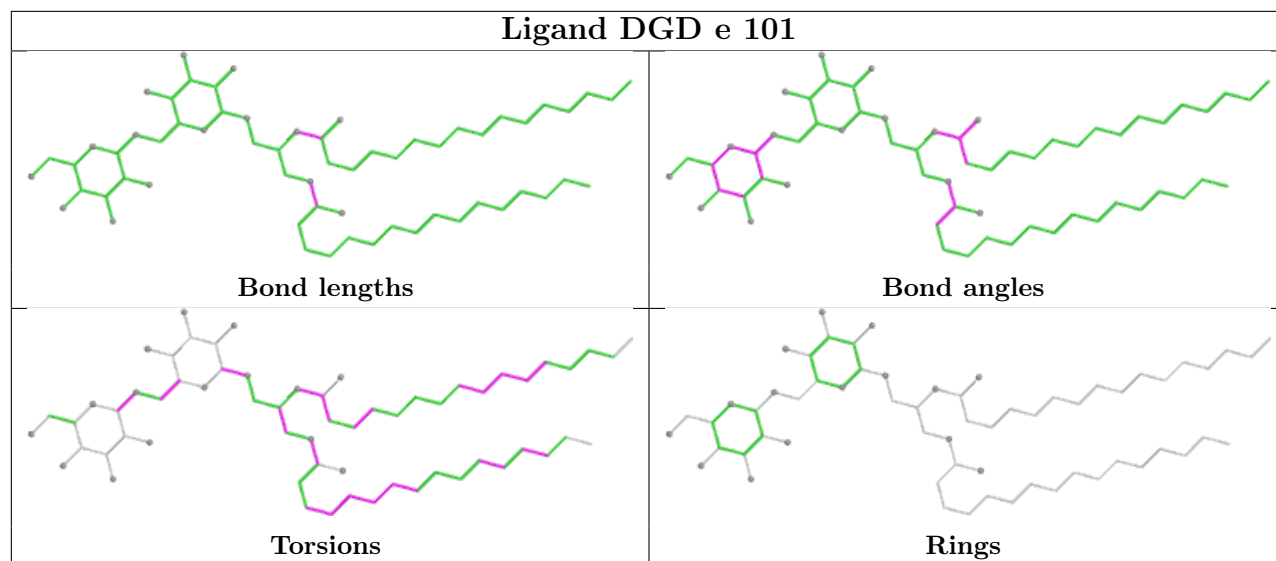
Ligand CLA b 622



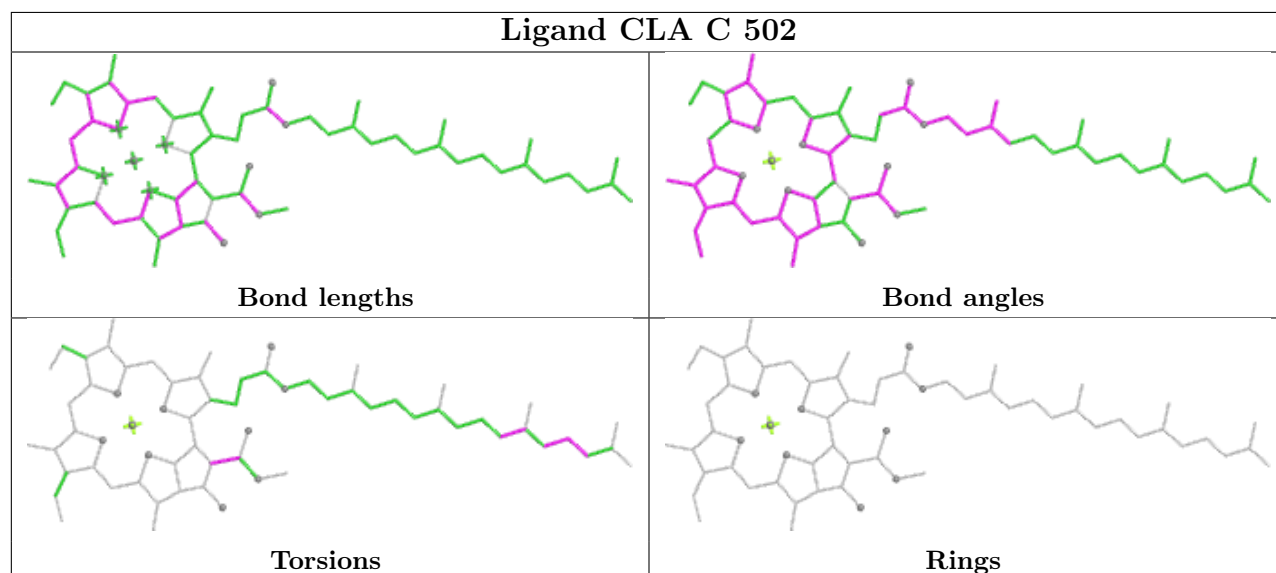
Ligand HEM e 103



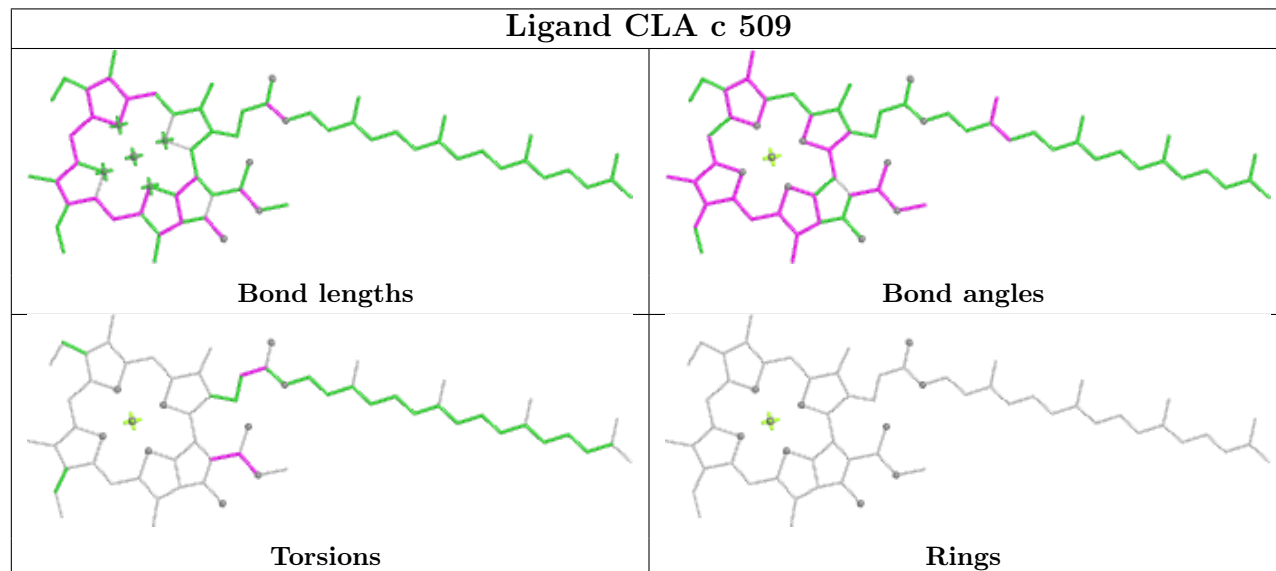
Ligand DGD e 101



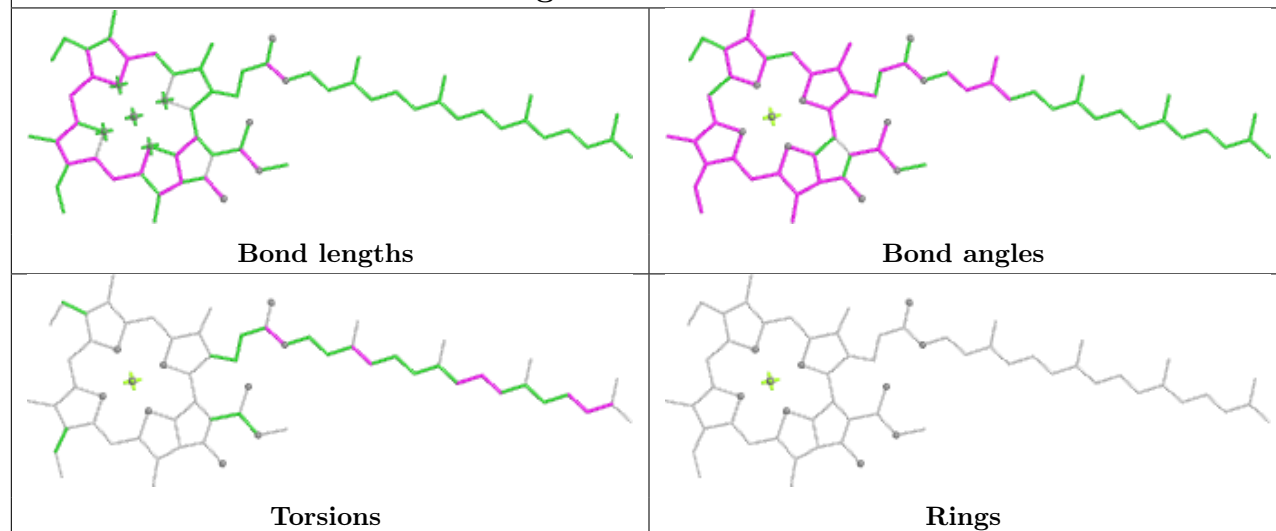
Ligand CLA C 502



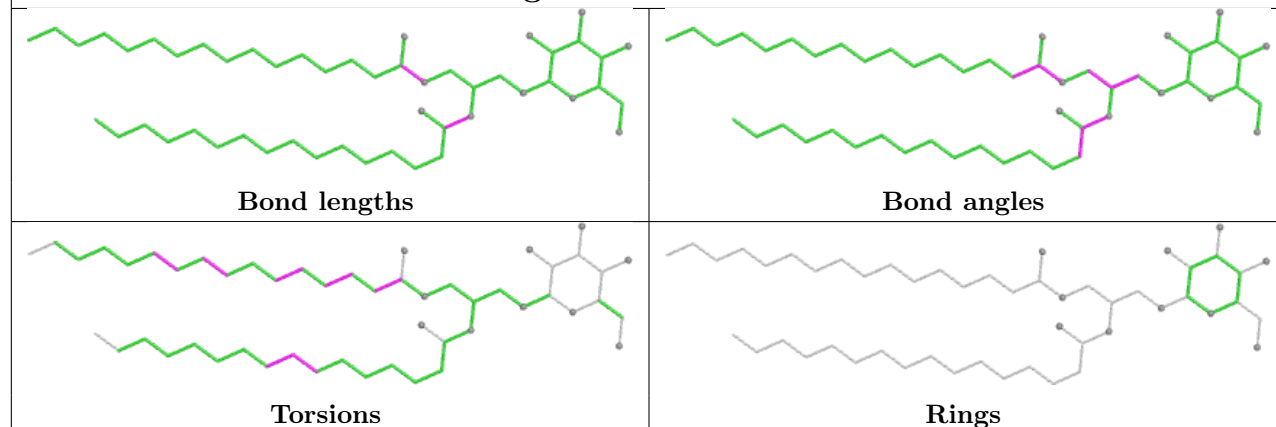
Ligand CLA c 509



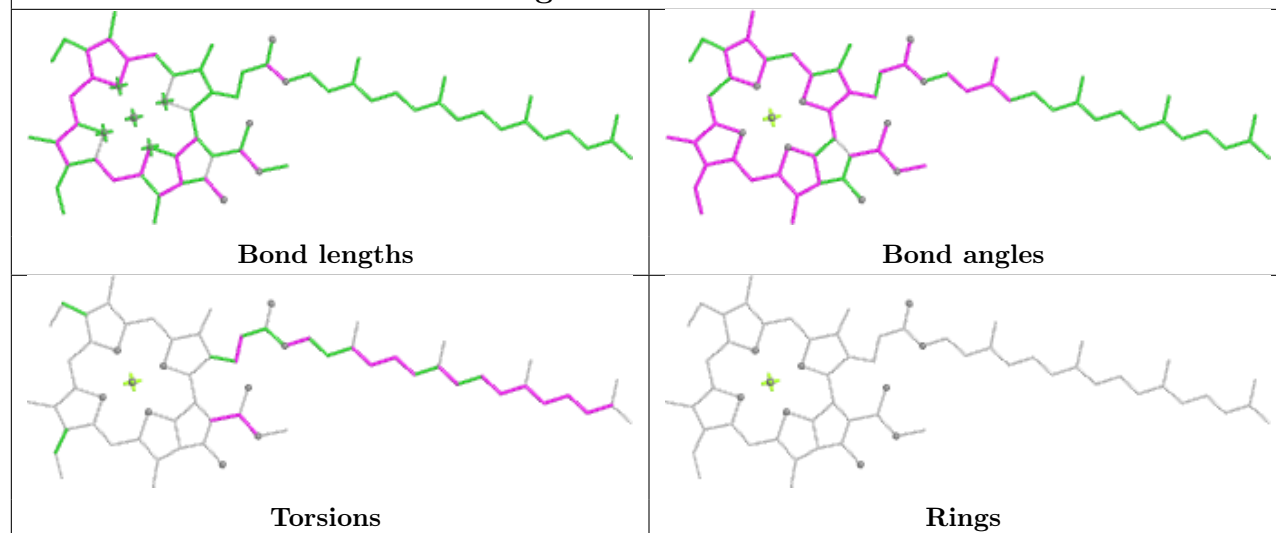
Ligand CLA a 412

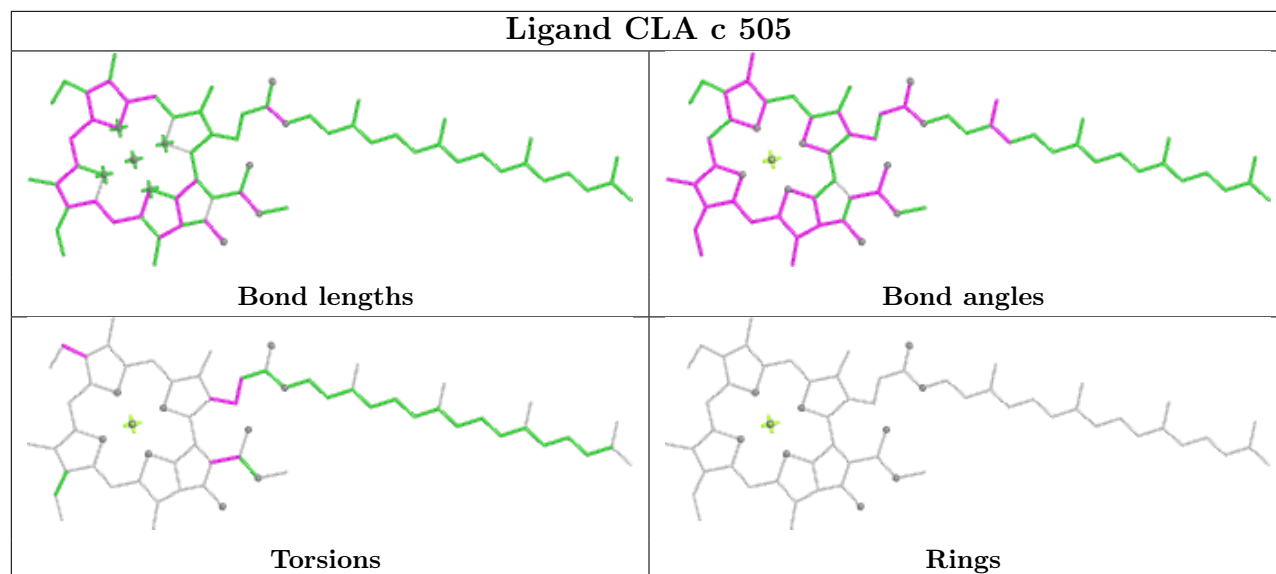
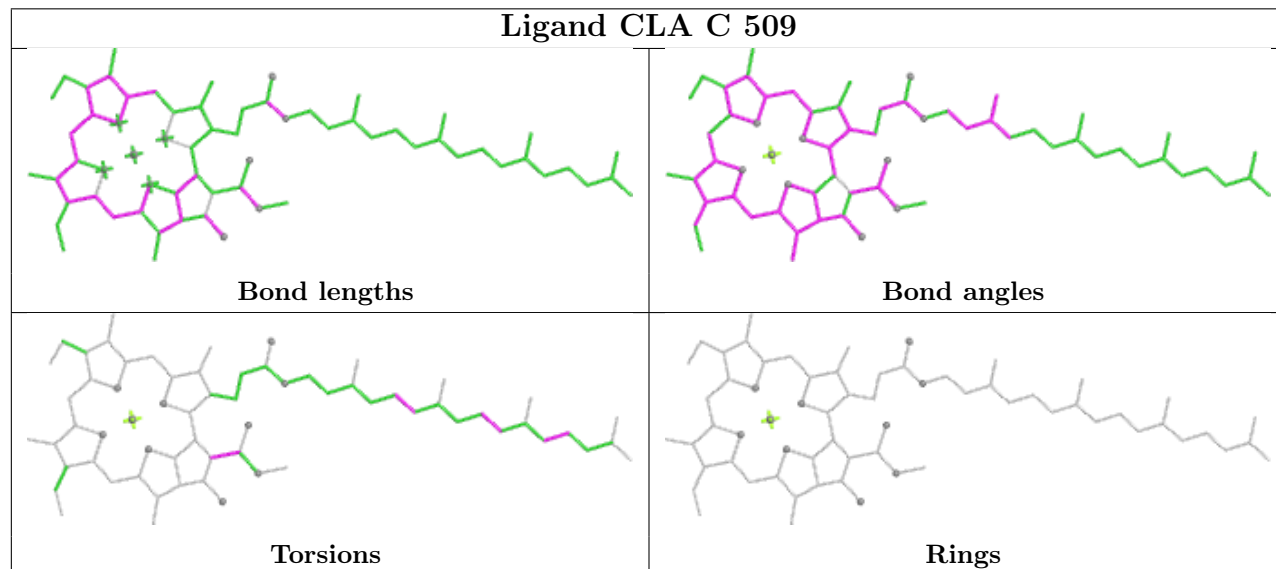


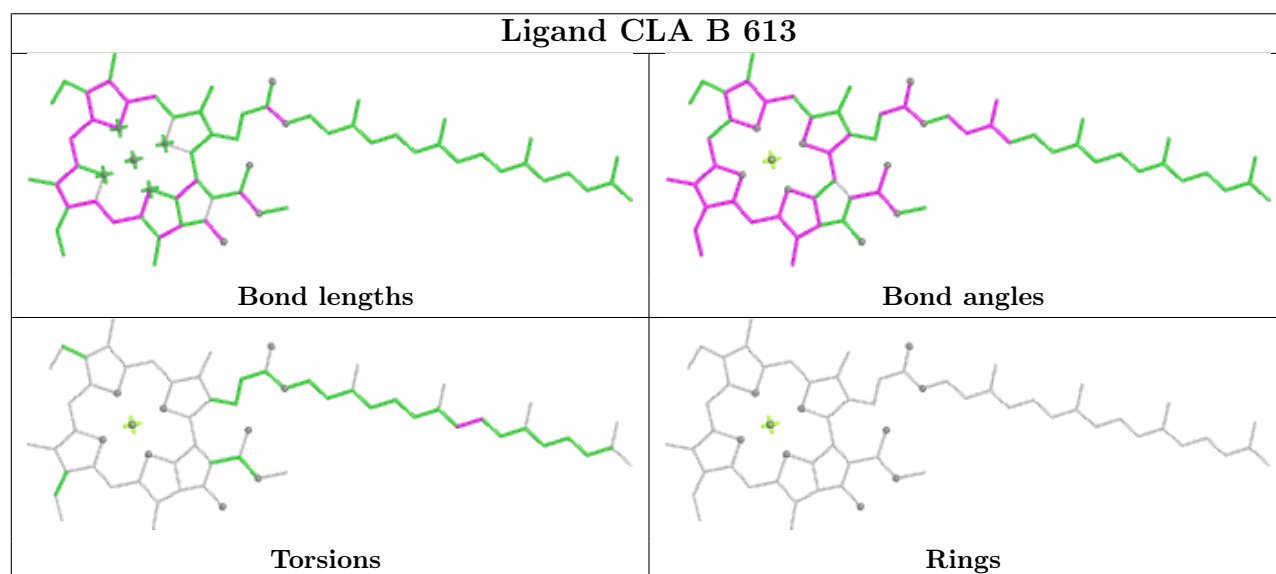
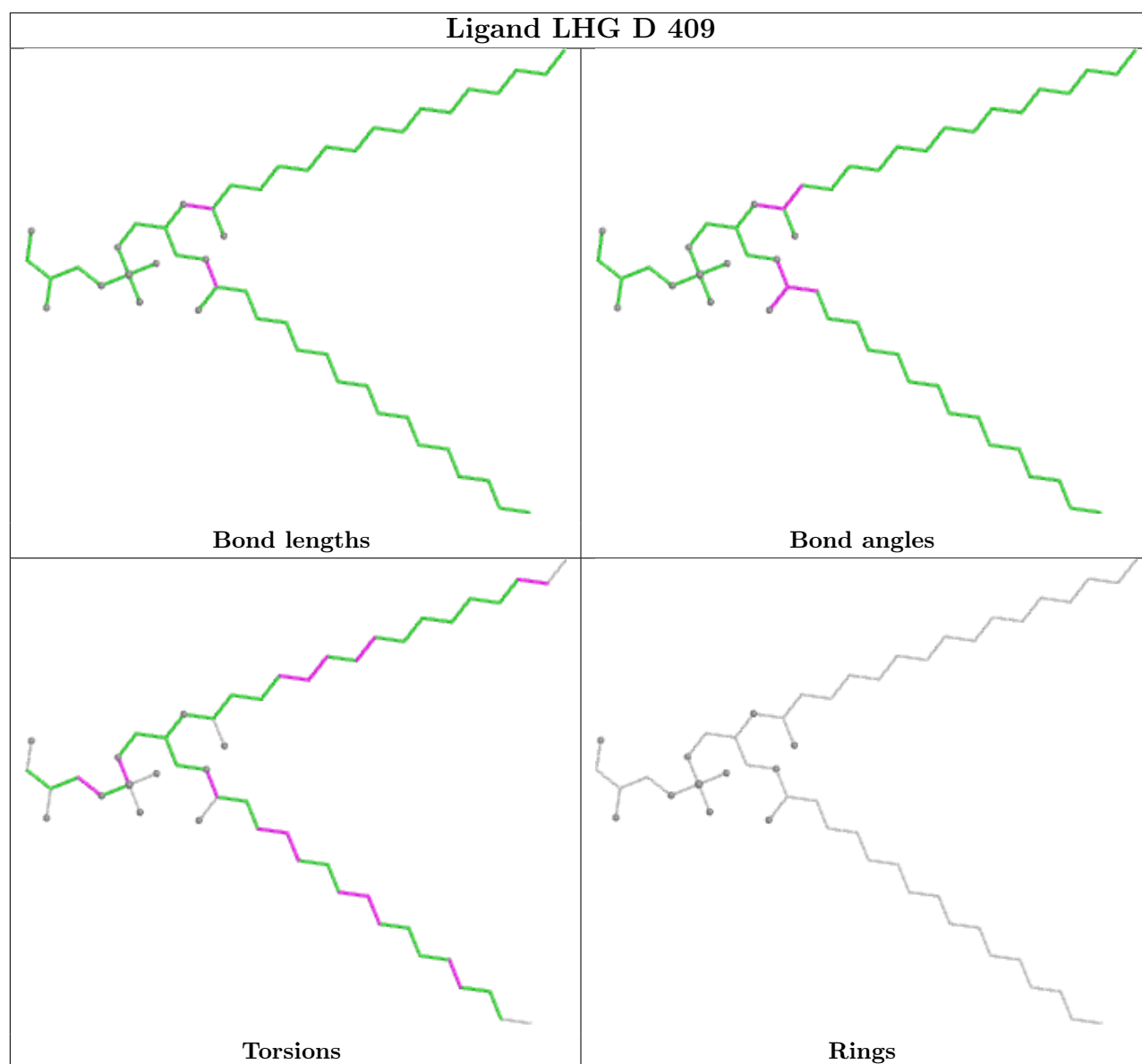
Ligand LMG M 101

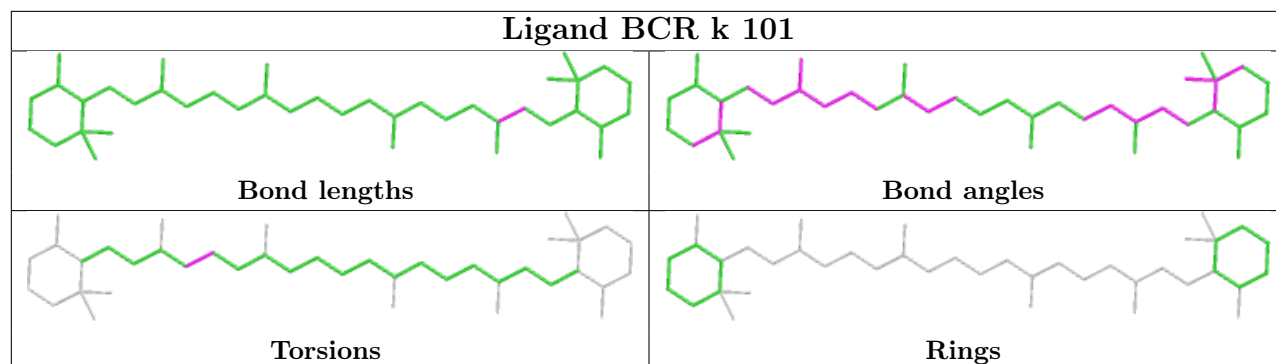
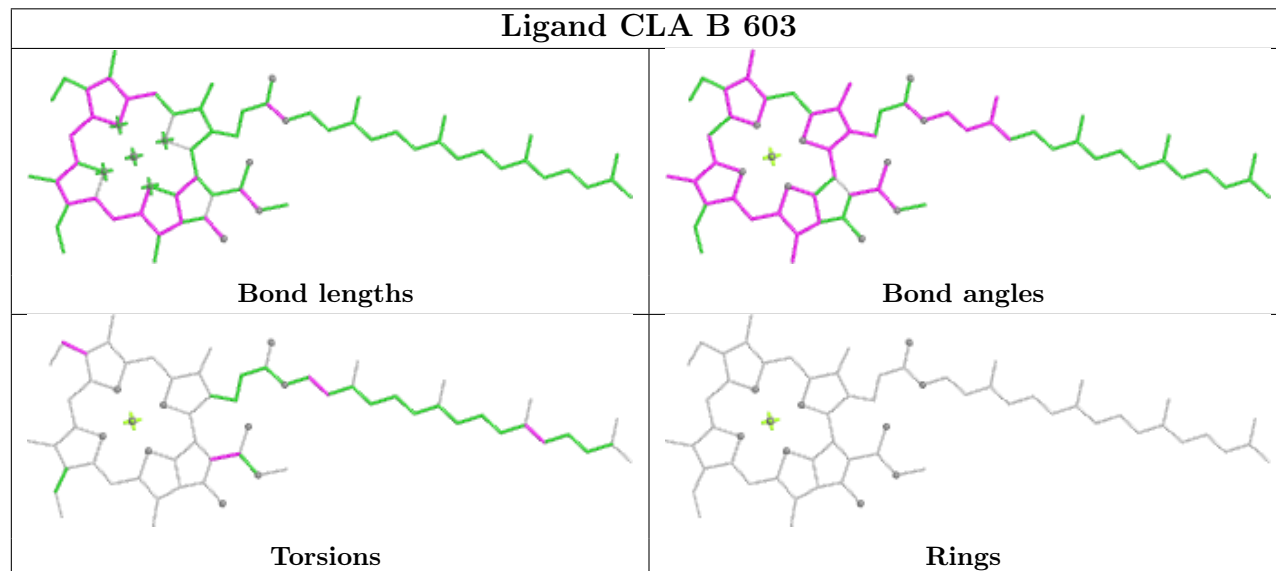
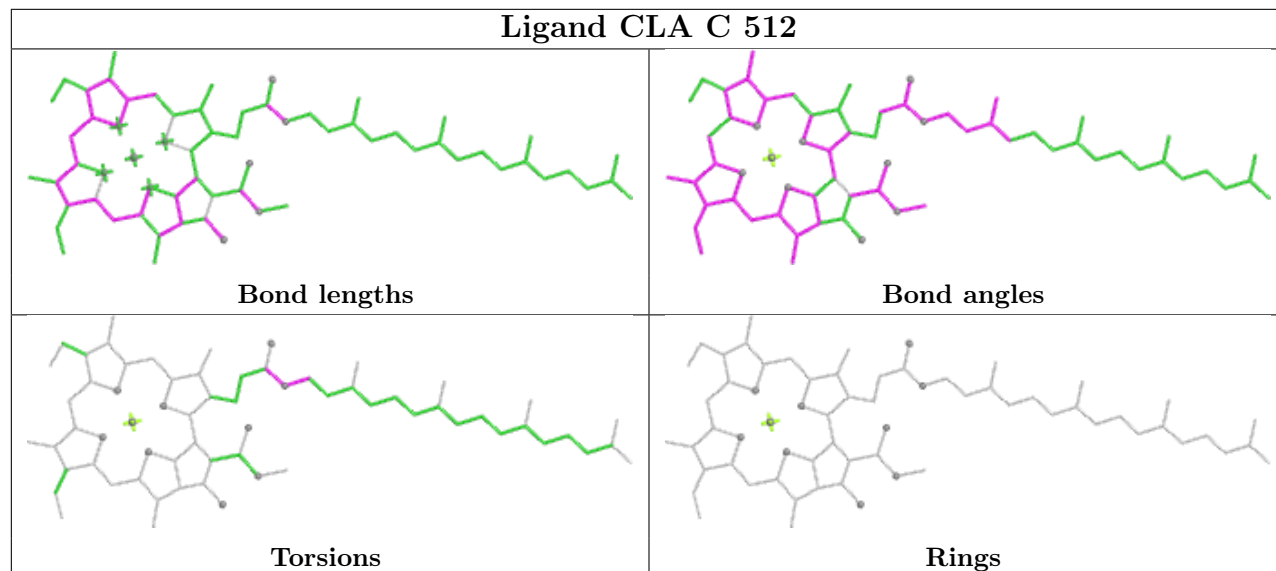


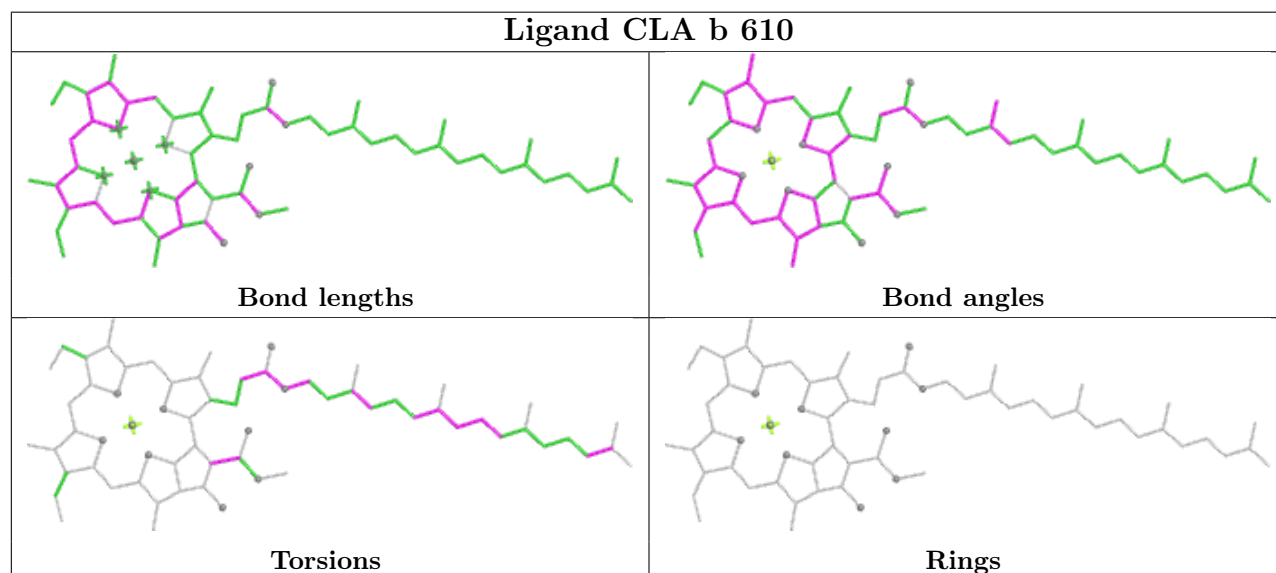
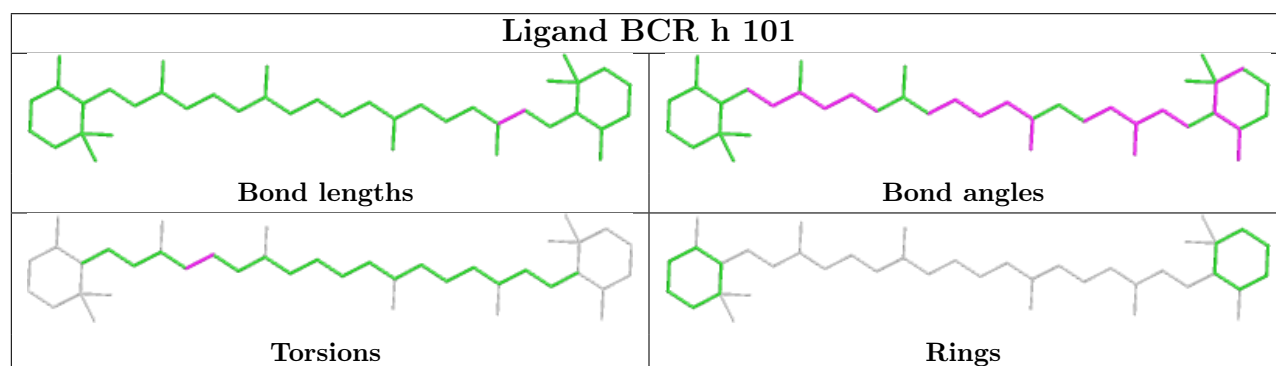
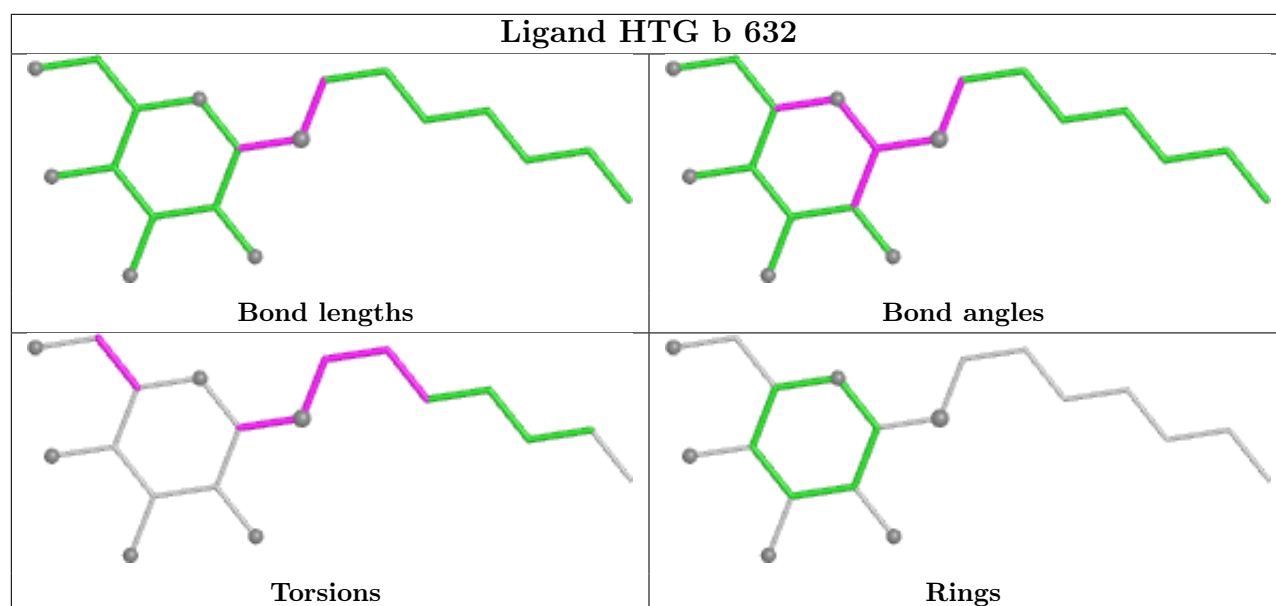
Ligand CLA b 623

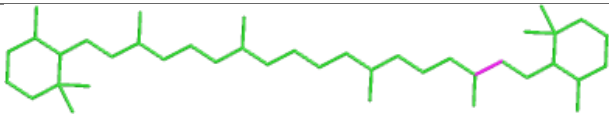
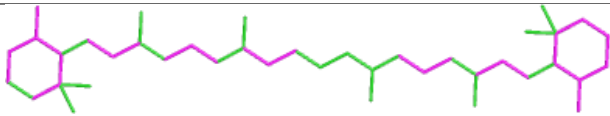
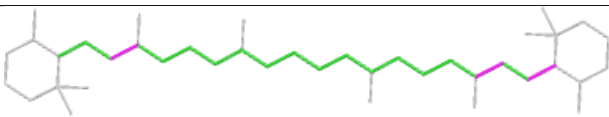
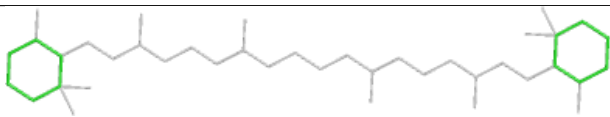


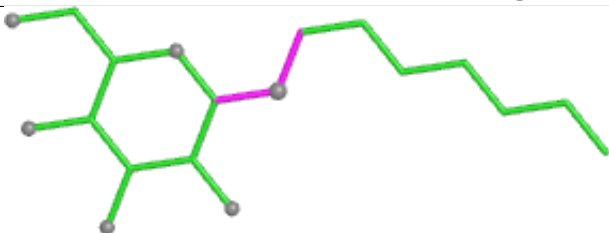
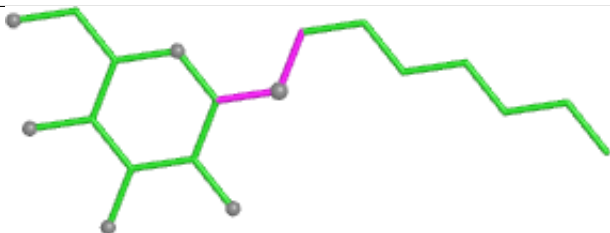
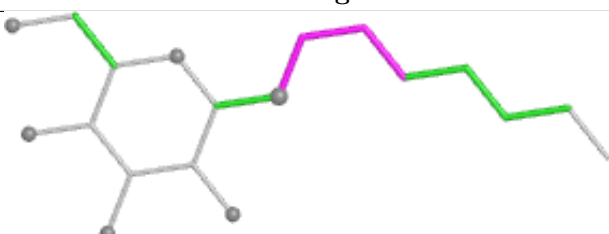
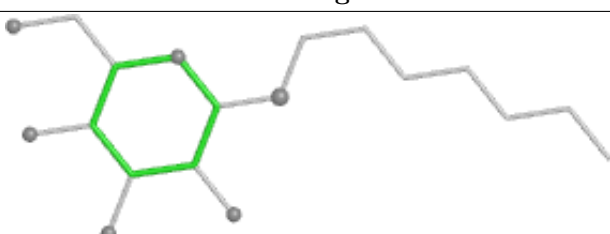
Ligand CLA c 505**Ligand CLA C 509**

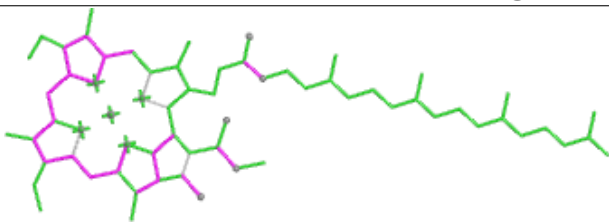
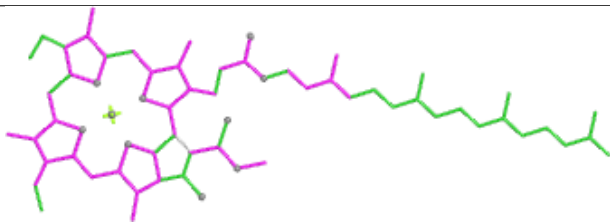
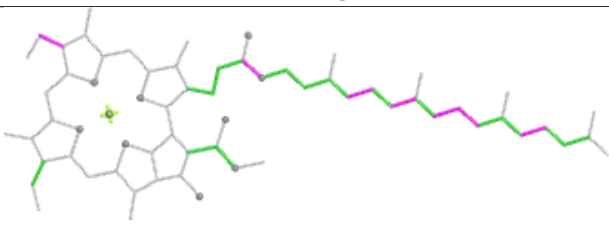
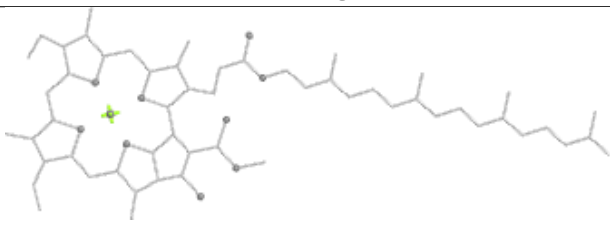


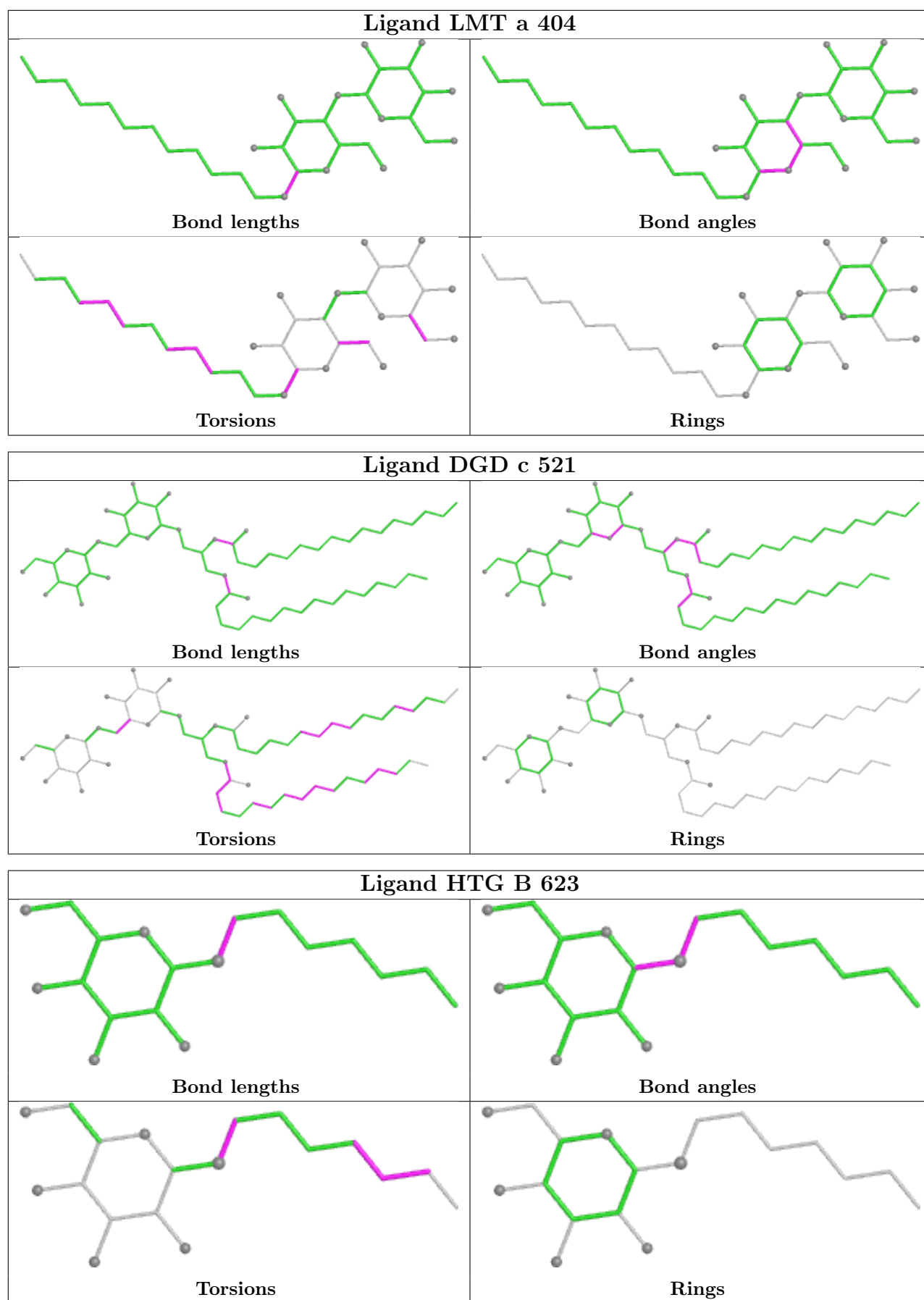
Ligand BCR k 101**Ligand CLA B 603****Ligand CLA C 512**



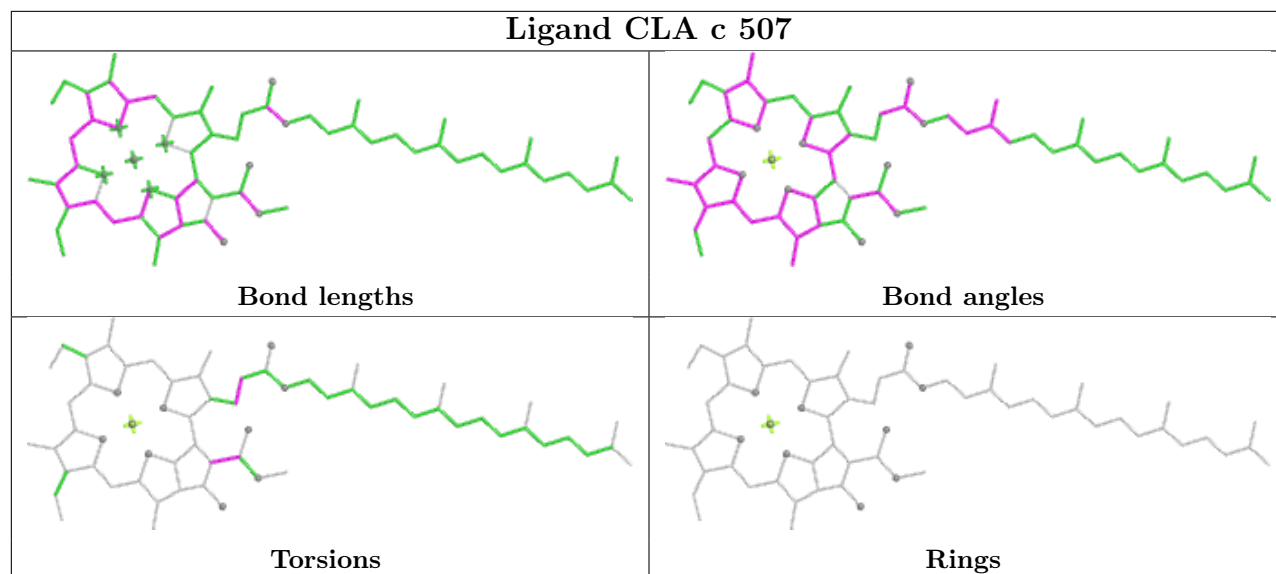
Ligand BCR d 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand HTG c 524	
	
Bond lengths	Bond angles
	
Torsions	Rings

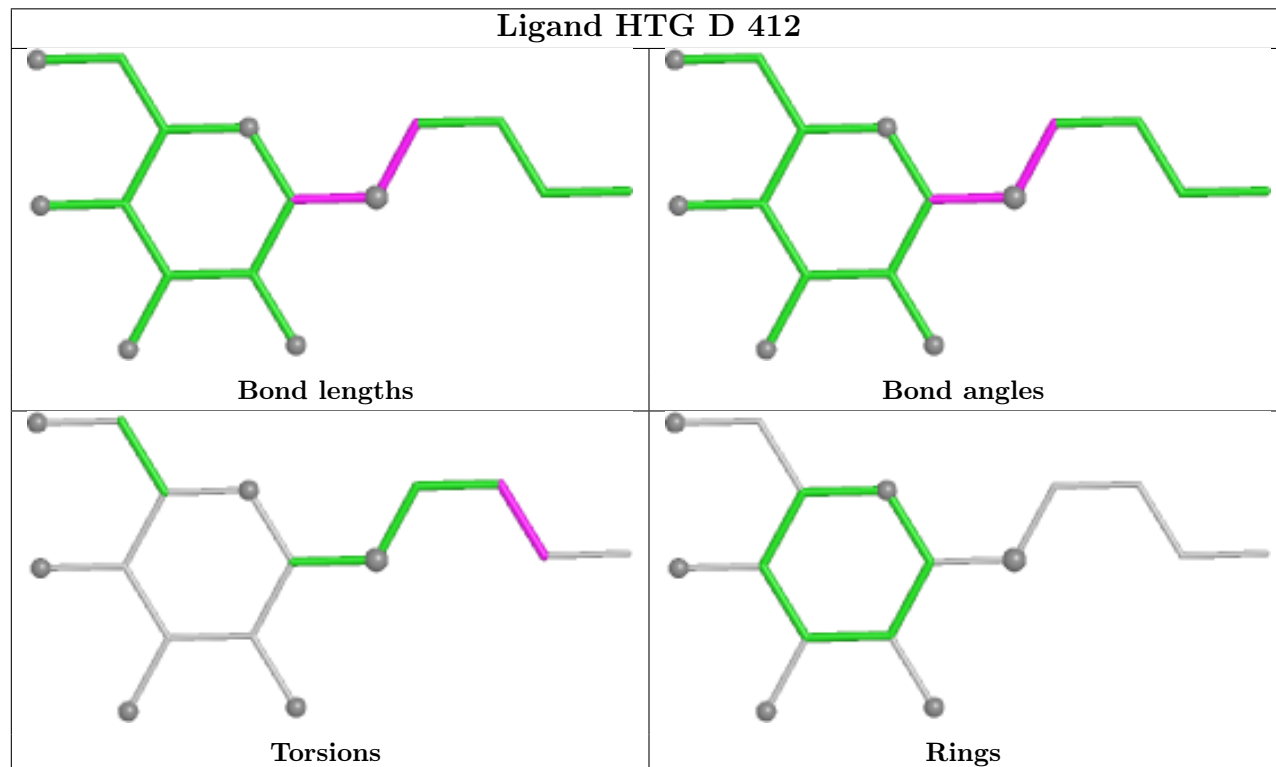
Ligand CLA A 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

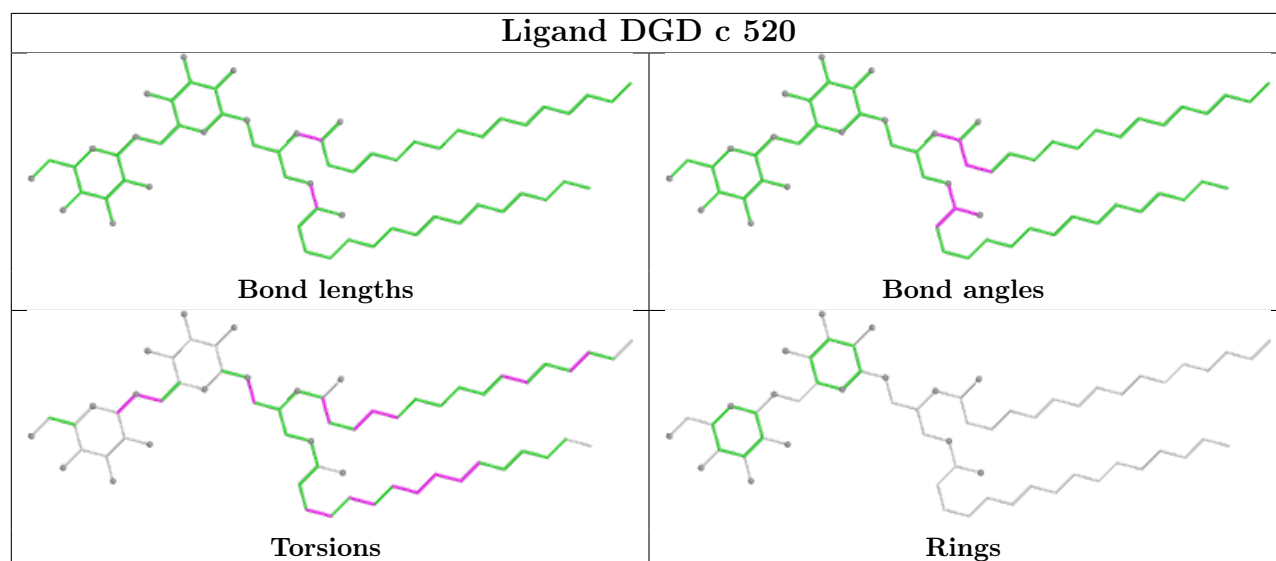
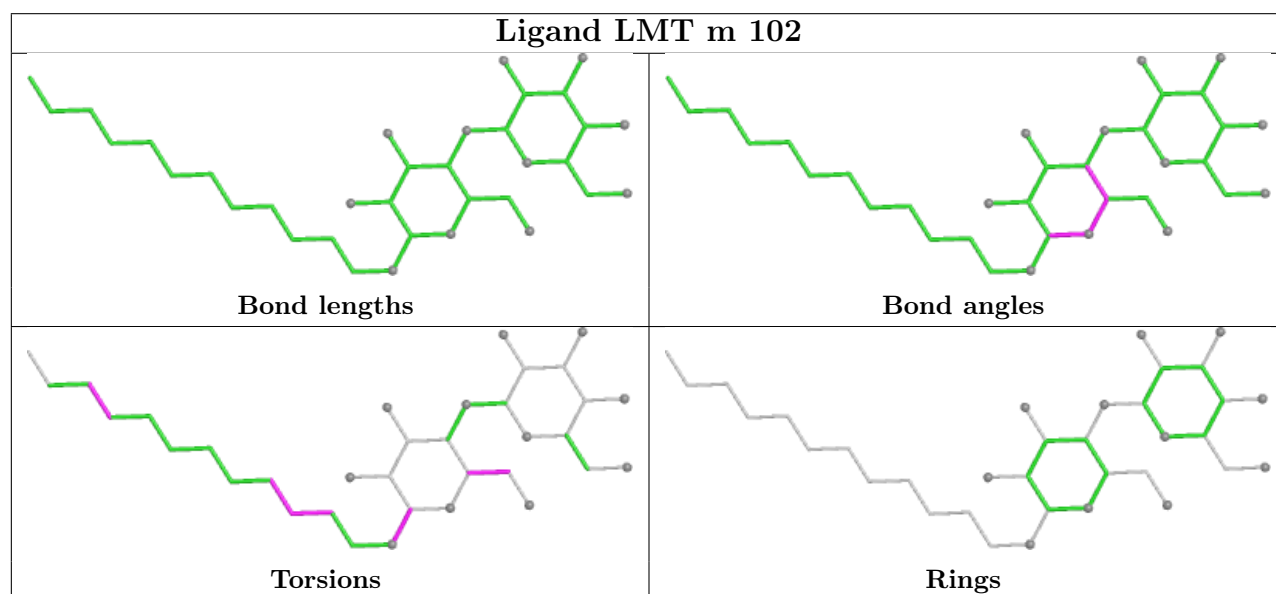
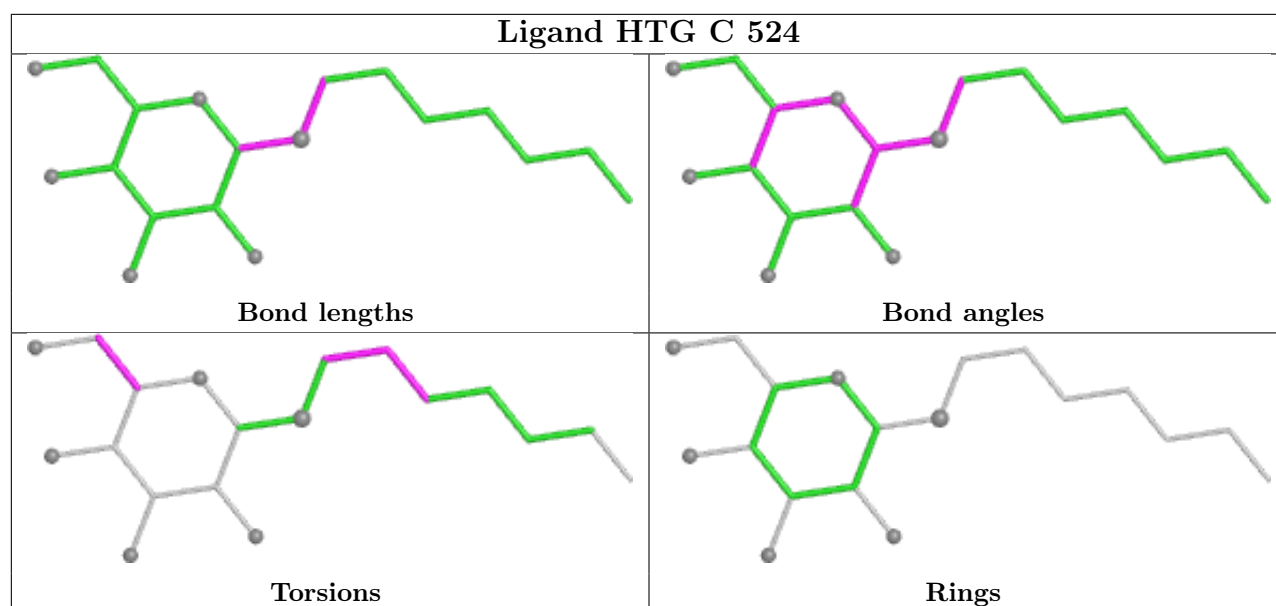


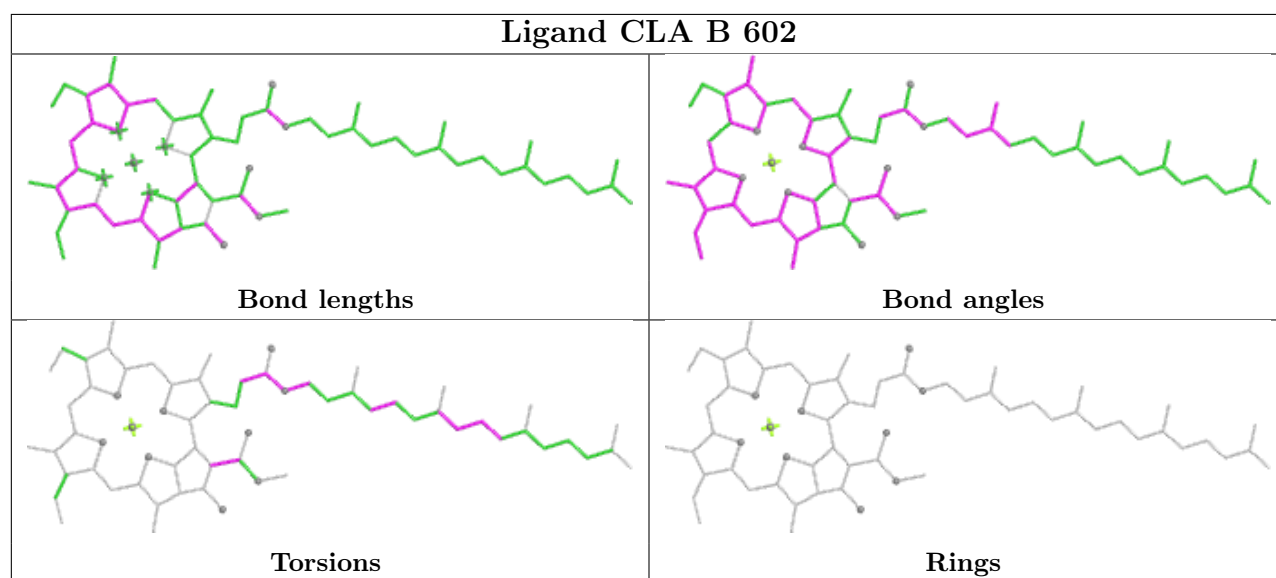
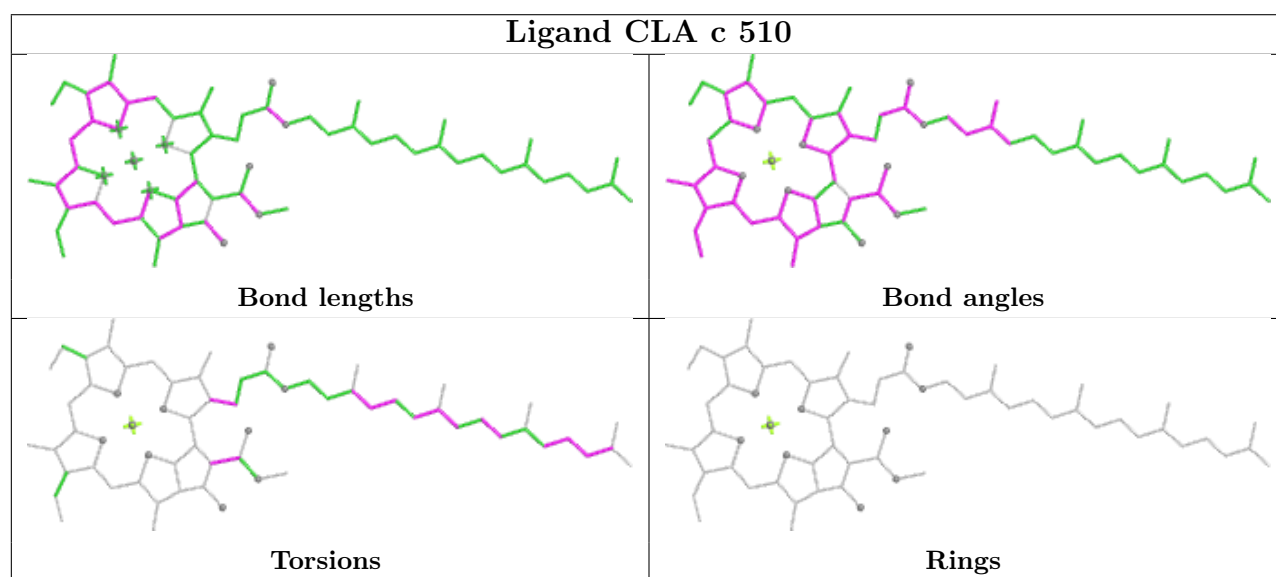
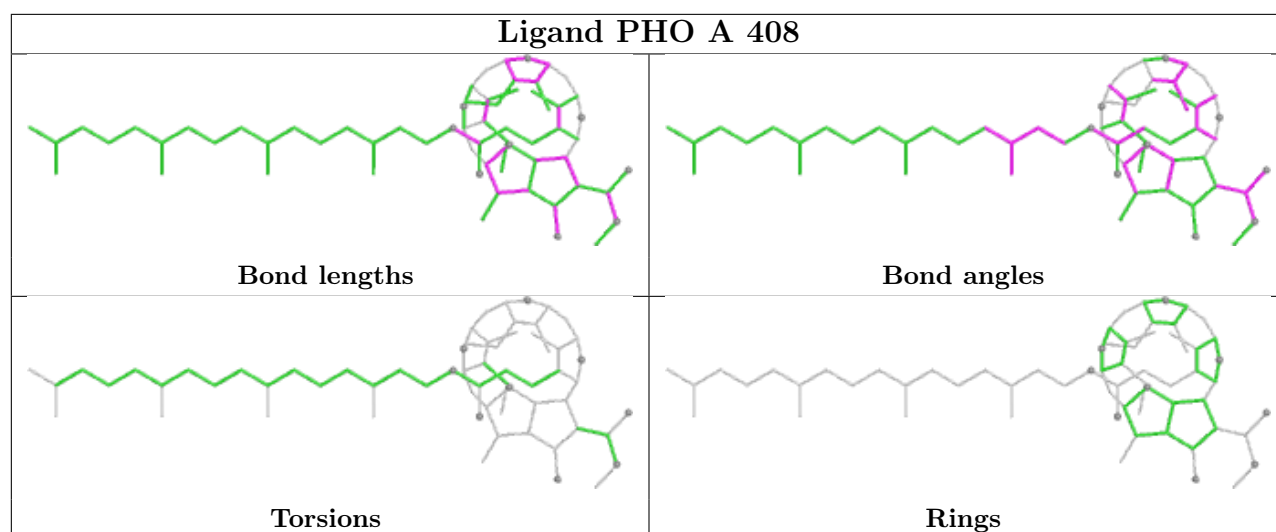
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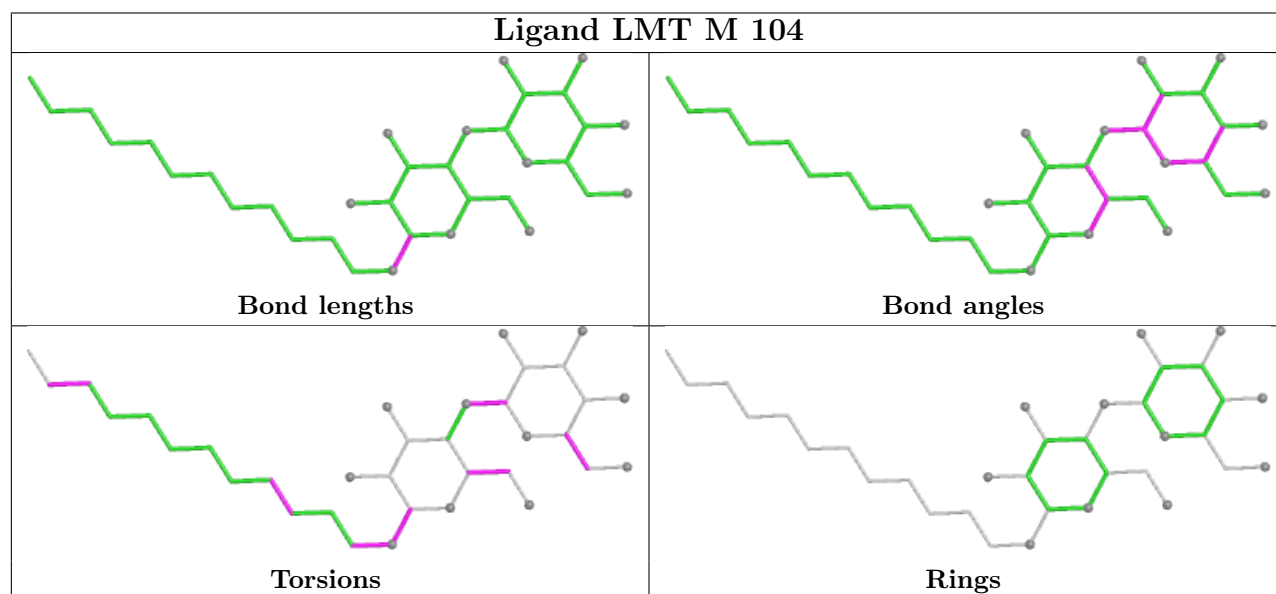
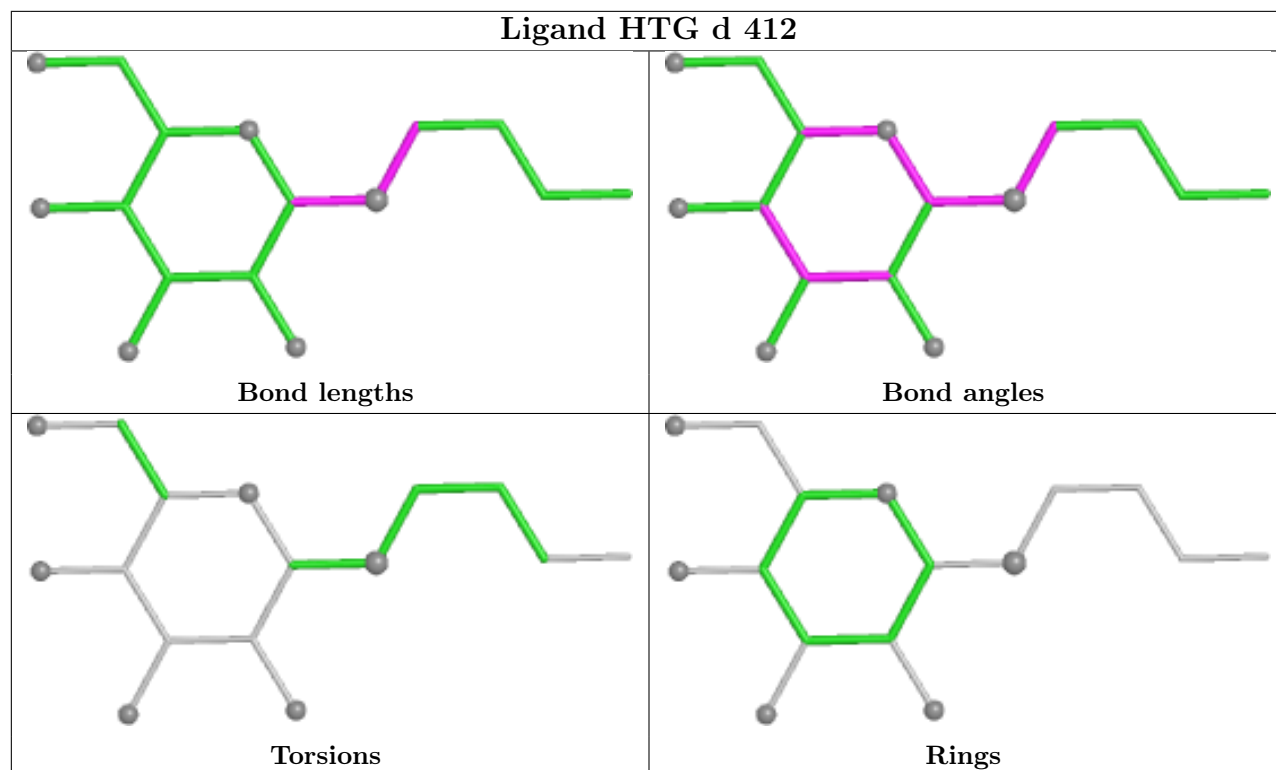


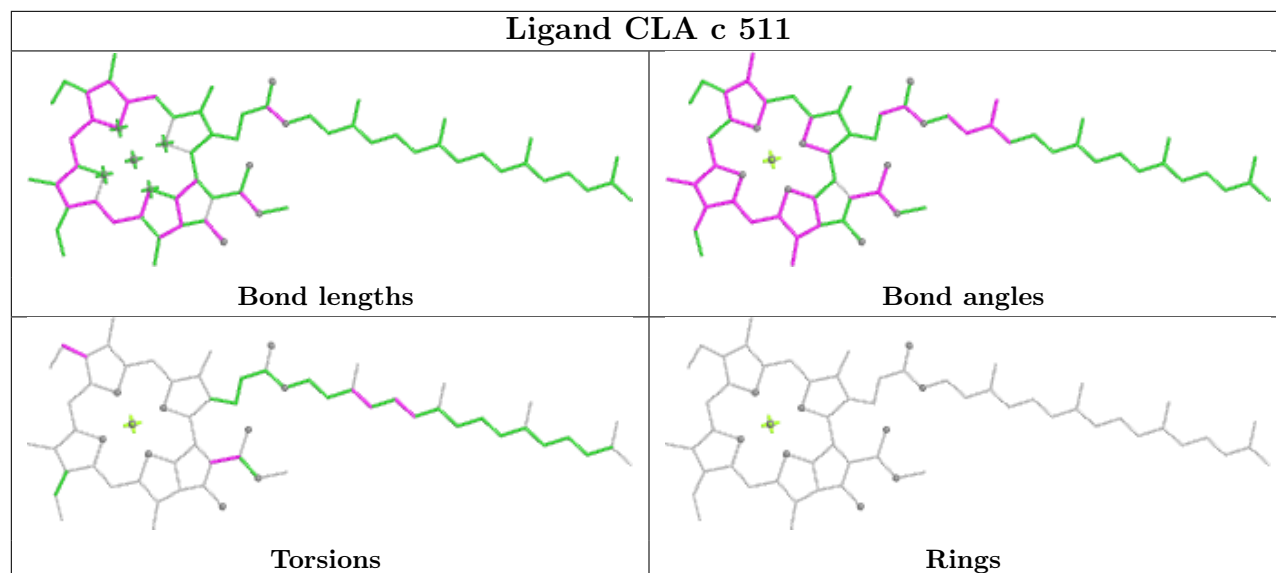
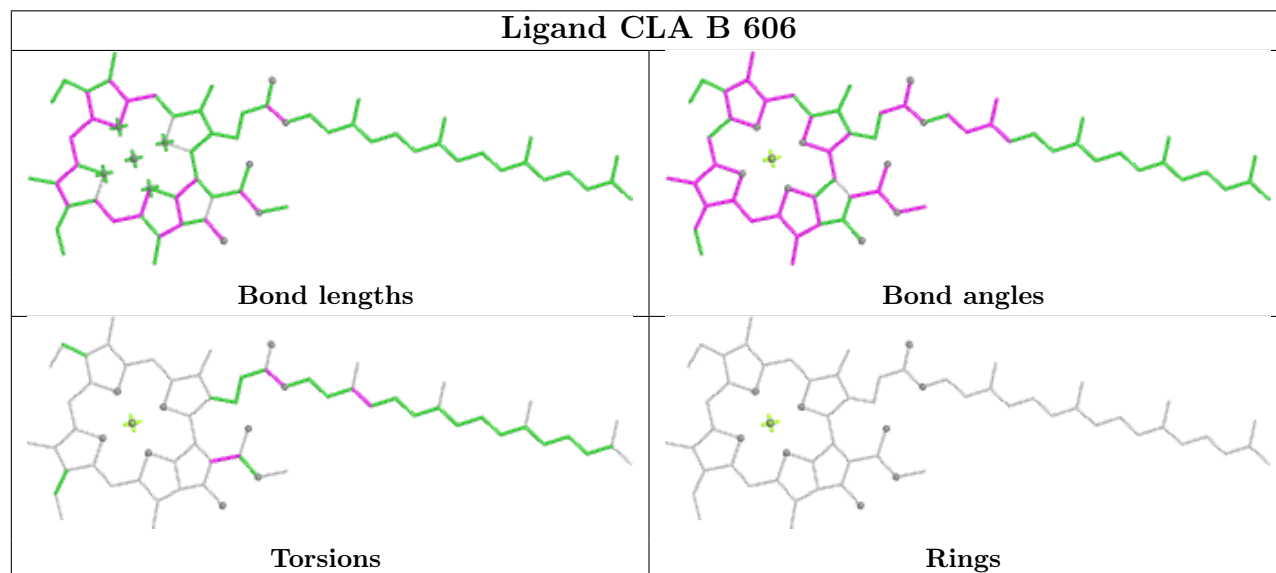
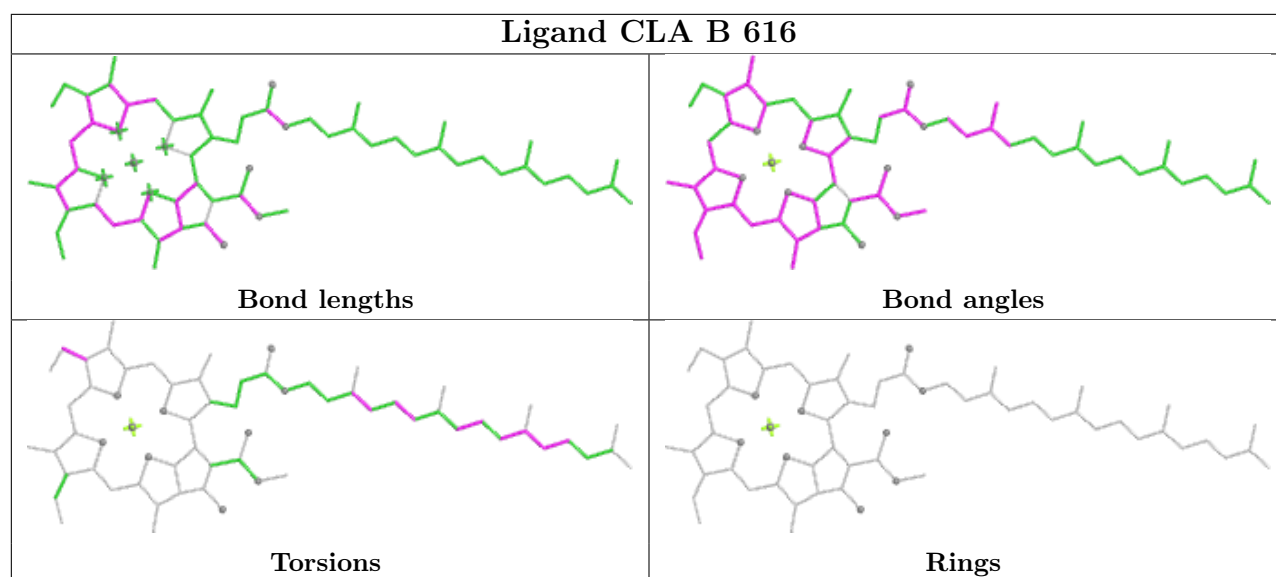
Ligand HTG D 412

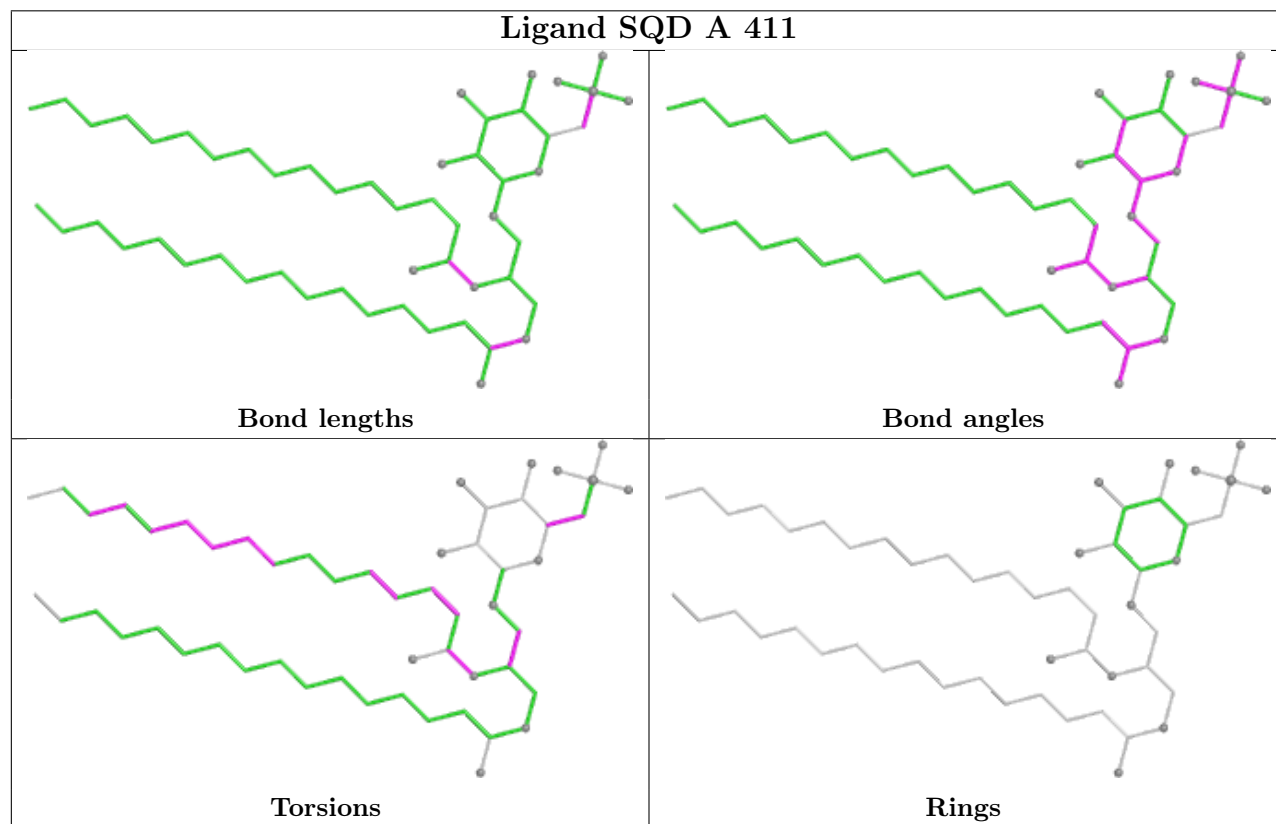
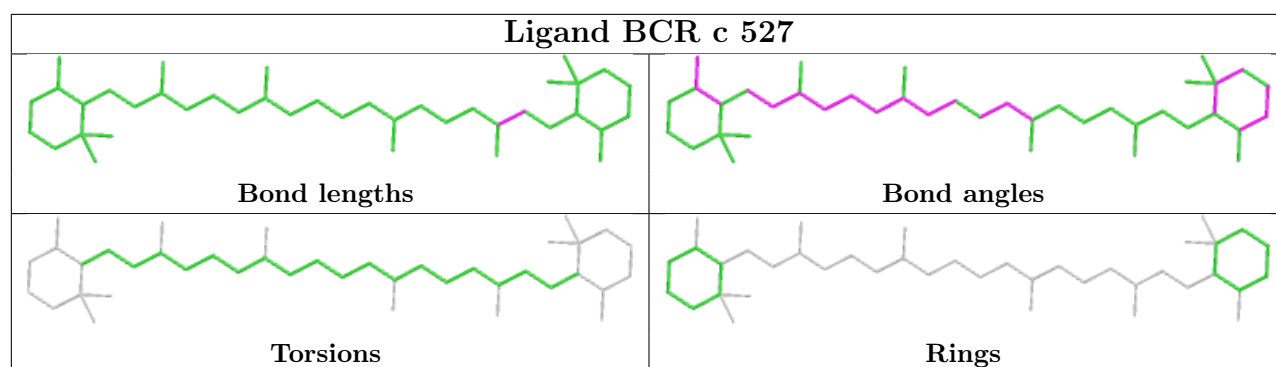


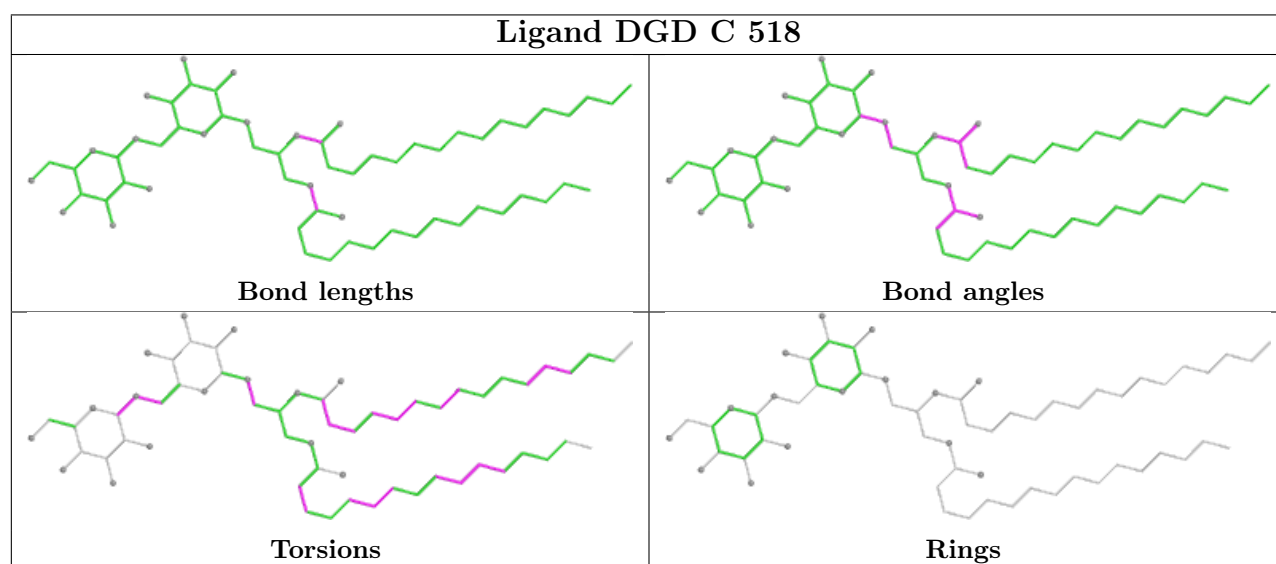
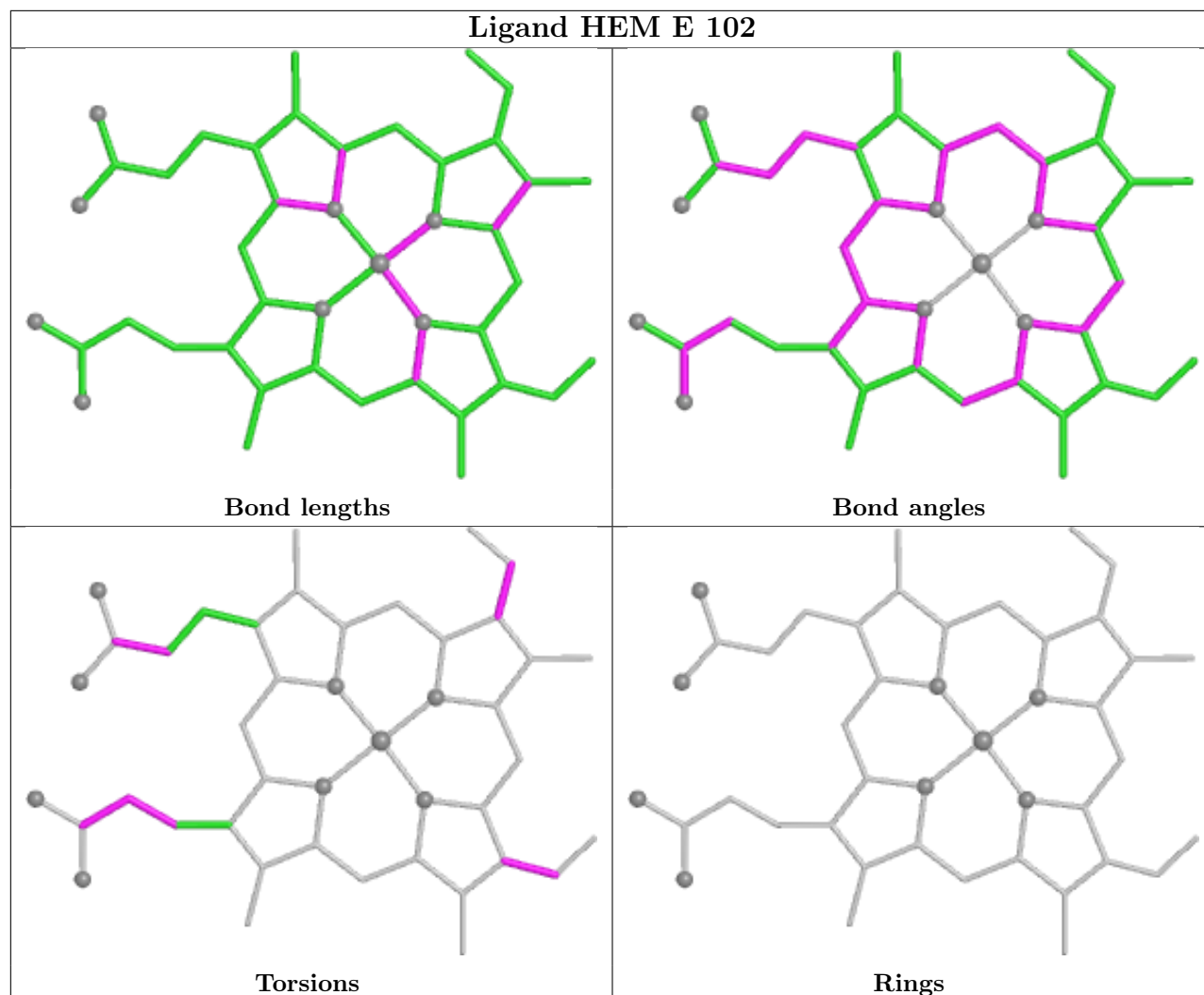


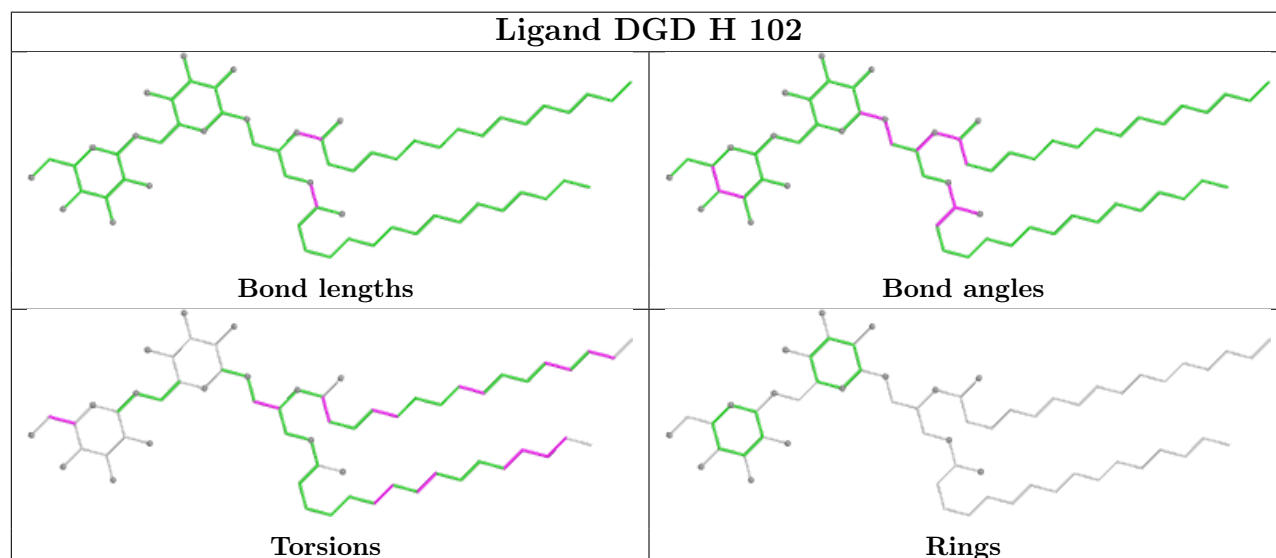
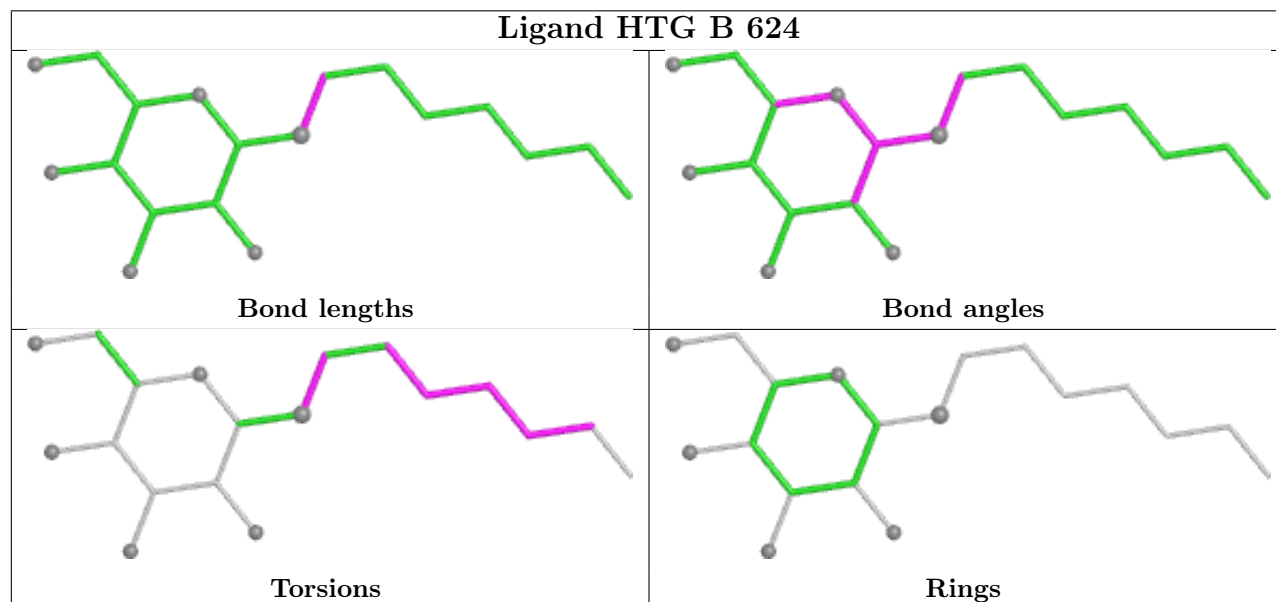
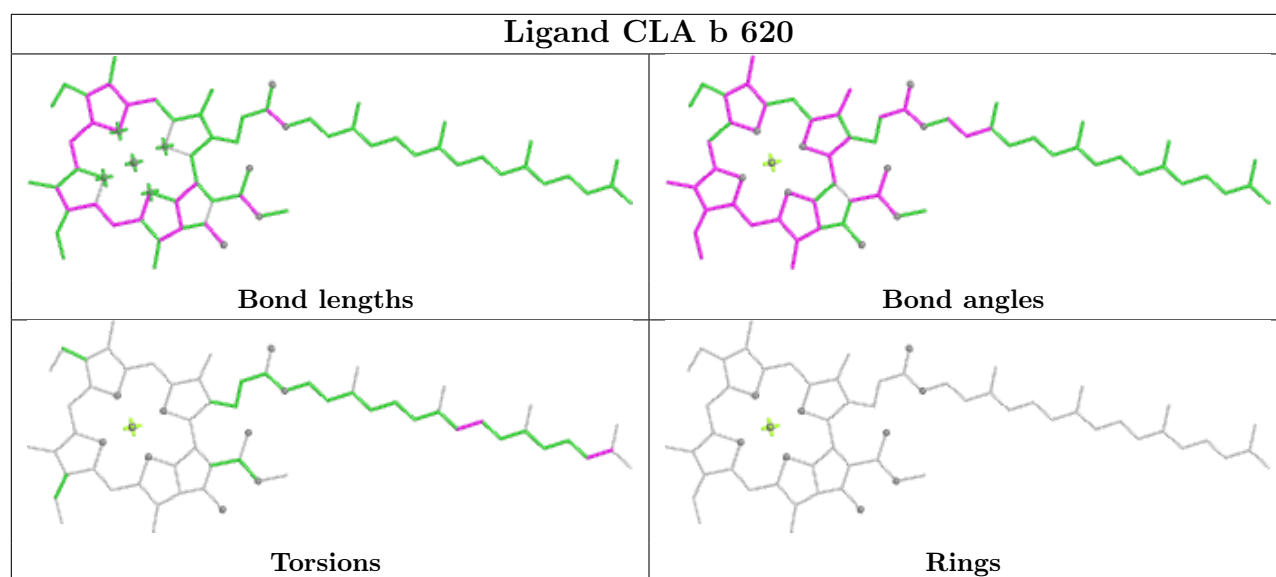


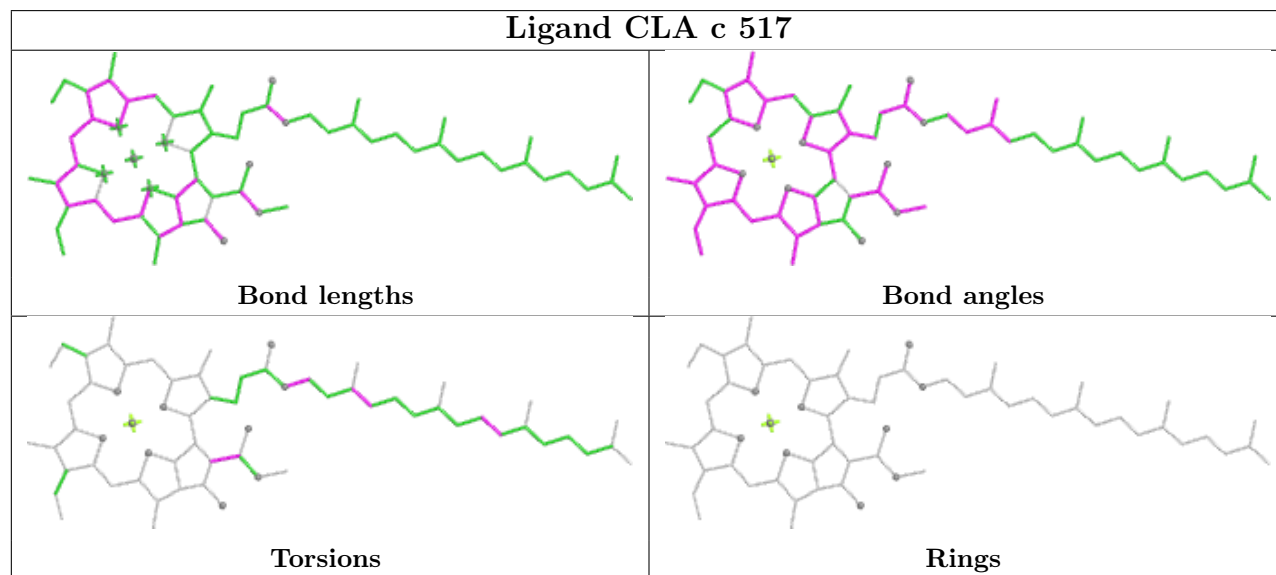
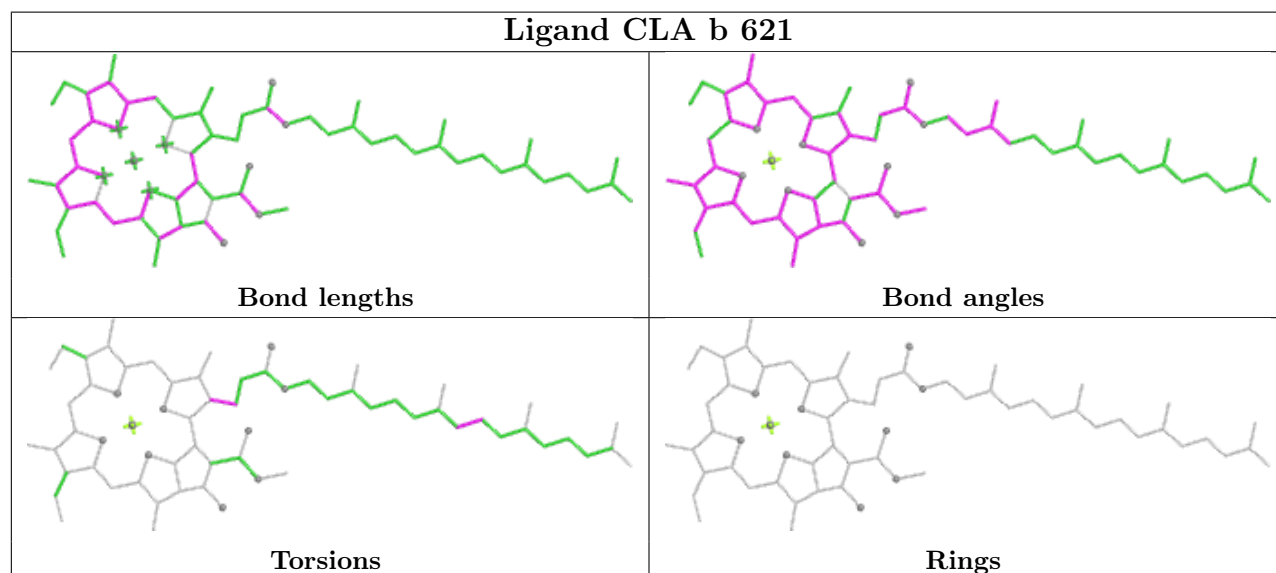
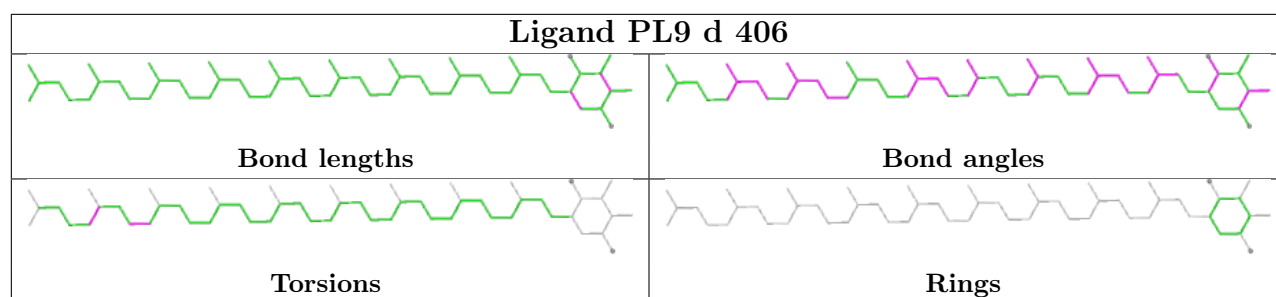




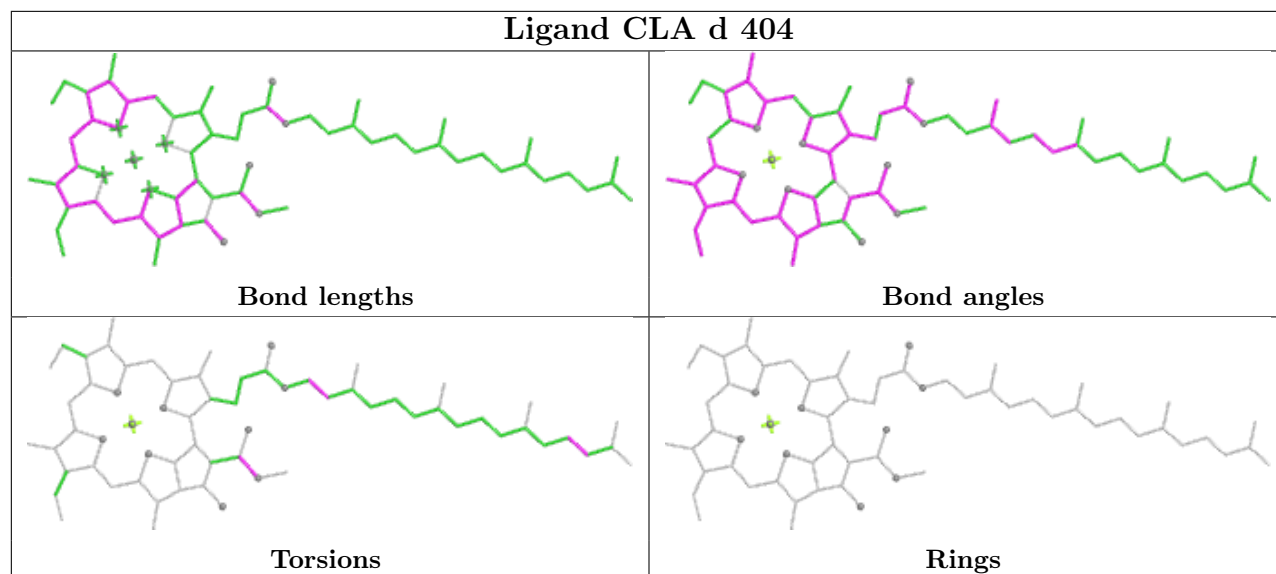




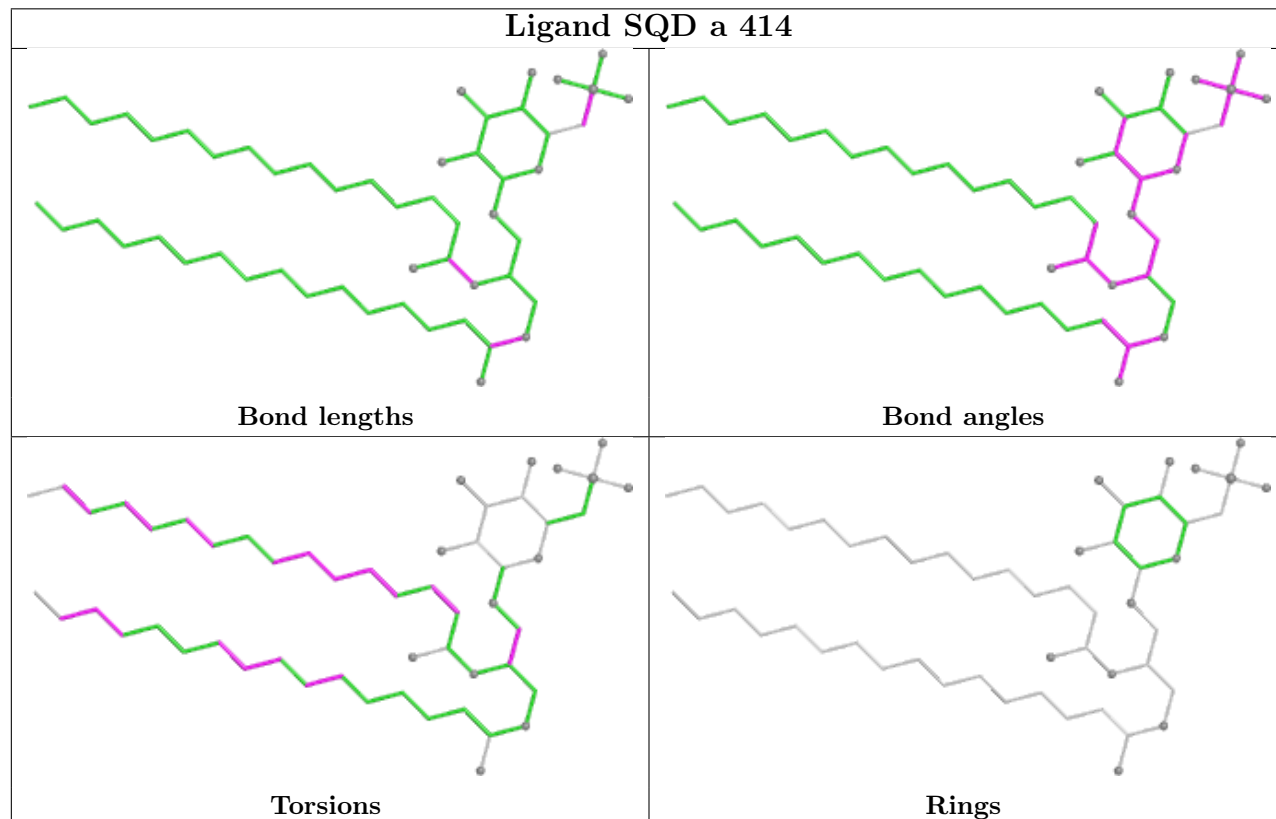


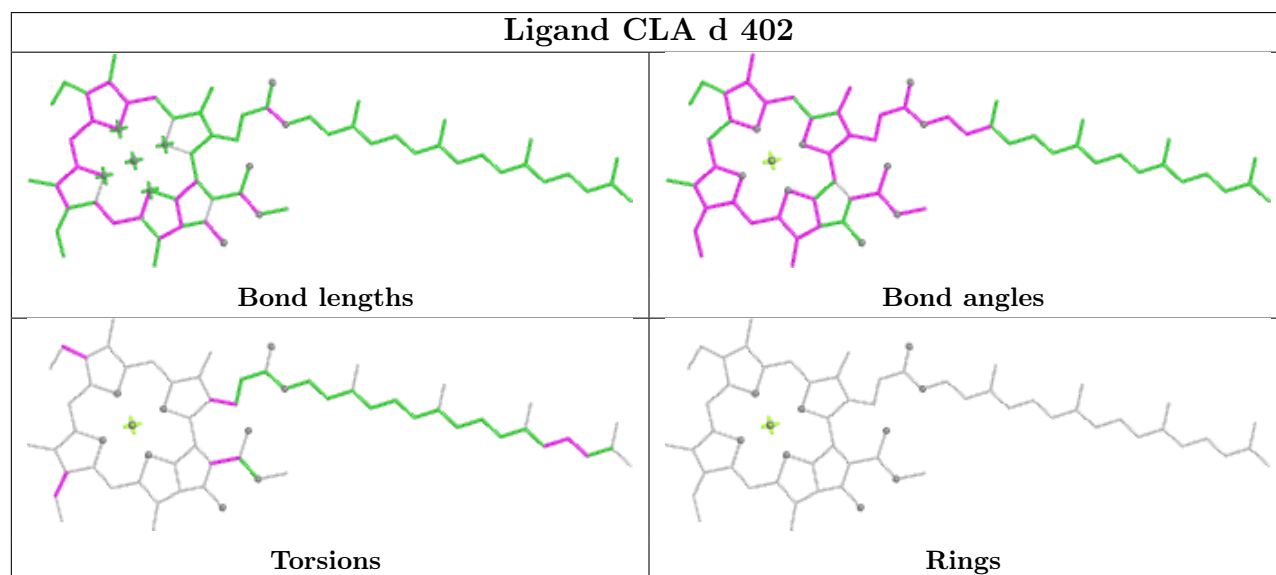
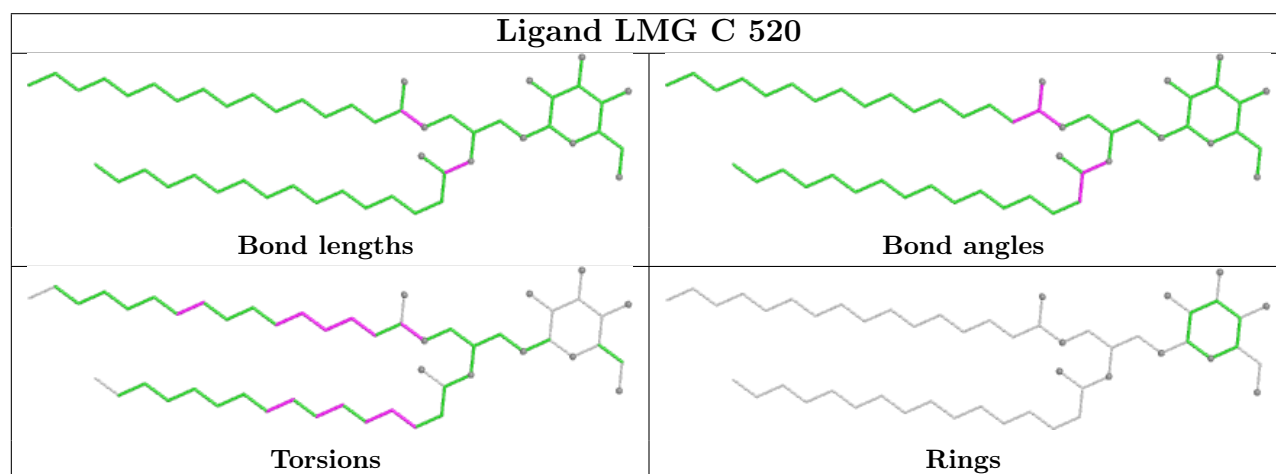
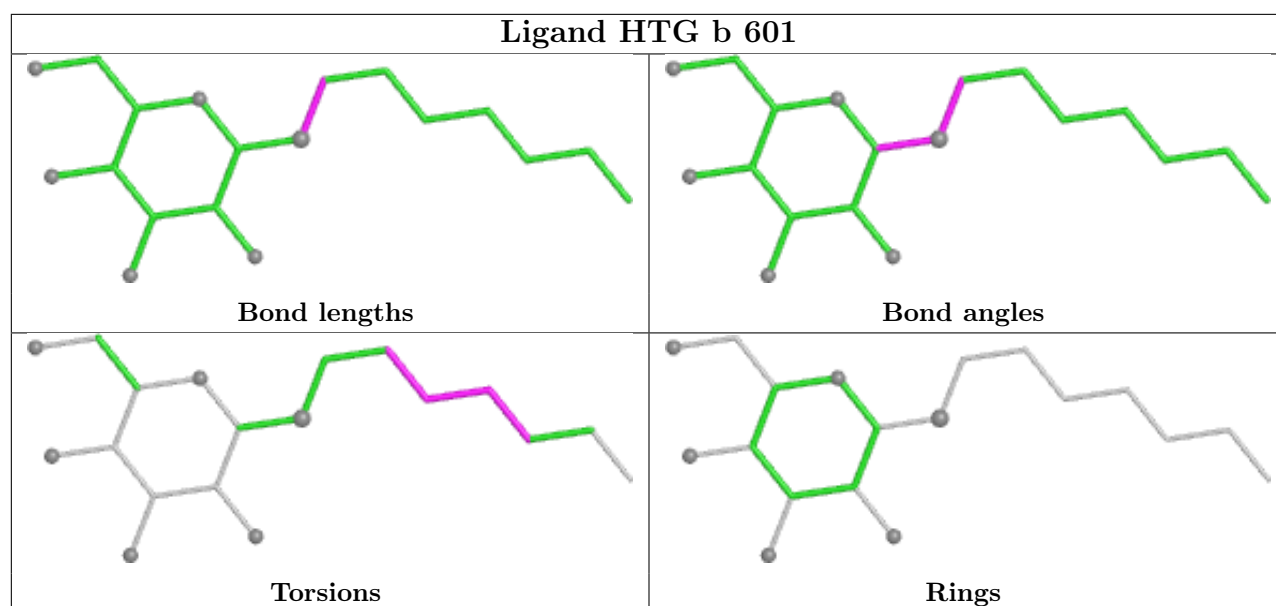


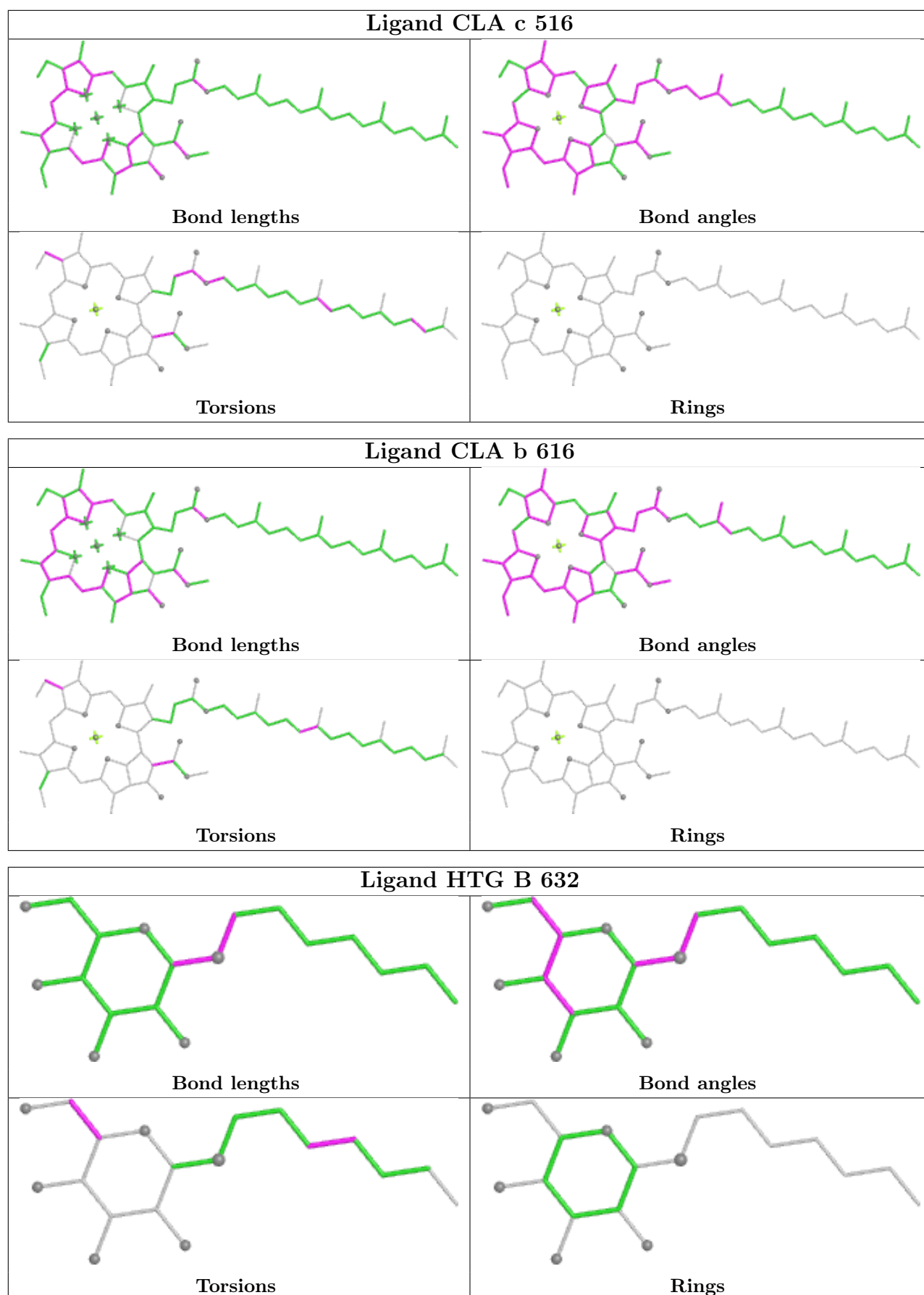
Ligand CLA d 404

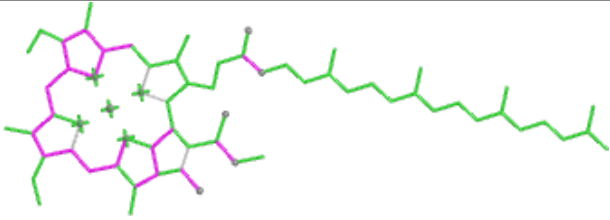
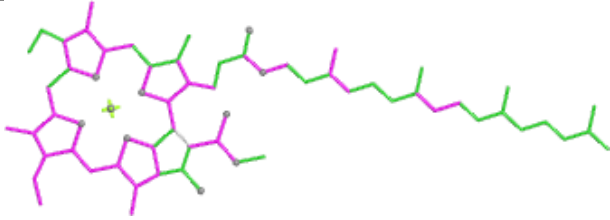
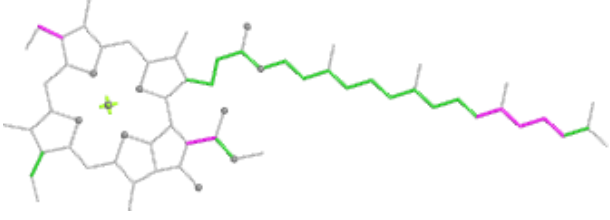
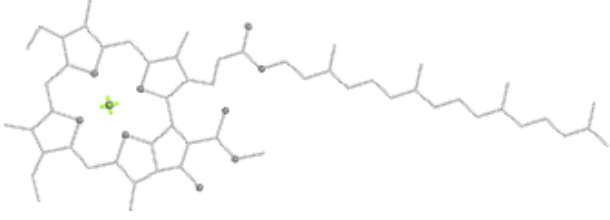
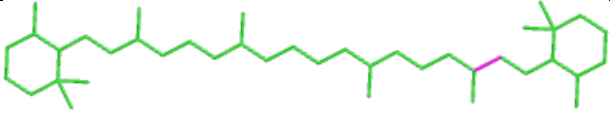
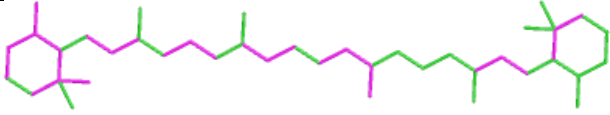
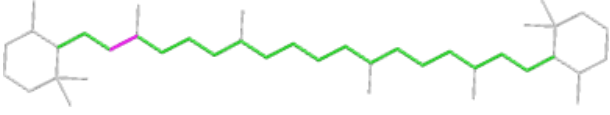
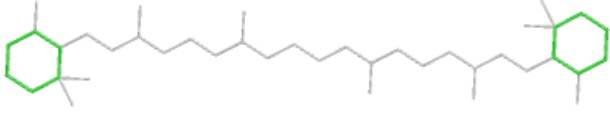
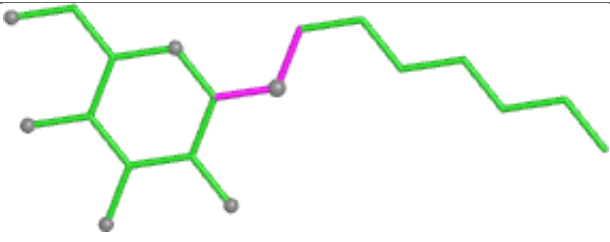
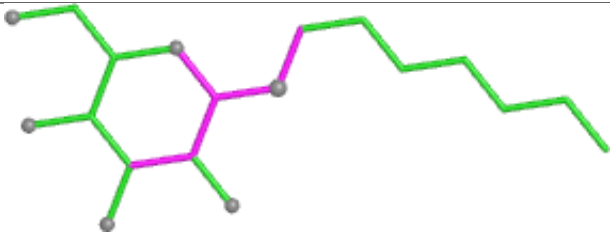
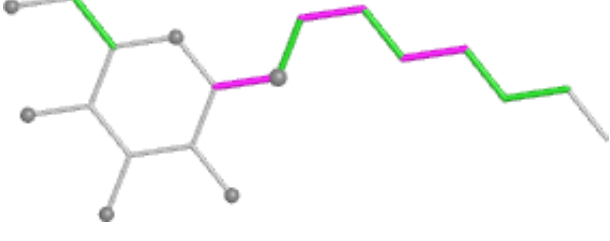
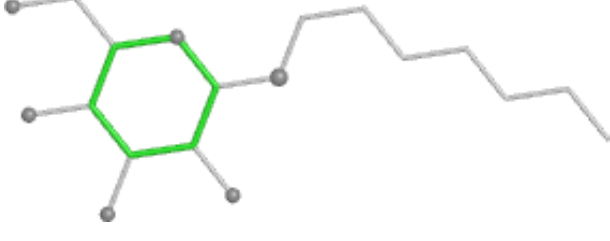


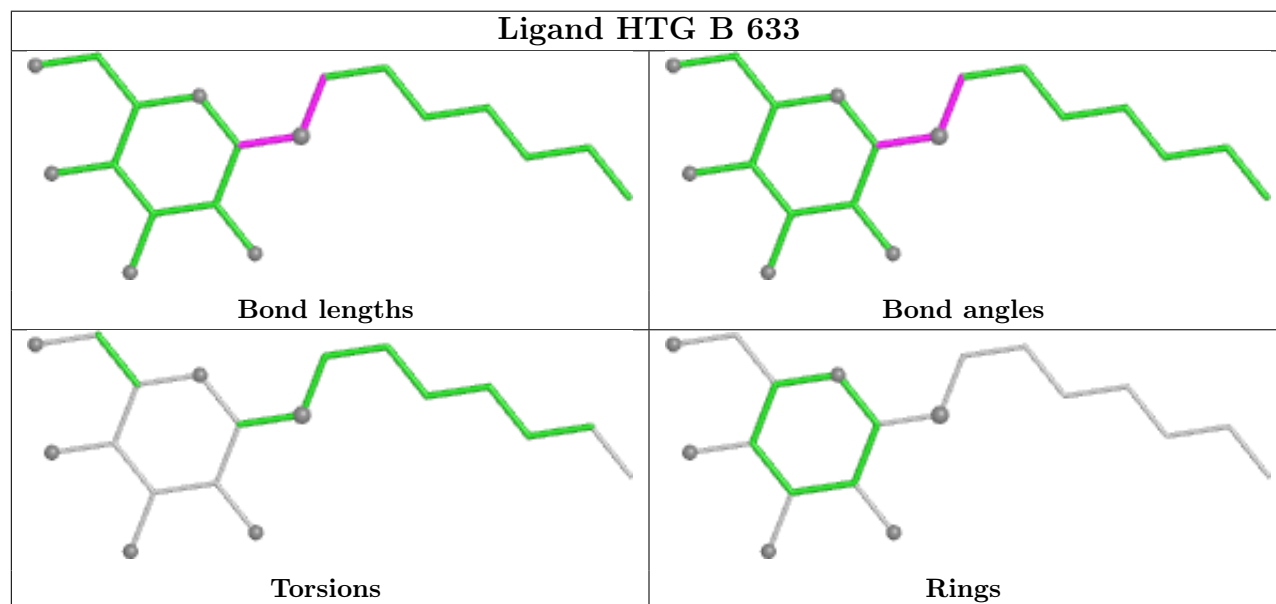
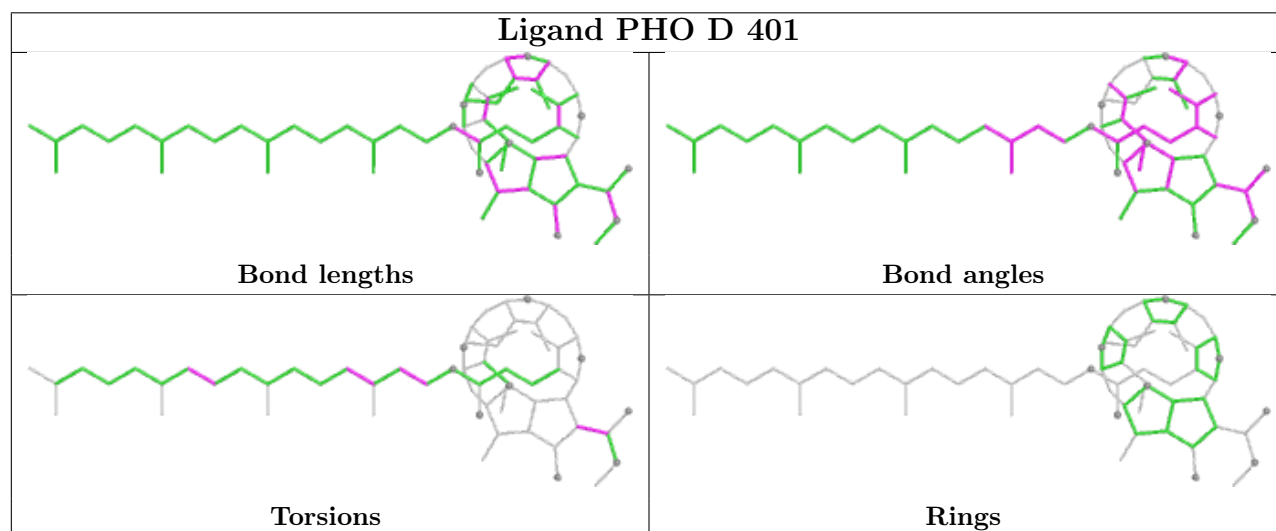
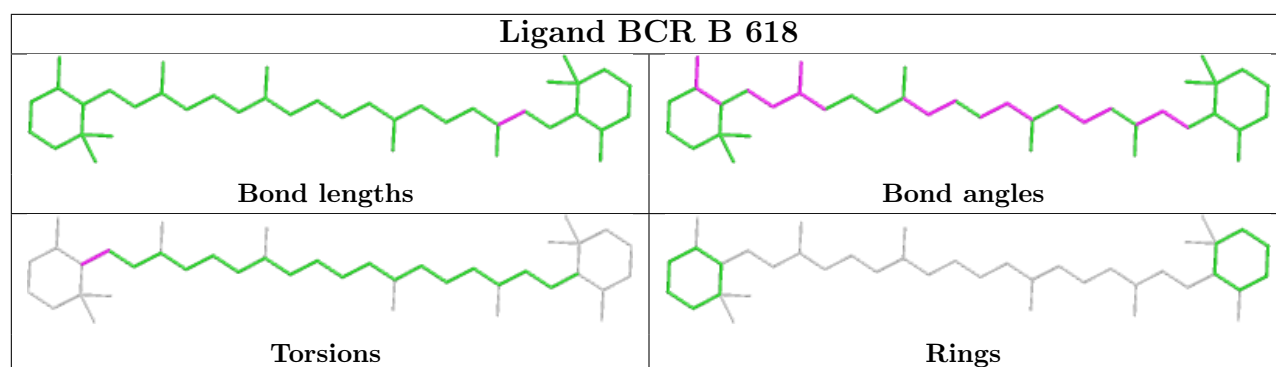
Ligand SQD a 414

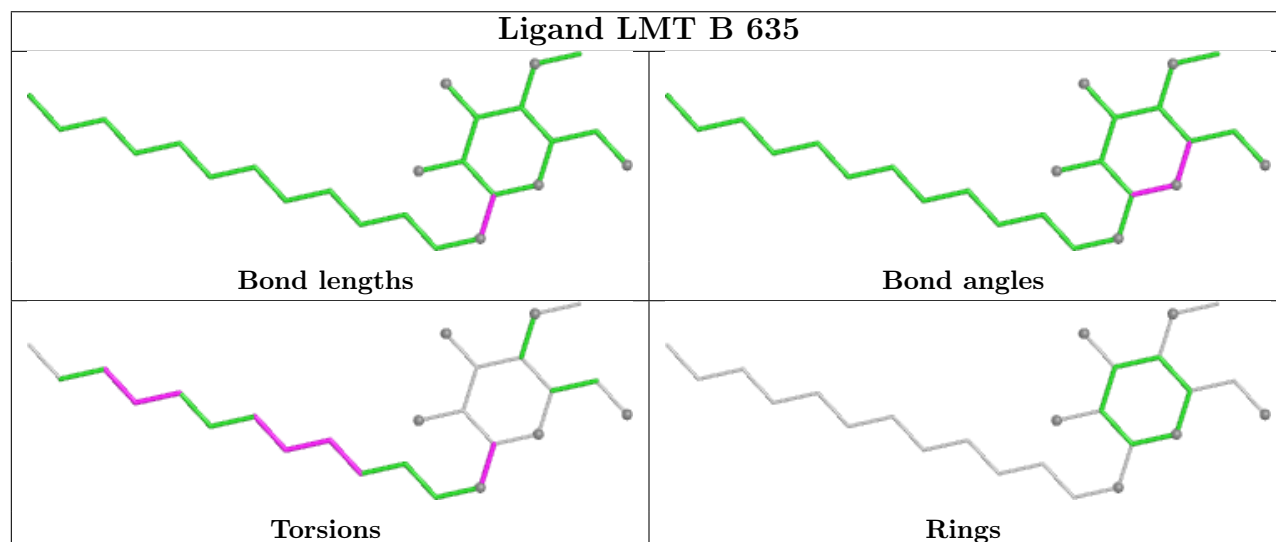
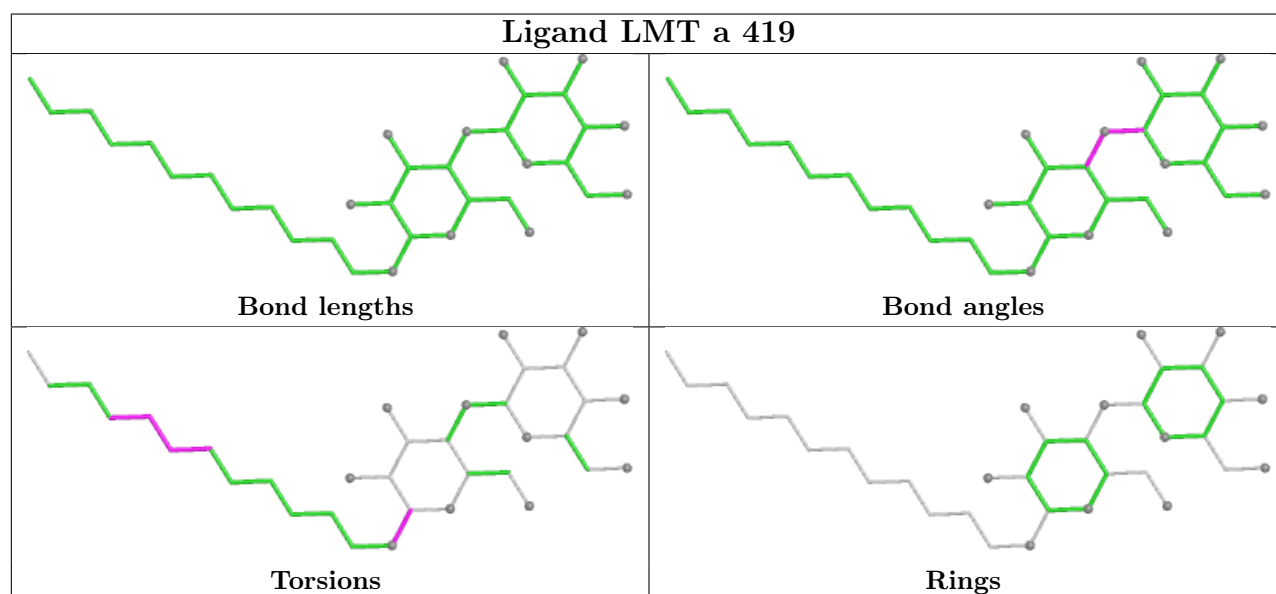
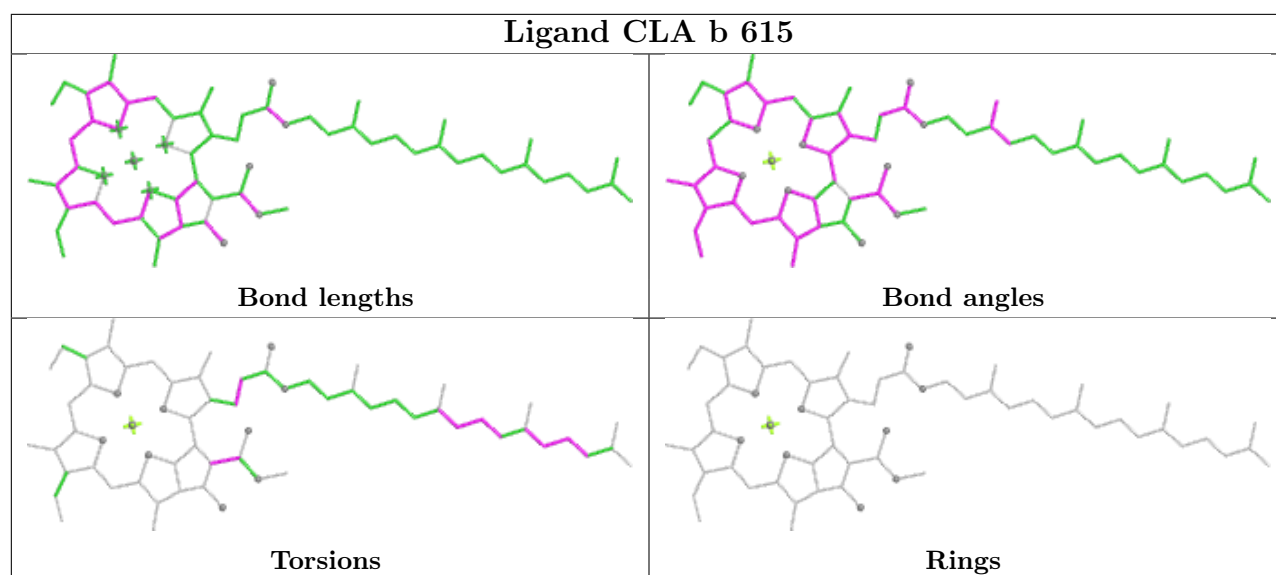


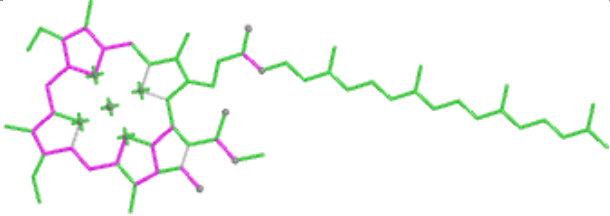
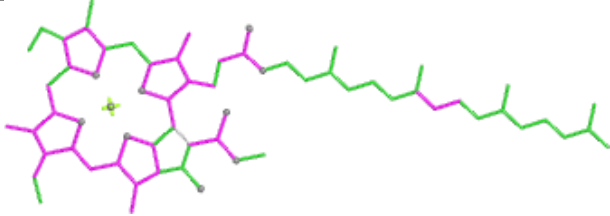
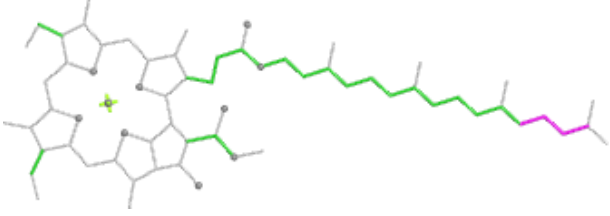
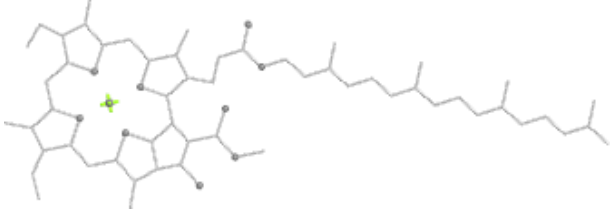
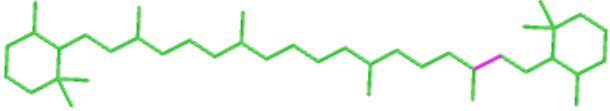
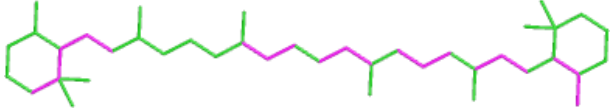
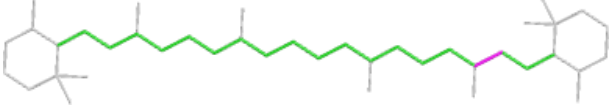
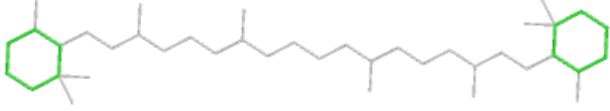




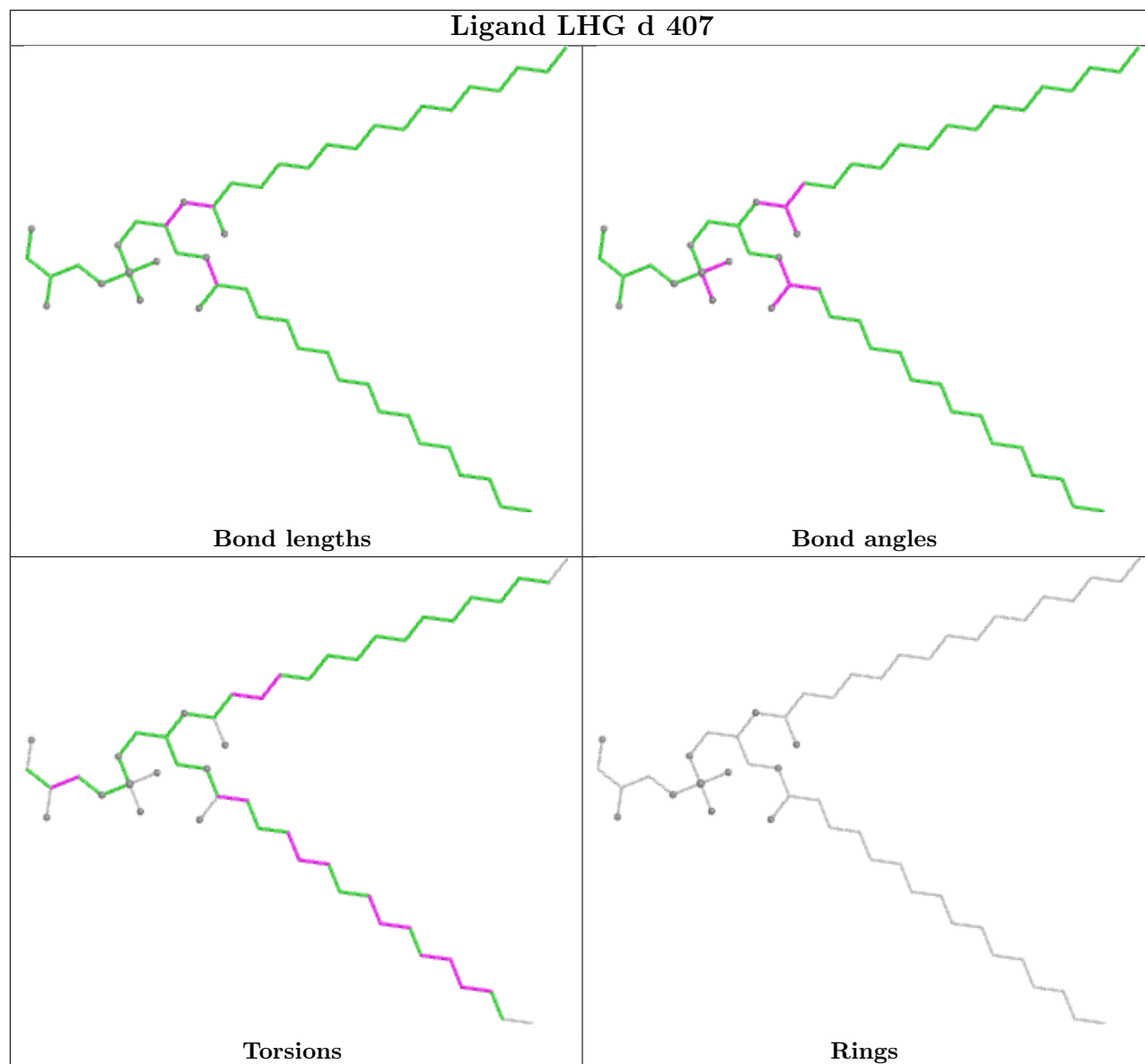
Ligand CLA C 505	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR K 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand HTG V 206	
 Bond lengths	 Bond angles
 Torsions	 Rings



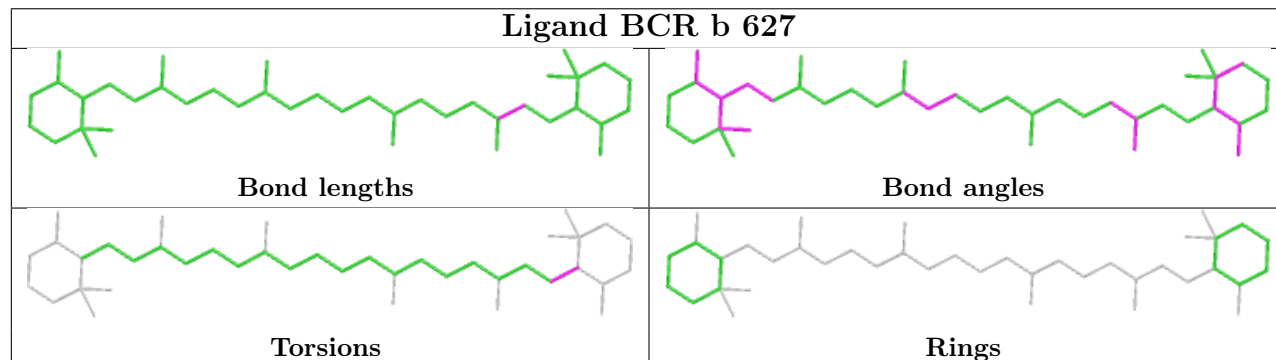


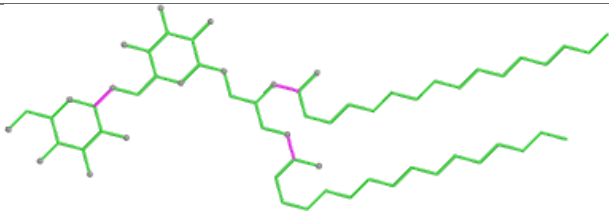
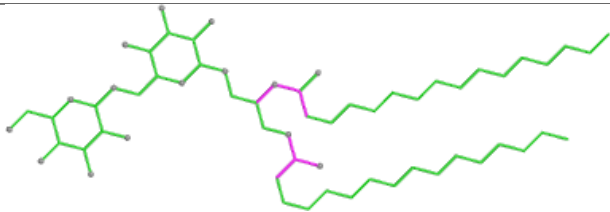
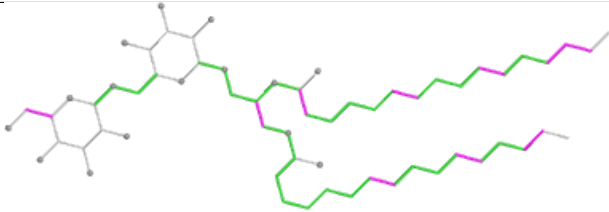
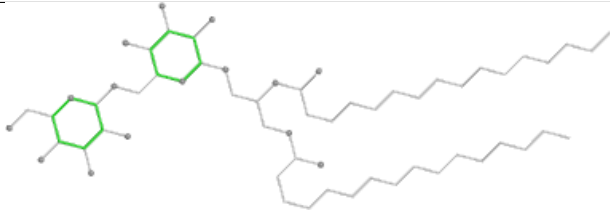
Ligand CLA A 405	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b 628	
 Bond lengths	 Bond angles
 Torsions	 Rings

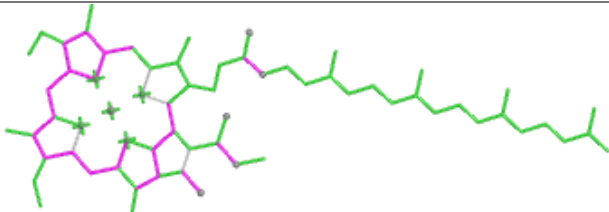
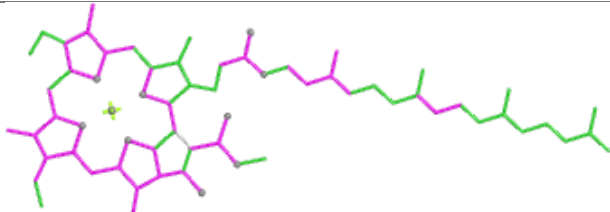
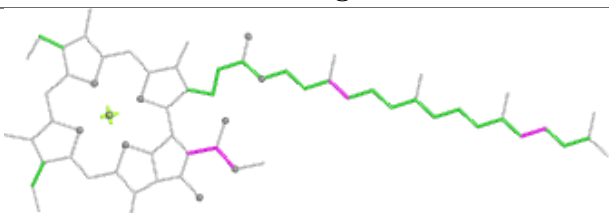
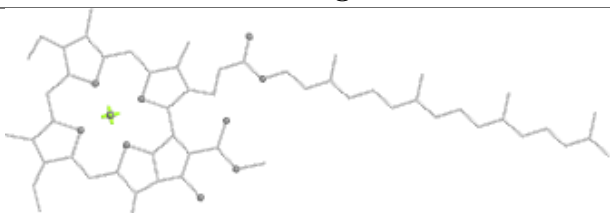
Ligand LHG d 407

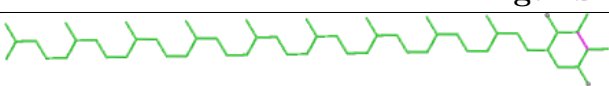
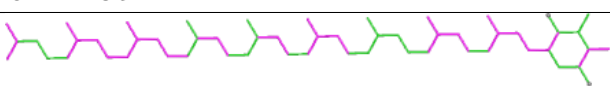
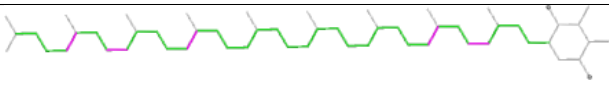
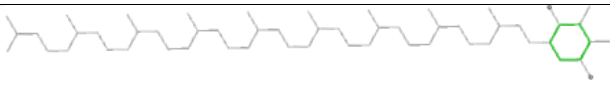


Ligand BCR b 627

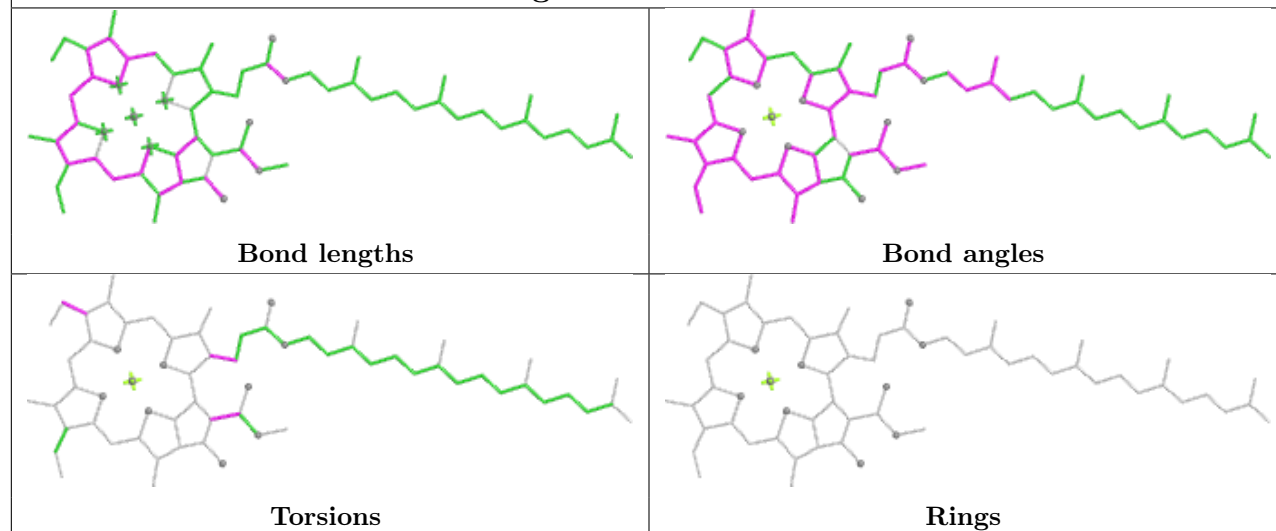


Ligand DGD h 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

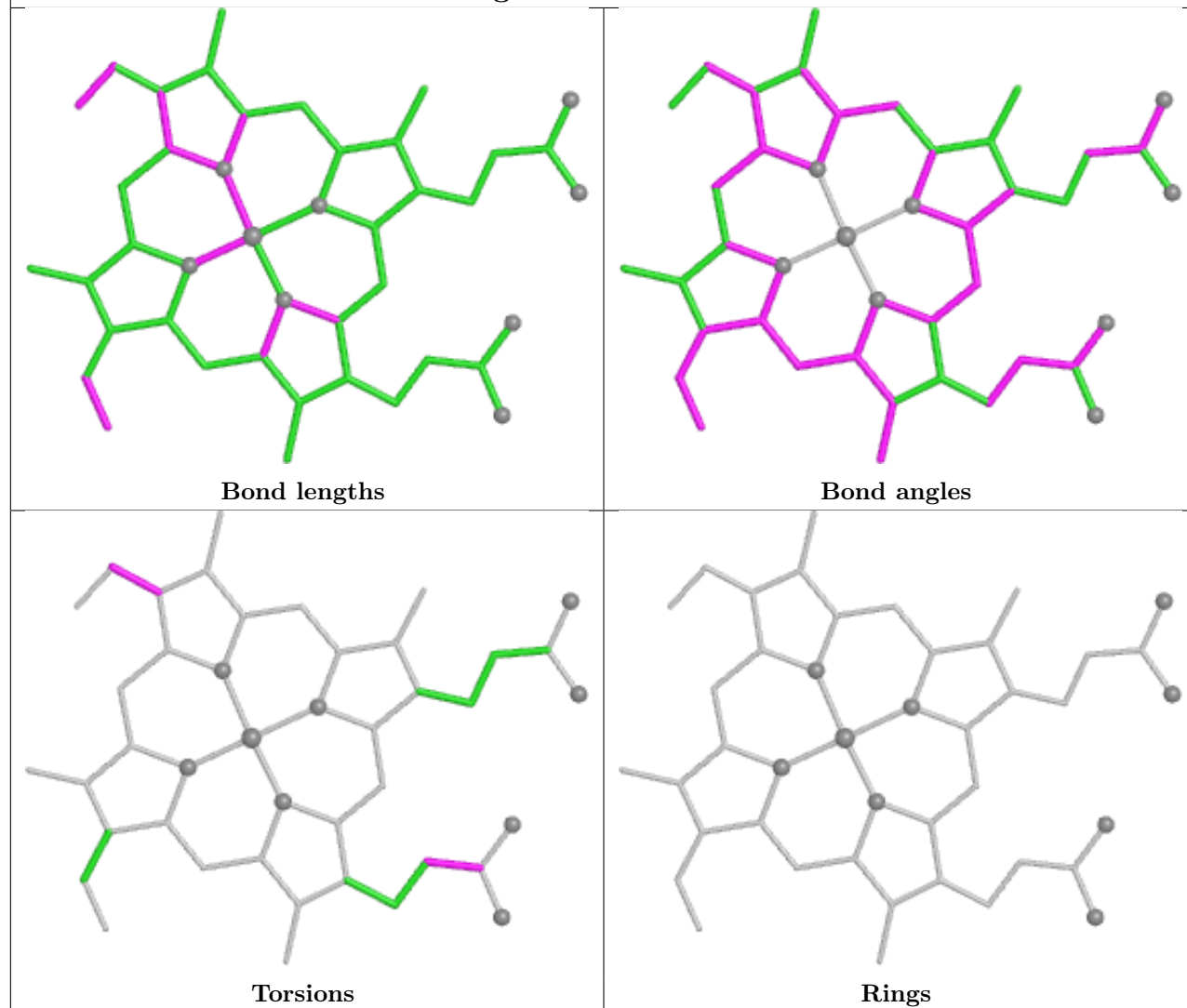
Ligand CLA B 605	
	
Bond lengths	Bond angles
	
Torsions	Rings

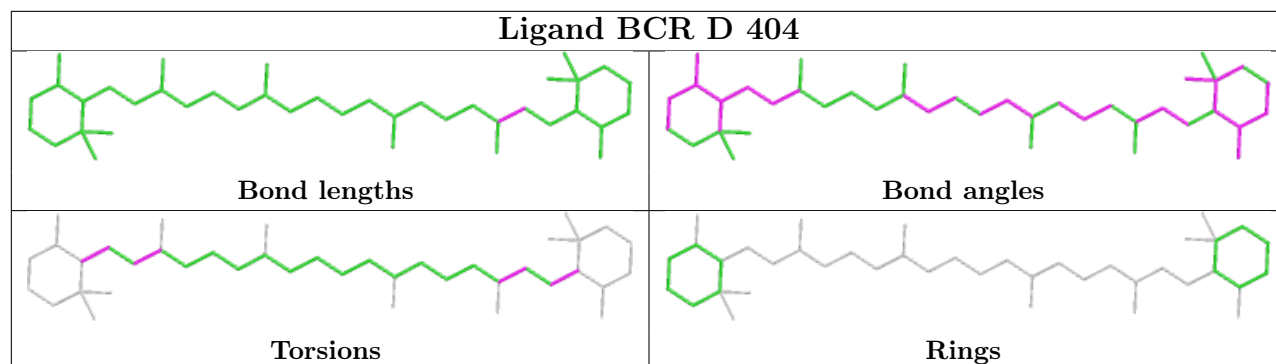
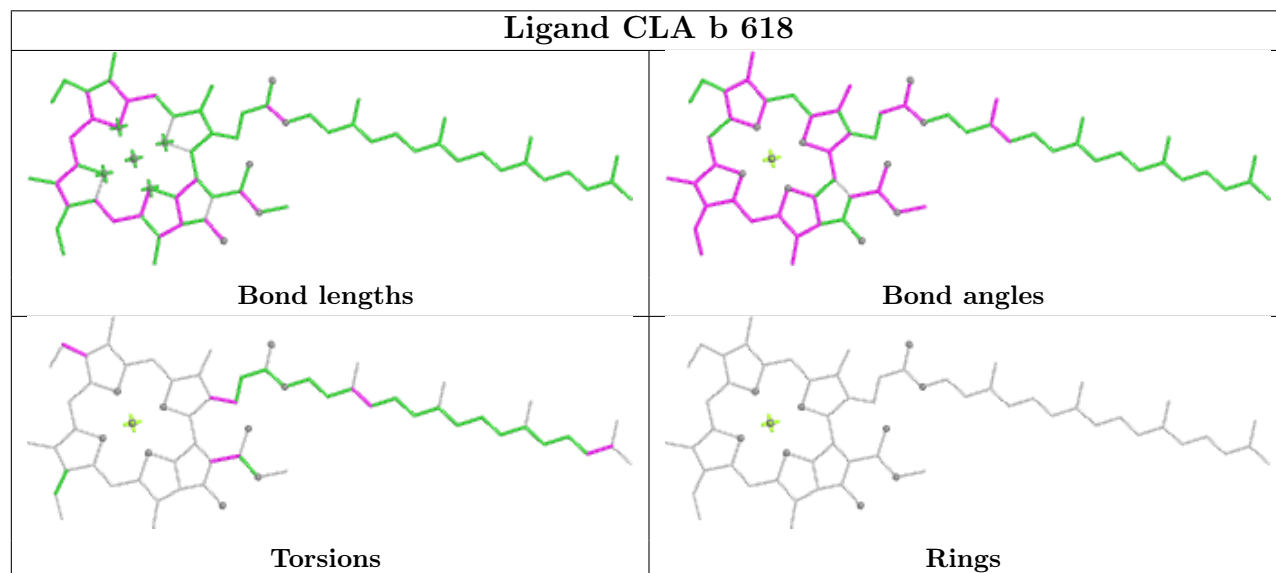
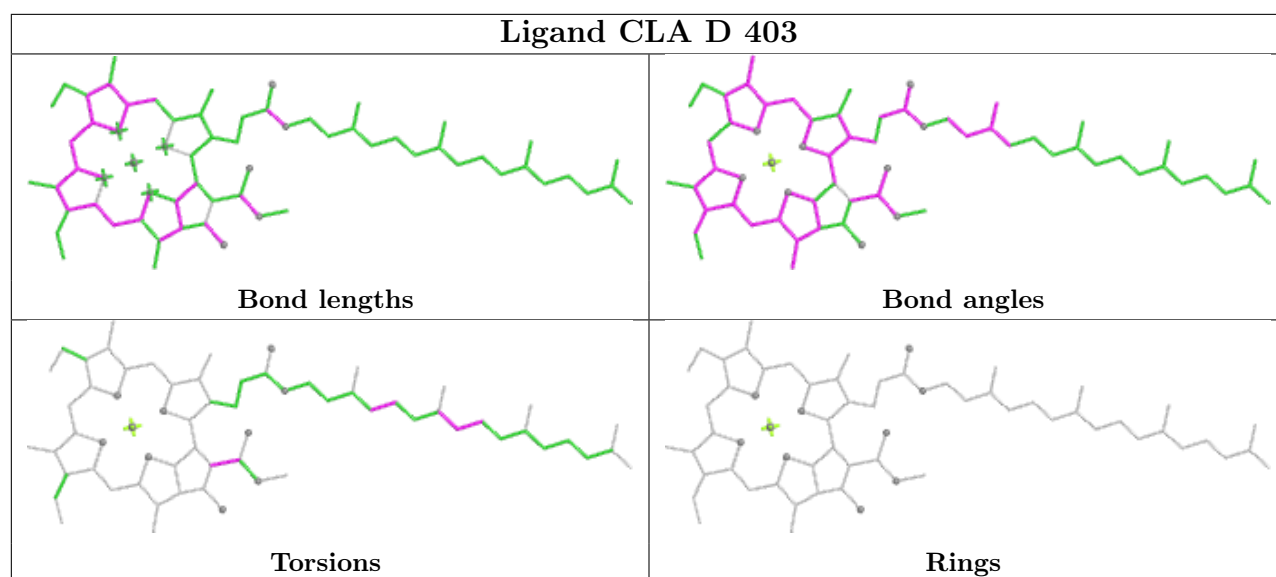
Ligand PL9 D 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

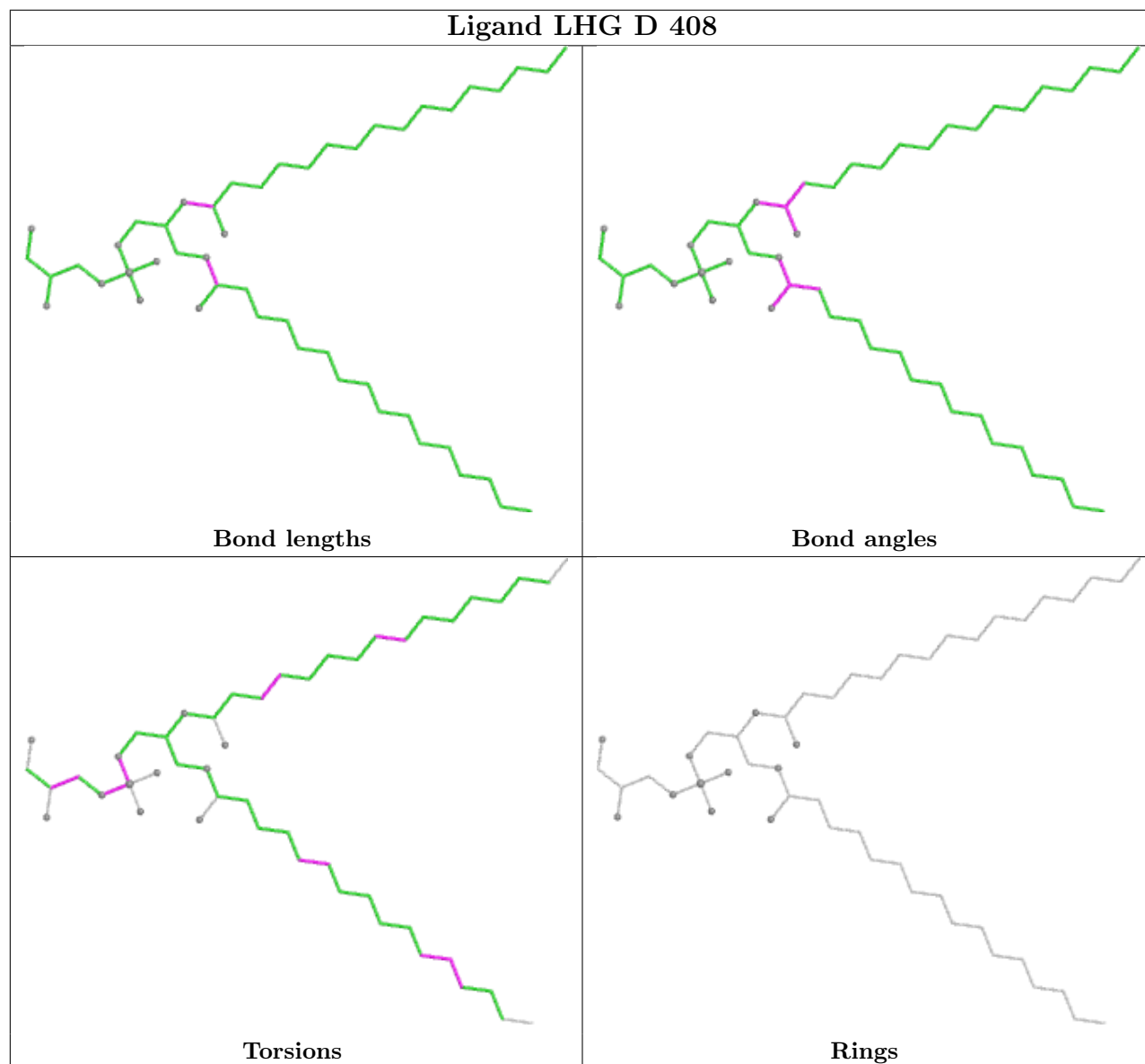
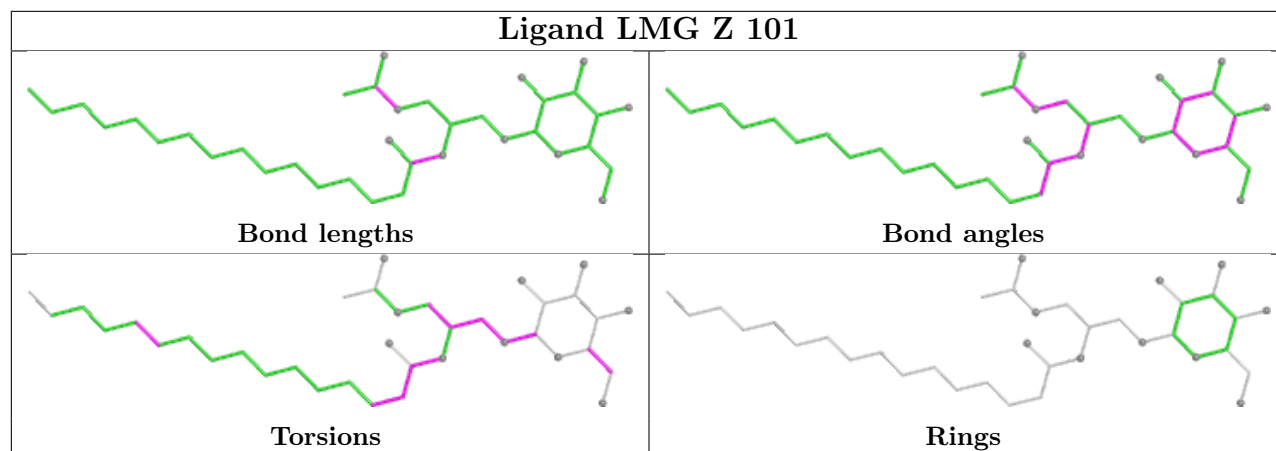
Ligand CLA B 608

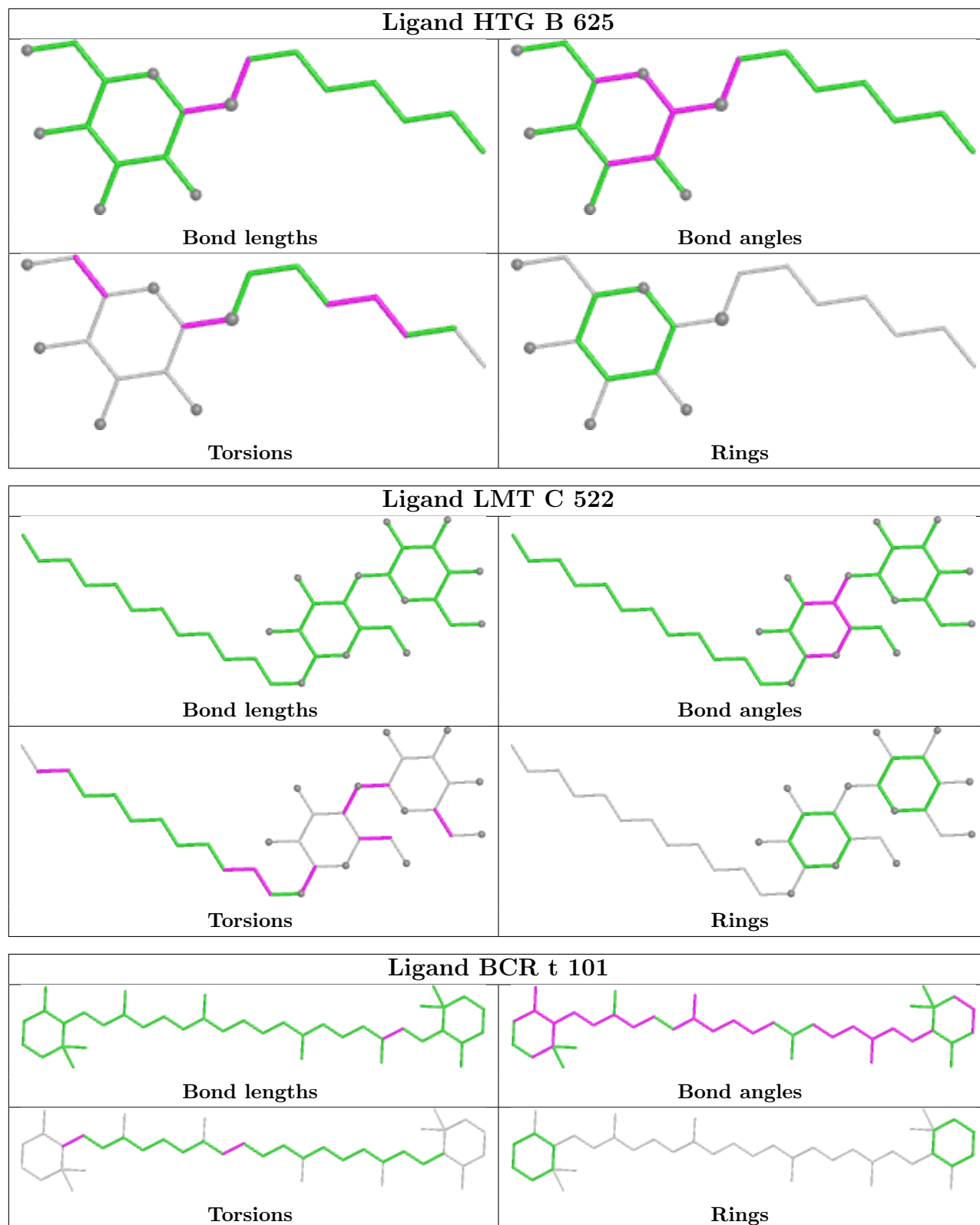


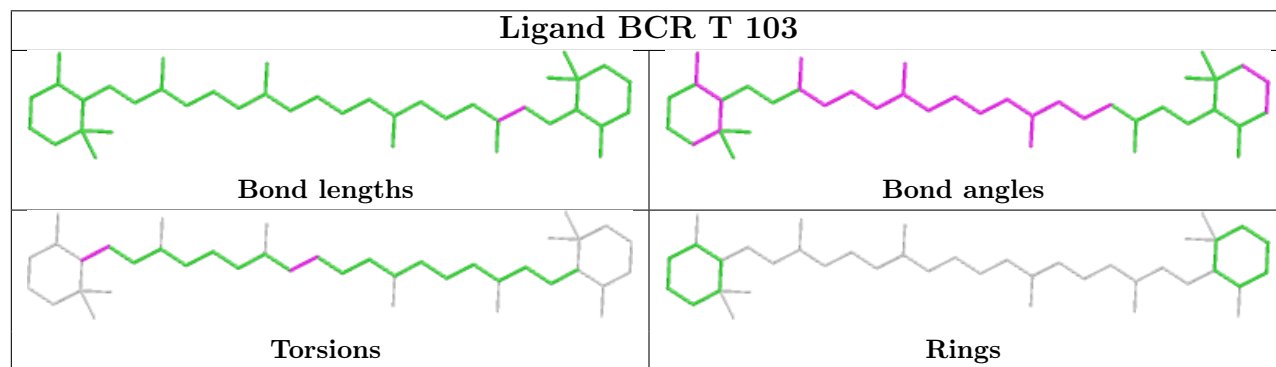
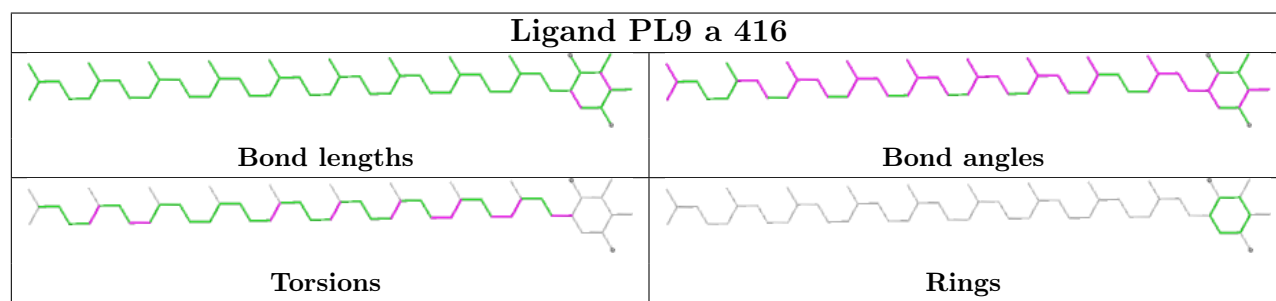
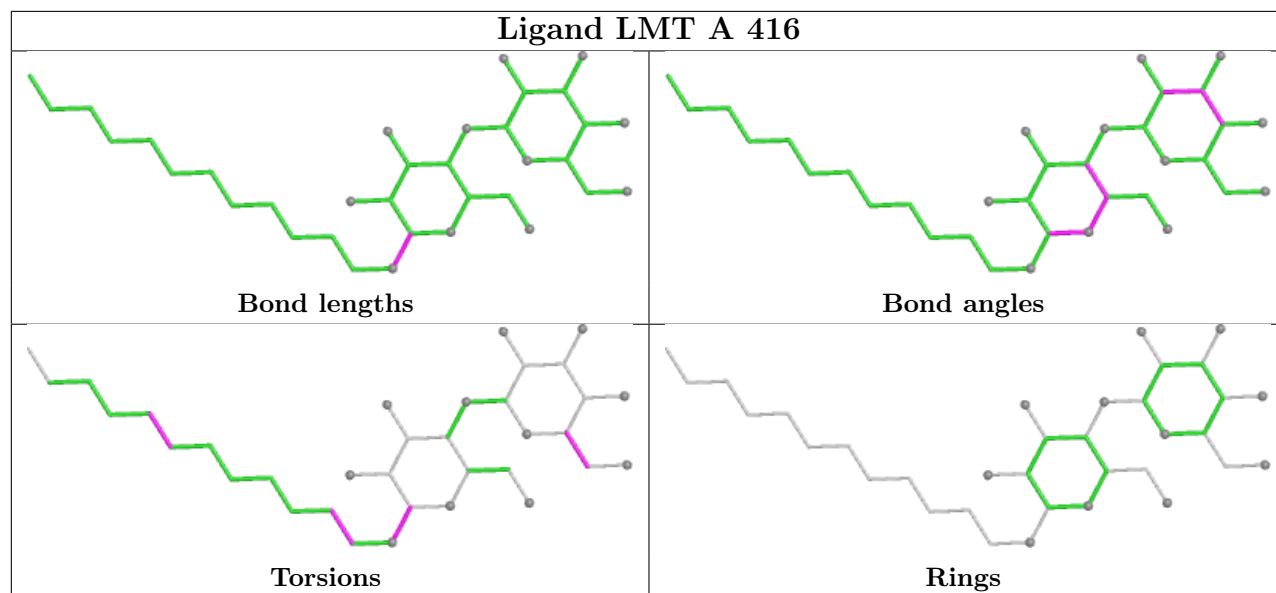
Ligand HEC V 205

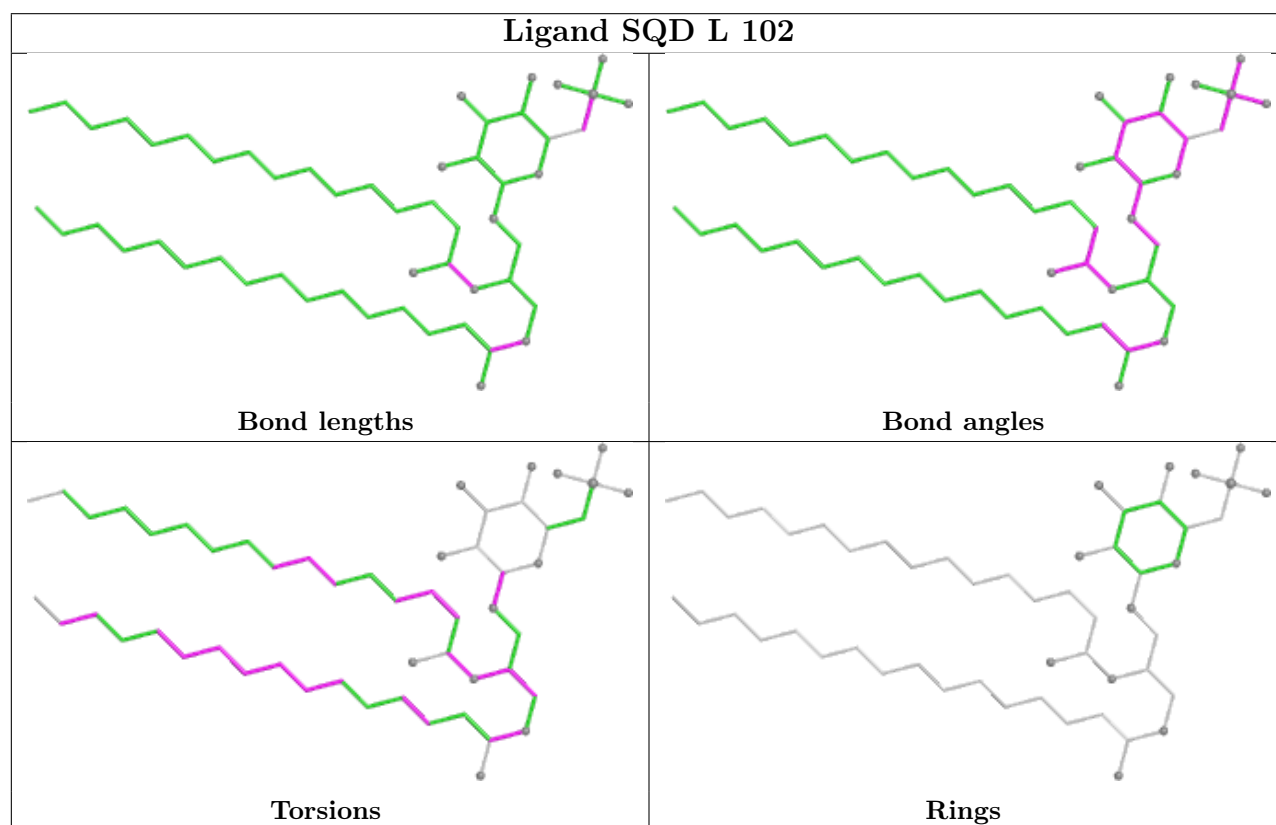
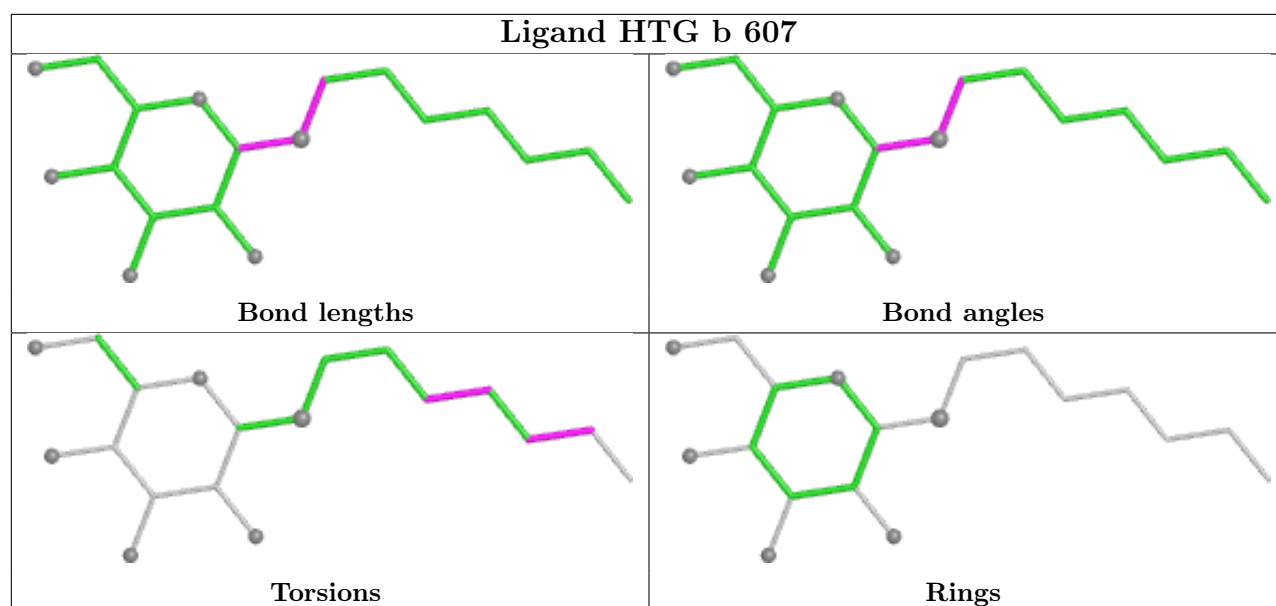


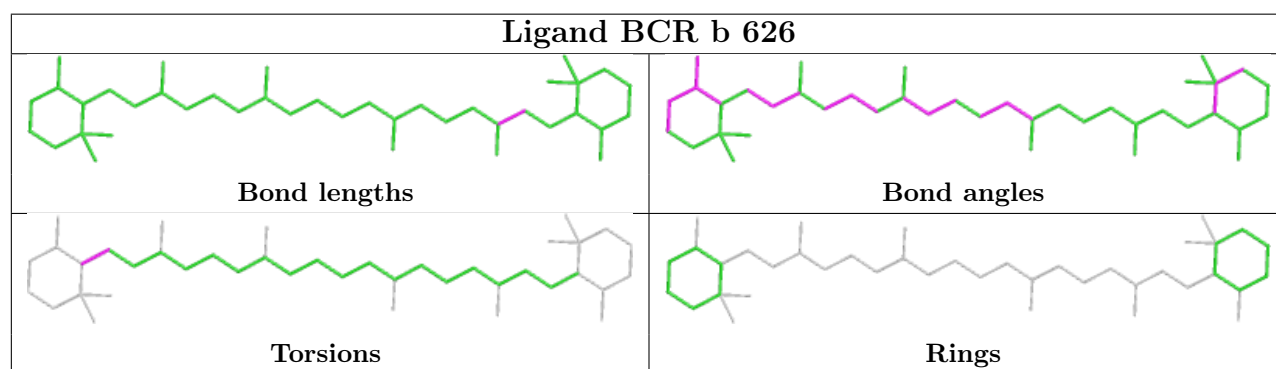
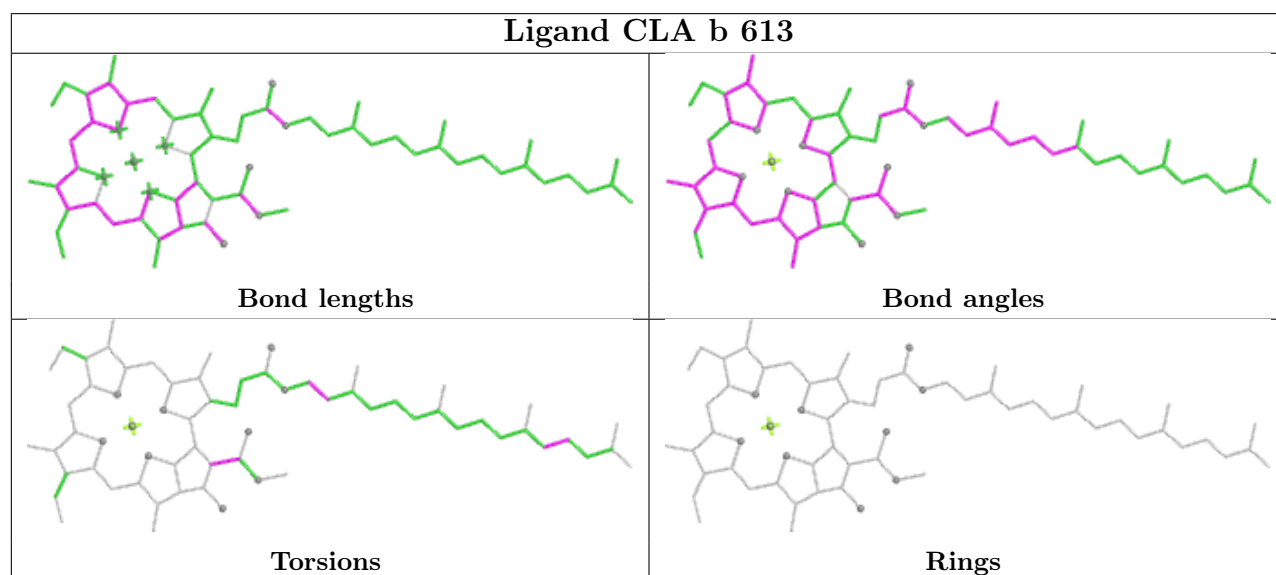
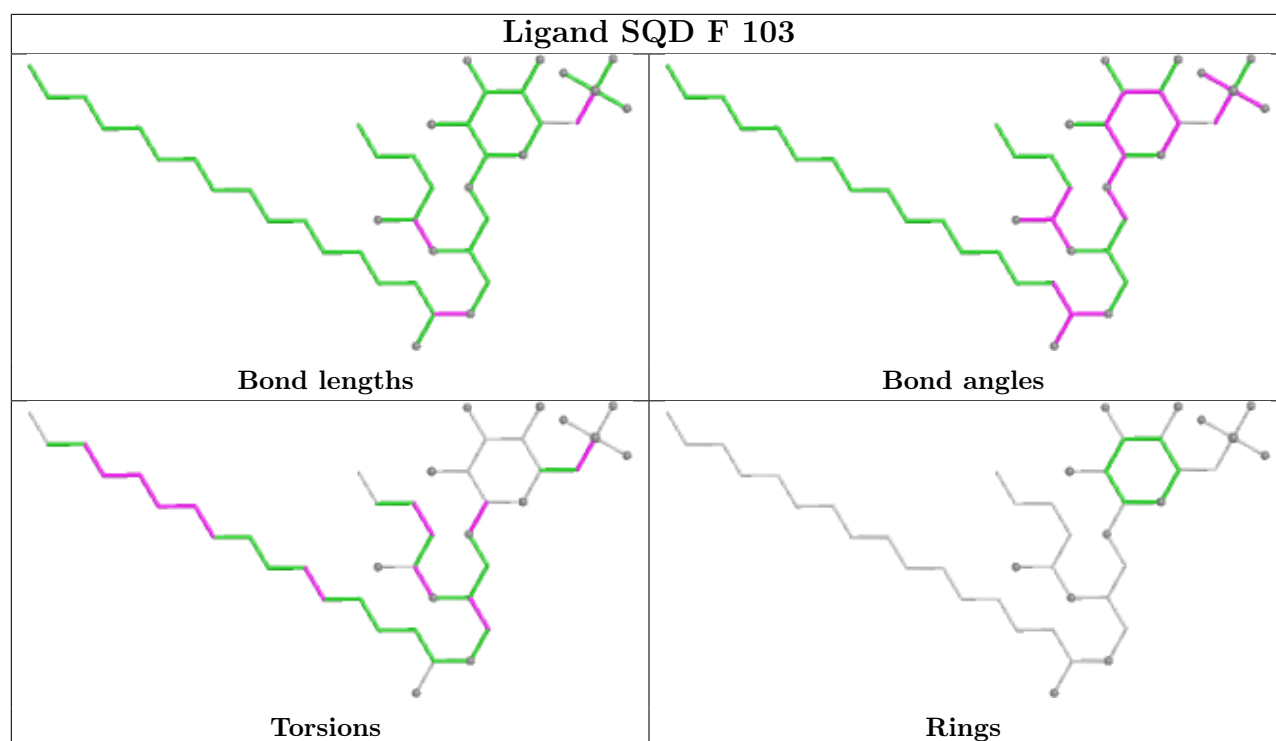


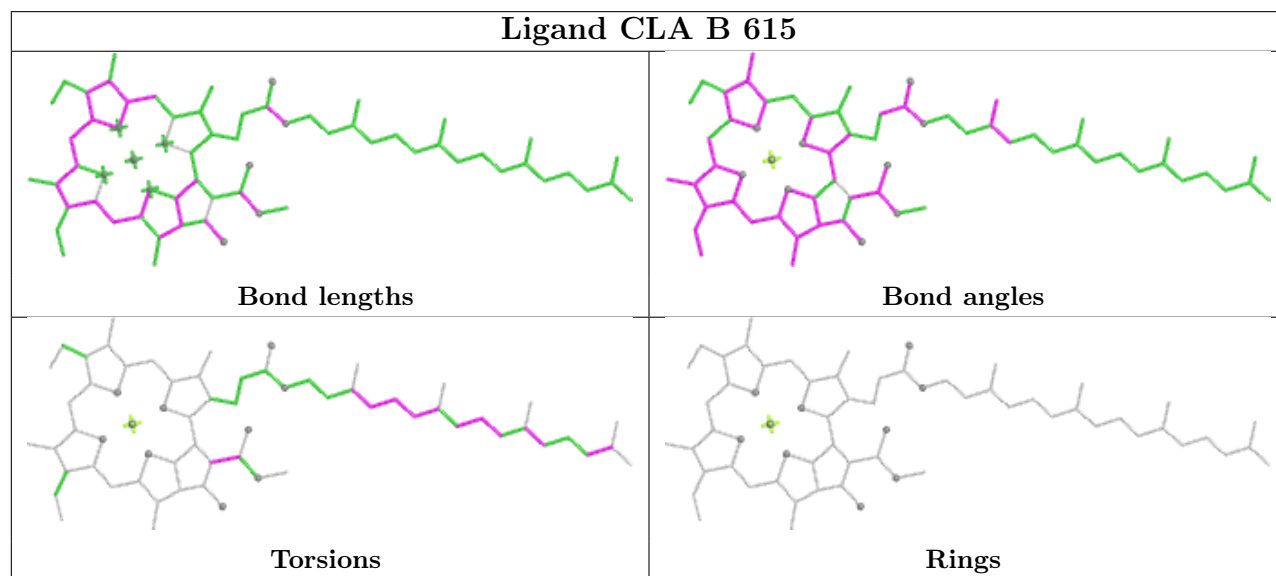
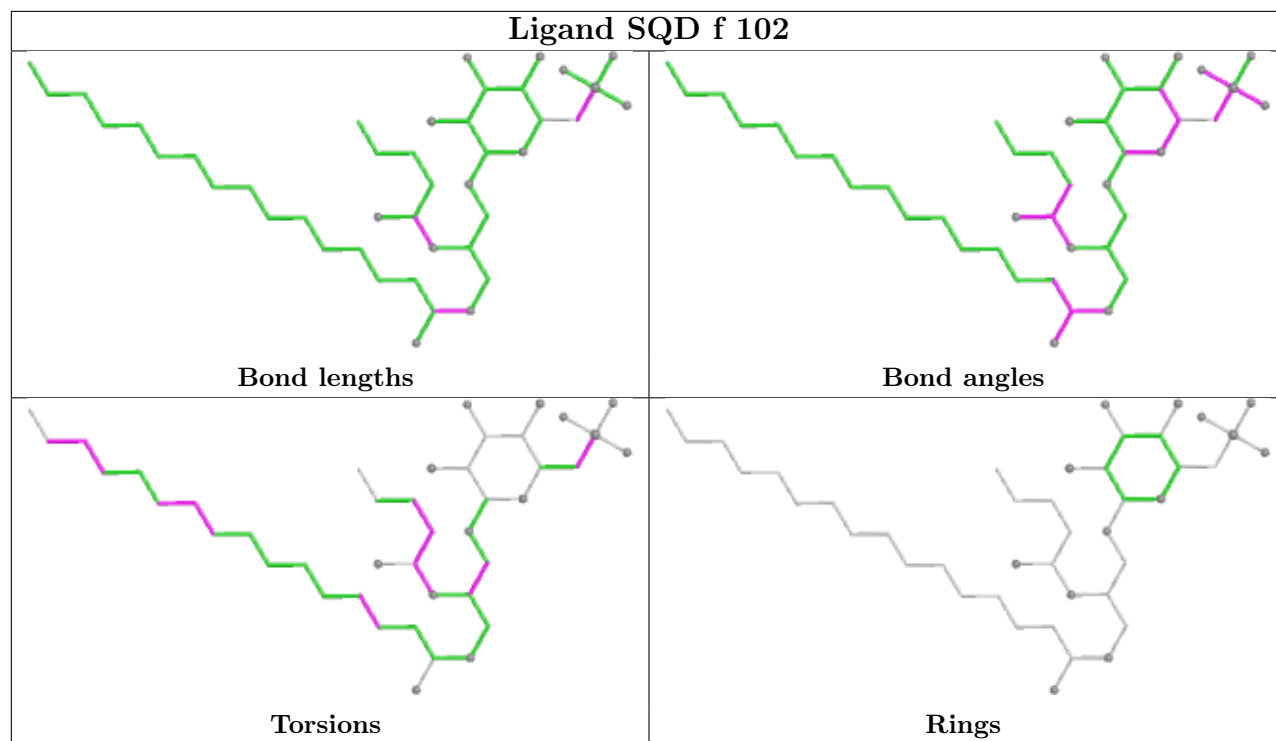


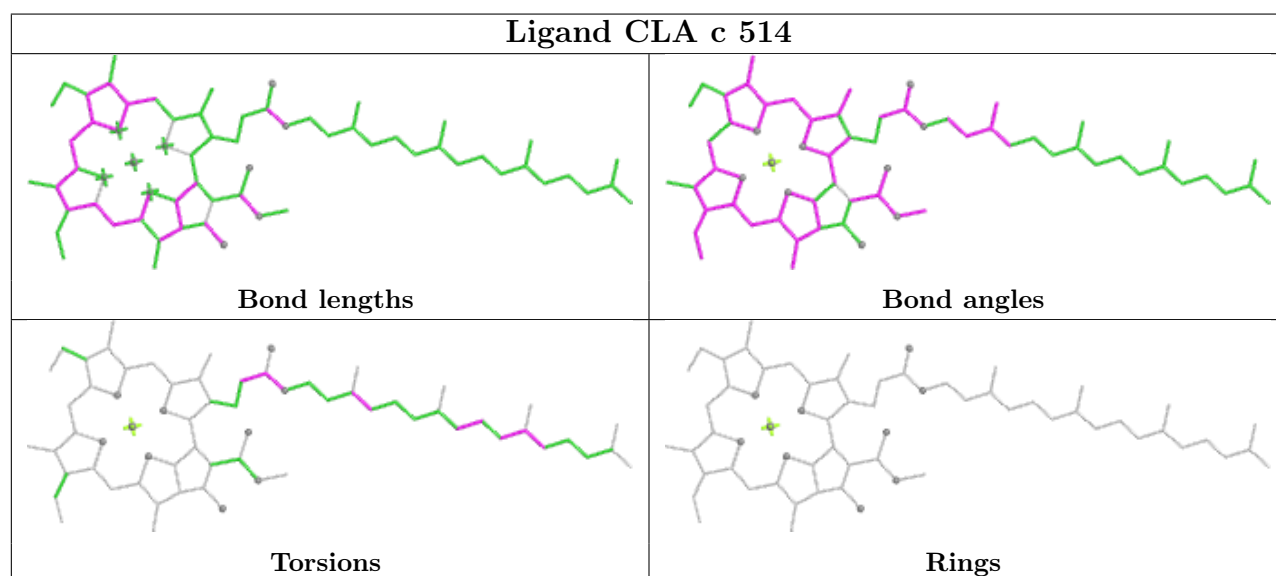
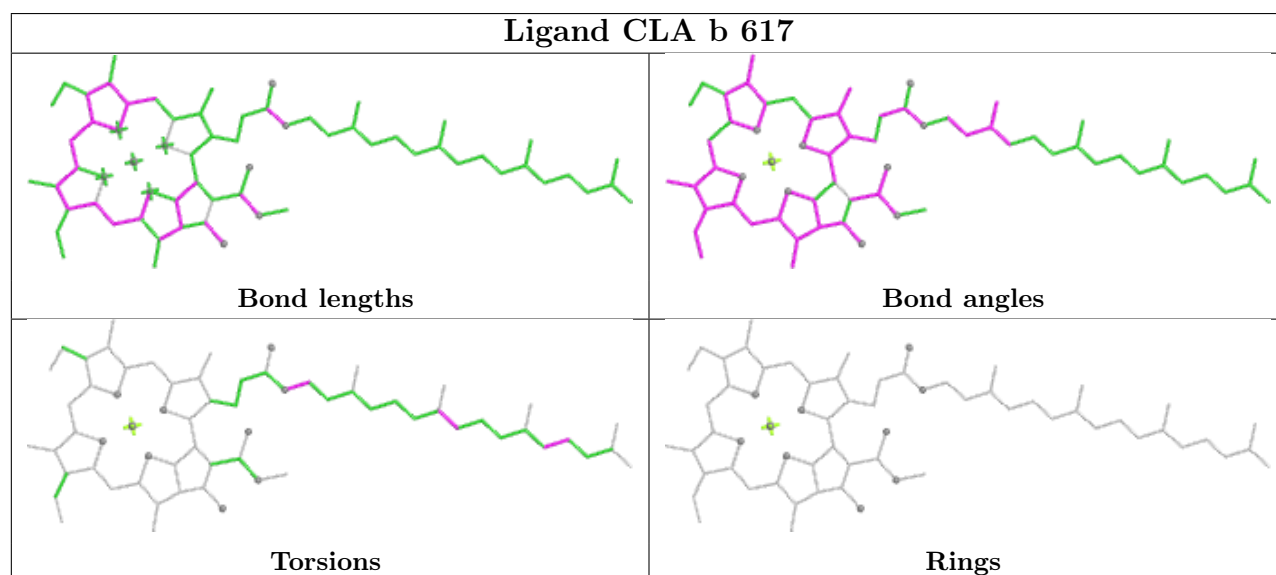
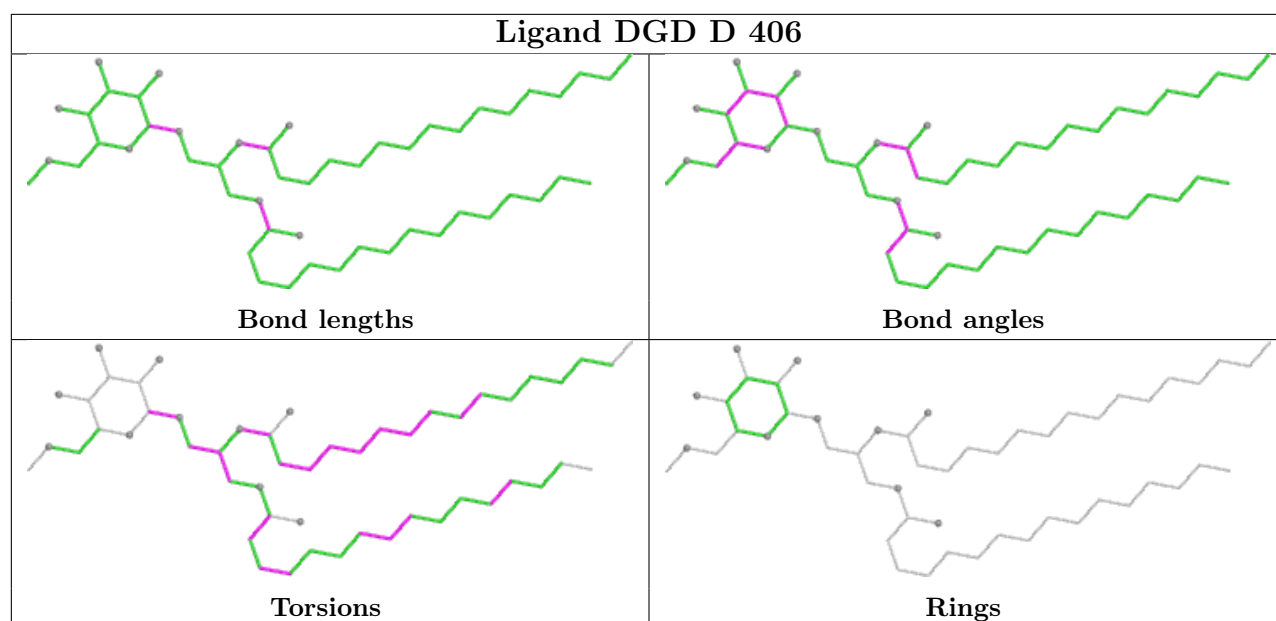


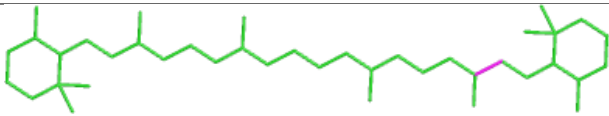
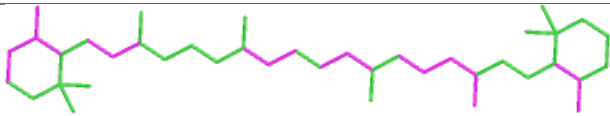
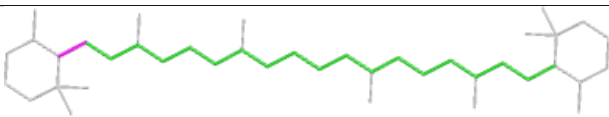
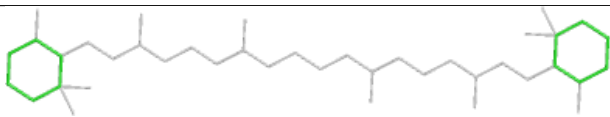


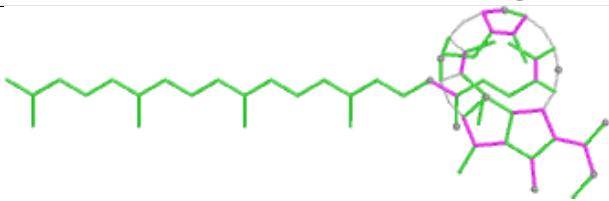
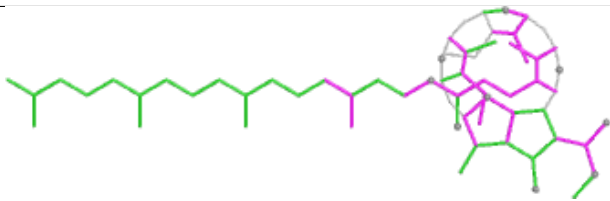
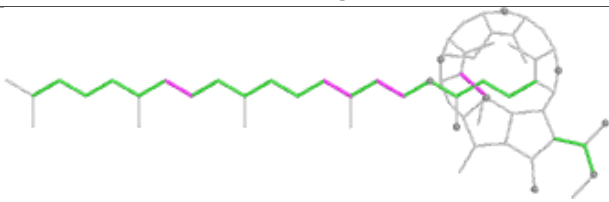
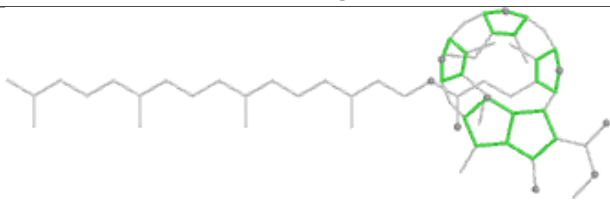


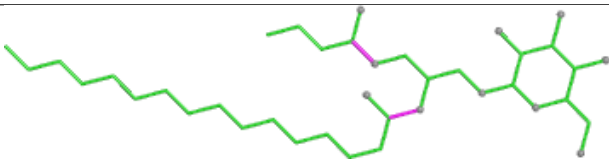
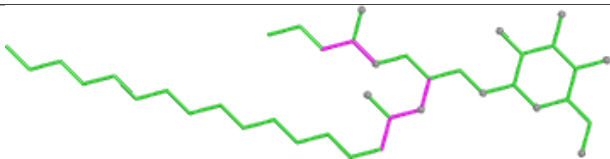
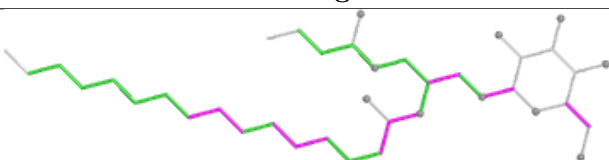
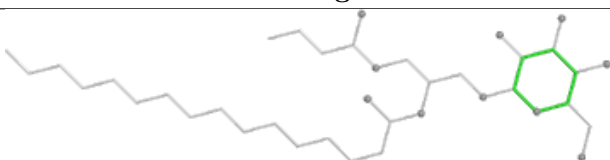


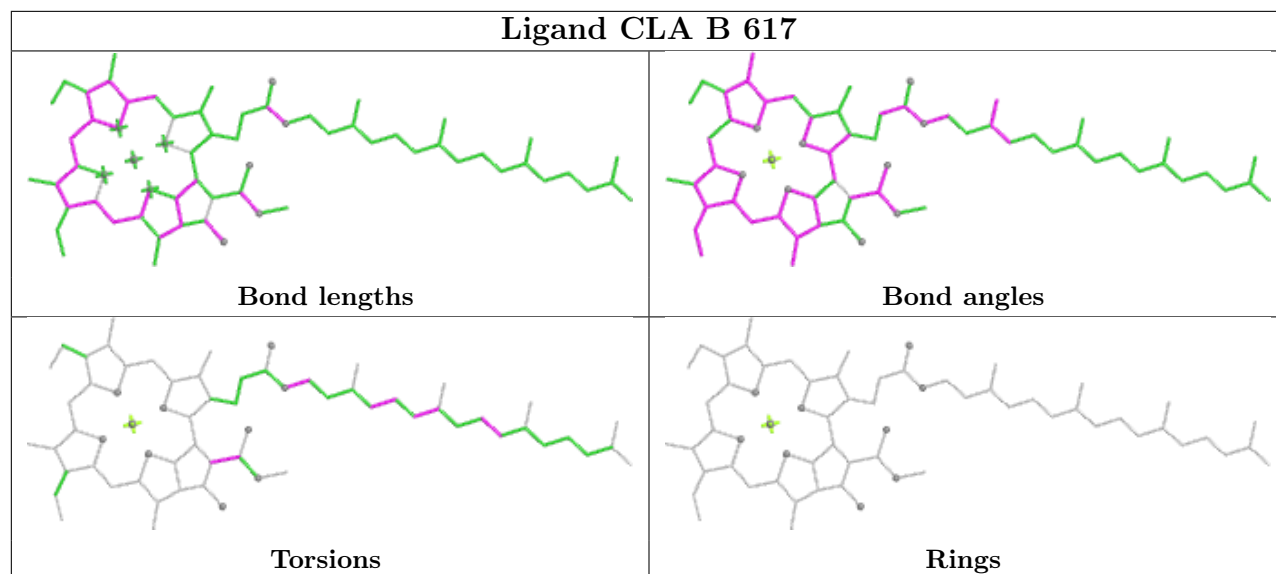
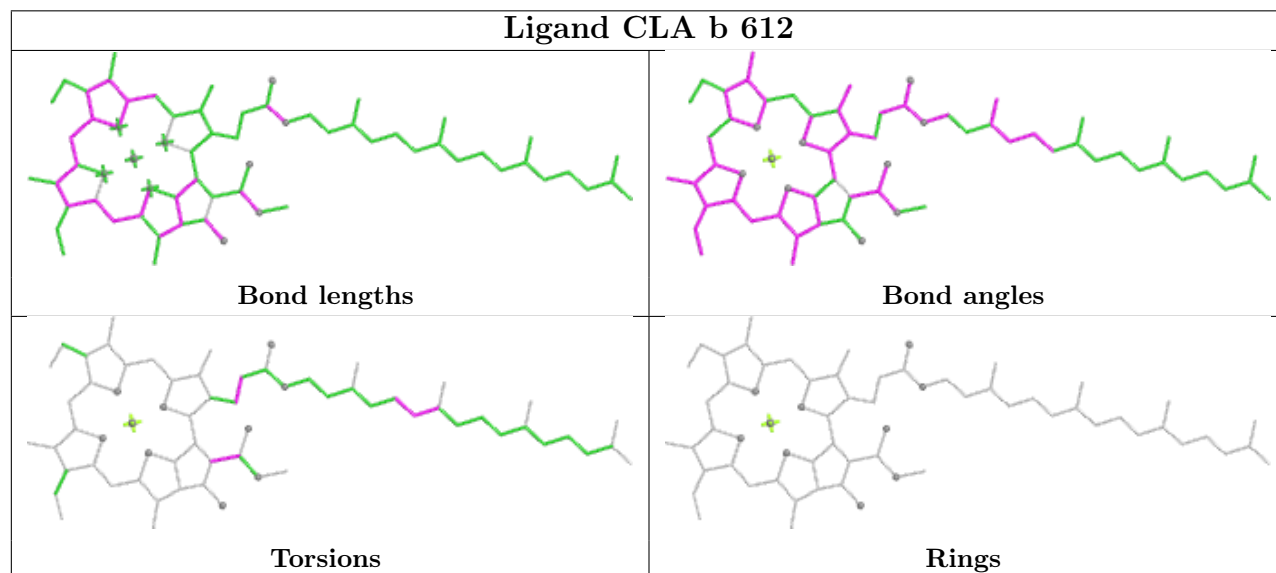
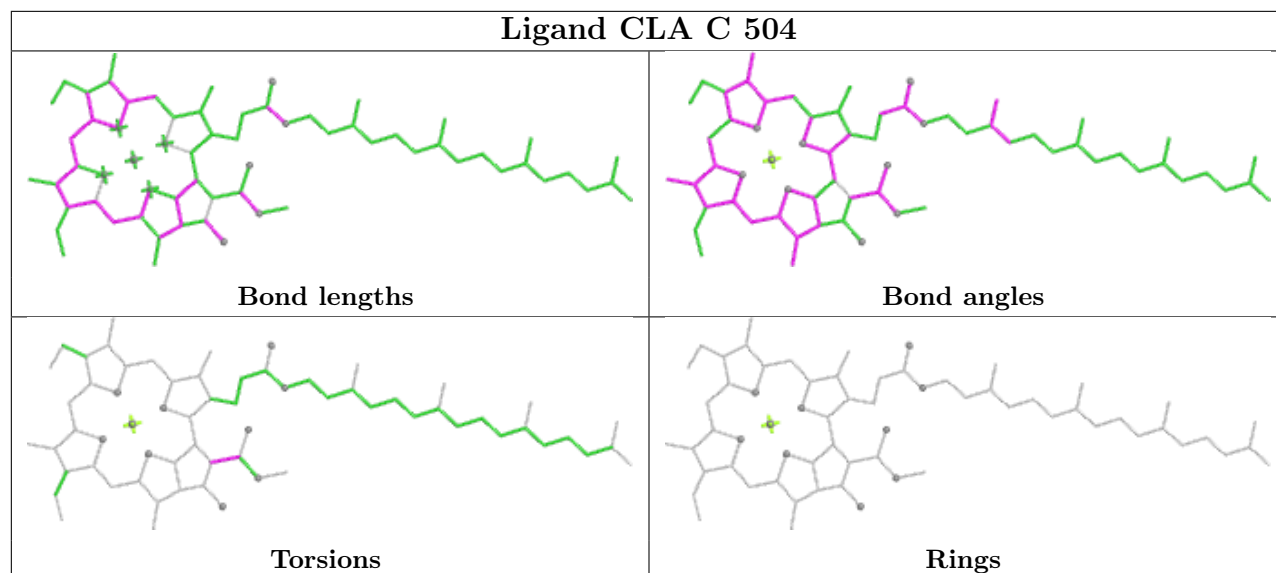




Ligand BCR c 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PHO a 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG z 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 617**Ligand CLA b 612****Ligand CLA C 504**

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%)	-0.70	0 100 100	25, 39, 69, 112	3 (0%)
1	a	334/344 (97%)	-0.69	1 (0%) 90 91	24, 40, 74, 141	6 (1%)
2	B	504/505 (99%)	-0.61	2 (0%) 88 90	22, 44, 78, 119	10 (1%)
2	b	503/505 (99%)	-0.52	6 (1%) 76 79	26, 44, 81, 174	12 (2%)
3	C	451/455 (99%)	-0.54	0 100 100	31, 51, 70, 120	4 (0%)
3	c	455/455 (100%)	-0.52	0 100 100	25, 53, 71, 124	6 (1%)
4	D	341/342 (99%)	-0.74	0 100 100	22, 41, 64, 131	1 (0%)
4	d	341/342 (99%)	-0.73	1 (0%) 90 91	24, 42, 65, 122	1 (0%)
5	E	81/84 (96%)	-0.16	1 (1%) 76 79	32, 63, 95, 127	2 (2%)
5	e	81/84 (96%)	0.01	2 (2%) 58 62	35, 65, 118, 172	2 (2%)
6	F	34/44 (77%)	-0.27	0 100 100	46, 57, 91, 98	0
6	f	32/44 (72%)	-0.21	1 (3%) 51 55	47, 57, 115, 139	0
7	H	65/65 (100%)	-0.37	2 (3%) 51 55	34, 53, 71, 154	1 (1%)
7	h	65/65 (100%)	-0.43	2 (3%) 51 55	43, 56, 77, 165	0
8	I	37/38 (97%)	-0.27	0 100 100	43, 53, 107, 152	0
8	i	37/38 (97%)	-0.28	1 (2%) 56 60	42, 53, 100, 129	0
9	J	38/39 (97%)	-0.01	2 (5%) 32 36	44, 61, 133, 171	0
9	j	39/39 (100%)	-0.10	1 (2%) 57 61	48, 61, 130, 168	0
10	K	37/37 (100%)	-0.27	0 100 100	53, 62, 77, 105	0
10	k	37/37 (100%)	-0.34	0 100 100	53, 62, 80, 105	0
11	L	37/37 (100%)	-0.63	0 100 100	18, 37, 101, 123	1 (2%)
11	l	37/37 (100%)	-0.64	0 100 100	22, 36, 99, 122	1 (2%)
12	M	33/36 (91%)	-0.66	0 100 100	23, 38, 63, 116	1 (3%)
12	m	33/36 (91%)	-0.65	0 100 100	33, 38, 71, 117	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.58	1 (0%) 88 90	25, 49, 95, 134	8 (3%)
13	o	243/244 (99%)	-0.50	2 (0%) 82 84	27, 50, 102, 167	5 (2%)
14	T	29/32 (90%)	-0.71	1 (3%) 48 52	31, 37, 65, 135	1 (3%)
14	t	29/32 (90%)	-0.69	1 (3%) 48 52	31, 38, 66, 135	1 (3%)
15	U	97/104 (93%)	-0.65	0 100 100	37, 48, 75, 118	0
15	u	97/104 (93%)	-0.60	0 100 100	41, 49, 72, 118	0
16	V	137/137 (100%)	-0.54	0 100 100	26, 49, 78, 121	1 (0%)
16	v	137/137 (100%)	-0.56	1 (0%) 84 85	40, 55, 82, 123	0
17	Y	29/30 (96%)	0.66	2 (6%) 23 26	64, 77, 135, 141	0
17	y	29/30 (96%)	0.32	2 (6%) 23 26	67, 80, 135, 142	0
18	X	39/40 (97%)	0.04	1 (2%) 57 61	53, 62, 114, 138	0
18	x	38/40 (95%)	0.22	2 (5%) 32 36	53, 62, 110, 130	0
19	Z	62/62 (100%)	0.23	4 (6%) 25 28	65, 77, 122, 164	0
19	z	62/62 (100%)	0.36	2 (3%) 50 54	68, 79, 122, 165	0
20	R	18/34 (52%)	2.72	13 (72%) 0 0	106, 139, 173, 174	0
All	All	5275/5384 (97%)	-0.51	54 (1%) 79 82	18, 48, 91, 174	67 (1%)

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	R	15	ALA	4.7
20	R	13	LEU	4.3
20	R	3	TRP	4.2
2	b	486	LEU	3.9
20	R	9	LEU	3.8

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	0.95	0.07	33,38,60,72	0
12	FME	m	1	10/11	0.96	0.09	35,47,107,124	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	0.97	0.07	33,52,85,91	0
14	FME	t	1	10/11	0.97	0.05	28,40,49,83	0
8	FME	I	1	10/11	0.98	0.06	36,49,53,57	0
8	FME	i	1	10/11	0.98	0.06	39,51,57,61	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	DGD	D	406	52/66	0.69	0.15	62,106,145,154	0
36	DGD	e	101	62/66	0.69	0.16	68,115,177,183	0
37	LHG	e	102	42/49	0.71	0.12	68,134,167,175	0
29	LMT	F	102	35/35	0.74	0.15	81,117,147,150	0
28	GOL	V	201	6/6	0.74	0.15	69,78,89,95	0
27	SQD	f	102	43/54	0.75	0.14	86,119,144,148	0
29	LMT	C	522	35/35	0.75	0.14	83,119,152,161	0
33	CA	b	609	1/1	0.77	0.13	137,137,137,137	0
29	LMT	b	630	25/35	0.77	0.13	70,95,151,153	0
32	UNL	m	101	10/-	0.77	0.15	54,59,86,88	0
33	CA	B	601	1/1	0.77	0.09	143,143,143,143	0
29	LMT	M	104	35/35	0.78	0.14	44,96,137,144	0
29	LMT	f	103	35/35	0.78	0.13	74,122,151,156	0
32	UNL	a	403	30/-	0.78	0.14	69,90,128,130	0
34	HTG	D	412	16/19	0.79	0.14	70,142,157,160	0
32	UNL	A	419	28/-	0.79	0.13	63,86,104,104	0
32	UNL	M	103	10/-	0.79	0.12	48,61,72,79	0
29	LMT	a	419	35/35	0.79	0.13	86,112,130,132	0
32	UNL	j	102	10/-	0.80	0.13	64,78,93,97	0
32	UNL	i	101	40/-	0.80	0.14	49,77,144,146	0
34	HTG	c	525	19/19	0.81	0.12	56,109,121,130	0
32	UNL	C	528	34/-	0.81	0.13	68,109,132,133	0
34	HTG	B	625	19/19	0.81	0.12	72,118,144,148	0
32	UNL	I	101	40/-	0.81	0.14	41,84,148,161	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	LMT	A	416	35/35	0.82	0.12	40,84,106,133	0
32	UNL	J	102	10/-	0.82	0.14	47,71,94,97	0
32	UNL	D	411	40/-	0.82	0.12	56,80,133,139	0
34	HTG	b	608	19/19	0.83	0.11	56,113,148,151	0
28	GOL	O	301	6/6	0.83	0.10	68,79,81,88	0
34	HTG	d	412	16/19	0.83	0.12	64,114,125,129	0
32	UNL	c	526	32/-	0.83	0.13	63,98,133,141	0
29	LMT	B	622	35/35	0.83	0.12	62,118,148,153	0
37	LHG	E	101	42/49	0.83	0.12	67,98,120,121	0
34	HTG	V	206	19/19	0.83	0.12	61,91,114,204	0
35	LMG	c	523	51/55	0.84	0.11	49,107,130,130	0
35	LMG	z	101	39/55	0.84	0.14	63,116,139,159	0
34	HTG	b	632	19/19	0.84	0.12	66,115,147,147	0
34	HTG	B	633	19/19	0.84	0.11	53,105,137,170	0
29	LMT	a	404	35/35	0.84	0.12	44,83,115,132	0
35	LMG	C	521	51/55	0.84	0.12	55,109,128,136	0
27	SQD	B	621	54/54	0.85	0.12	52,88,144,153	0
28	GOL	c	502	6/6	0.85	0.16	75,86,99,108	0
32	UNL	B	634	33/-	0.85	0.13	57,82,136,141	0
35	LMG	Z	101	37/55	0.85	0.14	50,111,133,137	0
32	UNL	b	633	33/-	0.85	0.14	41,94,159,162	0
28	GOL	C	525	6/6	0.86	0.13	54,60,75,81	0
27	SQD	F	103	43/54	0.86	0.11	75,102,123,134	0
31	PL9	A	418	55/55	0.86	0.13	56,99,114,133	0
31	PL9	a	416	55/55	0.86	0.14	64,103,126,128	0
32	UNL	d	411	36/-	0.86	0.11	54,77,132,138	0
28	GOL	T	101	6/6	0.86	0.18	51,78,96,104	0
34	HTG	C	524	19/19	0.86	0.10	82,92,128,134	0
27	SQD	L	102	54/54	0.87	0.10	46,74,126,143	0
27	SQD	a	405	54/54	0.87	0.10	43,78,123,126	0
29	LMT	B	635	25/35	0.87	0.12	42,86,138,141	0
27	SQD	A	415	54/54	0.87	0.10	48,74,114,132	0
28	GOL	A	414	6/6	0.87	0.12	53,77,82,88	0
28	GOL	B	630	6/6	0.87	0.12	51,67,75,83	0
34	HTG	b	631	19/19	0.87	0.12	58,68,84,96	0
28	GOL	t	102	6/6	0.87	0.15	54,82,93,98	0
34	HTG	B	624	19/19	0.87	0.12	48,66,92,98	0
29	LMT	m	102	35/35	0.88	0.10	35,98,128,134	0
34	HTG	c	524	19/19	0.88	0.09	89,95,108,128	0
28	GOL	a	402	6/6	0.88	0.11	73,83,89,92	0
28	GOL	b	606	6/6	0.88	0.12	63,79,87,89	0
29	LMT	M	105	35/35	0.89	0.10	41,84,106,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	GOL	v	201	6/6	0.89	0.13	71,93,96,100	0
28	GOL	T	102	6/6	0.90	0.12	106,113,118,120	0
29	LMT	M	102	35/35	0.90	0.10	41,85,110,112	0
34	HTG	C	523	19/19	0.90	0.09	72,86,102,106	0
29	LMT	T	104	25/35	0.90	0.12	34,84,134,140	0
33	CA	f	104	1/1	0.91	0.06	104,104,104,104	0
35	LMG	a	415	51/55	0.91	0.10	57,82,99,102	0
35	LMG	c	522	51/55	0.91	0.09	51,86,112,114	0
32	UNL	X	101	18/-	0.91	0.11	56,75,101,102	0
32	UNL	d	410	17/-	0.91	0.11	48,69,97,101	0
28	GOL	B	636	6/6	0.91	0.10	48,57,65,65	0
35	LMG	C	501	51/55	0.91	0.09	49,84,108,116	0
35	LMG	C	520	51/55	0.91	0.09	50,77,108,118	0
28	GOL	B	626	6/6	0.91	0.10	44,52,59,85	0
24	CLA	C	514	65/65	0.92	0.08	51,65,99,109	0
24	CLA	c	517	65/65	0.92	0.08	57,80,96,104	0
22	CL	U	201	1/1	0.92	0.11	92,92,92,92	0
28	GOL	b	605	6/6	0.92	0.14	67,80,108,110	0
32	UNL	d	413	18/-	0.92	0.11	52,71,109,110	0
28	GOL	v	202	6/6	0.92	0.10	74,80,100,114	0
28	GOL	o	301	6/6	0.93	0.10	71,80,88,106	0
27	SQD	A	411	54/54	0.93	0.09	45,78,99,103	0
28	GOL	B	628	6/6	0.93	0.10	52,71,84,87	0
35	LMG	b	629	51/55	0.93	0.08	41,51,73,89	0
28	GOL	B	629	6/6	0.93	0.12	48,57,63,72	0
24	CLA	B	602	65/65	0.93	0.09	43,60,100,128	0
24	CLA	b	610	65/65	0.93	0.08	43,69,104,133	0
34	HTG	B	632	19/19	0.93	0.08	48,69,99,103	0
28	GOL	A	413	6/6	0.93	0.14	51,54,63,67	0
37	LHG	D	409	49/49	0.93	0.09	36,54,115,128	0
24	CLA	C	507	65/65	0.93	0.08	46,64,107,116	0
28	GOL	f	101	6/6	0.93	0.08	76,84,86,91	0
24	CLA	c	510	65/65	0.94	0.07	44,63,92,115	0
24	CLA	C	505	65/65	0.94	0.07	34,48,82,94	0
26	BCR	C	515	40/40	0.94	0.07	49,65,78,83	0
35	LMG	J	101	51/55	0.94	0.10	38,58,111,127	0
35	LMG	M	101	51/55	0.94	0.07	35,52,78,95	0
28	GOL	v	203	6/6	0.94	0.10	47,53,61,71	0
26	BCR	D	404	40/40	0.94	0.07	38,51,93,99	0
27	SQD	a	414	54/54	0.94	0.08	49,79,106,110	0
26	BCR	b	627	40/40	0.94	0.06	31,41,60,69	0
26	BCR	c	527	40/40	0.94	0.08	57,74,86,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	LMG	j	101	51/55	0.94	0.08	46,58,105,117	0
26	BCR	d	405	40/40	0.94	0.07	40,55,77,83	0
26	BCR	t	101	40/40	0.94	0.06	31,46,62,64	0
32	UNL	D	410	17/-	0.94	0.08	37,68,83,91	0
26	BCR	y	101	40/40	0.94	0.07	44,61,74,84	0
23	BCT	a	418	4/4	0.94	0.08	60,63,70,83	0
24	CLA	b	625	65/65	0.94	0.08	35,54,102,112	0
24	CLA	C	508	65/65	0.95	0.07	42,54,68,76	0
28	GOL	B	631	6/6	0.95	0.08	40,73,74,83	0
26	BCR	H	101	40/40	0.95	0.06	36,51,67,73	0
26	BCR	K	101	40/40	0.95	0.07	43,55,63,69	0
28	GOL	F	101	6/6	0.95	0.07	70,74,77,77	0
26	BCR	T	103	40/40	0.95	0.06	28,47,64,68	0
26	BCR	Y	101	40/40	0.95	0.07	44,60,69,71	0
34	HTG	b	607	19/19	0.95	0.06	46,75,81,82	0
24	CLA	C	513	65/65	0.95	0.07	46,63,85,92	0
24	CLA	B	615	65/65	0.95	0.07	27,41,91,103	0
28	GOL	V	204	6/6	0.95	0.09	68,81,85,94	0
24	CLA	a	412	65/65	0.95	0.08	32,48,114,123	0
26	BCR	k	101	40/40	0.95	0.07	45,62,73,75	0
24	CLA	B	617	65/65	0.95	0.09	36,52,114,120	0
24	CLA	b	615	65/65	0.95	0.07	31,45,89,103	0
24	CLA	b	618	65/65	0.95	0.06	36,48,60,71	0
24	CLA	b	623	65/65	0.95	0.07	27,41,88,115	0
24	CLA	C	502	65/65	0.95	0.07	38,51,77,91	0
24	CLA	c	507	65/65	0.95	0.07	41,53,65,83	0
24	CLA	c	508	65/65	0.95	0.06	38,55,73,80	0
23	BCT	A	404	4/4	0.95	0.08	52,54,73,86	0
24	CLA	c	511	65/65	0.95	0.07	42,55,70,76	0
24	CLA	c	516	65/65	0.95	0.06	47,65,83,91	0
28	GOL	A	412	6/6	0.95	0.07	43,50,53,61	0
24	CLA	C	506	65/65	0.95	0.07	36,48,70,73	0
24	CLA	d	404	65/65	0.95	0.07	37,52,101,114	0
36	DGD	C	518	62/66	0.95	0.07	37,55,95,113	0
26	BCR	A	410	40/40	0.95	0.06	30,39,45,50	0
36	DGD	H	102	62/66	0.95	0.07	32,49,69,79	0
36	DGD	c	520	62/66	0.95	0.07	38,55,107,128	0
36	DGD	c	521	62/66	0.95	0.07	38,52,94,99	0
33	CA	F	104	1/1	0.95	0.05	84,84,84,84	0
37	LHG	D	407	49/49	0.95	0.07	31,49,67,73	0
28	GOL	B	627	6/6	0.95	0.09	47,62,83,99	0
26	BCR	B	620	40/40	0.95	0.06	32,46,59,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	LHG	d	409	49/49	0.95	0.09	34,55,108,115	0
24	CLA	B	607	65/65	0.95	0.07	31,43,93,105	0
24	CLA	D	403	65/65	0.96	0.07	38,52,104,119	0
24	CLA	B	614	65/65	0.96	0.06	26,37,63,84	0
26	BCR	c	518	40/40	0.96	0.06	40,55,67,69	0
24	CLA	C	509	65/65	0.96	0.06	36,50,110,126	0
24	CLA	c	512	65/65	0.96	0.06	36,49,116,129	0
26	BCR	h	101	40/40	0.96	0.06	42,56,70,74	0
24	CLA	c	513	65/65	0.96	0.07	42,54,74,88	0
24	CLA	c	514	65/65	0.96	0.06	41,53,63,77	0
24	CLA	c	515	65/65	0.96	0.07	43,54,75,87	0
24	CLA	C	510	65/65	0.96	0.07	41,54,76,80	0
24	CLA	b	616	65/65	0.96	0.06	24,36,48,52	0
24	CLA	C	511	65/65	0.96	0.06	39,49,62,82	0
28	GOL	V	202	6/6	0.96	0.08	40,47,51,59	0
28	GOL	V	203	6/6	0.96	0.08	59,61,61,68	0
24	CLA	b	620	65/65	0.96	0.06	28,40,52,59	0
26	BCR	B	619	40/40	0.96	0.05	29,41,56,60	0
36	DGD	C	517	62/66	0.96	0.07	32,47,94,98	0
28	GOL	b	602	6/6	0.96	0.09	56,60,69,93	0
36	DGD	C	519	62/66	0.96	0.06	36,48,73,86	0
31	PL9	D	405	55/55	0.96	0.06	26,38,51,69	0
28	GOL	b	603	6/6	0.96	0.07	47,56,83,87	0
36	DGD	c	519	62/66	0.96	0.06	38,48,98,105	0
24	CLA	b	622	65/65	0.96	0.05	26,39,55,61	0
24	CLA	C	512	65/65	0.96	0.06	41,57,68,83	0
26	BCR	C	516	40/40	0.96	0.05	39,54,64,65	0
36	DGD	h	102	62/66	0.96	0.07	34,50,68,82	0
24	CLA	A	409	65/65	0.96	0.07	33,47,119,128	0
34	HTG	b	601	19/19	0.96	0.07	40,50,74,83	0
24	CLA	c	505	65/65	0.96	0.06	42,55,66,70	0
37	LHG	d	407	49/49	0.96	0.06	37,51,64,71	0
24	CLA	c	506	65/65	0.96	0.06	39,54,67,74	0
24	CLA	C	504	65/65	0.96	0.06	39,50,60,64	0
24	CLA	B	603	65/65	0.97	0.05	33,44,51,54	0
26	BCR	a	413	40/40	0.97	0.05	30,41,52,56	0
26	BCR	b	626	40/40	0.97	0.05	30,42,49,49	0
24	CLA	B	604	65/65	0.97	0.05	34,44,53,61	0
31	PL9	d	406	55/55	0.97	0.05	26,38,48,58	0
26	BCR	b	628	40/40	0.97	0.05	39,50,66,77	0
24	CLA	C	503	65/65	0.97	0.05	37,46,61,71	0
24	CLA	a	409	65/65	0.97	0.05	28,35,51,55	0

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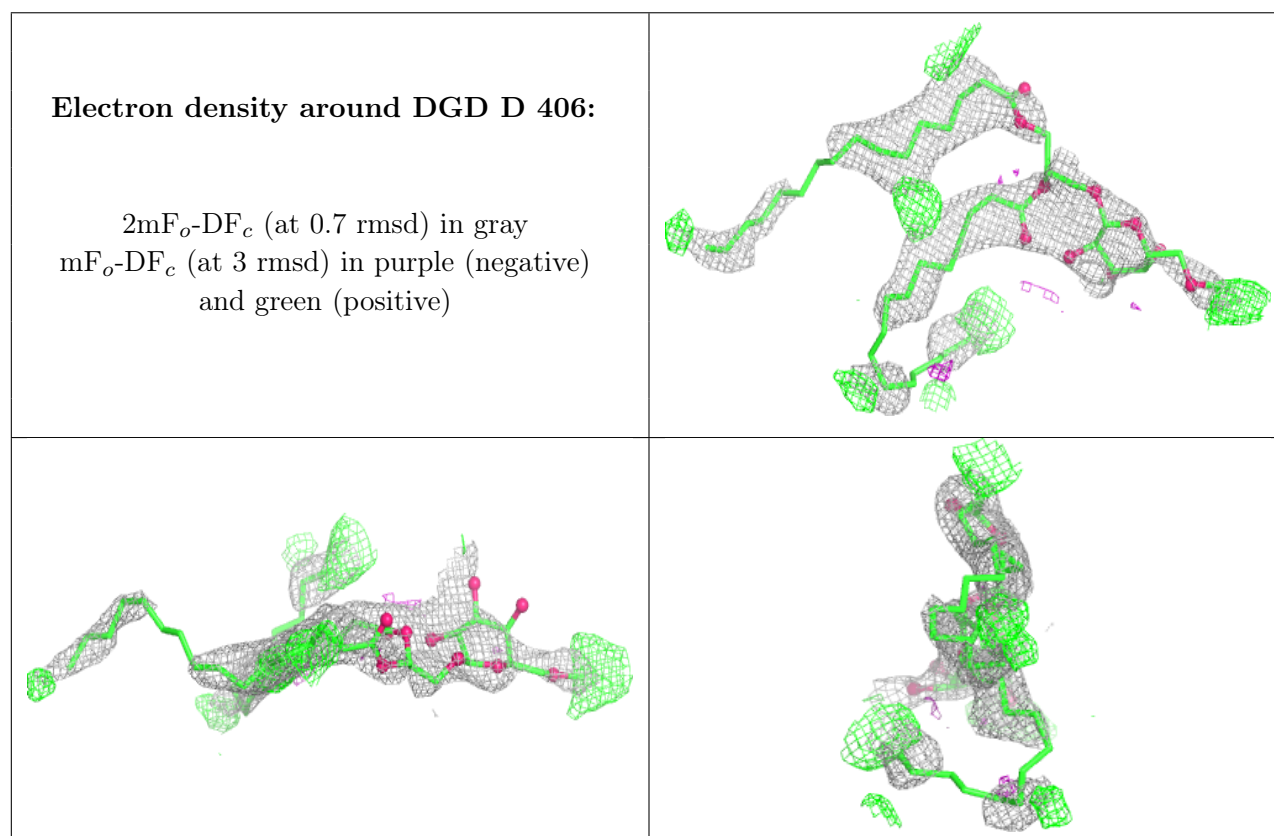
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	GOL	a	401	6/6	0.97	0.08	51,66,70,85	0
24	CLA	c	509	65/65	0.97	0.06	36,47,70,78	0
24	CLA	a	410	65/65	0.97	0.06	31,41,105,116	0
24	CLA	A	407	65/65	0.97	0.06	28,40,98,118	0
28	GOL	b	604	6/6	0.97	0.07	60,73,79,90	0
24	CLA	B	608	65/65	0.97	0.05	24,36,50,55	0
24	CLA	b	611	65/65	0.97	0.06	33,45,55,59	0
24	CLA	b	612	65/65	0.97	0.05	34,44,57,62	0
24	CLA	b	613	65/65	0.97	0.06	26,38,73,79	0
24	CLA	b	614	65/65	0.97	0.06	29,39,49,58	0
24	CLA	B	609	65/65	0.97	0.05	32,43,56,58	0
24	CLA	d	402	65/65	0.97	0.05	27,35,43,55	0
24	CLA	B	610	65/65	0.97	0.05	34,47,56,66	0
25	PHO	A	408	64/64	0.97	0.05	29,42,52,56	0
25	PHO	D	401	64/64	0.97	0.05	25,35,41,43	0
25	PHO	a	411	64/64	0.97	0.04	28,36,44,47	0
25	PHO	d	401	64/64	0.97	0.05	29,42,50,56	0
24	CLA	b	617	65/65	0.97	0.05	34,45,55,58	0
26	BCR	B	618	40/40	0.97	0.04	27,40,47,52	0
34	HTG	B	623	19/19	0.97	0.06	40,54,75,76	0
24	CLA	B	611	65/65	0.97	0.06	36,47,54,68	0
24	CLA	b	619	65/65	0.97	0.06	36,46,56,60	0
24	CLA	B	613	65/65	0.97	0.05	28,38,48,55	0
37	LHG	D	408	49/49	0.97	0.06	27,42,64,86	0
24	CLA	b	621	65/65	0.97	0.05	29,42,50,56	0
22	CL	v	204	1/1	0.97	0.06	94,94,94,94	0
37	LHG	L	101	49/49	0.97	0.06	31,44,56,61	0
24	CLA	A	405	65/65	0.97	0.05	25,33,49,67	0
37	LHG	d	408	49/49	0.97	0.06	32,41,57,86	0
24	CLA	b	624	65/65	0.97	0.05	34,46,60,73	0
24	CLA	B	616	65/65	0.97	0.06	34,47,65,76	0
37	LHG	l	101	49/49	0.97	0.06	37,46,58,66	0
38	HEM	e	103	43/43	0.97	0.09	55,78,123,153	0
24	CLA	B	612	65/65	0.98	0.05	26,37,51,59	0
28	GOL	c	501	6/6	0.98	0.05	43,45,47,48	0
28	GOL	C	526	6/6	0.98	0.05	33,42,47,49	0
22	CL	A	403	1/1	0.98	0.07	35,35,35,35	0
24	CLA	B	605	65/65	0.98	0.05	26,37,70,75	0
24	CLA	d	403	65/65	0.98	0.05	27,38,59,62	0
24	CLA	B	606	65/65	0.98	0.05	29,40,53,64	0
24	CLA	D	402	65/65	0.98	0.05	24,35,54,58	0
38	HEM	E	102	43/43	0.98	0.06	44,64,81,93	0

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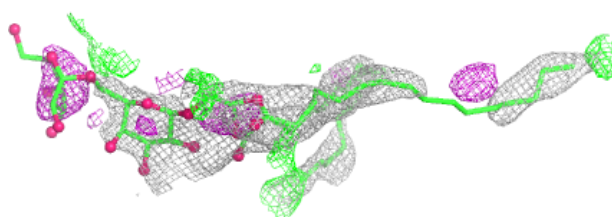
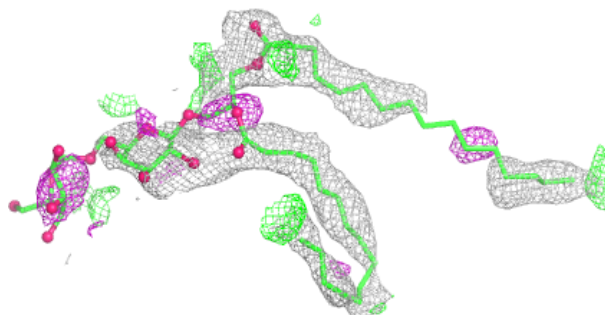
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	A	406	65/65	0.98	0.04	24,34,44,58	0
39	MG	j	103	1/1	0.98	0.07	57,57,57,57	0
33	CA	c	503	1/1	0.99	0.08	66,66,66,66	0
33	CA	c	504	1/1	0.99	0.03	74,74,74,74	0
33	CA	C	527	1/1	0.99	0.07	67,67,67,67	0
33	CA	o	302	1/1	0.99	0.04	91,91,91,91	0
22	CL	a	408	1/1	0.99	0.03	41,41,41,41	0
33	CA	O	302	1/1	0.99	0.02	84,84,84,84	0
39	MG	J	103	1/1	0.99	0.02	53,53,53,53	0
22	CL	a	407	1/1	0.99	0.05	36,36,36,36	0
40	HEC	V	205	43/43	0.99	0.04	35,41,50,53	0
40	HEC	v	205	43/43	0.99	0.05	42,52,61,62	0
22	CL	A	402	1/1	1.00	0.02	32,32,32,32	0
21	FE2	A	401	1/1	1.00	0.04	51,51,51,51	0
30	OEX	A	417	10/10	1.00	0.03	33,36,47,71	0
30	OEX	a	417	10/10	1.00	0.03	32,40,64,67	0
21	FE2	a	406	1/1	1.00	0.06	49,49,49,49	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.

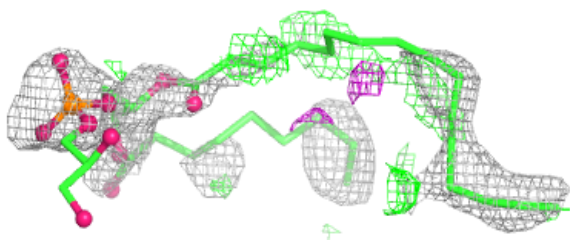
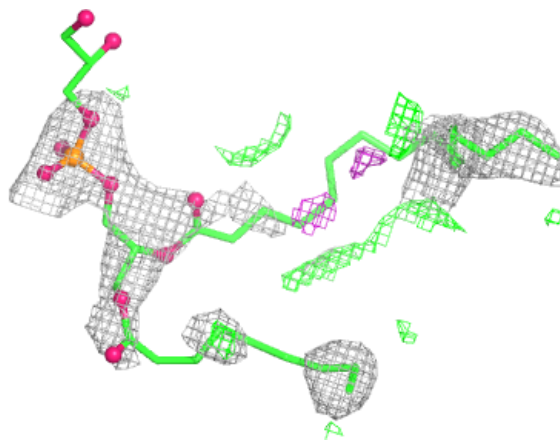


Electron density around DGD e 101:

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

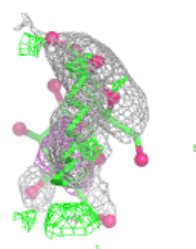
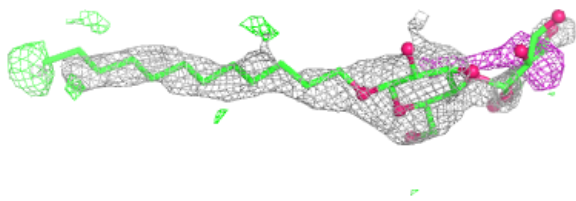
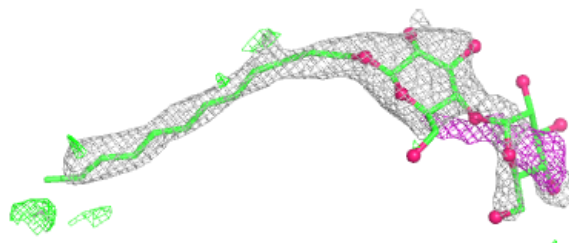
**Electron density around LHG e 102:**

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

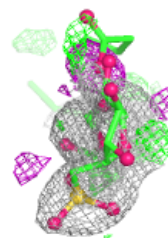
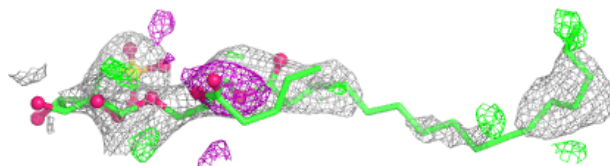
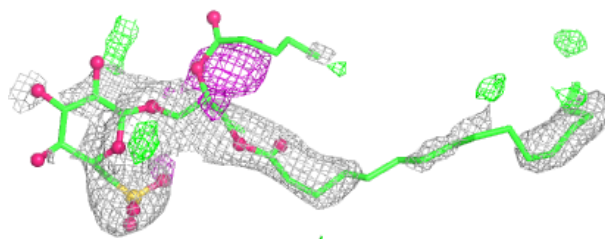


Electron density around LMT F 102:

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

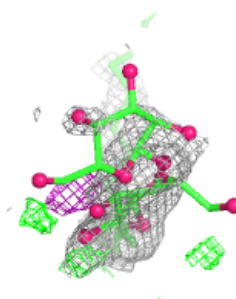
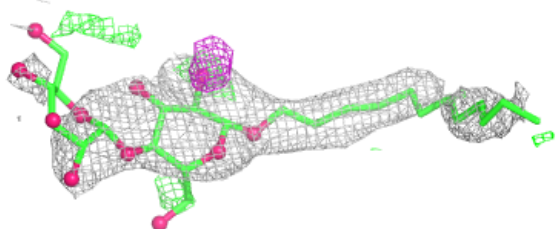
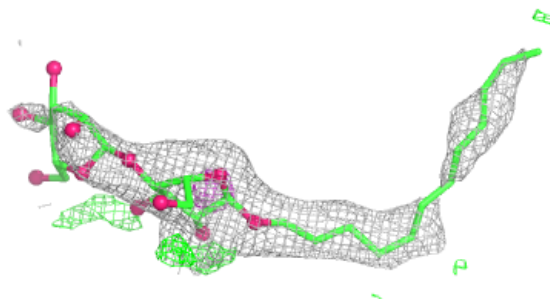
**Electron density around SQD f 102:**

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

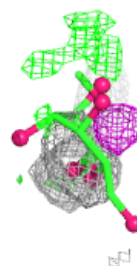
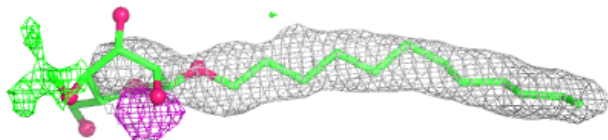
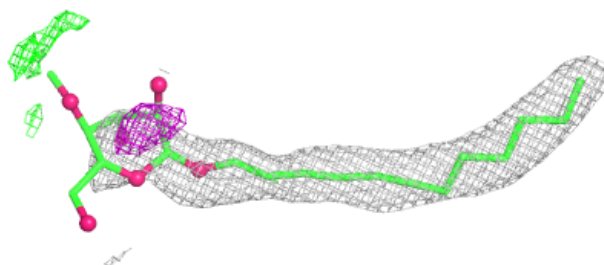


Electron density around LMT C 522:

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

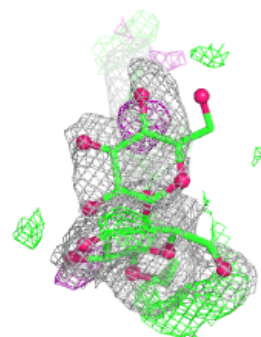
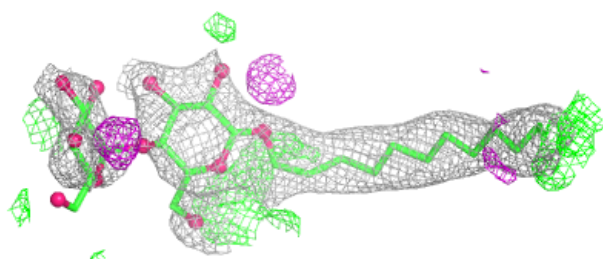
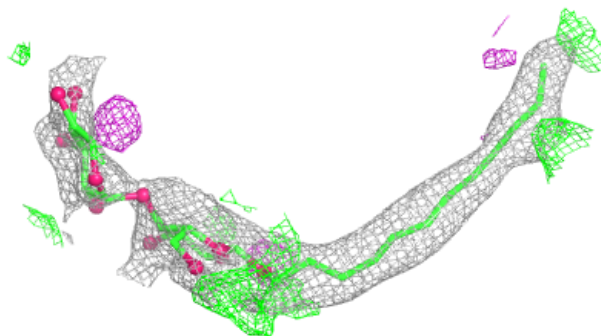
**Electron density around LMT b 630:**

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

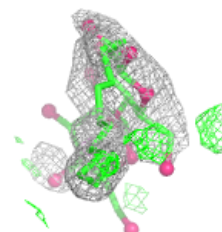
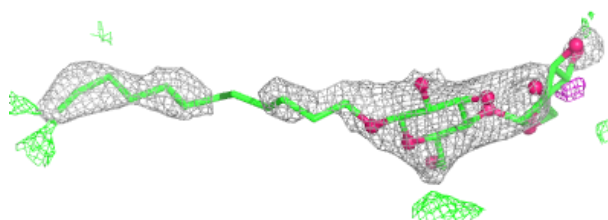
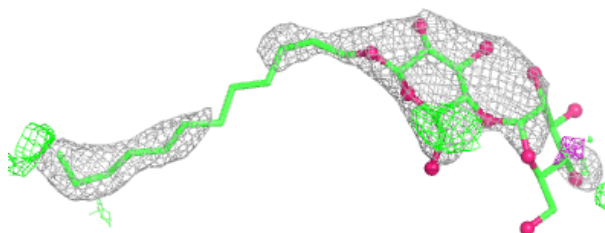


Electron density around LMT M 104:

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

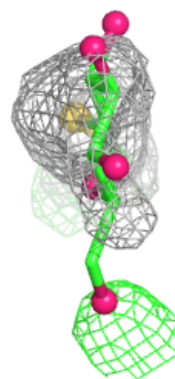
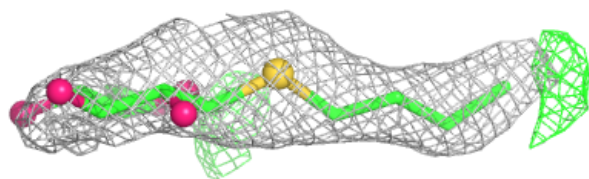
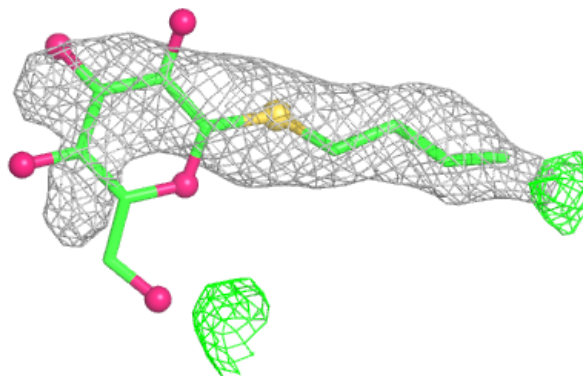
**Electron density around LMT f 103:**

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

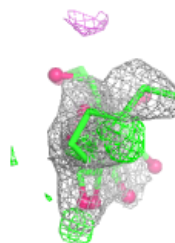
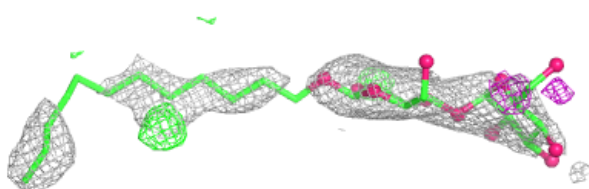
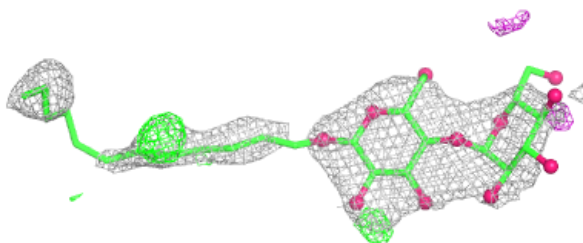


Electron density around HTG D 412:

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

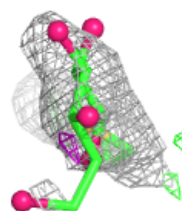
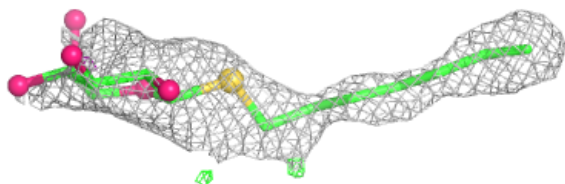
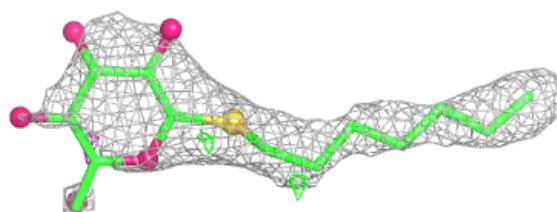
**Electron density around LMT a 419:**

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

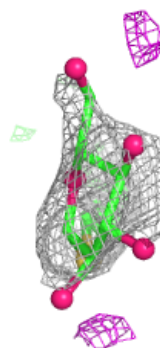
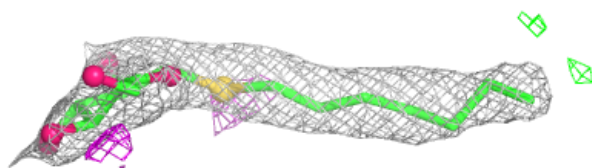
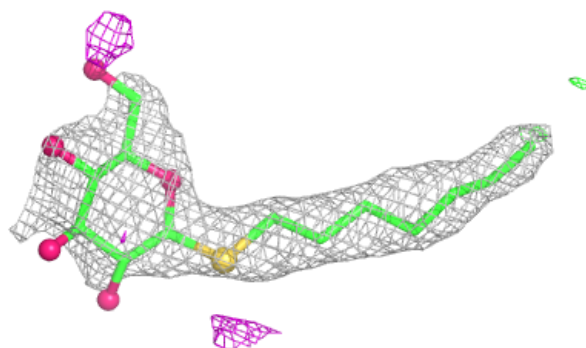


Electron density around HTG c 525:

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

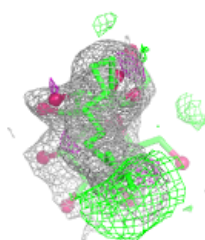
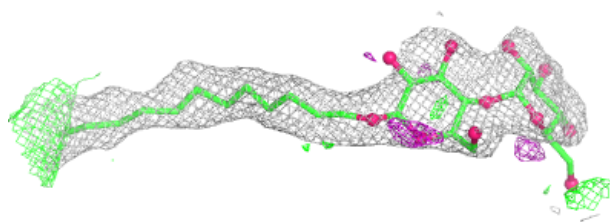
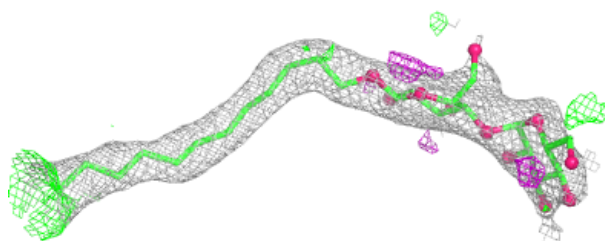
**Electron density around HTG B 625:**

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

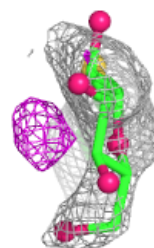
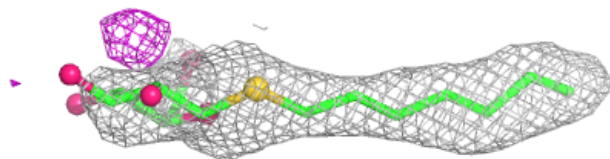
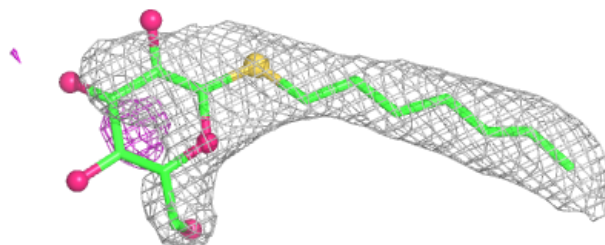


Electron density around LMT A 416:

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

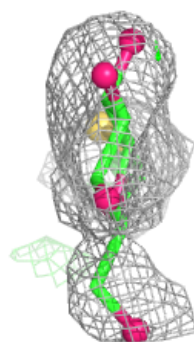
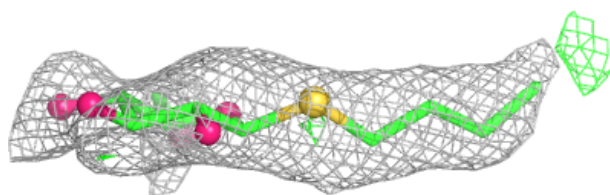
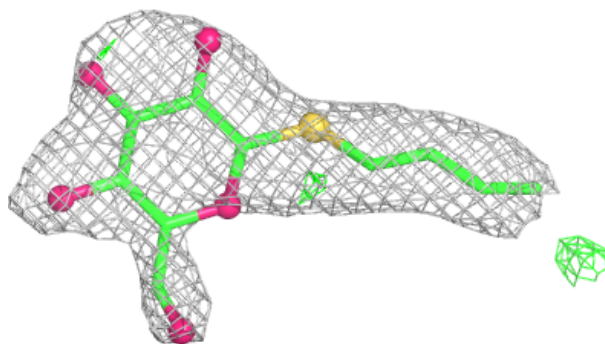
**Electron density around HTG b 608:**

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

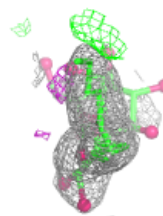
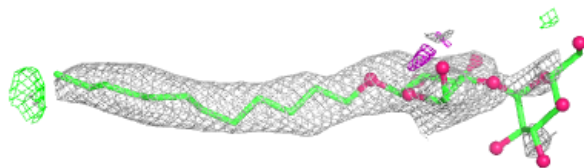
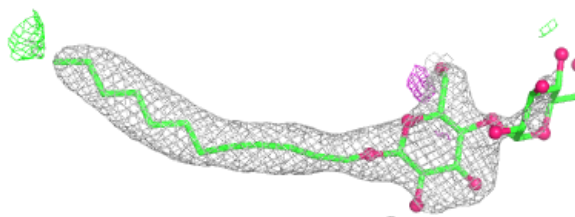


Electron density around HTG d 412:

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

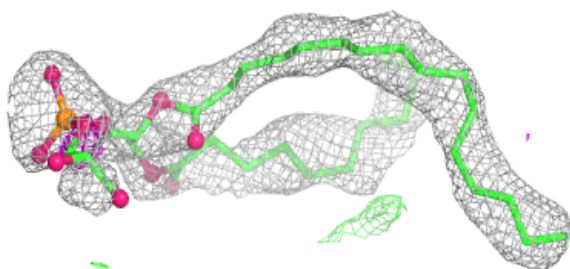
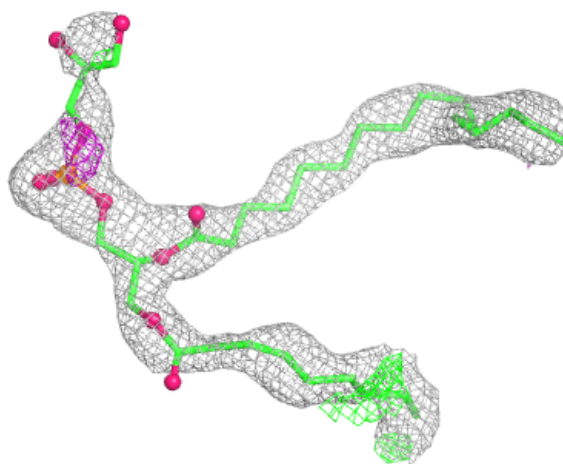
**Electron density around LMT B 622:**

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



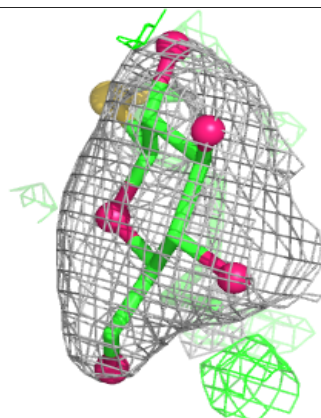
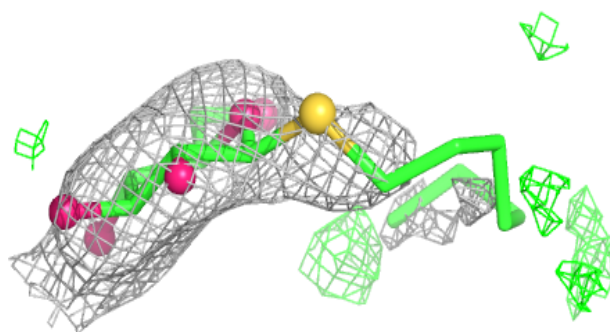
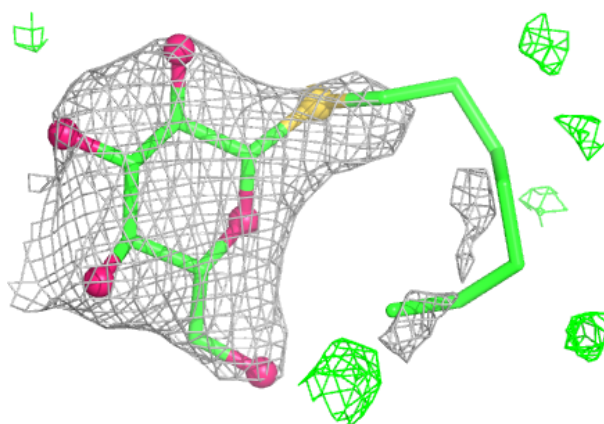
Electron density around LHG E 101:

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

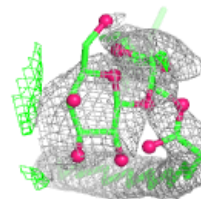
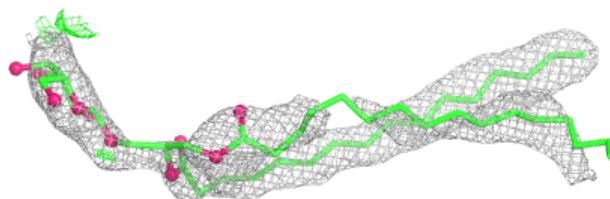
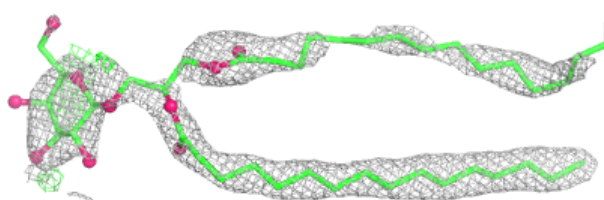


Electron density around HTG V 206:

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

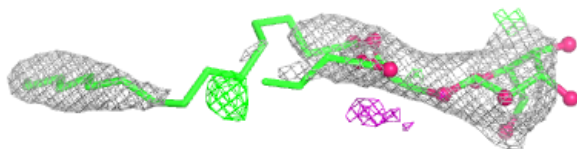
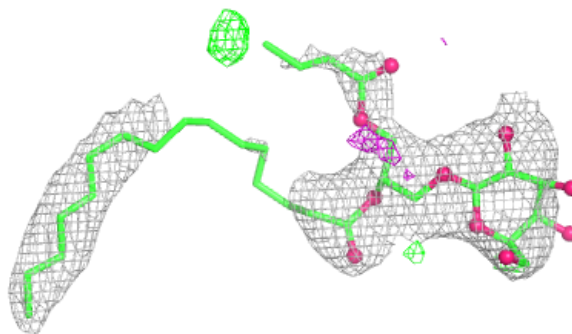
**Electron density around LMG c 523:**

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

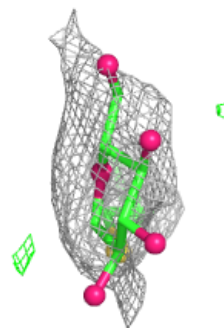
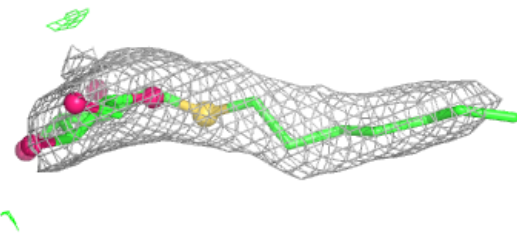
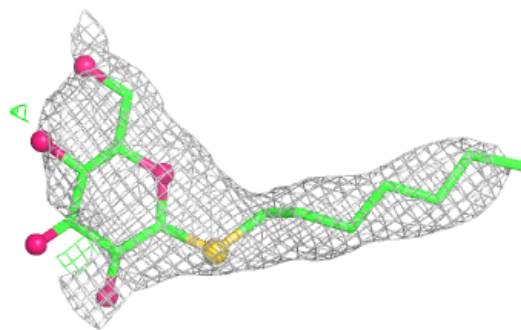


Electron density around LMG z 101:

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

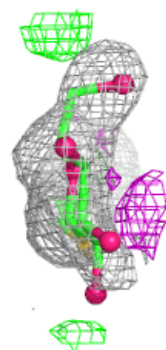
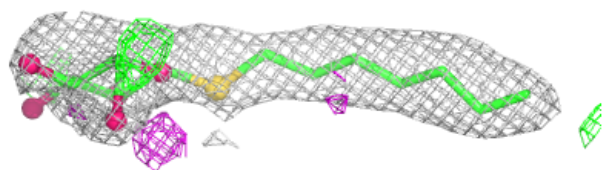
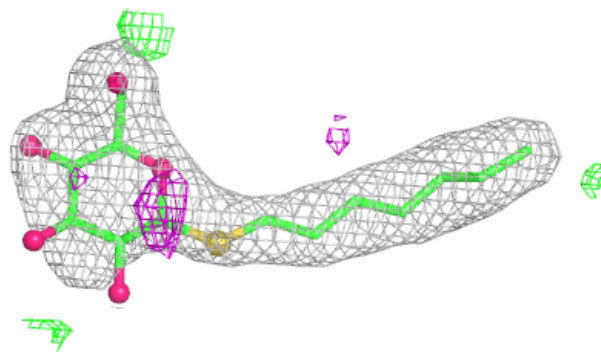
**Electron density around HTG b 632:**

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

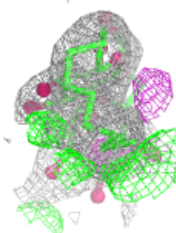
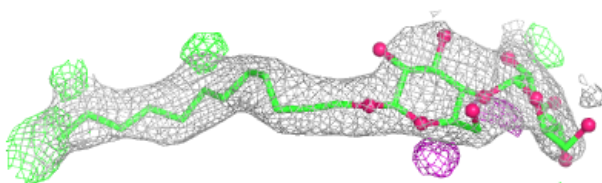
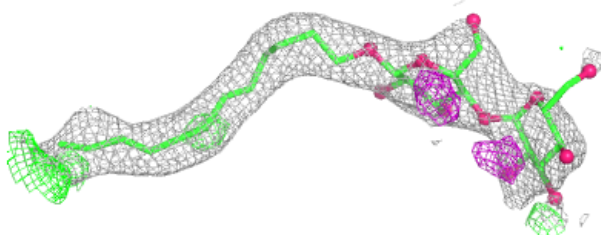


Electron density around HTG B 633:

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

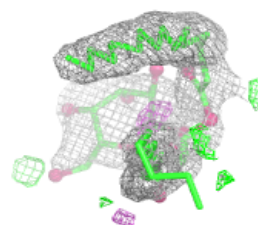
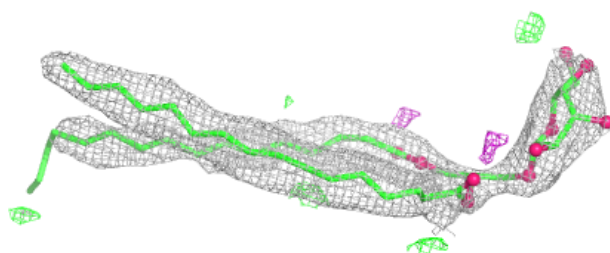
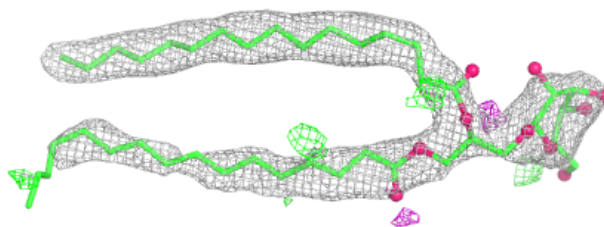
**Electron density around LMT a 404:**

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

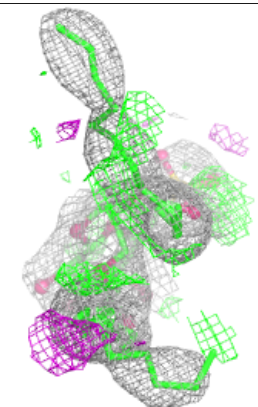
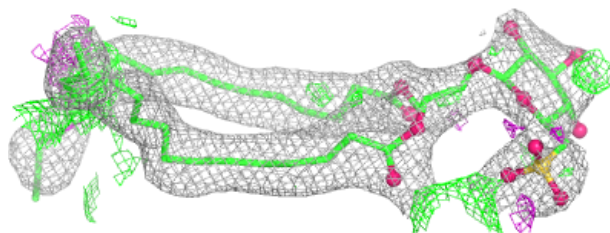
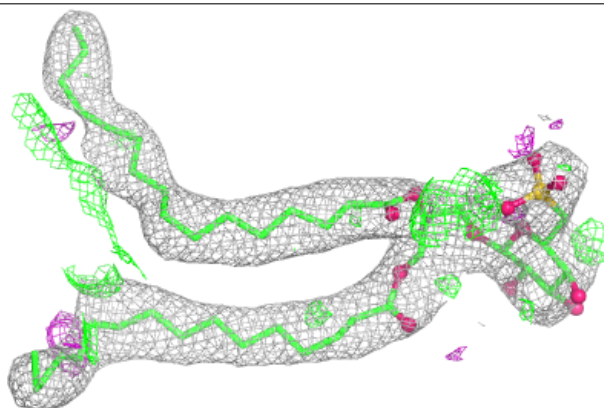


Electron density around LMG C 521:

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

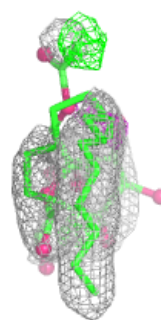
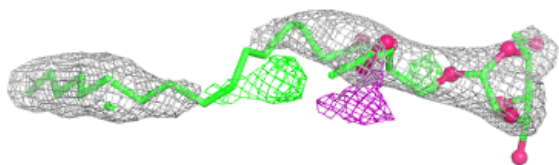
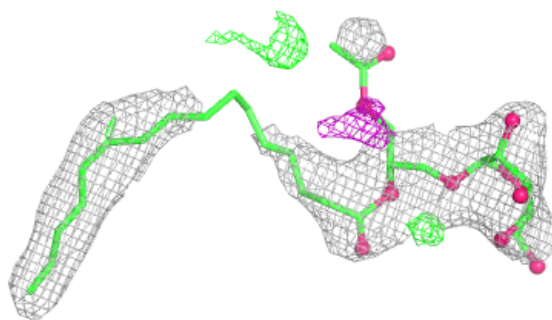
**Electron density around SQD B 621:**

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

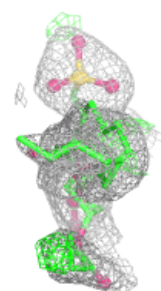
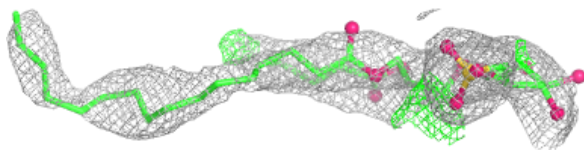
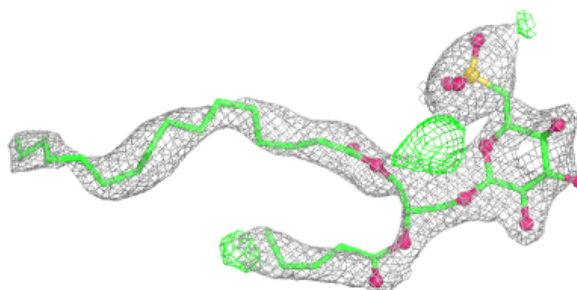


Electron density around LMG Z 101:

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

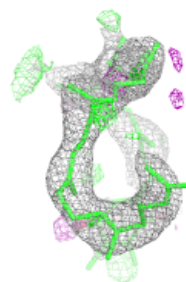
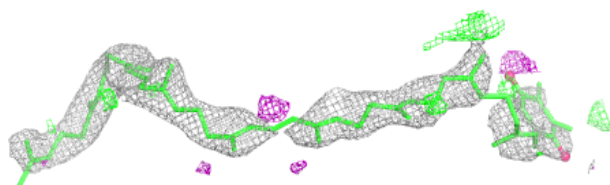
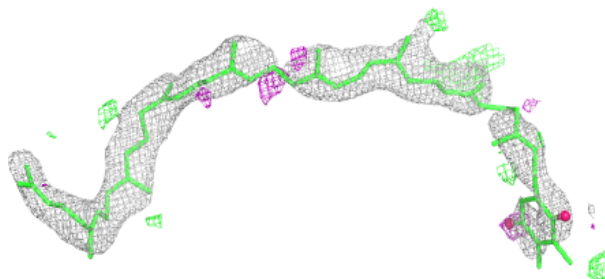
**Electron density around SQD F 103:**

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

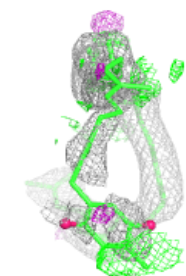
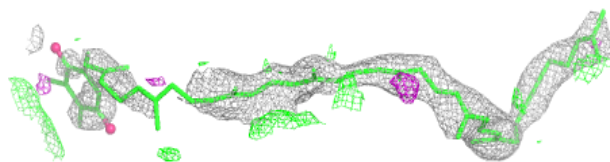
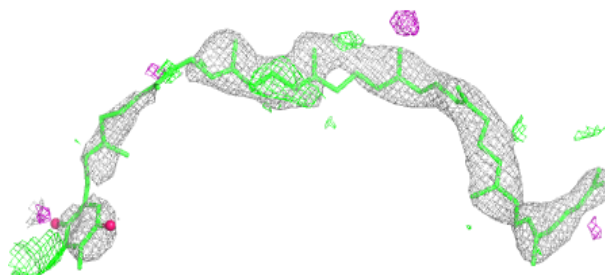


Electron density around PL9 A 418:

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

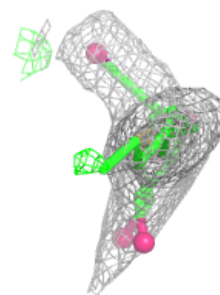
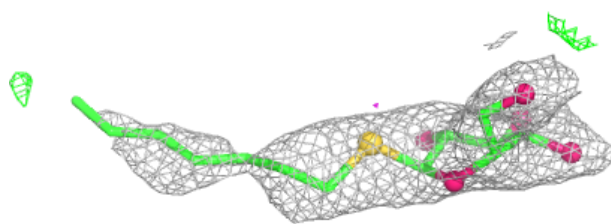
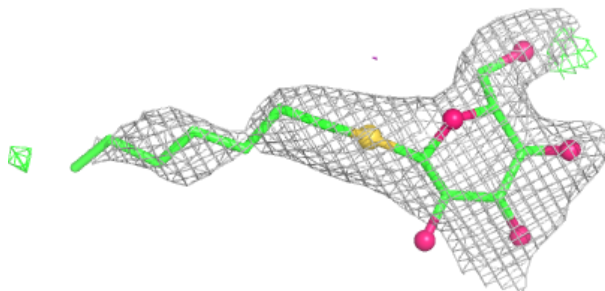
**Electron density around PL9 a 416:**

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

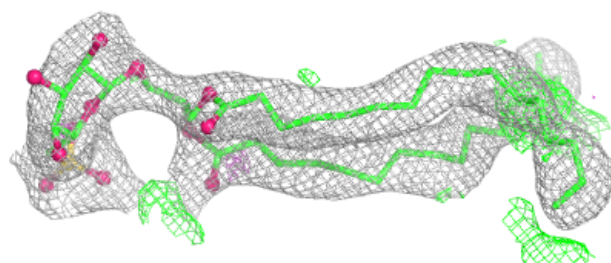
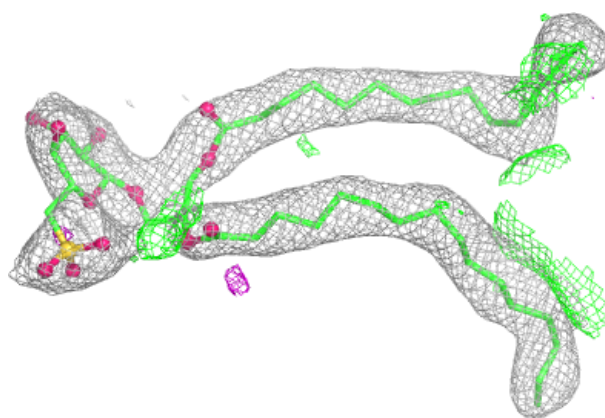


Electron density around HTG C 524:

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

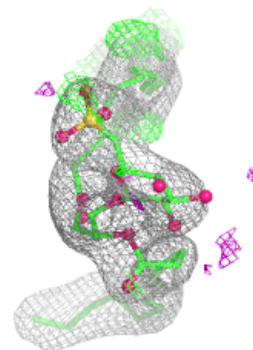
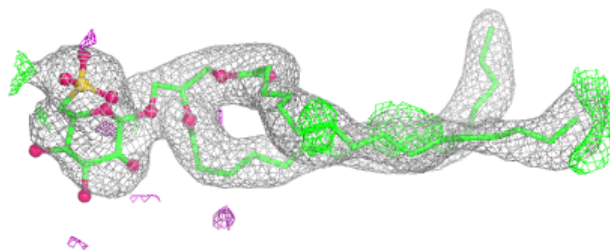
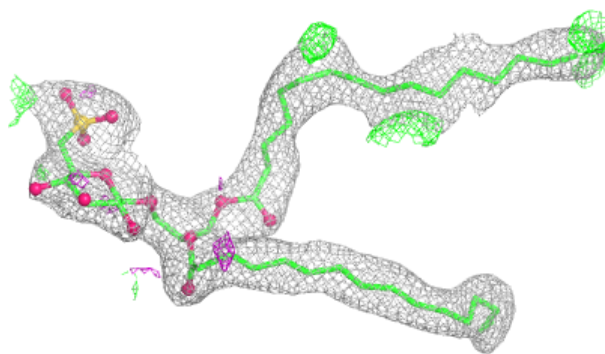
**Electron density around SQD L 102:**

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

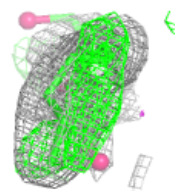
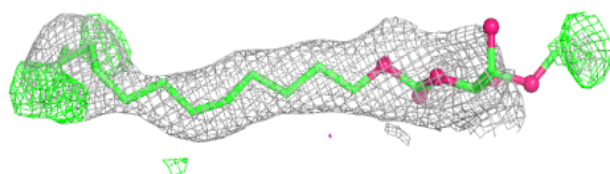
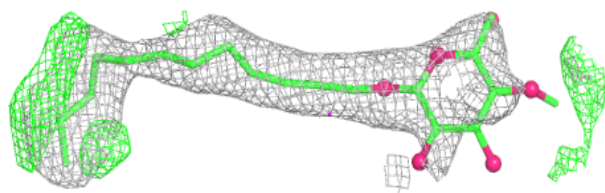


Electron density around SQD a 405:

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

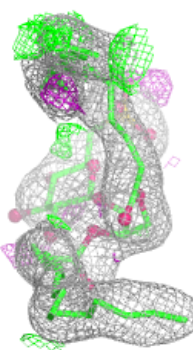
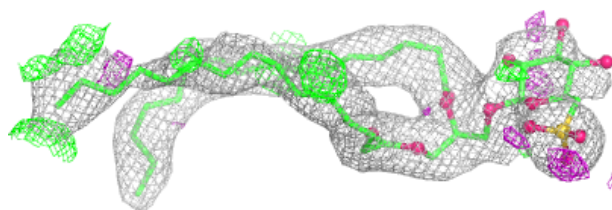
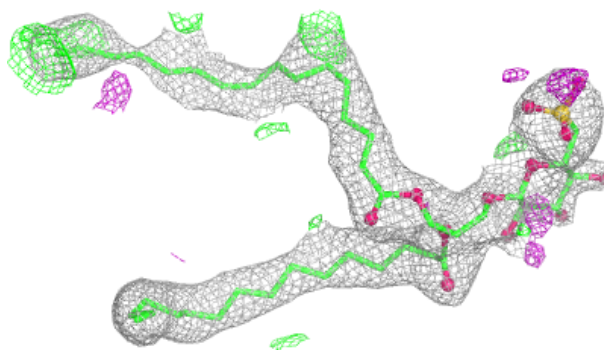
**Electron density around LMT B 635:**

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

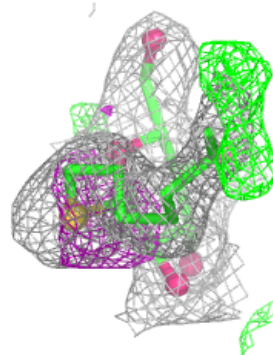
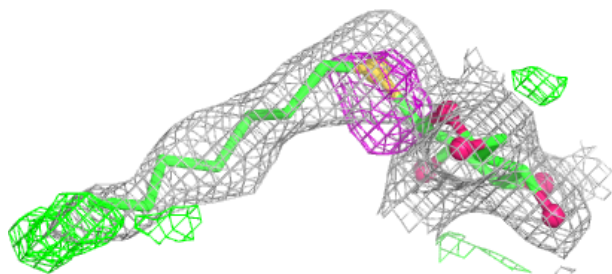
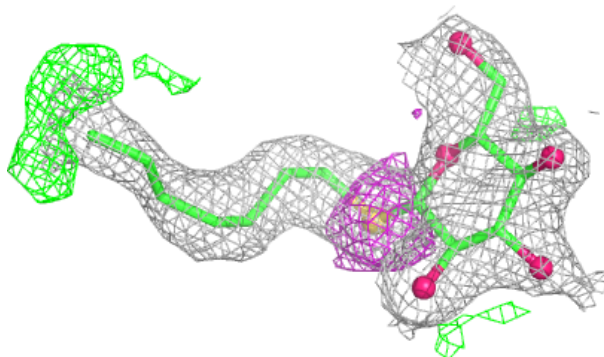


Electron density around SQD A 415:

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

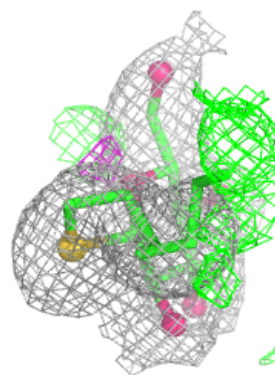
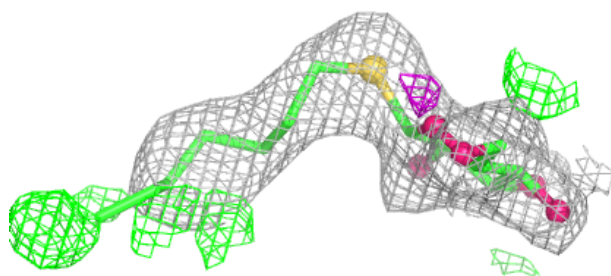
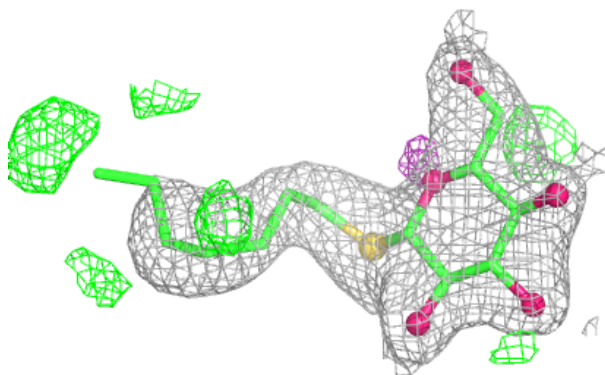
**Electron density around HTG b 631:**

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

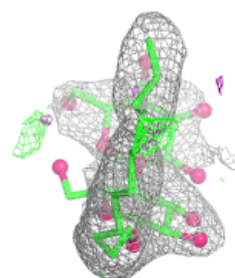
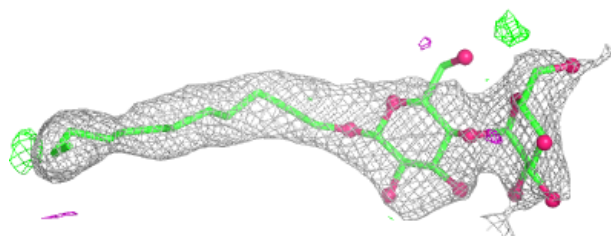
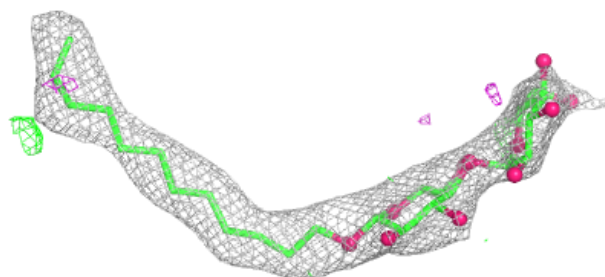


Electron density around HTG B 624:

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

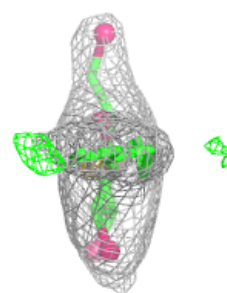
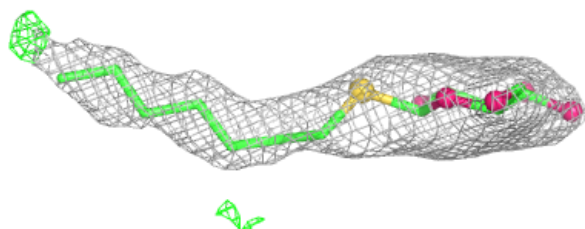
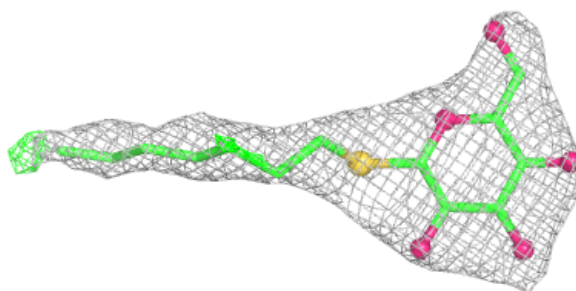
**Electron density around LMT m 102:**

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

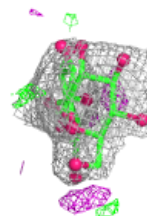
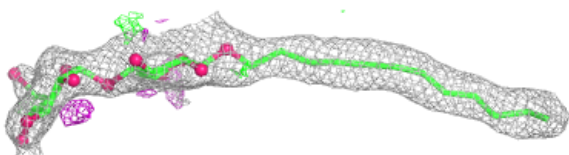
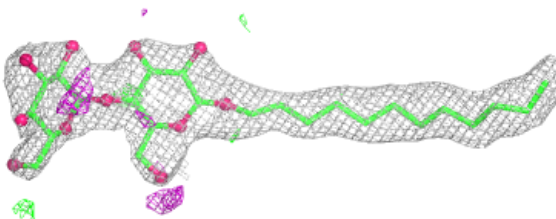


Electron density around HTG c 524:

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

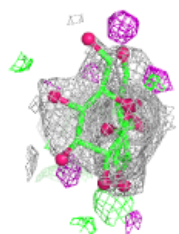
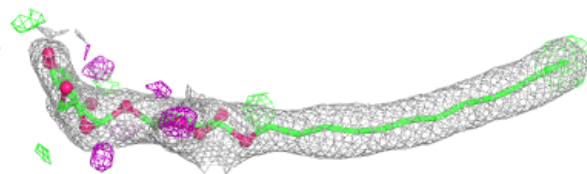
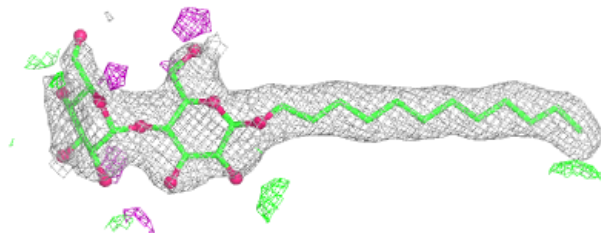
**Electron density around LMT M 105:**

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

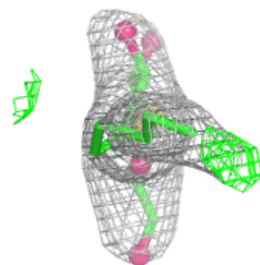
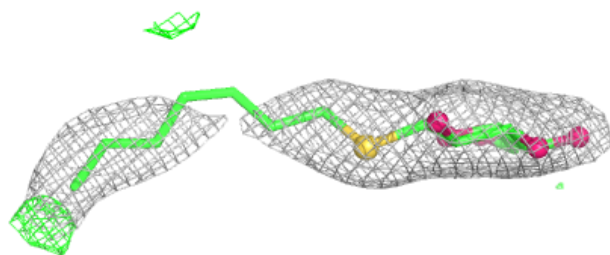
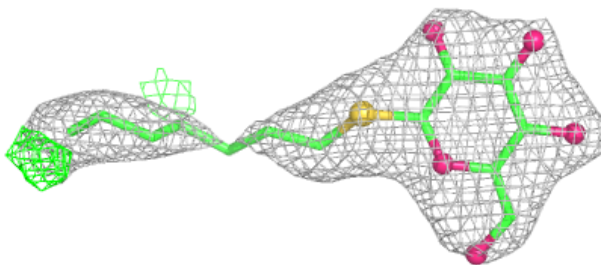


Electron density around LMT M 102:

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

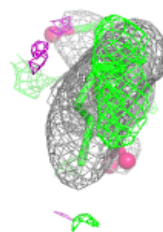
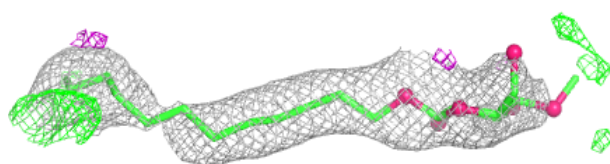
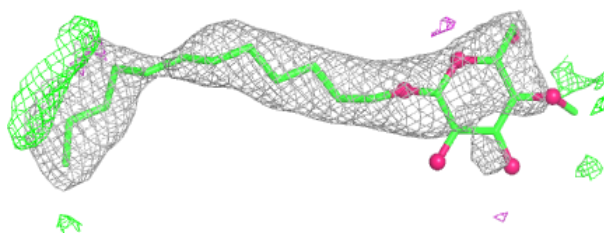
**Electron density around HTG C 523:**

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

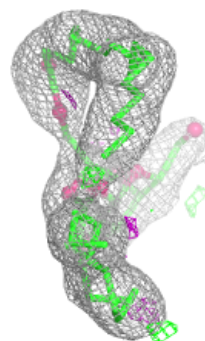
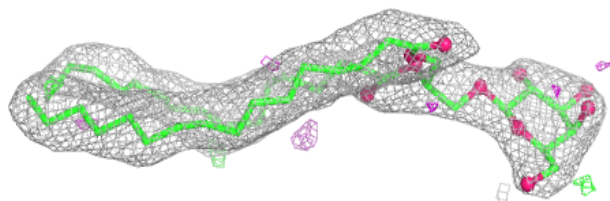
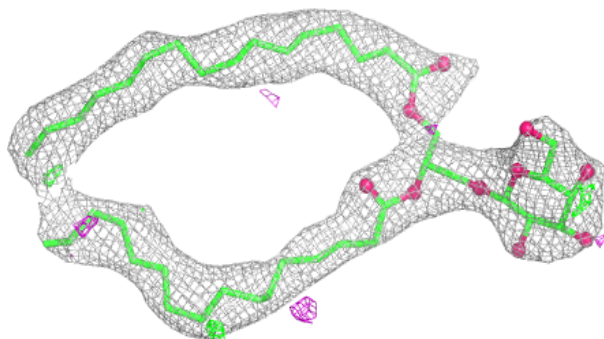


Electron density around LMT T 104:

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

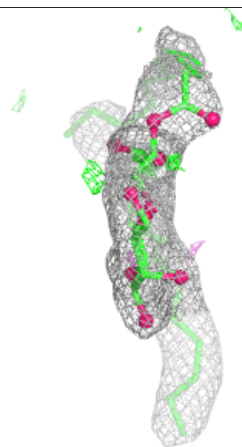
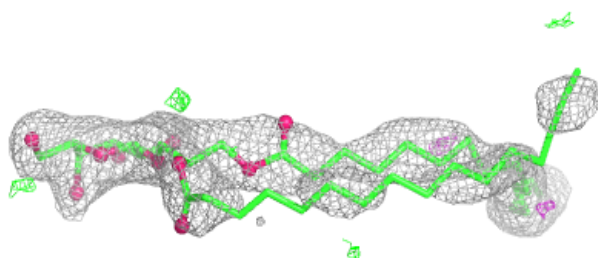
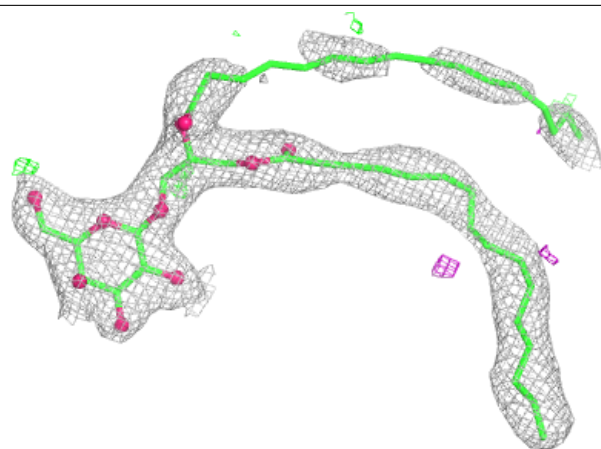
**Electron density around LMG a 415:**

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

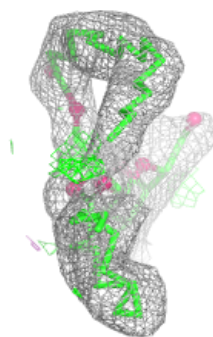
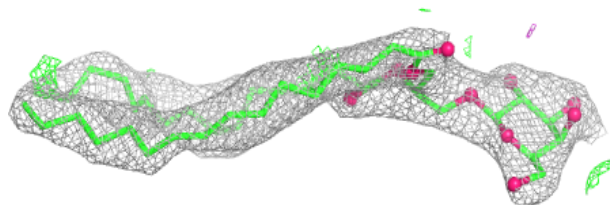
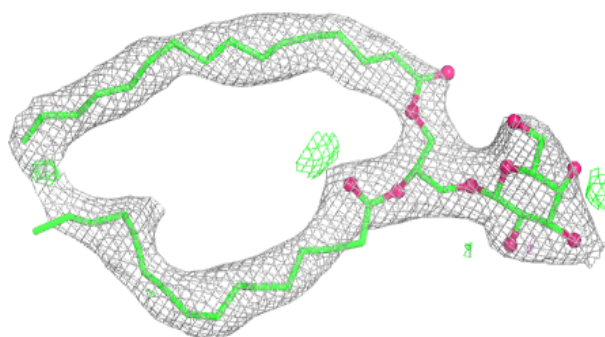


Electron density around LMG c 522:

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

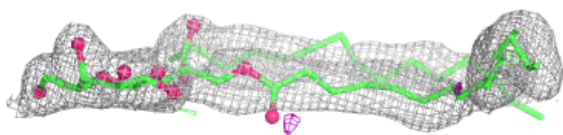
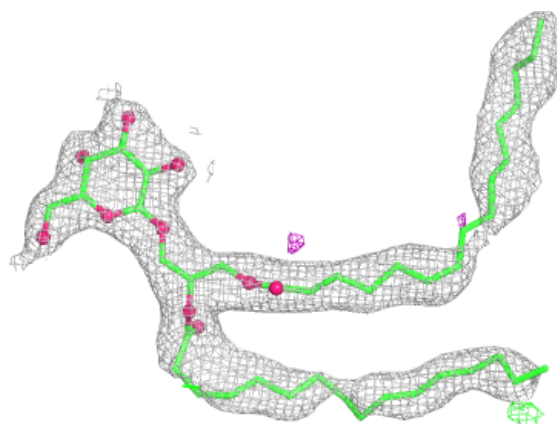
**Electron density around LMG C 501:**

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

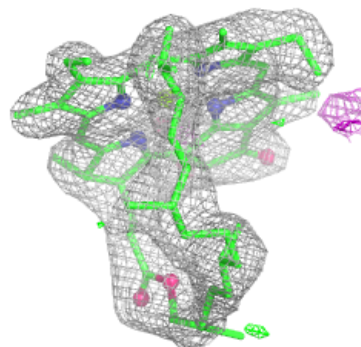
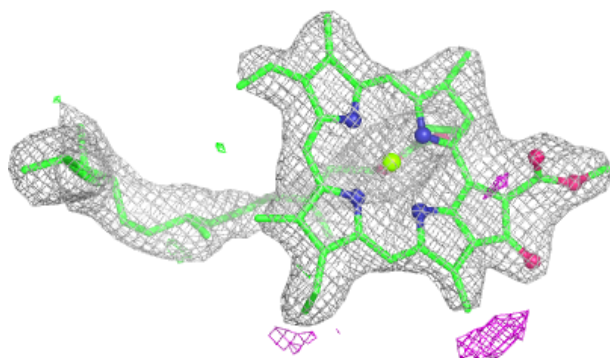
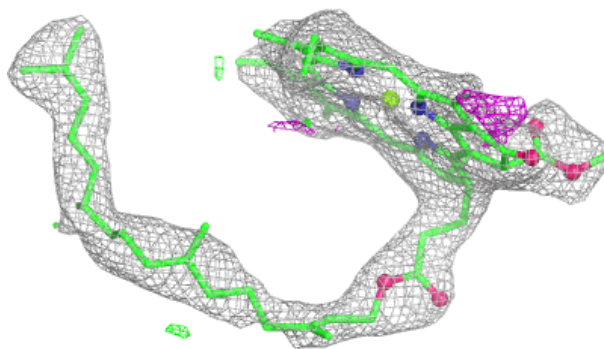


Electron density around LMG C 520:

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

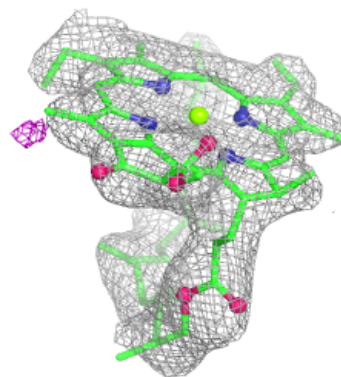
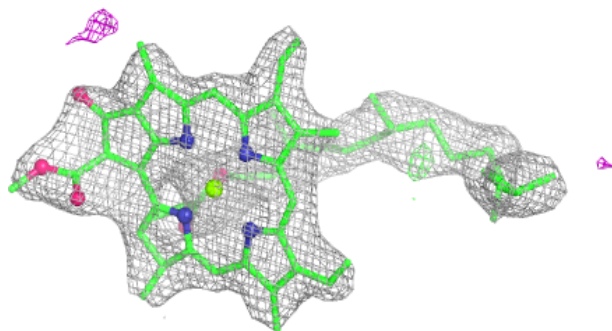
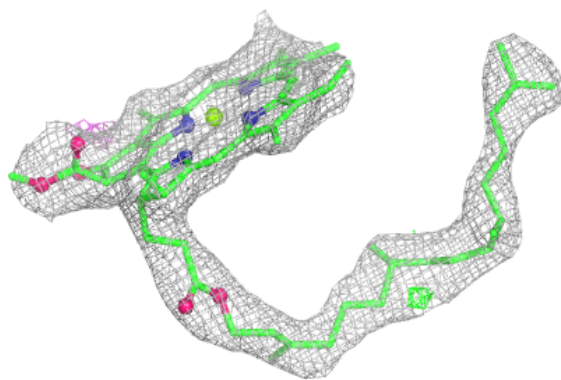
**Electron density around CLA C 514:**

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

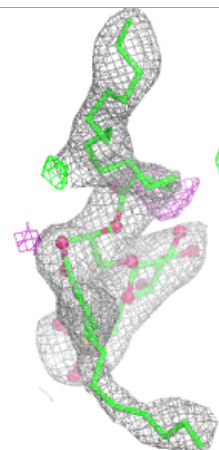
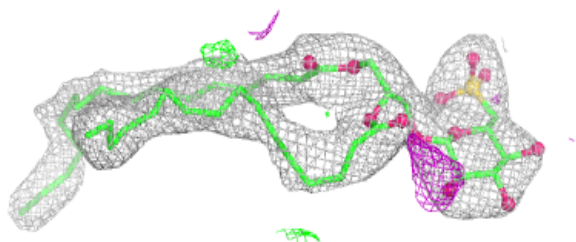
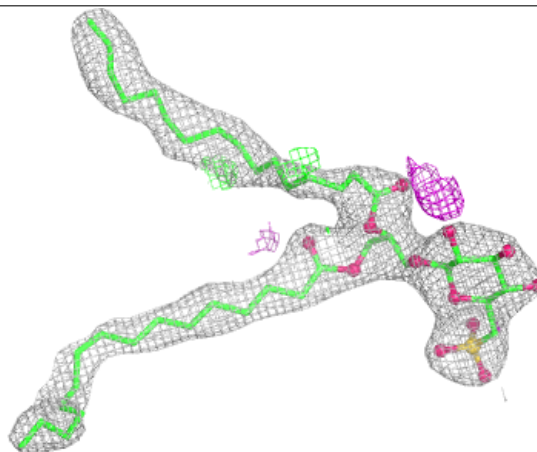


Electron density around CLA c 517:

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

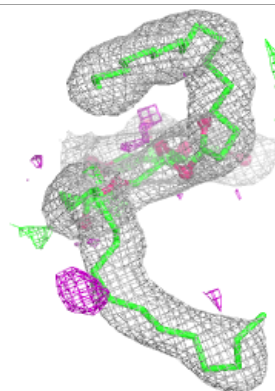
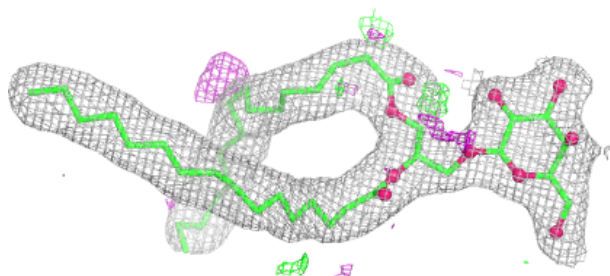
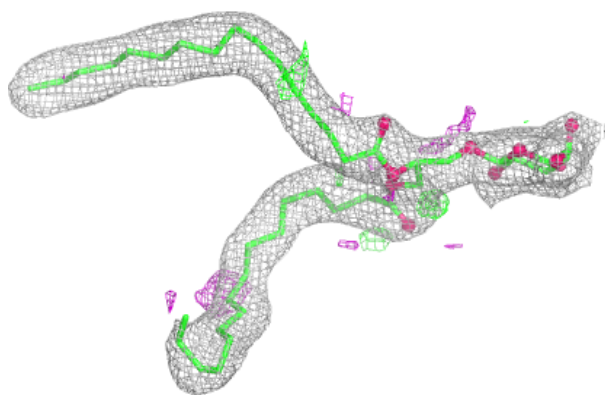
**Electron density around SQD A 411:**

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

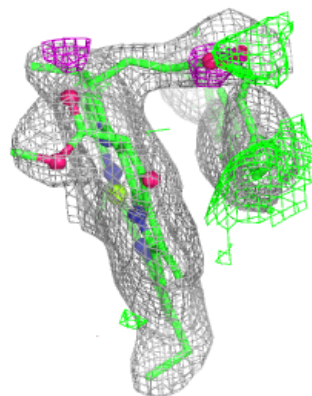
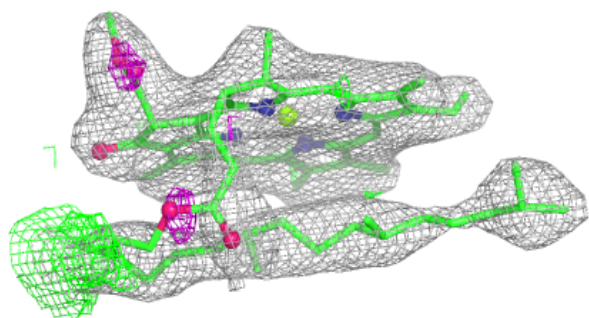
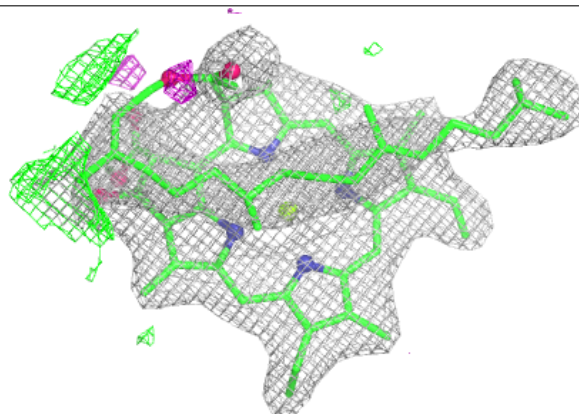


Electron density around LMG b 629:

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

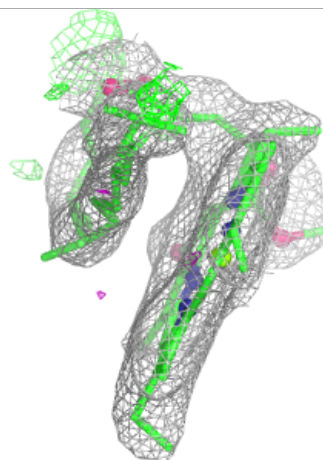
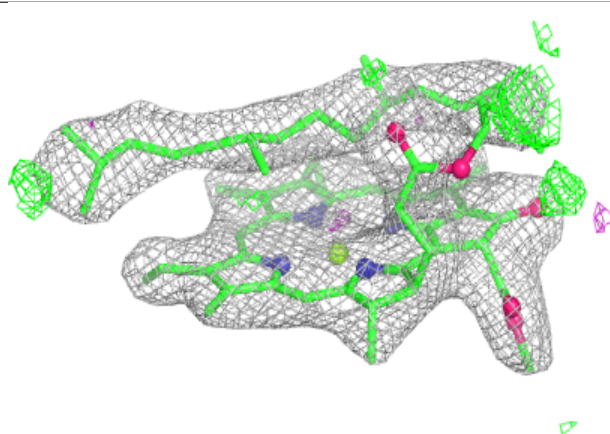
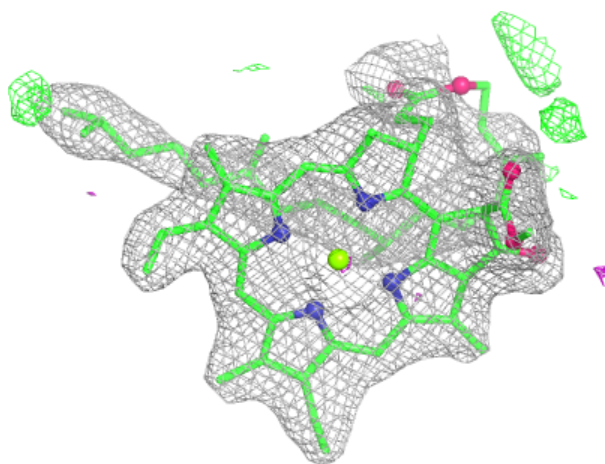
**Electron density around CLA B 602:**

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



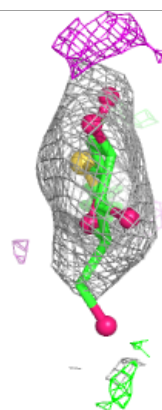
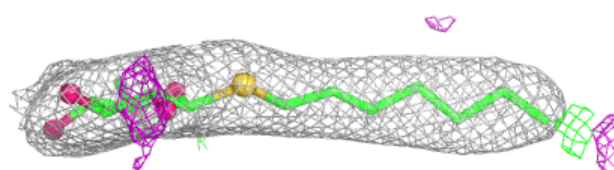
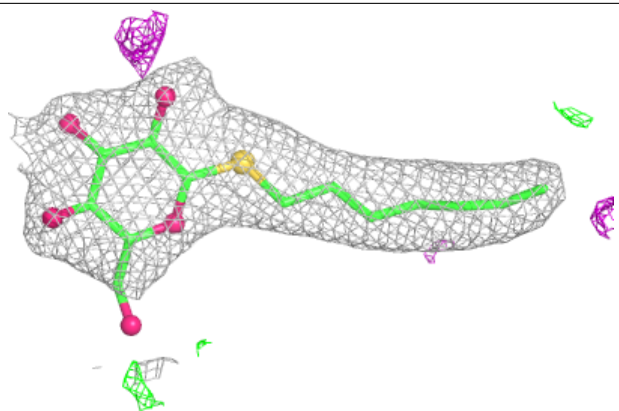
Electron density around CLA b 610:

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

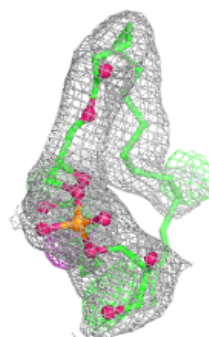
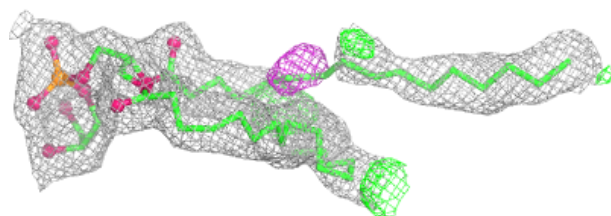
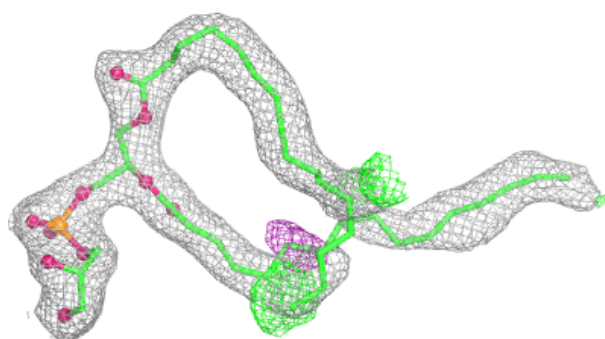


Electron density around HTG B 632:

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

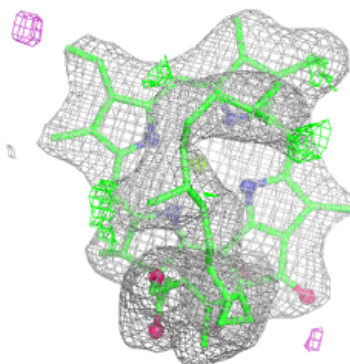
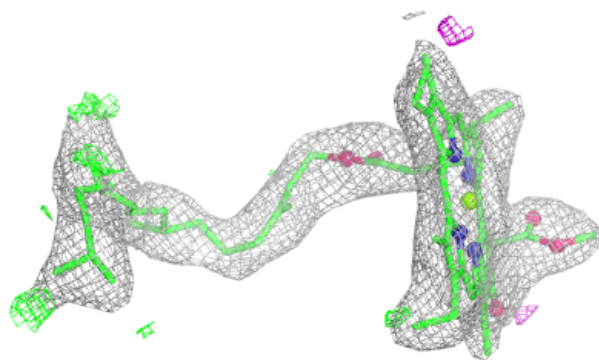
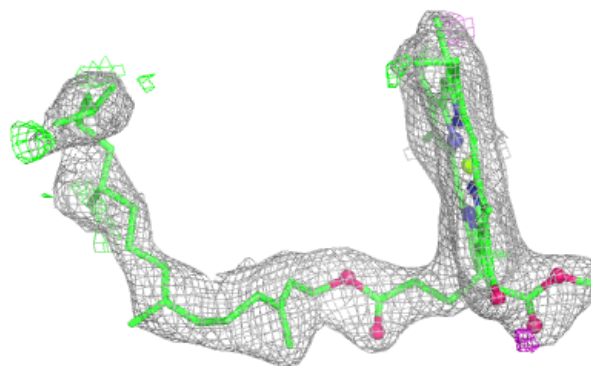
**Electron density around LHG D 409:**

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

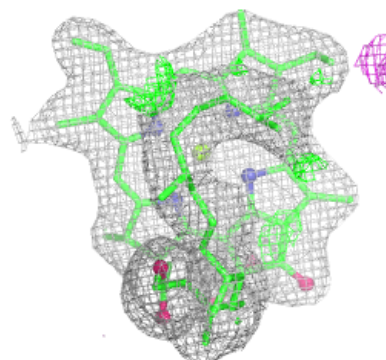
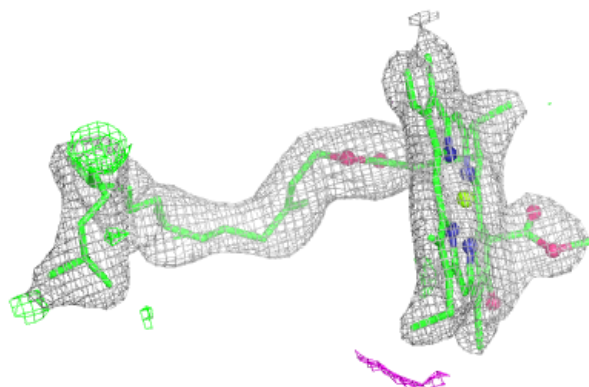
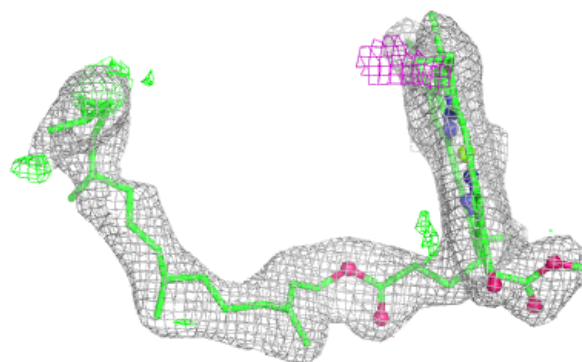


Electron density around CLA C 507:

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

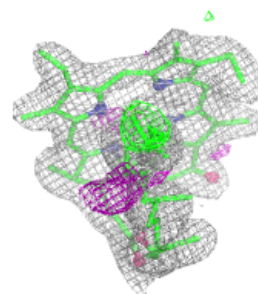
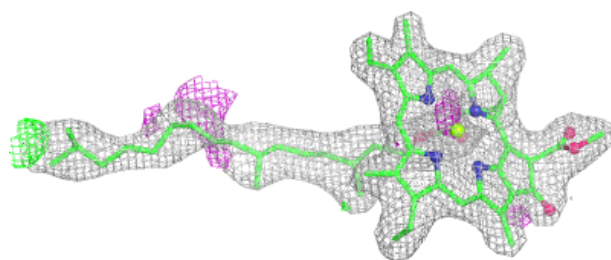
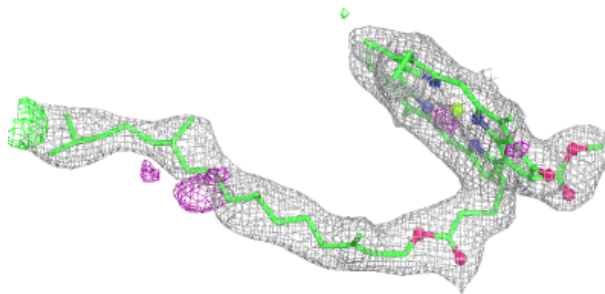
**Electron density around CLA c 510:**

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

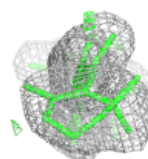
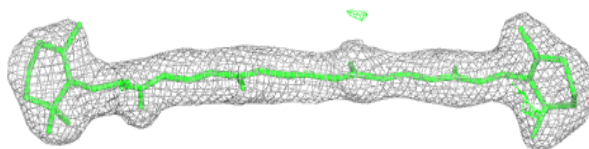
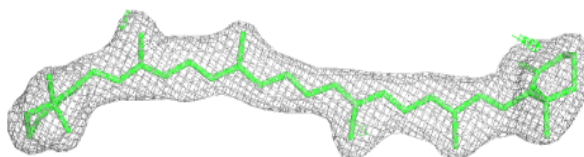


Electron density around CLA C 505:

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

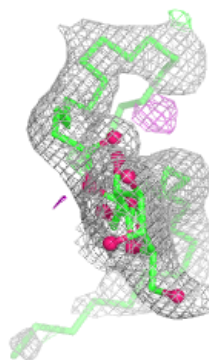
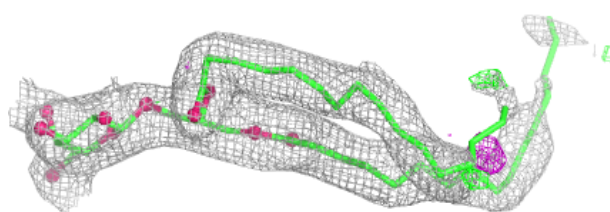
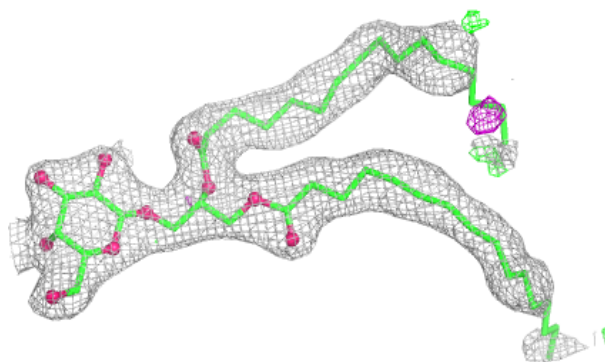
**Electron density around BCR C 515:**

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



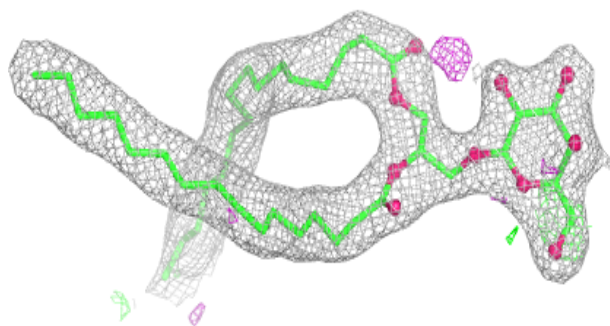
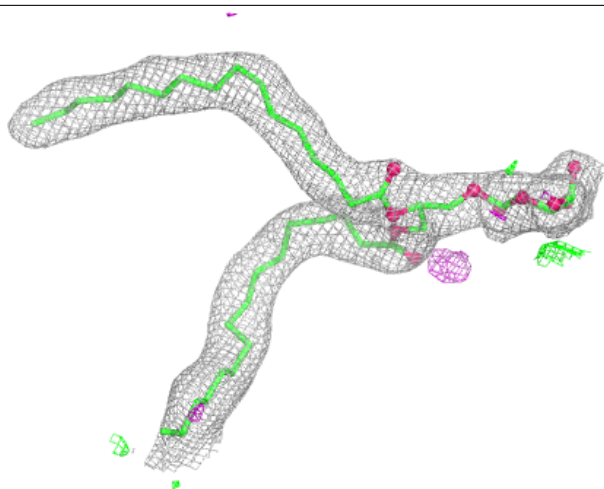
Electron density around LMG J 101:

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



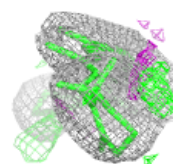
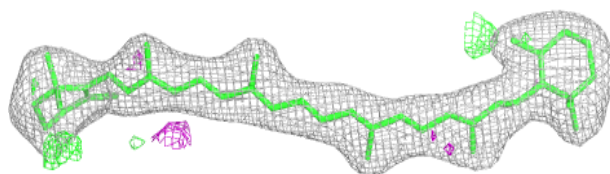
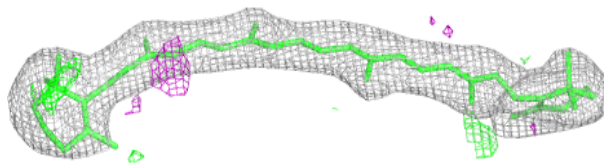
Electron density around LMG M 101:

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



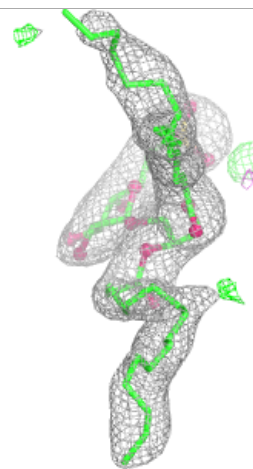
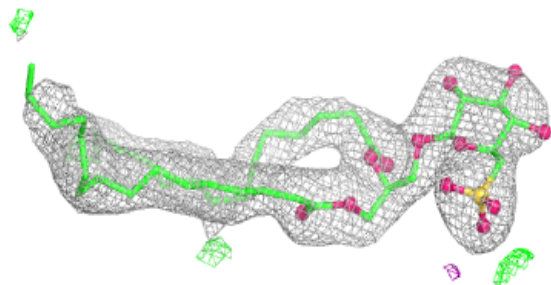
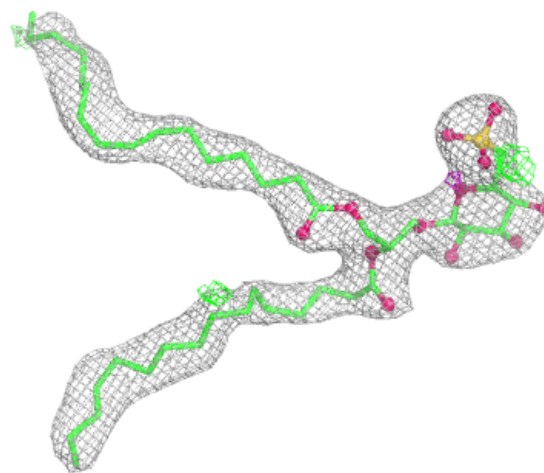
Electron density around BCR D 404:

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



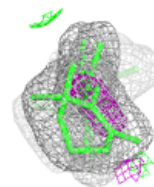
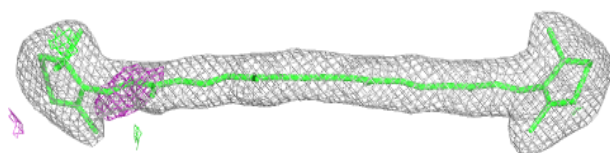
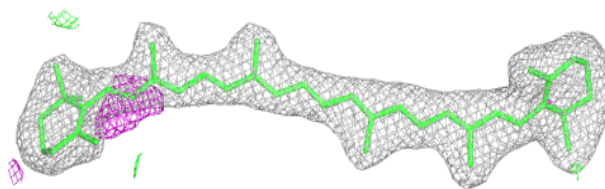
Electron density around SQD a 414:

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

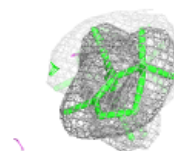
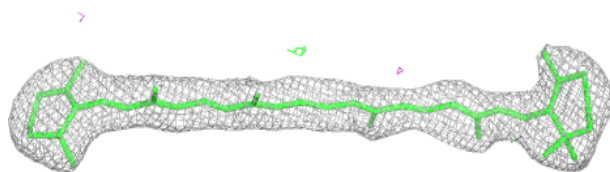
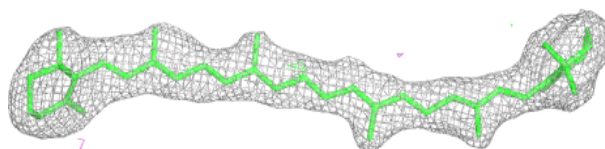


Electron density around BCR b 627:

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

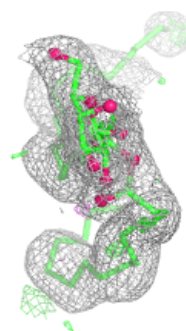
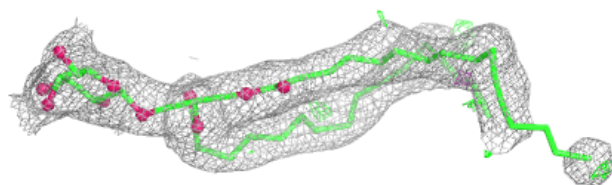
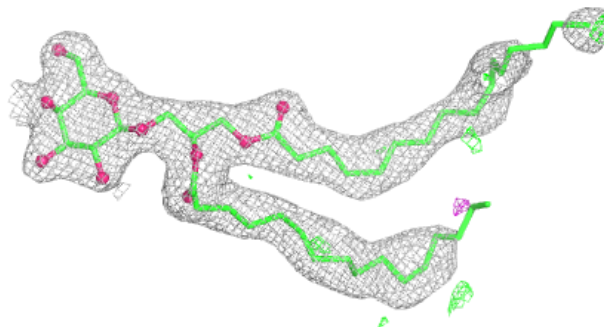
**Electron density around BCR c 527:**

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

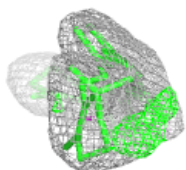
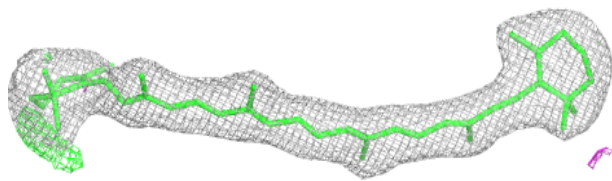
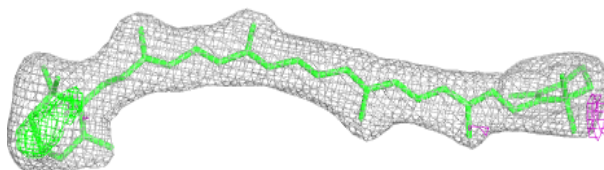


Electron density around LMG j 101:

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

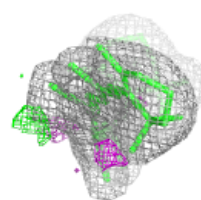
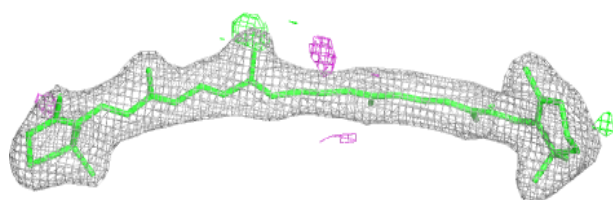
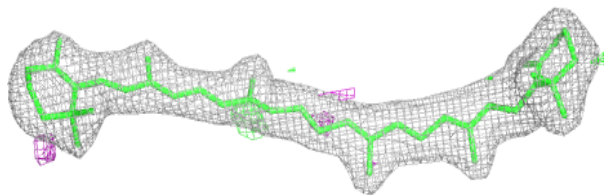
**Electron density around BCR d 405:**

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

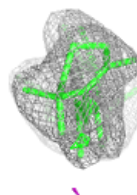
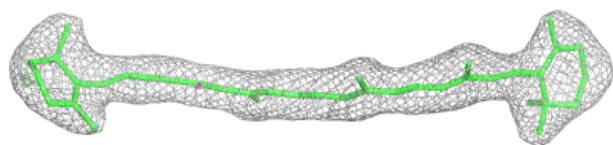
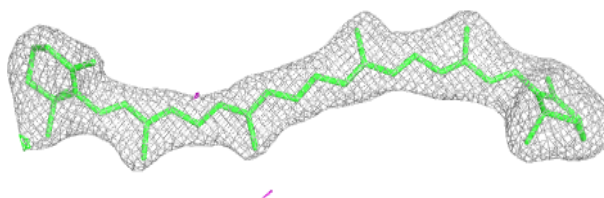


Electron density around BCR t 101:

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

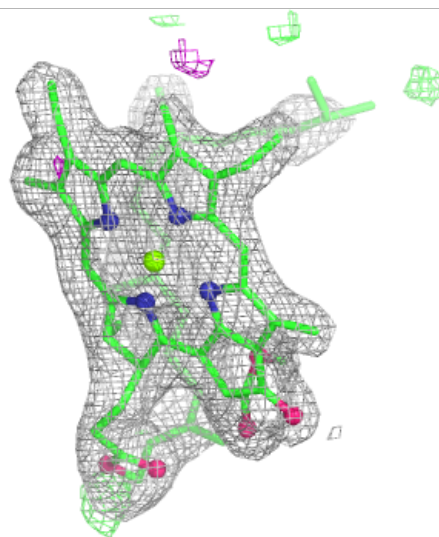
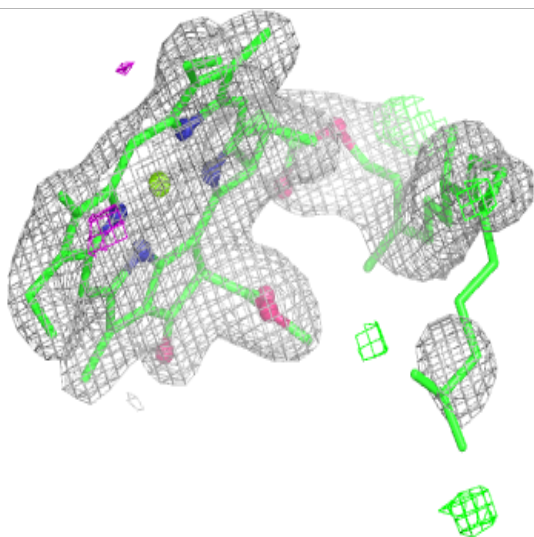
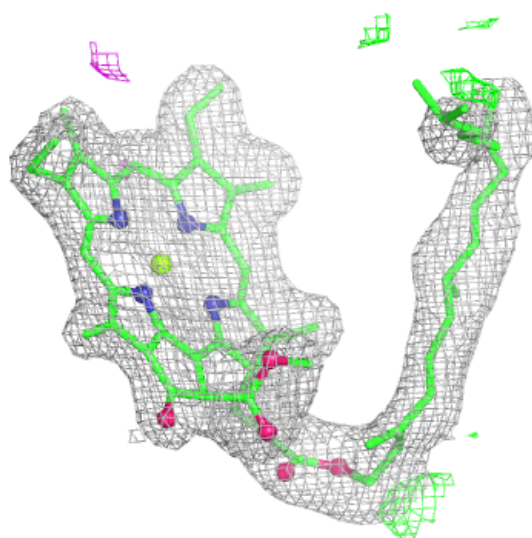
**Electron density around BCR y 101:**

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



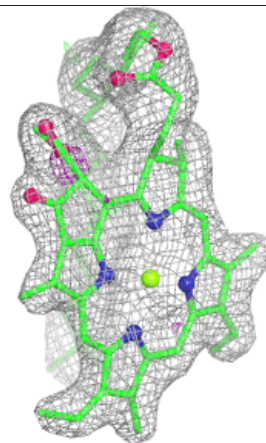
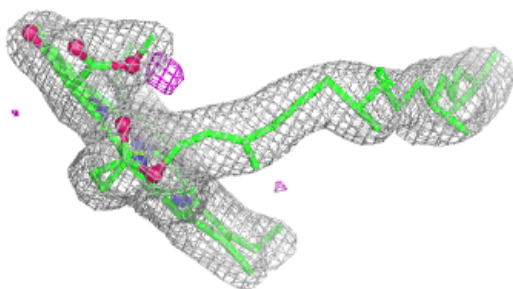
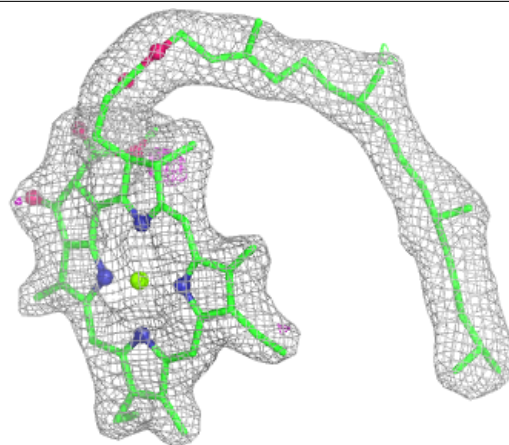
Electron density around CLA b 625:

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

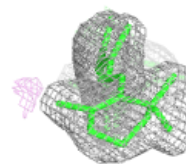
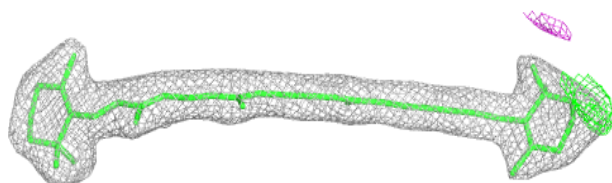
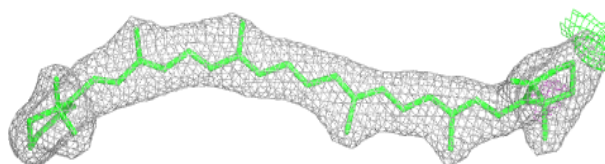


Electron density around CLA C 508:

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

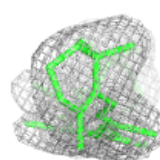
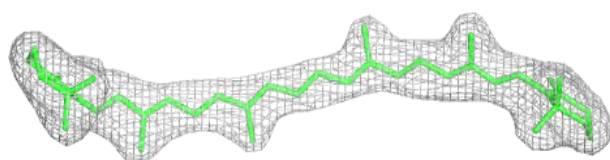
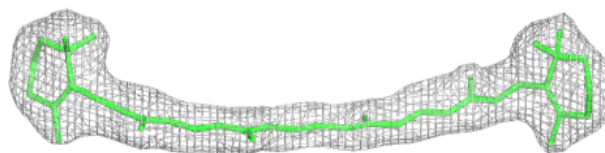
**Electron density around BCR H 101:**

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

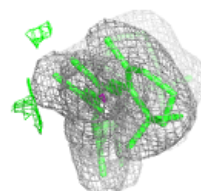
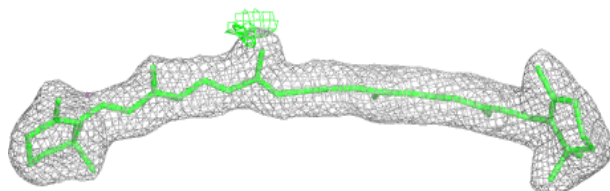
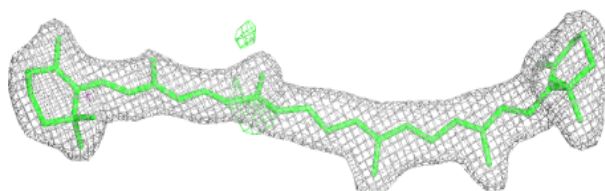


Electron density around BCR K 101:

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

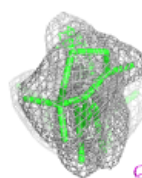
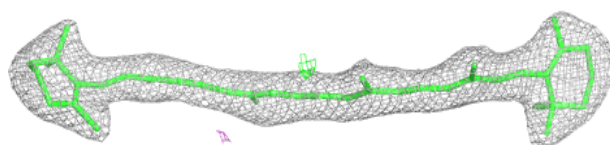
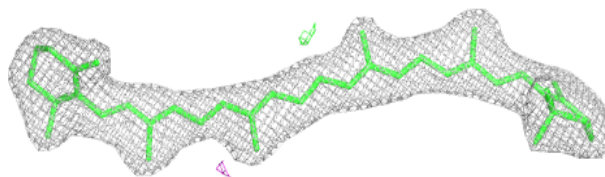
**Electron density around BCR T 103:**

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

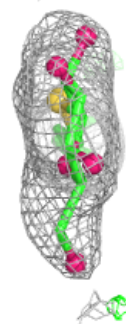
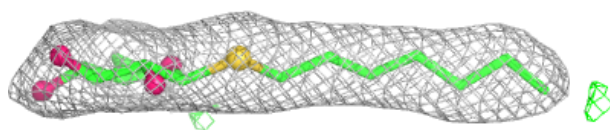
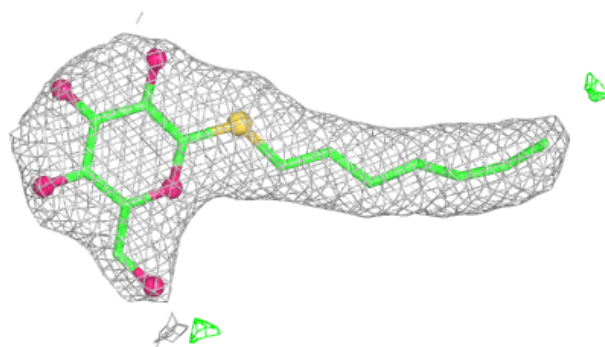


Electron density around BCR Y 101:

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

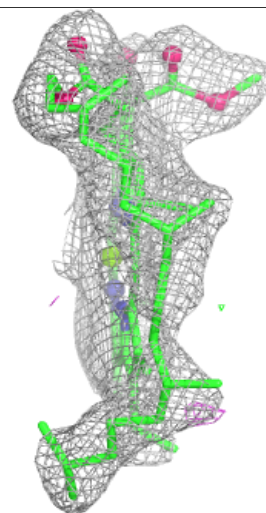
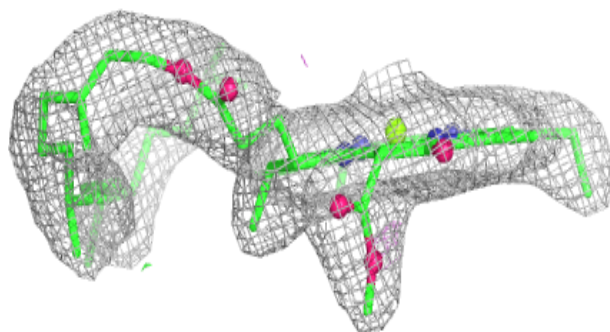
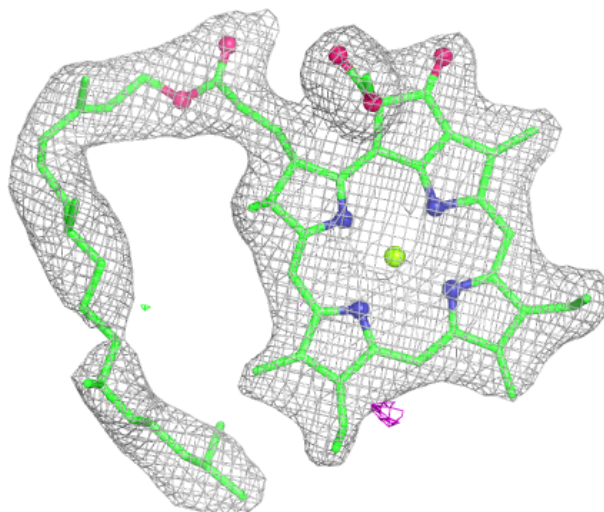
**Electron density around HTG b 607:**

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



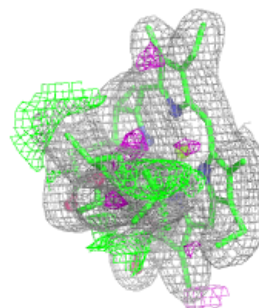
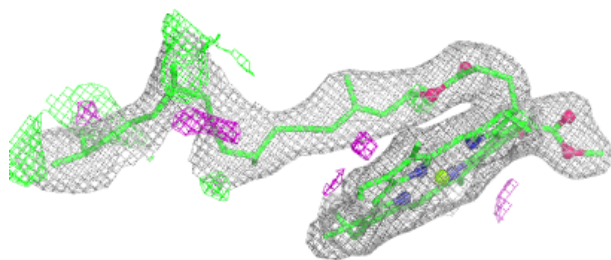
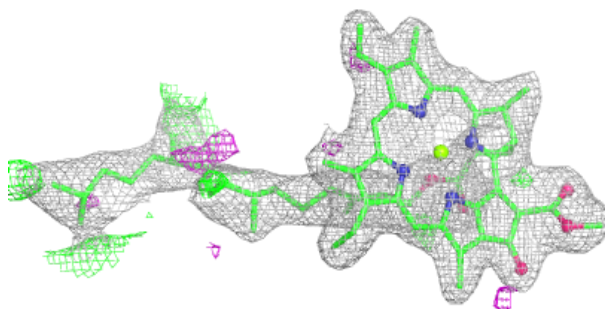
Electron density around CLA C 513:

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

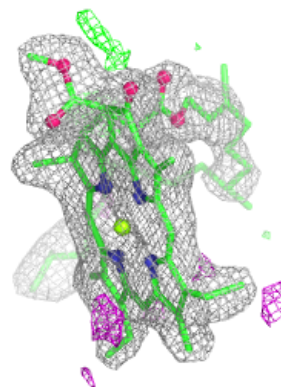
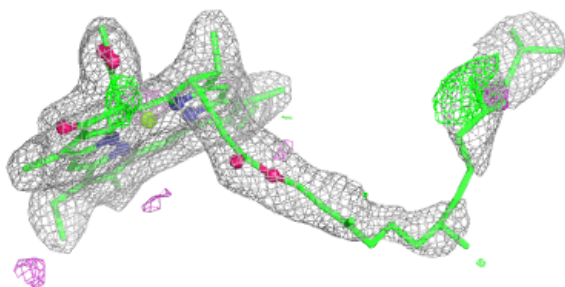
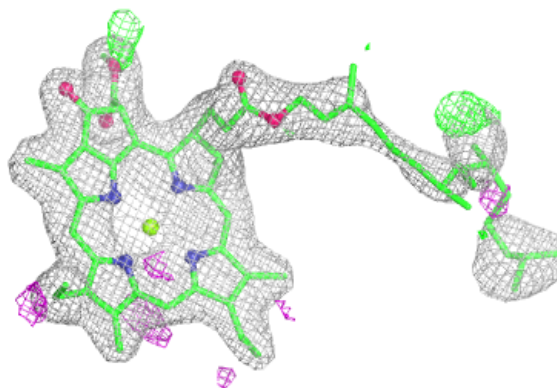


Electron density around CLA B 615:

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

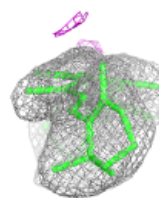
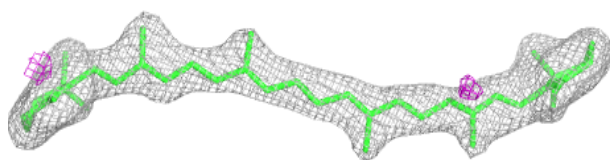
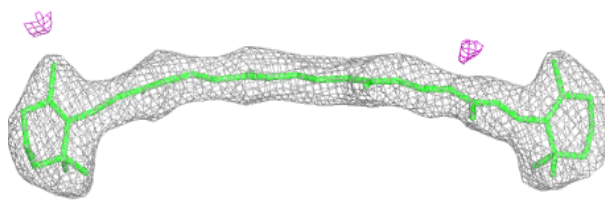
**Electron density around CLA a 412:**

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



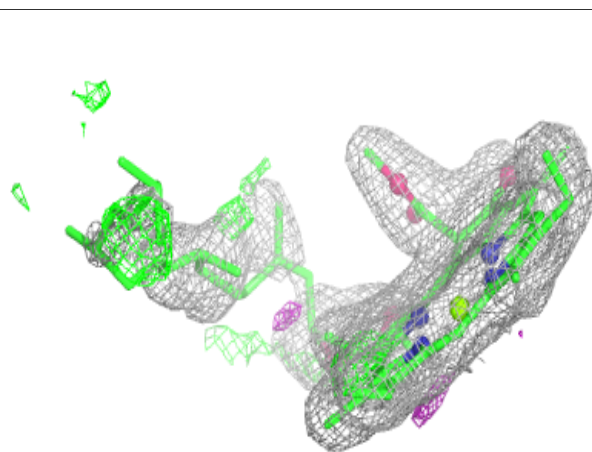
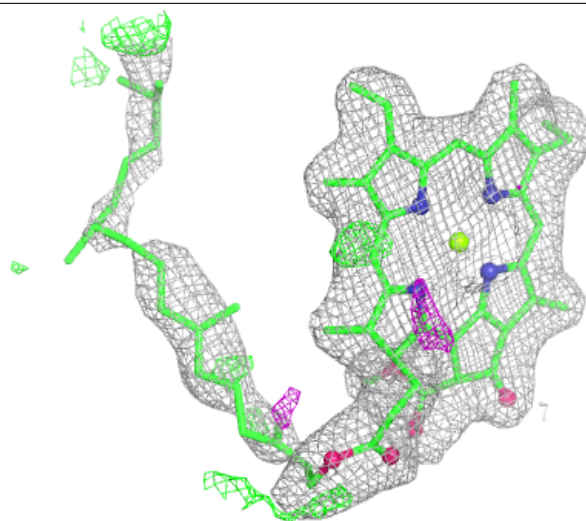
Electron density around BCR k 101:

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



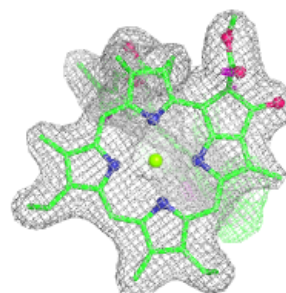
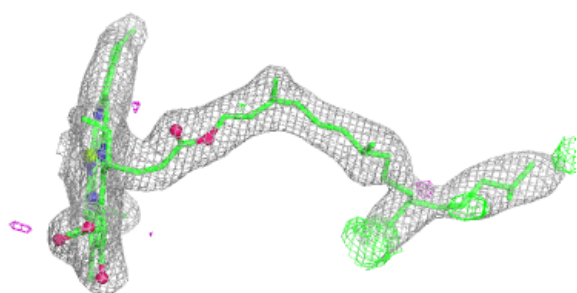
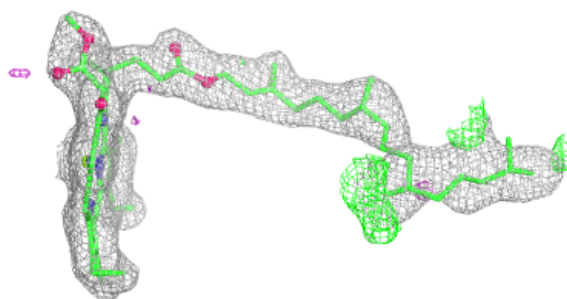
Electron density around CLA B 617:

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

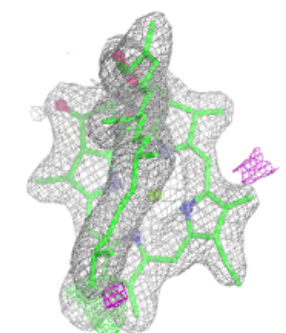
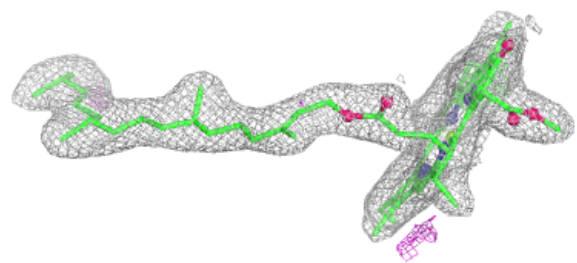
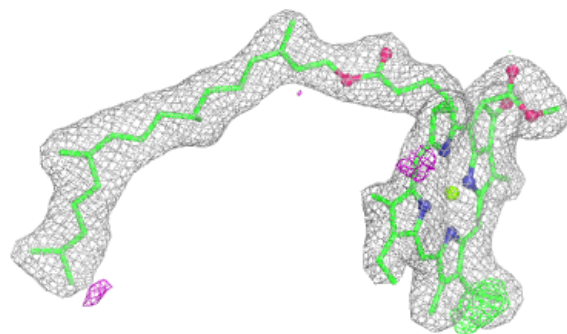


Electron density around CLA b 615:

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

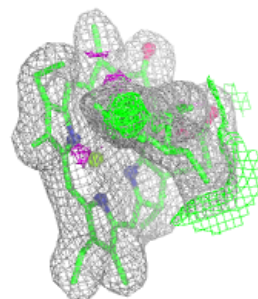
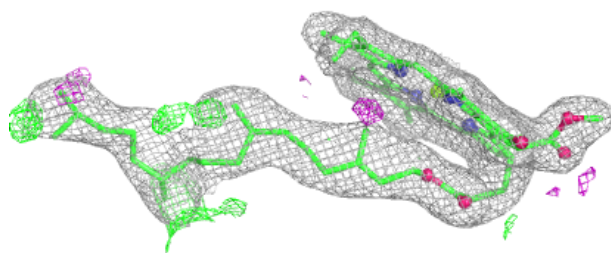
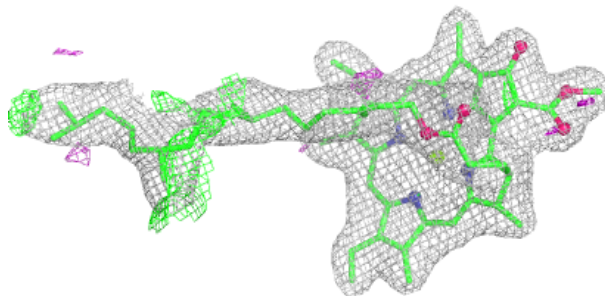
**Electron density around CLA b 618:**

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

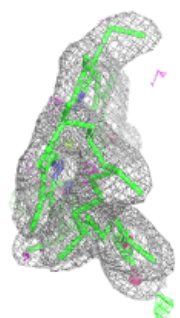
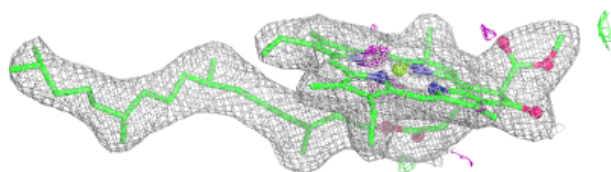
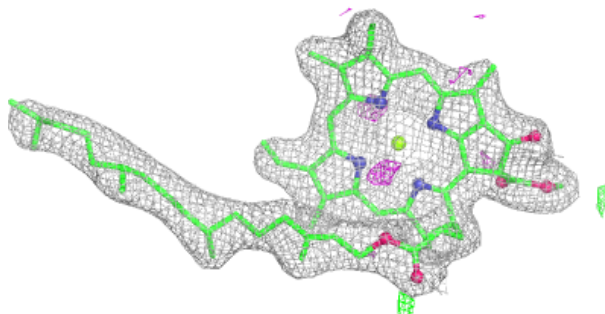


Electron density around CLA b 623:

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

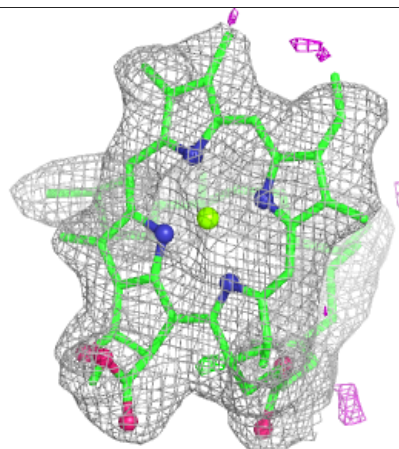
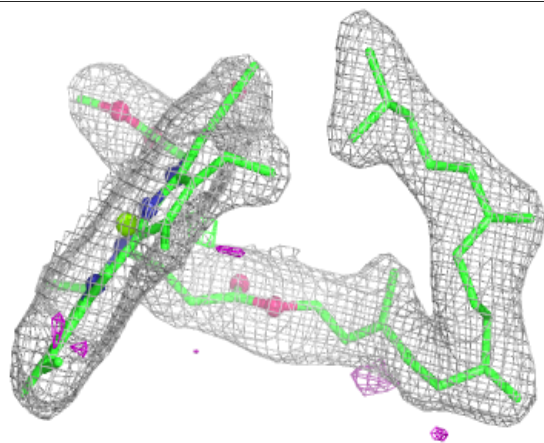
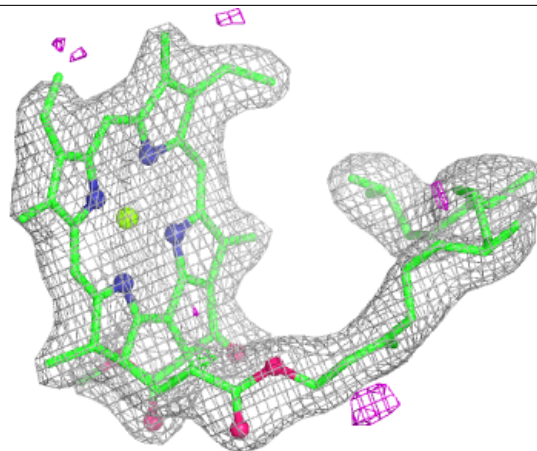
**Electron density around CLA C 502:**

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

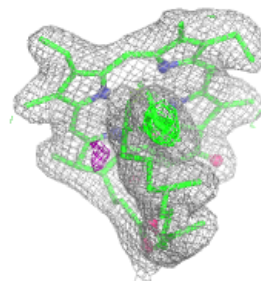
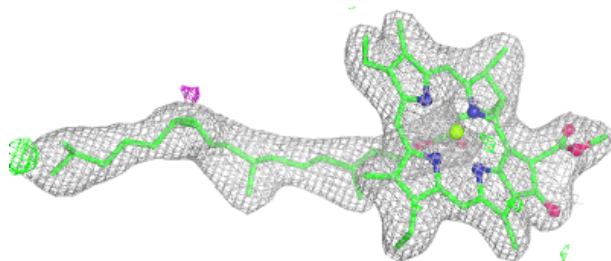
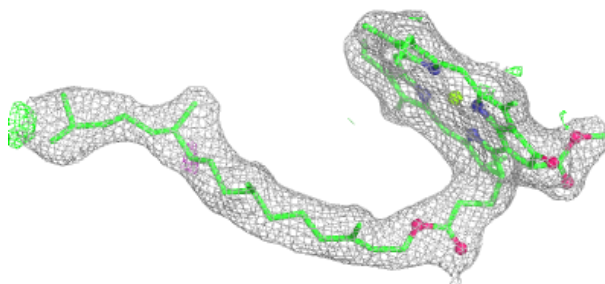


Electron density around CLA c 507:

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

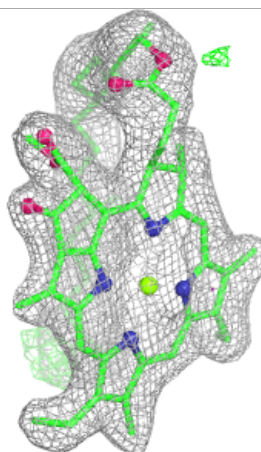
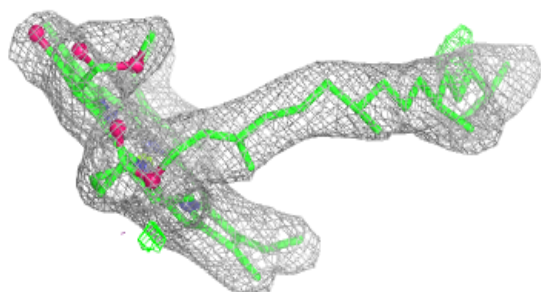
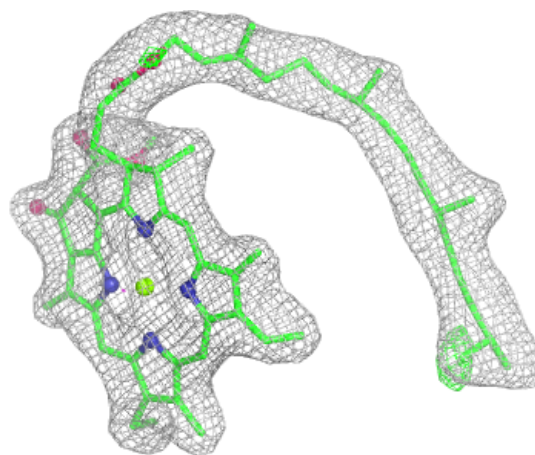
**Electron density around CLA c 508:**

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



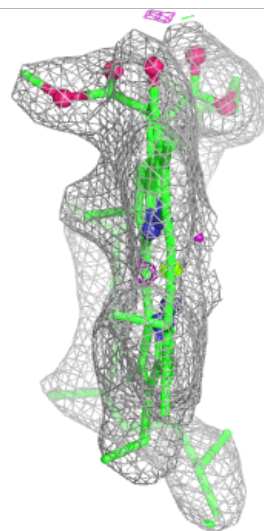
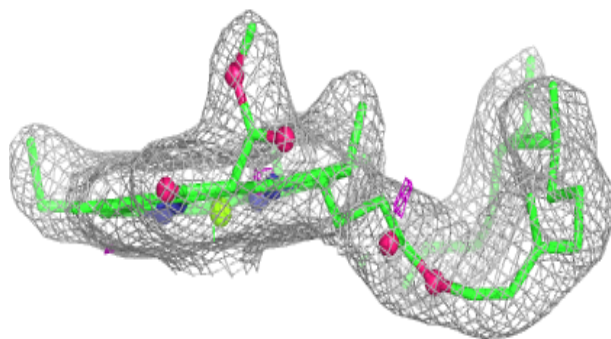
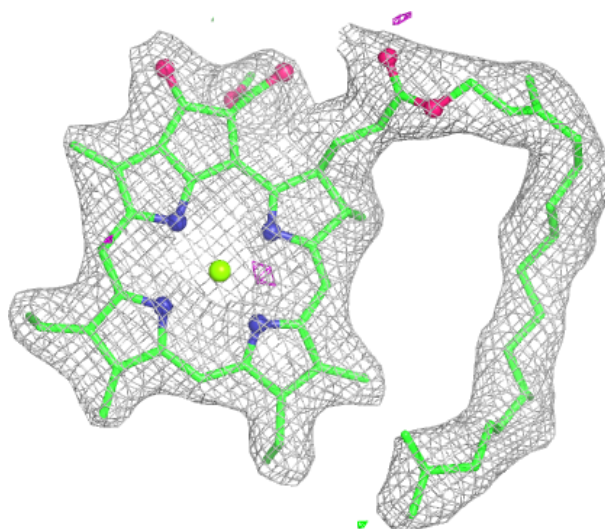
Electron density around CLA c 511:

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



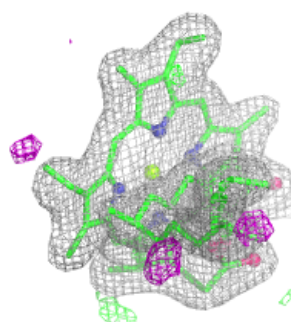
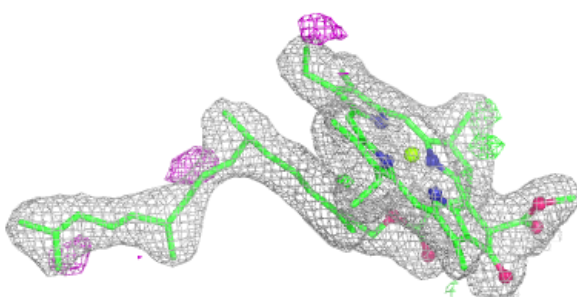
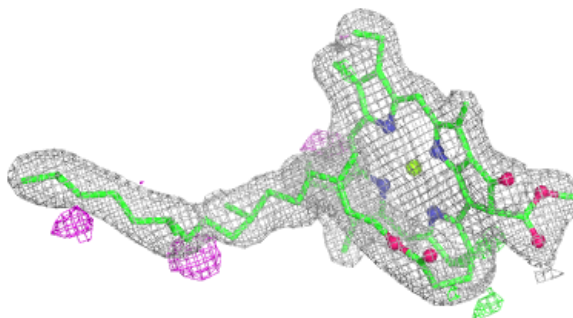
Electron density around CLA c 516:

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

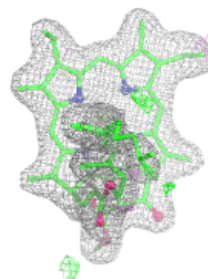
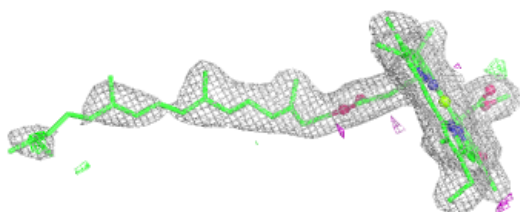
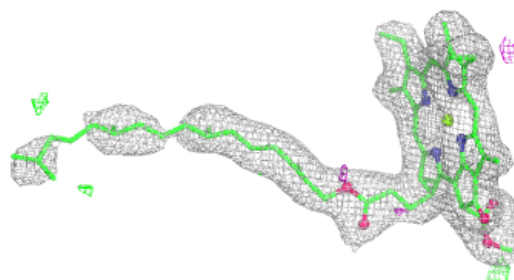


Electron density around CLA C 506:

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

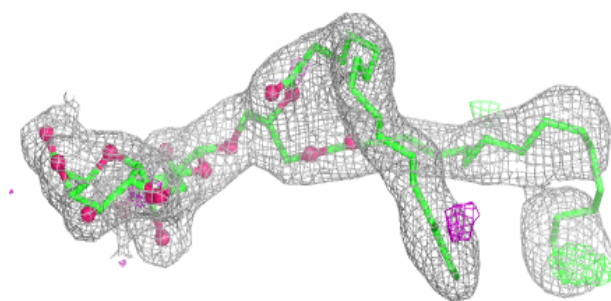
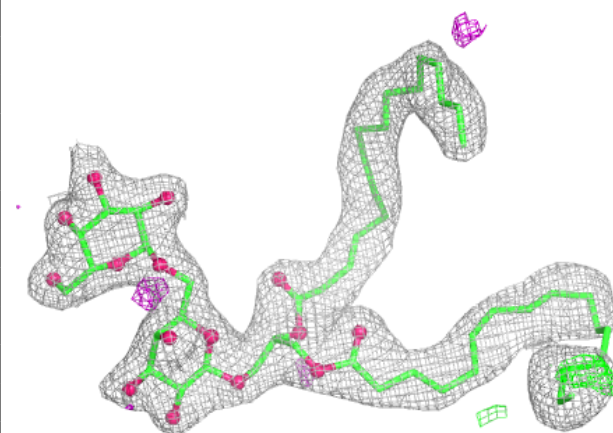
**Electron density around CLA d 404:**

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

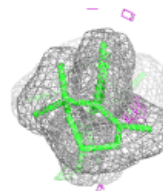
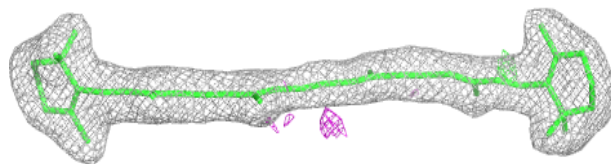
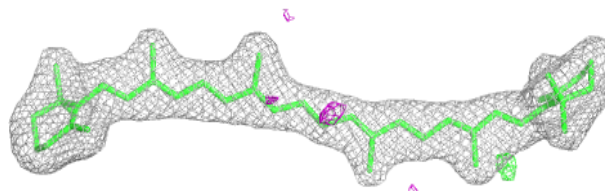


Electron density around DGD C 518:

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

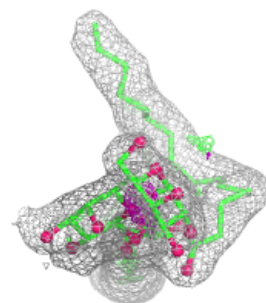
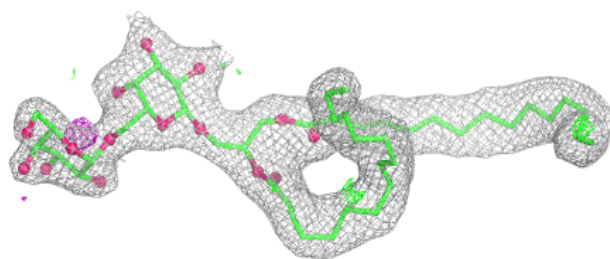
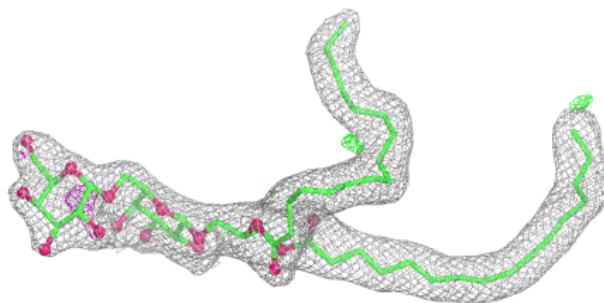
**Electron density around BCR A 410:**

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

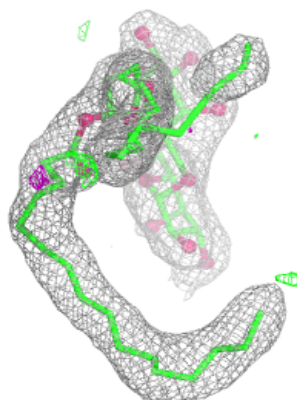
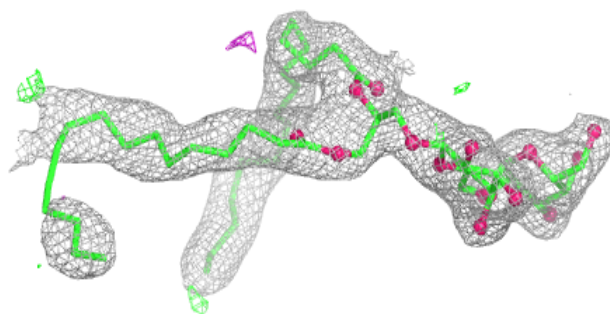
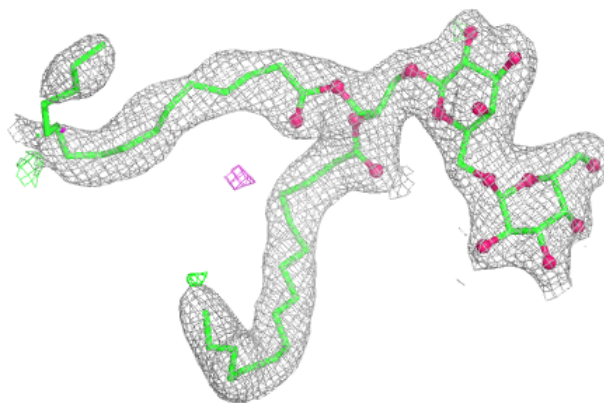


Electron density around DGD H 102:

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

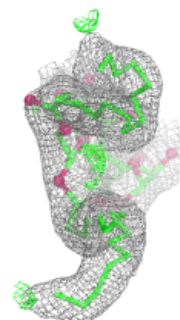
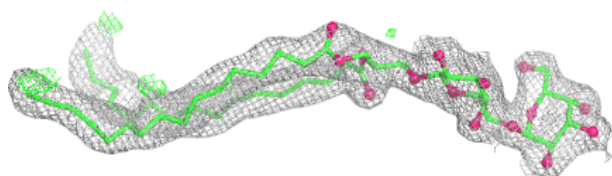
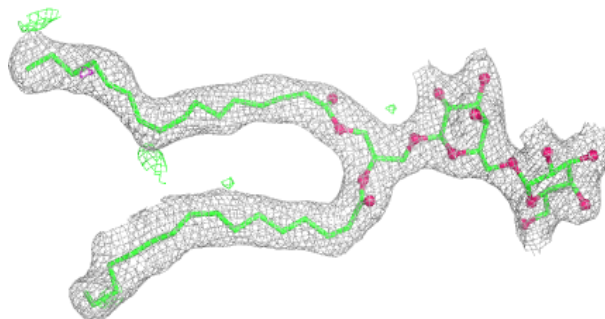
**Electron density around DGD c 520:**

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

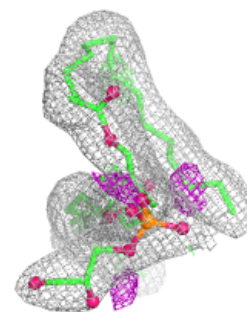
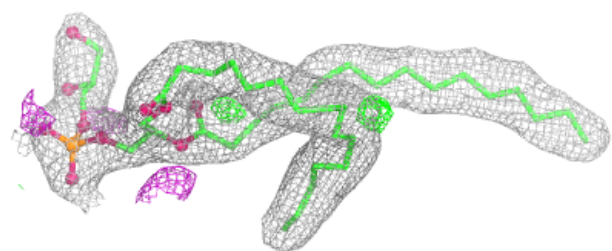
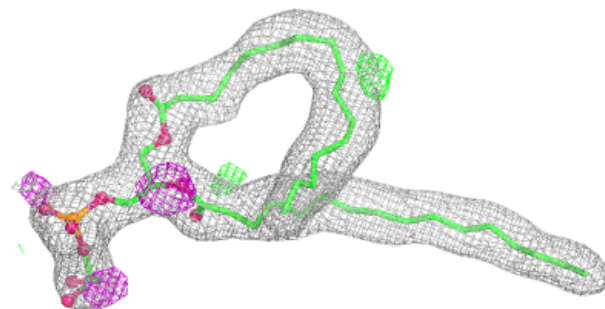


Electron density around DGD c 521:

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

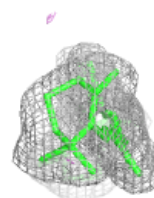
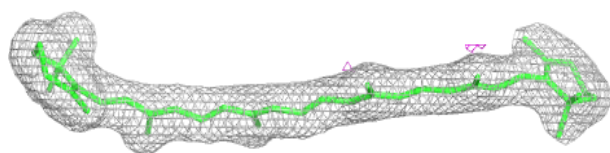
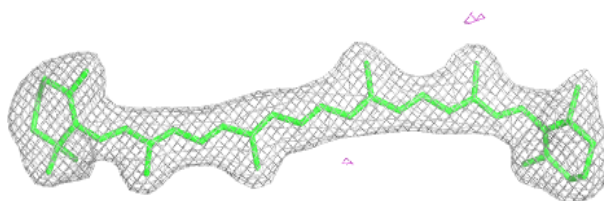
**Electron density around LHG D 407:**

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

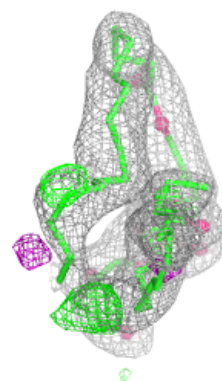
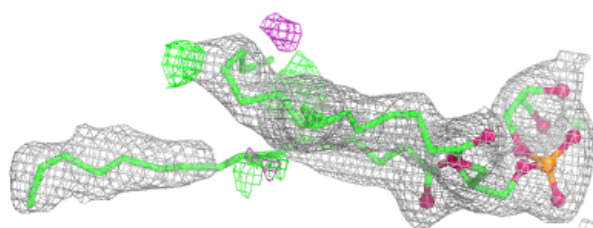
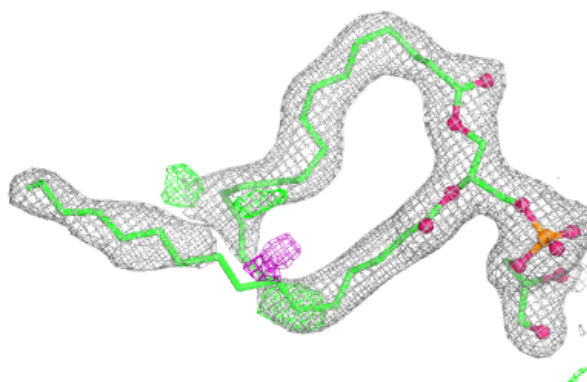


Electron density around BCR B 620:

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

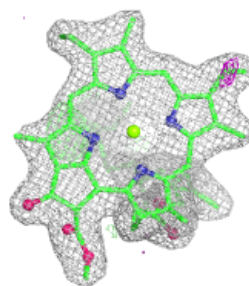
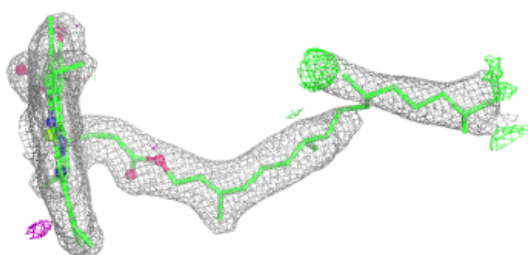
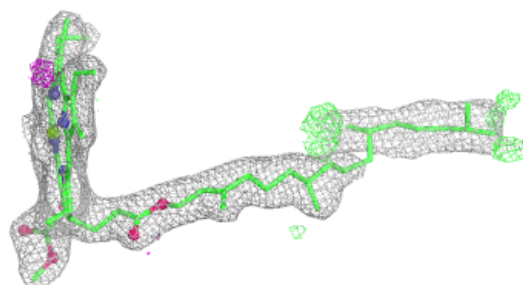
**Electron density around LHG d 409:**

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

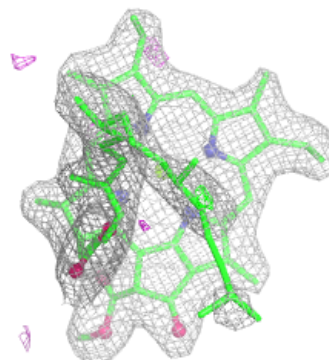
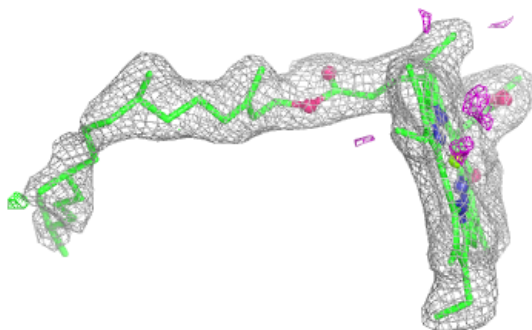
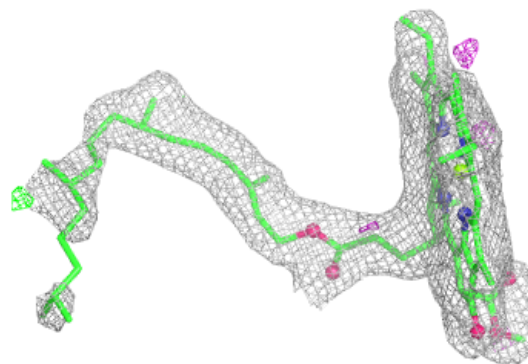


Electron density around CLA B 607:

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

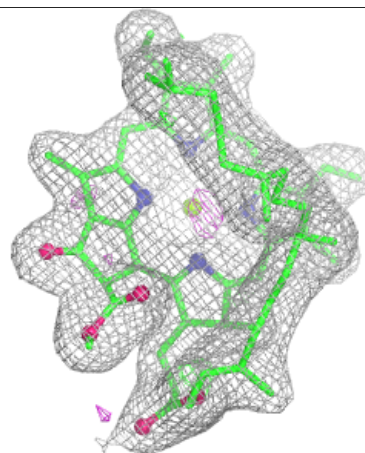
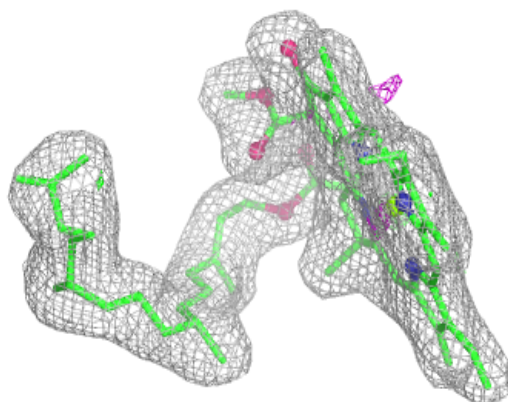
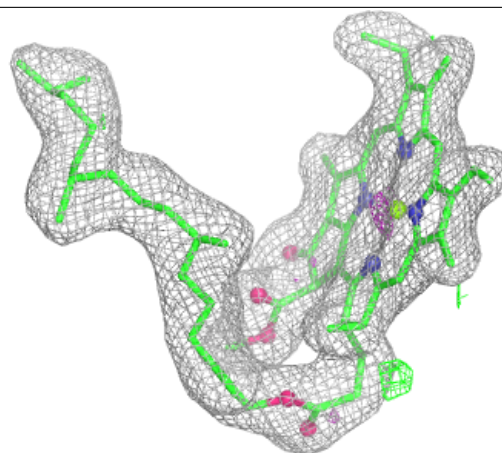
**Electron density around CLA D 403:**

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

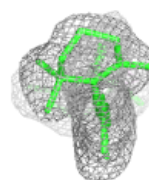
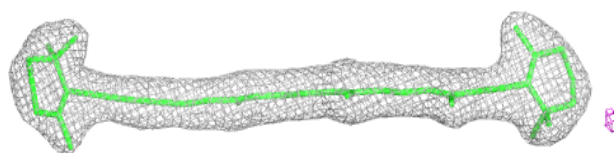
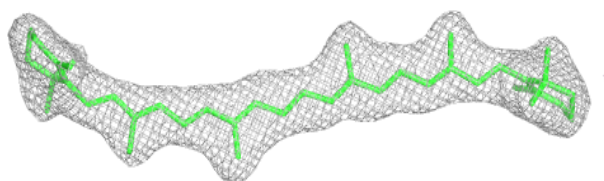


Electron density around CLA B 614:

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

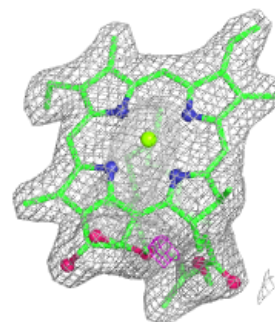
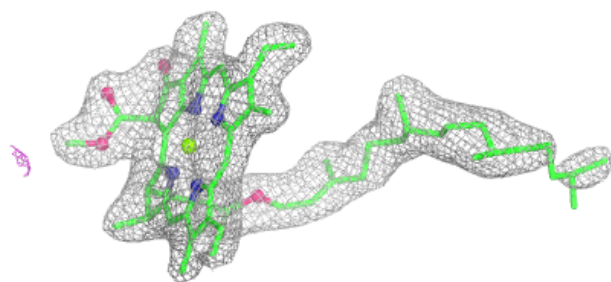
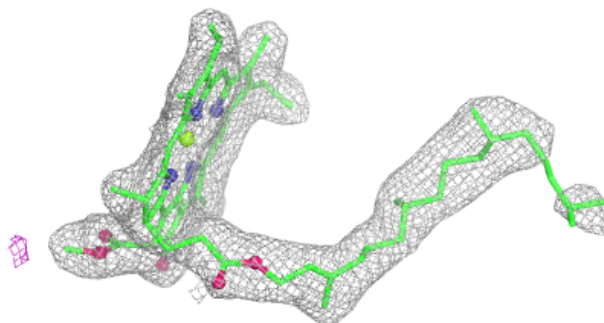
**Electron density around BCR c 518:**

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

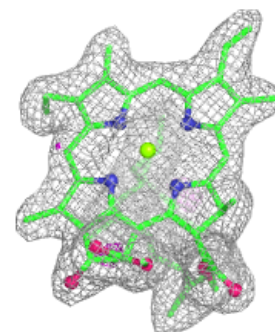
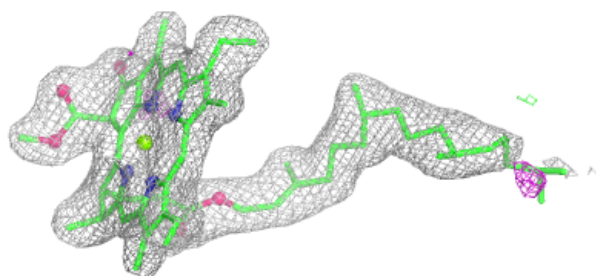
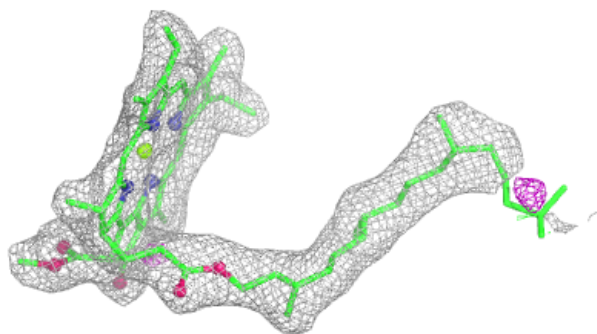


Electron density around CLA C 509:

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

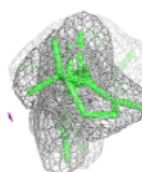
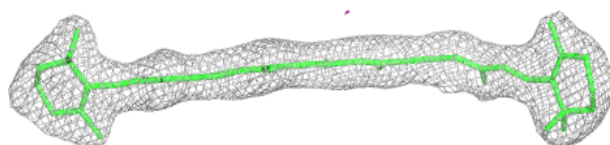
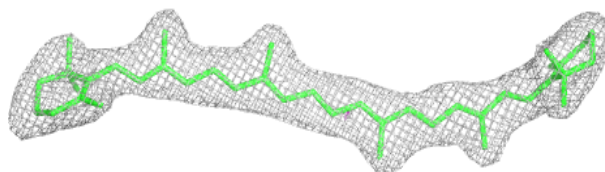
**Electron density around CLA c 512:**

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

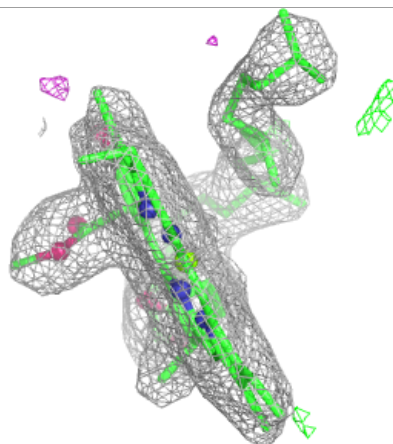
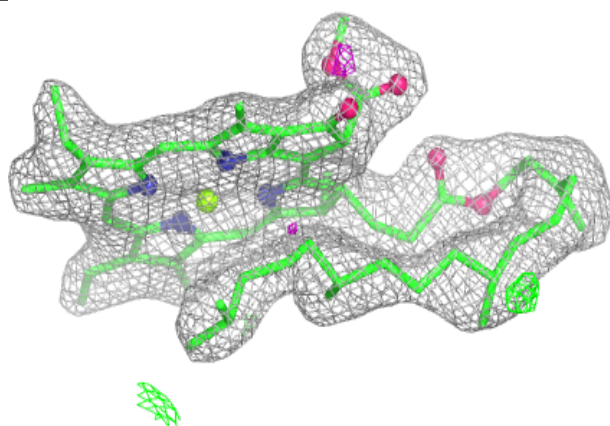
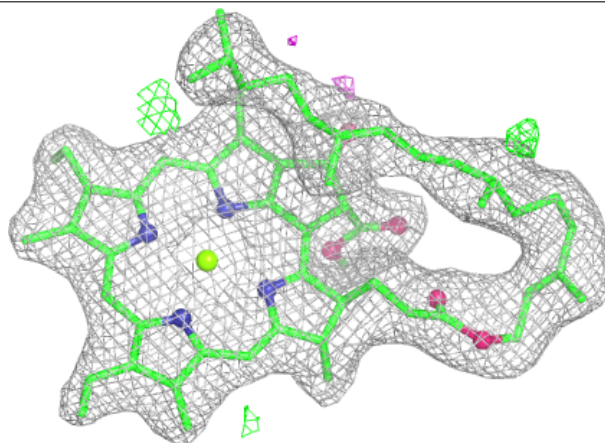


Electron density around BCR h 101:

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

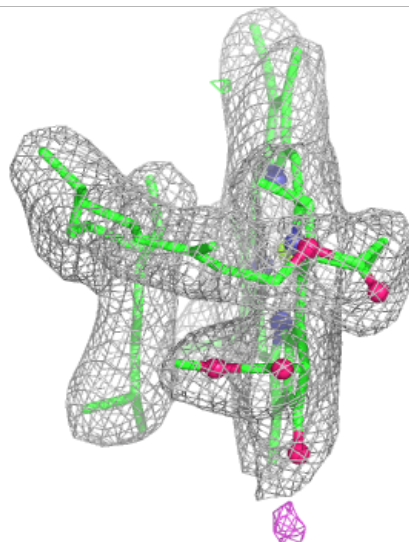
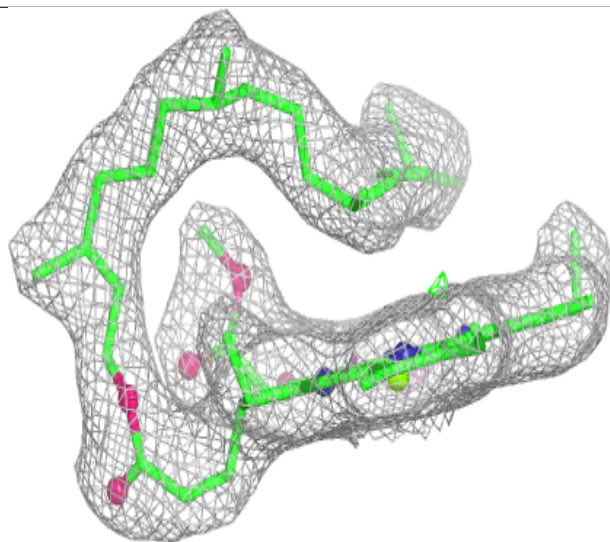
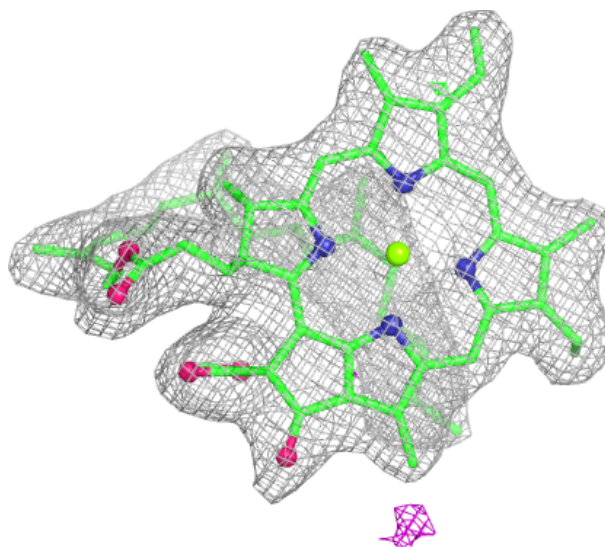
**Electron density around CLA c 513:**

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



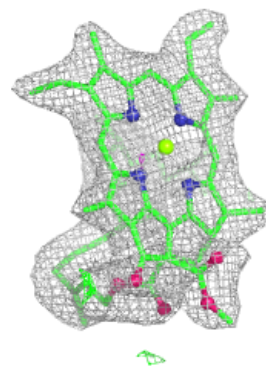
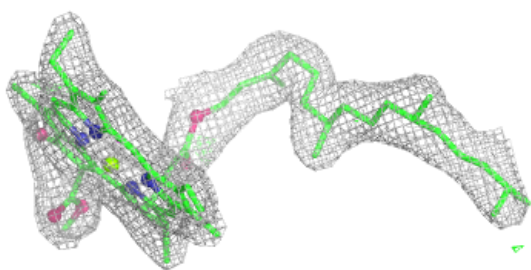
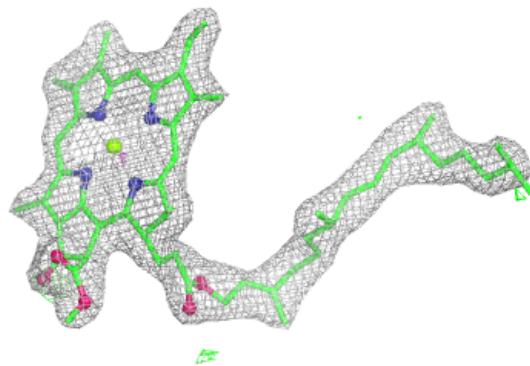
Electron density around CLA c 514:

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



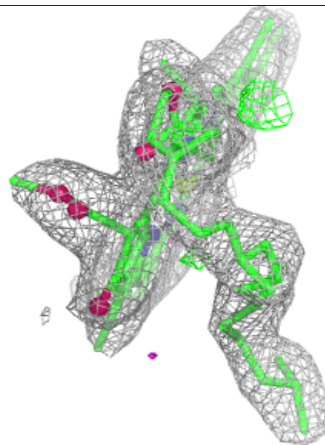
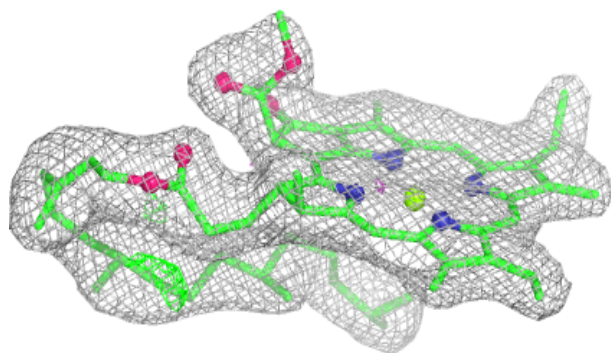
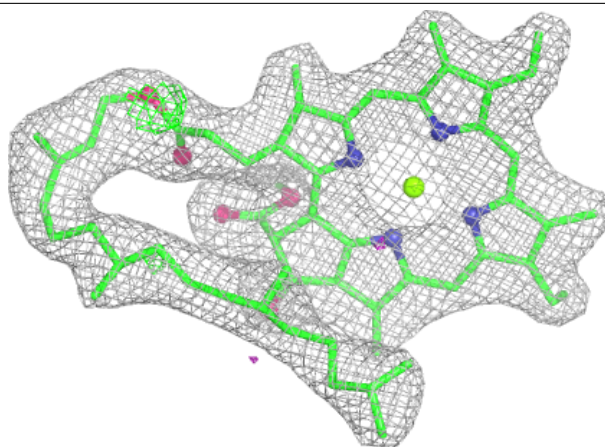
Electron density around CLA c 515:

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



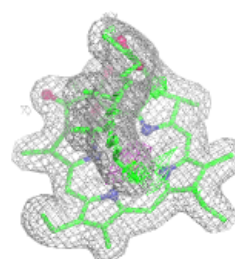
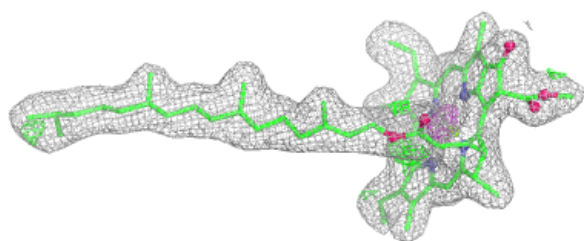
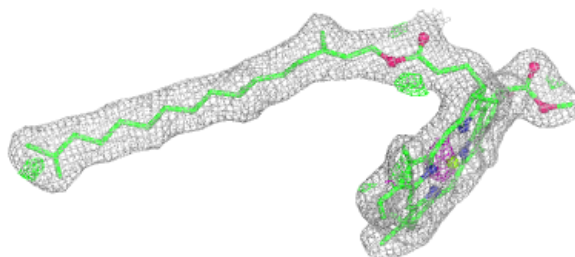
Electron density around CLA C 510:

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



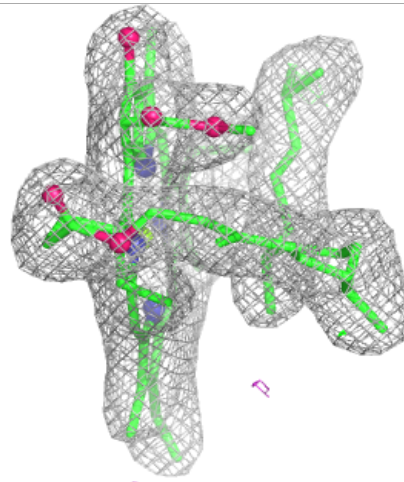
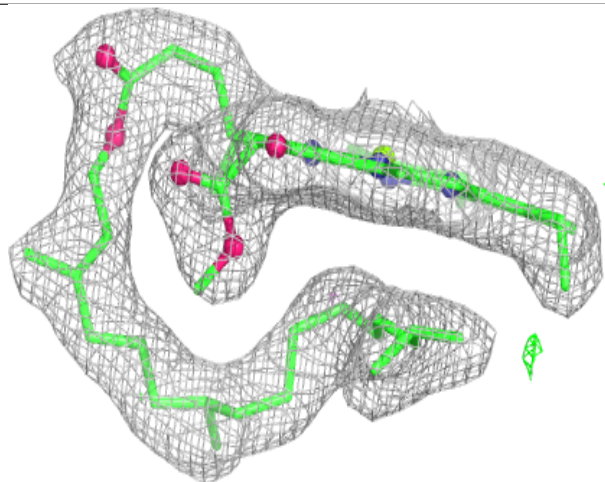
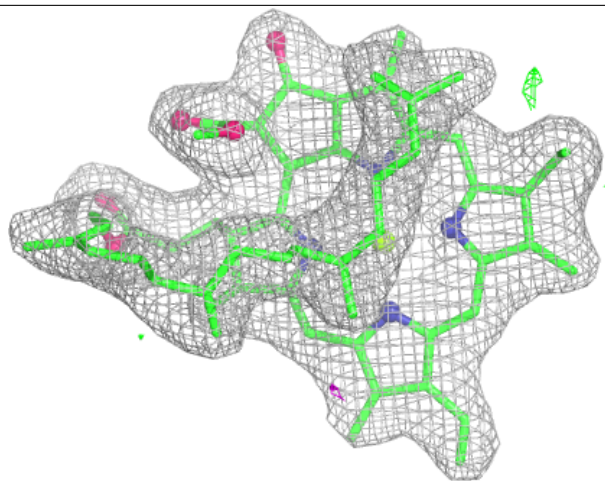
Electron density around CLA b 616:

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



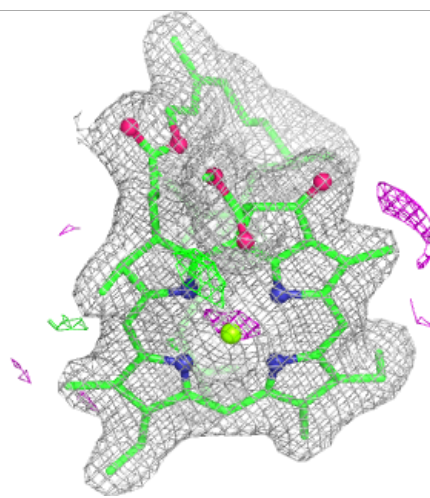
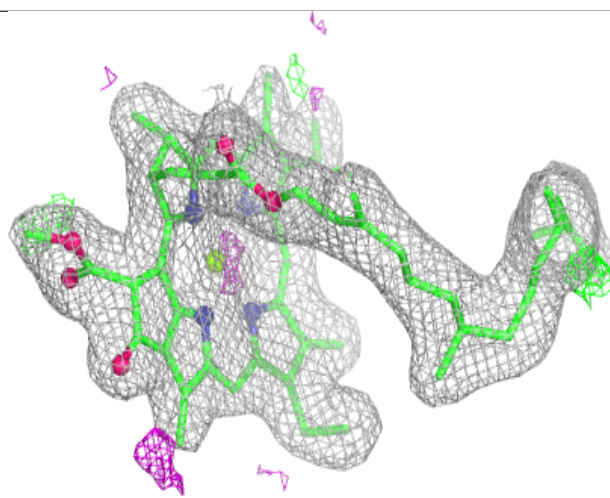
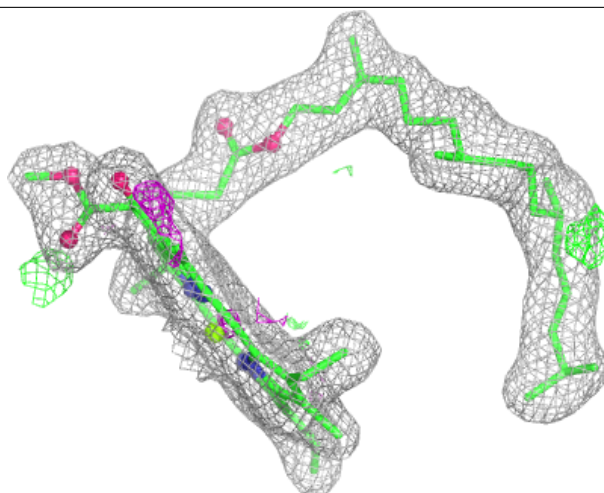
Electron density around CLA C 511:

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



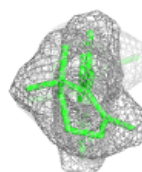
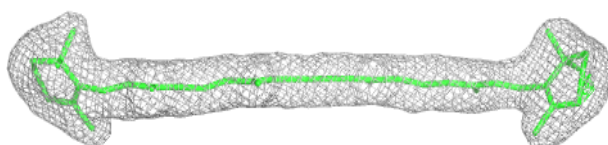
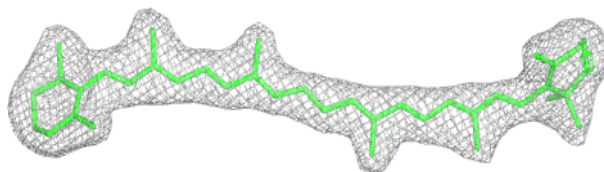
Electron density around CLA b 620:

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

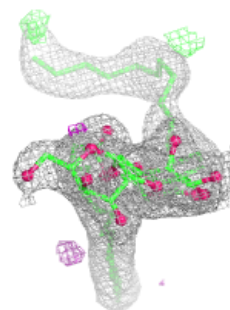
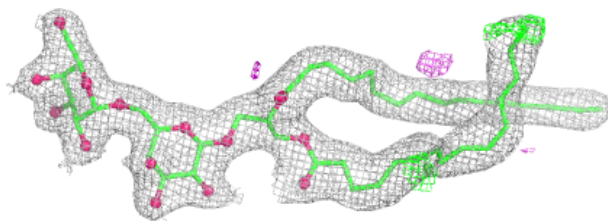
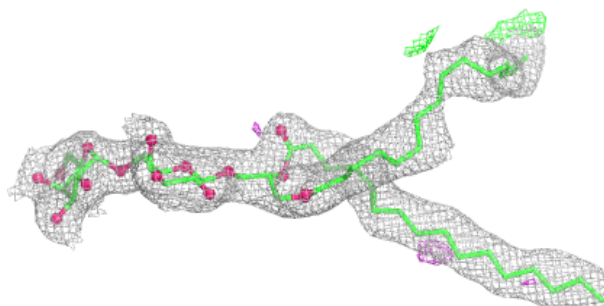


Electron density around BCR B 619:

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

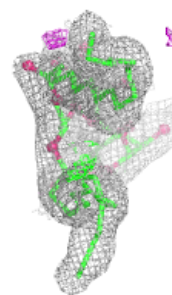
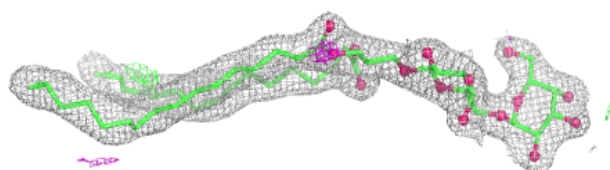
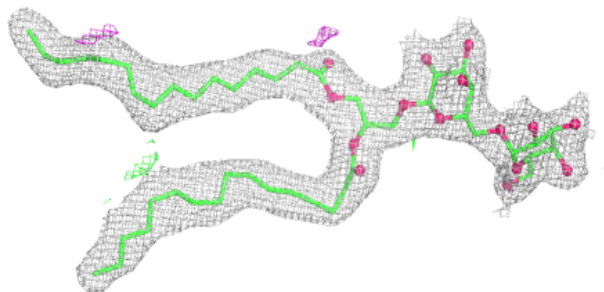
**Electron density around DGD C 517:**

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

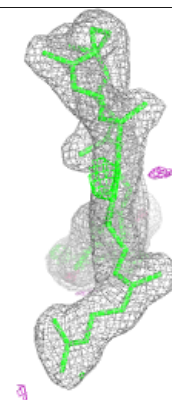
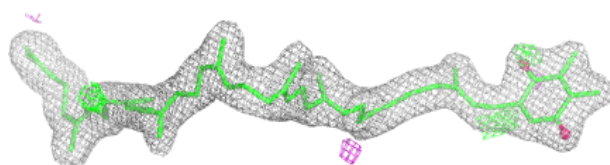
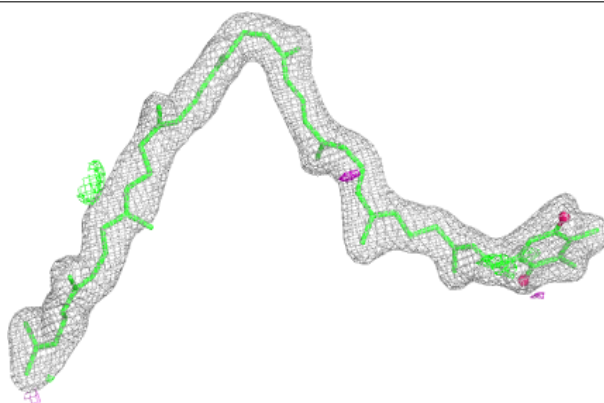


Electron density around DGD C 519:

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

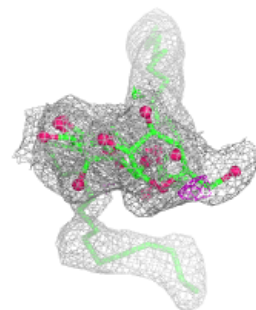
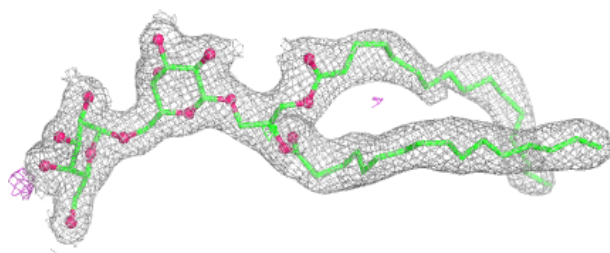
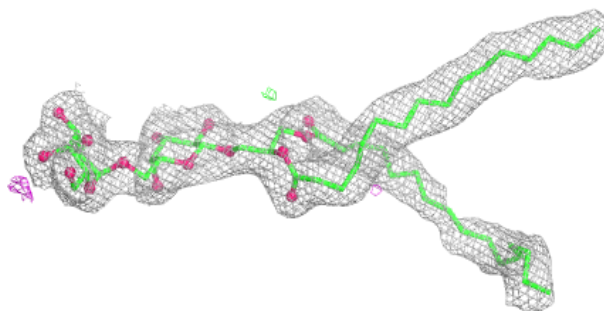
**Electron density around PL9 D 405:**

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



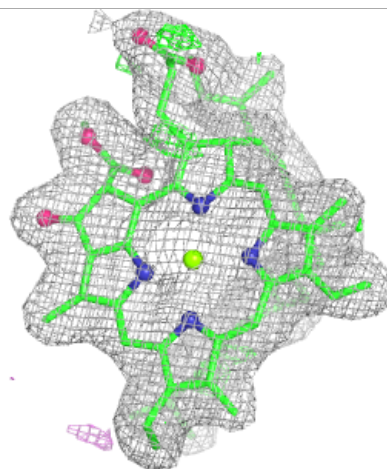
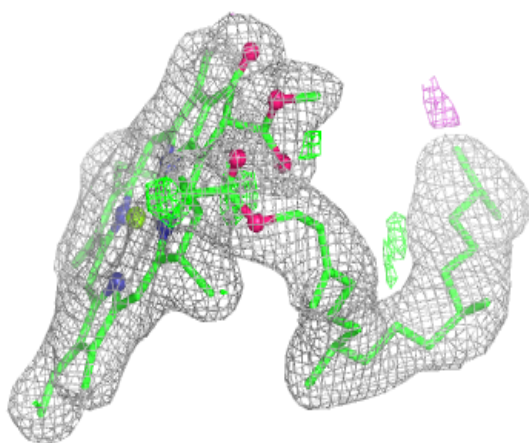
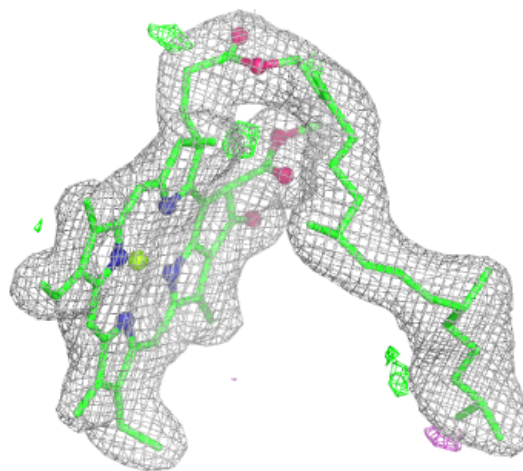
Electron density around DGD c 519:

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



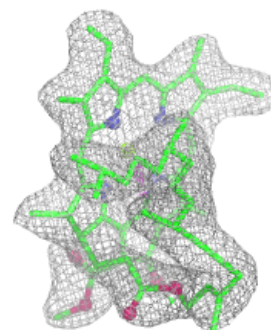
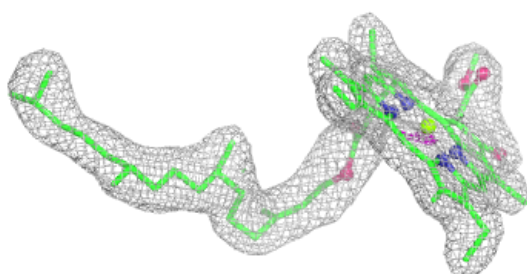
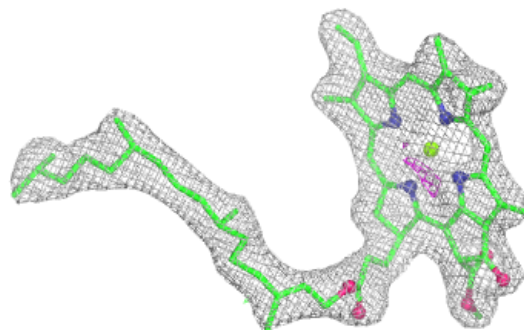
Electron density around CLA b 622:

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

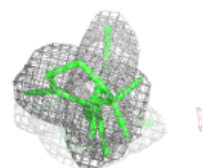
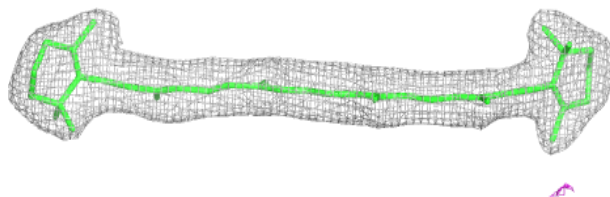
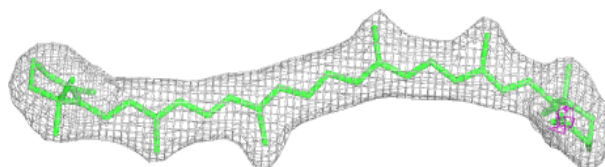


Electron density around CLA C 512:

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

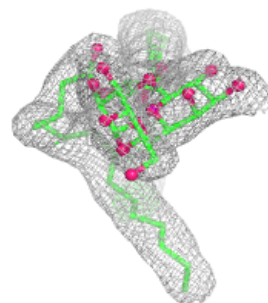
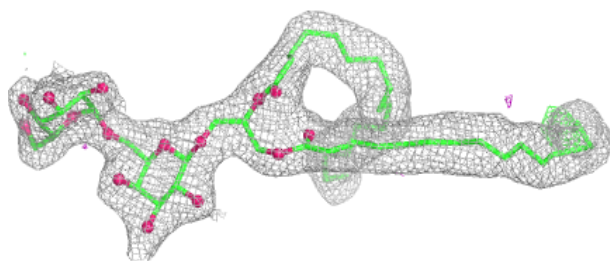
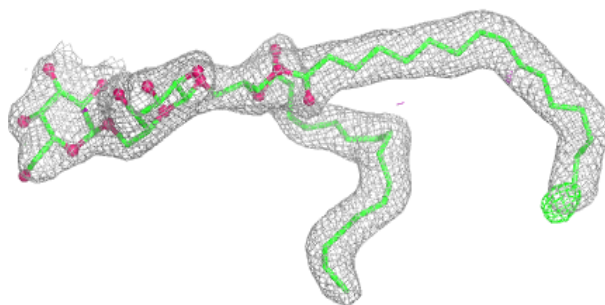
**Electron density around BCR C 516:**

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

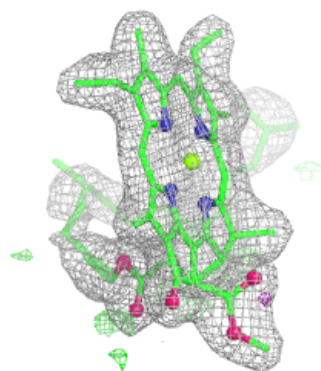
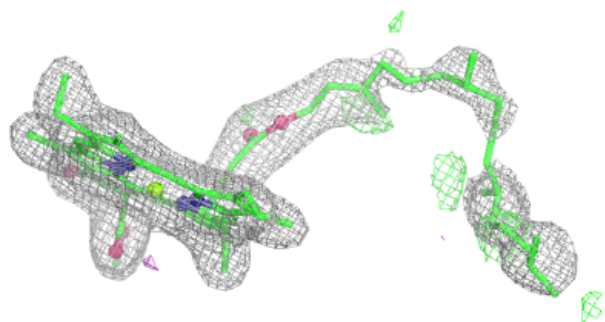
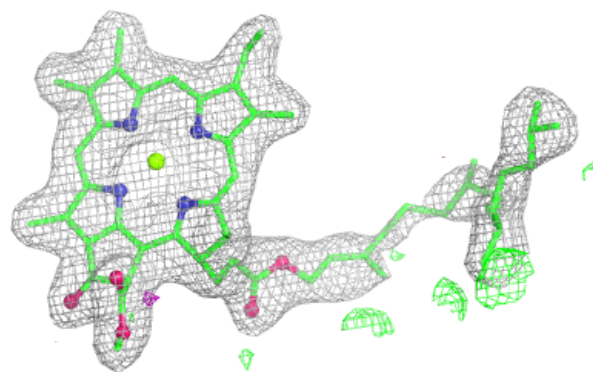


Electron density around DGD h 102:

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

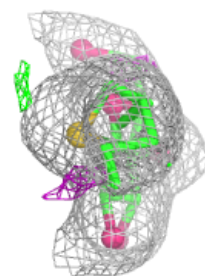
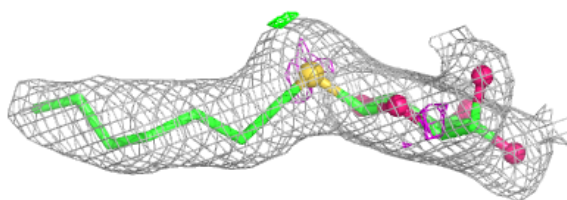
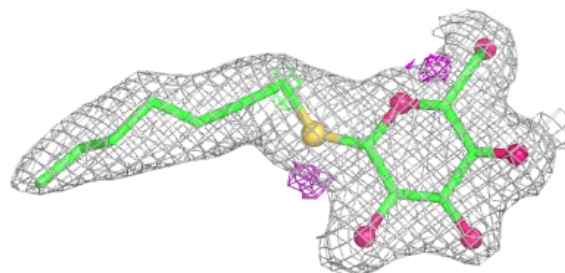
**Electron density around CLA A 409:**

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

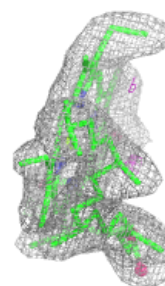
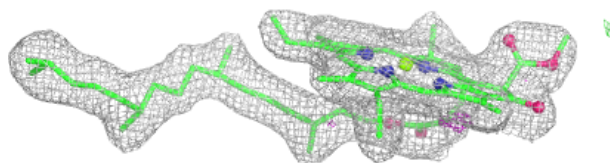
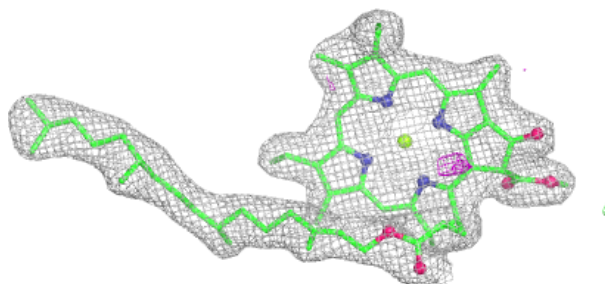


Electron density around HTG b 601:

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

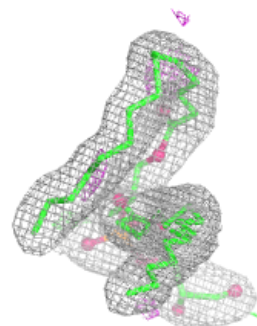
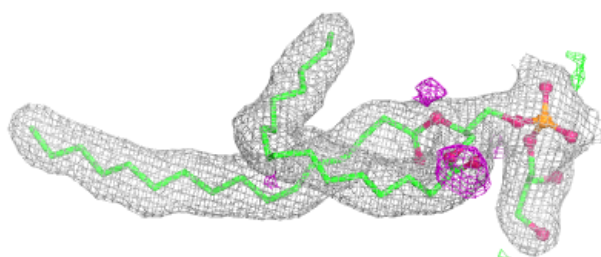
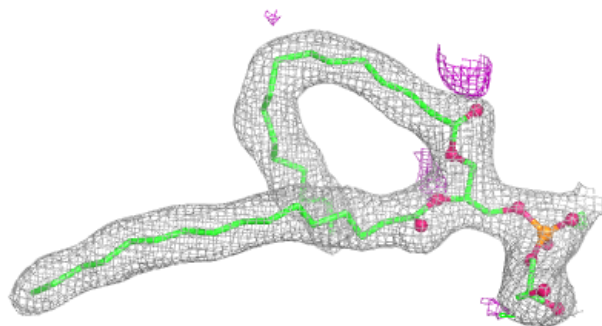
**Electron density around CLA c 505:**

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

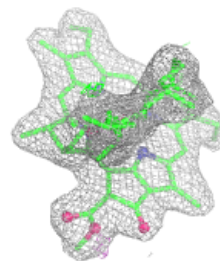
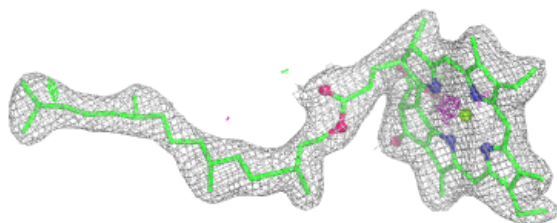
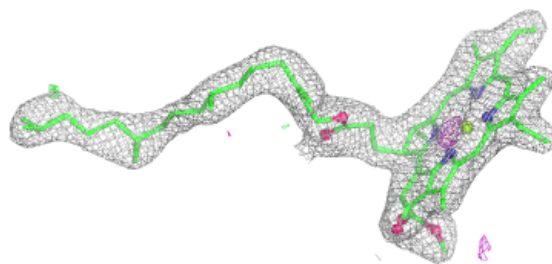


Electron density around LHG d 407:

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

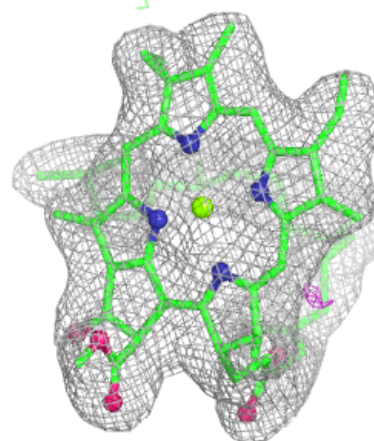
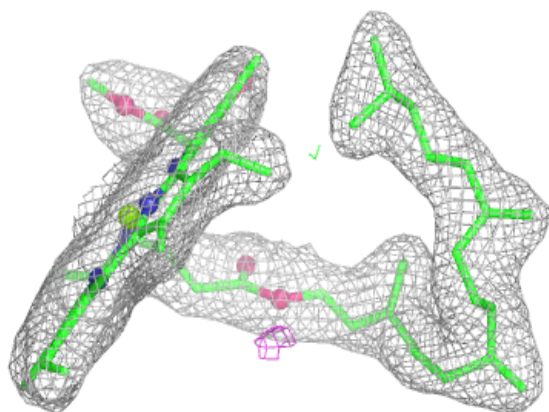
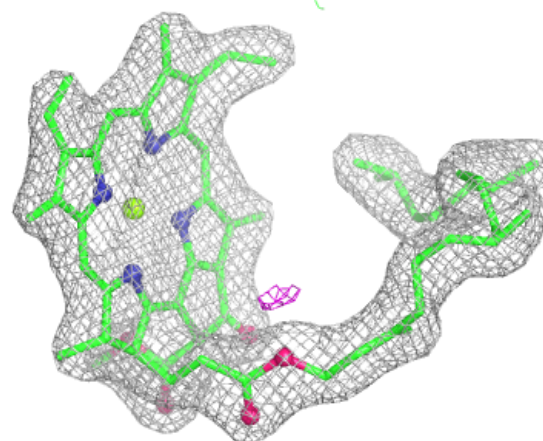
**Electron density around CLA c 506:**

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

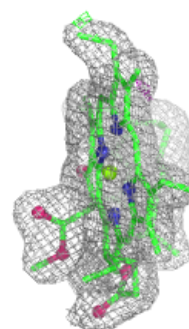
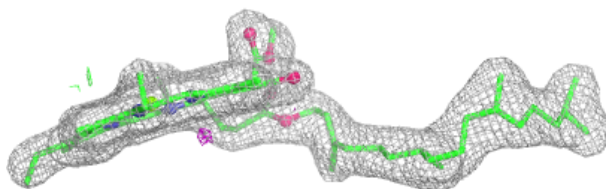
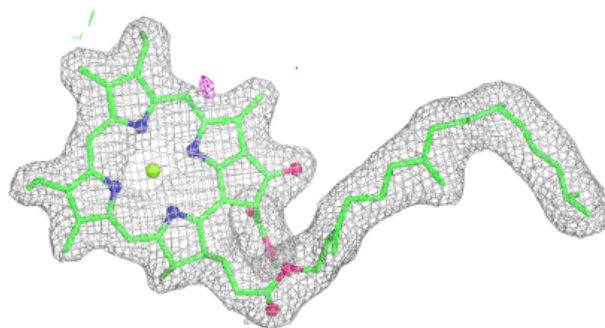


Electron density around CLA C 504:

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

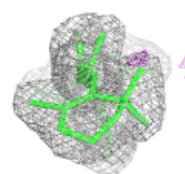
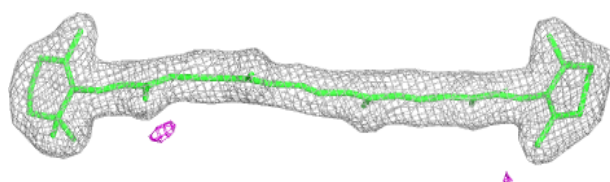
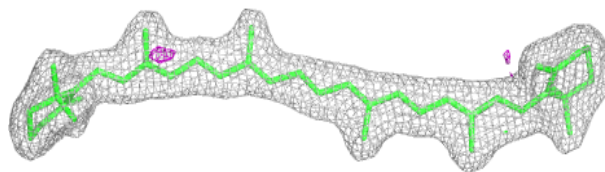
**Electron density around CLA B 603:**

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

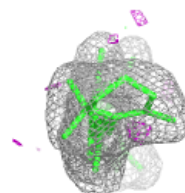
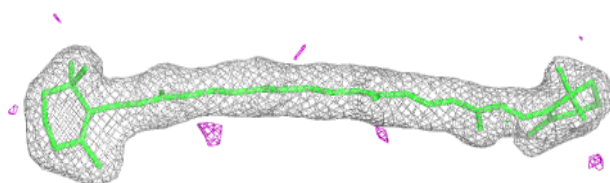
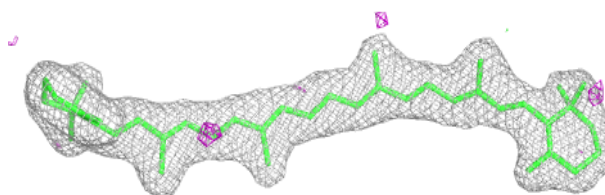


Electron density around BCR a 413:

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

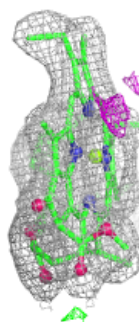
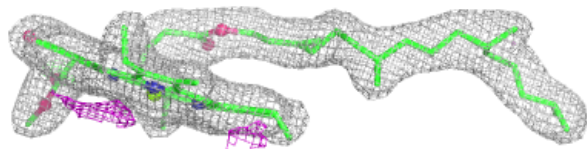
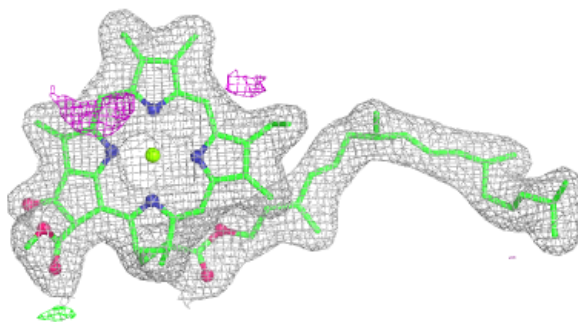
**Electron density around BCR b 626:**

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

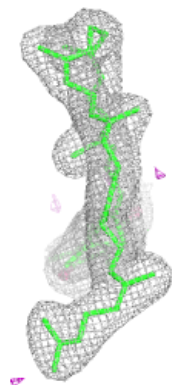
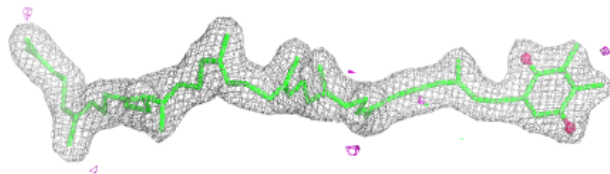
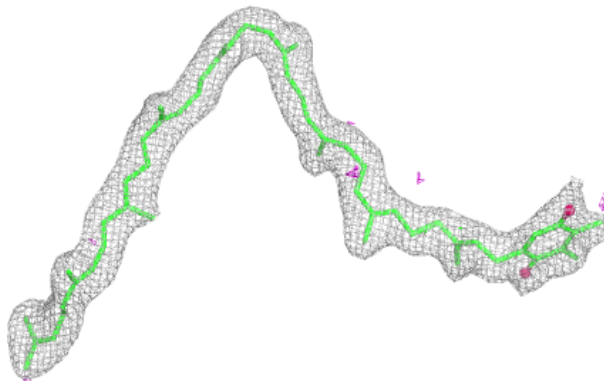


Electron density around CLA B 604:

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

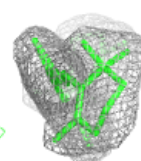
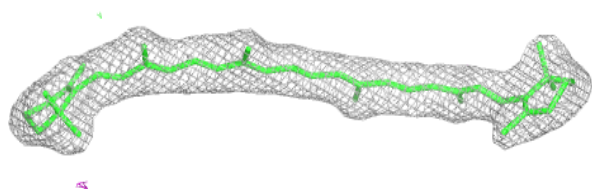
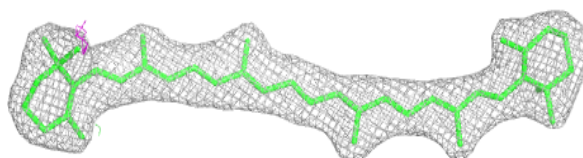
**Electron density around PL9 d 406:**

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

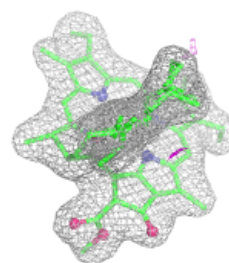
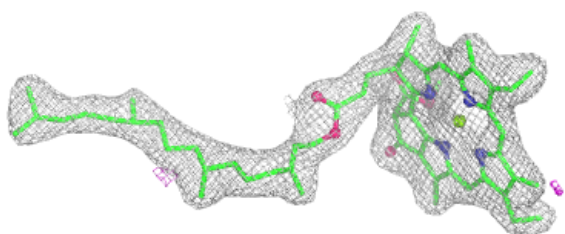
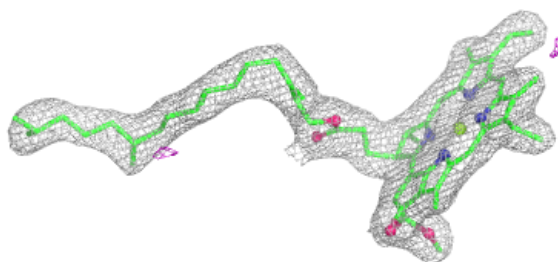


Electron density around BCR b 628:

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

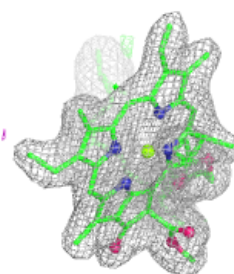
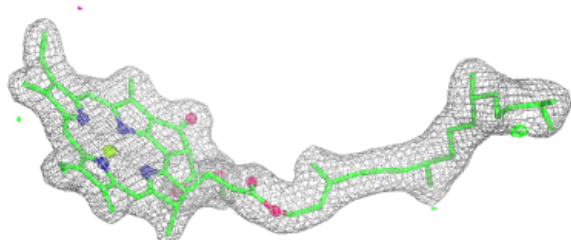
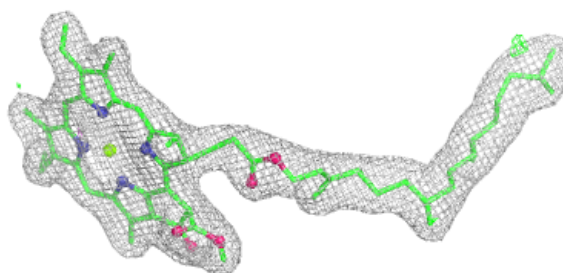
**Electron density around CLA C 503:**

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

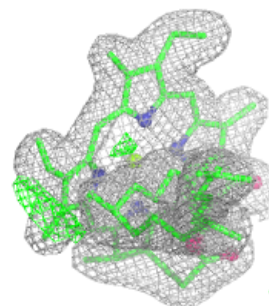
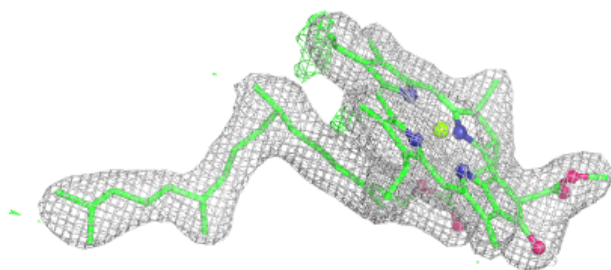
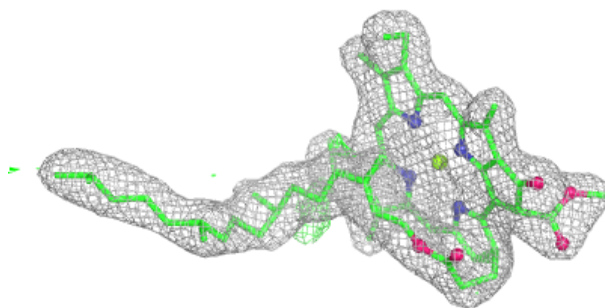


Electron density around CLA a 409:

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

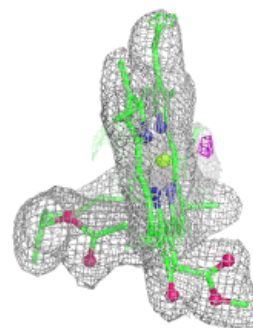
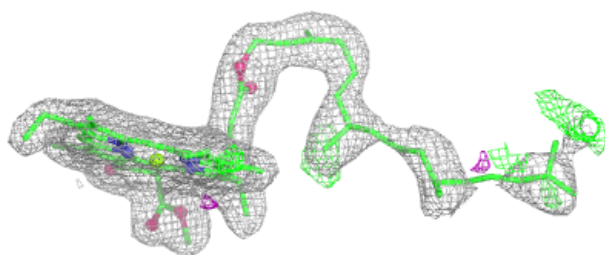
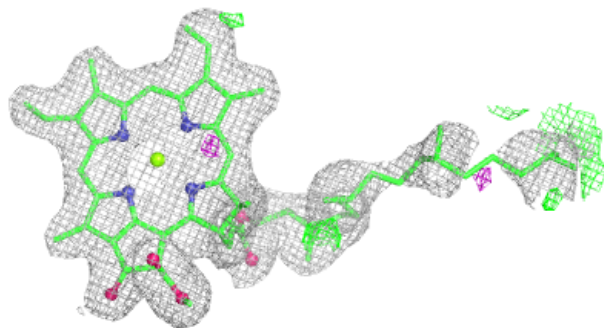
**Electron density around CLA c 509:**

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

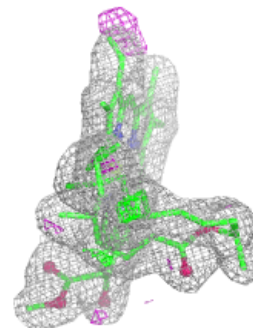
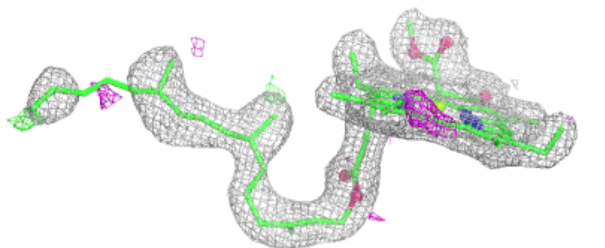
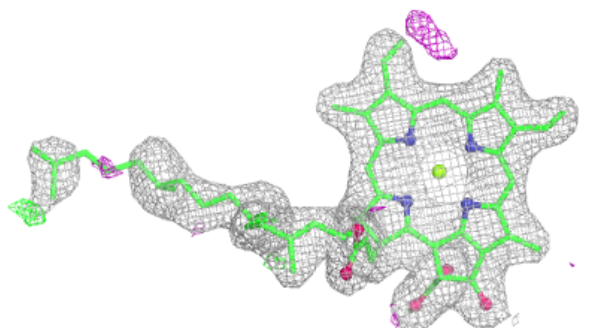


Electron density around CLA a 410:

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

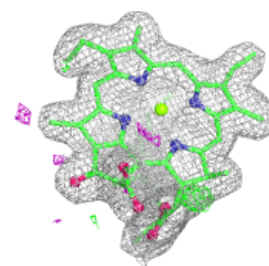
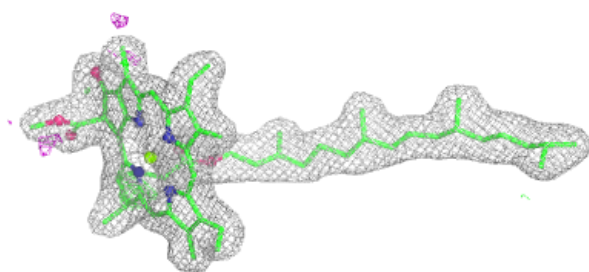
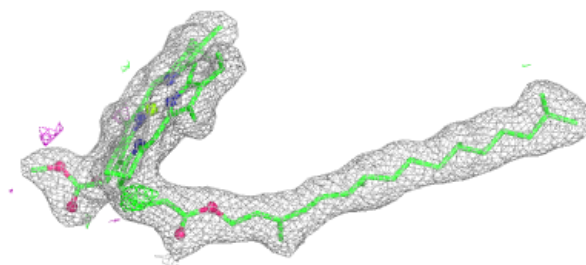
**Electron density around CLA A 407:**

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

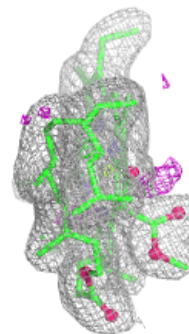
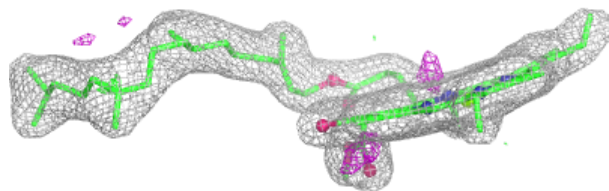
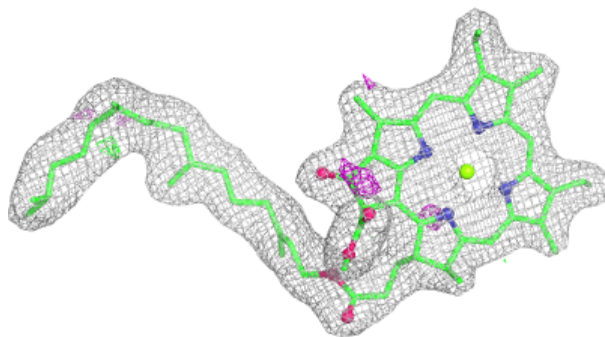


Electron density around CLA B 608:

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

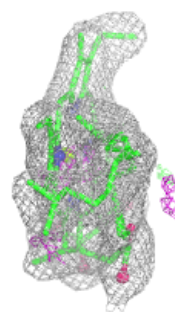
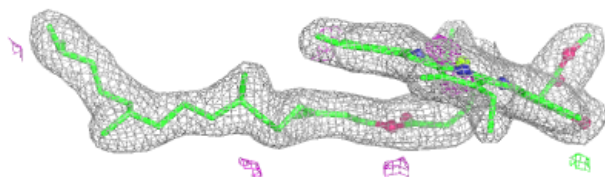
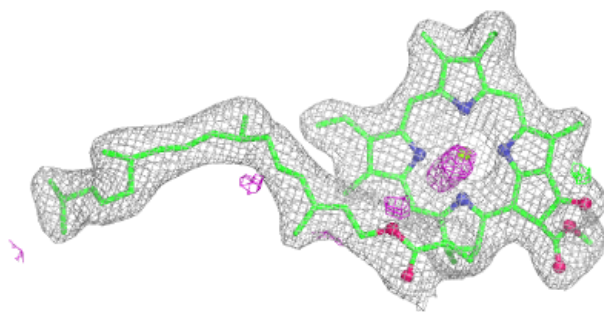
**Electron density around CLA b 611:**

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

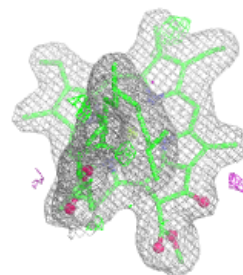
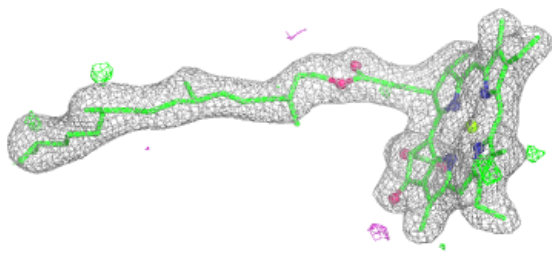
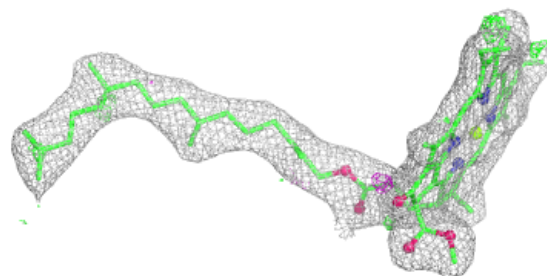


Electron density around CLA b 612:

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

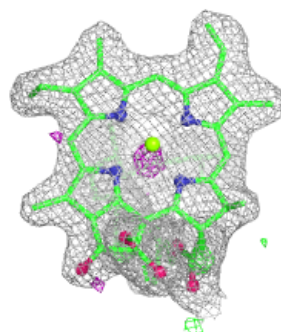
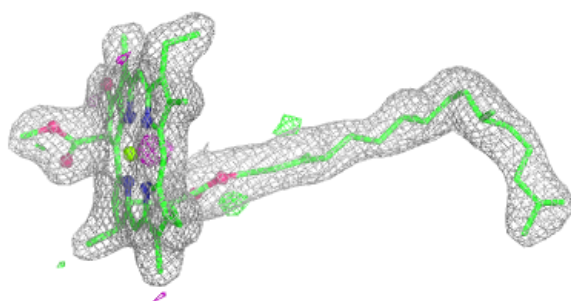
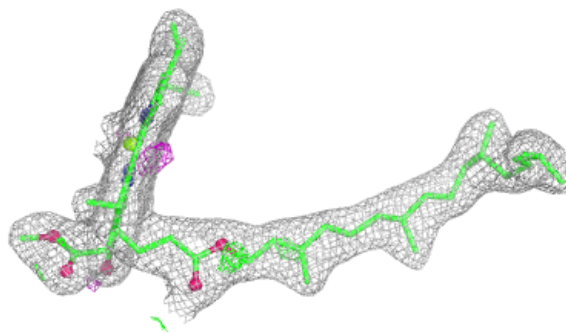
**Electron density around CLA b 613:**

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

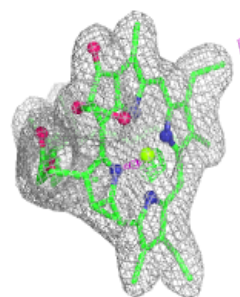
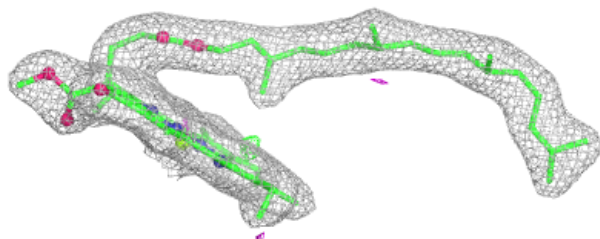
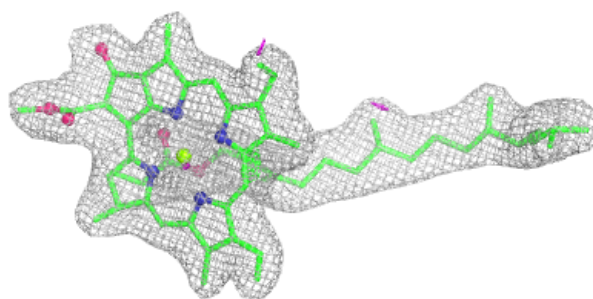


Electron density around CLA b 614:

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

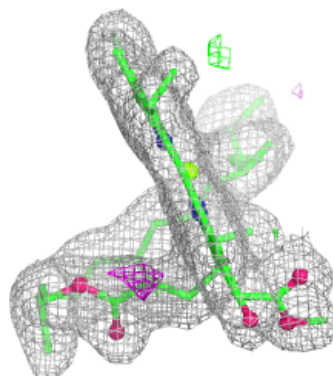
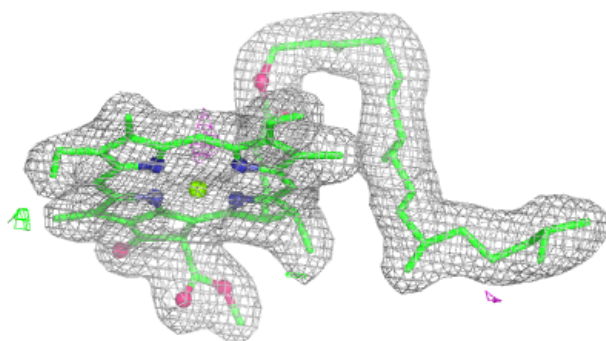
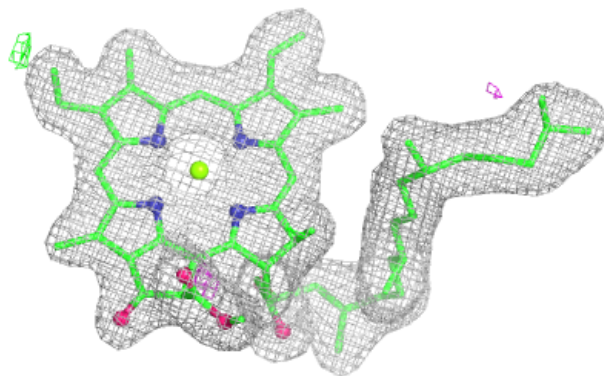
**Electron density around CLA B 609:**

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

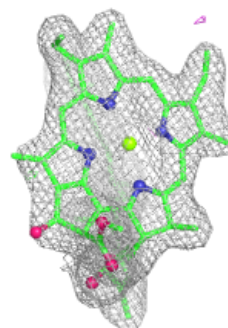
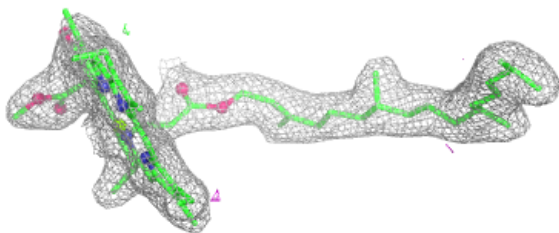
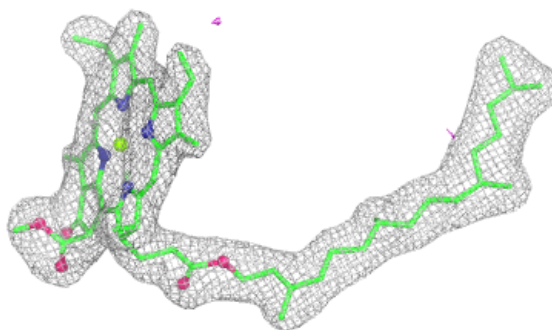


Electron density around CLA d 402:

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

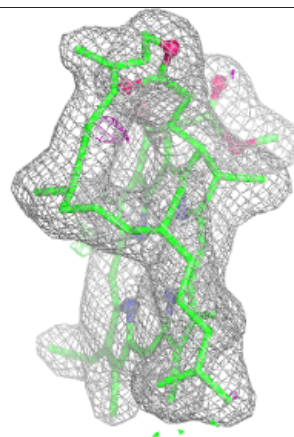
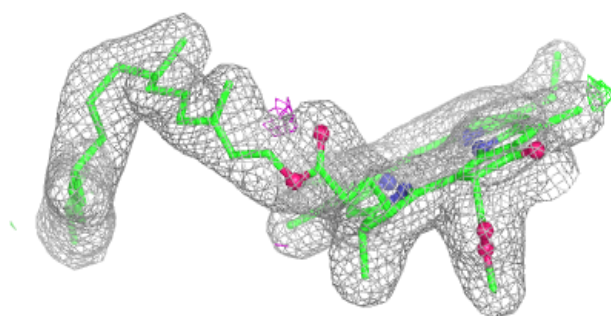
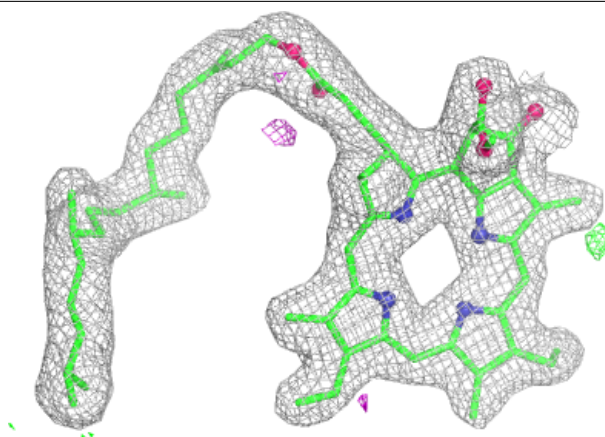
**Electron density around CLA B 610:**

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



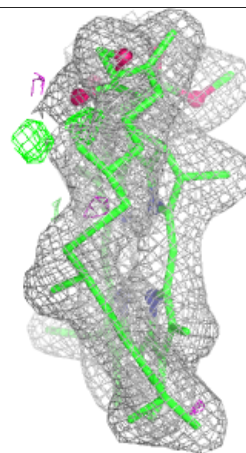
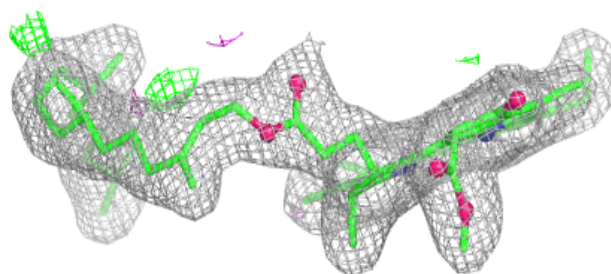
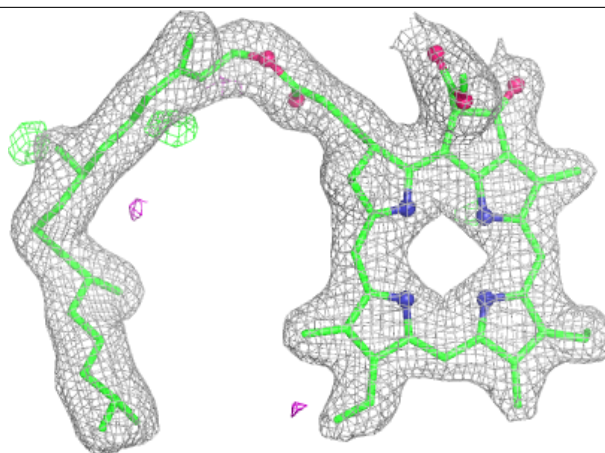
Electron density around PHO A 408:

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

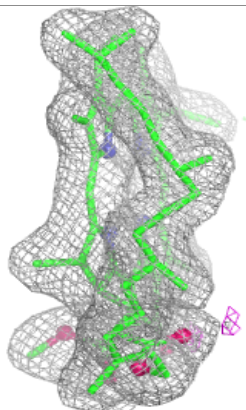
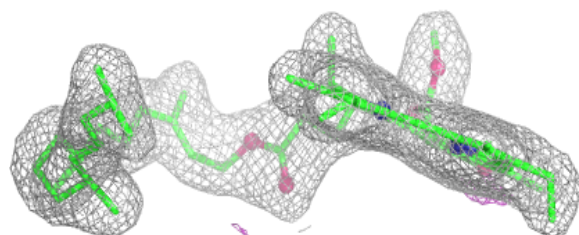
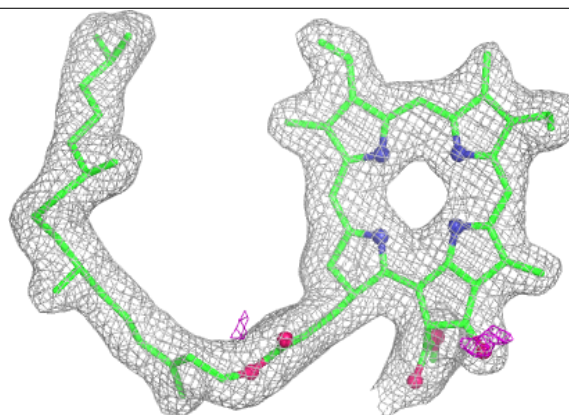


Electron density around PHO D 401:

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

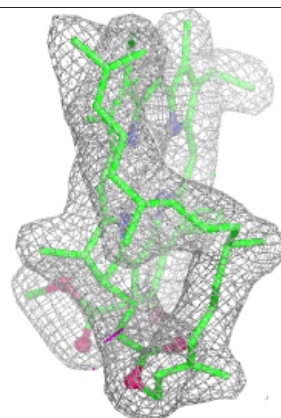
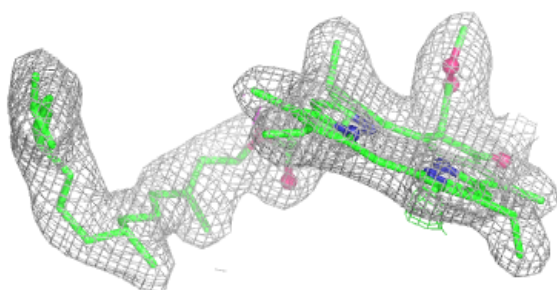
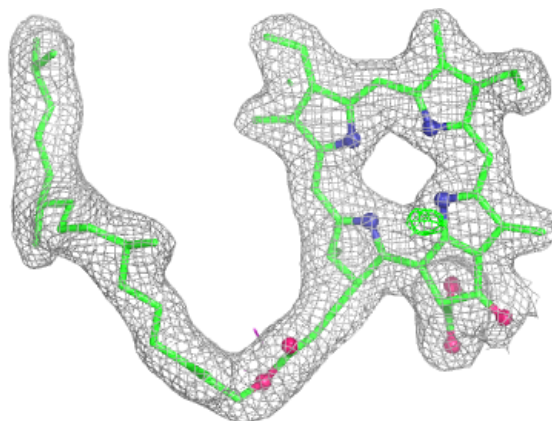
**Electron density around PHO a 411:**

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

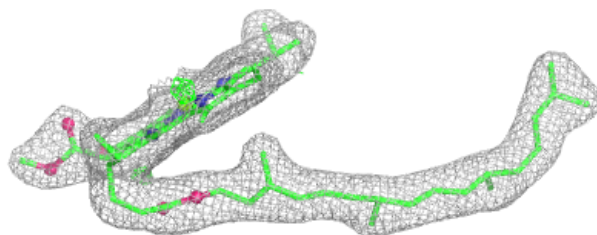
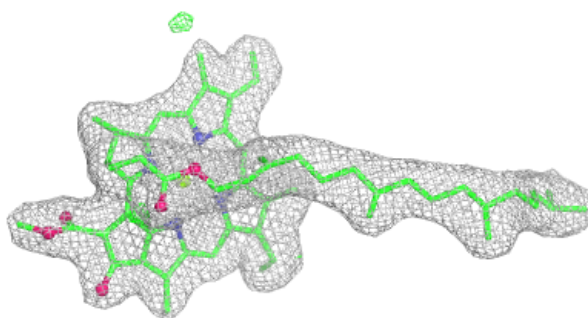


Electron density around PHO d 401:

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

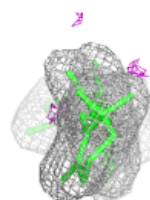
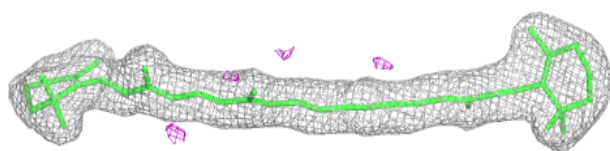
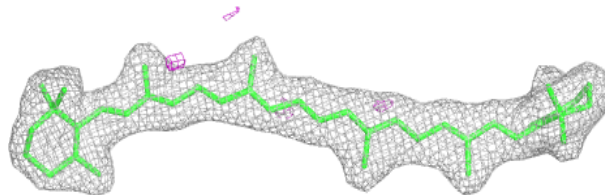
**Electron density around CLA b 617:**

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

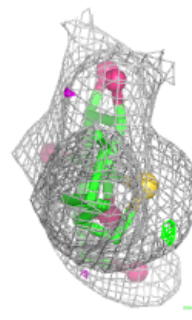
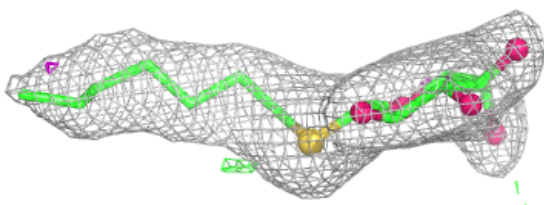
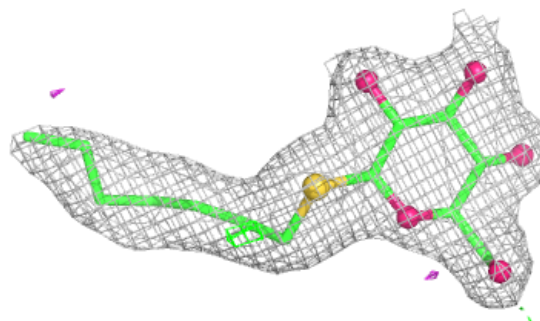


Electron density around BCR B 618:

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

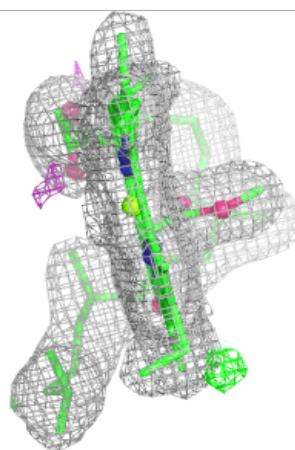
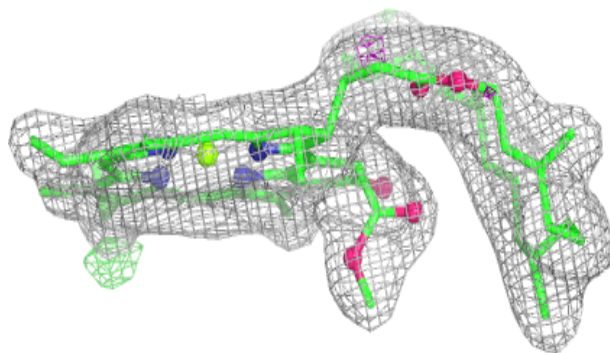
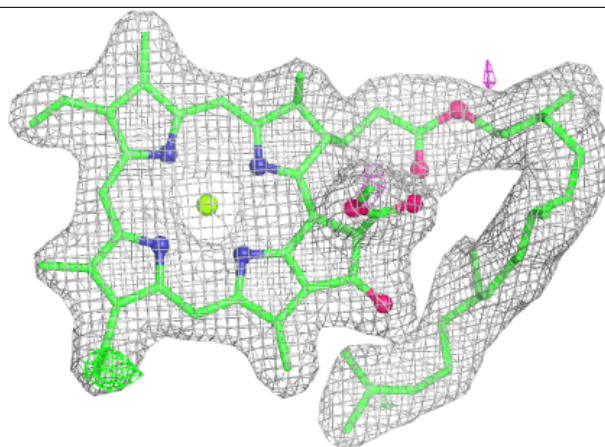
**Electron density around HTG B 623:**

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



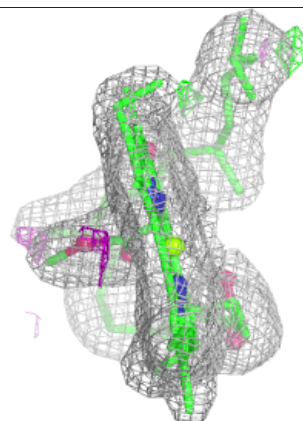
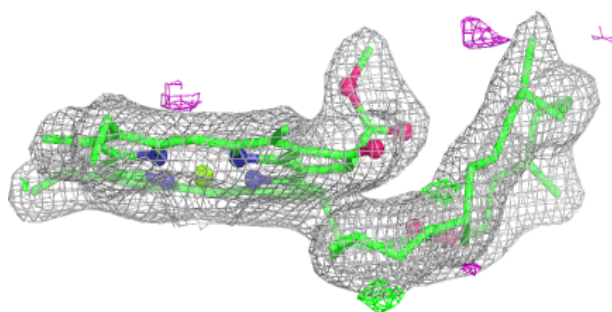
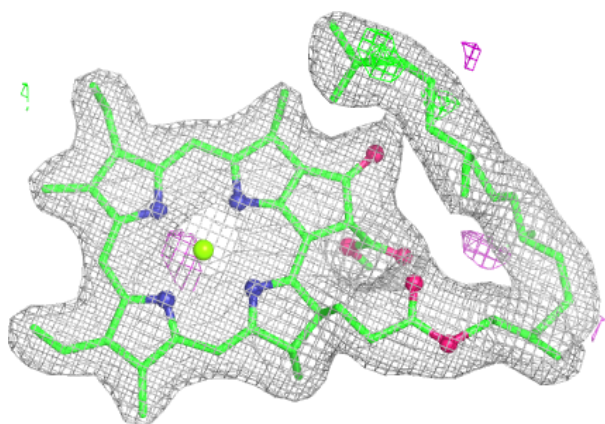
Electron density around CLA B 611:

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

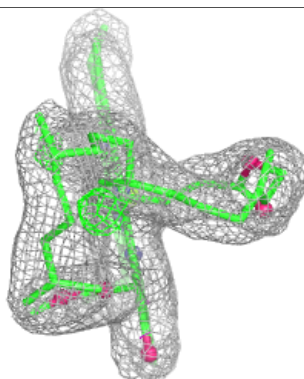
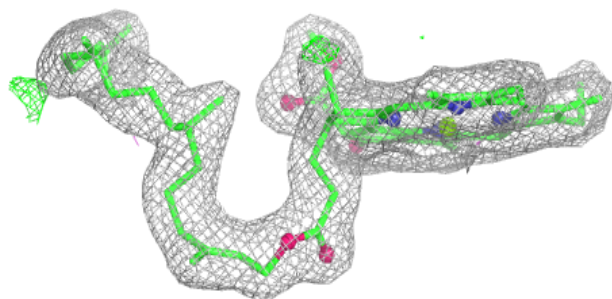
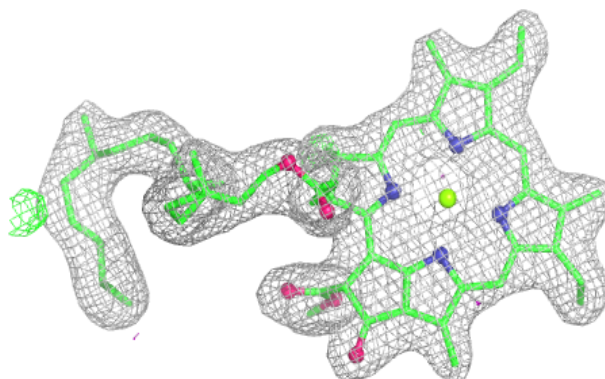


Electron density around CLA b 619:

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

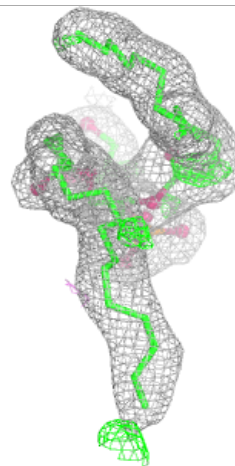
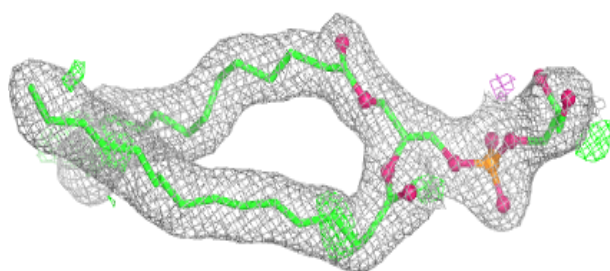
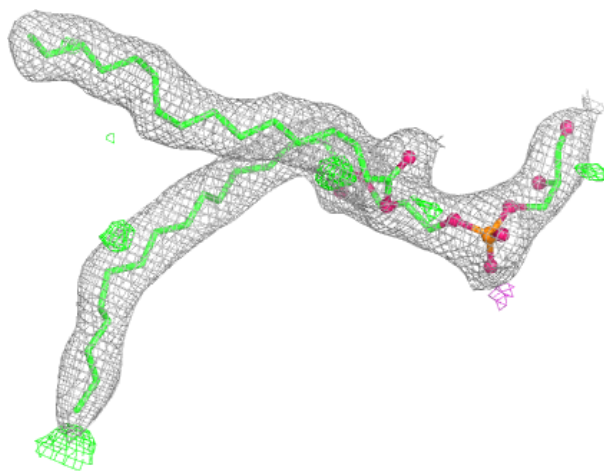
**Electron density around CLA B 613:**

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



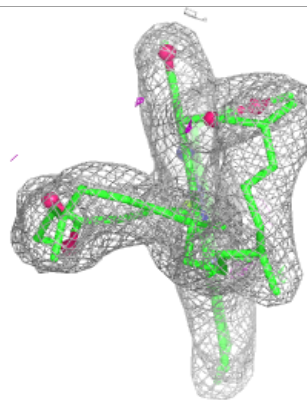
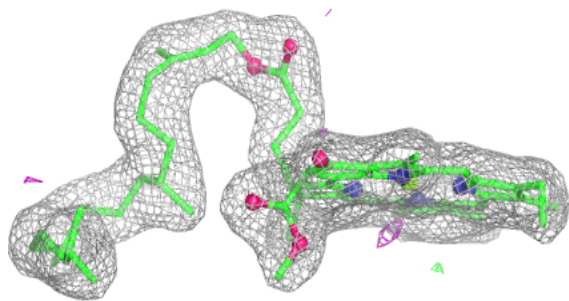
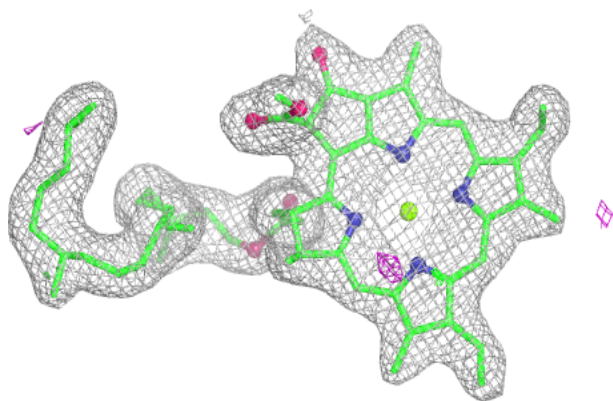
Electron density around LHG D 408:

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



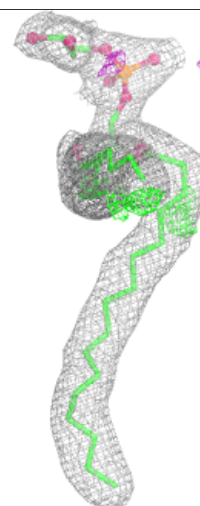
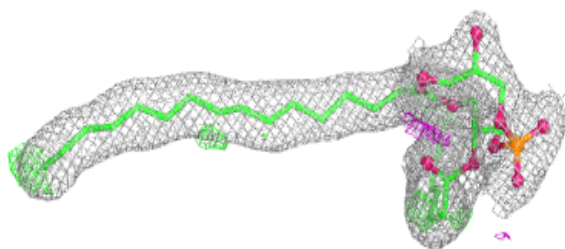
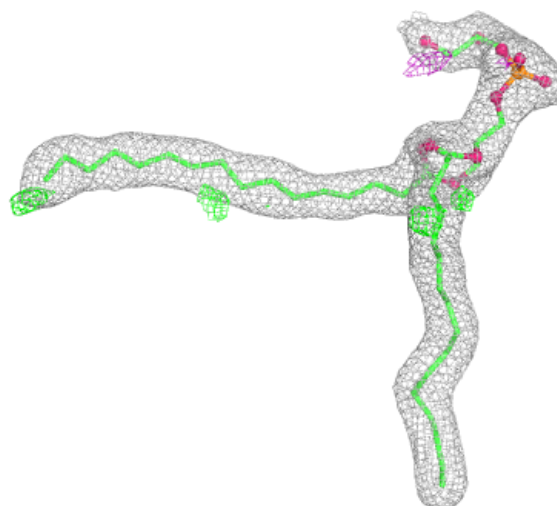
Electron density around CLA b 621:

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



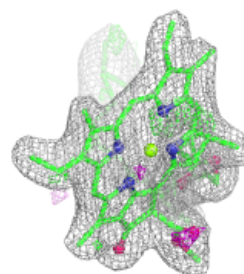
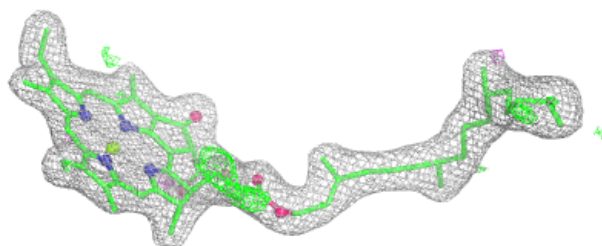
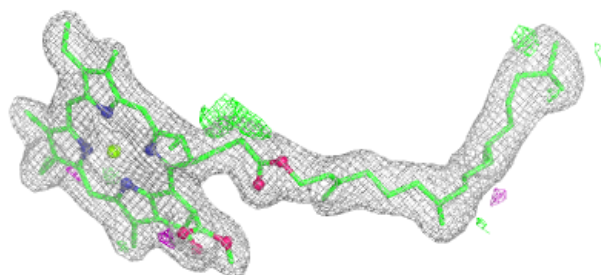
Electron density around LHG L 101:

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



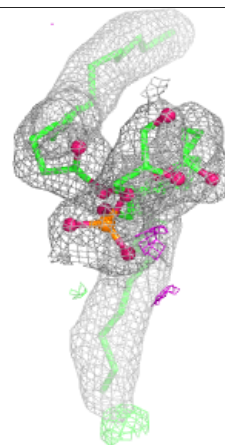
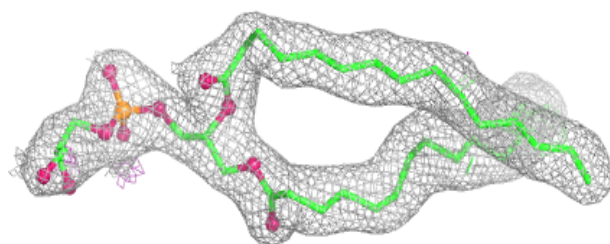
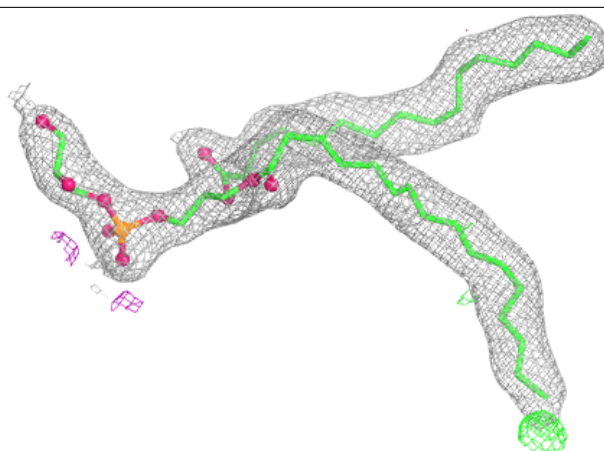
Electron density around CLA A 405:

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



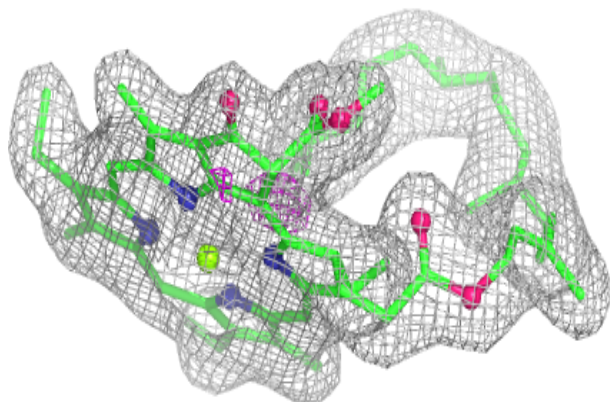
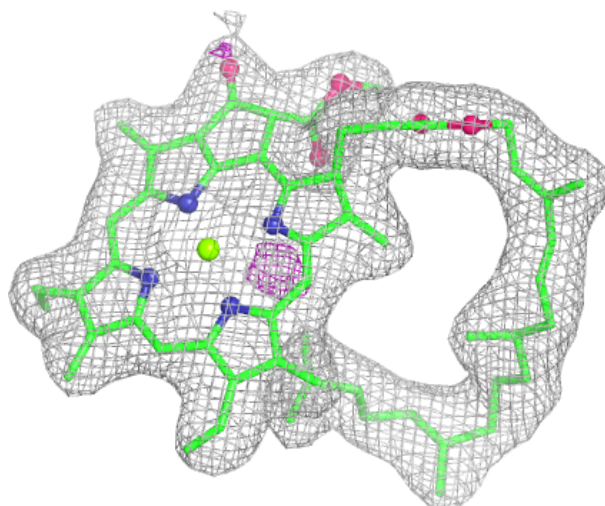
Electron density around LHG d 408:

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



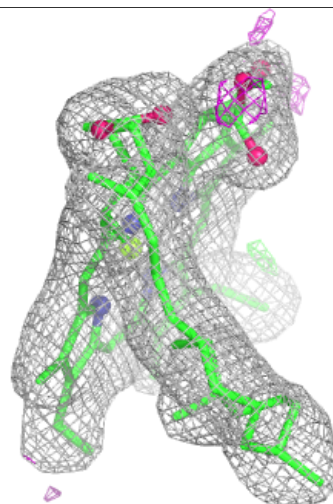
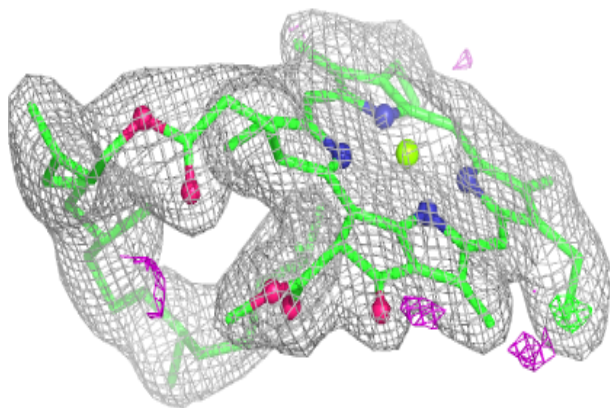
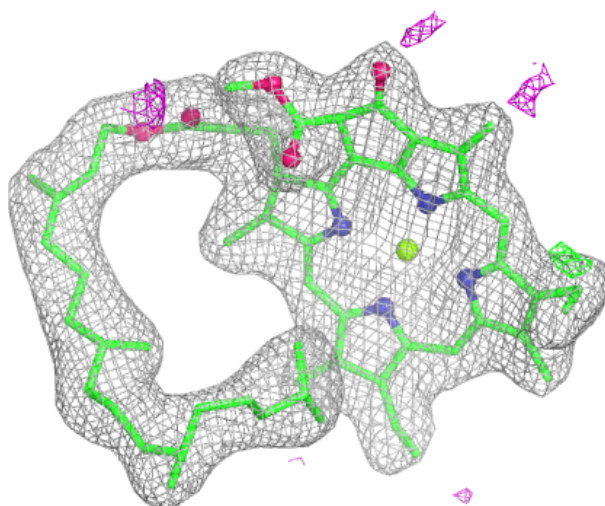
Electron density around CLA b 624:

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



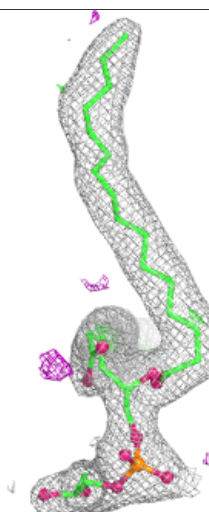
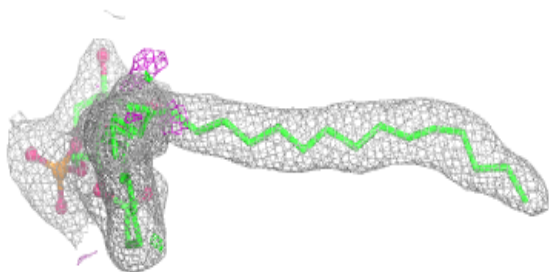
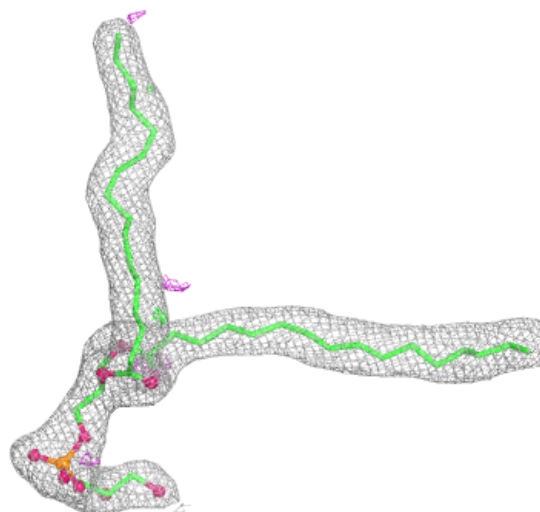
Electron density around CLA B 616:

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



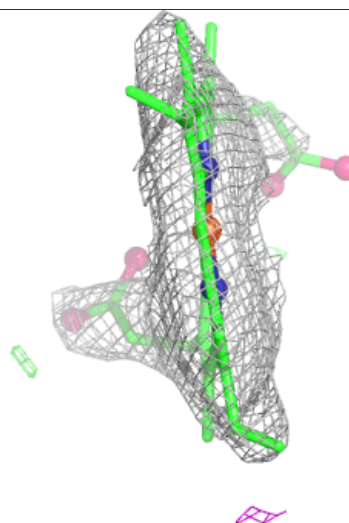
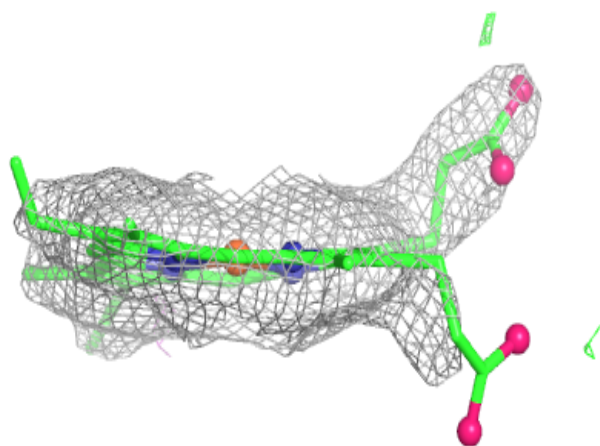
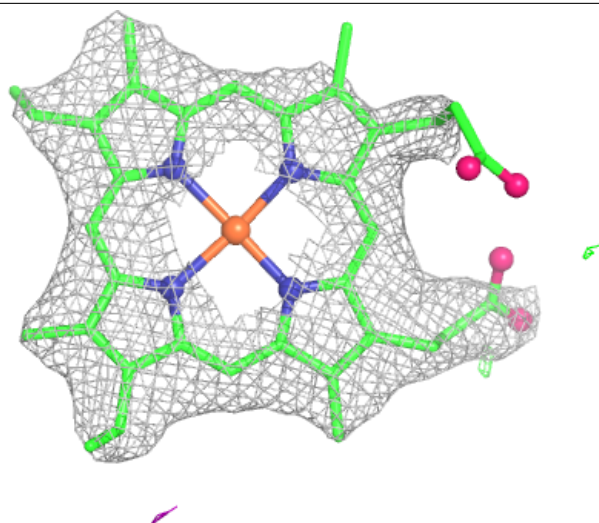
Electron density around LHG 1 101:

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



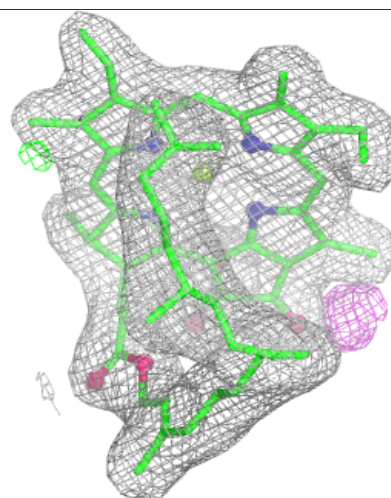
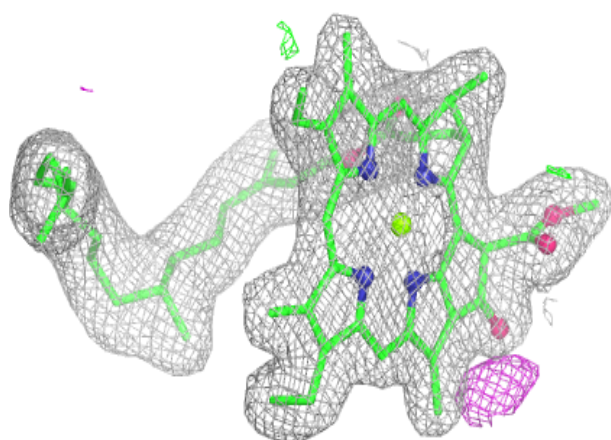
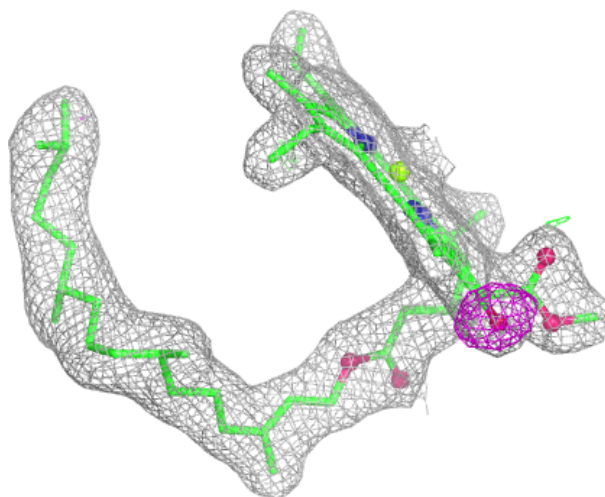
Electron density around HEM e 103:

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



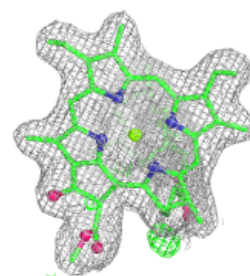
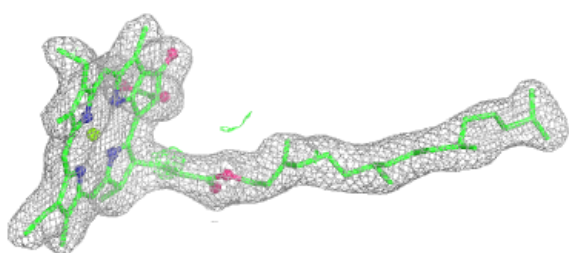
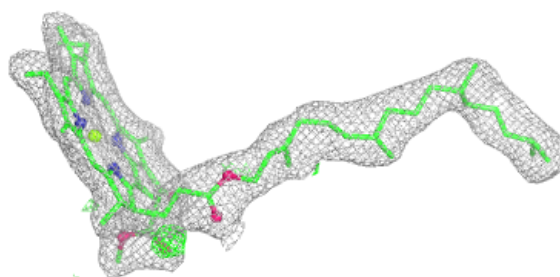
Electron density around CLA B 612:

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

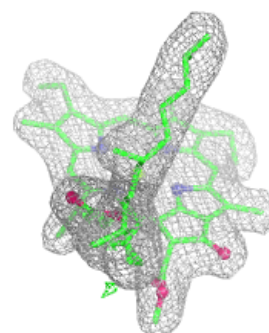
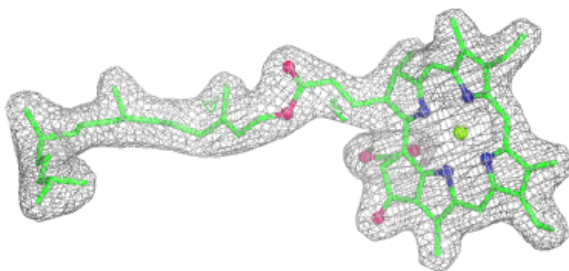
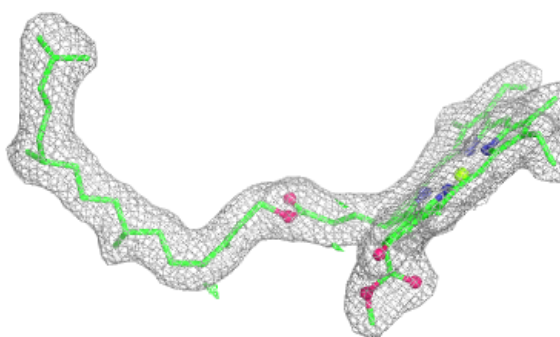


Electron density around CLA B 605:

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

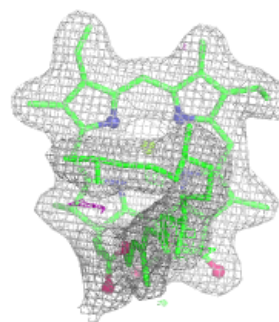
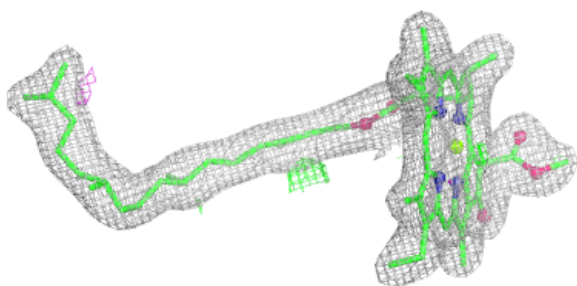
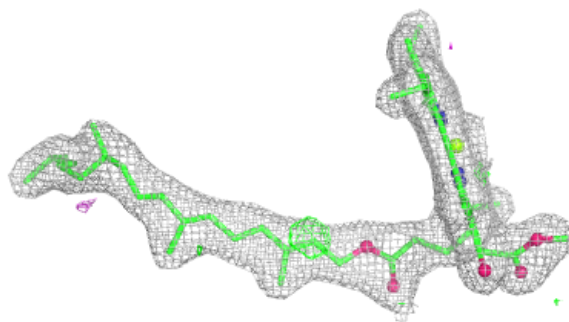
**Electron density around CLA d 403:**

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

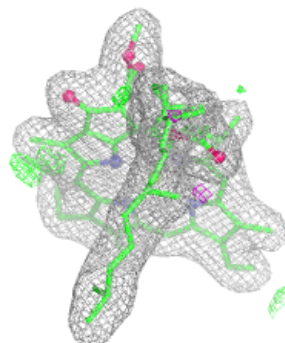
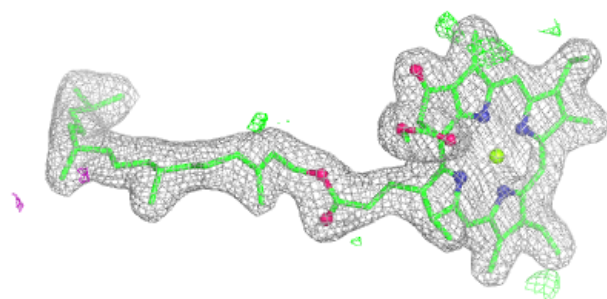
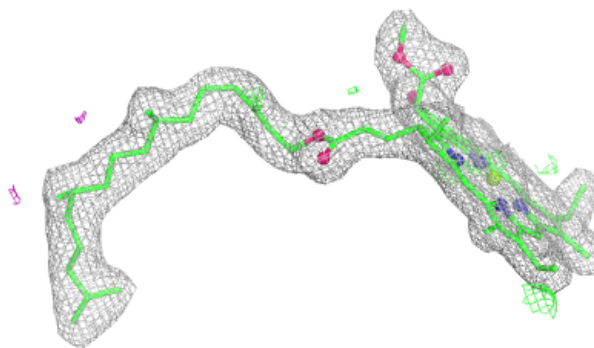


Electron density around CLA B 606:

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

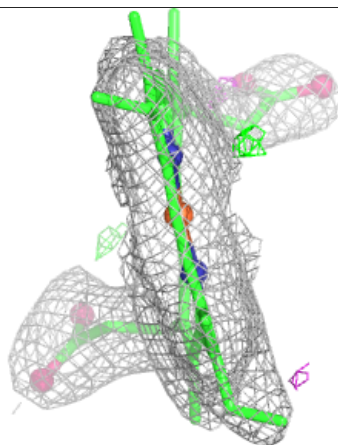
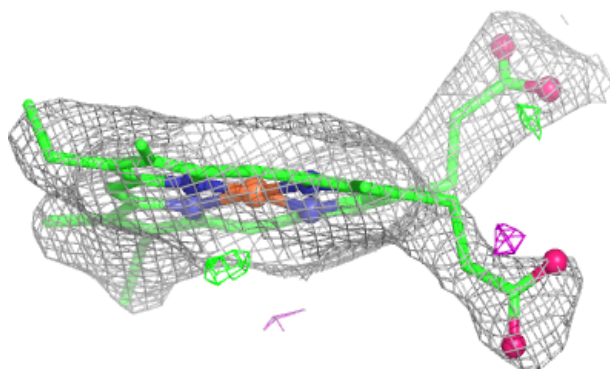
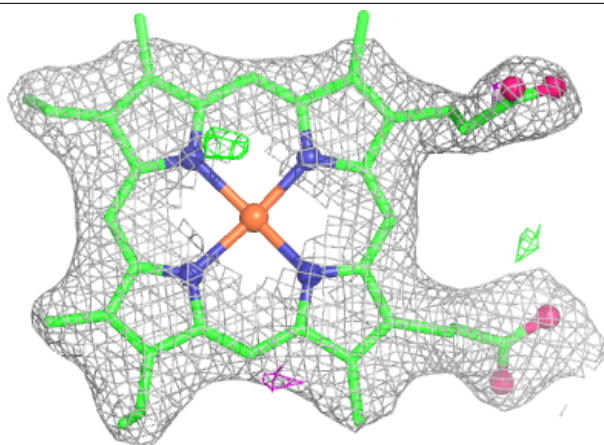
**Electron density around CLA D 402:**

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

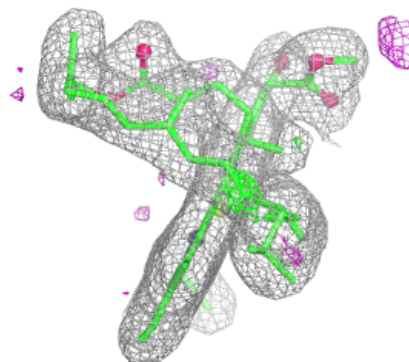
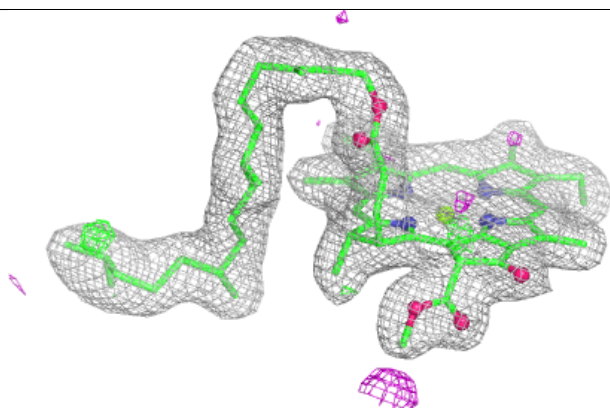
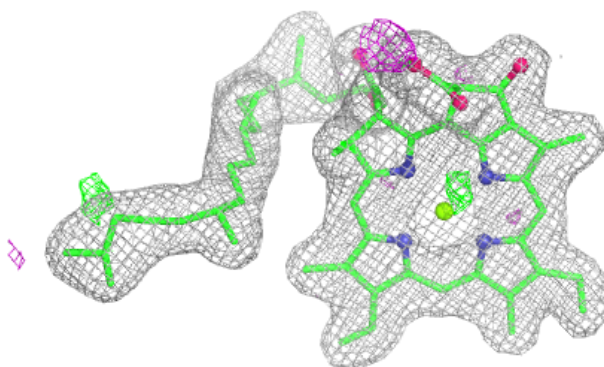


Electron density around HEM E 102:

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

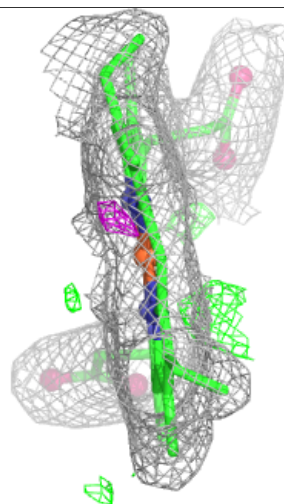
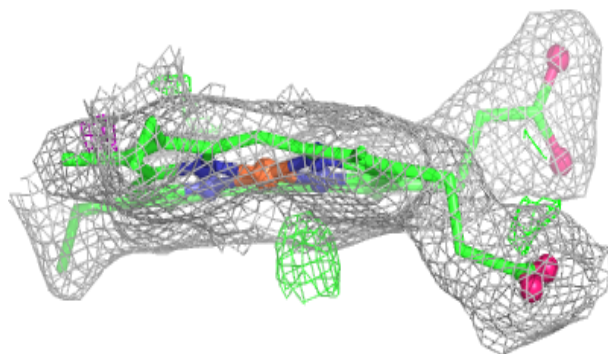
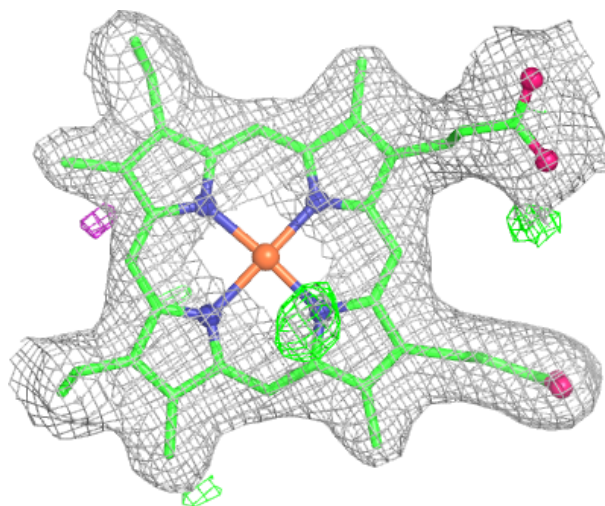
**Electron density around CLA A 406:**

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



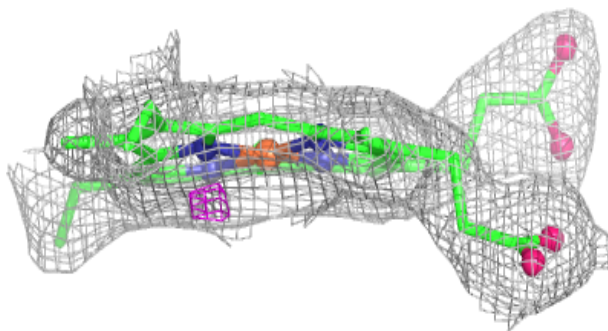
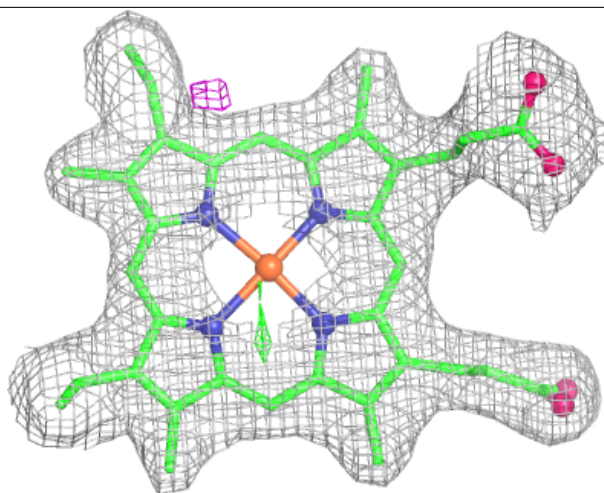
Electron density around HEC V 205:

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



Electron density around HEC v 205:

$2mF_o-DF_c$ (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.