



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 09:15 PM JST

PDB ID : 7COU / pdb_00007cou
Title : Structure of cyanobacterial photosystem II in the dark S1 state
Authors : Li, H.; Shen, J.-R.; Suga, M.
Deposited on : 2020-08-05
Resolution : 2.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

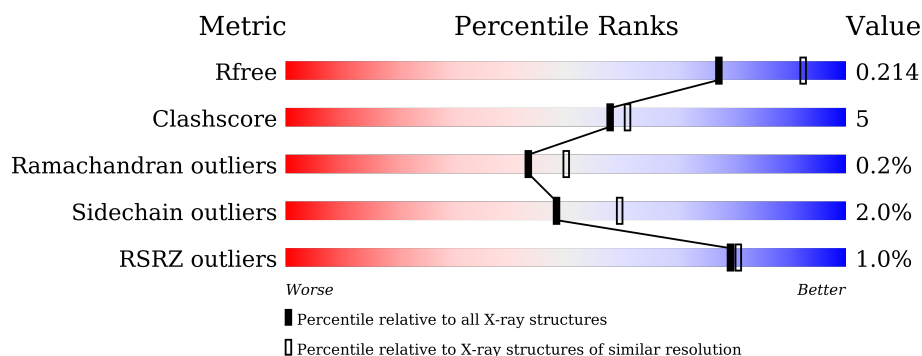
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 Å.

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



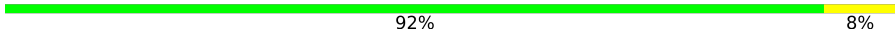
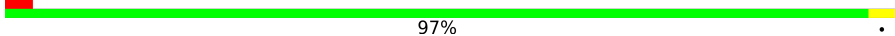
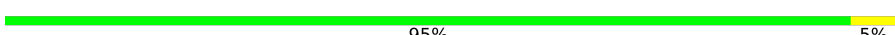
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	91% 6% .
1	a	344	% 89% 8% .
2	B	505	91% 9%
2	b	505	2% 90% 9% .
3	C	455	91% 8% .
3	c	455	91% 8%

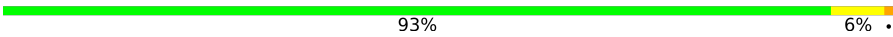
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Mol	Chain	Length	Quality of chain
4	D	342	
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V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

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Mol	Chain	Length	Quality of chain
16	v	137	
17	X	40	
17	x	40	
18	Y	30	
18	y	30	
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
38	HEC	E	103	X	-	-	-
38	HEC	V	201	X	-	-	-
38	HEC	e	102	X	-	-	-
38	HEC	v	202	X	-	-	-

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 53138 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	2	0
			2634	1725	433	461	15			
1	a	334	Total	C	N	O	S	0	3	0
			2642	1731	434	462	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	conflict	UNP P51765
a	279	PRO	ARG	conflict	UNP P51765

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	10	0
			4050	2650	677	710	13			
2	b	504	Total	C	N	O	S	0	4	0
			3998	2622	665	698	13			

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	4	0
			3513	2295	588	617	13			
3	c	455	Total	C	N	O	S	0	2	0
			3534	2311	591	619	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	0	0
			2726	1805	445	464	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	d	341	Total	C	N	O	S	0	0	0
			2717	1800	444	461	12			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	0	0
			293	204	43	46			
10	k	37	Total	C	N	O	0	0	0
			293	204	43	46			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	conflict	UNP P19054
K	39	TRP	VAL	conflict	UNP P19054
k	33	LEU	PHE	conflict	UNP P19054
k	39	TRP	VAL	conflict	UNP P19054

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	36	Total	C	N	O	0	1	0
			304	203	48	53			
11	l	36	Total	C	N	O	0	1	0
			304	203	48	53			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			268	179	39	49	1			
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	conflict	UNP P12312
m	8	LEU	PHE	conflict	UNP P12312

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	3	0
			1886	1177	318	386	5			

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

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

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

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

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

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

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

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

- Molecule 18 is a protein called Photosystem II reaction center protein Ycf12.

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	0	0	0
			273	186	47	40			

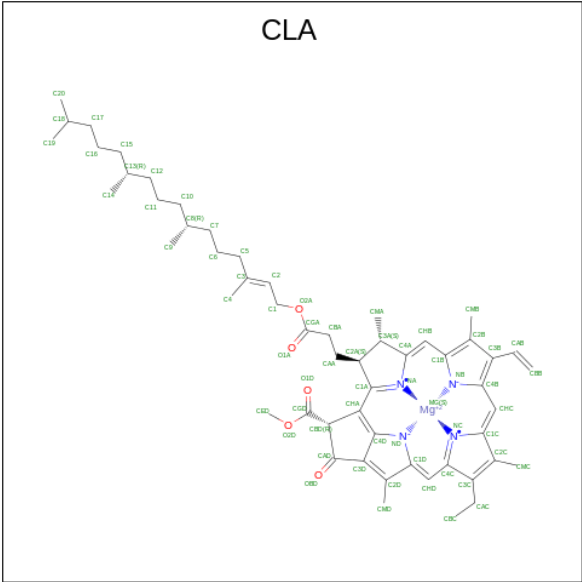
- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total	Fe	0	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	a	2	Total	Cl	0	0
			2	2		

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



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

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

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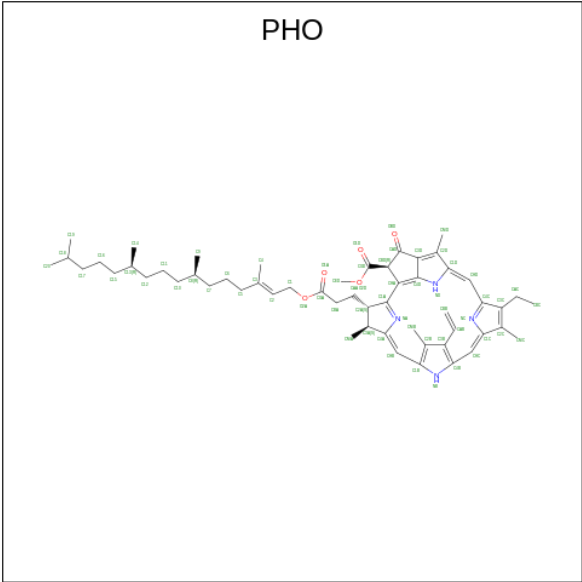
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N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

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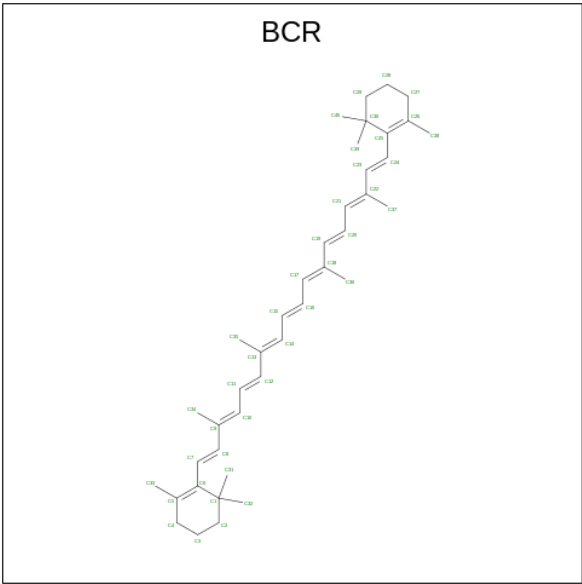
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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



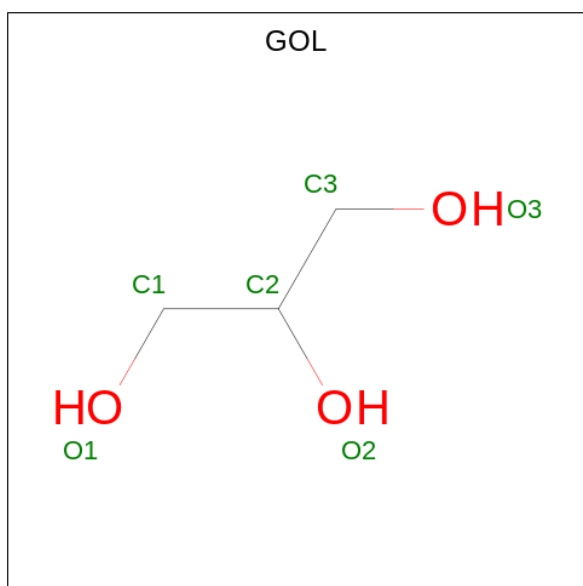
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		

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



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

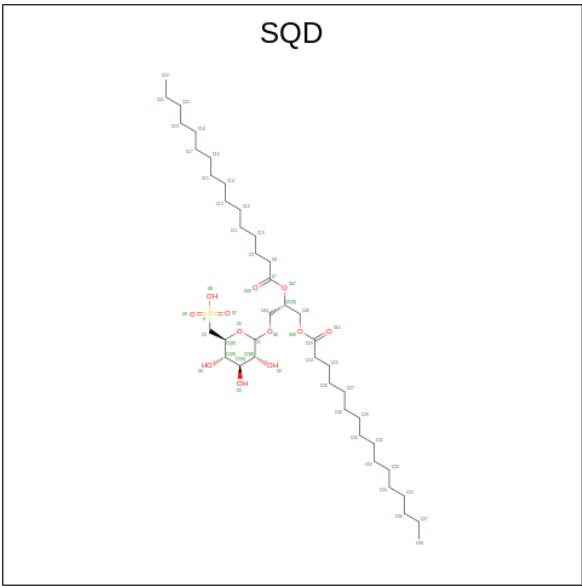
- Molecule 26 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

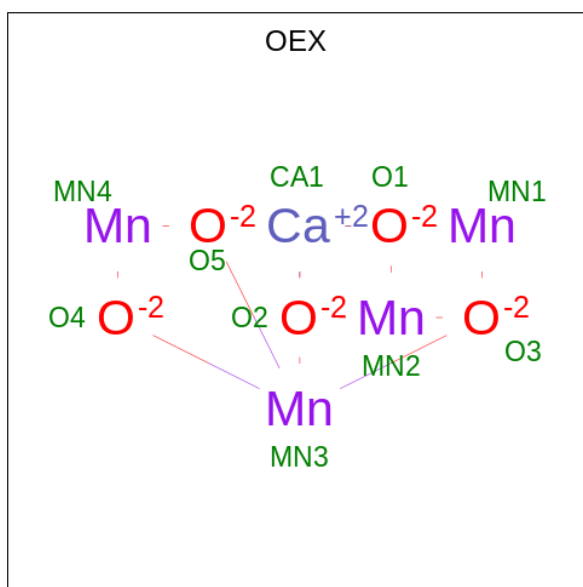
- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



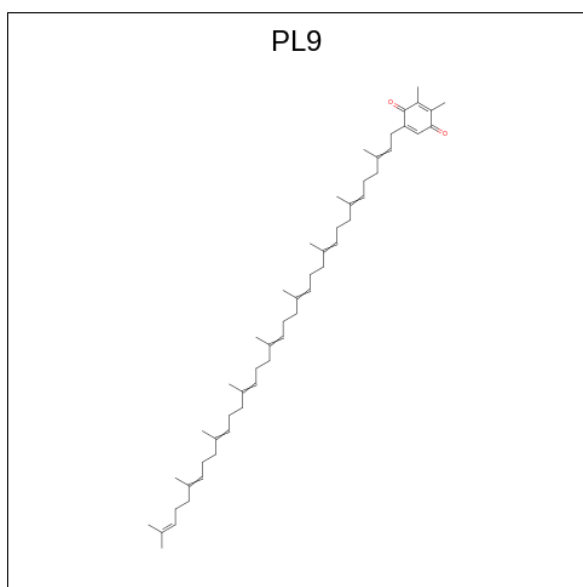
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	B	1	Total	C	O	S	0	0
			54	41	12	1		
27	C	1	Total	C	O	S	0	0
			54	41	12	1		
27	D	1	Total	C	O	S	0	0
			43	30	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	b	1	Total	C	O	S	0	0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

- Molecule 28 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn₄O₅).



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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			55	53	2		

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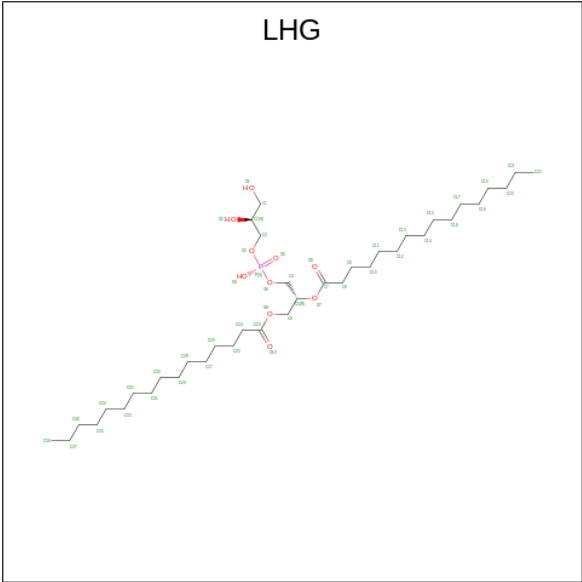
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	D	1	Total	C	O	0	0
			55	53	2		
29	a	1	Total	C	O	0	0
			55	53	2		
29	d	1	Total	C	O	0	0
			55	53	2		

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

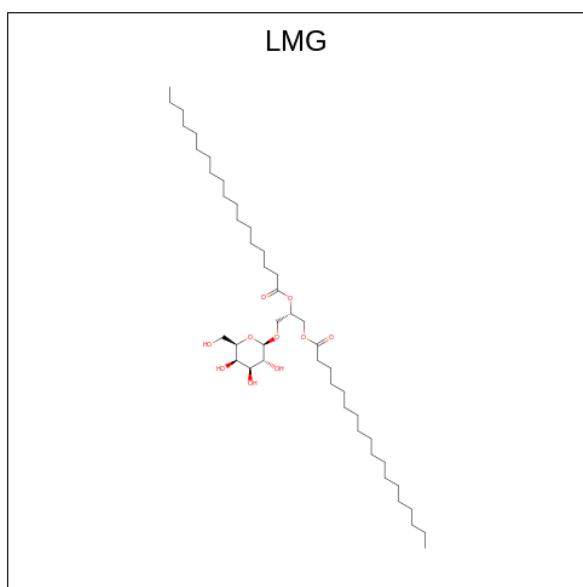
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			28	23	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	C	1	Total	C	O	0	0
			34	29	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	I	1	Total	C	O	0	0
			40	35	5		
30	J	1	Total	C		0	0
			10	10			
30	M	1	Total	C		0	0
			10	10			
30	X	1	Total	C	O	0	0
		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

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



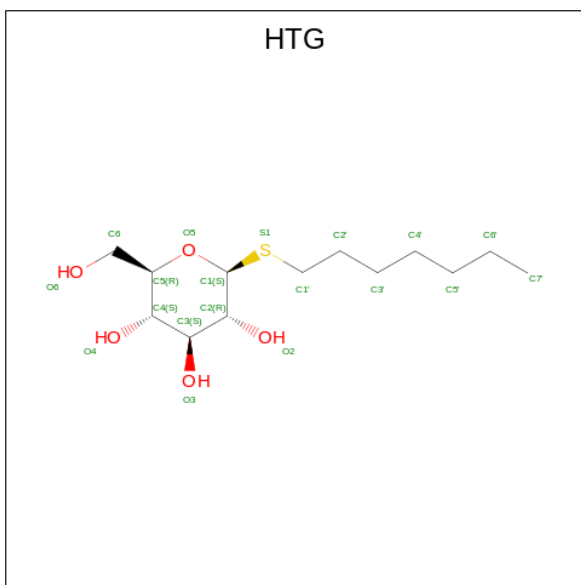
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	E	1	Total	C	O	P	0	0
			42	31	10	1		
31	L	1	Total	C	O	P	0	0
			49	38	10	1		
31	a	1	Total	C	O	P	0	0
			42	31	10	1		
31	b	1	Total	C	O	P	0	0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

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



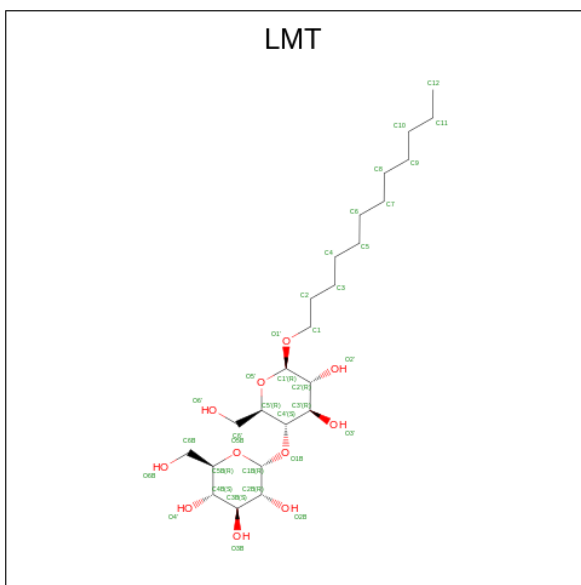
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	B	1	Total	C	O	0	0
			51	41	10		
32	C	1	Total	C	O	0	0
			51	41	10		
32	C	1	Total	C	O	0	0
			51	41	10		
32	C	1	Total	C	O	0	0
			51	41	10		
32	D	1	Total	C	O	0	0
			51	41	10		
32	Z	1	Total	C	O	0	0
			37	27	10		
32	c	1	Total	C	O	0	0
			51	41	10		
32	c	1	Total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

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



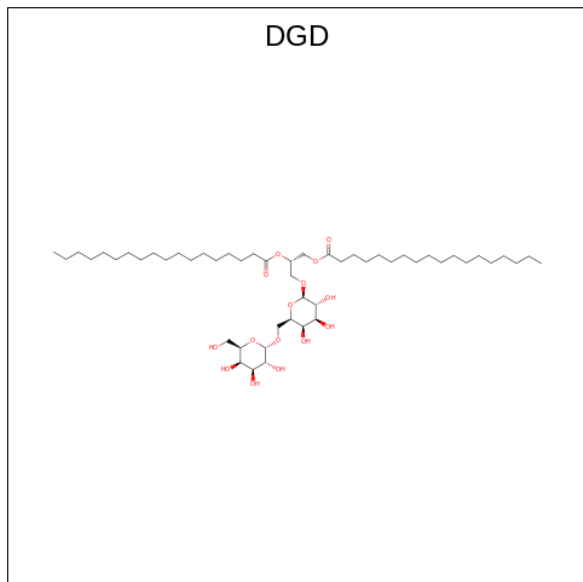
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	B	1	Total 19	C 13	O 5	S 1	0	0
33	B	1	Total 19	C 13	O 5	S 1	0	0
33	B	1	Total 19	C 13	O 5	S 1	0	0
33	C	1	Total 19	C 13	O 5	S 1	0	0
33	D	1	Total 16	C 10	O 5	S 1	0	0
33	V	1	Total 11	C 6	O 5		0	0
33	b	1	Total 19	C 13	O 5	S 1	0	0
33	b	1	Total 19	C 13	O 5	S 1	0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

- Molecule 34 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



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

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



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

- Molecule 36 is CALCIUM ION (CCD ID: CA) (formula: Ca).

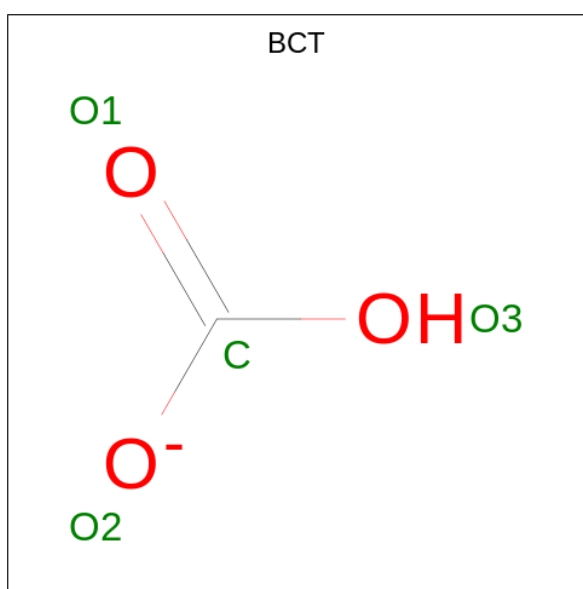
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	C	1	Total	Ca	0	0
			1	1		
36	F	1	Total	Ca	0	0
			1	1		

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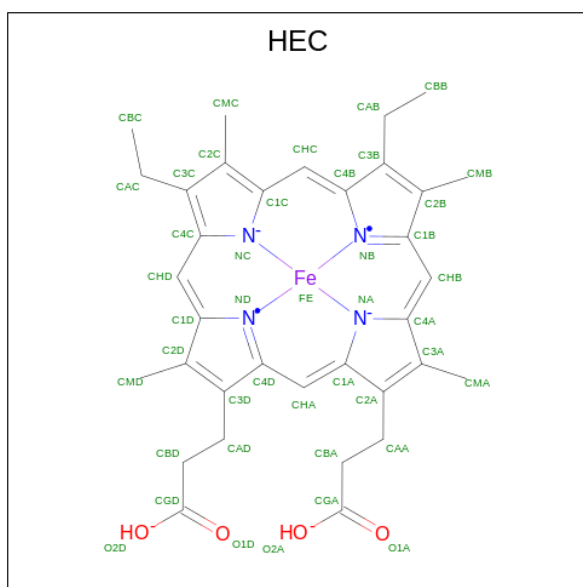
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	O	1	Total	Ca	0	0
			1	1		
36	a	1	Total	Ca	0	0
			1	1		
36	c	2	Total	Ca	0	0
			2	2		
36	o	1	Total	Ca	0	0
			1	1		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	D	1	Total	C	O	0	0
			4	1	3		
37	d	1	Total	C	O	0	0
			4	1	3		

- Molecule 38 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$).



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

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

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

- Molecule 40 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	A	143	Total O 143 143	0	0
40	B	223	Total O 223 223	0	0
40	C	203	Total O 203 203	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	D	136	Total O 136 136	0	0
40	E	27	Total O 27 27	0	0
40	F	9	Total O 9 9	0	0
40	H	26	Total O 26 26	0	0
40	I	5	Total O 5 5	0	0
40	J	5	Total O 5 5	0	0
40	K	7	Total O 7 7	0	0
40	L	6	Total O 6 6	0	0
40	M	17	Total O 17 17	0	0
40	O	125	Total O 125 125	0	0
40	T	16	Total O 16 16	0	0
40	U	56	Total O 56 56	0	0
40	V	102	Total O 102 102	0	0
40	X	9	Total O 9 9	0	0
40	Y	1	Total O 1 1	0	0
40	R	1	Total O 1 1	0	0
40	a	143	Total O 143 143	0	0
40	b	234	Total O 234 234	0	0
40	c	174	Total O 174 174	0	0
40	d	125	Total O 125 125	0	0
40	e	16	Total O 16 16	0	0

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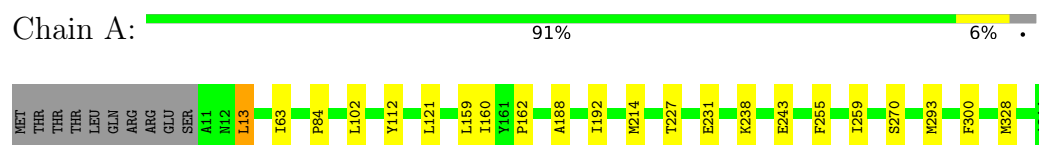
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	f	4	Total 4	O 4	0	0
40	h	23	Total 23	O 23	0	0
40	i	2	Total 2	O 2	0	0
40	j	3	Total 3	O 3	0	0
40	k	5	Total 5	O 5	0	0
40	l	7	Total 7	O 7	0	0
40	m	11	Total 11	O 11	0	0
40	o	99	Total 99	O 99	0	0
40	t	11	Total 11	O 11	0	0
40	u	71	Total 71	O 71	0	0
40	v	60	Total 60	O 60	0	0
40	x	9	Total 9	O 9	0	0
40	y	4	Total 4	O 4	0	0

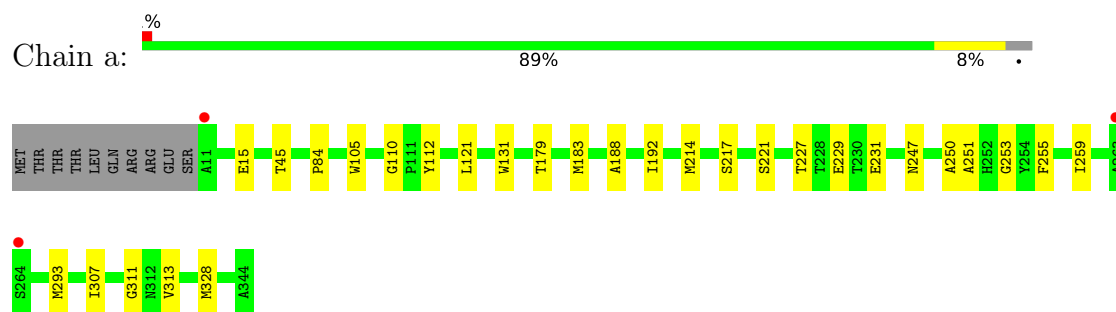
3 Residue-property plots [i](#)

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.

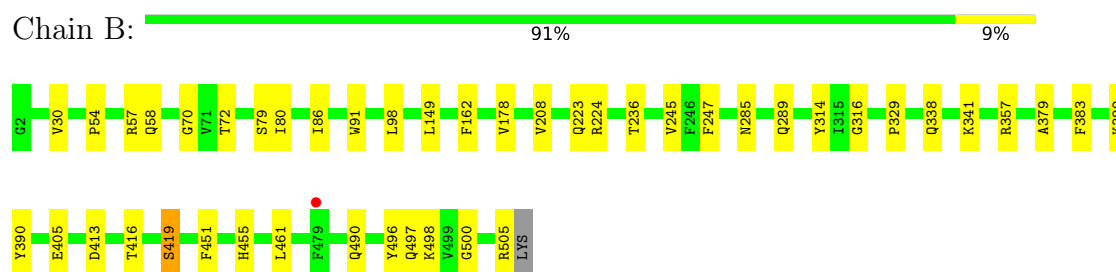
- Molecule 1: Photosystem II protein D1



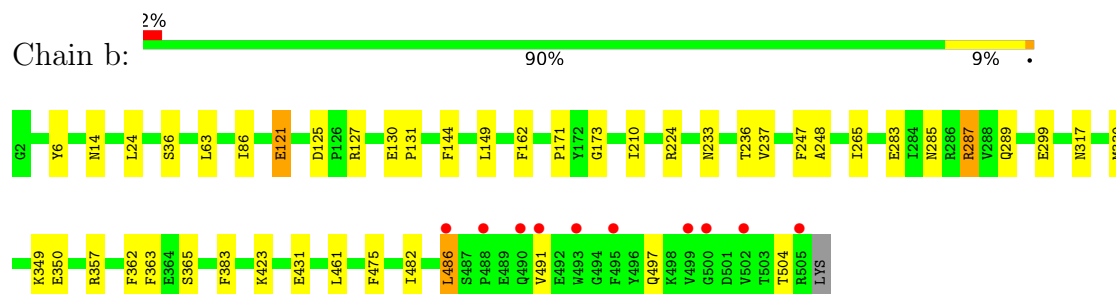
- Molecule 1: Photosystem II protein D1



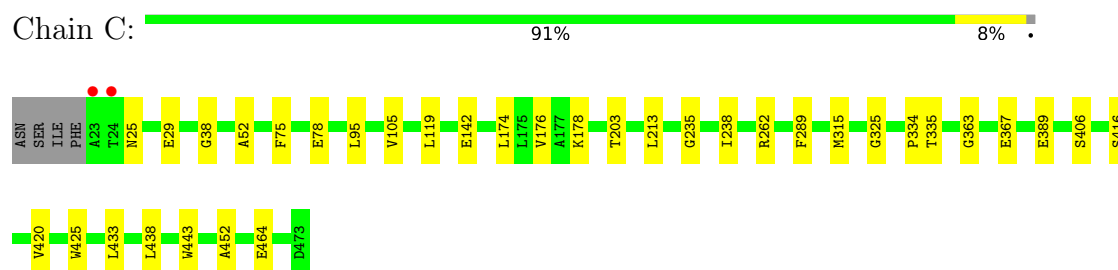
- Molecule 2: Photosystem II CP47 reaction center protein



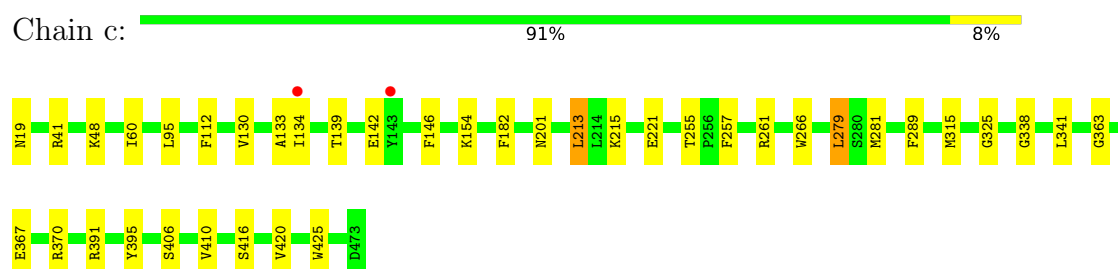
- Molecule 2: Photosystem II CP47 reaction center protein



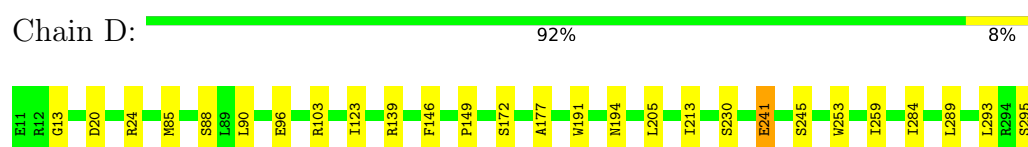
- Molecule 3: Photosystem II CP43 reaction center protein



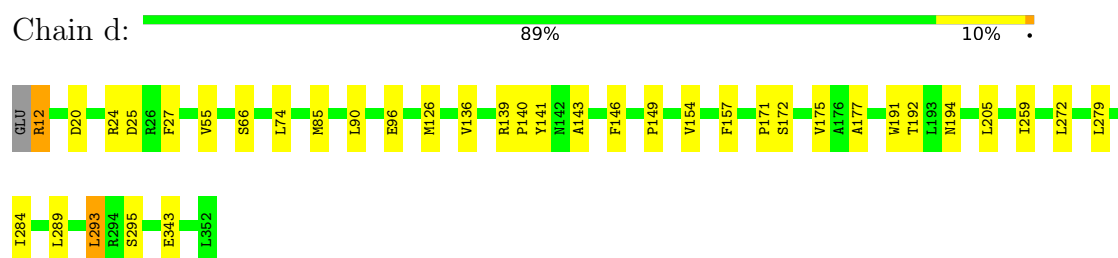
- Molecule 3: Photosystem II CP43 reaction center protein



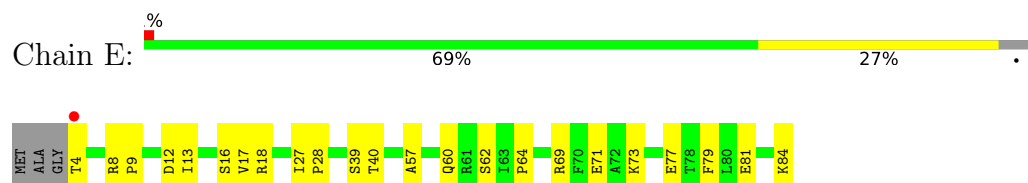
- Molecule 4: Photosystem II D2 protein



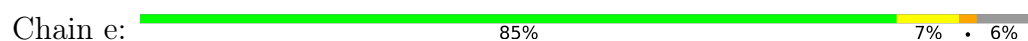
- Molecule 4: Photosystem II D2 protein



- Molecule 5: Cytochrome b559 subunit alpha

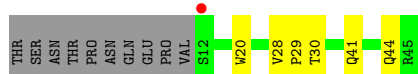


- Molecule 5: Cytochrome b559 subunit alpha

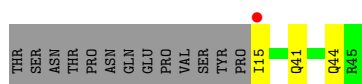




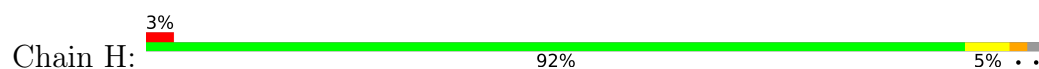
- Molecule 6: Cytochrome b559 subunit beta



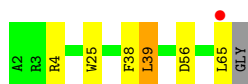
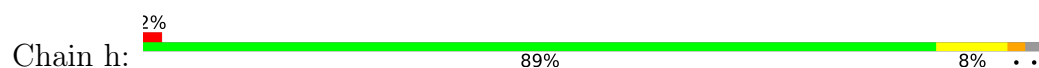
- Molecule 6: Cytochrome b559 subunit beta



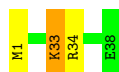
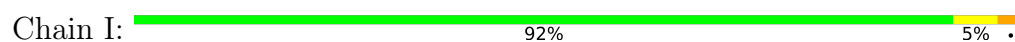
- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H



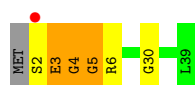
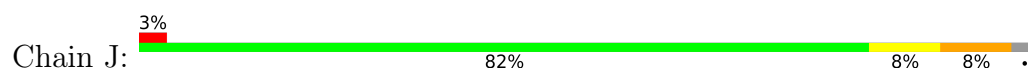
- Molecule 8: Photosystem II reaction center protein I



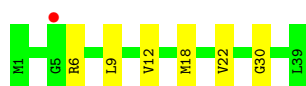
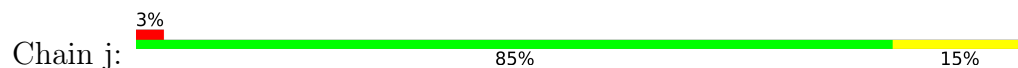
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



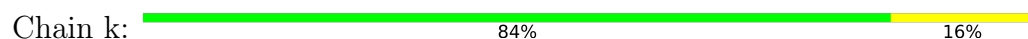
- Molecule 9: Photosystem II reaction center protein J



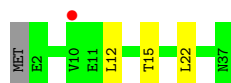
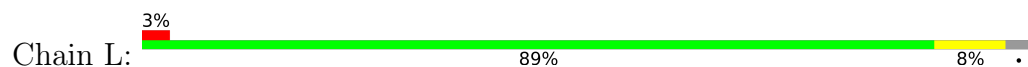
- Molecule 10: Photosystem II reaction center protein K



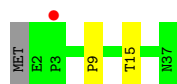
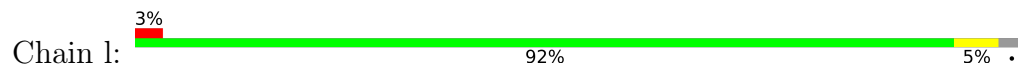
- Molecule 10: Photosystem II reaction center protein K



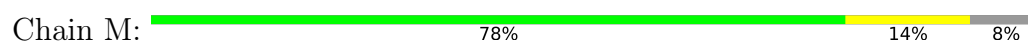
- Molecule 11: Photosystem II reaction center protein L



- 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:  75% 17% 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  90% 9%



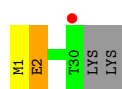
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  91% 8%



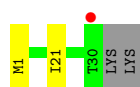
- Molecule 14: Photosystem II reaction center protein T

Chain T:  3% 88% 6% 6%



- Molecule 14: Photosystem II reaction center protein T

Chain t:  3% 88% 6% 6%



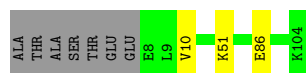
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  85% 7% 8%

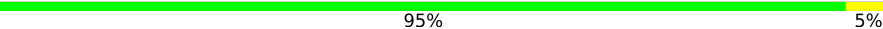


- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  90% 7%



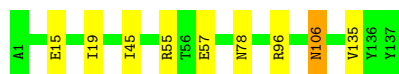
- Molecule 16: Cytochrome c-550

Chain V:  95% 5%



- Molecule 16: Cytochrome c-550

Chain v:  93% 6% .



- Molecule 17: Photosystem II reaction center protein X

Chain X:  88% 8% 5%



- Molecule 17: Photosystem II reaction center protein X

Chain x:  82% 12% 5%



- Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:  7% 73% 23% .



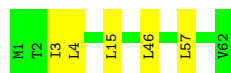
- Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:  77% 20% .

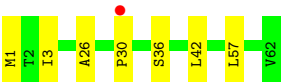
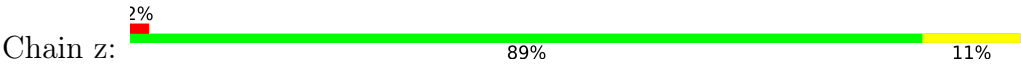


- Molecule 19: Photosystem II reaction center protein Z

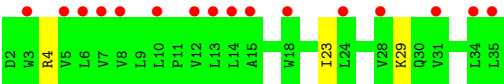
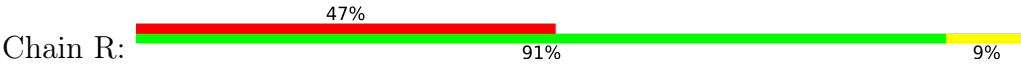
Chain Z:  92% 8%



- 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	126.15Å 232.70Å 288.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.97 – 2.25 39.97 – 2.25	Depositor EDS
% Data completeness (in resolution range)	96.0 (39.97-2.25) 85.6 (39.97-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.25Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.169 , 0.211 0.171 , 0.214	Depositor DCC
R_{free} test set	20023 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 72.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	53138	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.37	0/2719	0.55	0/3708
1	a	0.34	0/2727	0.50	0/3719
2	B	0.34	0/4190	0.49	0/5708
2	b	0.31	0/4138	0.49	0/5640
3	C	0.29	0/3626	0.46	0/4936
3	c	0.27	0/3648	0.43	0/4966
4	D	0.36	0/2821	0.52	0/3844
4	d	0.33	0/2812	0.49	0/3832
5	E	0.26	0/687	0.45	0/936
5	e	0.24	0/667	0.40	0/908
6	F	0.25	0/284	0.39	0/387
6	f	0.22	0/257	0.43	0/349
7	H	0.27	0/530	0.50	0/723
7	h	0.25	0/519	0.48	0/708
8	I	0.24	0/311	0.36	0/419
8	i	0.26	0/311	0.41	0/419
9	J	0.23	0/278	0.37	0/376
9	j	0.23	0/283	0.39	0/383
10	K	0.25	0/303	0.46	0/416
10	k	0.24	0/303	0.44	0/416
11	L	0.40	0/311	0.47	0/423
11	l	0.33	0/311	0.50	0/423
12	M	0.35	0/261	0.51	0/357
12	m	0.35	0/262	0.50	0/357
13	O	0.30	0/1917	0.48	0/2599
13	o	0.28	0/1910	0.46	0/2589
14	T	0.36	0/257	0.42	0/349
14	t	0.35	0/257	0.41	0/349
15	U	0.33	0/776	0.53	0/1052
15	u	0.29	0/785	0.52	0/1064
16	V	0.29	0/1085	0.46	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.26	0/1085	0.41	0/1473
17	X	0.22	0/284	0.36	0/384
17	x	0.18	0/284	0.31	0/384
18	Y	0.20	0/216	0.37	0/289
18	y	0.18	0/216	0.38	0/289
19	Z	0.18	0/490	0.33	0/669
19	z	0.18	0/490	0.33	0/669
20	R	0.19	0/279	0.33	0/383
All	All	0.31	0/42890	0.47	0/58368

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2634	0	2531	14	0
1	a	2642	0	2541	23	0
2	B	4050	0	3894	31	0
2	b	3998	0	3852	36	0
3	C	3513	0	3424	23	0
3	c	3534	0	3446	26	0
4	D	2726	0	2627	23	0
4	d	2717	0	2621	25	0
5	E	668	0	652	16	0
5	e	648	0	634	7	0
6	F	275	0	282	5	0
6	f	250	0	261	3	0
7	H	517	0	542	4	0
7	h	506	0	529	5	0
8	I	314	0	328	2	0
8	i	314	0	328	0	0
9	J	272	0	279	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	277	0	284	4	0
10	K	293	0	305	1	0
10	k	293	0	305	3	0
11	L	304	0	314	2	0
11	l	304	0	314	2	0
12	M	268	0	285	4	0
12	m	269	0	288	5	0
13	O	1886	0	1856	14	0
13	o	1879	0	1850	11	0
14	T	258	0	261	1	0
14	t	258	0	261	1	0
15	U	765	0	767	4	0
15	u	774	0	773	1	0
16	V	1064	0	1073	4	0
16	v	1064	0	1073	6	0
17	X	281	0	312	2	0
17	x	281	0	312	4	0
18	Y	215	0	246	4	0
18	y	215	0	246	3	0
19	Z	479	0	516	2	0
19	z	479	0	516	2	0
20	R	273	0	305	2	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0
23	A	260	0	288	10	0
23	B	1040	0	1152	32	0
23	C	845	0	936	30	0
23	D	130	0	144	2	0
23	a	260	0	288	9	0
23	b	1040	0	1152	32	0
23	c	845	0	936	30	0
23	d	130	0	144	1	0
24	A	128	0	148	3	0
24	a	128	0	148	5	0
25	A	40	0	56	2	0
25	B	120	0	168	7	0
25	C	80	0	112	1	0
25	D	40	0	56	0	0
25	H	40	0	56	3	0
25	K	40	0	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	T	40	0	56	4	0
25	Y	40	0	56	1	0
25	a	40	0	56	2	0
25	b	120	0	168	9	0
25	c	80	0	112	5	0
25	d	40	0	56	1	0
25	h	40	0	56	3	0
25	k	40	0	56	1	0
25	t	40	0	56	5	0
25	y	40	0	56	2	0
26	A	6	0	8	0	0
26	B	18	0	24	0	0
26	C	6	0	8	0	0
26	O	6	0	8	0	0
26	a	6	0	8	0	0
26	b	12	0	16	1	0
26	c	6	0	8	1	0
26	o	6	0	8	0	0
26	v	6	0	8	1	0
27	A	54	0	78	1	0
27	B	54	0	78	0	0
27	C	54	0	77	3	0
27	D	43	0	53	0	0
27	a	108	0	155	2	0
27	b	54	0	78	1	0
27	f	43	0	53	2	0
28	A	10	0	0	0	0
28	a	10	0	0	0	0
29	A	55	0	80	5	0
29	D	55	0	80	2	0
29	a	55	0	80	6	0
29	d	55	0	80	1	0
30	A	28	0	0	0	0
30	B	33	0	0	1	0
30	C	34	0	0	0	0
30	D	57	0	0	0	0
30	I	40	0	0	0	0
30	J	10	0	0	0	0
30	M	10	0	0	0	0
30	X	18	0	0	0	0
30	a	30	0	0	0	0
30	b	33	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	c	32	0	0	0	0
30	d	71	0	0	0	0
30	i	40	0	0	0	0
30	j	10	0	0	0	0
30	m	10	0	0	0	0
31	A	49	0	74	2	0
31	D	98	0	148	6	0
31	E	42	0	57	2	0
31	L	49	0	74	2	0
31	a	42	0	57	5	0
31	b	49	0	74	0	0
31	d	147	0	222	10	0
32	B	51	0	72	3	0
32	C	153	0	216	4	0
32	D	51	0	72	1	0
32	Z	37	0	44	0	0
32	c	153	0	216	5	0
32	d	51	0	71	2	0
32	m	51	0	72	2	0
32	z	39	0	48	2	0
33	B	57	0	78	4	0
33	C	19	0	26	0	0
33	D	16	0	17	1	0
33	V	11	0	10	0	0
33	b	57	0	78	3	0
33	c	19	0	26	1	0
33	h	16	0	17	1	0
34	B	60	0	81	0	0
34	C	35	0	46	2	0
34	D	35	0	46	2	0
34	E	35	0	46	1	0
34	M	70	0	92	3	0
34	a	70	0	92	3	0
34	b	50	0	70	1	0
34	e	35	0	46	0	0
34	m	35	0	46	0	0
34	t	26	0	35	0	0
35	C	186	0	246	9	0
35	H	62	0	82	1	0
35	c	186	0	246	3	0
35	h	62	0	82	0	0
36	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	F	1	0	0	0	0
36	O	1	0	0	0	0
36	a	1	0	0	0	0
36	c	2	0	0	0	0
36	o	1	0	0	0	0
37	D	4	0	0	0	0
37	d	4	0	0	0	0
38	E	43	0	32	1	0
38	V	43	0	30	1	0
38	e	43	0	32	2	0
38	v	43	0	30	0	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	A	143	0	0	0	0
40	B	223	0	0	1	0
40	C	203	0	0	1	0
40	D	136	0	0	3	0
40	E	27	0	0	0	0
40	F	9	0	0	1	0
40	H	26	0	0	1	0
40	I	5	0	0	0	0
40	J	5	0	0	0	0
40	K	7	0	0	0	0
40	L	6	0	0	0	0
40	M	17	0	0	0	0
40	O	125	0	0	1	0
40	R	1	0	0	0	0
40	T	16	0	0	0	0
40	U	56	0	0	0	0
40	V	102	0	0	0	0
40	X	9	0	0	0	0
40	Y	1	0	0	0	0
40	a	143	0	0	0	0
40	b	234	0	0	1	0
40	c	174	0	0	3	0
40	d	125	0	0	0	0
40	e	16	0	0	0	0
40	f	4	0	0	1	0
40	h	23	0	0	0	0
40	i	2	0	0	0	0
40	j	3	0	0	0	0
40	k	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	l	7	0	0	0	0
40	m	11	0	0	0	0
40	o	99	0	0	0	0
40	t	11	0	0	0	0
40	u	71	0	0	0	0
40	v	60	0	0	1	0
40	x	9	0	0	0	0
40	y	4	0	0	0	0
All	All	53138	0	51938	468	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 468 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)
23:c:515:CLA:HBB1	25:c:516:BCR:H24C	1.57	0.86
1:a:250:ALA:HA	2:b:491:VAL:HG11	1.58	0.83
4:D:85:MET:HE2	4:D:90:LEU:HD21	1.61	0.82
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.62	0.82
4:d:192:THR:HG23	23:d:402:CLA:HBC2	1.62	0.81

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	334/344 (97%)	330 (99%)	3 (1%)	1 (0%)	36	40
1	a	335/344 (97%)	328 (98%)	6 (2%)	1 (0%)	36	40
2	B	512/505 (101%)	505 (99%)	7 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	506/505 (100%)	497 (98%)	9 (2%)	0	100	100
3	C	453/455 (100%)	443 (98%)	8 (2%)	2 (0%)	30	31
3	c	455/455 (100%)	444 (98%)	10 (2%)	1 (0%)	43	50
4	D	340/342 (99%)	329 (97%)	11 (3%)	0	100	100
4	d	339/342 (99%)	331 (98%)	8 (2%)	0	100	100
5	E	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
5	e	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	29/44 (66%)	29 (100%)	0	0	100	100
7	H	63/65 (97%)	61 (97%)	2 (3%)	0	100	100
7	h	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
8	I	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
8	i	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
9	J	36/39 (92%)	33 (92%)	0	3 (8%)	0	0
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	32/36 (89%)	30 (94%)	2 (6%)	0	100	100
13	O	244/244 (100%)	237 (97%)	6 (2%)	1 (0%)	30	31
13	o	243/244 (100%)	236 (97%)	7 (3%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	94/104 (90%)	92 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
16	v	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
17	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
17	x	36/40 (90%)	35 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	Y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
18	y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	7	3
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	5246/5384 (97%)	5129 (98%)	107 (2%)	10 (0%)	43	50

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416	SER
9	J	4	GLY
9	J	5	GLY

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	271/279 (97%)	268 (99%)	3 (1%)	65	75
1	a	272/279 (98%)	271 (100%)	1 (0%)	84	89
2	B	412/403 (102%)	406 (98%)	6 (2%)	57	68
2	b	406/403 (101%)	399 (98%)	7 (2%)	53	65
3	C	356/356 (100%)	349 (98%)	7 (2%)	48	59
3	c	358/356 (101%)	352 (98%)	6 (2%)	53	65
4	D	277/277 (100%)	274 (99%)	3 (1%)	65	75
4	d	276/277 (100%)	271 (98%)	5 (2%)	51	63
5	E	73/73 (100%)	70 (96%)	3 (4%)	27	33
5	e	70/73 (96%)	67 (96%)	3 (4%)	26	31
6	F	28/38 (74%)	28 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	f	25/38 (66%)	25 (100%)	0	100	100
7	H	55/54 (102%)	52 (94%)	3 (6%)	19	20
7	h	54/54 (100%)	52 (96%)	2 (4%)	30	37
8	I	34/34 (100%)	33 (97%)	1 (3%)	37	47
8	i	34/34 (100%)	34 (100%)	0	100	100
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	26/27 (96%)	25 (96%)	1 (4%)	29	36
10	K	30/30 (100%)	26 (87%)	4 (13%)	4	2
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	5
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	47
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	30/32 (94%)	30 (100%)	0	100	100
12	m	30/32 (94%)	28 (93%)	2 (7%)	15	14
13	O	209/207 (101%)	206 (99%)	3 (1%)	59	70
13	o	208/207 (100%)	203 (98%)	5 (2%)	43	54
14	T	26/28 (93%)	25 (96%)	1 (4%)	29	36
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	83/89 (93%)	80 (96%)	3 (4%)	31	39
15	u	84/89 (94%)	82 (98%)	2 (2%)	43	54
16	V	117/117 (100%)	117 (100%)	0	100	100
16	v	117/117 (100%)	114 (97%)	3 (3%)	40	50
17	X	31/33 (94%)	30 (97%)	1 (3%)	34	43
17	x	31/33 (94%)	29 (94%)	2 (6%)	15	14
18	Y	22/23 (96%)	20 (91%)	2 (9%)	9	7
18	y	22/23 (96%)	20 (91%)	2 (9%)	9	7
19	Z	52/52 (100%)	51 (98%)	1 (2%)	50	61
19	z	52/52 (100%)	50 (96%)	2 (4%)	29	36
20	R	29/29 (100%)	28 (97%)	1 (3%)	32	40
All	All	4352/4403 (99%)	4263 (98%)	89 (2%)	48	59

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	d	12	ARG
12	m	5	GLN
4	d	154	VAL
7	h	39	LEU
13	o	69	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
3	c	19	ASN
13	o	80	GLN
4	D	186	GLN
13	O	231	HIS
15	U	78	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	FME	t	1	14	8,9,10	0.62	0	7,9,11	1.74	2 (28%)
14	FME	T	1	14	8,9,10	0.70	0	7,9,11	1.44	2 (28%)
12	FME	m	1	12	8,9,10	0.56	0	7,9,11	1.46	2 (28%)
12	FME	M	1	12	8,9,10	0.60	0	7,9,11	1.70	2 (28%)
8	FME	i	1	8	8,9,10	0.56	0	7,9,11	1.05	1 (14%)
8	FME	I	1	8	8,9,10	0.66	0	7,9,11	1.15	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

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

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	CA-N-CN	-3.25	117.82	122.82
12	M	1	FME	CA-N-CN	-3.08	118.08	122.82
14	t	1	FME	O-C-CA	-2.60	117.96	124.78
14	T	1	FME	O-C-CA	-2.48	118.29	124.78
12	m	1	FME	C-CA-N	2.39	114.04	109.73

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 216 ligands modelled in this entry, 15 are monoatomic and 18 are unknown - leaving 183 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LHG	d	408	-	48,48,48	0.90	2 (4%)	51,54,54	1.07	3 (5%)
31	LHG	D	407	-	48,48,48	0.88	2 (4%)	51,54,54	1.00	3 (5%)
25	BCR	c	517	-	41,41,41	1.06	1 (2%)	56,56,56	1.44	11 (19%)
32	LMG	C	521	-	51,51,55	0.99	2 (3%)	59,59,63	1.03	3 (5%)
23	CLA	b	608	2	69,73,73	2.06	20 (28%)	83,113,113	2.81	31 (37%)
25	BCR	b	618	-	41,41,41	1.03	1 (2%)	56,56,56	1.30	8 (14%)
33	HTG	B	623	-	19,19,19	0.81	1 (5%)	23,24,24	1.82	5 (21%)
23	CLA	B	608	2	69,73,73	1.99	20 (28%)	83,113,113	2.82	32 (38%)
35	DGD	c	518	-	63,63,67	0.89	2 (3%)	77,77,81	1.05	6 (7%)
23	CLA	c	507	3	69,73,73	2.03	19 (27%)	83,113,113	2.75	30 (36%)
23	CLA	A	405	40	69,73,73	2.04	19 (27%)	83,113,113	2.89	31 (37%)
23	CLA	b	607	40	69,73,73	2.03	19 (27%)	83,113,113	2.81	30 (36%)
34	LMT	B	628	-	36,36,36	0.42	0	47,47,47	1.10	3 (6%)
23	CLA	C	515	3	69,73,73	2.05	20 (28%)	83,113,113	2.83	30 (36%)
34	LMT	C	526	-	36,36,36	0.49	1 (2%)	47,47,47	1.04	3 (6%)
23	CLA	a	404	1	69,73,73	1.99	20 (28%)	83,113,113	2.86	32 (38%)
23	CLA	b	613	2	69,73,73	2.01	19 (27%)	83,113,113	2.85	30 (36%)
25	BCR	b	619	-	41,41,41	1.16	2 (4%)	56,56,56	1.50	11 (19%)
31	LHG	a	419	-	41,41,48	1.05	2 (4%)	44,47,54	0.97	2 (4%)
23	CLA	b	615	2	69,73,73	2.00	18 (26%)	83,113,113	2.81	30 (36%)
25	BCR	a	409	-	41,41,41	1.08	1 (2%)	56,56,56	1.47	10 (17%)
32	LMG	D	413	39	51,51,55	0.83	2 (3%)	59,59,63	0.96	4 (6%)
23	CLA	A	408	1	69,73,73	2.05	20 (28%)	83,113,113	2.80	32 (38%)
23	CLA	B	605	2	69,73,73	2.05	19 (27%)	83,113,113	2.85	28 (33%)
33	HTG	B	625	-	19,19,19	1.04	2 (10%)	23,24,24	1.11	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	a	408	1	69,73,73	2.00	19 (27%)	83,113,113	2.83	32 (38%)
38	HEC	V	201	16	50,50,50	1.83	9 (18%)	68,82,82	1.64	11 (16%)
25	BCR	d	404	-	41,41,41	1.12	1 (2%)	56,56,56	1.73	11 (19%)
25	BCR	C	516	-	41,41,41	1.00	1 (2%)	56,56,56	1.62	10 (17%)
23	CLA	B	610	40	69,73,73	2.04	20 (28%)	83,113,113	2.83	29 (34%)
34	LMT	a	413	-	36,36,36	0.59	1 (2%)	47,47,47	1.14	3 (6%)
23	CLA	D	403	4	69,73,73	1.99	20 (28%)	83,113,113	2.94	30 (36%)
23	CLA	D	404	4	69,73,73	2.07	18 (26%)	83,113,113	2.80	28 (33%)
25	BCR	B	617	-	41,41,41	1.06	1 (2%)	56,56,56	1.35	7 (12%)
26	GOL	B	627	-	5,5,5	0.99	0	5,5,5	1.15	0
33	HTG	D	411	-	16,16,19	1.06	2 (12%)	20,21,24	1.33	1 (5%)
35	DGD	C	519	-	63,63,67	0.90	2 (3%)	77,77,81	1.10	4 (5%)
26	GOL	b	628	-	5,5,5	0.97	0	5,5,5	1.07	0
33	HTG	c	523	-	19,19,19	0.96	2 (10%)	23,24,24	1.48	1 (4%)
34	LMT	b	621	-	25,25,36	0.51	0	30,30,47	0.58	0
28	OEX	a	414	1,40,3	0,14,14	-	-	-	-	-
33	HTG	b	623	-	19,19,19	1.00	1 (5%)	23,24,24	1.59	2 (8%)
35	DGD	H	102	-	63,63,67	0.83	3 (4%)	77,77,81	1.04	5 (6%)
38	HEC	E	103	6,5	50,50,50	1.73	9 (18%)	68,82,82	1.87	20 (29%)
23	CLA	b	609	-	69,73,73	2.02	22 (31%)	83,113,113	2.74	31 (37%)
25	BCR	t	102	-	41,41,41	1.06	1 (2%)	56,56,56	1.41	10 (17%)
38	HEC	e	102	6,5	50,50,50	1.73	9 (18%)	68,82,82	1.86	20 (29%)
23	CLA	b	611	2	69,73,73	1.96	20 (28%)	83,113,113	2.86	30 (36%)
23	CLA	b	612	2	69,73,73	2.01	20 (28%)	83,113,113	2.86	29 (34%)
25	BCR	H	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.36	7 (12%)
34	LMT	D	402	-	36,36,36	0.52	1 (2%)	47,47,47	0.85	1 (2%)
34	LMT	t	101	-	26,26,36	0.55	1 (3%)	31,31,47	1.14	4 (12%)
23	CLA	C	507	3	69,73,73	1.99	19 (27%)	83,113,113	2.75	29 (34%)
23	CLA	B	603	2	69,73,73	2.03	19 (27%)	83,113,113	2.93	29 (34%)
34	LMT	E	102	-	36,36,36	0.52	1 (2%)	47,47,47	0.85	1 (2%)
27	SQD	C	501	-	53,54,54	0.95	3 (5%)	62,65,65	1.90	10 (16%)
25	BCR	C	517	-	41,41,41	1.01	1 (2%)	56,56,56	1.56	12 (21%)
23	CLA	B	612	2	69,73,73	1.94	19 (27%)	83,113,113	2.96	29 (34%)
27	SQD	f	101	-	42,43,54	1.17	3 (7%)	51,54,65	1.30	8 (15%)
23	CLA	b	614	2	69,73,73	1.99	20 (28%)	83,113,113	2.93	32 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PL9	a	415	-	55,55,55	0.65	2 (3%)	68,69,69	1.98	22 (32%)
32	LMG	c	501	-	51,51,55	0.92	2 (3%)	59,59,63	1.09	3 (5%)
25	BCR	K	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.41	9 (16%)
32	LMG	c	521	-	51,51,55	0.92	2 (3%)	59,59,63	1.01	3 (5%)
33	HTG	b	622	-	19,19,19	1.10	1 (5%)	23,24,24	1.42	2 (8%)
32	LMG	B	621	-	51,51,55	0.91	2 (3%)	59,59,63	1.16	4 (6%)
23	CLA	B	615	2	69,73,73	1.95	17 (24%)	83,113,113	2.85	29 (34%)
32	LMG	C	522	-	51,51,55	1.01	3 (5%)	59,59,63	1.31	5 (8%)
29	PL9	d	405	-	55,55,55	0.64	1 (1%)	68,69,69	1.66	16 (23%)
23	CLA	B	607	40	69,73,73	2.02	19 (27%)	83,113,113	2.78	31 (37%)
25	BCR	c	516	-	41,41,41	1.03	1 (2%)	56,56,56	1.45	10 (17%)
25	BCR	B	618	-	41,41,41	0.93	1 (2%)	56,56,56	1.41	7 (12%)
23	CLA	A	404	1	69,73,73	2.03	20 (28%)	83,113,113	2.84	32 (38%)
26	GOL	c	502	-	5,5,5	1.06	0	5,5,5	0.89	0
23	CLA	b	601	40	69,73,73	2.13	20 (28%)	83,113,113	2.83	28 (33%)
23	CLA	B	614	2	69,73,73	1.98	19 (27%)	83,113,113	3.07	30 (36%)
23	CLA	C	503	3	69,73,73	1.99	20 (28%)	83,113,113	2.93	30 (36%)
23	CLA	b	602	2	69,73,73	2.08	20 (28%)	83,113,113	2.88	32 (38%)
34	LMT	e	101	-	36,36,36	0.53	1 (2%)	47,47,47	1.04	2 (4%)
23	CLA	B	616	2	69,73,73	1.97	20 (28%)	83,113,113	2.82	30 (36%)
26	GOL	b	624	-	5,5,5	0.95	0	5,5,5	1.06	0
23	CLA	b	605	2	69,73,73	2.01	20 (28%)	83,113,113	2.99	27 (32%)
23	CLA	C	510	3	69,73,73	2.02	21 (30%)	83,113,113	2.85	30 (36%)
23	CLA	c	509	40	69,73,73	2.09	18 (26%)	83,113,113	2.93	30 (36%)
23	CLA	c	506	40	69,73,73	2.06	21 (30%)	83,113,113	2.88	33 (39%)
35	DGD	c	519	-	63,63,67	0.85	2 (3%)	77,77,81	1.00	3 (3%)
23	CLA	a	406	40	69,73,73	1.95	18 (26%)	83,113,113	2.87	30 (36%)
32	LMG	c	522	-	51,51,55	0.96	2 (3%)	59,59,63	1.11	5 (8%)
37	BCT	D	401	21	2,3,3	0.55	0	2,3,3	1.18	0
32	LMG	Z	101	-	37,37,55	1.01	3 (8%)	45,45,63	1.53	6 (13%)
23	CLA	c	504	3	69,73,73	2.02	19 (27%)	83,113,113	2.76	27 (32%)
31	LHG	A	416	-	48,48,48	0.89	2 (4%)	51,54,54	1.12	6 (11%)
34	LMT	B	630	-	25,25,36	0.44	0	30,30,47	1.02	2 (6%)
25	BCR	k	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.45	11 (19%)
23	CLA	b	604	2	69,73,73	2.02	19 (27%)	83,113,113	2.72	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	A	409	-	41,41,41	1.03	1 (2%)	56,56,56	1.48	12 (21%)
23	CLA	c	514	3	69,73,73	2.05	19 (27%)	83,113,113	2.87	32 (38%)
23	CLA	B	604	2	69,73,73	2.02	21 (30%)	83,113,113	2.72	30 (36%)
23	CLA	c	511	3	69,73,73	2.09	20 (28%)	83,113,113	2.80	29 (34%)
23	CLA	c	515	3	69,73,73	2.07	20 (28%)	83,113,113	2.84	31 (37%)
23	CLA	C	514	3	69,73,73	2.04	20 (28%)	83,113,113	2.78	30 (36%)
32	LMG	m	101	-	51,51,55	0.89	2 (3%)	59,59,63	1.12	5 (8%)
37	BCT	d	401	21	2,3,3	0.58	0	2,3,3	1.69	1 (50%)
27	SQD	b	620	-	53,54,54	1.03	3 (5%)	62,65,65	1.55	8 (12%)
23	CLA	B	609	2	69,73,73	1.99	18 (26%)	83,113,113	2.89	29 (34%)
25	BCR	b	617	-	41,41,41	1.10	1 (2%)	56,56,56	1.50	7 (12%)
25	BCR	B	619	-	41,41,41	1.03	1 (2%)	56,56,56	1.30	9 (16%)
24	PHO	A	415	-	58,69,69	2.70	14 (24%)	56,99,99	2.71	18 (32%)
34	LMT	m	103	-	36,36,36	0.46	0	47,47,47	0.99	4 (8%)
27	SQD	B	620	-	53,54,54	1.04	3 (5%)	62,65,65	1.44	11 (17%)
27	SQD	a	410	-	53,54,54	0.98	3 (5%)	62,65,65	1.68	11 (17%)
23	CLA	d	402	4	69,73,73	1.97	20 (28%)	83,113,113	2.75	31 (37%)
24	PHO	A	407	-	58,69,69	2.64	14 (24%)	56,99,99	2.86	16 (28%)
23	CLA	c	513	3	69,73,73	2.02	19 (27%)	83,113,113	2.87	31 (37%)
32	LMG	d	412	39	51,51,55	0.92	2 (3%)	59,59,63	0.87	2 (3%)
33	HTG	B	622	-	19,19,19	1.00	1 (5%)	23,24,24	1.59	5 (21%)
33	HTG	V	202	-	11,11,19	0.21	0	15,15,24	1.25	2 (13%)
33	HTG	b	625	-	19,19,19	0.99	2 (10%)	23,24,24	1.30	3 (13%)
23	CLA	B	613	2	69,73,73	1.95	19 (27%)	83,113,113	2.80	29 (34%)
26	GOL	B	629	-	5,5,5	1.01	0	5,5,5	0.87	0
33	HTG	h	101	-	16,16,19	1.14	2 (12%)	20,21,24	2.11	5 (25%)
23	CLA	a	405	40	69,73,73	2.10	18 (26%)	83,113,113	2.87	32 (38%)
23	CLA	C	506	40	69,73,73	2.00	21 (30%)	83,113,113	2.80	32 (38%)
23	CLA	C	508	3	69,73,73	2.08	20 (28%)	83,113,113	2.79	32 (38%)
23	CLA	C	509	40	69,73,73	2.01	20 (28%)	83,113,113	2.78	27 (32%)
25	BCR	h	102	-	41,41,41	1.07	1 (2%)	56,56,56	1.31	7 (12%)
32	LMG	C	502	-	51,51,55	0.92	2 (3%)	59,59,63	1.02	2 (3%)
23	CLA	C	504	3	69,73,73	2.00	20 (28%)	83,113,113	2.78	30 (36%)
24	PHO	a	407	-	58,69,69	2.65	14 (24%)	56,99,99	2.95	15 (26%)
34	LMT	M	101	-	36,36,36	0.45	0	47,47,47	0.97	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	601	40	69,73,73	2.10	21 (30%)	83,113,113	2.84	29 (34%)
35	DGD	C	520	-	63,63,67	0.84	2 (3%)	77,77,81	1.04	5 (6%)
23	CLA	B	602	2	69,73,73	2.08	20 (28%)	83,113,113	2.90	32 (38%)
38	HEC	v	202	16	50,50,50	1.75	7 (14%)	68,82,82	1.38	8 (11%)
26	GOL	A	410	-	5,5,5	1.12	0	5,5,5	0.81	0
32	LMG	z	101	-	39,39,55	1.08	2 (5%)	47,47,63	1.10	3 (6%)
23	CLA	c	510	3	69,73,73	2.10	20 (28%)	83,113,113	2.87	30 (36%)
34	LMT	M	103	-	36,36,36	0.46	0	47,47,47	1.03	2 (4%)
23	CLA	c	505	3	69,73,73	2.06	19 (27%)	83,113,113	2.80	29 (34%)
27	SQD	D	412	-	42,43,54	1.15	3 (7%)	51,54,65	1.79	11 (21%)
25	BCR	T	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.57	12 (21%)
31	LHG	d	406	-	48,48,48	0.88	2 (4%)	51,54,54	1.12	5 (9%)
26	GOL	C	524	-	5,5,5	1.08	0	5,5,5	0.94	0
27	SQD	a	412	-	53,54,54	1.04	3 (5%)	62,65,65	1.28	6 (9%)
28	OEX	A	412	1,40,3	0,14,14	-	-	-	-	-
31	LHG	E	101	-	41,41,48	1.04	2 (4%)	44,47,54	1.03	2 (4%)
31	LHG	b	629	-	48,48,48	0.90	2 (4%)	51,54,54	1.04	3 (5%)
34	LMT	b	627	-	25,25,36	0.45	0	30,30,47	0.90	1 (3%)
25	BCR	Y	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.84	17 (30%)
35	DGD	C	518	-	63,63,67	0.88	2 (3%)	77,77,81	0.99	3 (3%)
26	GOL	a	411	-	5,5,5	0.87	0	5,5,5	1.04	0
26	GOL	O	302	-	5,5,5	0.86	0	5,5,5	1.01	0
26	GOL	B	624	-	5,5,5	0.89	0	5,5,5	1.02	0
27	SQD	A	411	-	53,54,54	1.04	3 (5%)	62,65,65	1.26	7 (11%)
33	HTG	C	523	-	19,19,19	0.92	1 (5%)	23,24,24	1.41	1 (4%)
23	CLA	b	610	40	69,73,73	2.05	20 (28%)	83,113,113	2.88	33 (39%)
23	CLA	B	606	2	69,73,73	2.01	20 (28%)	83,113,113	2.87	30 (36%)
35	DGD	c	520	-	63,63,67	0.88	2 (3%)	77,77,81	1.02	5 (6%)
23	CLA	A	406	40	69,73,73	2.05	21 (30%)	83,113,113	2.81	28 (33%)
23	CLA	C	512	3	69,73,73	2.06	20 (28%)	83,113,113	2.82	30 (36%)
24	PHO	a	417	-	58,69,69	2.78	13 (22%)	56,99,99	2.98	14 (25%)
23	CLA	C	511	3	69,73,73	2.11	20 (28%)	83,113,113	2.79	31 (37%)
23	CLA	b	606	2	69,73,73	1.97	20 (28%)	83,113,113	3.00	31 (37%)
23	CLA	C	513	3	69,73,73	2.05	22 (31%)	83,113,113	2.81	30 (36%)
23	CLA	b	616	2	69,73,73	1.99	19 (27%)	83,113,113	2.92	32 (38%)
25	BCR	D	405	-	41,41,41	1.06	1 (2%)	56,56,56	1.64	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	y	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.61	10 (17%)
23	CLA	c	508	3	69,73,73	2.04	20 (28%)	83,113,113	2.78	30 (36%)
23	CLA	B	611	2	69,73,73	2.03	19 (27%)	83,113,113	2.95	34 (40%)
23	CLA	c	503	3	69,73,73	2.03	20 (28%)	83,113,113	2.82	29 (34%)
31	LHG	D	408	-	48,48,48	0.90	2 (4%)	51,54,54	0.96	3 (5%)
23	CLA	c	512	3	69,73,73	1.98	20 (28%)	83,113,113	2.72	30 (36%)
29	PL9	A	413	-	55,55,55	0.66	2 (3%)	68,69,69	1.87	21 (30%)
31	LHG	d	407	-	48,48,48	0.89	2 (4%)	51,54,54	1.01	4 (7%)
35	DGD	h	103	-	63,63,67	0.91	3 (4%)	77,77,81	1.01	3 (3%)
23	CLA	d	403	4	69,73,73	2.11	20 (28%)	83,113,113	2.92	32 (38%)
23	CLA	C	505	3	69,73,73	2.05	19 (27%)	83,113,113	2.90	27 (32%)
29	PL9	D	406	-	55,55,55	0.67	2 (3%)	68,69,69	1.66	17 (25%)
34	LMT	a	418	-	36,36,36	0.45	0	47,47,47	0.92	1 (2%)
26	GOL	o	302	-	5,5,5	0.82	0	5,5,5	1.04	0
23	CLA	b	603	2	69,73,73	2.05	20 (28%)	83,113,113	2.91	31 (37%)
31	LHG	L	101	-	48,48,48	0.92	3 (6%)	51,54,54	1.11	3 (5%)
26	GOL	v	201	-	5,5,5	1.15	0	5,5,5	0.82	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LHG	d	408	-	-	10/53/53/53	-
31	LHG	D	407	-	-	12/53/53/53	-
25	BCR	c	517	-	-	0/29/63/63	0/2/2/2
32	LMG	C	521	-	-	10/46/66/70	0/1/1/1
23	CLA	b	608	2	-	2/39/115/115	-
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
33	HTG	B	623	-	-	4/10/30/30	0/1/1/1
23	CLA	B	608	2	-	2/39/115/115	-
35	DGD	c	518	-	-	18/51/91/95	0/2/2/2
23	CLA	c	507	3	-	6/39/115/115	-
23	CLA	A	405	40	-	5/39/115/115	-
23	CLA	b	607	40	-	1/39/115/115	-
34	LMT	B	628	-	-	10/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	515	3	-	15/39/115/115	-
34	LMT	C	526	-	-	8/21/61/61	0/2/2/2
23	CLA	a	404	1	-	6/39/115/115	-
23	CLA	b	613	2	-	7/39/115/115	-
25	BCR	b	619	-	-	4/29/63/63	0/2/2/2
31	LHG	a	419	-	-	18/46/46/53	-
23	CLA	b	615	2	-	8/39/115/115	-
25	BCR	a	409	-	-	2/29/63/63	0/2/2/2
32	LMG	D	413	39	-	8/46/66/70	0/1/1/1
23	CLA	A	408	1	-	9/39/115/115	-
23	CLA	B	605	2	-	4/39/115/115	-
33	HTG	B	625	-	-	3/10/30/30	0/1/1/1
23	CLA	a	408	1	-	16/39/115/115	-
38	HEC	V	201	16	1/1/3/7	6/14/54/54	-
25	BCR	d	404	-	-	4/29/63/63	0/2/2/2
25	BCR	C	516	-	-	3/29/63/63	0/2/2/2
23	CLA	B	610	40	-	8/39/115/115	-
34	LMT	a	413	-	-	7/21/61/61	0/2/2/2
23	CLA	D	403	4	-	6/39/115/115	-
23	CLA	D	404	4	-	10/39/115/115	-
25	BCR	B	617	-	-	0/29/63/63	0/2/2/2
26	GOL	B	627	-	-	0/4/4/4	-
33	HTG	D	411	-	-	2/7/27/30	0/1/1/1
35	DGD	C	519	-	-	16/51/91/95	0/2/2/2
26	GOL	b	628	-	-	0/4/4/4	-
33	HTG	c	523	-	-	3/10/30/30	0/1/1/1
34	LMT	b	621	-	-	7/17/37/61	0/1/1/2
33	HTG	b	623	-	-	2/10/30/30	0/1/1/1
38	HEC	E	103	6,5	1/1/3/7	7/14/54/54	-
35	DGD	H	102	-	-	11/51/91/95	0/2/2/2
23	CLA	b	609	-	-	8/39/115/115	-
25	BCR	t	102	-	-	4/29/63/63	0/2/2/2
38	HEC	e	102	6,5	1/1/3/7	5/14/54/54	-
23	CLA	b	611	2	-	5/39/115/115	-
23	CLA	b	612	2	-	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	H	101	-	-	1/29/63/63	0/2/2/2
34	LMT	D	402	-	-	8/21/61/61	0/2/2/2
34	LMT	t	101	-	-	6/17/38/61	0/1/1/2
23	CLA	C	507	3	-	9/39/115/115	-
23	CLA	B	603	2	-	6/39/115/115	-
34	LMT	E	102	-	-	7/21/61/61	0/2/2/2
27	SQD	C	501	-	-	12/49/69/69	0/1/1/1
25	BCR	C	517	-	-	2/29/63/63	0/2/2/2
23	CLA	B	612	2	-	3/39/115/115	-
27	SQD	f	101	-	-	19/38/58/69	0/1/1/1
23	CLA	b	614	2	-	13/39/115/115	-
29	PL9	a	415	-	-	13/53/73/73	0/1/1/1
32	LMG	c	501	-	-	18/46/66/70	0/1/1/1
25	BCR	K	101	-	-	1/29/63/63	0/2/2/2
32	LMG	c	521	-	-	6/46/66/70	0/1/1/1
33	HTG	b	622	-	-	2/10/30/30	0/1/1/1
32	LMG	B	621	-	-	11/46/66/70	0/1/1/1
23	CLA	B	615	2	-	9/39/115/115	-
32	LMG	C	522	-	-	12/46/66/70	0/1/1/1
29	PL9	d	405	-	-	7/53/73/73	0/1/1/1
23	CLA	B	607	40	-	4/39/115/115	-
25	BCR	c	516	-	-	0/29/63/63	0/2/2/2
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
23	CLA	A	404	1	-	3/39/115/115	-
26	GOL	c	502	-	-	0/4/4/4	-
23	CLA	b	601	40	-	16/39/115/115	-
23	CLA	B	614	2	-	14/39/115/115	-
23	CLA	C	503	3	-	4/39/115/115	-
23	CLA	b	602	2	-	5/39/115/115	-
34	LMT	e	101	-	-	9/21/61/61	0/2/2/2
23	CLA	B	616	2	-	8/39/115/115	-
26	GOL	b	624	-	-	3/4/4/4	-
23	CLA	b	605	2	-	5/39/115/115	-
23	CLA	C	510	3	-	5/39/115/115	-
23	CLA	c	509	40	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	506	40	-	6/39/115/115	-
35	DGD	c	519	-	-	17/51/91/95	0/2/2/2
23	CLA	a	406	40	-	8/39/115/115	-
32	LMG	c	522	-	-	11/46/66/70	0/1/1/1
32	LMG	Z	101	-	-	9/31/51/70	0/1/1/1
23	CLA	c	504	3	-	7/39/115/115	-
31	LHG	A	416	-	-	16/53/53/53	-
34	LMT	B	630	-	-	5/17/37/61	0/1/1/2
25	BCR	k	101	-	-	2/29/63/63	0/2/2/2
23	CLA	b	604	2	-	11/39/115/115	-
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
23	CLA	c	514	3	-	15/39/115/115	-
23	CLA	B	604	2	-	10/39/115/115	-
23	CLA	c	511	3	-	14/39/115/115	-
23	CLA	c	515	3	-	9/39/115/115	-
23	CLA	C	514	3	-	14/39/115/115	-
32	LMG	m	101	-	-	10/46/66/70	0/1/1/1
27	SQD	b	620	-	-	24/49/69/69	0/1/1/1
23	CLA	B	609	2	-	5/39/115/115	-
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
24	PHO	A	415	-	-	3/37/103/103	0/5/6/6
34	LMT	m	103	-	-	7/21/61/61	0/2/2/2
27	SQD	B	620	-	-	17/49/69/69	0/1/1/1
27	SQD	a	410	-	-	14/49/69/69	0/1/1/1
23	CLA	d	402	4	-	3/39/115/115	-
24	PHO	A	407	-	-	2/37/103/103	0/5/6/6
23	CLA	c	513	3	-	8/39/115/115	-
32	LMG	d	412	39	-	9/46/66/70	0/1/1/1
33	HTG	B	622	-	-	5/10/30/30	0/1/1/1
33	HTG	V	202	-	-	1/2/19/30	0/1/1/1
33	HTG	b	625	-	-	4/10/30/30	0/1/1/1
23	CLA	B	613	2	-	8/39/115/115	-
26	GOL	B	629	-	-	0/4/4/4	-
33	HTG	h	101	-	-	2/7/27/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	a	405	40	-	11/39/115/115	-
23	CLA	C	506	40	-	8/39/115/115	-
23	CLA	C	508	3	-	11/39/115/115	-
23	CLA	C	509	40	-	7/39/115/115	-
25	BCR	h	102	-	-	0/29/63/63	0/2/2/2
32	LMG	C	502	-	-	25/46/66/70	0/1/1/1
23	CLA	C	504	3	-	10/39/115/115	-
24	PHO	a	407	-	-	5/37/103/103	0/5/6/6
34	LMT	M	101	-	-	6/21/61/61	0/2/2/2
23	CLA	B	601	40	-	10/39/115/115	-
35	DGD	C	520	-	-	10/51/91/95	0/2/2/2
23	CLA	B	602	2	-	5/39/115/115	-
38	HEC	v	202	16	1/1/3/7	4/14/54/54	-
26	GOL	A	410	-	-	2/4/4/4	-
32	LMG	z	101	-	-	8/34/54/70	0/1/1/1
23	CLA	c	510	3	-	10/39/115/115	-
34	LMT	M	103	-	-	9/21/61/61	0/2/2/2
23	CLA	c	505	3	-	1/39/115/115	-
27	SQD	D	412	-	-	15/38/58/69	0/1/1/1
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
31	LHG	d	406	-	-	15/53/53/53	-
26	GOL	C	524	-	-	0/4/4/4	-
27	SQD	a	412	-	-	17/49/69/69	0/1/1/1
31	LHG	E	101	-	-	15/46/46/53	-
31	LHG	b	629	-	-	15/53/53/53	-
34	LMT	b	627	-	-	9/17/37/61	0/1/1/2
25	BCR	Y	101	-	-	6/29/63/63	0/2/2/2
35	DGD	C	518	-	-	14/51/91/95	0/2/2/2
26	GOL	a	411	-	-	4/4/4/4	-
26	GOL	O	302	-	-	4/4/4/4	-
26	GOL	B	624	-	-	2/4/4/4	-
27	SQD	A	411	-	-	11/49/69/69	0/1/1/1
33	HTG	C	523	-	-	1/10/30/30	0/1/1/1
23	CLA	b	610	40	-	9/39/115/115	-
23	CLA	B	606	2	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	DGD	c	520	-	-	10/51/91/95	0/2/2/2
23	CLA	A	406	40	-	6/39/115/115	-
23	CLA	C	512	3	-	10/39/115/115	-
24	PHO	a	417	-	-	3/37/103/103	0/5/6/6
23	CLA	C	511	3	-	5/39/115/115	-
23	CLA	b	606	2	-	13/39/115/115	-
23	CLA	C	513	3	-	2/39/115/115	-
23	CLA	b	616	2	-	9/39/115/115	-
25	BCR	D	405	-	-	8/29/63/63	0/2/2/2
25	BCR	y	101	-	-	6/29/63/63	0/2/2/2
23	CLA	c	508	3	-	10/39/115/115	-
23	CLA	B	611	2	-	3/39/115/115	-
23	CLA	c	503	3	-	7/39/115/115	-
31	LHG	D	408	-	-	13/53/53/53	-
23	CLA	c	512	3	-	7/39/115/115	-
29	PL9	A	413	-	-	16/53/73/73	0/1/1/1
31	LHG	d	407	-	-	20/53/53/53	-
35	DGD	h	103	-	-	14/51/91/95	0/2/2/2
23	CLA	d	403	4	-	8/39/115/115	-
23	CLA	C	505	3	-	4/39/115/115	-
29	PL9	D	406	-	-	8/53/73/73	0/1/1/1
34	LMT	a	418	-	-	4/21/61/61	0/2/2/2
26	GOL	o	302	-	-	2/4/4/4	-
23	CLA	b	603	2	-	3/39/115/115	-
31	LHG	L	101	-	-	14/53/53/53	-
26	GOL	v	201	-	-	2/4/4/4	-

The worst 5 of 1604 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	417	PHO	C1B-C2B	9.03	1.49	1.39
24	A	407	PHO	C1D-C2D	8.87	1.49	1.39
24	a	417	PHO	C1D-C2D	8.72	1.49	1.39
24	a	407	PHO	C1B-C2B	8.65	1.49	1.39
24	A	415	PHO	C1D-C2D	8.25	1.48	1.39

The worst 5 of 2778 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	407	PHO	C2D-C1D-ND	12.13	117.90	109.53
24	a	417	PHO	C2D-C1D-ND	11.78	117.66	109.53
24	A	415	PHO	C2D-C1D-ND	10.95	117.08	109.53
24	A	407	PHO	C2D-C1D-ND	10.88	117.04	109.53
23	B	614	CLA	C2D-C1D-ND	10.44	117.80	110.10

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
38	E	103	HEC	NA
38	V	201	HEC	NA
38	e	102	HEC	NA
38	v	202	HEC	NA

5 of 1332 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	605	CLA	C2-C3-C5-C6
23	B	605	CLA	C4-C3-C5-C6
23	B	606	CLA	CHA-CBD-CGD-O1D
23	B	606	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

138 monomers are involved in 270 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	d	408	LHG	5	0
31	D	407	LHG	1	0
25	c	517	BCR	1	0
32	C	521	LMG	1	0
23	b	608	CLA	3	0
25	b	618	BCR	3	0
33	B	623	HTG	2	0
35	c	518	DGD	1	0
23	c	507	CLA	6	0
23	A	405	CLA	2	0
23	C	515	CLA	1	0
34	C	526	LMT	2	0
23	a	404	CLA	1	0
23	b	613	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	b	619	BCR	5	0
31	a	419	LHG	5	0
23	b	615	CLA	2	0
25	a	409	BCR	2	0
32	D	413	LMG	1	0
23	A	408	CLA	4	0
23	B	605	CLA	4	0
23	a	408	CLA	2	0
38	V	201	HEC	1	0
25	d	404	BCR	1	0
23	B	610	CLA	2	0
34	a	413	LMT	1	0
23	D	403	CLA	2	0
25	B	617	BCR	2	0
33	D	411	HTG	1	0
35	C	519	DGD	2	0
26	b	628	GOL	1	0
33	c	523	HTG	1	0
34	b	621	LMT	1	0
35	H	102	DGD	1	0
38	E	103	HEC	1	0
23	b	609	CLA	2	0
25	t	102	BCR	5	0
38	e	102	HEC	2	0
25	H	101	BCR	3	0
34	D	402	LMT	2	0
23	C	507	CLA	2	0
23	B	603	CLA	1	0
34	E	102	LMT	1	0
27	C	501	SQD	3	0
25	C	517	BCR	1	0
23	B	612	CLA	1	0
27	f	101	SQD	2	0
23	b	614	CLA	1	0
29	a	415	PL9	6	0
32	c	501	LMG	4	0
25	K	101	BCR	1	0
32	c	521	LMG	1	0
33	b	622	HTG	2	0
32	B	621	LMG	3	0
23	B	615	CLA	5	0
29	d	405	PL9	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	607	CLA	2	0
25	c	516	BCR	4	0
25	B	618	BCR	4	0
23	A	404	CLA	3	0
26	c	502	GOL	1	0
23	b	601	CLA	1	0
23	B	614	CLA	3	0
23	C	503	CLA	5	0
23	B	616	CLA	5	0
23	b	605	CLA	6	0
23	C	510	CLA	3	0
23	c	509	CLA	3	0
23	c	506	CLA	2	0
35	c	519	DGD	1	0
23	a	406	CLA	1	0
31	A	416	LHG	2	0
25	k	101	BCR	1	0
23	b	604	CLA	2	0
25	A	409	BCR	2	0
23	c	514	CLA	4	0
23	B	604	CLA	4	0
23	c	511	CLA	3	0
23	c	515	CLA	4	0
23	C	514	CLA	1	0
32	m	101	LMG	2	0
27	b	620	SQD	1	0
23	B	609	CLA	1	0
25	b	617	BCR	1	0
25	B	619	BCR	1	0
24	A	415	PHO	1	0
27	a	410	SQD	2	0
23	d	402	CLA	1	0
24	A	407	PHO	2	0
23	c	513	CLA	3	0
32	d	412	LMG	2	0
33	B	622	HTG	2	0
33	b	625	HTG	1	0
23	B	613	CLA	3	0
33	h	101	HTG	1	0
23	a	405	CLA	5	0
23	C	506	CLA	2	0
23	C	508	CLA	6	0

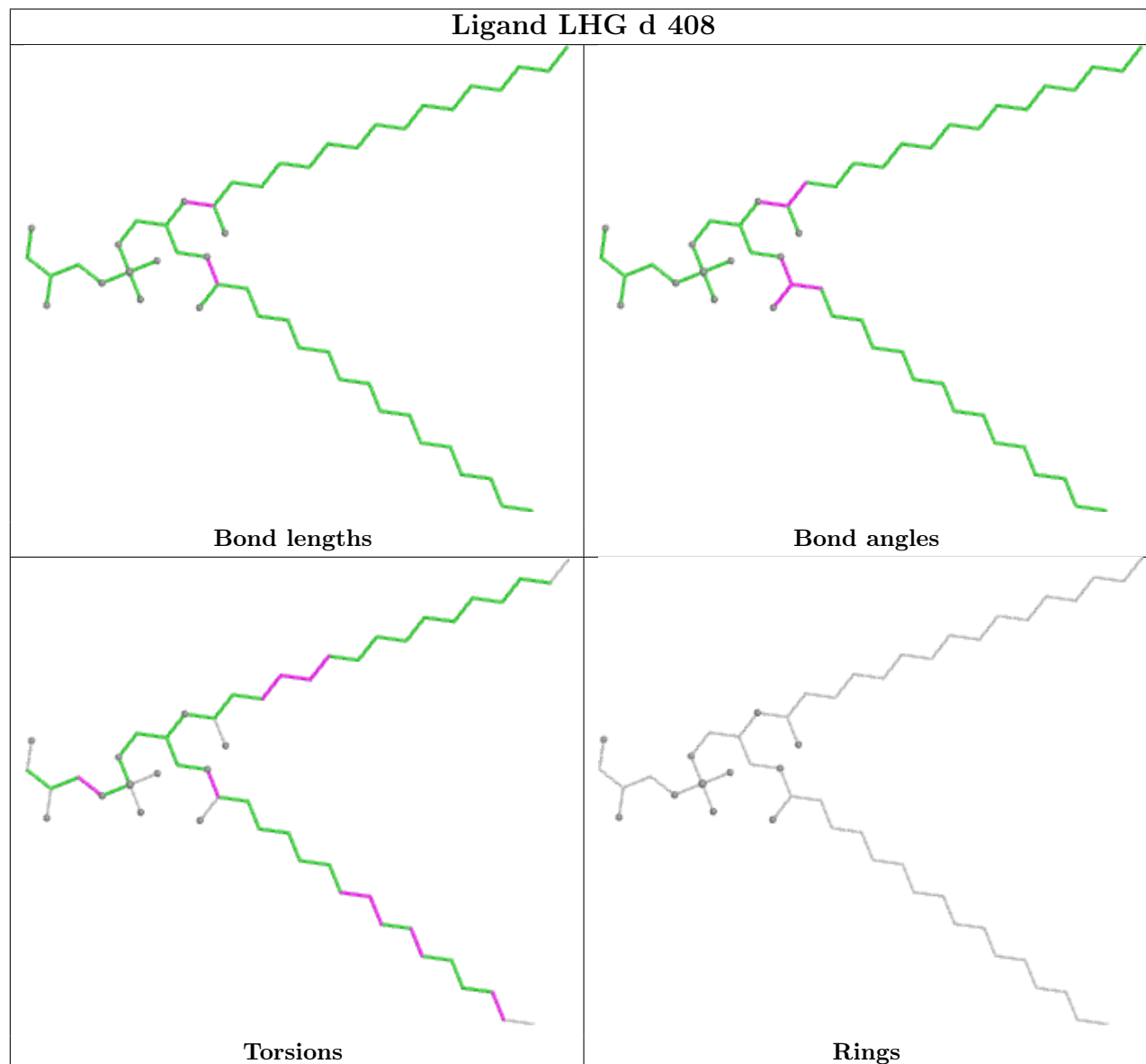
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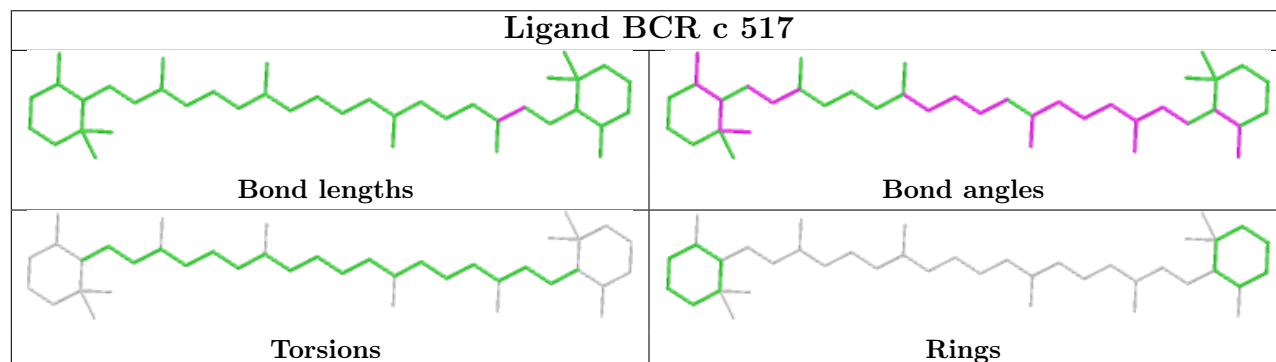
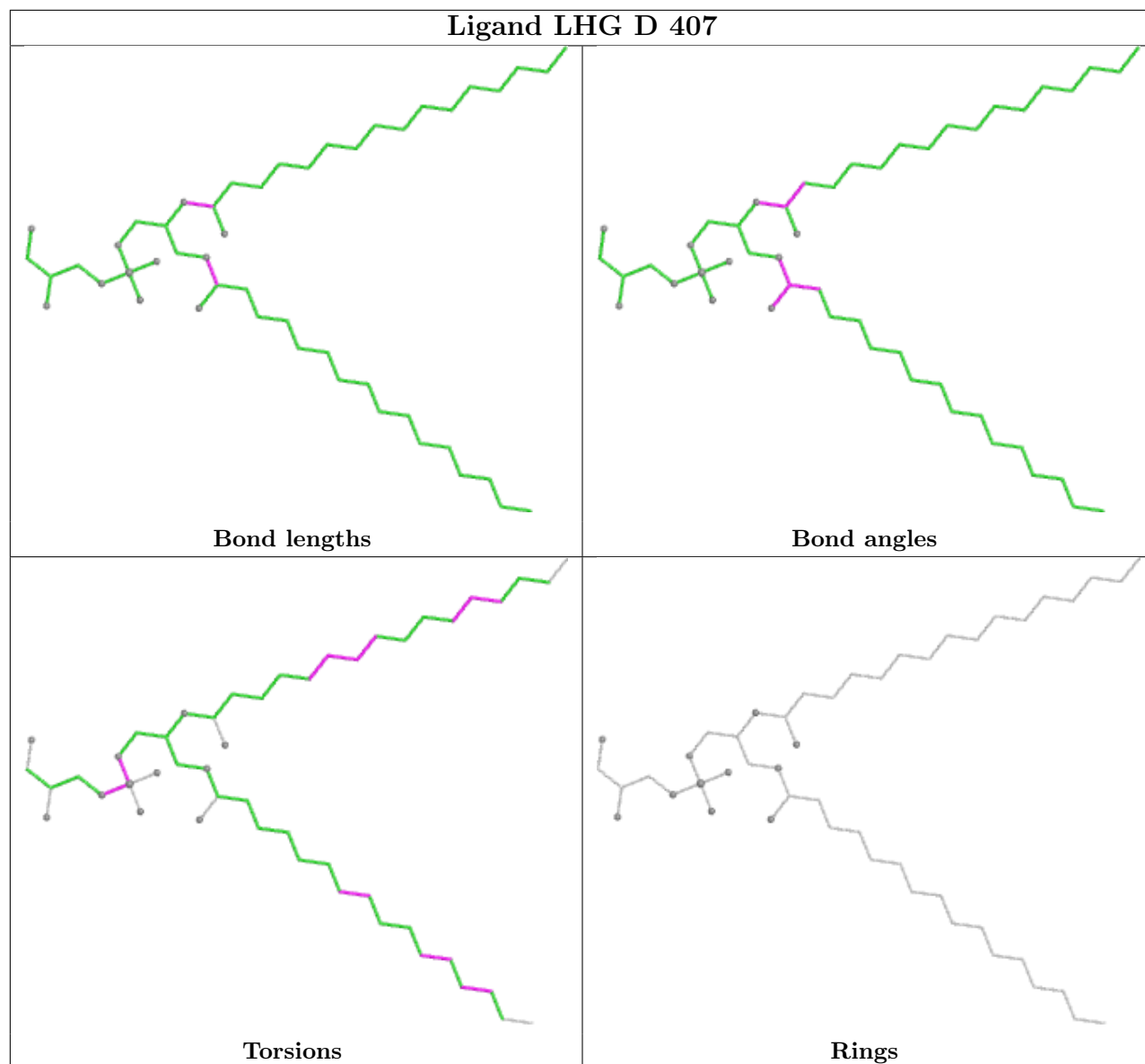
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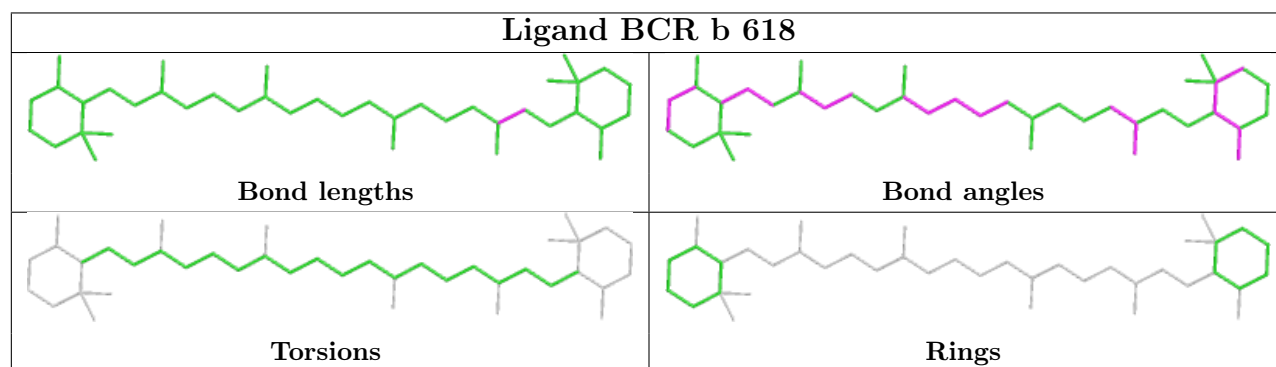
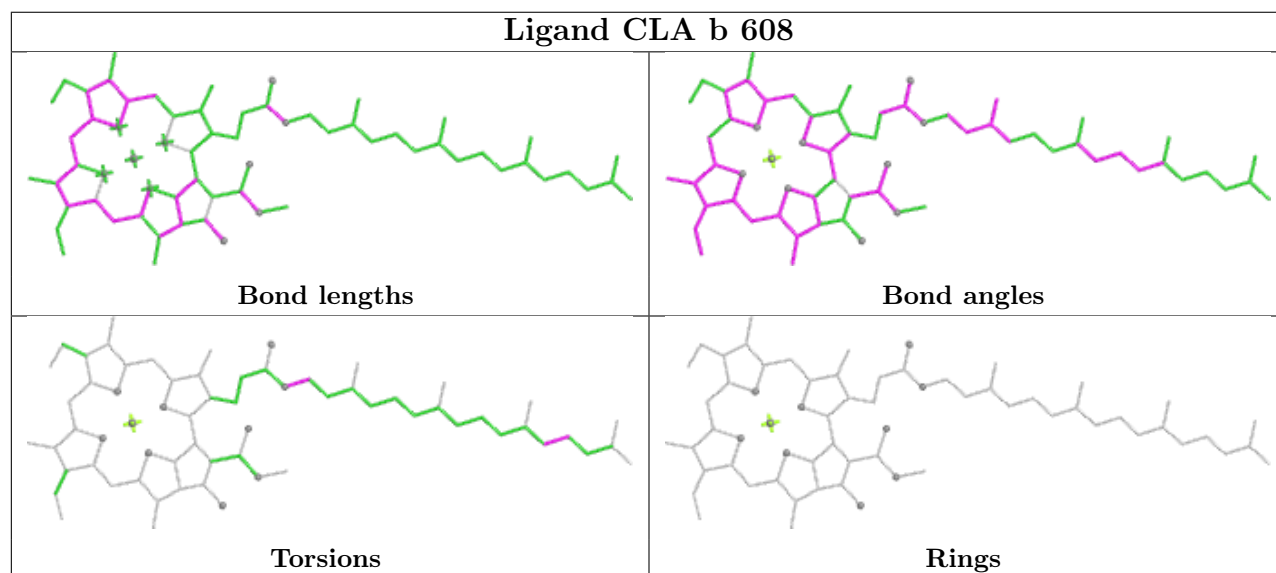
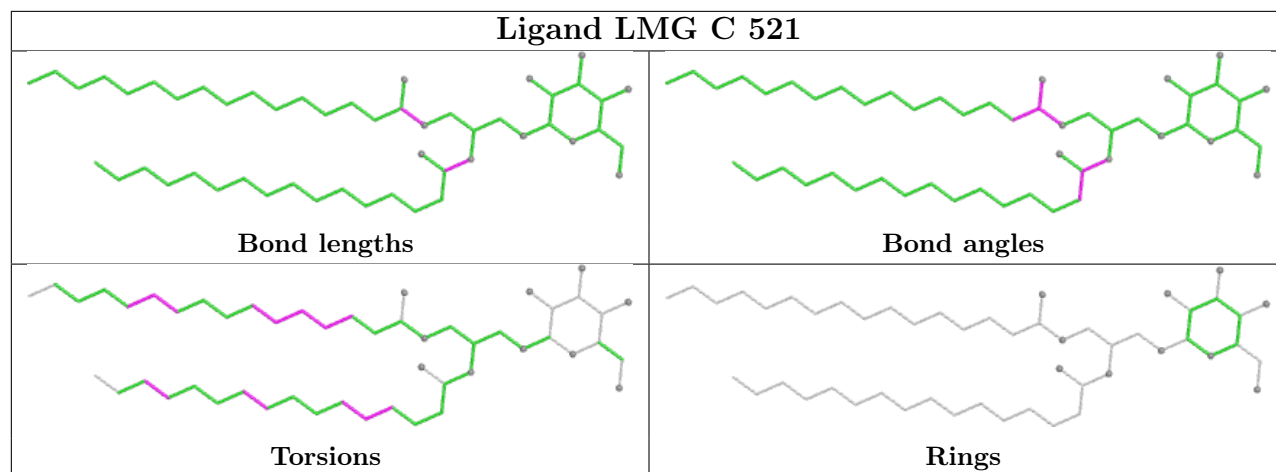
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	C	509	CLA	3	0
25	h	102	BCR	3	0
32	C	502	LMG	3	0
23	C	504	CLA	5	0
24	a	407	PHO	2	0
34	M	101	LMT	3	0
23	B	601	CLA	1	0
35	C	520	DGD	3	0
23	B	602	CLA	3	0
32	z	101	LMG	2	0
23	c	510	CLA	2	0
23	c	505	CLA	5	0
25	T	101	BCR	4	0
31	d	406	LHG	3	0
31	E	101	LHG	2	0
25	Y	101	BCR	1	0
35	C	518	DGD	4	0
27	A	411	SQD	1	0
23	b	610	CLA	1	0
23	B	606	CLA	2	0
35	c	520	DGD	2	0
23	A	406	CLA	2	0
23	C	512	CLA	2	0
24	a	417	PHO	3	0
23	b	606	CLA	7	0
23	C	513	CLA	2	0
23	b	616	CLA	5	0
25	y	101	BCR	2	0
23	c	508	CLA	1	0
23	c	503	CLA	3	0
31	D	408	LHG	5	0
23	c	512	CLA	1	0
29	A	413	PL9	5	0
31	d	407	LHG	2	0
23	C	505	CLA	4	0
29	D	406	PL9	2	0
34	a	418	LMT	2	0
23	b	603	CLA	3	0
31	L	101	LHG	2	0
26	v	201	GOL	1	0

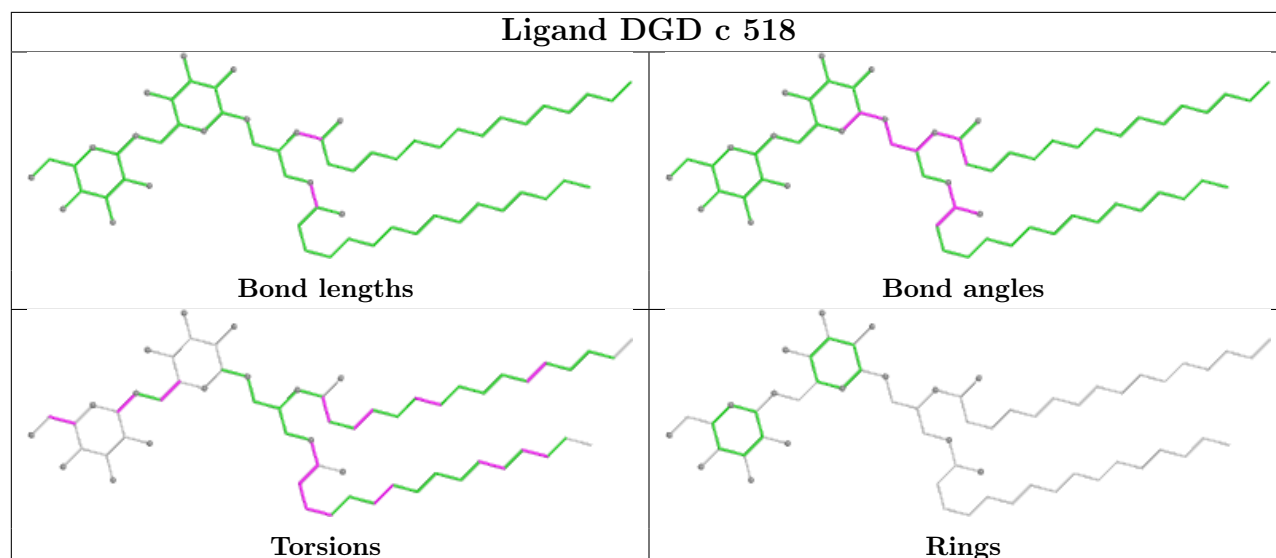
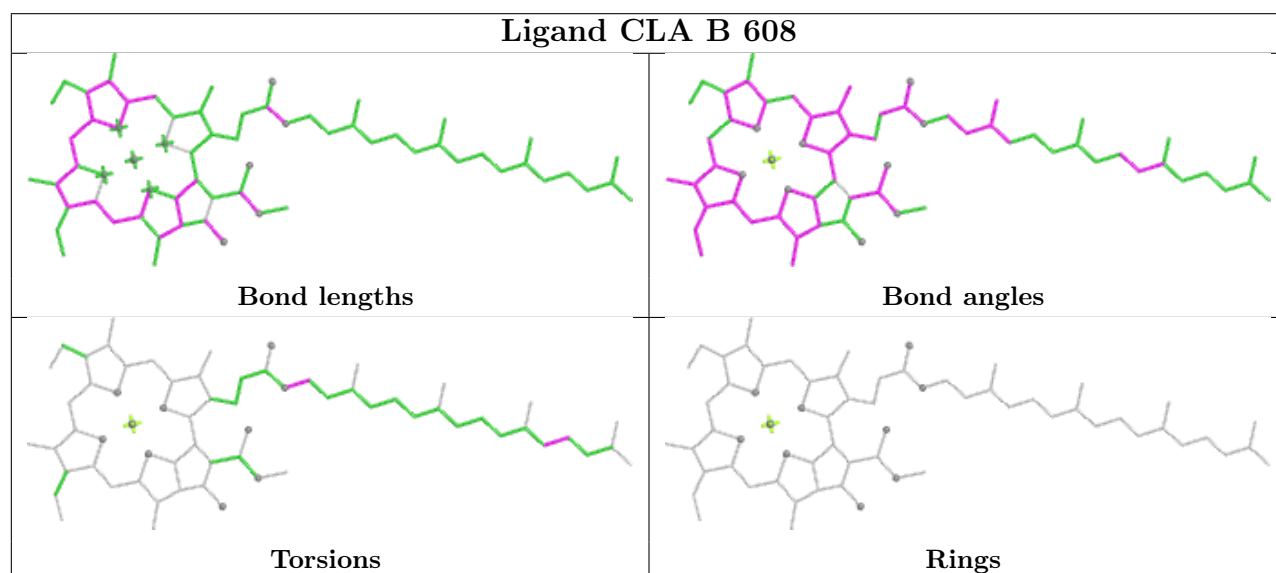
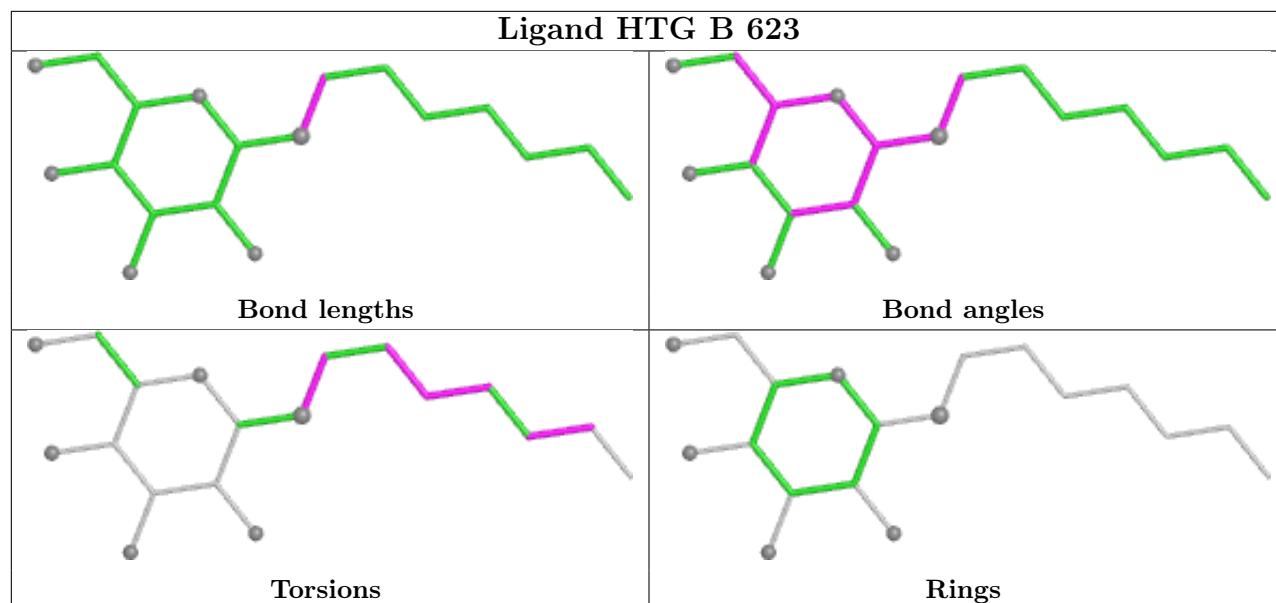
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

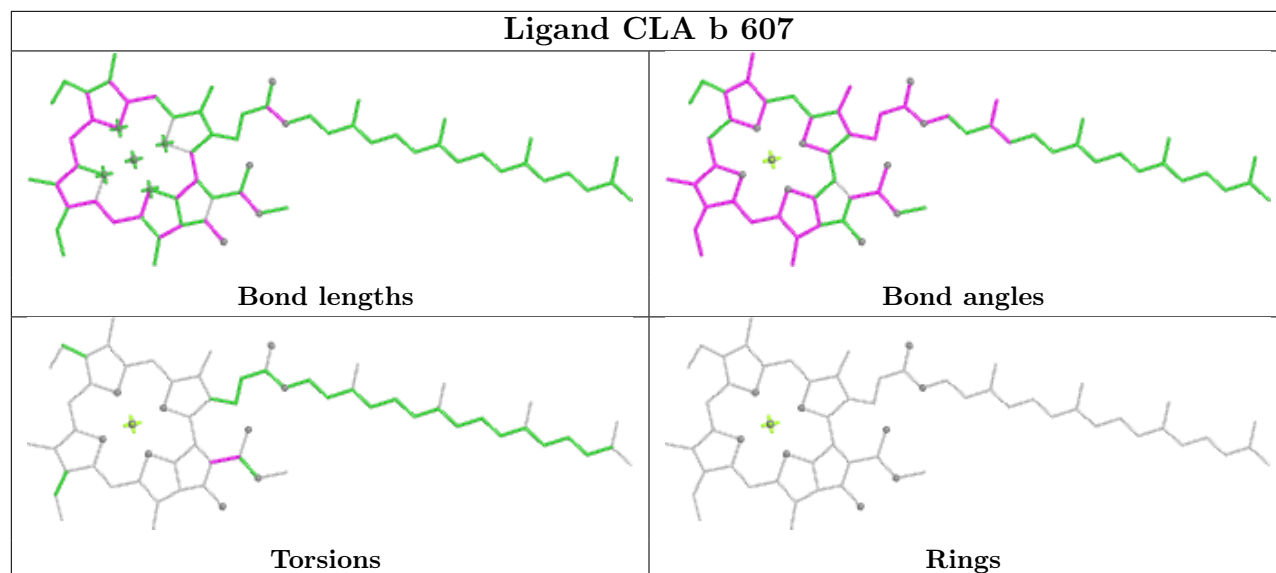
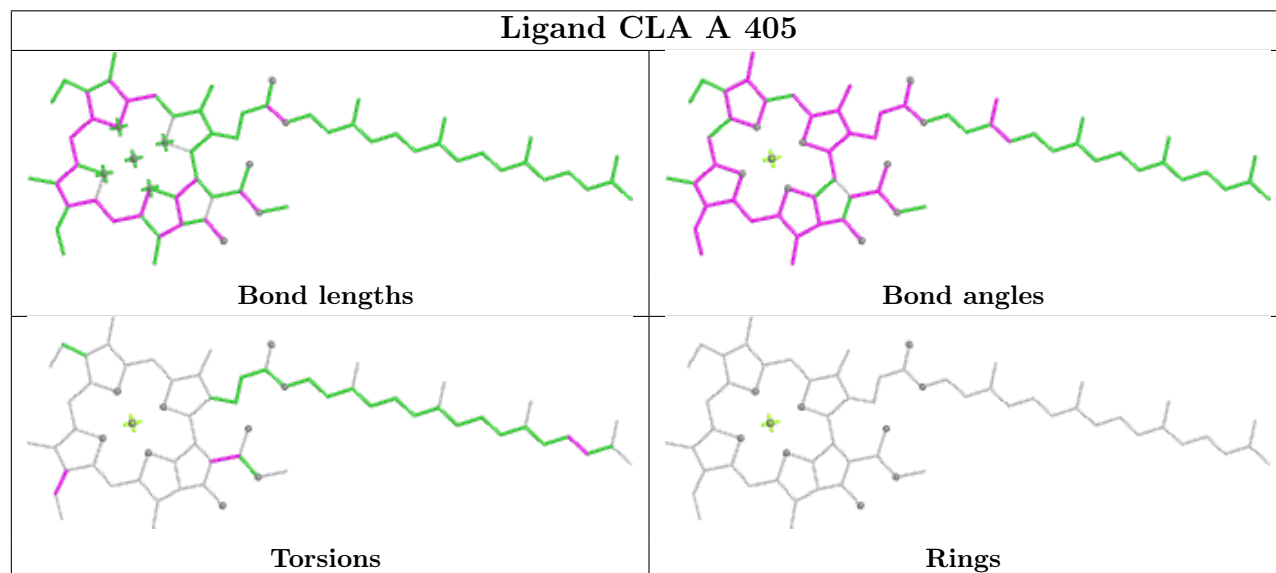
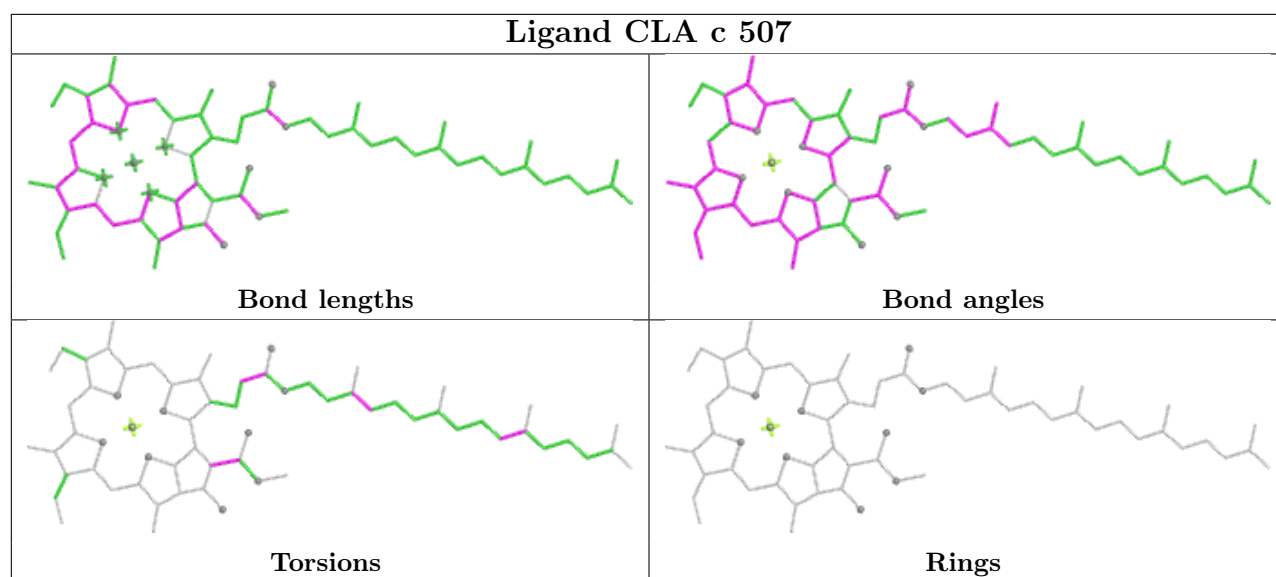
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

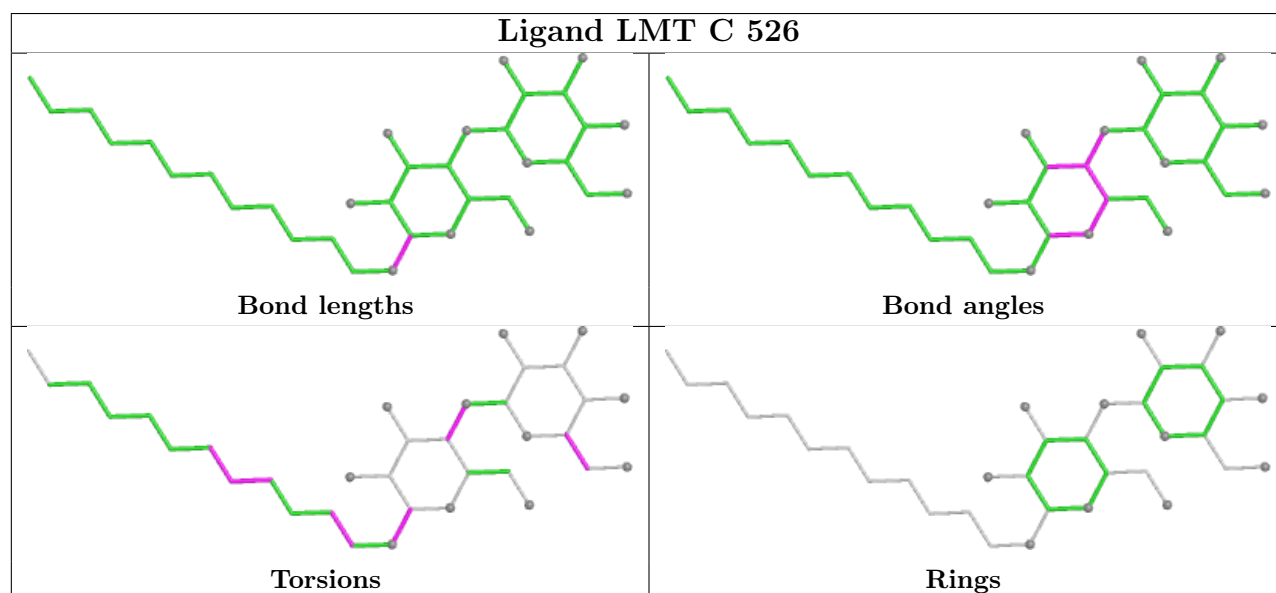
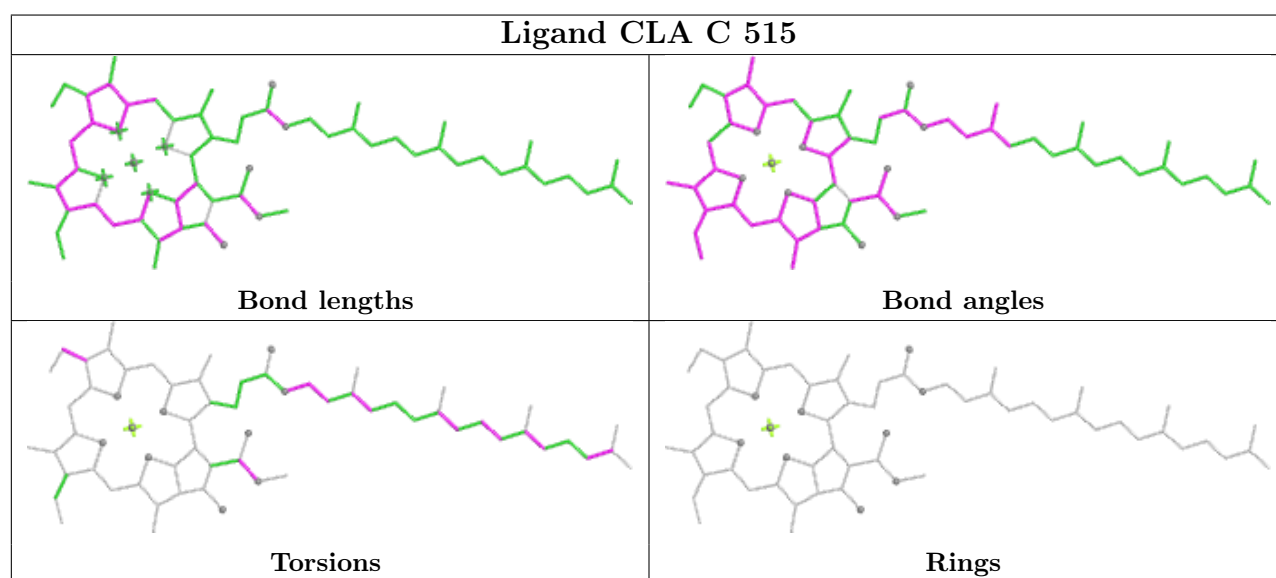
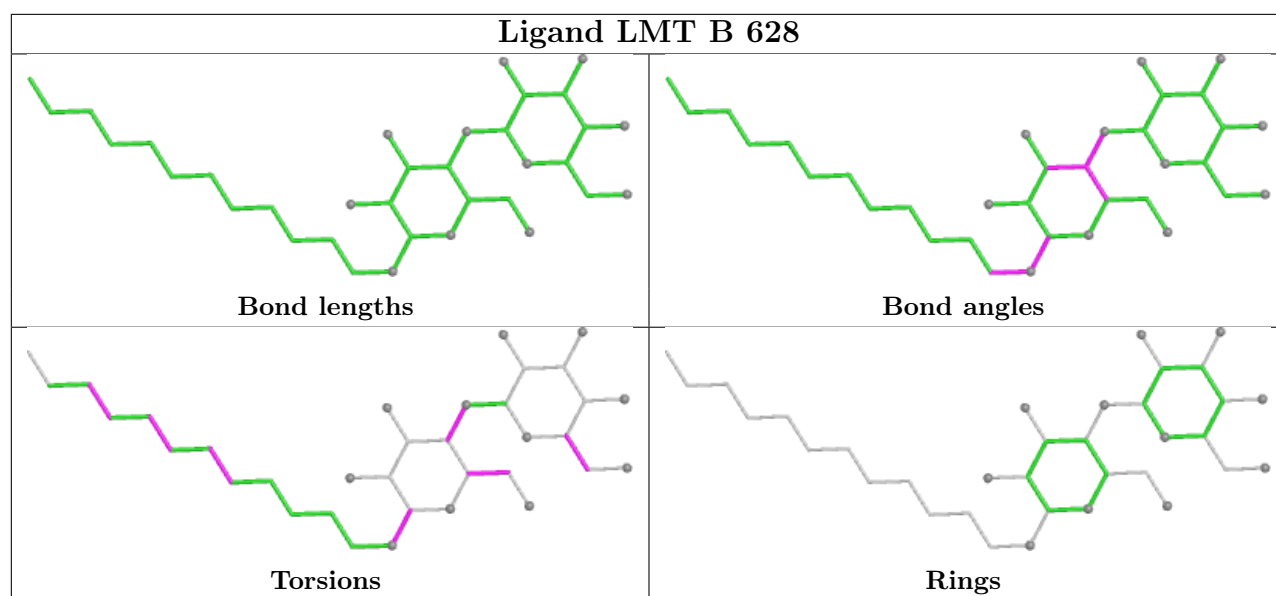


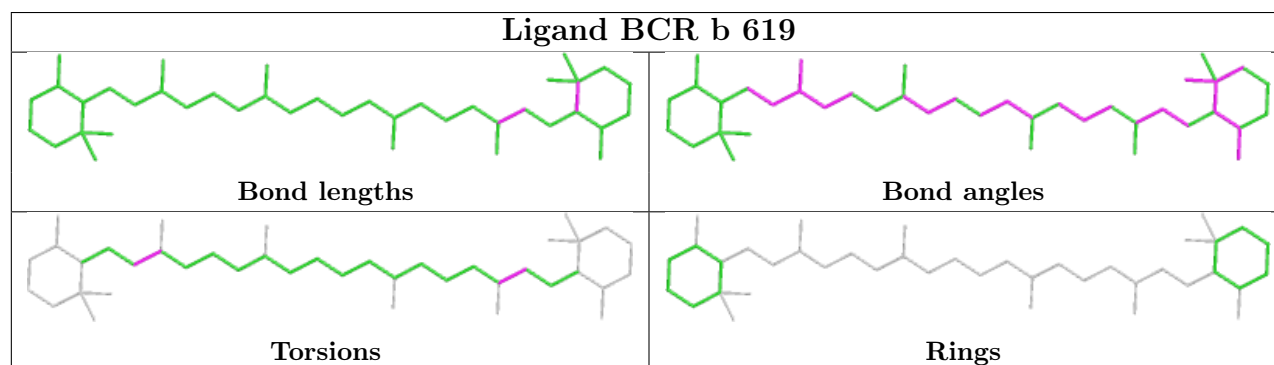
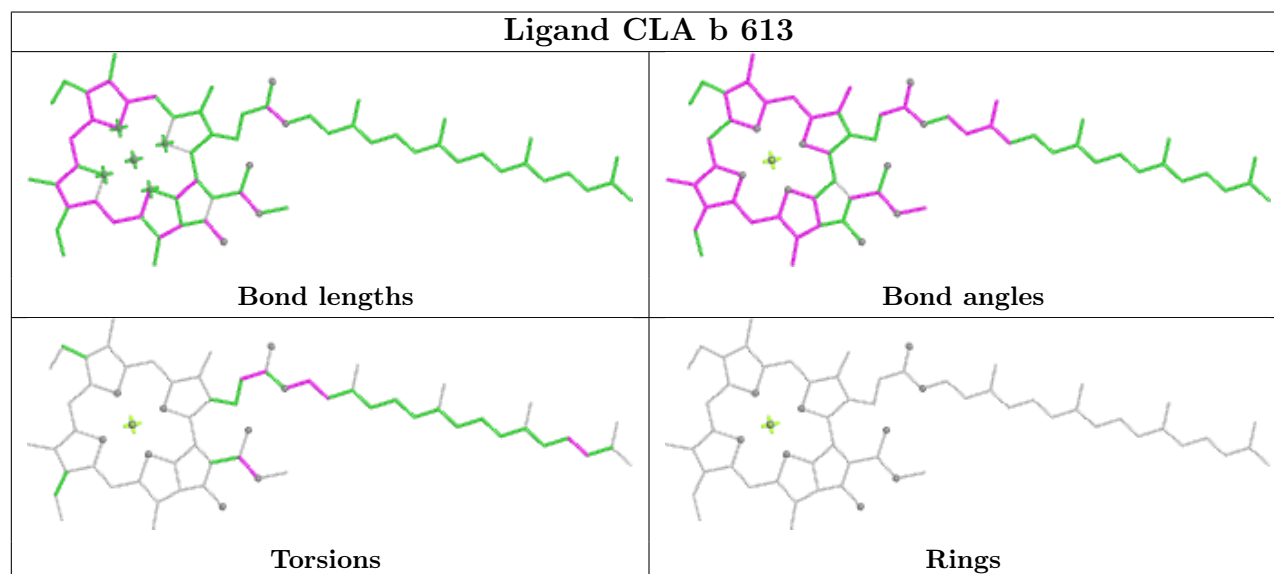
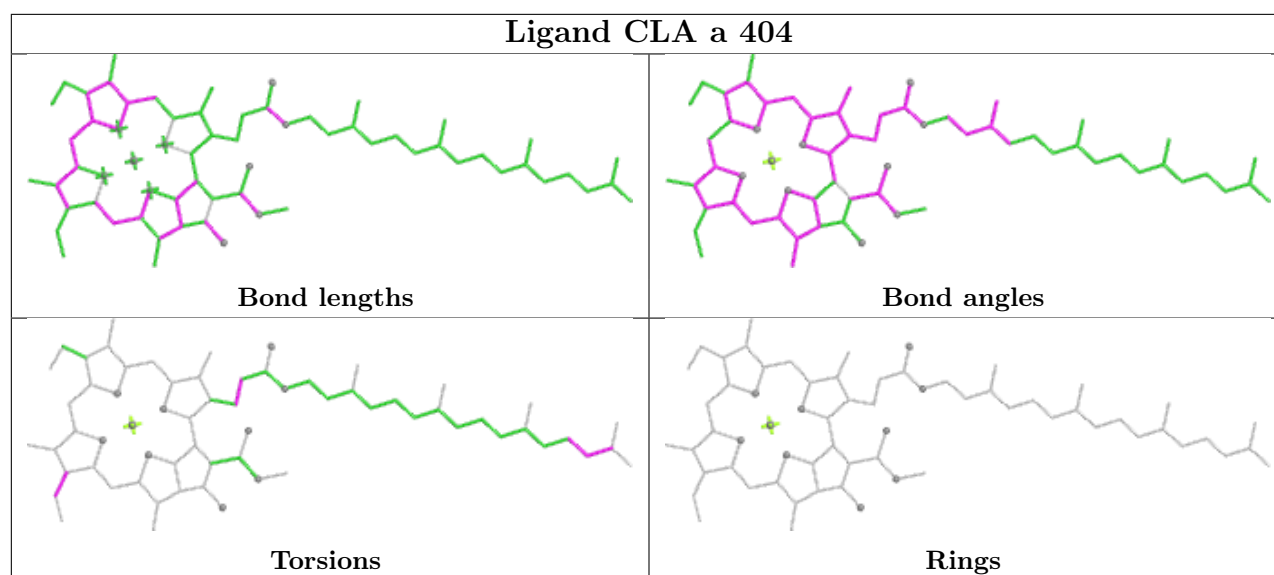


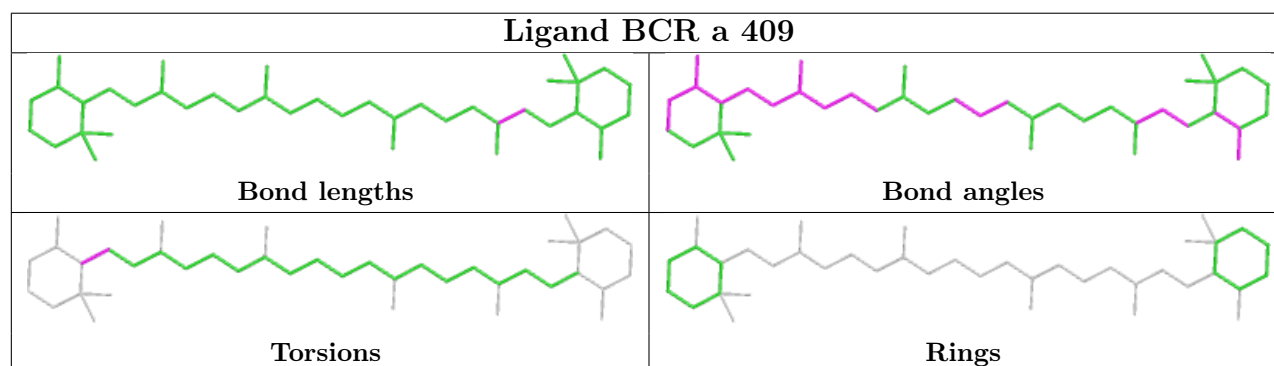
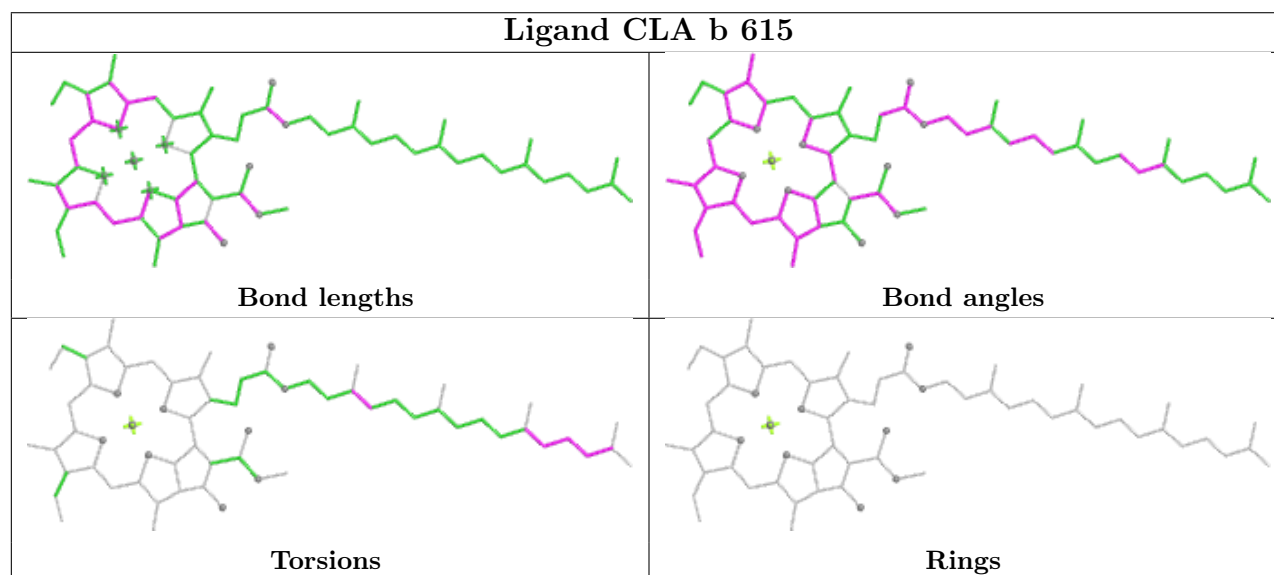
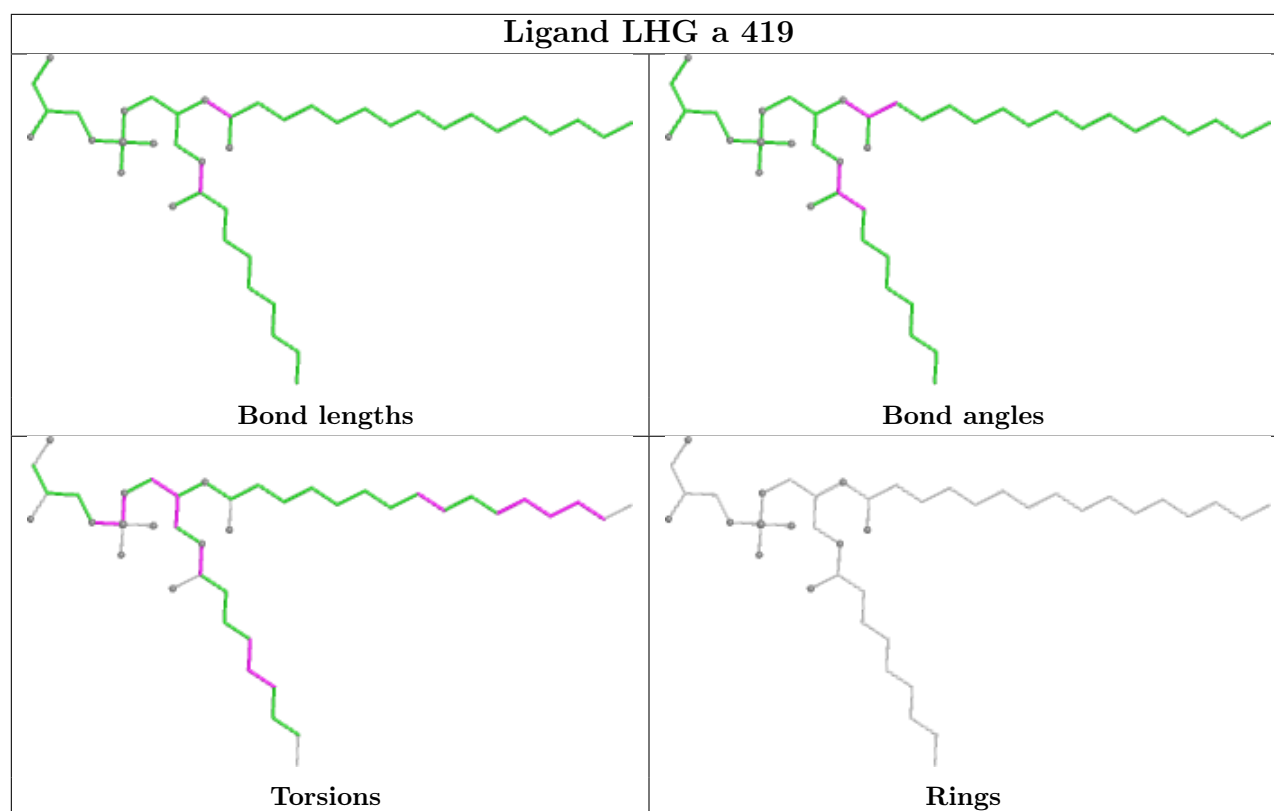


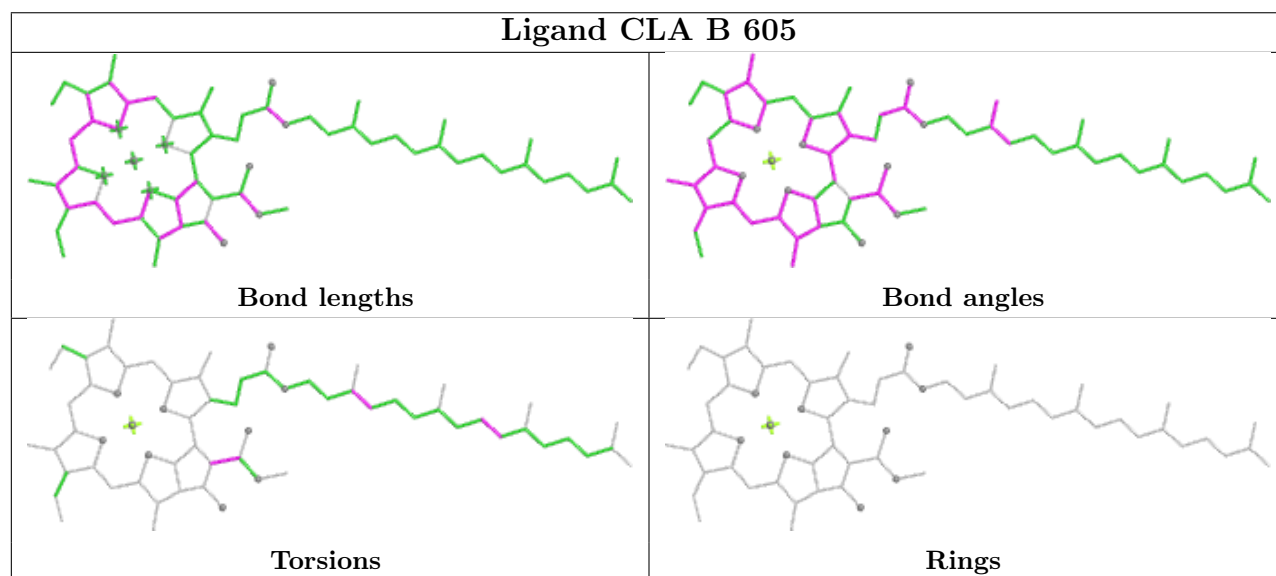
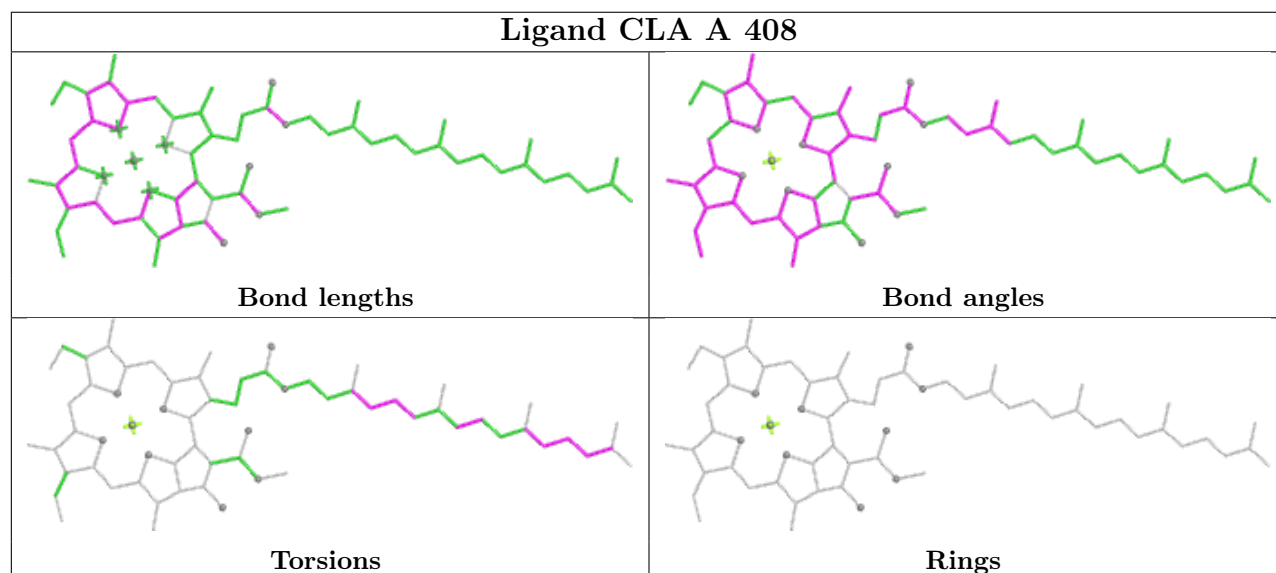
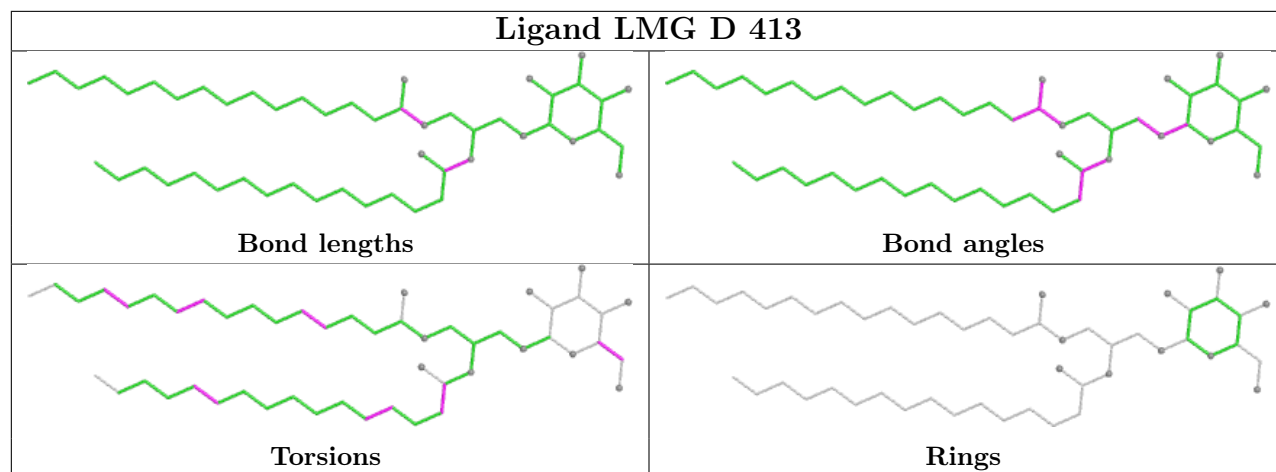


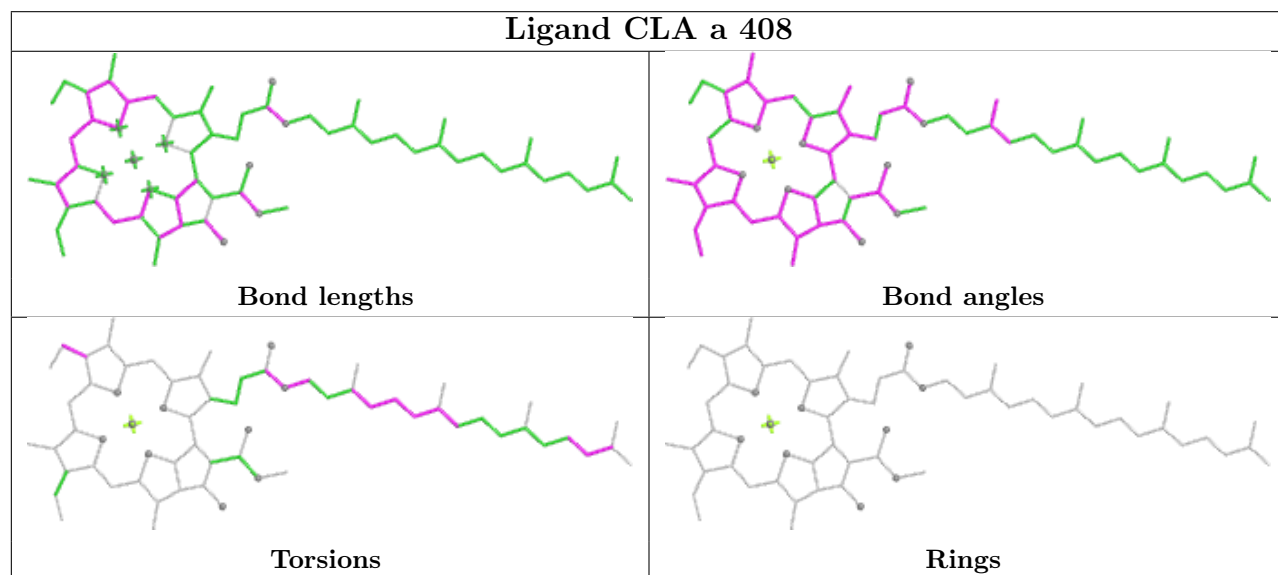
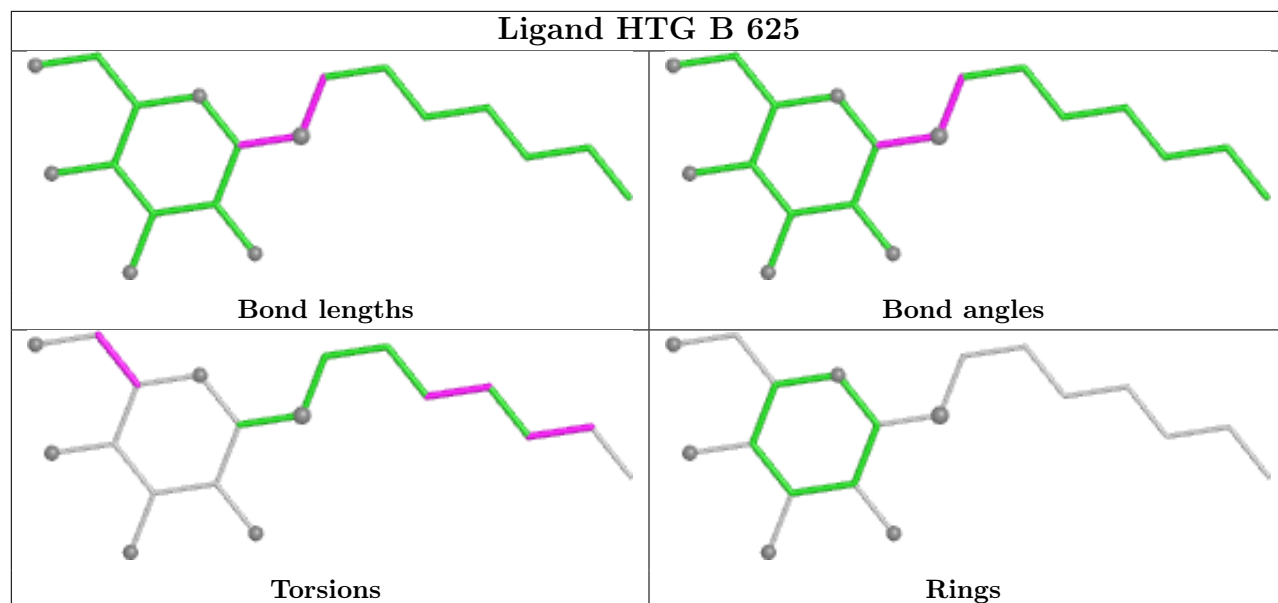




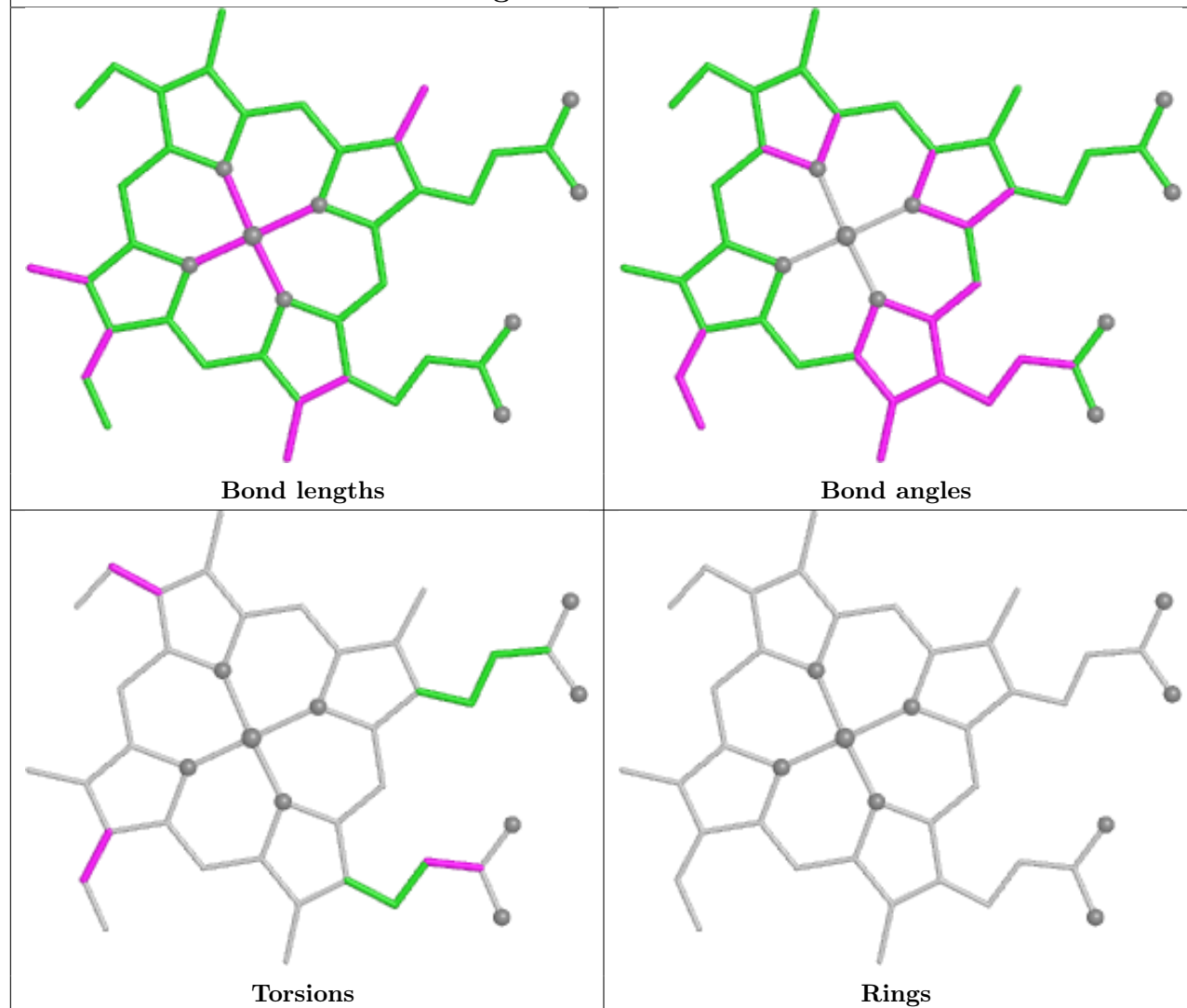




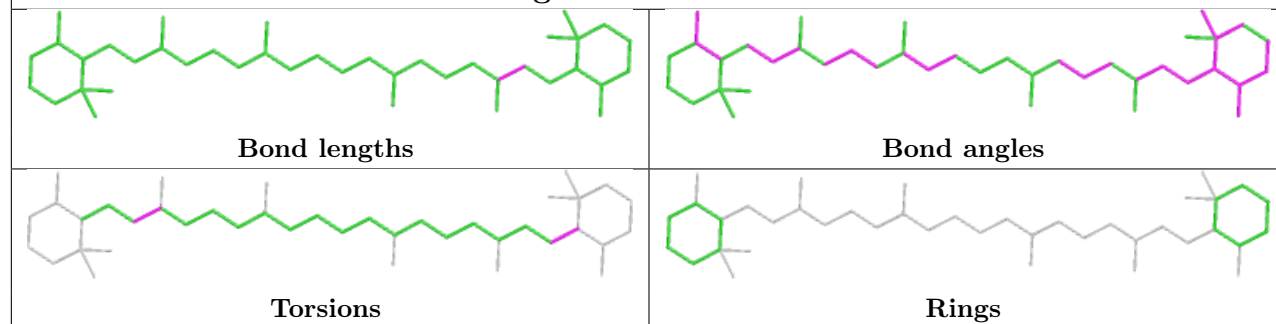


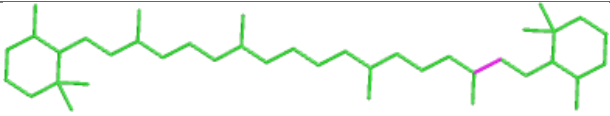
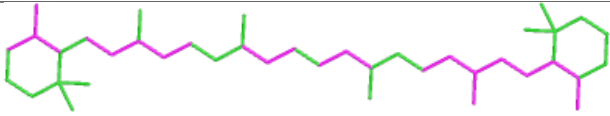
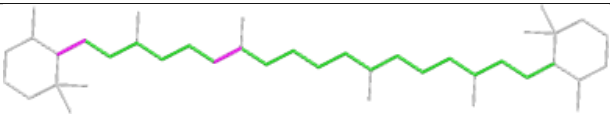
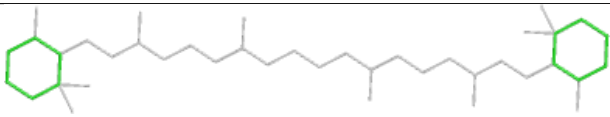
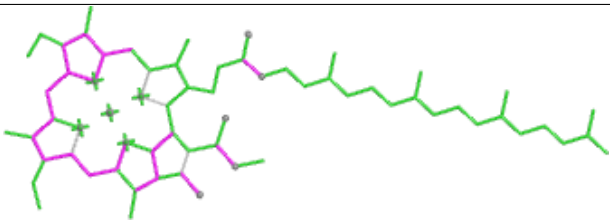
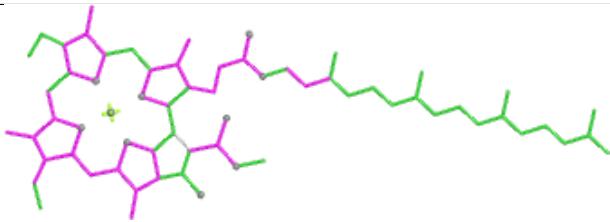
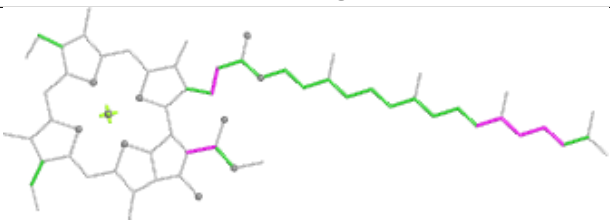
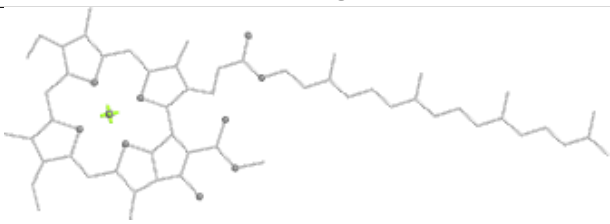
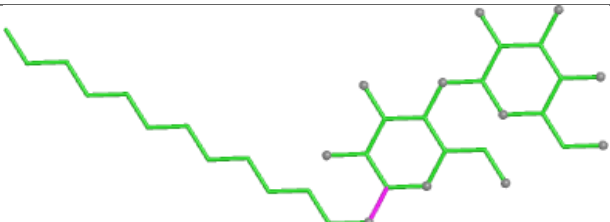
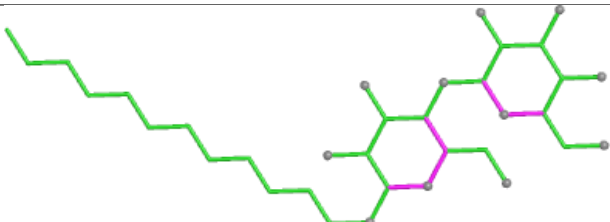
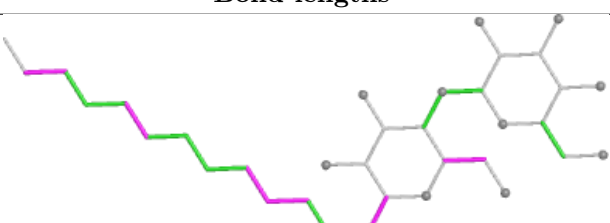
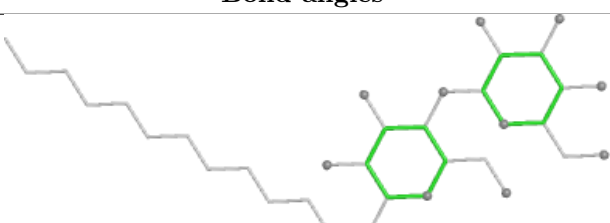


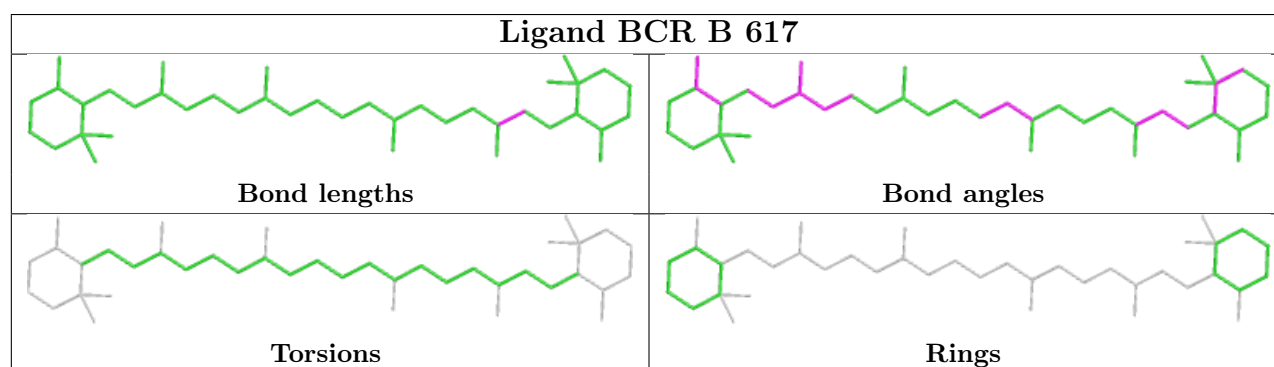
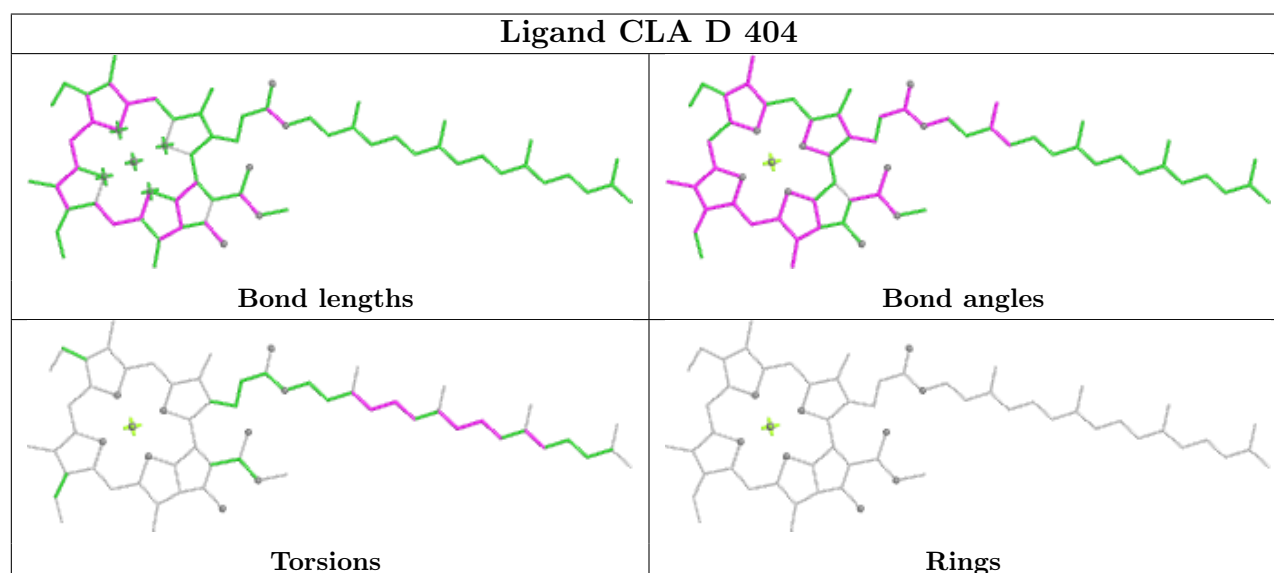
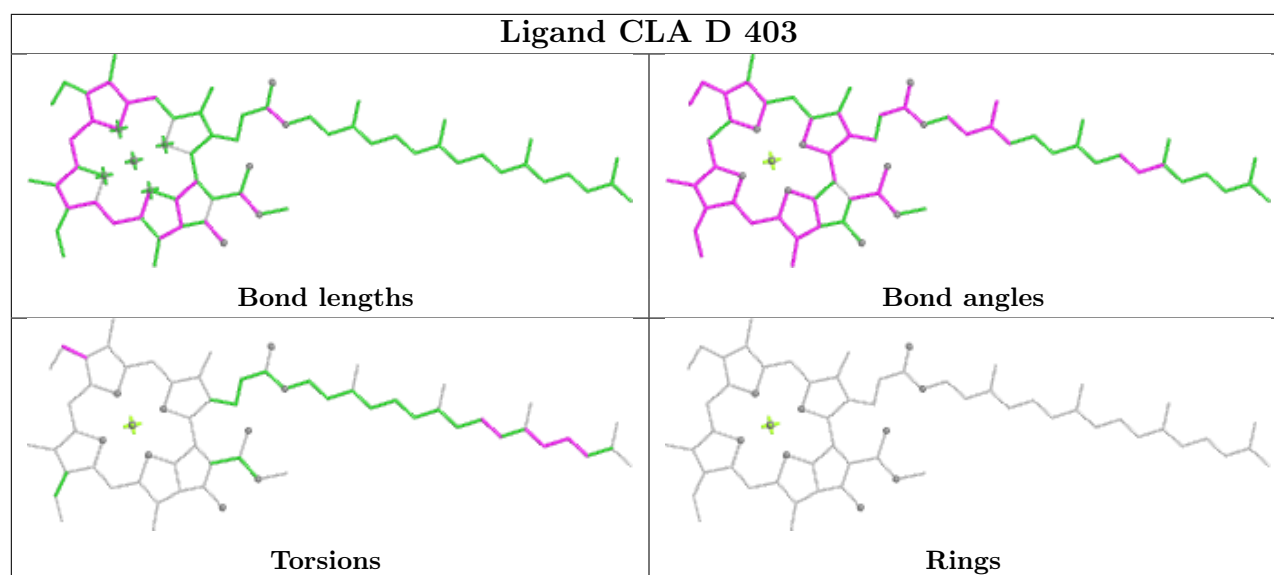
Ligand HEC V 201

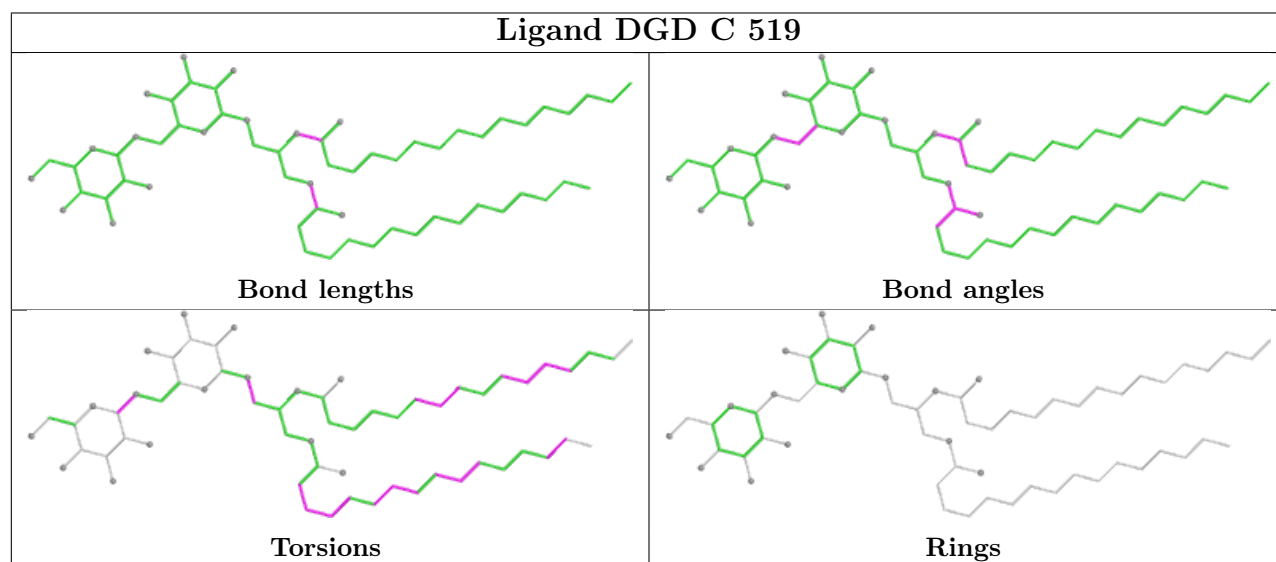
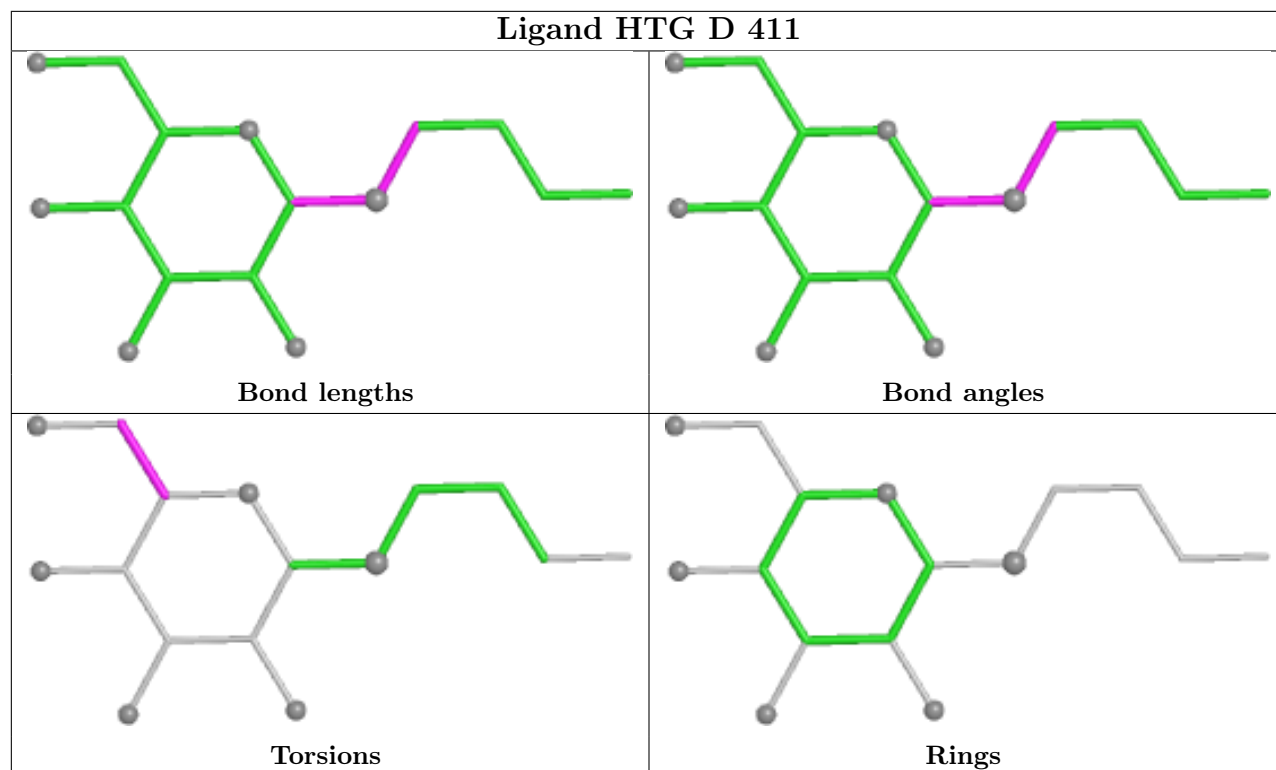


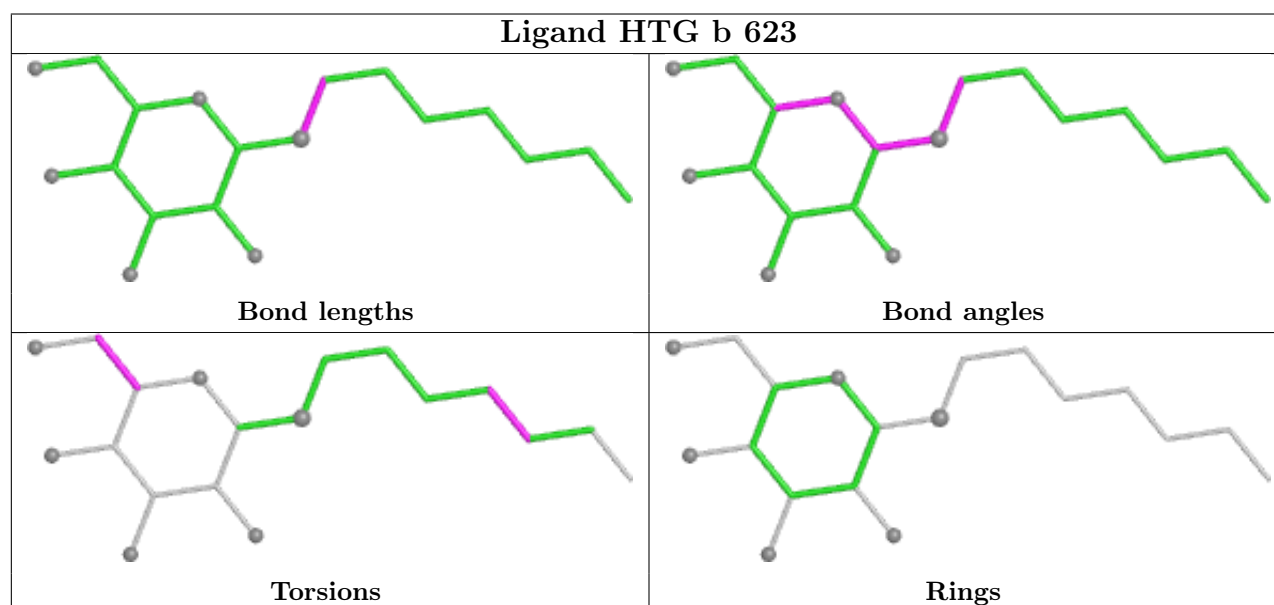
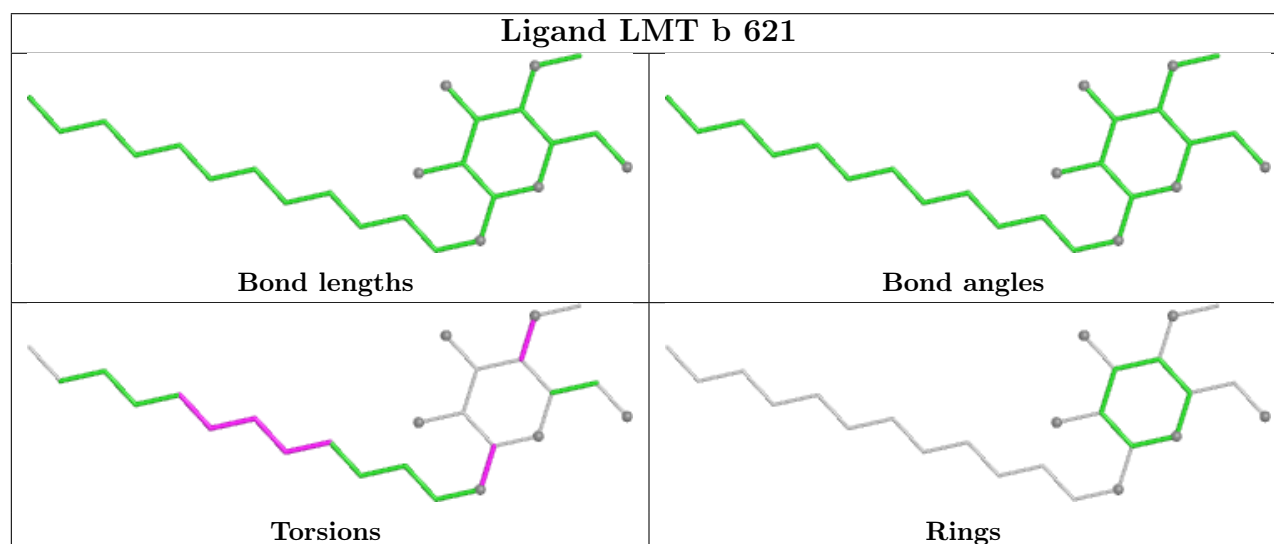
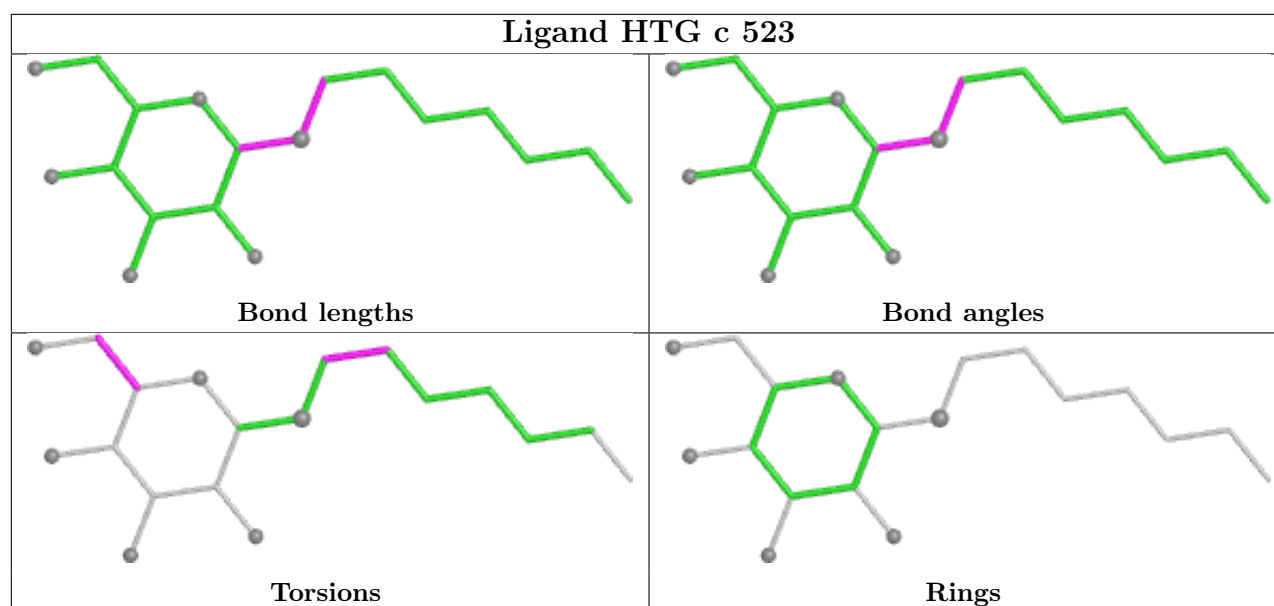
Ligand BCR d 404

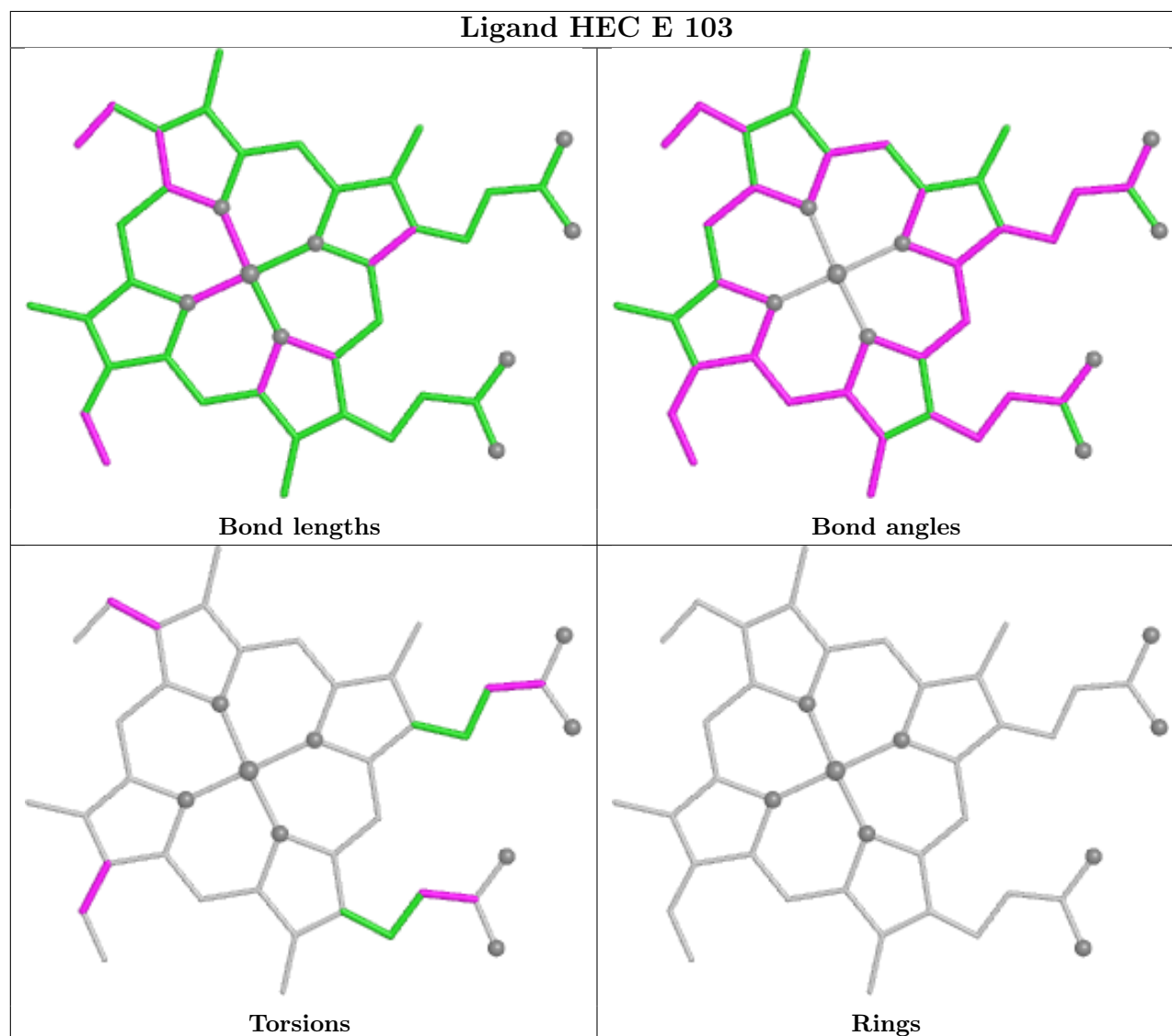
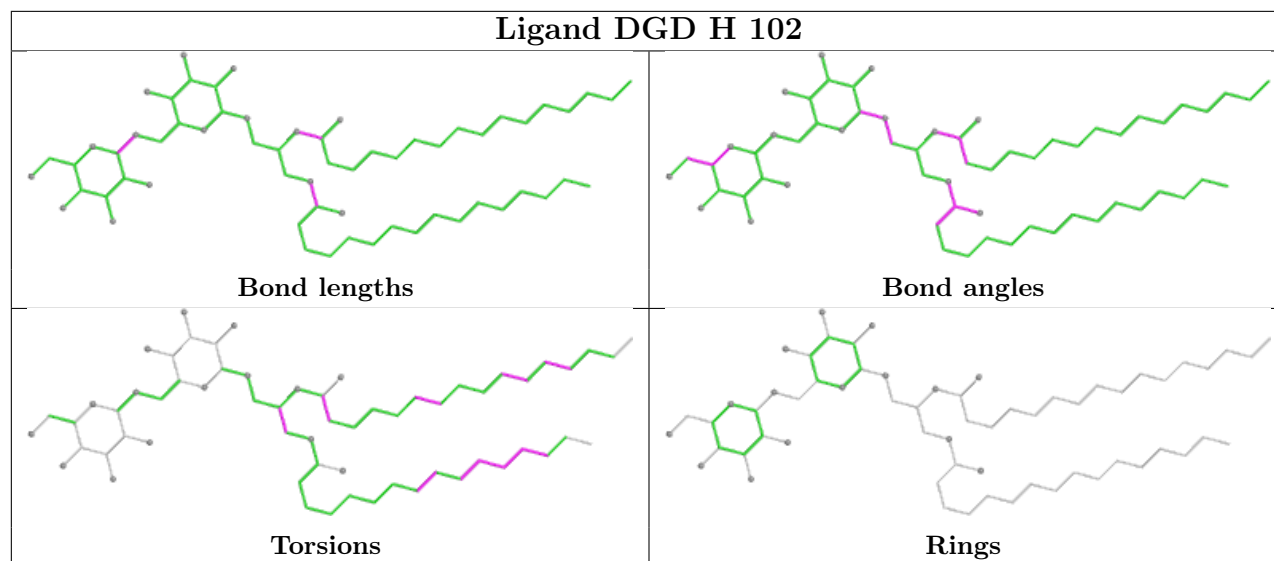


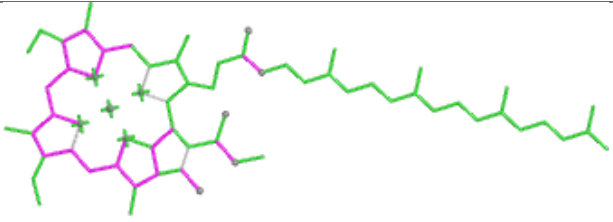
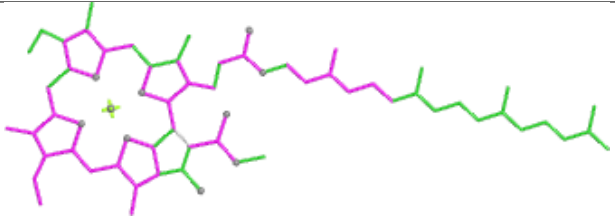
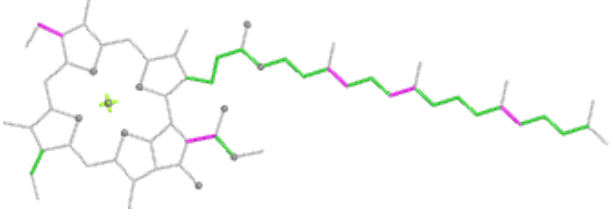
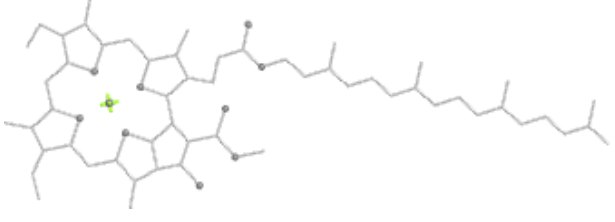
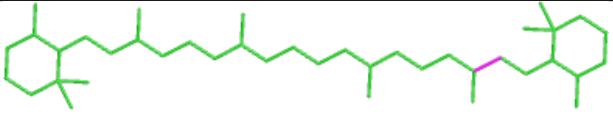
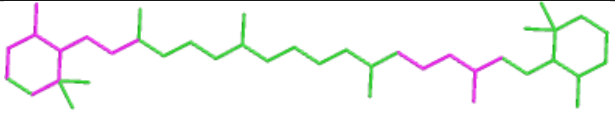
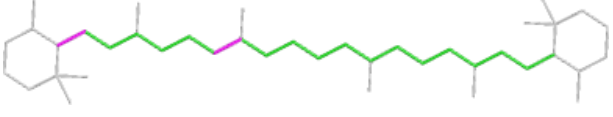
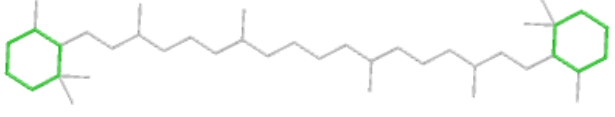
Ligand BCR C 516	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 610	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMT a 413	
 Bond lengths	 Bond angles
 Torsions	 Rings



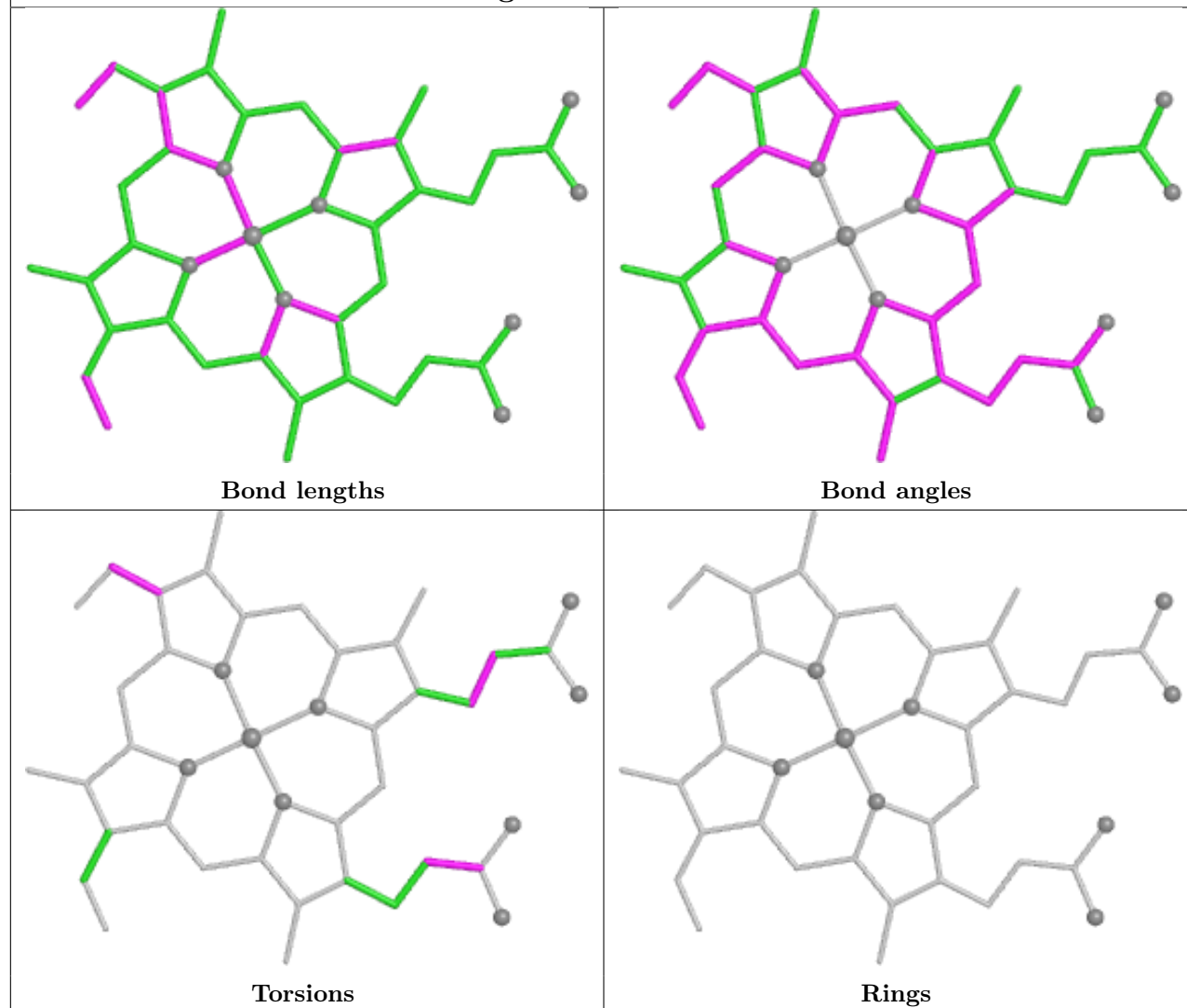




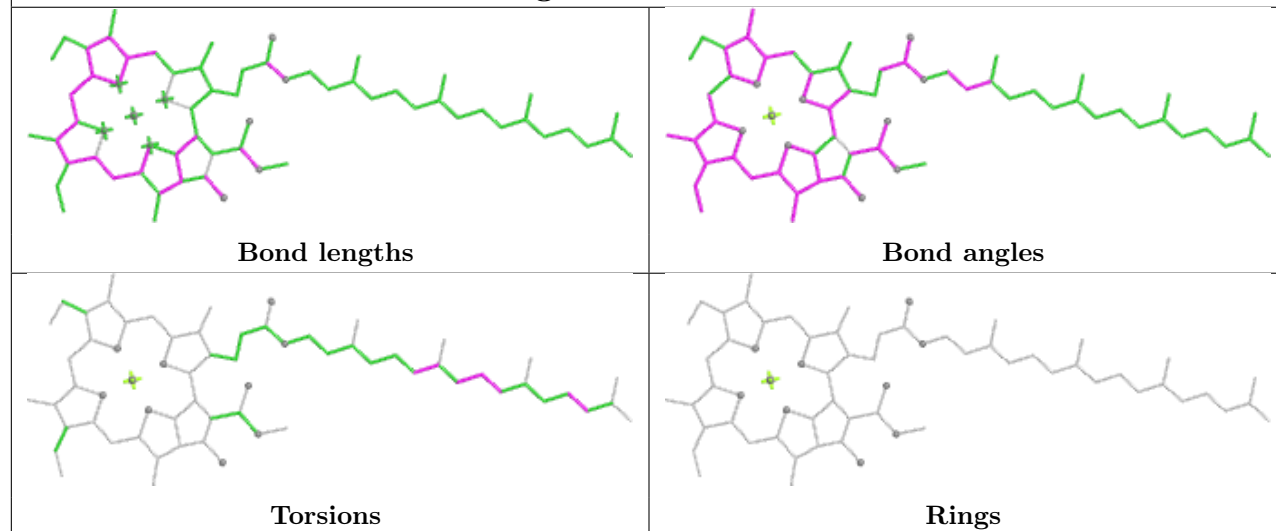


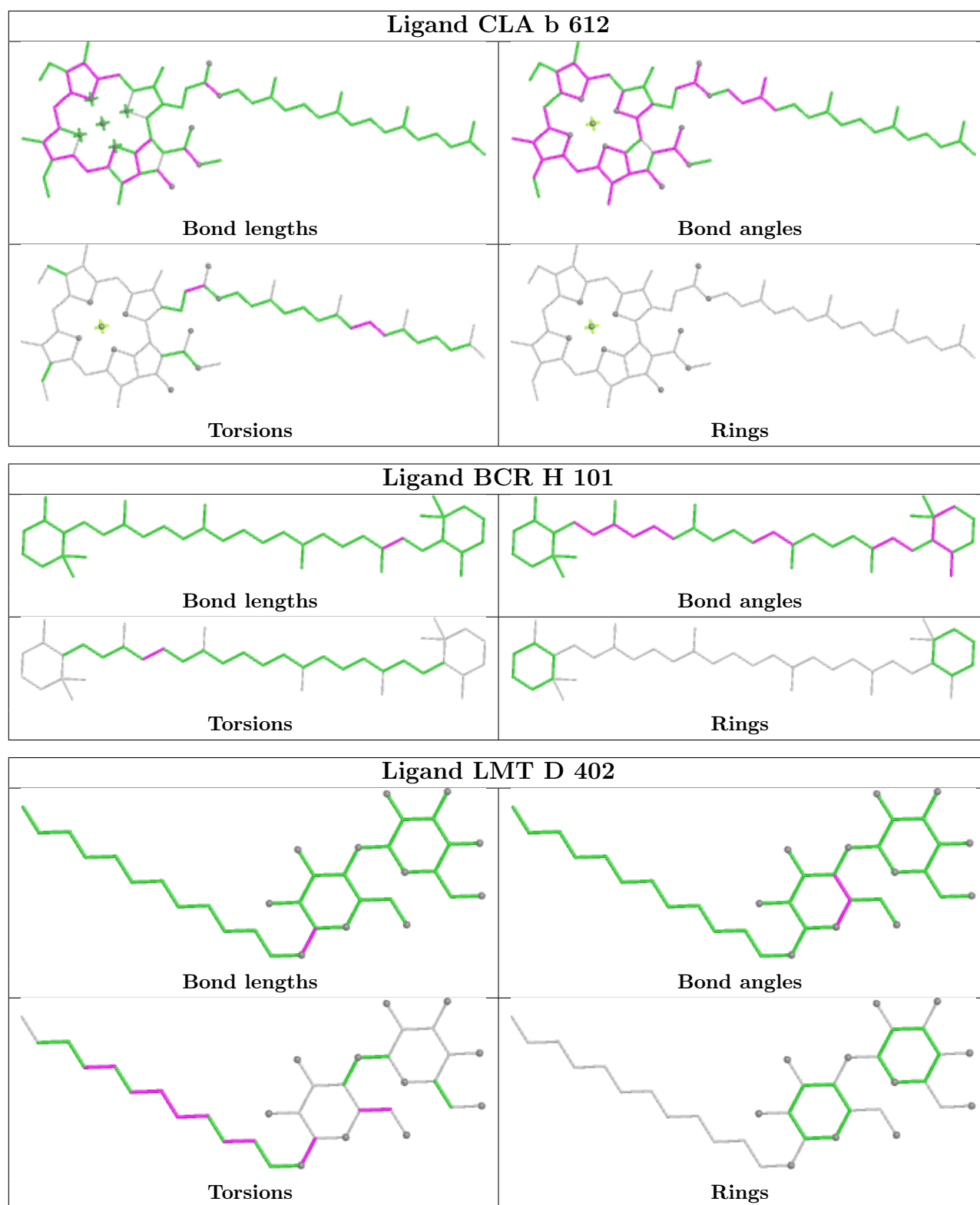
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 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR t 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

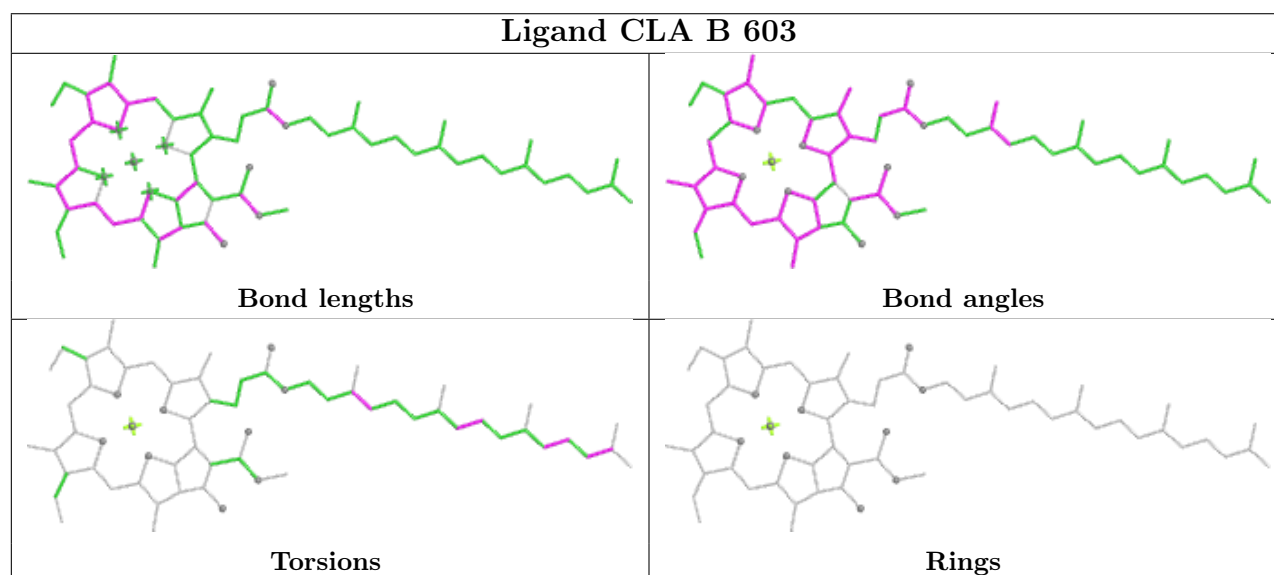
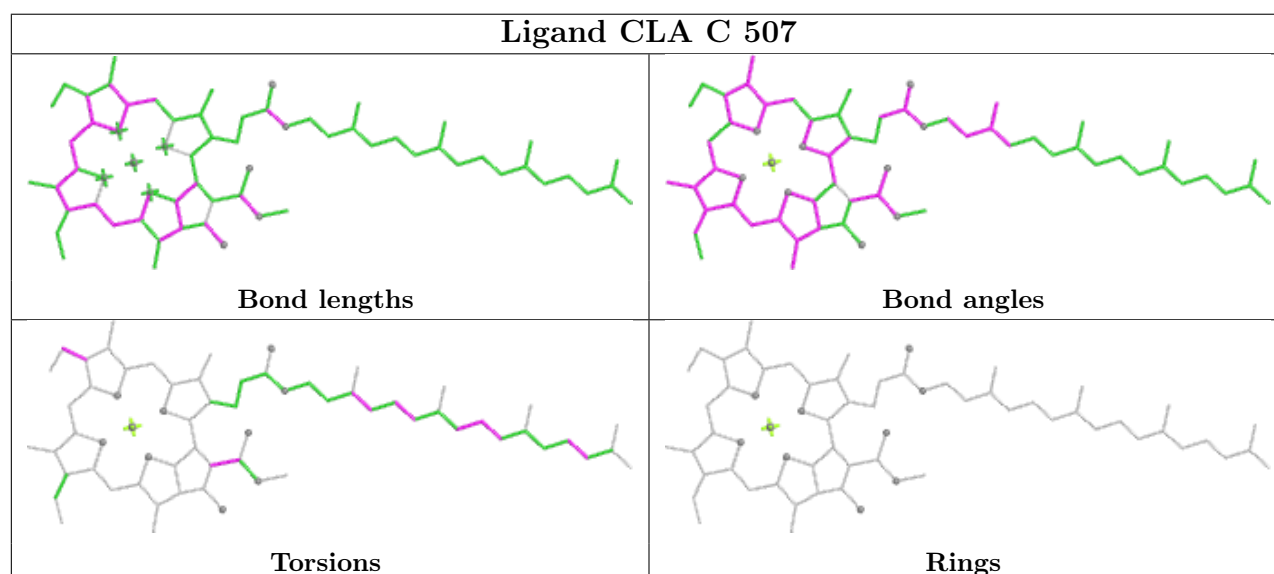
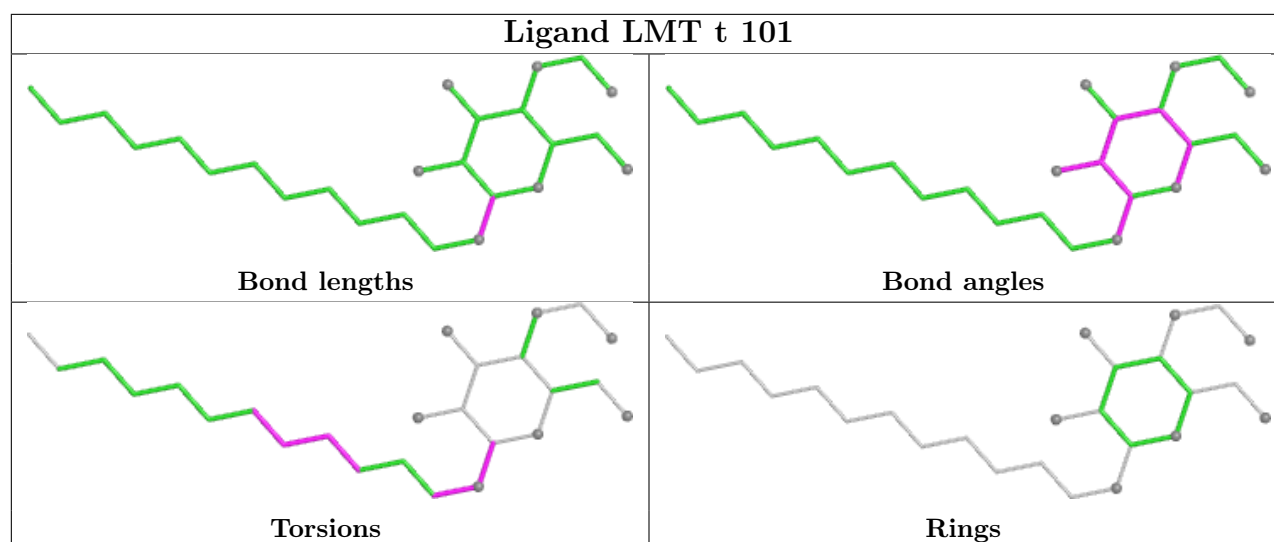
Ligand HEC e 102

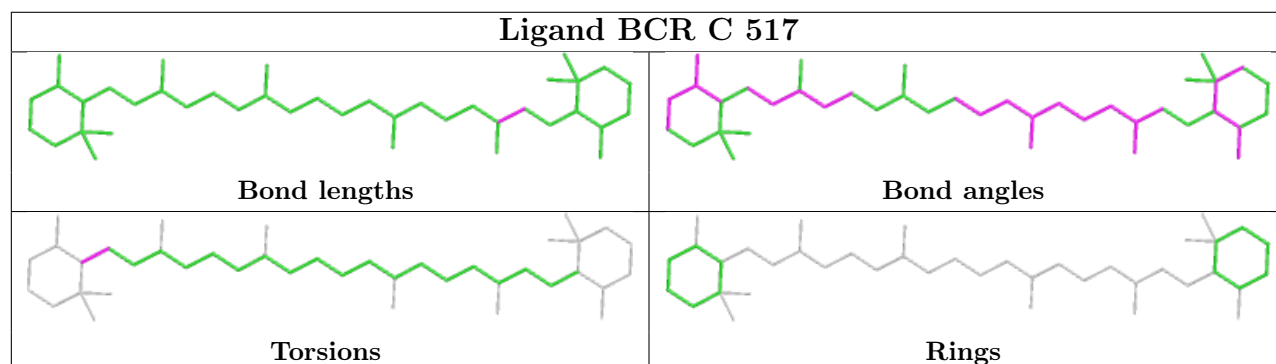
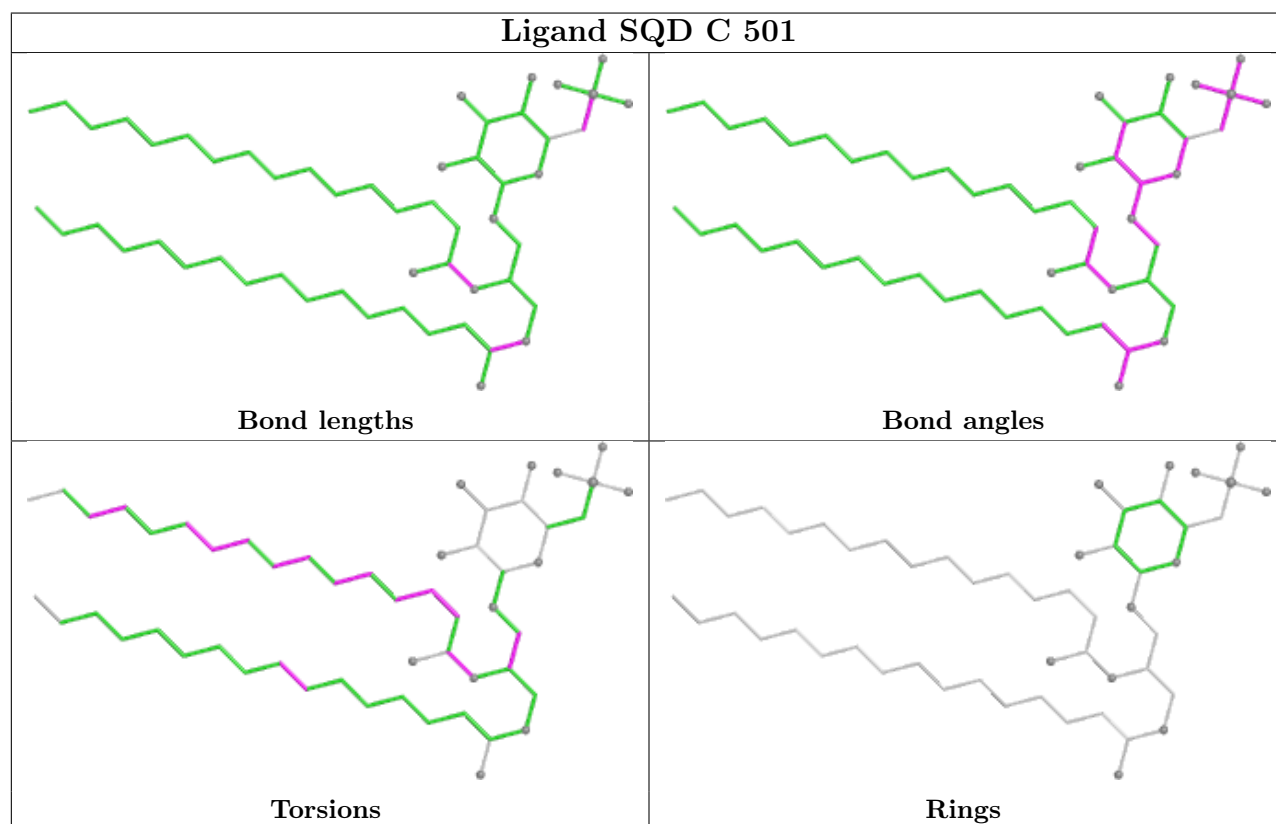
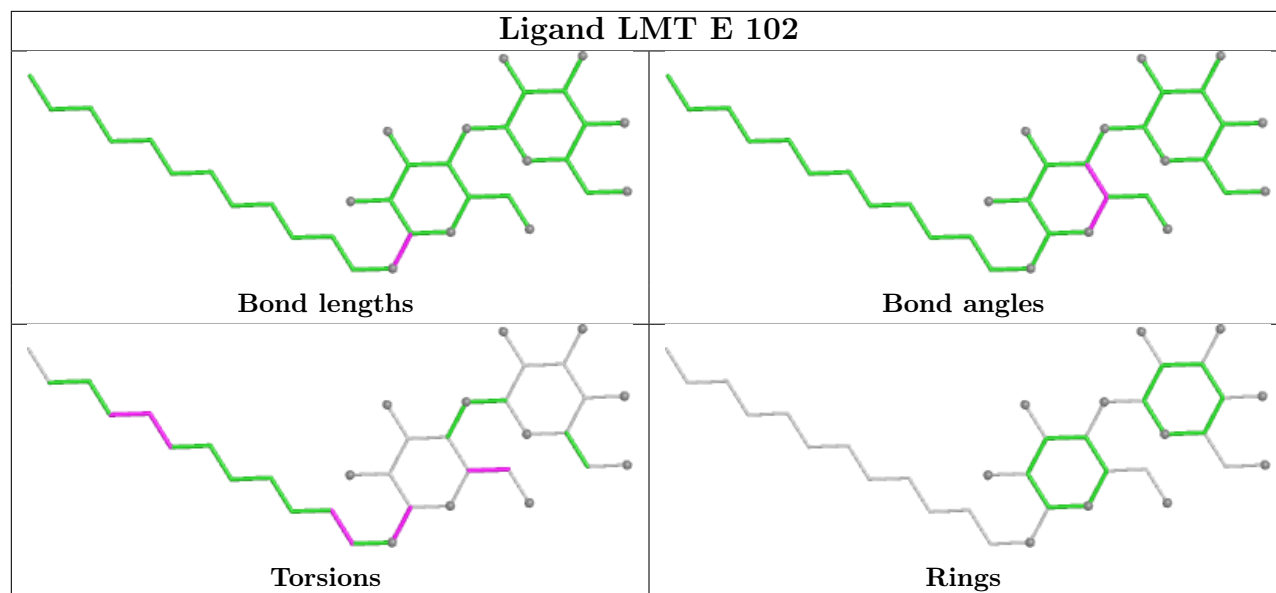


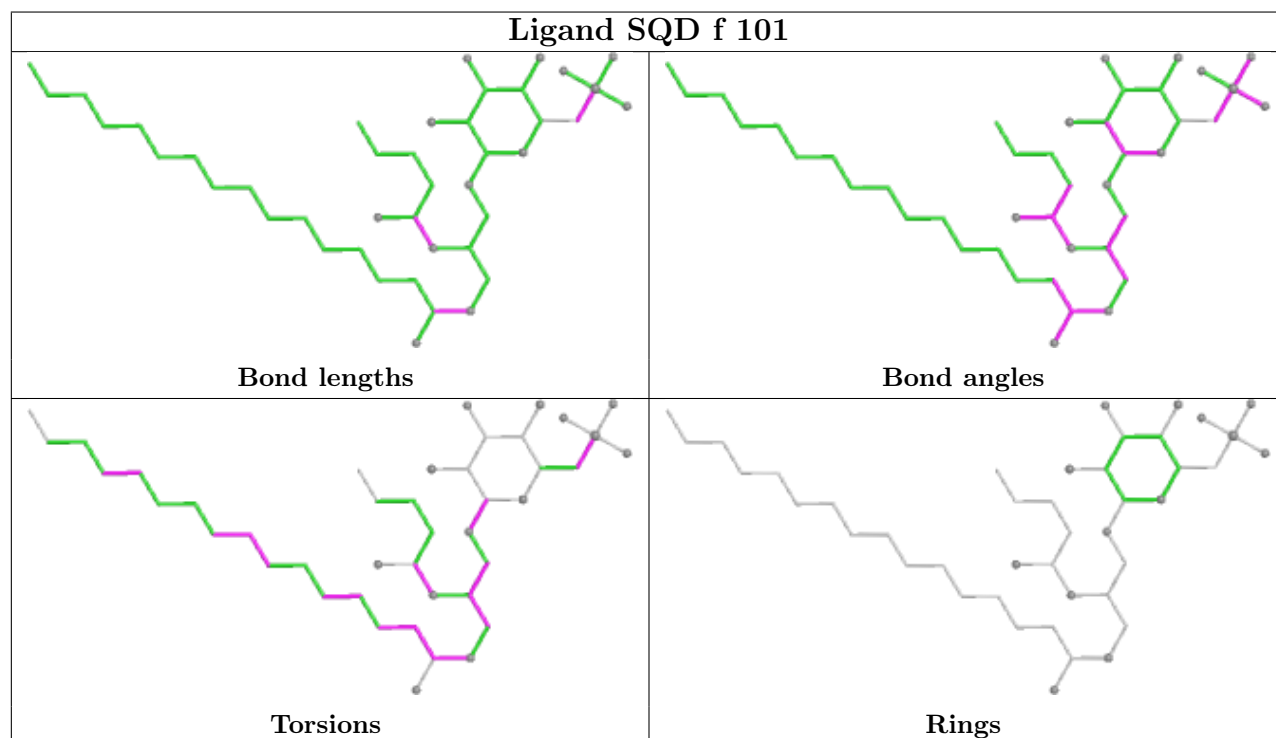
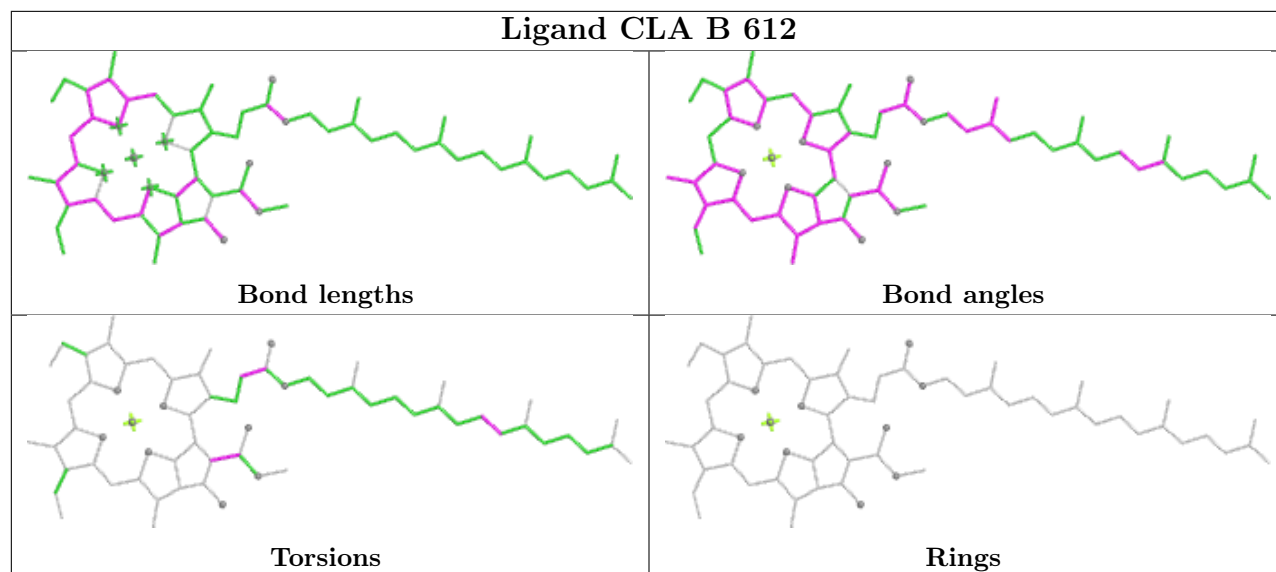
Ligand CLA b 611

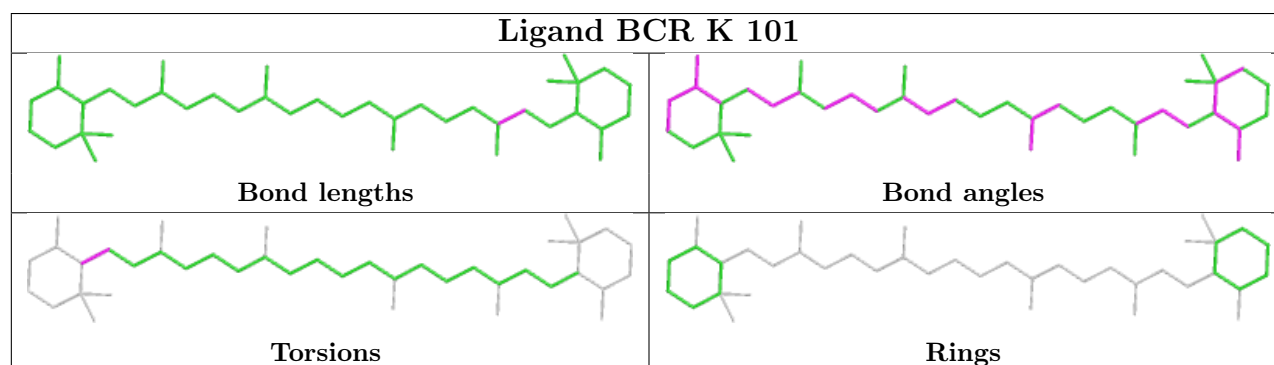
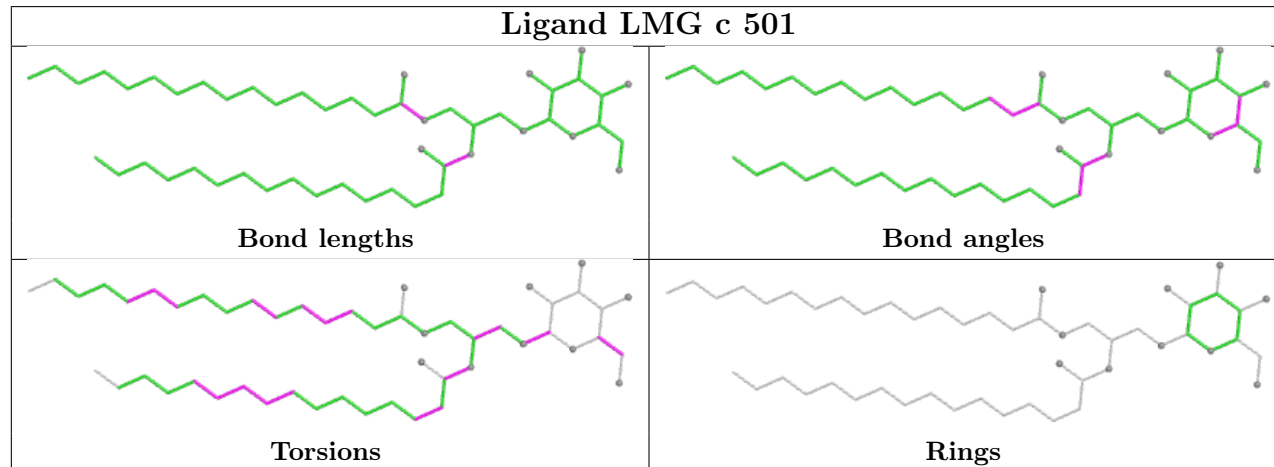
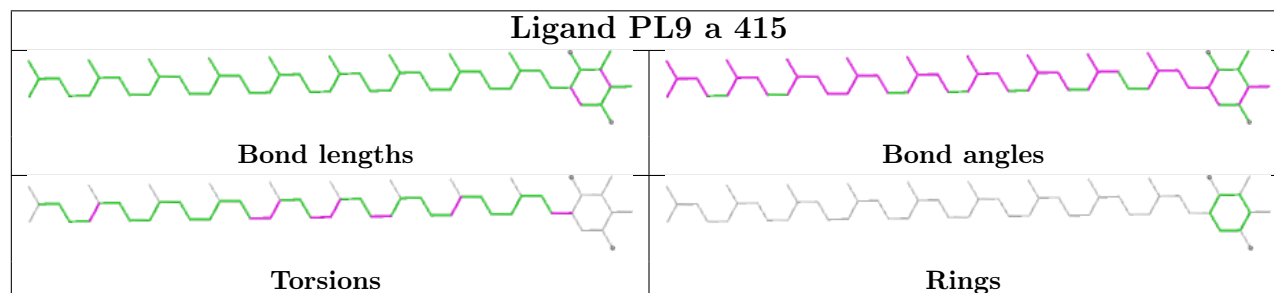
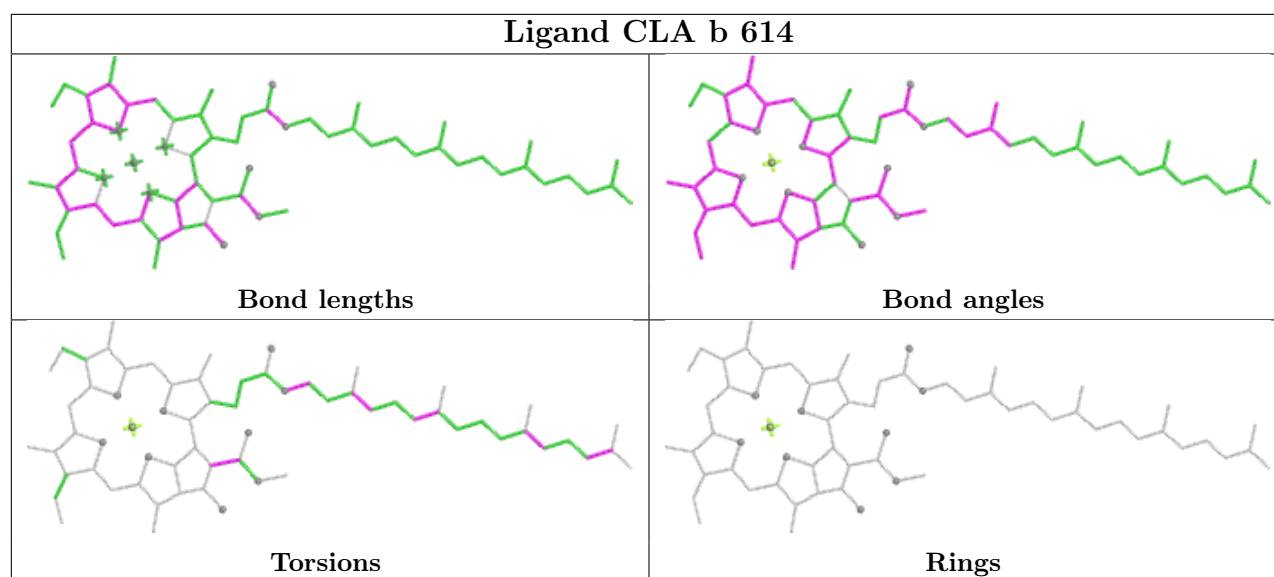


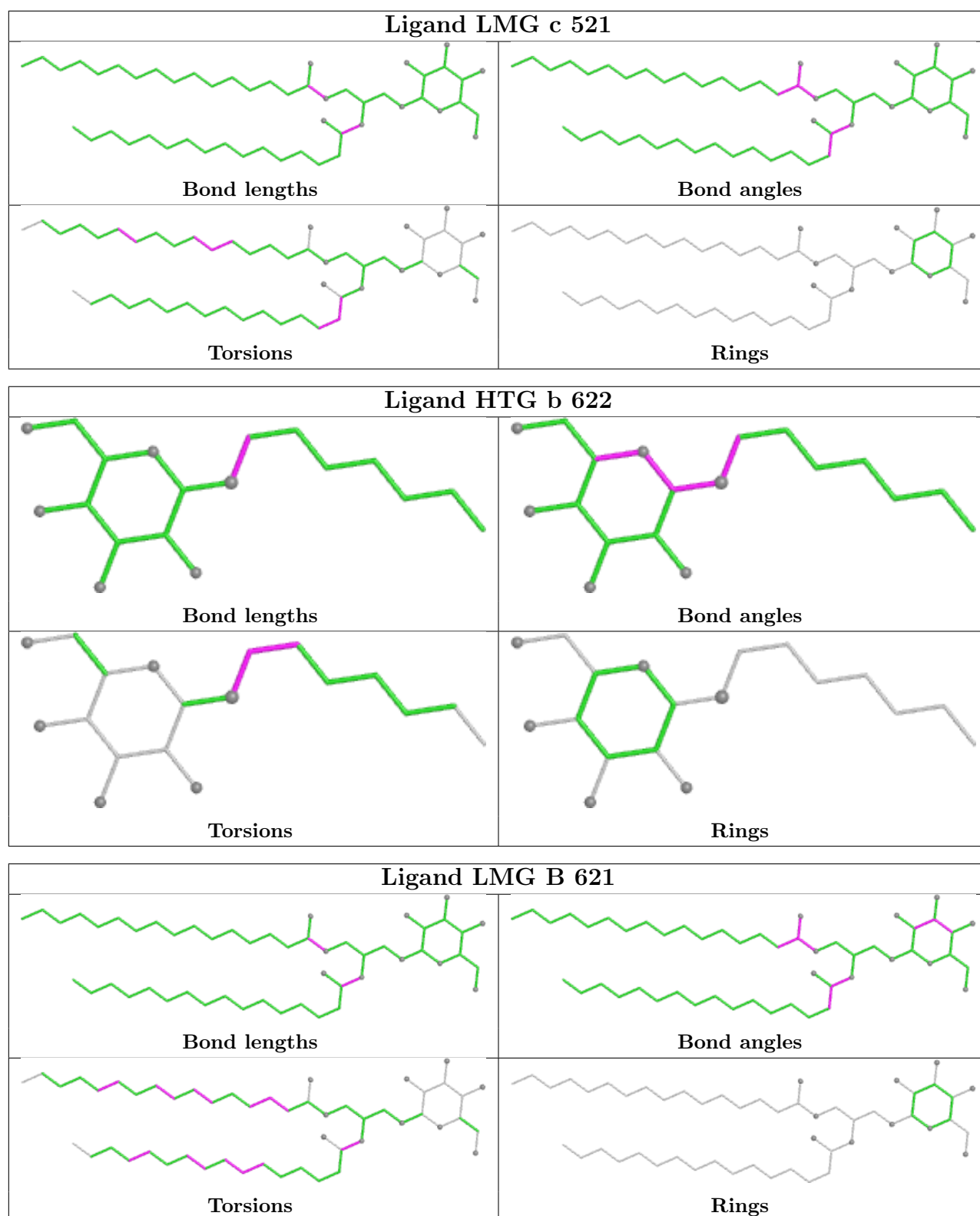


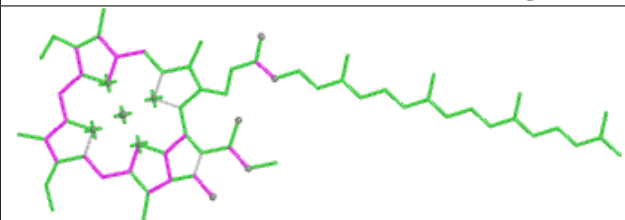
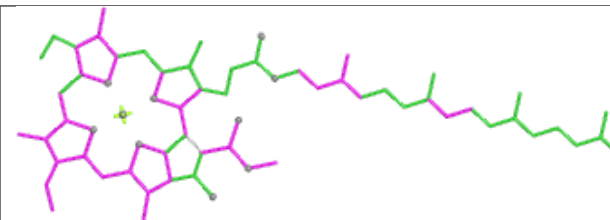
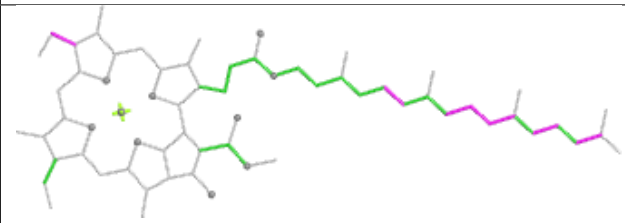
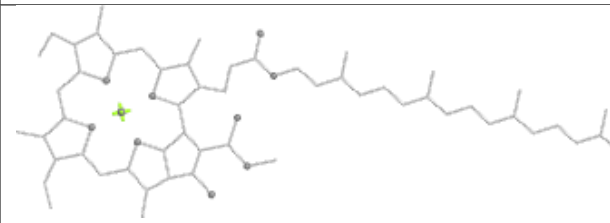


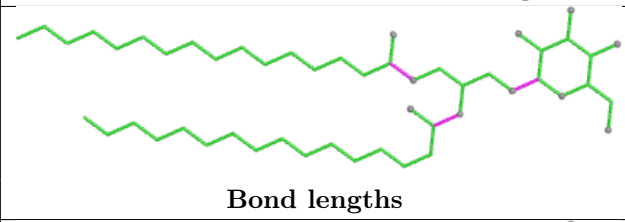
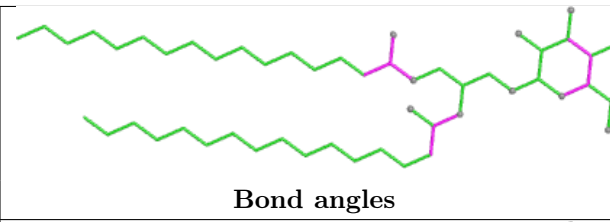
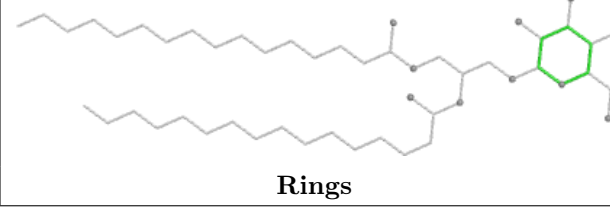


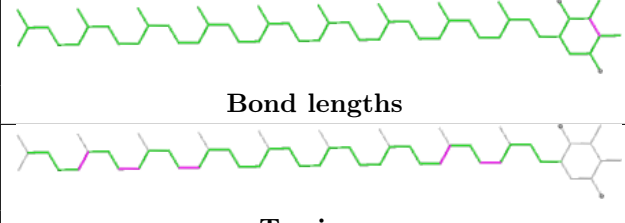
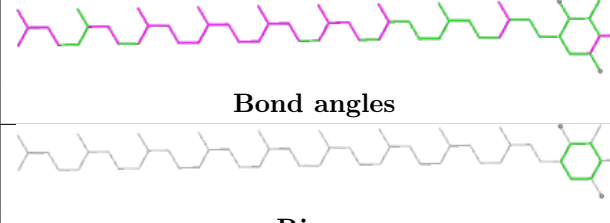
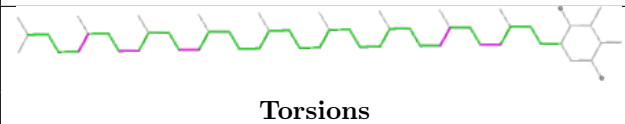
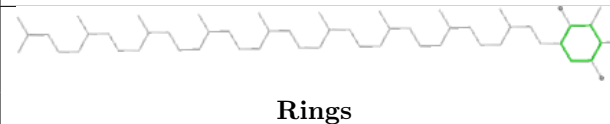


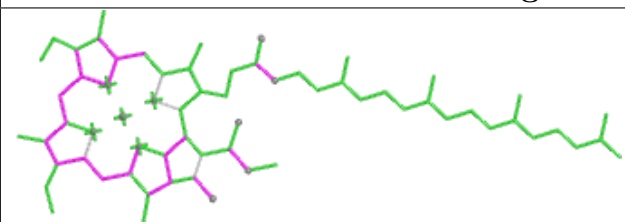
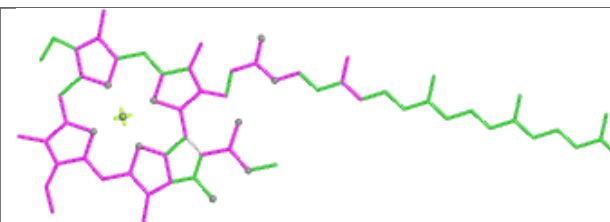
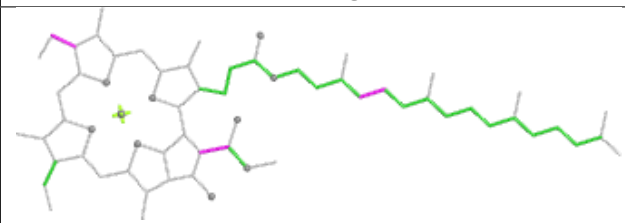
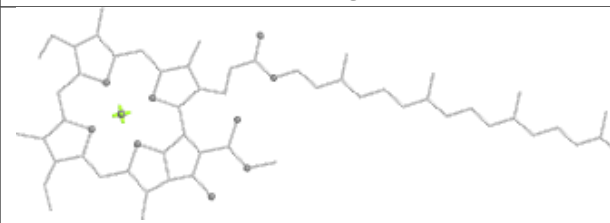


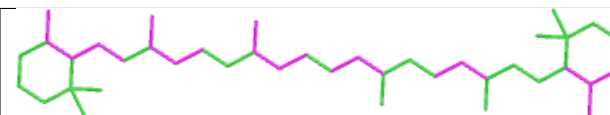
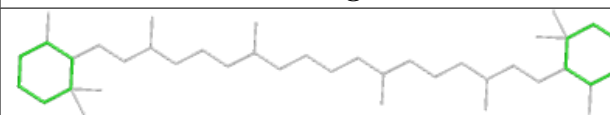


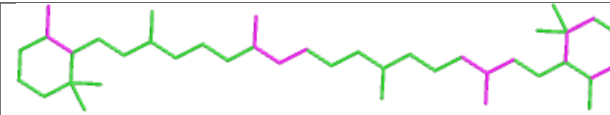
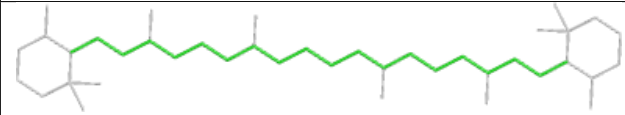
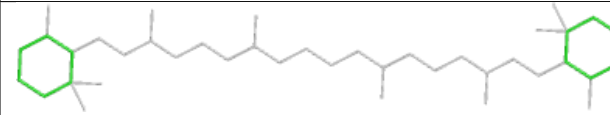
Ligand CLA B 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

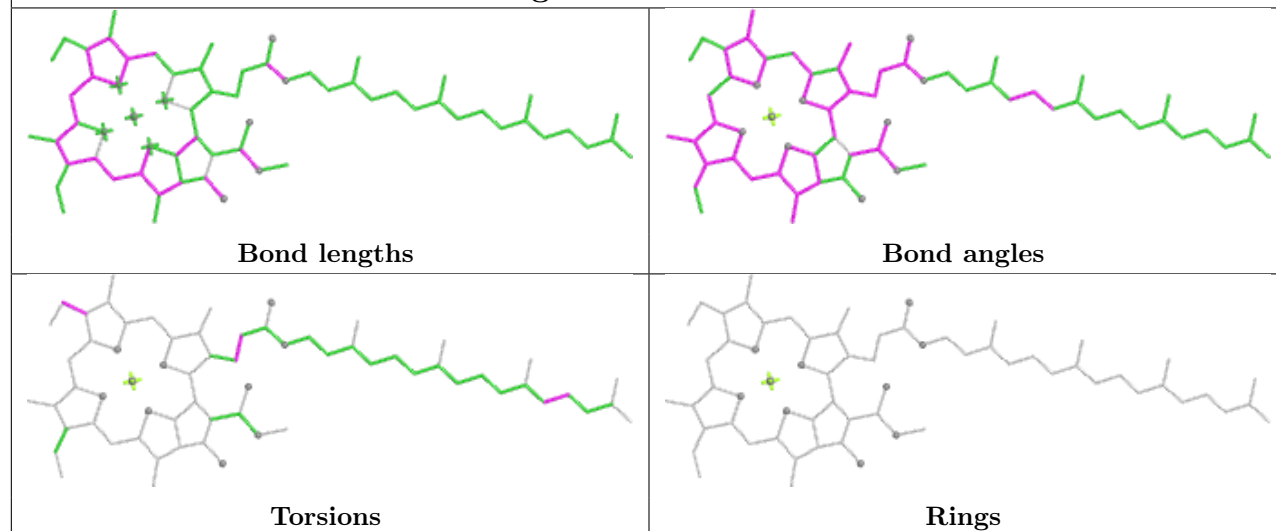
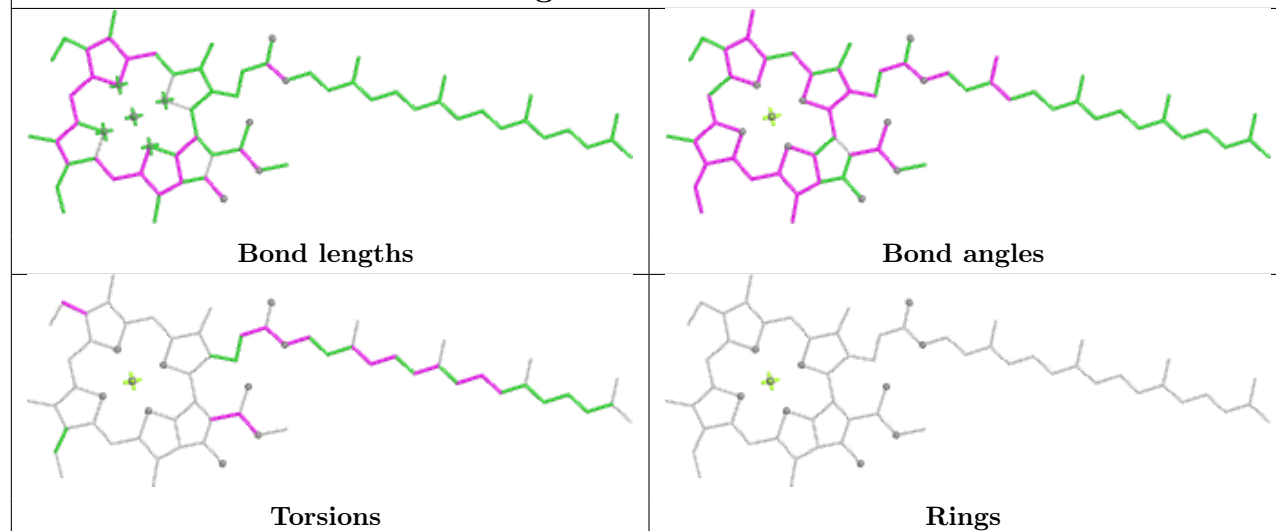
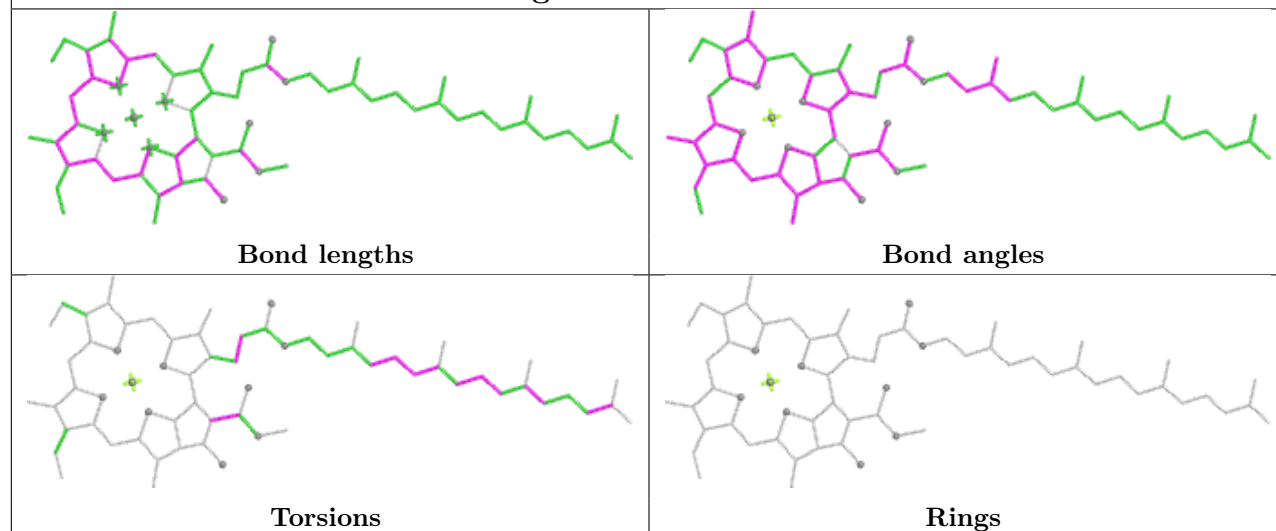
Ligand LMG C 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

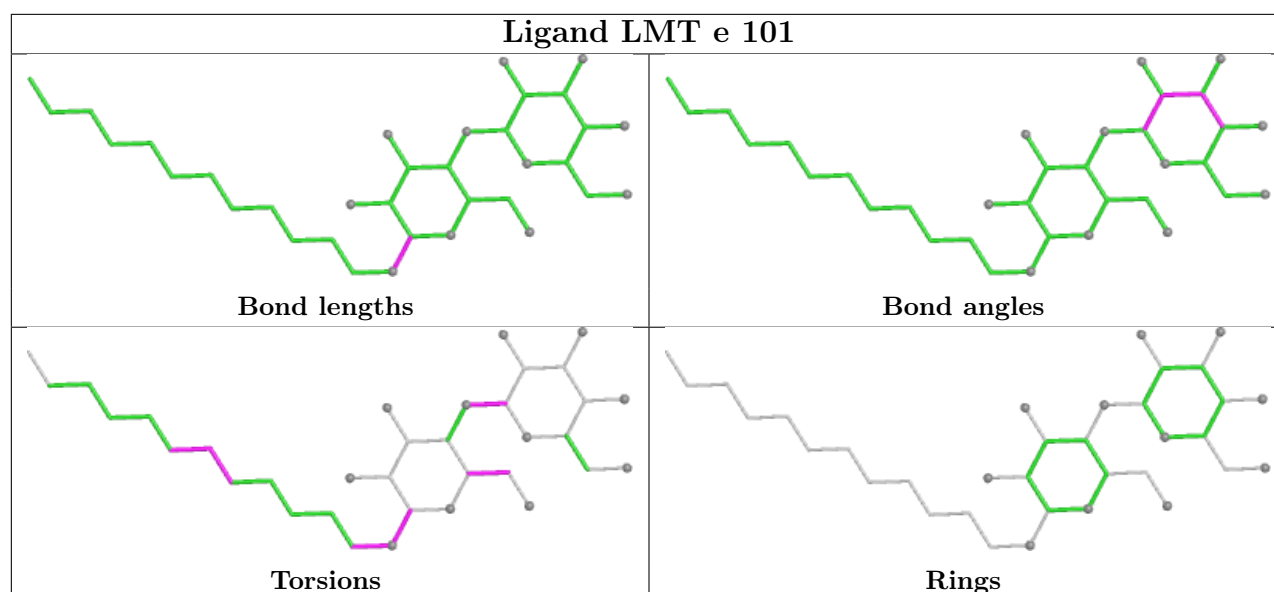
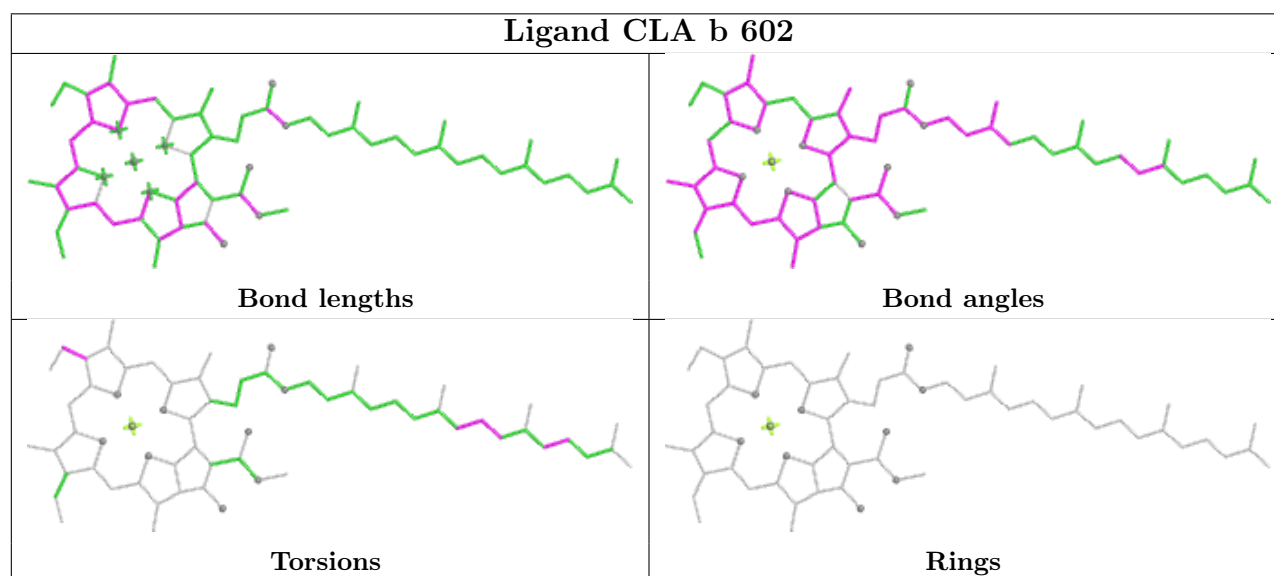
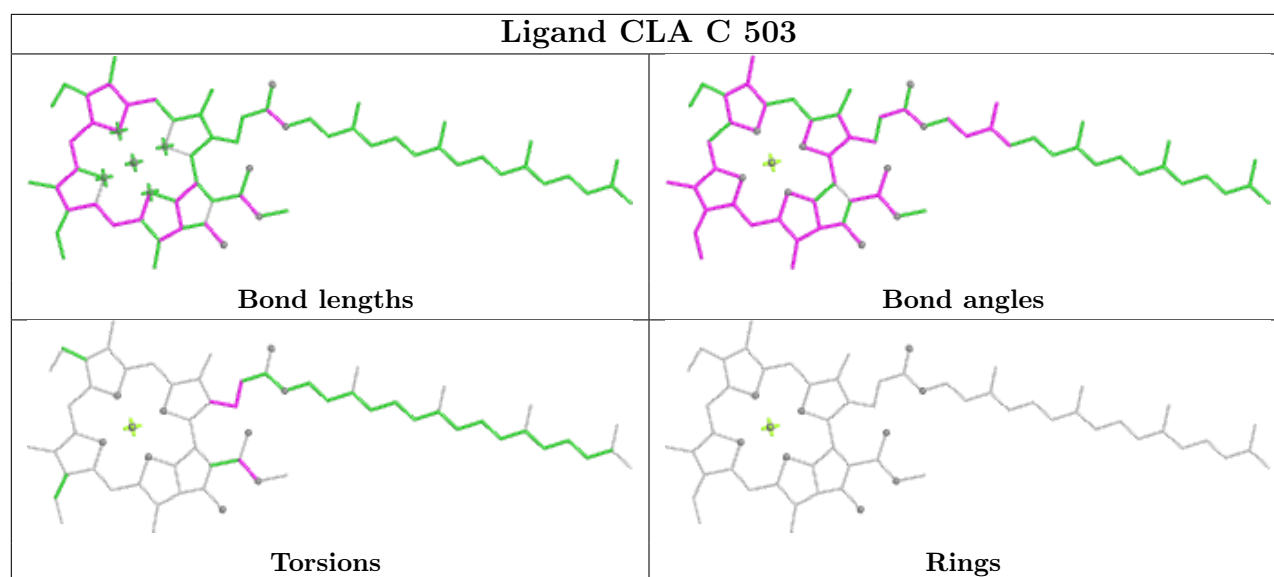
Ligand PL9 d 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

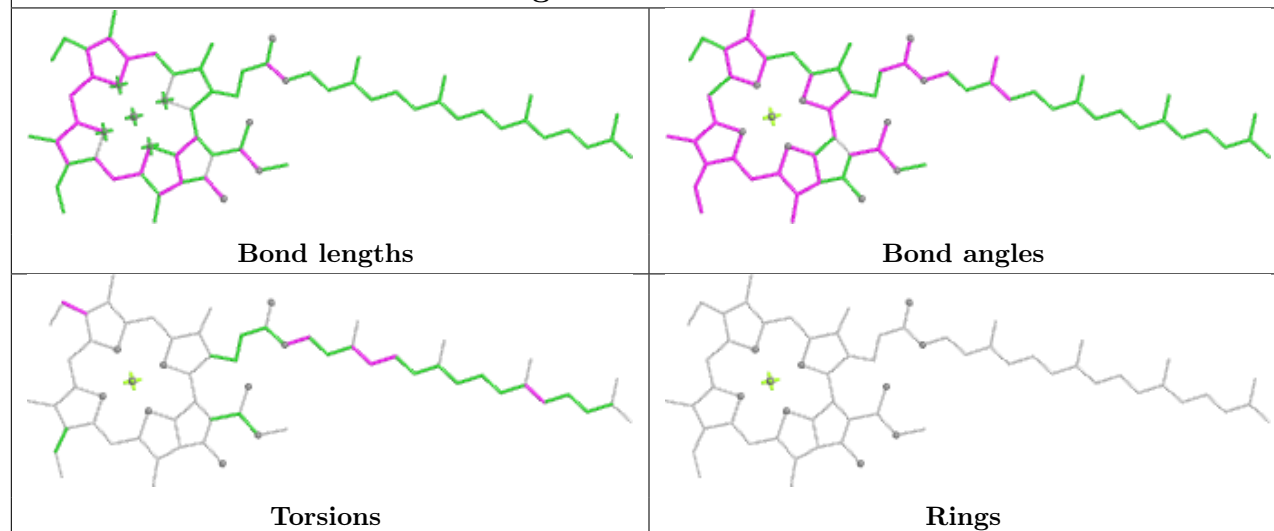
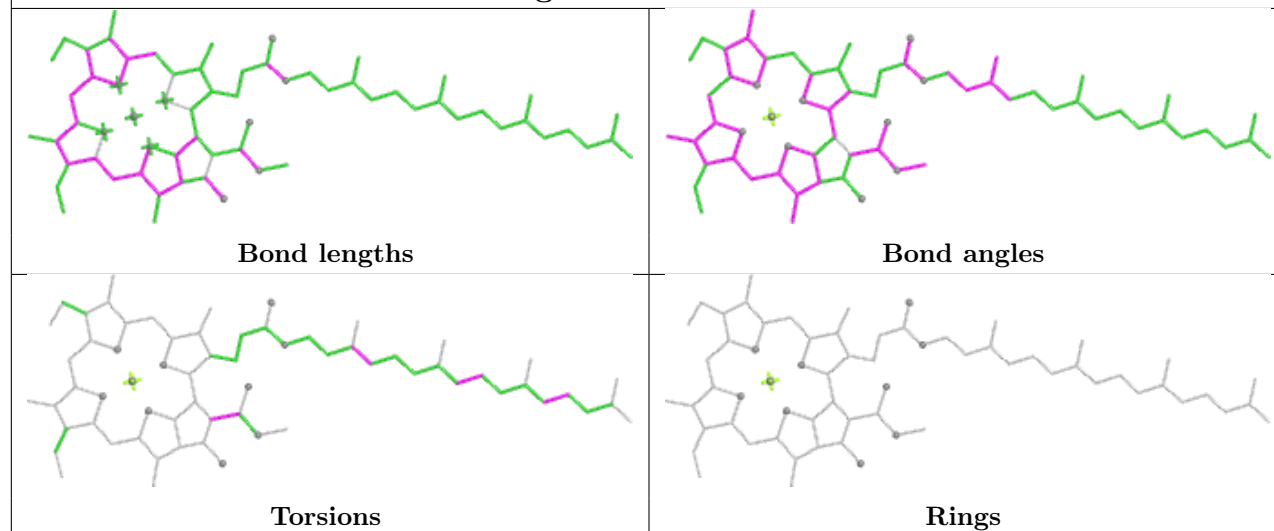
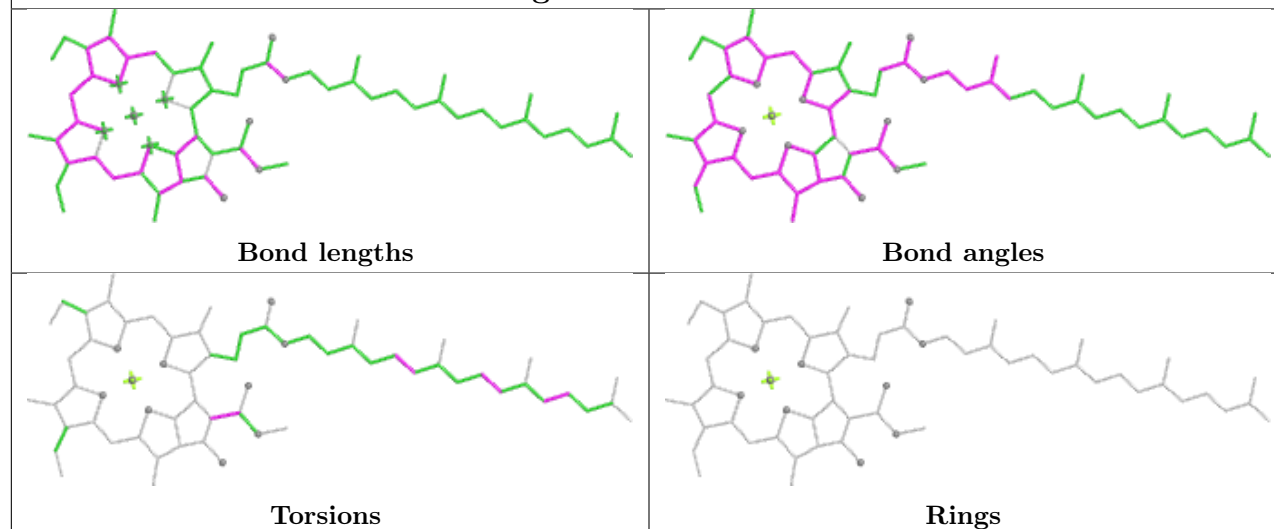
Ligand CLA B 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

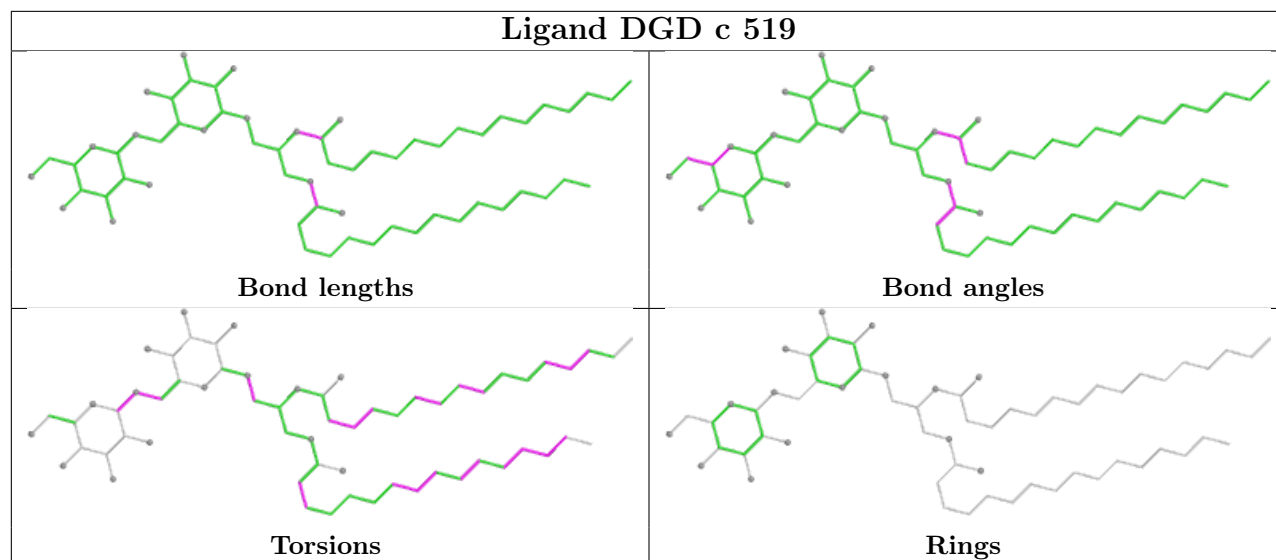
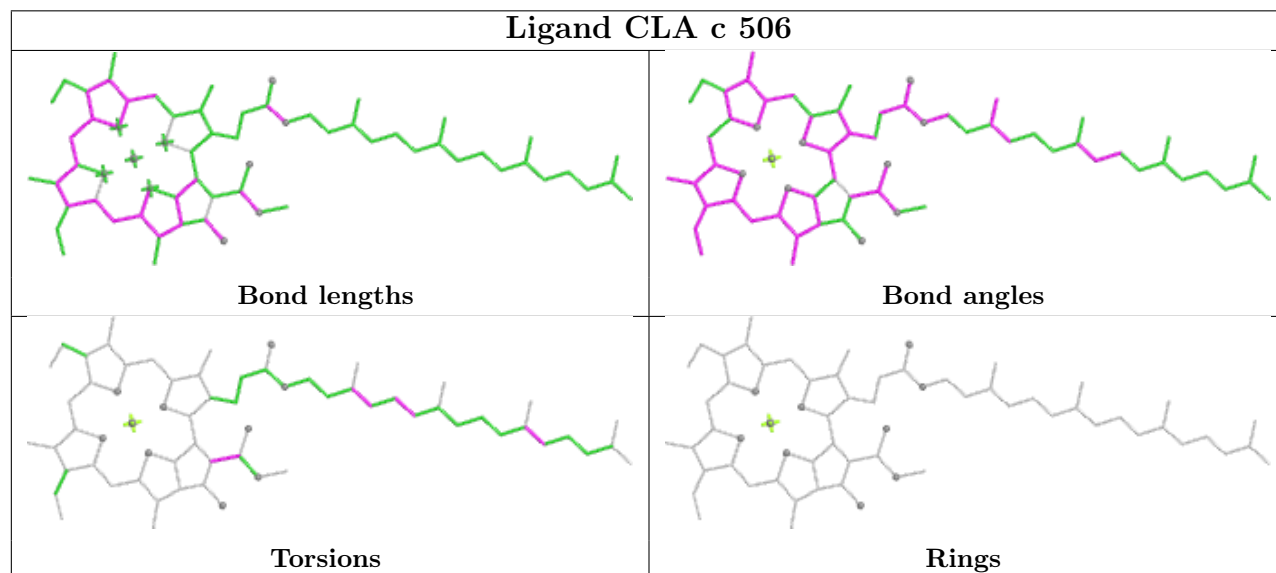
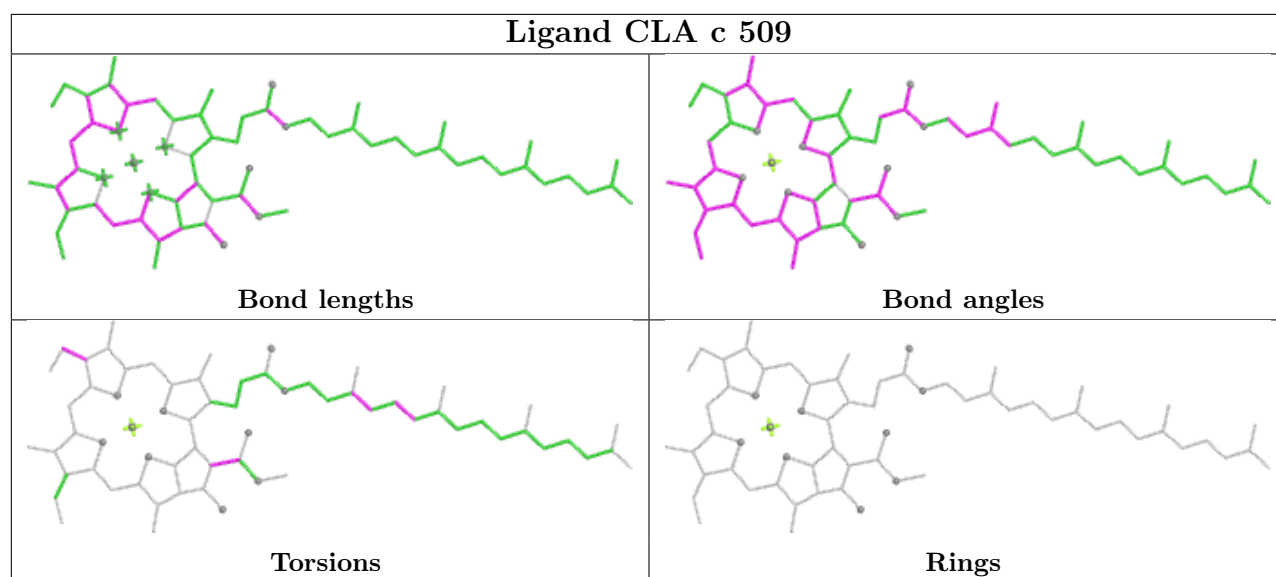
Ligand BCR c 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

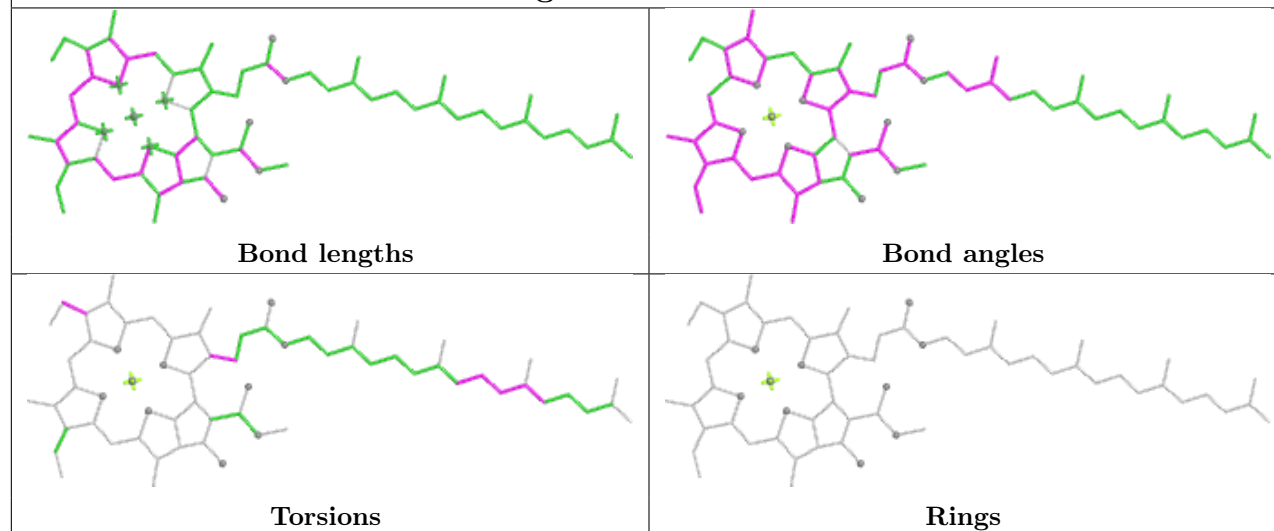
Ligand CLA A 404**Ligand CLA b 601****Ligand CLA B 614**



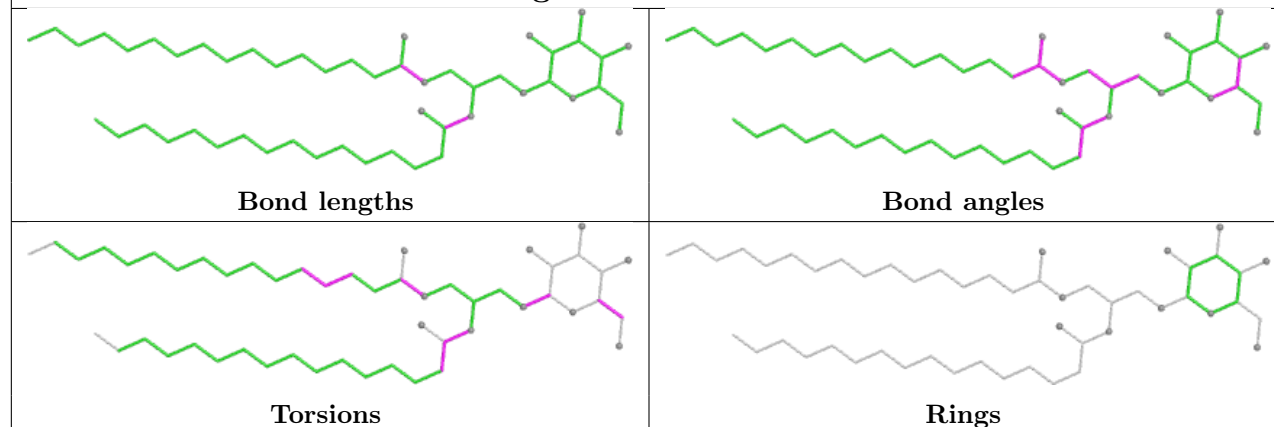
Ligand CLA B 616**Ligand CLA b 605****Ligand CLA C 510**



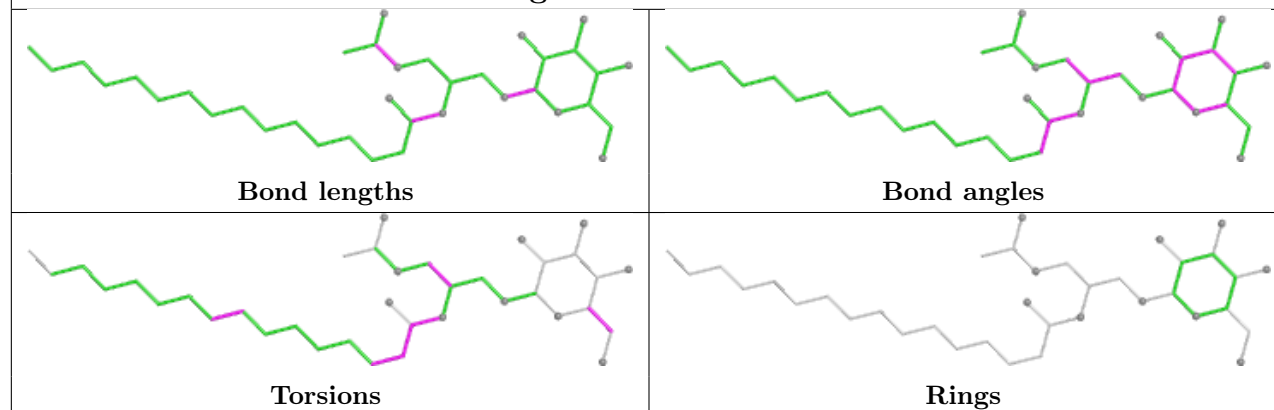
Ligand CLA a 406

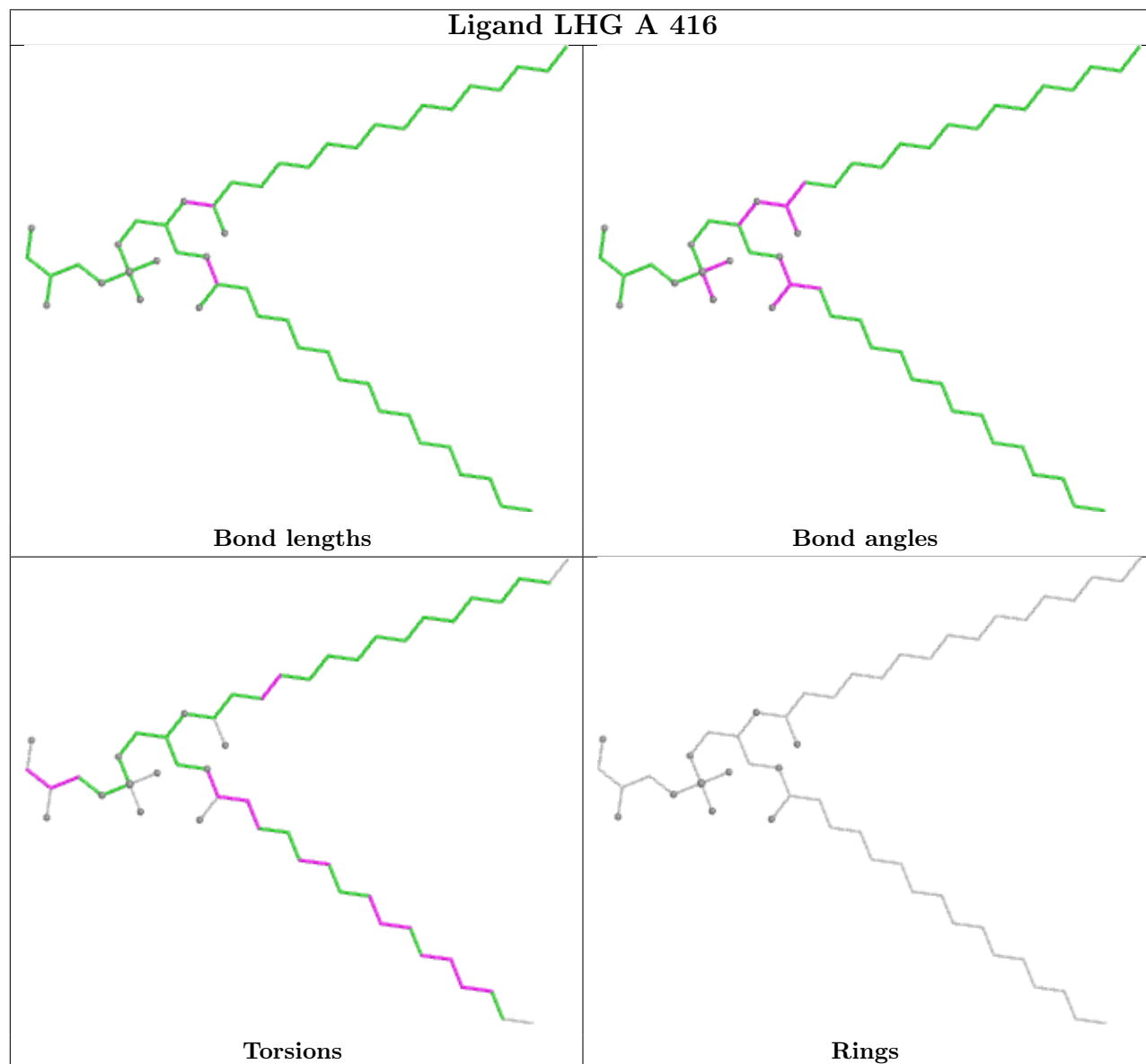
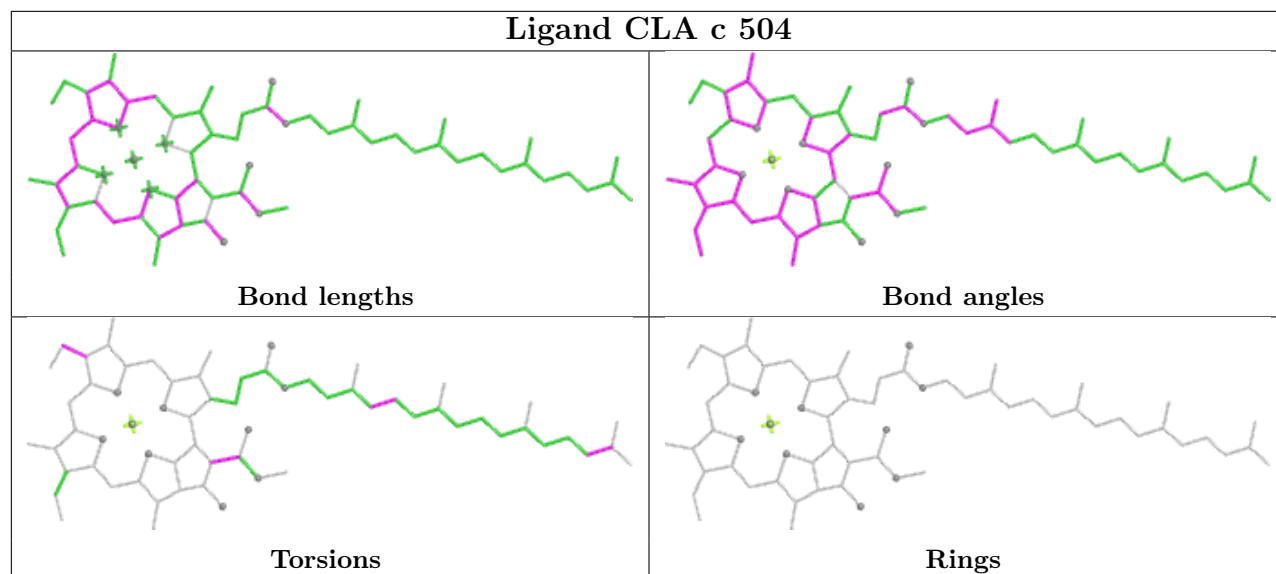


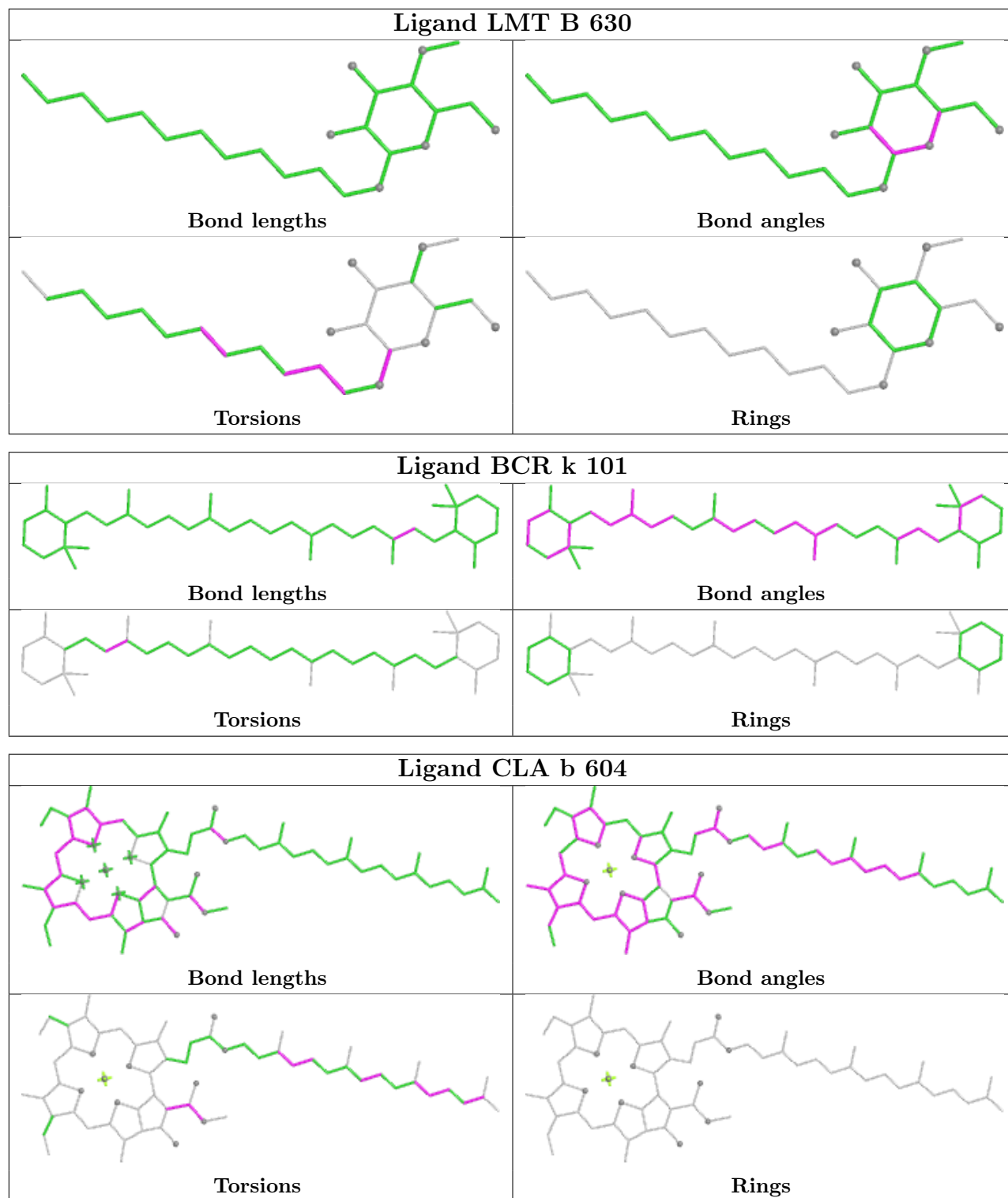
Ligand LMG c 522

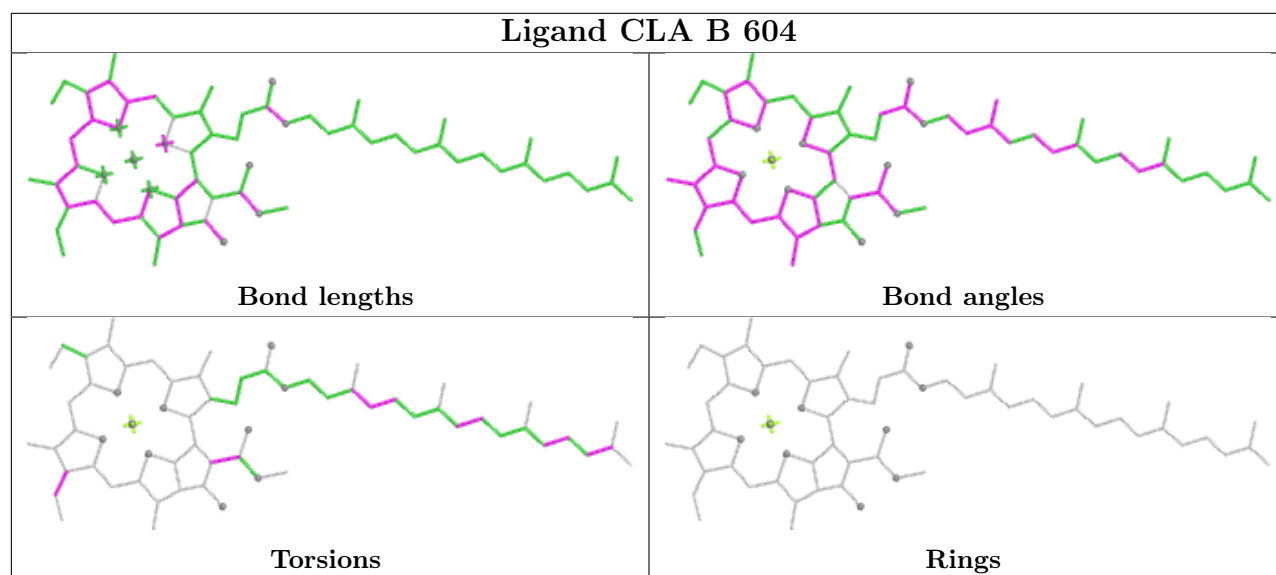
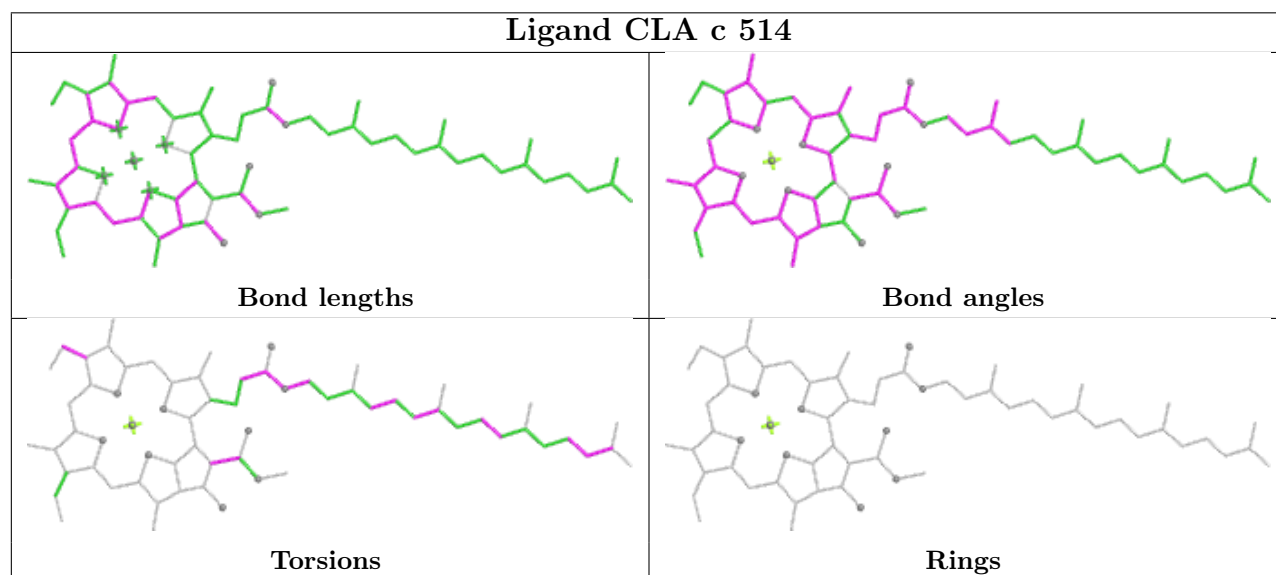
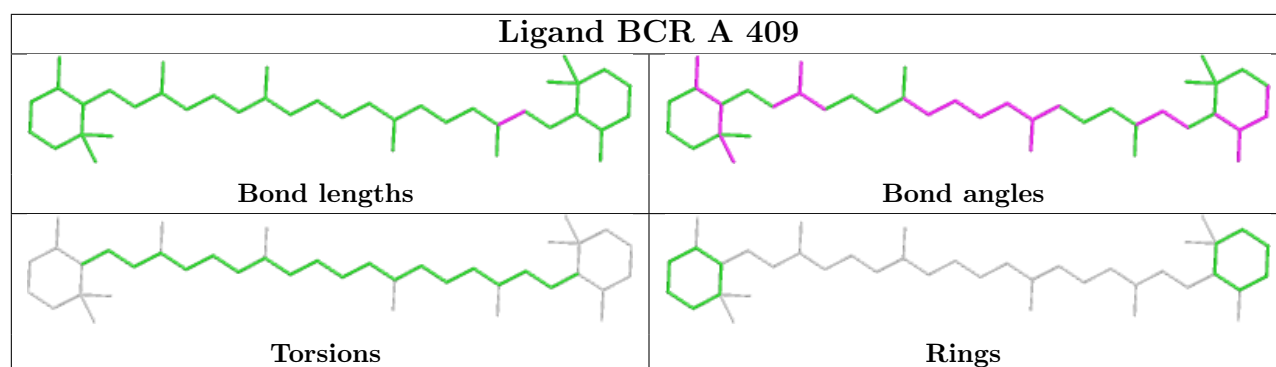


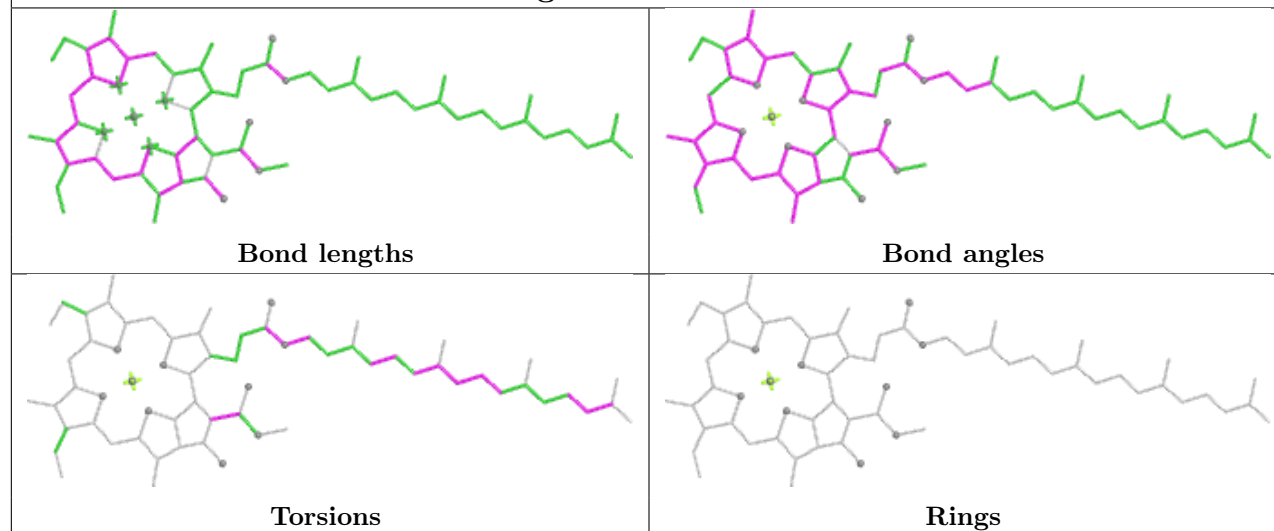
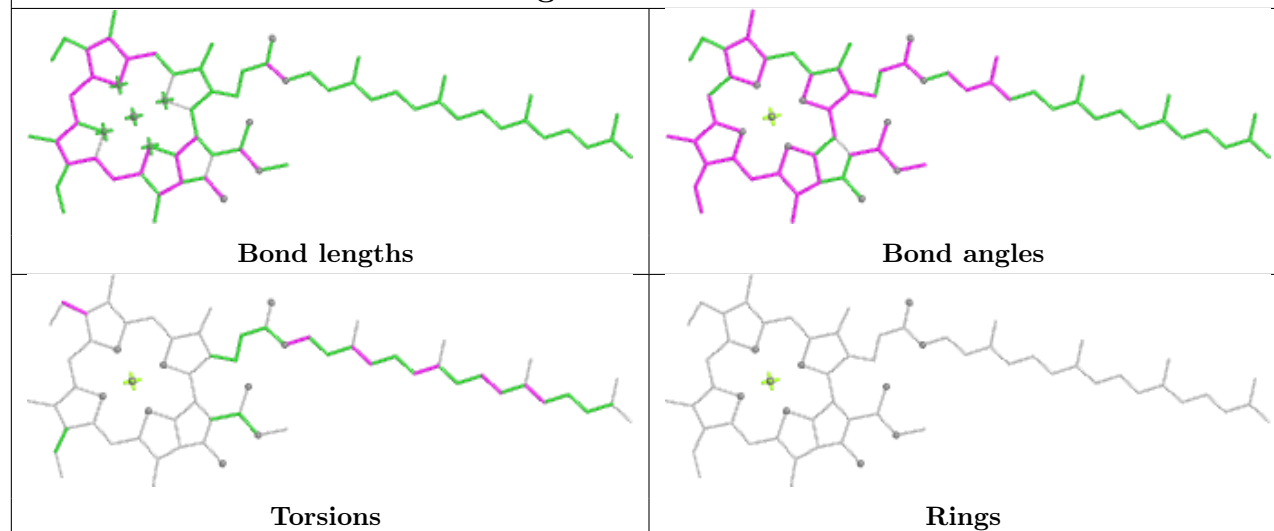
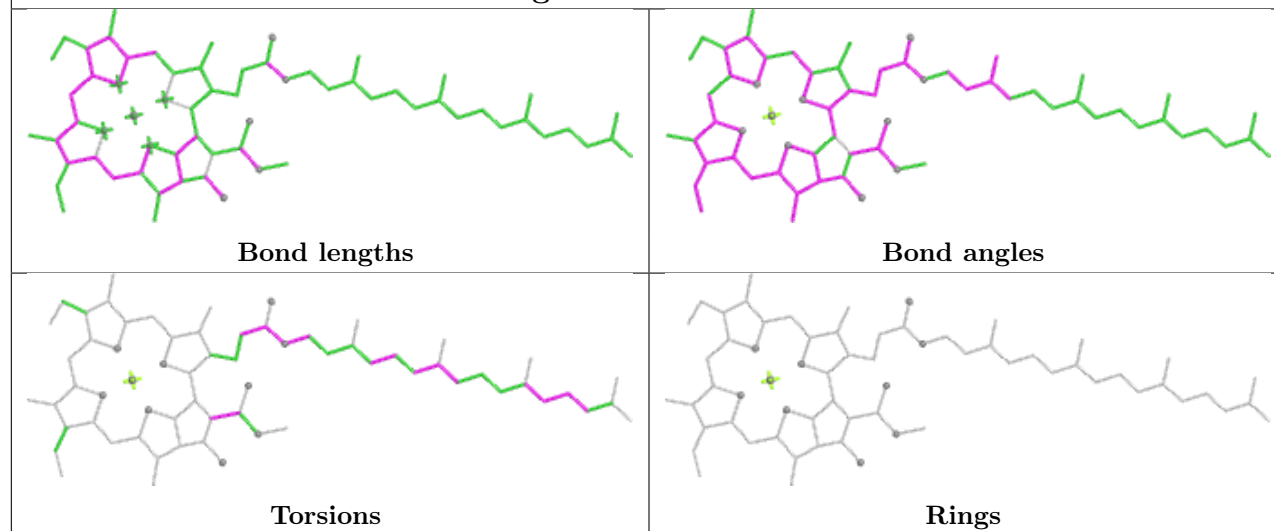
Ligand LMG Z 101

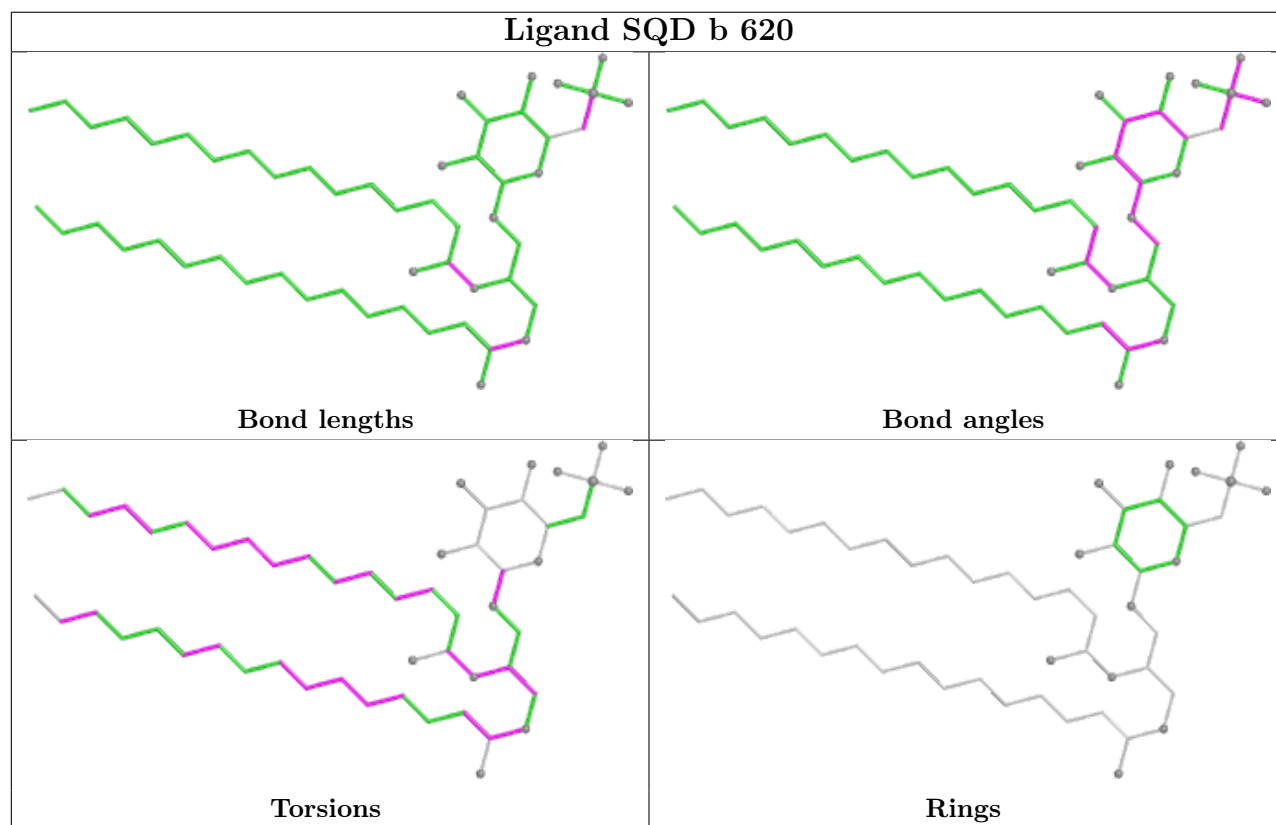
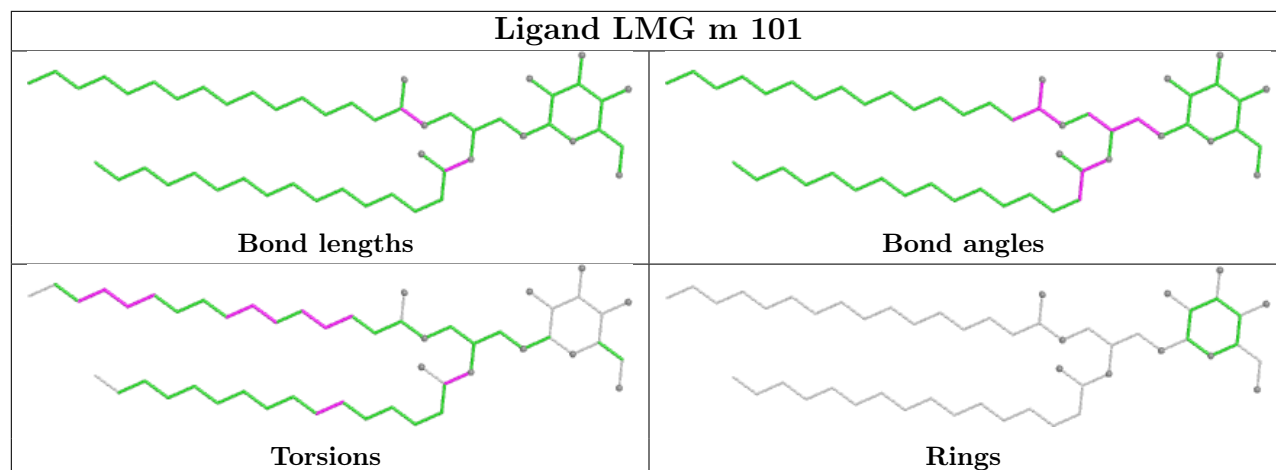


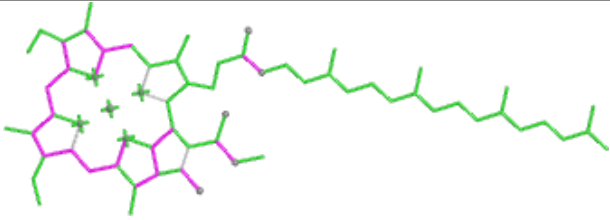
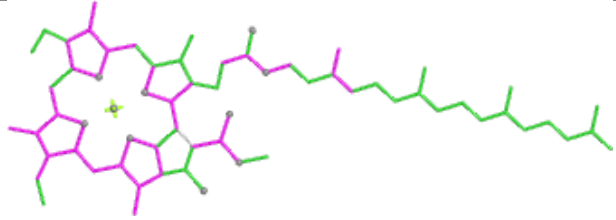
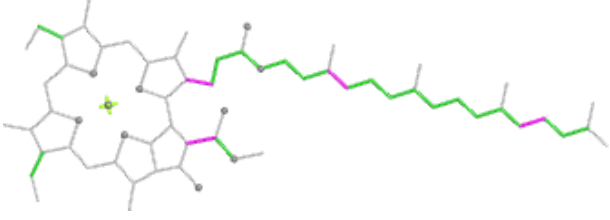
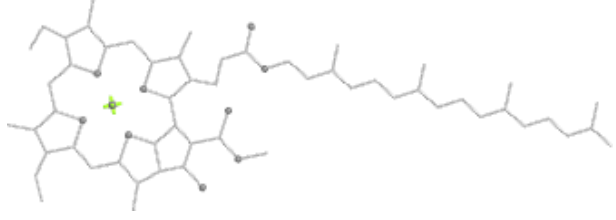
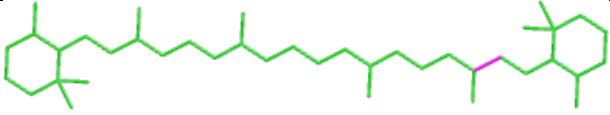
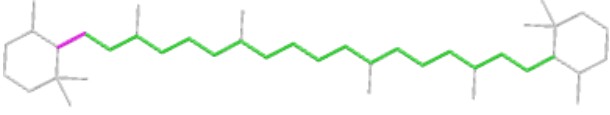
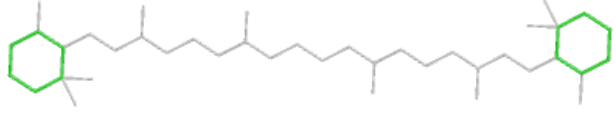
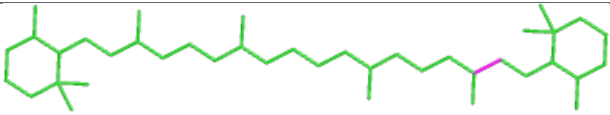
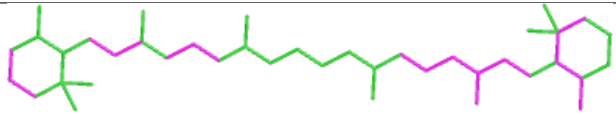
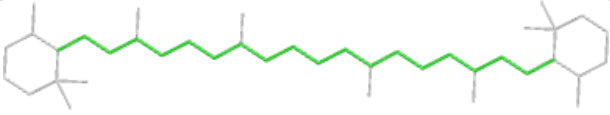
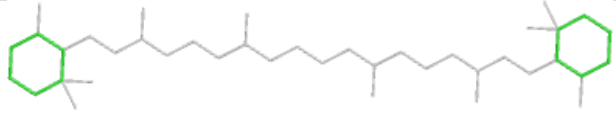


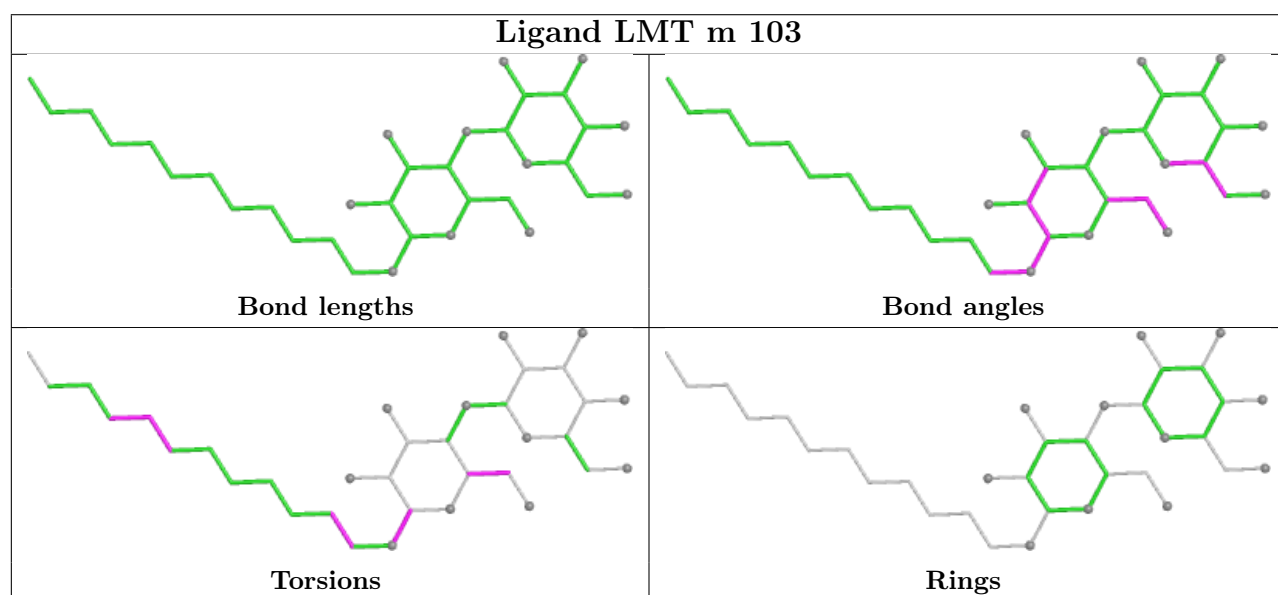
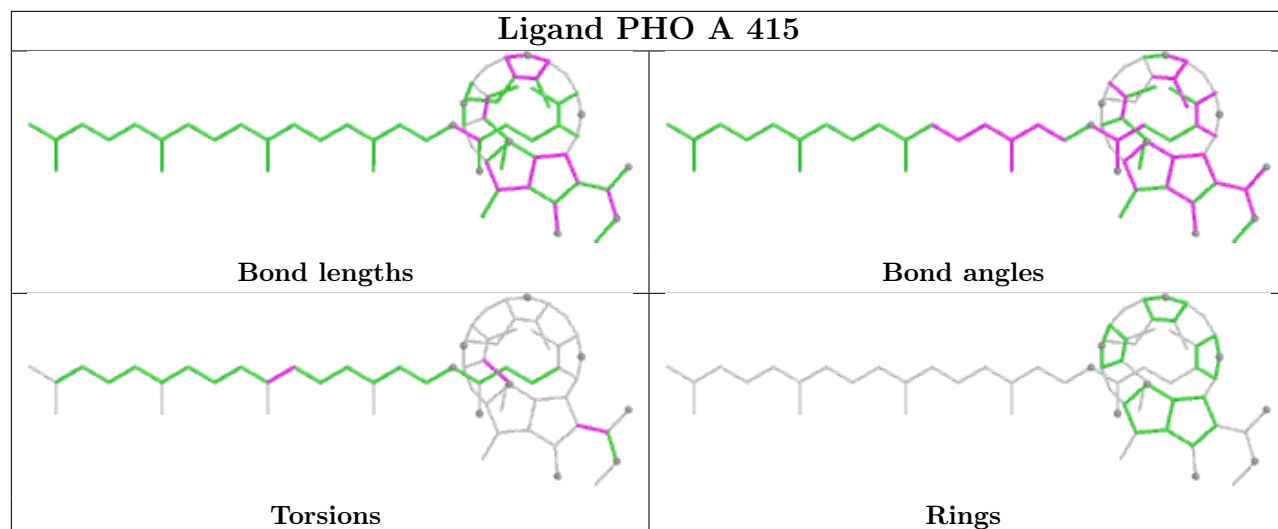


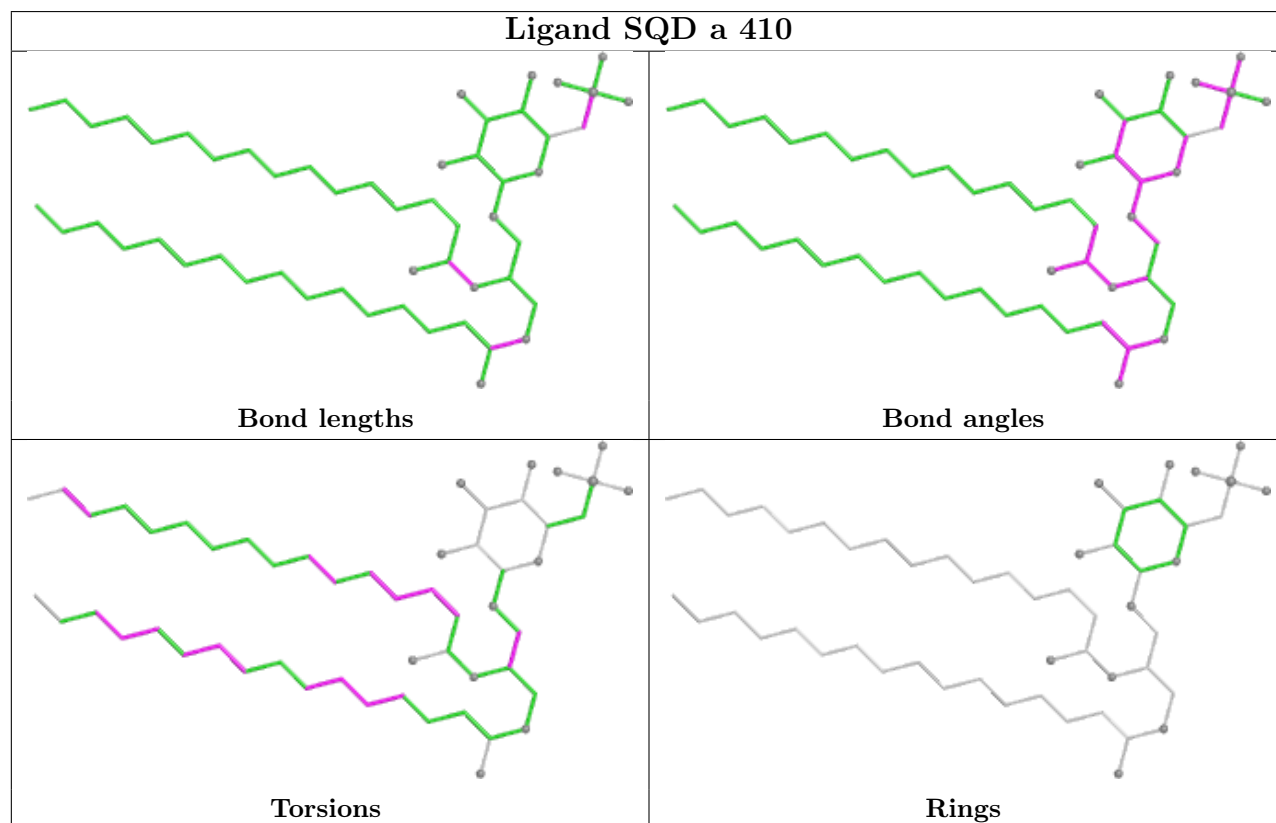
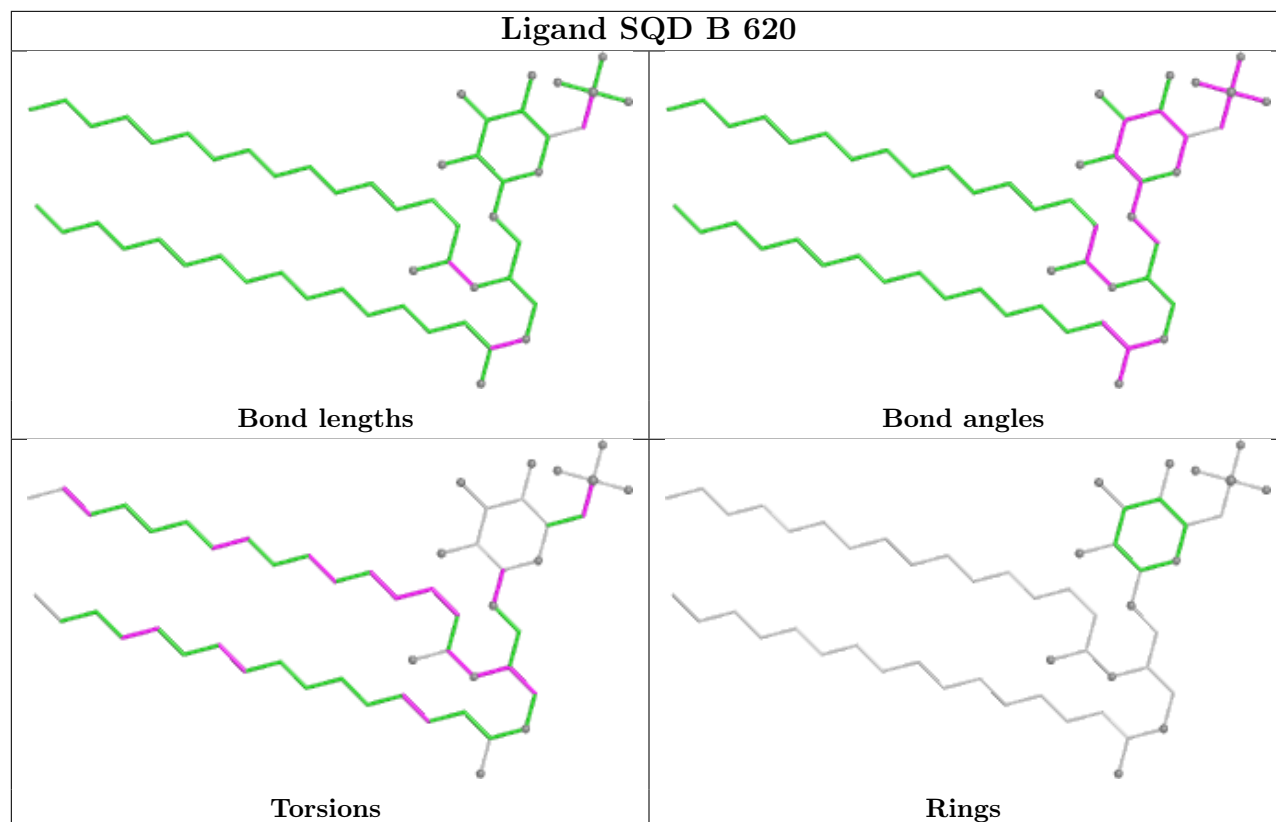


Ligand CLA c 511**Ligand CLA c 515****Ligand CLA C 514**

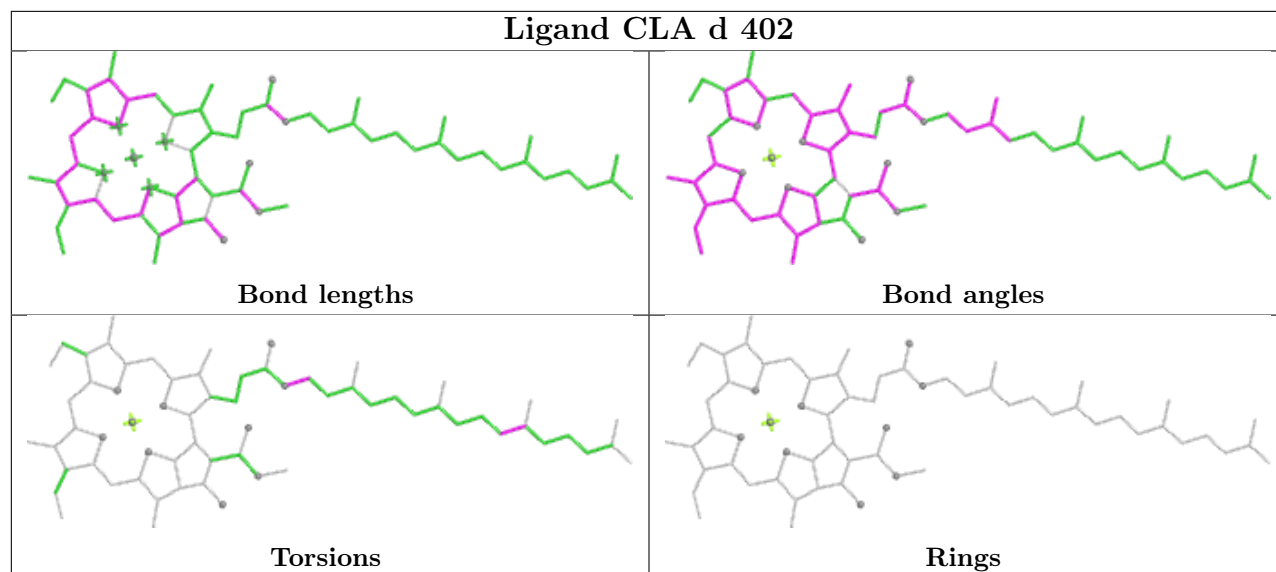


Ligand CLA B 609	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b 617	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

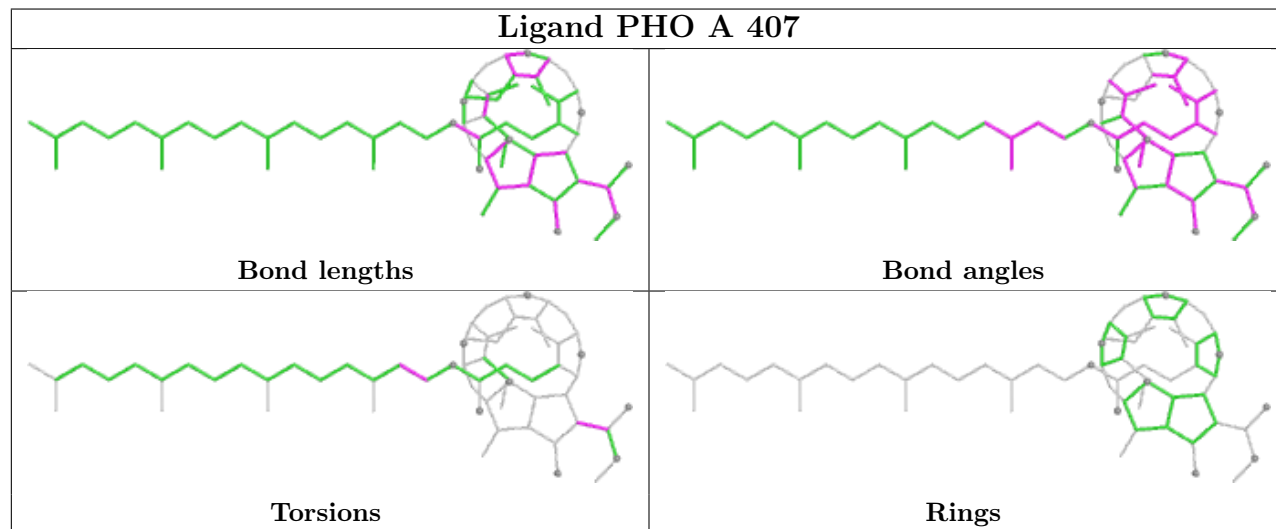




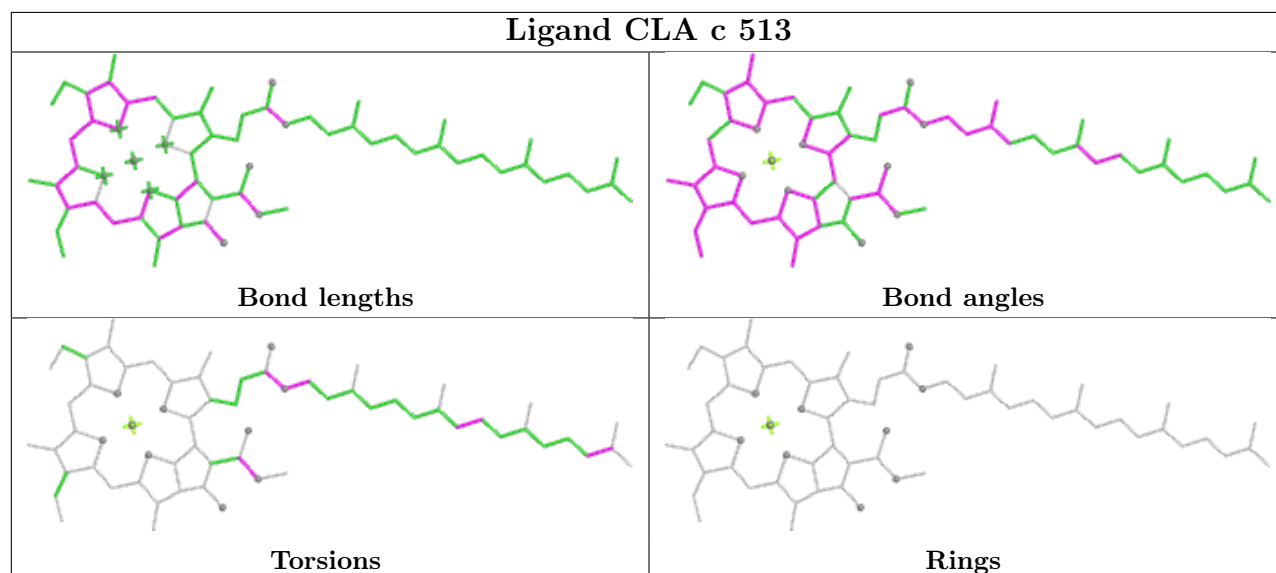
Ligand CLA d 402

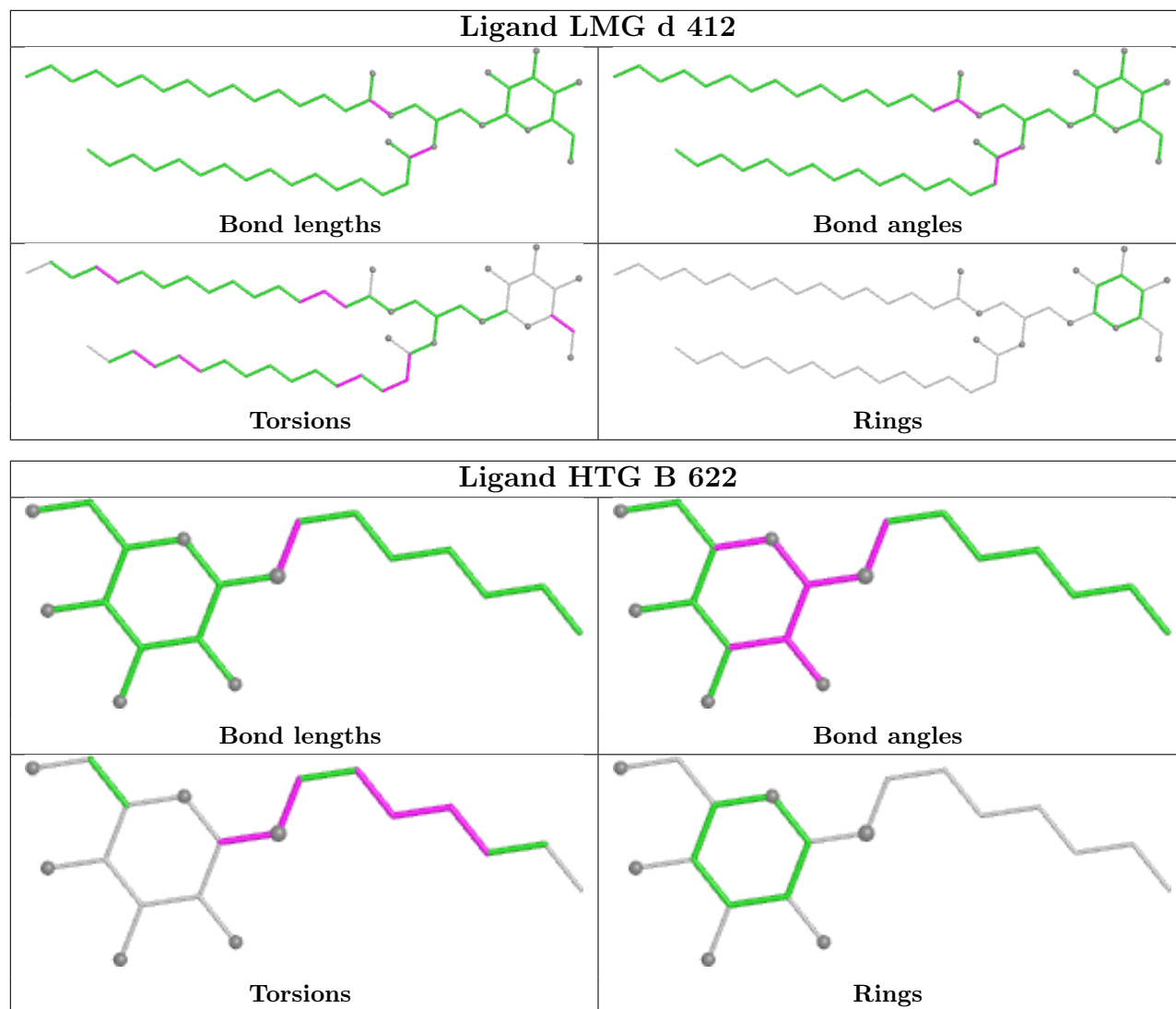


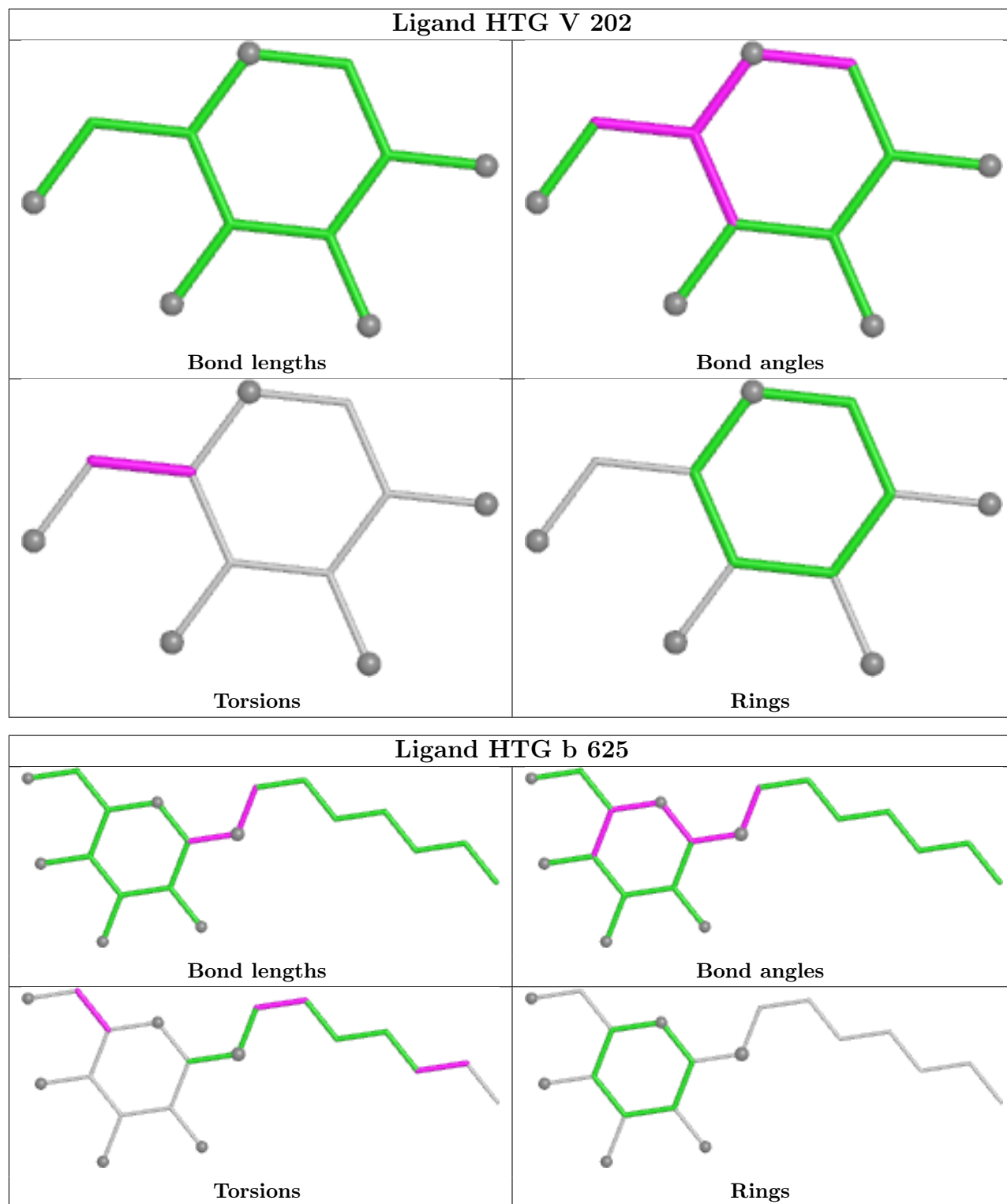
Ligand PHO A 407

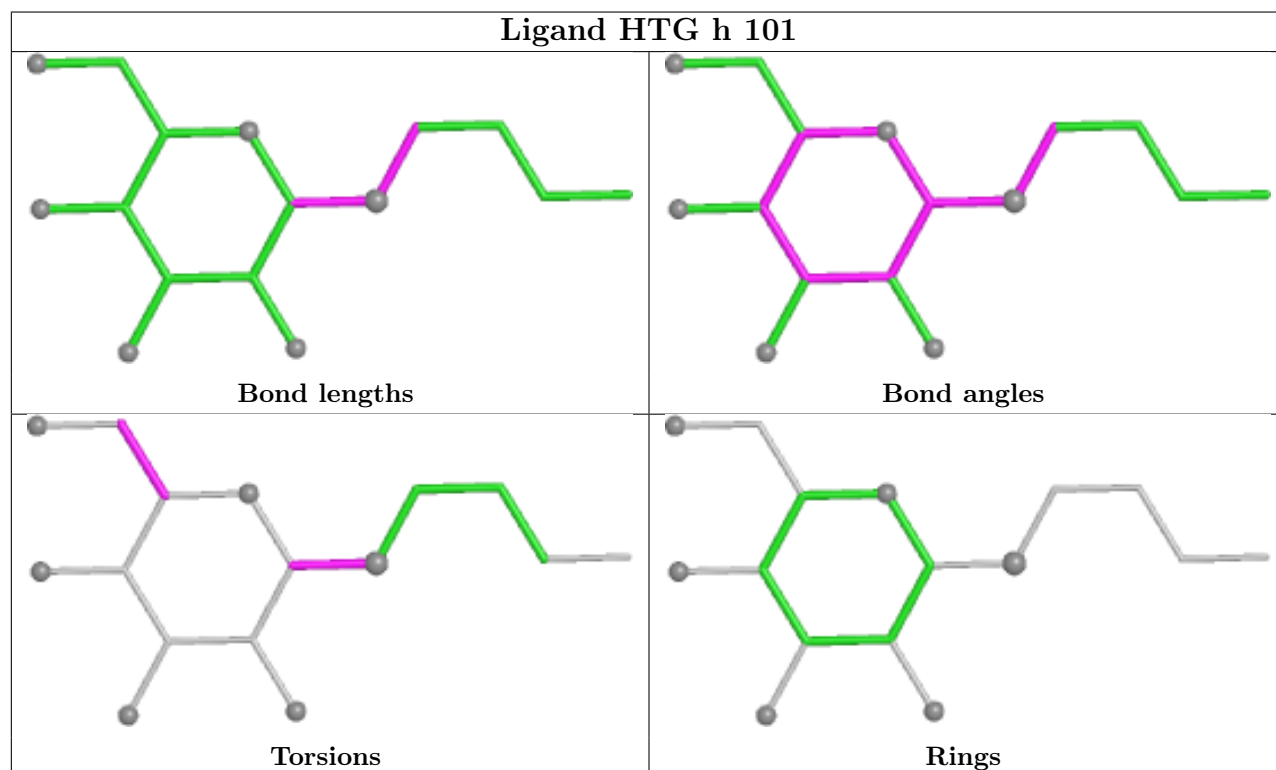
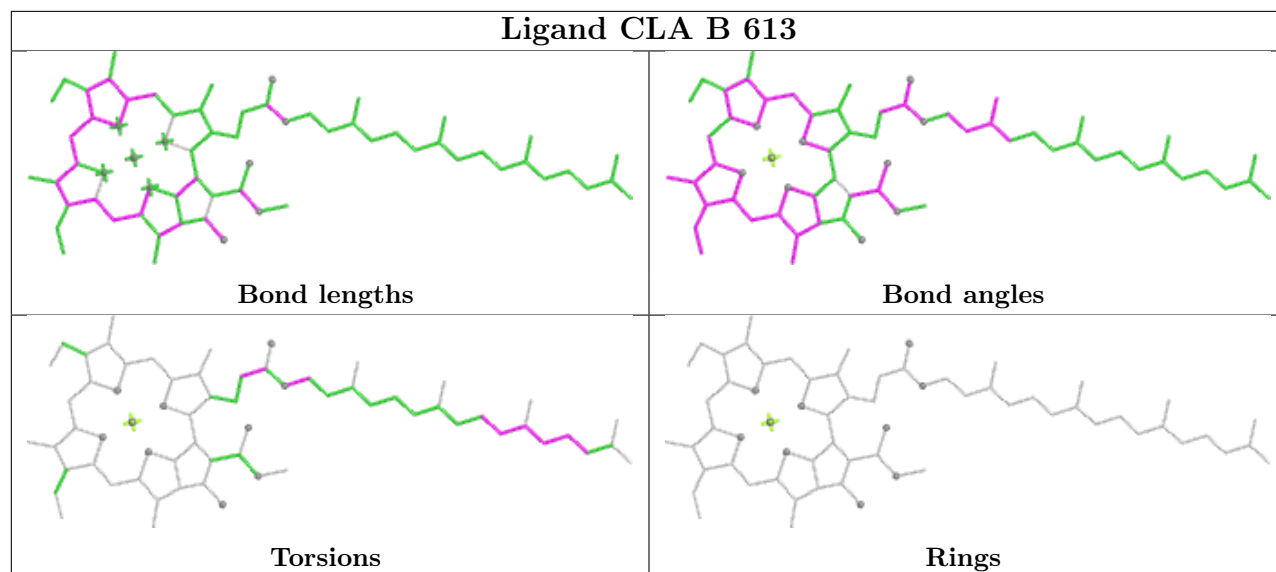


Ligand CLA c 513

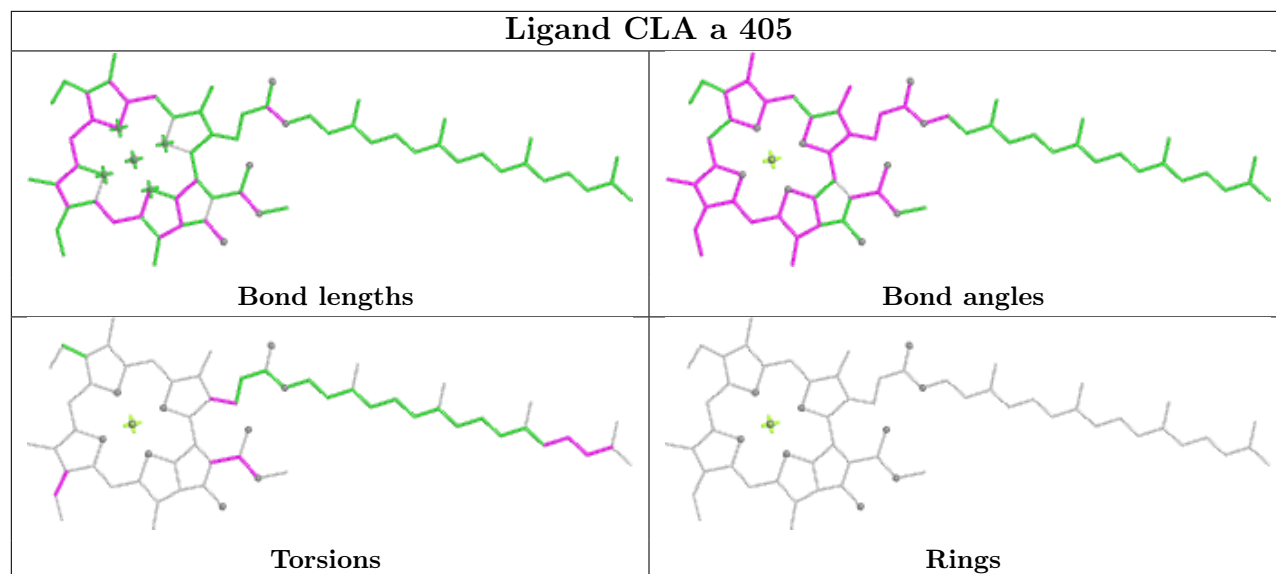




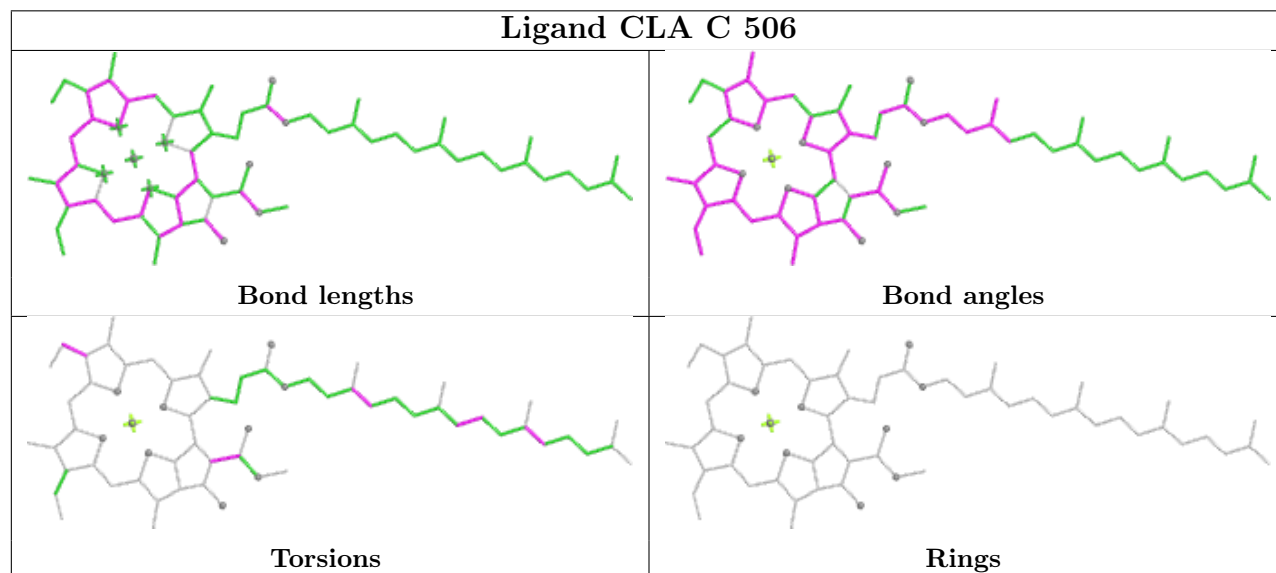




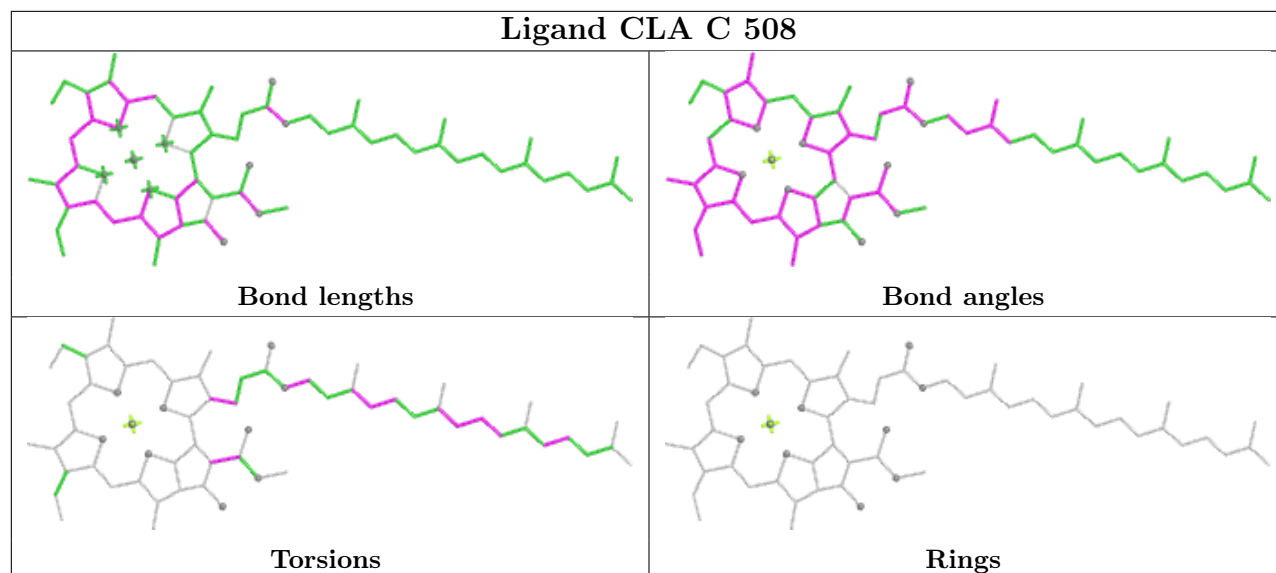
Ligand CLA a 405

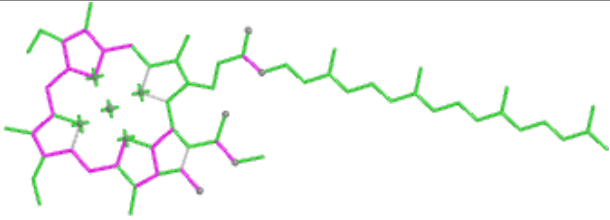
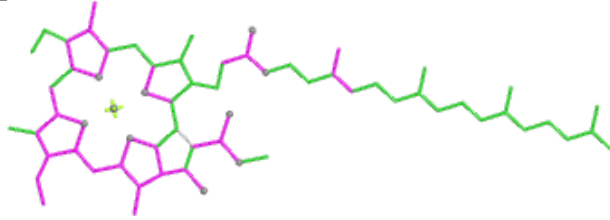
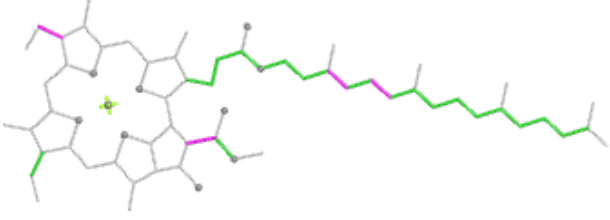
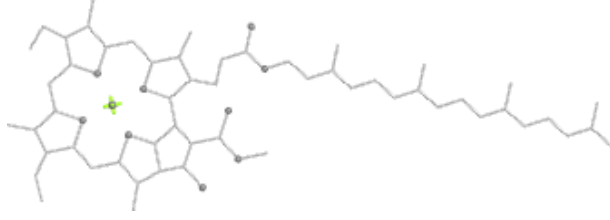
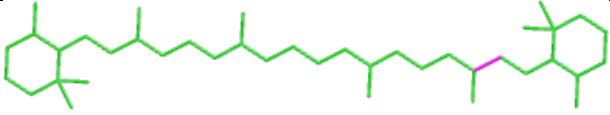
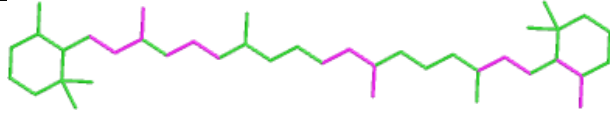
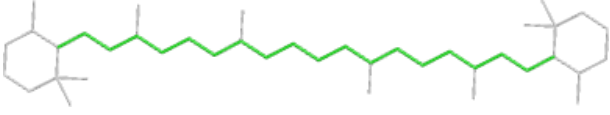
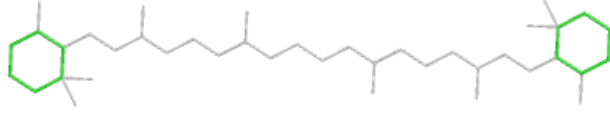
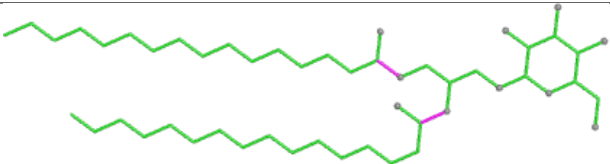
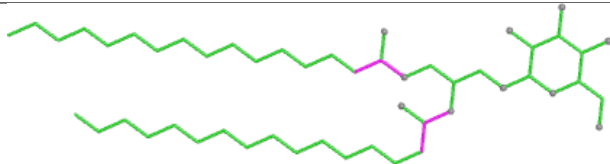
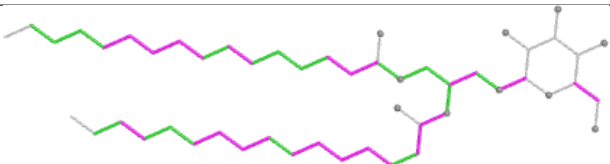
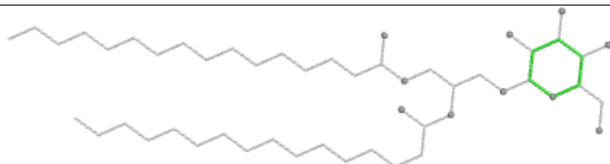


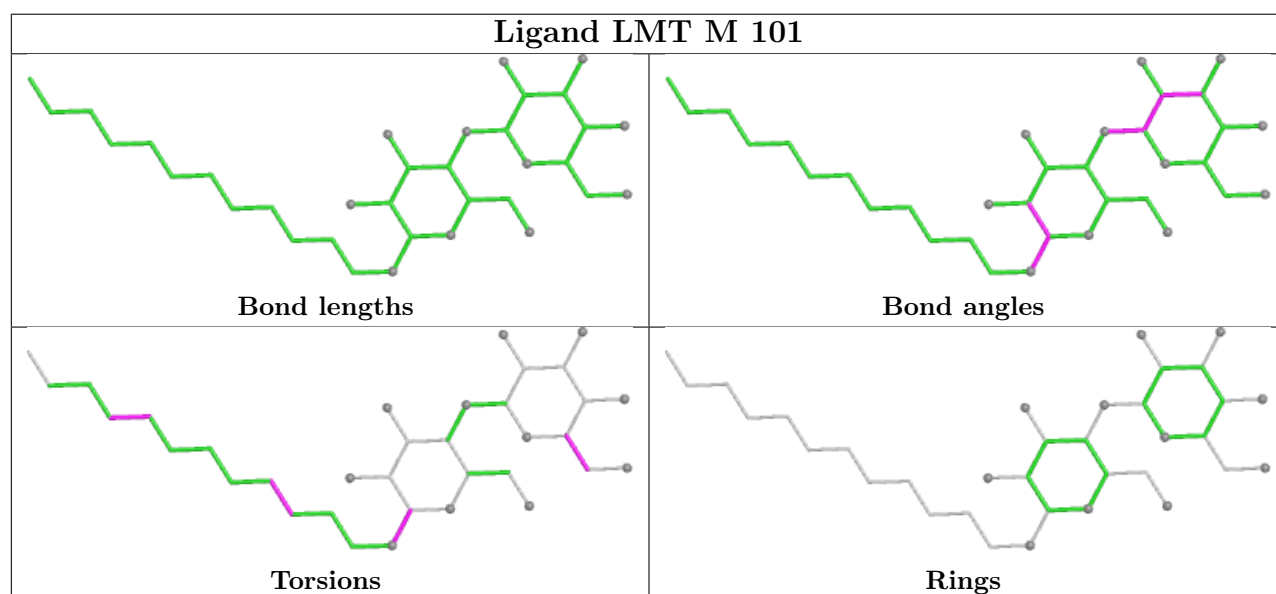
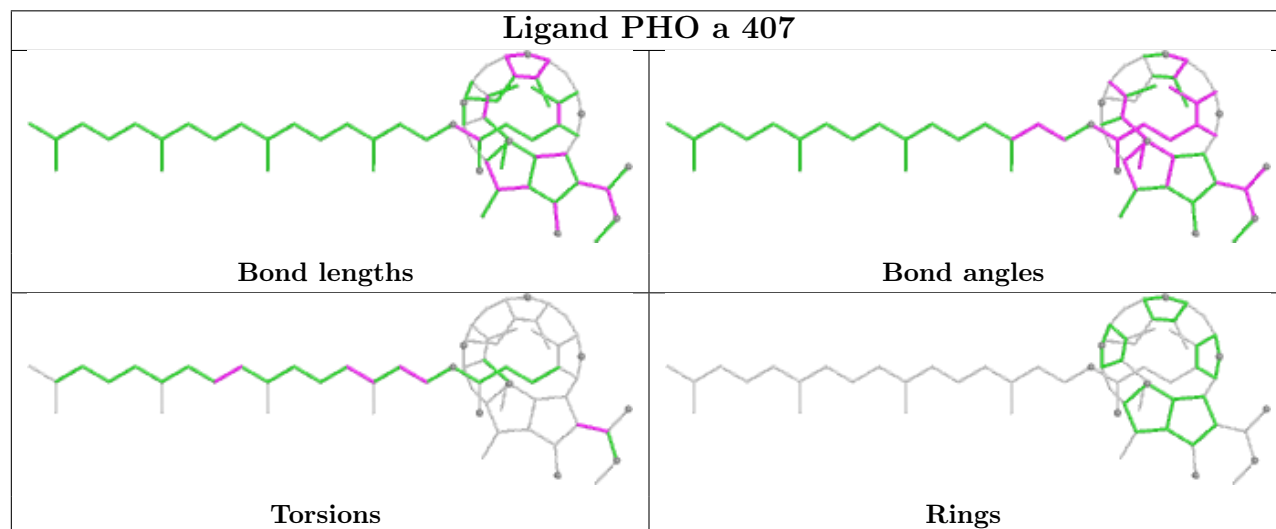
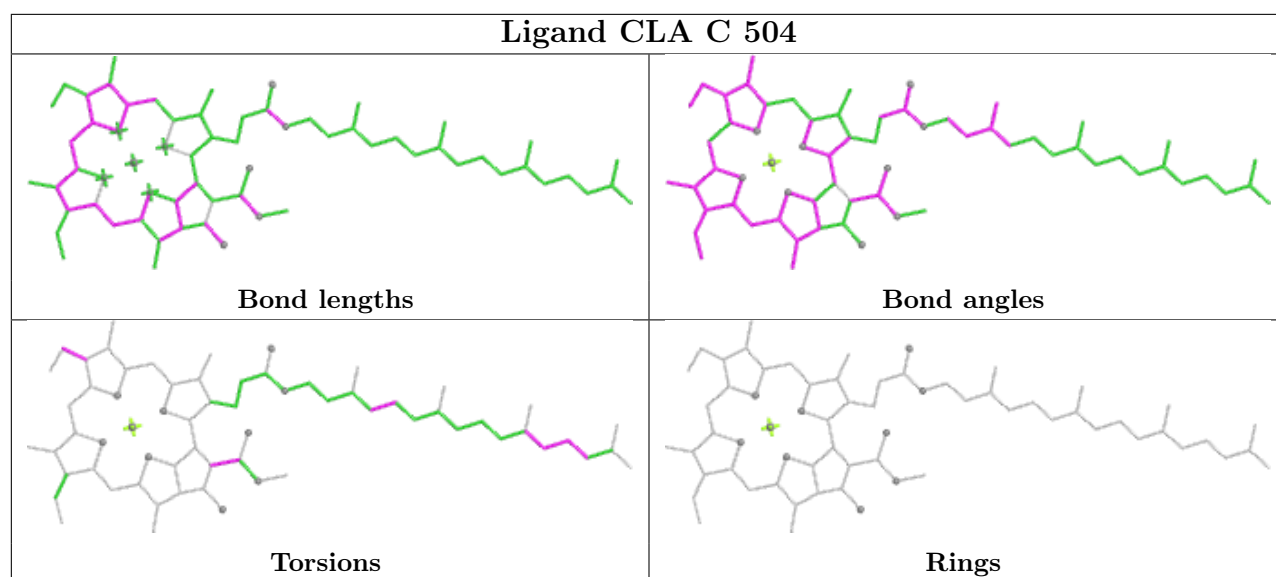
Ligand CLA C 506



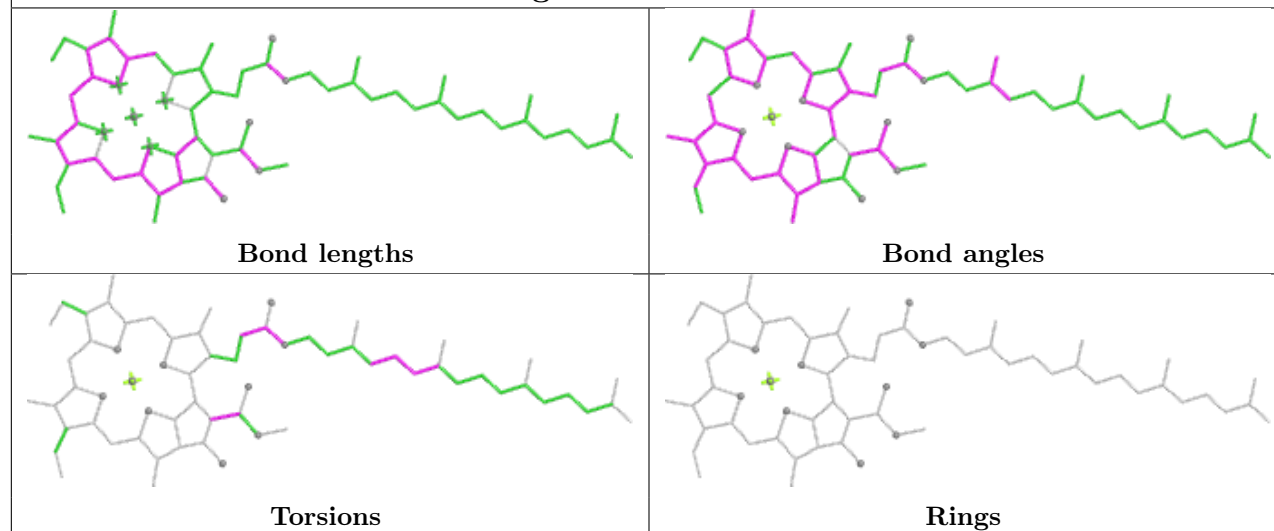
Ligand CLA C 508



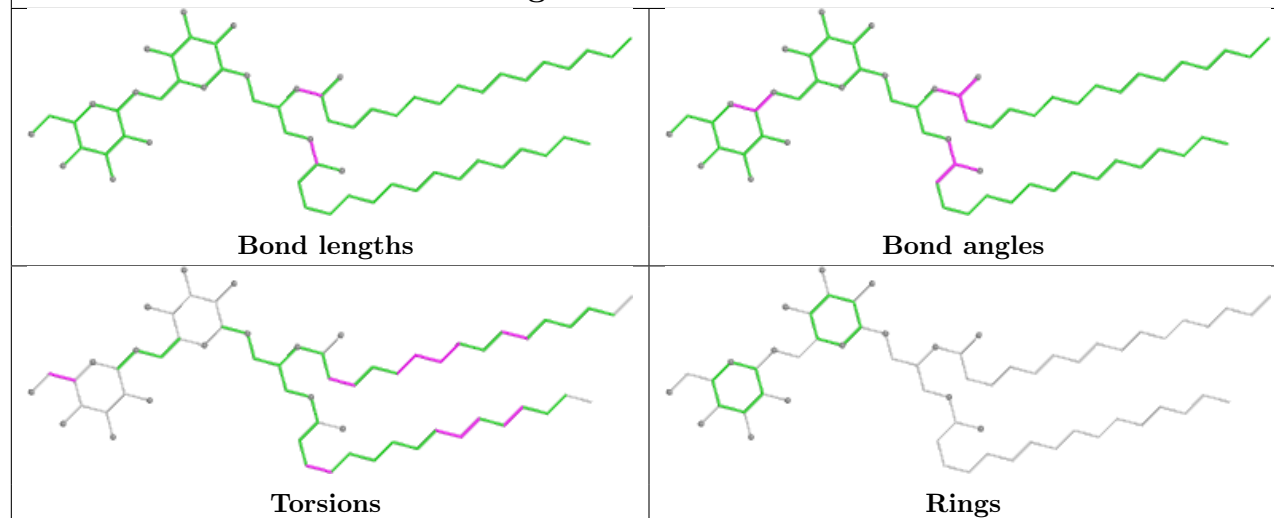
Ligand CLA C 509	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR h 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG C 502	
 Bond lengths	 Bond angles
 Torsions	 Rings



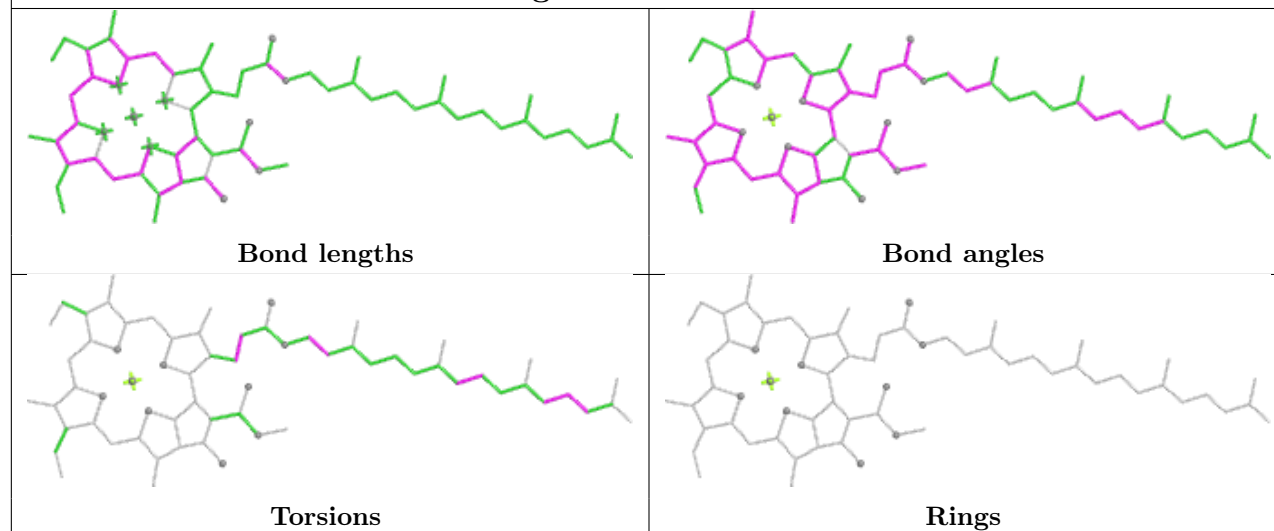
Ligand CLA B 601



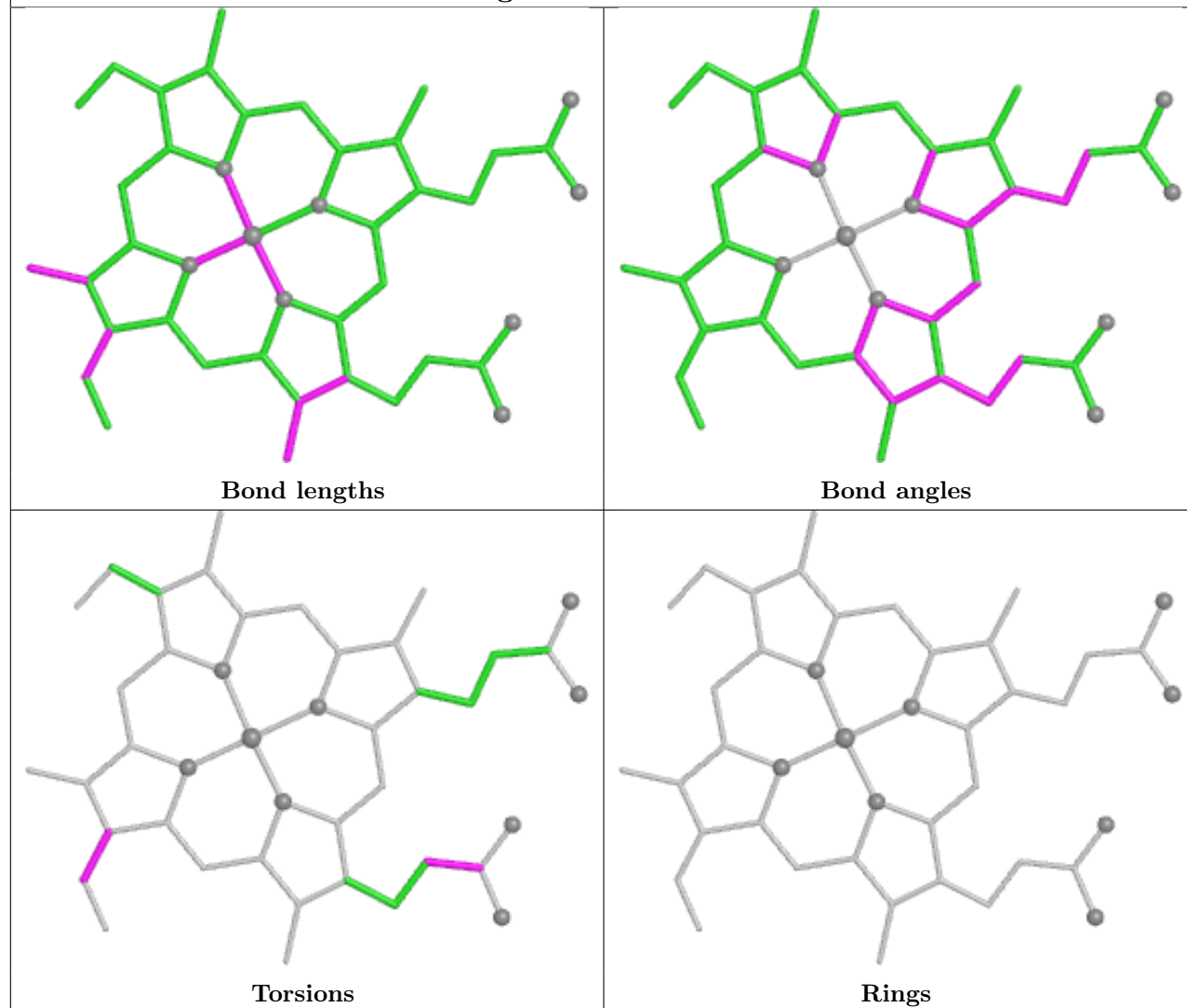
Ligand DGD C 520



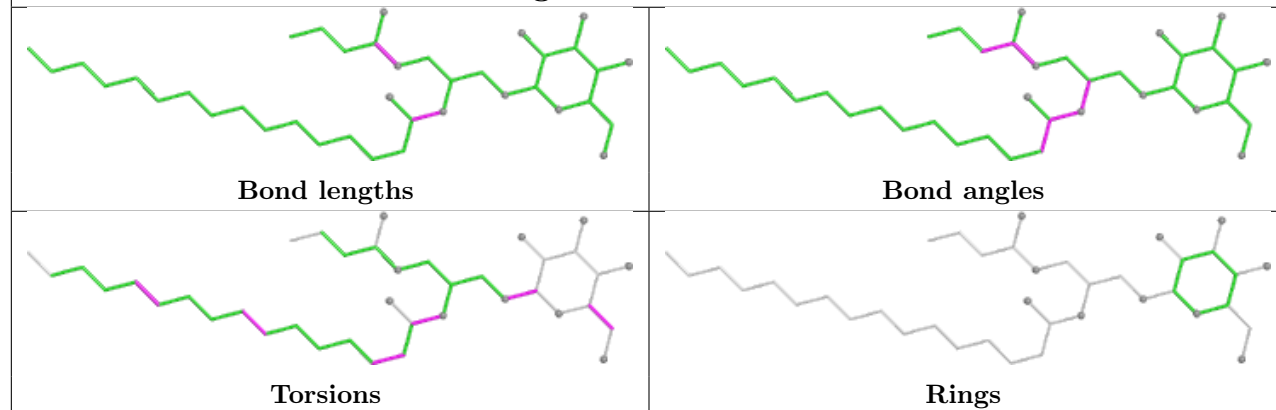
Ligand CLA B 602



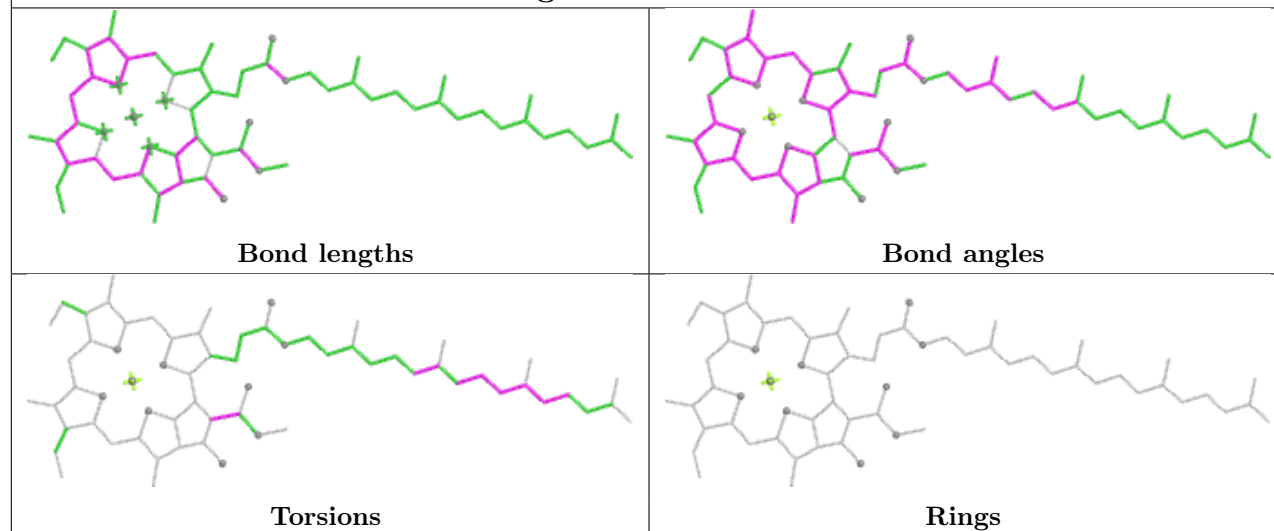
Ligand HEC v 202



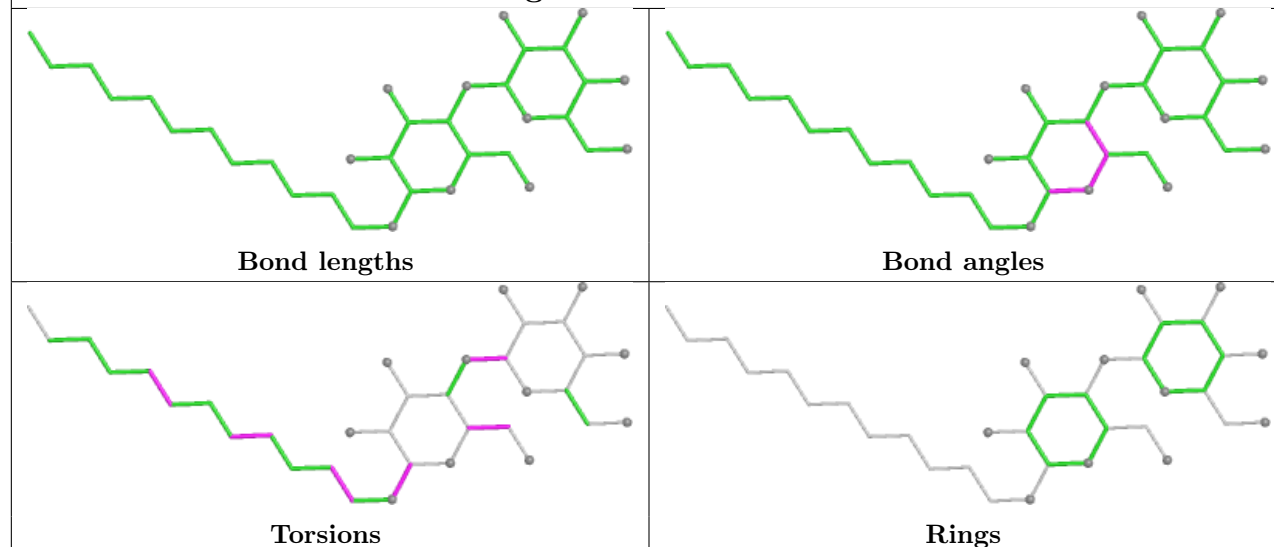
Ligand LMG z 101



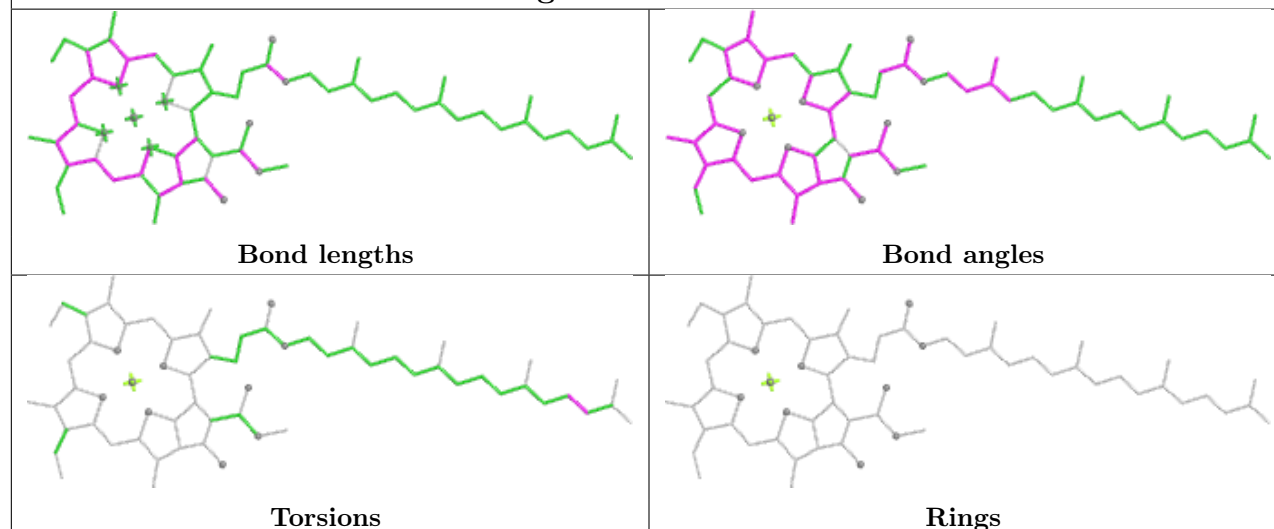
Ligand CLA c 510

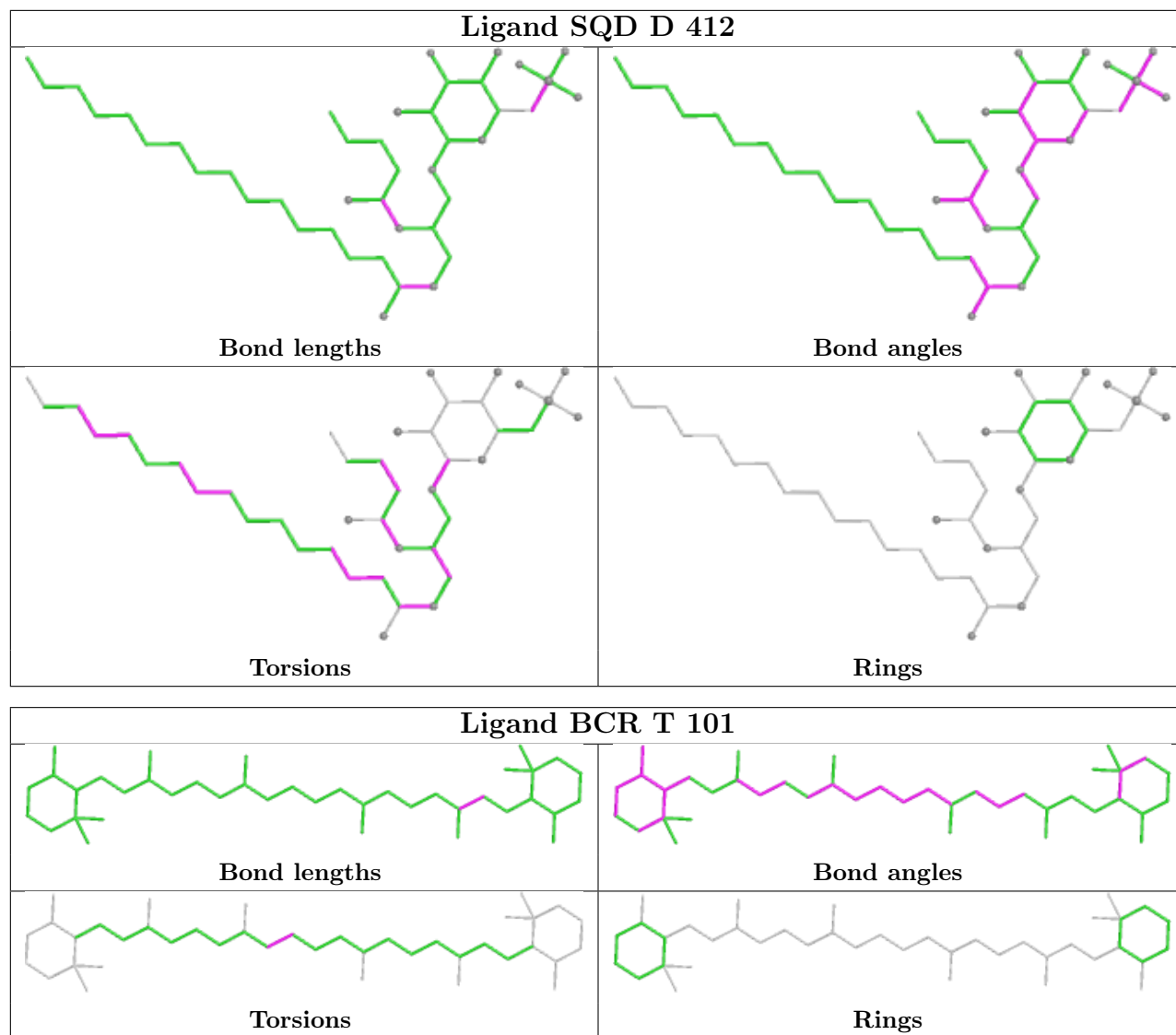


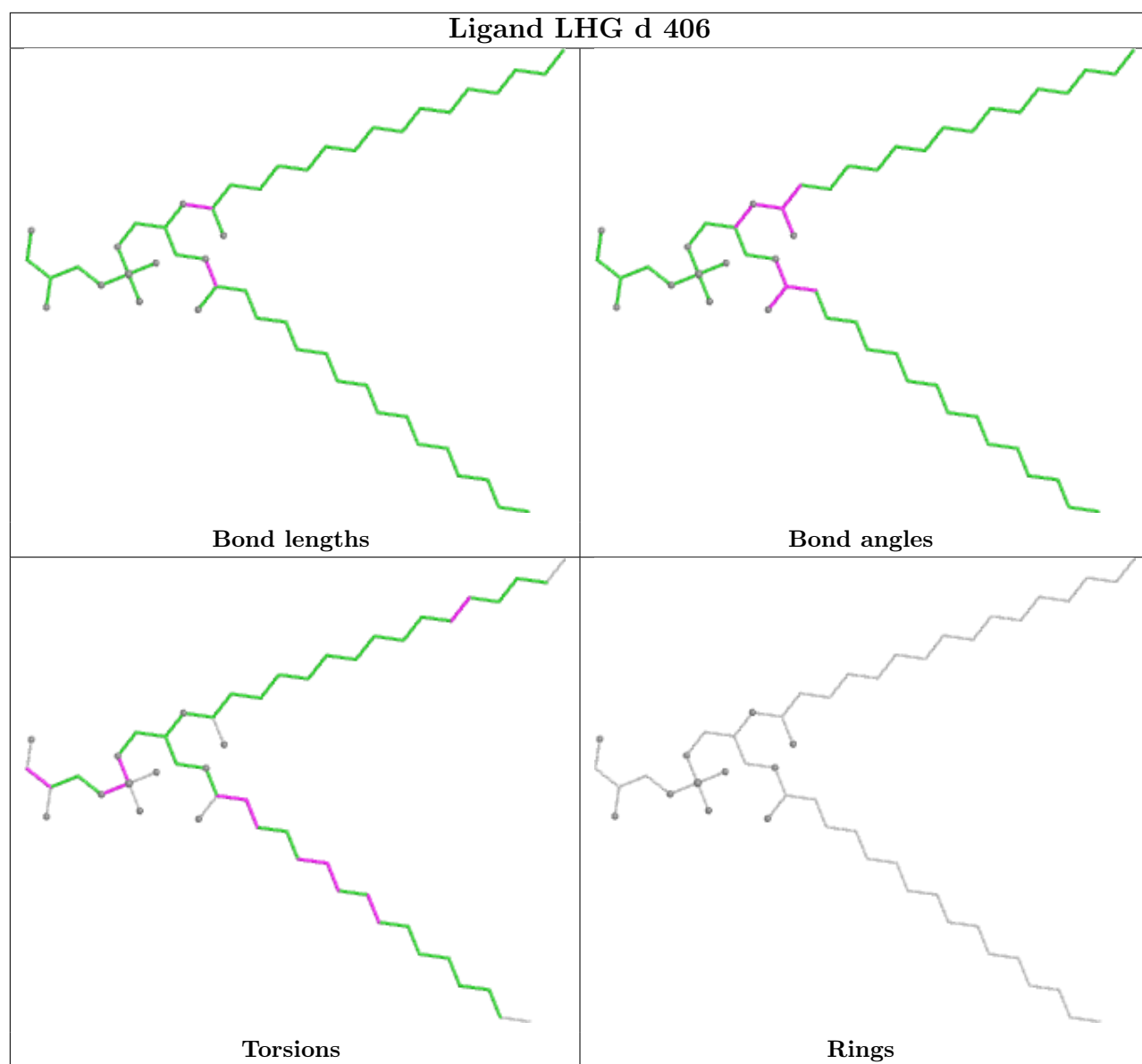
Ligand LMT M 103

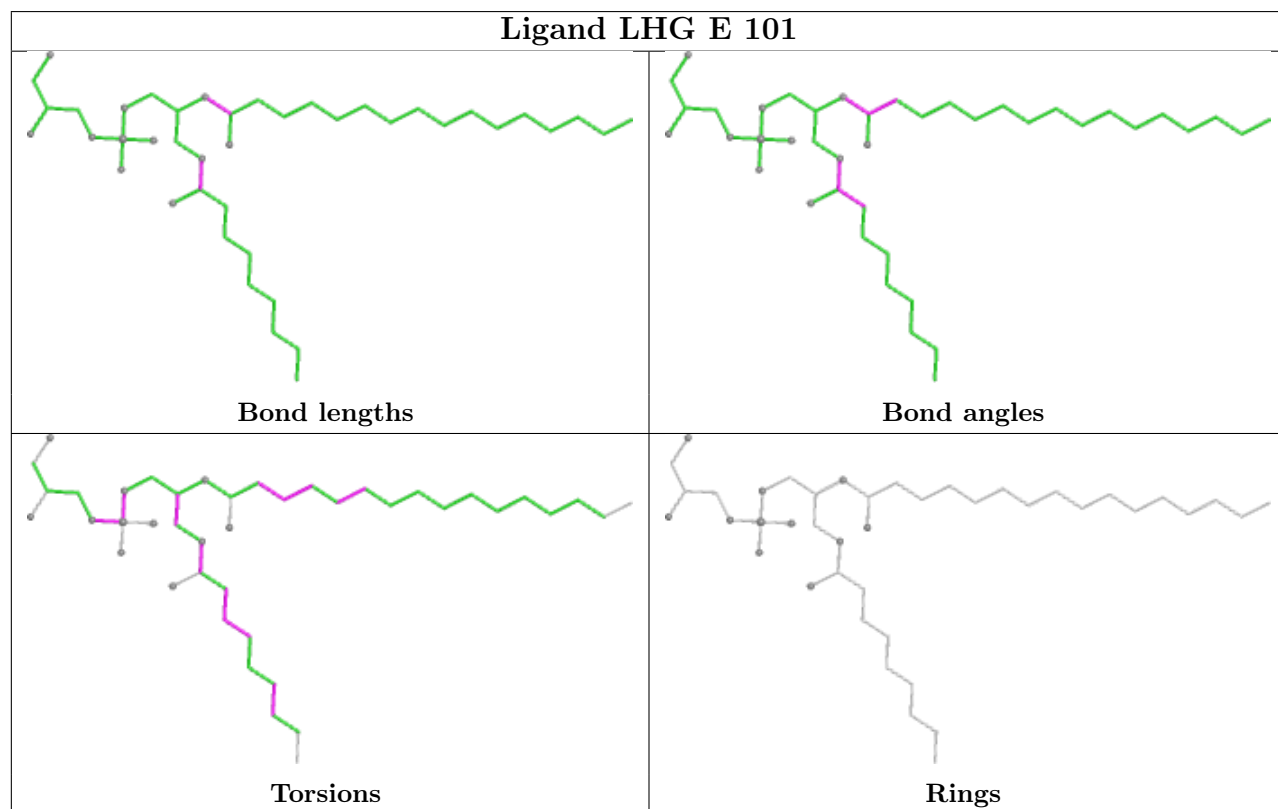
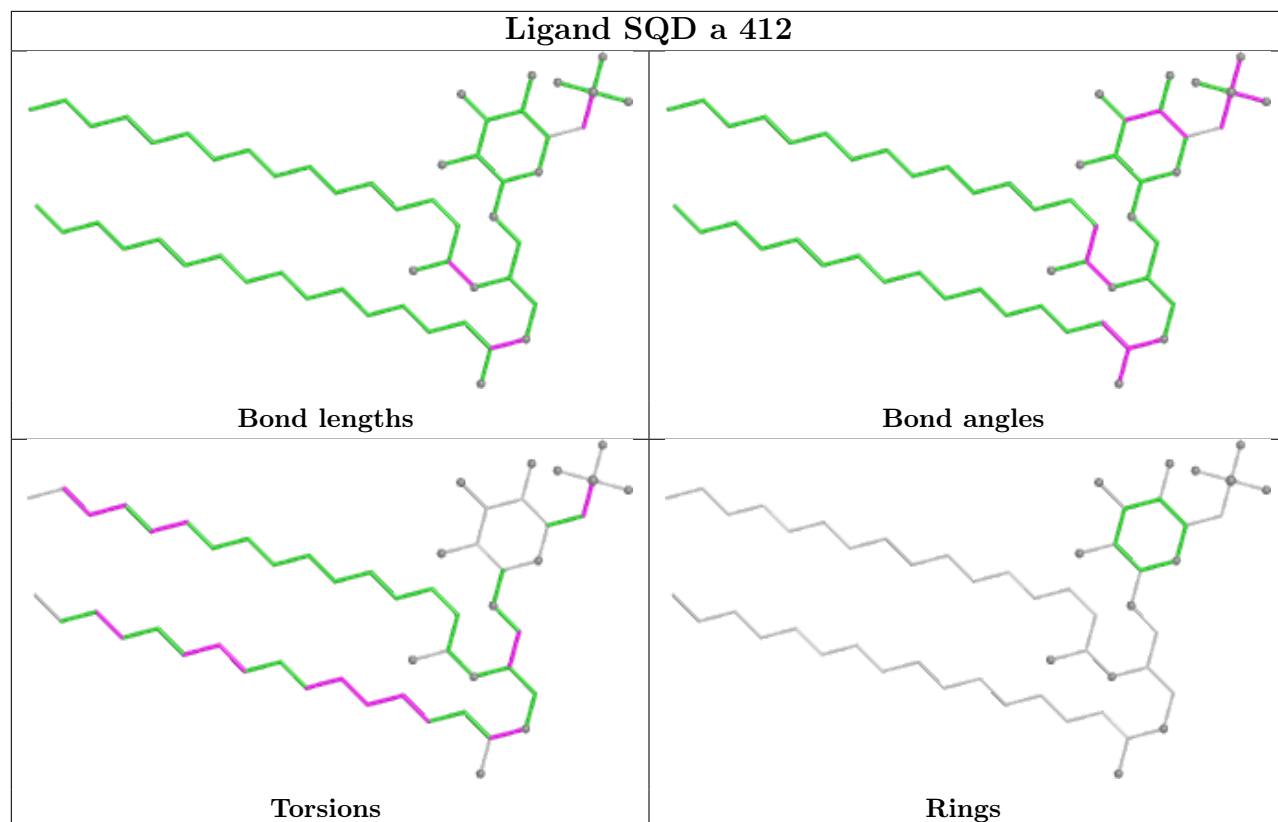


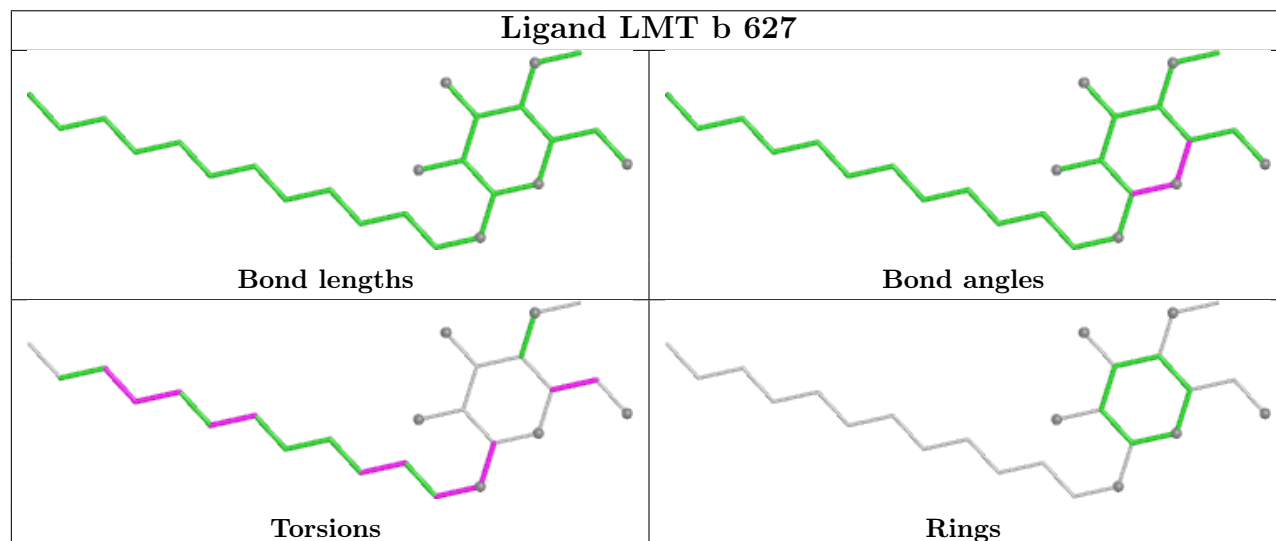
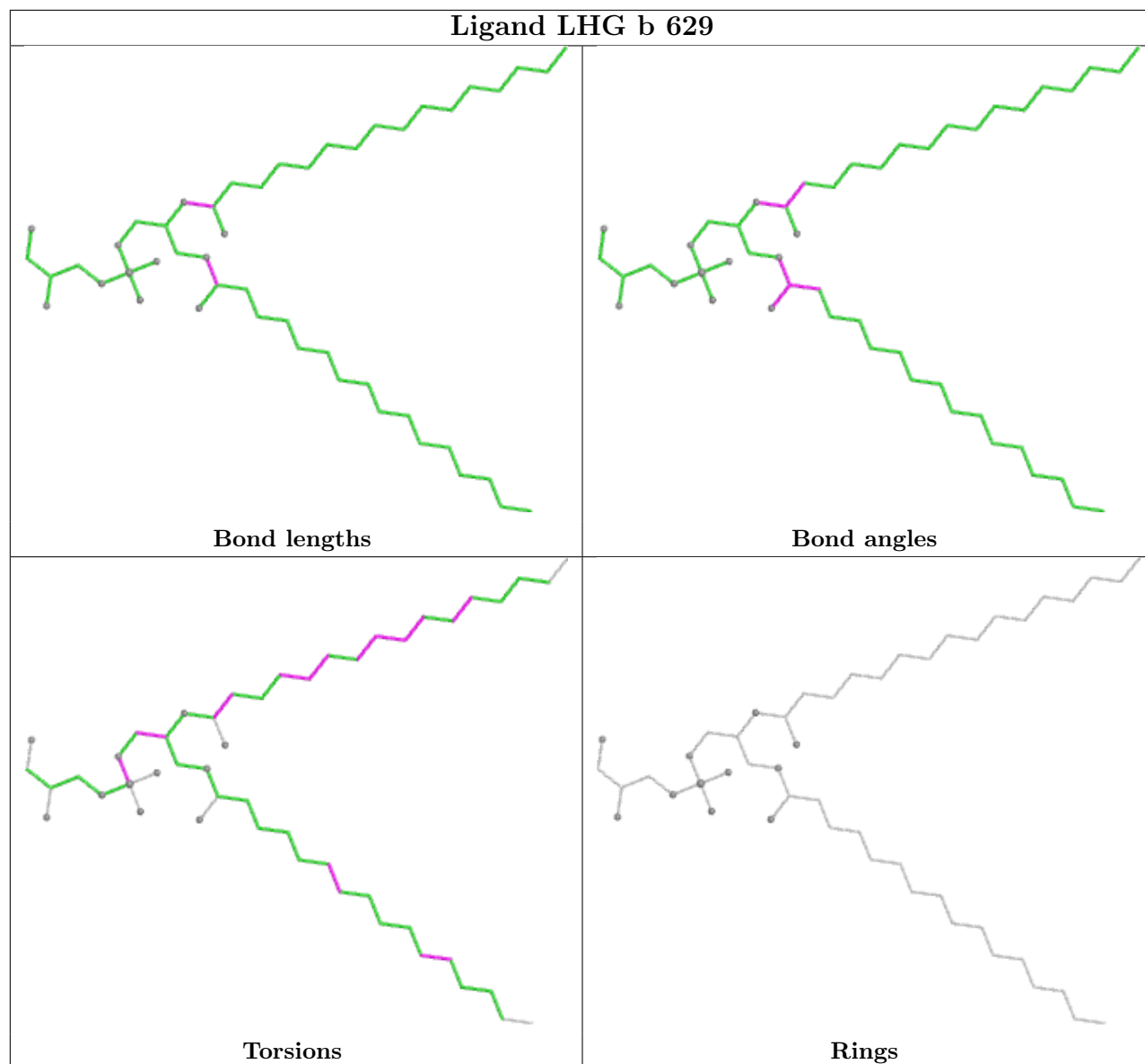
Ligand CLA c 505

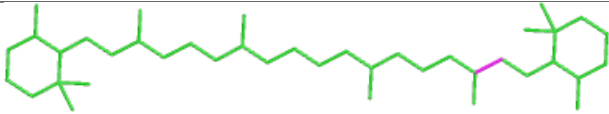
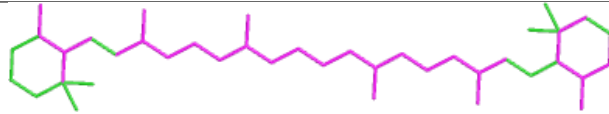
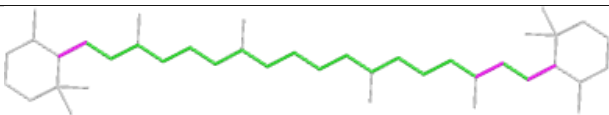
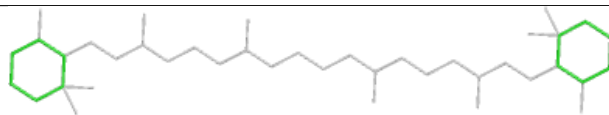


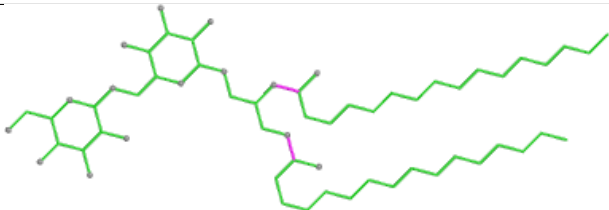
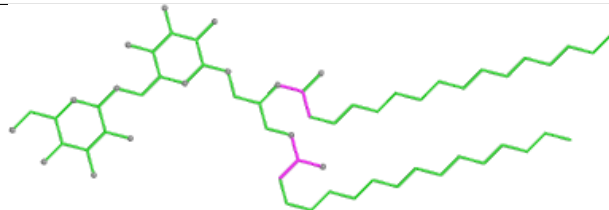
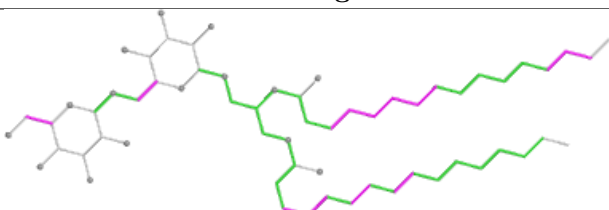
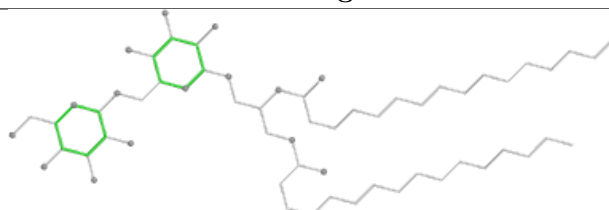


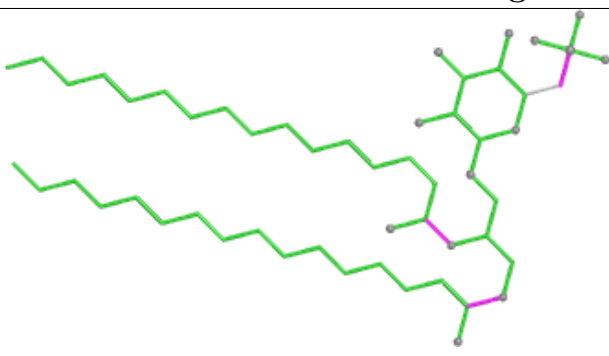
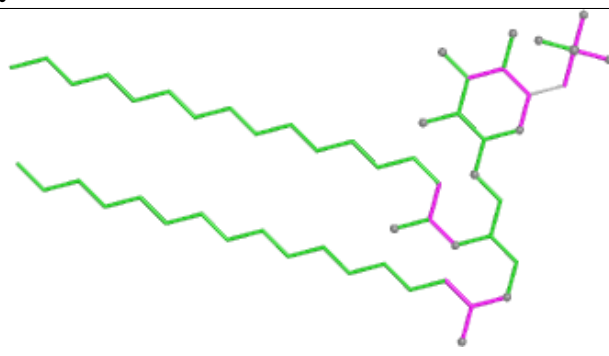
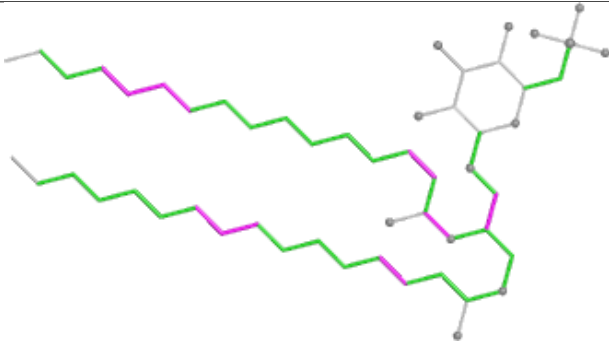
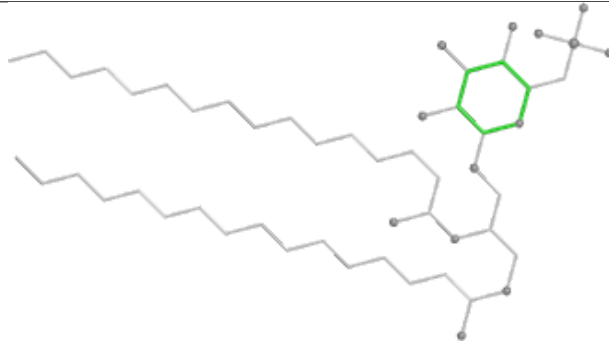


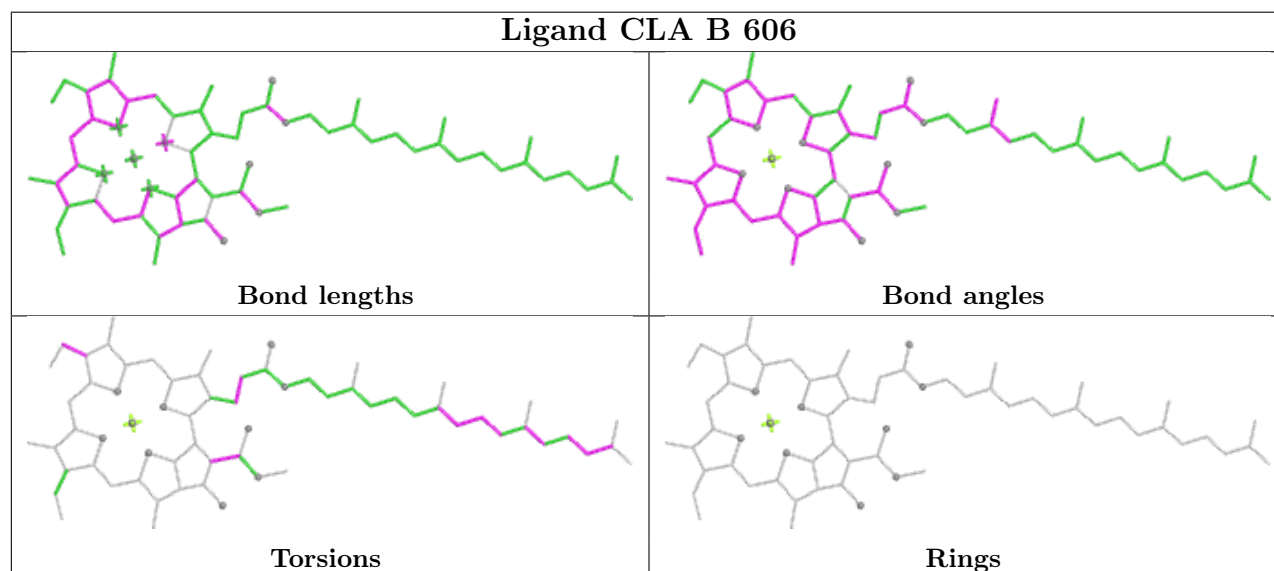
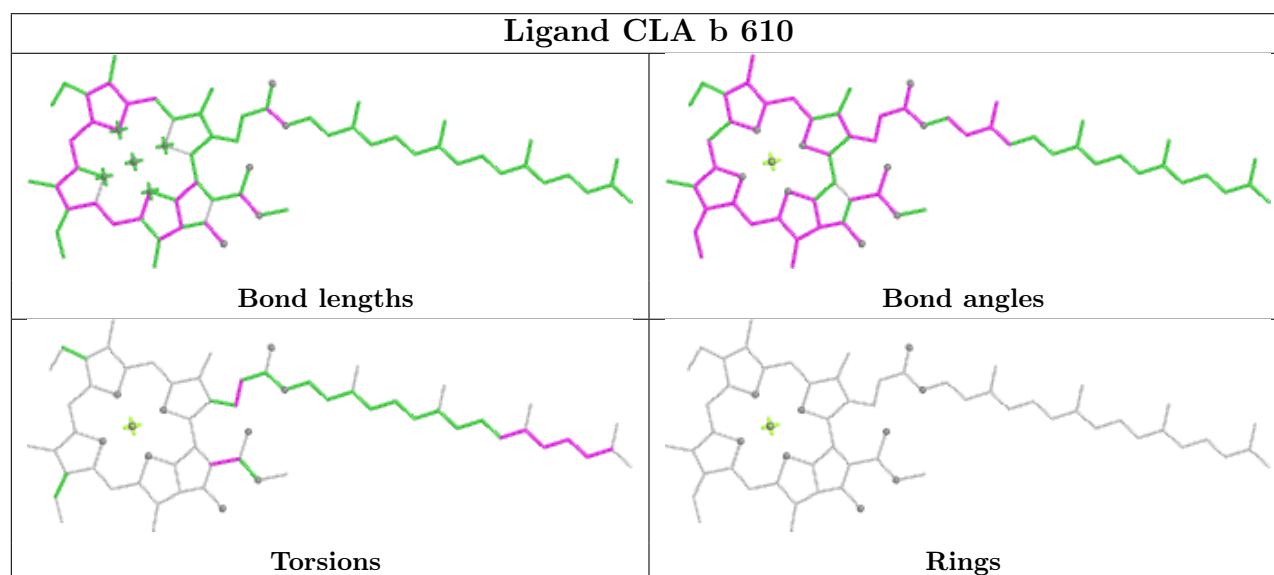
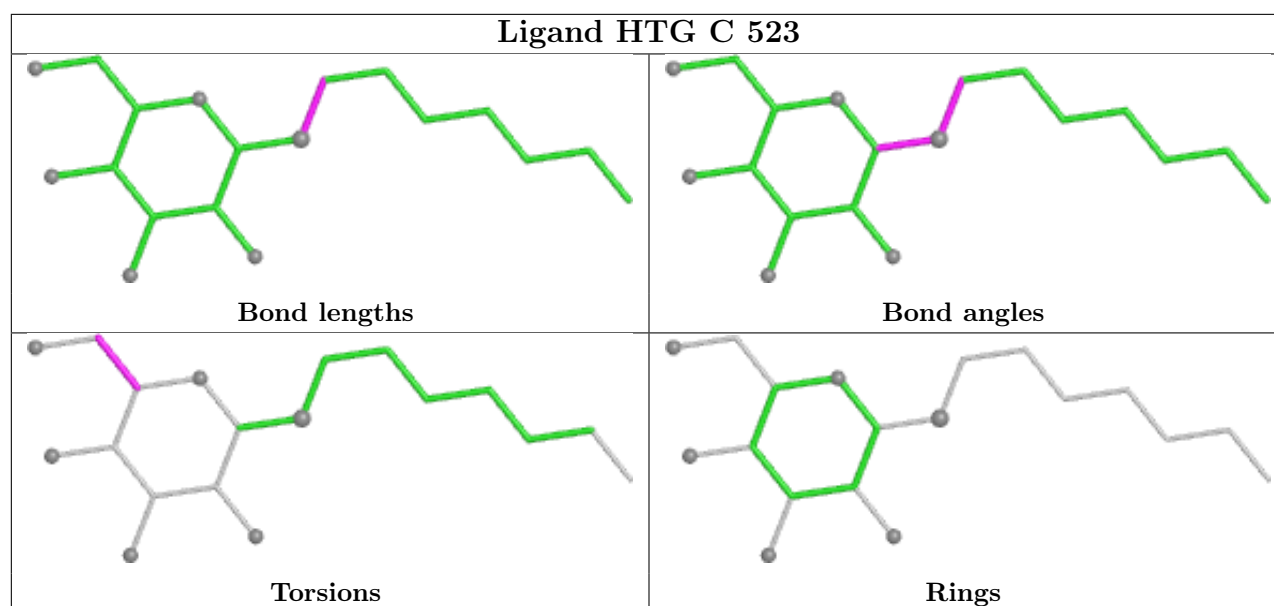


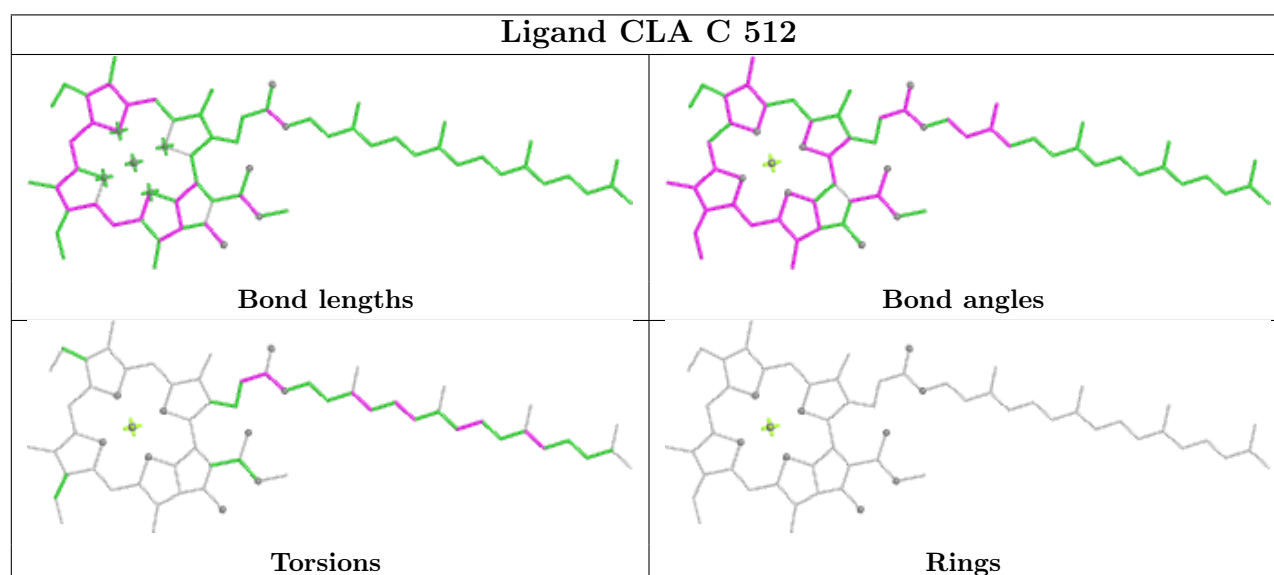
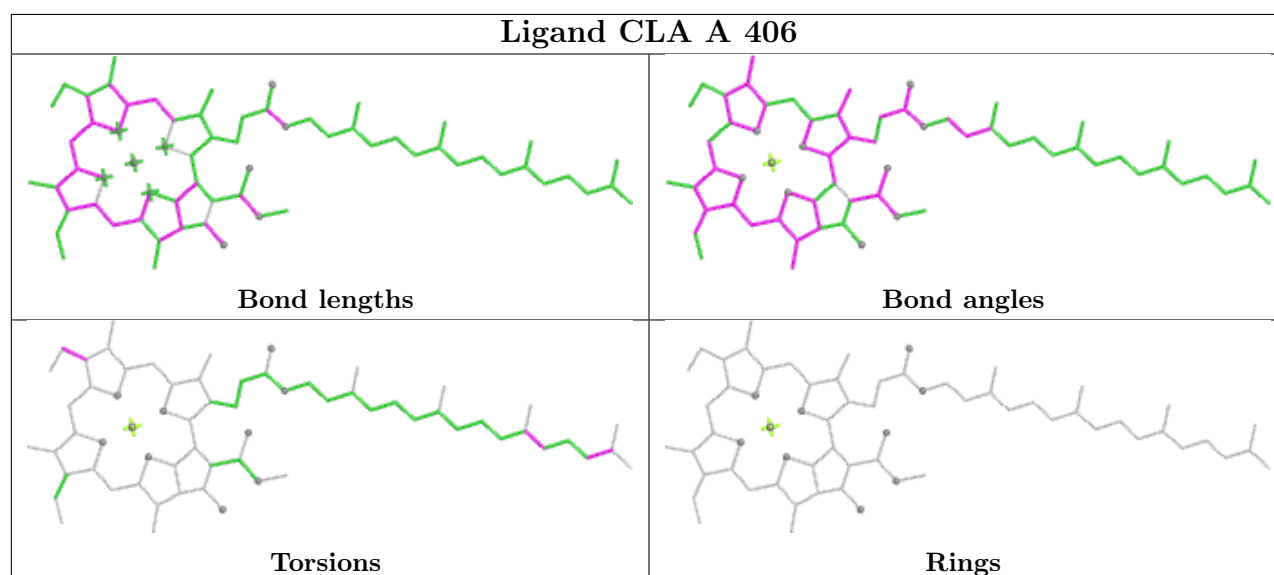
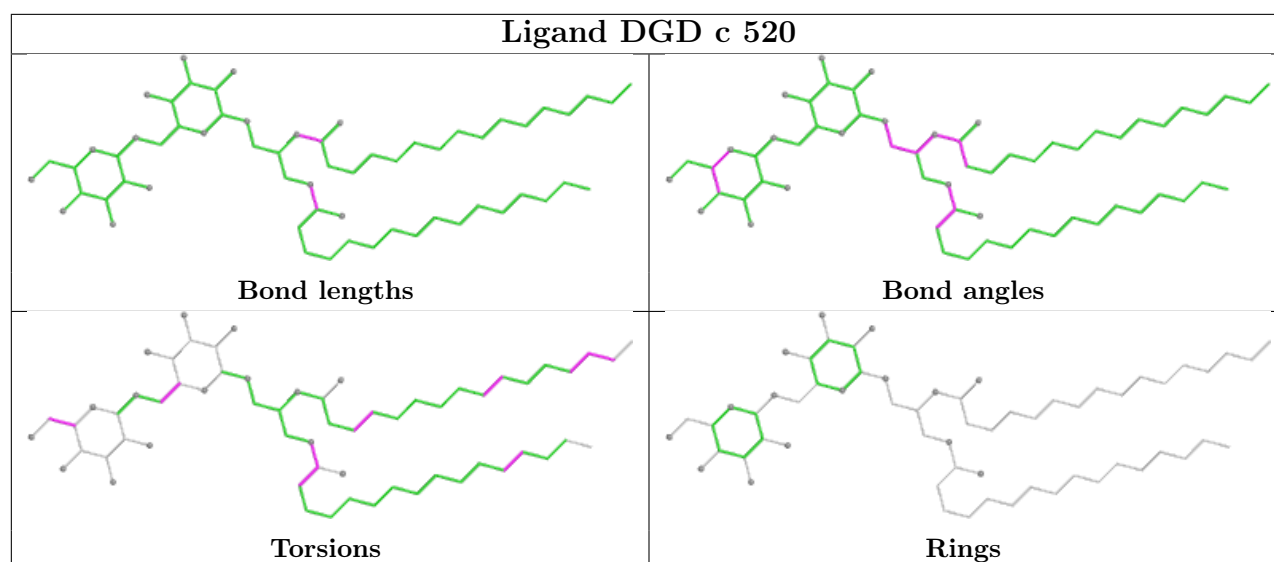


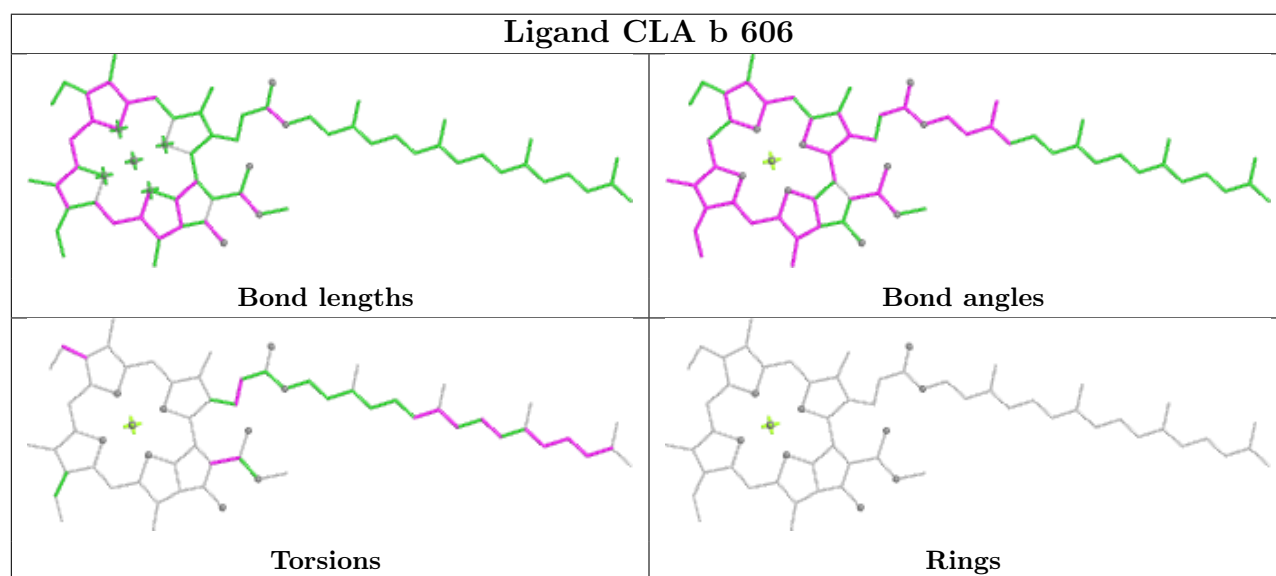
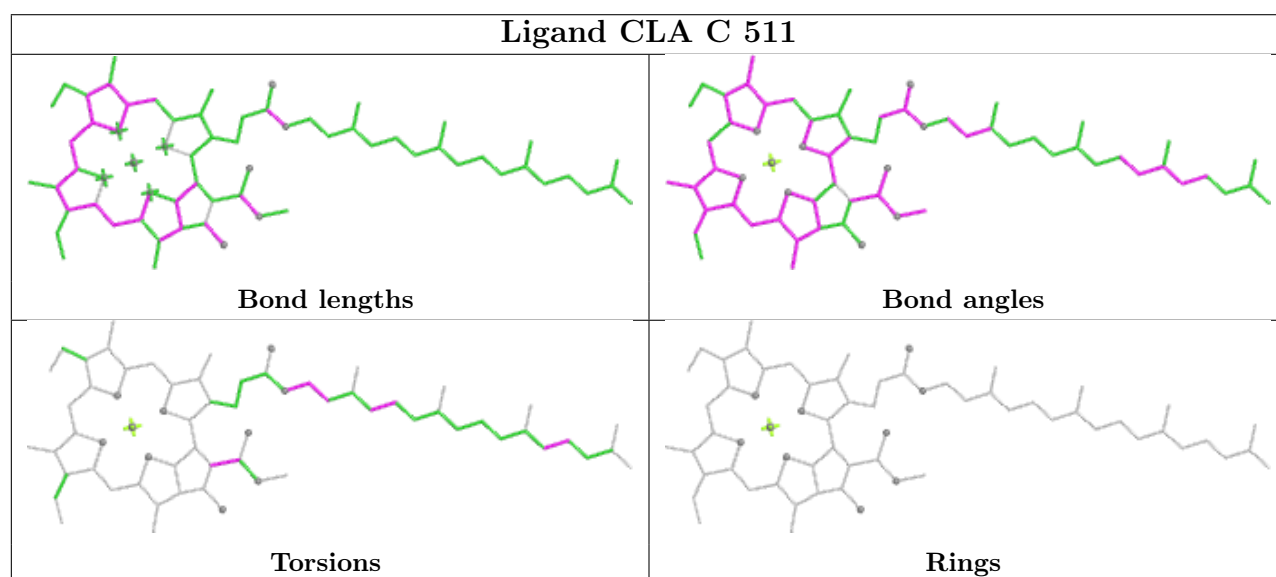
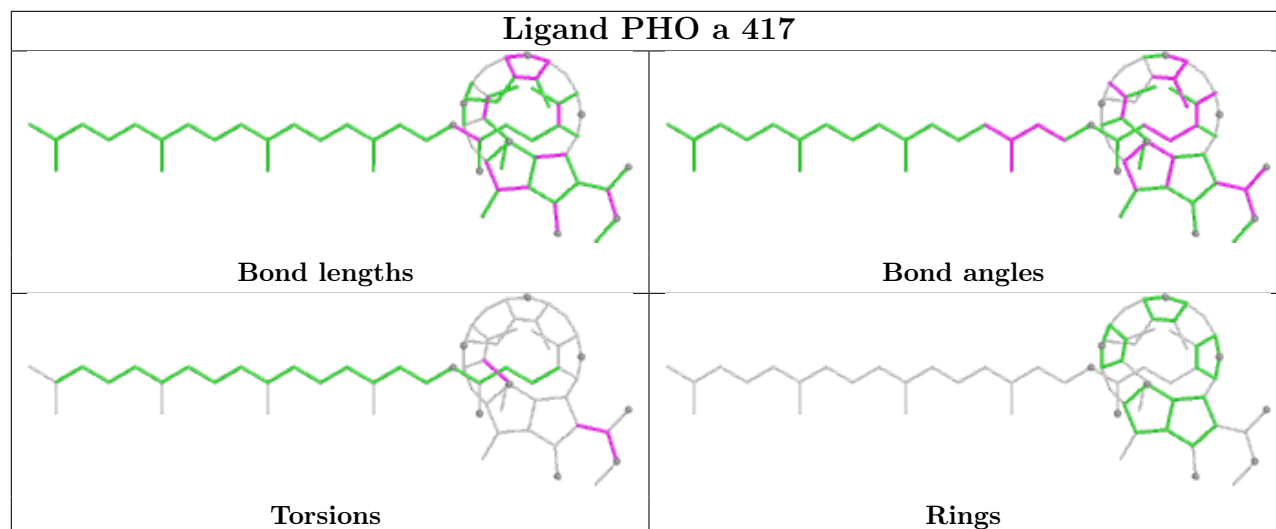
Ligand BCR Y 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

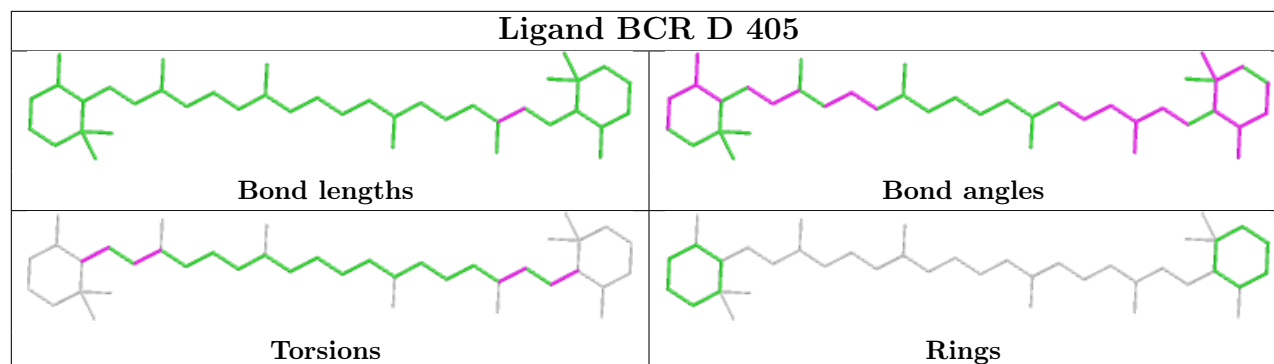
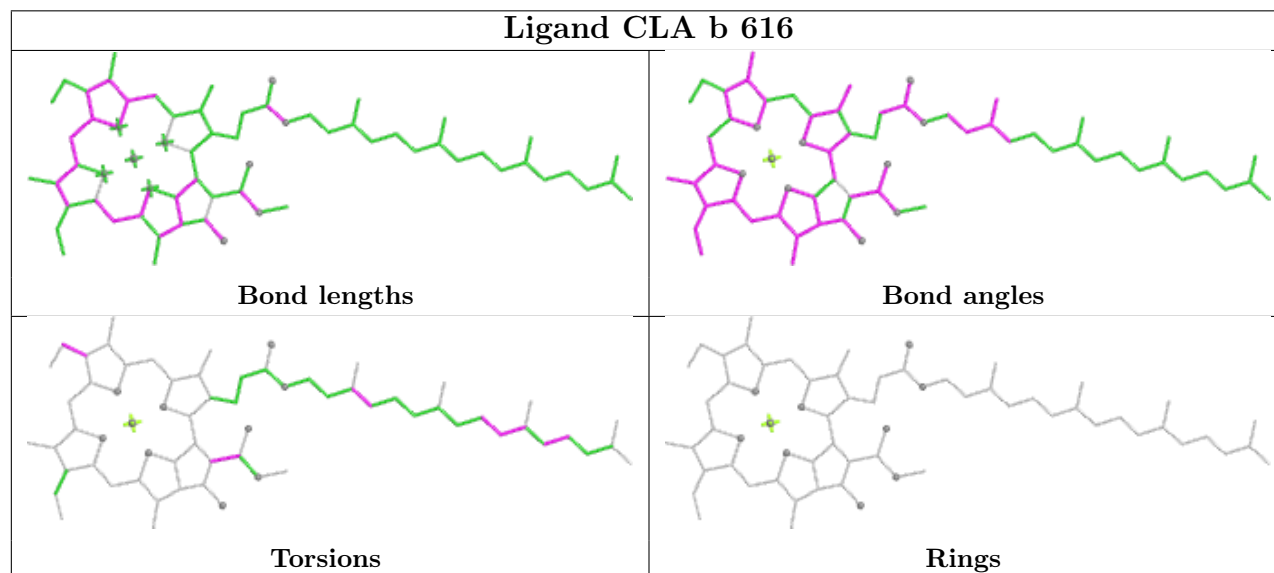
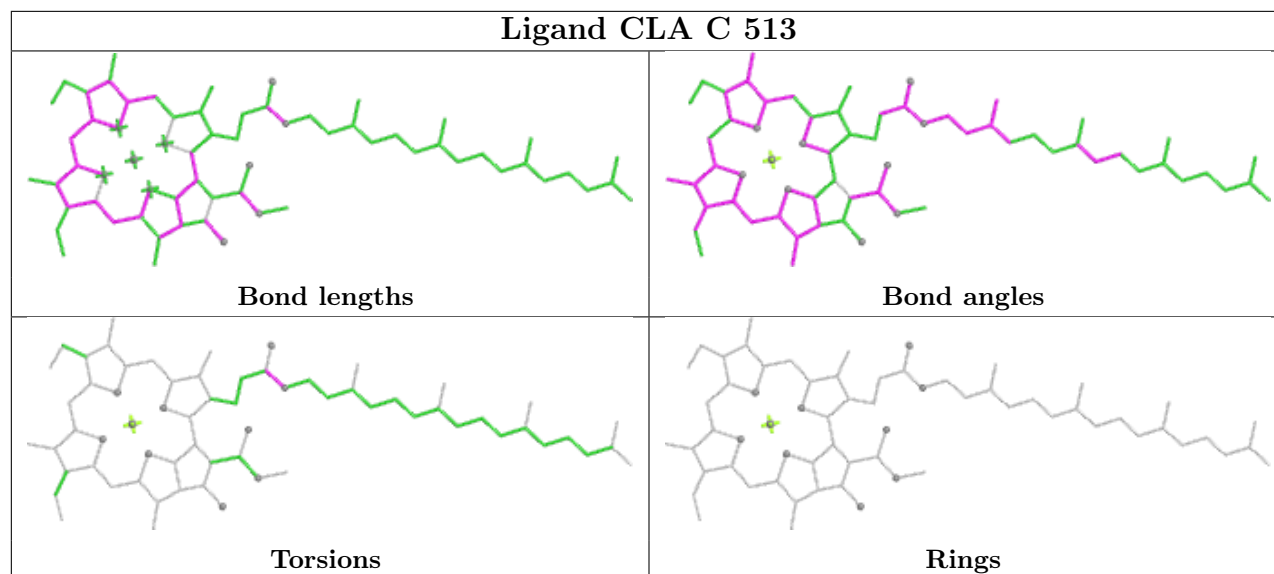
Ligand DGD C 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

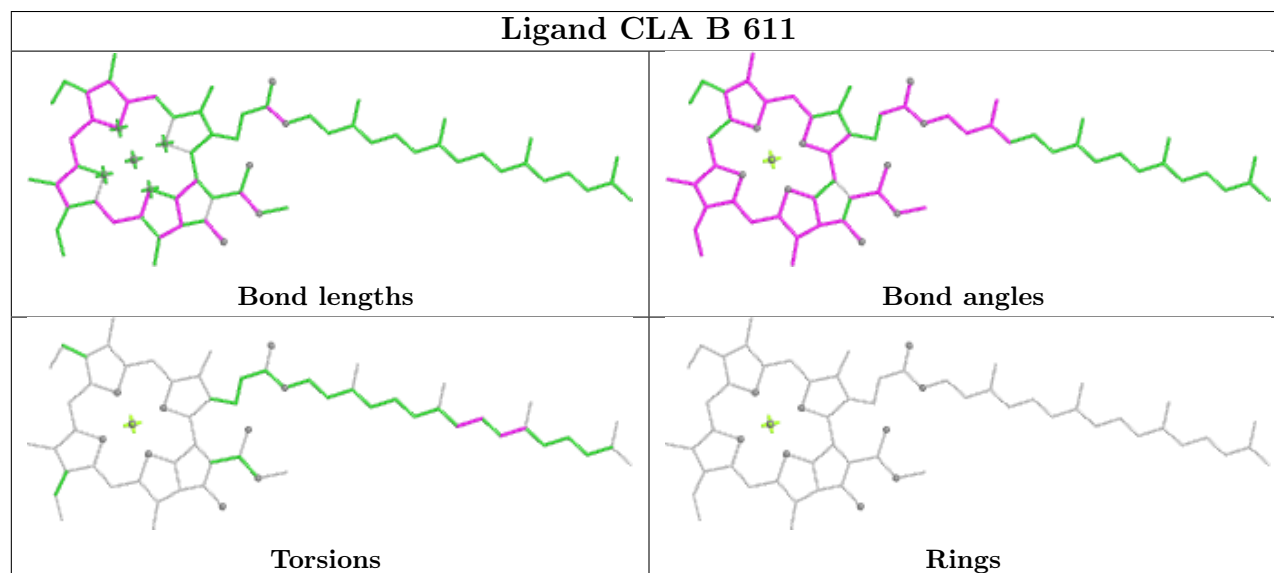
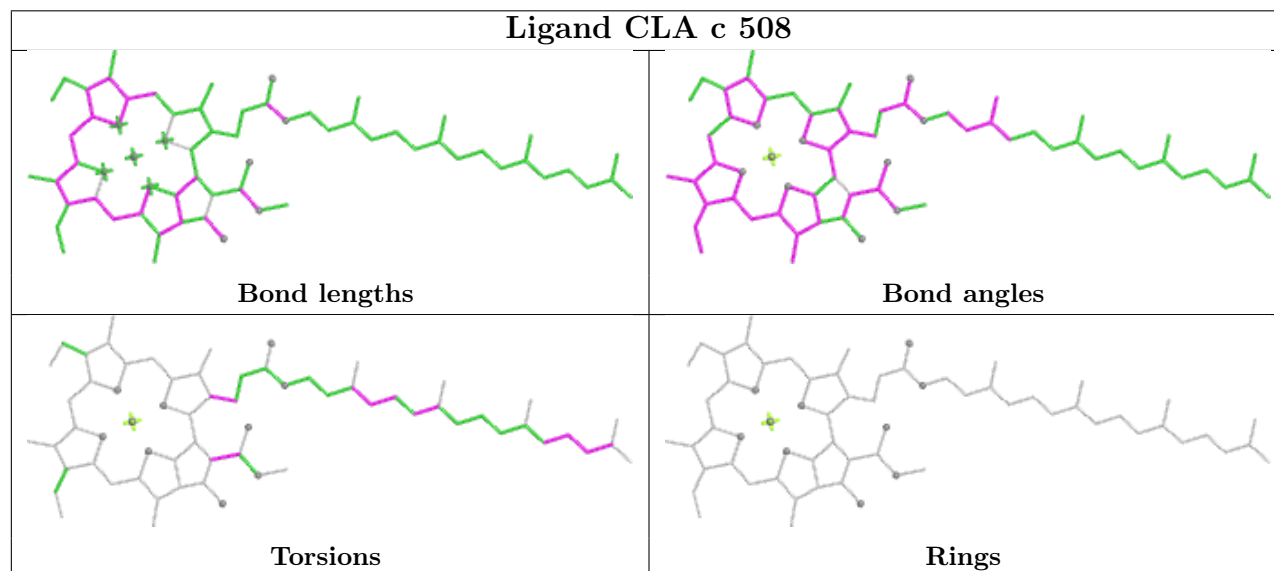
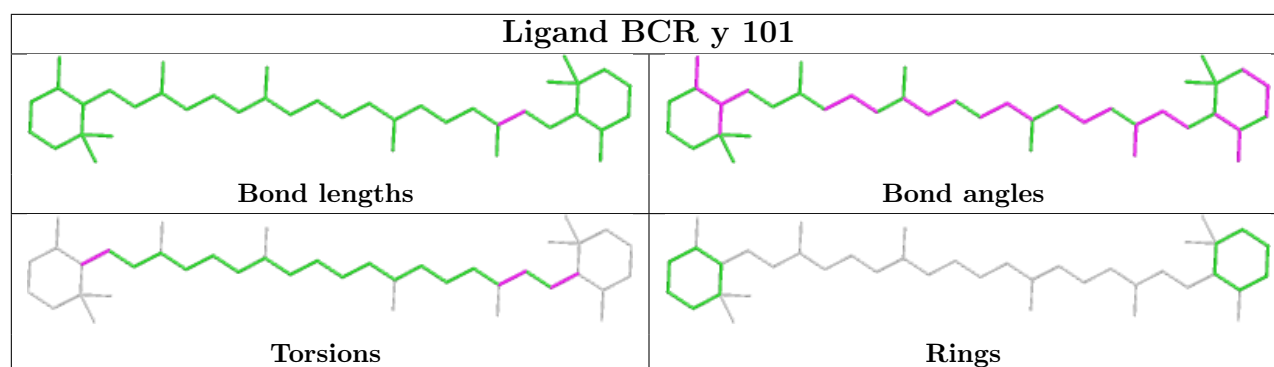
Ligand SQD A 411	
	
Bond lengths	Bond angles
	
Torsions	Rings



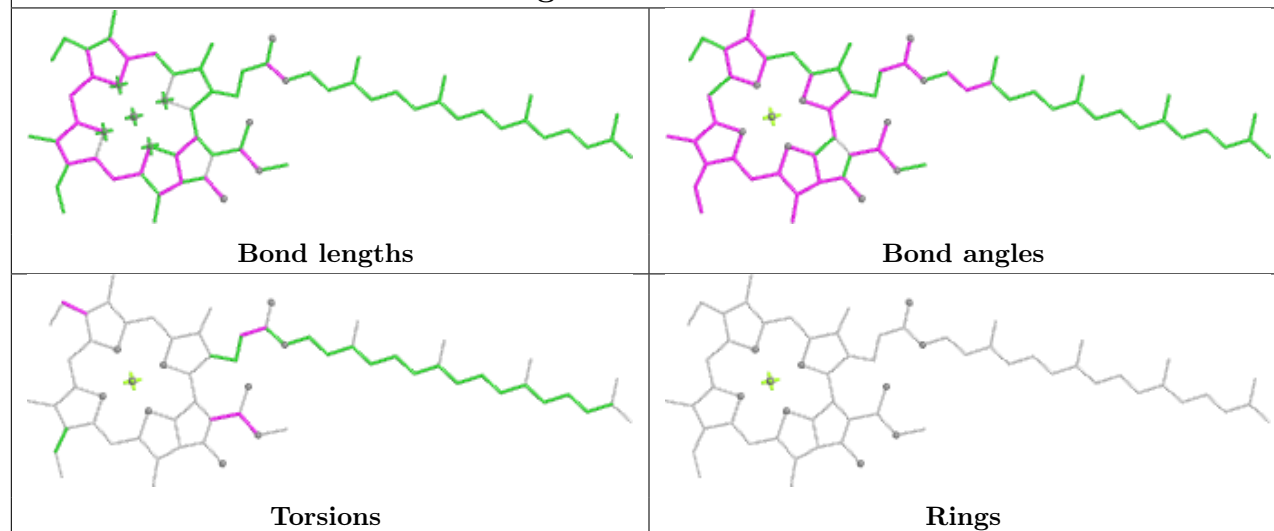




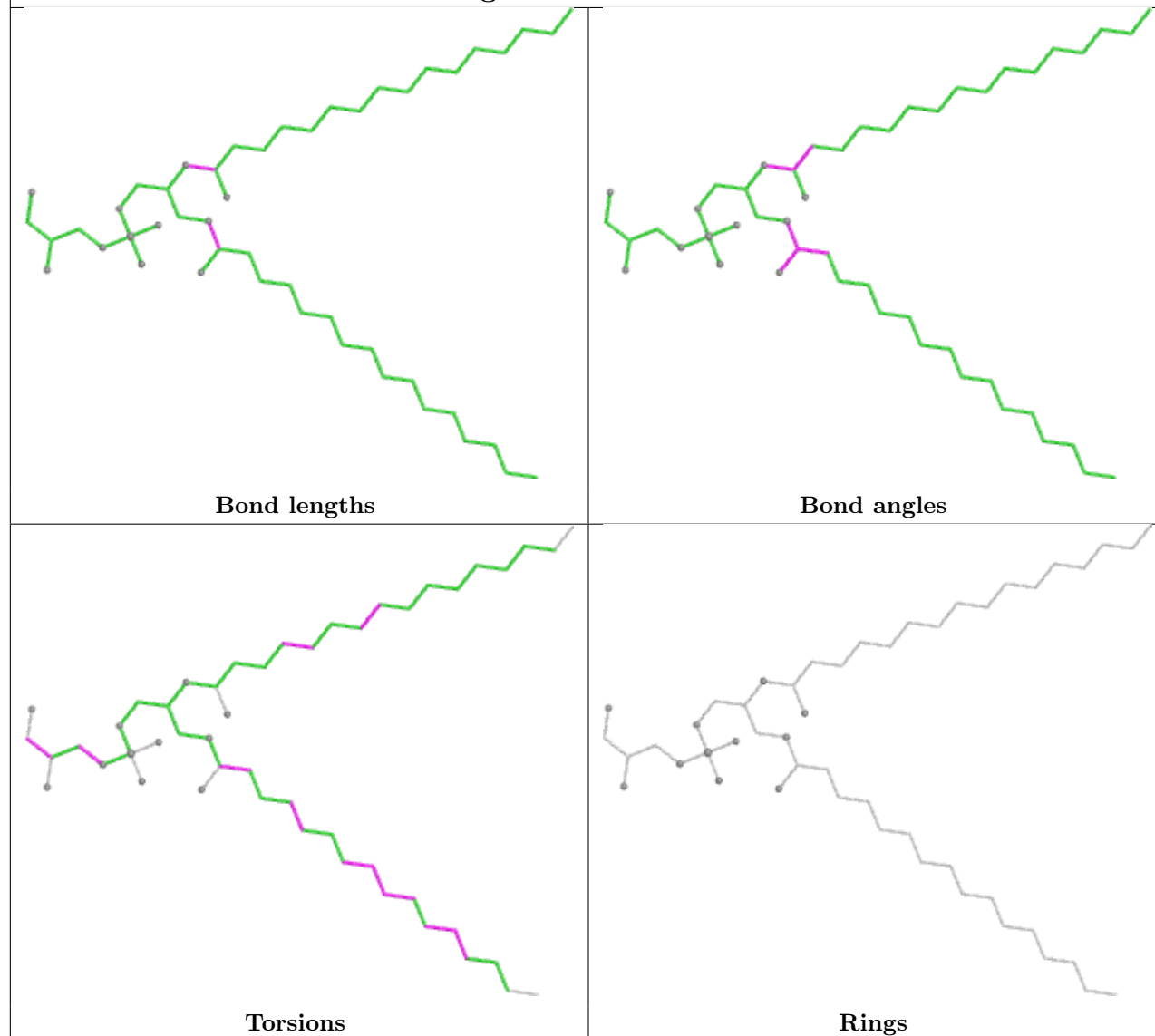


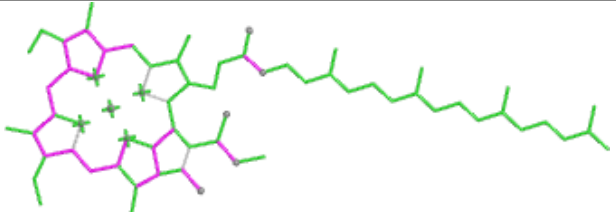
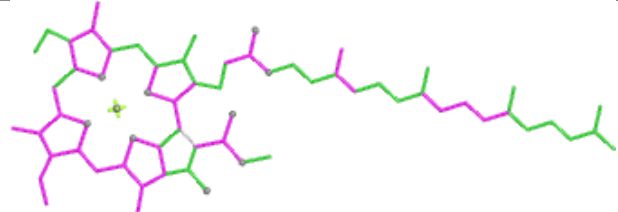
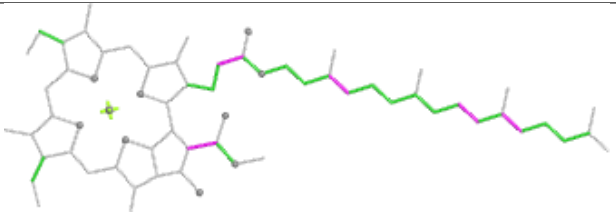
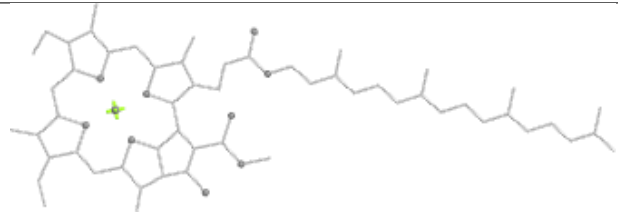


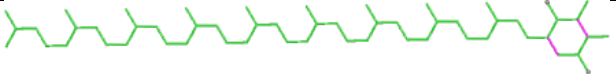
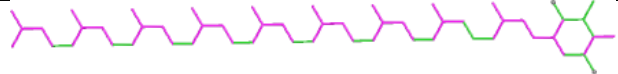
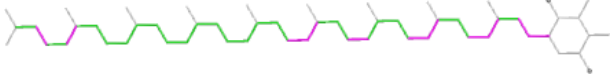
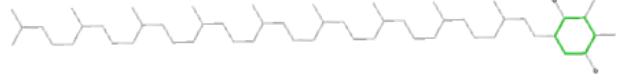
Ligand CLA c 503



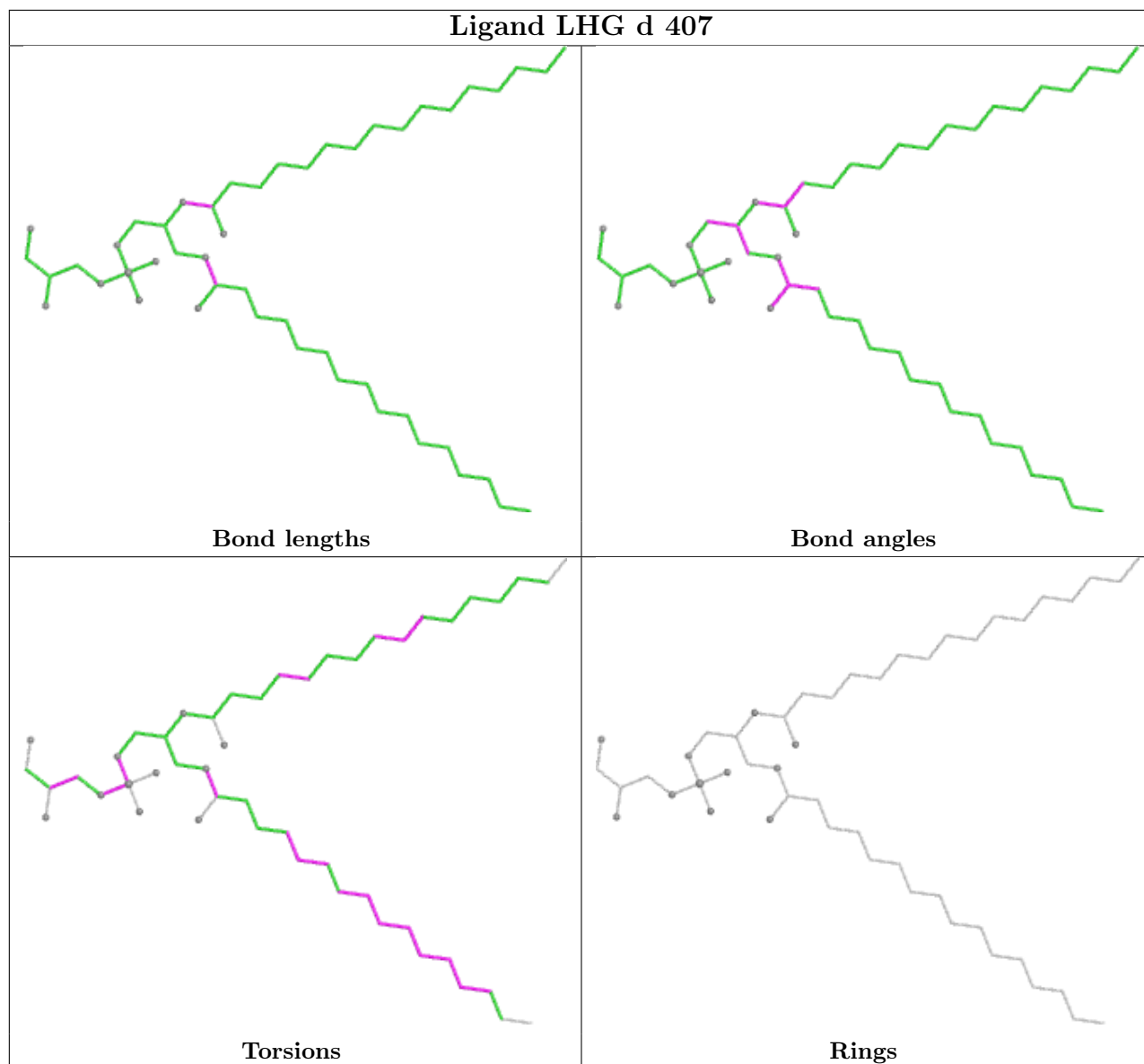
Ligand LHG D 408



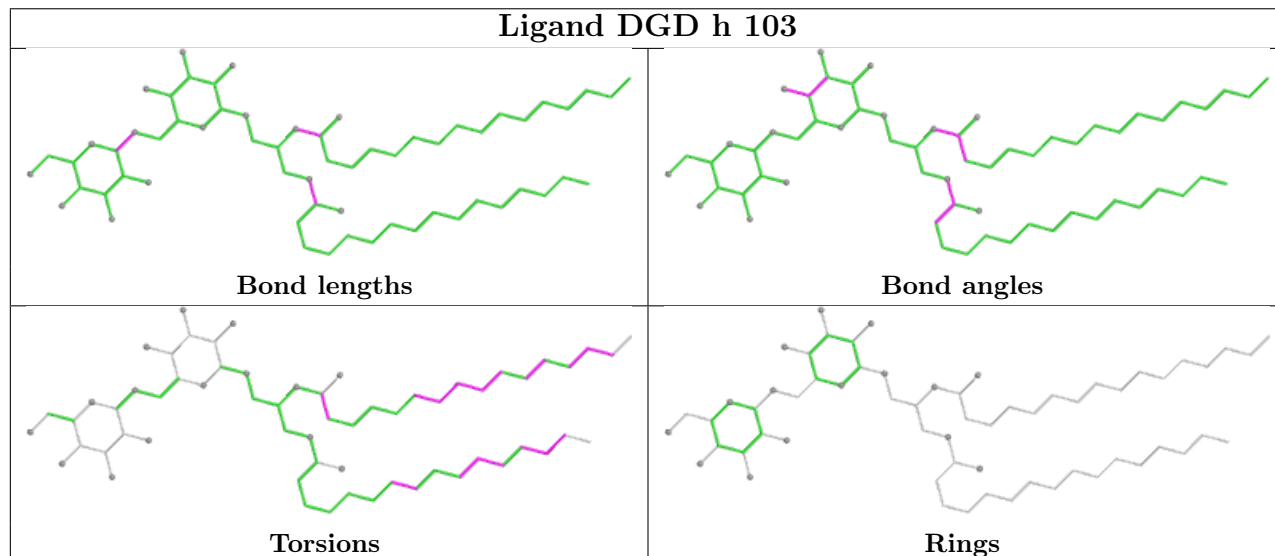
Ligand CLA c 512	
	
Bond lengths	Bond angles
	
Torsions	Rings

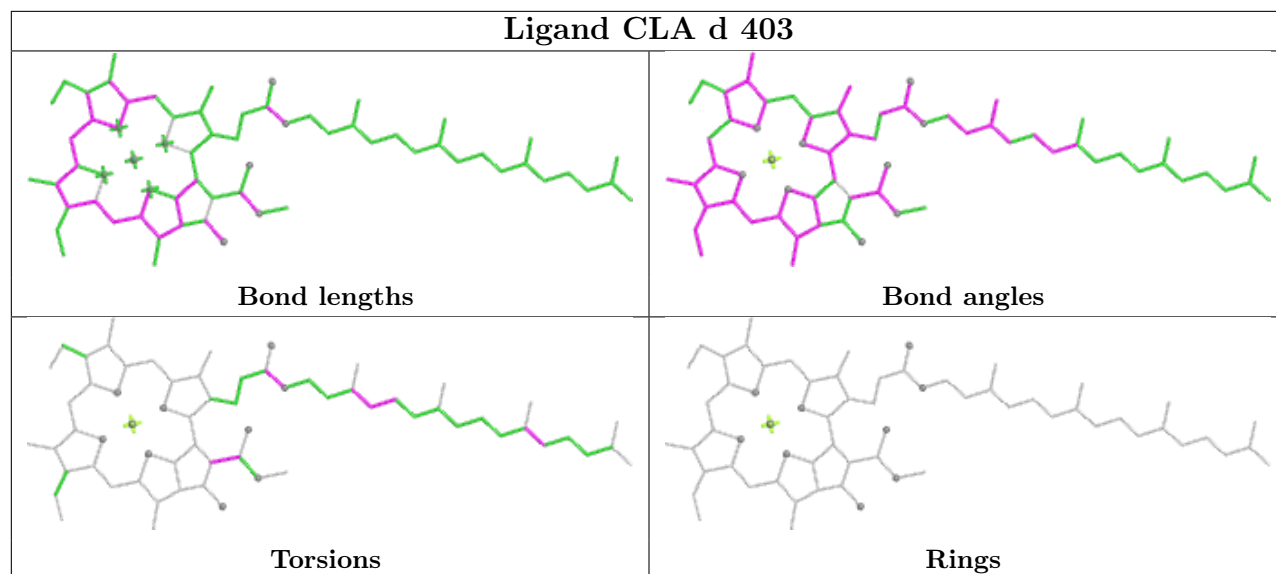
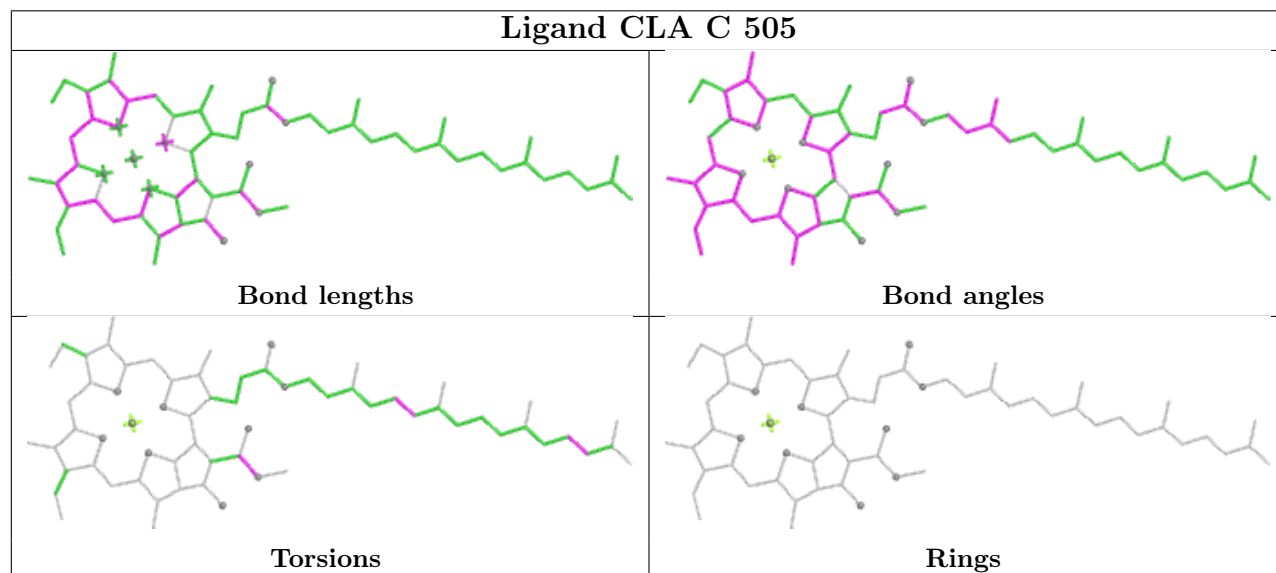
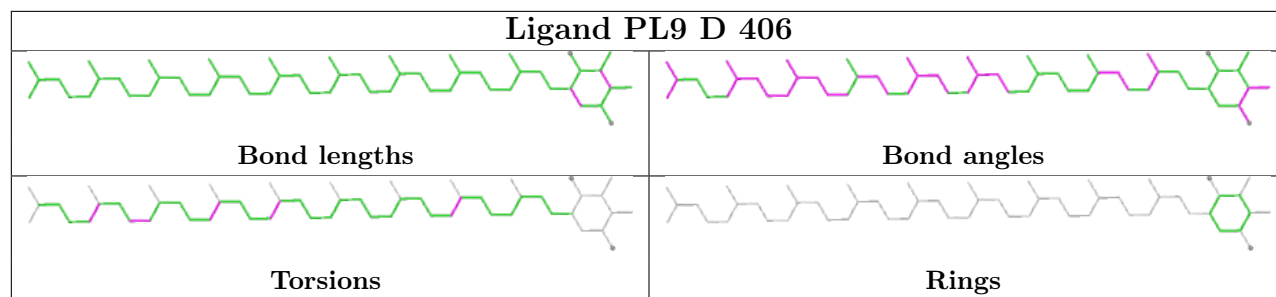
Ligand PL9 A 413	
	
Bond lengths	Bond angles
	
Torsions	Rings

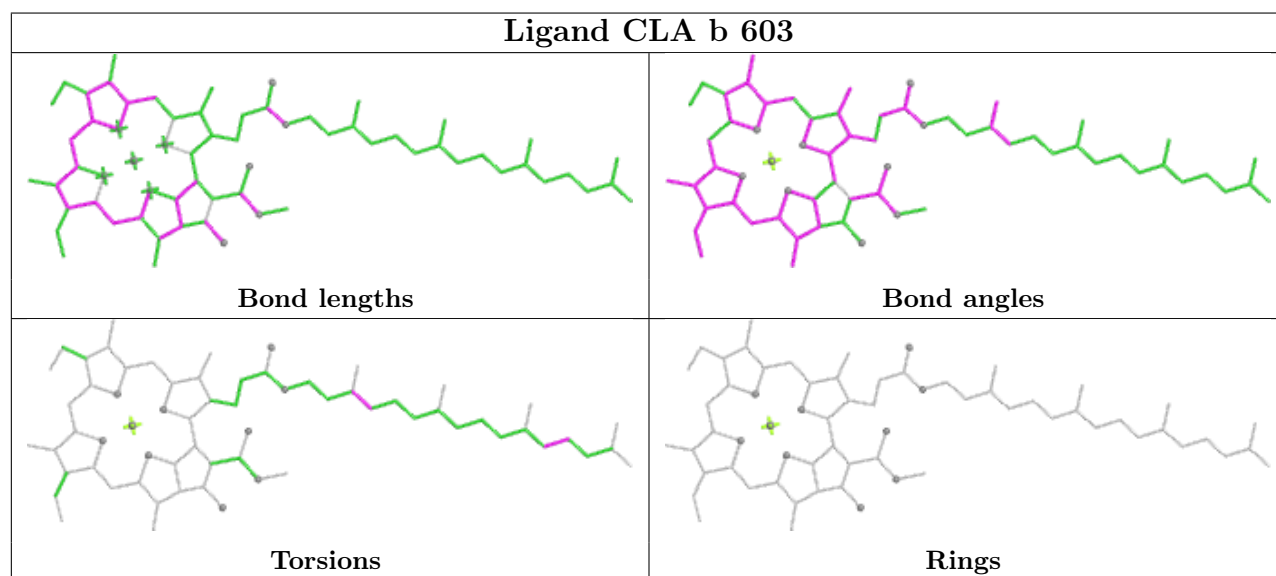
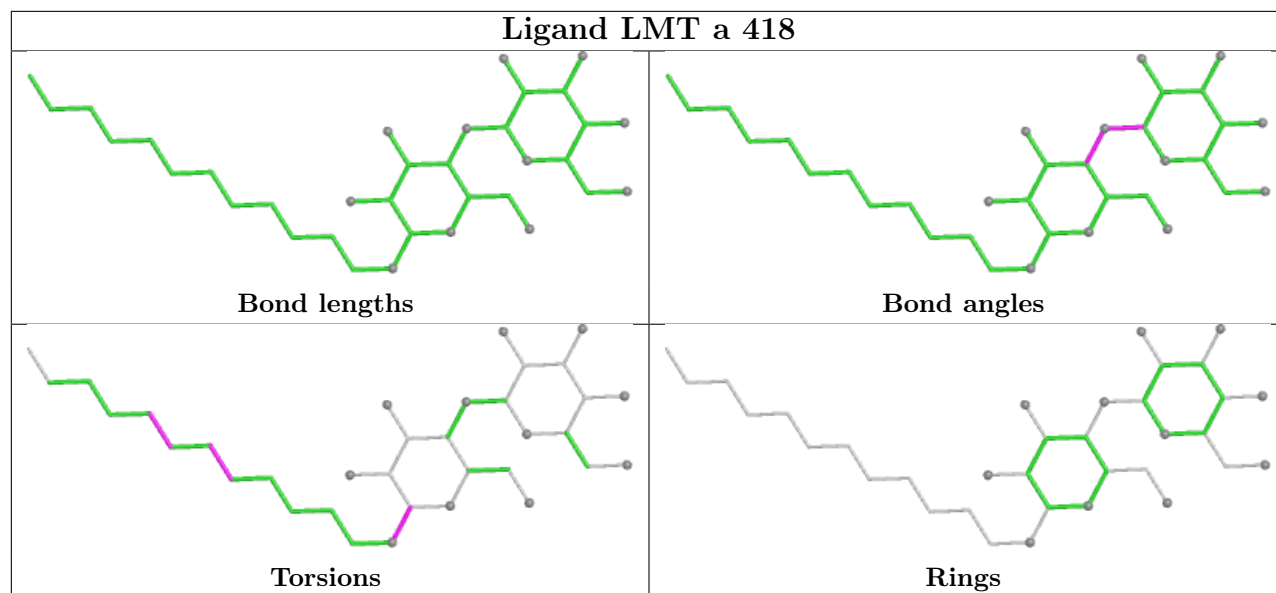
Ligand LHG d 407

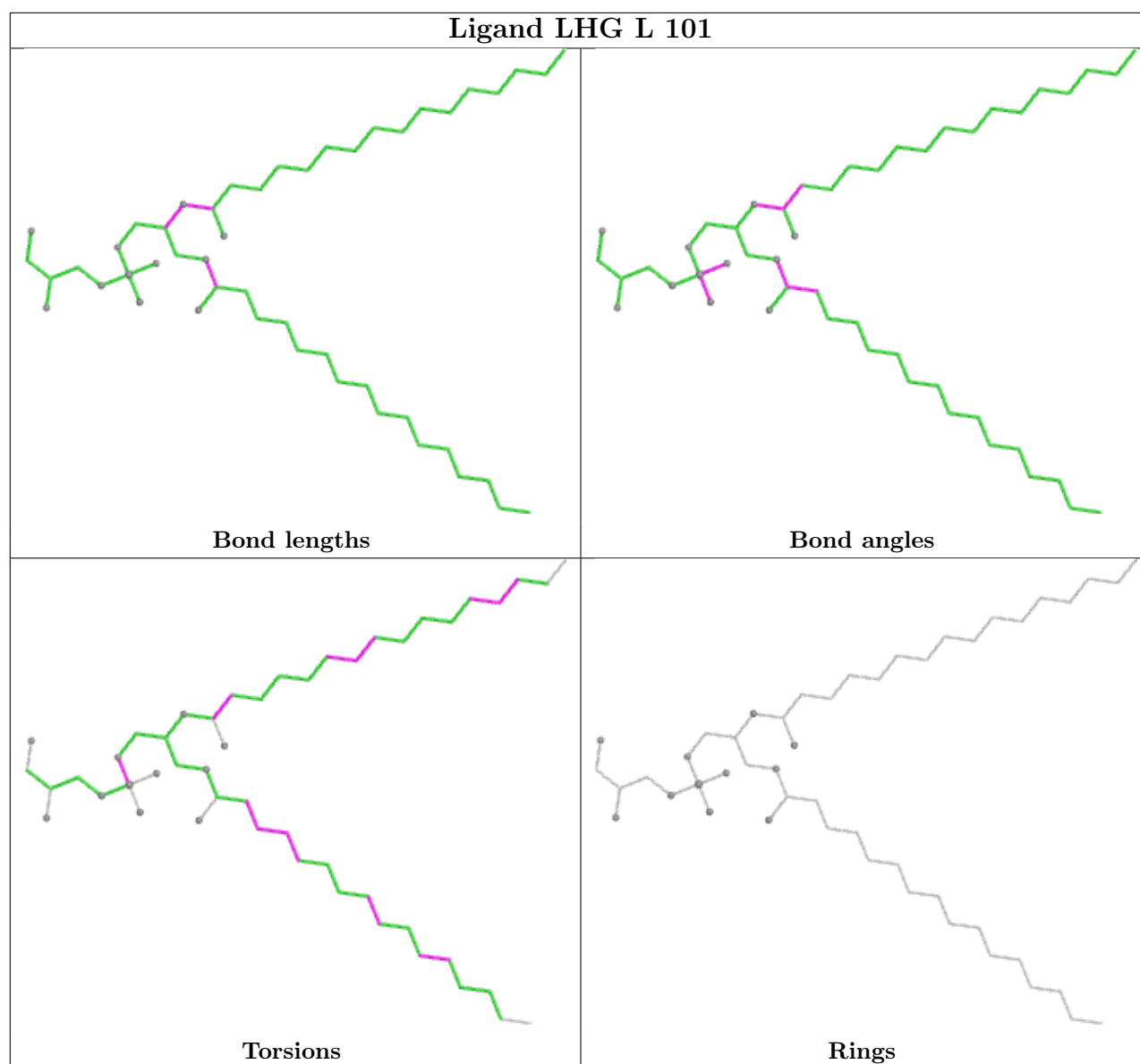


Ligand DGD h 103



Ligand CLA d 403**Ligand CLA C 505****Ligand PL9 D 406**





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%)	-0.38	0 100 100	22, 41, 67, 126	2 (0%)
1	a	334/344 (97%)	-0.36	3 (0%) 81 82	23, 46, 80, 122	3 (0%)
2	B	504/505 (99%)	-0.31	1 (0%) 91 92	19, 46, 79, 129	10 (1%)
2	b	504/505 (99%)	-0.19	10 (1%) 65 65	22, 50, 92, 164	4 (0%)
3	C	451/455 (99%)	-0.19	2 (0%) 88 89	23, 54, 77, 144	4 (0%)
3	c	455/455 (100%)	-0.18	2 (0%) 88 89	31, 62, 84, 127	2 (0%)
4	D	342/342 (100%)	-0.35	0 100 100	33, 43, 65, 134	0
4	d	341/342 (99%)	-0.39	0 100 100	35, 49, 74, 136	0
5	E	81/84 (96%)	-0.02	1 (1%) 76 77	32, 66, 95, 140	1 (1%)
5	e	79/84 (94%)	-0.02	0 100 100	57, 74, 117, 150	0
6	F	34/44 (77%)	-0.04	1 (2%) 53 54	48, 58, 92, 113	0
6	f	31/44 (70%)	0.04	1 (3%) 50 50	57, 66, 93, 154	0
7	H	64/65 (98%)	0.08	2 (3%) 51 51	29, 58, 77, 105	1 (1%)
7	h	64/65 (98%)	0.08	1 (1%) 70 71	51, 63, 85, 108	0
8	I	37/38 (97%)	0.08	0 100 100	47, 58, 120, 144	0
8	i	37/38 (97%)	-0.11	1 (2%) 56 57	49, 59, 117, 145	0
9	J	38/39 (97%)	-0.01	1 (2%) 57 58	47, 66, 127, 181	0
9	j	39/39 (100%)	0.16	1 (2%) 57 58	55, 74, 135, 179	0
10	K	37/37 (100%)	-0.27	0 100 100	53, 65, 88, 102	0
10	k	37/37 (100%)	-0.16	0 100 100	66, 72, 94, 109	0
11	L	36/37 (97%)	-0.18	1 (2%) 55 55	18, 39, 95, 137	1 (2%)
11	l	36/37 (97%)	-0.19	1 (2%) 55 55	19, 40, 96, 132	1 (2%)
12	M	32/36 (88%)	-0.33	0 100 100	19, 42, 66, 135	1 (3%)
12	m	33/36 (91%)	-0.42	0 100 100	36, 43, 78, 125	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.22	0 100 100	23, 57, 110, 186	3 (1%)
13	o	243/244 (99%)	-0.12	1 (0%) 88 89	24, 59, 124, 166	2 (0%)
14	T	29/32 (90%)	-0.31	1 (3%) 48 48	36, 40, 78, 109	0
14	t	29/32 (90%)	-0.30	1 (3%) 48 48	36, 43, 70, 137	0
15	U	96/104 (92%)	-0.37	0 100 100	41, 53, 85, 90	0
15	u	97/104 (93%)	-0.30	0 100 100	46, 58, 80, 132	0
16	V	137/137 (100%)	-0.39	0 100 100	40, 53, 79, 115	0
16	v	137/137 (100%)	-0.28	0 100 100	47, 68, 96, 138	0
17	X	38/40 (95%)	0.03	0 100 100	56, 68, 93, 110	0
17	x	38/40 (95%)	0.09	0 100 100	60, 74, 114, 163	0
18	Y	29/30 (96%)	0.31	2 (6%) 23 21	66, 82, 139, 159	0
18	y	29/30 (96%)	0.23	0 100 100	77, 89, 119, 120	0
19	Z	62/62 (100%)	0.06	0 100 100	66, 80, 132, 180	0
19	z	62/62 (100%)	0.39	1 (1%) 70 71	77, 94, 135, 178	0
20	R	34/34 (100%)	1.88	16 (47%) 0 0	102, 124, 154, 164	0
All	All	5283/5384 (98%)	-0.21	51 (0%) 79 81	18, 54, 98, 186	35 (0%)

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	5.3
14	t	30	THR	4.4
7	h	65	LEU	4.1
6	f	15	ILE	3.7
3	C	23	ALA	3.5

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	FME	I	1	10/11	0.95	0.08	44,65,72,73	0
14	FME	T	1	10/11	0.96	0.07	40,46,63,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	FME	t	1	10/11	0.96	0.07	36,43,68,73	0
8	FME	i	1	10/11	0.97	0.06	49,58,67,73	0
12	FME	m	1	10/11	0.97	0.06	41,53,62,76	0
12	FME	M	1	10/11	0.97	0.09	37,50,80,87	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
34	LMT	E	102	35/35	0.61	0.20	102,145,164,166	0
34	LMT	e	101	35/35	0.64	0.18	122,163,170,171	0
34	LMT	a	413	35/35	0.65	0.21	66,131,140,142	0
34	LMT	C	526	35/35	0.65	0.16	88,140,155,158	0
30	UNL	A	414	28/-	0.67	0.20	83,97,113,115	0
30	UNL	j	101	10/-	0.69	0.27	78,87,93,94	0
33	HTG	b	623	19/19	0.72	0.15	83,144,150,150	0
33	HTG	D	411	16/19	0.72	0.15	91,113,123,129	0
34	LMT	D	402	35/35	0.72	0.21	69,124,137,143	0
30	UNL	J	101	10/-	0.76	0.27	75,79,91,92	0
33	HTG	B	623	19/19	0.78	0.18	61,86,94,95	0
30	UNL	m	102	10/-	0.78	0.21	59,68,91,92	0
31	LHG	a	419	42/49	0.79	0.16	100,147,177,181	0
30	UNL	i	101	40/-	0.79	0.19	69,98,148,152	0
27	SQD	f	101	43/54	0.79	0.16	111,132,160,166	0
30	UNL	a	416	30/-	0.79	0.16	96,111,134,138	0
34	LMT	a	418	35/35	0.79	0.14	118,150,157,158	0
33	HTG	c	523	19/19	0.79	0.14	119,138,143,144	0
30	UNL	C	527	34/-	0.81	0.17	83,110,123,126	0
32	LMG	C	522	51/55	0.81	0.17	69,127,161,165	0
30	UNL	c	526	32/-	0.82	0.17	94,113,130,132	0
30	UNL	I	101	40/-	0.82	0.20	68,107,149,150	0
33	HTG	C	523	19/19	0.82	0.14	106,118,127,127	0
26	GOL	O	302	6/6	0.82	0.10	78,85,86,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	GOL	B	627	6/6	0.82	0.20	63,92,96,97	0
30	UNL	b	626	33/-	0.82	0.16	63,90,146,148	0
34	LMT	m	103	35/35	0.82	0.14	52,93,109,110	0
30	UNL	M	102	10/-	0.83	0.20	63,73,84,84	0
33	HTG	h	101	16/19	0.83	0.12	103,133,139,143	0
34	LMT	B	628	35/35	0.83	0.13	63,110,126,130	0
34	LMT	M	103	35/35	0.83	0.15	78,152,175,176	0
32	LMG	Z	101	37/55	0.84	0.16	72,123,156,161	0
34	LMT	b	621	25/35	0.84	0.16	89,129,154,154	0
26	GOL	c	502	6/6	0.84	0.18	61,75,77,81	0
33	HTG	V	202	11/19	0.84	0.13	110,119,121,121	0
31	LHG	E	101	42/49	0.85	0.16	72,126,138,141	0
32	LMG	c	522	51/55	0.85	0.15	72,129,152,157	0
33	HTG	b	622	19/19	0.85	0.16	64,71,105,109	0
26	GOL	b	624	6/6	0.85	0.21	86,95,99,105	0
26	GOL	v	201	6/6	0.85	0.20	51,70,78,80	0
34	LMT	M	101	35/35	0.85	0.12	53,98,131,139	0
36	CA	F	101	1/1	0.85	0.12	115,115,115,115	0
27	SQD	A	411	54/54	0.86	0.13	60,82,123,130	0
30	UNL	d	410	36/-	0.86	0.17	70,94,127,130	0
34	LMT	b	627	25/35	0.86	0.15	50,75,135,136	0
30	UNL	B	626	33/-	0.86	0.15	52,108,152,156	0
26	GOL	B	629	6/6	0.86	0.20	103,111,114,116	0
29	PL9	a	415	55/55	0.86	0.23	87,111,124,126	0
32	LMG	z	101	39/55	0.87	0.15	80,128,136,139	0
30	UNL	D	410	40/-	0.87	0.17	56,85,125,129	0
27	SQD	a	412	54/54	0.87	0.12	59,85,125,127	0
26	GOL	A	410	6/6	0.87	0.14	68,68,74,81	0
27	SQD	D	412	43/54	0.87	0.15	74,111,131,138	0
34	LMT	B	630	25/35	0.87	0.14	55,84,135,139	0
23	CLA	b	601	65/65	0.88	0.12	58,80,120,129	0
33	HTG	B	622	19/19	0.88	0.17	61,83,110,111	0
26	GOL	o	302	6/6	0.88	0.16	110,113,118,120	0
27	SQD	b	620	54/54	0.88	0.13	59,88,112,115	0
27	SQD	B	620	54/54	0.88	0.13	54,88,124,129	0
29	PL9	A	413	55/55	0.88	0.20	72,102,112,115	0
32	LMG	C	521	51/55	0.90	0.14	52,87,119,120	0
34	LMT	t	101	26/35	0.90	0.15	77,117,136,140	0
23	CLA	B	601	65/65	0.90	0.11	52,72,115,121	0
26	GOL	a	411	6/6	0.91	0.12	57,68,80,81	0
33	HTG	B	625	19/19	0.91	0.11	65,75,82,87	0
32	LMG	C	502	51/55	0.92	0.12	57,84,104,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	LMG	c	501	51/55	0.92	0.14	60,88,109,117	0
32	LMG	c	521	51/55	0.92	0.14	68,92,125,127	0
23	CLA	c	515	65/65	0.92	0.12	64,83,117,119	0
23	CLA	C	515	65/65	0.92	0.12	59,70,111,114	0
32	LMG	D	413	51/55	0.92	0.12	44,64,111,123	0
30	UNL	D	409	17/-	0.93	0.16	56,77,114,114	0
25	BCR	t	102	40/40	0.93	0.08	37,51,66,70	0
32	LMG	m	101	51/55	0.93	0.11	51,68,96,98	0
26	GOL	b	628	6/6	0.93	0.17	94,100,102,103	0
31	LHG	A	416	49/49	0.93	0.13	41,57,80,87	0
23	CLA	C	506	65/65	0.93	0.11	42,51,85,95	0
25	BCR	B	619	40/40	0.93	0.10	43,53,72,75	0
32	LMG	B	621	51/55	0.93	0.11	49,65,92,114	0
25	BCR	K	101	40/40	0.93	0.10	54,63,69,71	0
26	GOL	C	524	6/6	0.93	0.17	53,56,60,61	0
25	BCR	T	101	40/40	0.93	0.08	37,48,57,61	0
30	UNL	d	409	17/-	0.93	0.13	67,82,97,97	0
33	HTG	b	625	19/19	0.93	0.10	66,72,92,98	0
25	BCR	h	102	40/40	0.93	0.10	50,61,74,75	0
35	DGD	C	519	62/66	0.93	0.12	42,62,116,121	0
30	UNL	d	411	18/-	0.93	0.13	74,78,109,112	0
36	CA	a	420	1/1	0.93	0.10	105,105,105,105	0
27	SQD	C	501	54/54	0.94	0.11	59,79,105,107	0
25	BCR	d	404	40/40	0.94	0.10	52,63,87,92	0
27	SQD	a	410	54/54	0.94	0.12	64,83,117,118	0
23	CLA	b	612	65/65	0.94	0.09	38,46,61,70	0
23	CLA	b	614	65/65	0.94	0.09	35,44,102,105	0
25	BCR	y	101	40/40	0.94	0.09	57,70,83,86	0
23	CLA	b	616	65/65	0.94	0.10	43,55,114,116	0
29	PL9	D	406	55/55	0.94	0.09	32,42,54,60	0
31	LHG	b	629	49/49	0.94	0.11	40,55,71,78	0
26	GOL	B	624	6/6	0.94	0.12	76,87,95,97	0
29	PL9	d	405	55/55	0.94	0.10	35,46,56,61	0
23	CLA	c	509	65/65	0.94	0.10	53,63,73,83	0
23	CLA	c	514	65/65	0.94	0.11	64,77,112,122	0
23	CLA	C	508	65/65	0.94	0.12	51,63,123,130	0
25	BCR	B	618	40/40	0.94	0.08	35,50,63,72	0
23	CLA	B	614	65/65	0.94	0.10	33,43,93,97	0
25	BCR	D	405	40/40	0.94	0.11	45,58,95,103	0
25	BCR	H	101	40/40	0.94	0.09	44,61,71,74	0
23	CLA	a	408	65/65	0.94	0.11	40,48,128,132	0
30	UNL	X	101	18/-	0.94	0.12	60,68,98,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	B	610	65/65	0.94	0.10	41,48,59,77	0
25	BCR	b	617	40/40	0.94	0.08	35,43,56,58	0
25	BCR	b	618	40/40	0.94	0.08	37,50,67,72	0
25	BCR	c	516	40/40	0.94	0.11	68,83,90,94	0
23	CLA	b	605	65/65	0.95	0.09	35,43,66,75	0
23	CLA	b	606	65/65	0.95	0.09	38,49,110,115	0
25	BCR	c	517	40/40	0.95	0.10	53,65,71,71	0
23	CLA	b	610	65/65	0.95	0.09	43,50,62,73	0
32	LMG	d	412	51/55	0.95	0.11	53,67,111,119	0
23	CLA	C	503	65/65	0.95	0.09	45,53,68,78	0
23	CLA	C	505	65/65	0.95	0.08	47,55,67,72	0
23	CLA	B	606	65/65	0.95	0.09	38,46,101,108	0
23	CLA	c	505	65/65	0.95	0.09	53,63,73,77	0
23	CLA	c	506	65/65	0.95	0.10	49,58,103,110	0
23	CLA	c	507	65/65	0.95	0.09	43,56,83,86	0
23	CLA	c	508	65/65	0.95	0.10	56,69,121,126	0
23	CLA	A	408	65/65	0.95	0.10	38,45,111,119	0
23	CLA	c	510	65/65	0.95	0.09	47,57,127,132	0
23	CLA	C	509	65/65	0.95	0.09	50,57,76,80	0
23	CLA	C	510	65/65	0.95	0.09	43,51,117,130	0
23	CLA	d	403	65/65	0.95	0.09	48,58,115,123	0
24	PHO	A	415	64/64	0.95	0.07	35,43,52,54	0
25	BCR	A	409	40/40	0.95	0.07	33,42,54,58	0
23	CLA	C	513	65/65	0.95	0.09	49,62,77,78	0
23	CLA	C	514	65/65	0.95	0.11	55,65,114,119	0
25	BCR	C	516	40/40	0.95	0.10	59,74,81,83	0
31	LHG	D	407	49/49	0.95	0.09	40,48,64,76	0
31	LHG	D	408	49/49	0.95	0.13	45,57,124,134	0
25	BCR	C	517	40/40	0.95	0.08	49,56,64,73	0
31	LHG	L	101	49/49	0.95	0.10	39,51,65,84	0
23	CLA	B	611	65/65	0.95	0.08	34,39,61,68	0
23	CLA	D	404	65/65	0.95	0.10	44,54,126,133	0
31	LHG	d	406	49/49	0.95	0.11	50,61,76,81	0
31	LHG	d	408	49/49	0.95	0.12	53,65,117,122	0
23	CLA	a	406	65/65	0.95	0.10	39,49,114,118	0
23	CLA	B	603	65/65	0.95	0.09	38,46,62,66	0
35	DGD	C	518	62/66	0.95	0.10	40,54,93,96	0
25	BCR	Y	101	40/40	0.95	0.09	53,64,73,77	0
35	DGD	C	520	62/66	0.95	0.10	40,53,95,108	0
35	DGD	H	102	62/66	0.95	0.10	40,55,67,69	0
35	DGD	c	518	62/66	0.95	0.10	45,58,90,95	0
35	DGD	c	519	62/66	0.95	0.09	50,70,107,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	DGD	c	520	62/66	0.95	0.10	48,60,98,111	0
35	DGD	h	103	62/66	0.95	0.09	50,59,68,71	0
25	BCR	a	409	40/40	0.95	0.07	36,45,56,59	0
23	CLA	B	616	65/65	0.95	0.11	41,52,136,137	0
36	CA	o	301	1/1	0.95	0.05	100,100,100,100	0
37	BCT	d	401	4/4	0.95	0.07	52,54,62,64	0
23	CLA	A	406	65/65	0.96	0.09	34,42,114,117	0
23	CLA	b	611	65/65	0.96	0.08	36,44,70,76	0
23	CLA	B	607	65/65	0.96	0.07	31,40,64,69	0
23	CLA	B	609	65/65	0.96	0.07	43,51,74,81	0
23	CLA	D	403	65/65	0.96	0.07	32,37,53,62	0
23	CLA	c	503	65/65	0.96	0.09	53,61,74,82	0
23	CLA	c	504	65/65	0.96	0.08	48,56,73,83	0
23	CLA	B	602	65/65	0.96	0.08	39,48,72,77	0
23	CLA	a	404	65/65	0.96	0.07	37,41,64,73	0
31	LHG	d	407	49/49	0.96	0.09	41,51,68,78	0
25	BCR	b	619	40/40	0.96	0.08	46,53,74,84	0
23	CLA	a	405	65/65	0.96	0.07	34,40,57,62	0
23	CLA	A	404	65/65	0.96	0.08	33,36,61,75	0
23	CLA	B	613	65/65	0.96	0.08	34,41,89,94	0
23	CLA	B	605	65/65	0.96	0.08	35,41,61,73	0
25	BCR	k	101	40/40	0.96	0.09	58,70,81,81	0
23	CLA	c	511	65/65	0.96	0.09	54,62,86,88	0
23	CLA	c	512	65/65	0.96	0.08	52,59,73,76	0
23	CLA	c	513	65/65	0.96	0.08	55,65,81,85	0
23	CLA	b	602	65/65	0.96	0.08	43,54,70,80	0
23	CLA	b	603	65/65	0.96	0.08	41,50,70,88	0
23	CLA	b	604	65/65	0.96	0.09	34,43,111,119	0
24	PHO	A	407	64/64	0.96	0.07	32,37,47,52	0
23	CLA	C	511	65/65	0.96	0.09	48,56,77,79	0
24	PHO	a	417	64/64	0.96	0.07	39,47,55,60	0
23	CLA	C	512	65/65	0.96	0.08	46,56,78,87	0
25	BCR	B	617	40/40	0.96	0.07	34,45,55,58	0
36	CA	O	301	1/1	0.96	0.06	103,103,103,103	0
23	CLA	b	607	65/65	0.96	0.08	32,40,73,80	0
23	CLA	b	608	65/65	0.96	0.07	45,52,69,76	0
37	BCT	D	401	4/4	0.96	0.08	51,57,61,62	0
23	CLA	b	609	65/65	0.96	0.08	49,57,78,100	0
38	HEC	e	102	43/43	0.96	0.08	64,78,119,130	0
39	MG	J	102	1/1	0.96	0.08	50,50,50,50	0
23	CLA	B	612	65/65	0.97	0.07	35,44,54,59	0
36	CA	C	525	1/1	0.97	0.10	66,66,66,66	0

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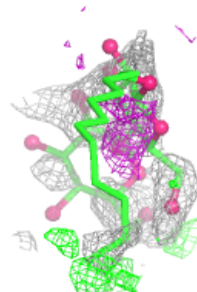
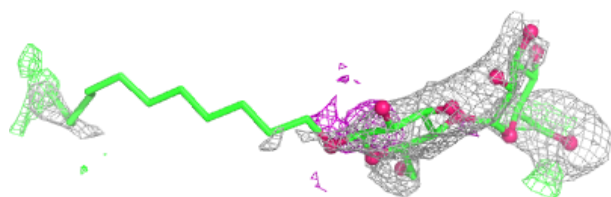
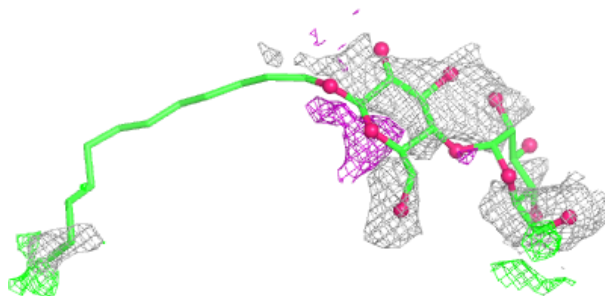
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	B	608	65/65	0.97	0.07	39,47,62,65	0
23	CLA	b	613	65/65	0.97	0.07	33,42,84,88	0
23	CLA	C	504	65/65	0.97	0.07	43,50,71,82	0
36	CA	c	524	1/1	0.97	0.07	73,73,73,73	0
23	CLA	b	615	65/65	0.97	0.08	42,50,74,79	0
23	CLA	A	405	65/65	0.97	0.07	31,37,52,56	0
24	PHO	a	407	64/64	0.97	0.06	35,42,47,50	0
38	HEC	E	103	43/43	0.97	0.07	57,65,80,93	0
38	HEC	V	201	43/43	0.97	0.07	43,46,51,54	0
23	CLA	B	615	65/65	0.97	0.07	40,46,77,83	0
38	HEC	v	202	43/43	0.97	0.08	52,58,63,64	0
23	CLA	C	507	65/65	0.97	0.08	43,52,86,93	0
23	CLA	d	402	65/65	0.98	0.06	36,40,68,77	0
22	CL	A	403	1/1	0.98	0.04	40,40,40,40	0
23	CLA	B	604	65/65	0.98	0.08	32,39,110,116	0
39	MG	j	102	1/1	0.98	0.04	60,60,60,60	0
22	CL	a	403	1/1	0.99	0.05	44,44,44,44	0
22	CL	A	402	1/1	0.99	0.04	35,35,35,35	0
36	CA	c	525	1/1	0.99	0.04	80,80,80,80	0
22	CL	a	402	1/1	0.99	0.04	42,42,42,42	0
28	OEX	A	412	10/10	0.99	0.04	35,38,45,46	0
28	OEX	a	414	10/10	0.99	0.03	39,45,49,49	0
21	FE2	A	401	1/1	1.00	0.04	53,53,53,53	0
21	FE2	a	401	1/1	1.00	0.04	57,57,57,57	0

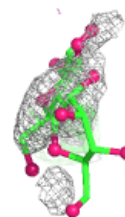
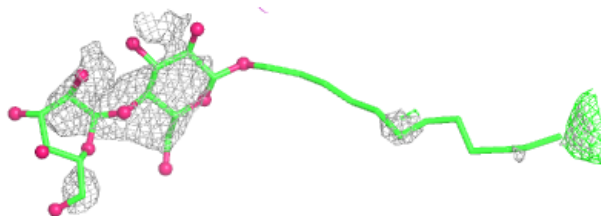
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT E 102:

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

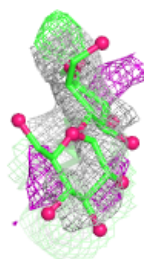
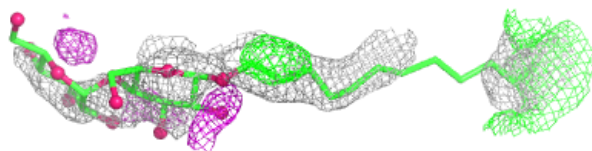
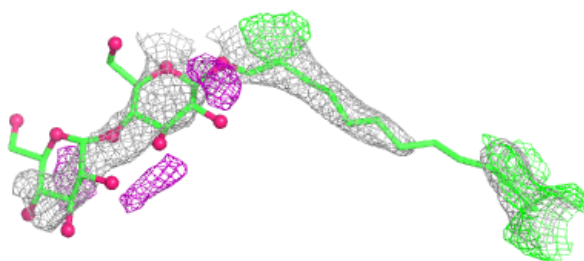
**Electron density around LMT e 101:**

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

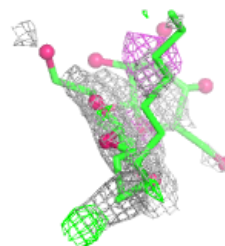
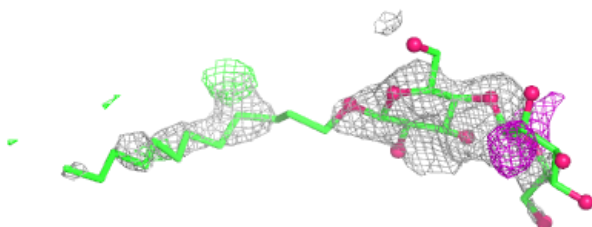
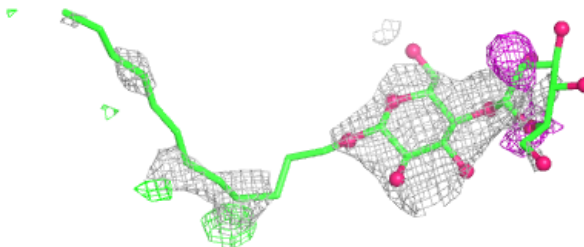


Electron density around LMT a 413:

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

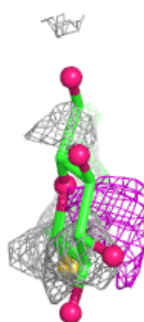
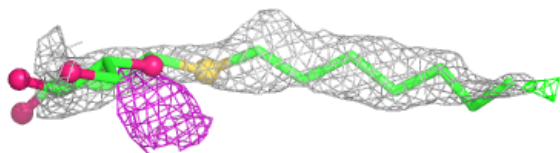
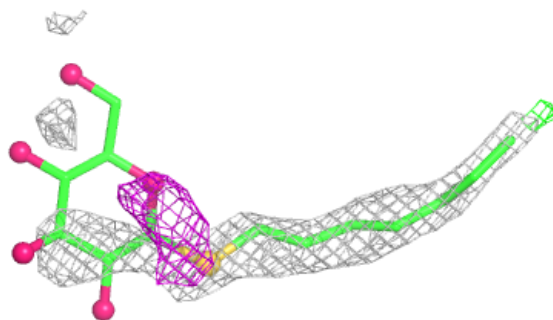
**Electron density around LMT C 526:**

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

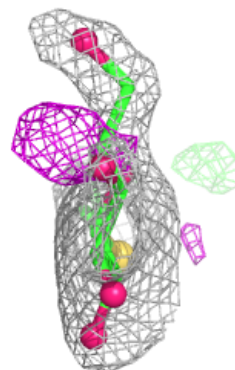
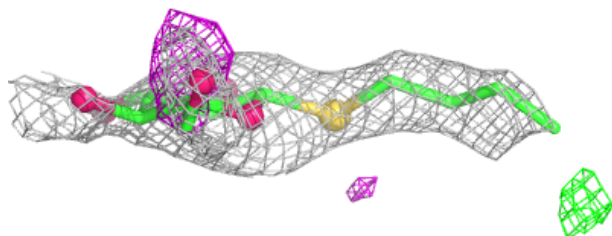
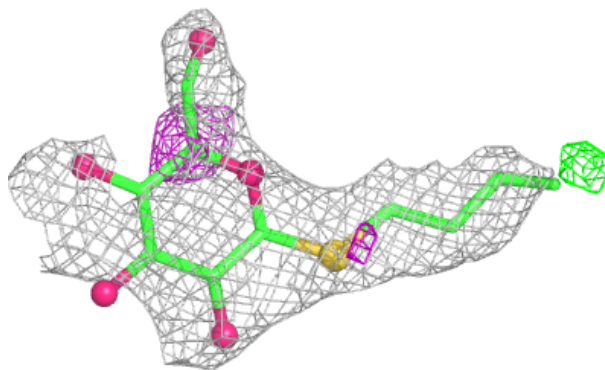


Electron density around HTG b 623:

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

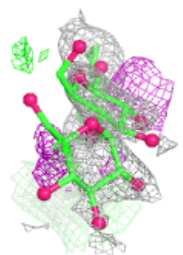
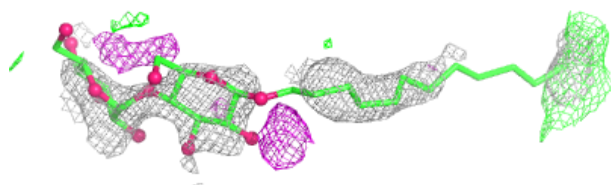
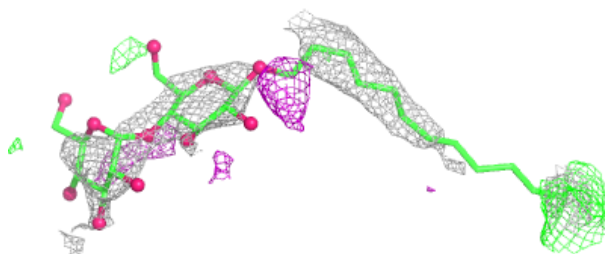
**Electron density around HTG D 411:**

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



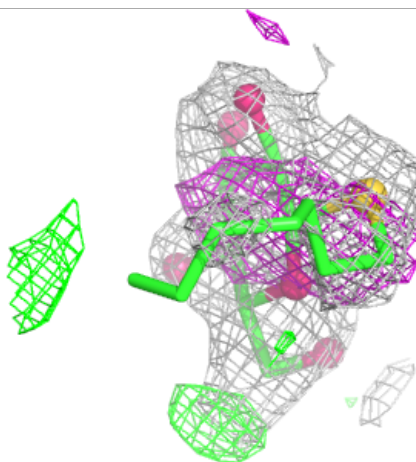
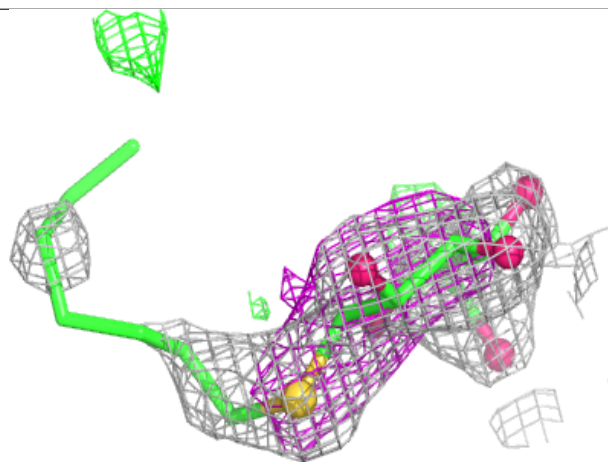
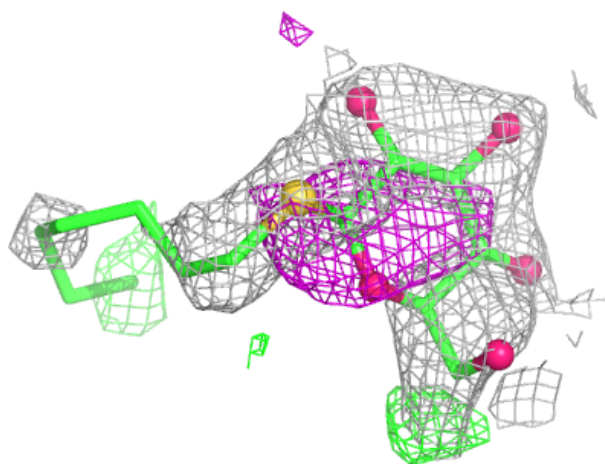
Electron density around LMT D 402:

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



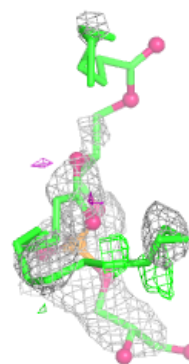
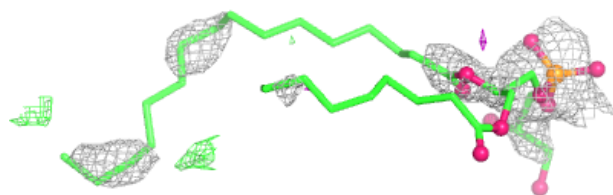
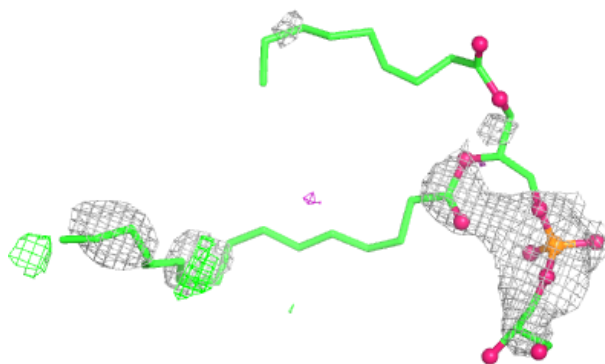
Electron density around HTG B 623:

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

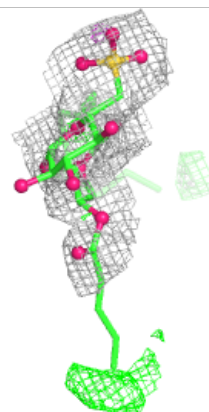
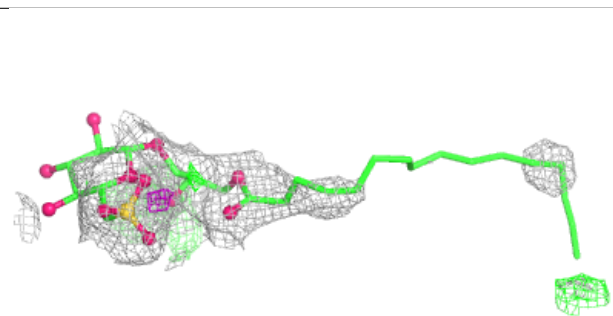
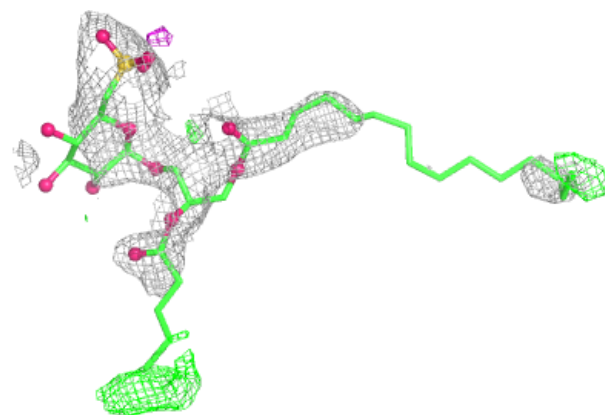


Electron density around LHG a 419:

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

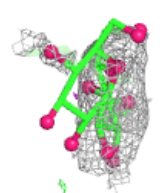
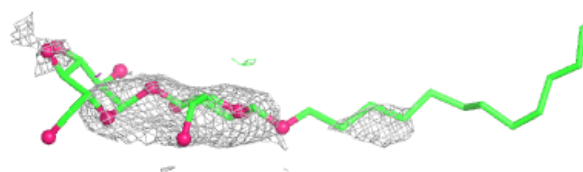
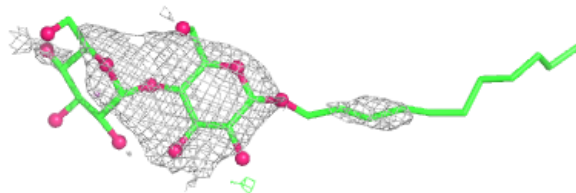
**Electron density around SQD f 101:**

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

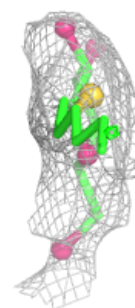
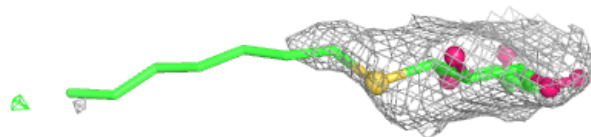
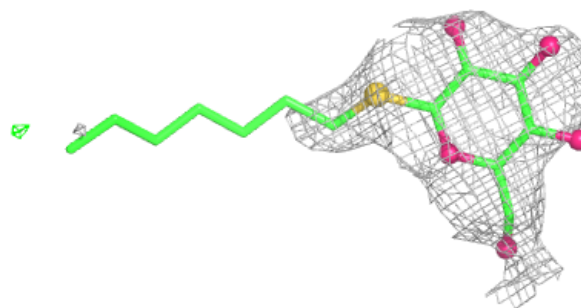


Electron density around LMT a 418:

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

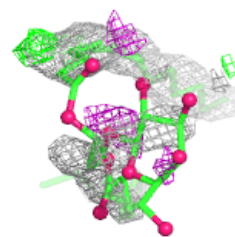
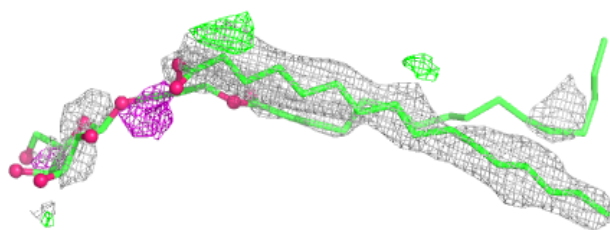
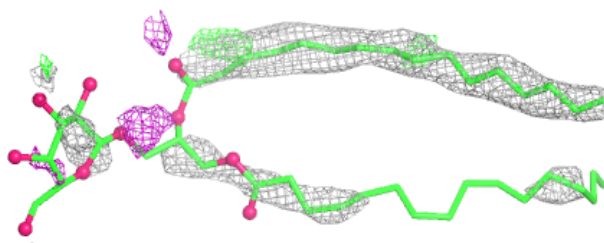
**Electron density around HTG c 523:**

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

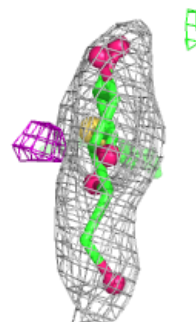
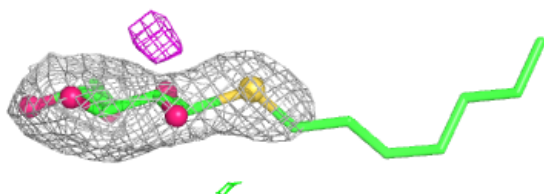
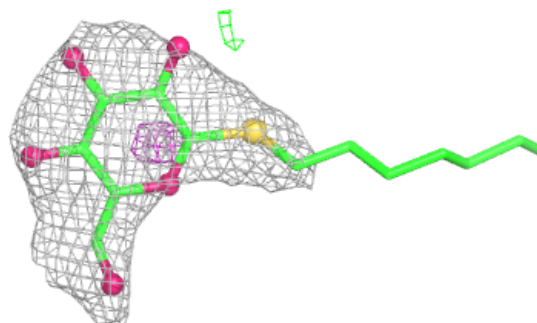


Electron density around LMG C 522:

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

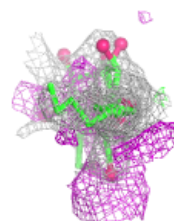
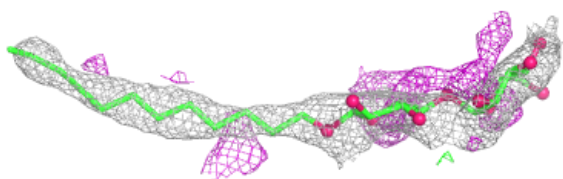
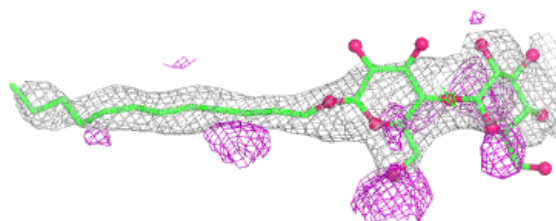
**Electron density around HTG C 523:**

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

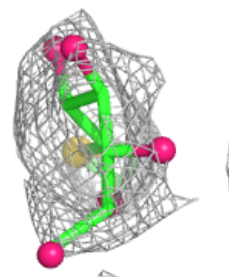
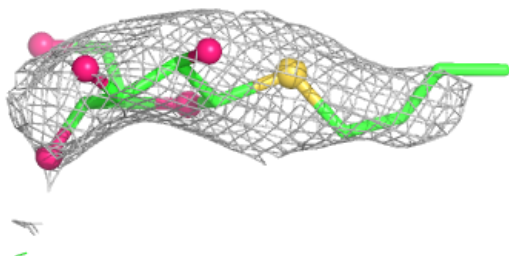
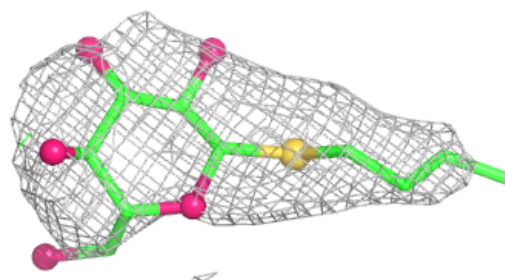


Electron density around LMT m 103:

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

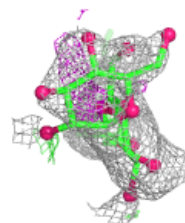
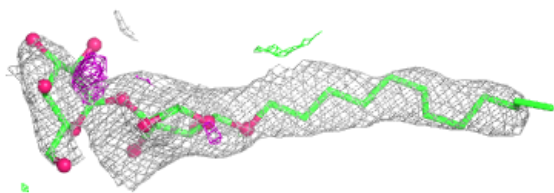
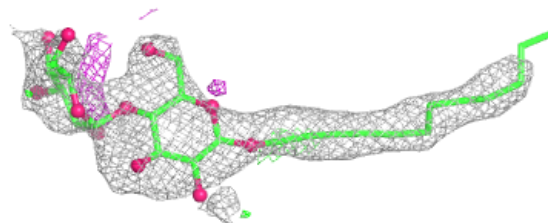
**Electron density around HTG h 101:**

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

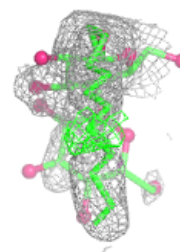
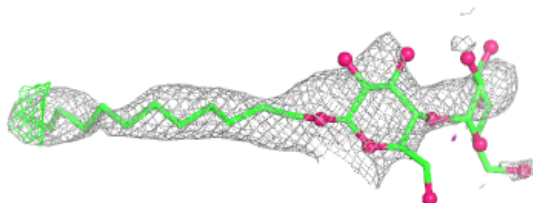
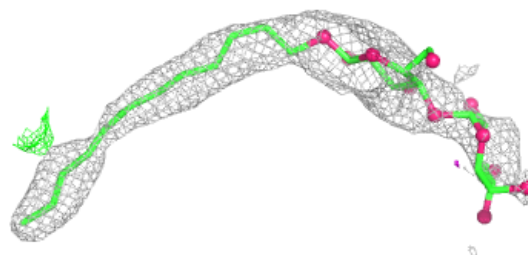


Electron density around LMT B 628:

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

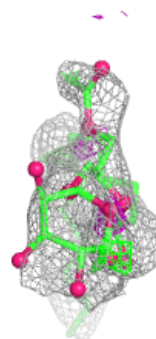
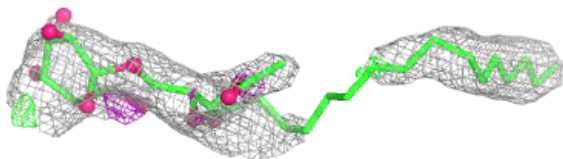
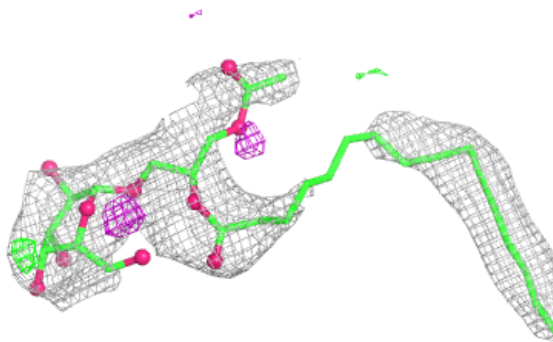
**Electron density around LMT M 103:**

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

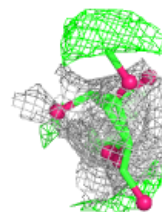
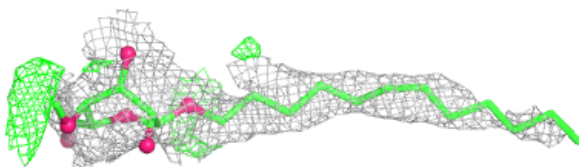
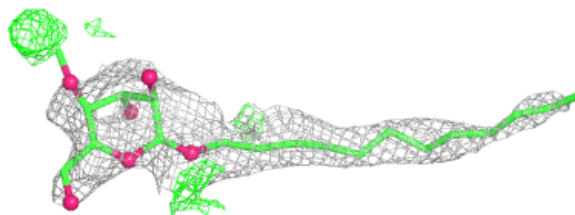


Electron density around LMG Z 101:

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

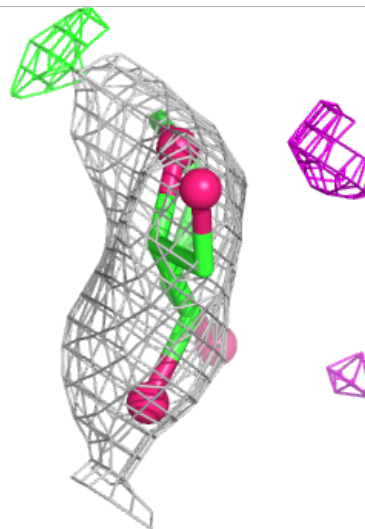
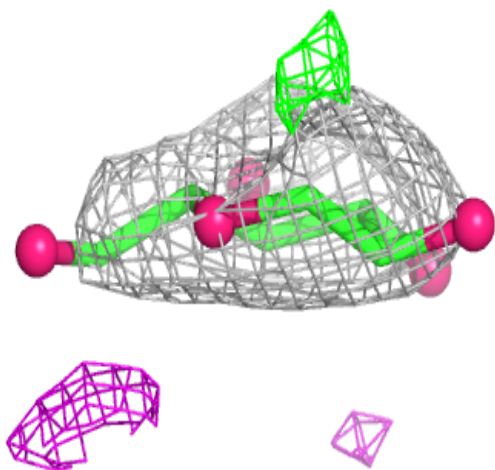
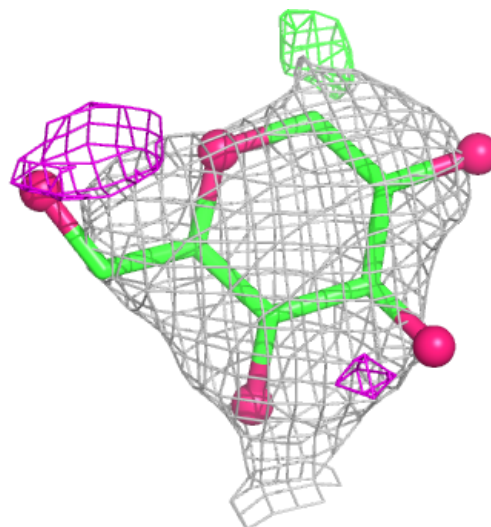
**Electron density around LMT b 621:**

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



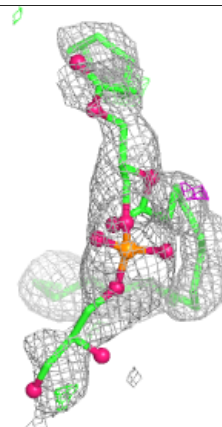
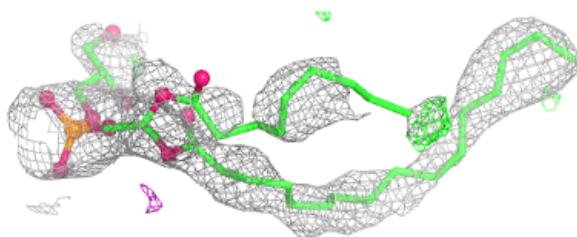
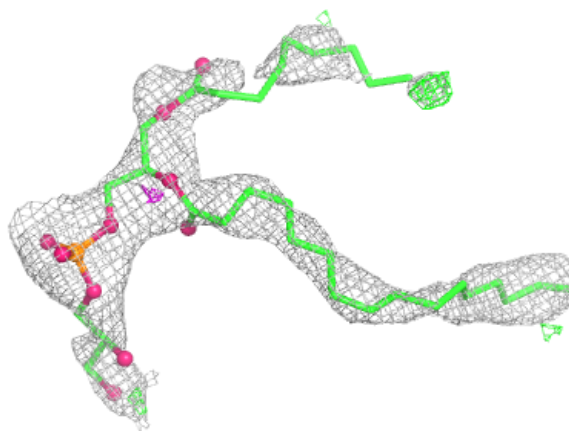
Electron density around HTG V 202:

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

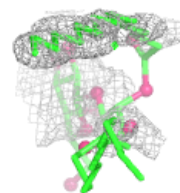
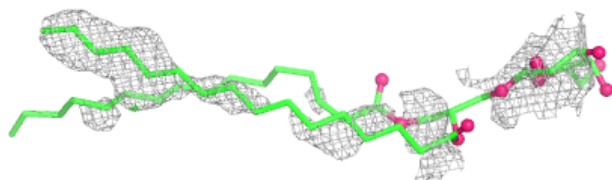
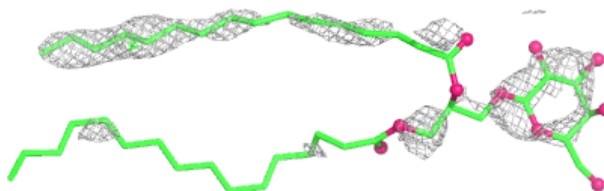


Electron density around LHG E 101:

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

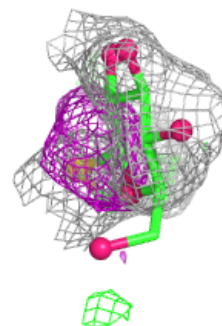
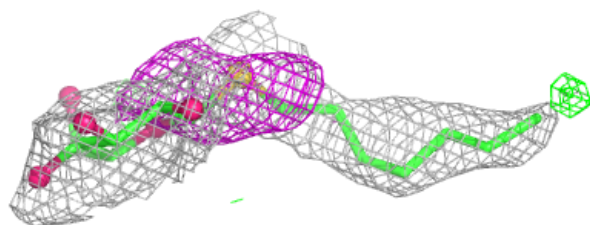
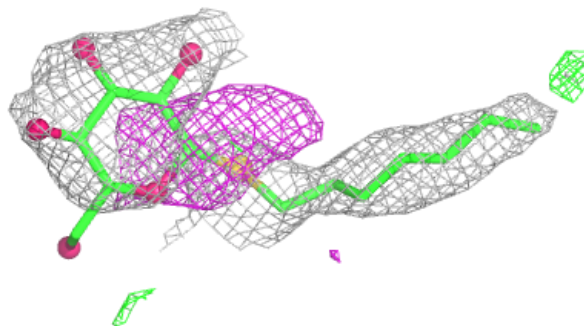
**Electron density around LMG c 522:**

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

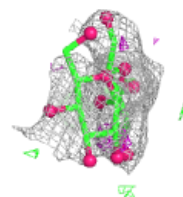
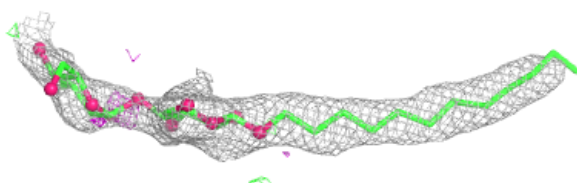
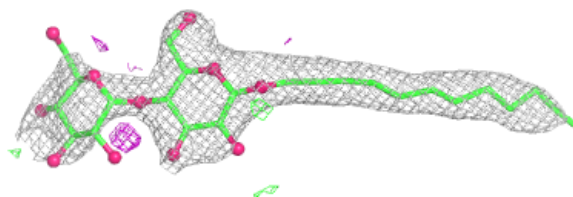


Electron density around HTG b 622:

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

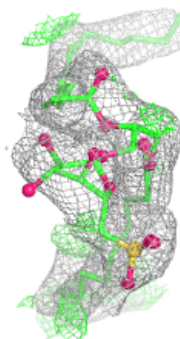
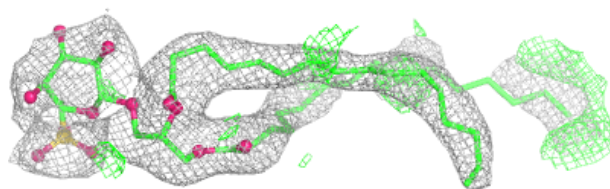
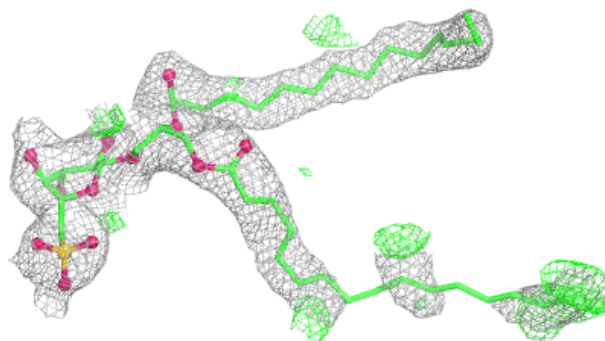
**Electron density around LMT M 101:**

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

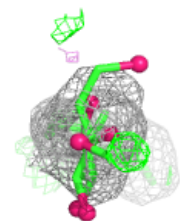
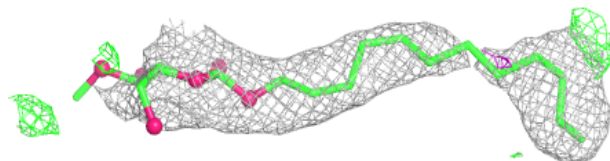
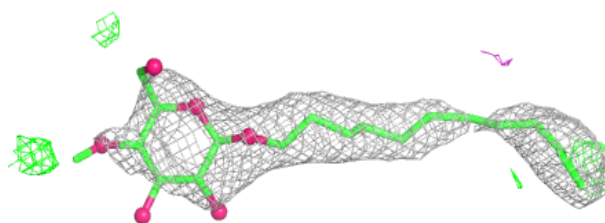


Electron density around SQD A 411:

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

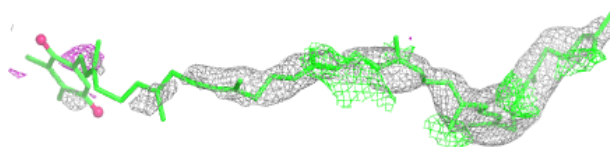
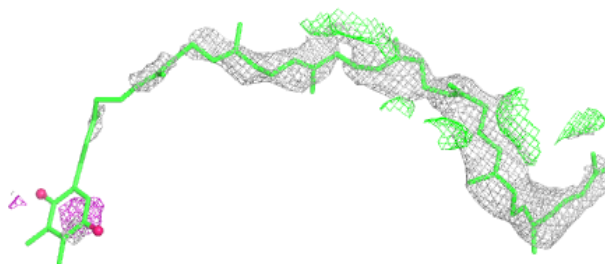
**Electron density around LMT b 627:**

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

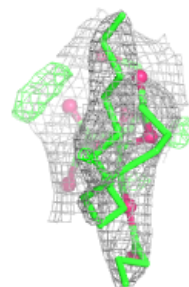
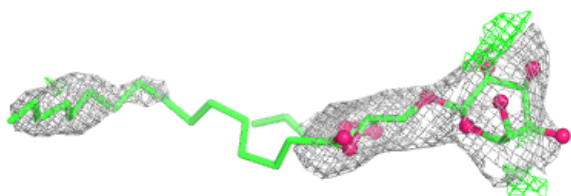
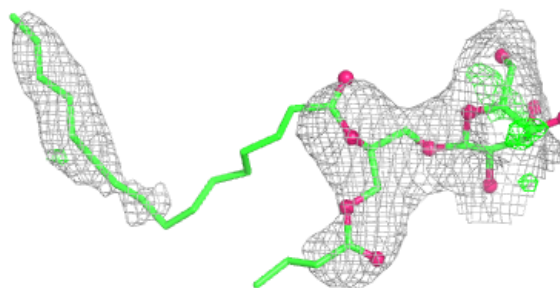


Electron density around PL9 a 415:

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

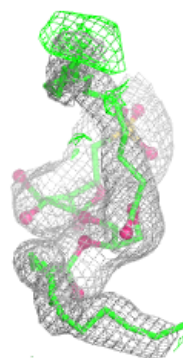
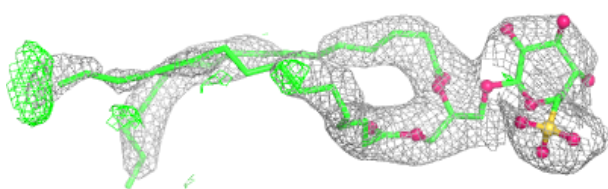
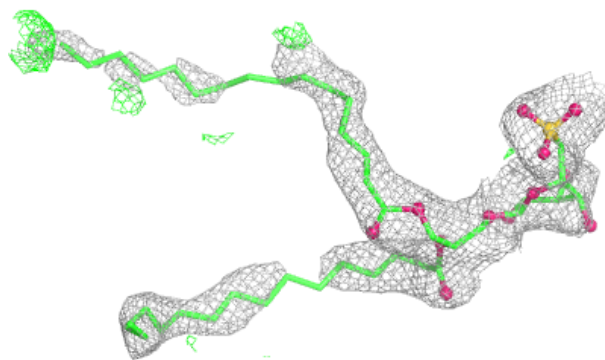
**Electron density around LMG z 101:**

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

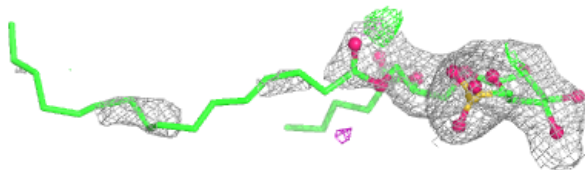
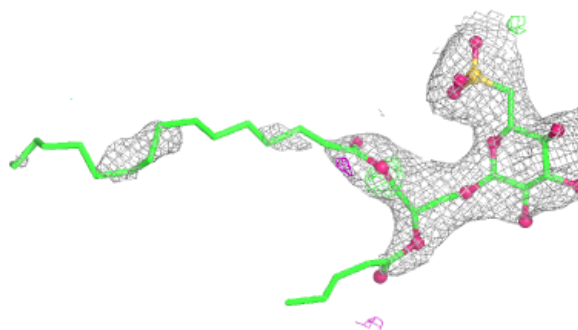


Electron density around SQD a 412:

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

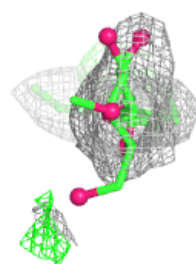
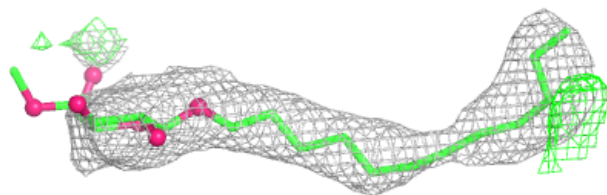
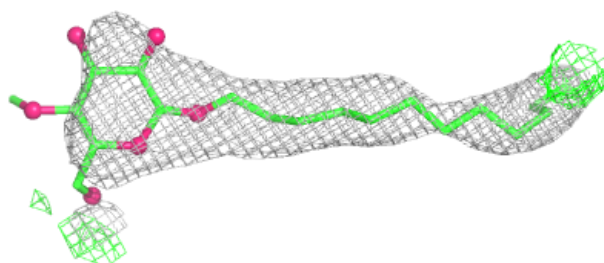
**Electron density around SQD D 412:**

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

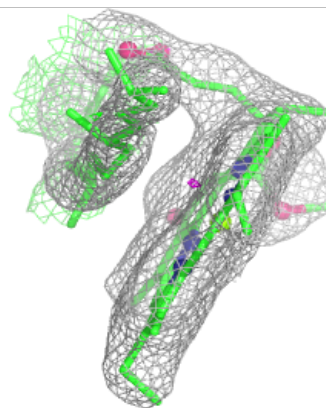
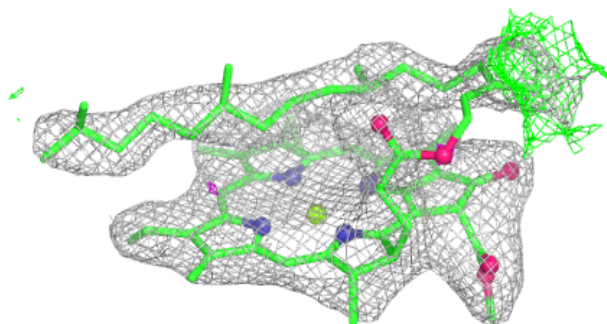
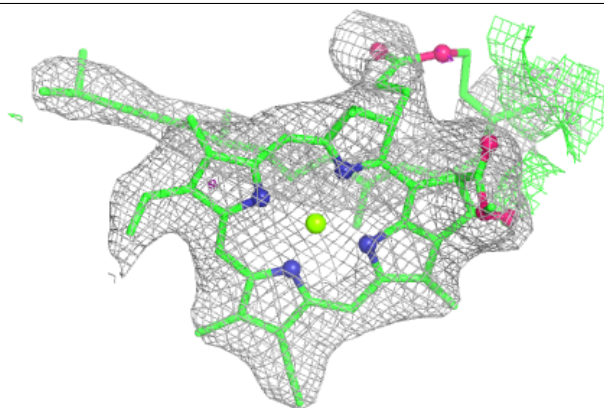


Electron density around LMT B 630:

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

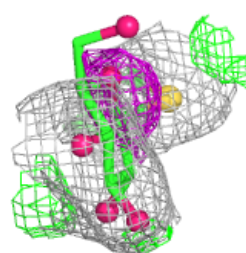
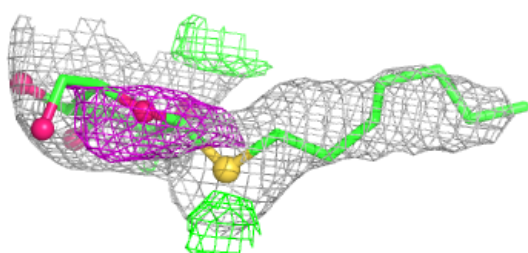
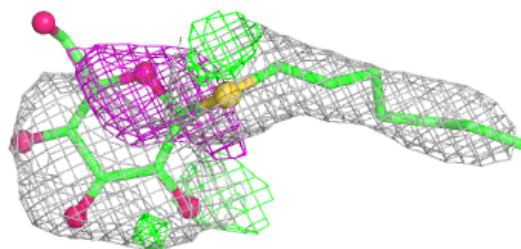
**Electron density around CLA b 601:**

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

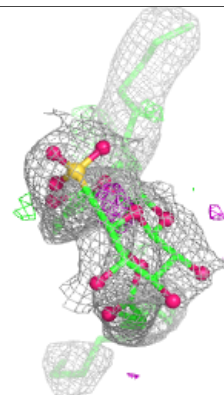
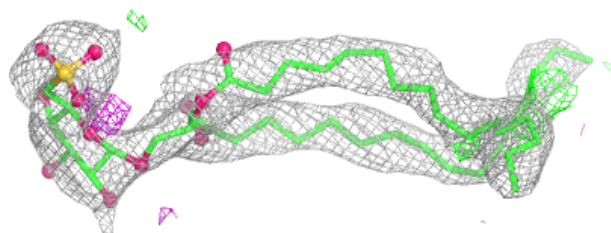
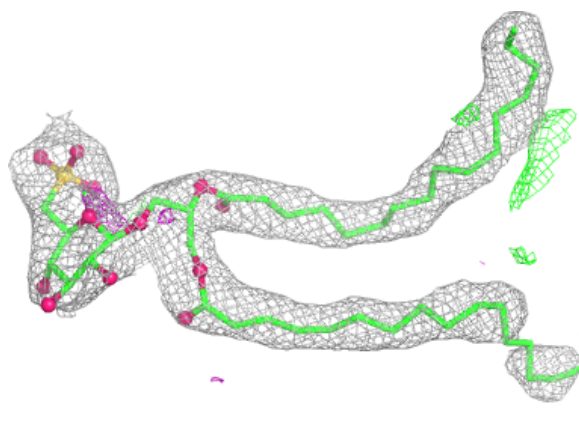


Electron density around HTG B 622:

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

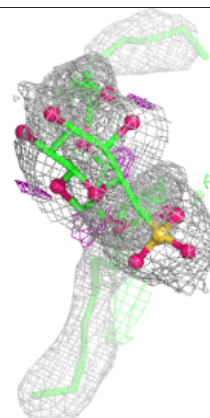
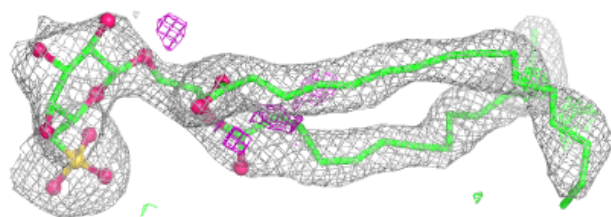
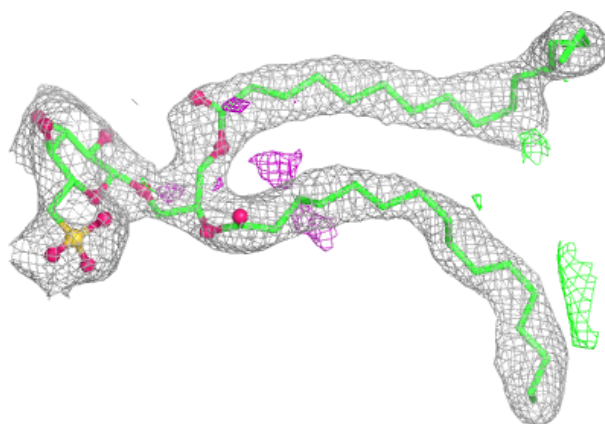
**Electron density around SQD b 620:**

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

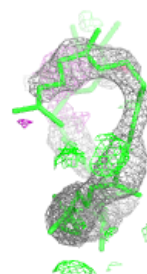
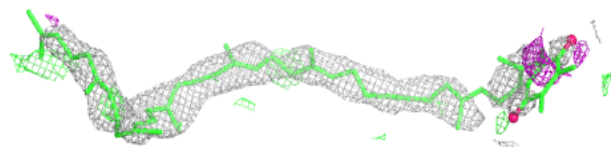
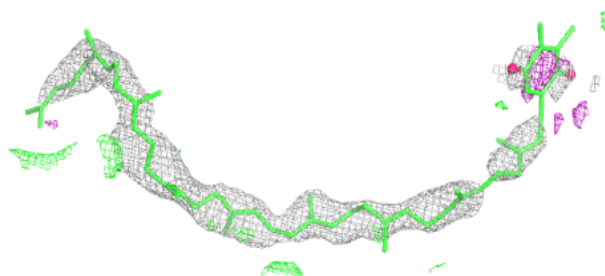


Electron density around SQD B 620:

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

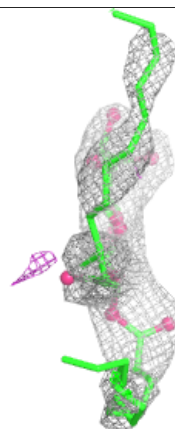
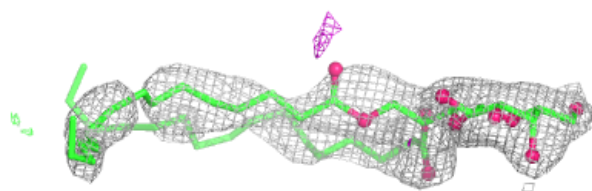
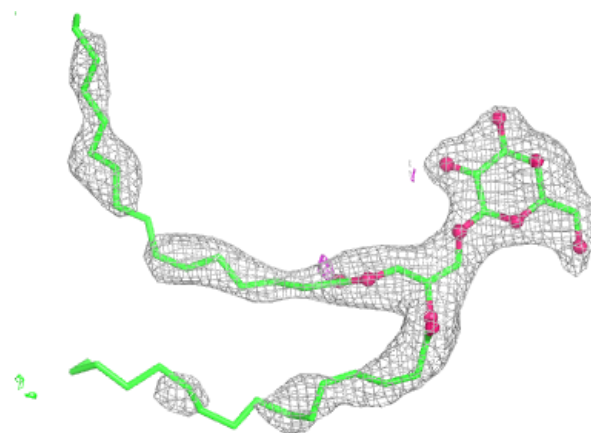
**Electron density around PL9 A 413:**

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

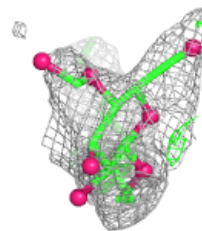
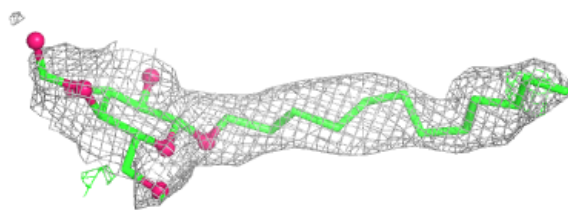
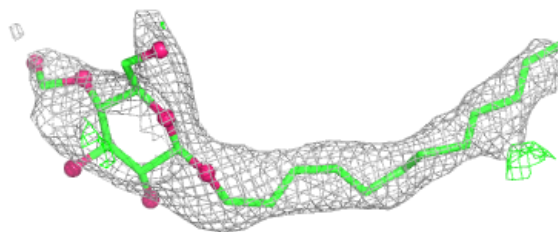


Electron density around LMG C 521:

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

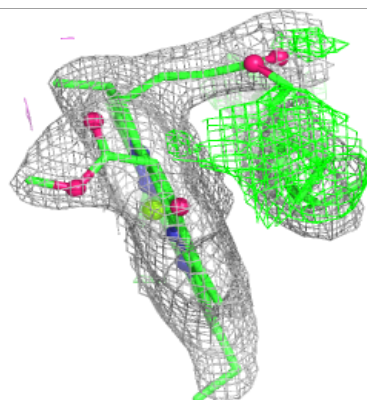
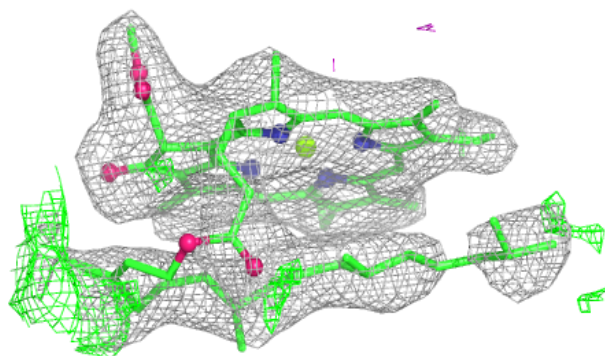
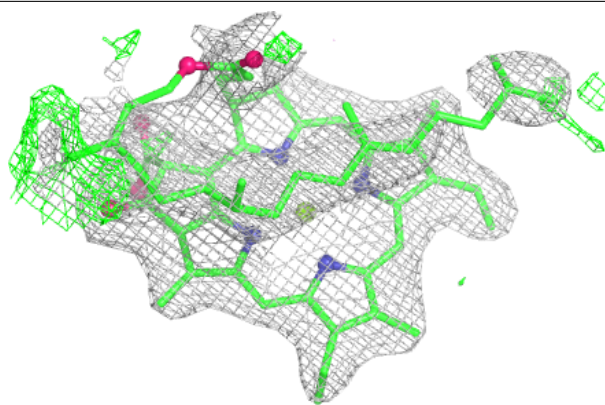
**Electron density around LMT t 101:**

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

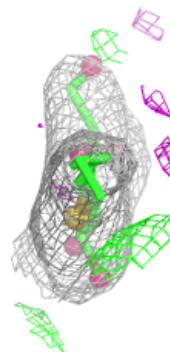
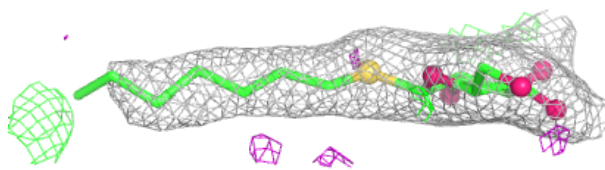
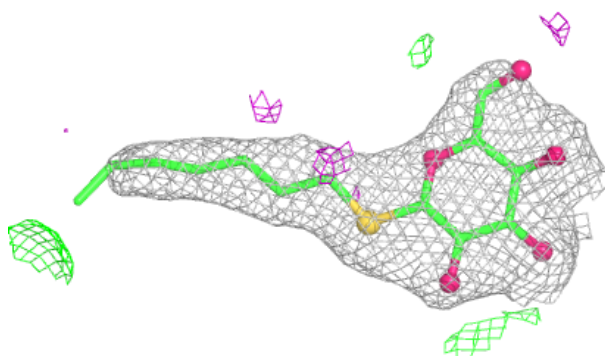


Electron density around CLA B 601:

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

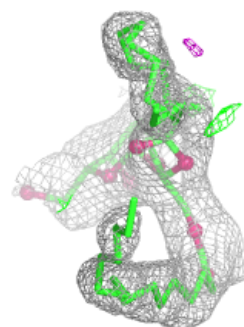
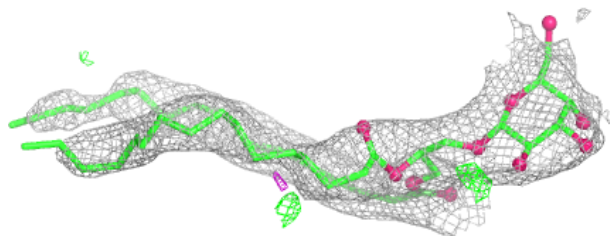
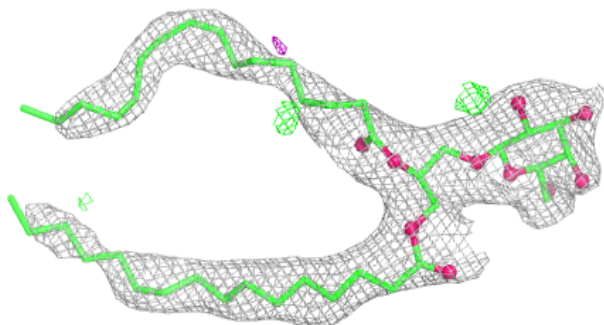
**Electron density around HTG B 625:**

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

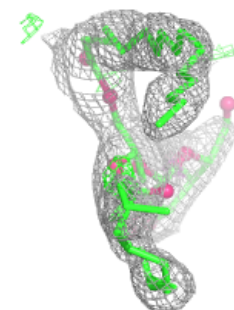
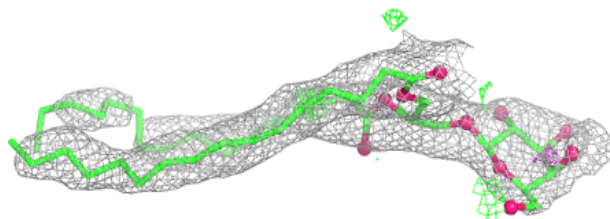
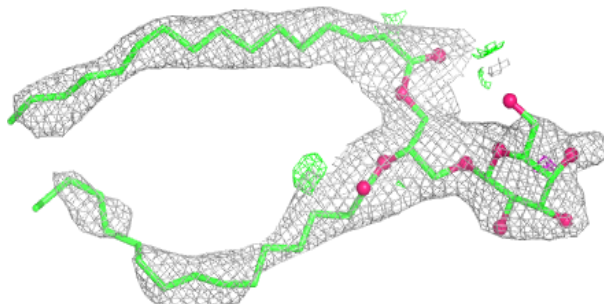


Electron density around LMG C 502:

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

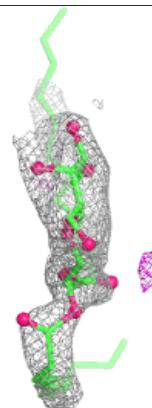
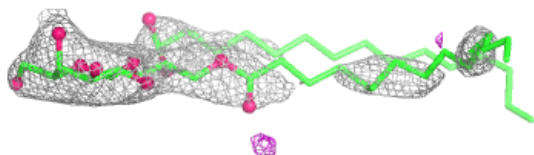
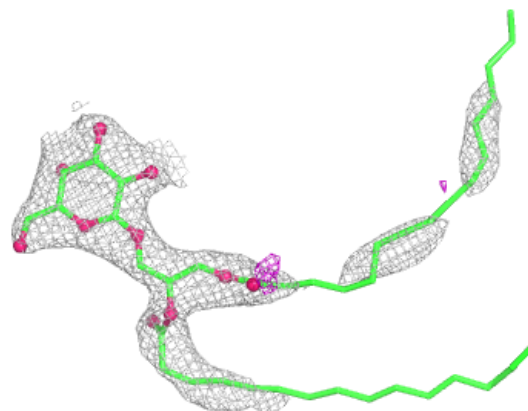
**Electron density around LMG c 501:**

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

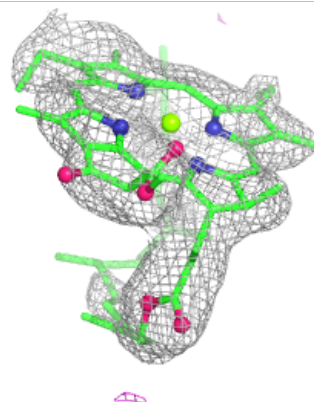
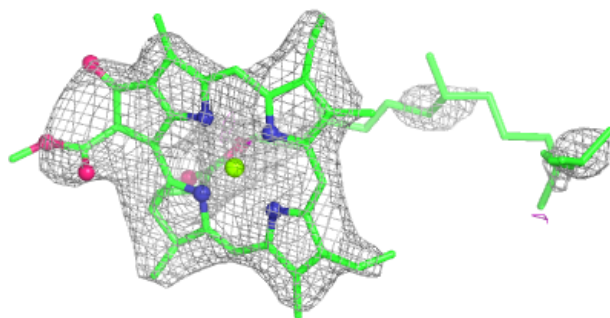
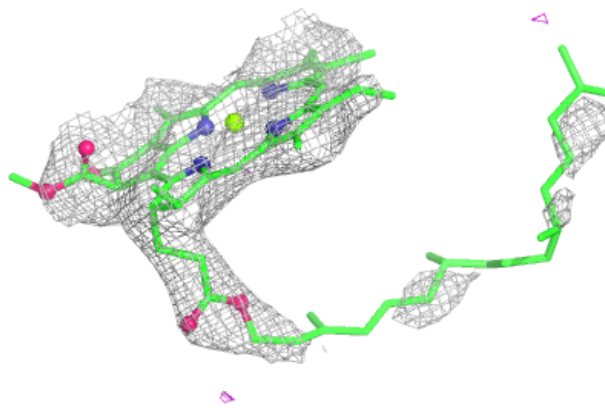


Electron density around LMG c 521:

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

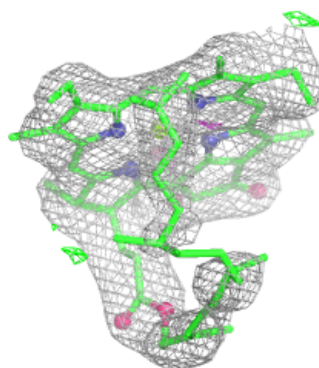
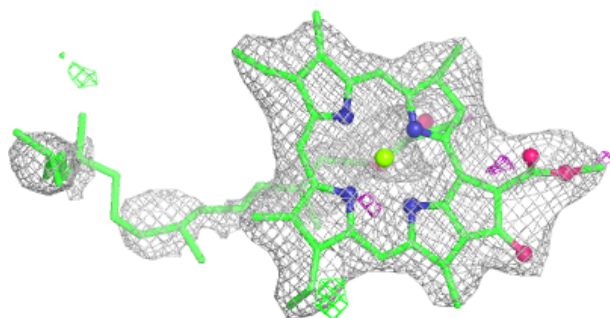
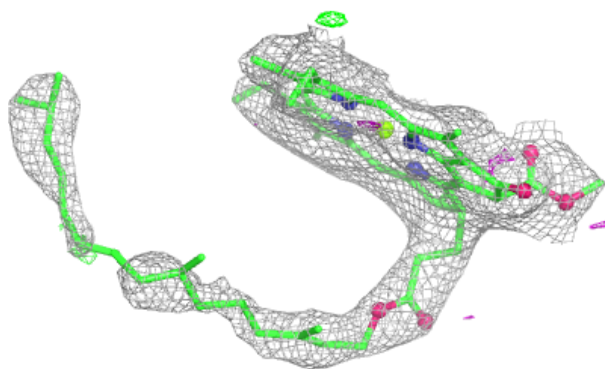
**Electron density around CLA c 515:**

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

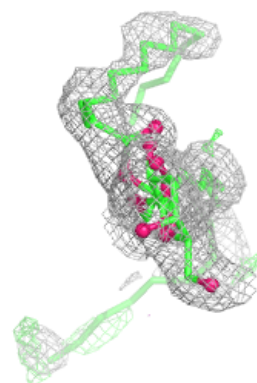
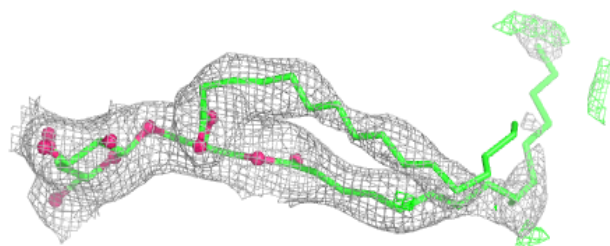
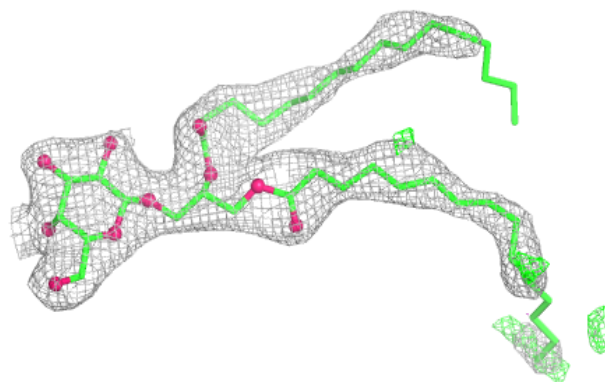


Electron density around CLA C 515:

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

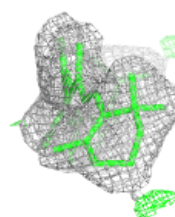
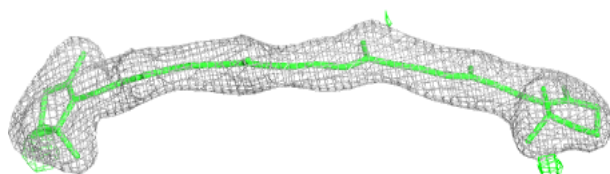
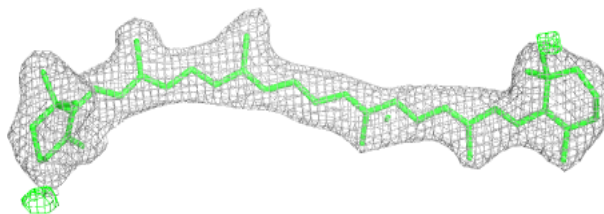
**Electron density around LMG D 413:**

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

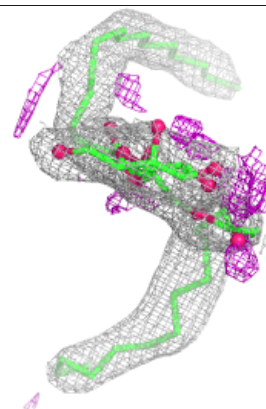
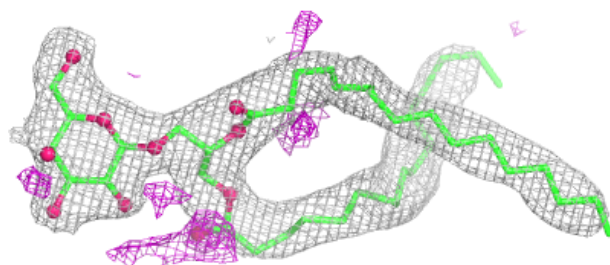
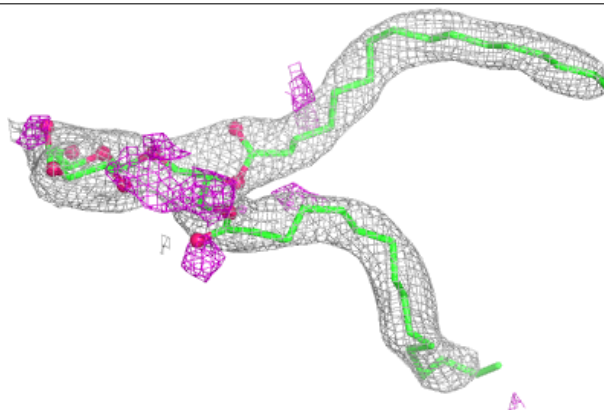


Electron density around BCR t 102:

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

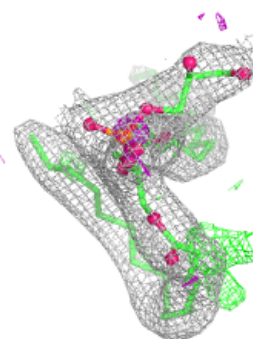
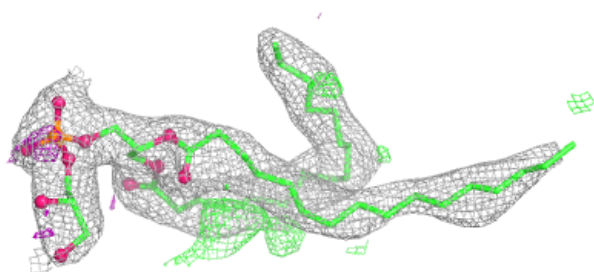
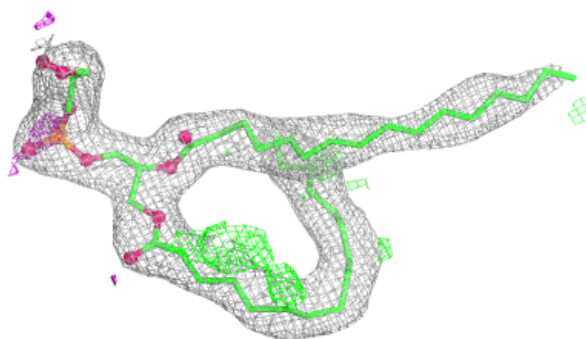
**Electron density around LMG m 101:**

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

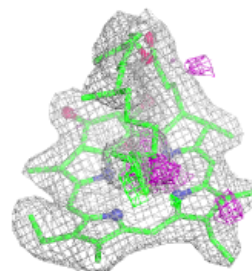
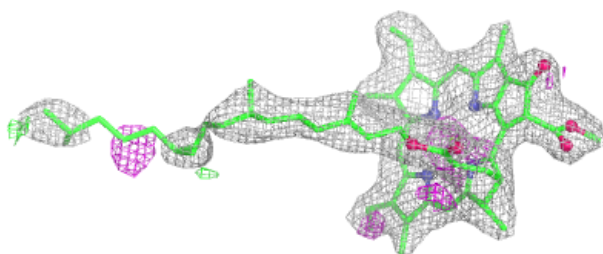
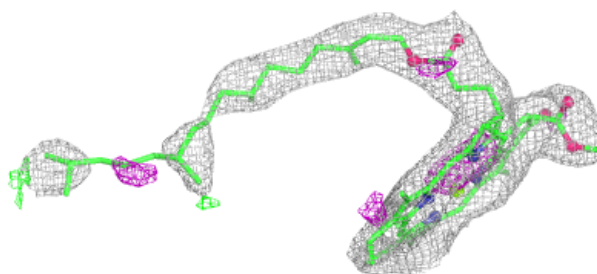


Electron density around LHG A 416:

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

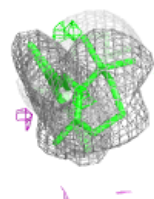
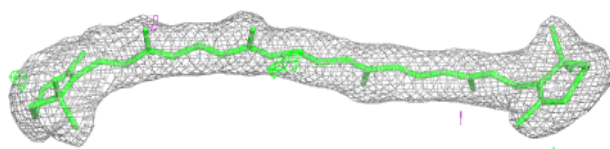
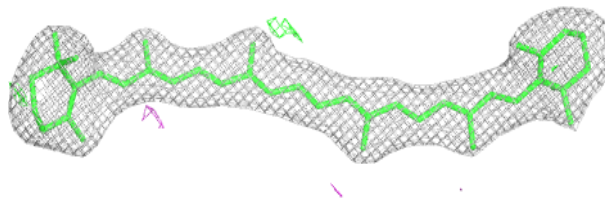
**Electron density around CLA C 506:**

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

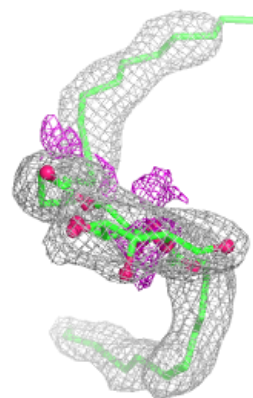
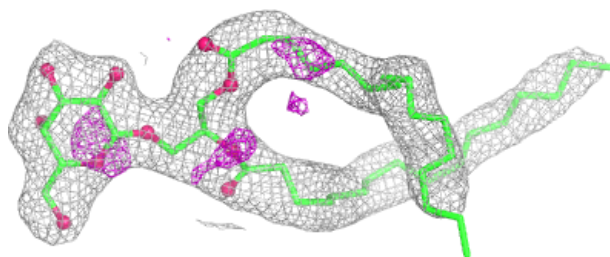
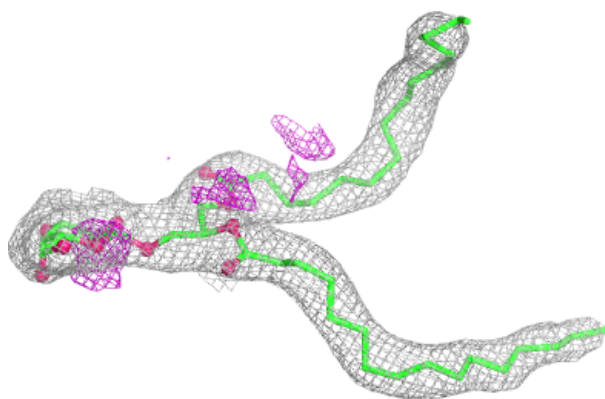


Electron density around BCR B 619:

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

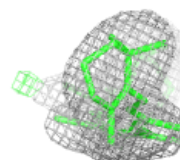
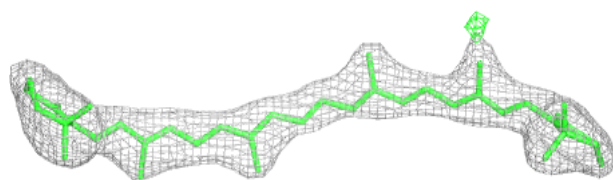
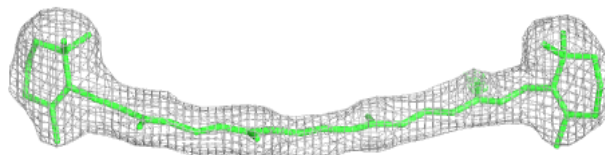
**Electron density around LMG B 621:**

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

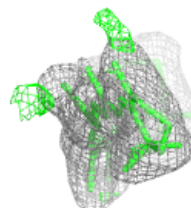
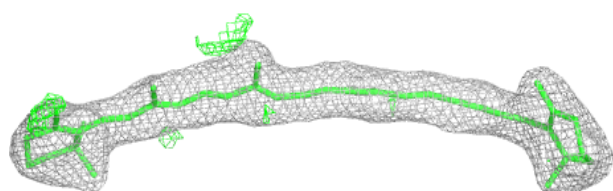
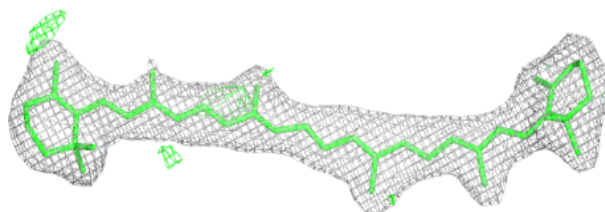


Electron density around BCR K 101:

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

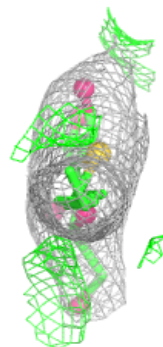
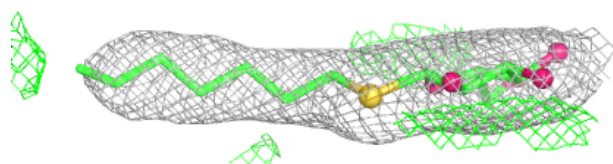
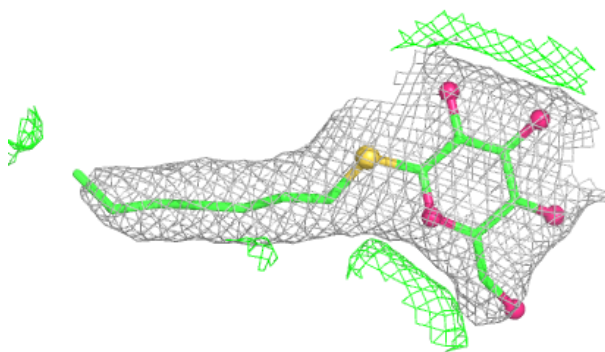
**Electron density around BCR T 101:**

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

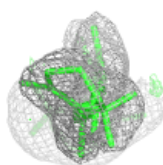
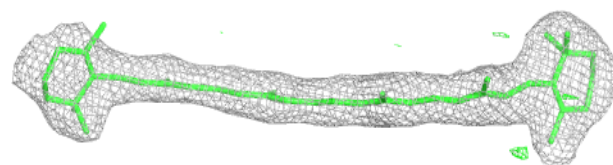


Electron density around HTG b 625:

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

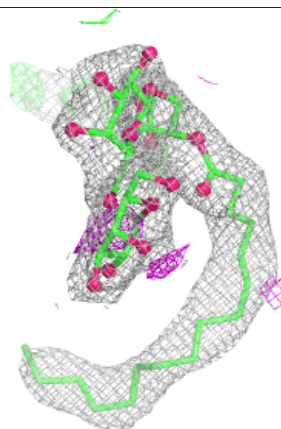
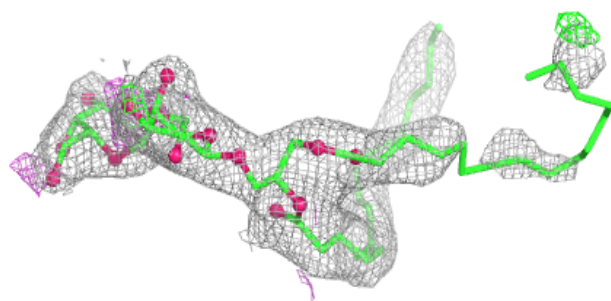
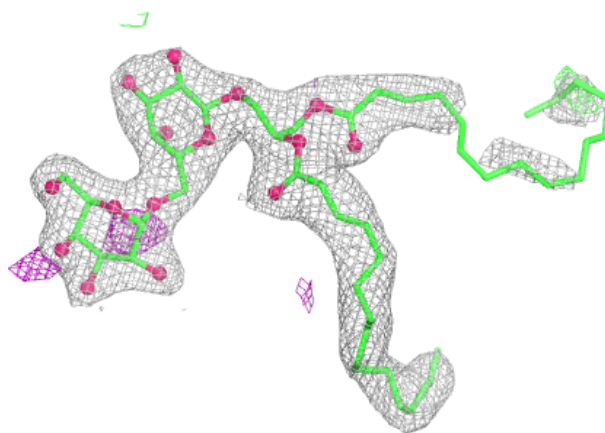
**Electron density around BCR h 102:**

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



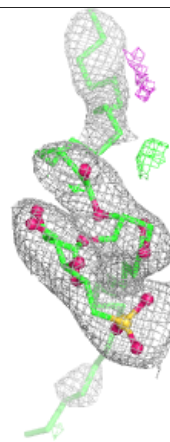
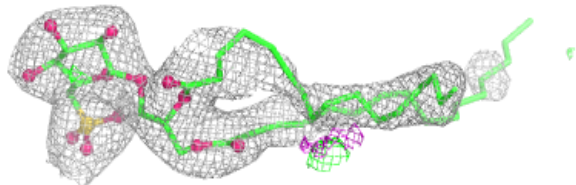
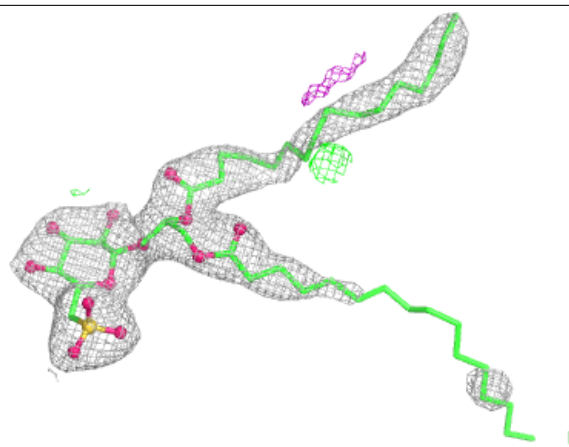
Electron density around DGD C 519:

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

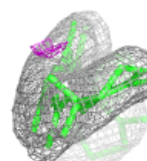
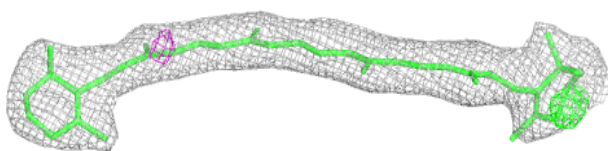
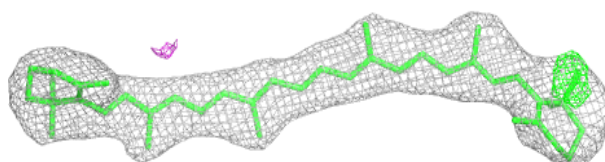


Electron density around SQD C 501:

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

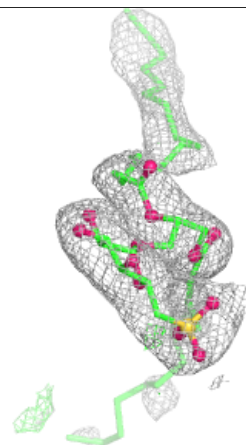
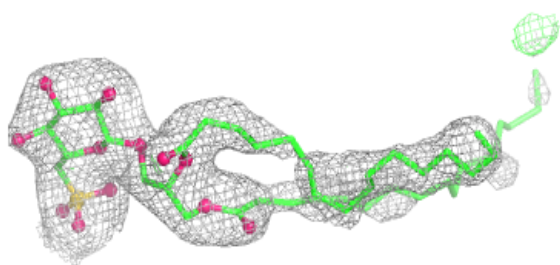
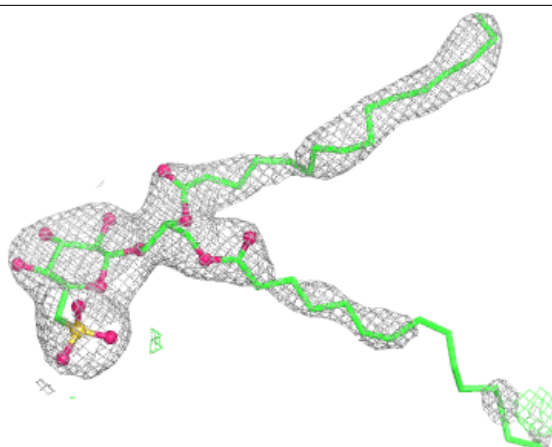
**Electron density around BCR d 404:**

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

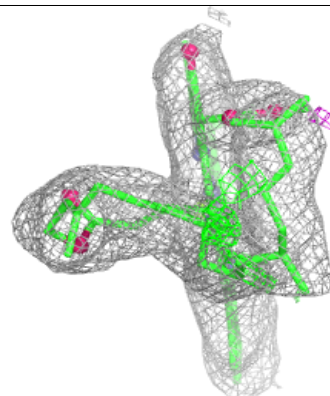
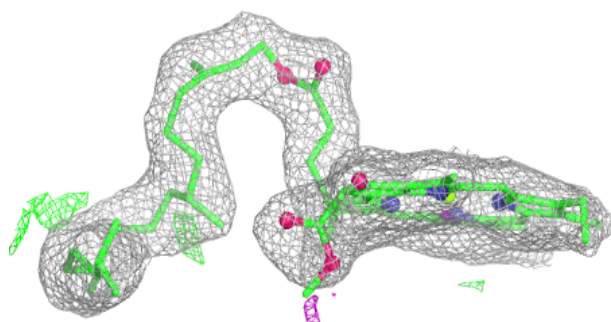
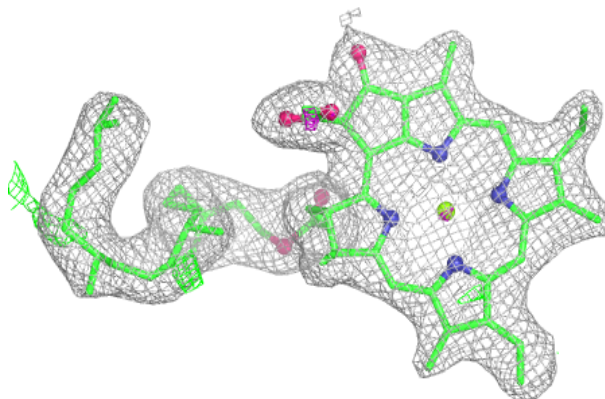


Electron density around SQD a 410:

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

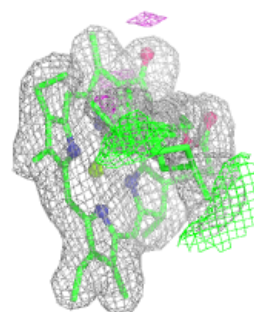
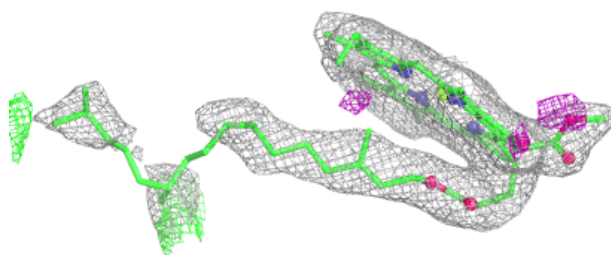
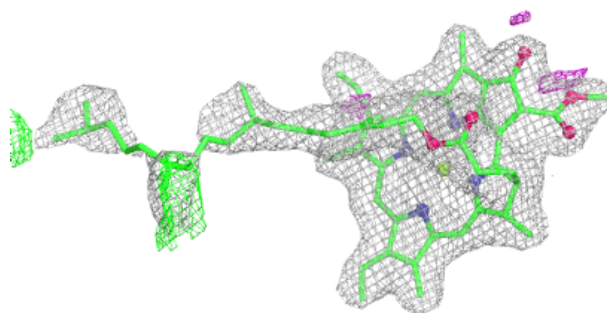
**Electron density around CLA b 612:**

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

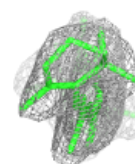
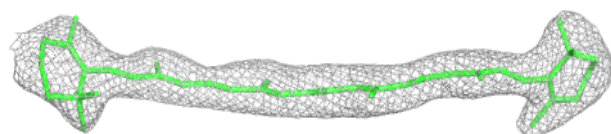
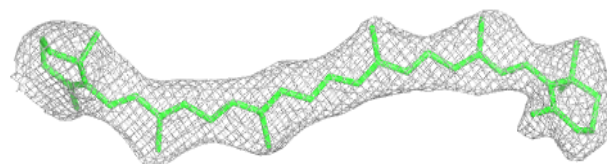


Electron density around CLA b 614:

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

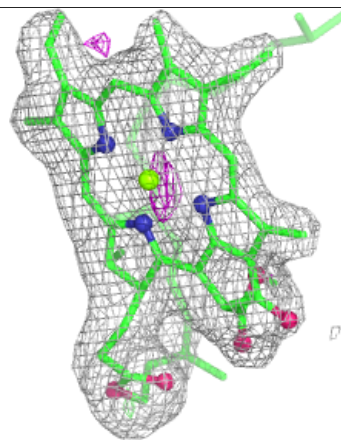
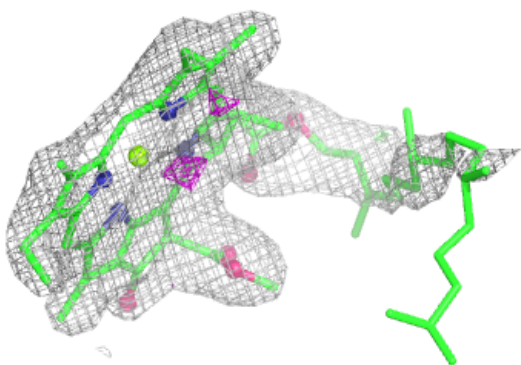
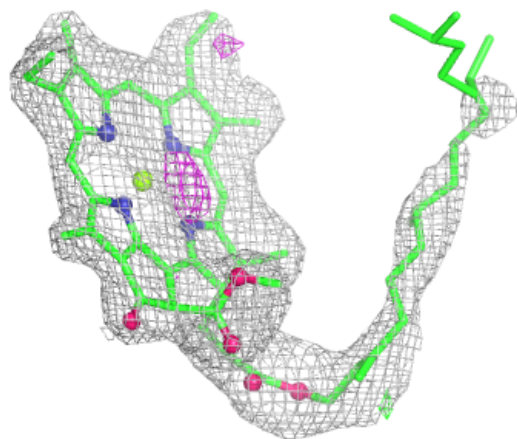
**Electron density around BCR y 101:**

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

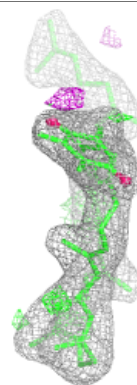
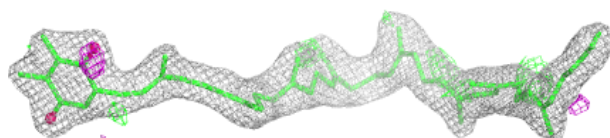
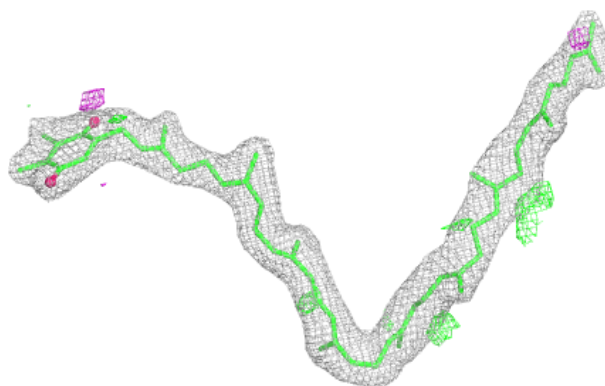


Electron density around CLA b 616:

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

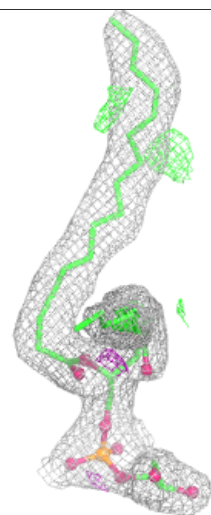
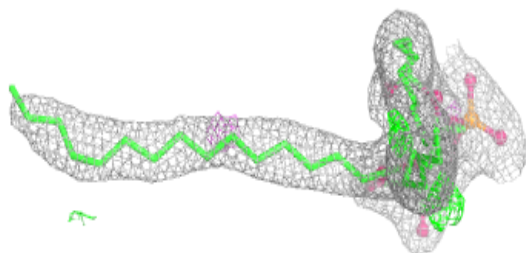
**Electron density around PL9 D 406:**

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



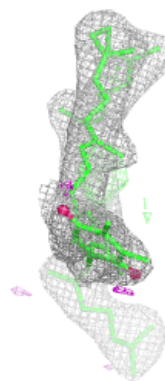
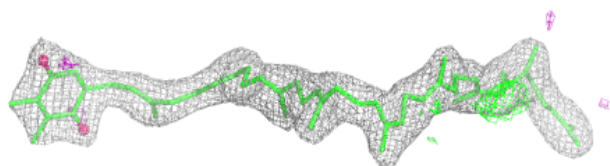
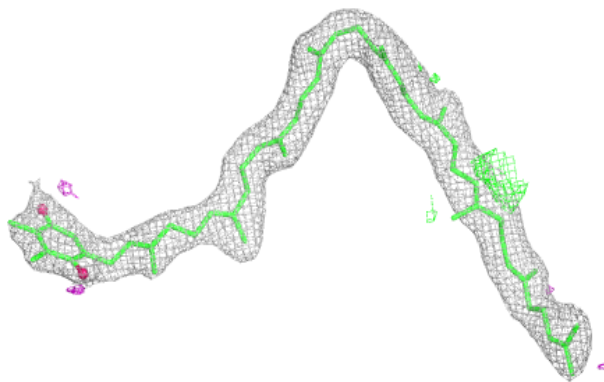
Electron density around LHG b 629:

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



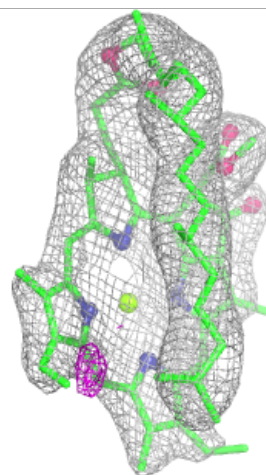
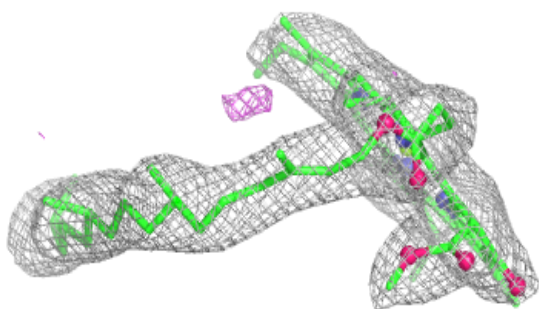
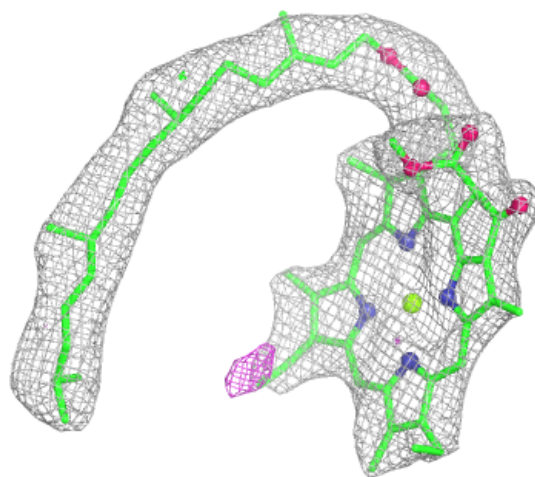
Electron density around PL9 d 405:

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



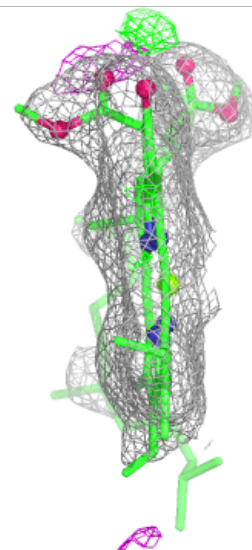
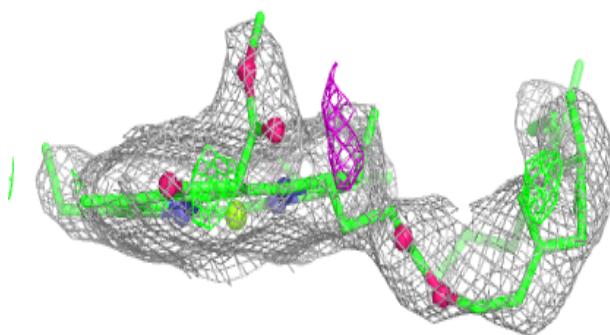
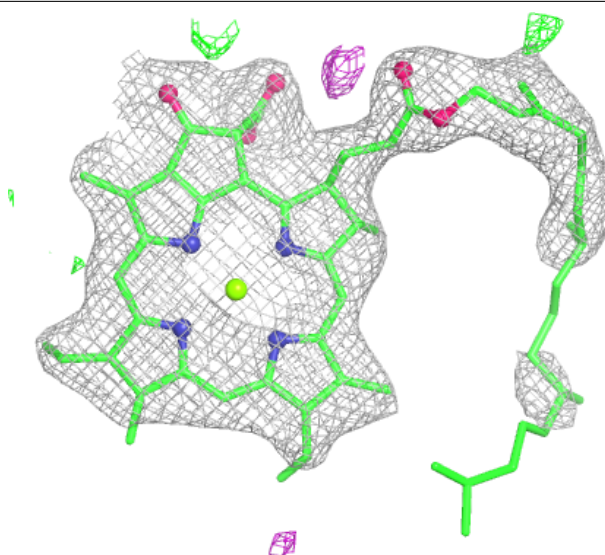
Electron density around CLA c 509:

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



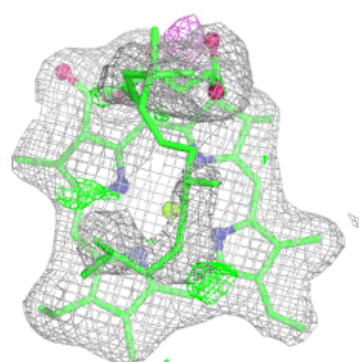
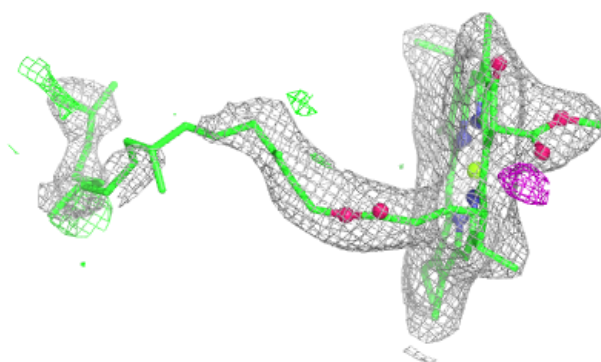
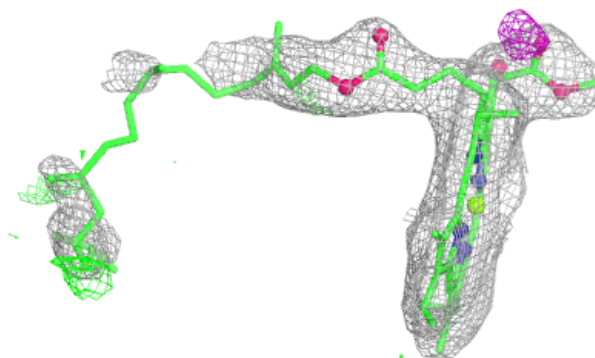
Electron density around CLA c 514:

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

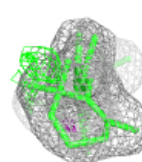
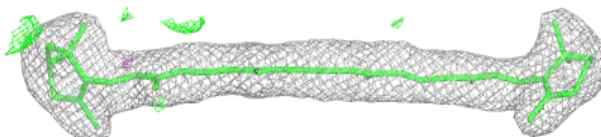
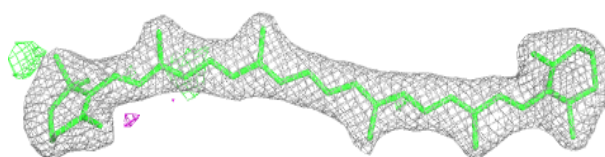


Electron density around CLA C 508:

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

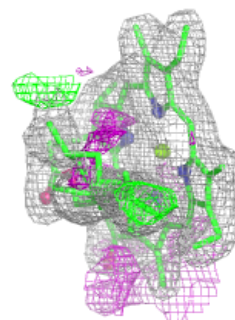
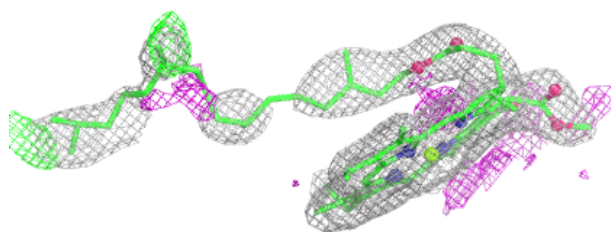
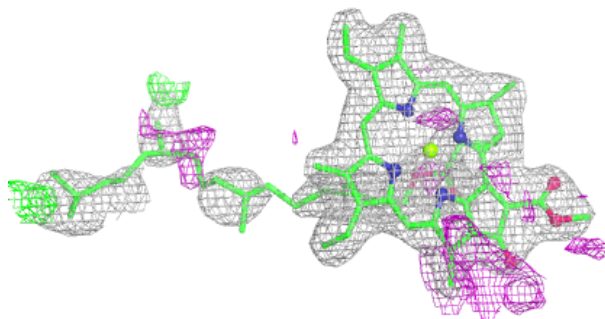
**Electron density around BCR B 618:**

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

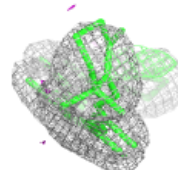
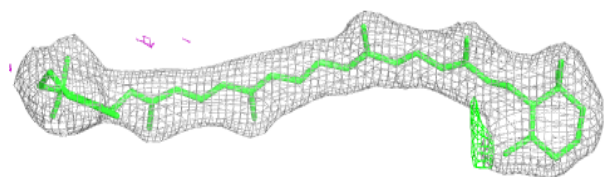
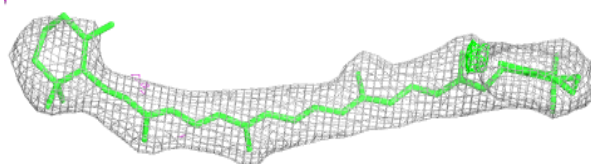


Electron density around CLA B 614:

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

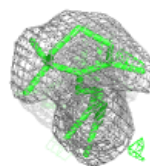
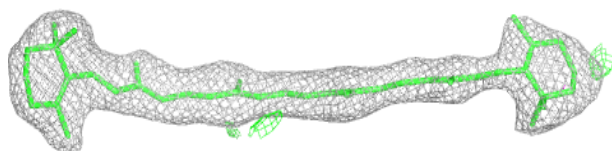
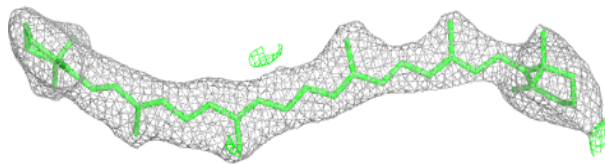
**Electron density around BCR D 405:**

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

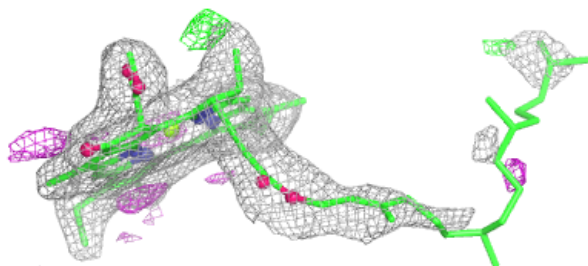
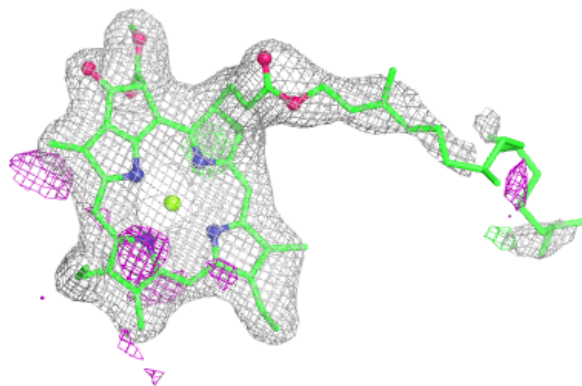


Electron density around BCR H 101:

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

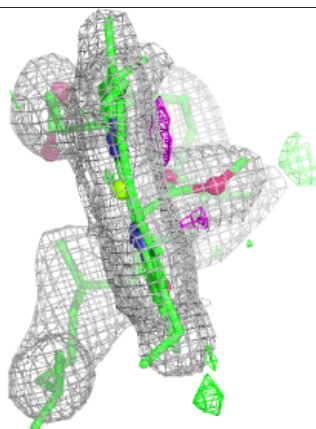
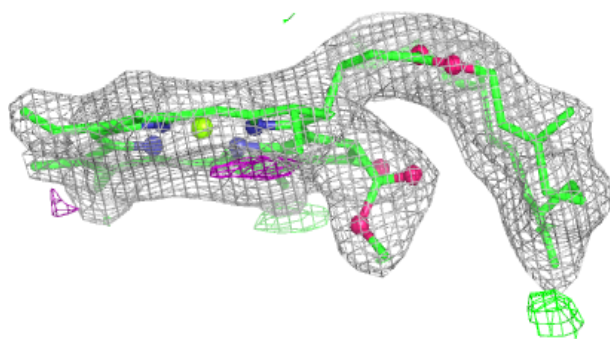
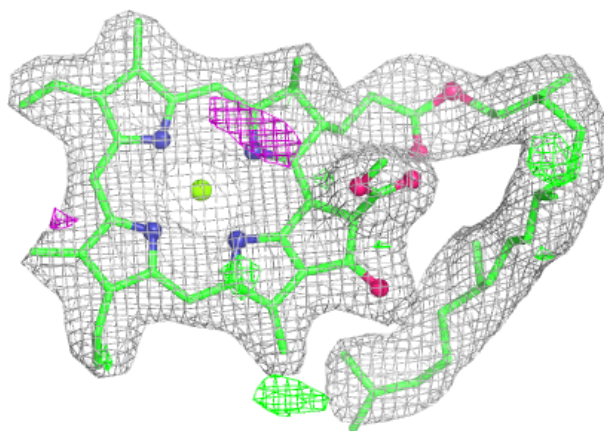
**Electron density around CLA a 408:**

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

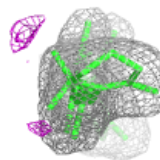
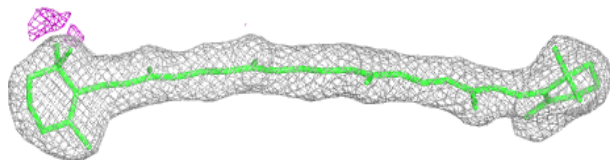
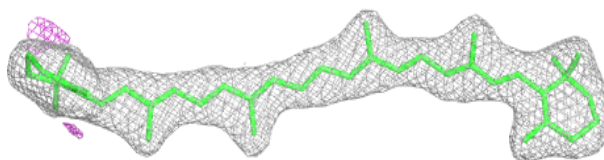


Electron density around CLA B 610:

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

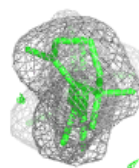
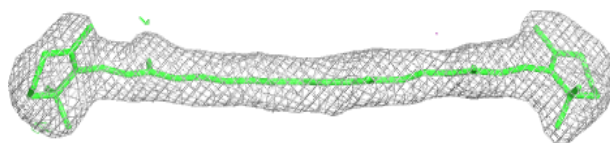
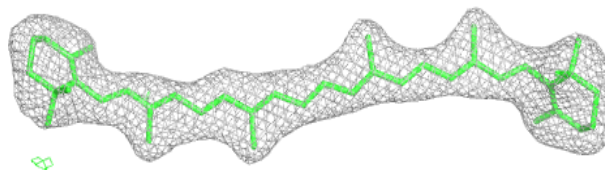
**Electron density around BCR b 617:**

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

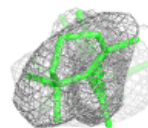
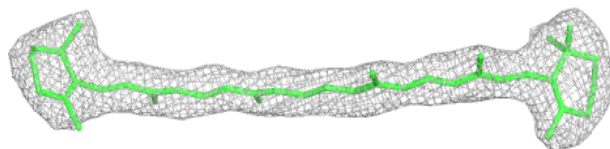
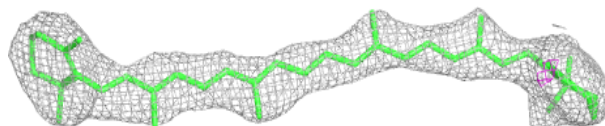


Electron density around BCR b 618:

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

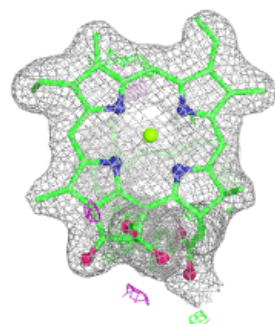
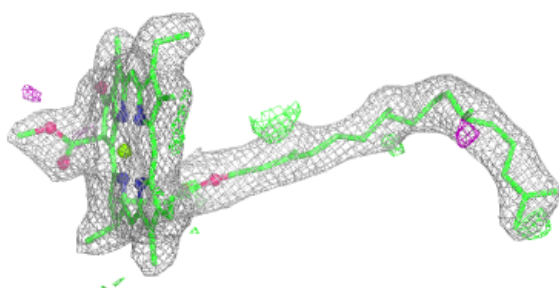
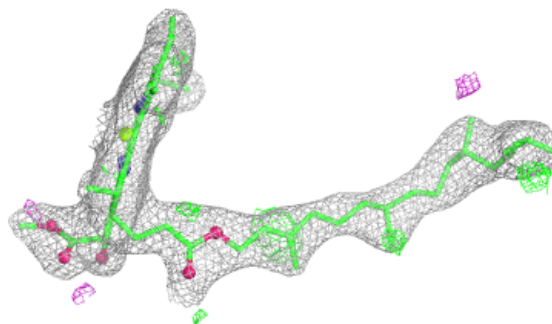
**Electron density around BCR c 516:**

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

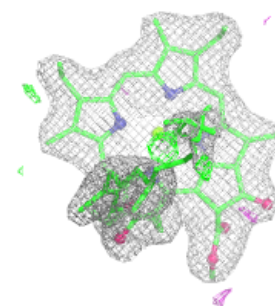
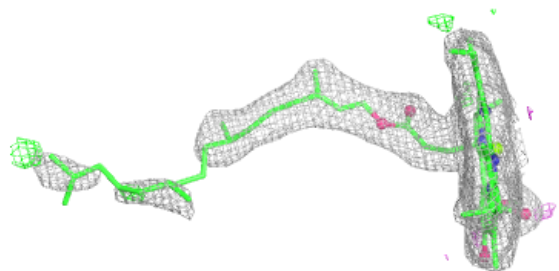
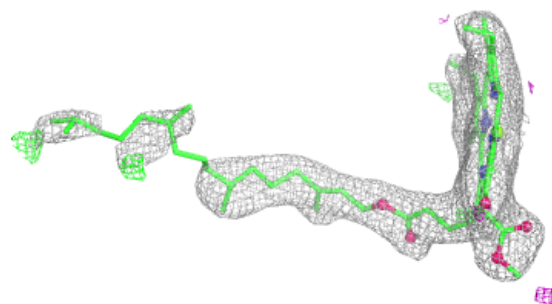


Electron density around CLA b 605:

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

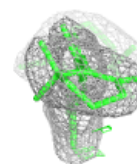
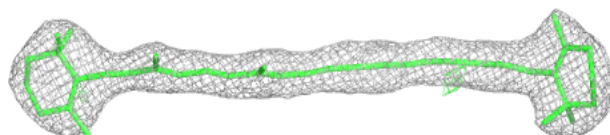
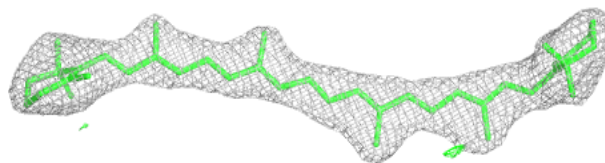
**Electron density around CLA b 606:**

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

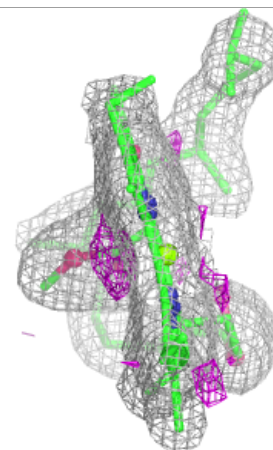
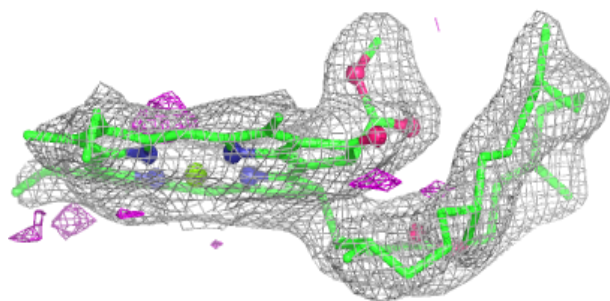
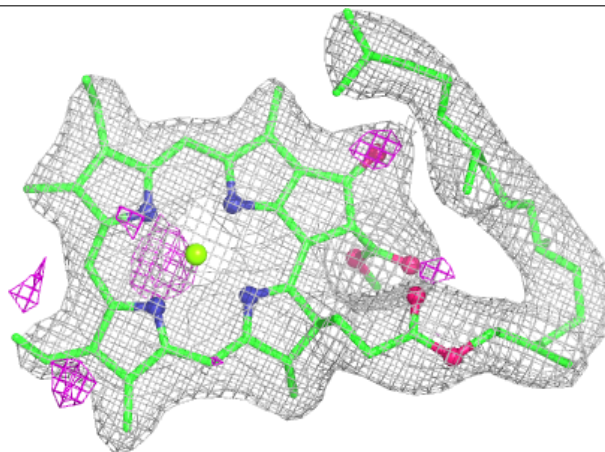


Electron density around BCR c 517:

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

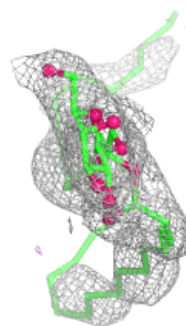
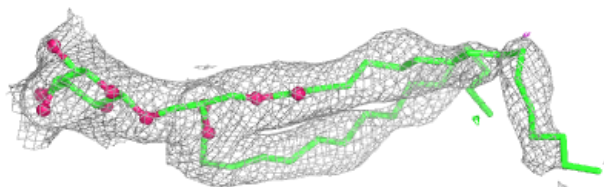
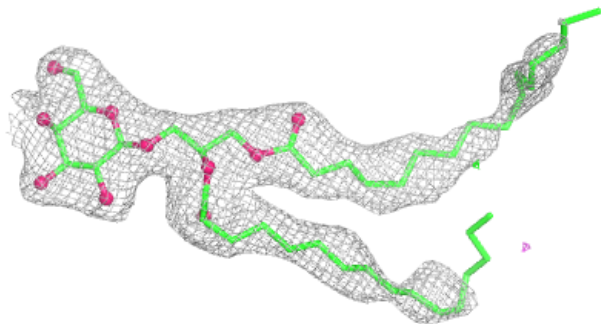
**Electron density around CLA b 610:**

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

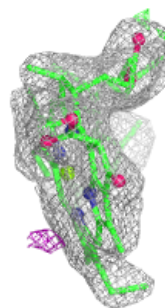
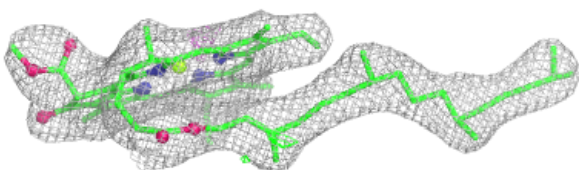
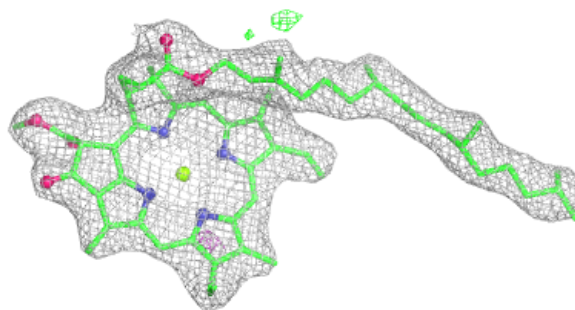


Electron density around LMG d 412:

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

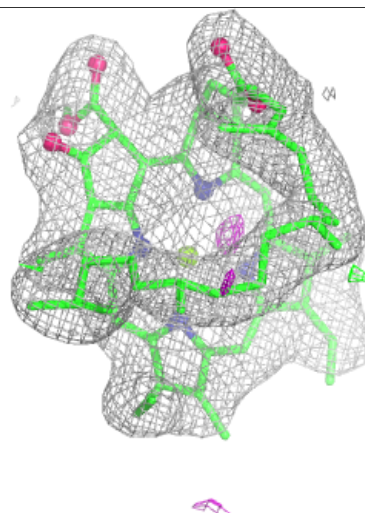
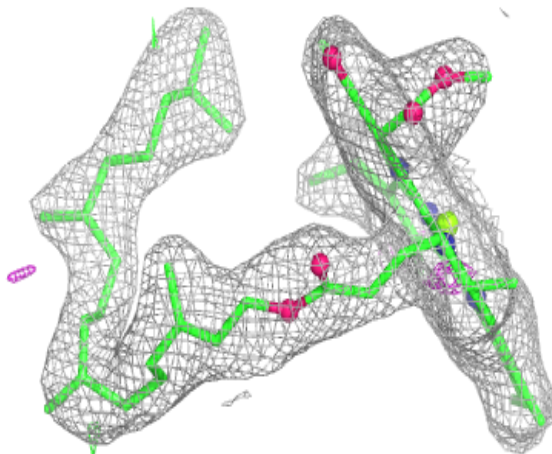
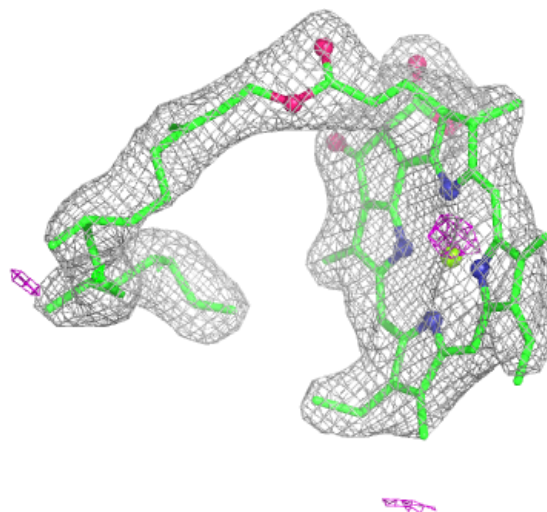
**Electron density around CLA C 503:**

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



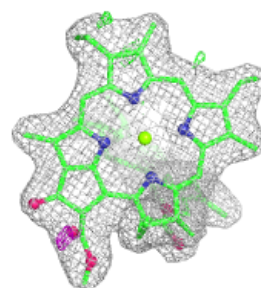
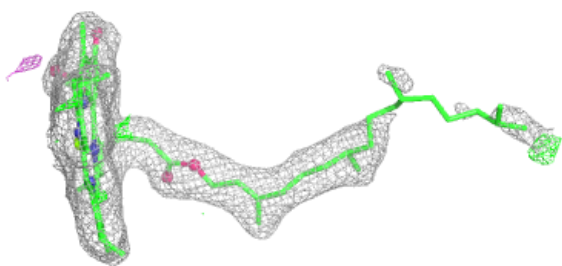
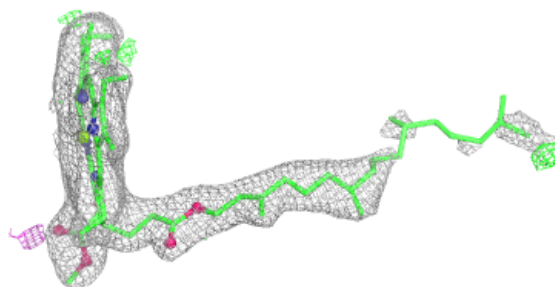
Electron density around CLA C 505:

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

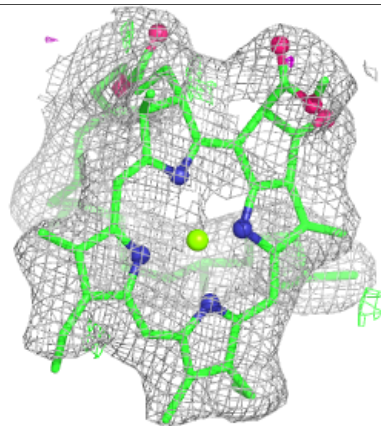
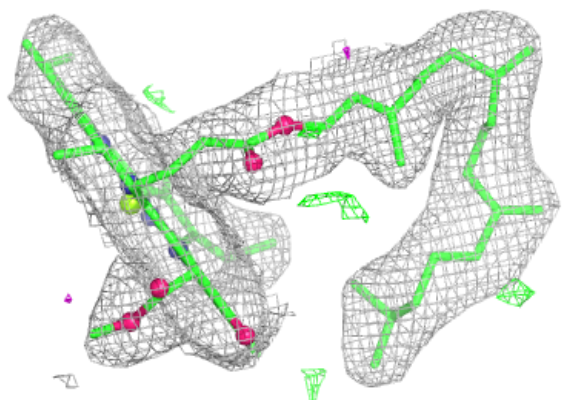
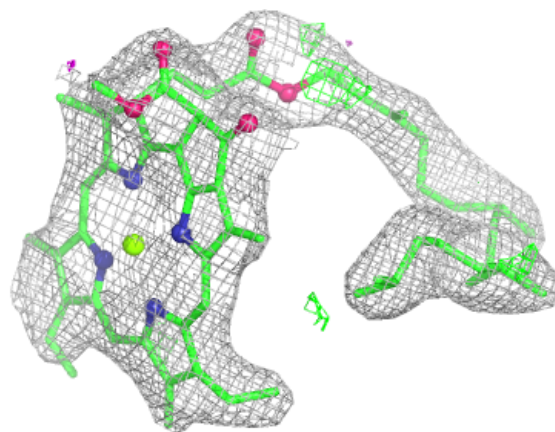


Electron density around CLA B 606:

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

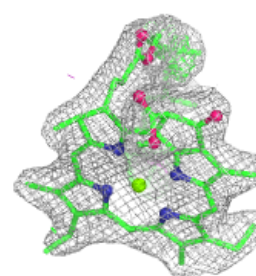
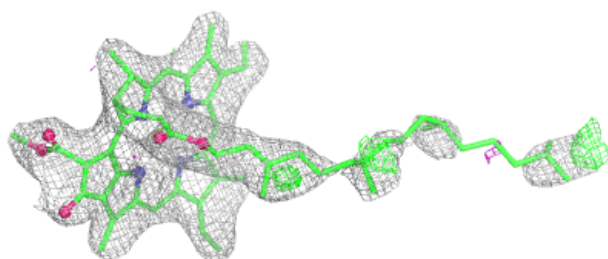
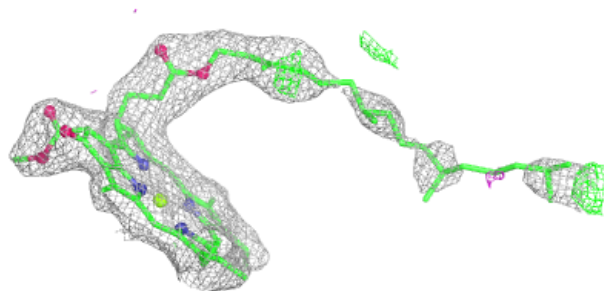
**Electron density around CLA c 505:**

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

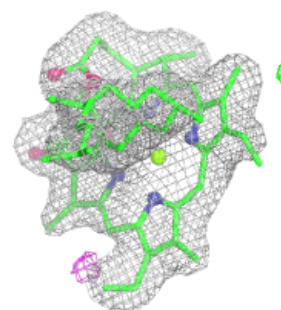
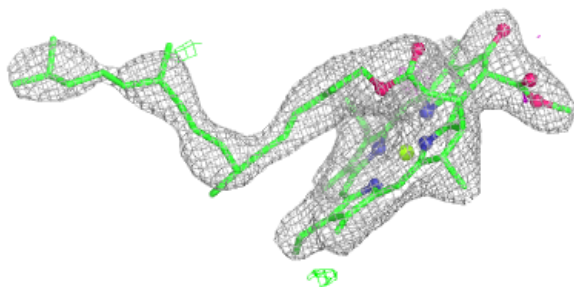
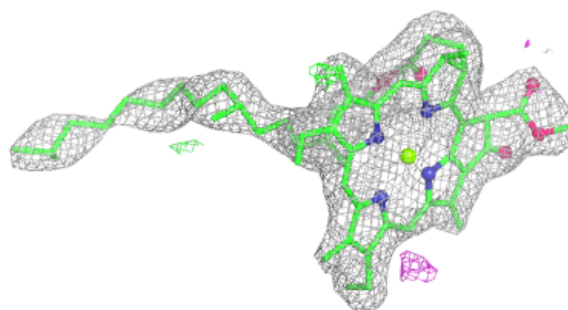


Electron density around CLA c 506:

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

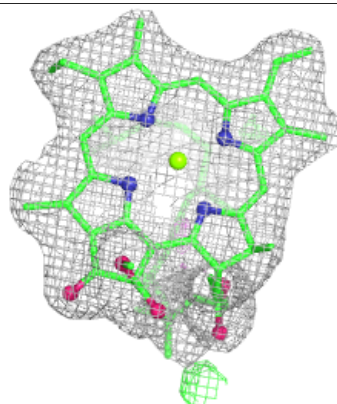
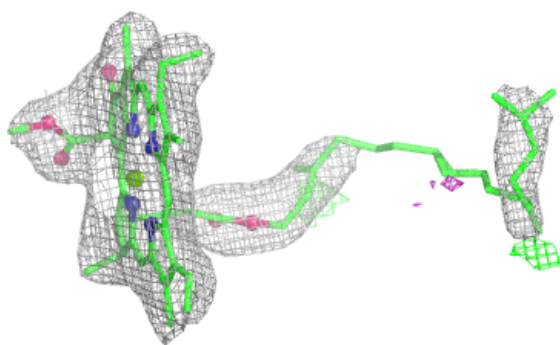
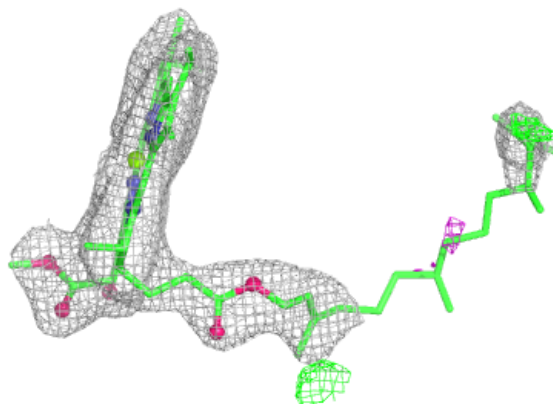
**Electron density around CLA c 507:**

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

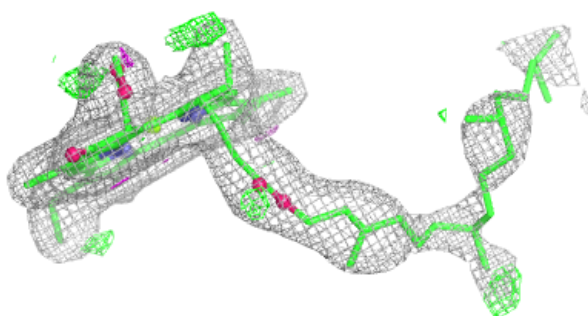
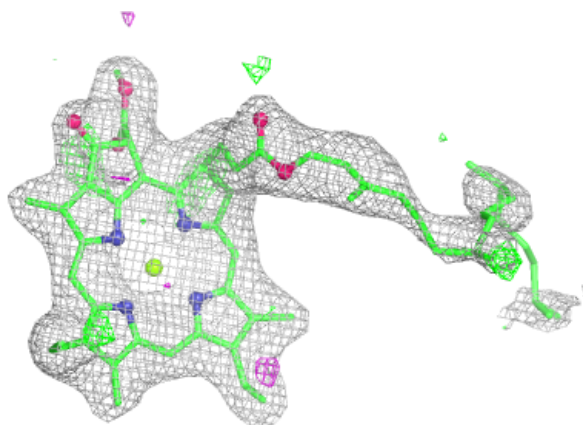


Electron density around CLA c 508:

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

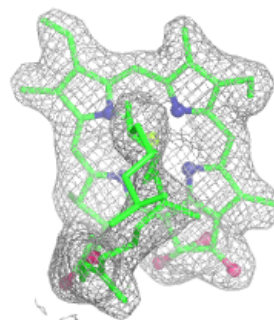
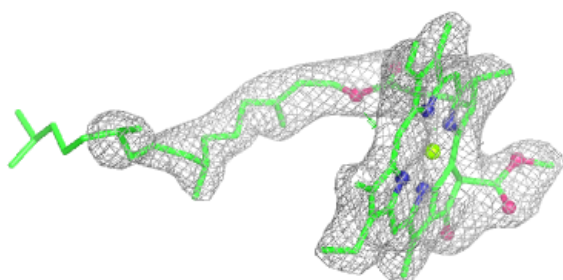
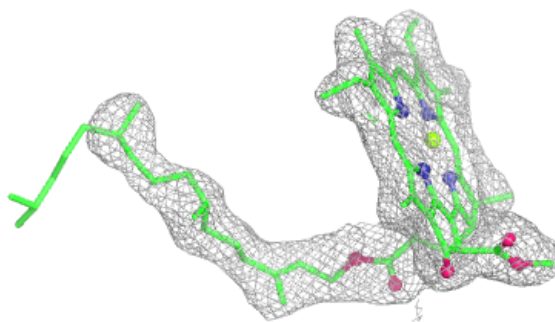
**Electron density around CLA A 408:**

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



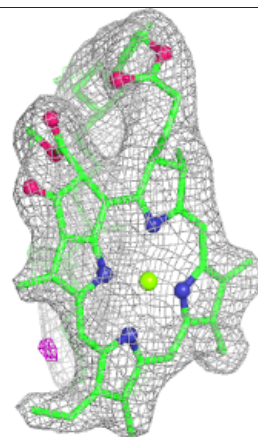
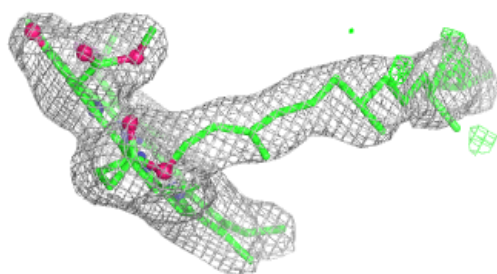
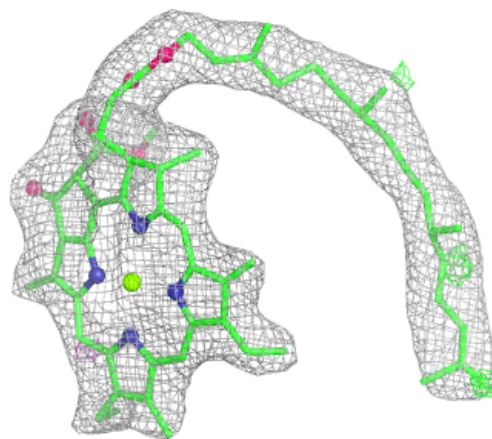
Electron density around CLA c 510:

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



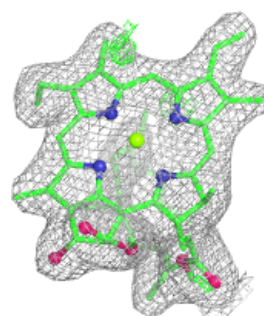
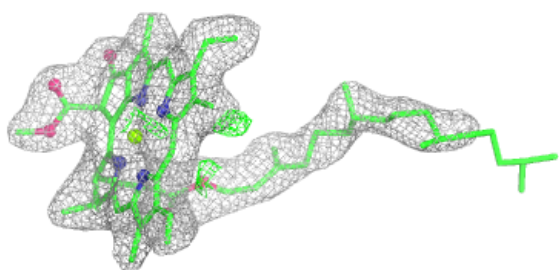
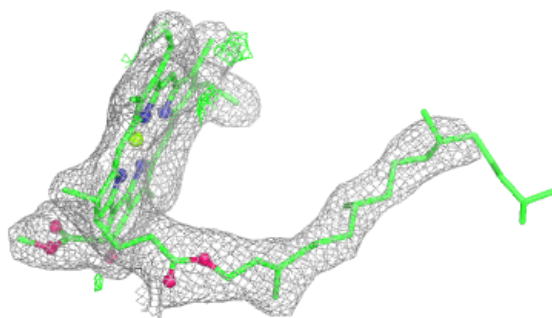
Electron density around CLA C 509:

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

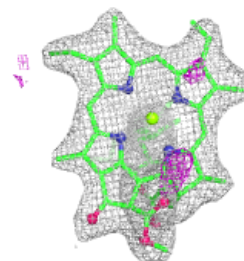
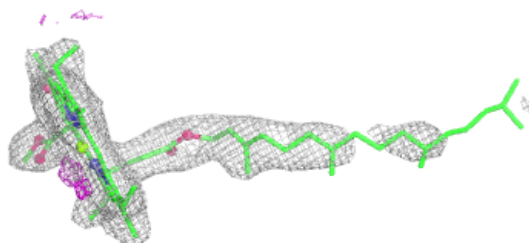
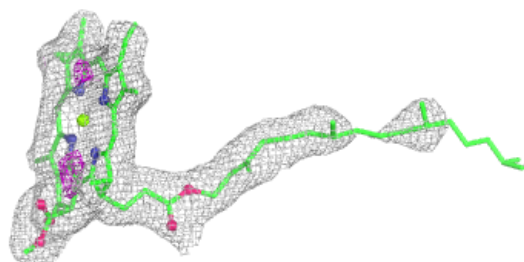


Electron density around CLA C 510:

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

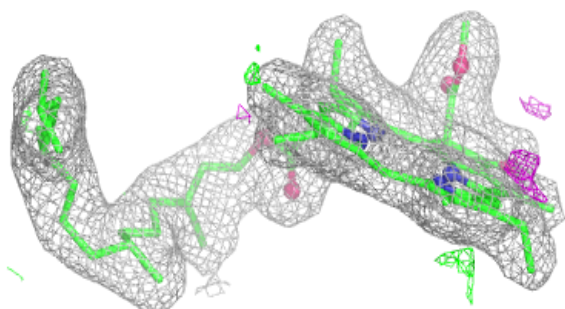
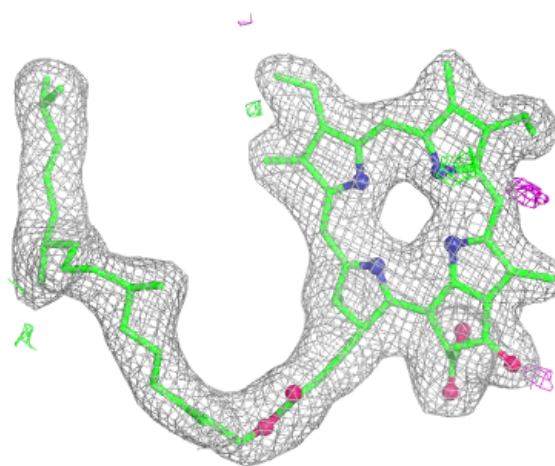
**Electron density around CLA d 403:**

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



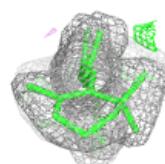
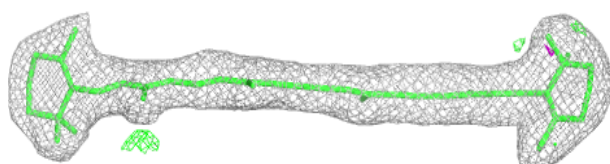
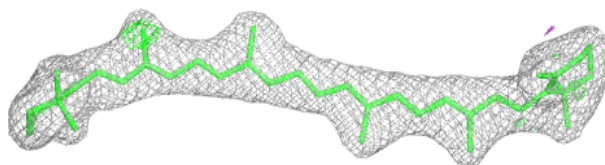
Electron density around PHO A 415:

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

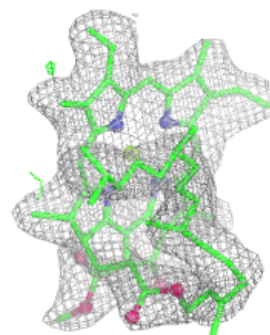
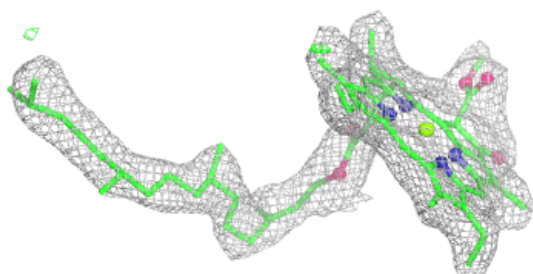
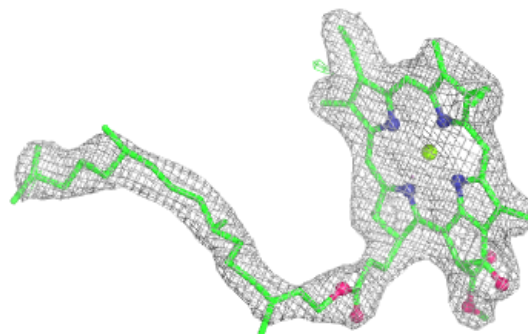


Electron density around BCR A 409:

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

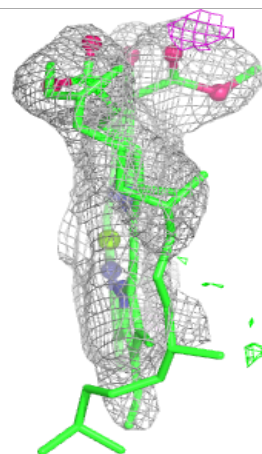
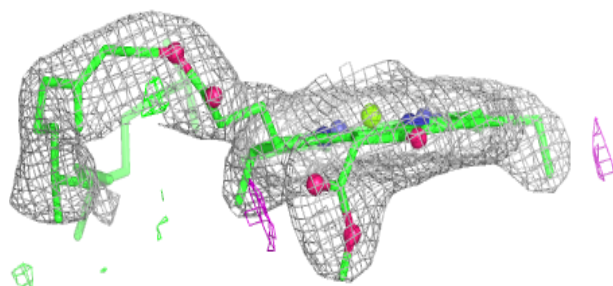
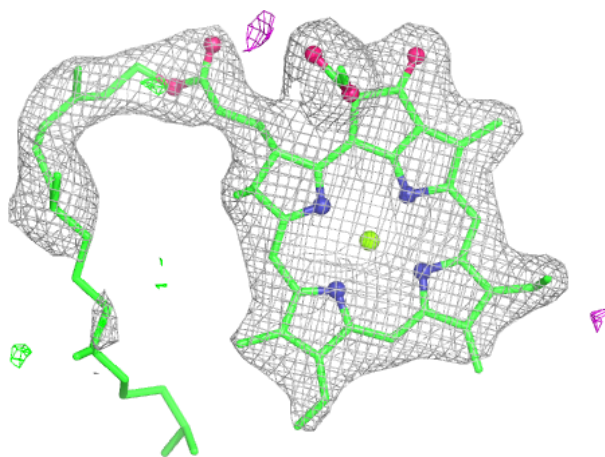
**Electron density around CLA C 513:**

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



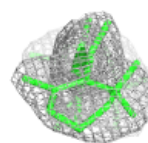
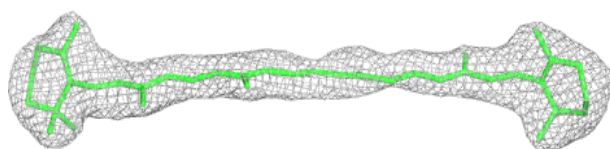
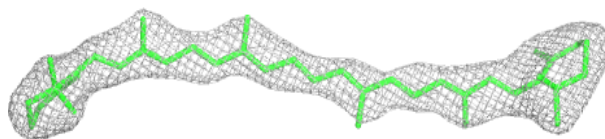
Electron density around CLA C 514:

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



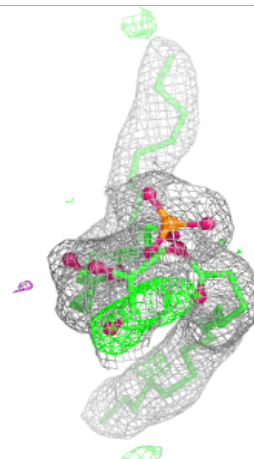
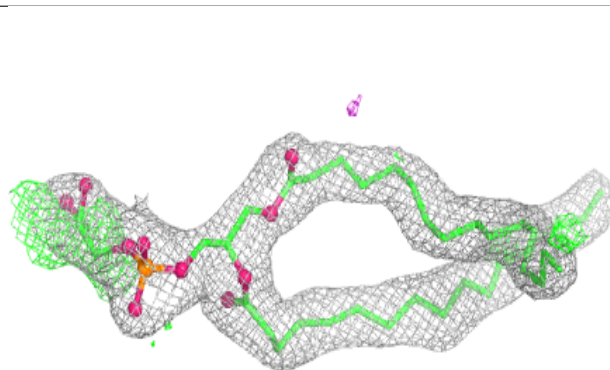
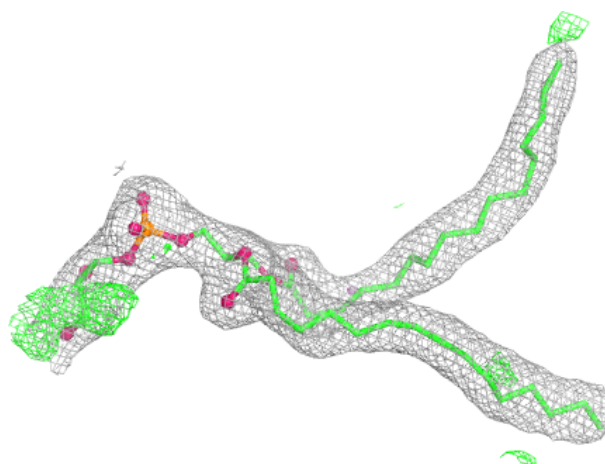
Electron density around BCR C 516:

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



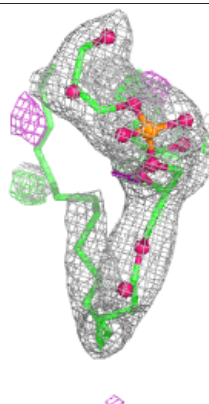
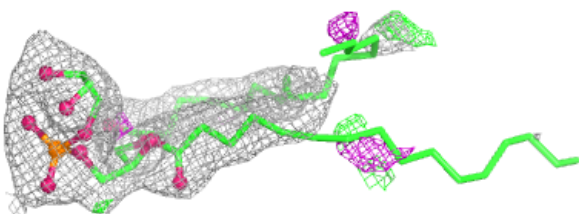
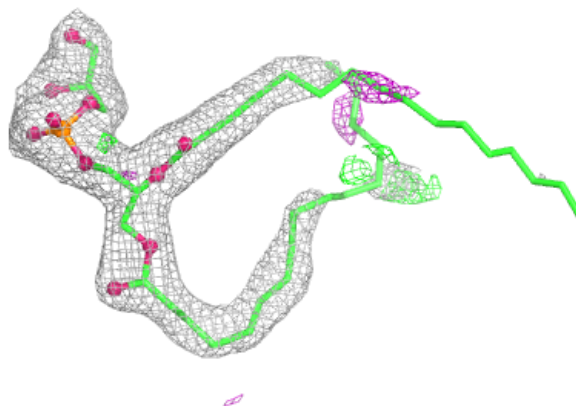
Electron density around LHG D 407:

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

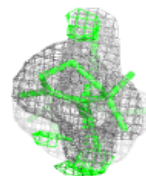
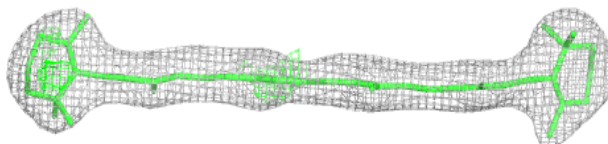
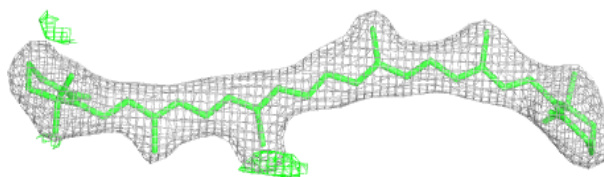


Electron density around LHG D 408:

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

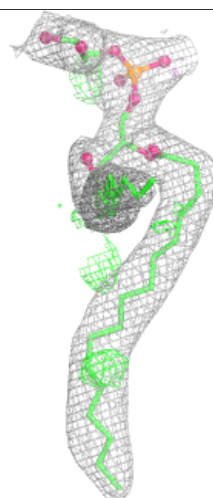
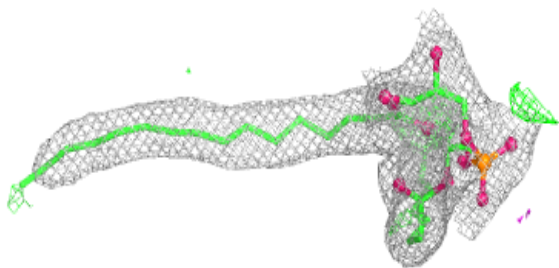
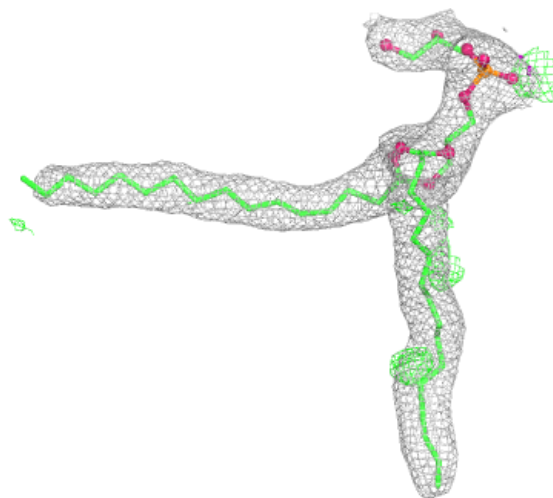
**Electron density around BCR C 517:**

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



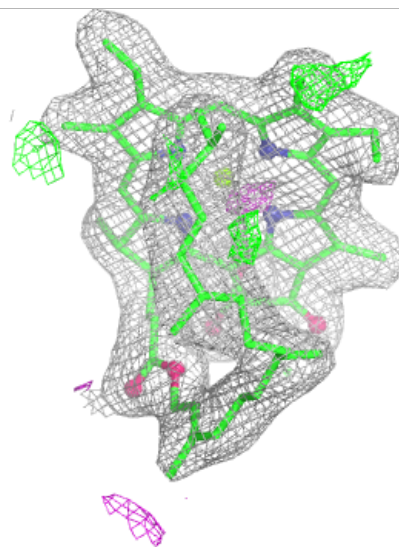
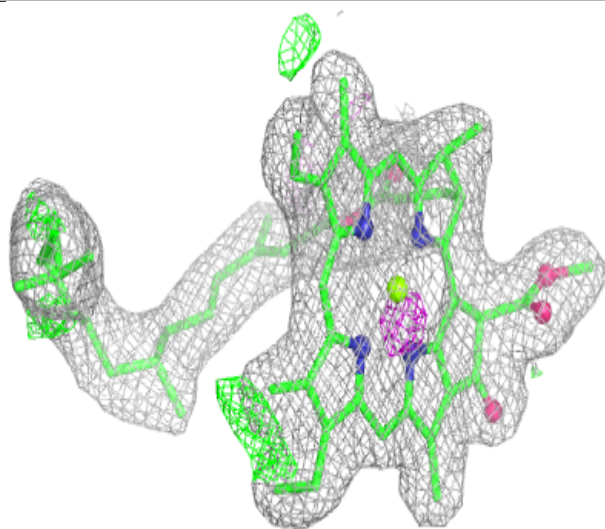
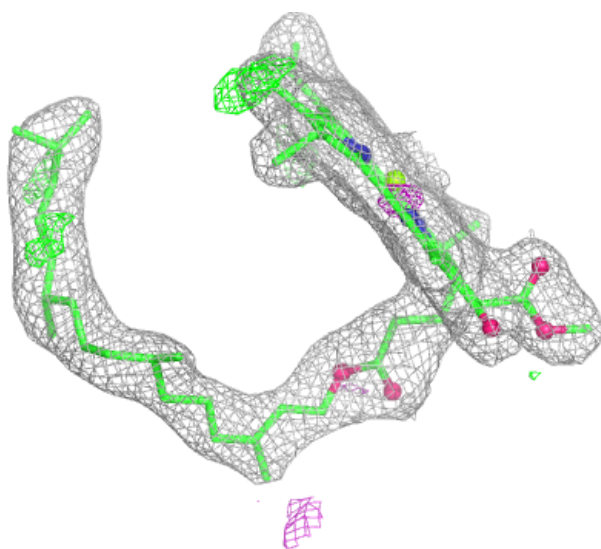
Electron density around LHG L 101:

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



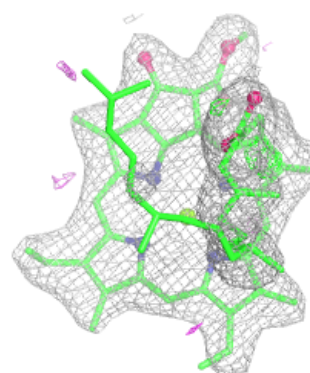
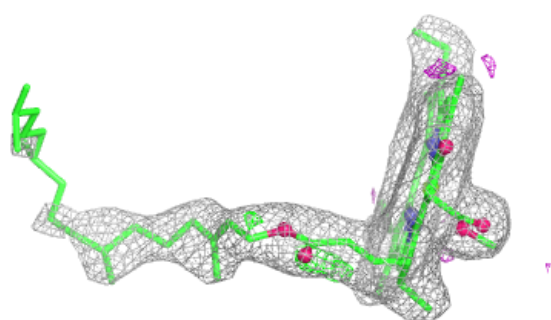
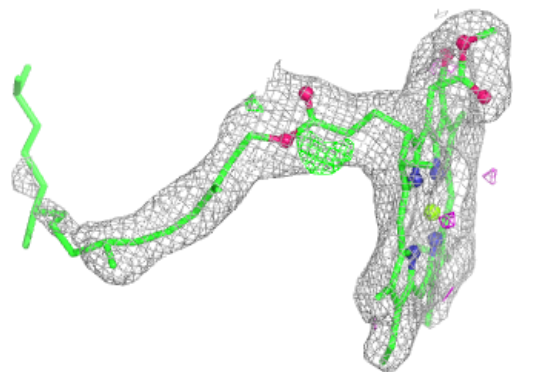
Electron density around CLA B 611:

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

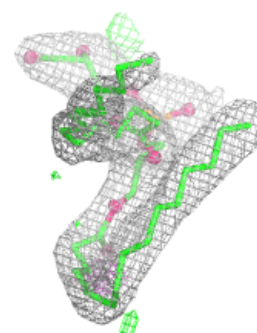
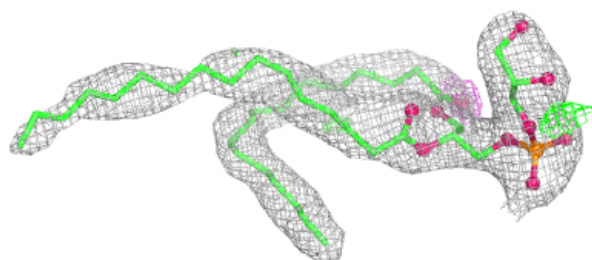
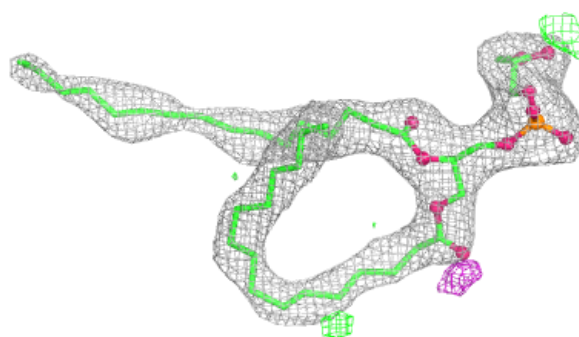


Electron density around CLA D 404:

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

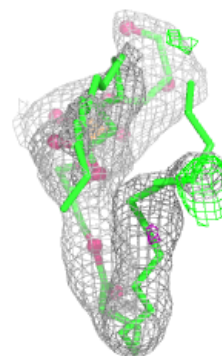
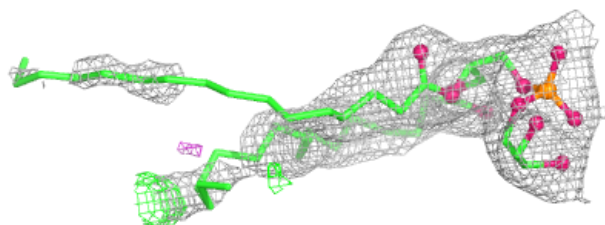
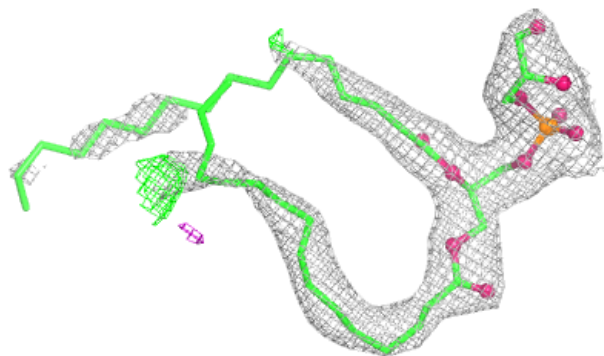
**Electron density around LHG d 406:**

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

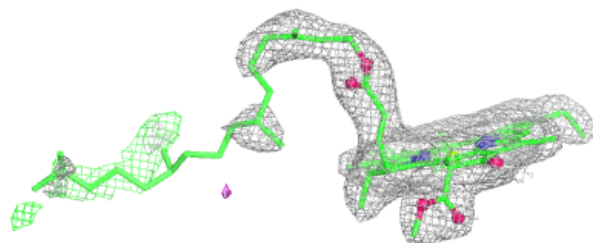
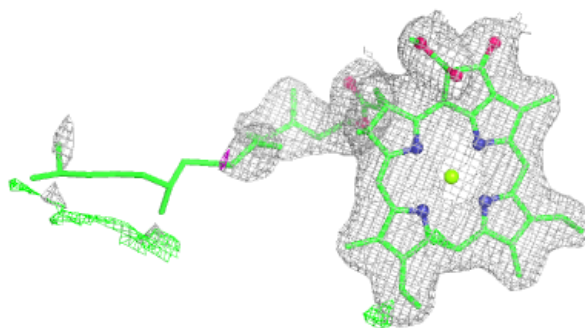


Electron density around LHG d 408:

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

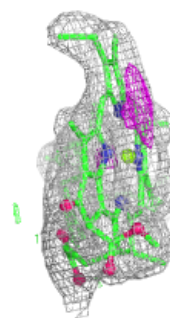
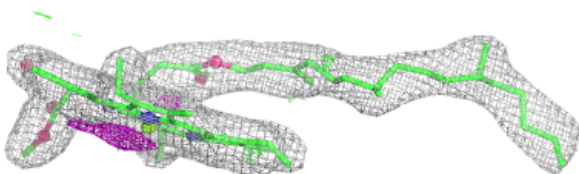
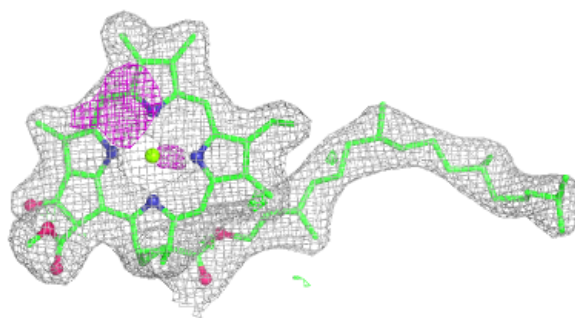
**Electron density around CLA a 406:**

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

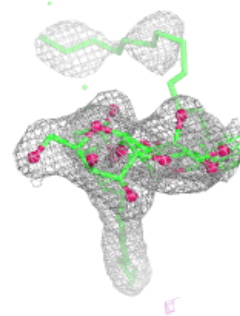
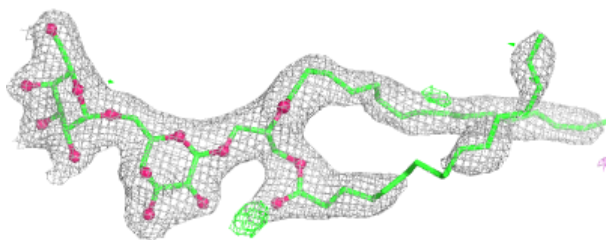
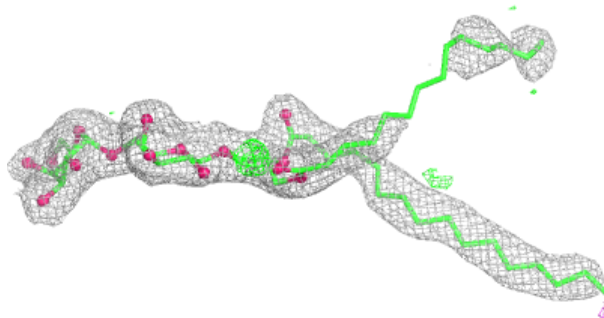


Electron density around CLA B 603:

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

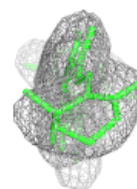
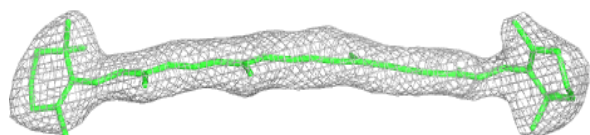
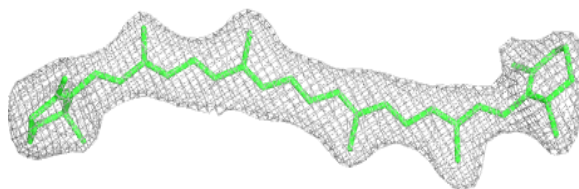
**Electron density around DGD C 518:**

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

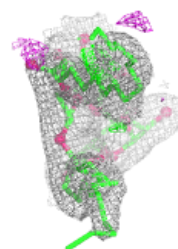
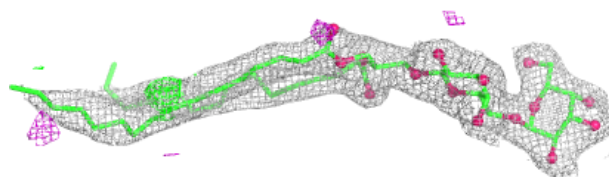
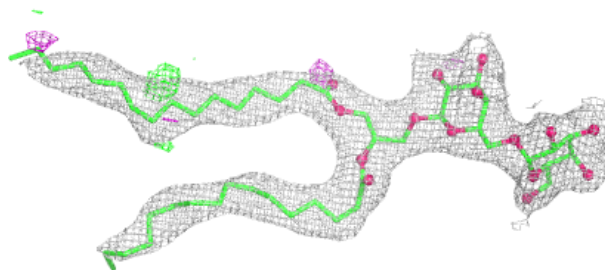


Electron density around BCR Y 101:

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

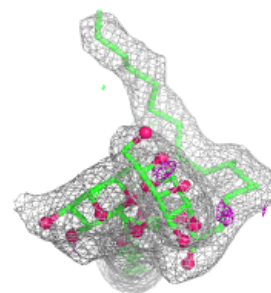
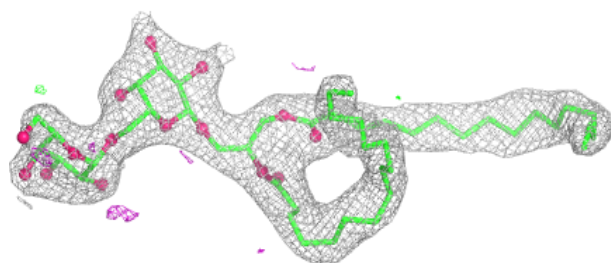
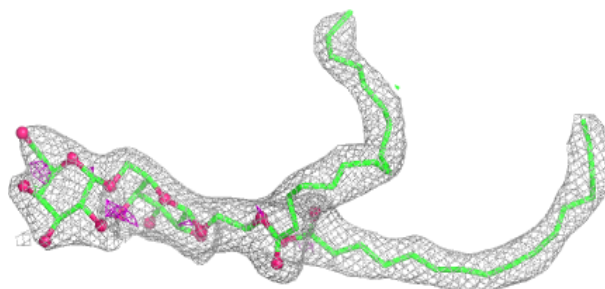
**Electron density around DGD C 520:**

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

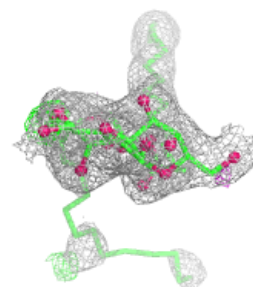
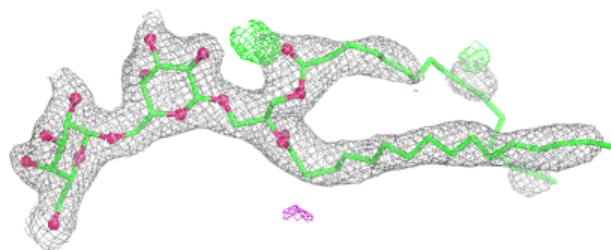
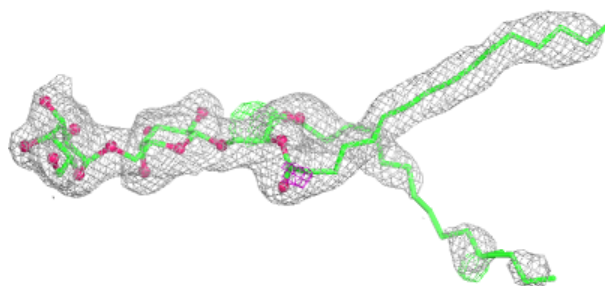


Electron density around DGD H 102:

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

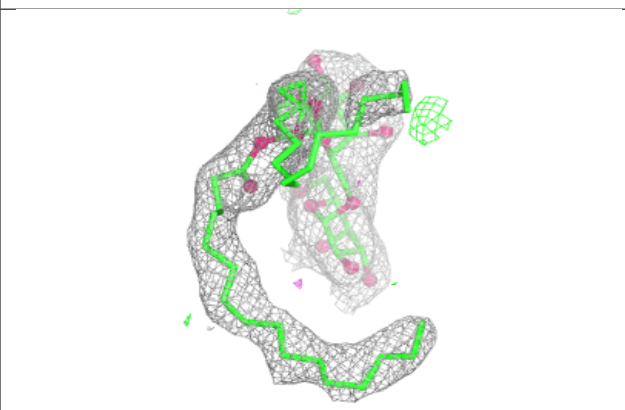
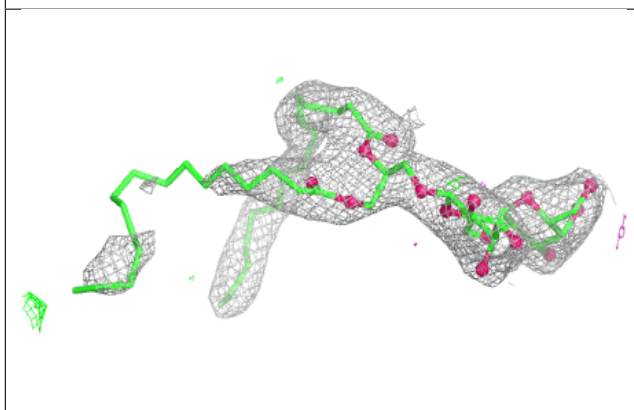
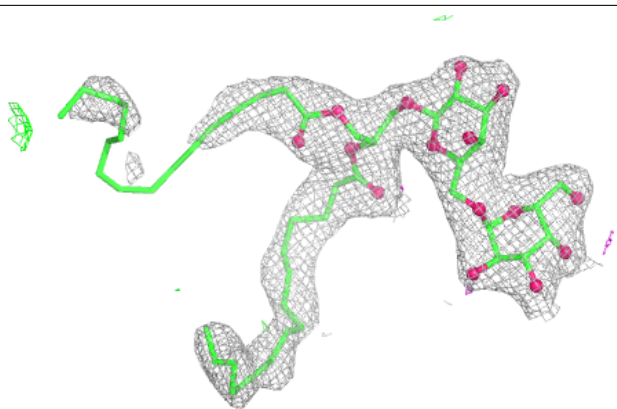
**Electron density around DGD c 518:**

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

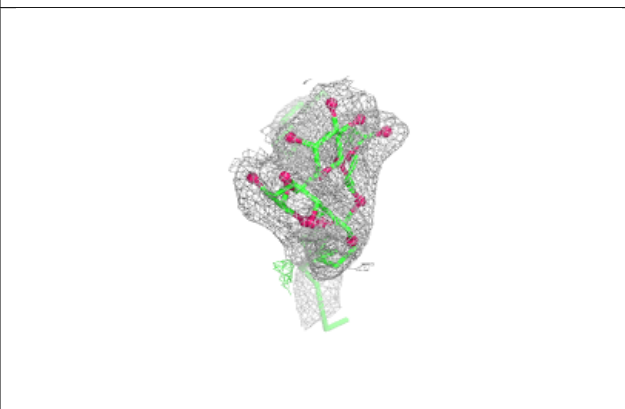
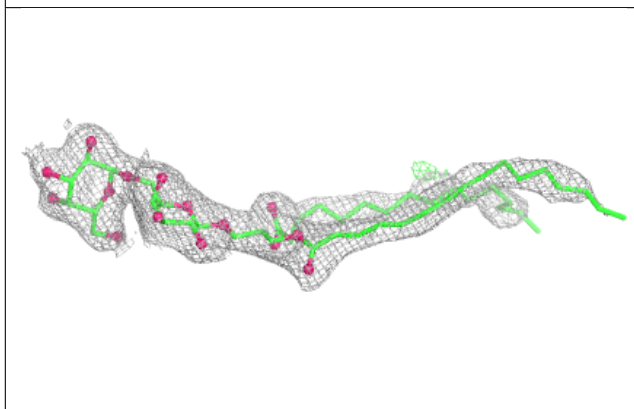
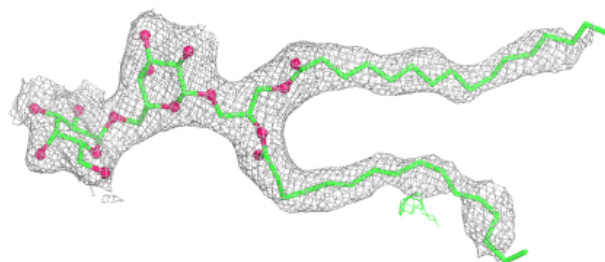


Electron density around DGD c 519:

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

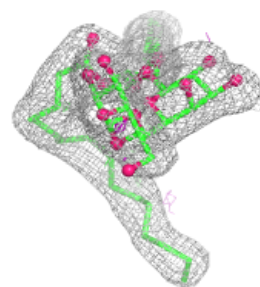
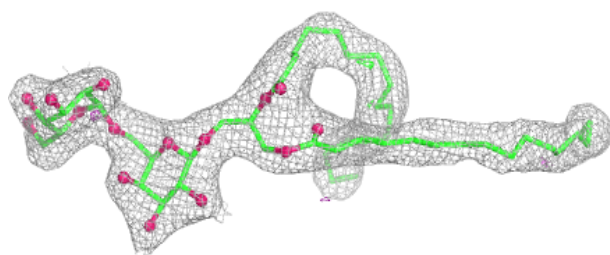
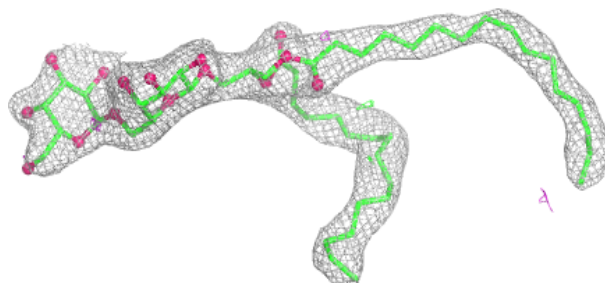
**Electron density around DGD c 520:**

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

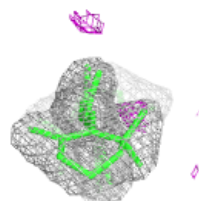
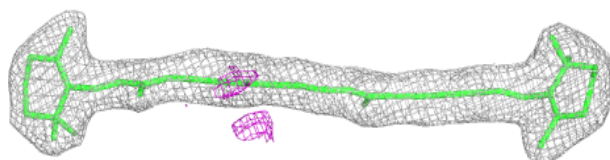
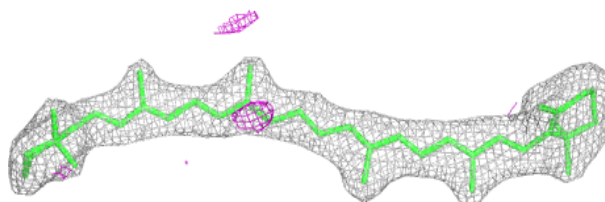


Electron density around DGD h 103:

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

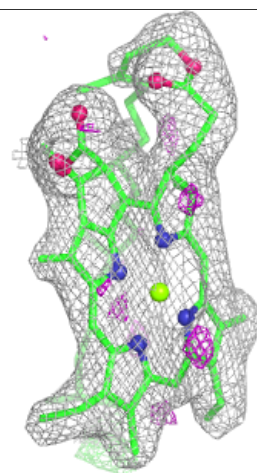
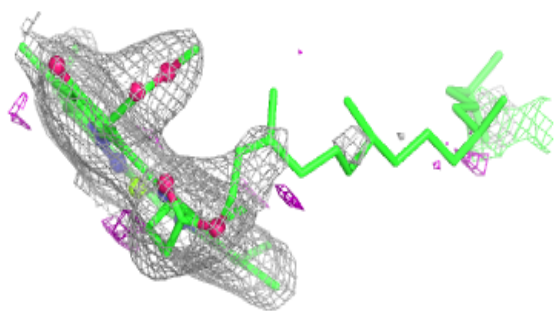
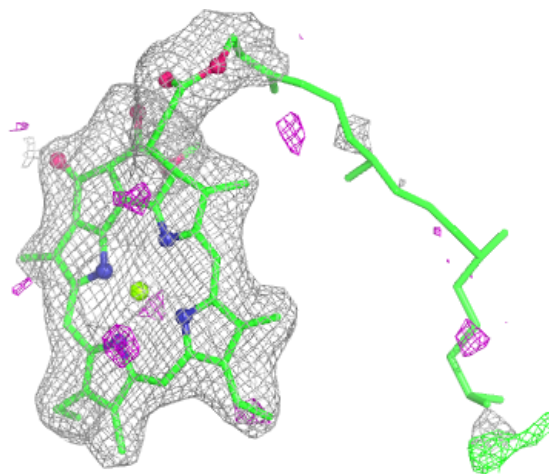
**Electron density around BCR a 409:**

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



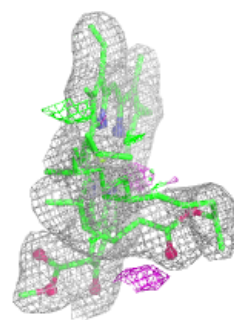
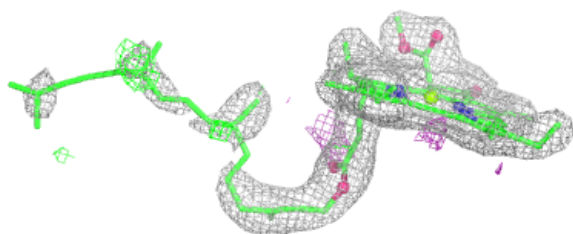
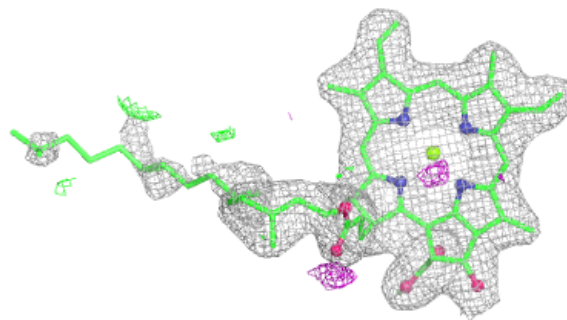
Electron density around CLA B 616:

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



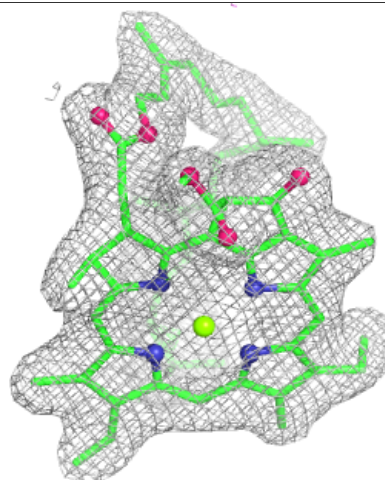
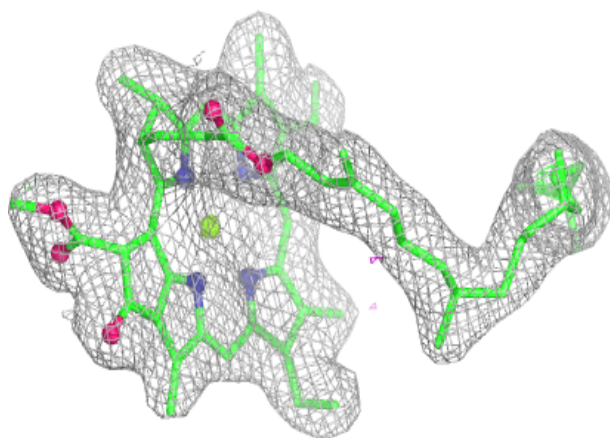
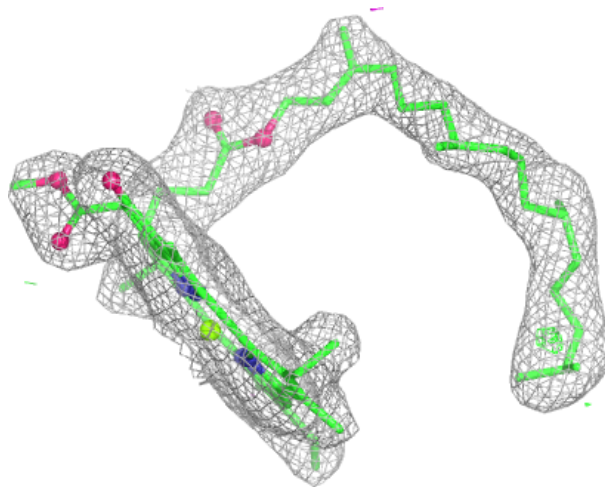
Electron density around CLA A 406:

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



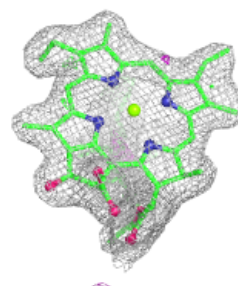
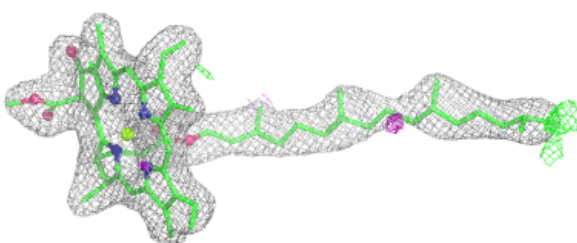
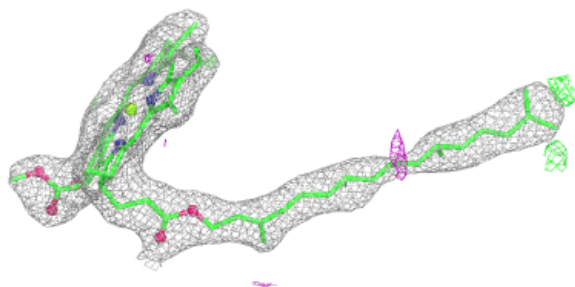
Electron density around CLA b 611:

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

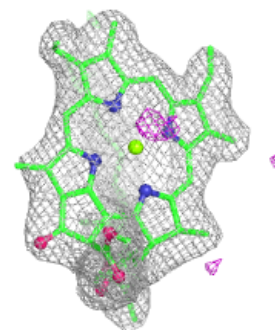
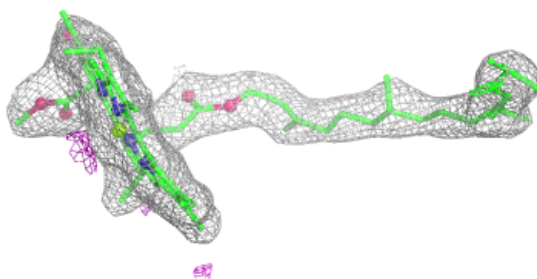
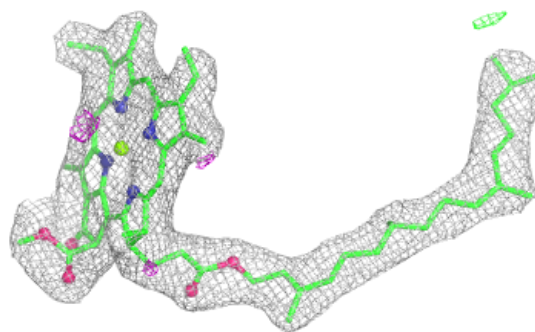


Electron density around CLA B 607:

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

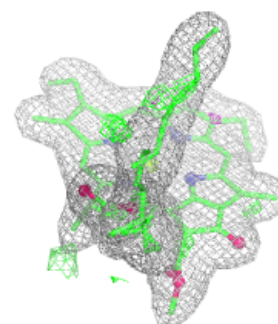
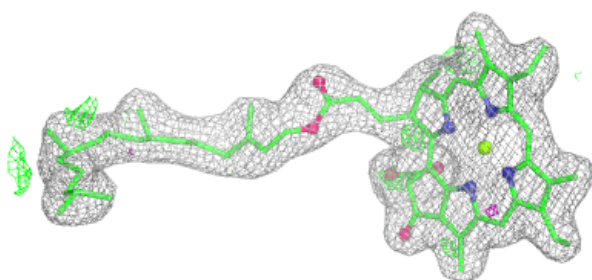
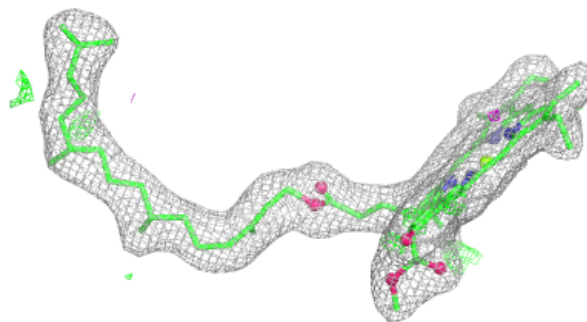
**Electron density around CLA B 609:**

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

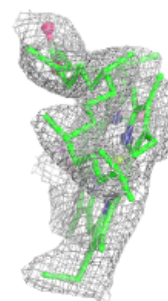
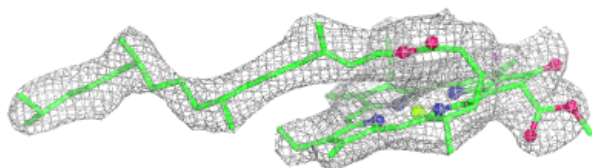
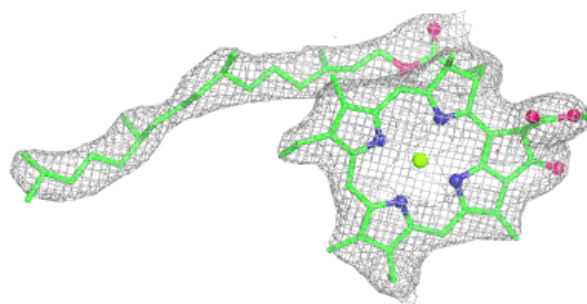


Electron density around CLA D 403:

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

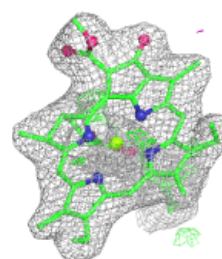
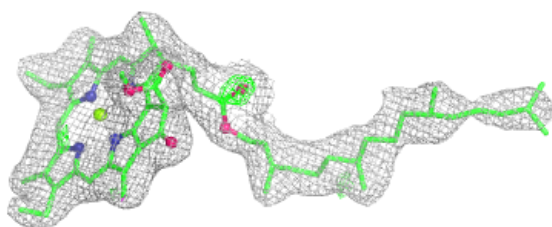
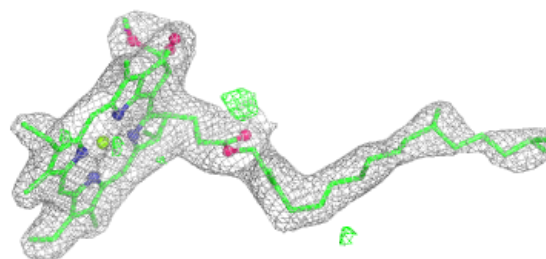
**Electron density around CLA c 503:**

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

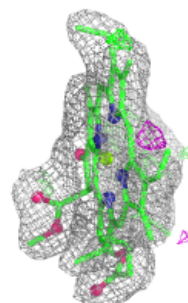
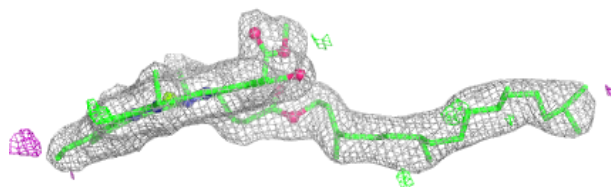
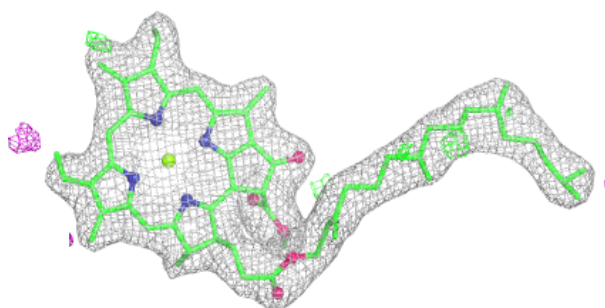


Electron density around CLA c 504:

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

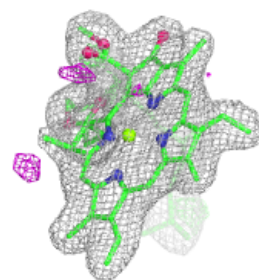
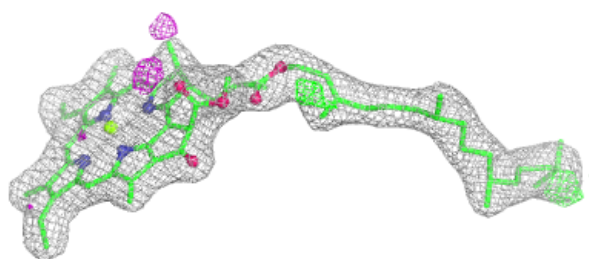
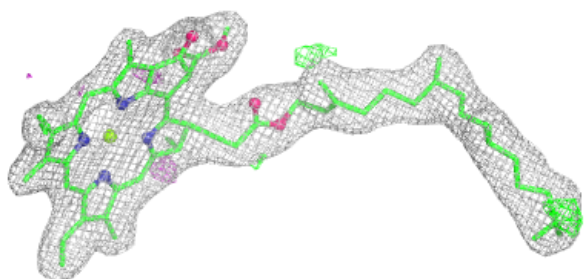
**Electron density around CLA B 602:**

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



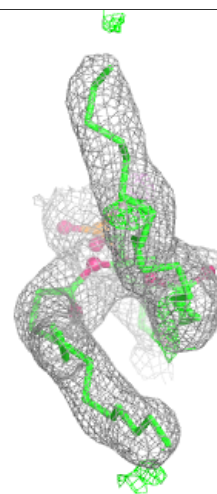
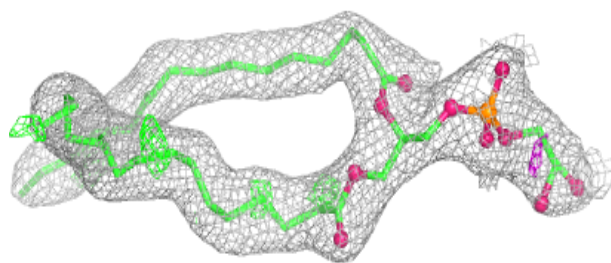
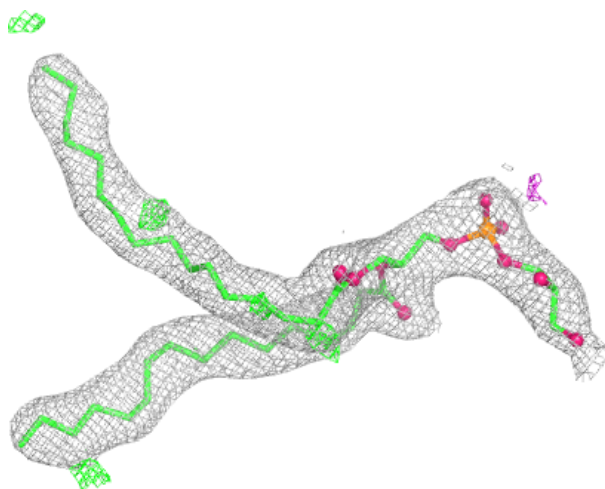
Electron density around CLA a 404:

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



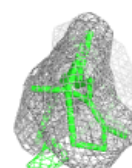
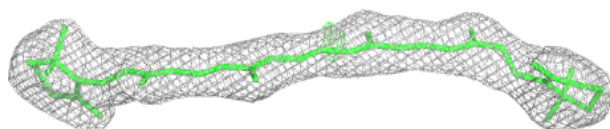
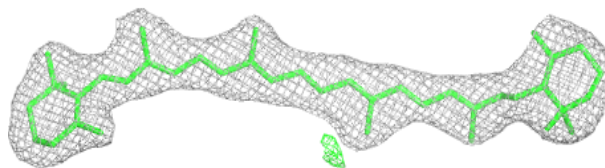
Electron density around LHG d 407:

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

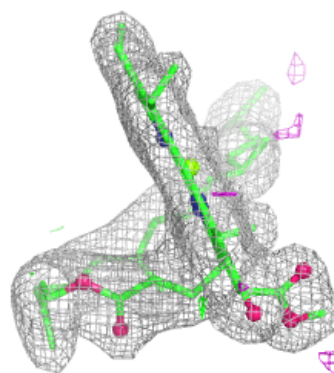
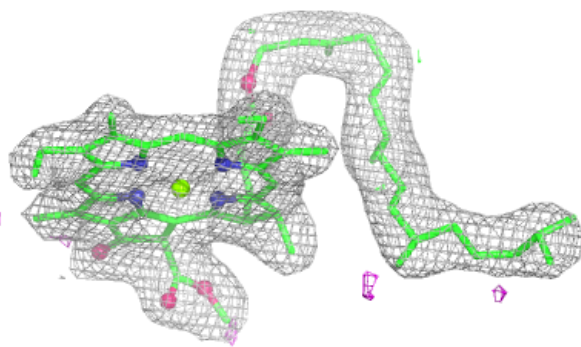
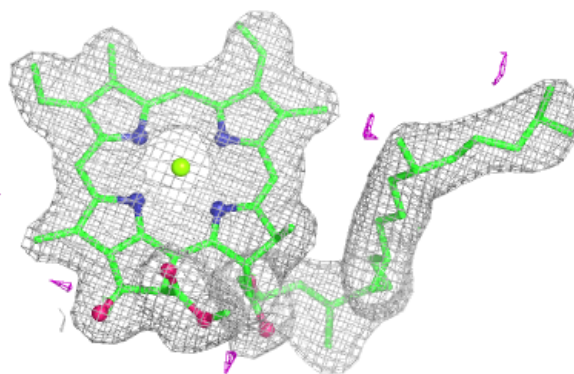


Electron density around BCR b 619:

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

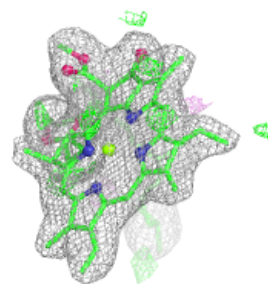
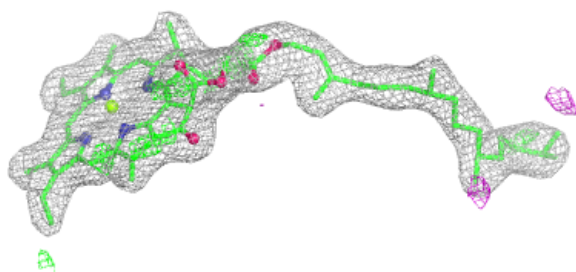
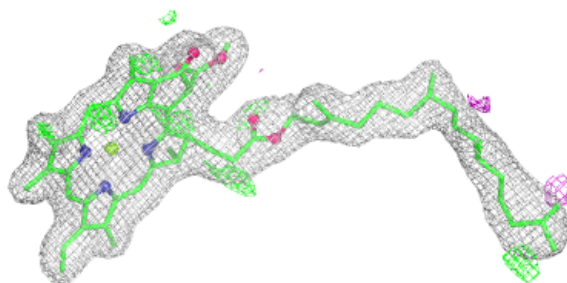
**Electron density around CLA a 405:**

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



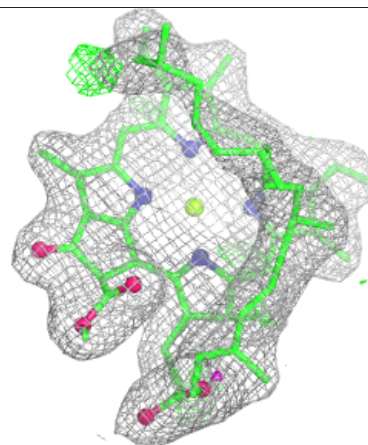
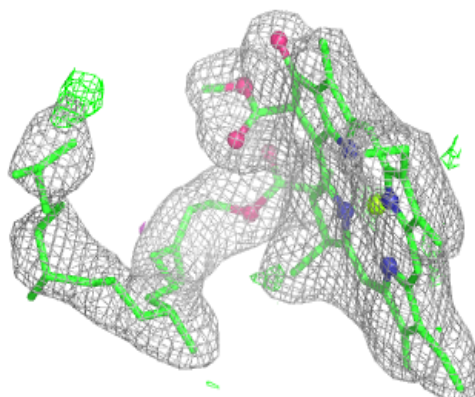
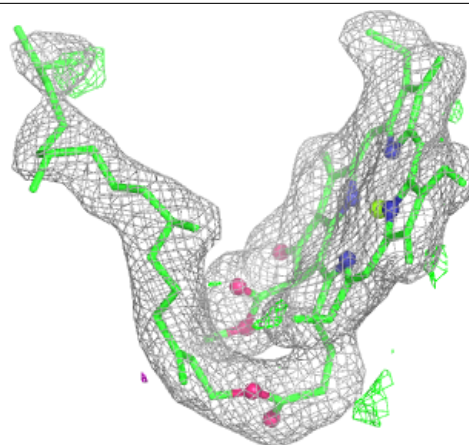
Electron density around CLA A 404:

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



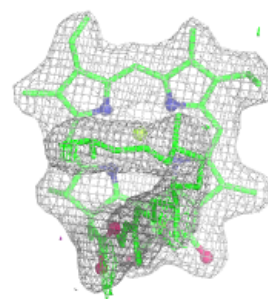
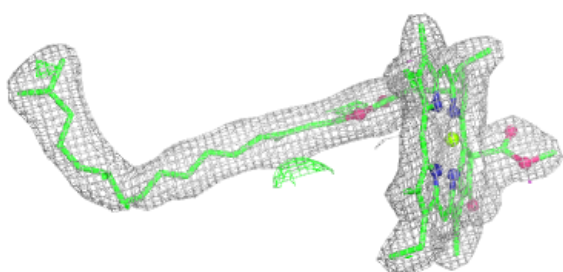
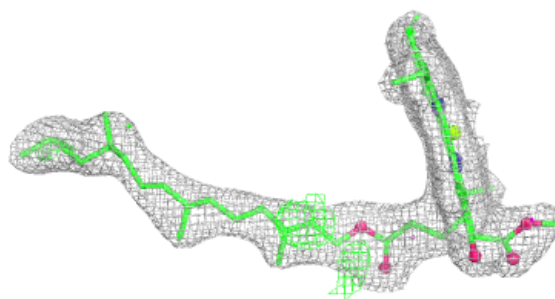
Electron density around CLA B 613:

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

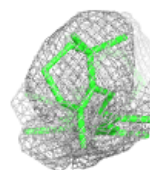
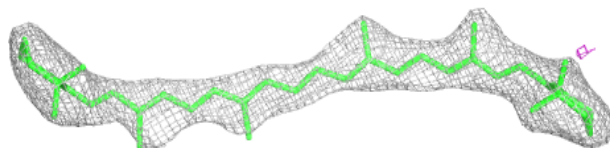
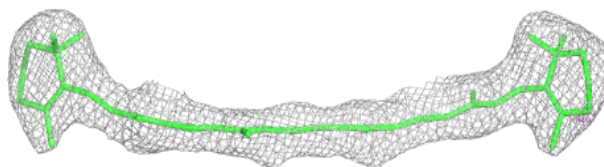


Electron density around CLA B 605:

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

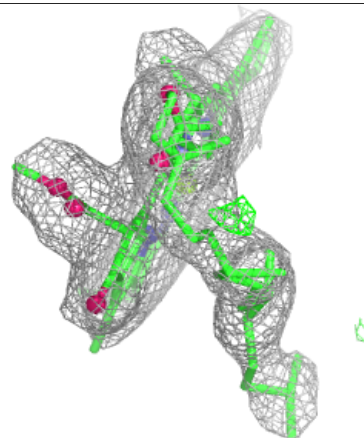
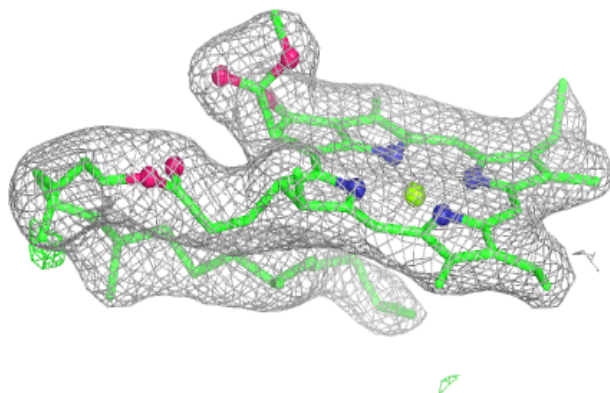
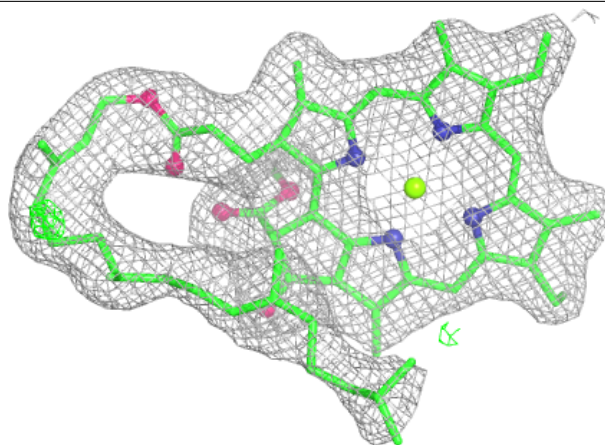
**Electron density around BCR k 101:**

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



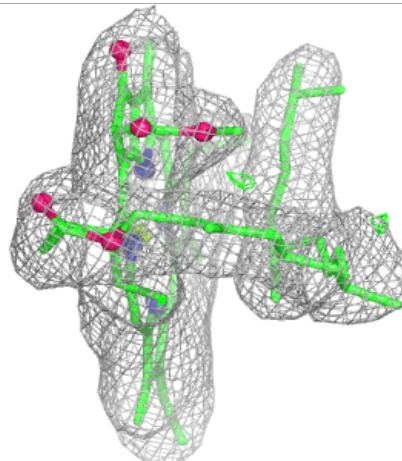
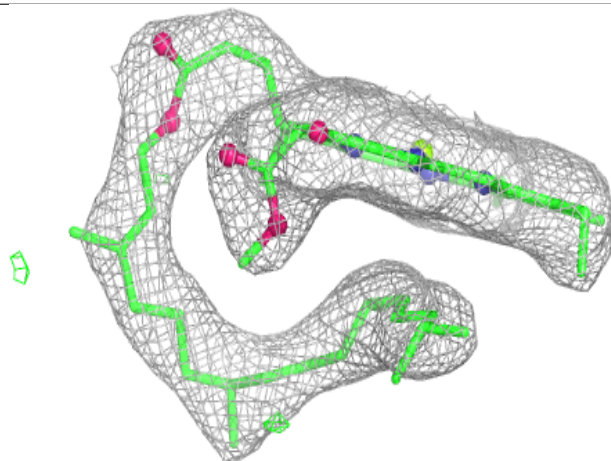
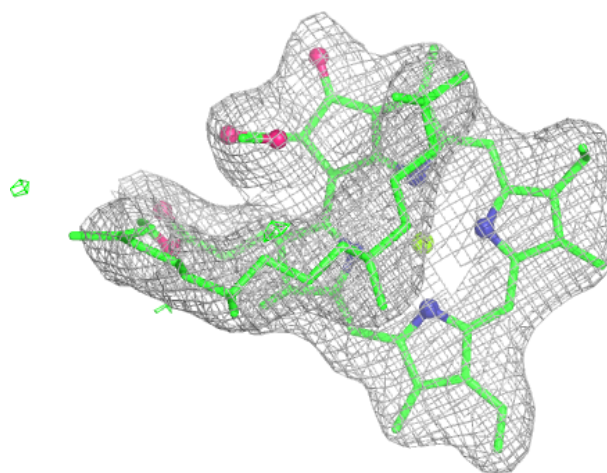
Electron density around CLA c 511:

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



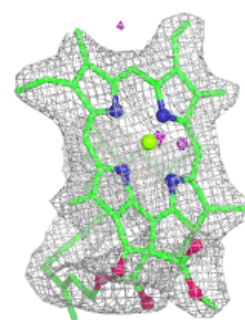
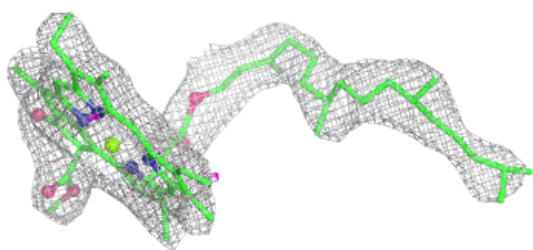
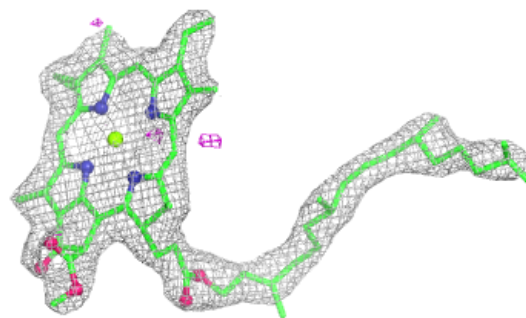
Electron density around CLA c 512:

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

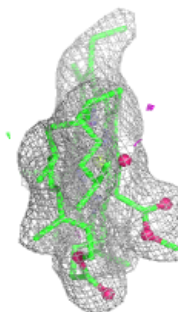
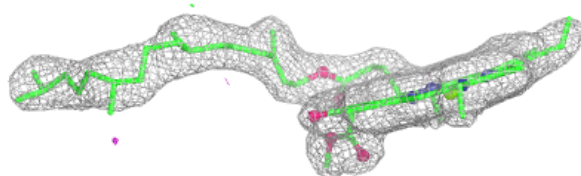
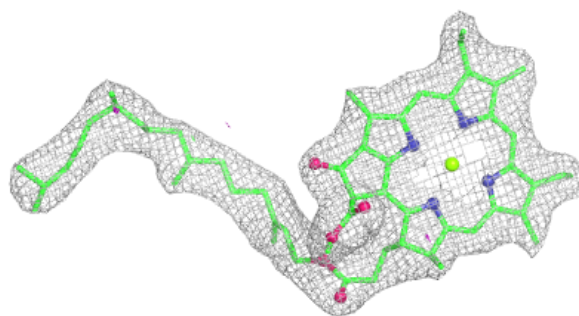


Electron density around CLA c 513:

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

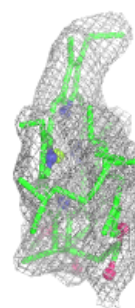
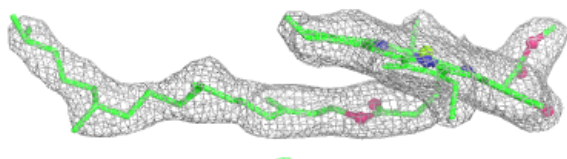
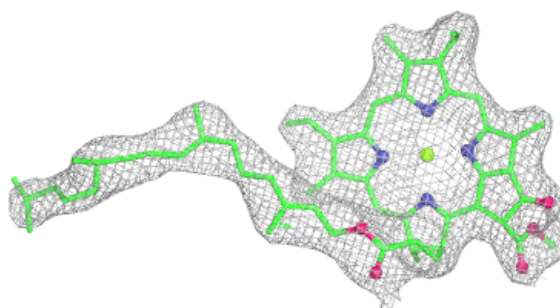
**Electron density around CLA b 602:**

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

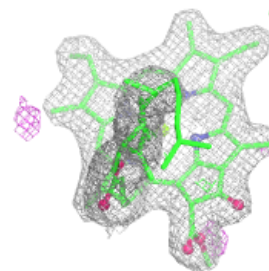
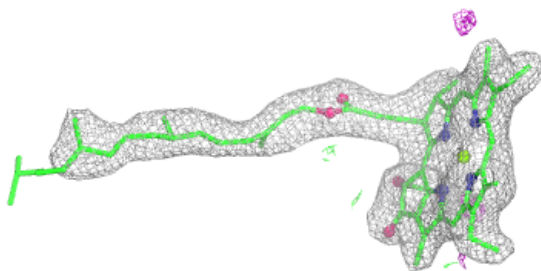
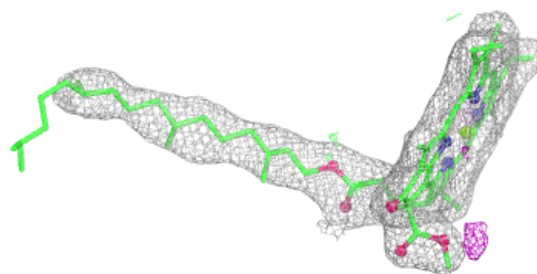


Electron density around CLA b 603:

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

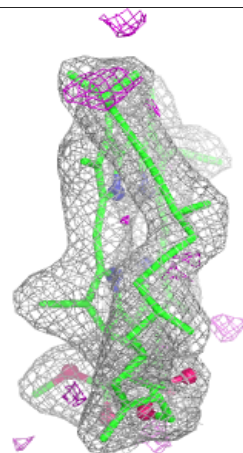
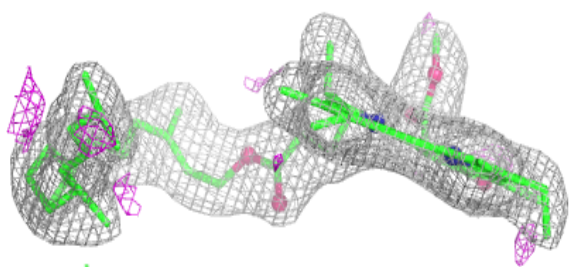
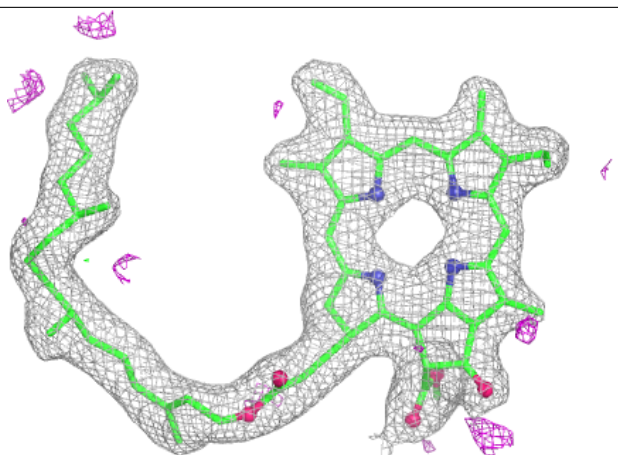
**Electron density around CLA b 604:**

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



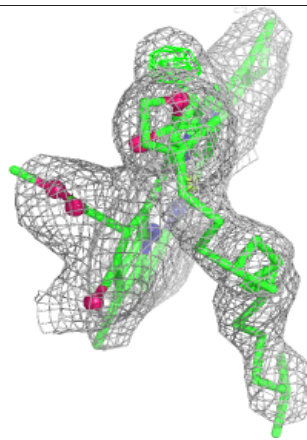
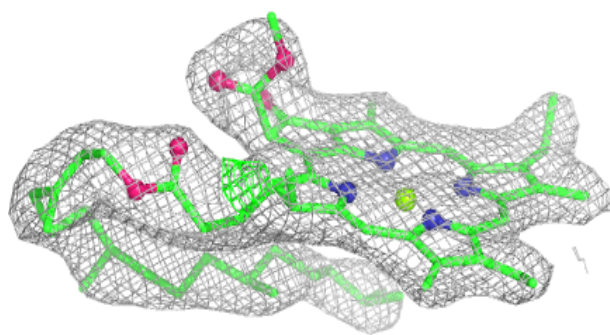
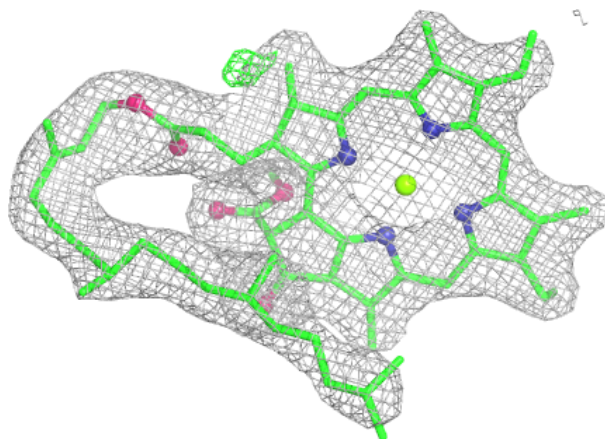
Electron density around PHO A 407:

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



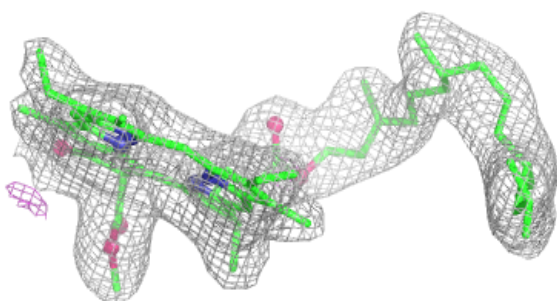
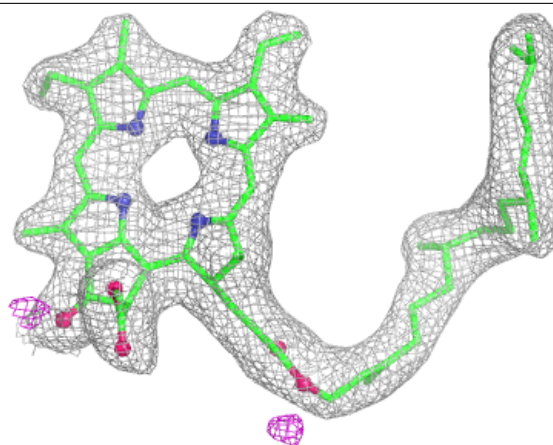
Electron density around CLA C 511:

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



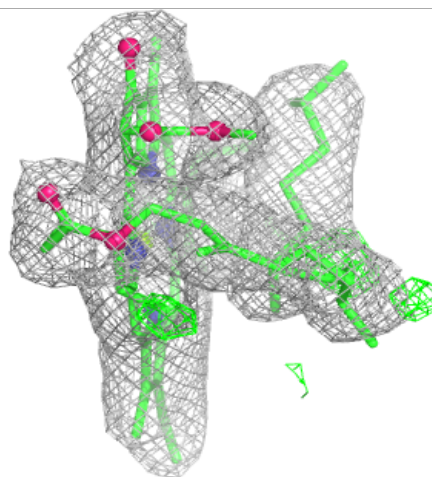
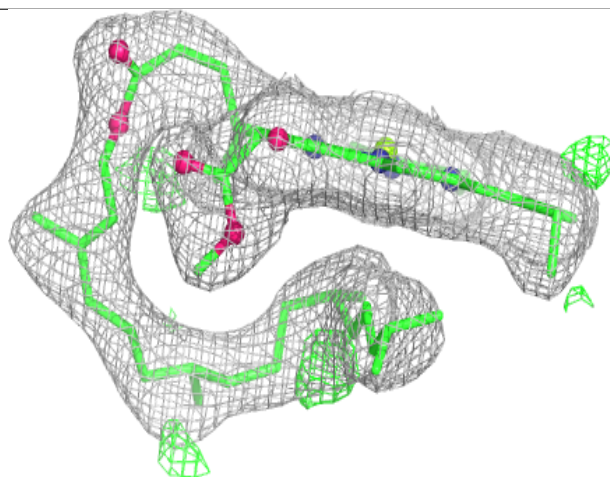
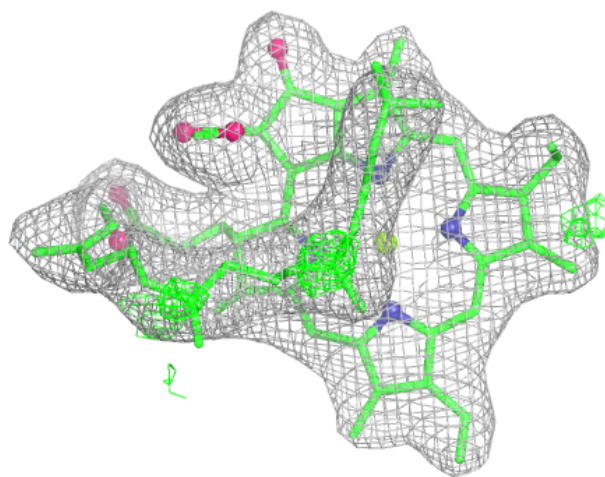
Electron density around PHO a 417:

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



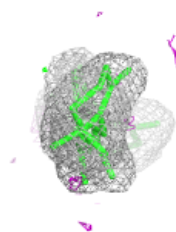
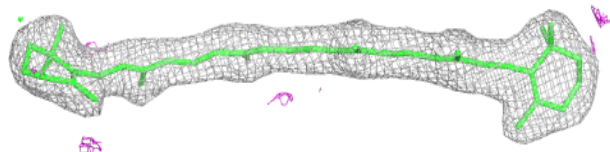
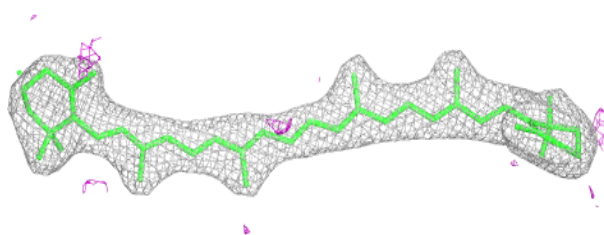
Electron density around CLA C 512:

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

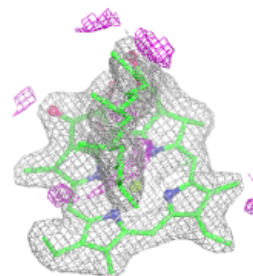
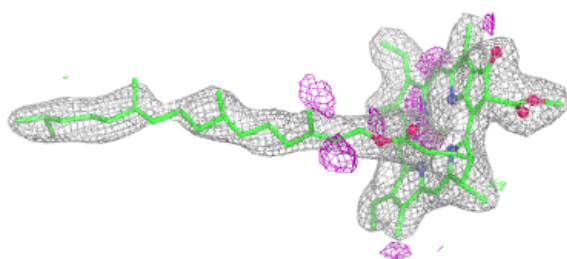
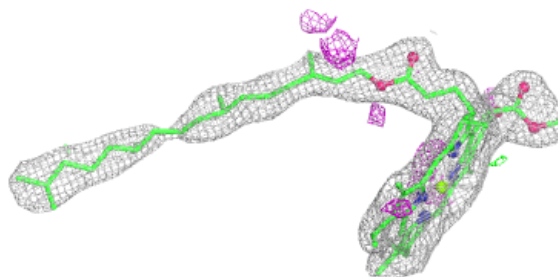


Electron density around BCR B 617:

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

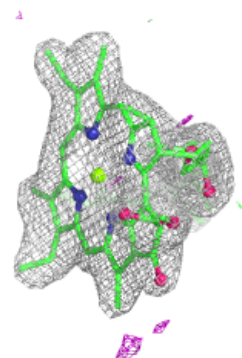
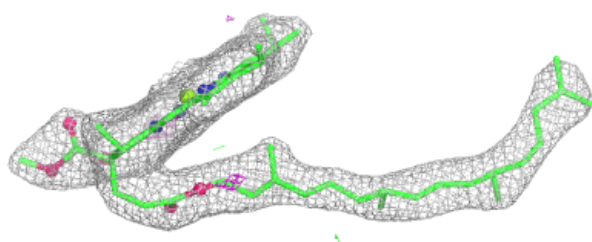
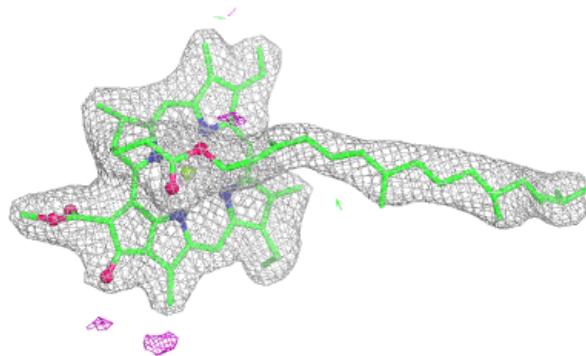
**Electron density around CLA b 607:**

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

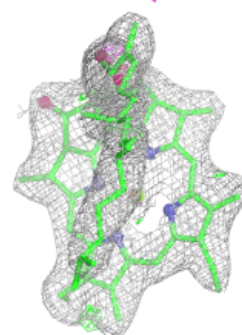
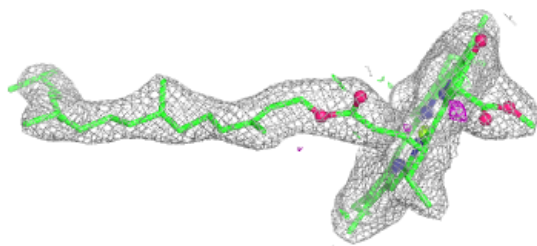
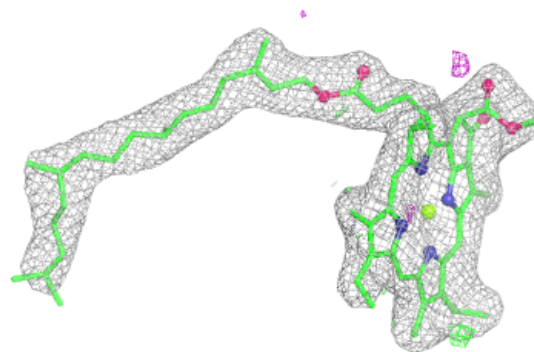


Electron density around CLA b 608:

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

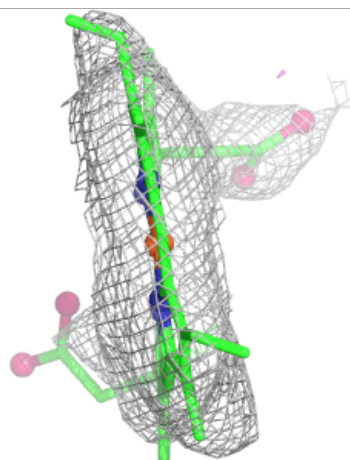
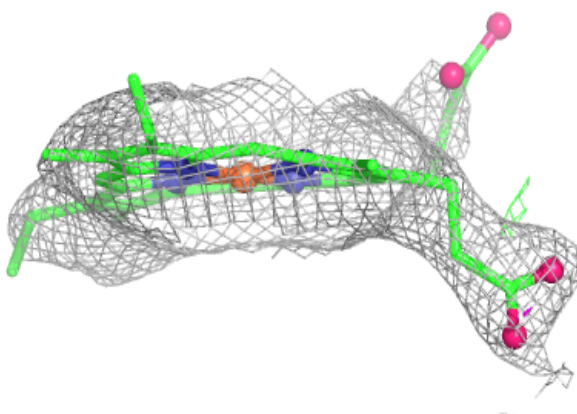
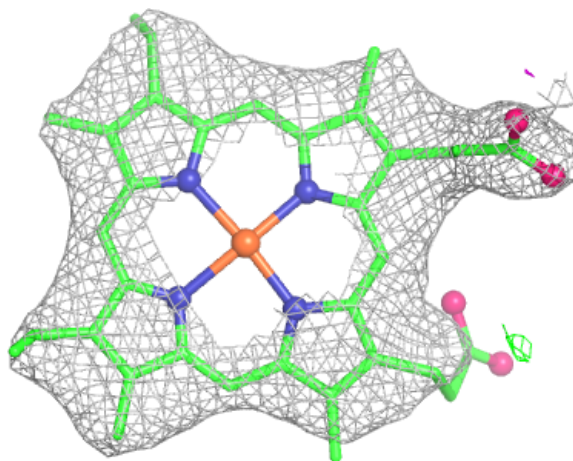
**Electron density around CLA b 609:**

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



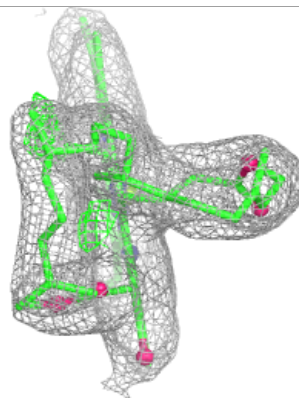
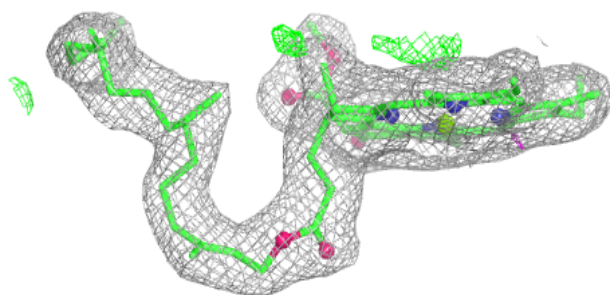
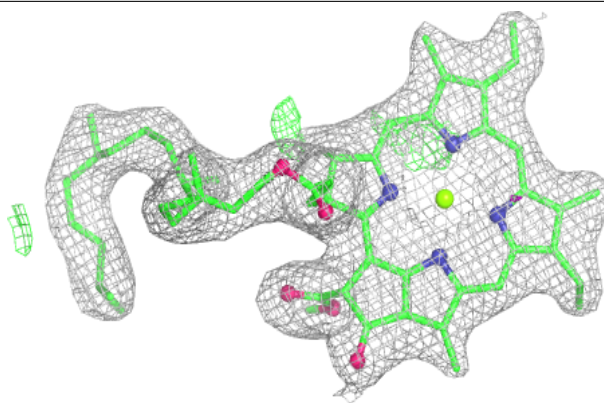
Electron density around HEC e 102:

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

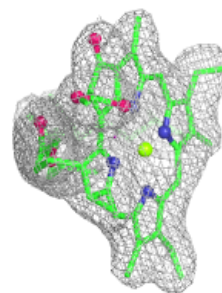
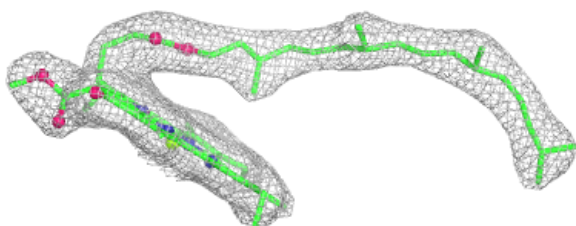
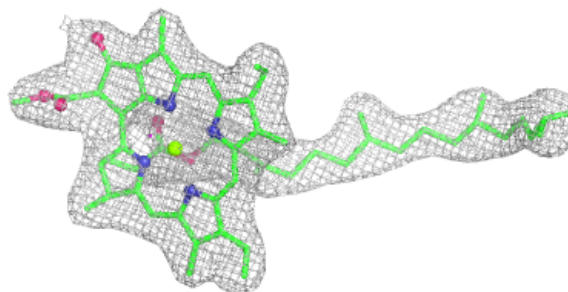


Electron density around CLA B 612:

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

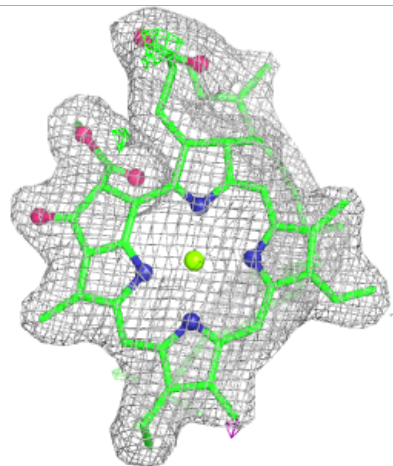
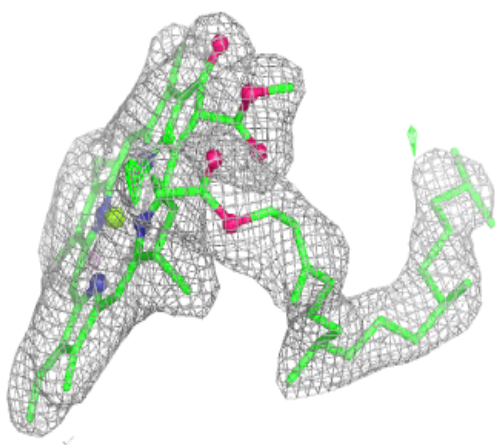
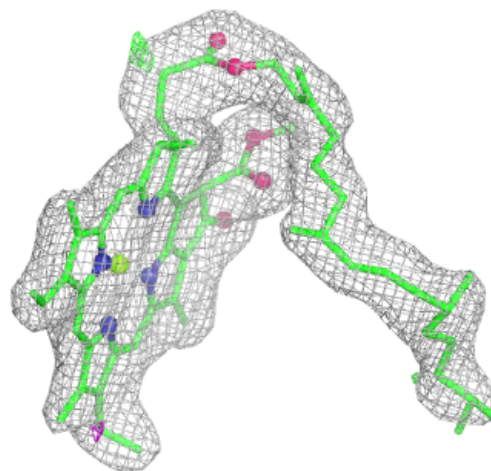
**Electron density around CLA B 608:**

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



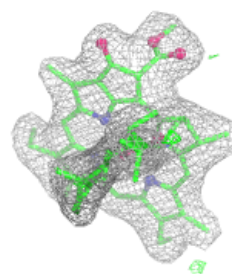
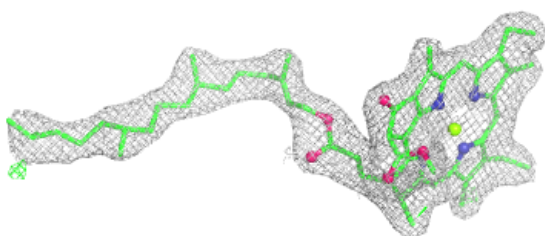
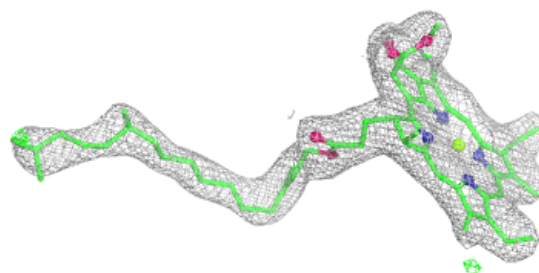
Electron density around CLA b 613:

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



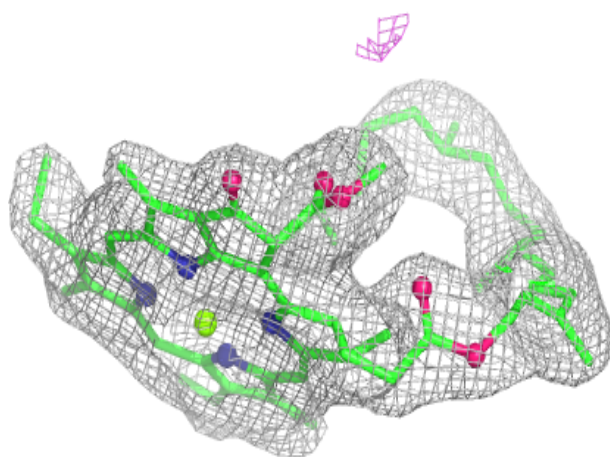
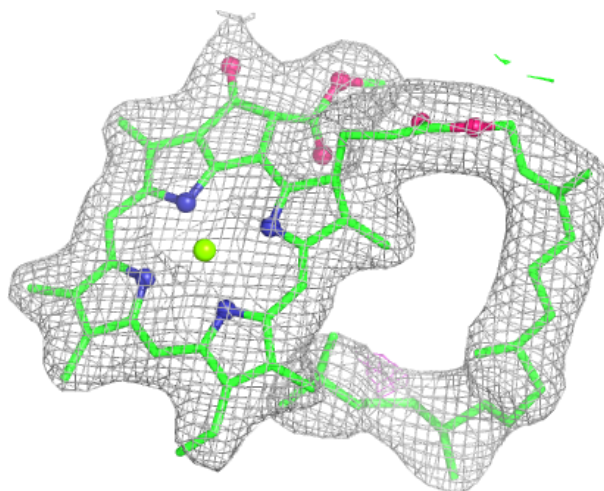
Electron density around CLA C 504:

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



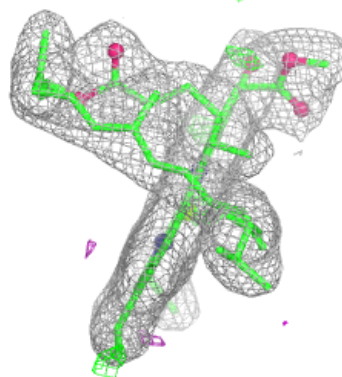
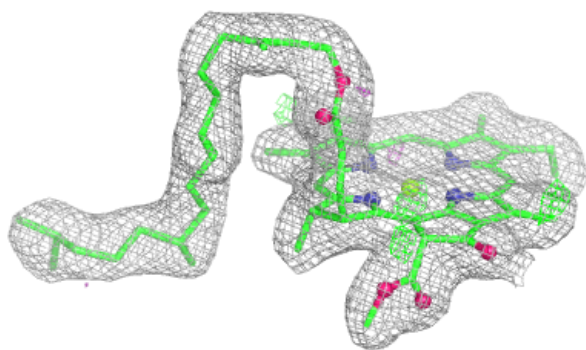
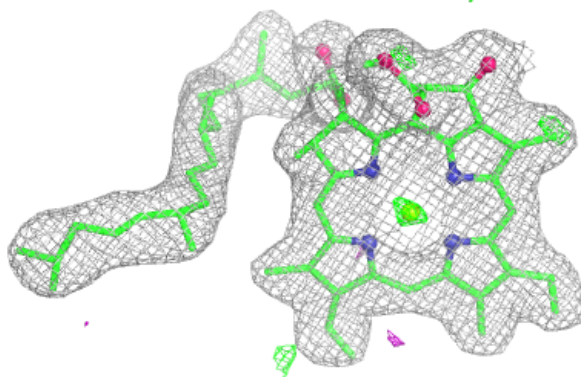
Electron density around CLA b 615:

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



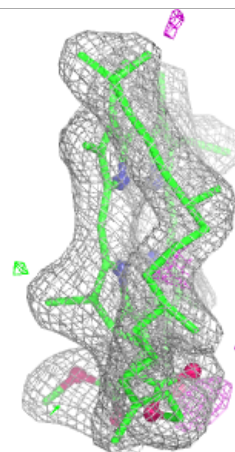
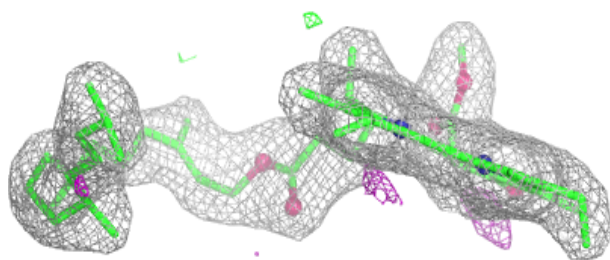
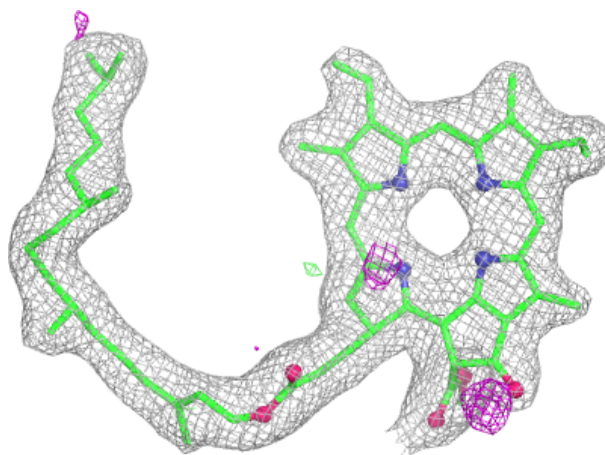
Electron density around CLA A 405:

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



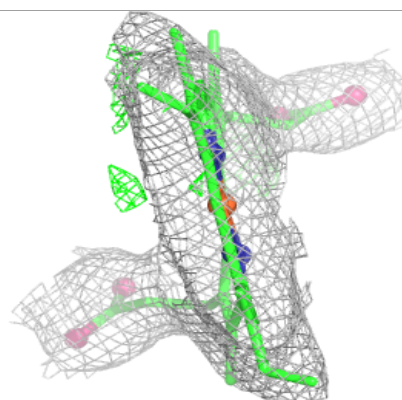
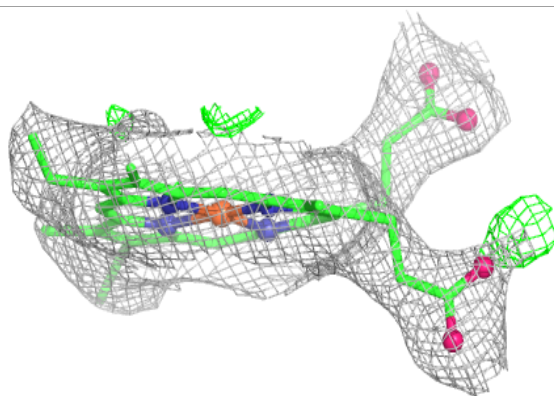
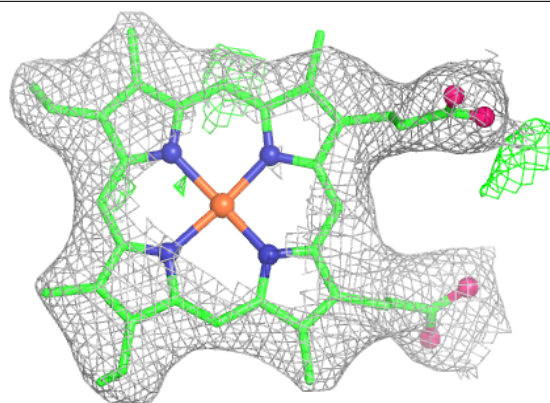
Electron density around PHO a 407:

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



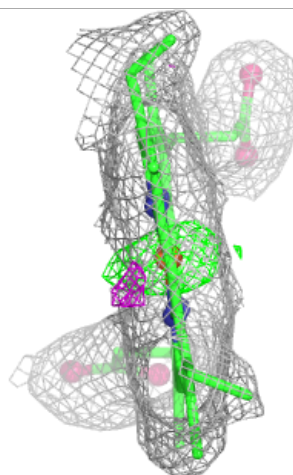
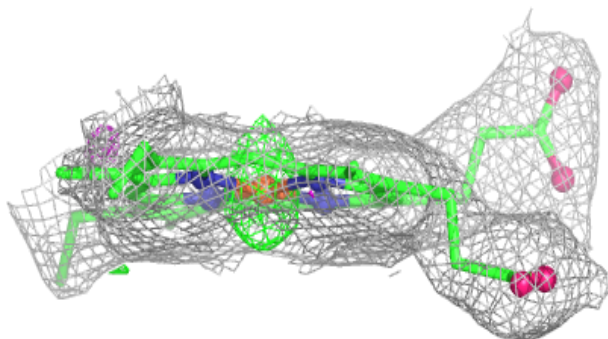
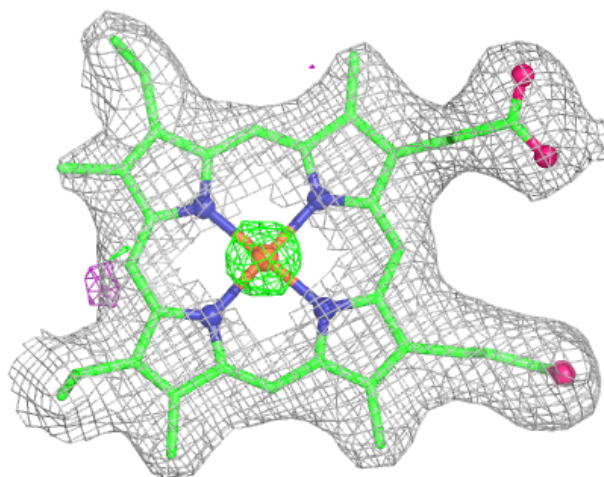
Electron density around HEC E 103:

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



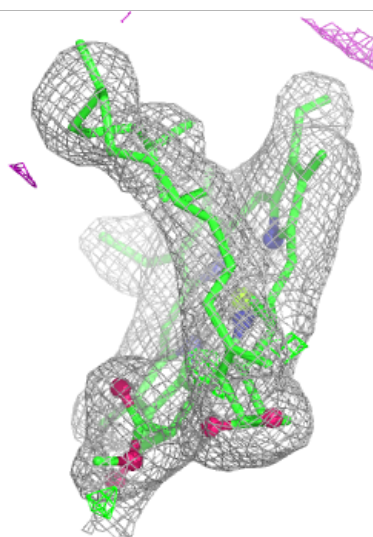
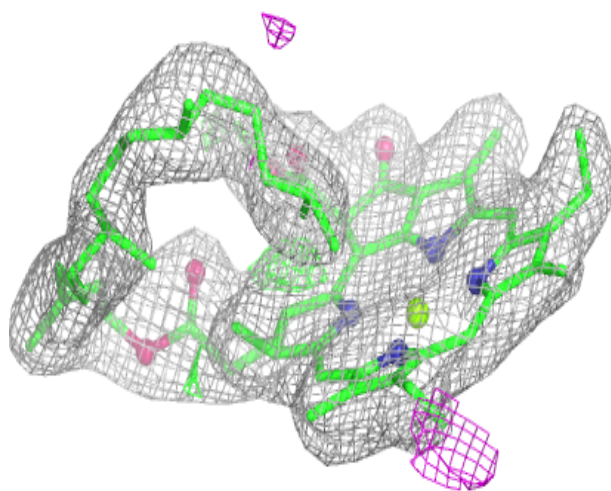
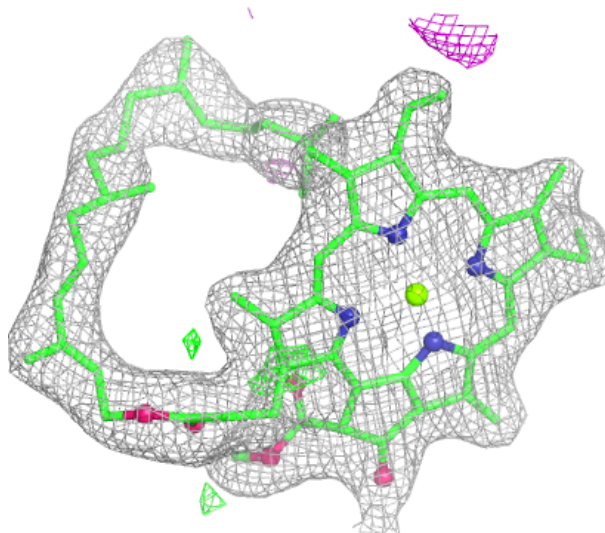
Electron density around HEC V 201:

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



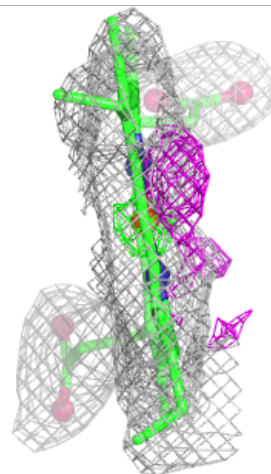
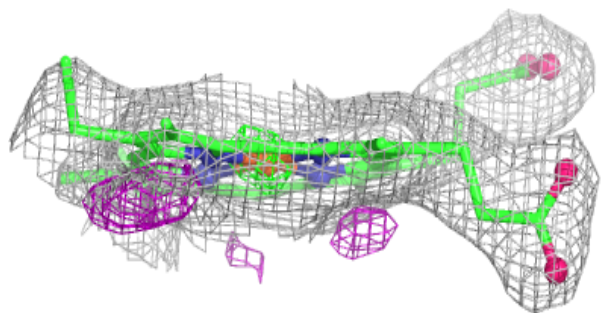
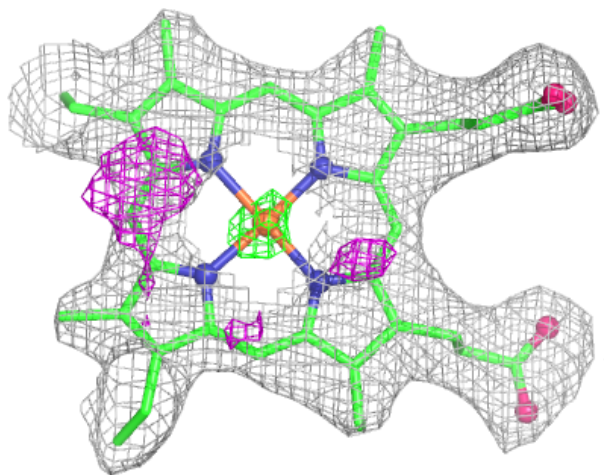
Electron density around CLA B 615:

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



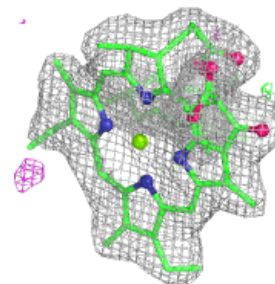
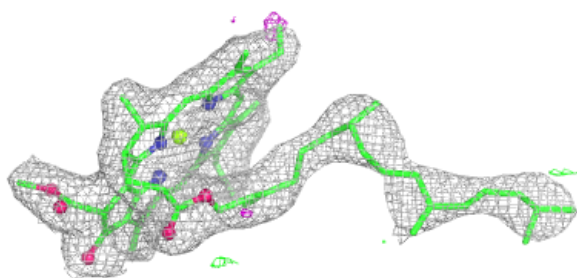
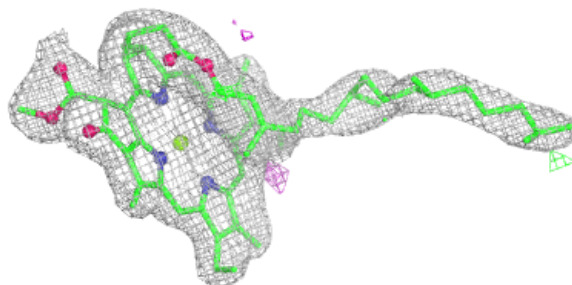
Electron density around HEC v 202:

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

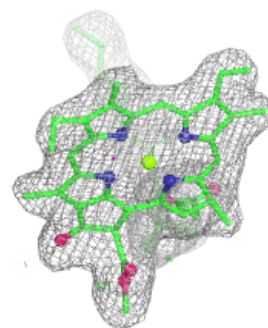
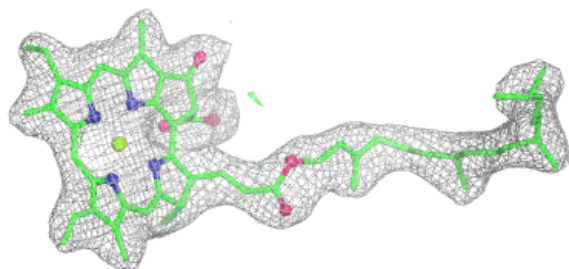
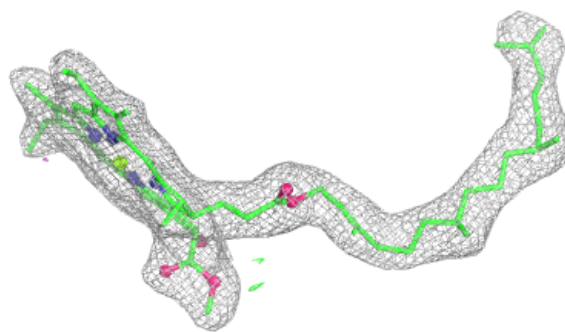


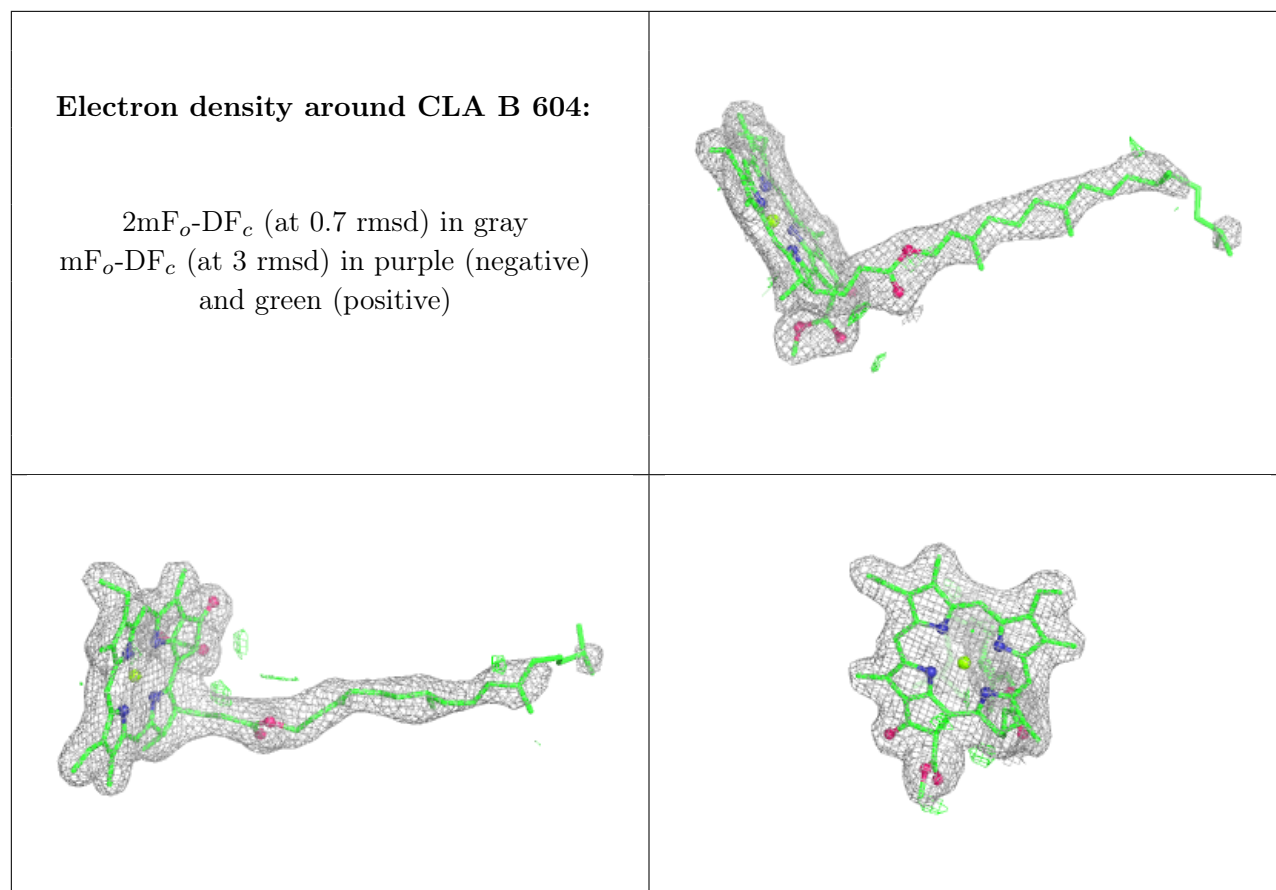
Electron density around CLA C 507:

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

**Electron density around CLA 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.