



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 07:23 AM JST

PDB ID : 5GTI / pdb_00005gti
Title : Native XFEL structure of photosystem II (two flash dataset)
Authors : Suga, M.; Shen, J.R.
Deposited on : 2016-08-20
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

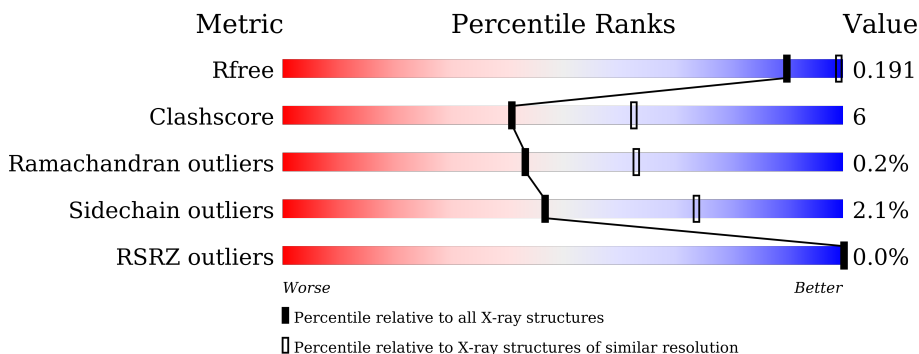
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

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X-RAY DIFFRACTION

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



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

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

Mol	Chain	Length	Quality of chain
1	A	344	87%10%.
1	a	344	87%10%.
2	B	505	87%13%
2	b	505	88%11%.
3	C	455	89%9%.
3	c	455	87%12%.

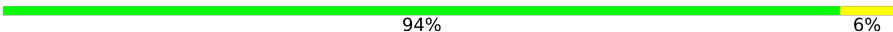
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Mol	Chain	Length	Quality of chain
4	D	342	
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V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

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Mol	Chain	Length	Quality of chain
16	v	137	 94% 6%
17	X	40	 85% 10% 5%
17	x	40	 82% 12% 5%
18	Y	30	 73% 23% .
18	y	30	 77% 17% . .
19	Z	62	 85% 15%
19	z	62	 89% 11%
20	R	34	 79% 21%

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
27	GOL	B	628	-	-	X	-
40	HEC	V	202	X	-	-	-
40	HEC	v	201	X	-	-	-

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 52752 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 D1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2620	1716	431	458	15			
1	a	334	Total	C	N	O	S	0	0	0
			2620	1716	431	458	15			

- 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	0	0
			3969	2605	661	690	13			
2	b	504	Total	C	N	O	S	0	0	0
			3969	2605	661	690	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	0	0
			3486	2281	584	608	13			
3	c	455	Total	C	N	O	S	0	0	0
			3519	2303	589	614	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			
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	0	0
			662	432	107	123			
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	0	0
			506	339	81	84	2			
7	h	65	Total	C	N	O	S	0	0	0
			511	341	82	86	2			

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

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

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

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

- Molecule 10 is a protein called Photosystem II PsbK protein.

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

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

- 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	0	0
			296	197	47	52			
11	l	36	Total	C	N	O	0	0	0
			296	197	47	52			

- Molecule 12 is a protein called Photosystem II PsbM protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	0	0
			260	173	38	48	1			
12	m	34	Total	C	N	O	S	0	0	0
			269	179	40	49	1			

- 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	0	0
			1865	1165	315	381	4			
13	o	243	Total	C	N	O	S	0	0	0
			1865	1165	315	381	4			

- 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	0	0	0
			765	486	128	151			
15	u	97	Total	C	N	O	0	0	0
			774	491	129	154			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	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	0	0	0
			281	188	45	48			
17	x	38	Total	C	N	O	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		

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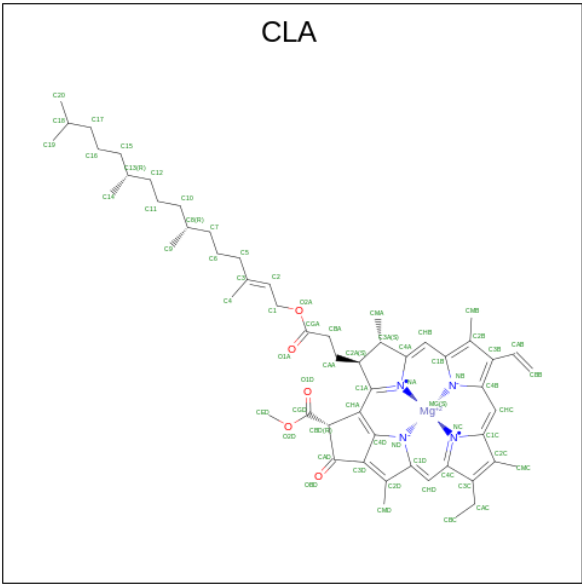
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	a	1	Total	Fe	0	0
			1	1		

- 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 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

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

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

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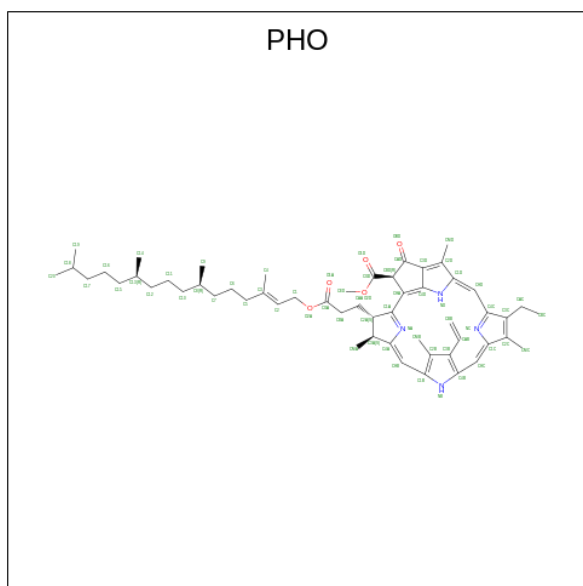
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N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

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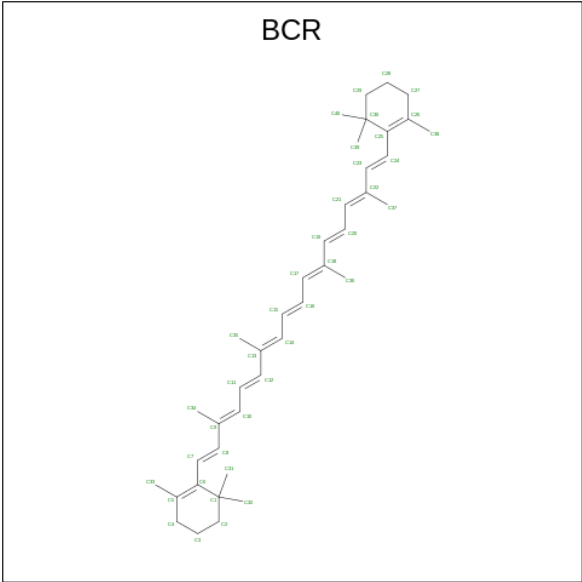
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- 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	D	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: $C_{40}H_{56}$).



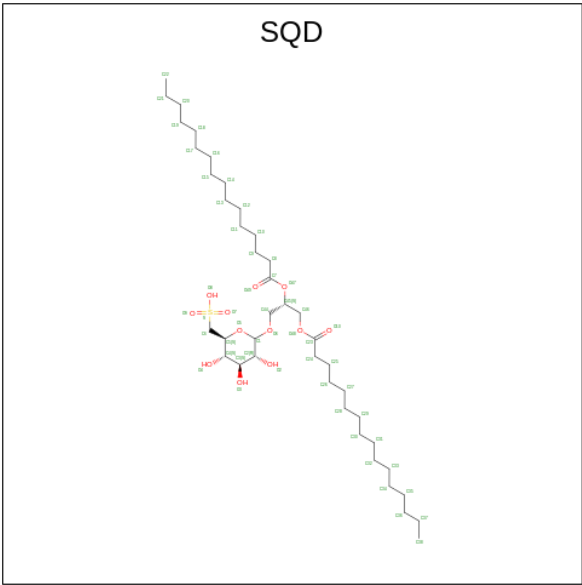
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total 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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY L]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



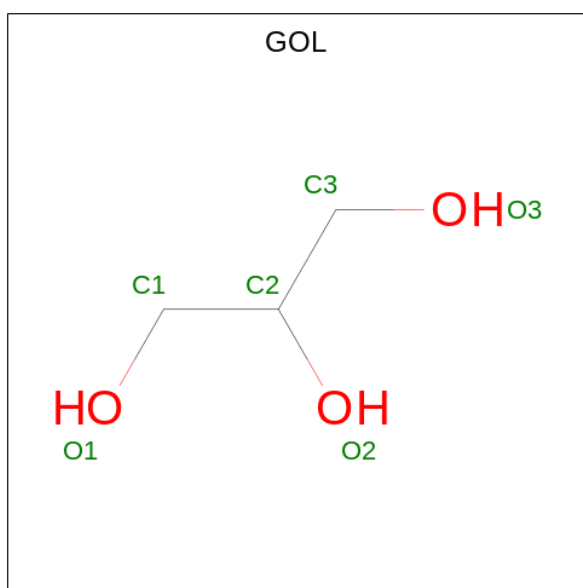
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O S 54 41 12 1	0	0
26	A	1	Total C O S 54 41 12 1	0	0
26	B	1	Total C O S 54 41 12 1	0	0

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

- Molecule 27 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



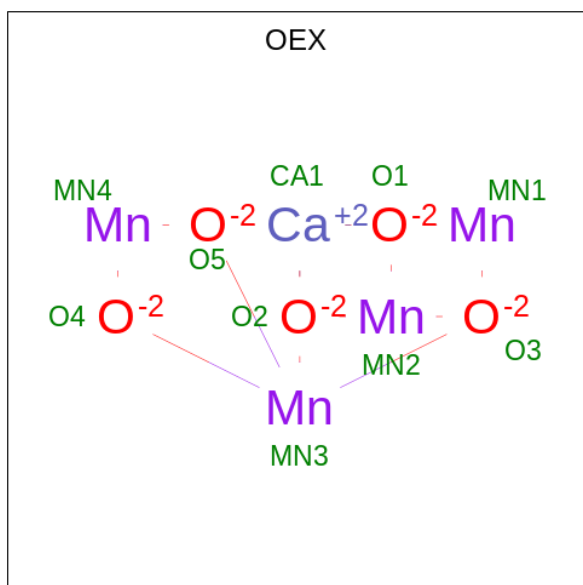
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	0
			6	3	3		
27	O	1	Total	C	O	0	0
			6	3	3		
27	a	1	Total	C	O	0	0
			6	3	3		

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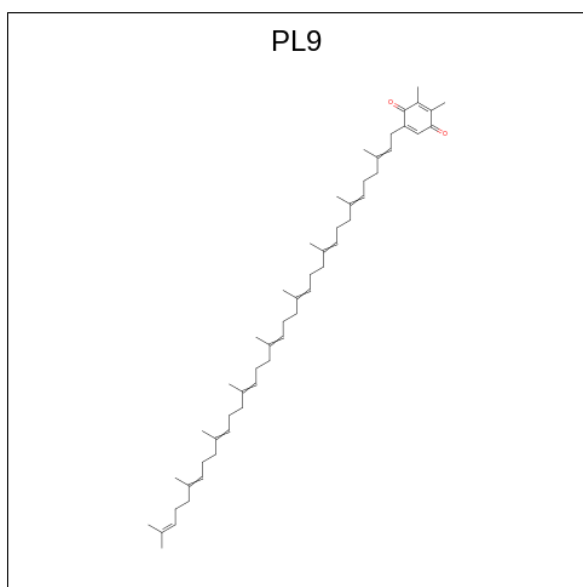
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	b	1	Total	C	O	0	0
			6	3	3		
27	d	1	Total	C	O	0	0
			6	3	3		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	Ca	Mn	O	0	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: $\text{C}_{53}\text{H}_{80}\text{O}_2$).



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

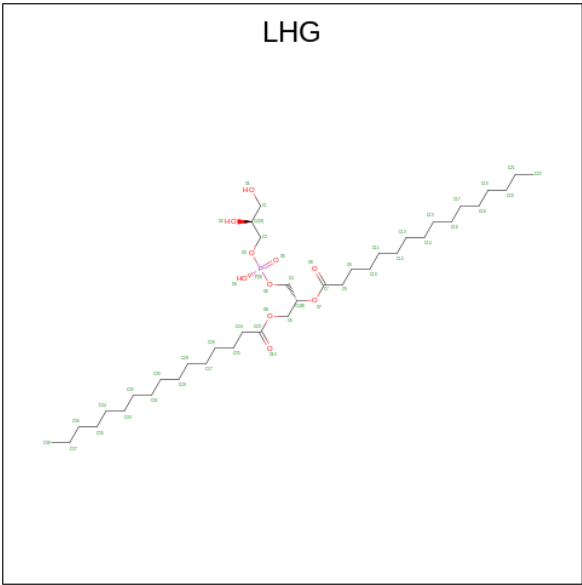
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			28	23	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	I	1	Total	C	O	0	0
			40	35	5		
30	J	1	Total	C		0	0
			10	10			
30	K	1	Total	C	O	0	0
			34	29	5		
30	M	1	Total	C		0	0
			10	10			
30	X	1	Total	C	O	0	0
		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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	a	1	Total	C	O	0	0
			30	25	5		
30	b	2	Total	C	O	0	0
			69	59	10		
30	c	1	Total	C	O	0	0
			32	27	5		
30	d	1	Total	C	O	0	0
			17	16	1		
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		

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



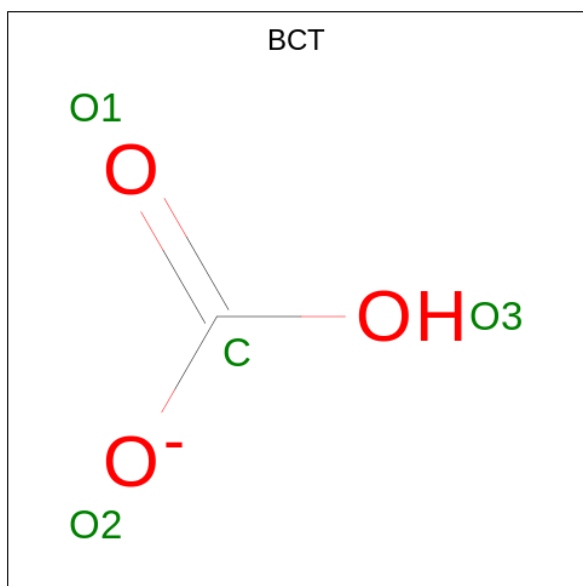
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		

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

- Molecule 32 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).

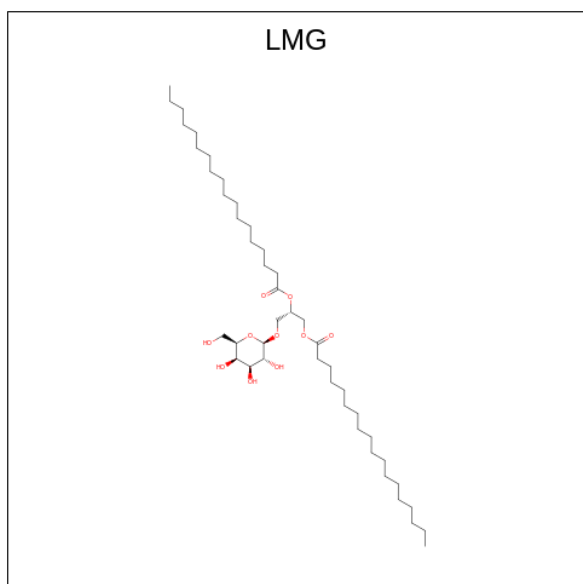


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			4	1	3		
32	a	1	Total	C	O	0	0
			4	1	3		

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

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

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



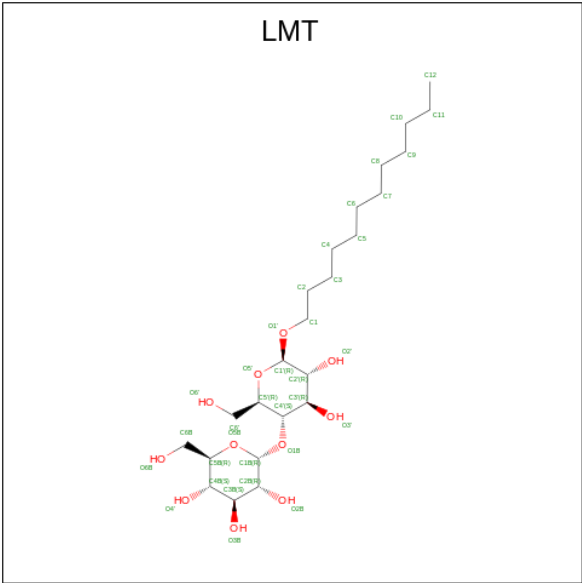
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	B	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	J	1	Total	C	O	0	0
			51	41	10		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	Z	1	Total	C	O	0	0
			37	27	10		
34	a	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total	C	O	0	0
			51	41	10		
34	j	1	Total	C	O	0	0
			51	41	10		
34	m	1	Total	C	O	0	0
			51	41	10		
34	z	1	Total	C	O	0	0
			39	29	10		

- Molecule 35 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



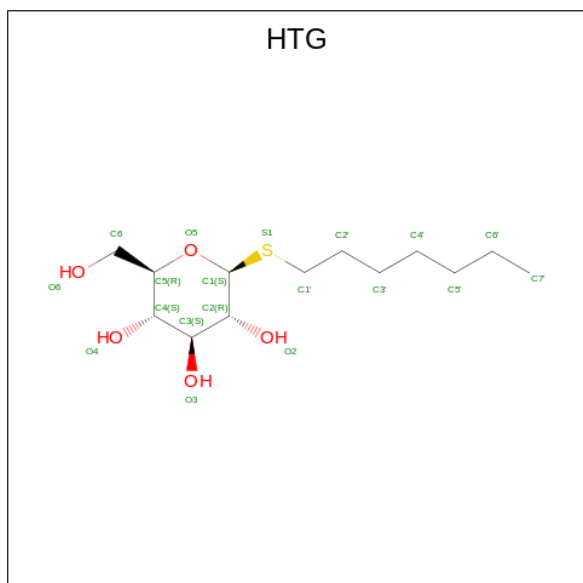
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	B	1	Total	C	O	0	0
			35	24	11		
35	B	1	Total	C	O	0	0
			25	19	6		
35	B	1	Total	C	O	0	0
			35	24	11		
35	B	1	Total	C	O	0	0
			26	19	7		

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

- Molecule 36 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C₁₃H₂₆O₅S).



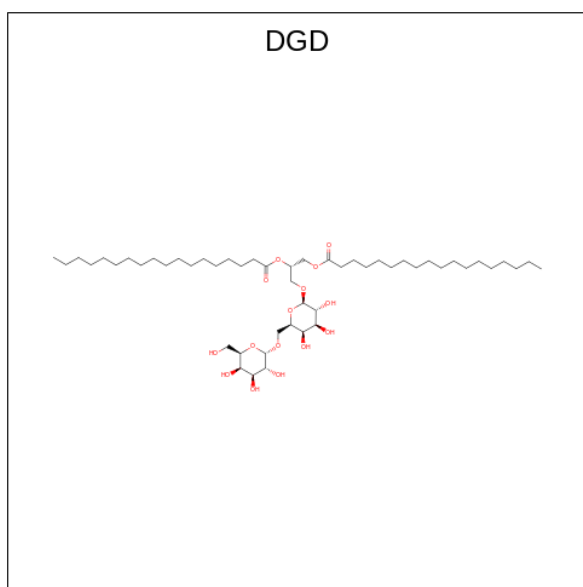
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	B	1	Total	C	O	S	0	0
			19	13	5	1		

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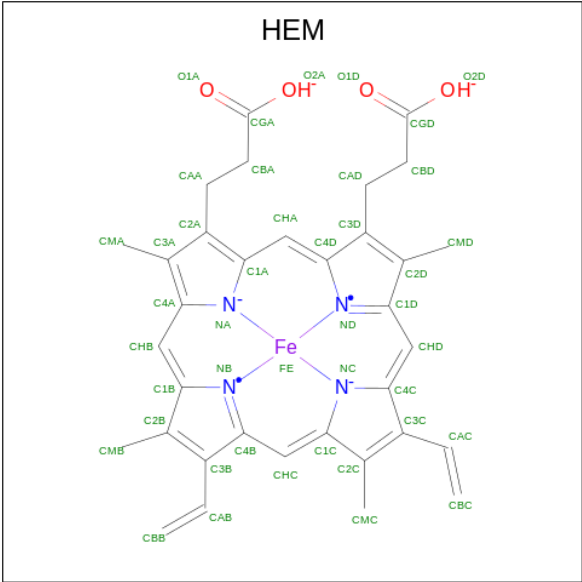
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	S		0	0
			9	8	1			
36	D	1	Total	C	O	S	0	0
			16	10	5	1		
36	V	1	Total	C	O		0	0
			11	6	5			
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	h	1	Total	C	O	S	0	0
			16	10	5	1		

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



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

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

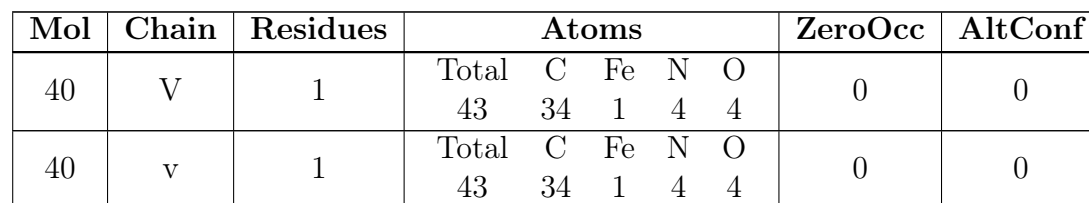


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
38	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
38	e	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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

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

- Molecule 40 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₆FeN₄O₄).



- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 41 | A | 135 | Total O
135 135 | 0 | 0 |
| 41 | B | 195 | Total O
195 195 | 0 | 0 |
| 41 | C | 151 | Total O
151 151 | 0 | 0 |
| 41 | D | 118 | Total O
118 118 | 0 | 0 |
| 41 | E | 25 | Total O
25 25 | 0 | 0 |
| 41 | F | 5 | Total O
5 5 | 0 | 0 |
| 41 | H | 22 | Total O
22 22 | 0 | 0 |
| 41 | I | 6 | Total O
6 6 | 0 | 0 |
| 41 | J | 4 | Total O
4 4 | 0 | 0 |
| 41 | K | 6 | Total O
6 6 | 0 | 0 |



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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	L	6	Total 6	O 6	0	0
41	M	15	Total 15	O 15	0	0
41	O	105	Total 105	O 105	0	0
41	T	13	Total 13	O 13	0	0
41	U	51	Total 51	O 51	0	0
41	V	81	Total 81	O 81	0	0
41	X	4	Total 4	O 4	0	0
41	Y	1	Total 1	O 1	0	0
41	Z	1	Total 1	O 1	0	0
41	R	1	Total 1	O 1	0	0
41	a	132	Total 132	O 132	0	0
41	b	206	Total 206	O 206	0	0
41	c	153	Total 153	O 153	0	0
41	d	115	Total 115	O 115	0	0
41	e	16	Total 16	O 16	0	0
41	f	5	Total 5	O 5	0	0
41	h	27	Total 27	O 27	0	0
41	i	3	Total 3	O 3	0	0
41	j	3	Total 3	O 3	0	0
41	k	6	Total 6	O 6	0	0
41	l	9	Total 9	O 9	0	0

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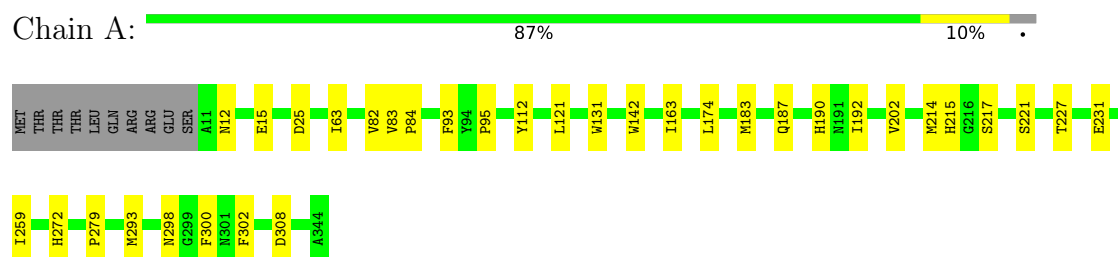
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	m	18	Total 18	O 18	0	0
41	o	115	Total 115	O 115	0	0
41	t	9	Total 9	O 9	0	0
41	u	62	Total 62	O 62	0	0
41	v	78	Total 78	O 78	0	0
41	x	8	Total 8	O 8	0	0
41	z	1	Total 1	O 1	0	0

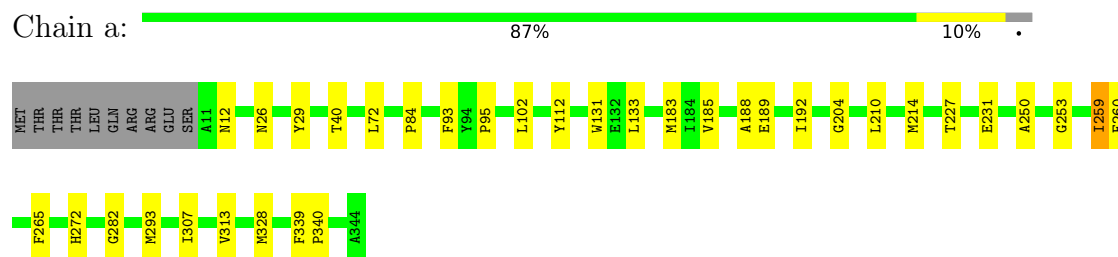
3 Residue-property plots

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

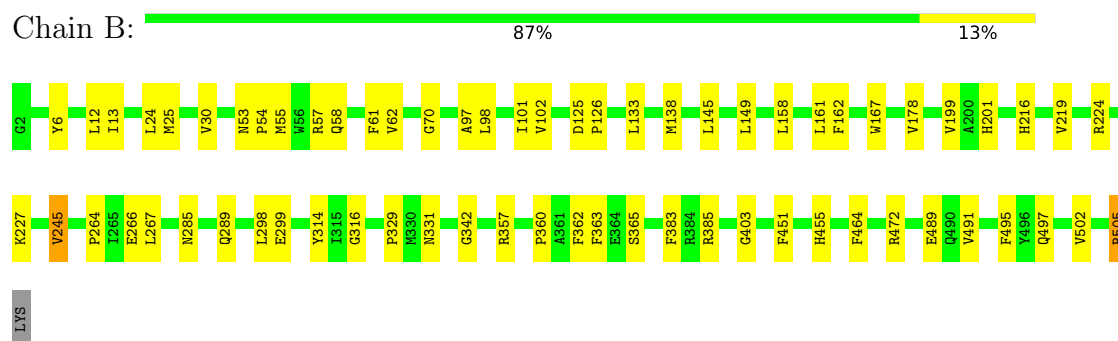
• Molecule 1: Photosystem II D1 protein



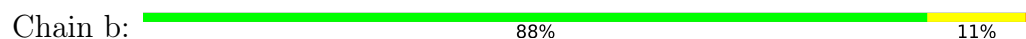
• Molecule 1: Photosystem II D1 protein

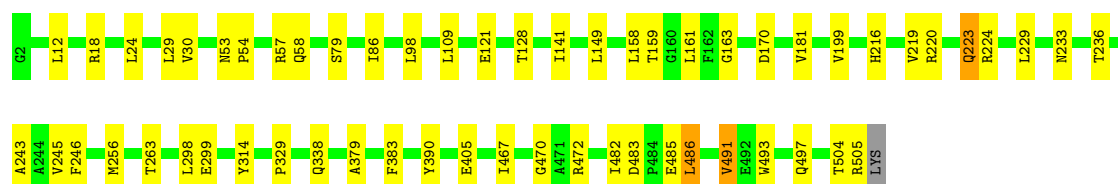


• Molecule 2: Photosystem II CP47 reaction center protein



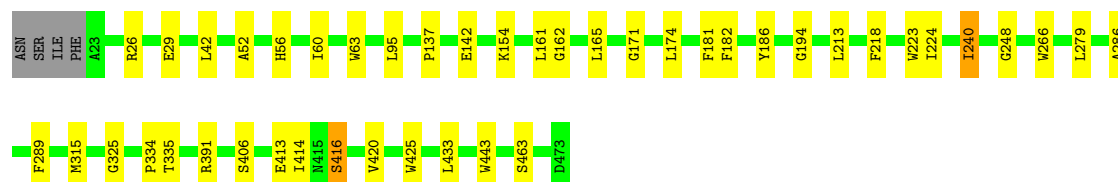
• Molecule 2: Photosystem II CP47 reaction center protein





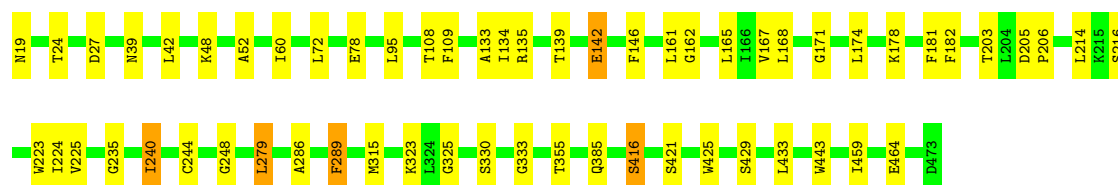
• Molecule 3: Photosystem II CP43 protein

Chain C: 89% 9% .



• Molecule 3: Photosystem II CP43 protein

Chain c: 87% 12% .



• Molecule 4: Photosystem II D2 protein

Chain D: 91% 9% .



• Molecule 4: Photosystem II D2 protein

Chain d: 92% 8% .



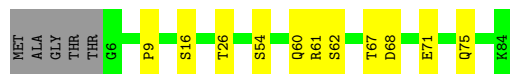
• Molecule 5: Cytochrome b559 subunit alpha

Chain E: 81% 15% .



- Molecule 5: Cytochrome b559 subunit alpha

Chain e:  81% 13% 6%



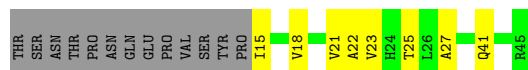
- Molecule 6: Cytochrome b559 subunit beta

Chain F:  61% 16% 23%

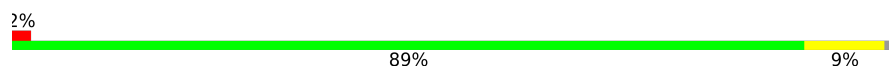


- Molecule 6: Cytochrome b559 subunit beta

Chain f:  52% 18% 30%



- Molecule 7: Photosystem II reaction center protein H

Chain H:  2% 89% 9%



- Molecule 7: Photosystem II reaction center protein H

Chain h:  2% 85% 15%



- Molecule 8: Photosystem II reaction center protein I

Chain I:  79% 18% 3%



- Molecule 8: Photosystem II reaction center protein I

Chain i:  76% 21% 3%



- Molecule 9: Photosystem II reaction center protein J

Chain J:  79% 18%



- Molecule 9: Photosystem II reaction center protein J

Chain j:  82% 18%



- Molecule 10: Photosystem II PsbK protein

Chain K:  81% 19%



- Molecule 10: Photosystem II PsbK protein

Chain k:  78% 19%



- Molecule 11: Photosystem II reaction center protein L

Chain L:  89% 8%



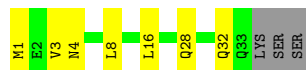
- Molecule 11: Photosystem II reaction center protein L

Chain l:  92% 5%



- Molecule 12: Photosystem II PsbM protein

Chain M:  72% 19% 8%



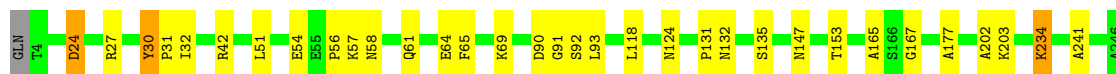
- Molecule 12: Photosystem II PsbM protein

Chain m:  67% 25% 6%



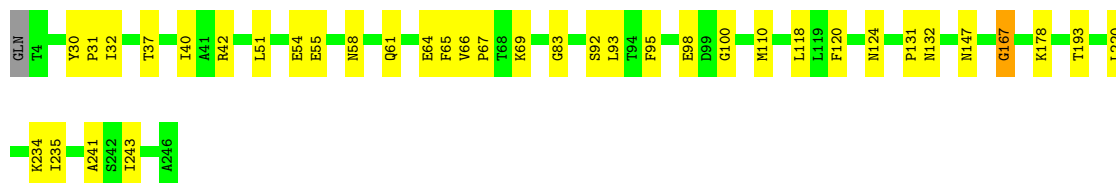
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  86% 12%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  84% 15%



- Molecule 14: Photosystem II reaction center protein T

Chain T:  81% 9% 6%



- Molecule 14: Photosystem II reaction center protein T

Chain t:  78% 12% 6%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  82% 11% 8%

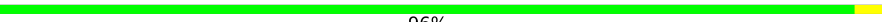


- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  85% 9% 7%



- Molecule 16: Cytochrome c-550

Chain V:  96% .



- Molecule 16: Cytochrome c-550

Chain v:  94% 6%



- Molecule 17: Photosystem II reaction center protein X

Chain X:  85% 10% 5%



- Molecule 17: Photosystem II reaction center protein X

Chain x:  82% 12% 5%



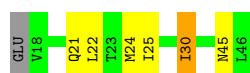
- Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:  73% 23% .



- Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:  77% 17% . .

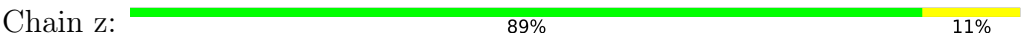


- Molecule 19: Photosystem II reaction center protein Z

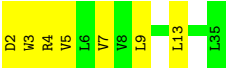
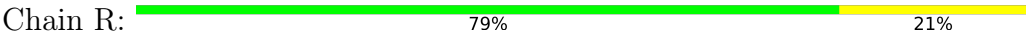
Chain Z:  85% 15%



- 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	126.52Å 231.23Å 287.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.50 19.98 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.98-2.50) 99.7 (19.98-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.139 , 0.187 0.145 , 0.191	Depositor DCC
R_{free} test set	14615 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	71.4	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 66.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	52752	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.55	0/2705	0.85	1/3689 (0.0%)
1	a	0.55	0/2705	0.83	0/3689
2	B	0.52	0/4109	0.82	0/5600
2	b	0.51	0/4109	0.82	4/5600 (0.1%)
3	C	0.48	0/3599	0.83	0/4900
3	c	0.49	0/3633	0.84	4/4946 (0.1%)
4	D	0.54	0/2821	0.84	4/3844 (0.1%)
4	d	0.53	0/2812	0.83	4/3832 (0.1%)
5	E	0.46	0/681	0.81	0/928
5	e	0.46	0/667	0.78	0/908
6	F	0.52	0/284	0.75	0/387
6	f	0.50	0/257	0.74	0/349
7	H	0.45	0/519	0.82	0/708
7	h	0.44	0/524	0.77	0/713
8	I	0.43	0/311	0.88	2/419 (0.5%)
8	i	0.45	0/311	0.84	0/419
9	J	0.43	0/278	0.84	0/376
9	j	0.45	0/283	0.77	0/383
10	K	0.48	0/303	0.85	0/416
10	k	0.48	0/303	0.88	0/416
11	L	0.51	0/303	0.73	0/412
11	l	0.45	0/303	0.79	0/412
12	M	0.59	0/253	0.84	0/346
12	m	0.56	0/262	0.93	2/357 (0.6%)
13	O	0.46	0/1896	0.83	2/2571 (0.1%)
13	o	0.48	0/1896	0.86	3/2571 (0.1%)
14	T	0.61	0/257	0.77	0/349
14	t	0.56	0/257	0.77	0/349
15	U	0.50	0/776	0.80	0/1052
15	u	0.51	0/785	0.79	0/1064
16	V	0.53	0/1085	0.81	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.49	0/1085	0.83	0/1473
17	X	0.42	0/284	0.79	0/384
17	x	0.42	0/284	0.77	0/384
18	Y	0.45	0/216	0.80	0/289
18	y	0.42	0/216	0.87	0/289
19	Z	0.43	0/490	0.86	1/669 (0.1%)
19	z	0.42	0/490	0.84	0/669
20	R	0.42	0/279	0.75	0/383
All	All	0.50	0/42631	0.83	27/58018 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	30	TYR	CA-C-N	7.12	126.88	119.76
13	O	30	TYR	C-N-CA	7.12	126.88	119.76
4	D	170	ALA	CA-C-N	-6.73	113.05	119.85
4	D	170	ALA	C-N-CA	-6.73	113.05	119.85
13	o	55	GLU	CA-C-N	6.36	126.31	119.76

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	2620	0	2517	28	0
1	a	2620	0	2517	25	0
2	B	3969	0	3828	54	0
2	b	3969	0	3828	44	0
3	C	3486	0	3407	39	0
3	c	3519	0	3437	46	0
4	D	2726	0	2627	28	0
4	d	2717	0	2621	17	0
5	E	662	0	648	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	e	648	0	634	10	0
6	F	275	0	282	6	0
6	f	250	0	261	7	0
7	H	506	0	529	4	0
7	h	511	0	532	12	0
8	I	314	0	328	4	0
8	i	314	0	328	4	0
9	J	272	0	279	4	0
9	j	277	0	284	4	0
10	K	293	0	305	3	0
10	k	293	0	305	4	0
11	L	296	0	304	2	0
11	l	296	0	304	3	0
12	M	260	0	275	4	0
12	m	269	0	288	5	0
13	O	1865	0	1838	21	0
13	o	1865	0	1838	24	0
14	T	258	0	261	6	0
14	t	258	0	261	4	0
15	U	765	0	767	6	0
15	u	774	0	773	4	0
16	V	1064	0	1073	3	0
16	v	1064	0	1073	4	0
17	X	281	0	312	4	0
17	x	281	0	312	5	0
18	Y	215	0	246	4	0
18	y	215	0	246	4	0
19	Z	479	0	516	2	0
19	z	479	0	516	1	0
20	R	273	0	305	4	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	195	0	216	14	0
23	B	1040	0	1152	49	0
23	C	845	0	936	38	0
23	D	195	0	216	9	0
23	a	260	0	288	12	0
23	b	1040	0	1152	48	0
23	c	845	0	936	61	0
23	d	130	0	144	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	A	64	0	74	1	0
24	D	64	0	74	3	0
24	a	128	0	148	5	0
25	A	40	0	56	2	0
25	B	120	0	168	10	0
25	C	120	0	168	6	0
25	D	40	0	56	2	0
25	H	40	0	56	5	0
25	T	40	0	56	4	0
25	Y	40	0	56	3	0
25	a	40	0	56	1	0
25	b	120	0	168	5	0
25	c	80	0	112	4	0
25	d	40	0	56	1	0
25	h	40	0	56	4	0
25	k	40	0	56	5	0
25	t	40	0	56	4	0
25	y	40	0	56	1	0
26	A	108	0	156	3	0
26	B	54	0	78	2	0
26	D	43	0	53	2	0
26	L	54	0	78	4	0
26	a	108	0	156	5	0
26	f	43	0	53	2	0
27	A	6	0	8	0	0
27	B	12	0	16	5	0
27	C	6	0	8	0	0
27	O	6	0	8	0	0
27	a	6	0	8	1	0
27	b	6	0	8	0	0
27	d	6	0	8	0	0
28	A	10	0	0	0	0
28	a	10	0	0	1	0
29	A	55	0	80	5	0
29	D	55	0	80	1	0
29	a	55	0	80	8	0
29	d	55	0	80	2	0
30	A	28	0	0	0	0
30	B	33	0	0	0	0
30	D	57	0	0	1	0
30	I	40	0	0	0	0
30	J	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	K	34	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	69	0	0	0	0
30	c	32	0	0	0	0
30	d	17	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
31	A	49	0	74	4	0
31	D	98	0	148	7	0
31	E	42	0	57	0	0
31	L	49	0	74	0	0
31	b	49	0	74	0	0
31	d	147	0	222	8	0
31	e	42	0	57	3	0
32	A	4	0	0	0	0
32	a	4	0	0	0	0
33	B	1	0	0	0	0
33	C	1	0	0	0	0
33	O	1	0	0	0	0
33	V	1	0	0	0	0
33	c	2	0	0	0	0
33	o	1	0	0	0	0
34	B	51	0	72	2	0
34	C	153	0	216	4	0
34	J	51	0	72	2	0
34	Z	37	0	44	2	0
34	a	51	0	72	3	0
34	c	102	0	144	5	0
34	j	51	0	71	5	0
34	m	51	0	72	2	0
34	z	39	0	48	1	0
35	B	121	0	162	9	0
35	C	35	0	46	1	0
35	D	35	0	46	2	0
35	E	35	0	46	1	0
35	M	70	0	92	2	0
35	a	35	0	46	0	0
35	b	50	0	70	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	e	35	0	46	0	0
35	m	35	0	46	2	0
36	B	95	0	130	6	0
36	C	28	0	41	2	0
36	D	16	0	17	1	0
36	V	11	0	10	0	0
36	b	95	0	130	5	0
36	c	38	0	52	2	0
36	h	16	0	17	1	0
37	C	186	0	246	6	0
37	H	62	0	82	0	0
37	c	186	0	246	8	0
37	h	62	0	82	0	0
38	E	43	0	30	4	0
38	e	43	0	30	3	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	V	43	0	30	0	0
40	v	43	0	30	0	0
41	A	135	0	0	2	0
41	B	195	0	0	11	0
41	C	151	0	0	6	0
41	D	118	0	0	7	0
41	E	25	0	0	2	0
41	F	5	0	0	0	0
41	H	22	0	0	3	0
41	I	6	0	0	1	0
41	J	4	0	0	0	0
41	K	6	0	0	0	0
41	L	6	0	0	0	0
41	M	15	0	0	1	0
41	O	105	0	0	0	0
41	R	1	0	0	0	0
41	T	13	0	0	0	0
41	U	51	0	0	0	0
41	V	81	0	0	1	0
41	X	4	0	0	0	0
41	Y	1	0	0	0	0
41	Z	1	0	0	1	0
41	a	132	0	0	1	0
41	b	206	0	0	7	0
41	c	153	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	d	115	0	0	1	0
41	e	16	0	0	1	0
41	f	5	0	0	0	0
41	h	27	0	0	0	0
41	i	3	0	0	0	0
41	j	3	0	0	0	0
41	k	6	0	0	0	0
41	l	9	0	0	0	0
41	m	18	0	0	3	0
41	o	115	0	0	0	0
41	t	9	0	0	0	0
41	u	62	0	0	0	0
41	v	78	0	0	2	0
41	x	8	0	0	0	0
41	z	1	0	0	0	0
All	All	52752	0	51821	667	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 6.

The worst 5 of 667 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:250:ALA:HA	2:b:491:VAL:HG11	1.48	0.94
23:B:605:CLA:H42	23:B:606:CLA:H2	1.48	0.93
4:D:199:MET:O	41:D:501:HOH:O	1.96	0.83
13:o:124:ASN:HD22	13:o:147:ASN:HD22	1.28	0.81
25:T:101:BCR:H19C	25:b:618:BCR:H363	1.62	0.80

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	332/344 (96%)	326 (98%)	5 (2%)	1 (0%)	36	55
1	a	332/344 (96%)	327 (98%)	4 (1%)	1 (0%)	36	55
2	B	502/505 (99%)	498 (99%)	4 (1%)	0	100	100
2	b	502/505 (99%)	494 (98%)	8 (2%)	0	100	100
3	C	449/455 (99%)	440 (98%)	8 (2%)	1 (0%)	43	63
3	c	453/455 (100%)	442 (98%)	10 (2%)	1 (0%)	43	63
4	D	340/342 (99%)	330 (97%)	10 (3%)	0	100	100
4	d	339/342 (99%)	333 (98%)	6 (2%)	0	100	100
5	E	79/84 (94%)	78 (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	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
7	h	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
8	I	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	i	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	4	6
9	J	36/39 (92%)	36 (100%)	0	0	100	100
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	34/37 (92%)	34 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
13	O	241/244 (99%)	232 (96%)	9 (4%)	0	100	100
13	o	241/244 (99%)	232 (96%)	9 (4%)	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%)	89 (95%)	5 (5%)	0	100	100
15	u	95/104 (91%)	91 (96%)	4 (4%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	X	36/40 (90%)	36 (100%)	0	0	100	100
17	x	36/40 (90%)	36 (100%)	0	0	100	100
18	Y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
18	y	27/30 (90%)	25 (93%)	1 (4%)	1 (4%)	2	3
19	Z	60/62 (97%)	59 (98%)	0	1 (2%)	7	13
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	7	13
20	R	32/34 (94%)	32 (100%)	0	0	100	100
All	All	5212/5384 (97%)	5097 (98%)	107 (2%)	8 (0%)	43	63

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	i	36	ASP
3	C	416	SER
3	c	416	SER
19	Z	30	PRO
1	a	259	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/279 (96%)	269 (100%)	0	100	100
1	a	269/279 (96%)	268 (100%)	1 (0%)	84	93
2	B	402/403 (100%)	396 (98%)	6 (2%)	57	80
2	b	402/403 (100%)	392 (98%)	10 (2%)	42	69
3	C	352/356 (99%)	346 (98%)	6 (2%)	53	78
3	c	356/356 (100%)	347 (98%)	9 (2%)	42	69
4	D	277/277 (100%)	276 (100%)	1 (0%)	84	93
4	d	276/277 (100%)	275 (100%)	1 (0%)	84	93
5	E	72/73 (99%)	71 (99%)	1 (1%)	59	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	e	70/73 (96%)	68 (97%)	2 (3%)	37	65
6	F	28/38 (74%)	27 (96%)	1 (4%)	31	58
6	f	25/38 (66%)	23 (92%)	2 (8%)	11	24
7	H	54/54 (100%)	52 (96%)	2 (4%)	30	57
7	h	54/54 (100%)	54 (100%)	0	100	100
8	I	34/34 (100%)	33 (97%)	1 (3%)	37	65
8	i	34/34 (100%)	32 (94%)	2 (6%)	18	37
9	J	26/27 (96%)	24 (92%)	2 (8%)	12	25
9	j	26/27 (96%)	25 (96%)	1 (4%)	29	56
10	K	30/30 (100%)	26 (87%)	4 (13%)	4	8
10	k	30/30 (100%)	26 (87%)	4 (13%)	4	8
11	L	34/35 (97%)	34 (100%)	0	100	100
11	l	34/35 (97%)	34 (100%)	0	100	100
12	M	29/32 (91%)	28 (97%)	1 (3%)	32	60
12	m	30/32 (94%)	27 (90%)	3 (10%)	7	15
13	O	206/207 (100%)	201 (98%)	5 (2%)	43	70
13	o	206/207 (100%)	203 (98%)	3 (2%)	57	80
14	T	26/28 (93%)	25 (96%)	1 (4%)	29	56
14	t	26/28 (93%)	25 (96%)	1 (4%)	29	56
15	U	83/89 (93%)	81 (98%)	2 (2%)	43	70
15	u	84/89 (94%)	82 (98%)	2 (2%)	43	70
16	V	117/117 (100%)	116 (99%)	1 (1%)	70	87
16	v	117/117 (100%)	116 (99%)	1 (1%)	70	87
17	X	31/33 (94%)	30 (97%)	1 (3%)	34	62
17	x	31/33 (94%)	31 (100%)	0	100	100
18	Y	22/23 (96%)	21 (96%)	1 (4%)	24	49
18	y	22/23 (96%)	21 (96%)	1 (4%)	24	49
19	Z	52/52 (100%)	47 (90%)	5 (10%)	8	17
19	z	52/52 (100%)	48 (92%)	4 (8%)	12	25
20	R	29/29 (100%)	28 (97%)	1 (3%)	32	60
All	All	4317/4403 (98%)	4228 (98%)	89 (2%)	47	74

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

Mol	Chain	Res	Type
3	c	279	LEU
10	k	17	ILE
3	c	315	MET
6	f	15	ILE
12	m	5	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
15	U	73	GLN
6	f	44	GLN
2	b	53	ASN
13	o	124	ASN
4	d	186	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	i	1	8	8,9,10	0.61	0	7,9,11	1.26	1 (14%)
12	FME	m	1	12	8,9,10	0.61	0	7,9,11	1.64	3 (42%)
12	FME	M	1	12	8,9,10	0.55	0	7,9,11	1.35	1 (14%)
8	FME	I	1	8	8,9,10	0.64	0	7,9,11	1.00	1 (14%)
14	FME	T	1	14	8,9,10	0.64	0	7,9,11	1.22	0
14	FME	t	1	14	8,9,10	0.68	0	7,9,11	1.72	2 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	i	1	8	-	2/7/9/11	-
12	FME	m	1	12	-	2/7/9/11	-
12	FME	M	1	12	-	0/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
14	FME	T	1	14	-	3/7/9/11	-
14	FME	t	1	14	-	0/7/9/11	-

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	CA-N-CN	-2.74	118.61	122.82
14	t	1	FME	O-C-CA	-2.68	117.76	124.78
12	M	1	FME	O-C-CA	-2.52	118.17	124.78
12	m	1	FME	CA-N-CN	-2.39	119.15	122.82
8	i	1	FME	O-C-CA	-2.30	118.75	124.78

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	T	1	FME	2	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 218 ligands modelled in this entry, 15 are monoatomic and 18 are unknown - leaving 185 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
37	DGD	c	516	-	63,63,67	0.85	2 (3%)	77,77,81	1.08	6 (7%)
36	HTG	b	626	-	19,19,19	1.08	2 (10%)	23,24,24	1.28	2 (8%)
23	CLA	B	609	2	69,73,73	1.97	19 (27%)	83,113,113	2.80	30 (36%)
38	HEM	e	103	6,5	50,50,50	1.55	8 (16%)	66,82,82	1.74	13 (19%)
23	CLA	C	508	41	69,73,73	2.06	19 (27%)	83,113,113	2.76	30 (36%)
31	LHG	d	408	-	48,48,48	0.96	2 (4%)	51,54,54	0.99	3 (5%)
29	PL9	A	413	-	55,55,55	0.63	2 (3%)	68,69,69	1.96	22 (32%)
23	CLA	B	613	2	69,73,73	2.00	20 (28%)	83,113,113	2.75	30 (36%)
36	HTG	B	629	-	19,19,19	0.97	2 (10%)	23,24,24	1.35	3 (13%)
34	LMG	C	501	-	51,51,55	0.95	2 (3%)	59,59,63	1.26	6 (10%)
36	HTG	V	203	-	11,11,19	0.28	0	15,15,24	1.35	1 (6%)
26	SQD	f	101	-	42,43,54	1.18	3 (7%)	51,54,65	1.53	8 (15%)
23	CLA	c	501	3	69,73,73	2.05	21 (30%)	83,113,113	2.75	29 (34%)
25	BCR	c	514	-	41,41,41	1.01	1 (2%)	56,56,56	1.87	15 (26%)
25	BCR	B	620	-	41,41,41	1.06	1 (2%)	56,56,56	1.50	12 (21%)
36	HTG	B	630	-	19,19,19	1.01	2 (10%)	23,24,24	1.33	1 (4%)
25	BCR	B	619	-	41,41,41	0.97	1 (2%)	56,56,56	1.56	13 (23%)
25	BCR	D	406	-	41,41,41	1.03	1 (2%)	56,56,56	1.77	13 (23%)
31	LHG	b	630	-	48,48,48	0.93	2 (4%)	51,54,54	1.06	2 (3%)
23	CLA	B	604	2	69,73,73	2.02	20 (28%)	83,113,113	2.85	31 (37%)
35	LMT	b	628	-	25,25,36	0.54	1 (4%)	30,30,47	1.21	4 (13%)
23	CLA	c	507	41	69,73,73	2.08	20 (28%)	83,113,113	2.86	33 (39%)
24	PHO	A	406	-	58,69,69	2.74	12 (20%)	56,99,99	2.83	20 (35%)
36	HTG	b	625	-	19,19,19	0.99	2 (10%)	23,24,24	1.48	3 (13%)
24	PHO	a	407	-	58,69,69	2.77	12 (20%)	56,99,99	2.93	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	B	618	-	41,41,41	1.04	1 (2%)	56,56,56	1.63	10 (17%)
34	LMG	m	101	-	51,51,55	0.89	2 (3%)	59,59,63	1.17	6 (10%)
23	CLA	c	513	3	69,73,73	2.08	21 (30%)	83,113,113	2.90	31 (37%)
26	SQD	B	621	-	53,54,54	1.04	3 (5%)	62,65,65	1.45	8 (12%)
23	CLA	B	615	2	69,73,73	2.00	19 (27%)	83,113,113	2.93	29 (34%)
23	CLA	c	504	41	69,73,73	2.06	21 (30%)	83,113,113	2.87	31 (37%)
23	CLA	D	405	4	69,73,73	2.09	18 (26%)	83,113,113	2.92	31 (37%)
27	GOL	B	627	-	5,5,5	0.35	0	5,5,5	0.37	0
32	BCT	A	416	21	2,3,3	0.66	0	2,3,3	0.33	0
26	SQD	D	413	-	42,43,54	1.14	3 (7%)	51,54,65	1.63	12 (23%)
37	DGD	C	517	-	63,63,67	0.85	2 (3%)	77,77,81	1.19	7 (9%)
27	GOL	A	410	-	5,5,5	0.37	0	5,5,5	0.25	0
23	CLA	d	403	4	69,73,73	2.06	20 (28%)	83,113,113	2.91	30 (36%)
23	CLA	b	613	2	69,73,73	2.06	20 (28%)	83,113,113	2.79	29 (34%)
23	CLA	B	605	2	69,73,73	2.00	19 (27%)	83,113,113	2.82	30 (36%)
23	CLA	B	614	2	69,73,73	2.01	20 (28%)	83,113,113	2.72	28 (33%)
23	CLA	C	502	3	69,73,73	2.02	20 (28%)	83,113,113	2.81	29 (34%)
23	CLA	C	509	3	69,73,73	2.03	21 (30%)	83,113,113	2.82	31 (37%)
35	LMT	M	103	-	36,36,36	0.46	0	47,47,47	0.78	1 (2%)
23	CLA	C	513	3	69,73,73	2.04	19 (27%)	83,113,113	2.79	32 (38%)
23	CLA	A	405	41	69,73,73	2.07	19 (27%)	83,113,113	2.85	31 (37%)
25	BCR	a	410	-	41,41,41	0.99	1 (2%)	56,56,56	1.57	13 (23%)
25	BCR	H	101	-	41,41,41	1.08	1 (2%)	56,56,56	1.59	11 (19%)
31	LHG	A	415	-	48,48,48	0.86	2 (4%)	51,54,54	1.18	6 (11%)
23	CLA	c	502	3	69,73,73	2.02	19 (27%)	83,113,113	2.81	26 (31%)
23	CLA	C	506	3	69,73,73	2.04	20 (28%)	83,113,113	2.78	30 (36%)
23	CLA	c	503	3	69,73,73	2.07	20 (28%)	83,113,113	2.82	30 (36%)
36	HTG	b	621	-	19,19,19	1.24	2 (10%)	23,24,24	1.76	5 (21%)
34	LMG	a	417	-	51,51,55	0.96	3 (5%)	59,59,63	1.11	4 (6%)
36	HTG	C	523	-	19,19,19	0.96	1 (5%)	23,24,24	1.50	3 (13%)
38	HEM	E	103	6,5	50,50,50	1.55	7 (14%)	66,82,82	1.76	16 (24%)
25	BCR	C	527	-	41,41,41	1.01	1 (2%)	56,56,56	1.57	12 (21%)
27	GOL	B	628	-	5,5,5	0.54	0	5,5,5	0.49	0
35	LMT	B	633	-	36,36,36	0.56	1 (2%)	47,47,47	0.97	1 (2%)
36	HTG	B	626	-	19,19,19	0.96	1 (5%)	23,24,24	1.59	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	511	3	69,73,73	2.04	19 (27%)	83,113,113	2.83	30 (36%)
35	LMT	b	620	-	25,25,36	0.46	0	30,30,47	0.66	0
24	PHO	D	402	-	58,69,69	2.78	14 (24%)	56,99,99	2.97	16 (28%)
25	BCR	y	101	-	41,41,41	1.09	1 (2%)	56,56,56	1.66	12 (21%)
31	LHG	E	101	-	41,41,48	1.02	2 (4%)	44,47,54	1.09	3 (6%)
36	HTG	c	521	-	19,19,19	0.93	1 (5%)	23,24,24	1.46	1 (4%)
35	LMT	B	623	-	36,36,36	0.42	0	47,47,47	1.14	4 (8%)
37	DGD	H	102	-	63,63,67	0.89	2 (3%)	77,77,81	0.98	3 (3%)
34	LMG	C	520	-	51,51,55	0.94	2 (3%)	59,59,63	1.08	3 (5%)
31	LHG	d	407	-	48,48,48	0.91	2 (4%)	51,54,54	0.93	3 (5%)
23	CLA	c	505	3	69,73,73	2.05	19 (27%)	83,113,113	2.74	29 (34%)
23	CLA	B	617	2	69,73,73	2.03	20 (28%)	83,113,113	2.86	30 (36%)
37	DGD	h	103	-	63,63,67	0.89	3 (4%)	77,77,81	0.96	3 (3%)
34	LMG	c	520	-	51,51,55	0.97	2 (3%)	59,59,63	1.21	7 (11%)
23	CLA	D	404	4	69,73,73	2.02	20 (28%)	83,113,113	2.88	30 (36%)
23	CLA	b	605	2	69,73,73	2.04	21 (30%)	83,113,113	2.85	31 (37%)
25	BCR	d	404	-	41,41,41	1.12	1 (2%)	56,56,56	1.68	13 (23%)
35	LMT	E	102	-	36,36,36	0.51	1 (2%)	47,47,47	0.86	0
31	LHG	e	101	-	41,41,48	1.03	2 (4%)	44,47,54	0.94	2 (4%)
23	CLA	b	604	2	69,73,73	2.00	19 (27%)	83,113,113	2.80	30 (36%)
23	CLA	c	506	3	69,73,73	2.04	19 (27%)	83,113,113	2.69	31 (37%)
23	CLA	a	405	41	69,73,73	2.08	19 (27%)	83,113,113	2.88	33 (39%)
40	HEC	V	202	16	50,50,50	1.74	9 (18%)	68,82,82	1.82	16 (23%)
23	CLA	B	607	2	69,73,73	2.00	18 (26%)	83,113,113	2.88	31 (37%)
23	CLA	b	602	2	69,73,73	2.04	20 (28%)	83,113,113	2.90	33 (39%)
26	SQD	a	413	-	53,54,54	1.09	4 (7%)	62,65,65	1.23	8 (12%)
24	PHO	a	408	-	58,69,69	2.81	15 (25%)	56,99,99	2.77	17 (30%)
25	BCR	k	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.61	13 (23%)
23	CLA	b	610	41	69,73,73	2.09	20 (28%)	83,113,113	2.84	30 (36%)
35	LMT	M	101	-	36,36,36	0.56	0	47,47,47	1.10	3 (6%)
28	OEX	A	412	1,41,3	0,14,14	-	-	-	-	-
37	DGD	c	518	-	63,63,67	0.86	3 (4%)	77,77,81	1.09	4 (5%)
27	GOL	b	624	-	5,5,5	0.36	0	5,5,5	0.41	0
31	LHG	D	408	-	48,48,48	0.90	2 (4%)	51,54,54	1.00	3 (5%)
23	CLA	C	503	3	69,73,73	2.06	19 (27%)	83,113,113	2.72	28 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	614	2	69,73,73	2.02	20 (28%)	83,113,113	2.82	30 (36%)
23	CLA	B	608	41	69,73,73	2.07	20 (28%)	83,113,113	2.78	31 (37%)
23	CLA	b	601	41	69,73,73	2.10	20 (28%)	83,113,113	2.75	28 (33%)
26	SQD	a	411	-	53,54,54	0.98	3 (5%)	62,65,65	1.60	11 (17%)
23	CLA	C	505	41	69,73,73	2.06	20 (28%)	83,113,113	2.77	32 (38%)
23	CLA	d	402	4	69,73,73	2.00	20 (28%)	83,113,113	2.77	32 (38%)
34	LMG	Z	101	-	37,37,55	0.99	3 (8%)	45,45,63	1.54	8 (17%)
35	LMT	D	403	-	36,36,36	0.57	1 (2%)	47,47,47	1.20	4 (8%)
23	CLA	a	406	41	69,73,73	1.99	19 (27%)	83,113,113	2.88	29 (34%)
23	CLA	b	611	2	69,73,73	2.01	19 (27%)	83,113,113	2.82	30 (36%)
27	GOL	C	525	-	5,5,5	0.39	0	5,5,5	0.20	0
36	HTG	h	101	-	16,16,19	1.09	2 (12%)	20,21,24	1.30	1 (5%)
35	LMT	B	634	-	26,26,36	0.49	0	31,31,47	0.90	1 (3%)
36	HTG	b	622	-	19,19,19	1.01	2 (10%)	23,24,24	1.39	2 (8%)
23	CLA	b	616	2	69,73,73	2.05	20 (28%)	83,113,113	2.73	32 (38%)
28	OEX	a	414	1,41,3	0,14,14	-	-	-	-	-
34	LMG	C	521	-	51,51,55	0.98	3 (5%)	59,59,63	1.21	4 (6%)
40	HEC	v	201	16	50,50,50	1.69	8 (16%)	68,82,82	1.79	18 (26%)
23	CLA	b	612	2	69,73,73	2.03	20 (28%)	83,113,113	2.79	28 (33%)
25	BCR	C	515	-	41,41,41	1.03	1 (2%)	56,56,56	1.54	7 (12%)
23	CLA	b	607	41	69,73,73	1.97	19 (27%)	83,113,113	2.77	29 (34%)
23	CLA	B	616	2	69,73,73	2.03	18 (26%)	83,113,113	2.73	31 (37%)
34	LMG	c	519	-	51,51,55	0.96	3 (5%)	59,59,63	1.05	5 (8%)
36	HTG	c	522	-	19,19,19	1.00	2 (10%)	23,24,24	1.47	3 (13%)
36	HTG	b	623	-	19,19,19	1.08	2 (10%)	23,24,24	1.63	3 (13%)
27	GOL	O	302	-	5,5,5	0.34	0	5,5,5	0.34	0
31	LHG	D	409	-	48,48,48	0.94	2 (4%)	51,54,54	1.06	3 (5%)
23	CLA	B	612	2	69,73,73	2.03	19 (27%)	83,113,113	2.86	32 (38%)
23	CLA	B	602	41	69,73,73	2.05	20 (28%)	83,113,113	2.83	32 (38%)
35	LMT	e	102	-	36,36,36	0.48	0	47,47,47	0.84	3 (6%)
26	SQD	A	411	-	53,54,54	1.03	3 (5%)	62,65,65	1.11	4 (6%)
23	CLA	a	409	1	69,73,73	2.09	19 (27%)	83,113,113	2.79	34 (40%)
34	LMG	B	622	-	51,51,55	0.90	2 (3%)	59,59,63	1.15	5 (8%)
32	BCT	a	419	21	2,3,3	0.65	0	2,3,3	0.46	0
37	DGD	c	517	-	63,63,67	0.91	3 (4%)	77,77,81	0.98	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	512	3	69,73,73	2.05	21 (30%)	83,113,113	2.77	29 (34%)
35	LMT	m	103	-	36,36,36	0.50	0	47,47,47	0.93	1 (2%)
36	HTG	C	524	-	8,8,19	0.39	0	7,7,24	1.15	1 (14%)
27	GOL	d	401	-	5,5,5	0.35	0	5,5,5	0.52	0
34	LMG	J	101	39	51,51,55	0.91	3 (5%)	59,59,63	1.07	5 (8%)
36	HTG	B	625	-	19,19,19	0.83	1 (5%)	23,24,24	1.60	1 (4%)
25	BCR	t	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.84	13 (23%)
25	BCR	b	618	-	41,41,41	0.98	1 (2%)	56,56,56	1.53	12 (21%)
25	BCR	h	102	-	41,41,41	1.05	1 (2%)	56,56,56	1.47	10 (17%)
23	CLA	B	603	2	69,73,73	2.10	21 (30%)	83,113,113	2.81	29 (34%)
23	CLA	c	512	3	69,73,73	2.05	19 (27%)	83,113,113	2.87	30 (36%)
25	BCR	T	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.85	10 (17%)
23	CLA	c	510	3	69,73,73	2.01	20 (28%)	83,113,113	2.82	34 (40%)
31	LHG	L	101	-	48,48,48	0.91	2 (4%)	51,54,54	1.17	4 (7%)
23	CLA	A	407	1	69,73,73	2.05	20 (28%)	83,113,113	2.91	28 (33%)
23	CLA	C	514	3	69,73,73	2.06	21 (30%)	83,113,113	2.90	30 (36%)
23	CLA	B	606	2	69,73,73	2.07	20 (28%)	83,113,113	2.86	32 (38%)
25	BCR	b	619	-	41,41,41	1.08	2 (4%)	56,56,56	1.81	12 (21%)
23	CLA	a	404	1	69,73,73	2.01	19 (27%)	83,113,113	2.79	33 (39%)
37	DGD	C	519	-	63,63,67	0.83	2 (3%)	77,77,81	0.99	4 (5%)
27	GOL	a	412	-	5,5,5	0.43	0	5,5,5	0.27	0
25	BCR	C	516	-	41,41,41	1.05	1 (2%)	56,56,56	1.50	11 (19%)
37	DGD	C	518	-	63,63,67	0.86	2 (3%)	77,77,81	0.98	5 (6%)
23	CLA	b	608	2	69,73,73	2.03	20 (28%)	83,113,113	2.81	30 (36%)
34	LMG	z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.12	4 (8%)
23	CLA	b	603	2	69,73,73	2.05	19 (27%)	83,113,113	2.93	30 (36%)
23	CLA	c	508	3	69,73,73	2.07	20 (28%)	83,113,113	2.79	26 (31%)
23	CLA	B	611	41	69,73,73	2.06	20 (28%)	83,113,113	2.87	31 (37%)
23	CLA	b	615	2	69,73,73	2.01	19 (27%)	83,113,113	2.81	31 (37%)
36	HTG	D	412	-	16,16,19	1.03	2 (12%)	20,21,24	1.40	1 (5%)
34	LMG	j	101	39	51,51,55	0.91	2 (3%)	59,59,63	1.08	6 (10%)
35	LMT	C	522	-	36,36,36	0.53	1 (2%)	47,47,47	1.02	4 (8%)
23	CLA	c	511	3	69,73,73	2.07	19 (27%)	83,113,113	2.79	28 (33%)
31	LHG	d	406	-	48,48,48	0.87	3 (6%)	51,54,54	1.09	5 (9%)
35	LMT	a	418	-	36,36,36	0.49	1 (2%)	47,47,47	0.74	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	Y	101	-	41,41,41	0.98	1 (2%)	56,56,56	1.82	17 (30%)
23	CLA	D	401	41	69,73,73	2.08	19 (27%)	83,113,113	2.90	32 (38%)
23	CLA	A	404	1	69,73,73	2.07	20 (28%)	83,113,113	2.82	31 (37%)
29	PL9	D	407	-	55,55,55	0.67	2 (3%)	68,69,69	1.66	19 (27%)
29	PL9	a	415	-	55,55,55	0.65	1 (1%)	68,69,69	2.00	20 (29%)
25	BCR	c	515	-	41,41,41	0.98	1 (2%)	56,56,56	1.67	14 (25%)
26	SQD	L	102	-	53,54,54	1.03	3 (5%)	62,65,65	1.53	10 (16%)
23	CLA	C	510	3	69,73,73	2.07	21 (30%)	83,113,113	2.87	29 (34%)
35	LMT	B	632	-	25,25,36	0.45	0	30,30,47	0.71	0
25	BCR	A	408	-	41,41,41	0.99	1 (2%)	56,56,56	1.65	16 (28%)
23	CLA	b	606	2	69,73,73	2.00	20 (28%)	83,113,113	2.87	29 (34%)
23	CLA	b	609	2	69,73,73	2.06	21 (30%)	83,113,113	2.82	29 (34%)
29	PL9	d	405	-	55,55,55	0.64	2 (3%)	68,69,69	1.86	22 (32%)
23	CLA	C	504	3	69,73,73	2.05	19 (27%)	83,113,113	2.84	26 (31%)
25	BCR	b	617	-	41,41,41	1.06	1 (2%)	56,56,56	1.39	6 (10%)
36	HTG	B	624	-	19,19,19	0.98	1 (5%)	23,24,24	1.38	4 (17%)
26	SQD	A	409	-	53,54,54	0.98	3 (5%)	62,65,65	1.84	13 (20%)
23	CLA	c	509	3	69,73,73	2.10	20 (28%)	83,113,113	2.82	30 (36%)
23	CLA	C	507	3	69,73,73	2.05	21 (30%)	83,113,113	2.78	32 (38%)
23	CLA	B	610	2	69,73,73	2.03	19 (27%)	83,113,113	2.79	26 (31%)

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
37	DGD	c	516	-	-	15/51/91/95	0/2/2/2
36	HTG	b	626	-	-	0/10/30/30	0/1/1/1
23	CLA	B	609	2	-	5/39/115/115	-
38	HEM	e	103	6,5	-	8/14/54/54	-
23	CLA	C	508	41	-	9/39/115/115	-
31	LHG	d	408	-	-	17/53/53/53	-
29	PL9	A	413	-	-	11/53/73/73	0/1/1/1
23	CLA	B	613	2	-	4/39/115/115	-
36	HTG	B	629	-	-	1/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMG	C	501	-	-	11/46/66/70	0/1/1/1
36	HTG	V	203	-	-	0/2/19/30	0/1/1/1
26	SQD	f	101	-	-	16/38/58/69	0/1/1/1
23	CLA	c	501	3	-	10/39/115/115	-
25	BCR	c	514	-	-	2/29/63/63	0/2/2/2
25	BCR	B	620	-	-	0/29/63/63	0/2/2/2
36	HTG	B	630	-	-	1/10/30/30	0/1/1/1
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
25	BCR	D	406	-	-	7/29/63/63	0/2/2/2
31	LHG	b	630	-	-	19/53/53/53	-
23	CLA	B	604	2	-	8/39/115/115	-
35	LMT	b	628	-	-	9/17/37/61	0/1/1/2
23	CLA	c	507	41	-	10/39/115/115	-
24	PHO	A	406	-	-	5/37/103/103	0/5/6/6
36	HTG	b	625	-	-	5/10/30/30	0/1/1/1
24	PHO	a	407	-	-	5/37/103/103	0/5/6/6
25	BCR	B	618	-	-	2/29/63/63	0/2/2/2
34	LMG	m	101	-	-	16/46/66/70	0/1/1/1
23	CLA	c	513	3	-	6/39/115/115	-
26	SQD	B	621	-	-	21/49/69/69	0/1/1/1
23	CLA	B	615	2	-	14/39/115/115	-
23	CLA	c	504	41	-	12/39/115/115	-
23	CLA	D	405	4	-	7/39/115/115	-
27	GOL	B	627	-	-	4/4/4/4	-
26	SQD	D	413	-	-	14/38/58/69	0/1/1/1
37	DGD	C	517	-	-	15/51/91/95	0/2/2/2
27	GOL	A	410	-	-	4/4/4/4	-
23	CLA	d	403	4	-	8/39/115/115	-
23	CLA	b	613	2	-	7/39/115/115	-
23	CLA	B	605	2	-	13/39/115/115	-
23	CLA	B	614	2	-	5/39/115/115	-
23	CLA	C	502	3	-	7/39/115/115	-
23	CLA	C	509	3	-	6/39/115/115	-
35	LMT	M	103	-	-	14/21/61/61	0/2/2/2
23	CLA	C	513	3	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	A	405	41	-	10/39/115/115	-
25	BCR	a	410	-	-	0/29/63/63	0/2/2/2
25	BCR	H	101	-	-	4/29/63/63	0/2/2/2
31	LHG	A	415	-	-	11/53/53/53	-
23	CLA	c	502	3	-	10/39/115/115	-
23	CLA	C	506	3	-	9/39/115/115	-
23	CLA	c	503	3	-	5/39/115/115	-
36	HTG	b	621	-	-	2/10/30/30	0/1/1/1
34	LMG	a	417	-	-	14/46/66/70	0/1/1/1
36	HTG	C	523	-	-	0/10/30/30	0/1/1/1
38	HEM	E	103	6,5	-	6/14/54/54	-
25	BCR	C	527	-	-	1/29/63/63	0/2/2/2
27	GOL	B	628	-	-	4/4/4/4	-
35	LMT	B	633	-	-	5/21/61/61	0/2/2/2
36	HTG	B	626	-	-	4/10/30/30	0/1/1/1
23	CLA	C	511	3	-	13/39/115/115	-
35	LMT	b	620	-	-	5/17/37/61	0/1/1/2
24	PHO	D	402	-	-	5/37/103/103	0/5/6/6
25	BCR	y	101	-	-	4/29/63/63	0/2/2/2
31	LHG	E	101	-	-	17/46/46/53	-
36	HTG	c	521	-	-	3/10/30/30	0/1/1/1
35	LMT	B	623	-	-	8/21/61/61	0/2/2/2
37	DGD	H	102	-	-	10/51/91/95	0/2/2/2
34	LMG	C	520	-	-	16/46/66/70	0/1/1/1
31	LHG	d	407	-	-	23/53/53/53	-
23	CLA	c	505	3	-	7/39/115/115	-
23	CLA	B	617	2	-	9/39/115/115	-
37	DGD	h	103	-	-	11/51/91/95	0/2/2/2
34	LMG	c	520	-	-	8/46/66/70	0/1/1/1
23	CLA	D	404	4	-	4/39/115/115	-
23	CLA	b	605	2	-	13/39/115/115	-
25	BCR	d	404	-	-	8/29/63/63	0/2/2/2
35	LMT	E	102	-	-	10/21/61/61	0/2/2/2
31	LHG	e	101	-	-	14/46/46/53	-
23	CLA	b	604	2	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	506	3	-	12/39/115/115	-
23	CLA	a	405	41	-	5/39/115/115	-
40	HEC	V	202	16	1/1/3/7	4/14/54/54	-
23	CLA	B	607	2	-	5/39/115/115	-
23	CLA	b	602	2	-	4/39/115/115	-
26	SQD	a	413	-	-	16/49/69/69	0/1/1/1
24	PHO	a	408	-	-	2/37/103/103	0/5/6/6
25	BCR	k	101	-	-	1/29/63/63	0/2/2/2
23	CLA	b	610	41	-	7/39/115/115	-
35	LMT	M	101	-	-	2/21/61/61	0/2/2/2
37	DGD	c	518	-	-	6/51/91/95	0/2/2/2
27	GOL	b	624	-	-	2/4/4/4	-
31	LHG	D	408	-	-	18/53/53/53	-
23	CLA	C	503	3	-	11/39/115/115	-
23	CLA	b	614	2	-	15/39/115/115	-
23	CLA	B	608	41	-	5/39/115/115	-
23	CLA	b	601	41	-	21/39/115/115	-
26	SQD	a	411	-	-	14/49/69/69	0/1/1/1
23	CLA	C	505	41	-	6/39/115/115	-
23	CLA	d	402	4	-	3/39/115/115	-
34	LMG	Z	101	-	-	14/31/51/70	0/1/1/1
35	LMT	D	403	-	-	8/21/61/61	0/2/2/2
23	CLA	a	406	41	-	10/39/115/115	-
23	CLA	b	611	2	-	10/39/115/115	-
27	GOL	C	525	-	-	2/4/4/4	-
36	HTG	h	101	-	-	3/7/27/30	0/1/1/1
35	LMT	B	634	-	-	6/17/38/61	0/1/1/2
36	HTG	b	622	-	-	1/10/30/30	0/1/1/1
23	CLA	b	616	2	-	13/39/115/115	-
40	HEC	v	201	16	1/1/3/7	4/14/54/54	-
34	LMG	C	521	-	-	9/46/66/70	0/1/1/1
23	CLA	b	612	2	-	5/39/115/115	-
25	BCR	C	515	-	-	1/29/63/63	0/2/2/2
23	CLA	b	607	41	-	11/39/115/115	-
23	CLA	B	616	2	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMG	c	519	-	-	13/46/66/70	0/1/1/1
36	HTG	c	522	-	-	2/10/30/30	0/1/1/1
36	HTG	b	623	-	-	2/10/30/30	0/1/1/1
27	GOL	O	302	-	-	2/4/4/4	-
31	LHG	D	409	-	-	14/53/53/53	-
23	CLA	B	612	2	-	4/39/115/115	-
23	CLA	B	602	41	-	13/39/115/115	-
35	LMT	e	102	-	-	8/21/61/61	0/2/2/2
26	SQD	A	411	-	-	14/49/69/69	0/1/1/1
23	CLA	a	409	1	-	9/39/115/115	-
34	LMG	B	622	-	-	12/46/66/70	0/1/1/1
37	DGD	c	517	-	-	14/51/91/95	0/2/2/2
23	CLA	C	512	3	-	6/39/115/115	-
35	LMT	m	103	-	-	8/21/61/61	0/2/2/2
36	HTG	C	524	-	-	1/6/6/30	-
27	GOL	d	401	-	-	2/4/4/4	-
34	LMG	J	101	39	-	10/46/66/70	0/1/1/1
36	HTG	B	625	-	-	5/10/30/30	0/1/1/1
25	BCR	t	101	-	-	1/29/63/63	0/2/2/2
25	BCR	b	618	-	-	2/29/63/63	0/2/2/2
25	BCR	h	102	-	-	0/29/63/63	0/2/2/2
23	CLA	B	603	2	-	10/39/115/115	-
23	CLA	c	512	3	-	9/39/115/115	-
25	BCR	T	101	-	-	5/29/63/63	0/2/2/2
23	CLA	c	510	3	-	8/39/115/115	-
31	LHG	L	101	-	-	16/53/53/53	-
23	CLA	A	407	1	-	10/39/115/115	-
23	CLA	C	514	3	-	10/39/115/115	-
23	CLA	B	606	2	-	11/39/115/115	-
25	BCR	b	619	-	-	0/29/63/63	0/2/2/2
23	CLA	a	404	1	-	5/39/115/115	-
37	DGD	C	519	-	-	7/51/91/95	0/2/2/2
27	GOL	a	412	-	-	2/4/4/4	-
25	BCR	C	516	-	-	1/29/63/63	0/2/2/2
37	DGD	C	518	-	-	15/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	608	2	-	5/39/115/115	-
34	LMG	z	101	-	-	15/34/54/70	0/1/1/1
23	CLA	b	603	2	-	6/39/115/115	-
23	CLA	c	508	3	-	7/39/115/115	-
23	CLA	B	611	41	-	8/39/115/115	-
23	CLA	b	615	2	-	7/39/115/115	-
36	HTG	D	412	-	-	1/7/27/30	0/1/1/1
34	LMG	j	101	39	-	8/46/66/70	0/1/1/1
35	LMT	C	522	-	-	9/21/61/61	0/2/2/2
23	CLA	c	511	3	-	5/39/115/115	-
31	LHG	d	406	-	-	12/53/53/53	-
35	LMT	a	418	-	-	3/21/61/61	0/2/2/2
25	BCR	Y	101	-	-	3/29/63/63	0/2/2/2
23	CLA	D	401	41	-	8/39/115/115	-
23	CLA	A	404	1	-	3/39/115/115	-
29	PL9	D	407	-	-	7/53/73/73	0/1/1/1
29	PL9	a	415	-	-	16/53/73/73	0/1/1/1
25	BCR	c	515	-	-	0/29/63/63	0/2/2/2
26	SQD	L	102	-	-	22/49/69/69	0/1/1/1
23	CLA	C	510	3	-	16/39/115/115	-
35	LMT	B	632	-	-	7/17/37/61	0/1/1/2
25	BCR	A	408	-	-	1/29/63/63	0/2/2/2
23	CLA	b	606	2	-	10/39/115/115	-
23	CLA	b	609	2	-	8/39/115/115	-
29	PL9	d	405	-	-	6/53/73/73	0/1/1/1
23	CLA	C	504	3	-	5/39/115/115	-
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
36	HTG	B	624	-	-	4/10/30/30	0/1/1/1
26	SQD	A	409	-	-	14/49/69/69	0/1/1/1
23	CLA	c	509	3	-	15/39/115/115	-
23	CLA	C	507	3	-	16/39/115/115	-
23	CLA	B	610	2	-	9/39/115/115	-

The worst 5 of 1619 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	402	PHO	C1D-C2D	9.46	1.50	1.39
24	a	407	PHO	C1B-C2B	9.27	1.49	1.39
24	A	406	PHO	C1D-C2D	9.19	1.49	1.39
24	a	408	PHO	C1D-C2D	8.76	1.49	1.39
24	a	407	PHO	C1D-C2D	8.67	1.49	1.39

The worst 5 of 2866 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	402	PHO	C2D-C1D-ND	12.17	117.93	109.53
24	a	407	PHO	C2D-C1D-ND	12.13	117.90	109.53
24	A	406	PHO	C2D-C1D-ND	10.95	117.09	109.53
24	a	408	PHO	C2D-C1D-ND	10.67	116.90	109.53
23	D	405	CLA	C1D-ND-C4D	-10.30	99.02	106.33

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
40	V	202	HEC	NA
40	v	201	HEC	NA

5 of 1421 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	603	CLA	C2B-C3B-CAB-CBB
23	B	603	CLA	C4B-C3B-CAB-CBB
23	B	604	CLA	C2B-C3B-CAB-CBB
23	B	604	CLA	C4B-C3B-CAB-CBB
23	B	604	CLA	C2-C3-C5-C6

There are no ring outliers.

162 monomers are involved in 390 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	c	516	DGD	3	0
36	b	626	HTG	1	0
23	B	609	CLA	1	0
38	e	103	HEM	3	0
23	C	508	CLA	4	0
31	d	408	LHG	4	0
29	A	413	PL9	5	0
23	B	613	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	B	629	HTG	1	0
34	C	501	LMG	3	0
26	f	101	SQD	2	0
23	c	501	CLA	3	0
25	c	514	BCR	3	0
25	B	620	BCR	2	0
25	B	619	BCR	3	0
25	D	406	BCR	2	0
23	B	604	CLA	4	0
35	b	628	LMT	1	0
23	c	507	CLA	8	0
24	A	406	PHO	1	0
36	b	625	HTG	1	0
25	B	618	BCR	5	0
34	m	101	LMG	2	0
23	c	513	CLA	7	0
26	B	621	SQD	2	0
23	B	615	CLA	8	0
23	c	504	CLA	3	0
23	D	405	CLA	1	0
27	B	627	GOL	1	0
26	D	413	SQD	2	0
37	C	517	DGD	4	0
23	d	403	CLA	2	0
23	b	613	CLA	2	0
23	B	605	CLA	3	0
23	B	614	CLA	2	0
23	C	502	CLA	4	0
23	C	509	CLA	3	0
35	M	103	LMT	1	0
23	C	513	CLA	1	0
23	A	405	CLA	3	0
25	a	410	BCR	1	0
25	H	101	BCR	5	0
31	A	415	LHG	4	0
23	c	502	CLA	6	0
23	C	506	CLA	4	0
23	c	503	CLA	4	0
36	b	621	HTG	2	0
34	a	417	LMG	3	0
36	C	523	HTG	1	0
38	E	103	HEM	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	527	BCR	1	0
27	B	628	GOL	4	0
35	B	633	LMT	3	0
23	C	511	CLA	1	0
35	b	620	LMT	1	0
24	D	402	PHO	3	0
25	y	101	BCR	1	0
36	c	521	HTG	1	0
35	B	623	LMT	3	0
31	d	407	LHG	3	0
23	c	505	CLA	4	0
23	B	617	CLA	5	0
34	c	520	LMG	3	0
23	D	404	CLA	3	0
23	b	605	CLA	8	0
25	d	404	BCR	1	0
35	E	102	LMT	1	0
31	e	101	LHG	3	0
23	b	604	CLA	3	0
23	c	506	CLA	6	0
23	a	405	CLA	2	0
23	B	607	CLA	5	0
23	b	602	CLA	4	0
26	a	413	SQD	3	0
24	a	408	PHO	5	0
25	k	101	BCR	5	0
23	b	610	CLA	2	0
35	M	101	LMT	1	0
37	c	518	DGD	2	0
31	D	408	LHG	3	0
23	C	503	CLA	4	0
23	b	614	CLA	2	0
23	B	608	CLA	2	0
23	b	601	CLA	4	0
26	a	411	SQD	2	0
23	C	505	CLA	2	0
23	d	402	CLA	7	0
34	Z	101	LMG	2	0
35	D	403	LMT	2	0
23	a	406	CLA	4	0
23	b	611	CLA	3	0
36	h	101	HTG	1	0

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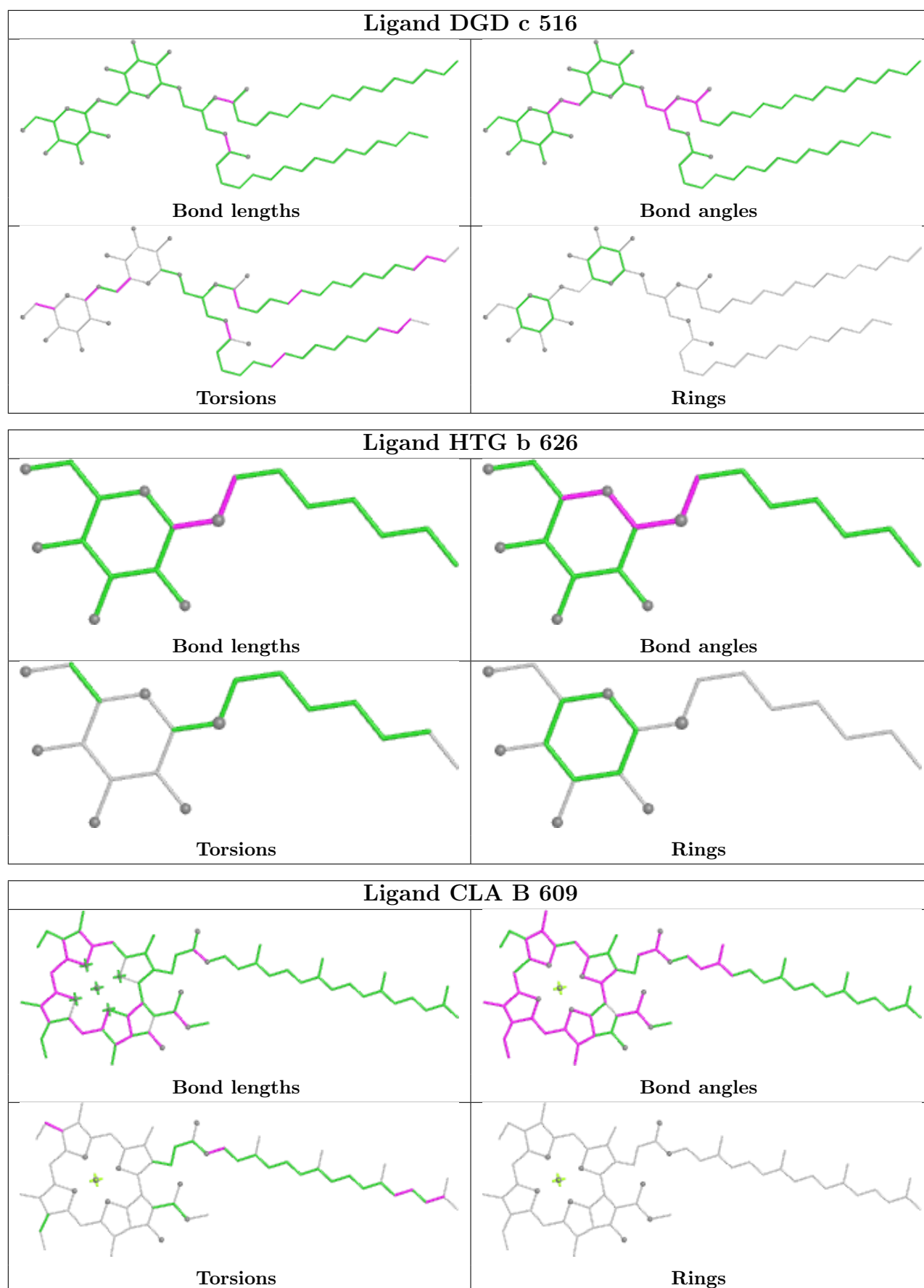
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	B	634	LMT	2	0
36	b	622	HTG	2	0
23	b	616	CLA	3	0
28	a	414	OEX	1	0
34	C	521	LMG	1	0
23	b	612	CLA	5	0
25	C	515	BCR	1	0
23	b	607	CLA	2	0
23	B	616	CLA	4	0
34	c	519	LMG	2	0
36	c	522	HTG	1	0
31	D	409	LHG	4	0
23	B	612	CLA	2	0
23	B	602	CLA	2	0
26	A	411	SQD	1	0
23	a	409	CLA	3	0
34	B	622	LMG	2	0
37	c	517	DGD	3	0
23	C	512	CLA	2	0
35	m	103	LMT	2	0
36	C	524	HTG	1	0
34	J	101	LMG	2	0
36	B	625	HTG	1	0
25	t	101	BCR	4	0
25	b	618	BCR	3	0
25	h	102	BCR	4	0
23	B	603	CLA	3	0
23	c	512	CLA	8	0
25	T	101	BCR	4	0
23	c	510	CLA	3	0
23	A	407	CLA	5	0
23	C	514	CLA	3	0
23	B	606	CLA	9	0
25	b	619	BCR	1	0
23	a	404	CLA	4	0
37	C	519	DGD	1	0
27	a	412	GOL	1	0
25	C	516	BCR	4	0
37	C	518	DGD	1	0
23	b	608	CLA	3	0
34	z	101	LMG	1	0
23	b	603	CLA	3	0

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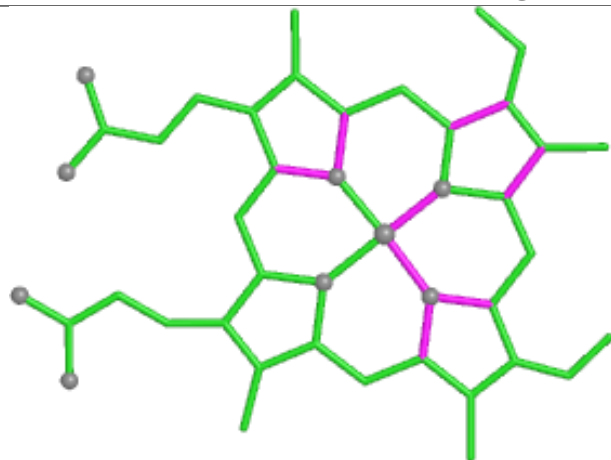
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	c	508	CLA	7	0
23	B	611	CLA	1	0
23	b	615	CLA	6	0
36	D	412	HTG	1	0
34	j	101	LMG	5	0
35	C	522	LMT	1	0
23	c	511	CLA	8	0
31	d	406	LHG	1	0
25	Y	101	BCR	3	0
23	D	401	CLA	5	0
23	A	404	CLA	6	0
29	D	407	PL9	1	0
29	a	415	PL9	8	0
25	c	515	BCR	1	0
26	L	102	SQD	4	0
23	C	510	CLA	3	0
35	B	632	LMT	1	0
25	A	408	BCR	2	0
23	b	606	CLA	3	0
23	b	609	CLA	3	0
29	d	405	PL9	2	0
23	C	504	CLA	4	0
25	b	617	BCR	1	0
36	B	624	HTG	4	0
26	A	409	SQD	2	0
23	c	509	CLA	5	0
23	C	507	CLA	9	0
23	B	610	CLA	4	0

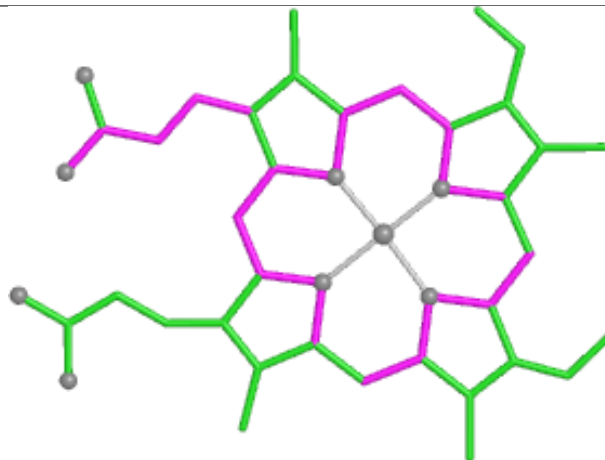
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



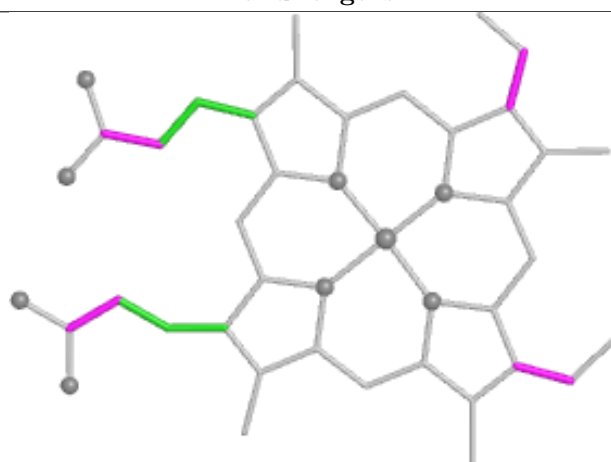
Ligand HEM e 103



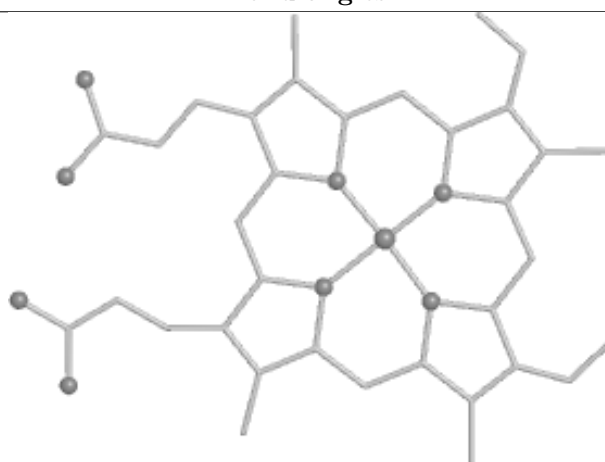
Bond lengths



Bond angles

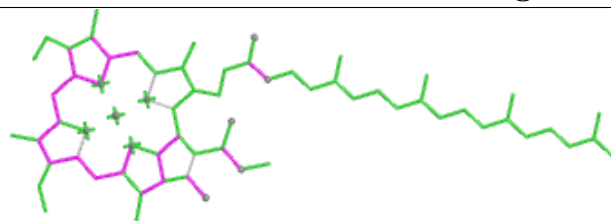


Torsions

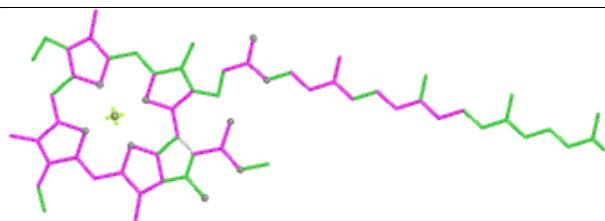


Rings

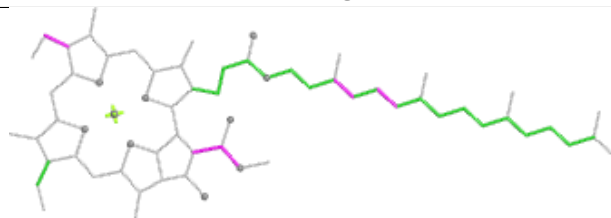
Ligand CLA C 508



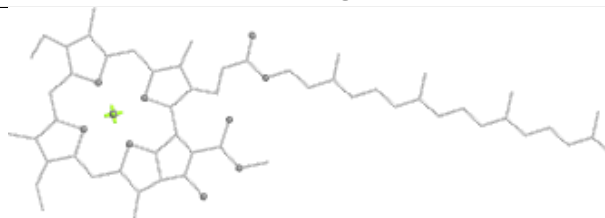
Bond lengths



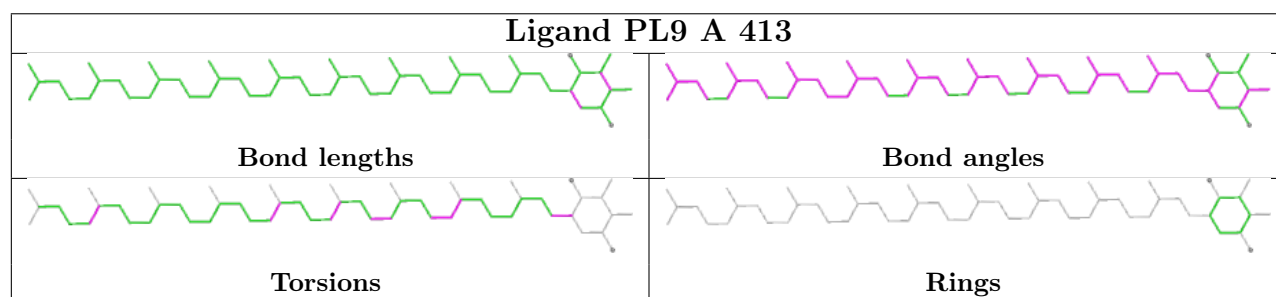
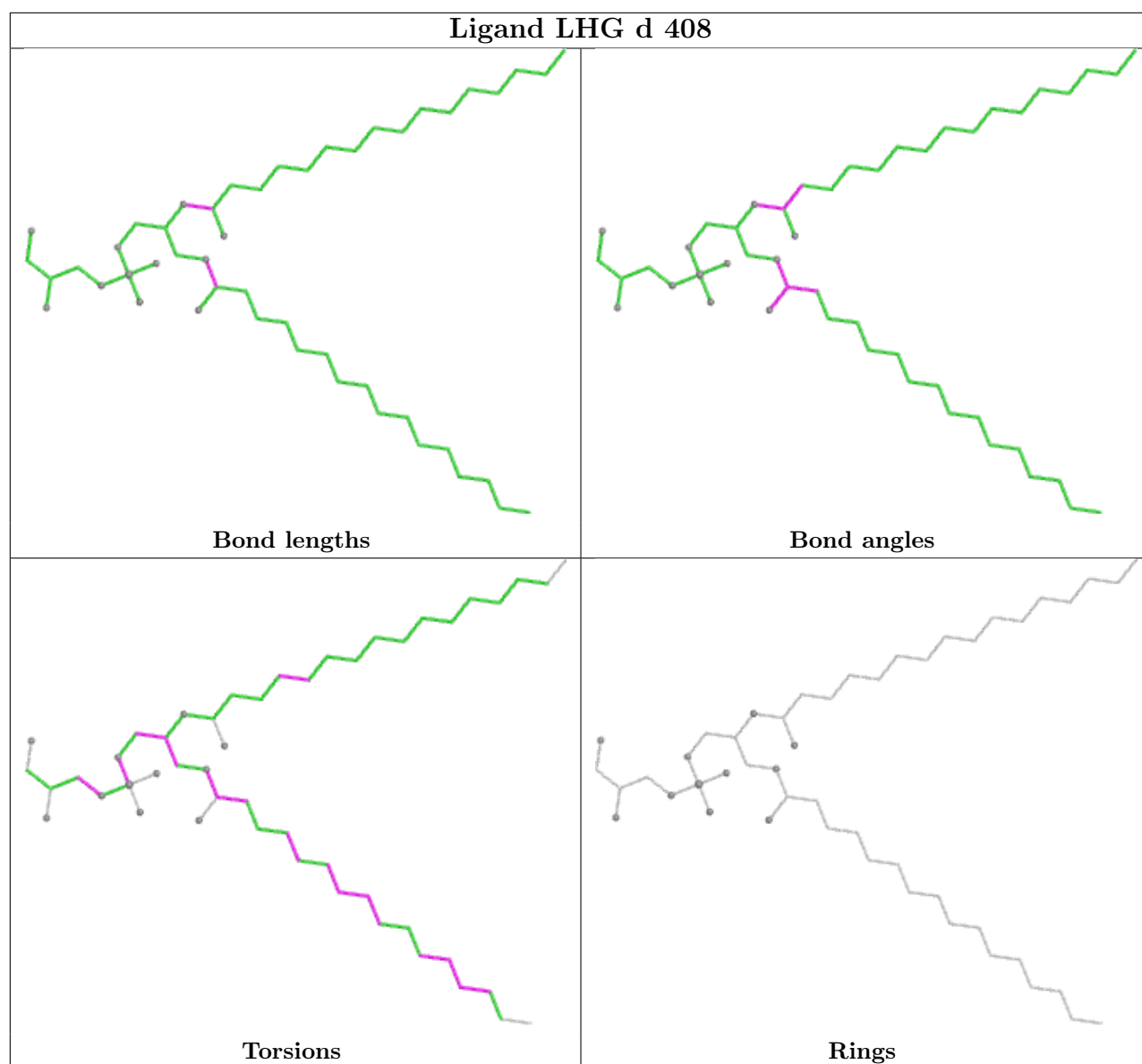
Bond angles

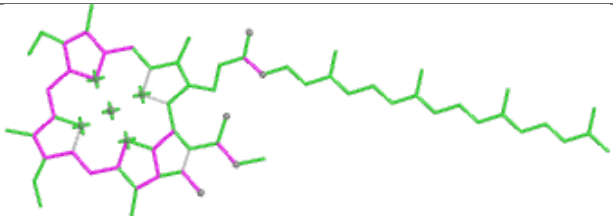
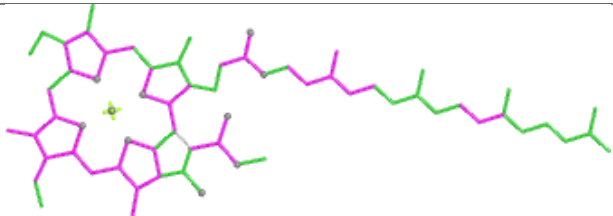
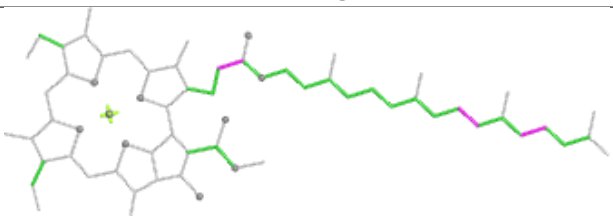
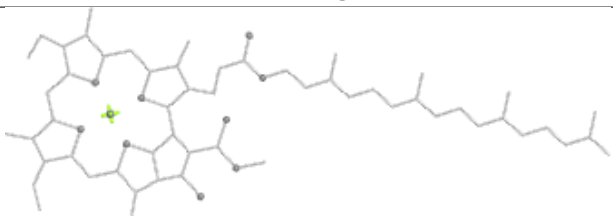


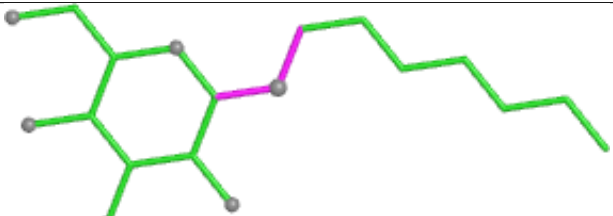
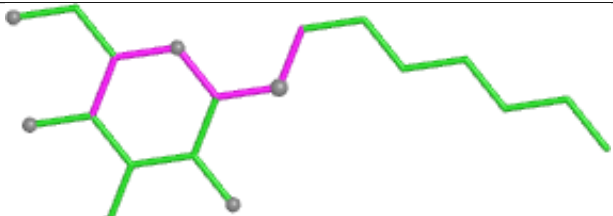
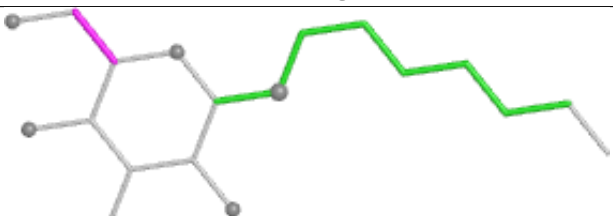
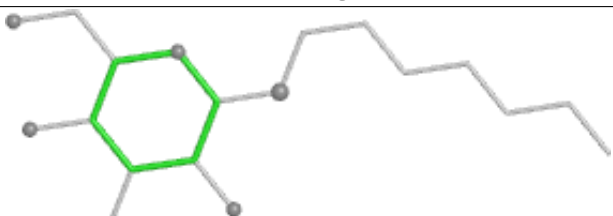
Torsions

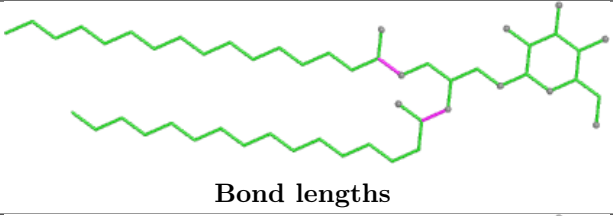
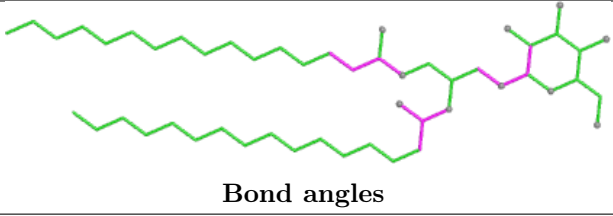
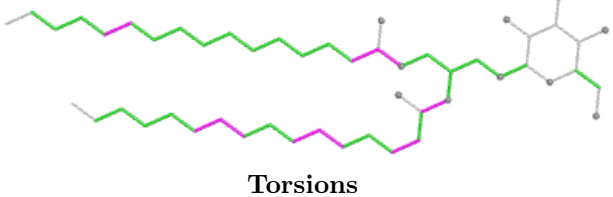
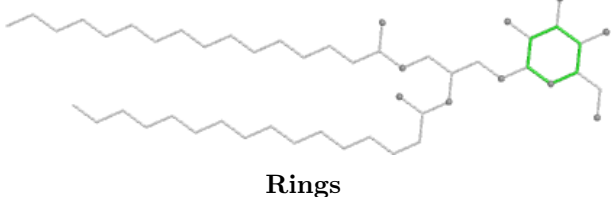


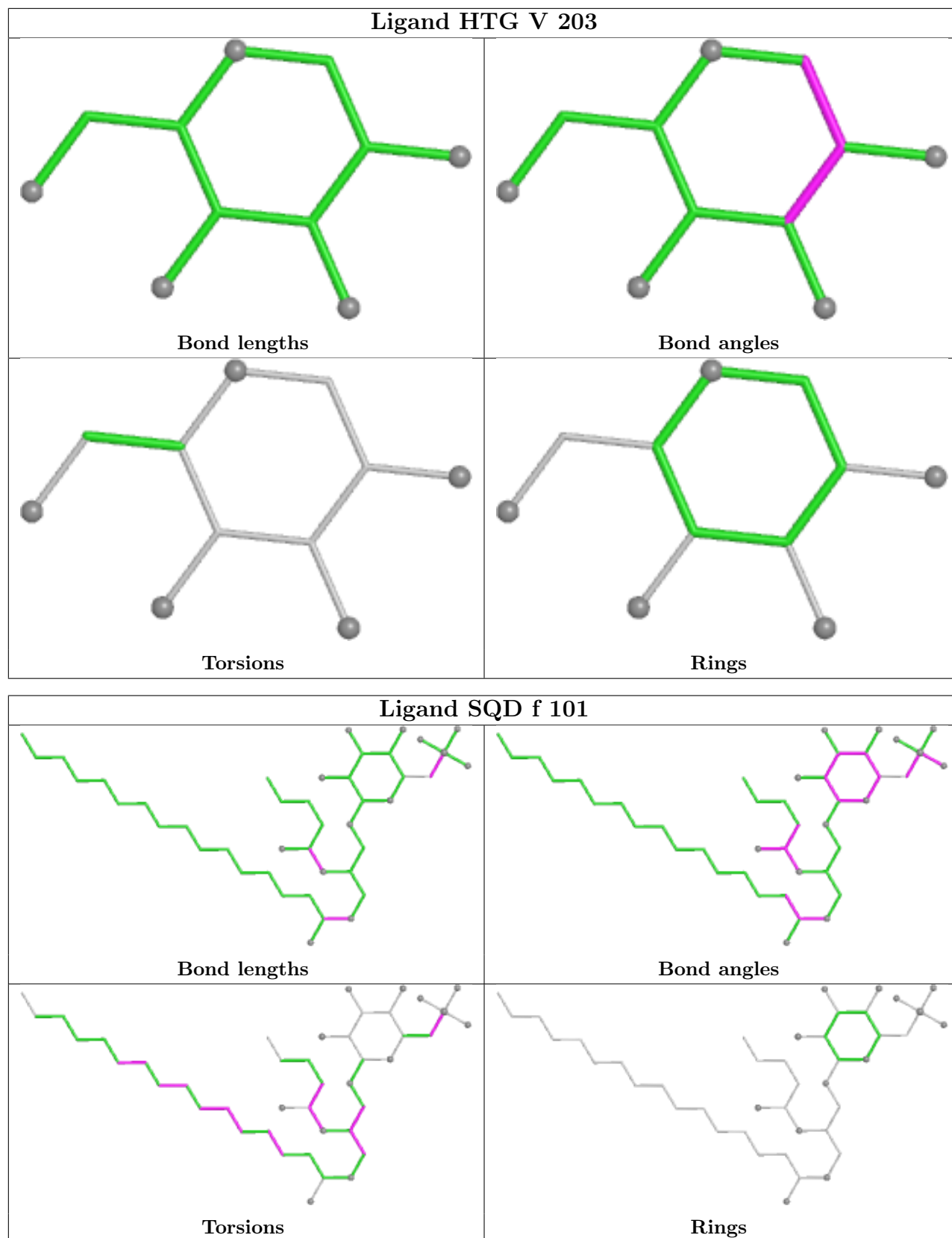
Rings

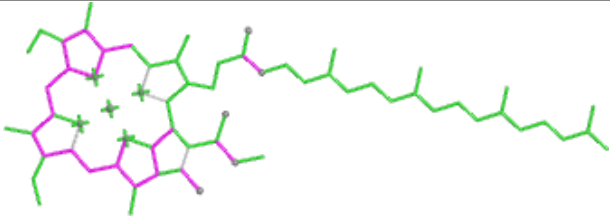
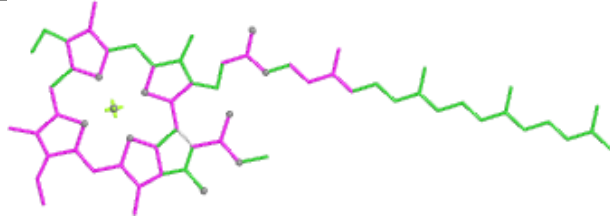
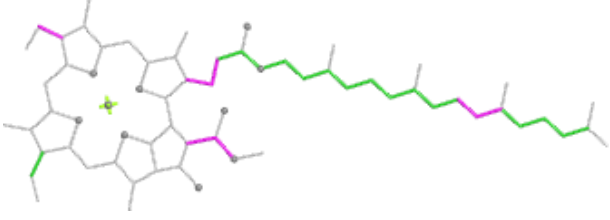
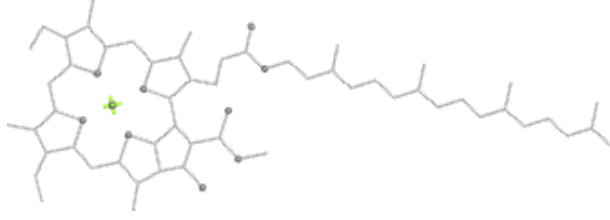
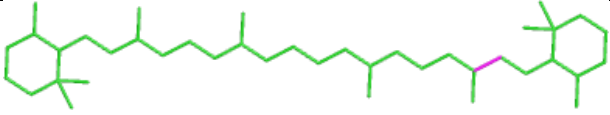
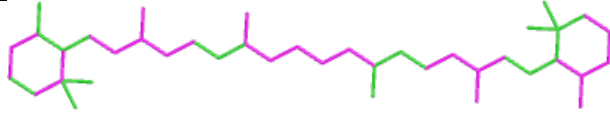
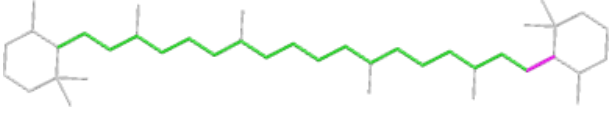
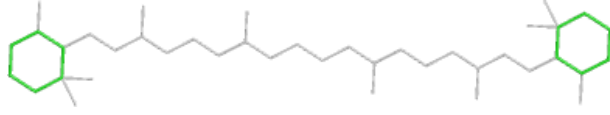
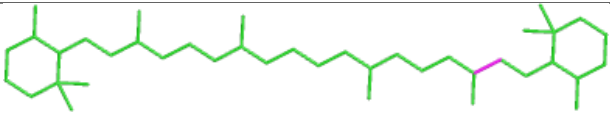
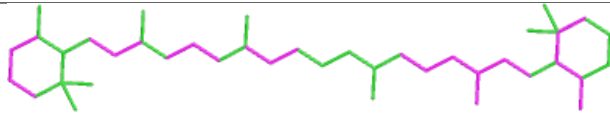
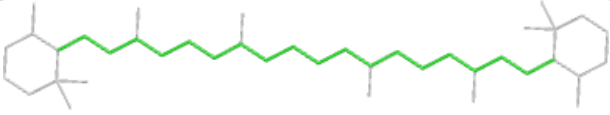
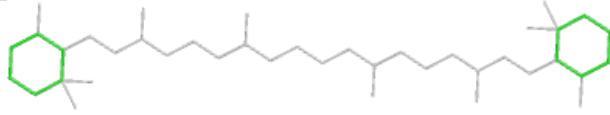


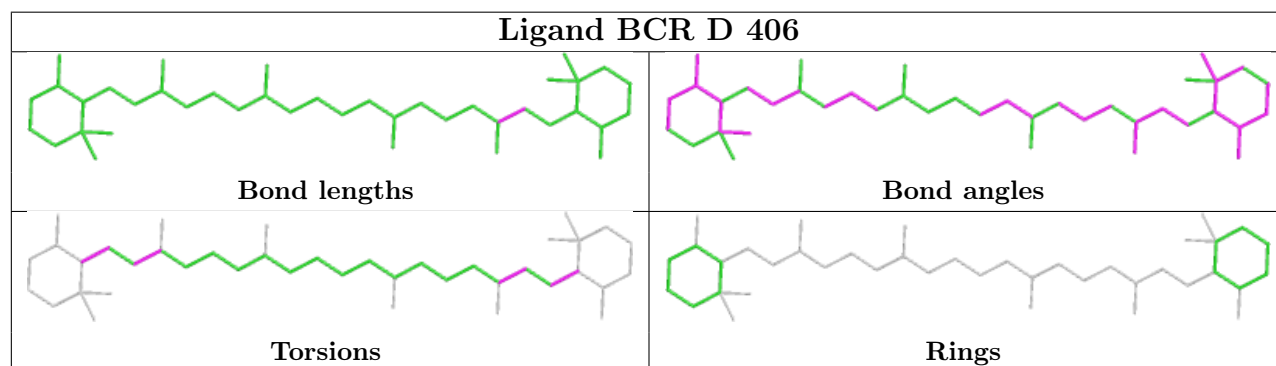
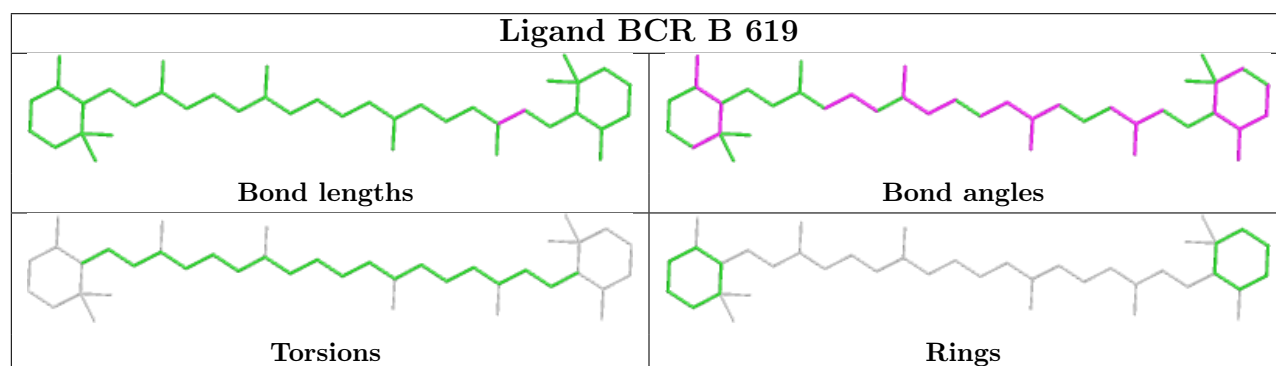
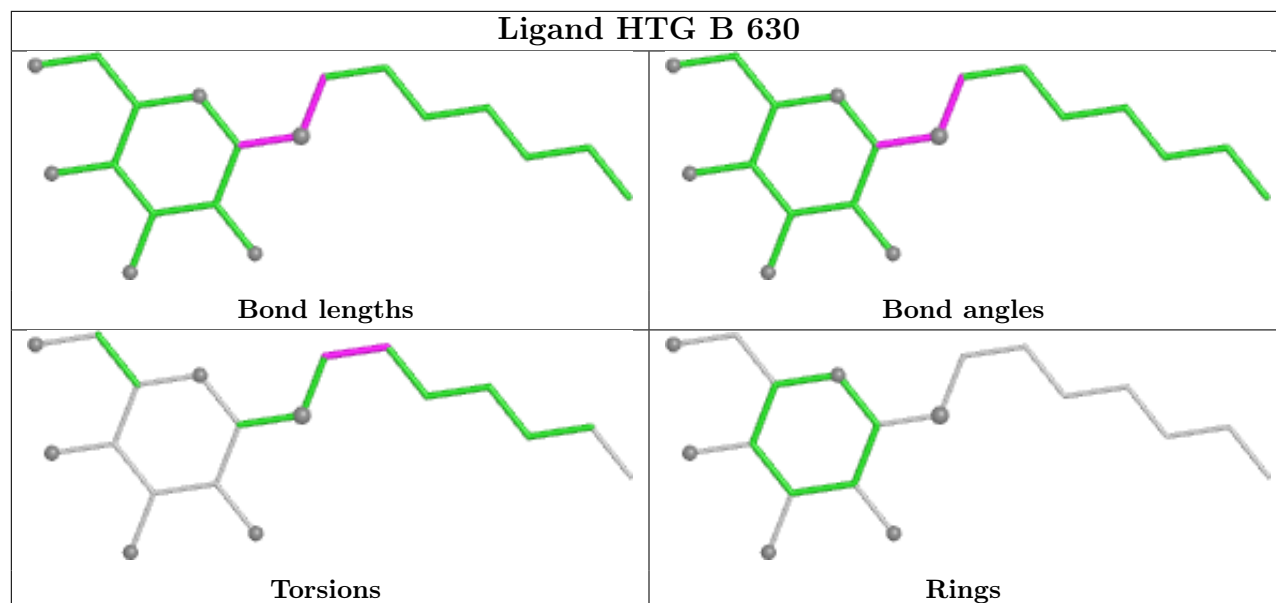
Ligand CLA B 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

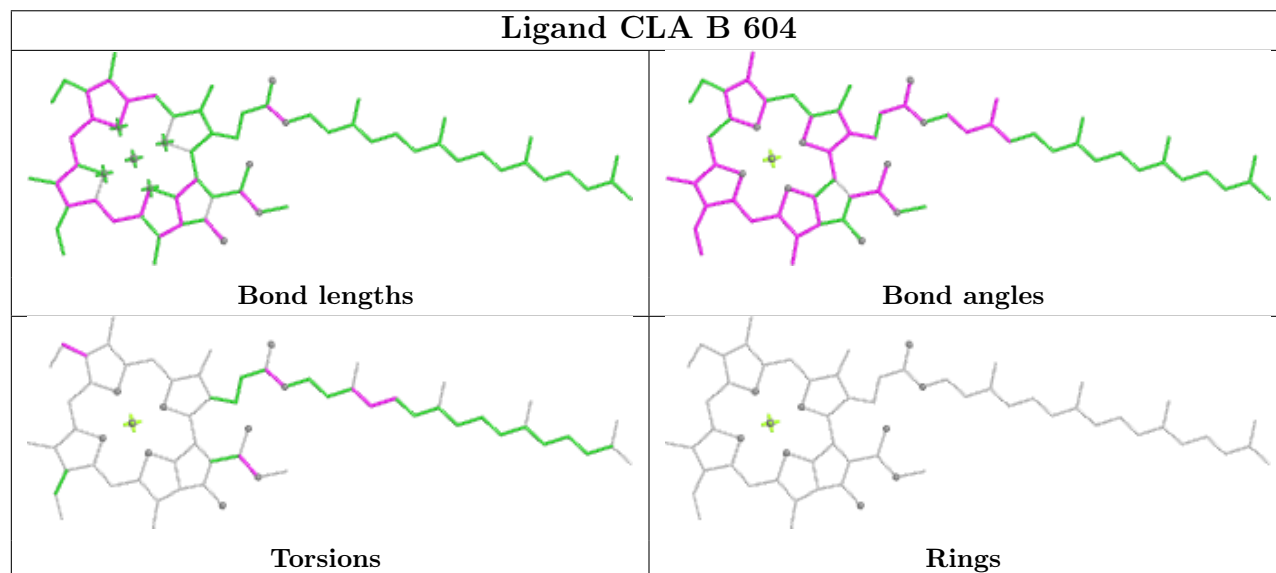
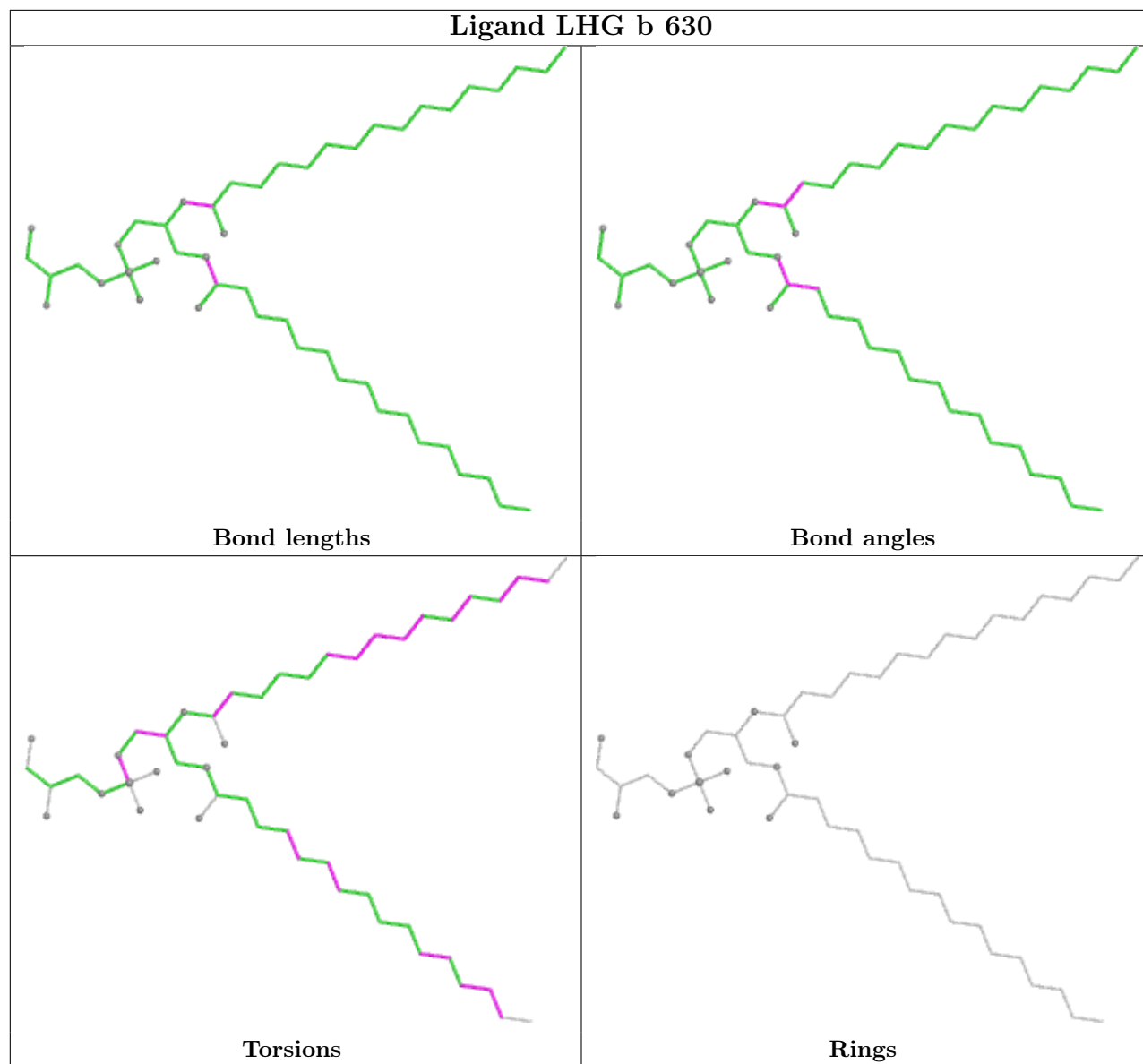
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Bond lengths	Bond angles
	
Torsions	Rings

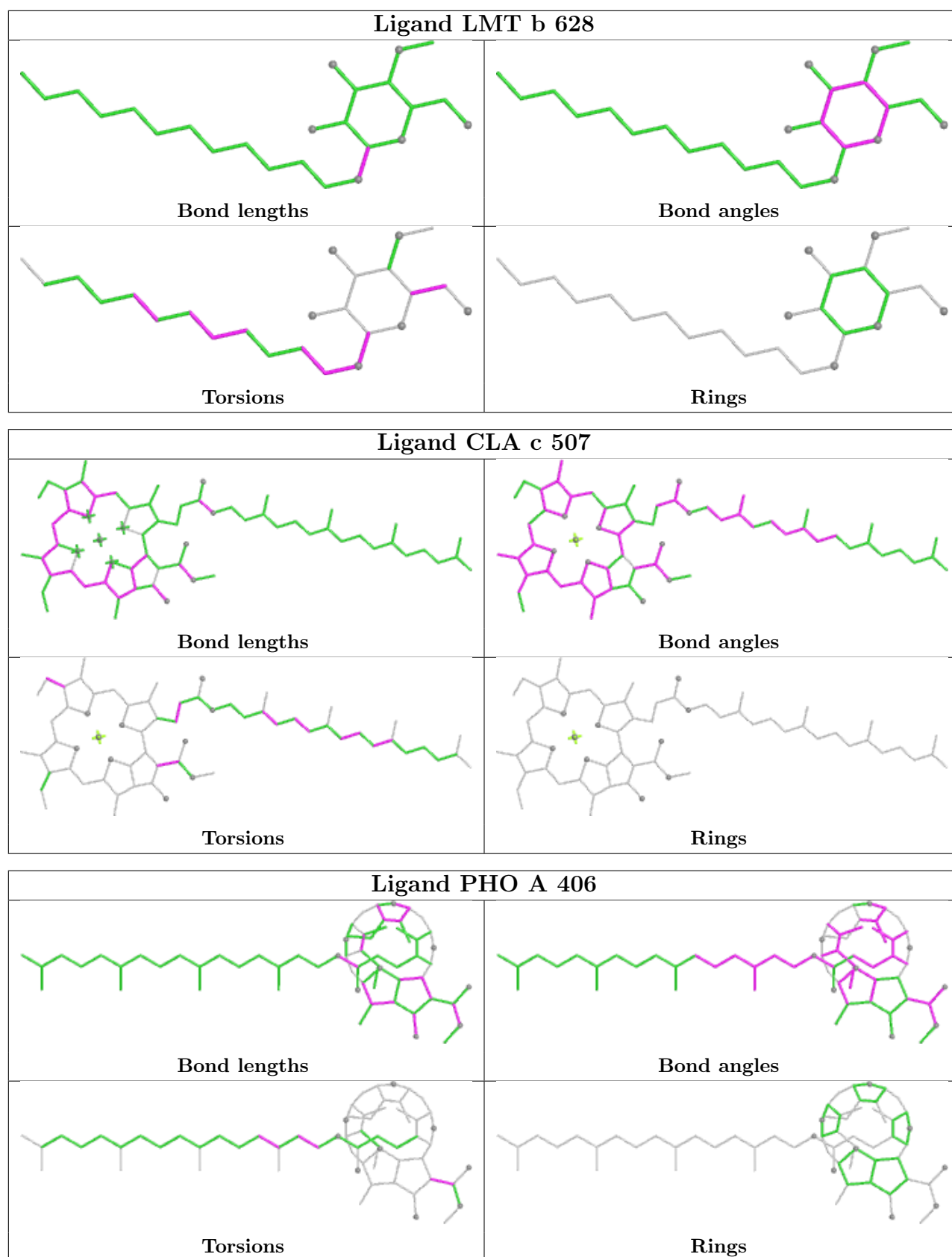
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Bond lengths	Bond angles
	
Torsions	Rings

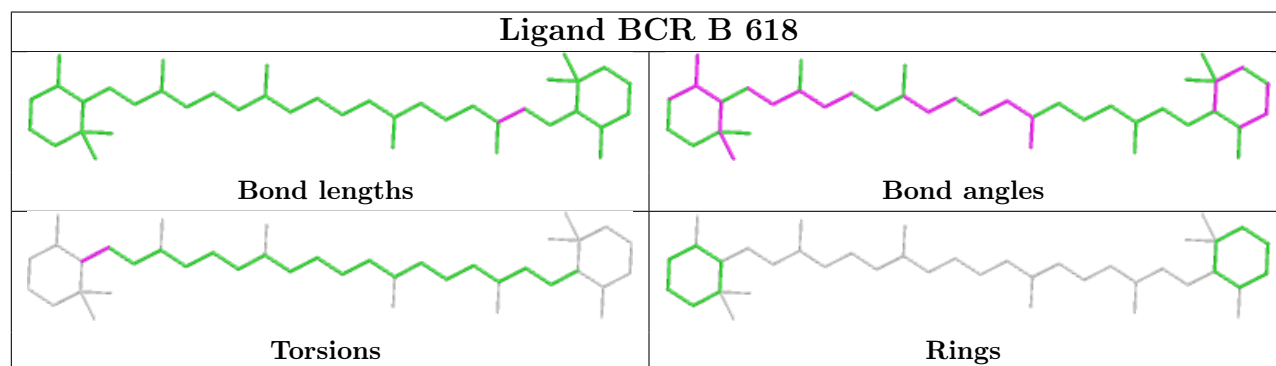
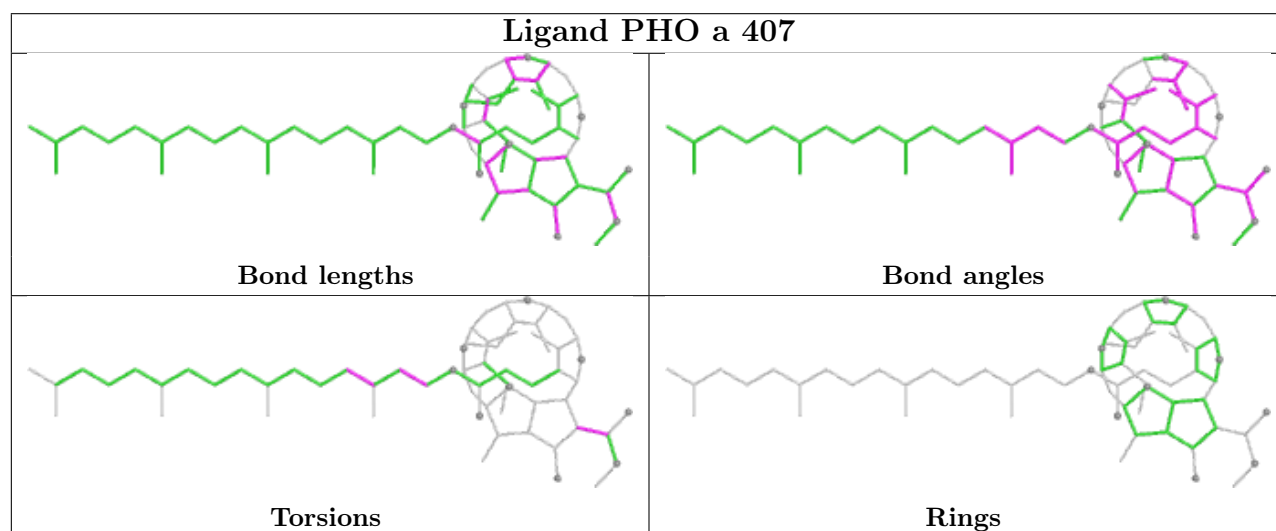
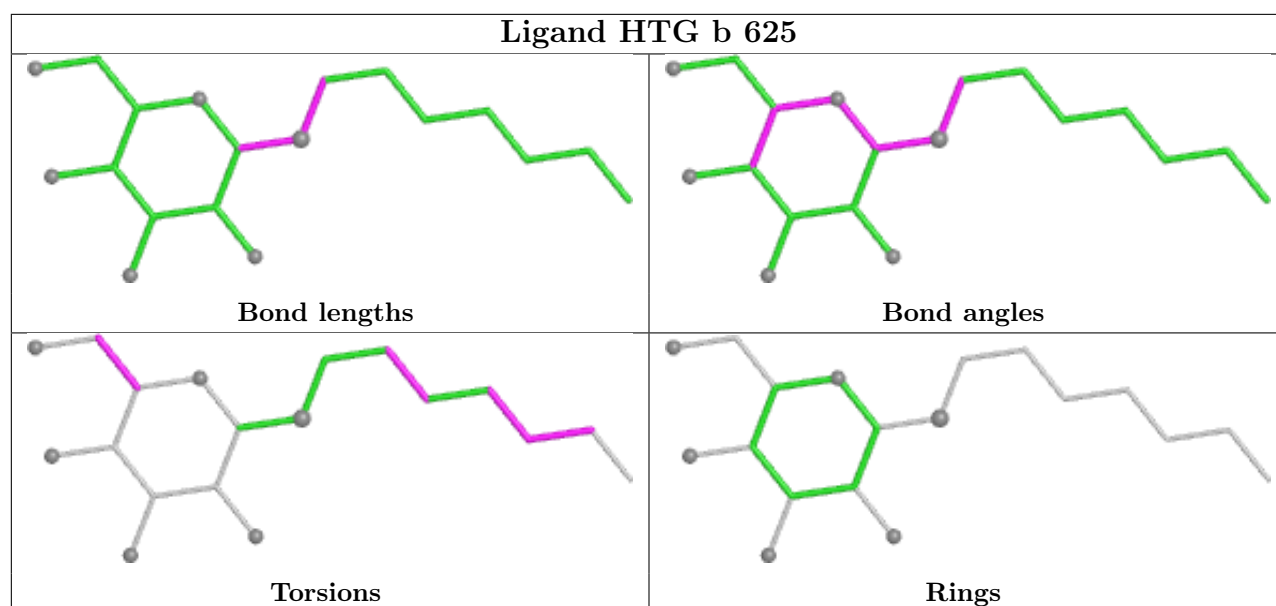


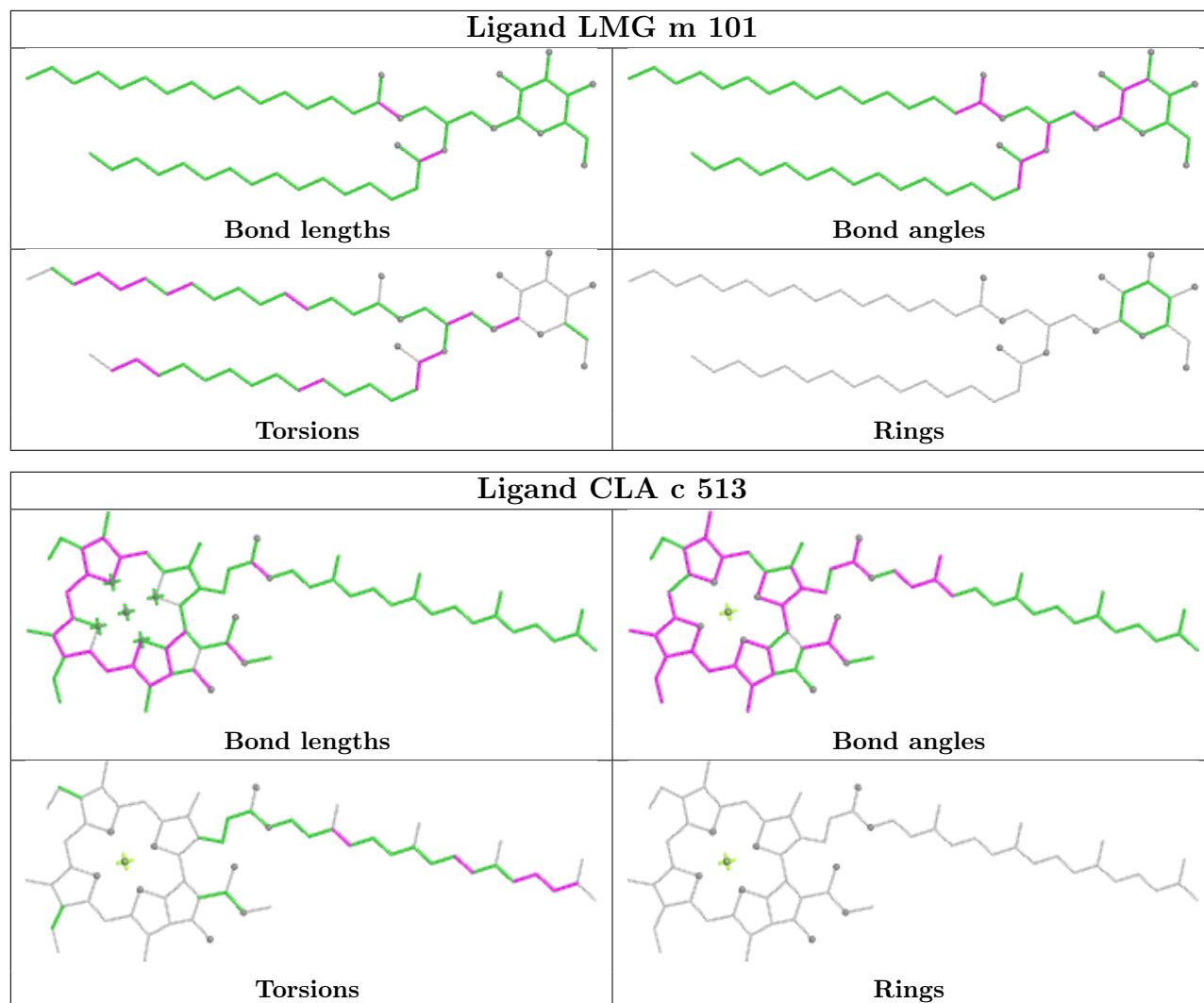
Ligand CLA c 501	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR c 514	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 620	
 Bond lengths	 Bond angles
 Torsions	 Rings

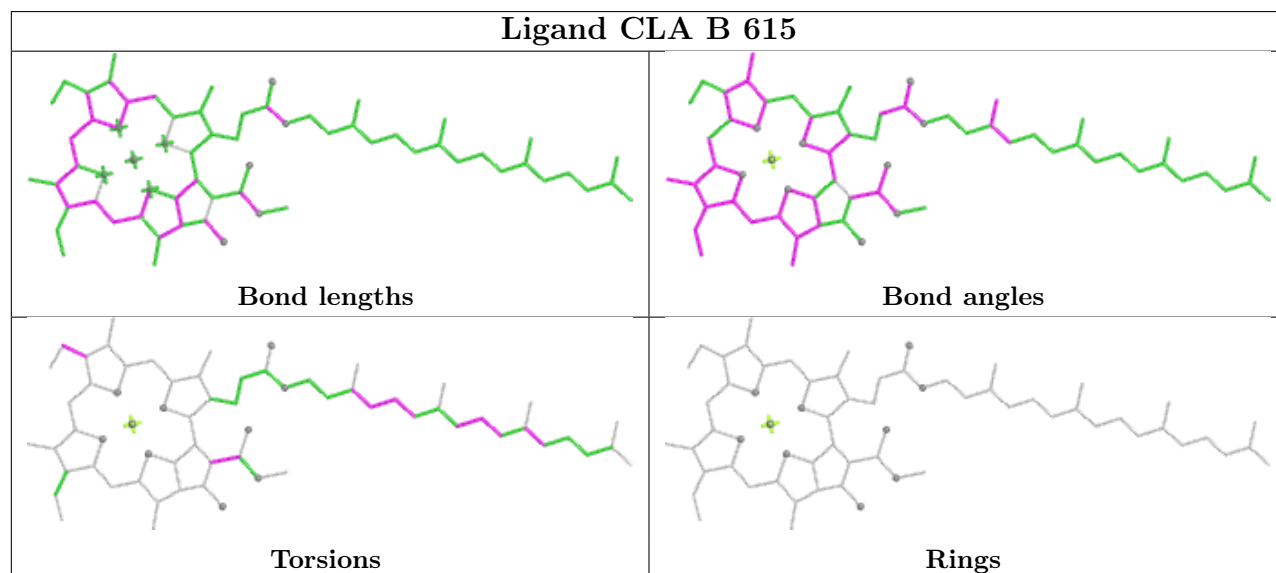
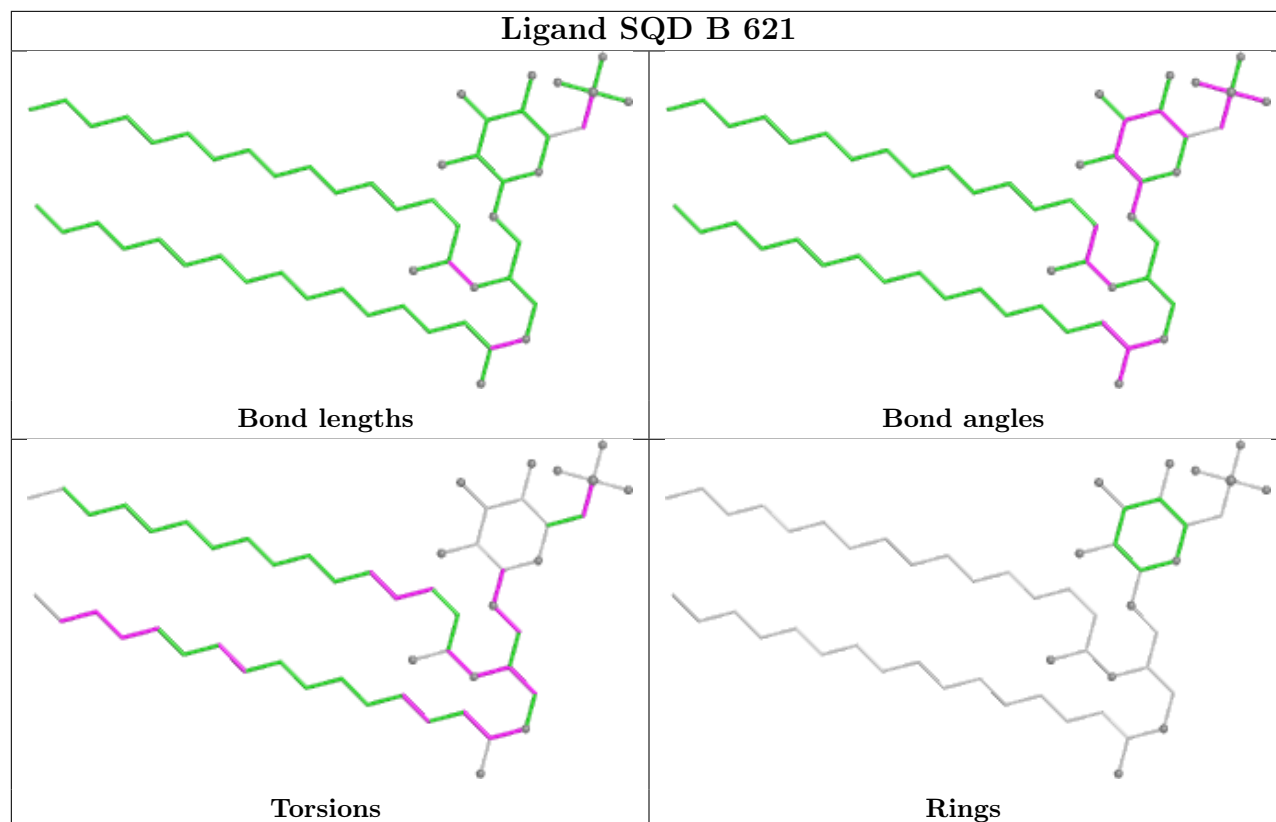




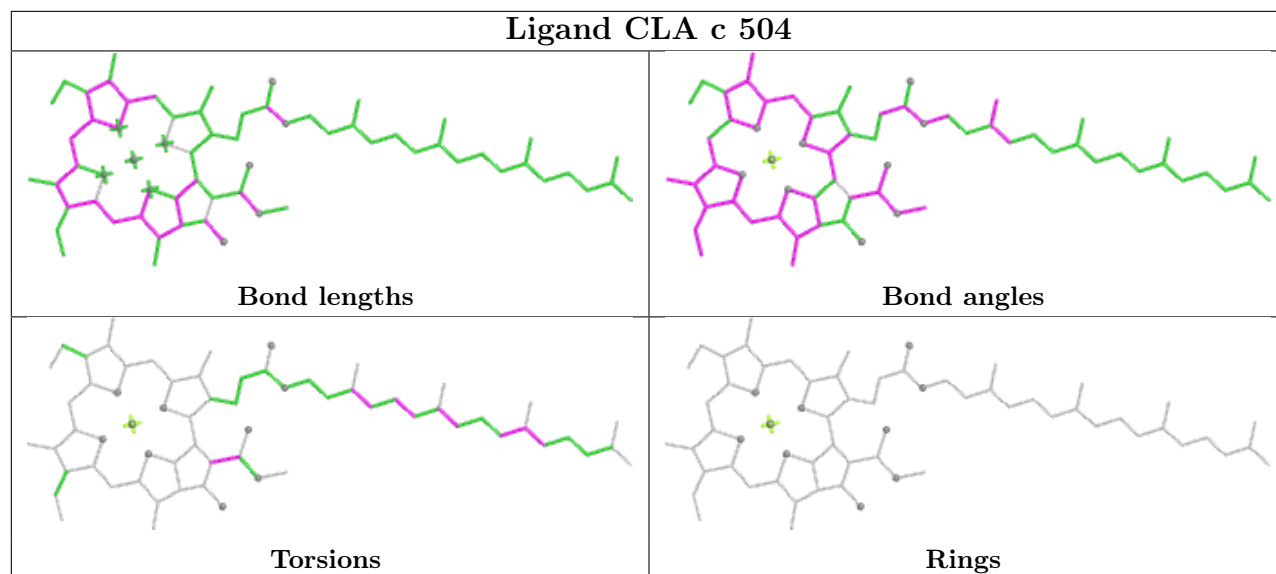




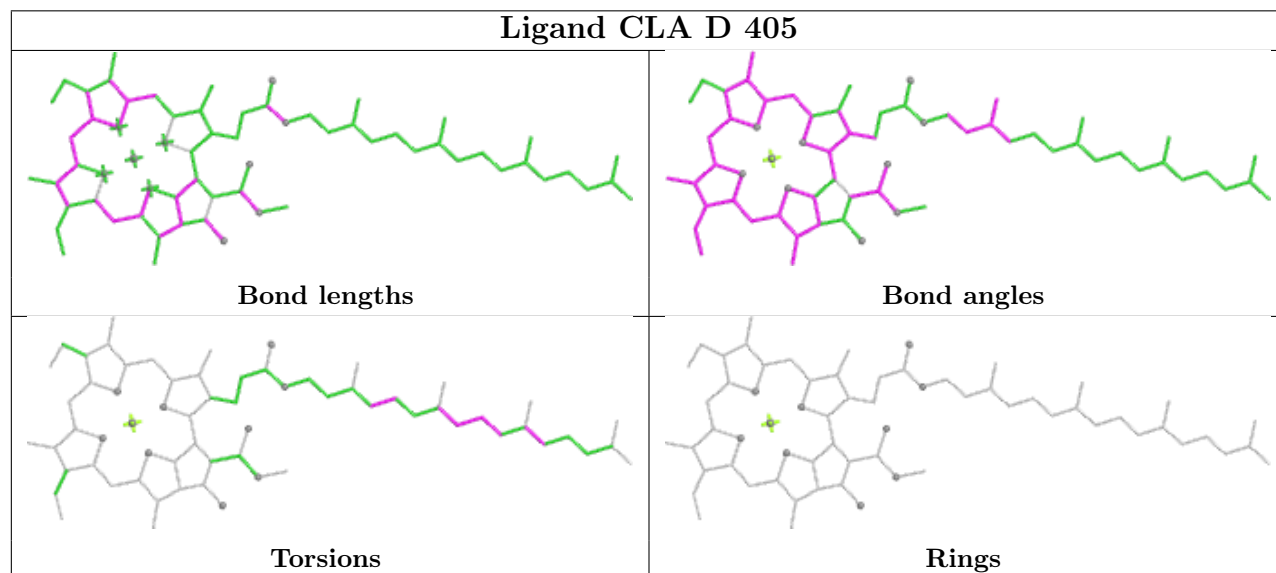


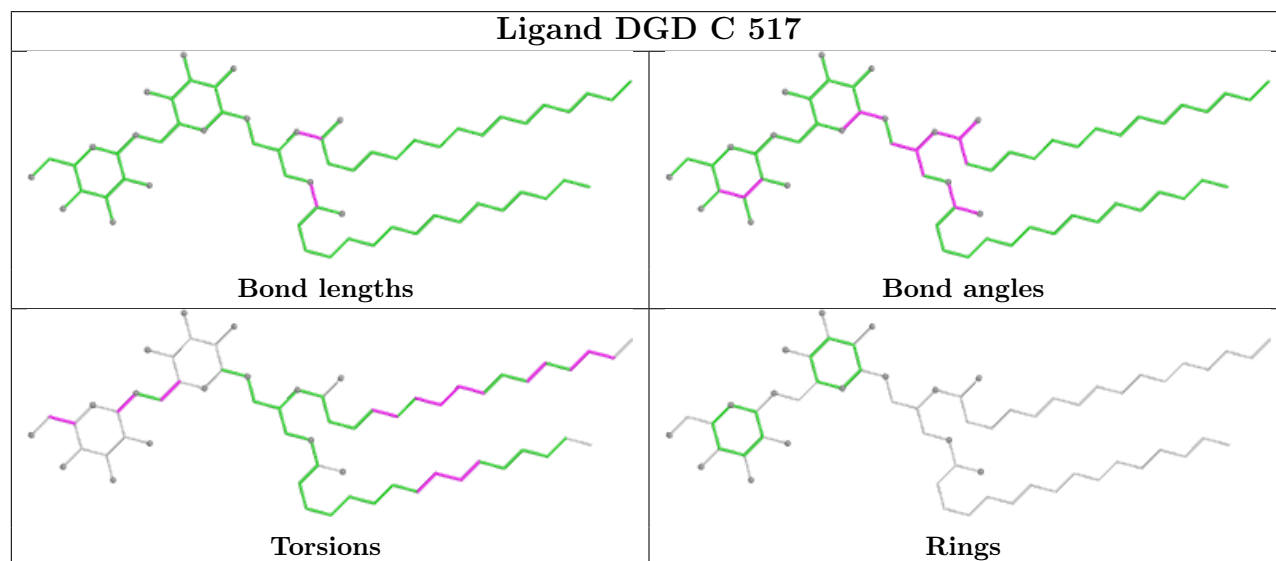
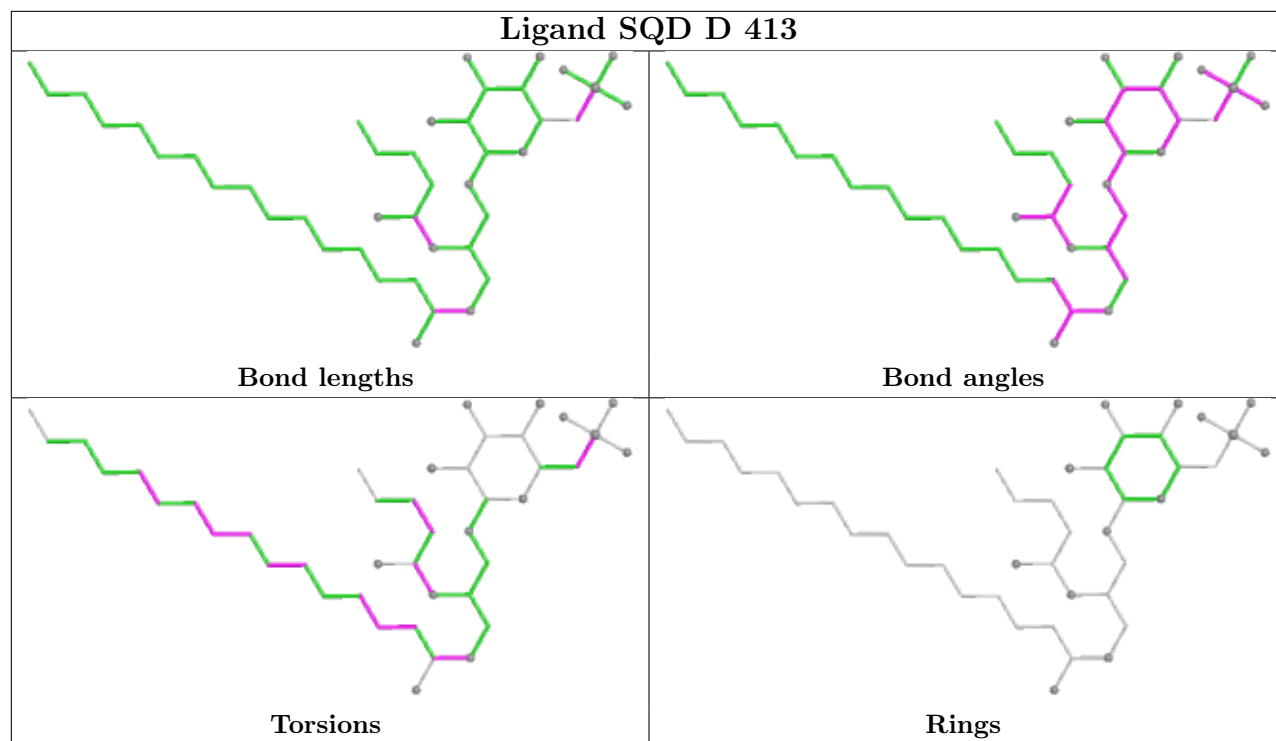


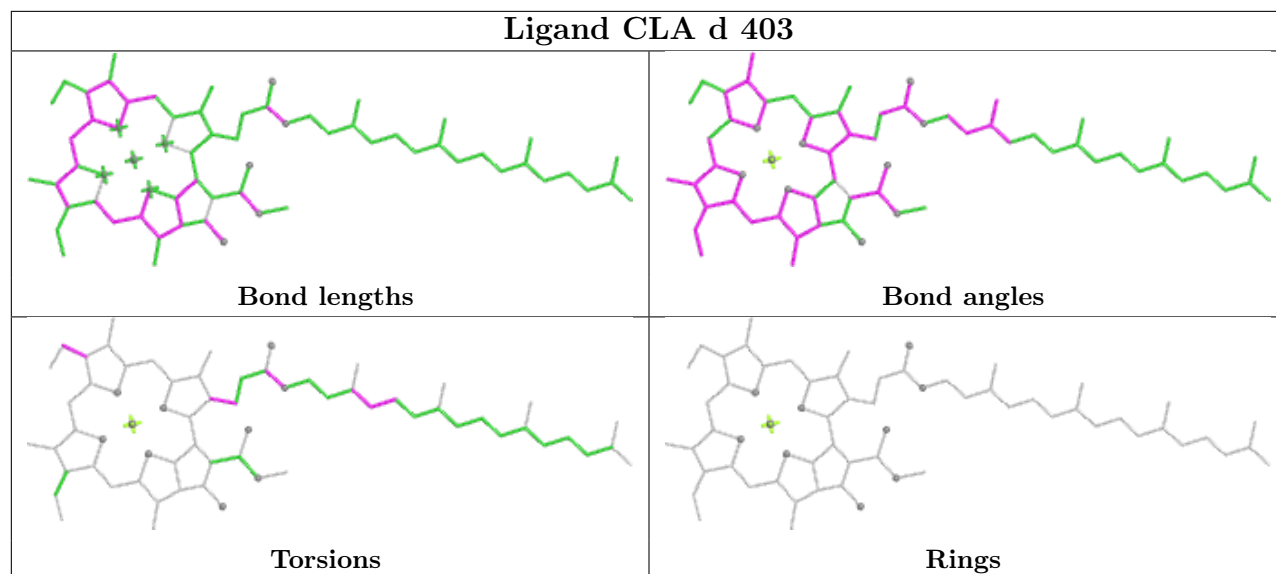
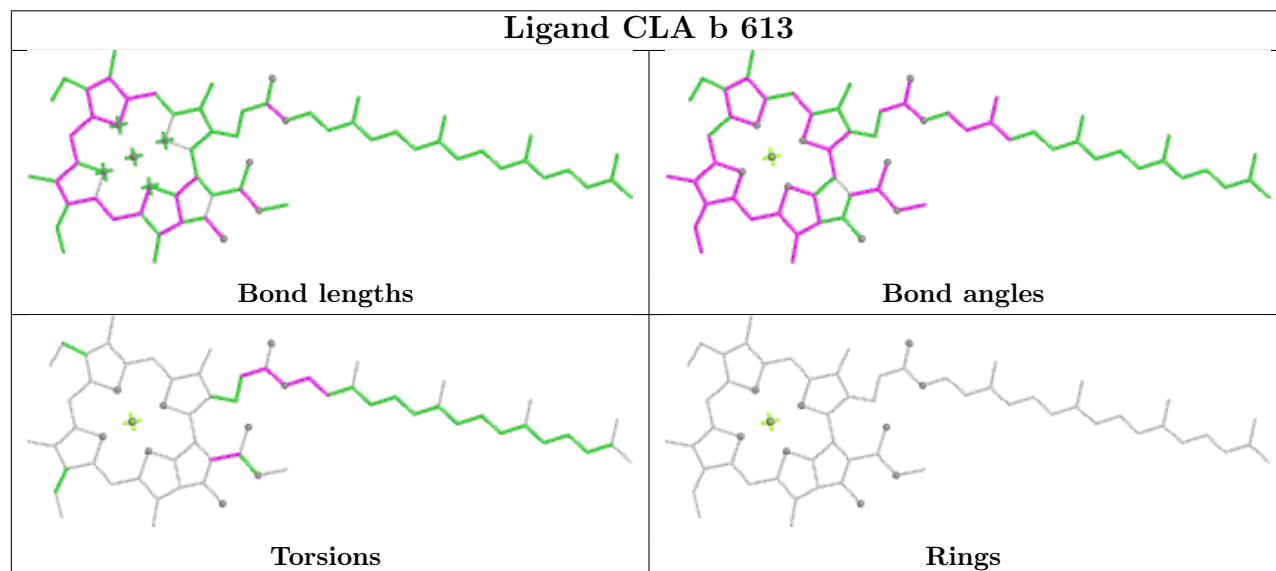
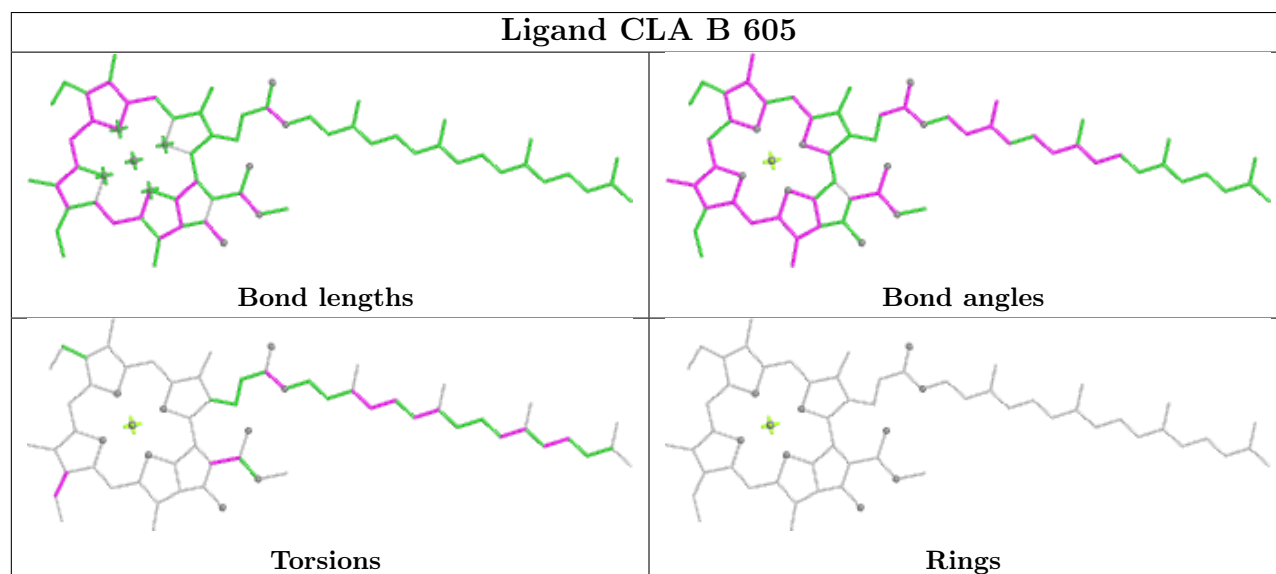
Ligand CLA c 504

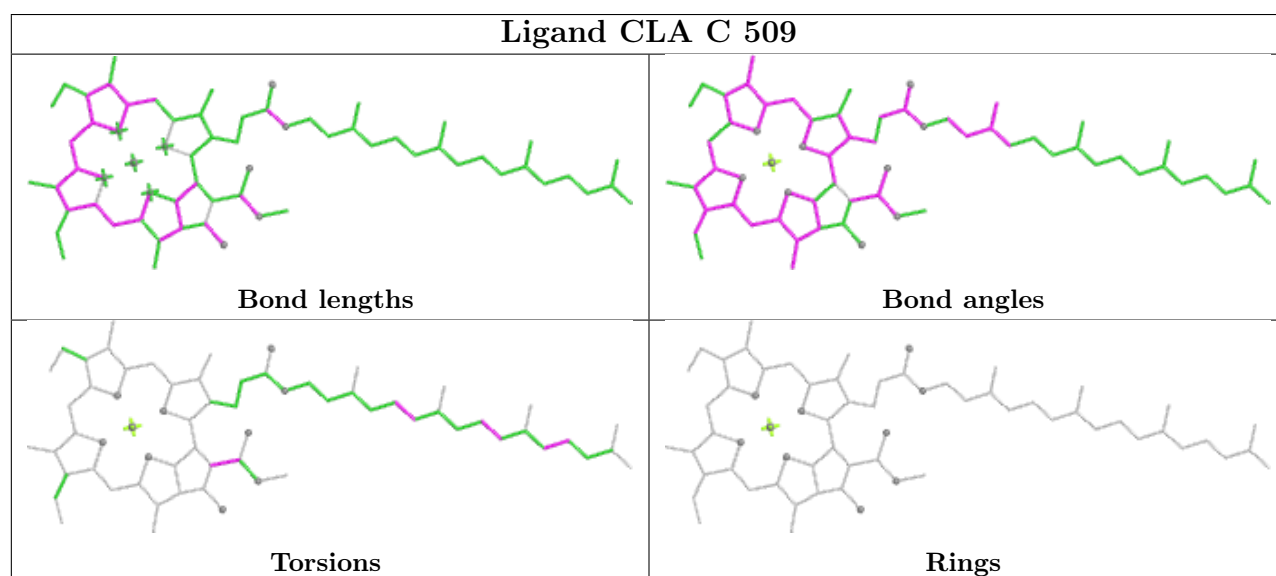
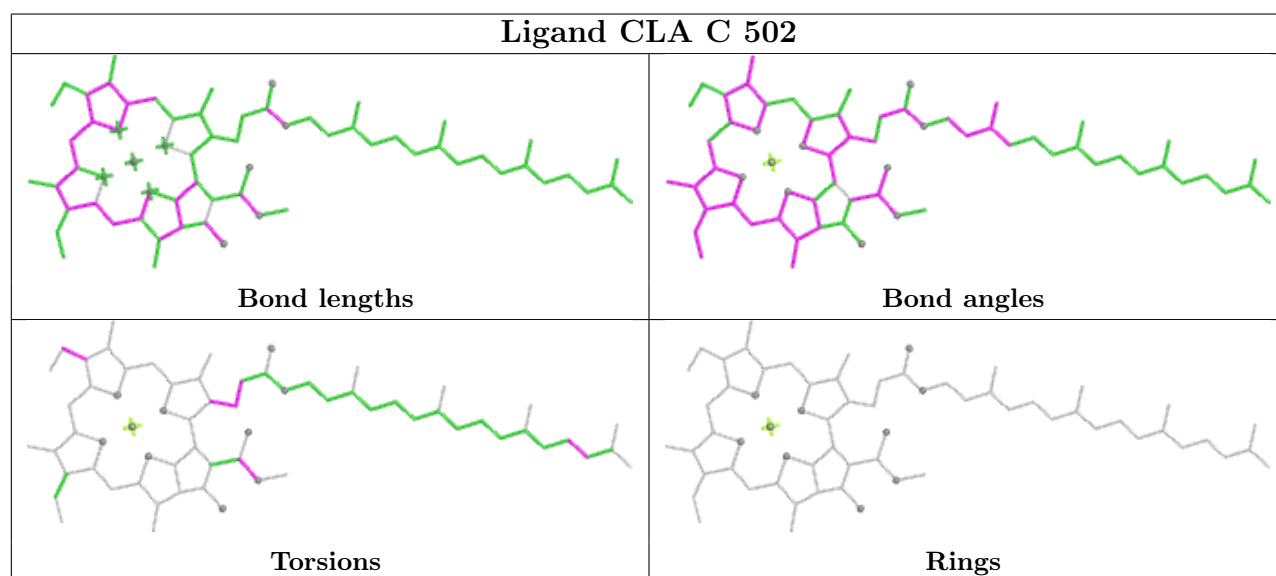
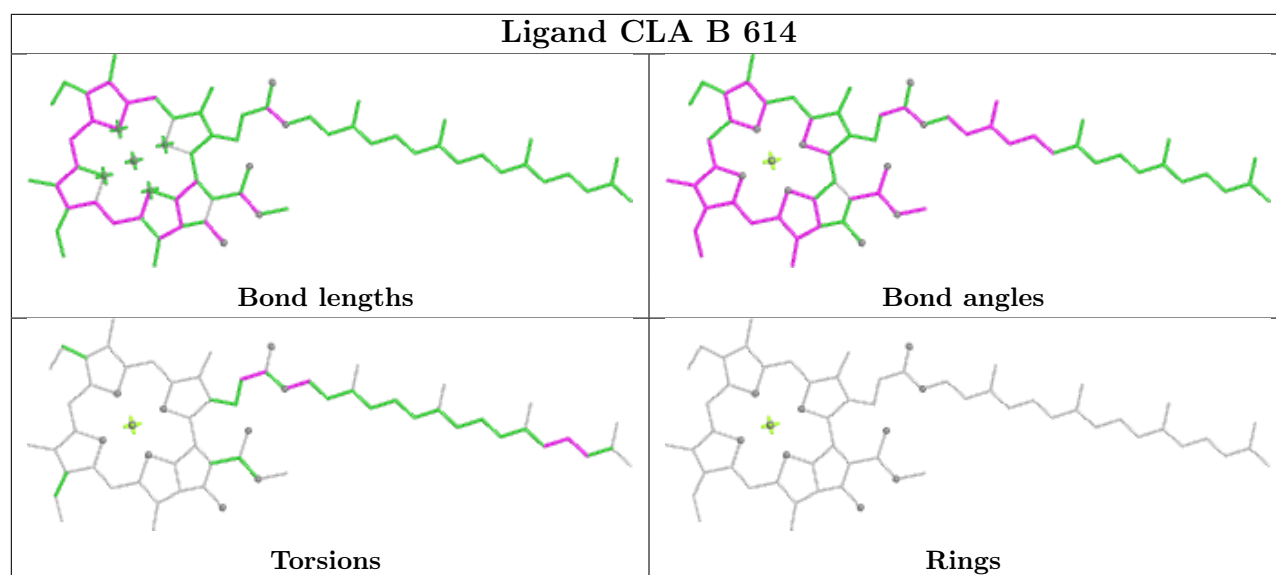


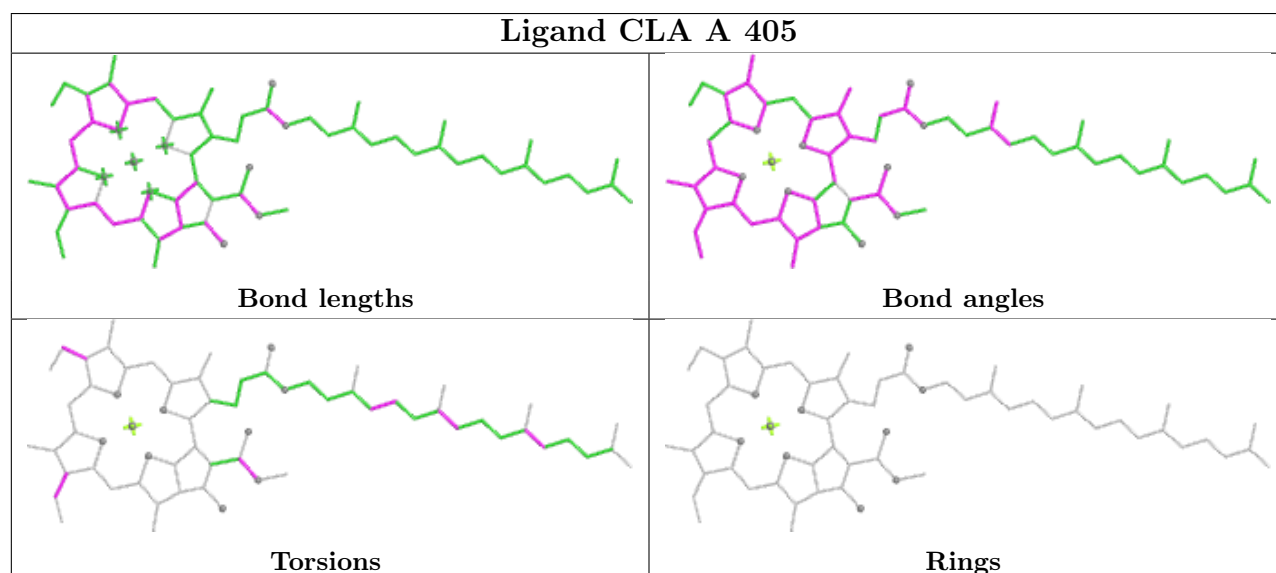
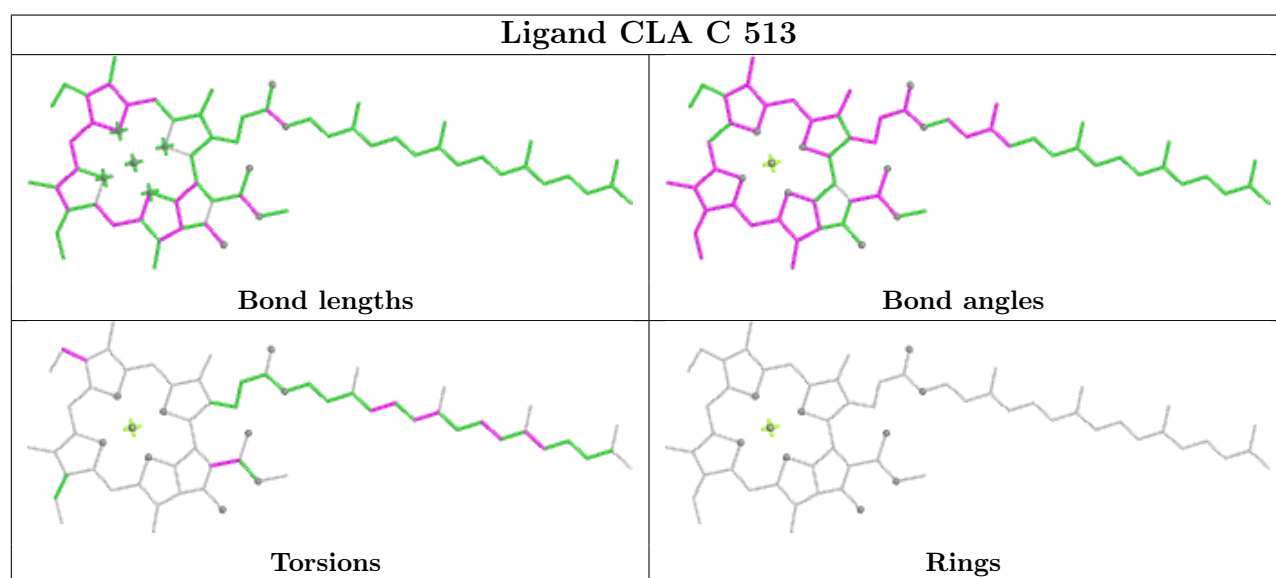
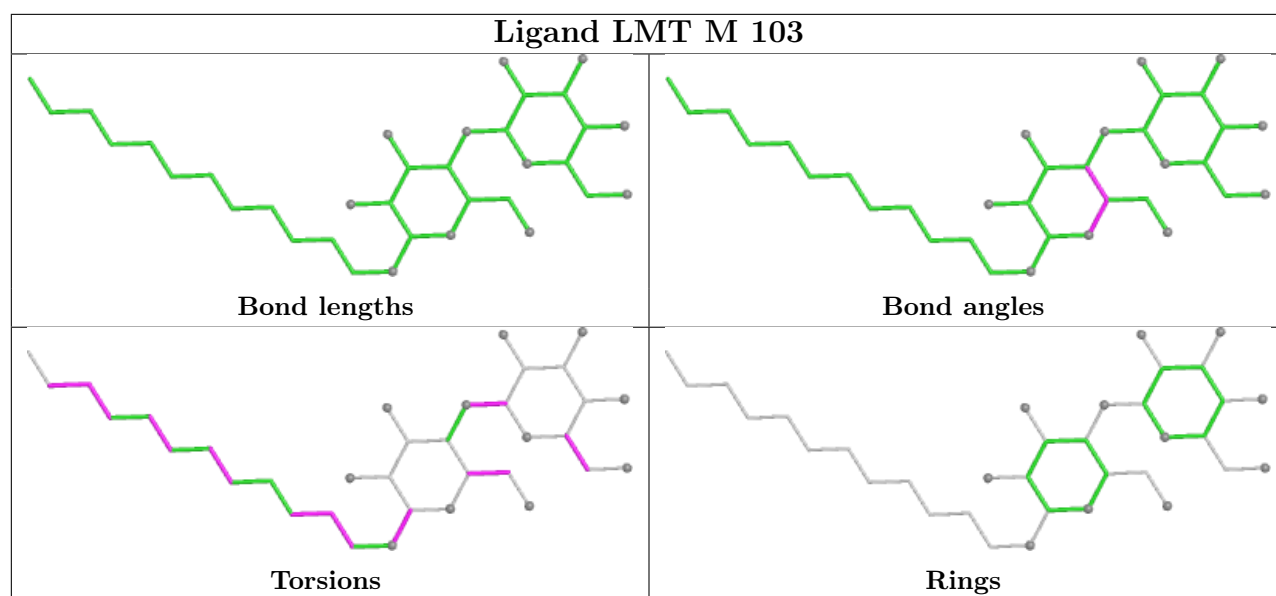
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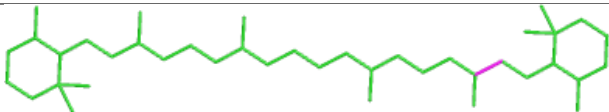
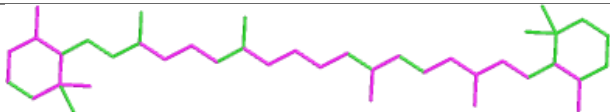
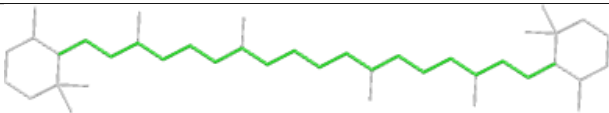
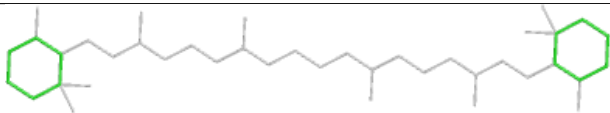


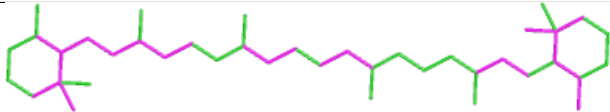
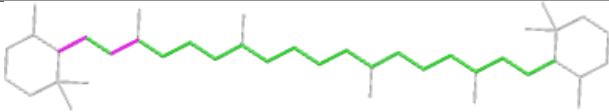
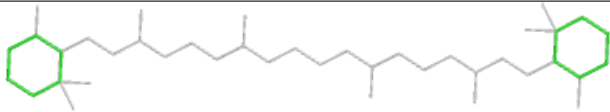


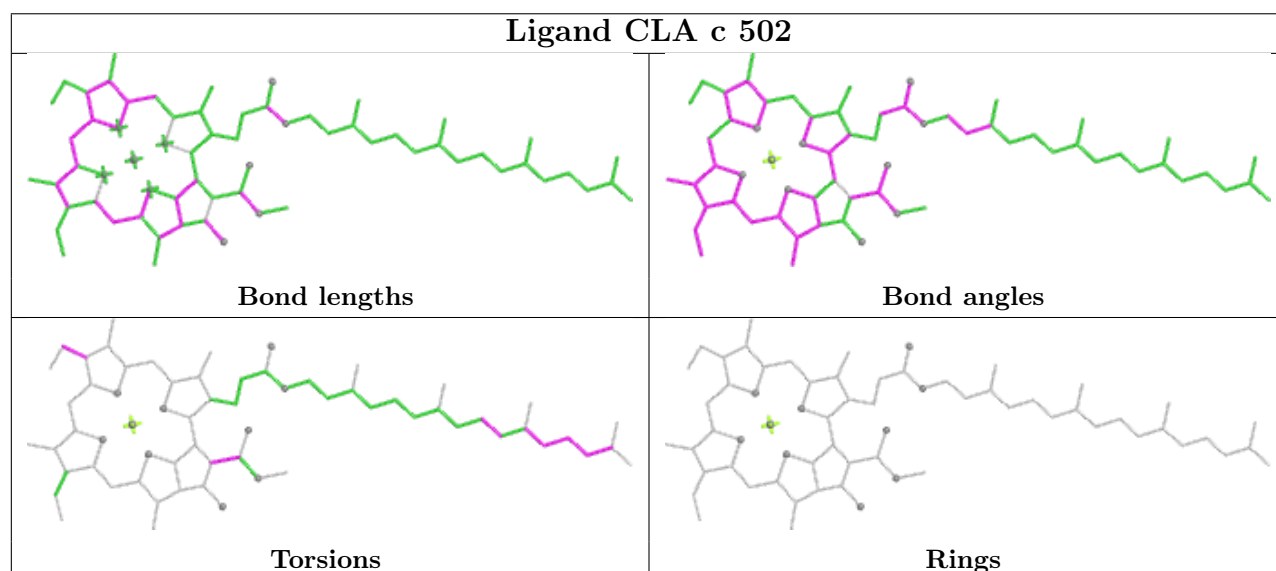
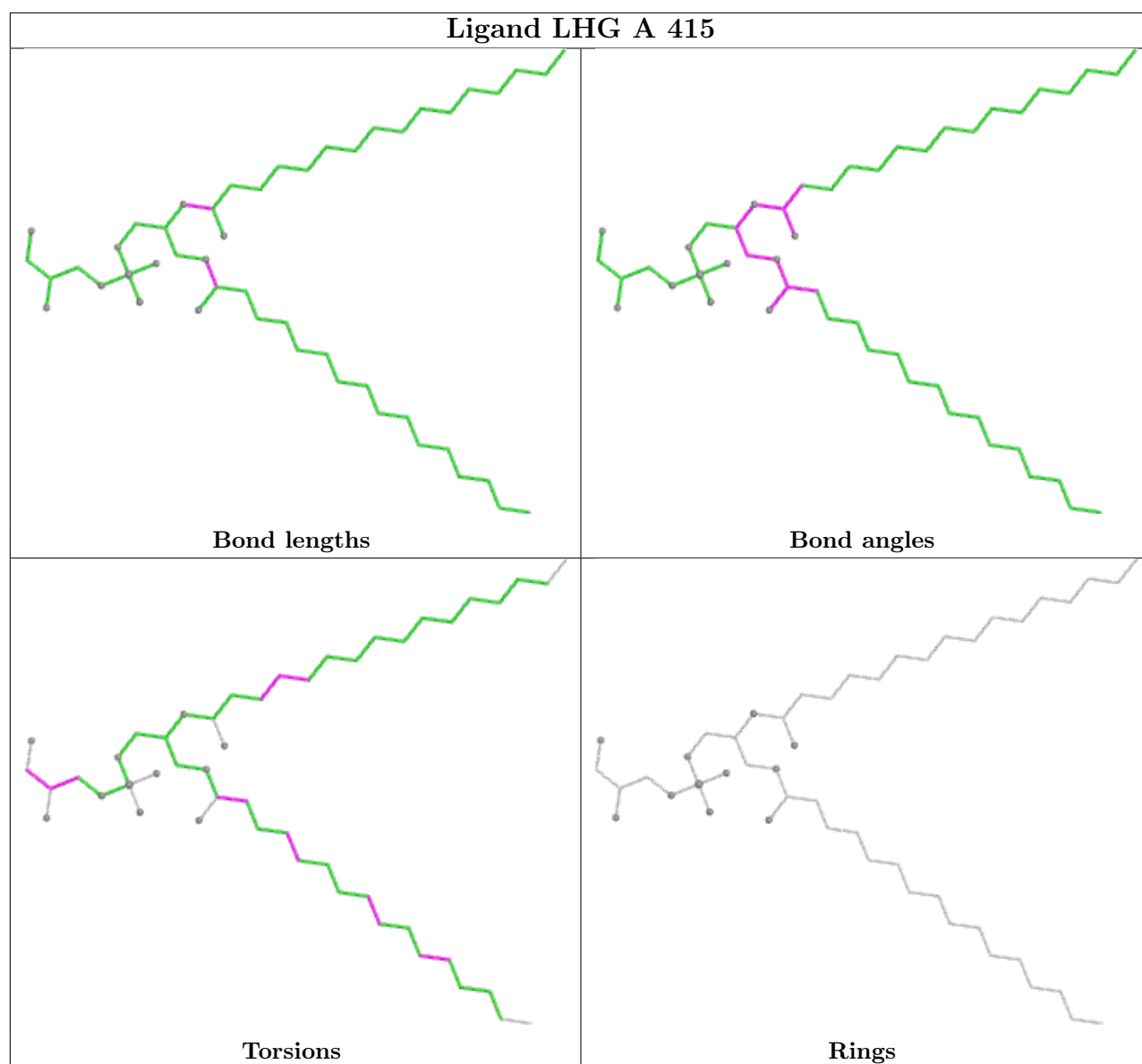
Ligand CLA d 403**Ligand CLA b 613****Ligand CLA B 605**

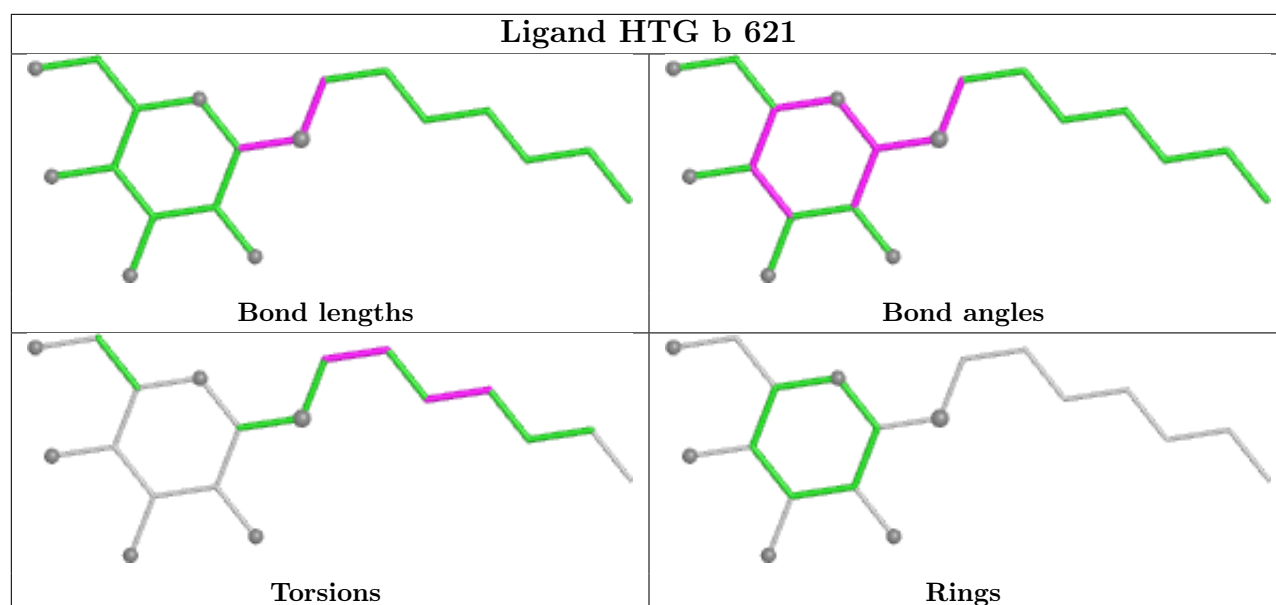
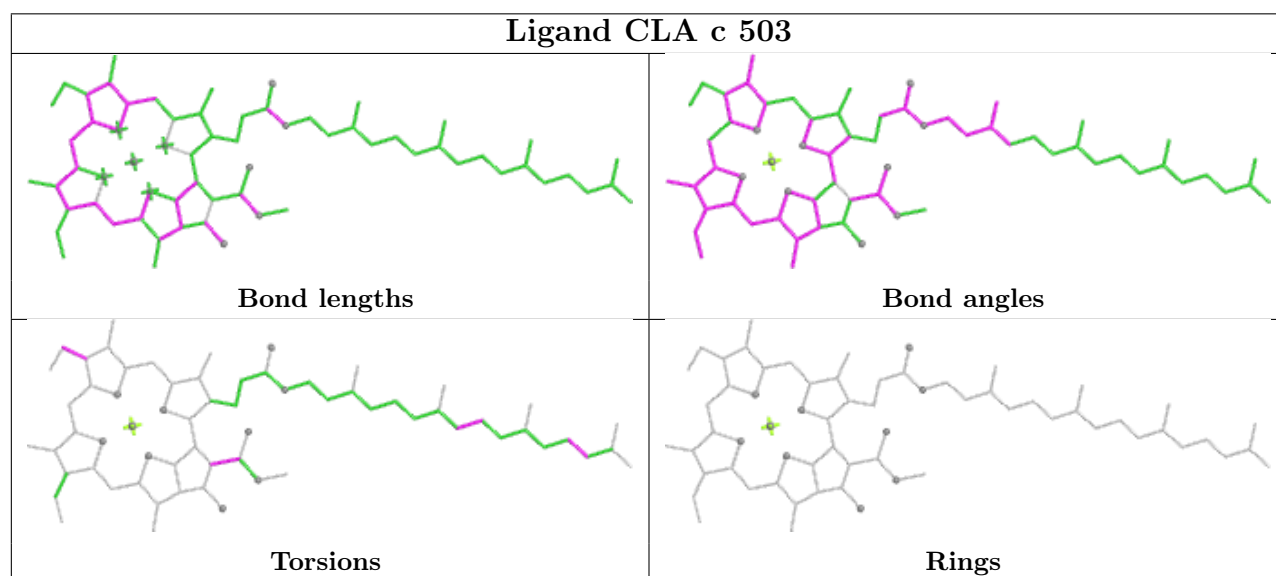
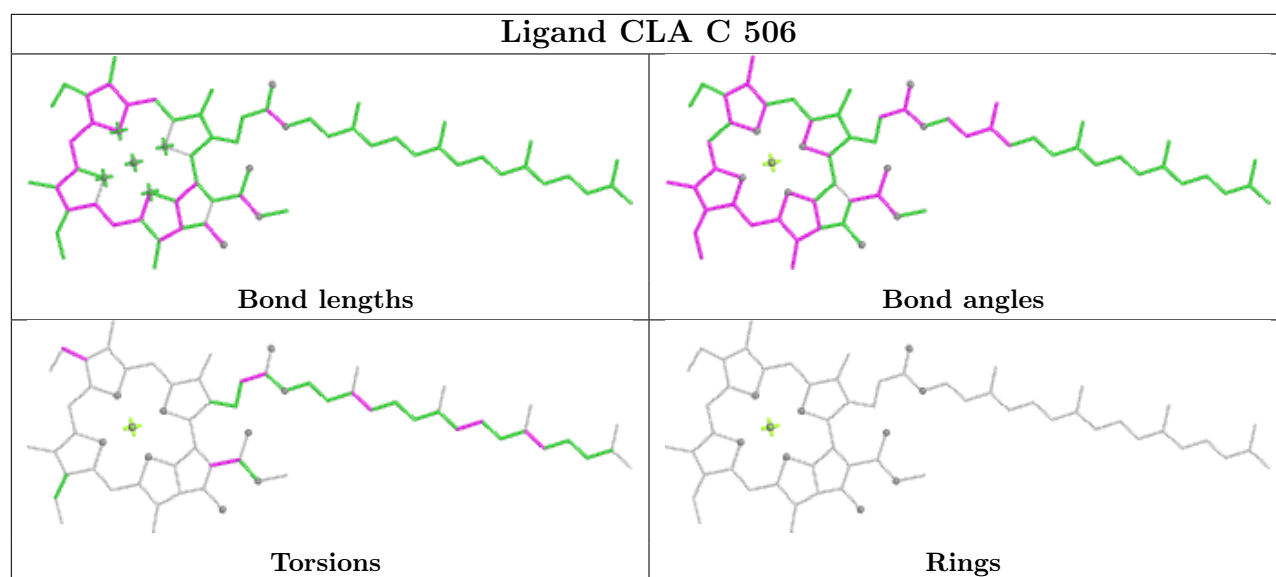


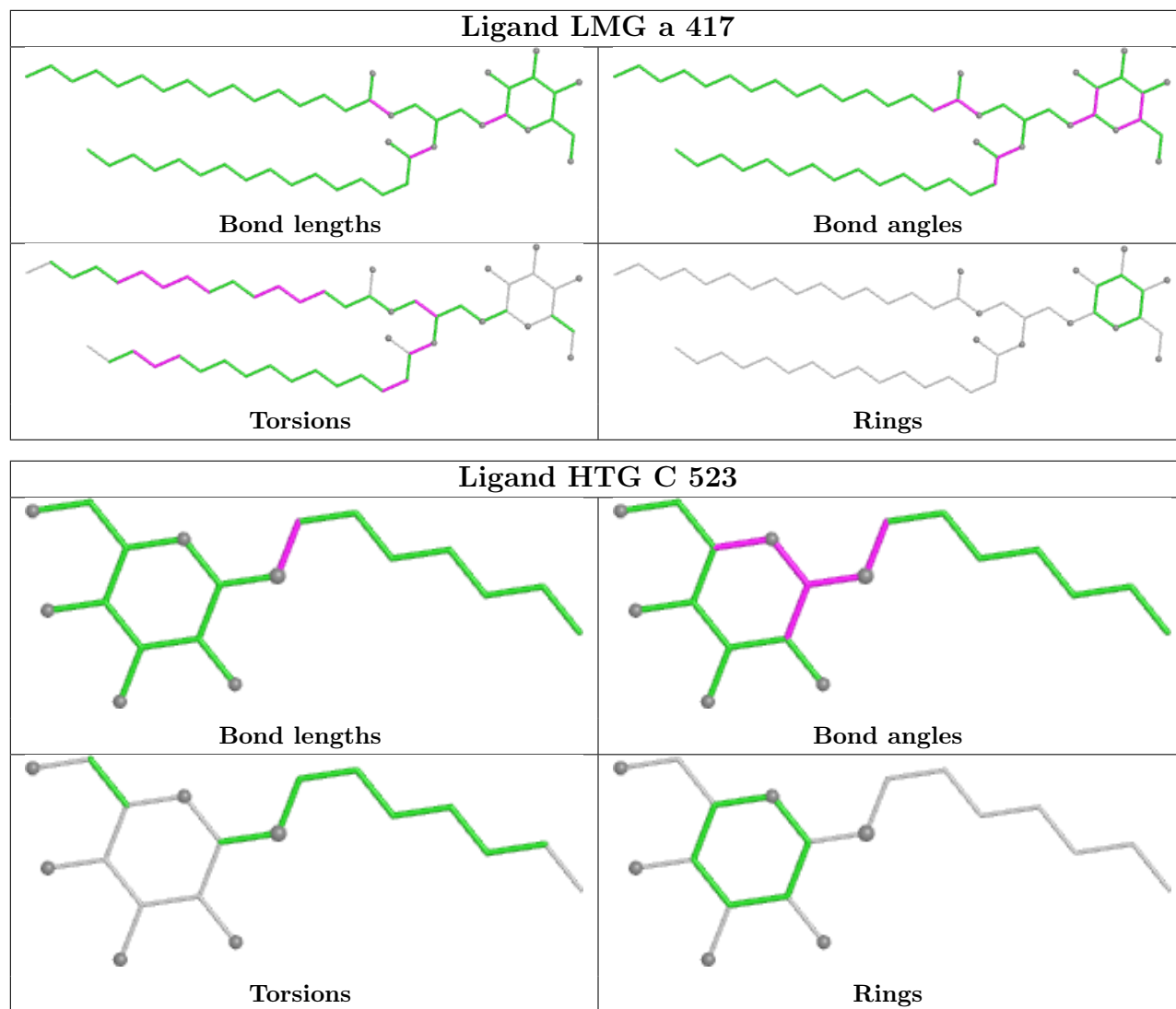


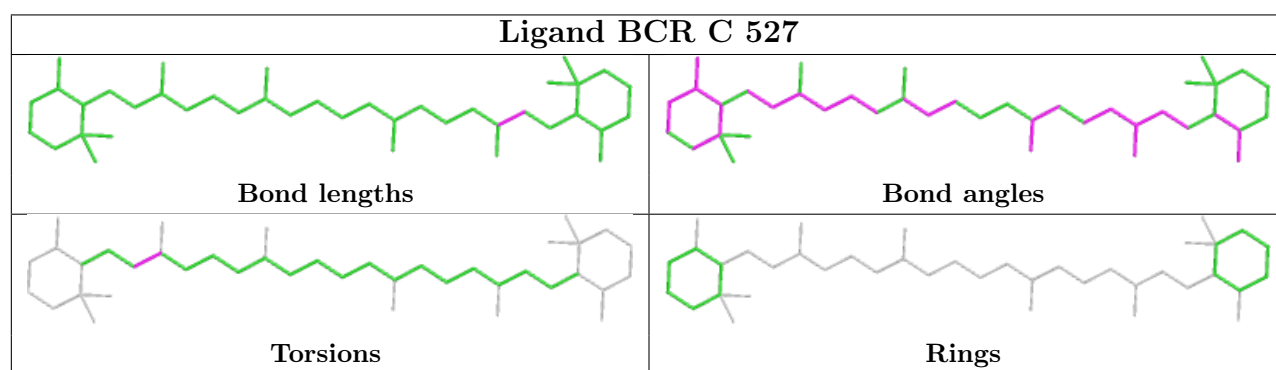
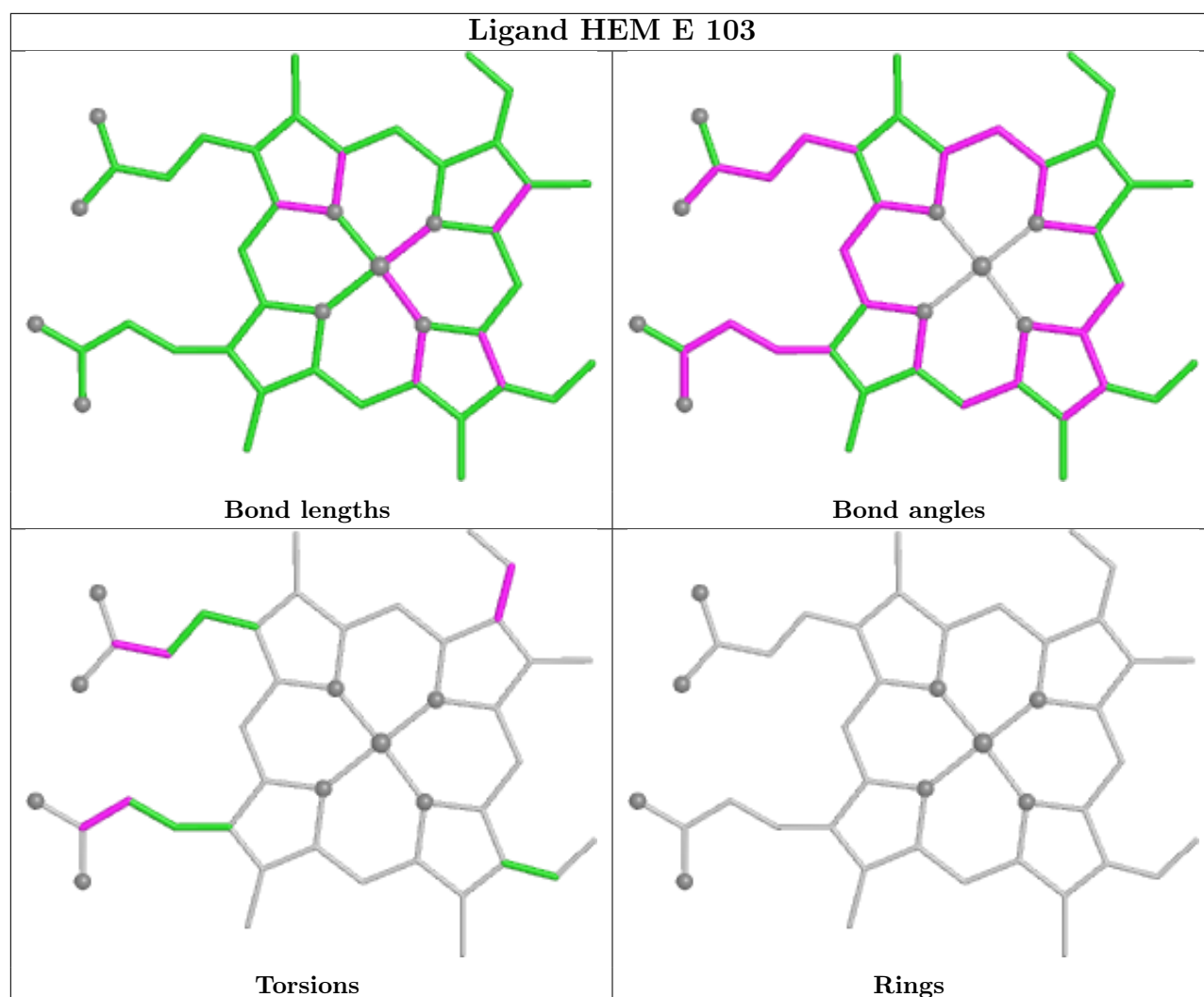
Ligand BCR a 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

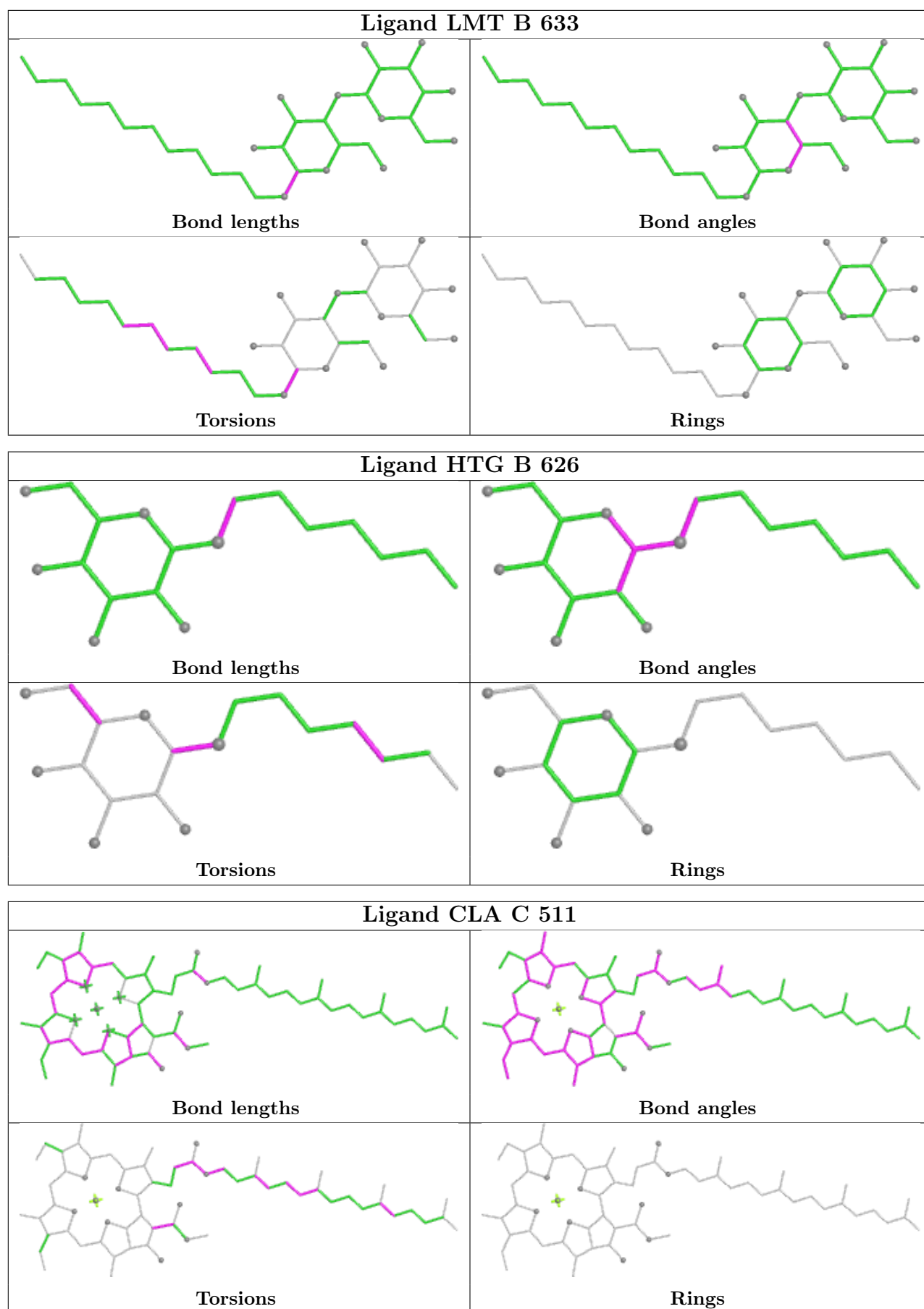
Ligand BCR H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

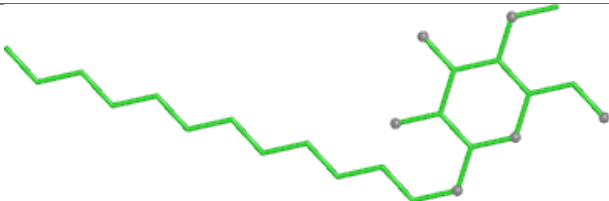
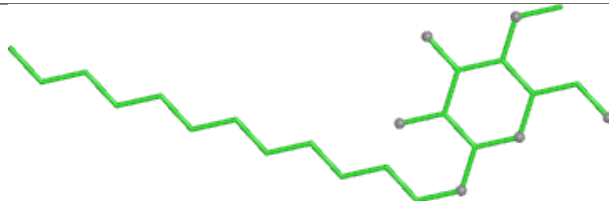
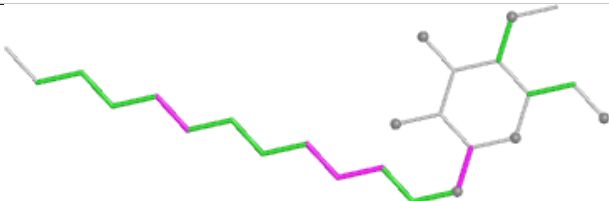
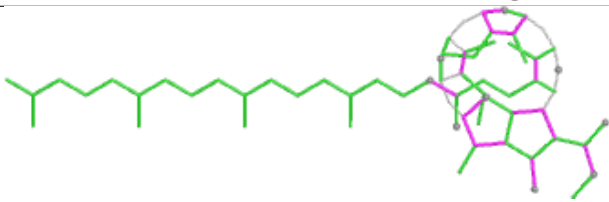
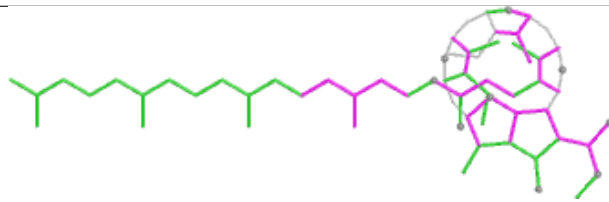
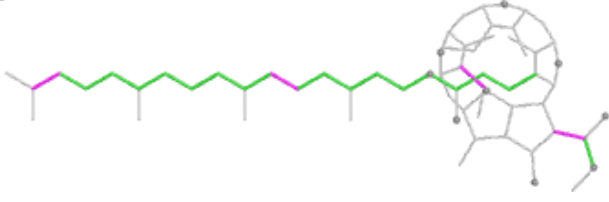
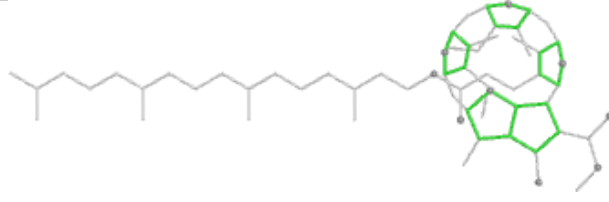
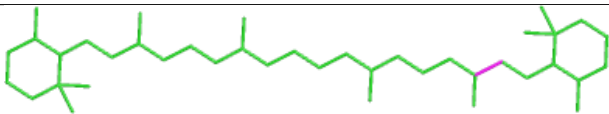
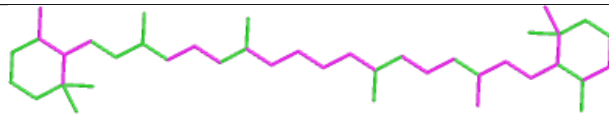
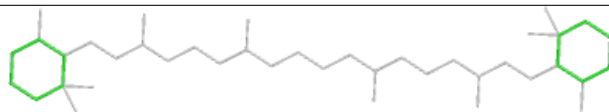


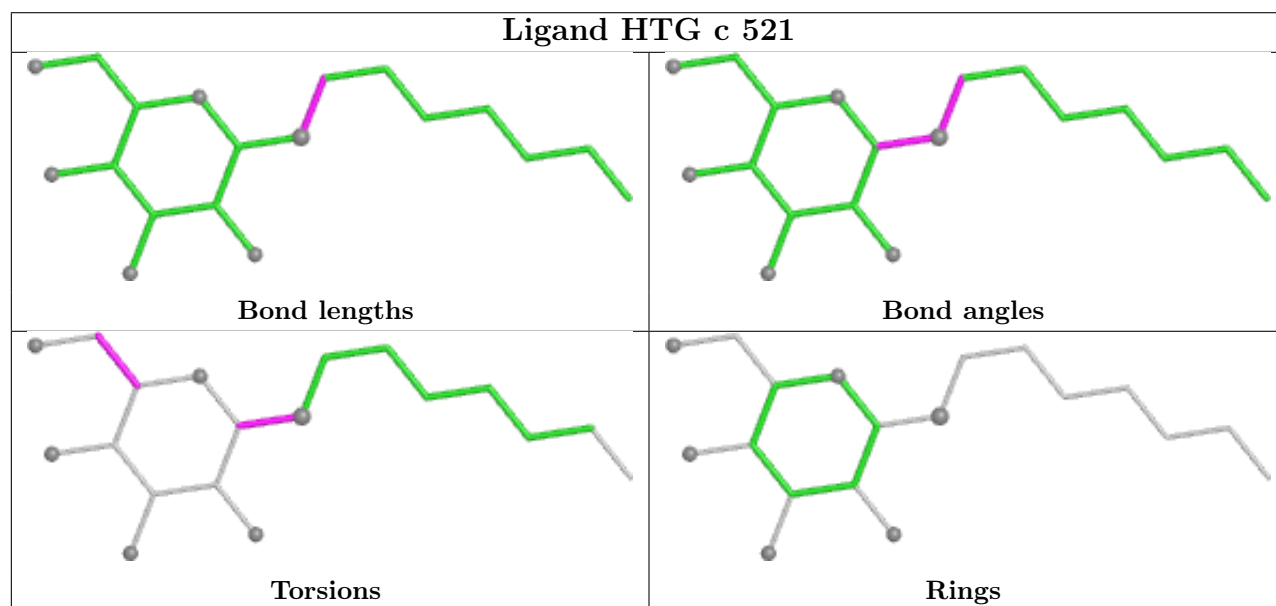
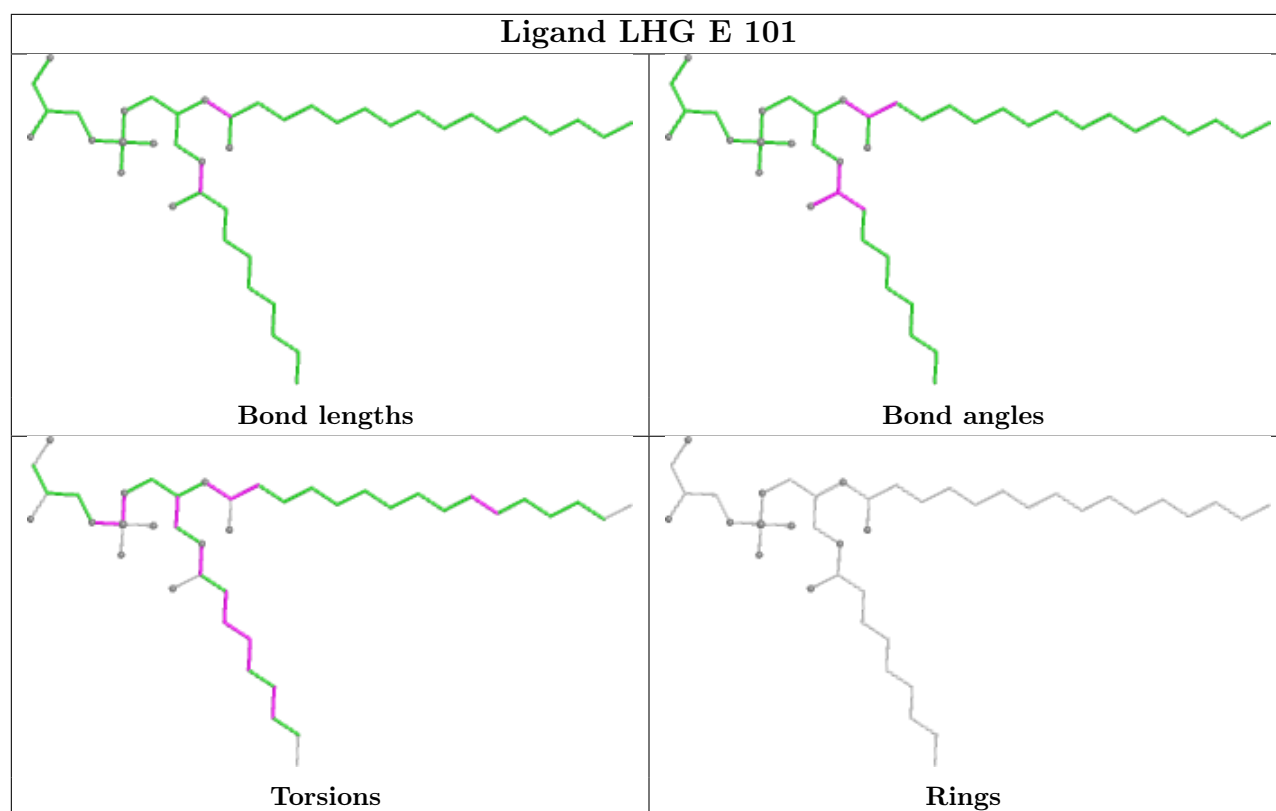


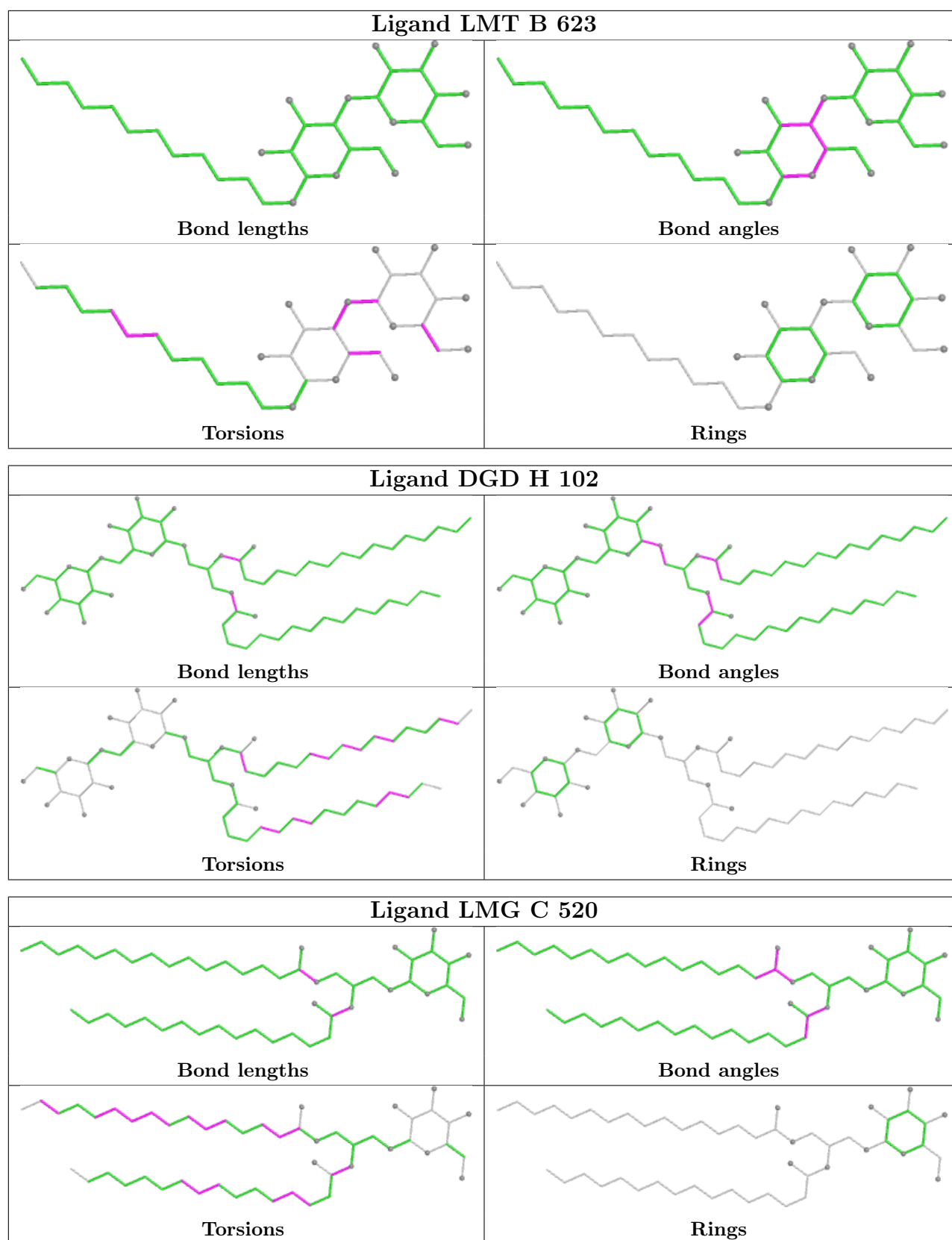


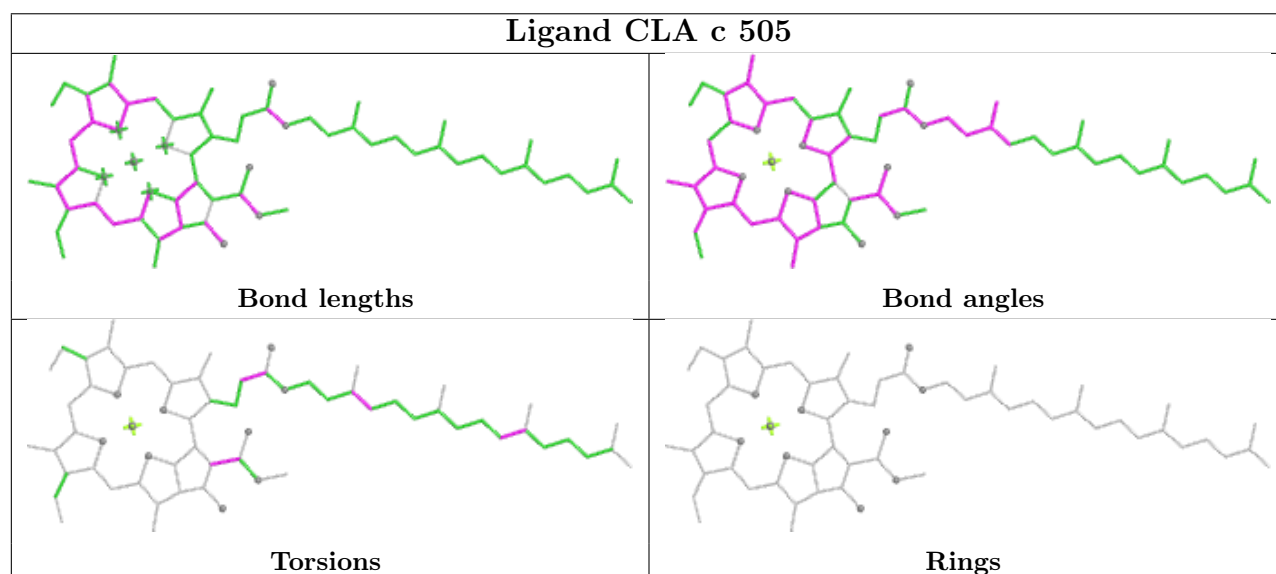
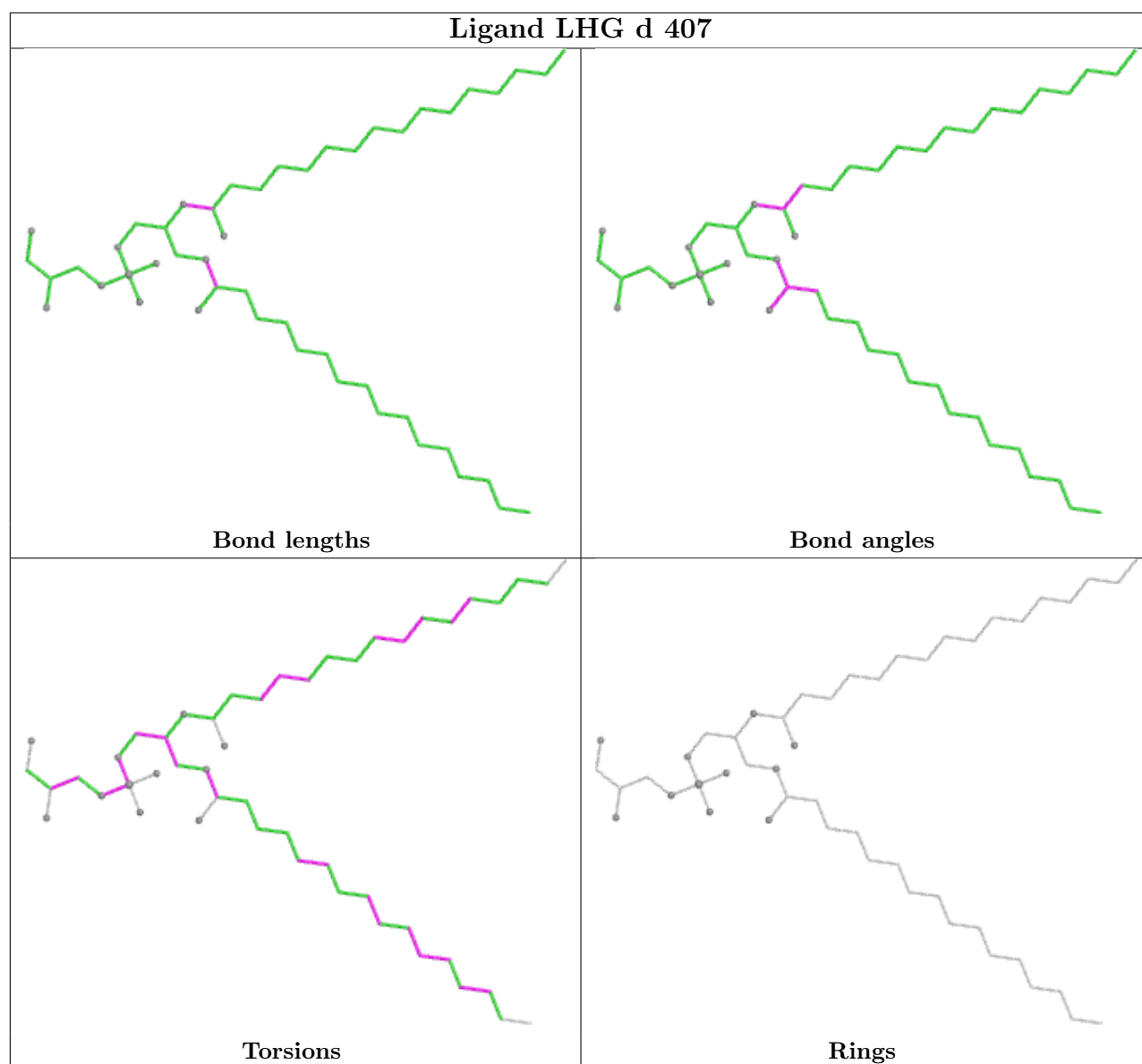


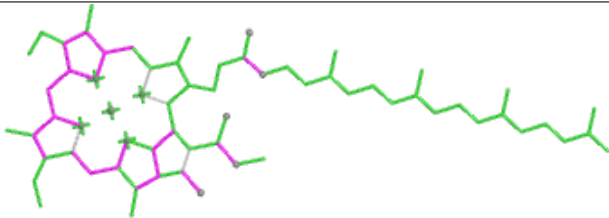
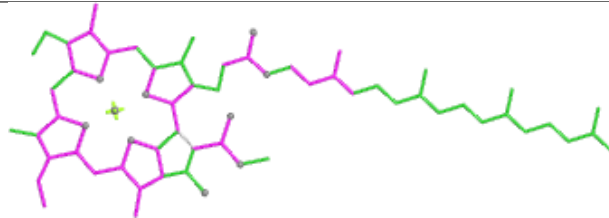
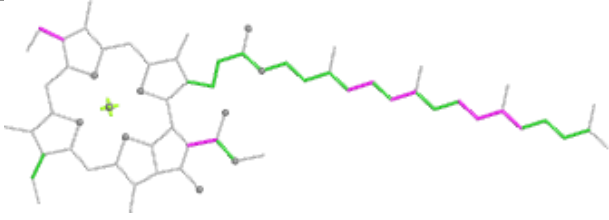
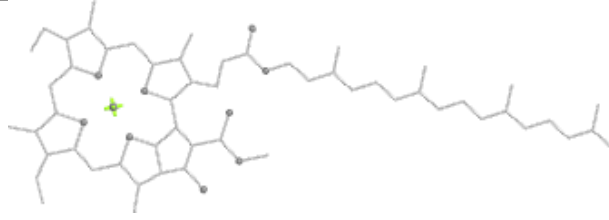


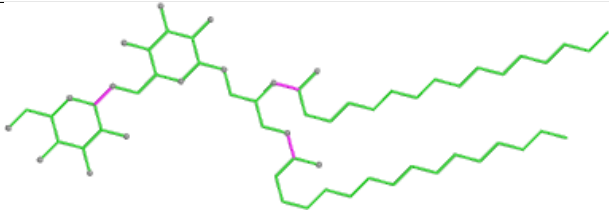
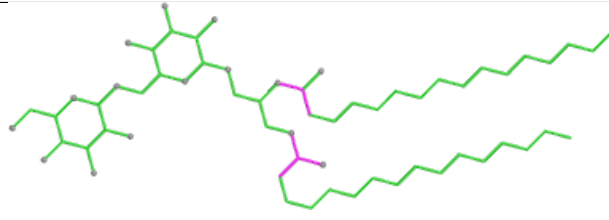
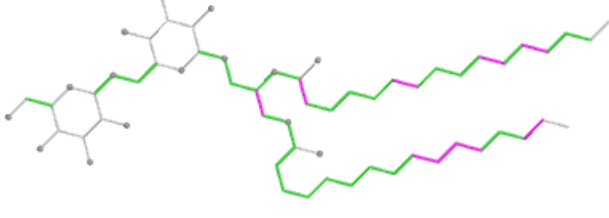
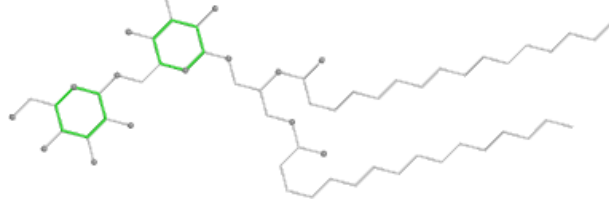
Ligand LMT b 620	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PHO D 402	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR y 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

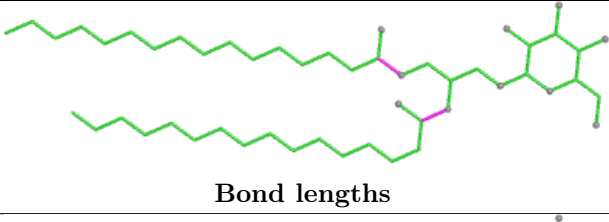
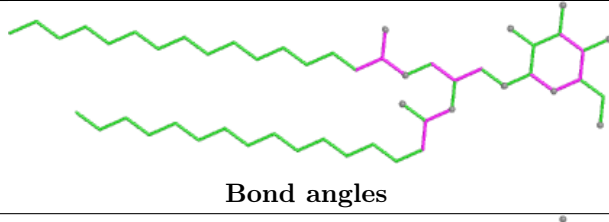
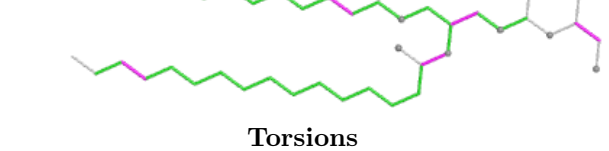


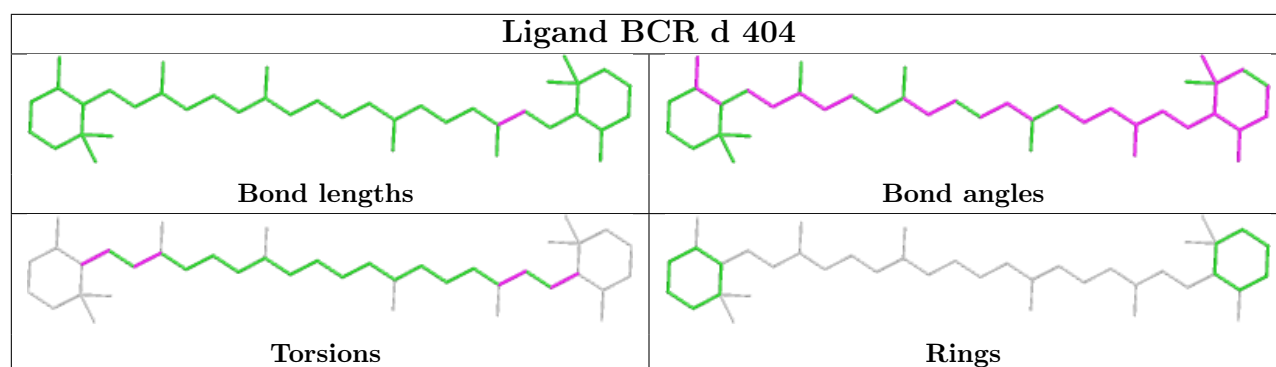
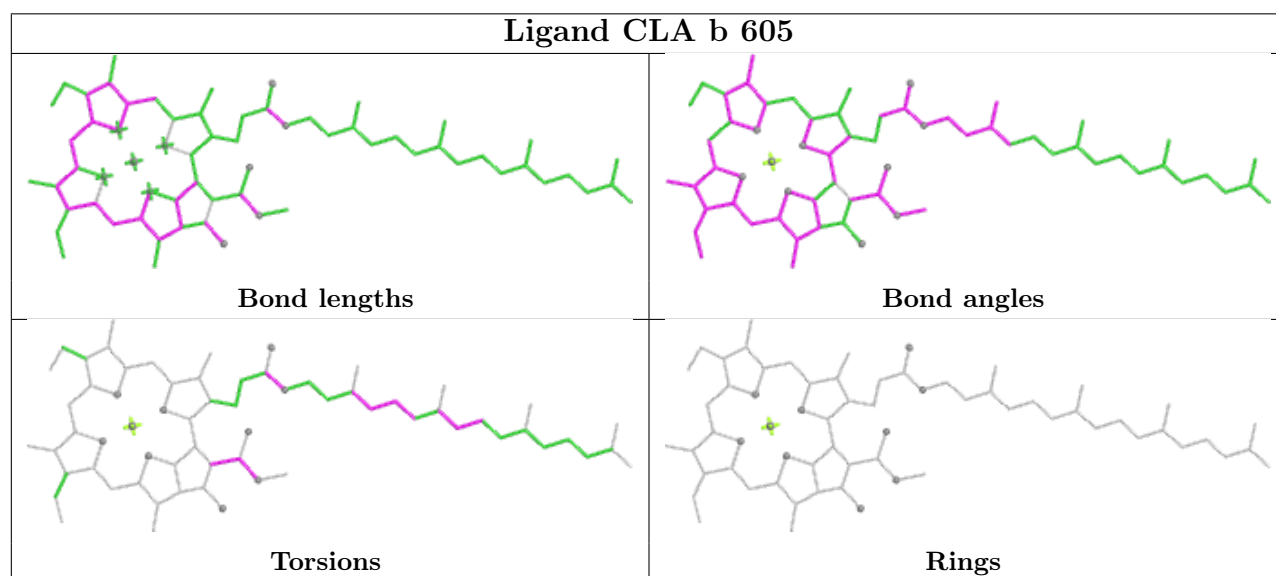
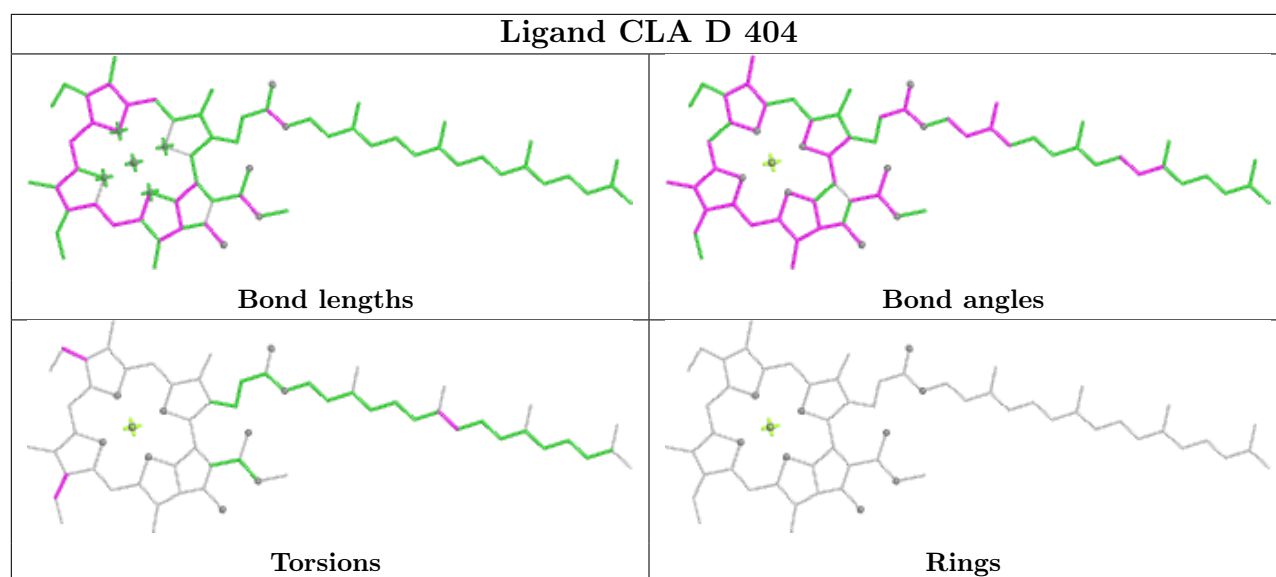


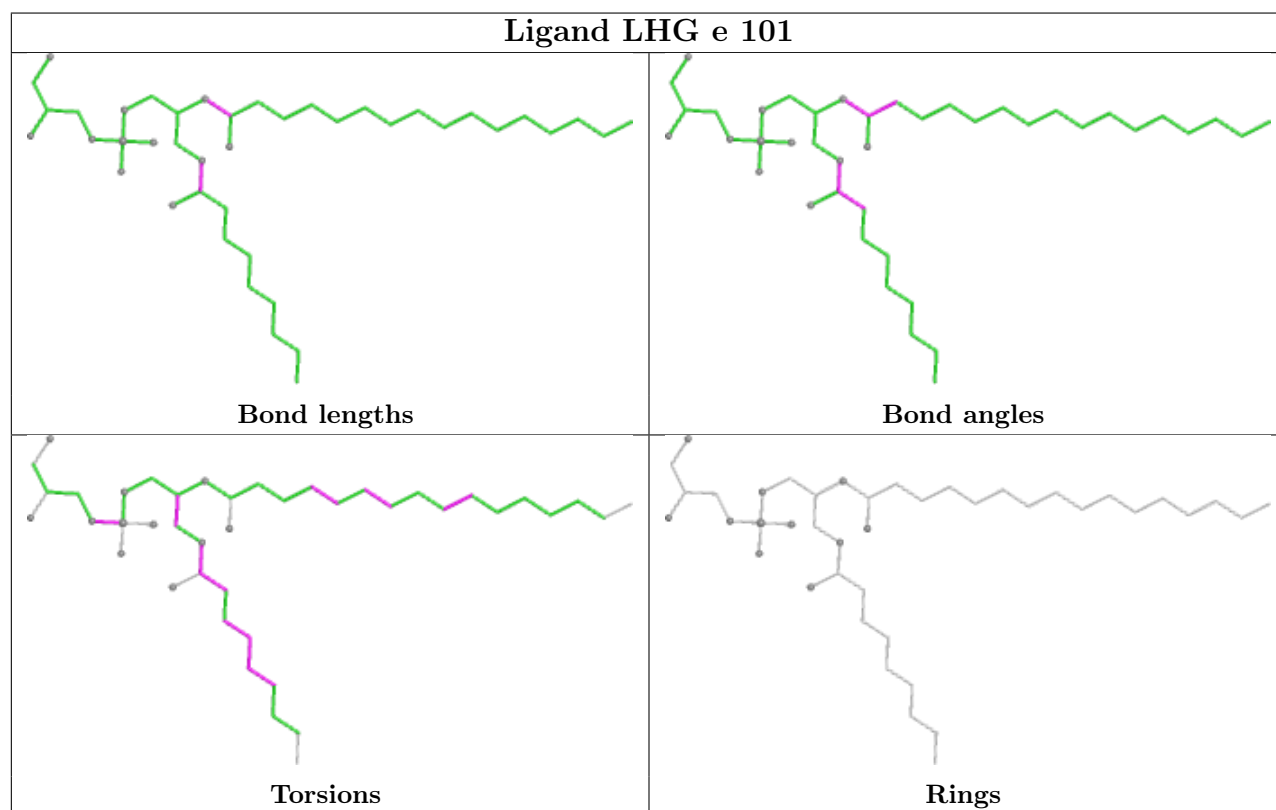
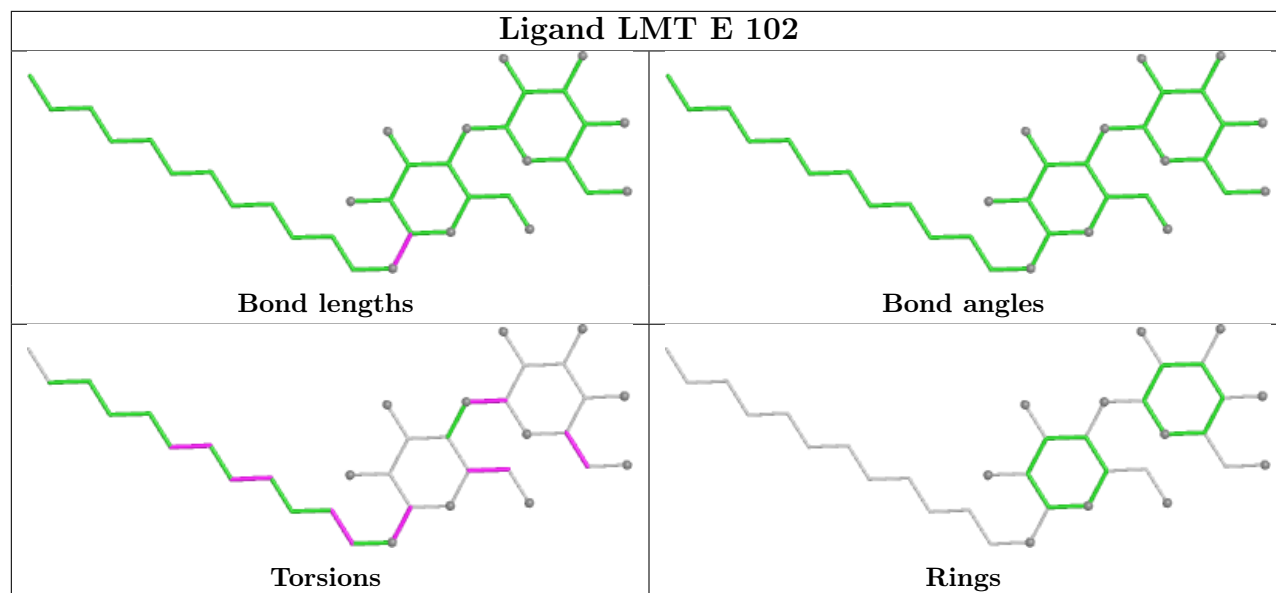


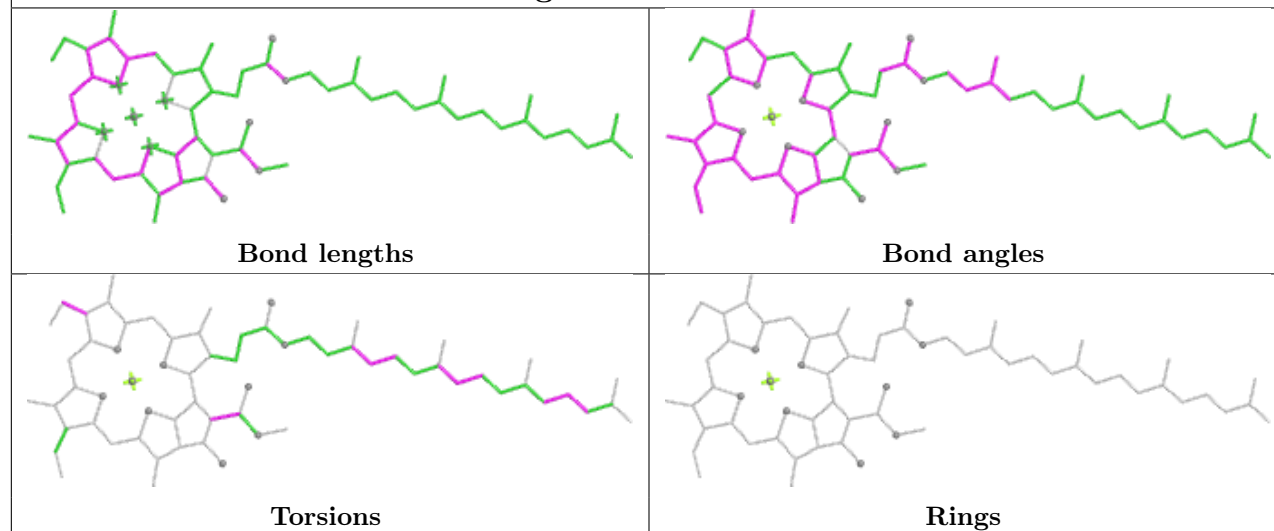
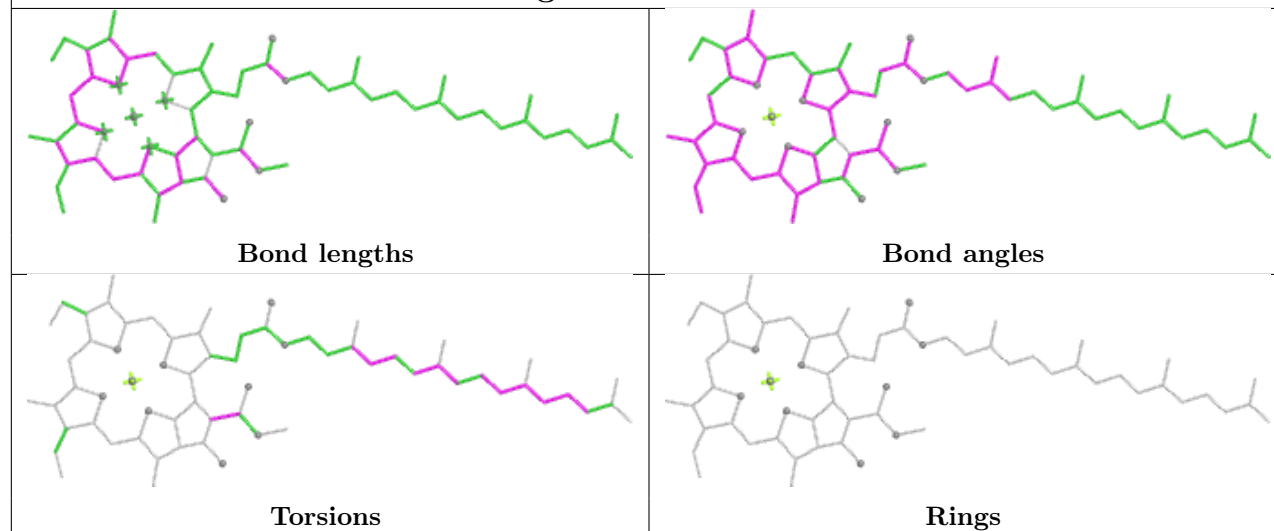
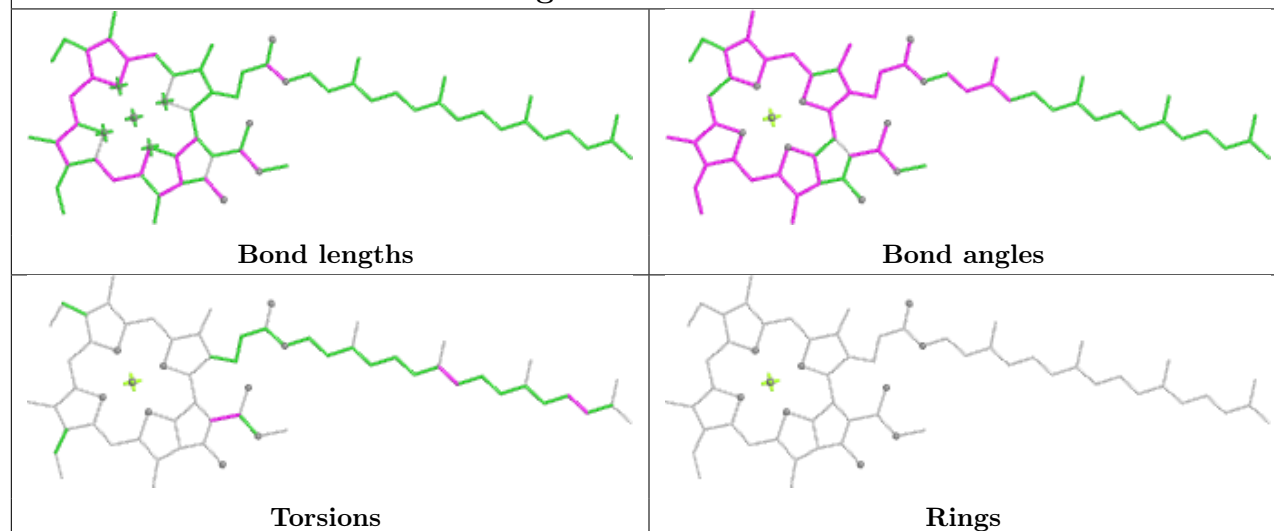
Ligand CLA B 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGD h 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

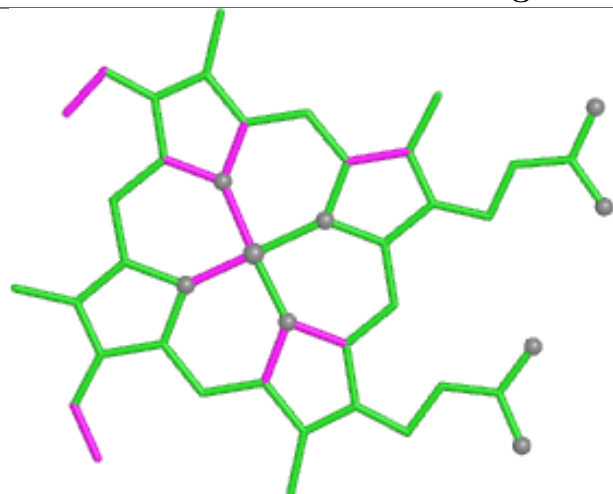
Ligand LMG c 520	
	
Bond lengths	Bond angles
	
Torsions	Rings



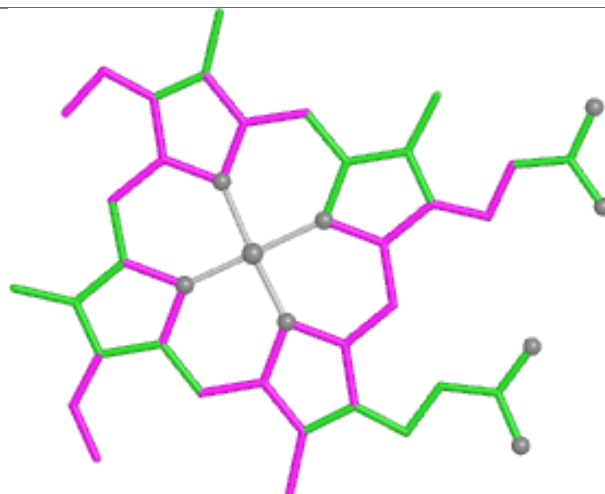


Ligand CLA b 604**Ligand CLA c 506****Ligand CLA a 405**

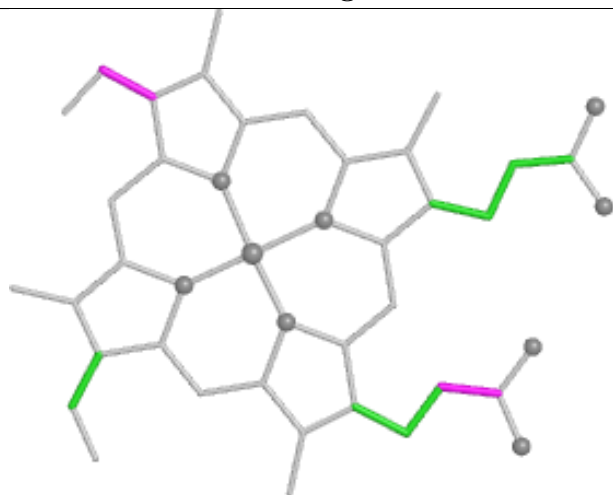
Ligand HEC V 202



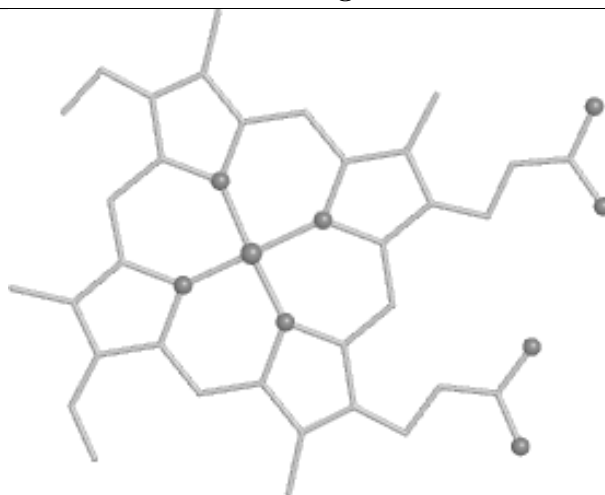
Bond lengths



Bond angles

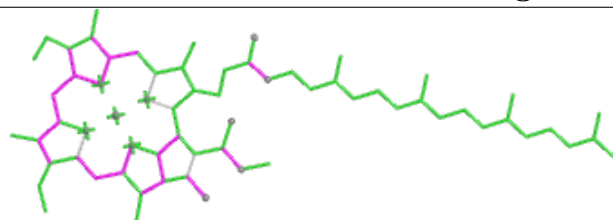


Torsions

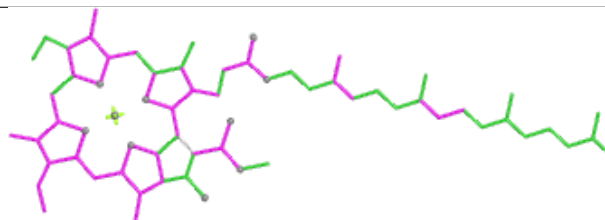


Rings

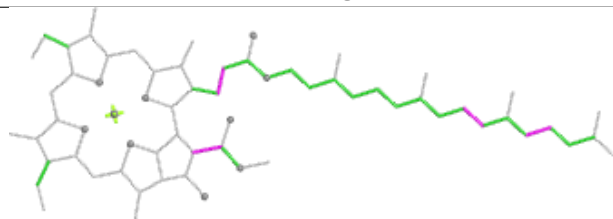
Ligand CLA B 607



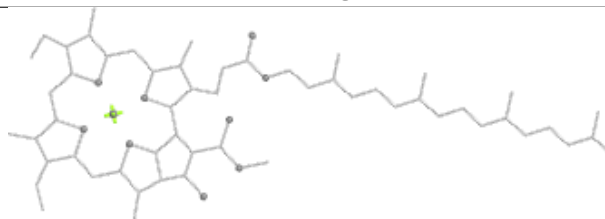
Bond lengths



Bond angles

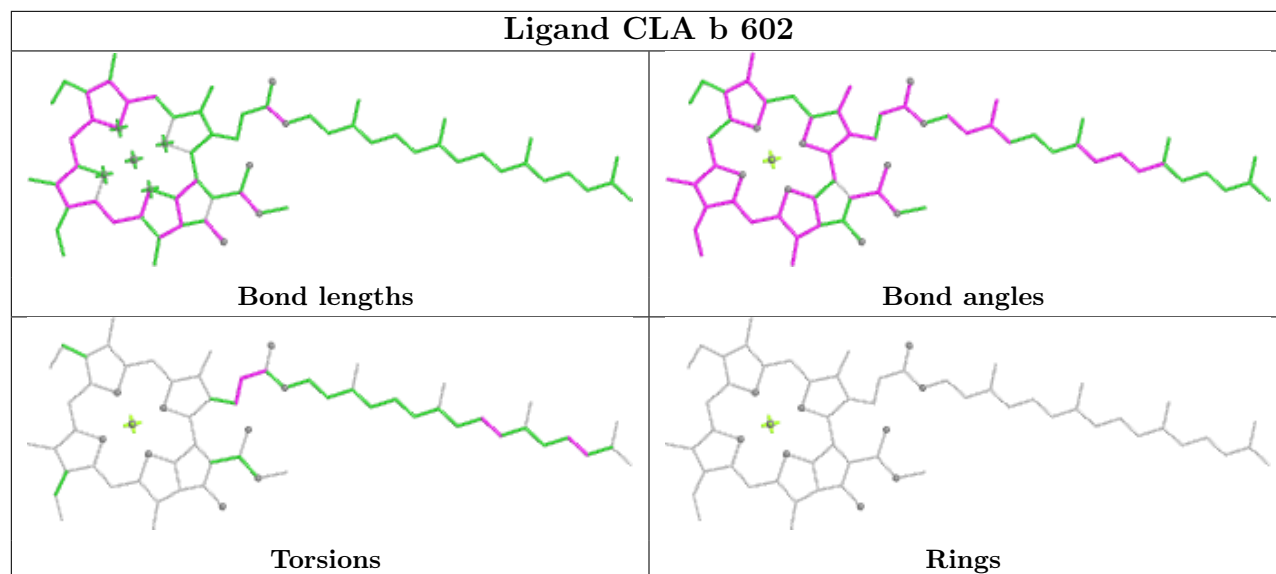


Torsions

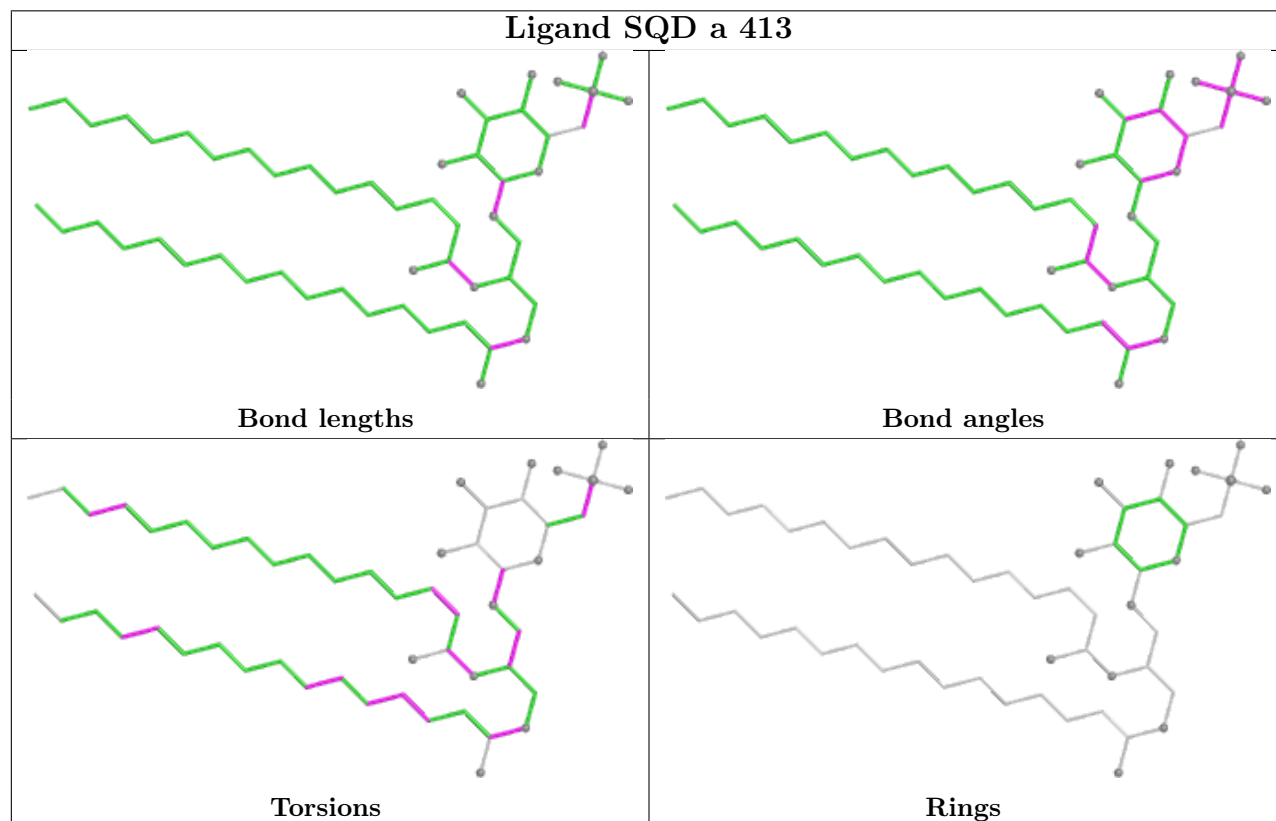


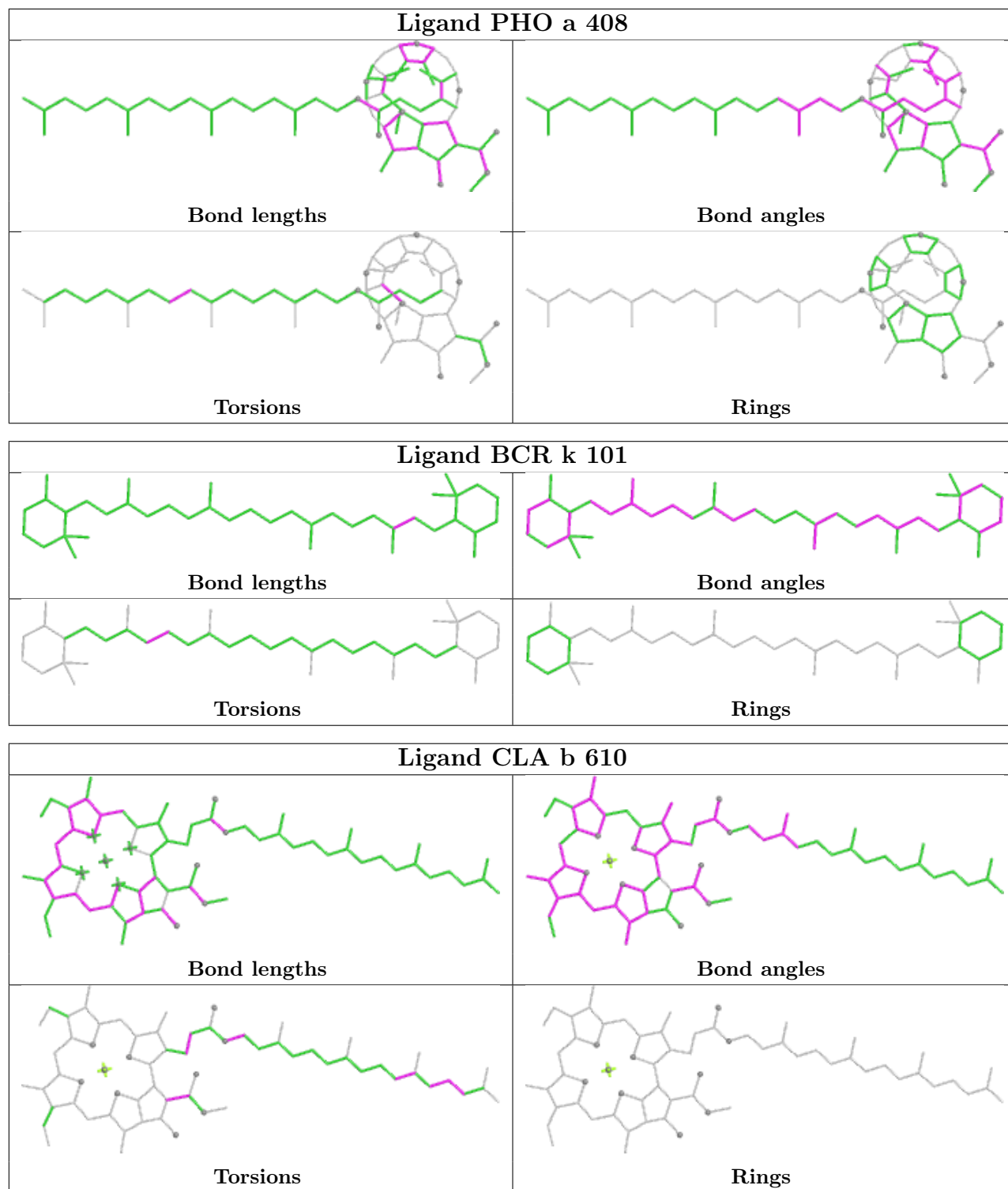
Rings

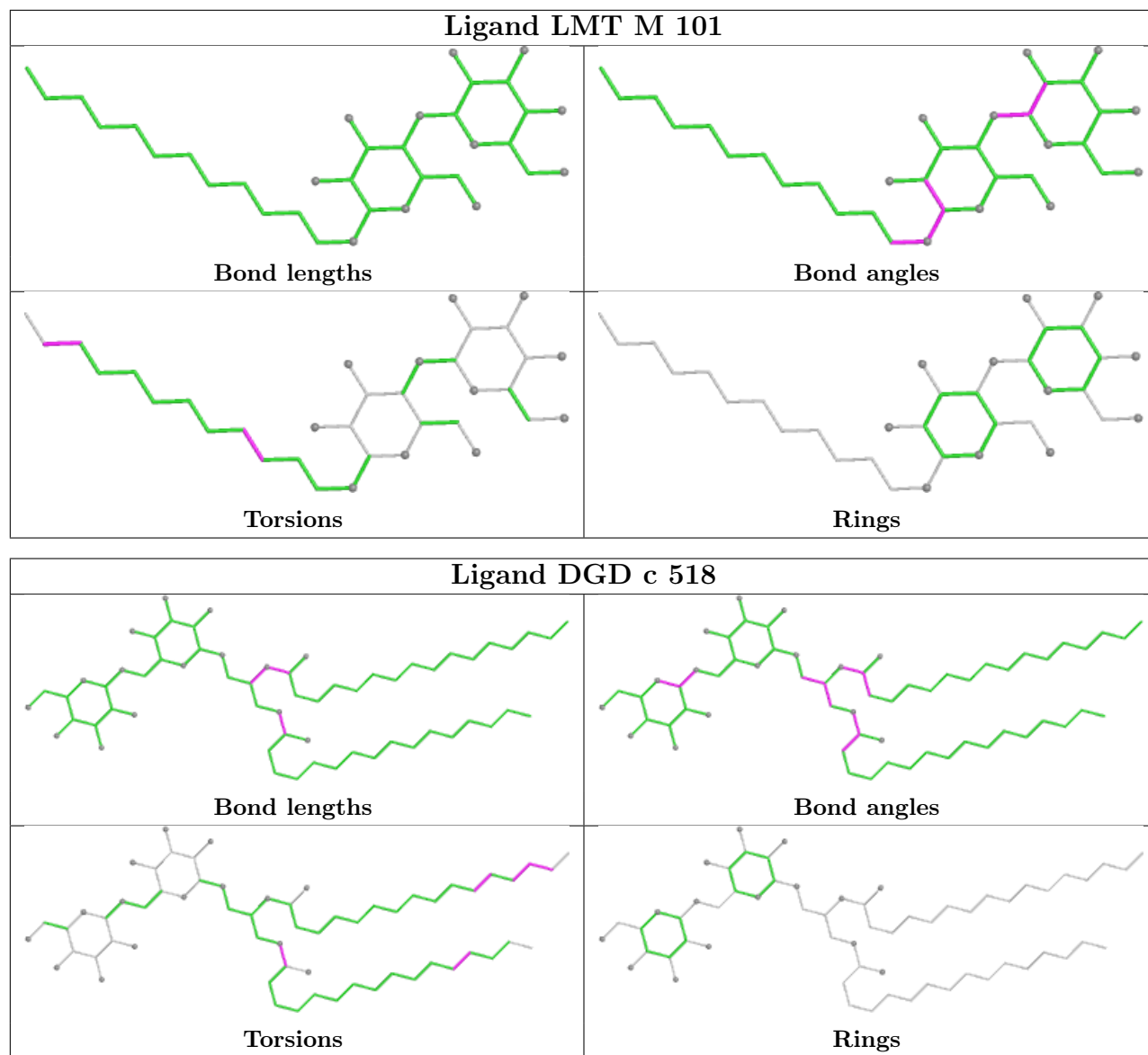
Ligand CLA b 602

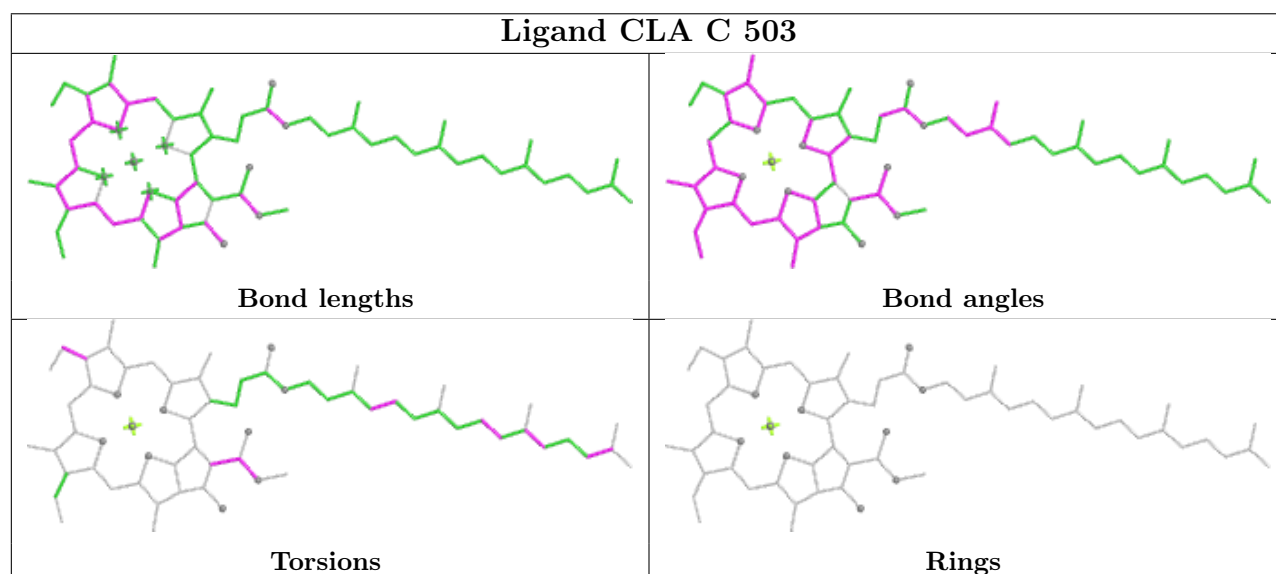
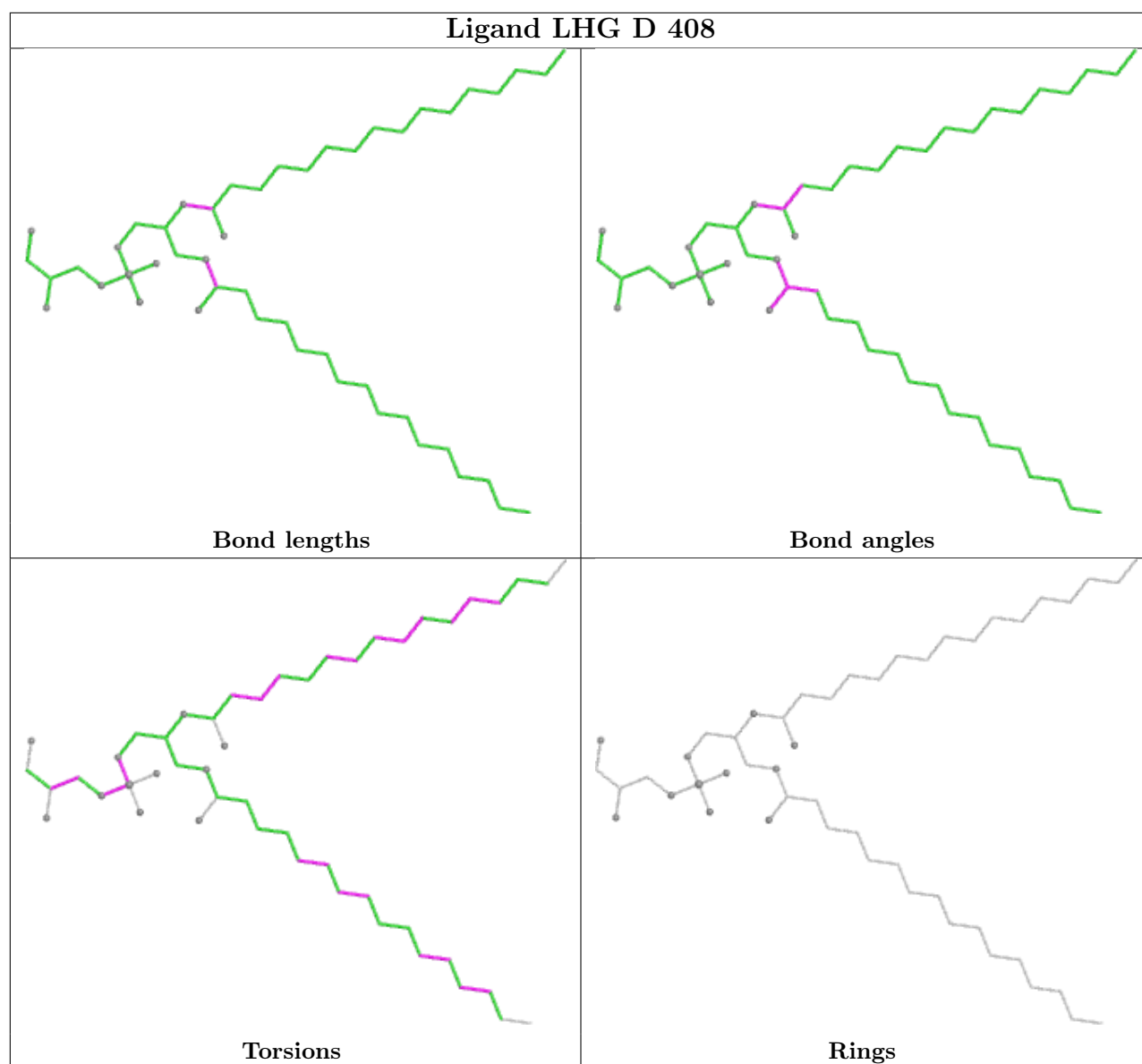


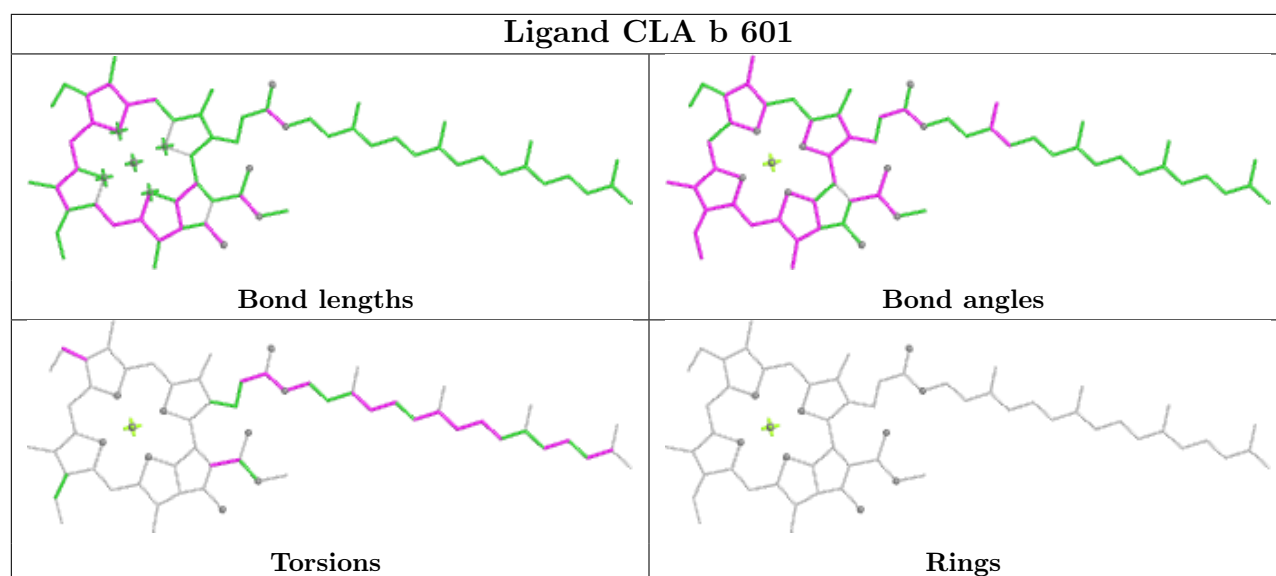
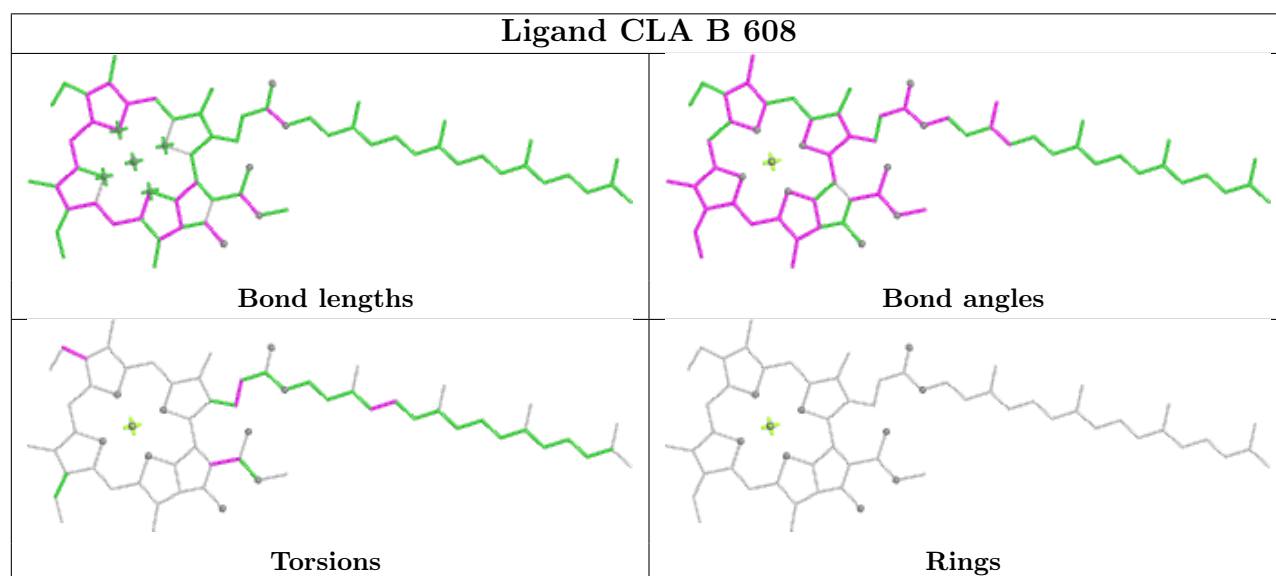
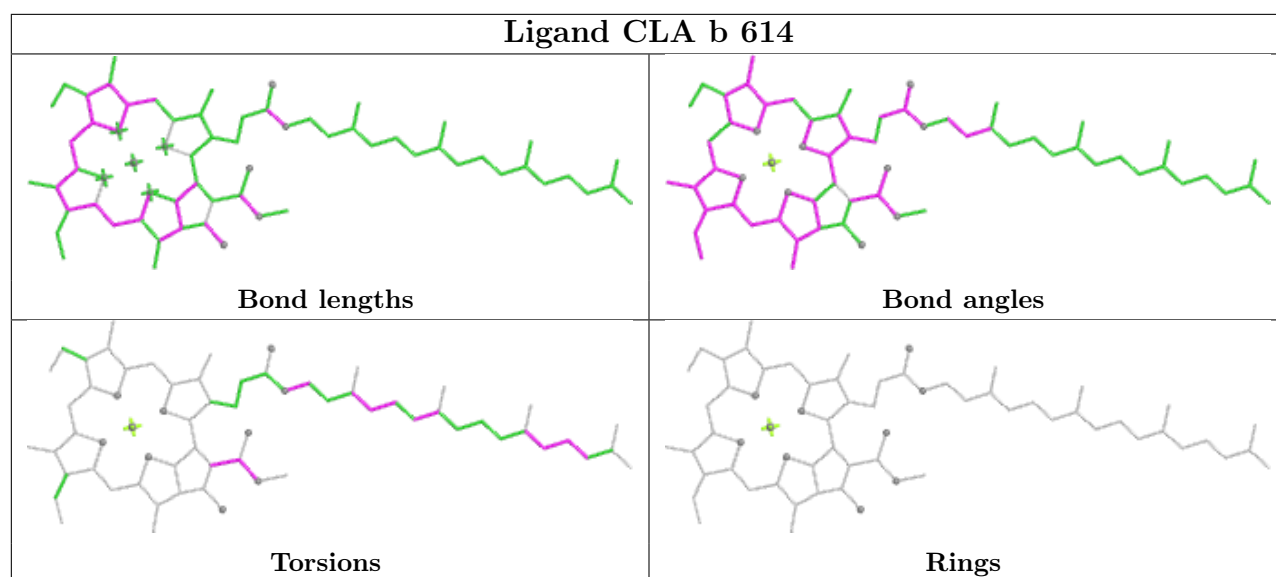
Ligand SQD a 413

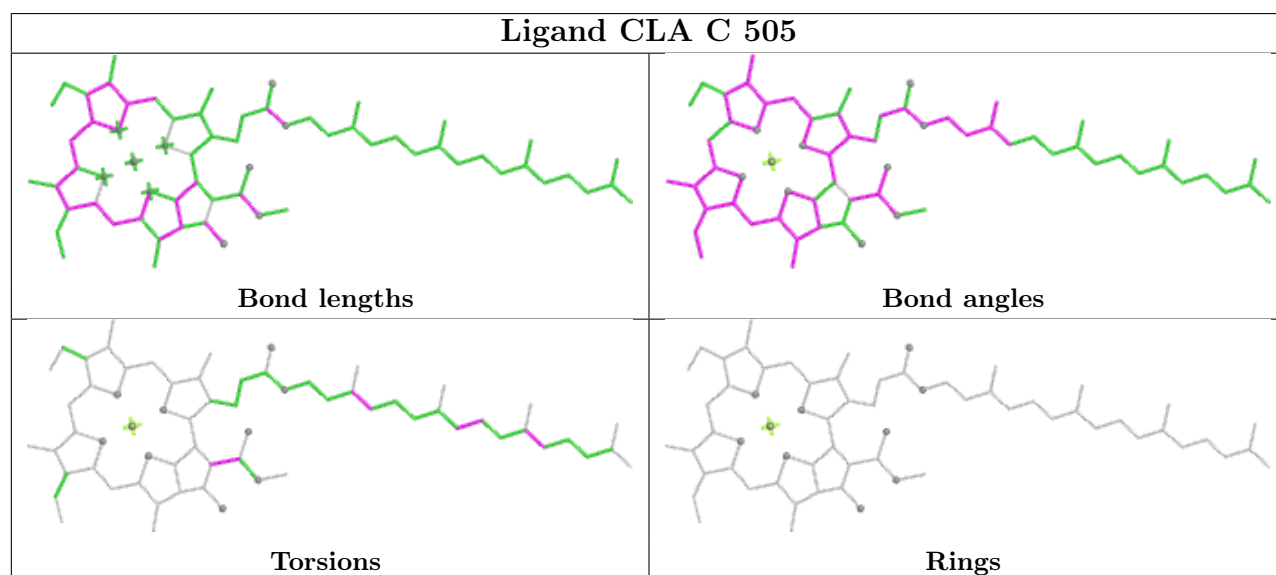
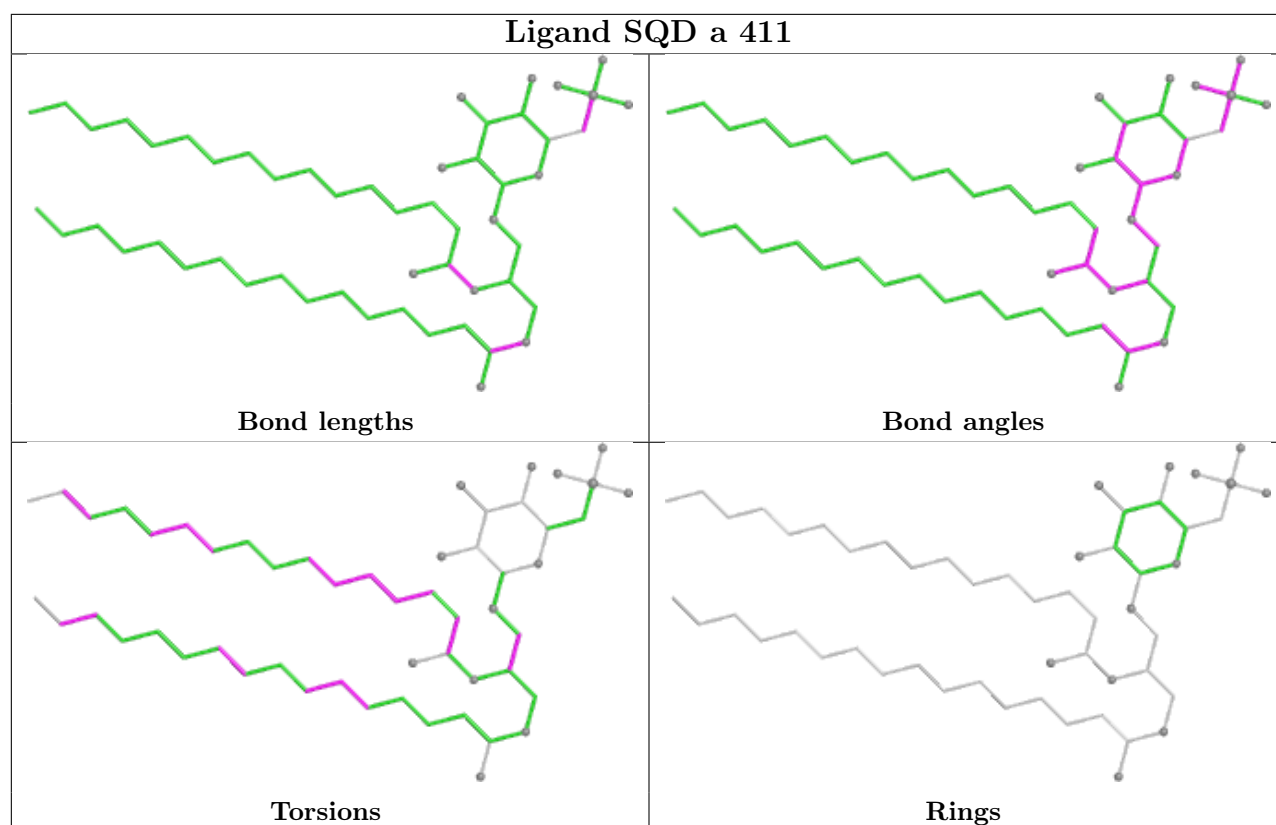


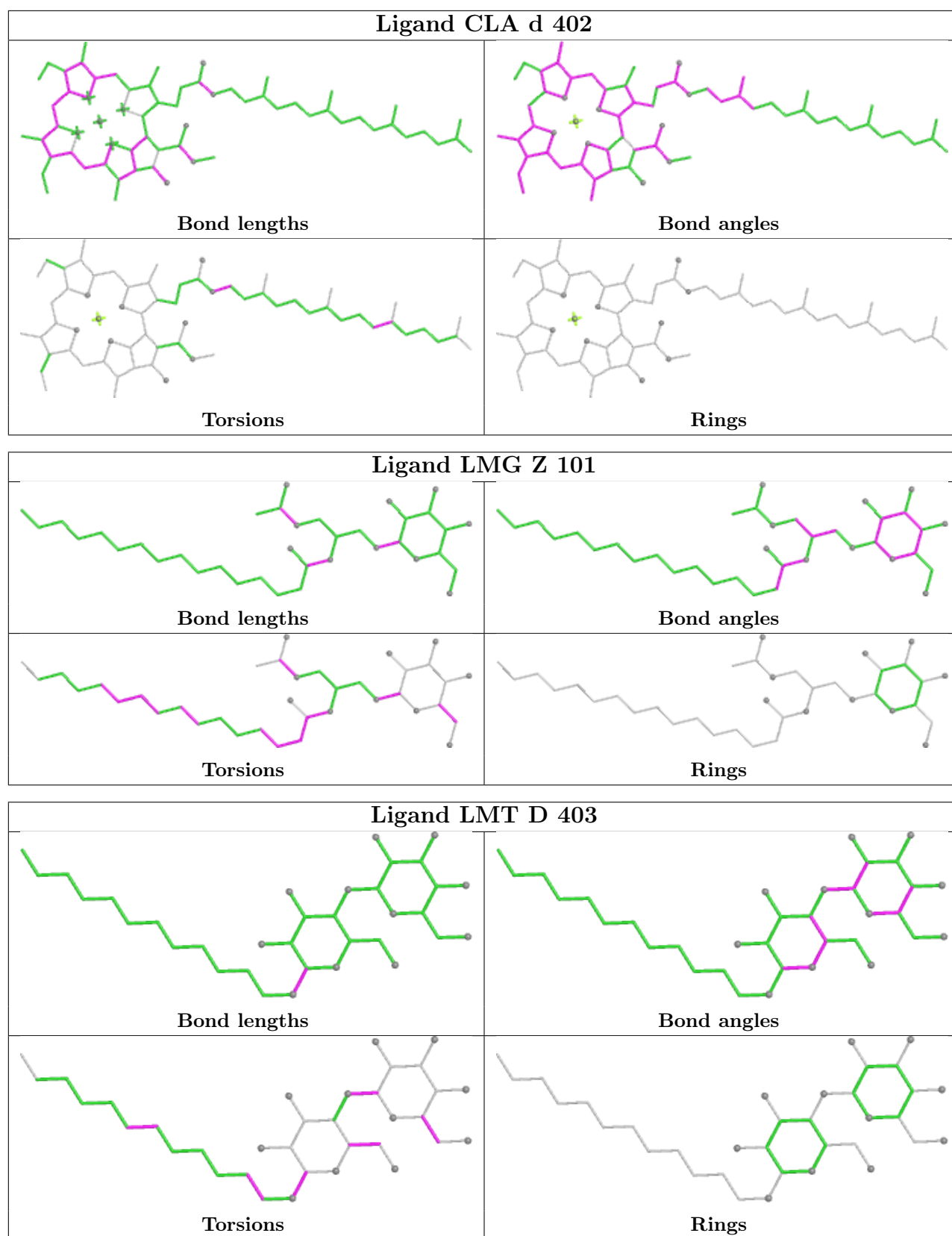


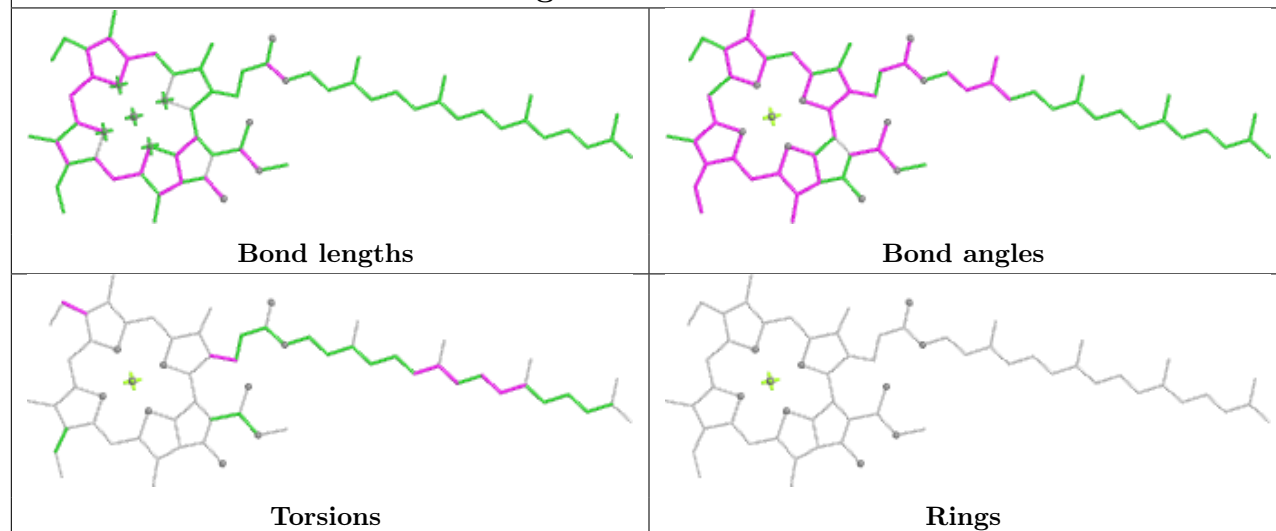
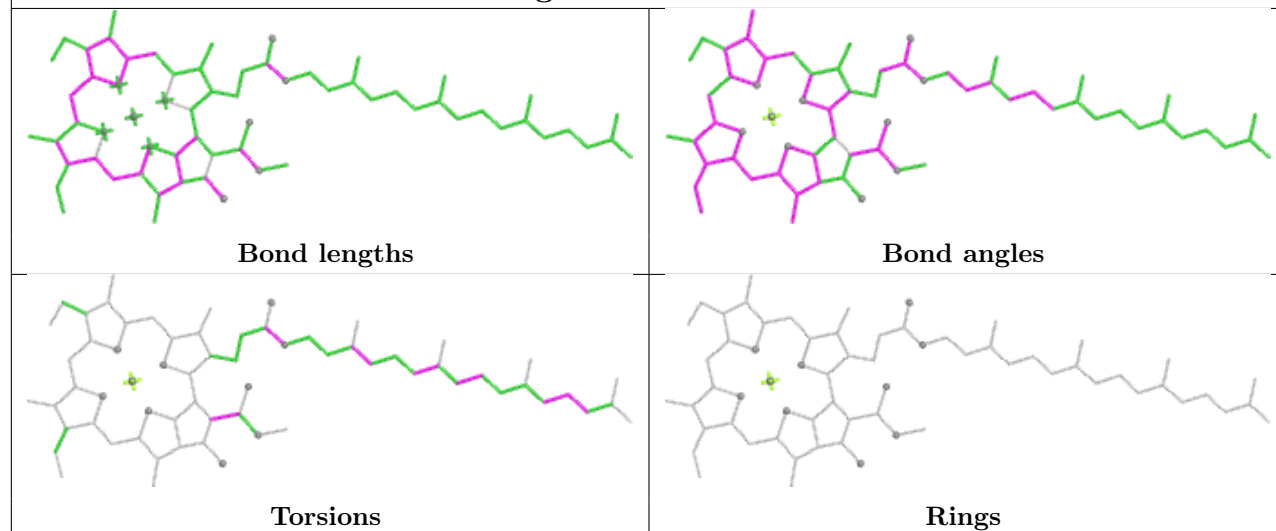


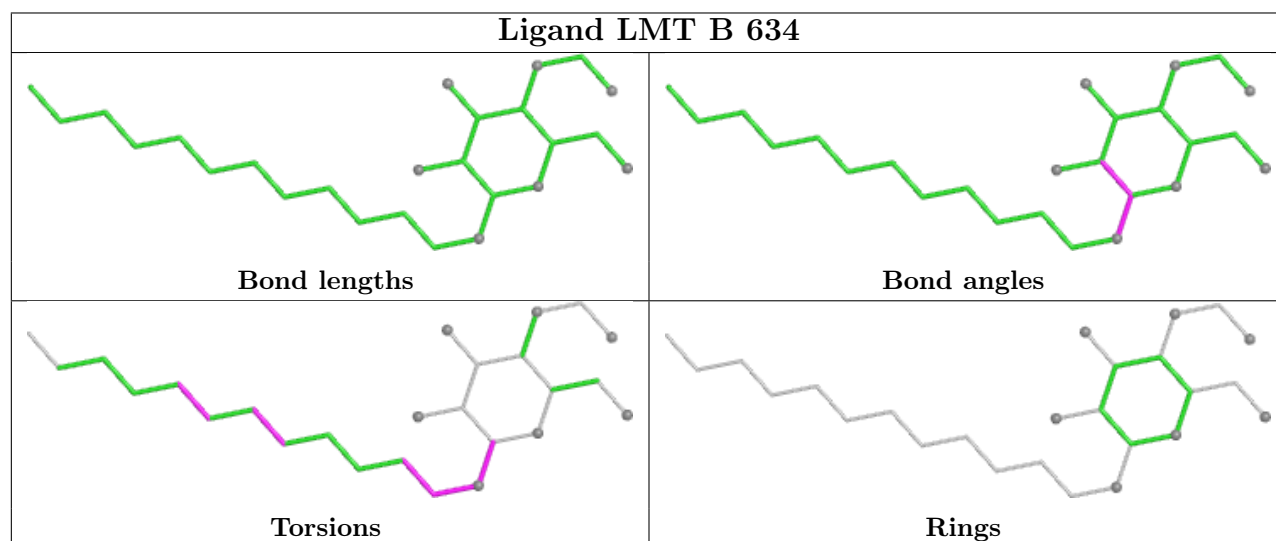
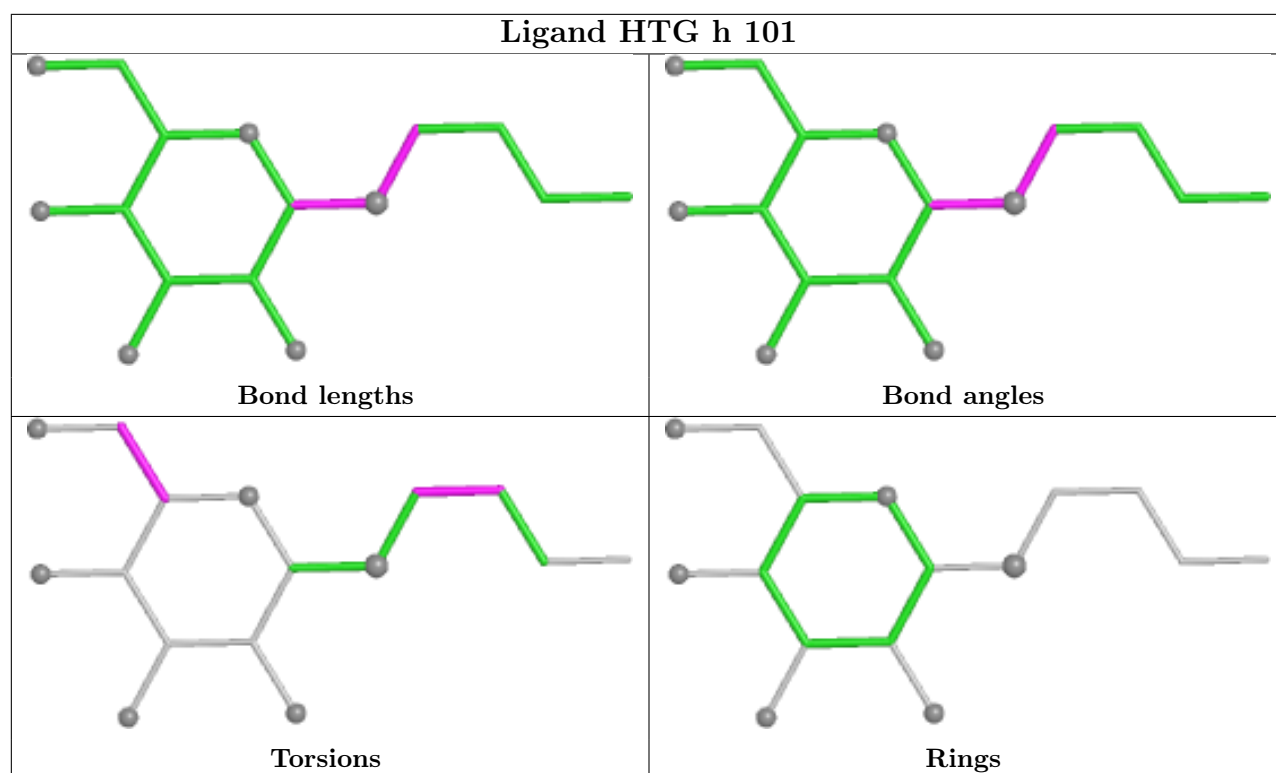


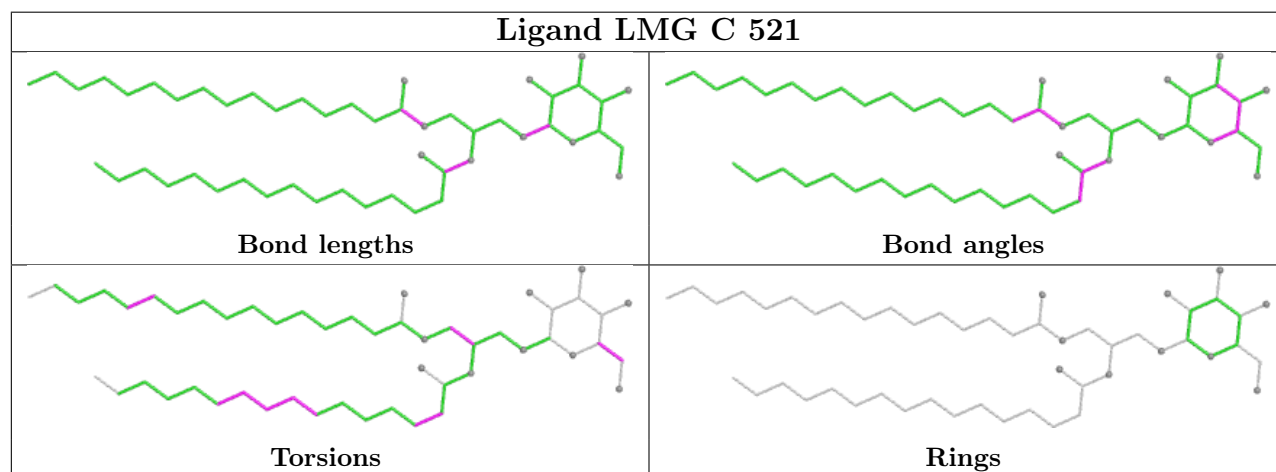
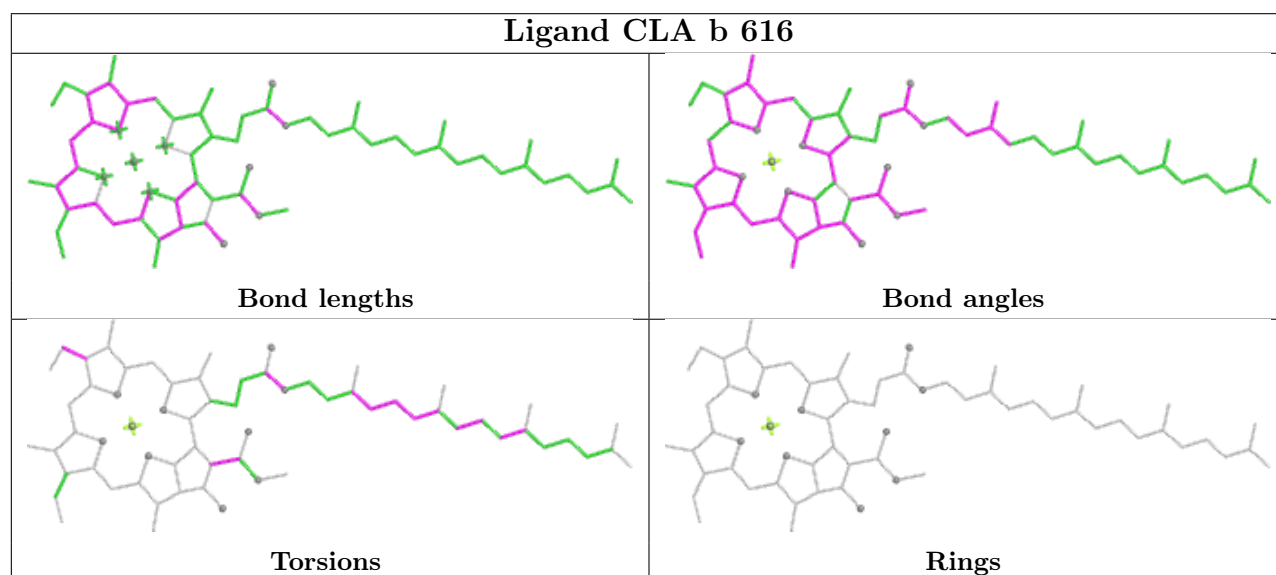
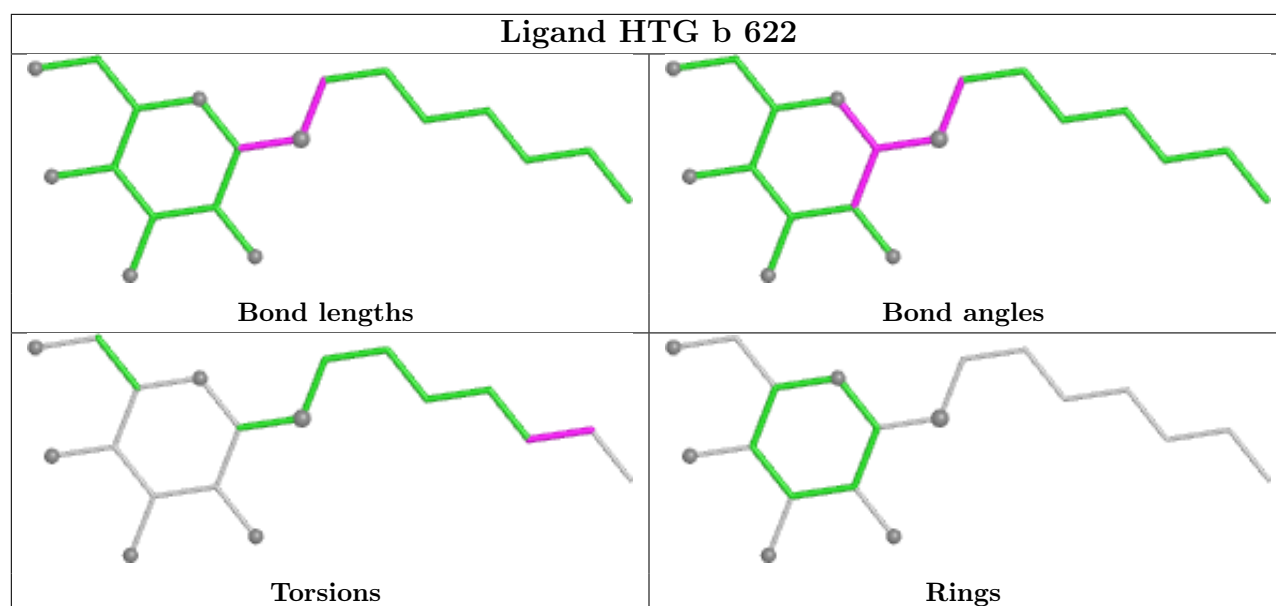




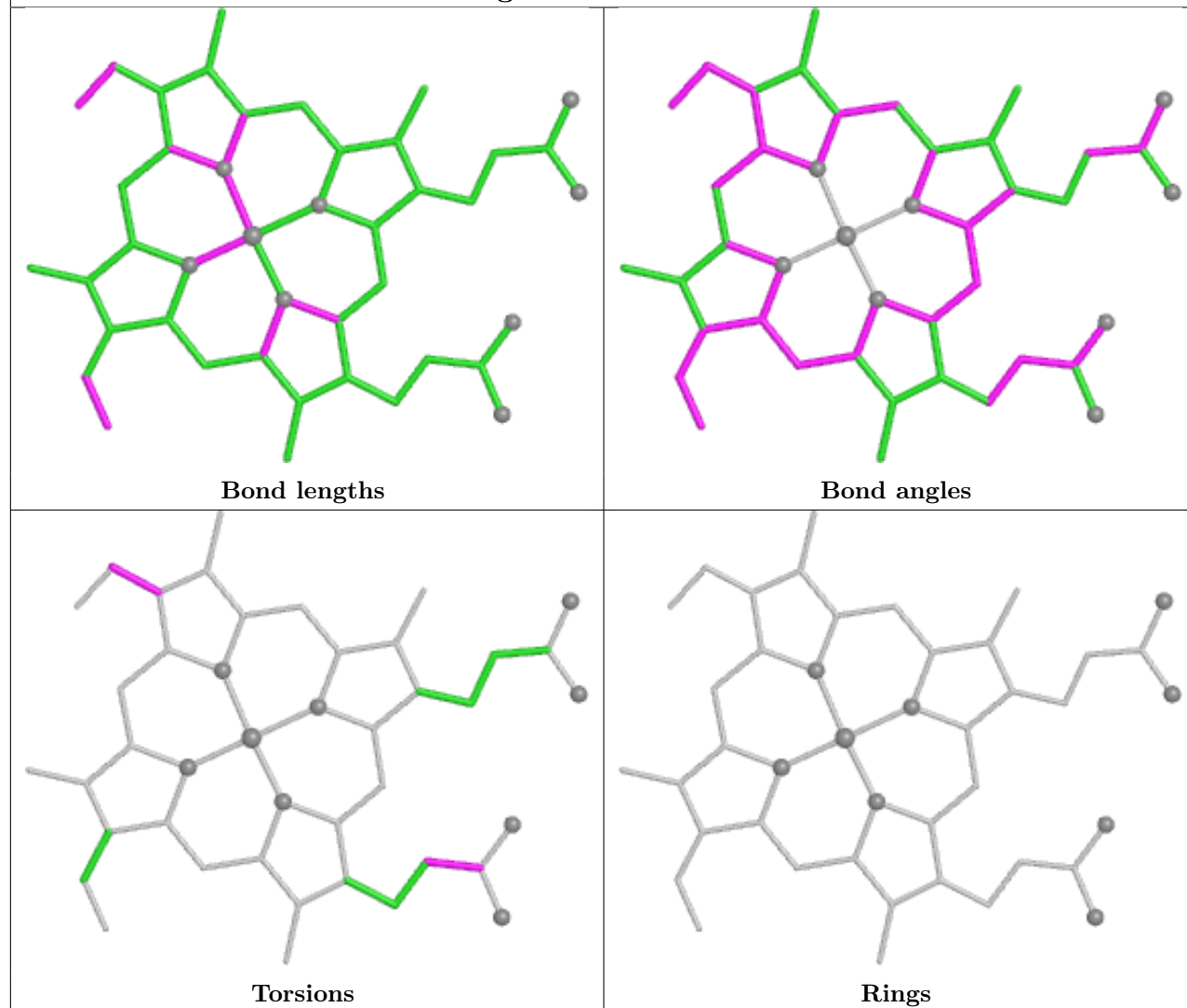


Ligand CLA a 406**Ligand CLA b 611**

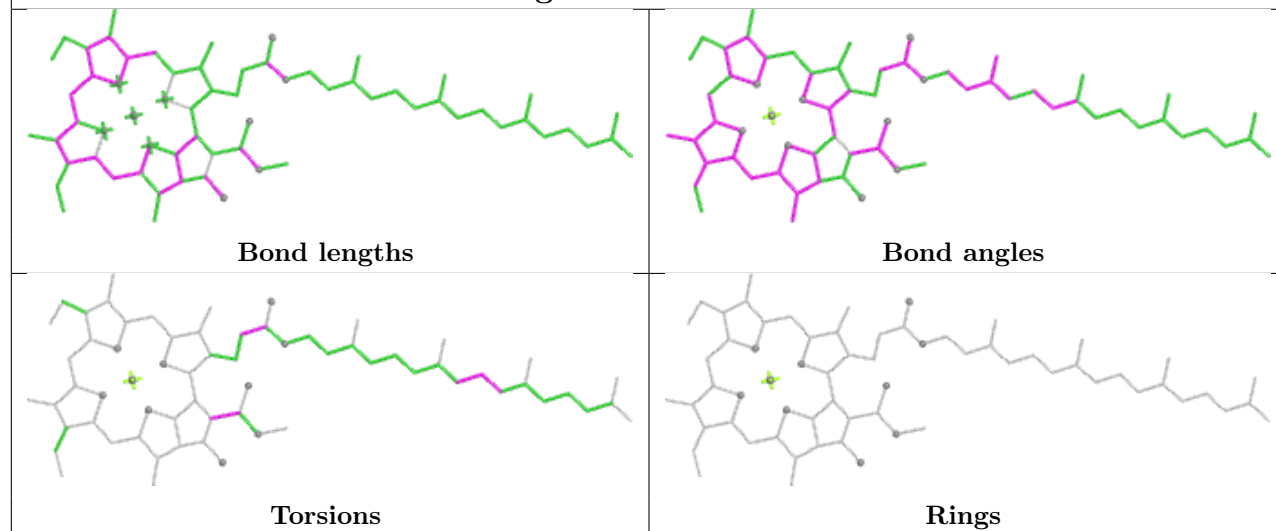


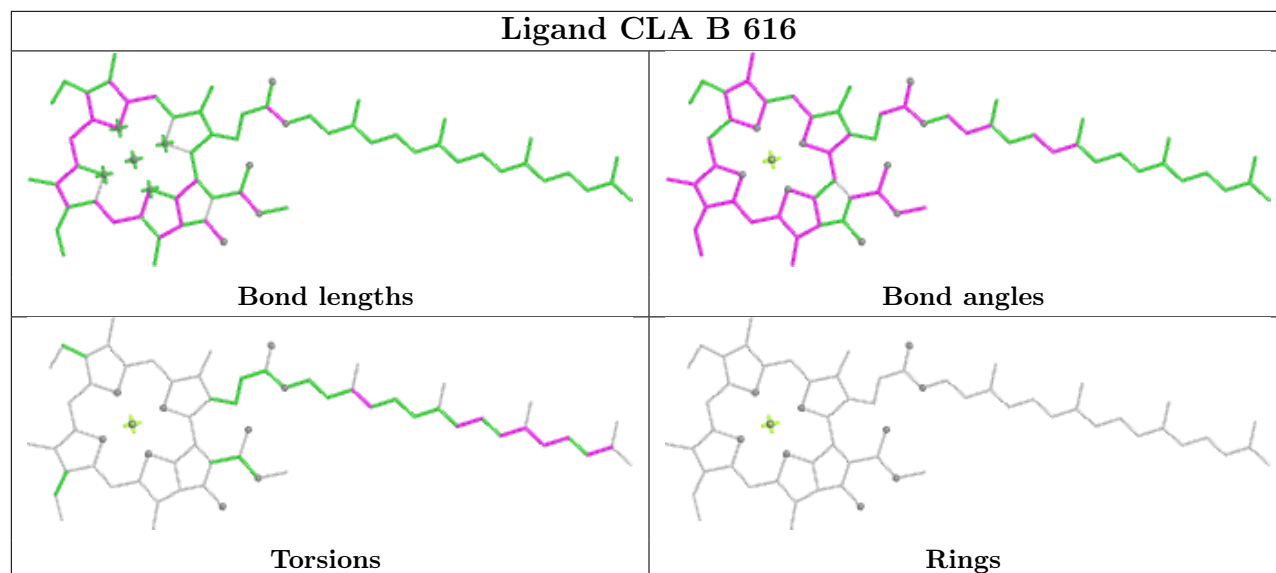
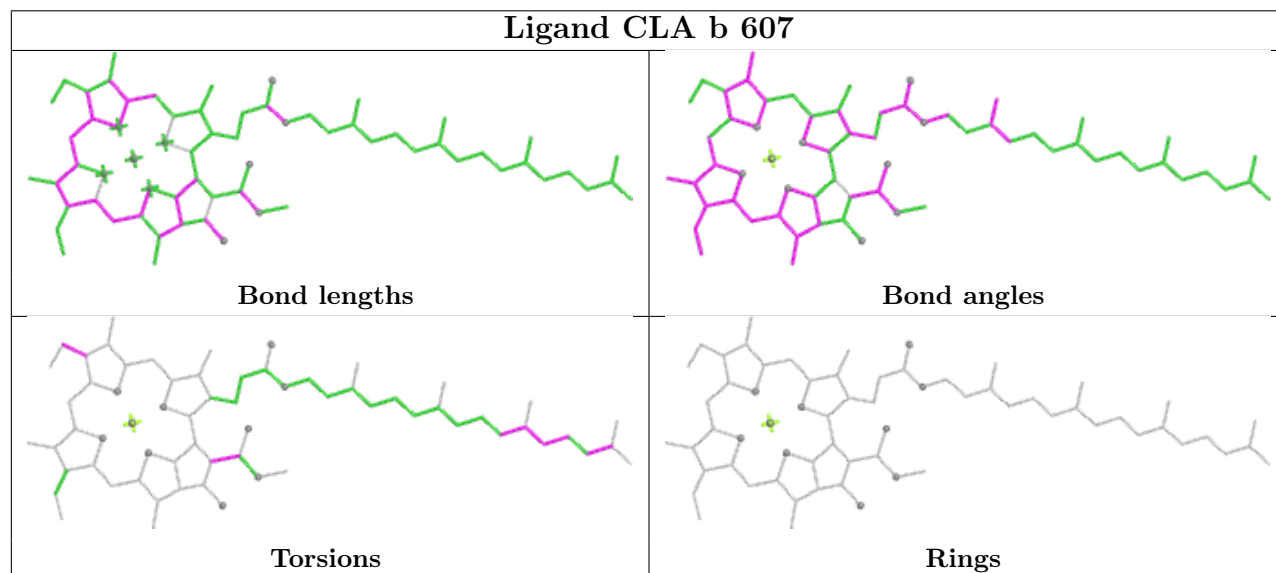
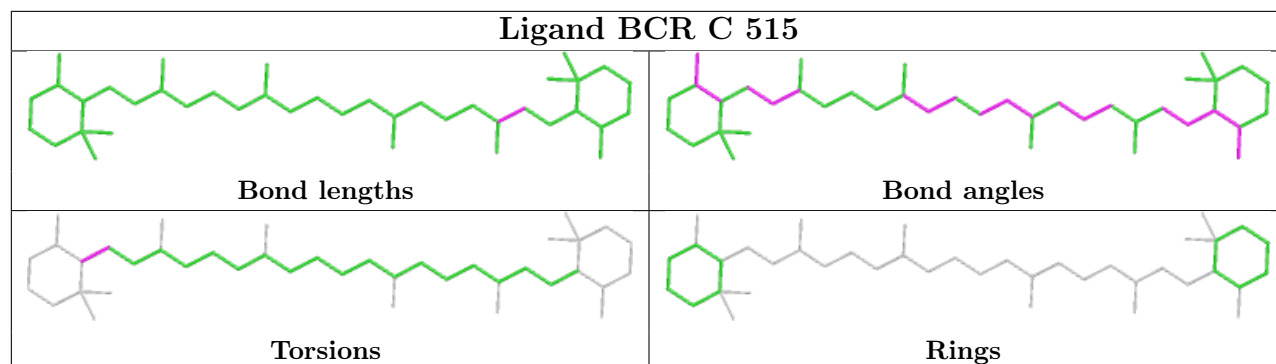


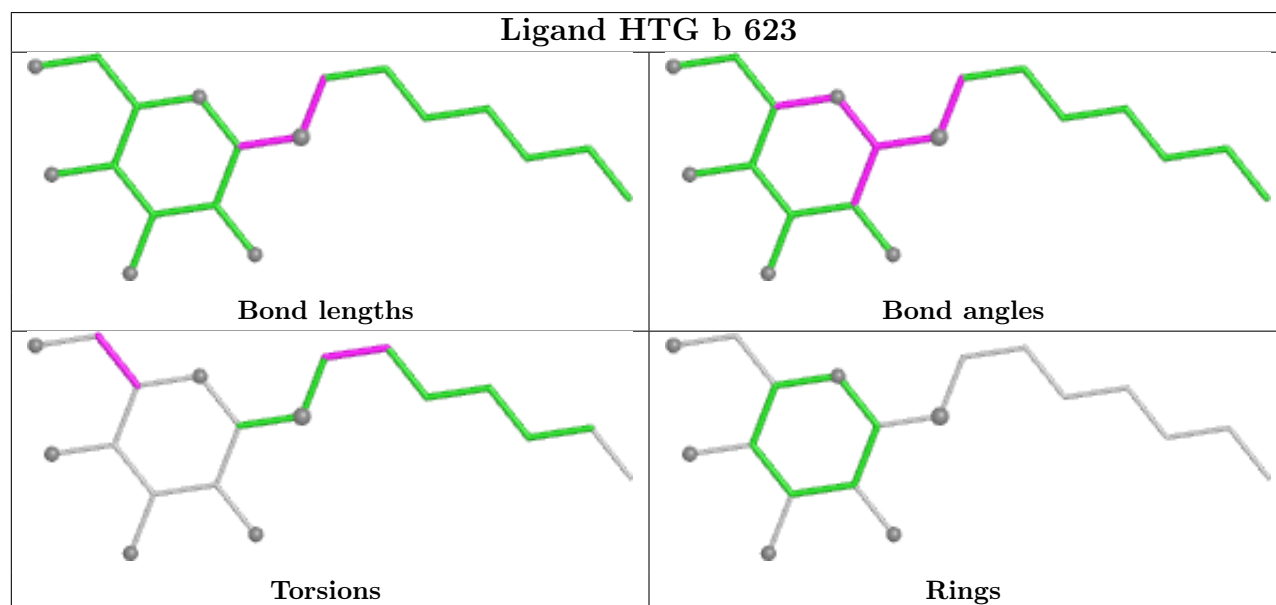
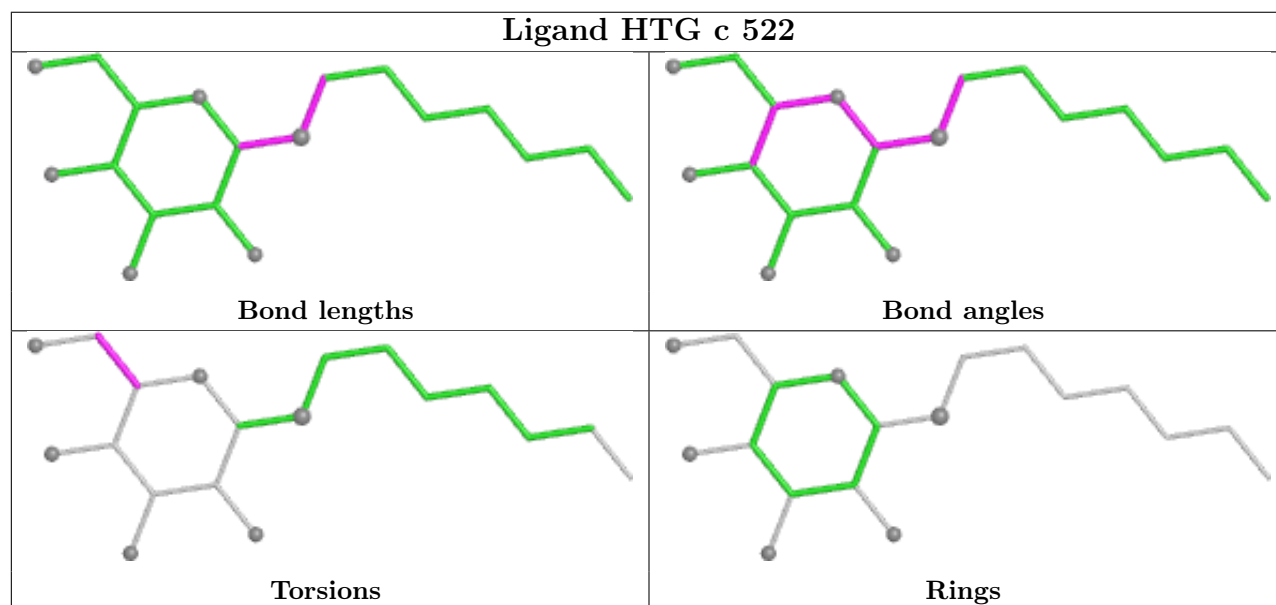
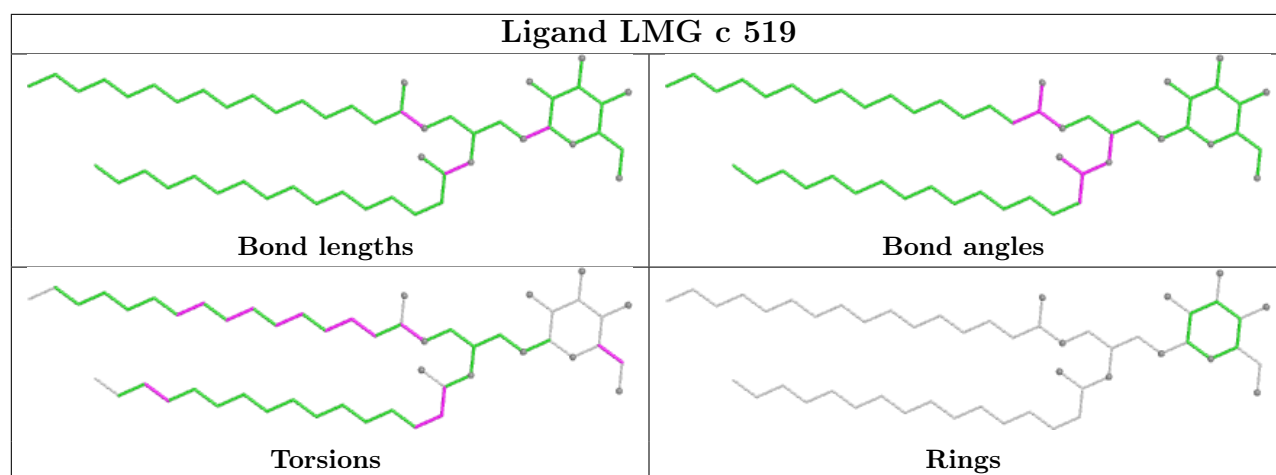
Ligand HEC v 201

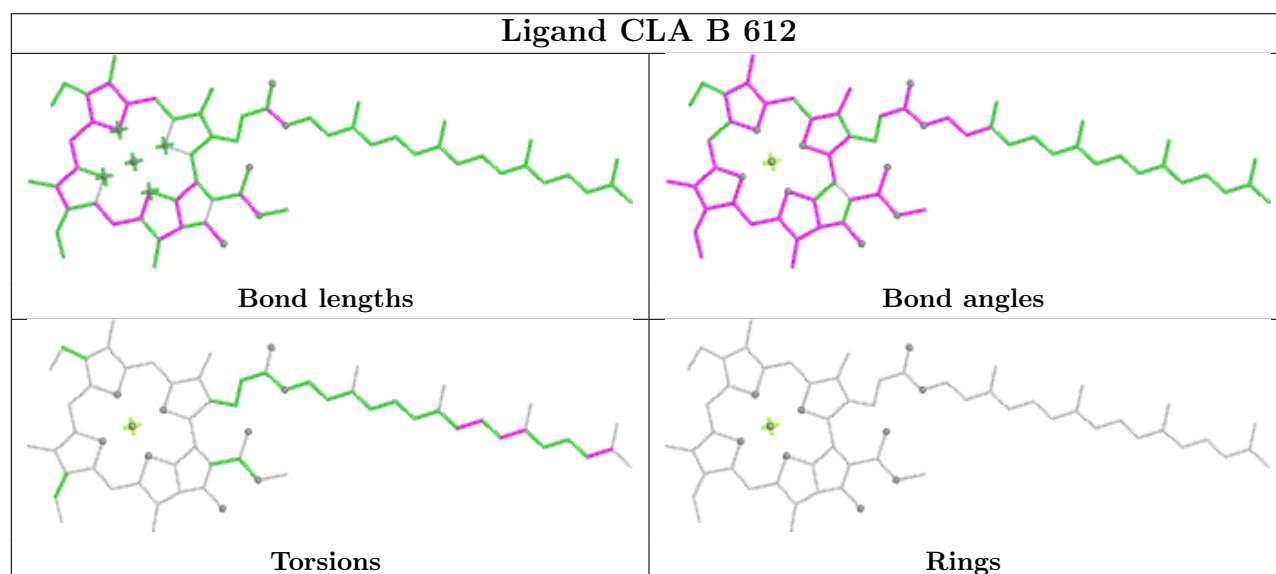
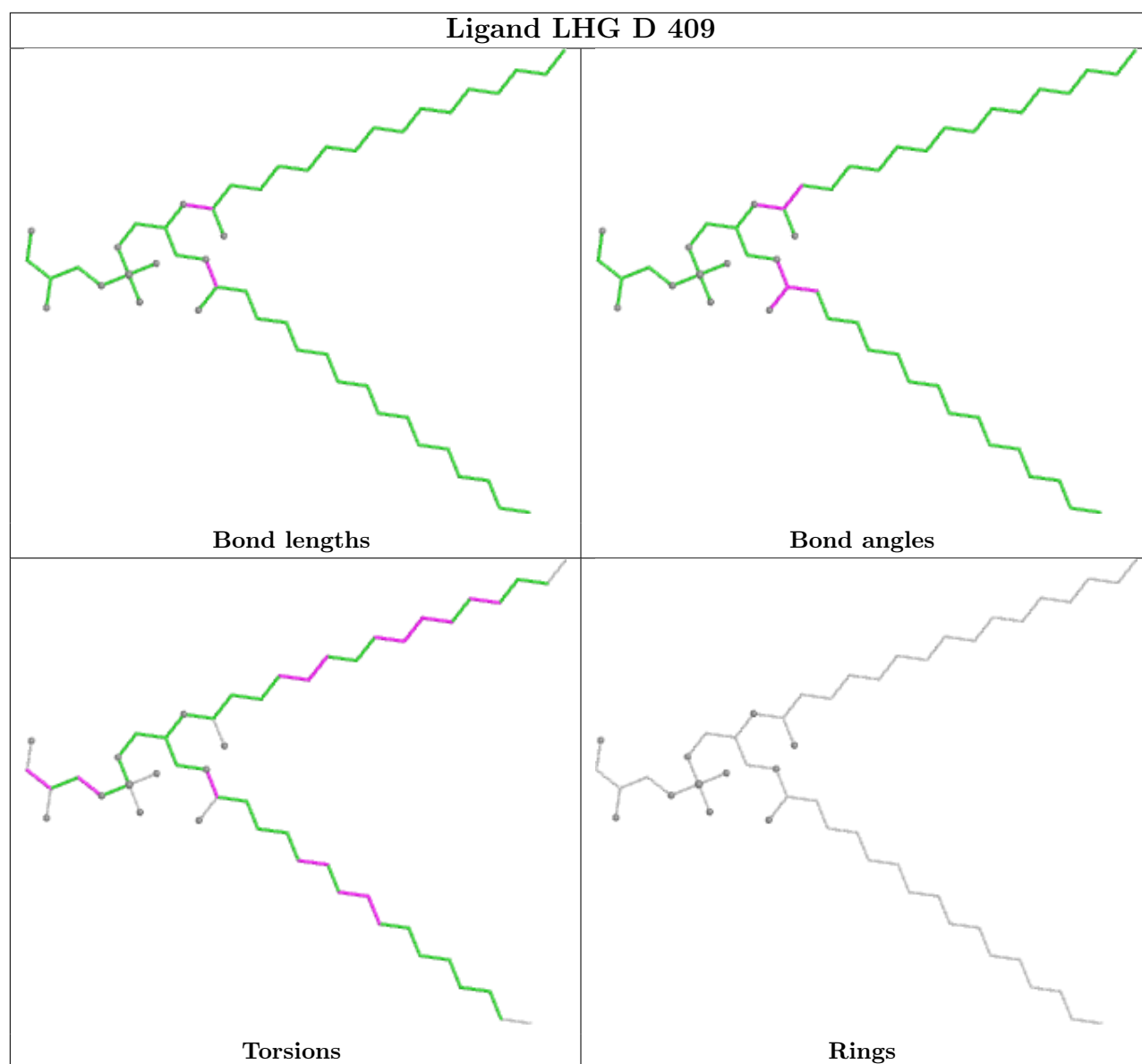


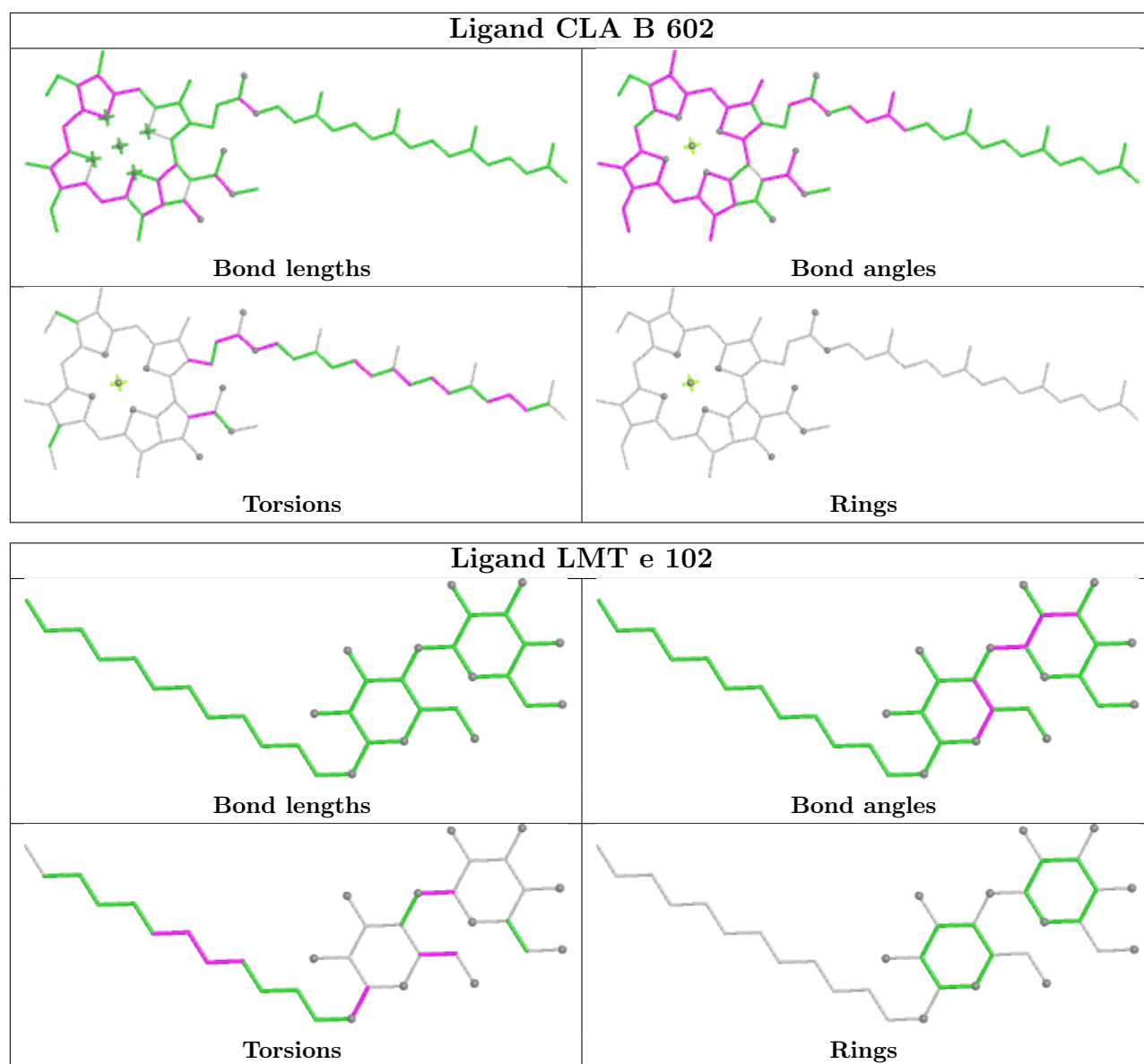
Ligand CLA b 612

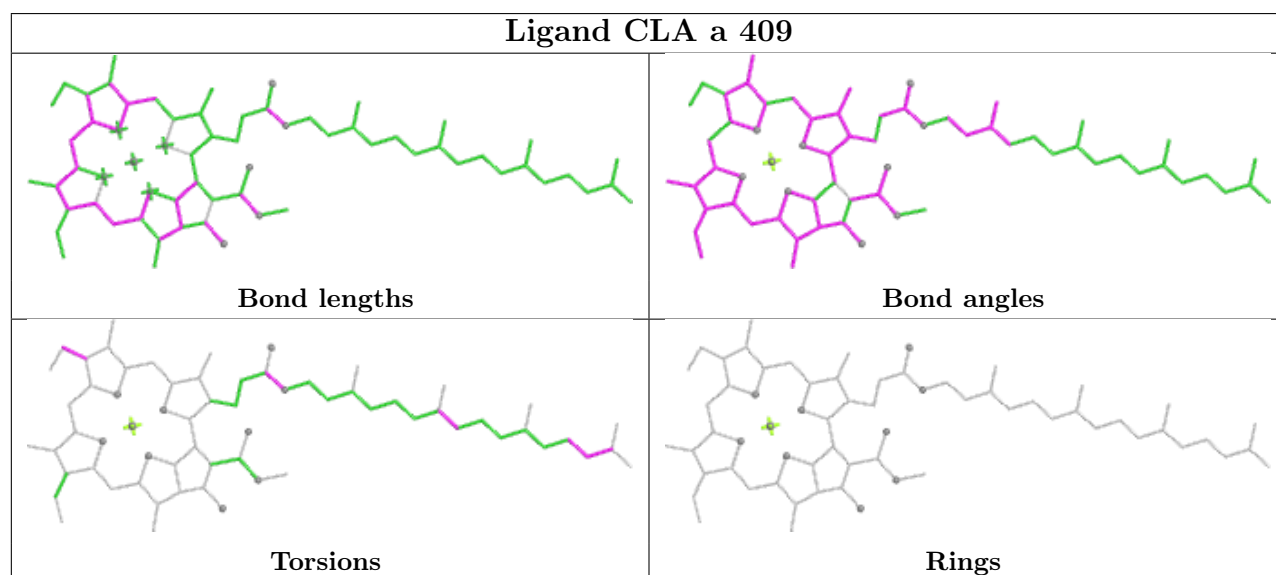
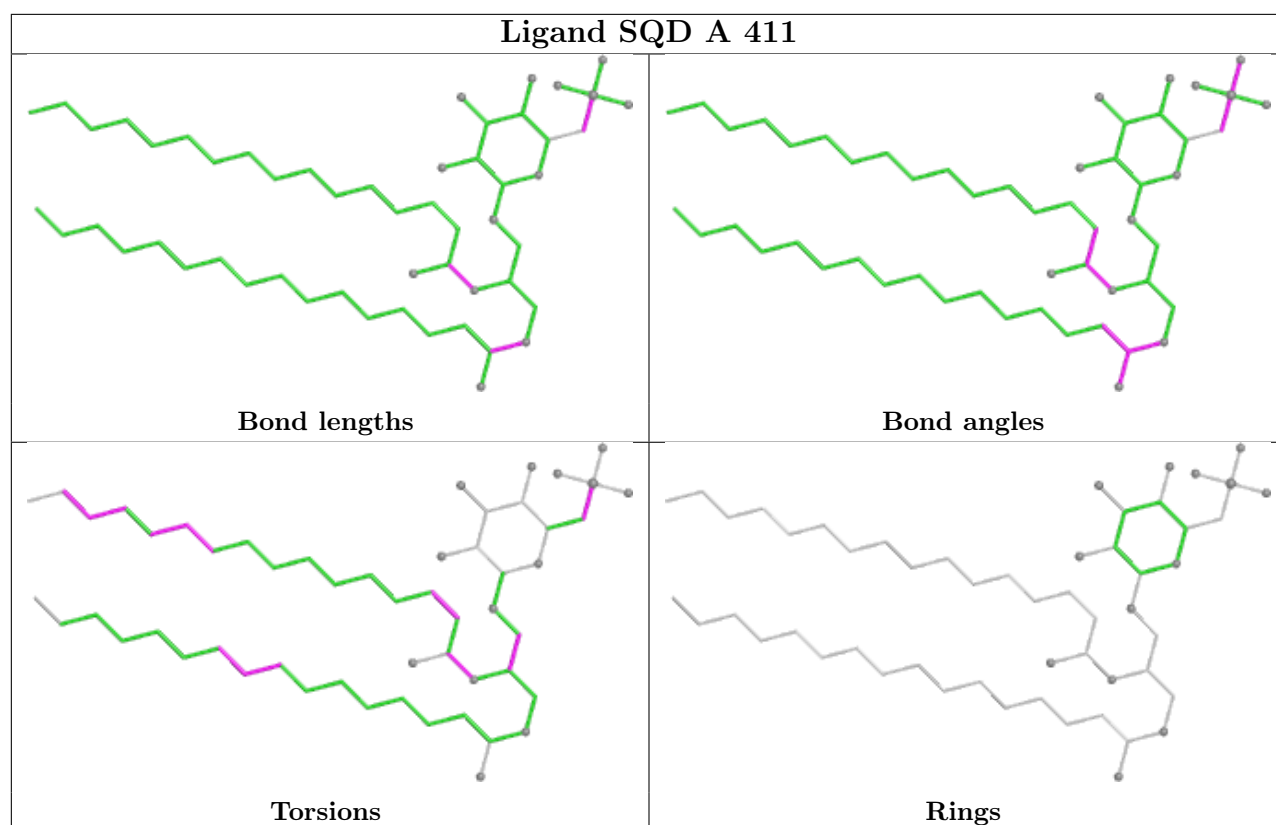


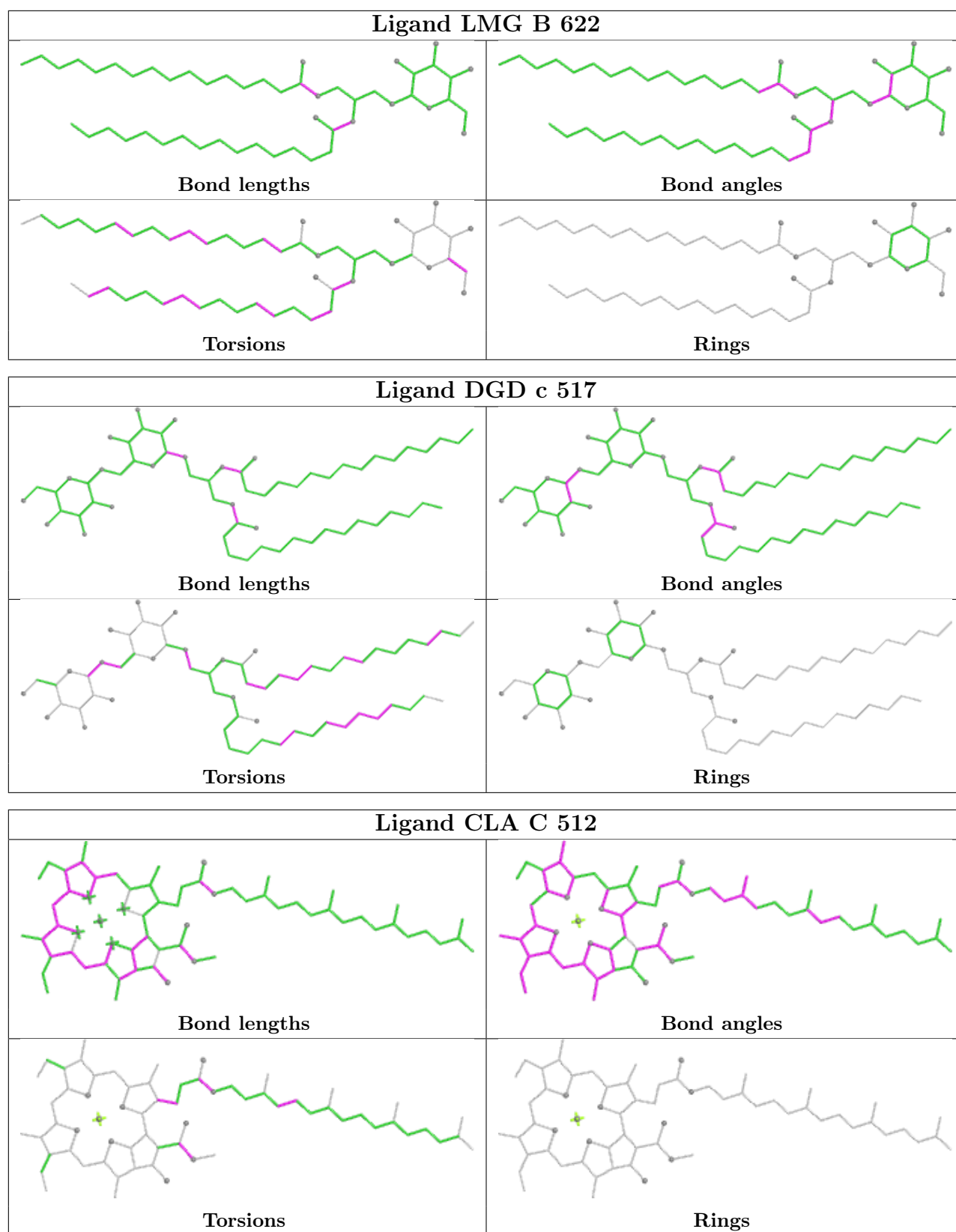


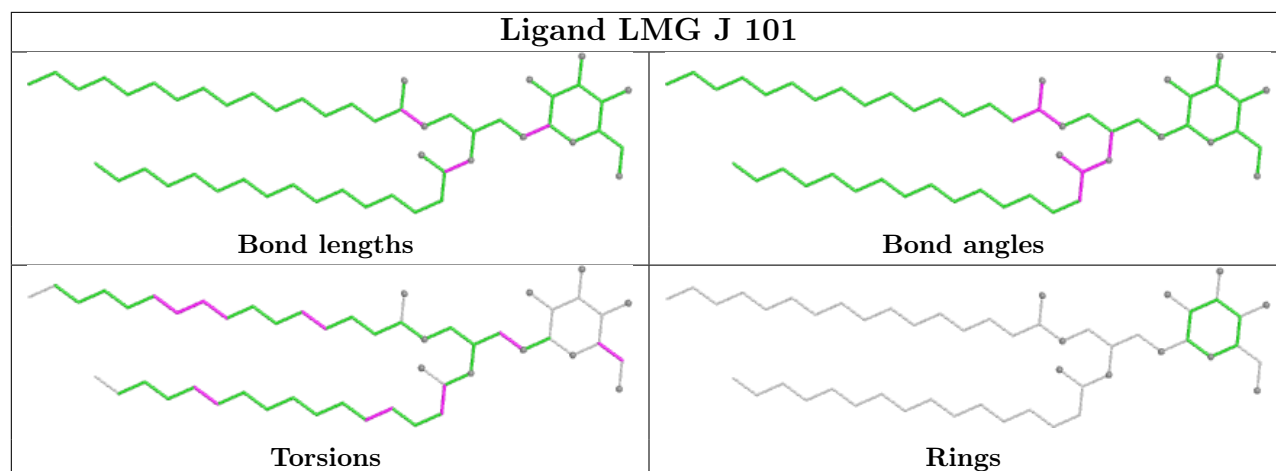
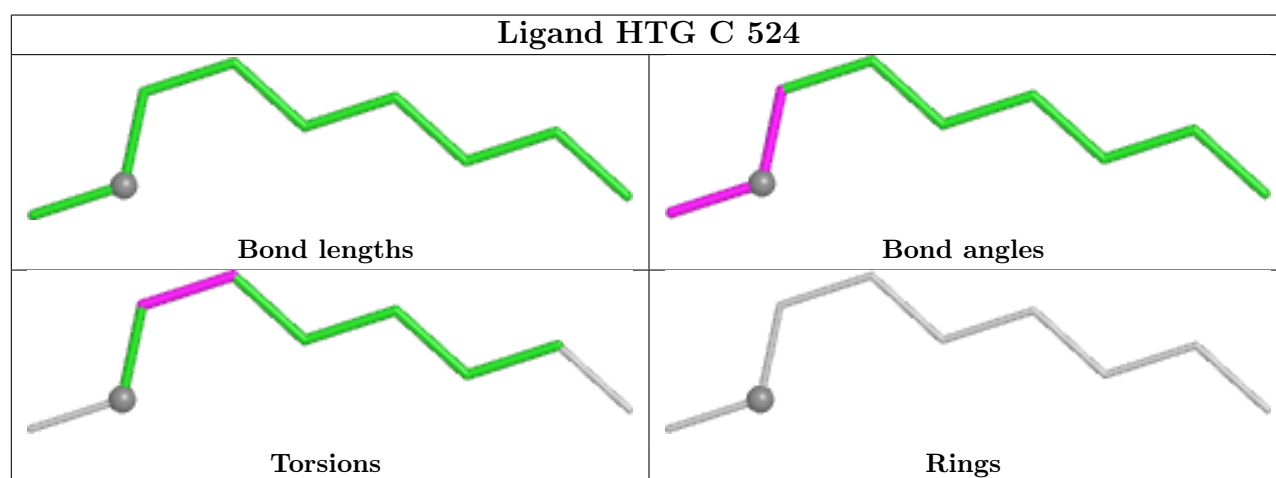
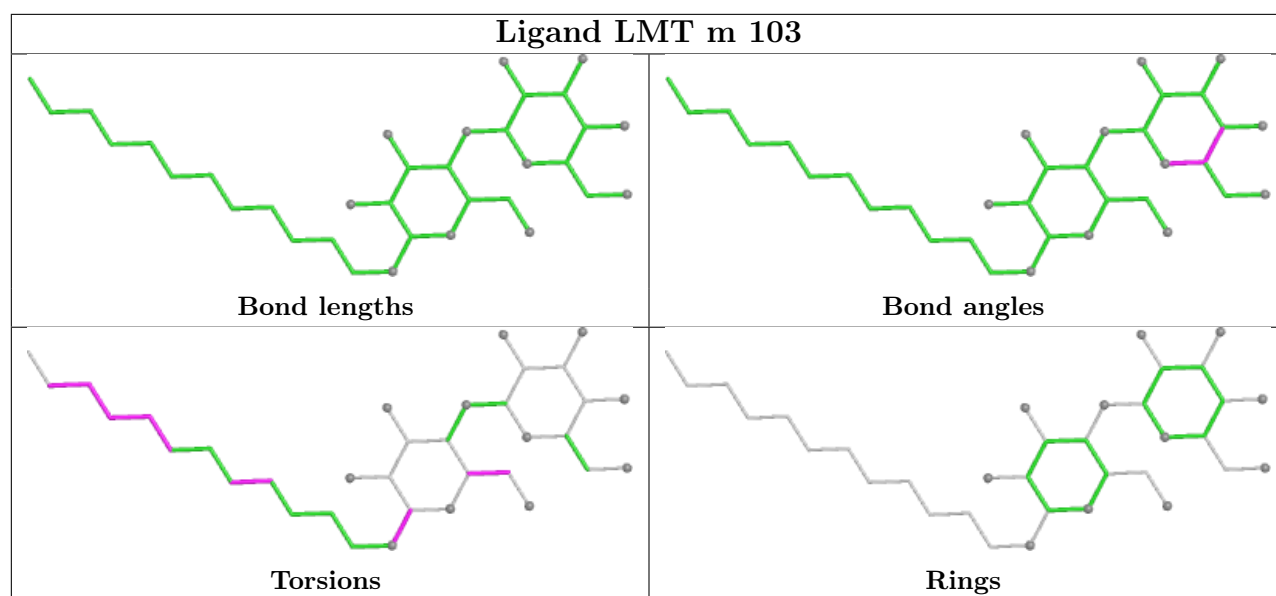


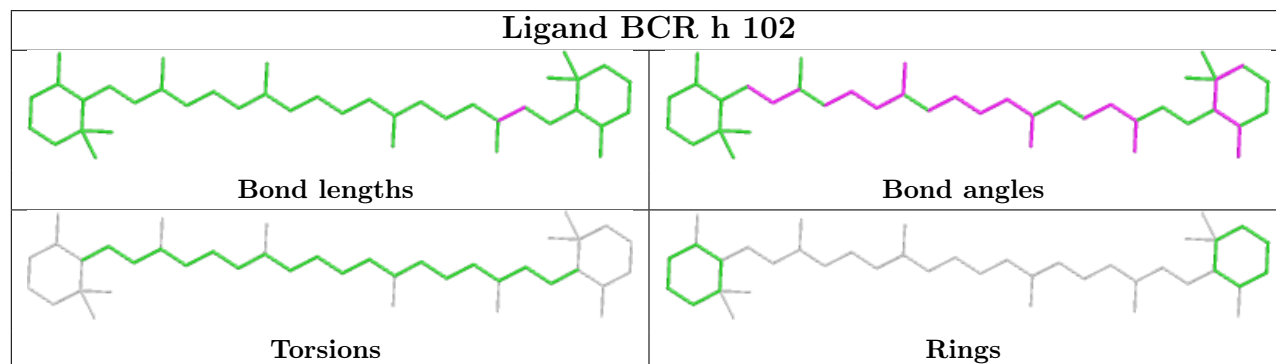
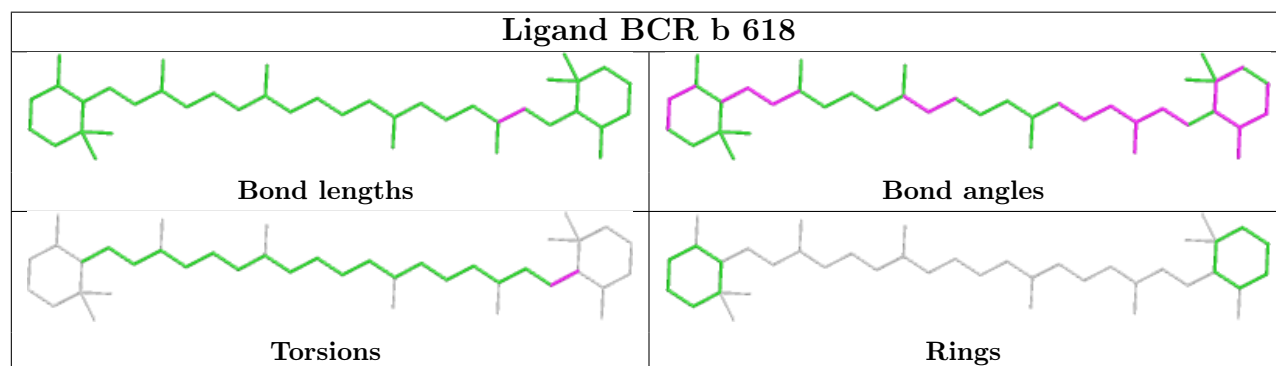
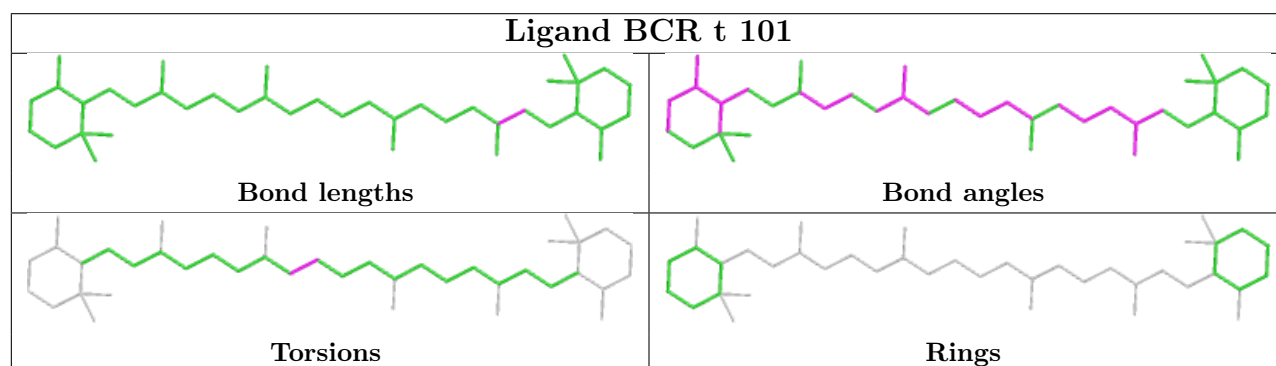
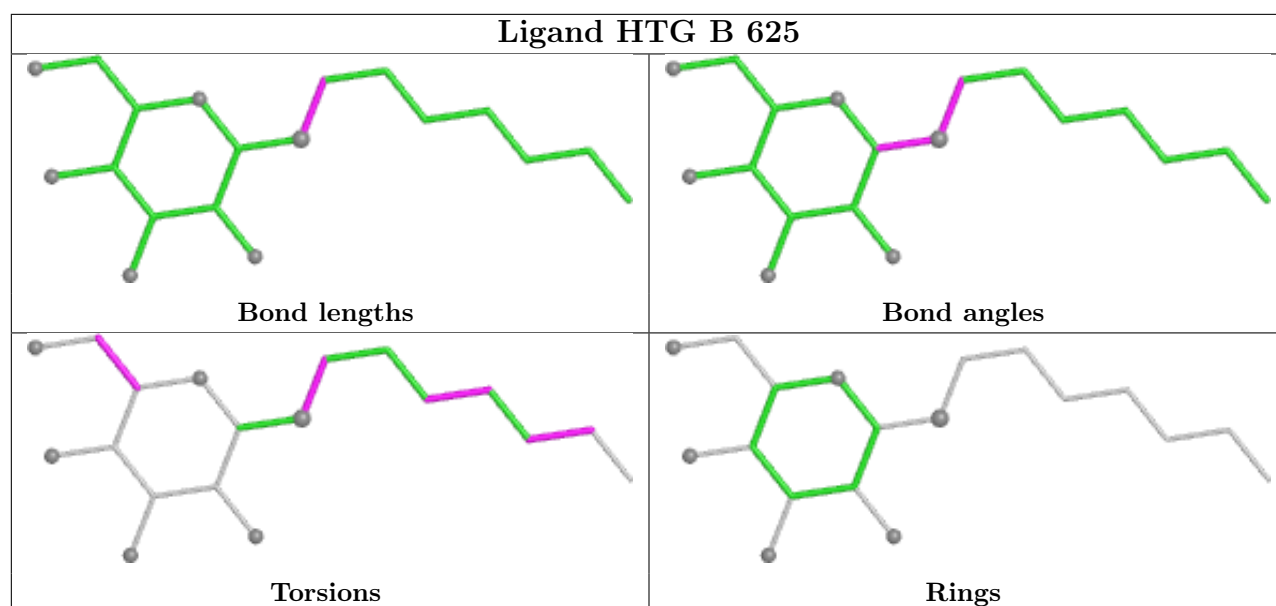


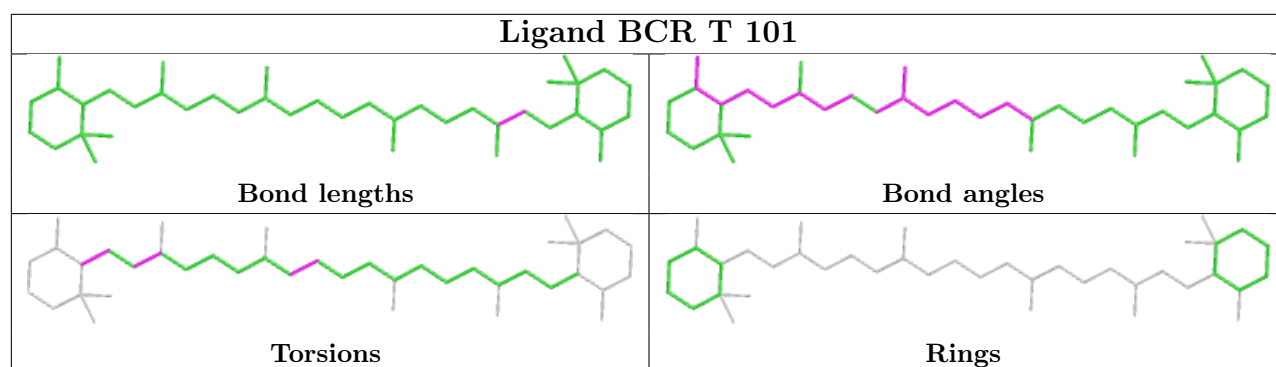
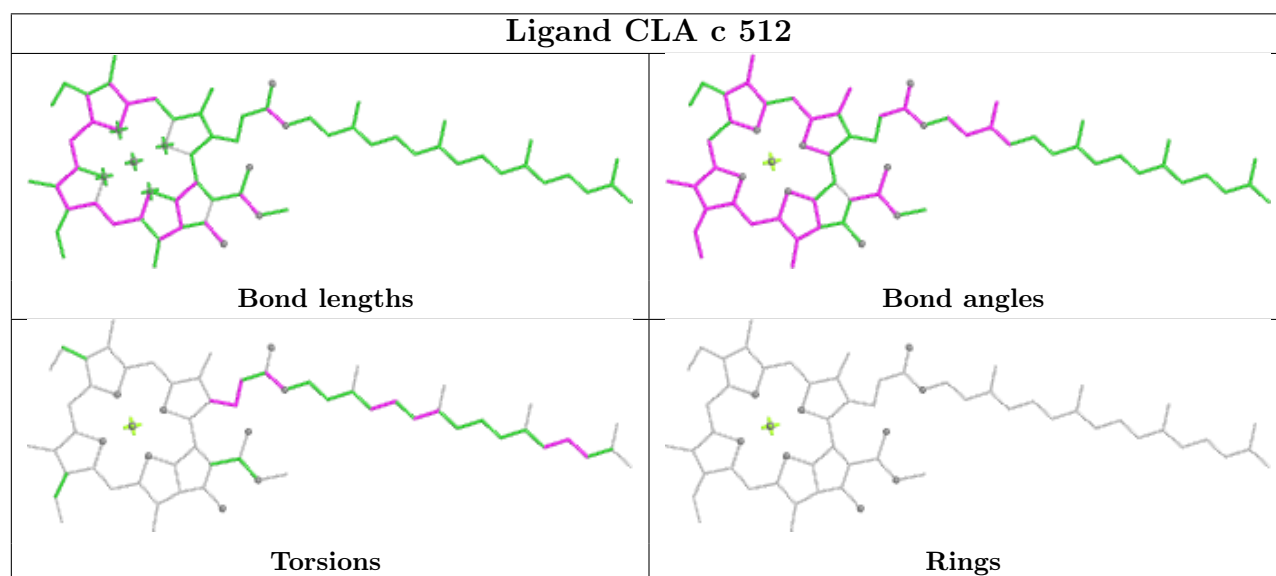
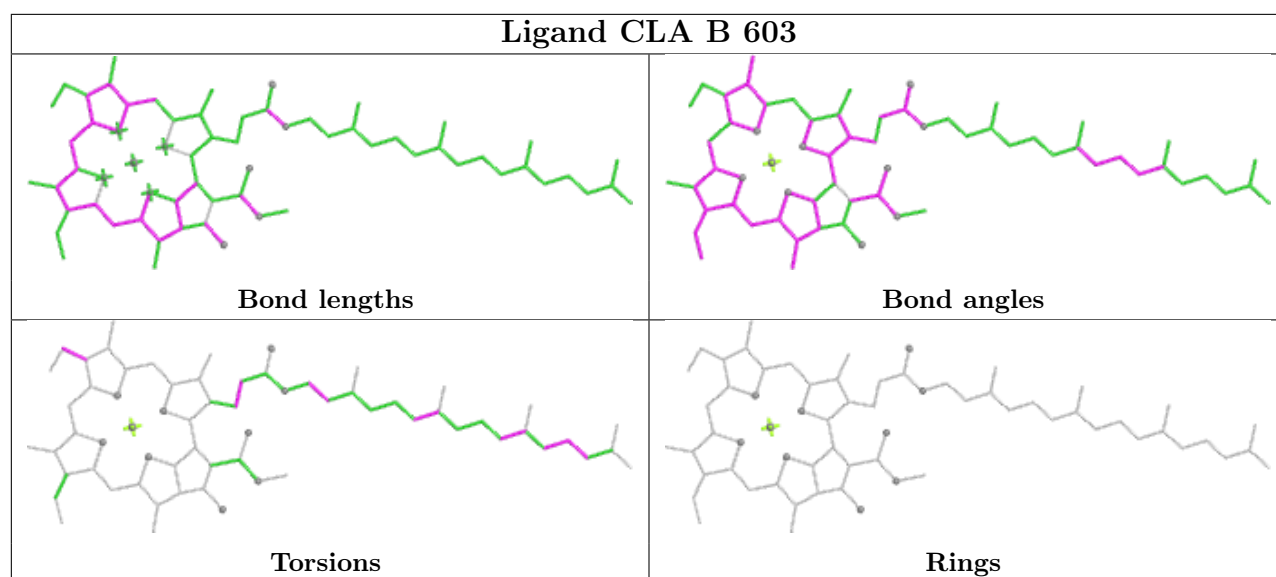


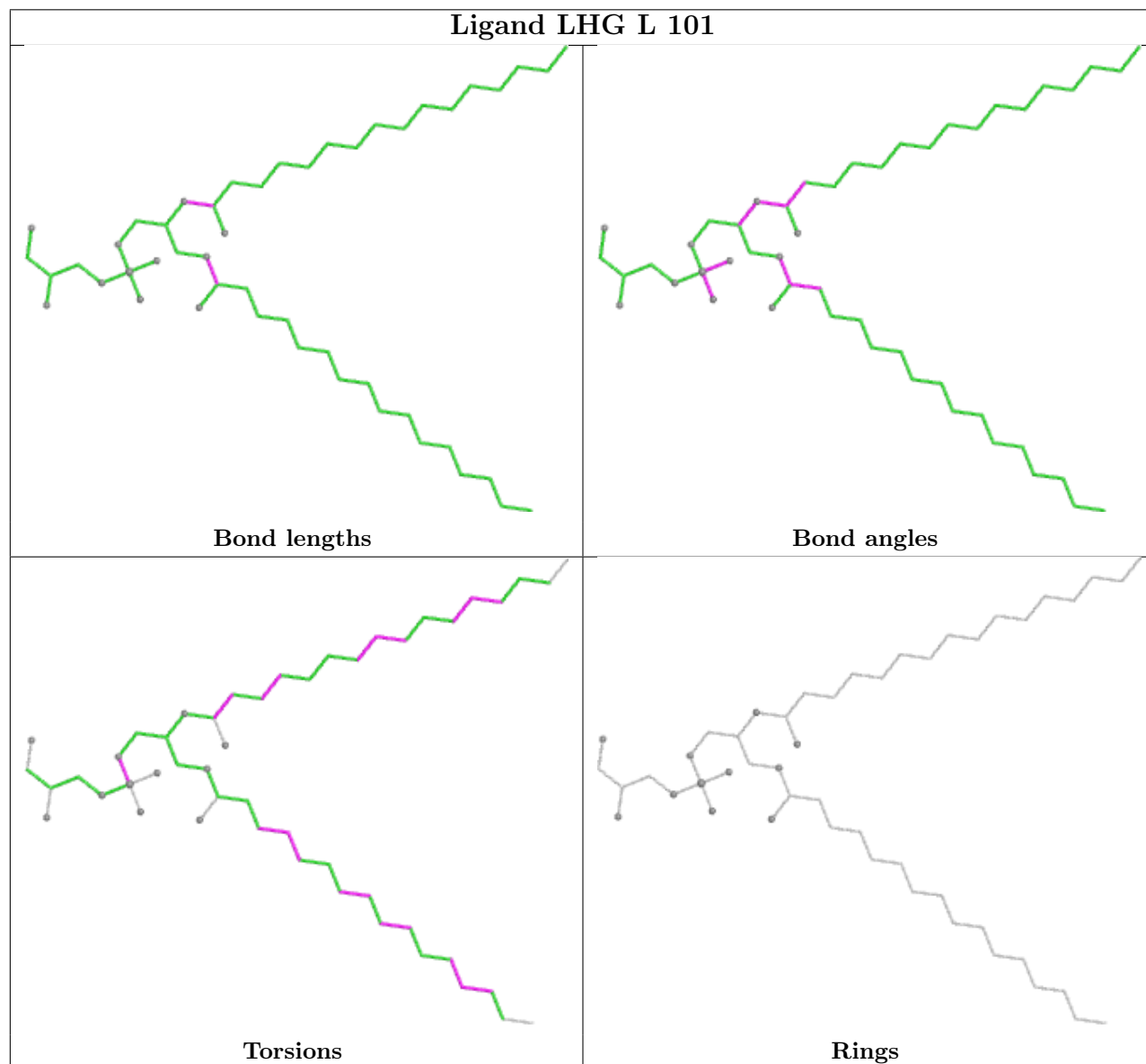
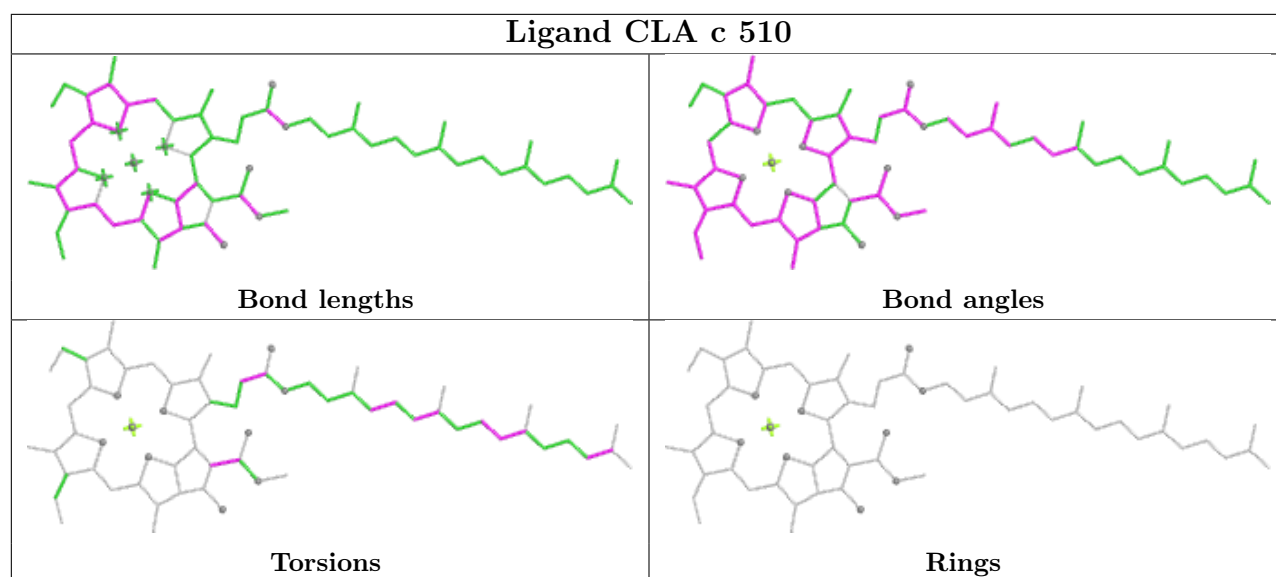


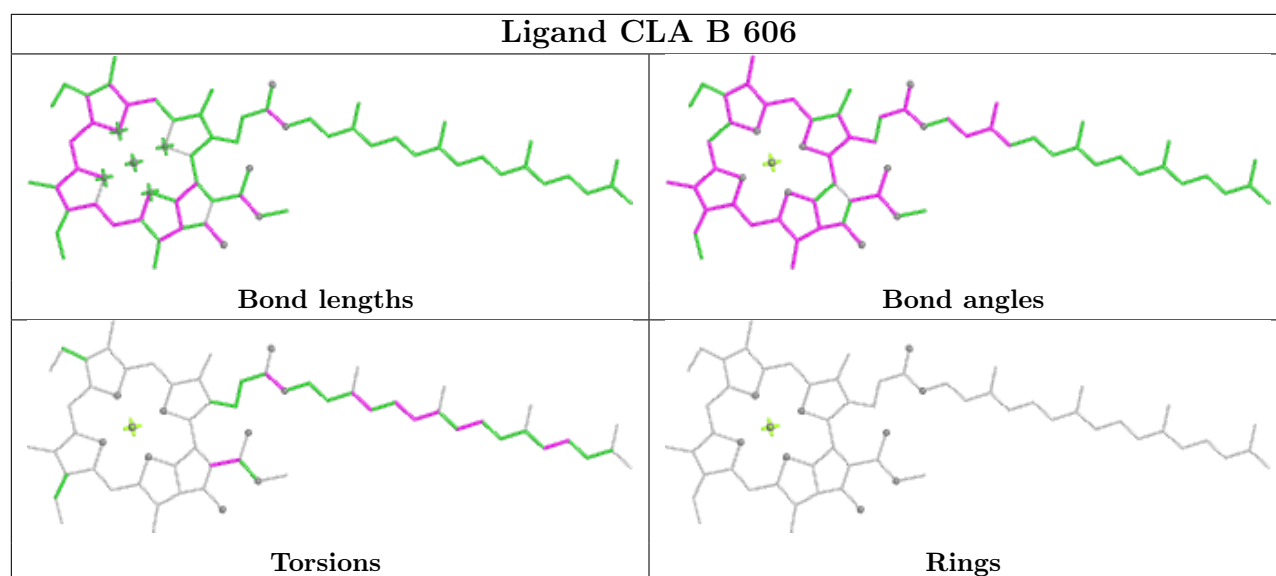
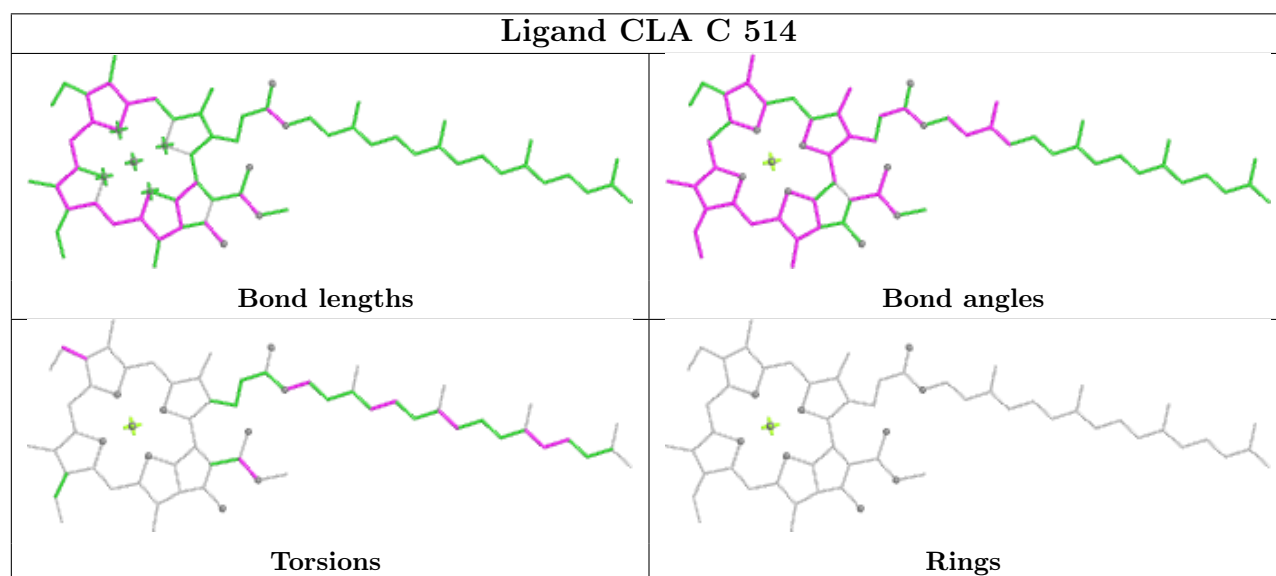
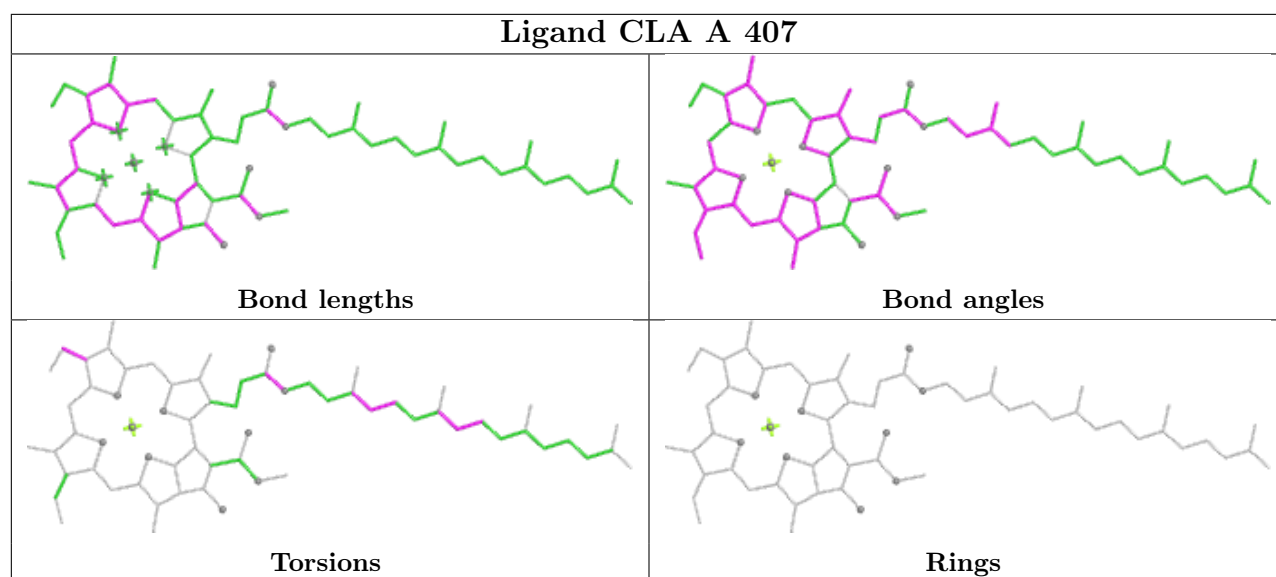


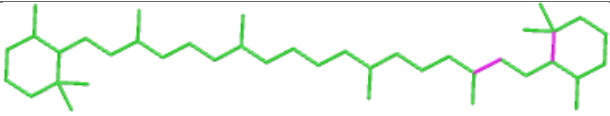
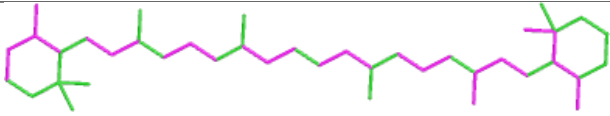
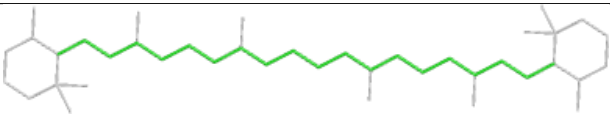
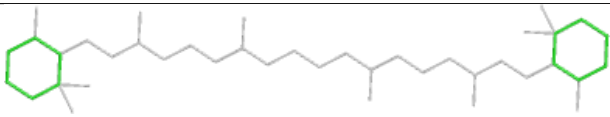
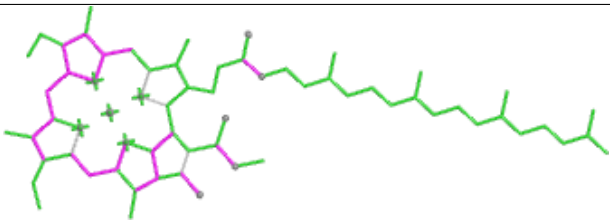
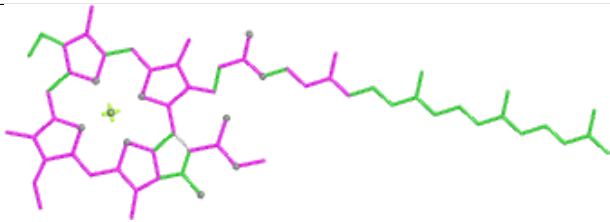
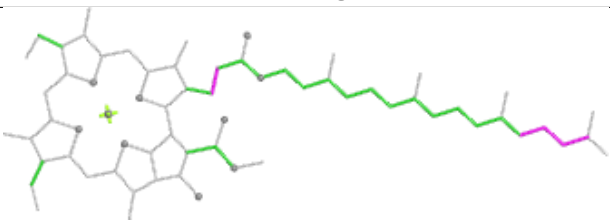
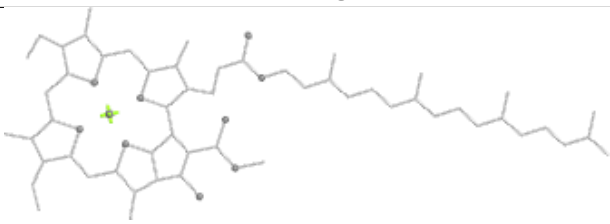
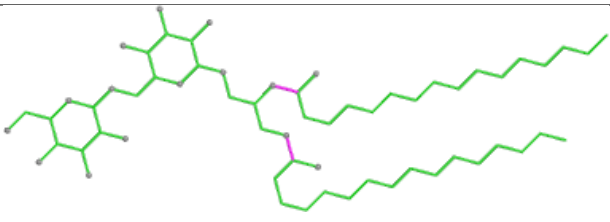
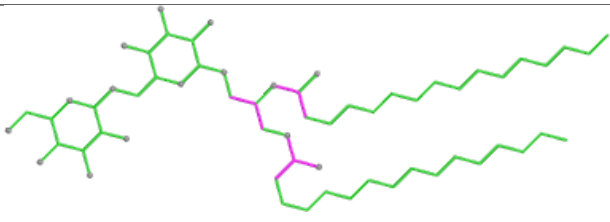
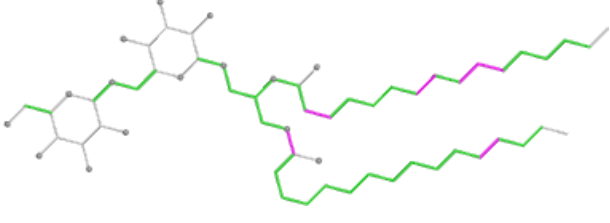
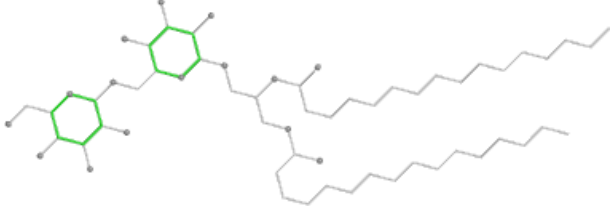


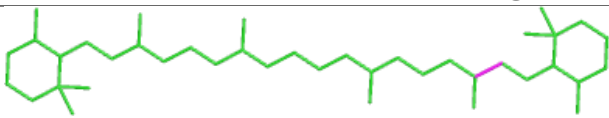
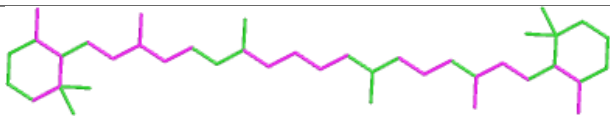
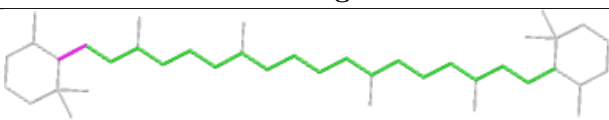
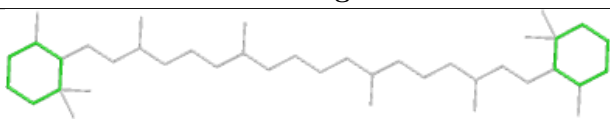


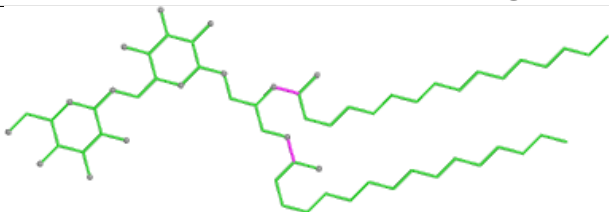
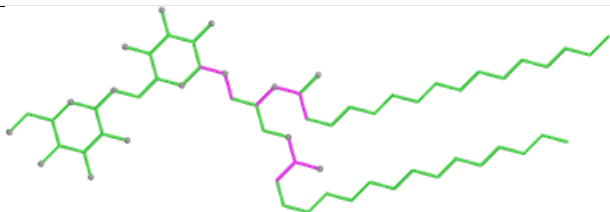
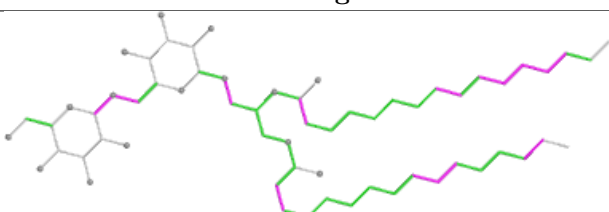
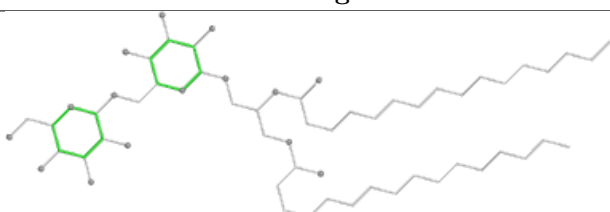


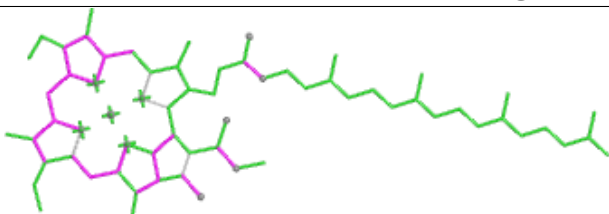
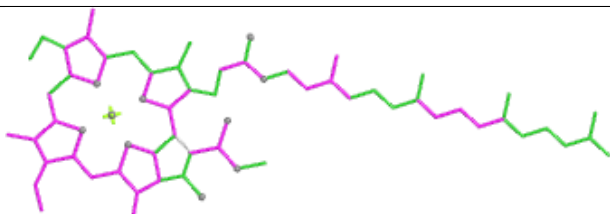
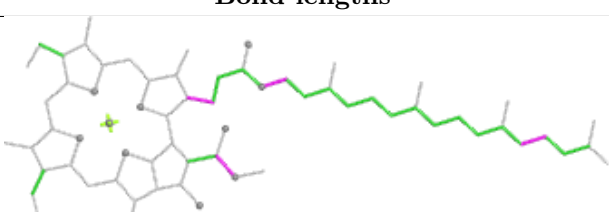
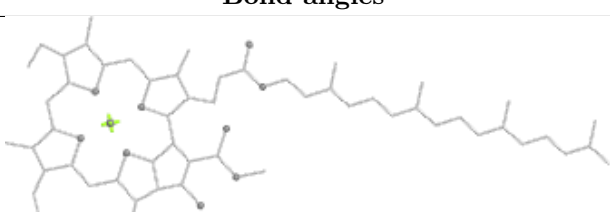


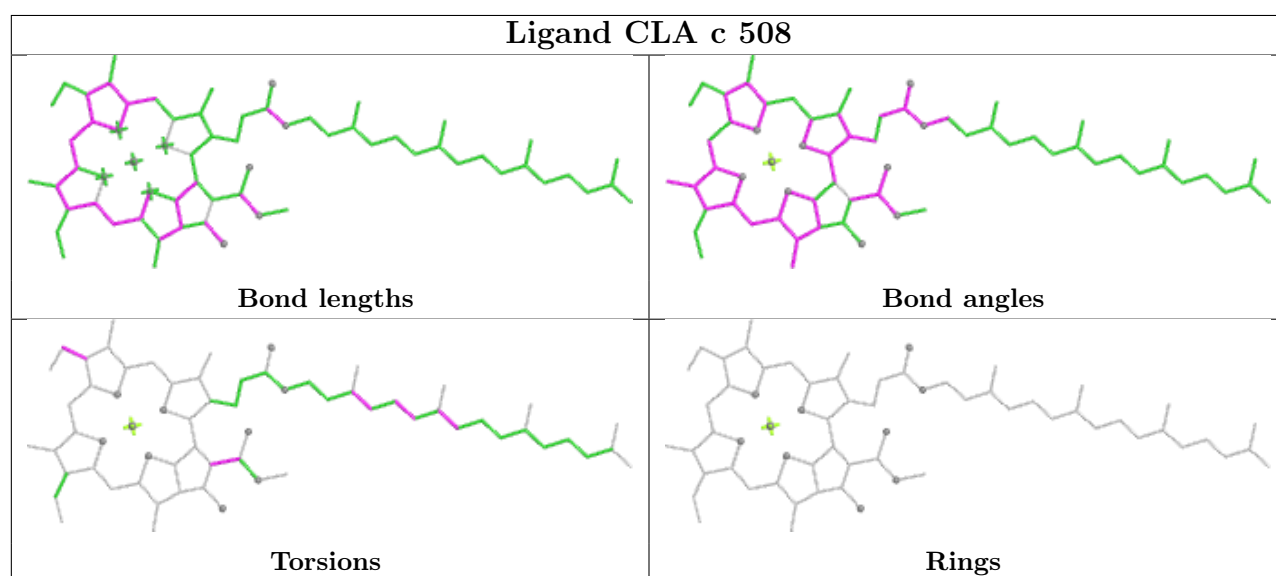
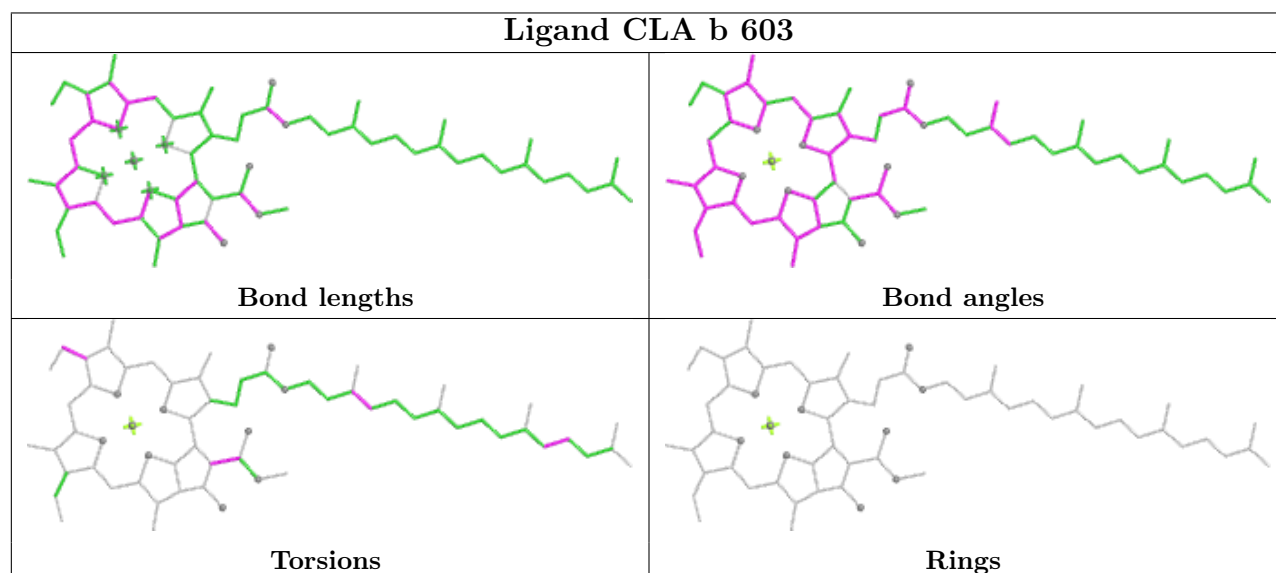
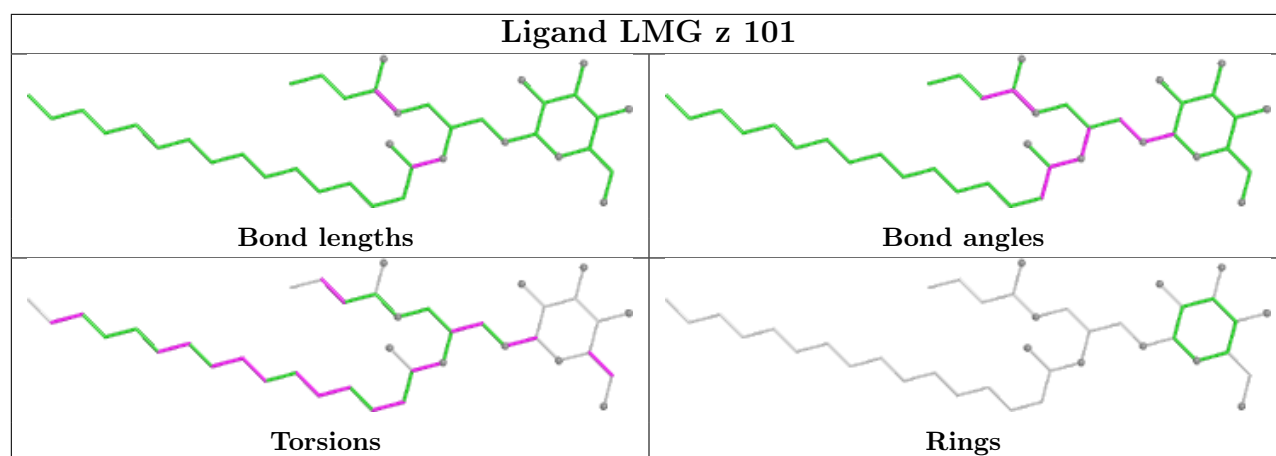


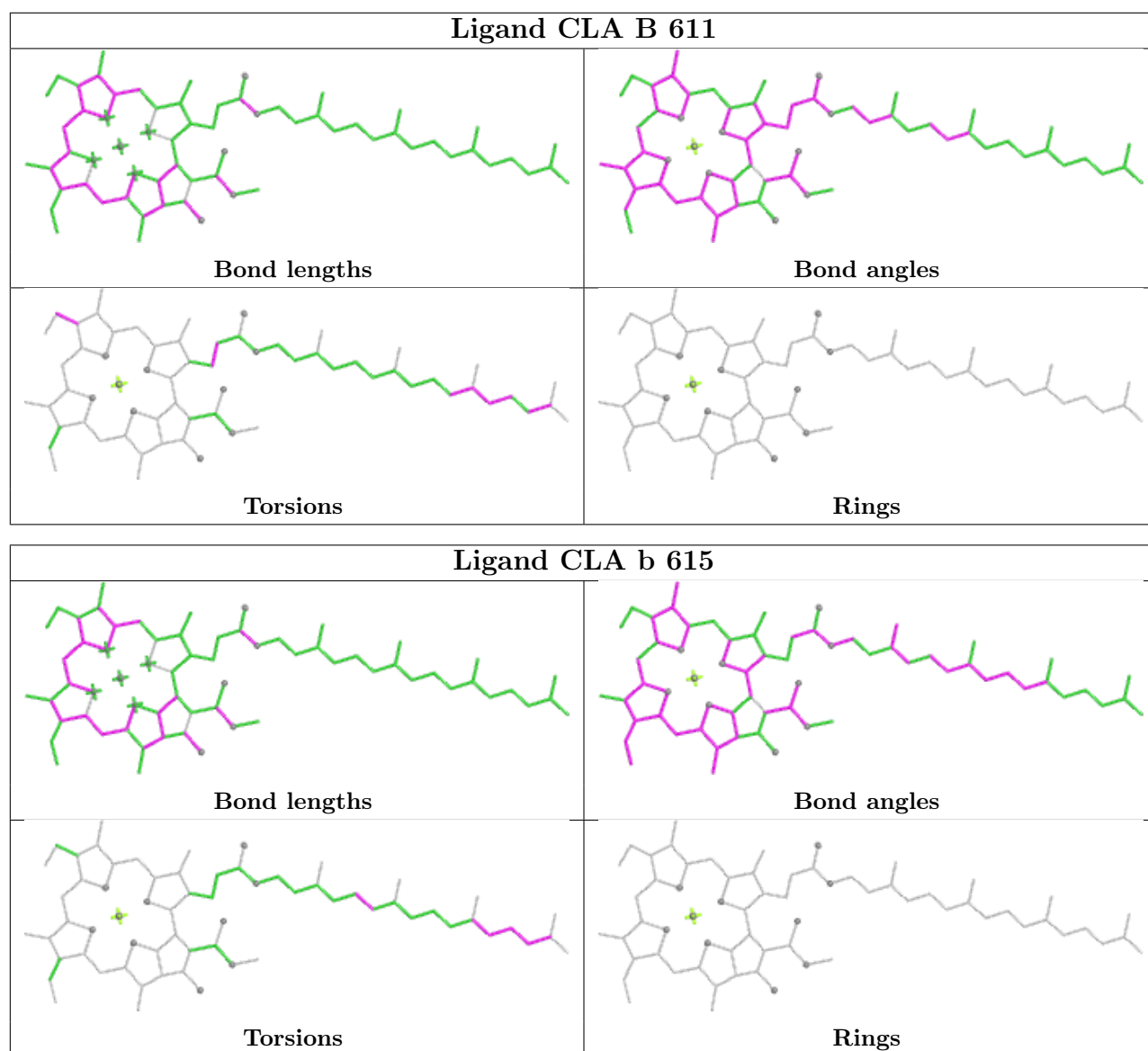
Ligand BCR b 619	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA a 404	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand DGD C 519	
 Bond lengths	 Bond angles
 Torsions	 Rings

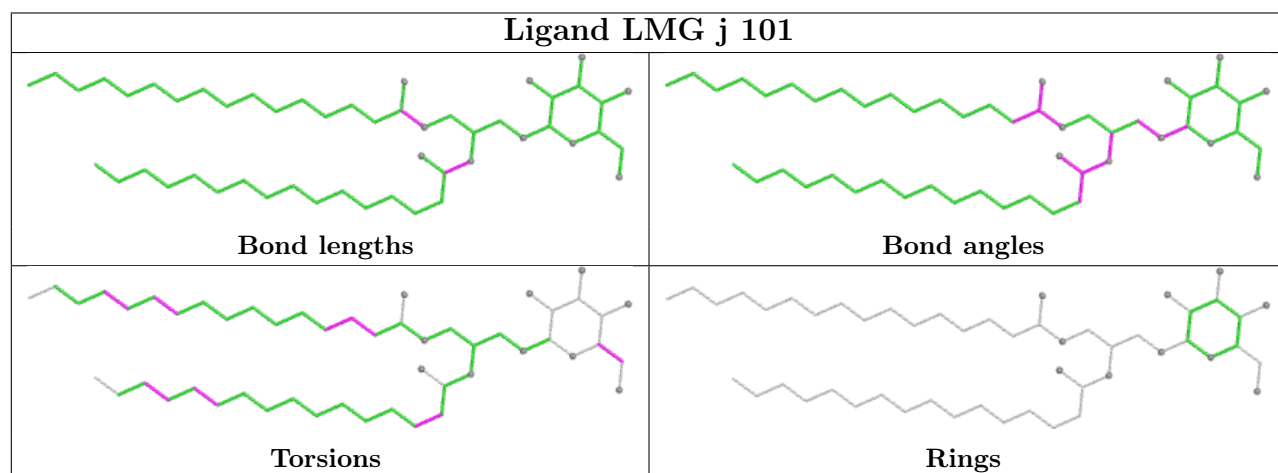
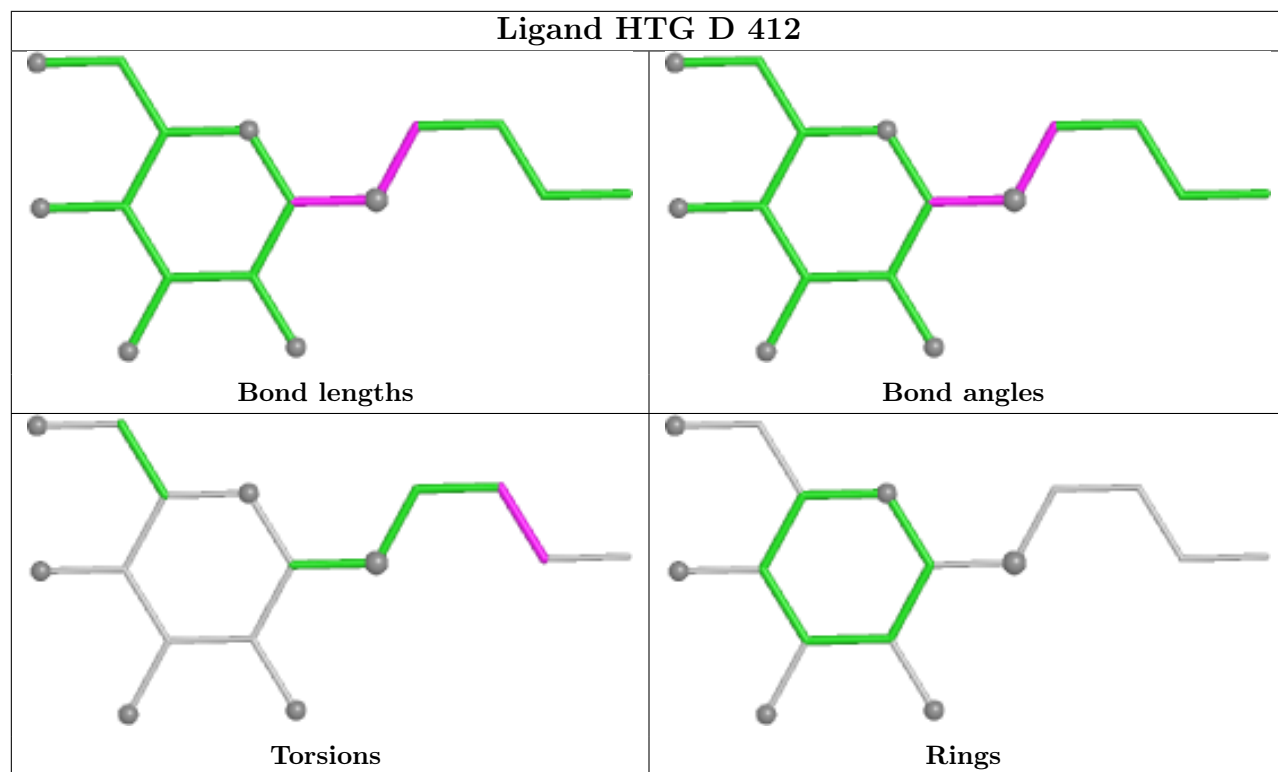
Ligand BCR C 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

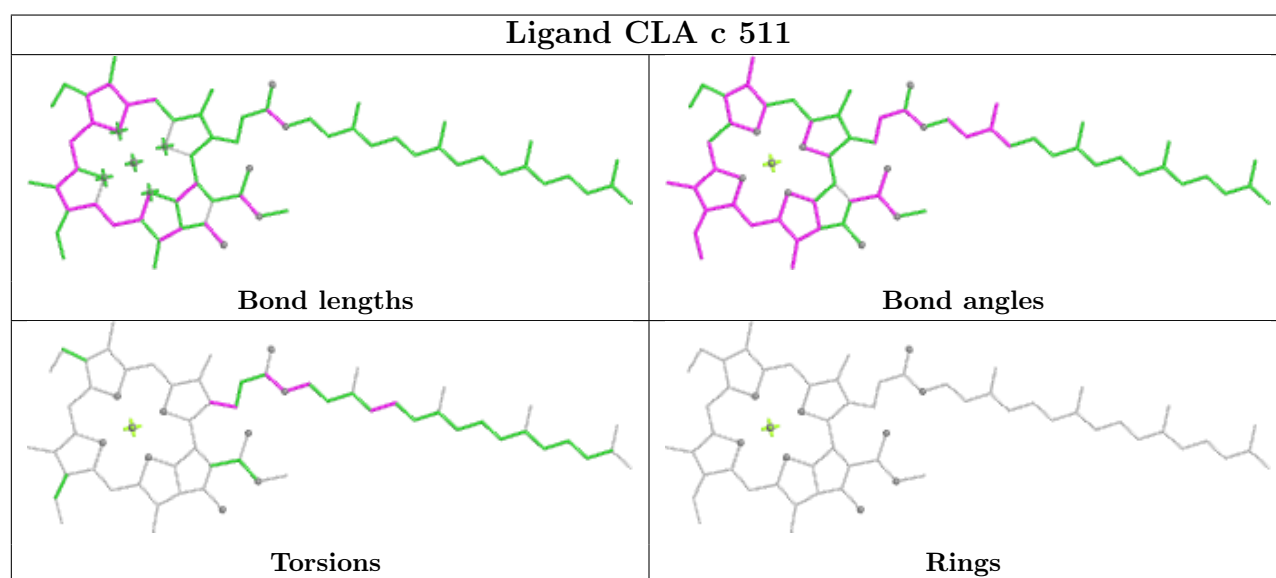
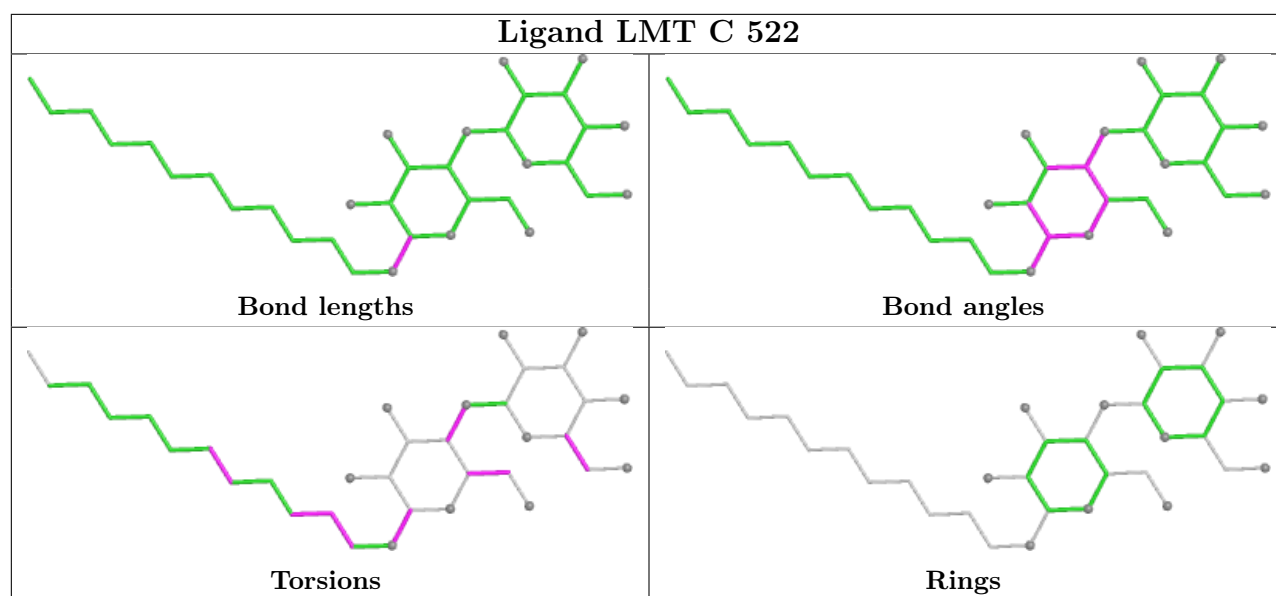
Ligand DGD C 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

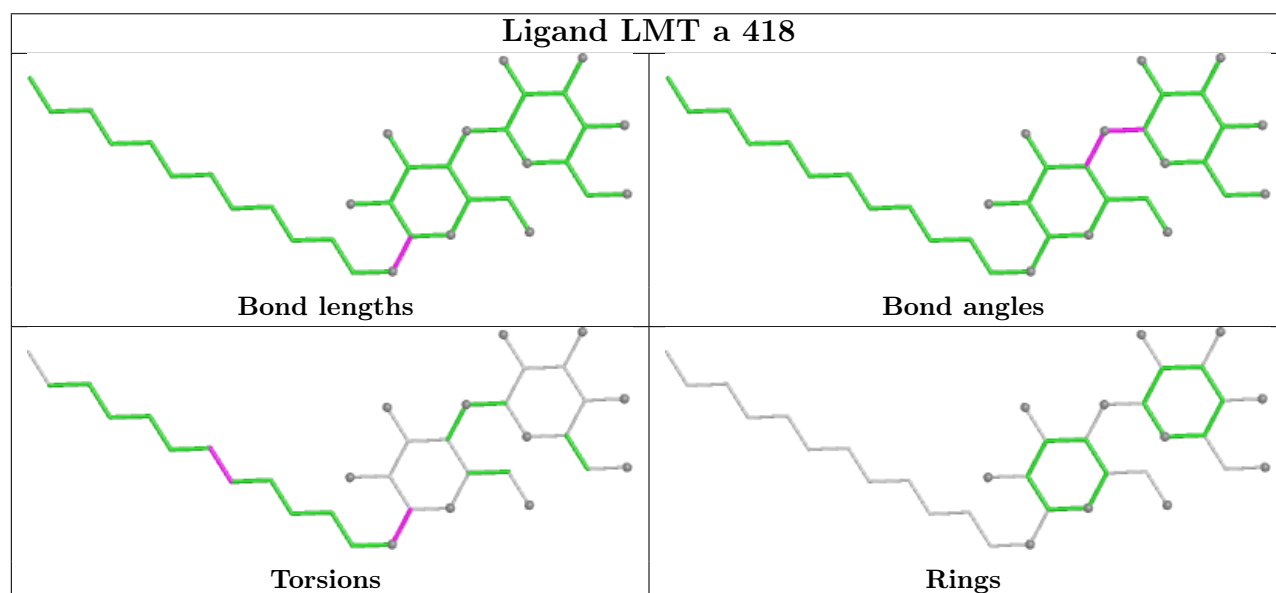
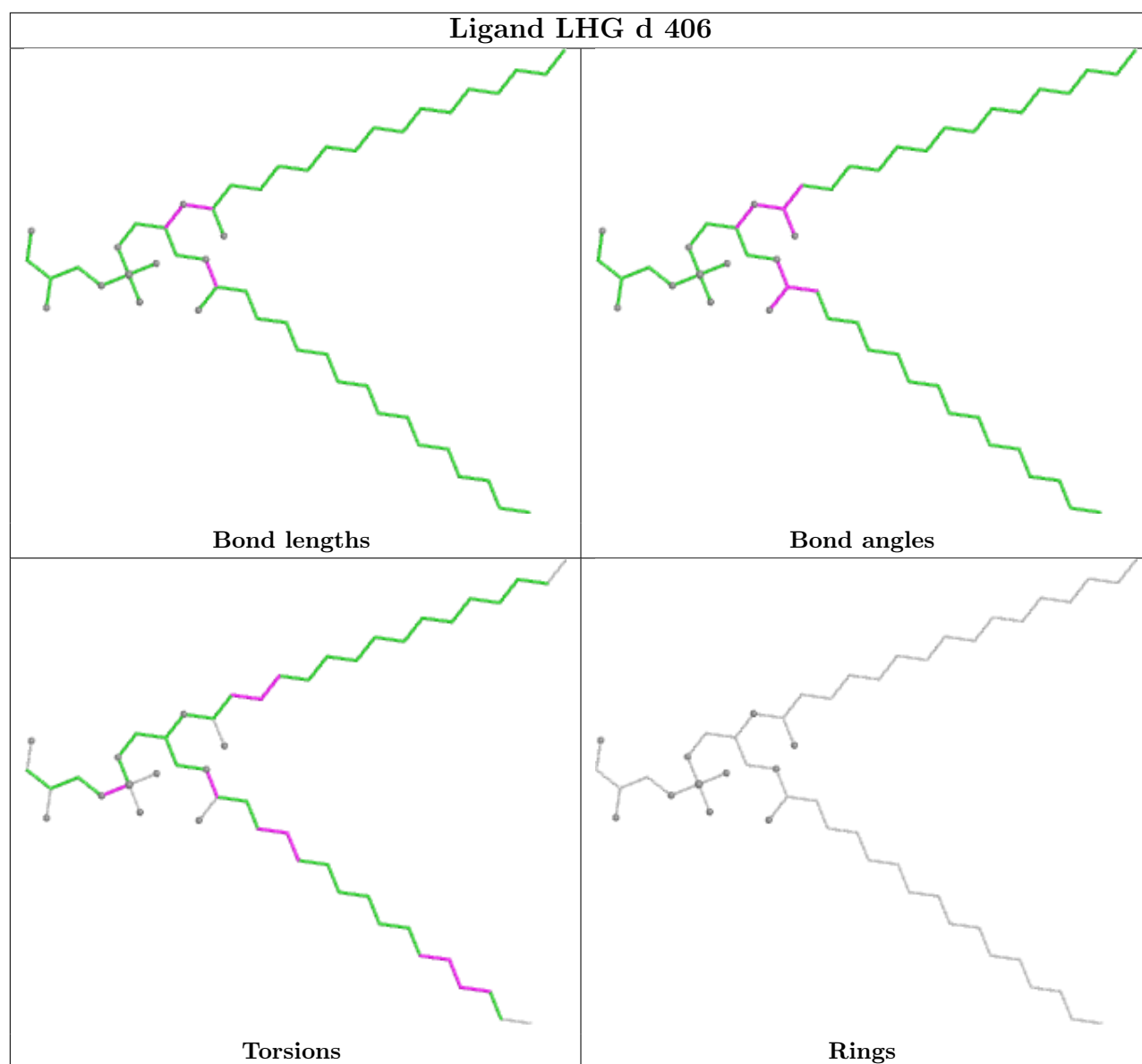
Ligand CLA b 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

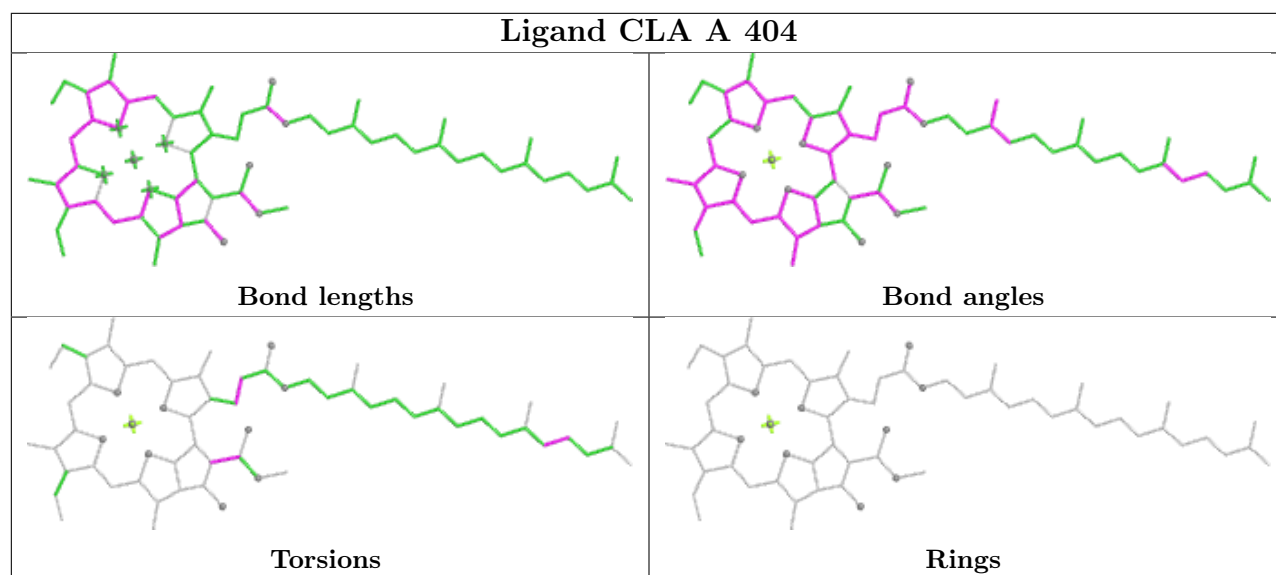
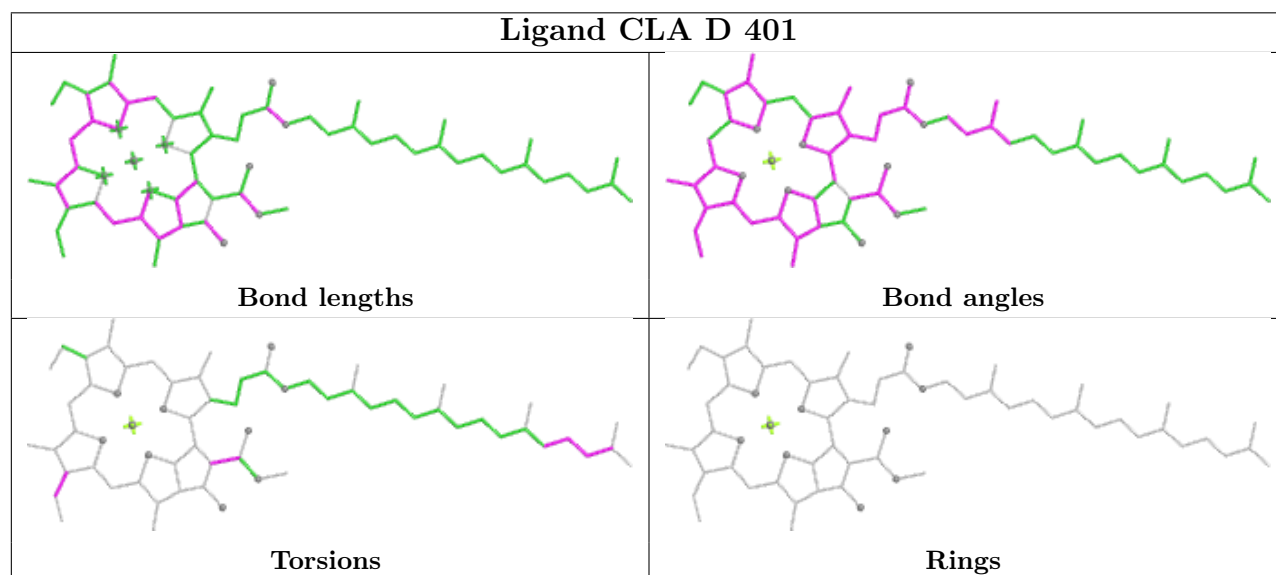
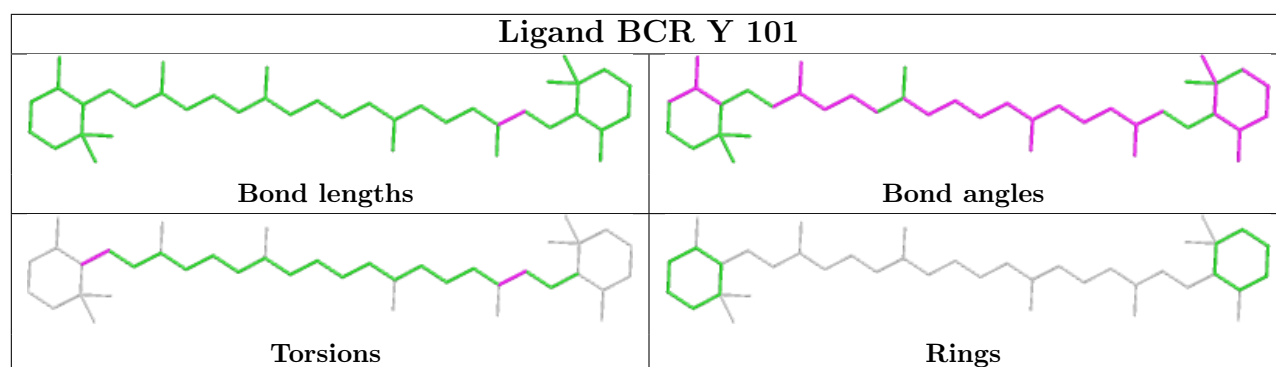


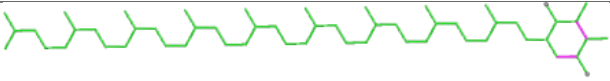
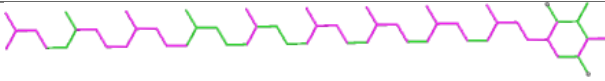
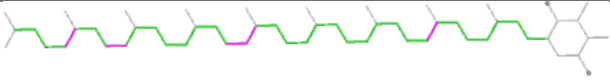
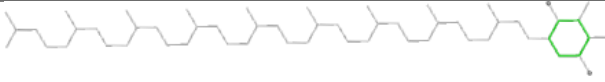
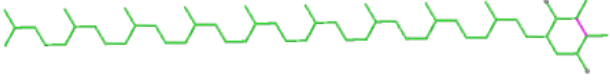
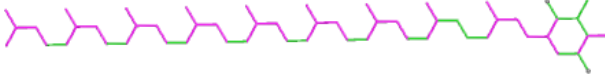
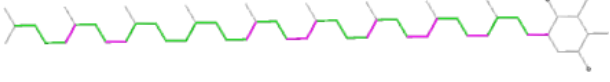
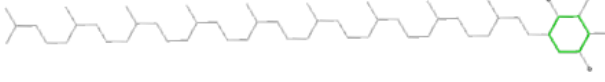
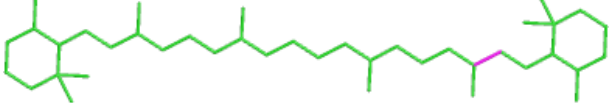
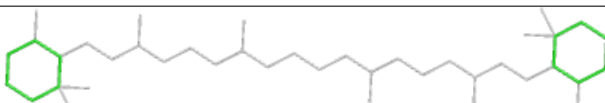


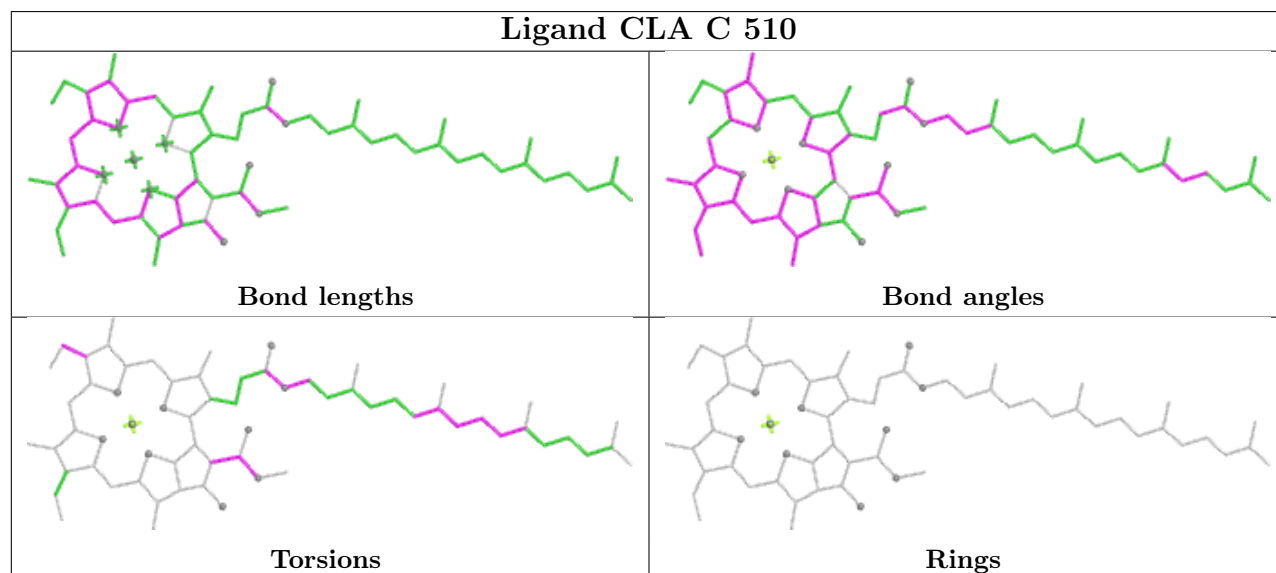
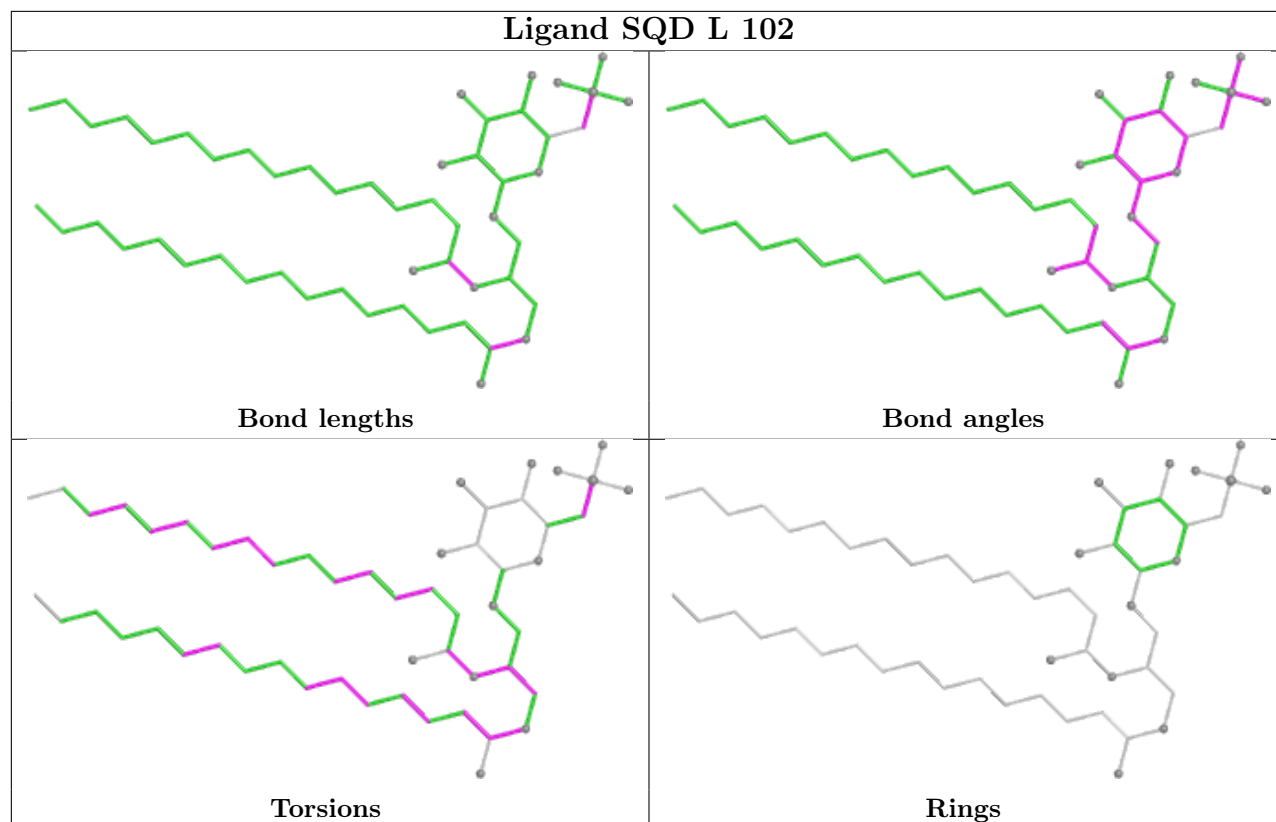


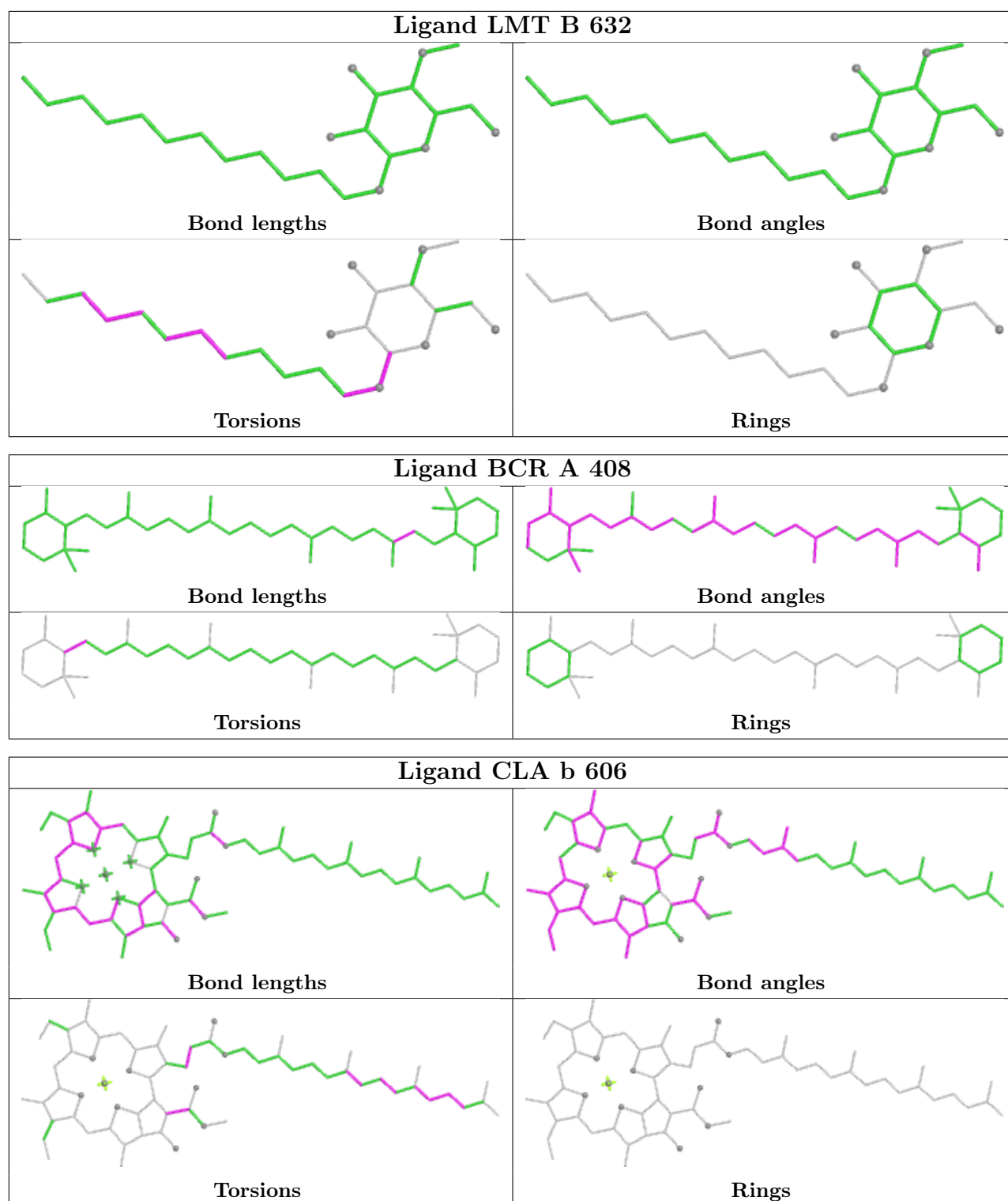


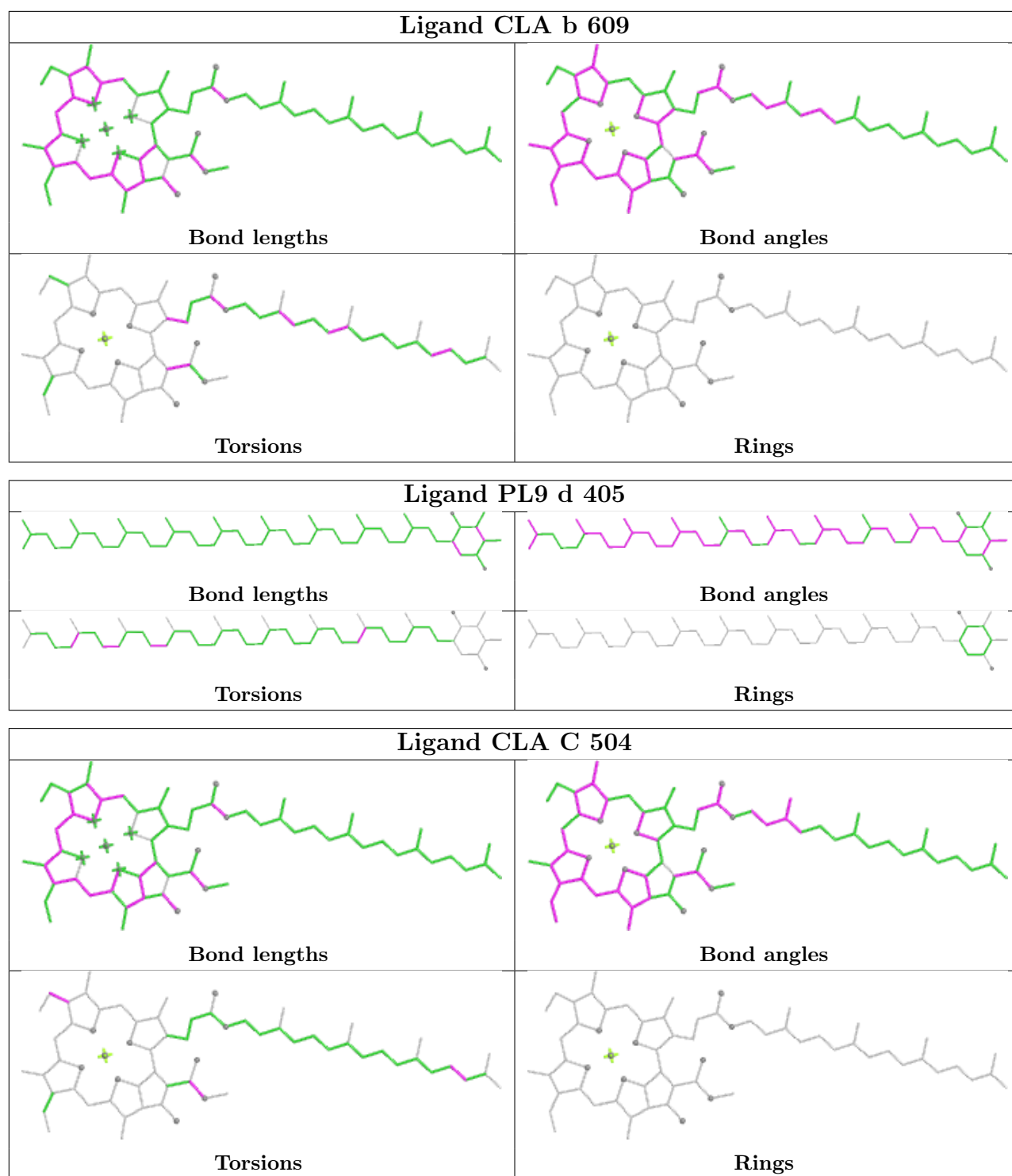


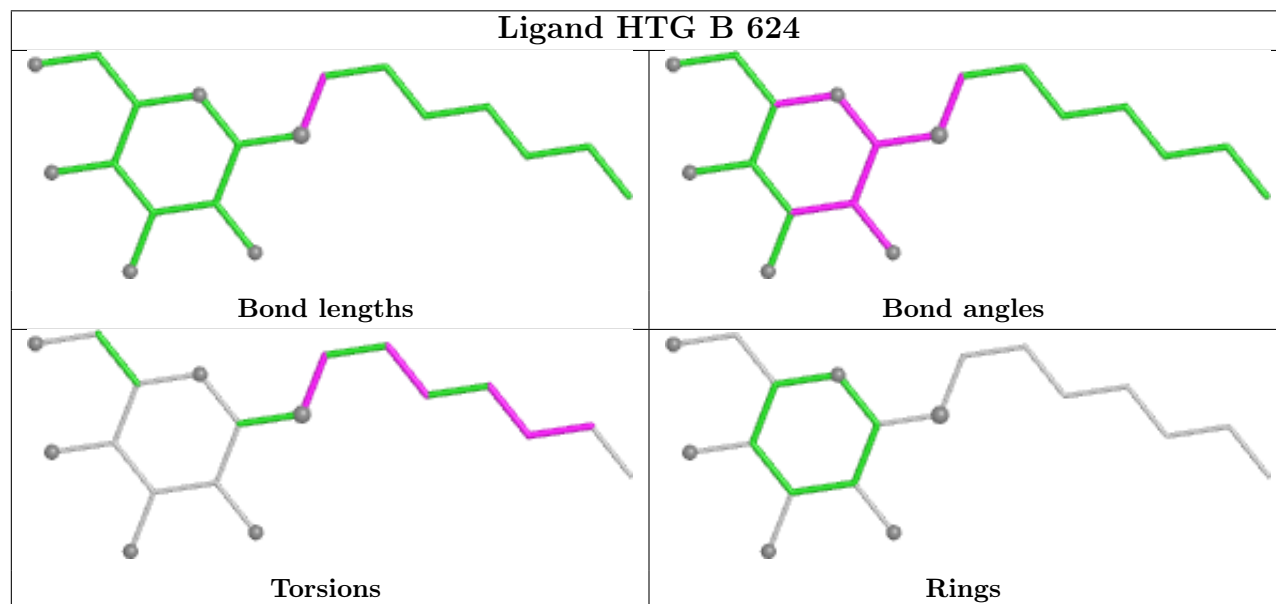
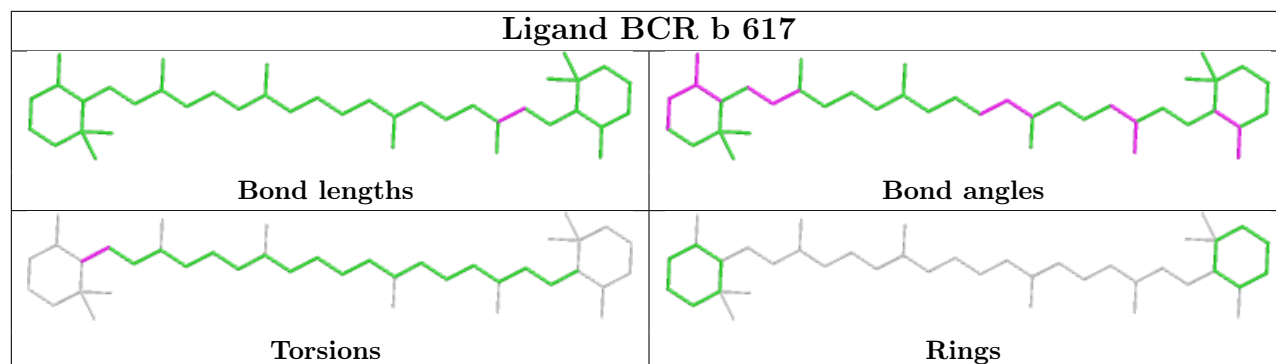


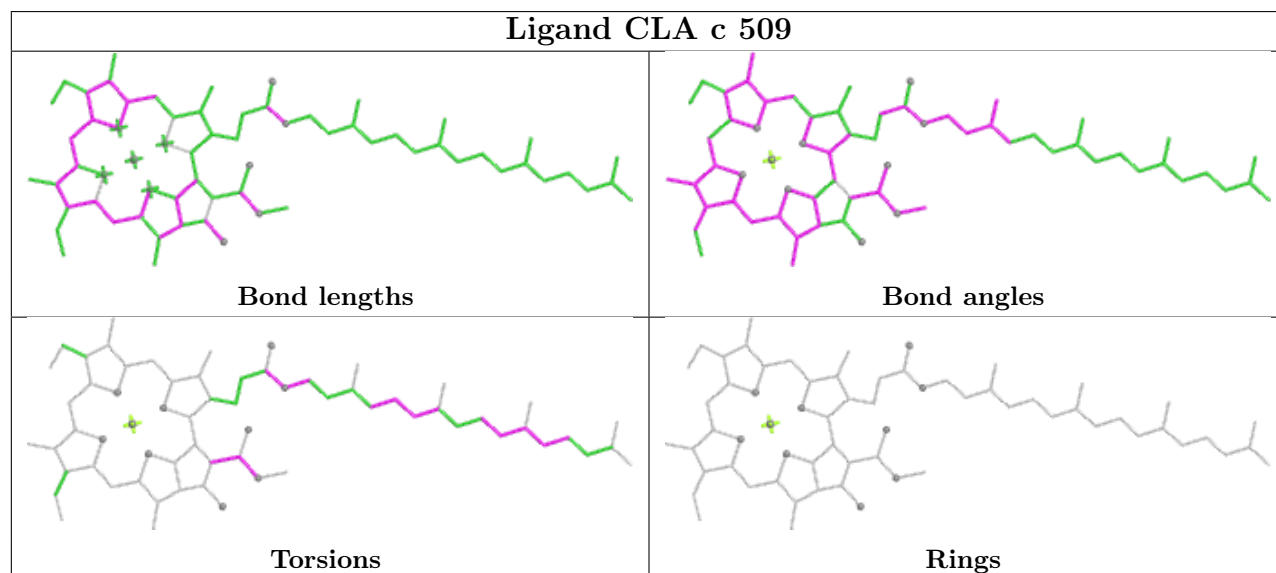
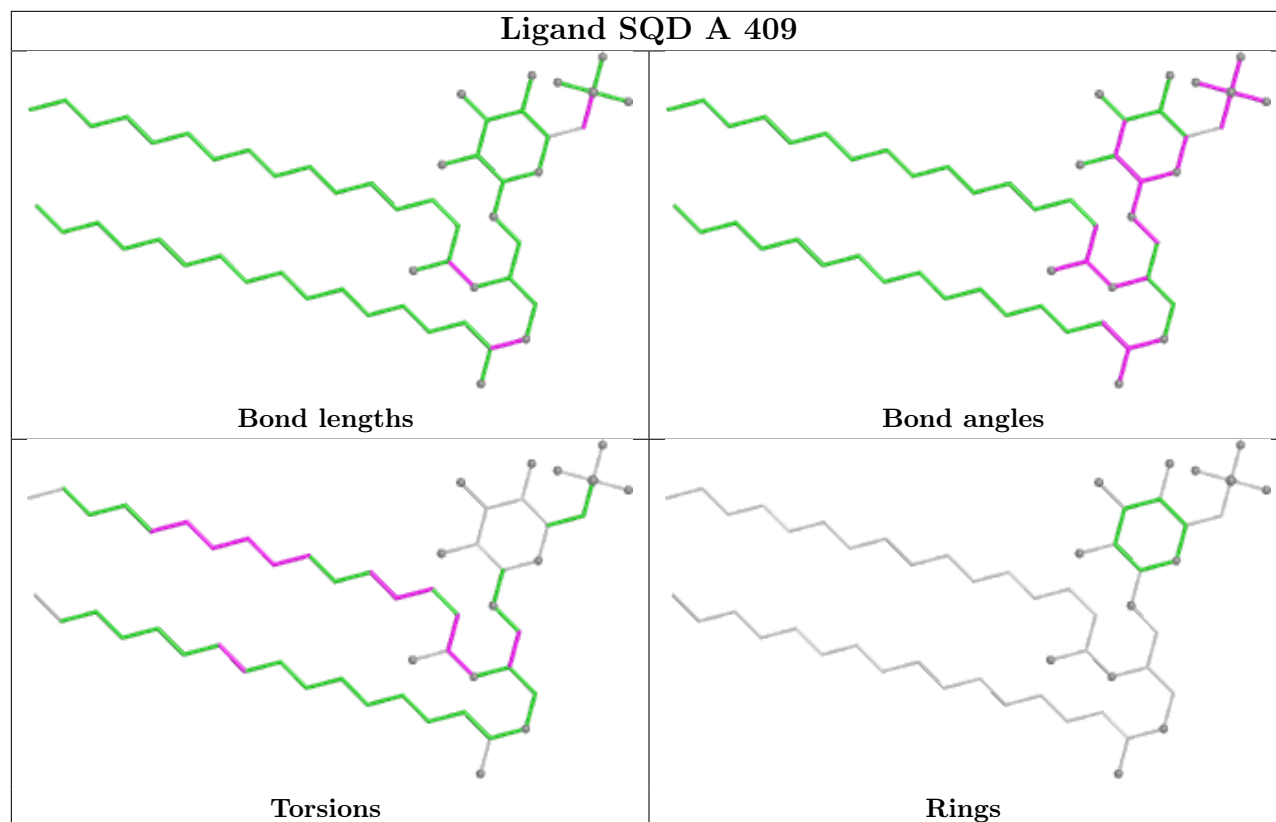
Ligand PL9 D 407	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 a 415	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR c 515	
 Bond lengths	 Bond angles
 Torsions	 Rings

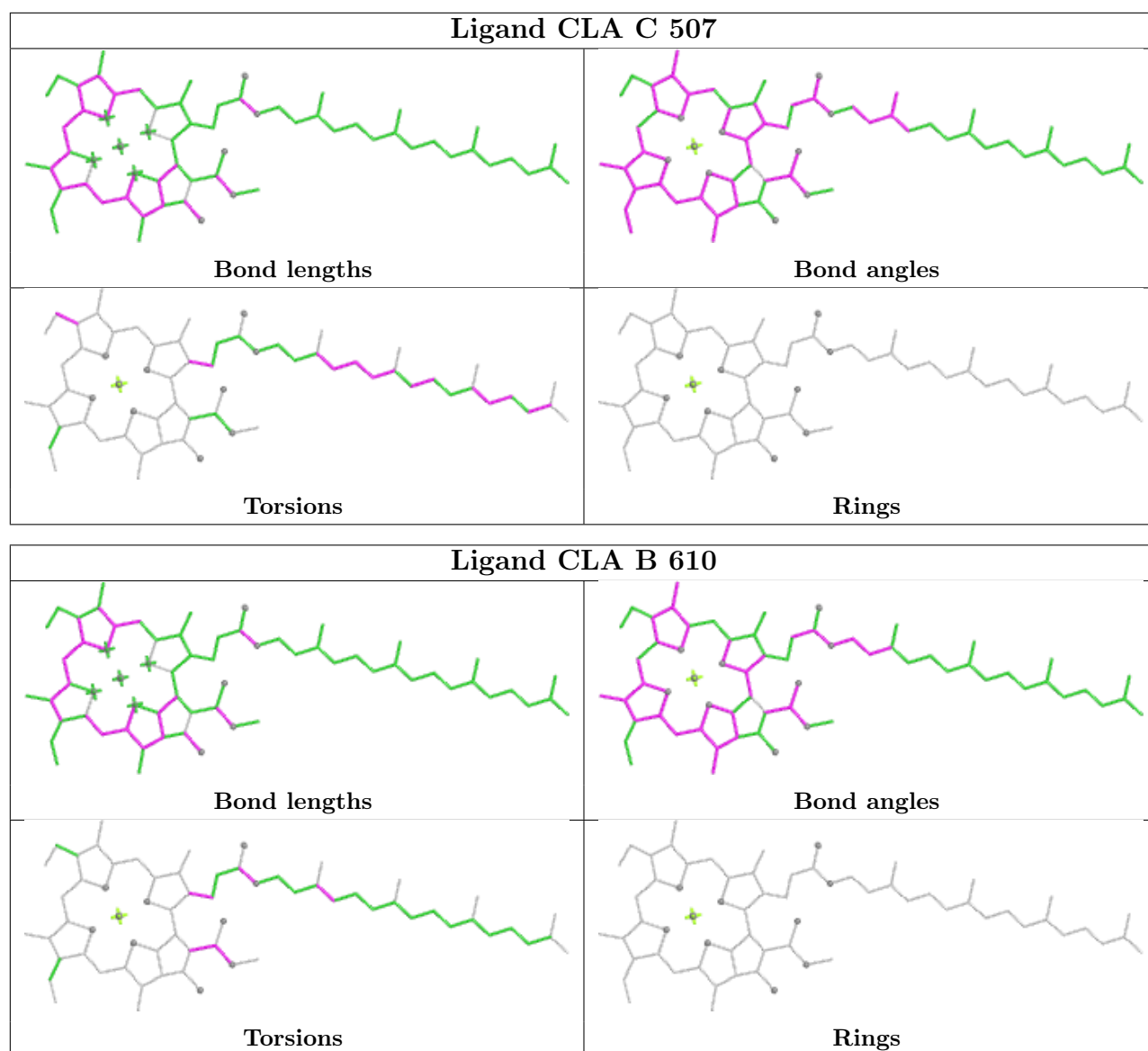












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	334/344 (97%)	-1.11	0	100	100	22, 33, 58, 97	0
1	a	334/344 (97%)	-1.11	0	100	100	24, 36, 65, 113	0
2	B	504/505 (99%)	-1.05	0	100	100	24, 38, 68, 118	0
2	b	504/505 (99%)	-1.02	0	100	100	25, 40, 77, 122	0
3	C	451/455 (99%)	-1.00	0	100	100	27, 48, 70, 108	0
3	c	455/455 (100%)	-0.99	0	100	100	32, 52, 72, 118	0
4	D	342/342 (100%)	-1.11	0	100	100	22, 35, 58, 113	0
4	d	341/342 (99%)	-1.11	0	100	100	24, 39, 59, 124	0
5	E	81/84 (96%)	-0.89	0	100	100	40, 59, 90, 125	0
5	e	79/84 (94%)	-0.87	0	100	100	45, 62, 100, 125	0
6	F	34/44 (77%)	-0.92	0	100	100	41, 51, 81, 96	0
6	f	31/44 (70%)	-0.82	0	100	100	48, 53, 84, 128	0
7	H	64/65 (98%)	-0.88	1 (1%)	70	67	37, 51, 72, 104	0
7	h	65/65 (100%)	-0.98	1 (1%)	72	68	40, 54, 79, 152	0
8	I	37/38 (97%)	-0.93	0	100	100	36, 48, 98, 129	0
8	i	37/38 (97%)	-0.78	0	100	100	38, 49, 107, 137	0
9	J	38/39 (97%)	-0.96	0	100	100	37, 55, 113, 156	0
9	j	39/39 (100%)	-0.86	0	100	100	46, 56, 109, 137	0
10	K	37/37 (100%)	-1.06	0	100	100	49, 58, 81, 98	0
10	k	37/37 (100%)	-1.04	0	100	100	52, 60, 82, 99	0
11	L	36/37 (97%)	-1.16	0	100	100	23, 30, 98, 143	0
11	l	36/37 (97%)	-1.15	0	100	100	24, 31, 97, 143	0
12	M	32/36 (88%)	-1.12	0	100	100	24, 31, 53, 125	0
12	m	33/36 (91%)	-1.10	0	100	100	24, 32, 66, 126	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-1.01	0 100 100	22, 50, 103, 163	0
13	o	243/244 (99%)	-1.01	0 100 100	26, 50, 108, 151	0
14	T	29/32 (90%)	-1.11	0 100 100	26, 31, 68, 97	0
14	t	29/32 (90%)	-1.11	0 100 100	26, 31, 69, 98	0
15	U	96/104 (92%)	-1.07	0 100 100	32, 44, 72, 86	0
15	u	97/104 (93%)	-1.15	0 100 100	37, 47, 72, 105	0
16	V	137/137 (100%)	-1.03	0 100 100	30, 46, 74, 111	0
16	v	137/137 (100%)	-1.02	0 100 100	37, 54, 79, 112	0
17	X	38/40 (95%)	-0.77	0 100 100	49, 58, 80, 121	0
17	x	38/40 (95%)	-0.59	0 100 100	50, 60, 84, 123	0
18	Y	29/30 (96%)	-0.51	0 100 100	60, 76, 112, 120	0
18	y	29/30 (96%)	-0.74	0 100 100	63, 76, 107, 118	0
19	Z	62/62 (100%)	-0.83	0 100 100	57, 77, 127, 161	0
19	z	62/62 (100%)	-0.59	0 100 100	61, 79, 127, 161	0
20	R	34/34 (100%)	0.46	0 100 100	92, 116, 145, 149	0
All	All	5284/5384 (98%)	-1.01	2 (0%) 100 100	22, 45, 88, 163	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	2.2
7	h	65	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
12	FME	m	1	10/11	0.96	0.06	26,43,69,74	0
14	FME	t	1	10/11	0.97	0.04	22,34,47,66	0
14	FME	T	1	10/11	0.97	0.05	19,37,45,52	0
8	FME	I	1	10/11	0.98	0.04	29,49,53,54	0
12	FME	M	1	10/11	0.98	0.06	33,41,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	FME	i	1	10/11	0.98	0.04	38,50,63,74	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
30	UNL	m	102	10/-	0.70	0.13	36,47,64,66	0
36	HTG	D	412	16/19	0.72	0.11	43,118,136,138	0
35	LMT	E	102	35/35	0.73	0.13	91,129,157,163	0
36	HTG	B	626	19/19	0.73	0.11	51,135,163,189	0
30	UNL	J	102	10/-	0.73	0.17	59,66,85,90	0
36	HTG	b	622	19/19	0.73	0.15	77,105,127,134	0
34	LMG	C	521	51/55	0.74	0.11	50,107,149,153	0
36	HTG	B	630	19/19	0.74	0.09	67,116,145,154	0
36	HTG	C	524	9/19	0.74	0.18	70,90,106,139	0
35	LMT	D	403	35/35	0.74	0.11	40,112,125,126	0
30	UNL	A	414	28/-	0.74	0.13	66,93,121,126	0
27	GOL	O	302	6/6	0.75	0.09	63,68,72,78	0
30	UNL	i	101	40/-	0.76	0.12	56,91,147,151	0
35	LMT	B	633	35/35	0.76	0.12	39,117,133,139	0
30	UNL	a	416	30/-	0.76	0.11	86,102,121,129	0
35	LMT	a	418	35/35	0.77	0.11	97,118,139,139	0
35	LMT	e	102	35/35	0.77	0.11	75,139,161,171	0
36	HTG	C	523	19/19	0.77	0.10	95,107,121,133	0
30	UNL	j	102	10/-	0.78	0.11	57,81,94,94	0
30	UNL	K	101	34/-	0.78	0.10	62,102,116,137	0
36	HTG	b	626	19/19	0.78	0.09	66,114,151,181	0
36	HTG	B	625	19/19	0.79	0.15	43,101,109,111	0
35	LMT	C	522	35/35	0.79	0.10	83,119,141,151	0
30	UNL	M	102	10/-	0.81	0.09	38,51,60,60	0
36	HTG	c	521	19/19	0.81	0.08	71,125,137,163	0
26	SQD	f	101	43/54	0.82	0.10	86,117,154,157	0
30	UNL	B	631	33/-	0.83	0.12	36,92,134,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	UNL	b	629	36/-	0.83	0.09	46,85,130,141	0
35	LMT	M	103	35/35	0.83	0.09	37,128,152,157	0
34	LMG	c	520	51/55	0.83	0.09	62,104,135,147	0
35	LMT	B	623	35/35	0.83	0.09	50,95,120,122	0
36	HTG	b	623	19/19	0.83	0.10	73,116,140,180	0
30	UNL	D	411	40/-	0.83	0.10	49,76,125,128	0
30	UNL	I	101	40/-	0.83	0.10	39,89,141,148	0
36	HTG	c	522	19/19	0.83	0.10	83,139,149,158	0
31	LHG	e	101	42/49	0.84	0.09	63,119,140,150	0
30	UNL	b	627	33/-	0.85	0.09	53,80,145,147	0
35	LMT	b	620	25/35	0.85	0.09	55,88,143,147	0
35	LMT	M	101	35/35	0.85	0.08	40,85,105,107	0
35	LMT	m	103	35/35	0.85	0.10	40,85,113,117	0
30	UNL	c	525	32/-	0.85	0.10	74,104,124,132	0
36	HTG	h	101	16/19	0.85	0.09	71,110,125,143	0
27	GOL	a	412	6/6	0.86	0.12	56,70,85,86	0
31	LHG	E	101	42/49	0.86	0.09	47,95,114,121	0
36	HTG	b	621	19/19	0.86	0.10	33,91,127,144	0
34	LMG	Z	101	37/55	0.87	0.10	57,103,134,149	0
26	SQD	B	621	54/54	0.87	0.09	44,82,109,118	0
26	SQD	a	413	54/54	0.87	0.07	37,73,134,146	0
27	GOL	d	401	6/6	0.87	0.24	36,51,76,77	0
36	HTG	V	203	11/19	0.87	0.08	88,101,107,108	0
26	SQD	A	411	54/54	0.87	0.07	41,71,114,129	0
33	CA	B	601	1/1	0.88	0.07	144,144,144,144	0
35	LMT	B	632	25/35	0.88	0.10	41,68,135,136	0
30	UNL	D	410	17/-	0.89	0.09	46,64,94,102	0
27	GOL	B	628	6/6	0.89	0.12	47,58,65,72	0
29	PL9	a	415	55/55	0.89	0.10	56,82,108,115	0
26	SQD	D	413	43/54	0.90	0.10	58,106,117,124	0
35	LMT	b	628	25/35	0.90	0.08	37,63,135,142	0
36	HTG	B	629	19/19	0.90	0.07	47,59,78,83	0
26	SQD	L	102	54/54	0.90	0.07	39,73,114,123	0
34	LMG	z	101	39/55	0.90	0.10	69,117,144,151	0
29	PL9	A	413	55/55	0.91	0.10	44,83,100,110	0
27	GOL	b	624	6/6	0.91	0.10	75,92,97,104	0
34	LMG	C	501	51/55	0.91	0.09	40,81,110,113	0
30	UNL	x	101	18/-	0.91	0.09	47,66,104,105	0
25	BCR	D	406	40/40	0.91	0.07	35,46,78,84	0
35	LMT	B	634	26/35	0.92	0.08	48,90,109,115	0
34	LMG	C	520	51/55	0.92	0.08	43,75,125,134	0
23	CLA	b	601	65/65	0.92	0.07	46,70,107,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	UNL	X	101	18/-	0.92	0.10	39,66,83,87	0
34	LMG	a	417	51/55	0.92	0.07	42,79,99,115	0
36	HTG	B	624	19/19	0.92	0.07	33,71,128,130	0
34	LMG	c	519	51/55	0.92	0.08	47,78,122,143	0
27	GOL	C	525	6/6	0.93	0.12	45,56,66,73	0
23	CLA	C	507	65/65	0.93	0.07	42,57,106,115	0
23	CLA	B	602	65/65	0.93	0.08	39,61,93,123	0
36	HTG	b	625	19/19	0.93	0.06	40,60,90,94	0
23	CLA	c	513	65/65	0.93	0.07	58,74,112,119	0
27	GOL	A	410	6/6	0.93	0.08	45,57,60,90	0
25	BCR	C	515	40/40	0.93	0.07	49,60,74,82	0
34	LMG	J	101	51/55	0.93	0.07	33,54,96,105	0
23	CLA	C	505	65/65	0.94	0.07	32,46,91,111	0
25	BCR	C	527	40/40	0.94	0.07	43,55,71,72	0
23	CLA	C	514	65/65	0.94	0.07	50,65,100,107	0
25	BCR	Y	101	40/40	0.94	0.06	40,51,62,71	0
25	BCR	y	101	40/40	0.94	0.06	48,60,74,77	0
25	BCR	B	620	40/40	0.94	0.06	30,43,67,78	0
27	GOL	B	627	6/6	0.94	0.09	60,77,93,95	0
34	LMG	j	101	51/55	0.94	0.06	41,56,92,119	0
34	LMG	B	622	51/55	0.94	0.06	35,53,83,101	0
30	UNL	d	409	17/-	0.94	0.06	48,58,94,99	0
37	DGD	c	517	62/66	0.94	0.06	42,55,110,126	0
23	CLA	C	513	65/65	0.95	0.06	46,60,106,112	0
31	LHG	d	406	49/49	0.95	0.07	27,48,81,84	0
26	SQD	A	409	54/54	0.95	0.07	41,66,99,109	0
23	CLA	b	616	65/65	0.95	0.06	34,51,101,111	0
23	CLA	c	504	65/65	0.95	0.06	41,52,94,117	0
23	CLA	c	506	65/65	0.95	0.06	47,65,98,117	0
23	CLA	c	507	65/65	0.95	0.07	43,57,70,72	0
29	PL9	D	407	55/55	0.95	0.05	20,30,44,53	0
26	SQD	a	411	54/54	0.95	0.07	44,69,108,113	0
23	CLA	c	512	65/65	0.95	0.07	53,66,96,104	0
25	BCR	b	619	40/40	0.95	0.05	33,46,69,80	0
25	BCR	d	404	40/40	0.95	0.06	43,55,79,81	0
25	BCR	k	101	40/40	0.95	0.07	50,60,84,87	0
25	BCR	t	101	40/40	0.95	0.05	23,43,64,68	0
34	LMG	m	101	51/55	0.95	0.05	33,52,85,99	0
37	DGD	C	518	62/66	0.95	0.06	35,51,111,119	0
37	DGD	c	516	62/66	0.95	0.06	35,47,74,93	0
31	LHG	A	415	49/49	0.95	0.06	29,46,67,82	0
37	DGD	c	518	62/66	0.95	0.05	39,50,74,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	C	508	65/65	0.96	0.06	40,51,66,78	0
23	CLA	C	509	65/65	0.96	0.05	33,46,93,103	0
23	CLA	d	403	65/65	0.96	0.06	41,52,102,116	0
24	PHO	a	408	64/64	0.96	0.05	30,40,53,60	0
25	BCR	A	408	40/40	0.96	0.05	23,34,48,56	0
25	BCR	B	619	40/40	0.96	0.04	21,36,52,60	0
23	CLA	C	511	65/65	0.96	0.05	36,48,61,67	0
23	CLA	B	607	65/65	0.96	0.06	28,37,76,93	0
31	LHG	D	409	49/49	0.96	0.07	32,50,107,117	0
25	BCR	C	516	40/40	0.96	0.06	38,50,63,68	0
31	LHG	b	630	49/49	0.96	0.05	26,43,59,64	0
23	CLA	B	617	65/65	0.96	0.07	33,45,121,132	0
31	LHG	d	408	49/49	0.96	0.07	40,55,105,111	0
23	CLA	D	405	65/65	0.96	0.07	33,48,111,119	0
25	BCR	H	101	40/40	0.96	0.05	35,46,66,73	0
25	BCR	T	101	40/40	0.96	0.04	21,37,55,60	0
23	CLA	a	409	65/65	0.96	0.07	30,44,124,130	0
25	BCR	b	617	40/40	0.96	0.04	21,35,45,51	0
25	BCR	b	618	40/40	0.96	0.04	22,36,51,56	0
29	PL9	d	405	55/55	0.96	0.05	24,33,49,66	0
23	CLA	C	502	65/65	0.96	0.06	36,45,67,70	0
25	BCR	c	514	40/40	0.96	0.05	58,68,80,83	0
25	BCR	c	515	40/40	0.96	0.05	41,54,66,70	0
23	CLA	b	602	65/65	0.96	0.06	36,48,68,77	0
25	BCR	h	102	40/40	0.96	0.06	42,57,71,74	0
23	CLA	C	503	65/65	0.96	0.06	33,43,60,67	0
23	CLA	c	501	65/65	0.96	0.05	43,53,67,72	0
23	CLA	C	504	65/65	0.96	0.06	37,47,66,75	0
37	DGD	C	519	62/66	0.96	0.05	30,44,80,109	0
37	DGD	H	102	62/66	0.96	0.06	29,42,64,68	0
23	CLA	A	407	65/65	0.96	0.06	28,38,98,117	0
23	CLA	B	603	65/65	0.96	0.05	31,41,57,69	0
23	CLA	c	511	65/65	0.96	0.06	47,56,78,89	0
23	CLA	b	605	65/65	0.97	0.05	26,34,51,76	0
23	CLA	b	606	65/65	0.97	0.05	29,42,91,110	0
23	CLA	b	607	65/65	0.97	0.05	21,30,58,67	0
23	CLA	b	608	65/65	0.97	0.05	34,44,67,72	0
23	CLA	b	609	65/65	0.97	0.05	39,48,63,74	0
25	BCR	a	410	40/40	0.97	0.05	28,38,55,58	0
23	CLA	b	610	65/65	0.97	0.05	35,44,56,61	0
23	CLA	b	611	65/65	0.97	0.05	27,35,57,62	0
23	CLA	b	612	65/65	0.97	0.06	28,35,48,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	b	613	65/65	0.97	0.05	24,36,79,89	0
23	CLA	b	614	65/65	0.97	0.05	25,35,93,107	0
23	CLA	b	615	65/65	0.97	0.05	33,43,65,87	0
23	CLA	C	506	65/65	0.97	0.05	33,44,75,82	0
23	CLA	B	611	65/65	0.97	0.06	29,41,55,70	0
23	CLA	c	502	65/65	0.97	0.05	40,55,70,74	0
23	CLA	c	503	65/65	0.97	0.05	44,55,67,84	0
23	CLA	B	612	65/65	0.97	0.05	24,32,49,54	0
23	CLA	c	505	65/65	0.97	0.06	36,46,76,82	0
23	CLA	B	613	65/65	0.97	0.05	26,33,45,65	0
23	CLA	B	614	65/65	0.97	0.04	23,31,72,87	0
31	LHG	D	408	49/49	0.97	0.06	25,37,56,78	0
23	CLA	c	508	65/65	0.97	0.05	39,53,121,131	0
23	CLA	c	509	65/65	0.97	0.06	46,56,73,79	0
31	LHG	L	101	49/49	0.97	0.04	26,39,54,75	0
23	CLA	c	510	65/65	0.97	0.05	39,51,67,71	0
23	CLA	C	512	65/65	0.97	0.06	39,54,77,85	0
31	LHG	d	407	49/49	0.97	0.06	24,38,58,65	0
23	CLA	B	615	65/65	0.97	0.05	23,32,86,95	0
23	CLA	B	604	65/65	0.97	0.05	30,43,56,67	0
32	BCT	a	419	4/4	0.97	0.05	41,45,48,58	0
23	CLA	B	605	65/65	0.97	0.05	22,31,101,111	0
33	CA	O	301	1/1	0.97	0.06	101,101,101,101	0
33	CA	V	201	1/1	0.97	0.04	94,94,94,94	0
24	PHO	D	402	64/64	0.97	0.04	25,31,44,55	0
23	CLA	a	406	65/65	0.97	0.05	30,38,98,103	0
37	DGD	C	517	62/66	0.97	0.05	30,41,77,88	0
23	CLA	A	405	65/65	0.97	0.05	24,33,85,94	0
25	BCR	B	618	40/40	0.97	0.04	24,37,48,49	0
23	CLA	B	608	65/65	0.97	0.05	20,28,59,67	0
23	CLA	B	610	65/65	0.97	0.05	31,42,53,89	0
23	CLA	b	603	65/65	0.97	0.05	32,44,61,70	0
23	CLA	b	604	65/65	0.97	0.05	24,33,95,101	0
37	DGD	h	103	62/66	0.97	0.05	34,46,67,76	0
23	CLA	D	404	65/65	0.98	0.05	21,29,50,56	0
22	CL	a	403	1/1	0.98	0.04	41,41,41,41	0
23	CLA	a	404	65/65	0.98	0.05	27,33,52,66	0
32	BCT	A	416	4/4	0.98	0.05	32,45,46,51	0
23	CLA	a	405	65/65	0.98	0.04	23,29,52,60	0
23	CLA	C	510	65/65	0.98	0.06	39,53,71,79	0
23	CLA	d	402	65/65	0.98	0.05	27,32,58,72	0
23	CLA	B	616	65/65	0.98	0.04	29,38,60,67	0

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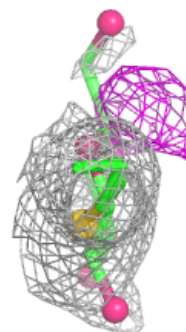
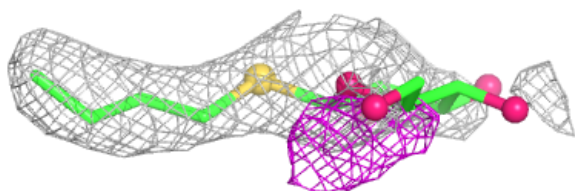
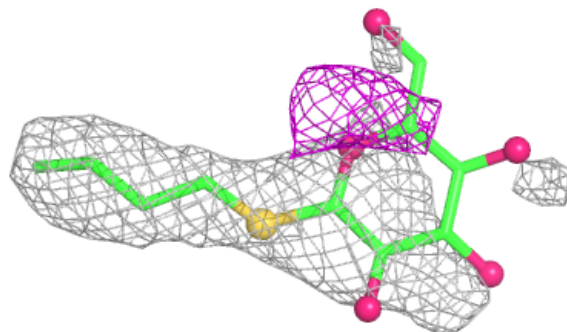
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	CA	c	523	1/1	0.98	0.10	68,68,68,68	0
24	PHO	A	406	64/64	0.98	0.04	22,29,39,46	0
23	CLA	A	404	65/65	0.98	0.04	22,25,39,58	0
24	PHO	a	407	64/64	0.98	0.04	24,31,45,50	0
23	CLA	B	609	65/65	0.98	0.04	30,42,56,66	0
23	CLA	B	606	65/65	0.98	0.05	24,33,46,51	0
23	CLA	D	401	65/65	0.98	0.04	21,28,43,47	0
38	HEM	E	103	43/43	0.98	0.06	43,56,69,83	0
38	HEM	e	103	43/43	0.98	0.06	52,78,106,116	0
39	MG	J	103	1/1	0.98	0.10	43,43,43,43	0
40	HEC	v	201	43/43	0.98	0.05	44,53,63,82	0
33	CA	o	301	1/1	0.99	0.02	89,89,89,89	0
21	FE2	a	401	1/1	0.99	0.03	47,47,47,47	0
22	CL	A	402	1/1	0.99	0.07	24,24,24,24	0
33	CA	C	526	1/1	0.99	0.10	59,59,59,59	0
22	CL	A	403	1/1	0.99	0.03	27,27,27,27	0
22	CL	a	402	1/1	0.99	0.06	28,28,28,28	0
21	FE2	A	401	1/1	0.99	0.03	46,46,46,46	0
39	MG	j	103	1/1	0.99	0.06	48,48,48,48	0
40	HEC	V	202	43/43	0.99	0.05	33,36,48,70	0
33	CA	c	524	1/1	0.99	0.03	66,66,66,66	0
28	OEX	A	412	10/10	1.00	0.03	23,32,46,47	0
28	OEX	a	414	10/10	1.00	0.02	29,36,46,48	0

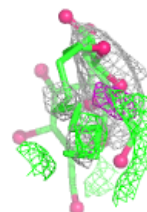
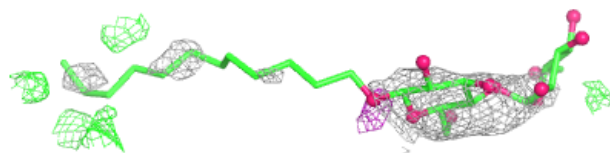
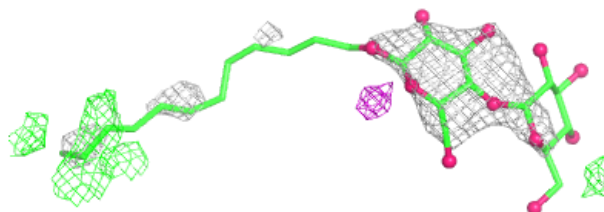
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HTG D 412:

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

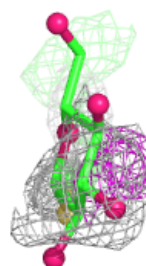
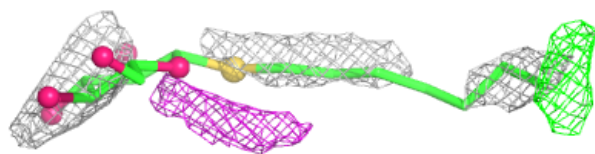
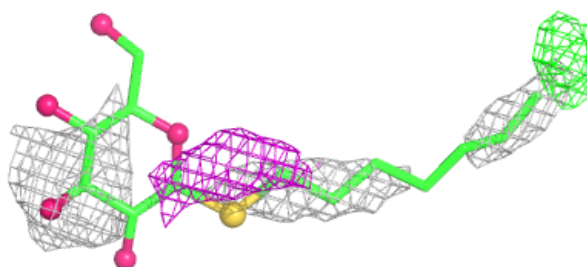
**Electron density around LMT E 102:**

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

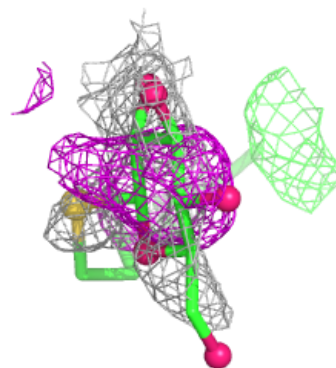
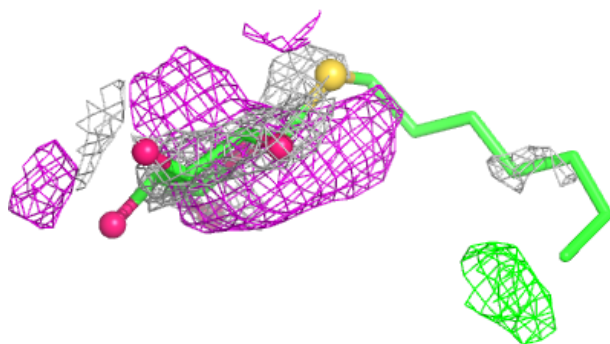
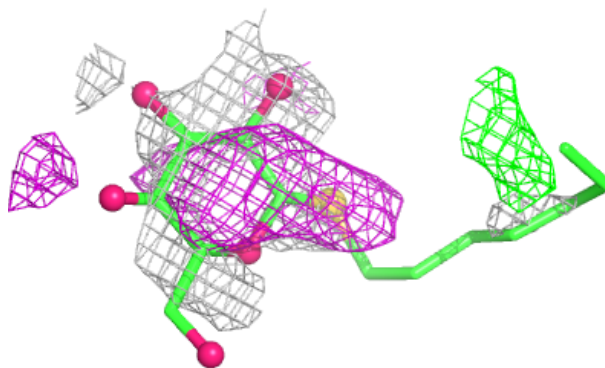


Electron density around HTG B 626:

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

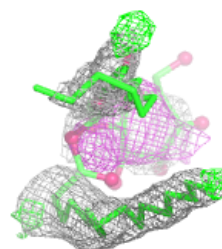
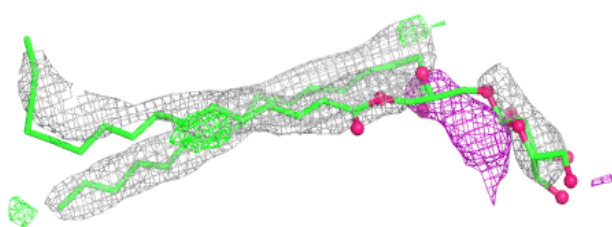
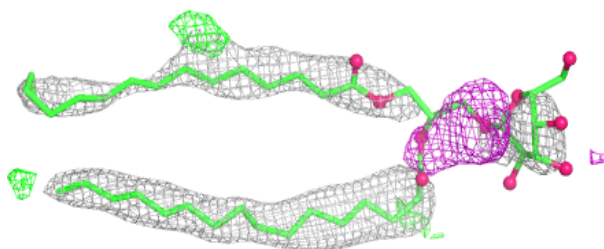
**Electron density around HTG b 622:**

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

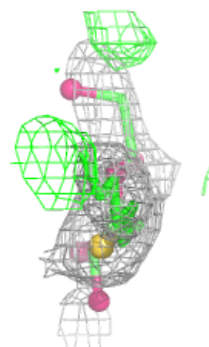
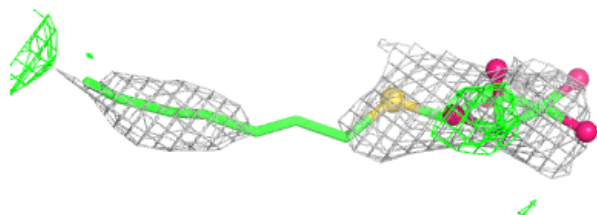
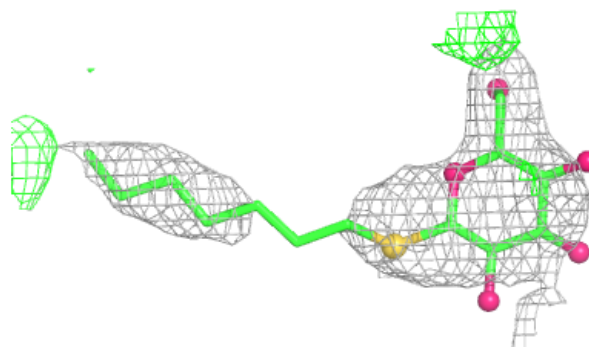


Electron density around LMG C 521:

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

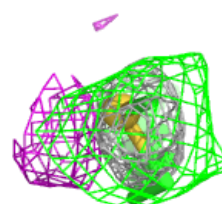
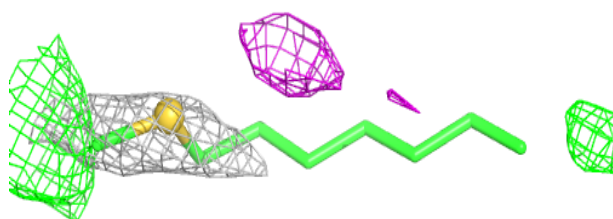
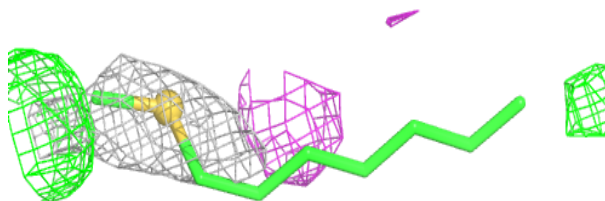
**Electron density around HTG B 630:**

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

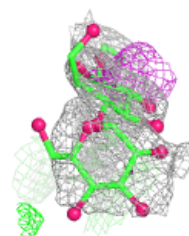
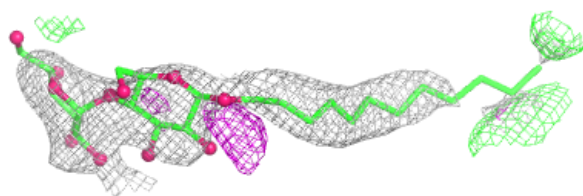
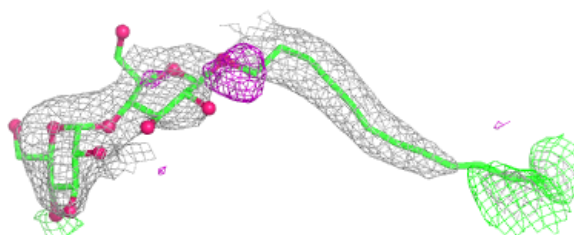


Electron density around HTG C 524:

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

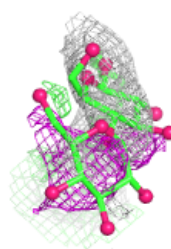
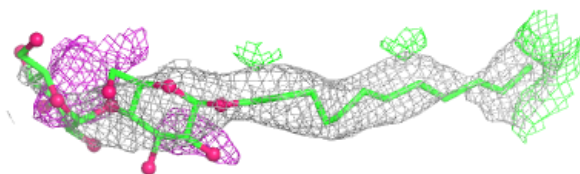
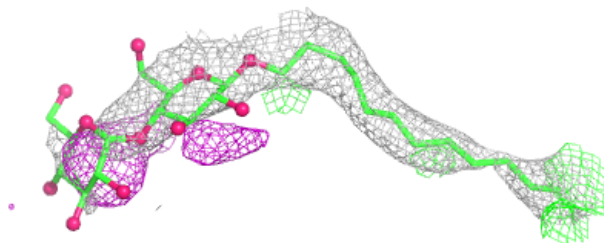
**Electron density around LMT D 403:**

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

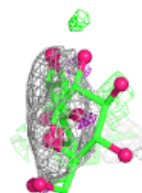
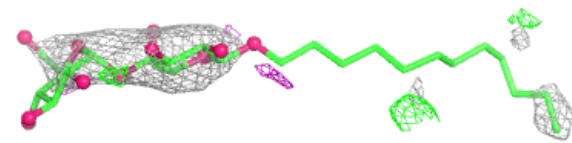
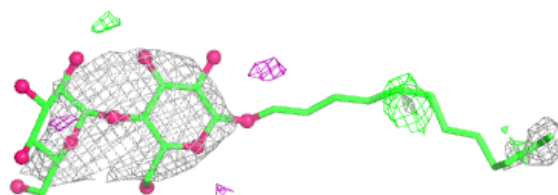


Electron density around LMT B 633:

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

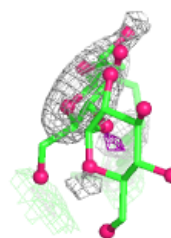
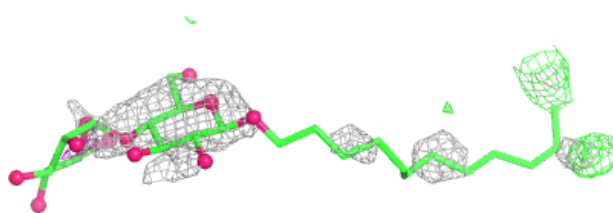
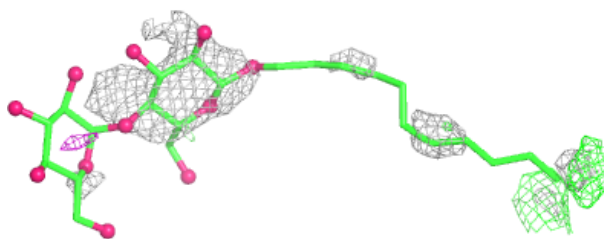
**Electron density around LMT a 418:**

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

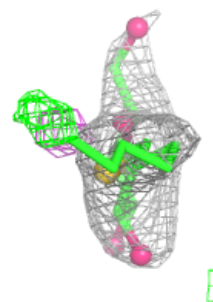
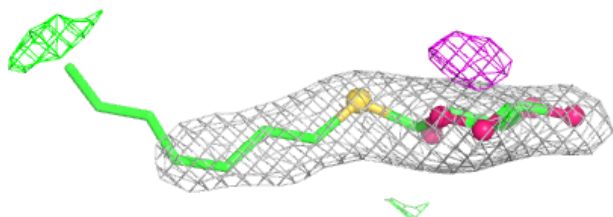
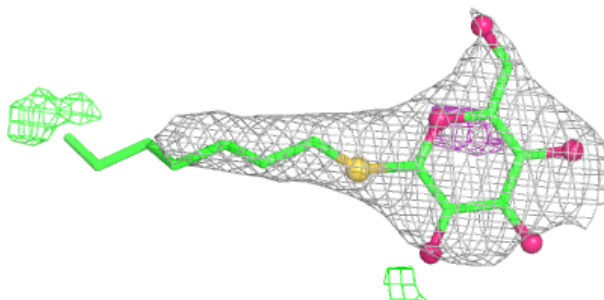


Electron density around LMT e 102:

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

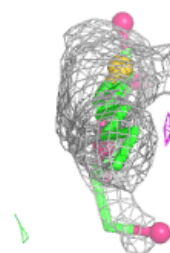
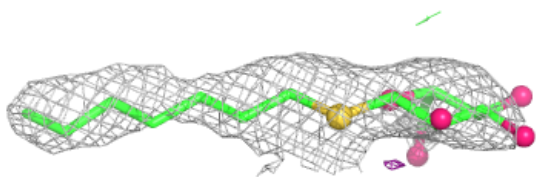
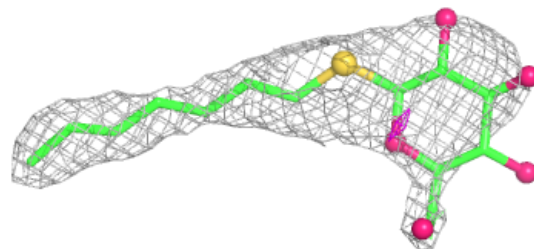
**Electron density around HTG C 523:**

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

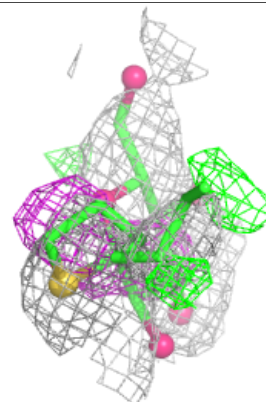
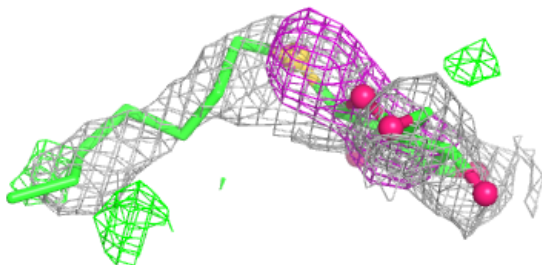
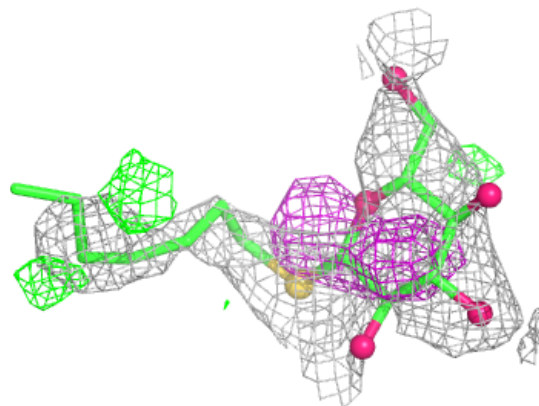


Electron density around HTG b 626:

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

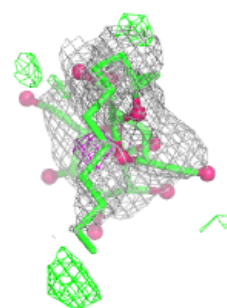
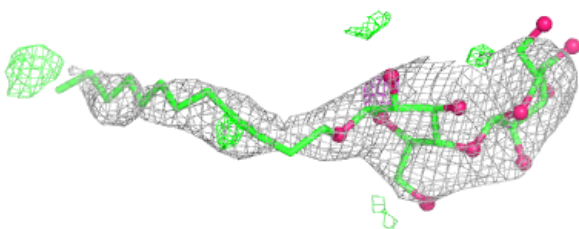
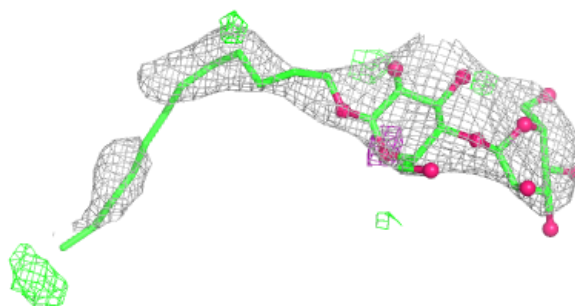
**Electron density around HTG B 625:**

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

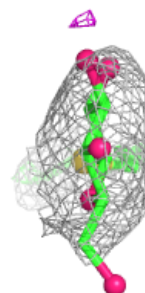
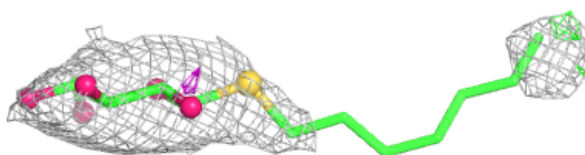
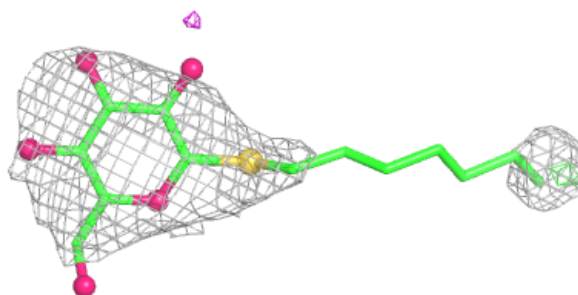


Electron density around LMT C 522:

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

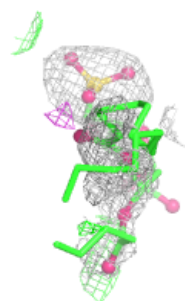
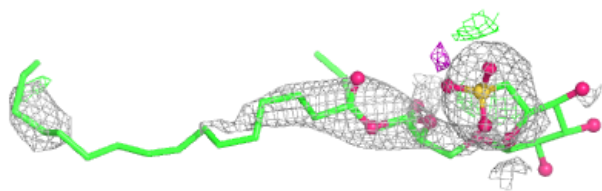
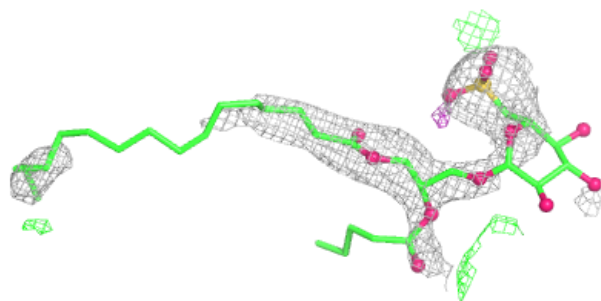
**Electron density around HTG c 521:**

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

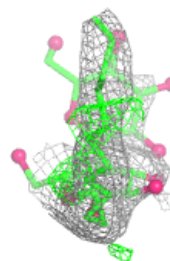
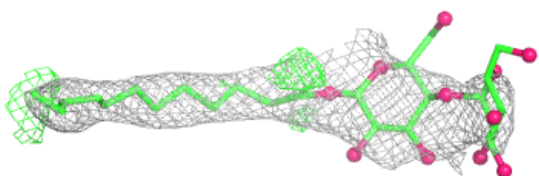
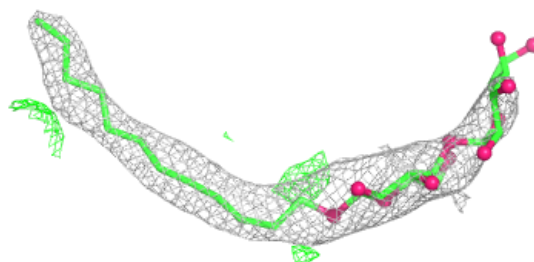


Electron density around SQD f 101:

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

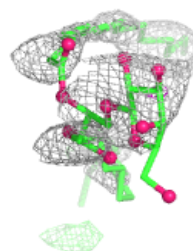
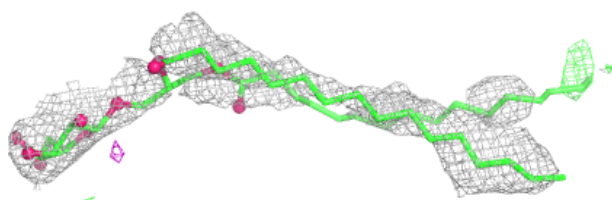
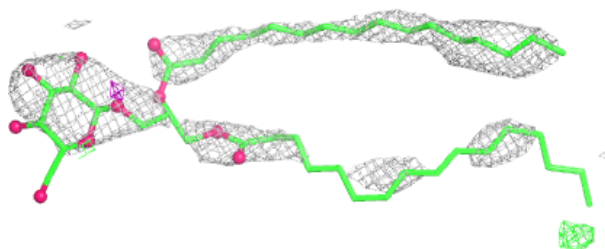
**Electron density around LMT M 103:**

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

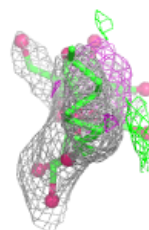
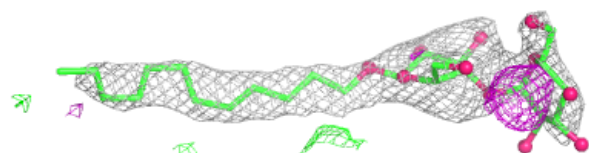
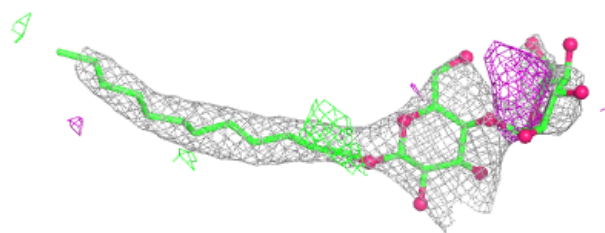


Electron density around LMG c 520:

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

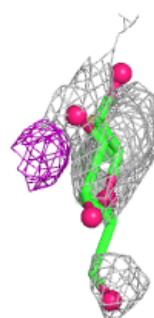
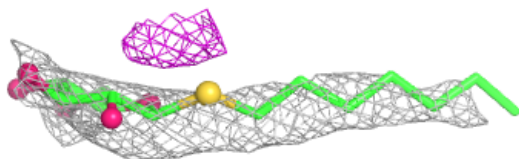
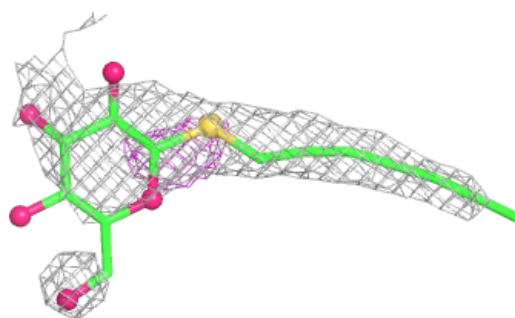
**Electron density around LMT B 623:**

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

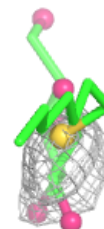
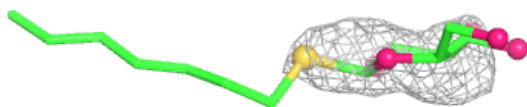
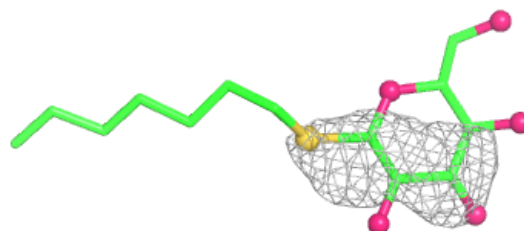


Electron density around HTG b 623:

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

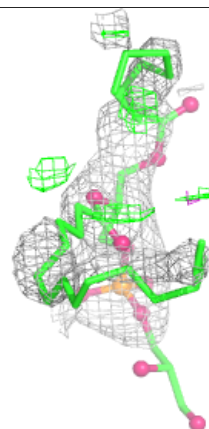
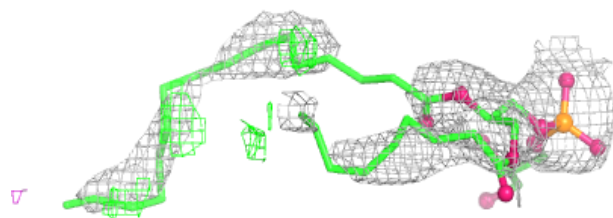
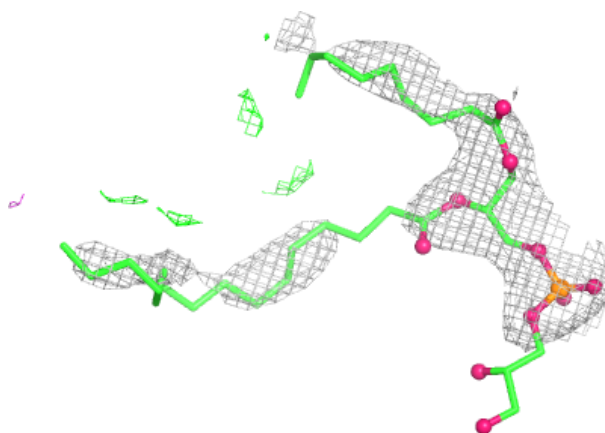
**Electron density around HTG c 522:**

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

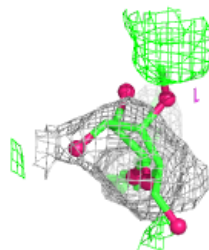
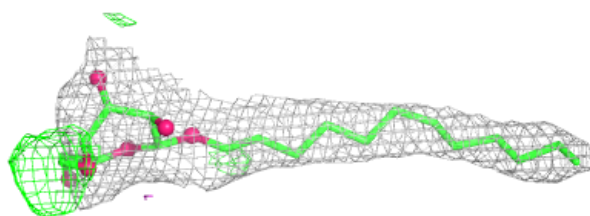
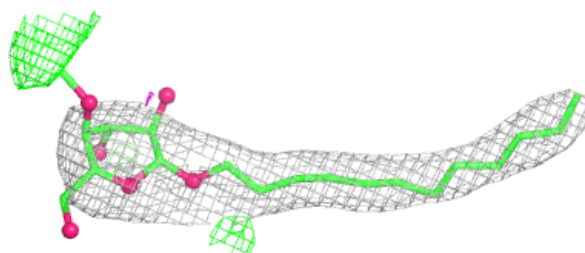


Electron density around LHG e 101:

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

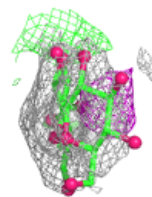
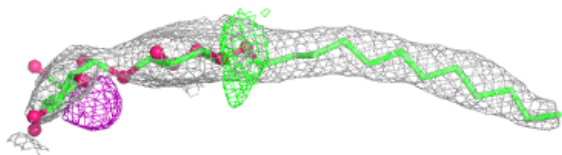
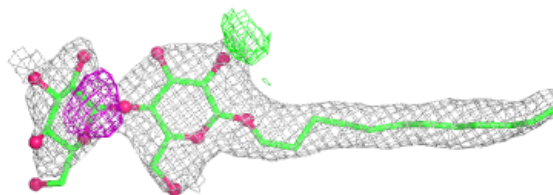
**Electron density around LMT b 620:**

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

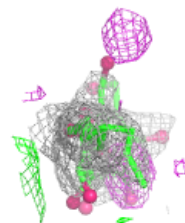
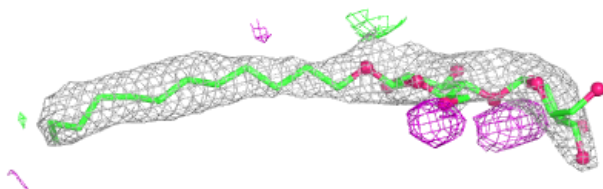
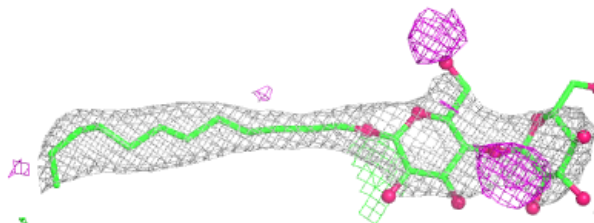


Electron density around LMT M 101:

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

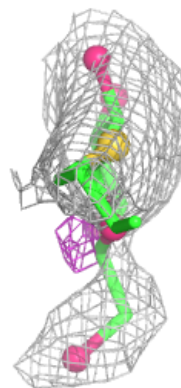
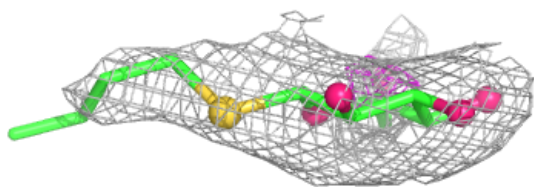
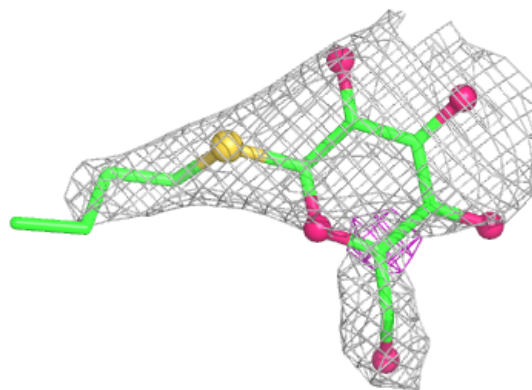
**Electron density around LMT m 103:**

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

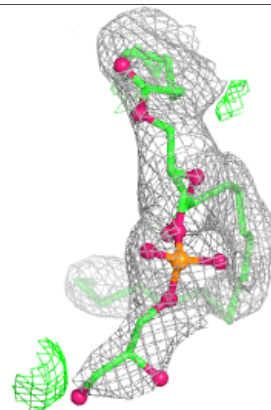
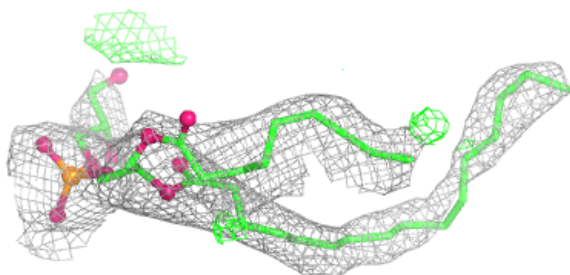
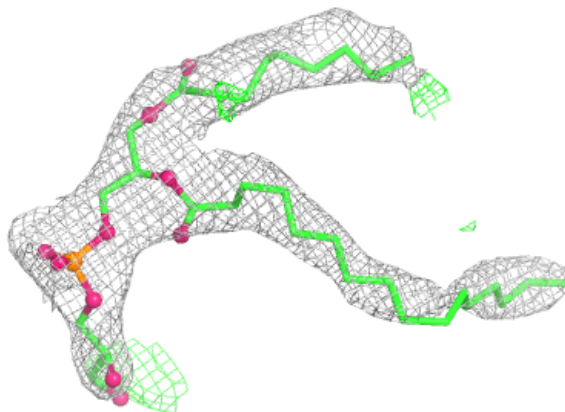


Electron density around HTG h 101:

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

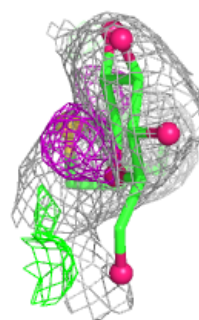
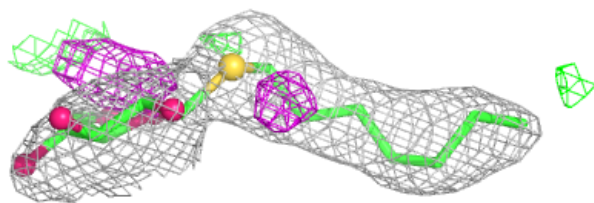
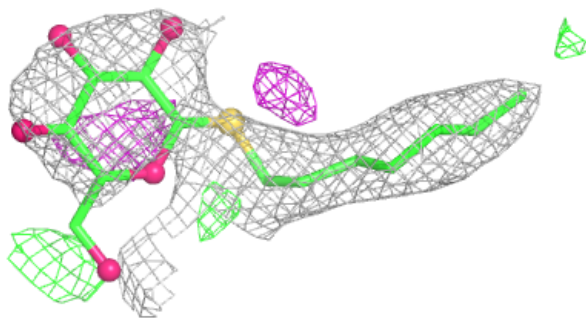
**Electron density around LHG E 101:**

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

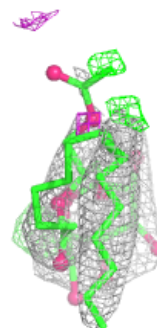
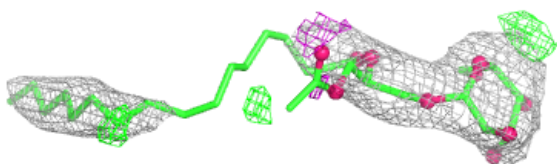
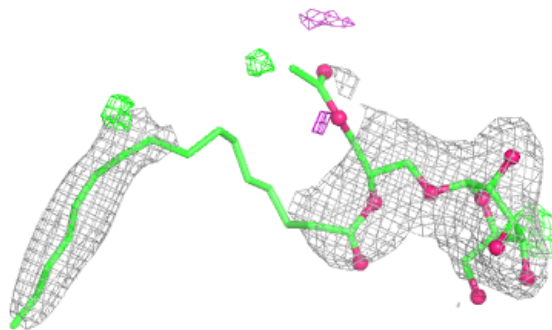


Electron density around HTG b 621:

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

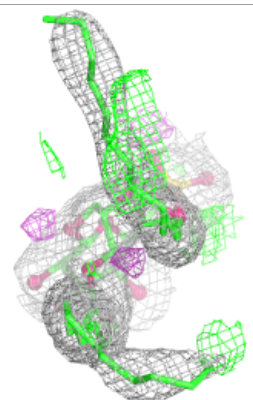
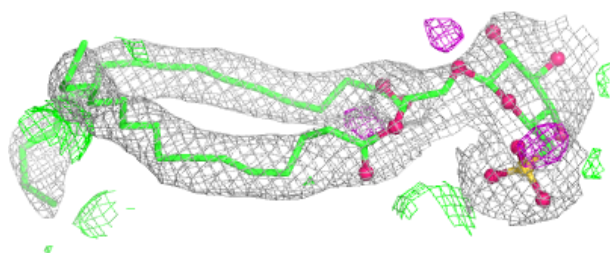
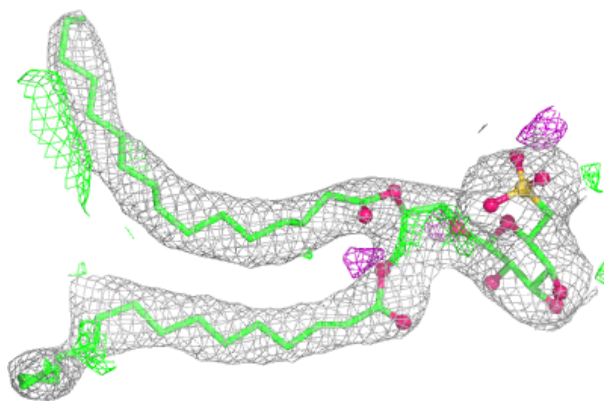
**Electron density around LMG Z 101:**

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

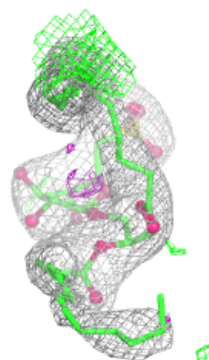
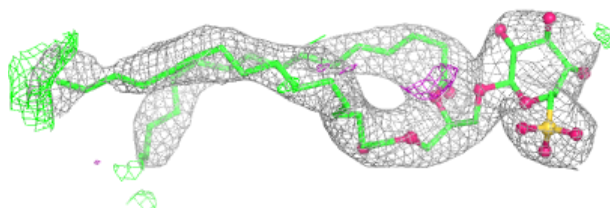
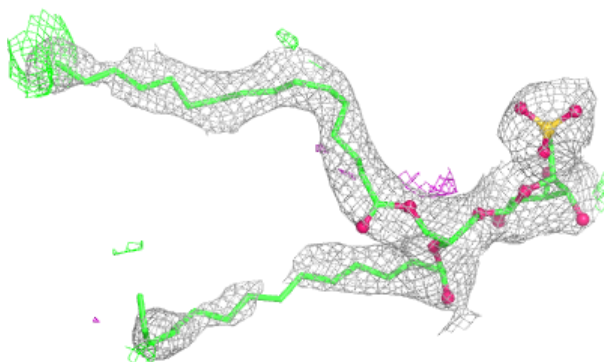


Electron density around SQD B 621:

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

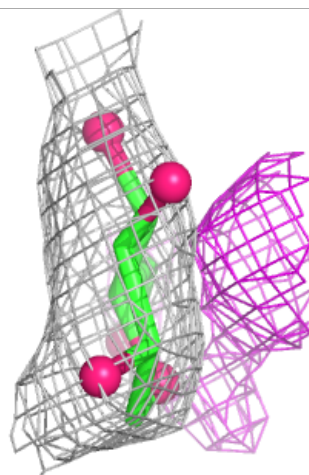
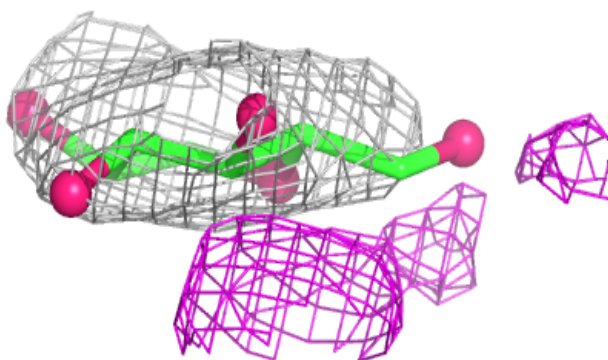
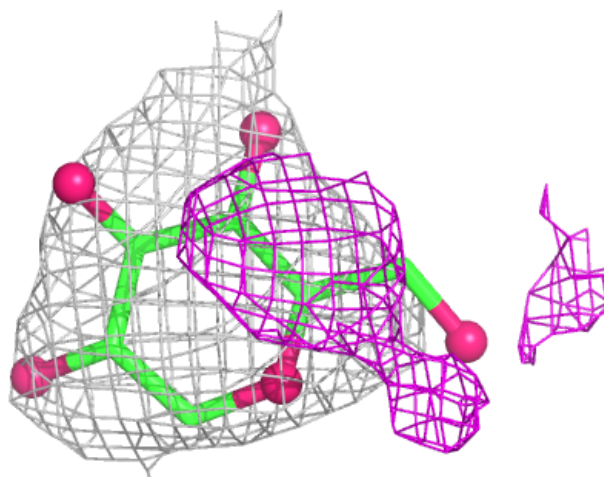
**Electron density around SQD a 413:**

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



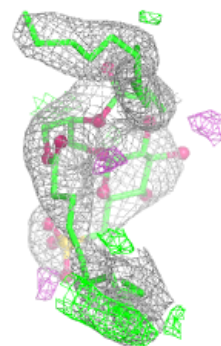
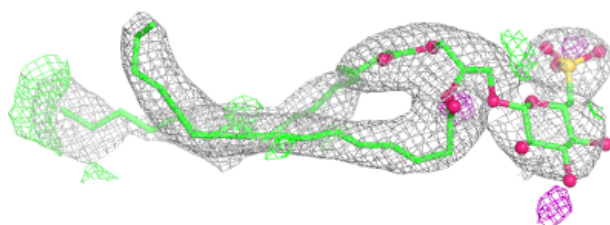
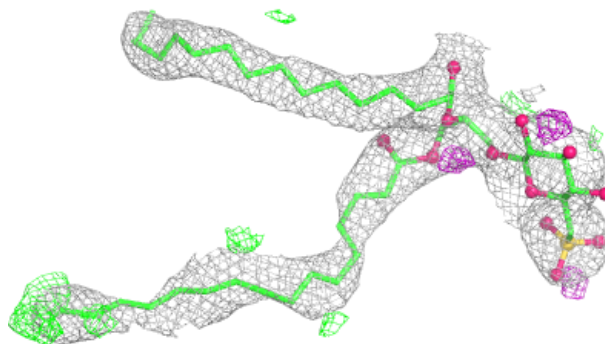
Electron density around HTG V 203:

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

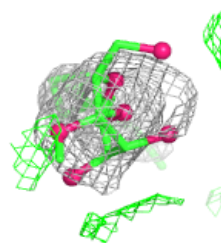
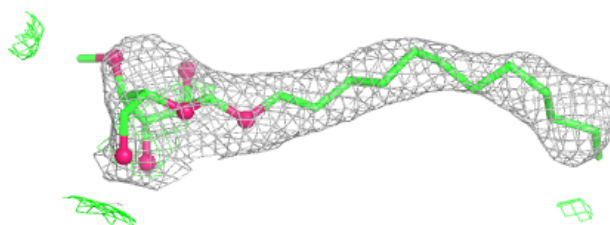
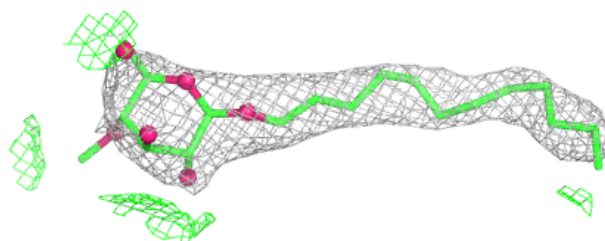


Electron density around SQD A 411:

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

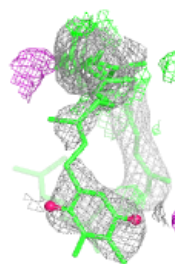
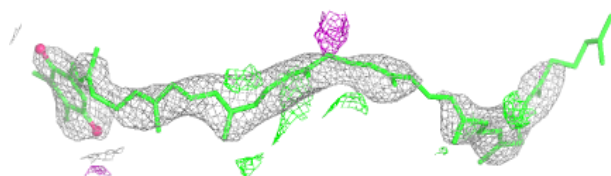
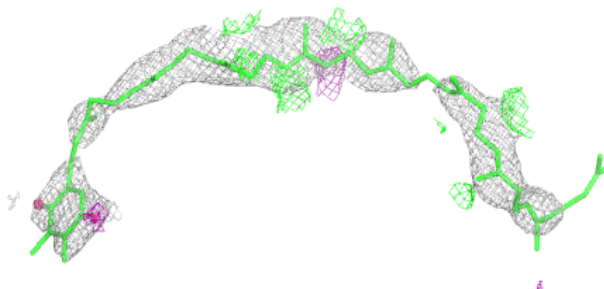
**Electron density around LMT B 632:**

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

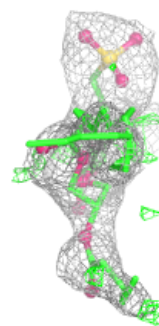
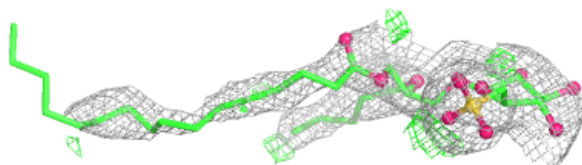
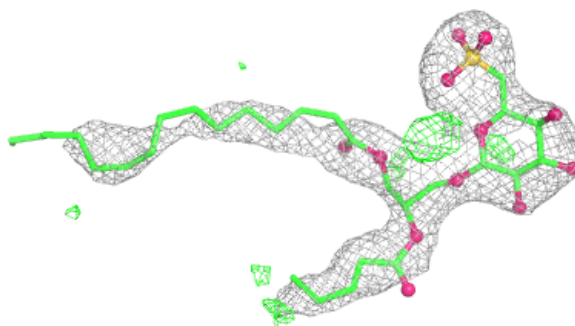


Electron density around PL9 a 415:

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

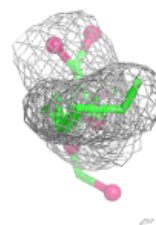
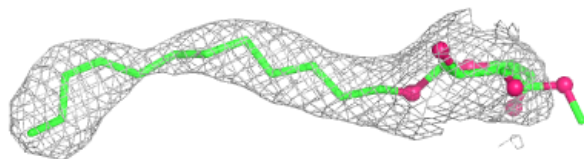
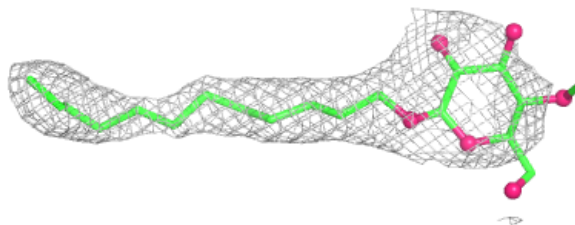
**Electron density around SQD D 413:**

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

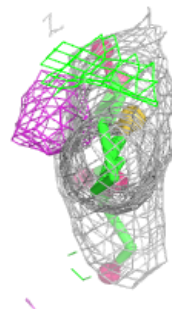
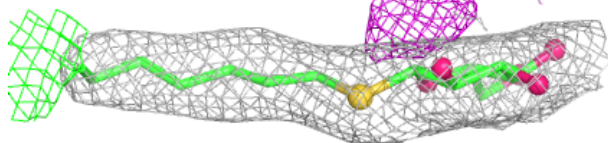
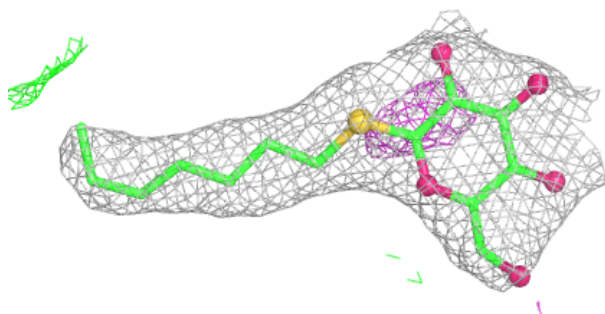


Electron density around LMT b 628:

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

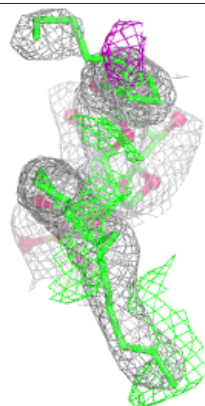
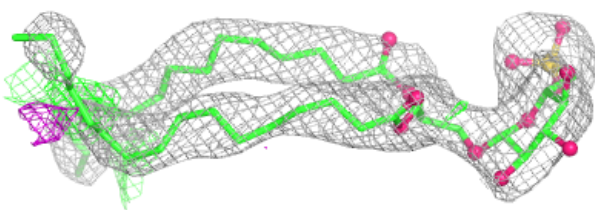
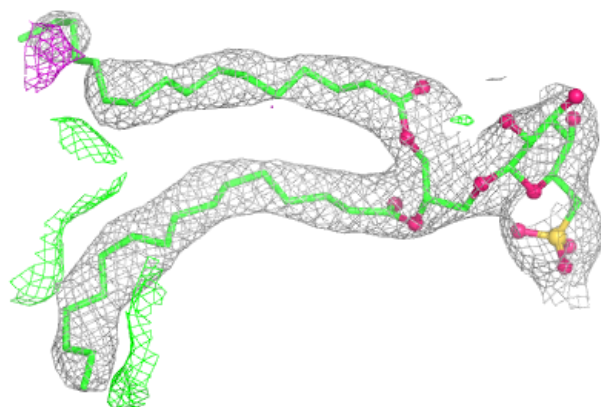
**Electron density around HTG B 629:**

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

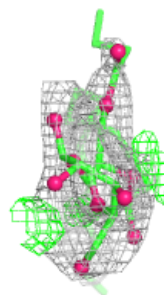
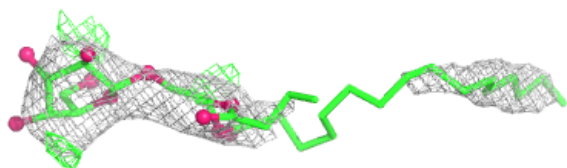
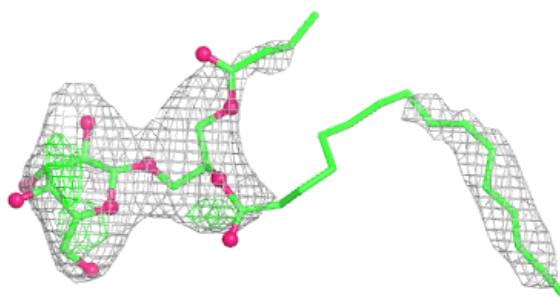


Electron density around SQD L 102:

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

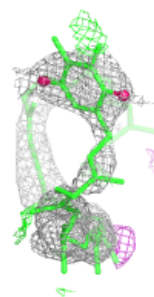
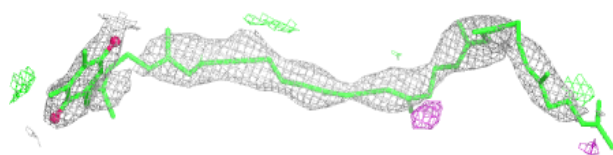
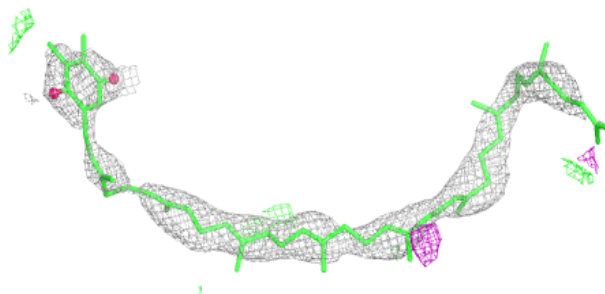
**Electron density around LMG z 101:**

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

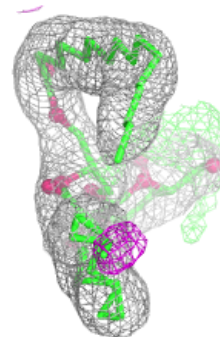
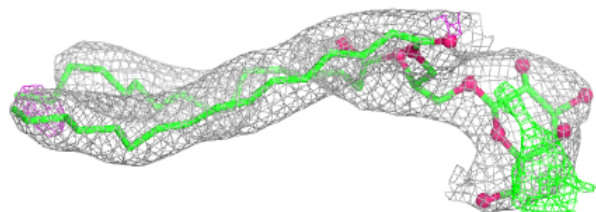
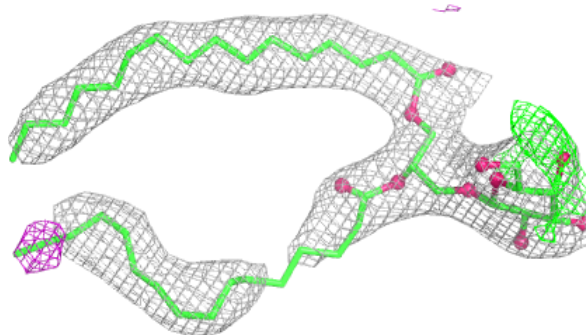


Electron density around PL9 A 413:

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

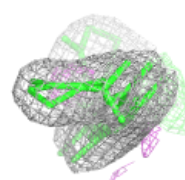
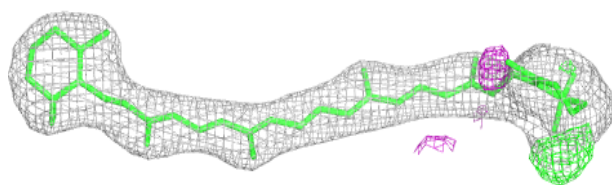
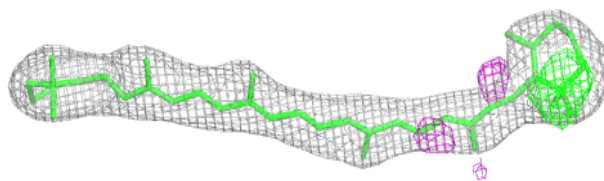
**Electron density around LMG C 501:**

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

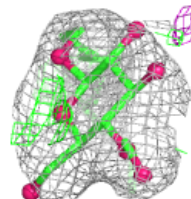
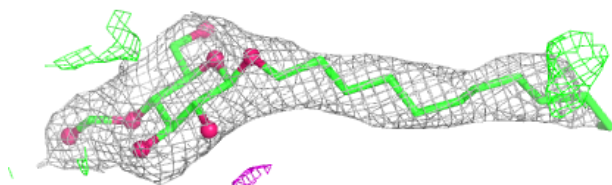
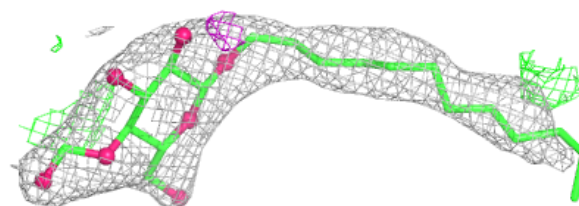


Electron density around BCR D 406:

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

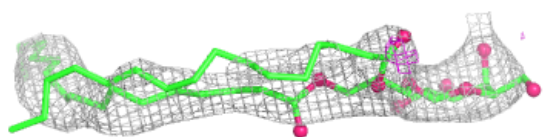
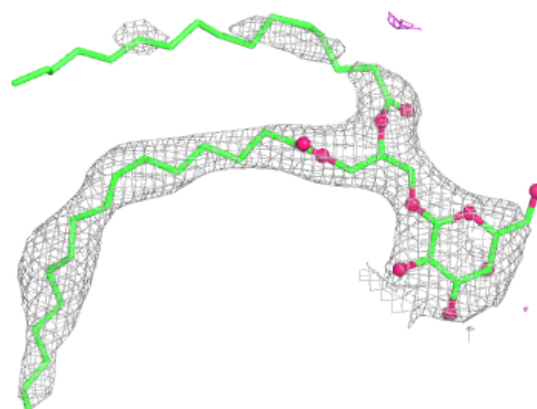
**Electron density around LMT B 634:**

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

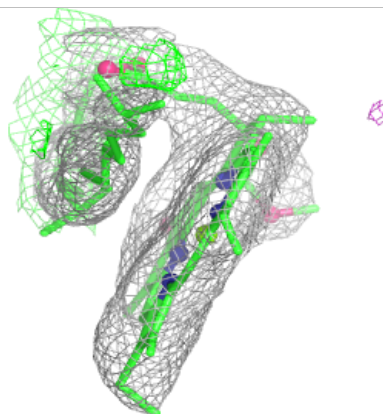
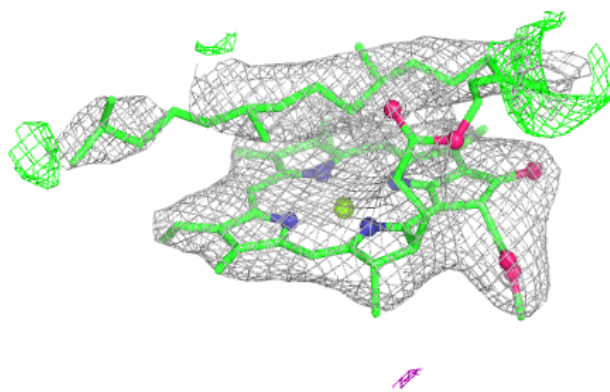
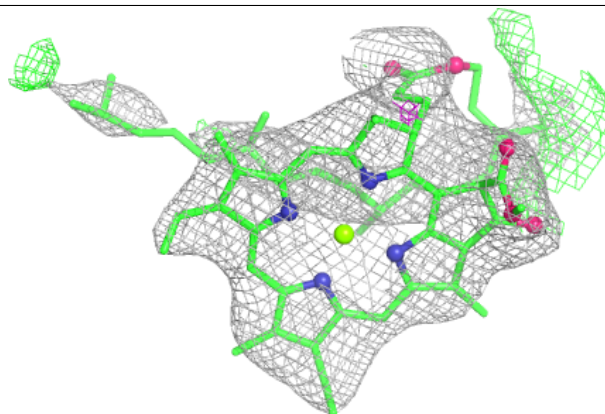


Electron density around LMG C 520:

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

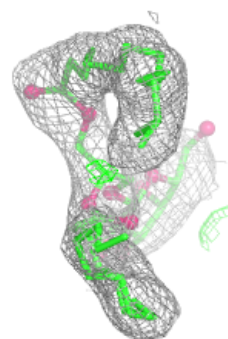
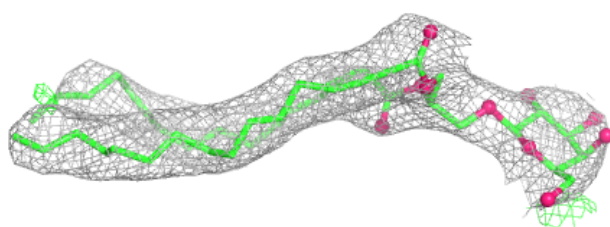
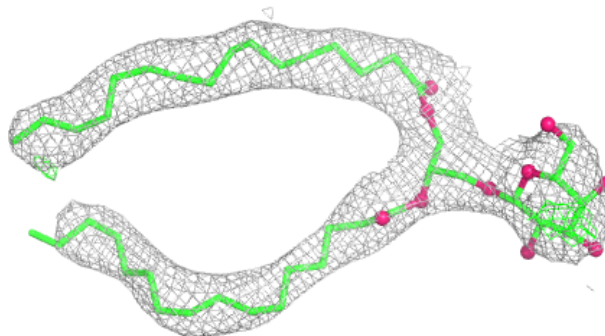
**Electron density around CLA b 601:**

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

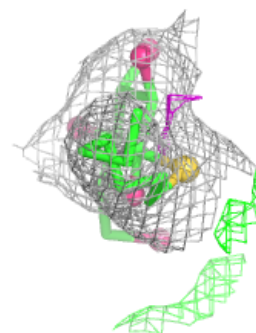
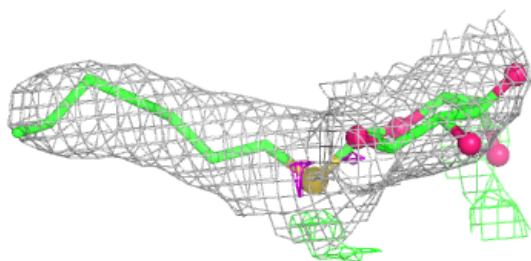
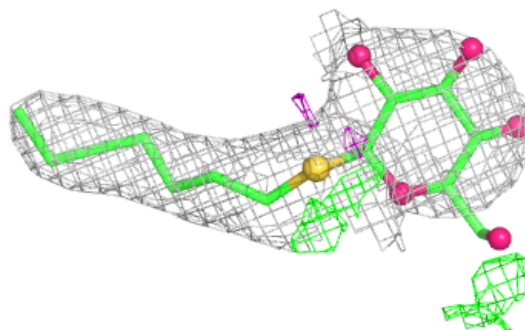


Electron density around LMG a 417:

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

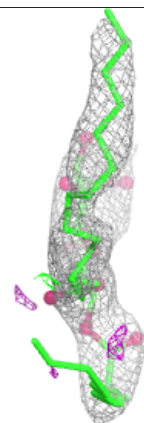
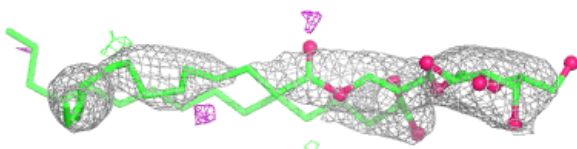
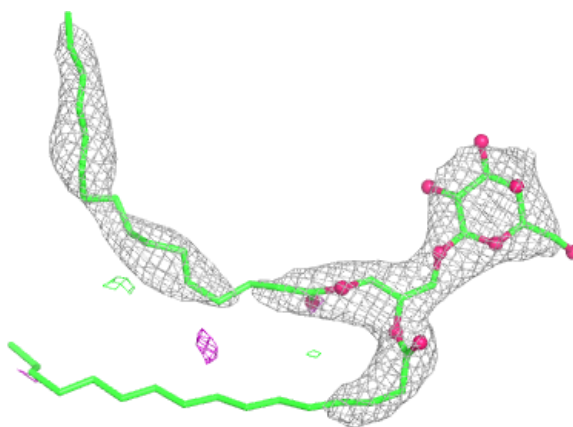
**Electron density around HTG B 624:**

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

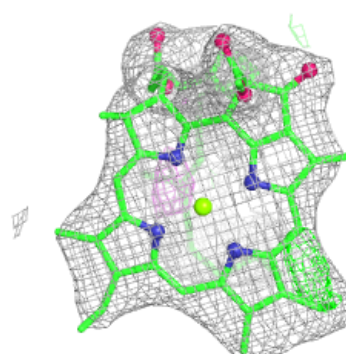
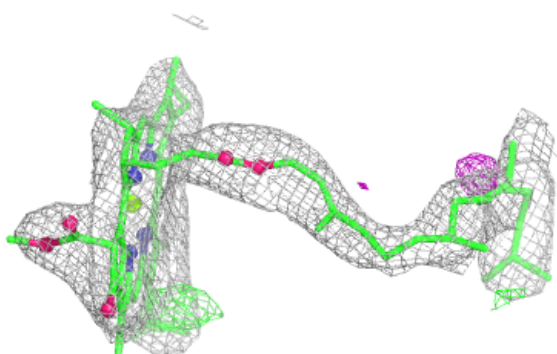
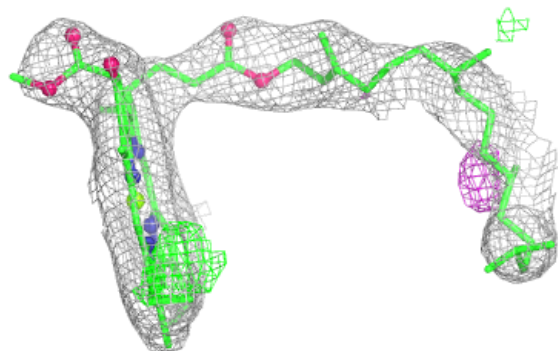


Electron density around LMG c 519:

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

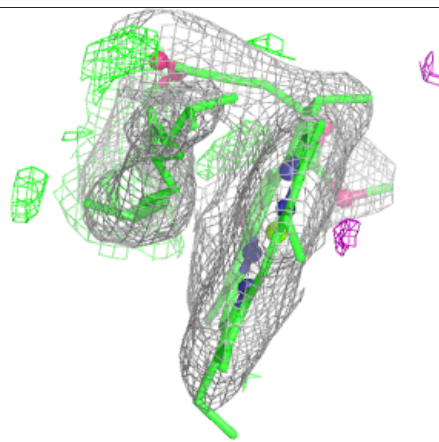
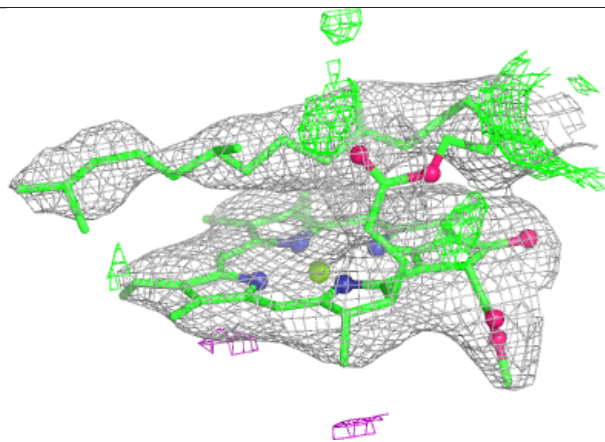
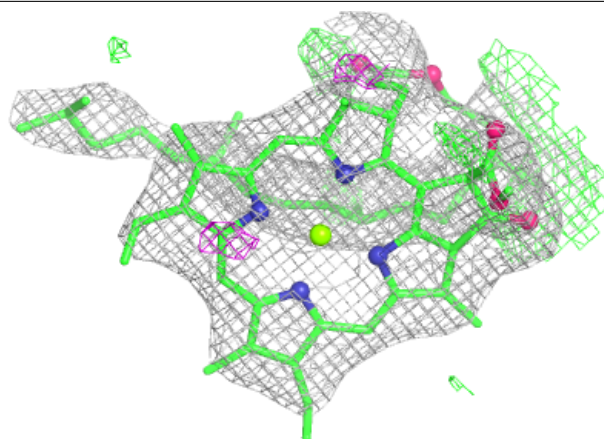
**Electron density around CLA C 507:**

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

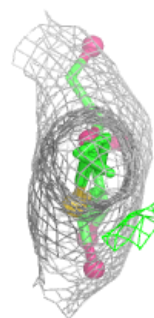
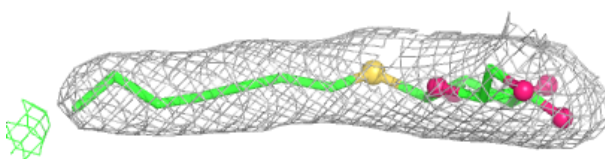
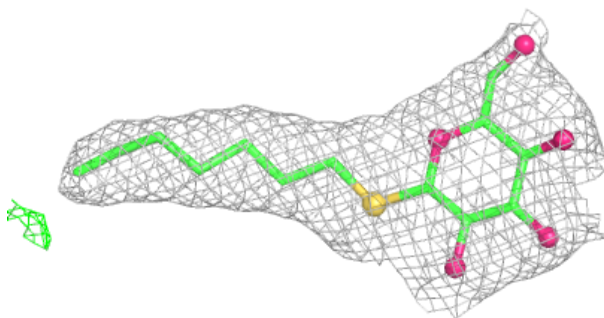


Electron density around CLA B 602:

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

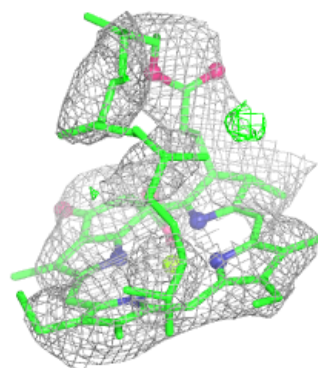
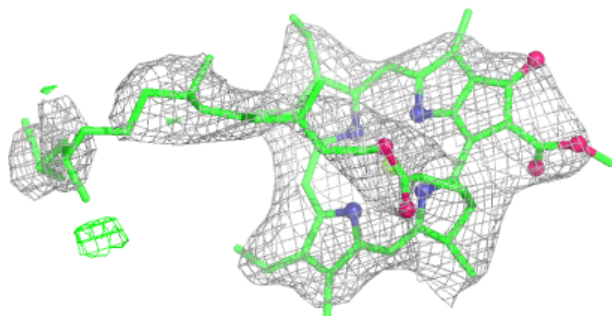
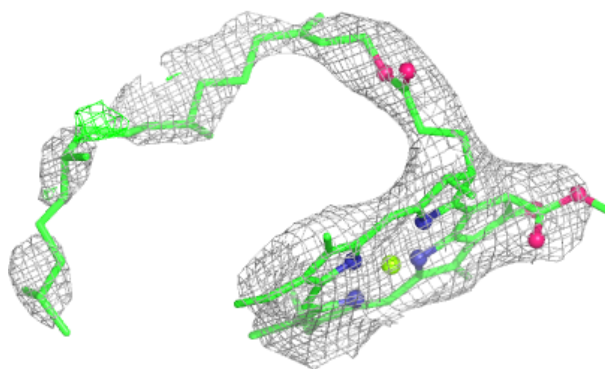
**Electron density around HTG b 625:**

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

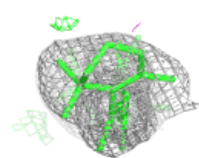
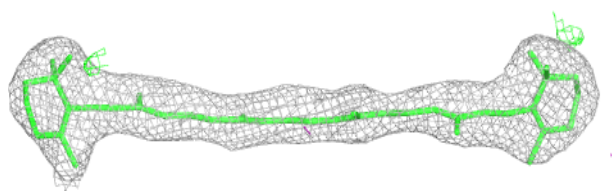
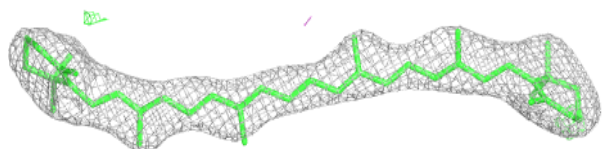


Electron density around CLA c 513:

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

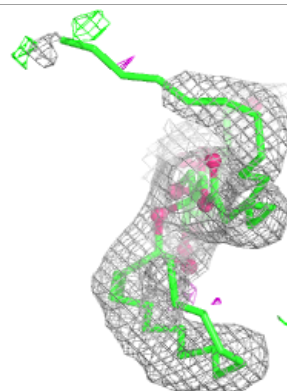
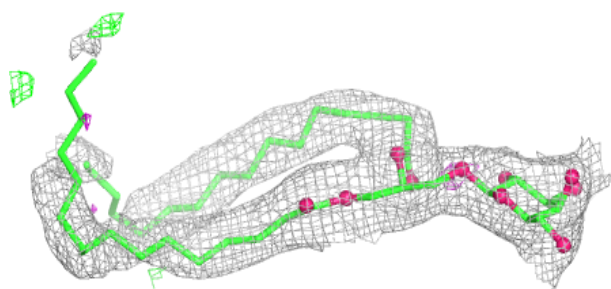
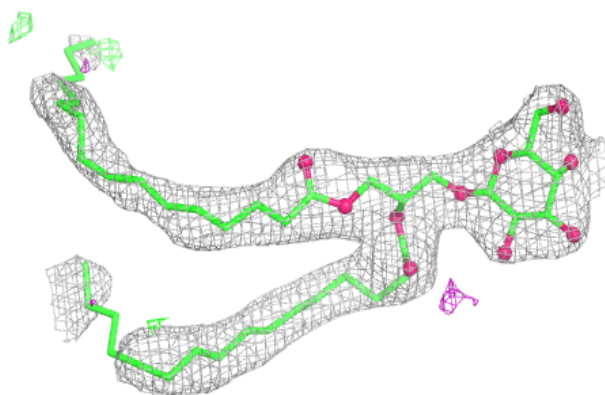
**Electron density around BCR C 515:**

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

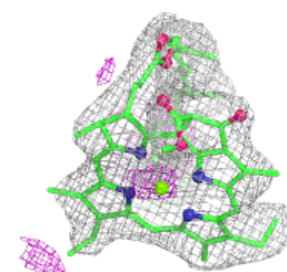
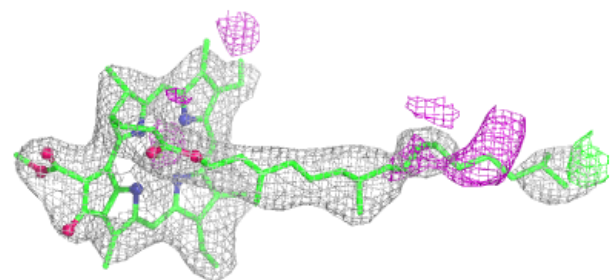
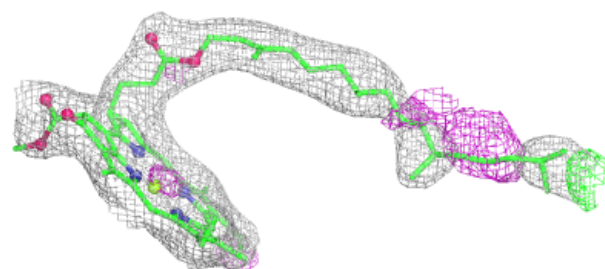


Electron density around LMG J 101:

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

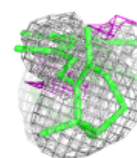
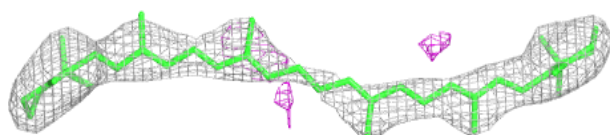
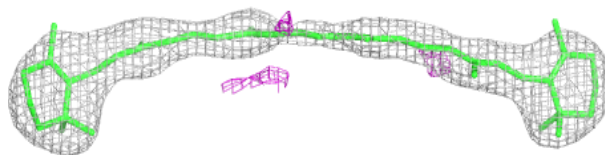
**Electron density around CLA C 505:**

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

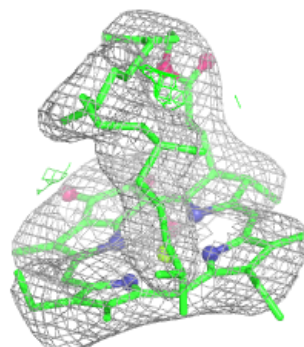
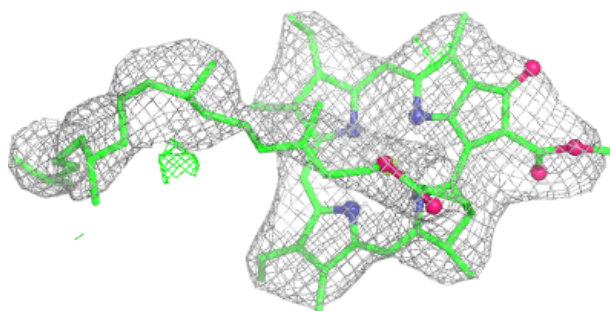
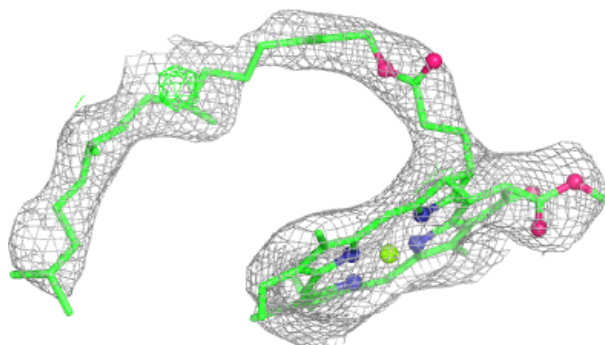


Electron density around BCR C 527:

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

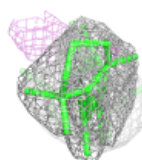
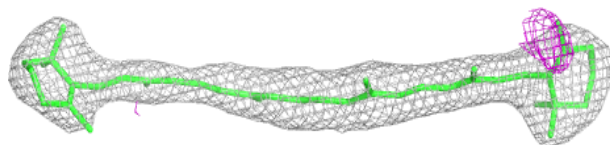
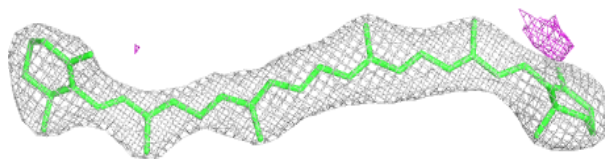
**Electron density around CLA C 514:**

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

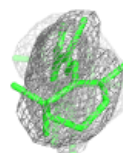
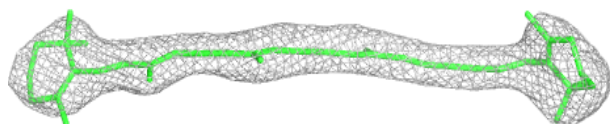
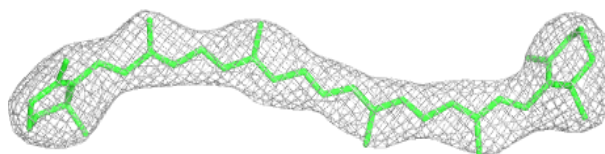


Electron density around BCR Y 101:

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

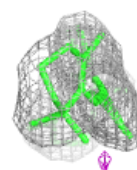
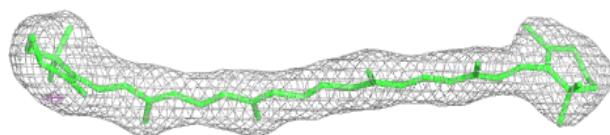
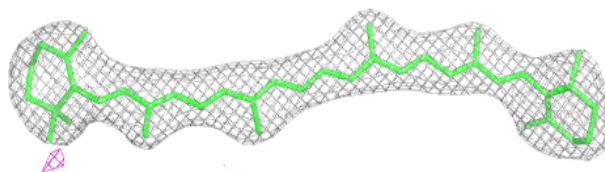
**Electron density around BCR y 101:**

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

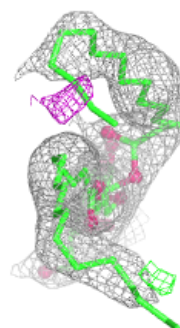
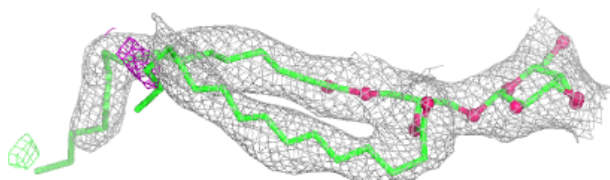
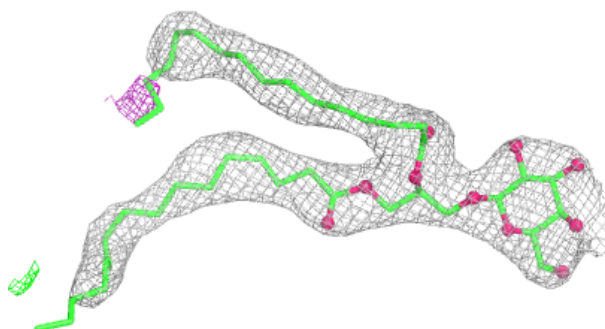


Electron density around BCR B 620:

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

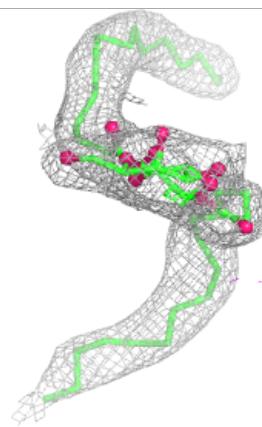
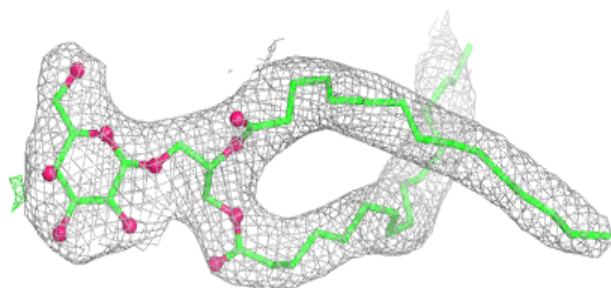
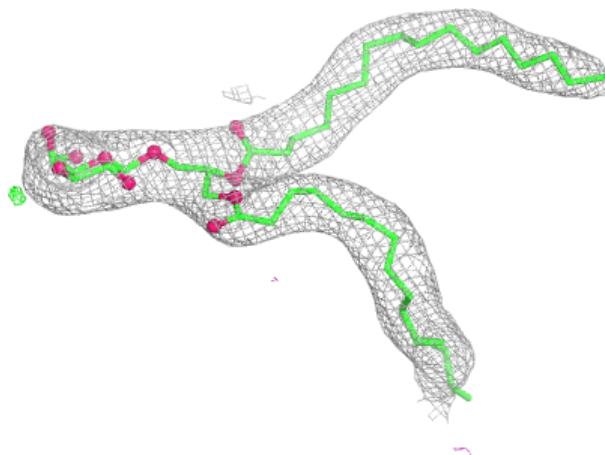
**Electron density around LMG j 101:**

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



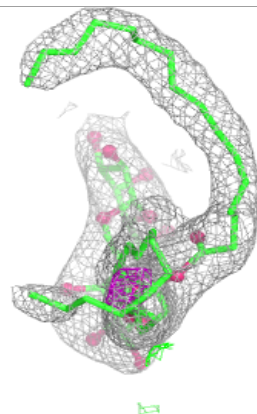
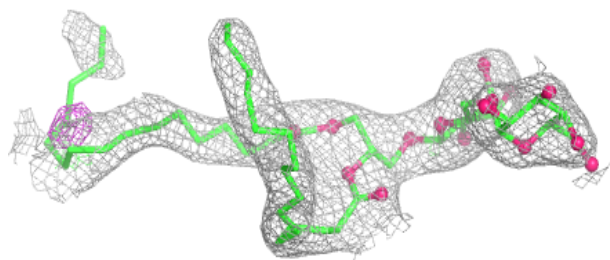
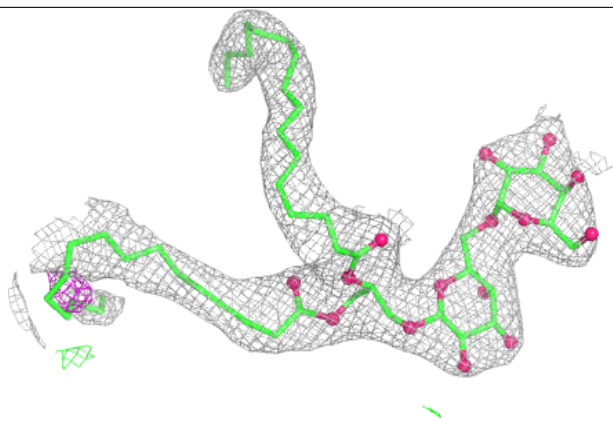
Electron density around LMG B 622:

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



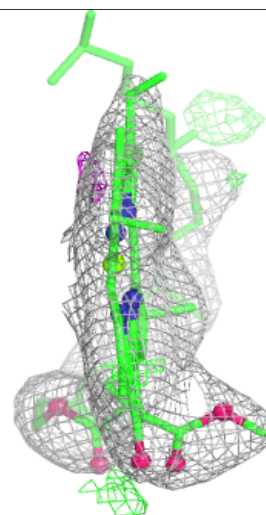
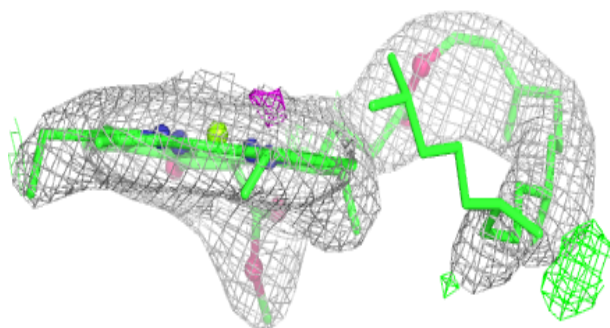
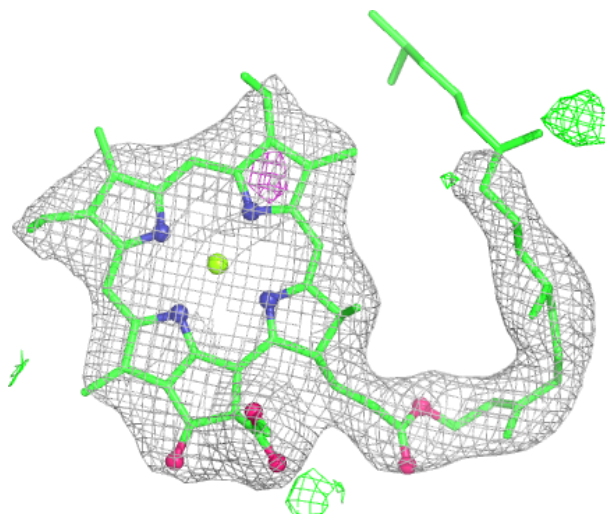
Electron density around DGD c 517:

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



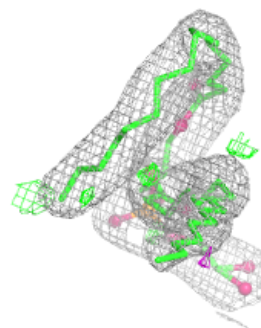
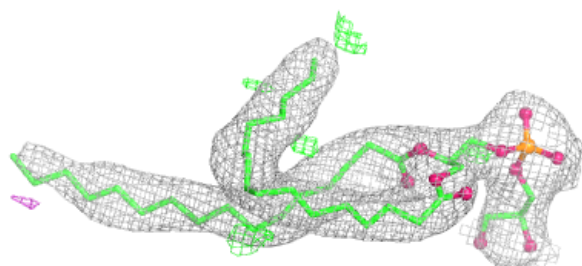
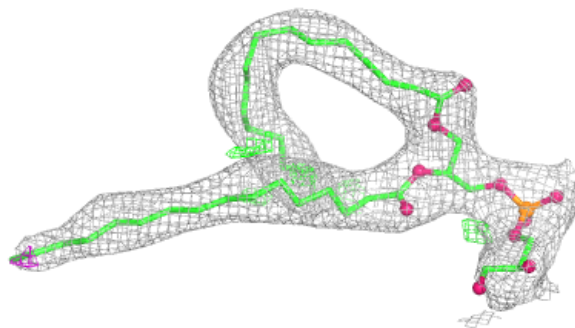
Electron density around CLA C 513:

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



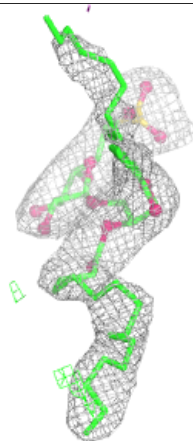
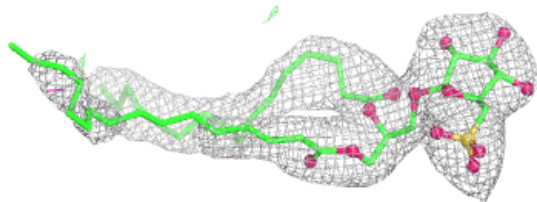
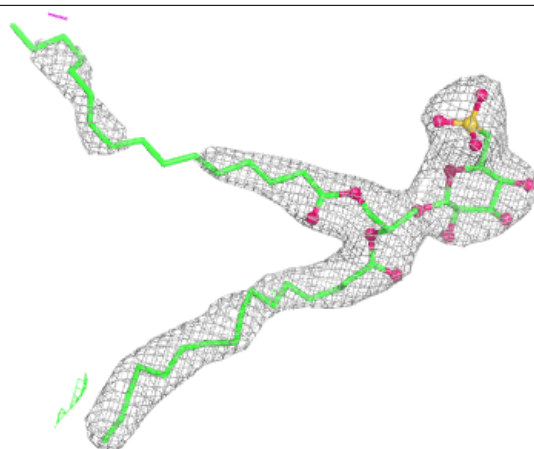
Electron density around LHG d 406:

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



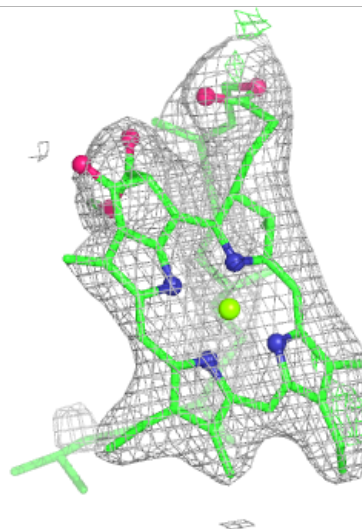
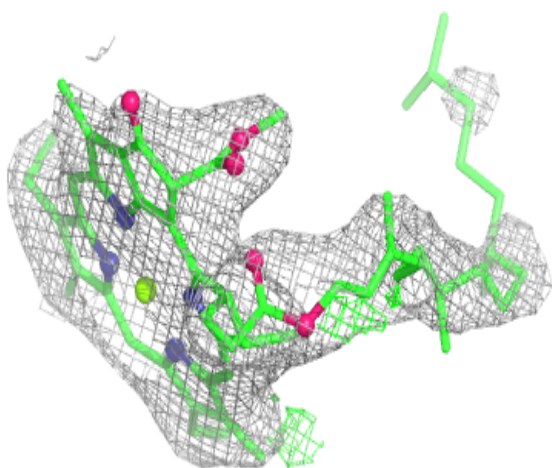
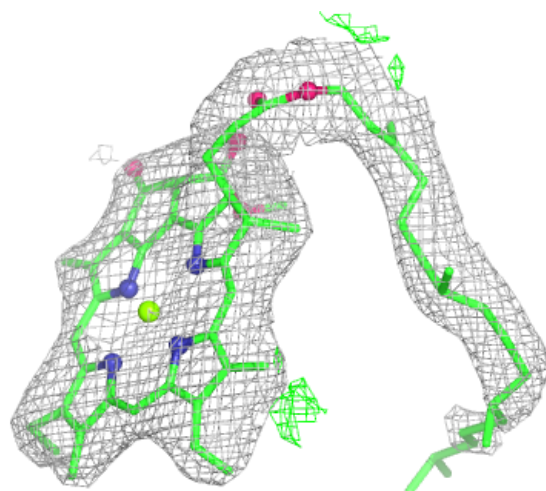
Electron density around SQD A 409:

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



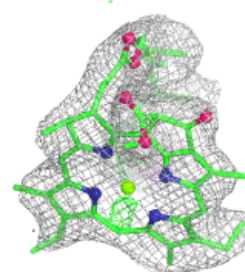
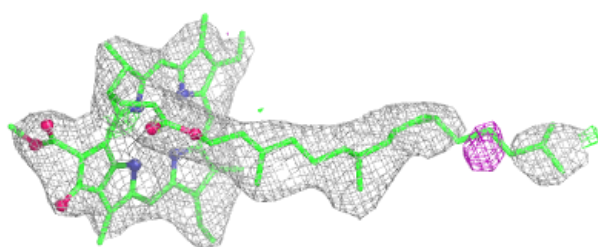
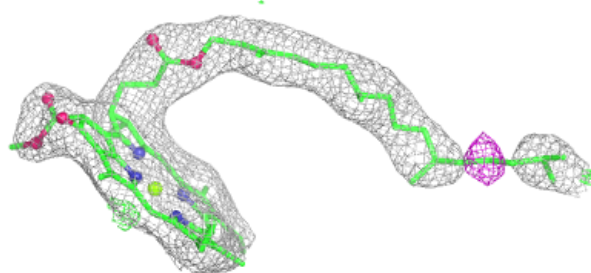
Electron density around CLA b 616:

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

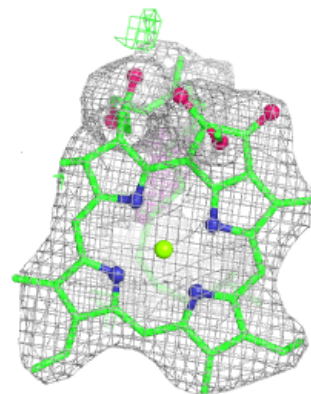
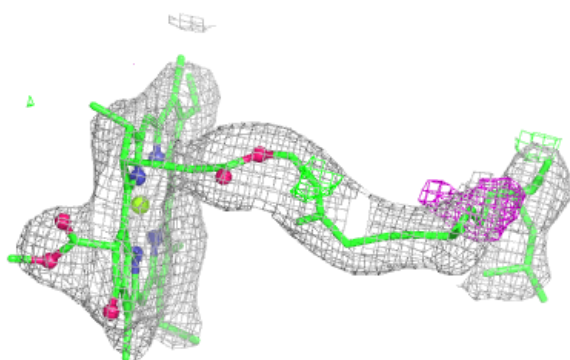
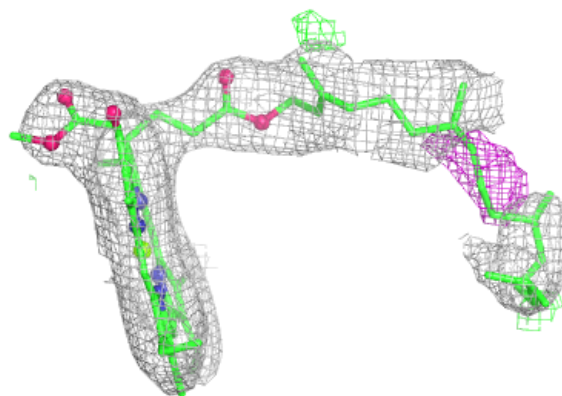


Electron density around CLA c 504:

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

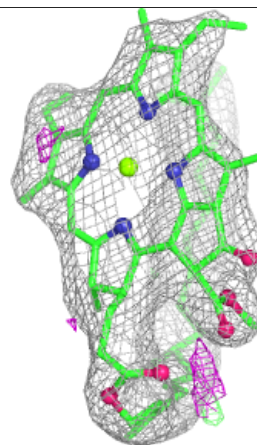
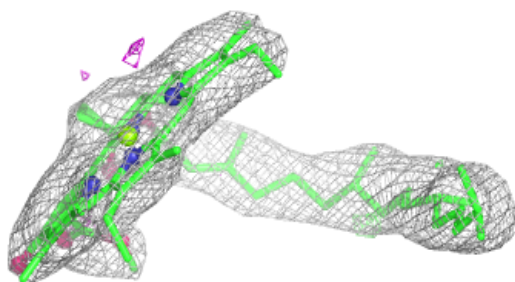
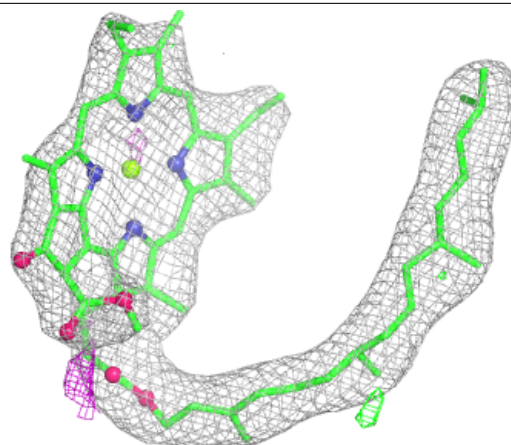
**Electron density around CLA c 506:**

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

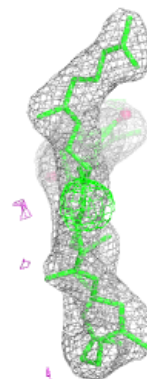
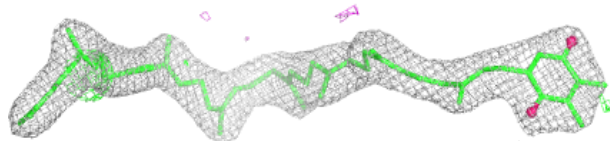
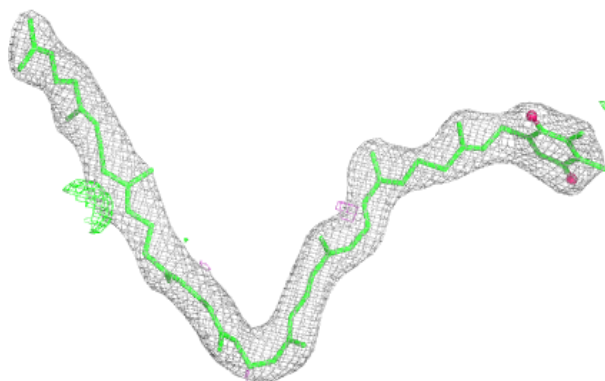


Electron density around CLA c 507:

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

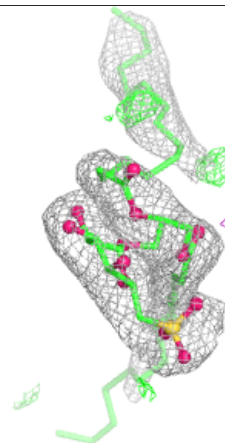
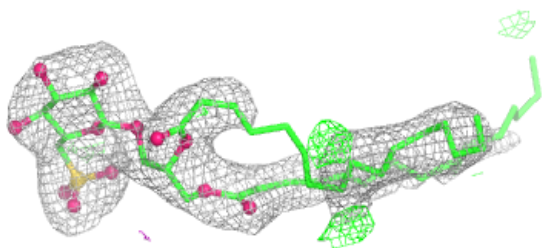
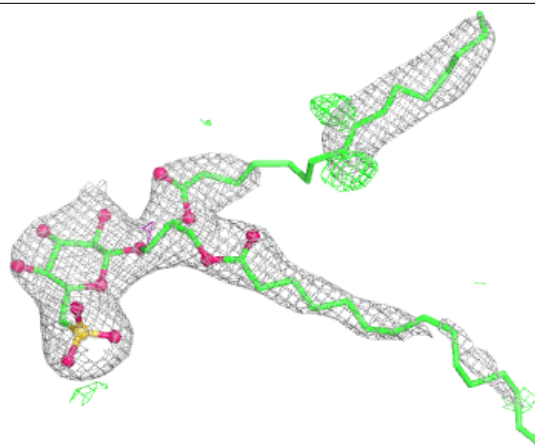
**Electron density around PL9 D 407:**

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



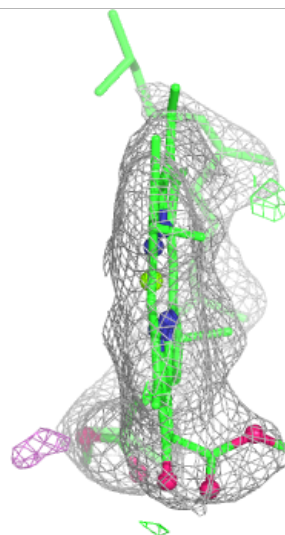
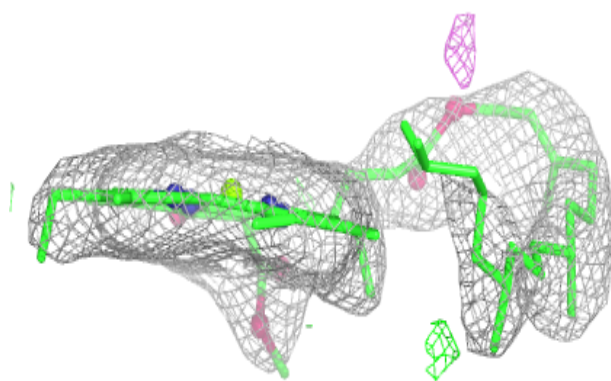
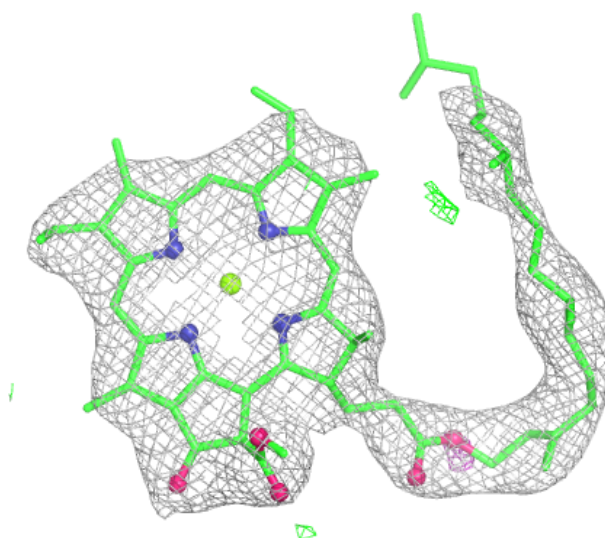
Electron density around SQD a 411:

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



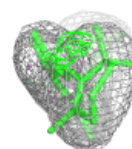
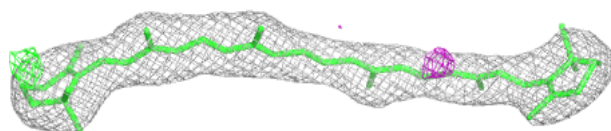
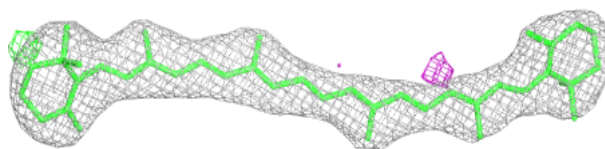
Electron density around CLA c 512:

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

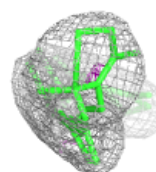
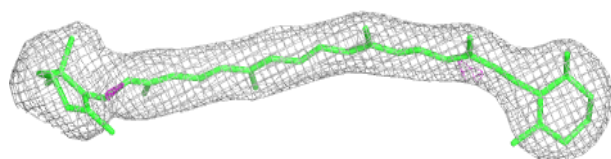
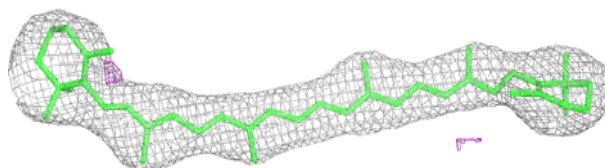


Electron density around BCR b 619:

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

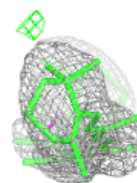
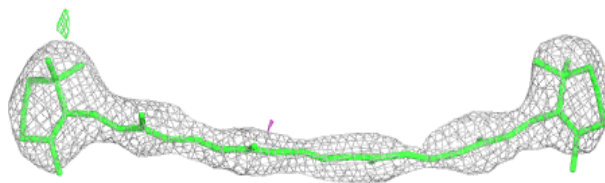
**Electron density around BCR d 404:**

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

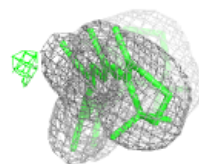
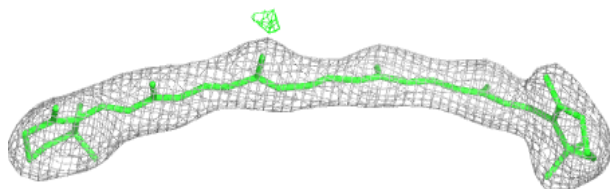
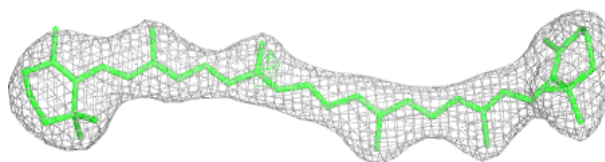


Electron density around BCR k 101:

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

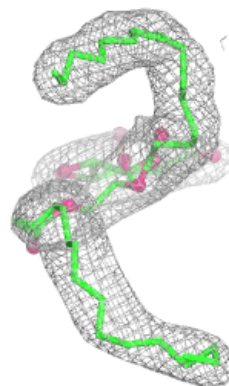
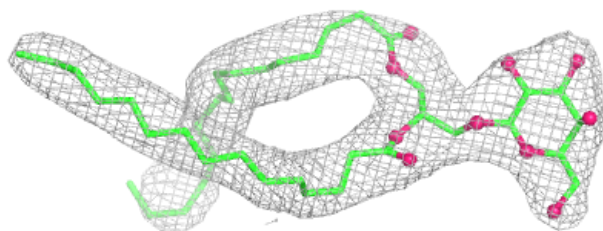
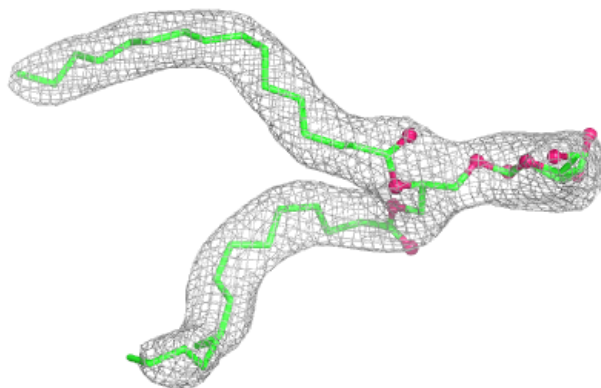
**Electron density around BCR t 101:**

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

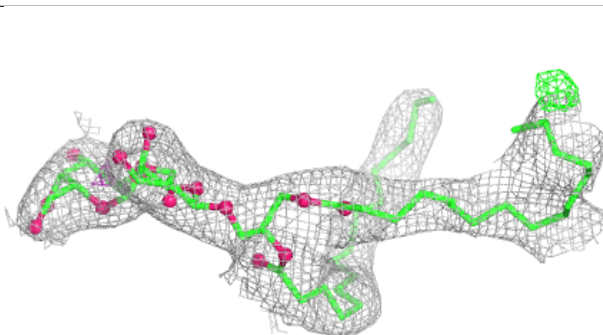
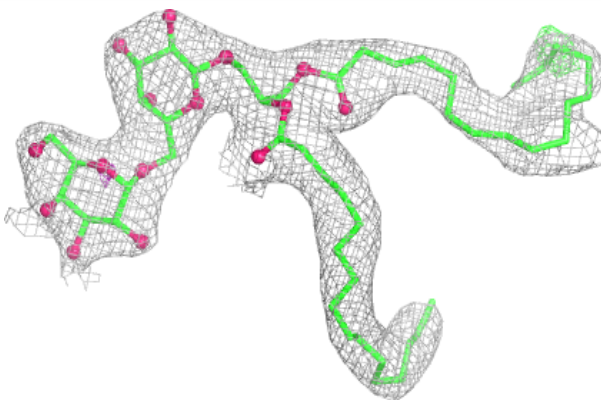


Electron density around LMG m 101:

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

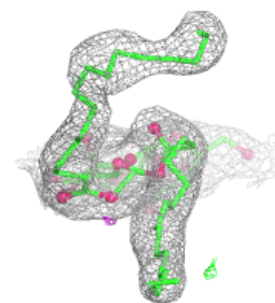
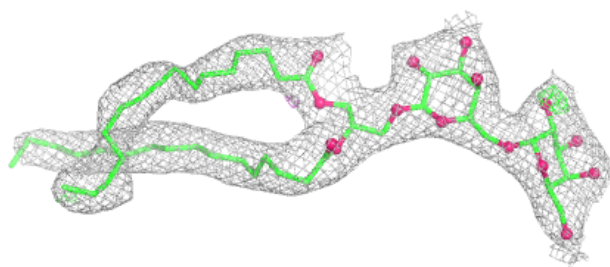
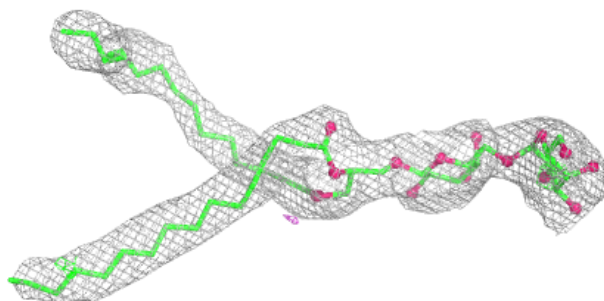
**Electron density around DGD C 518:**

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

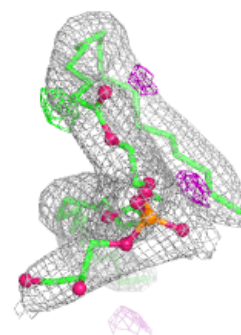
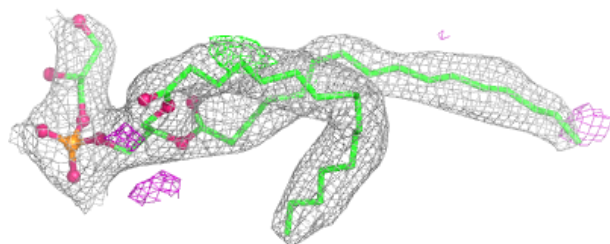
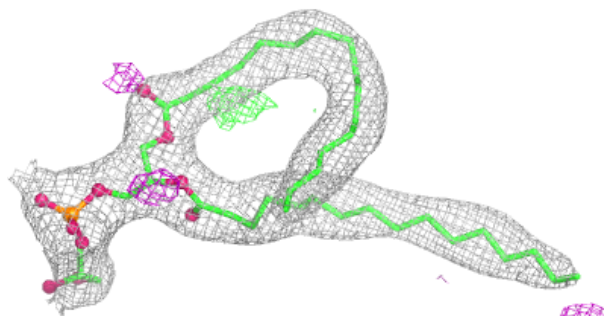


Electron density around DGD c 516:

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

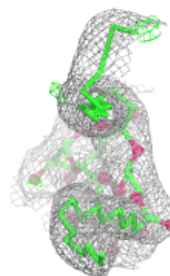
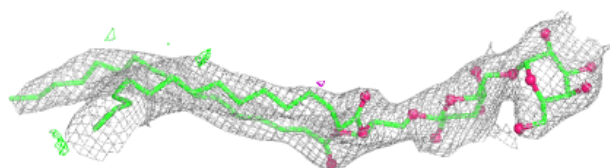
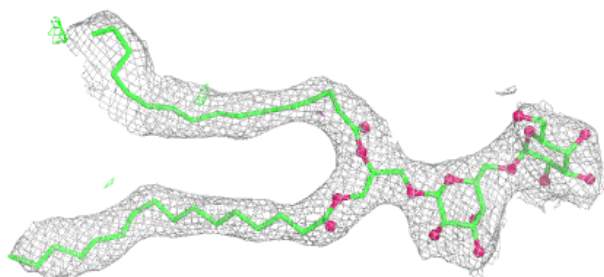
**Electron density around LHG A 415:**

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

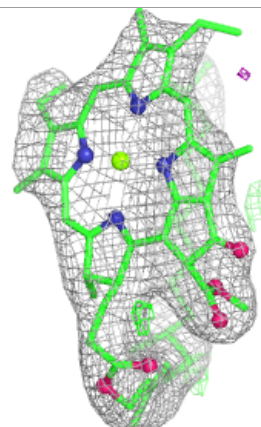
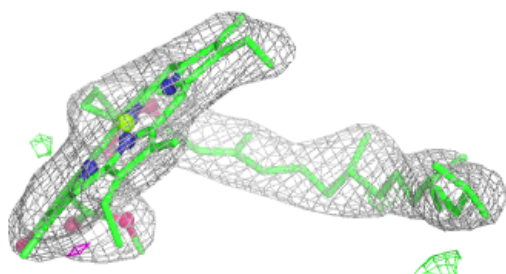
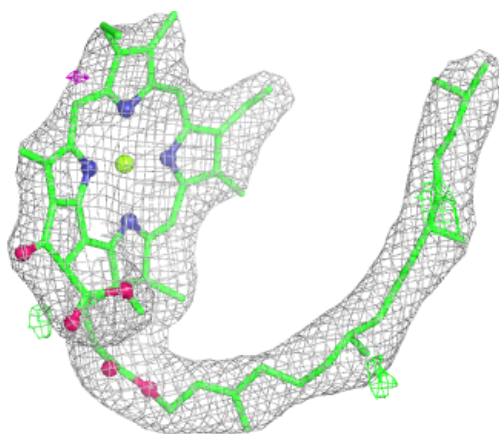


Electron density around DGD c 518:

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

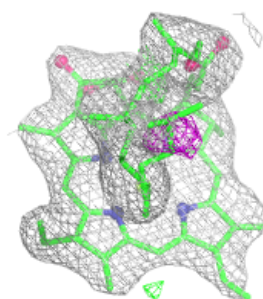
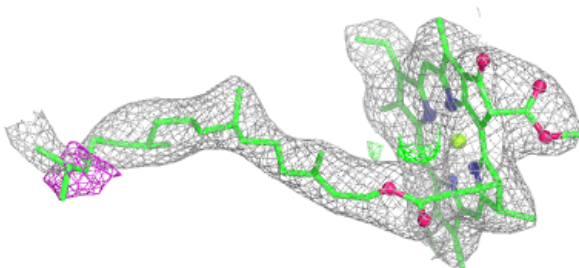
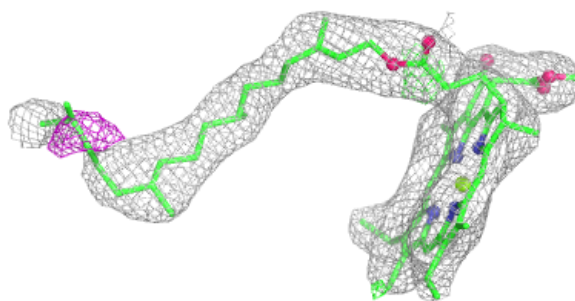
**Electron density around CLA C 508:**

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

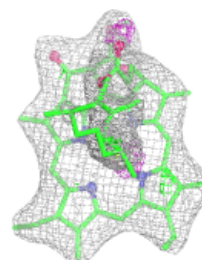
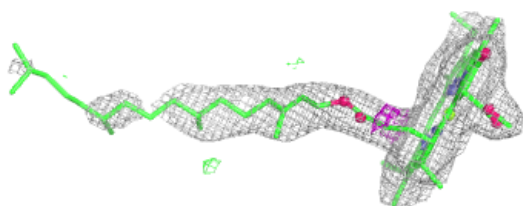
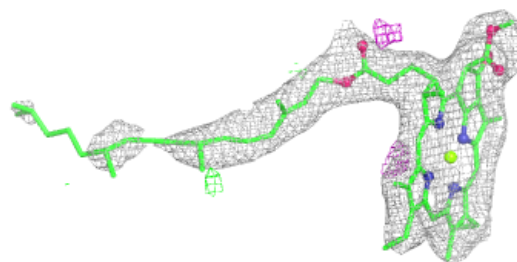


Electron density around CLA C 509:

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

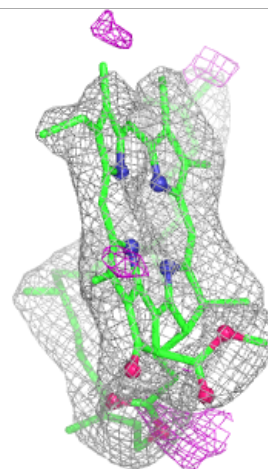
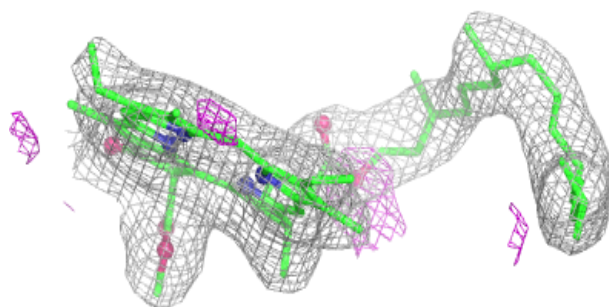
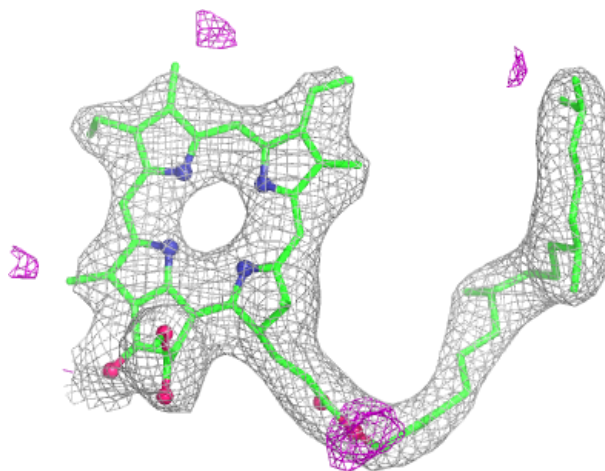
**Electron density around CLA d 403:**

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



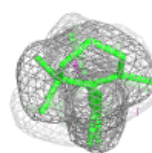
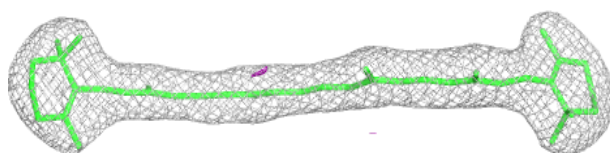
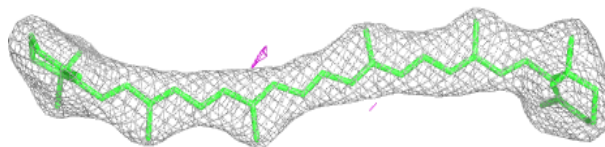
Electron density around PHO a 408:

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

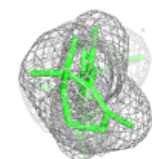
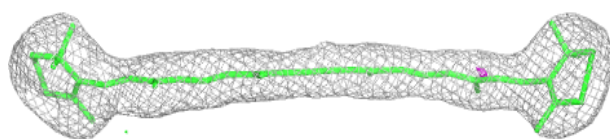
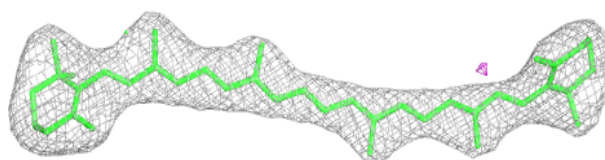


Electron density around BCR A 408:

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

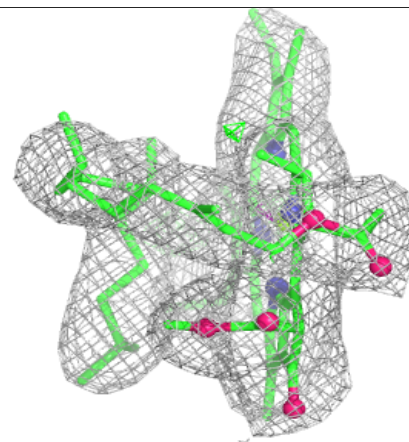
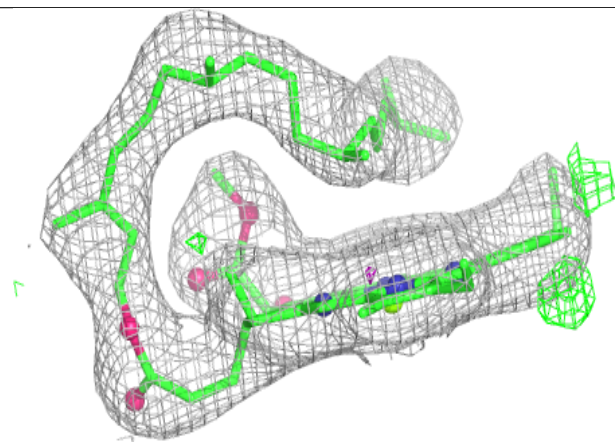
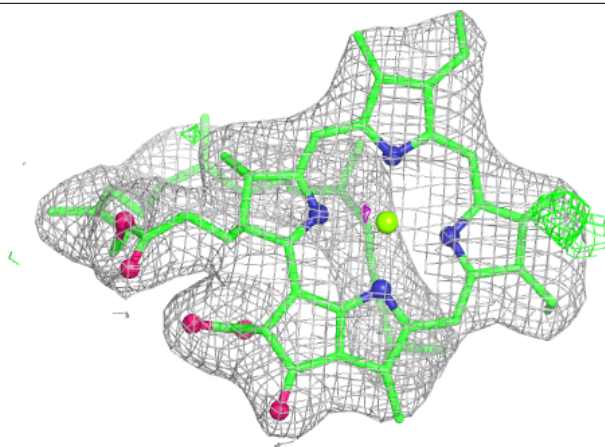
**Electron density around BCR B 619:**

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



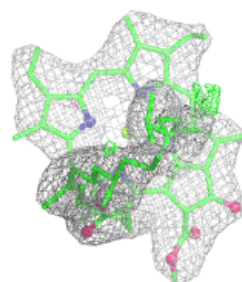
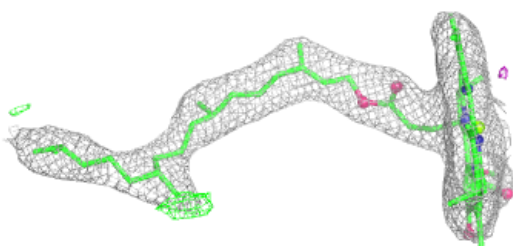
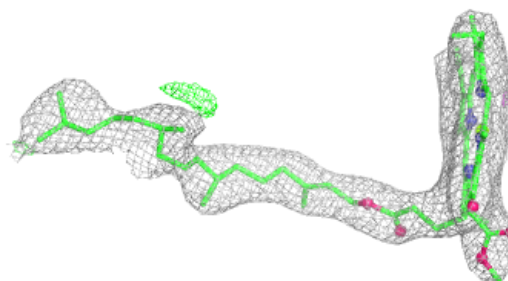
Electron density around CLA C 511:

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

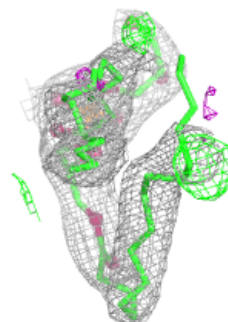
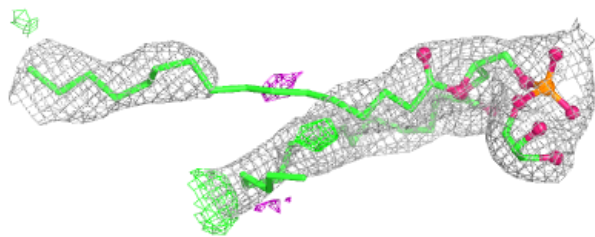
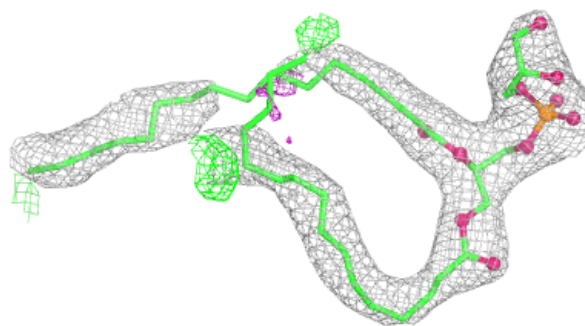


Electron density around CLA B 607:

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

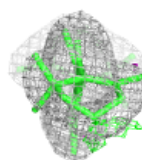
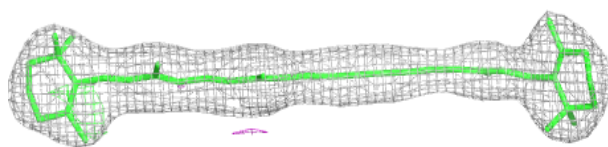
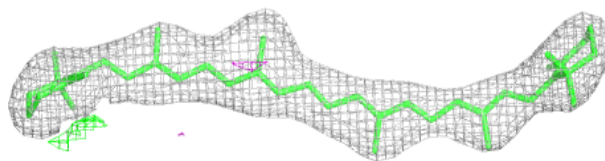
**Electron density around LHG D 409:**

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



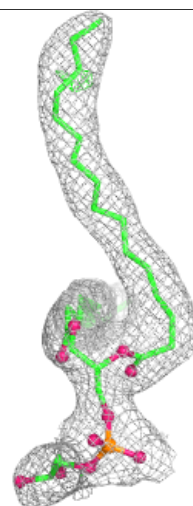
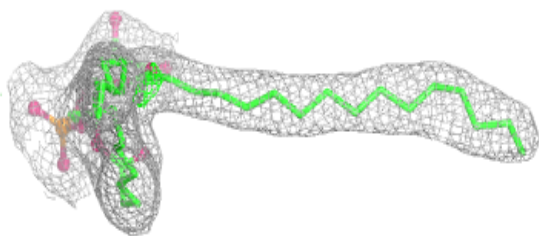
Electron density around BCR C 516:

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



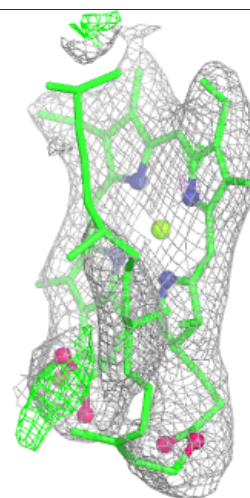
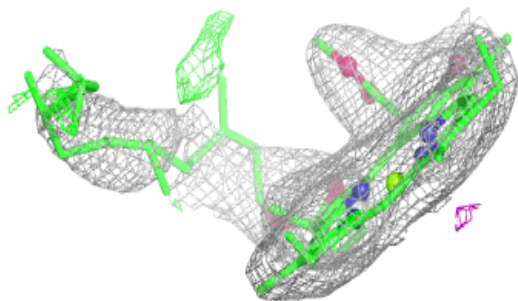
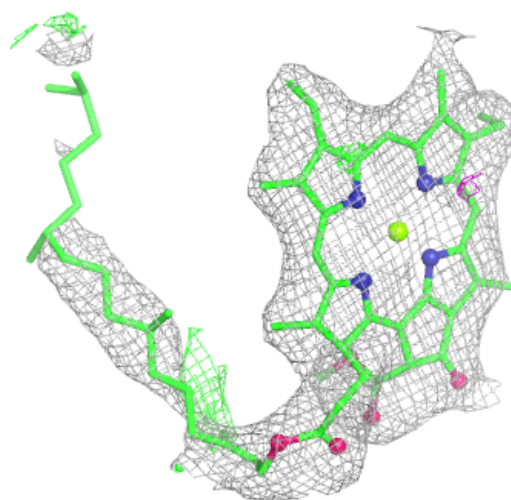
Electron density around LHG b 630:

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



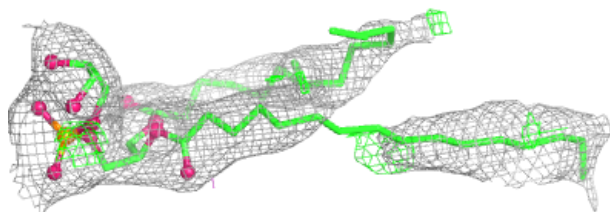
Electron density around CLA B 617:

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

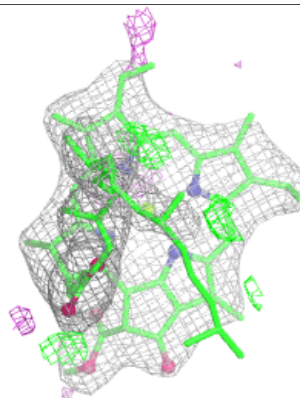
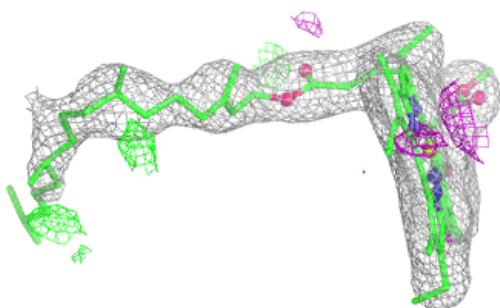
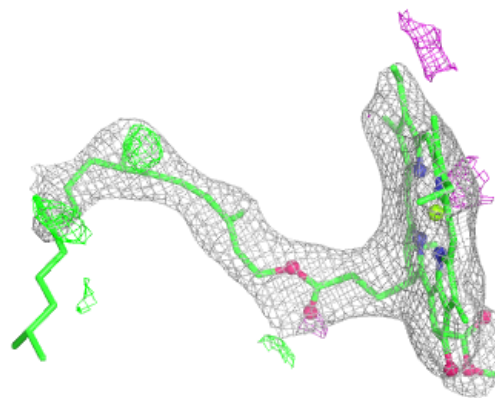


Electron density around LHG d 408:

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

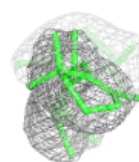
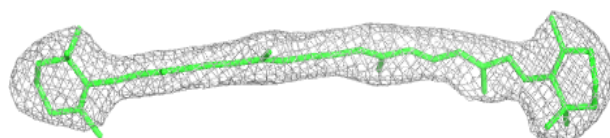
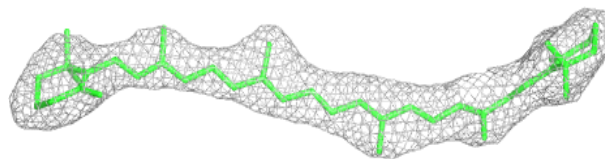
**Electron density around CLA D 405:**

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

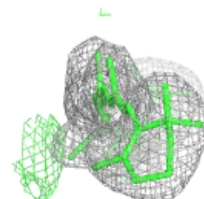
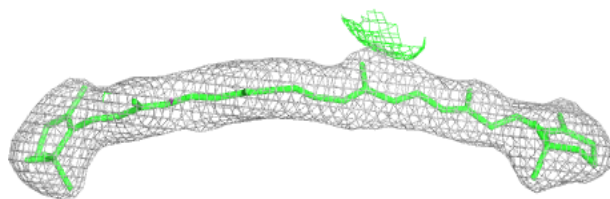
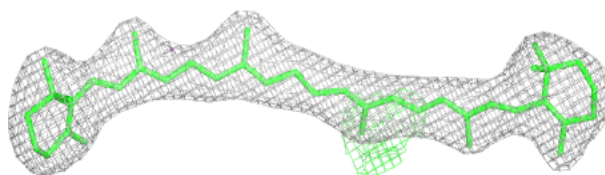


Electron density around BCR H 101:

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

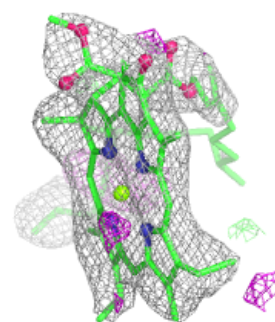
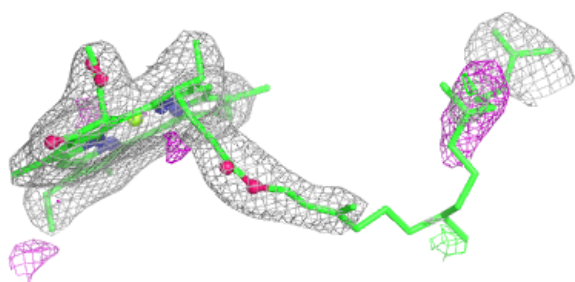
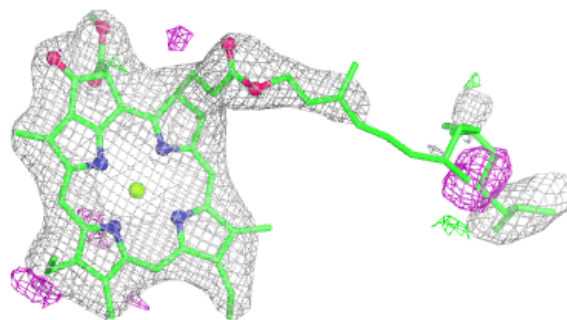
**Electron density around BCR T 101:**

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

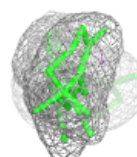
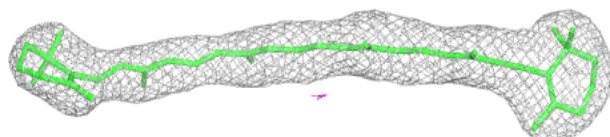
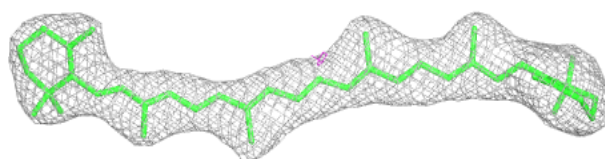


Electron density around CLA a 409:

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

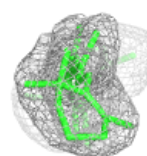
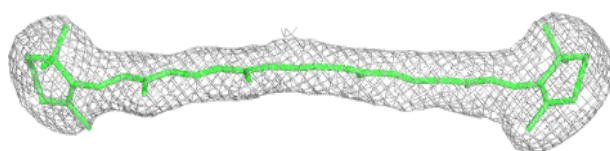
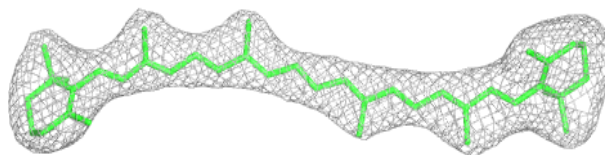
**Electron density around BCR b 617:**

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

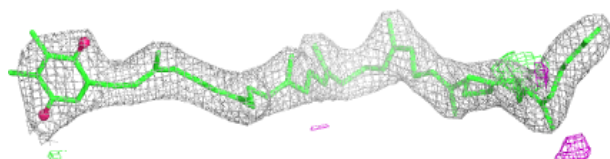
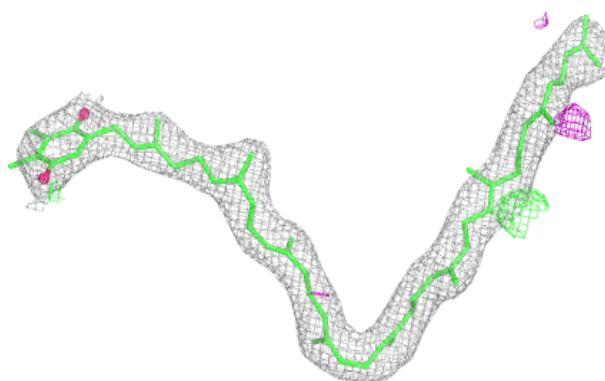


Electron density around BCR b 618:

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

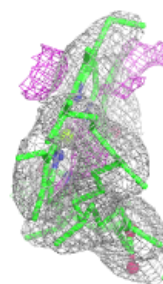
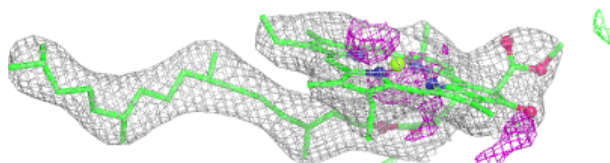
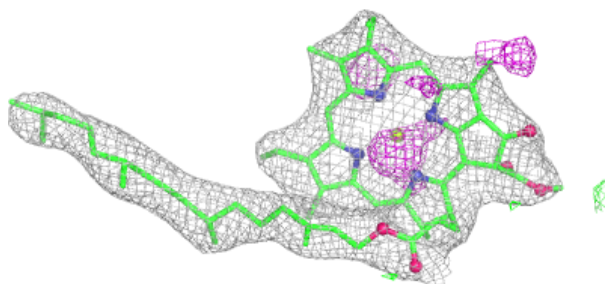
**Electron density around PL9 d 405:**

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

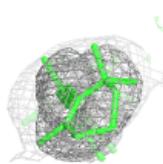
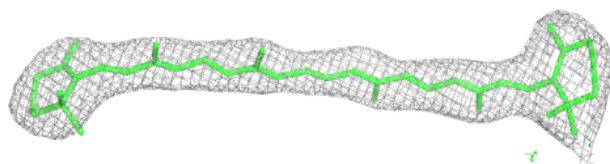
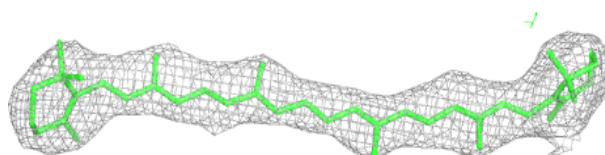


Electron density around CLA C 502:

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

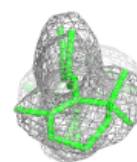
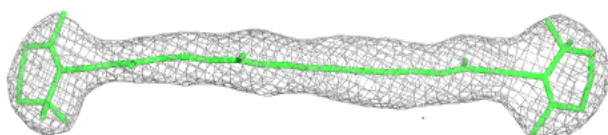
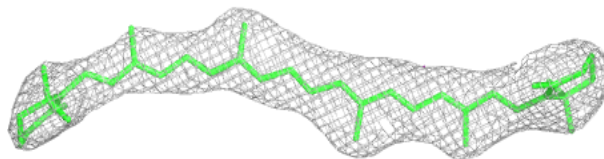
**Electron density around BCR c 514:**

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

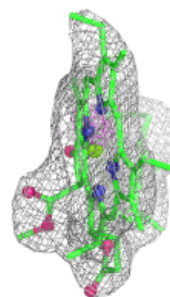
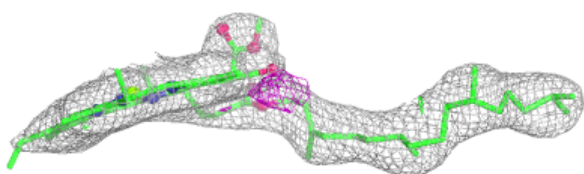
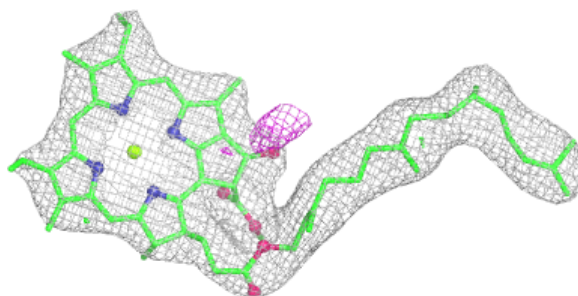


Electron density around BCR c 515:

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

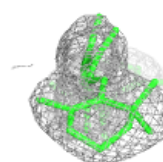
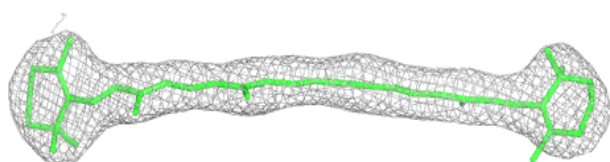
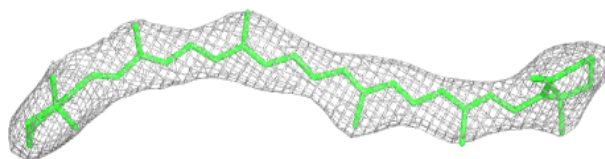
**Electron density around CLA b 602:**

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

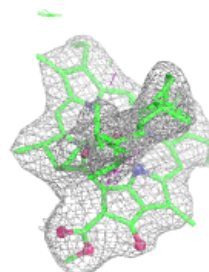
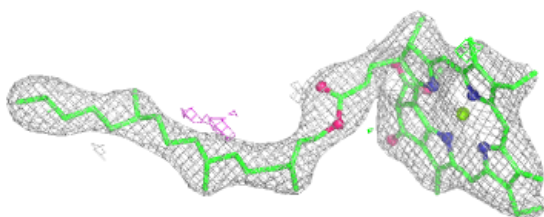
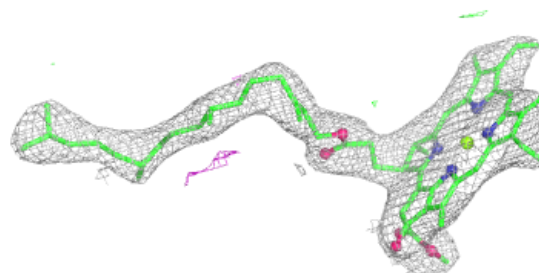


Electron density around BCR h 102:

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

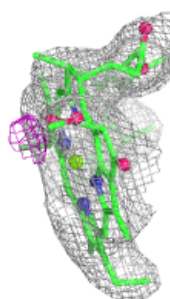
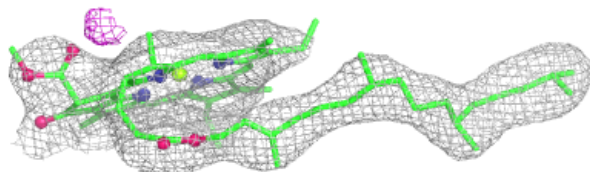
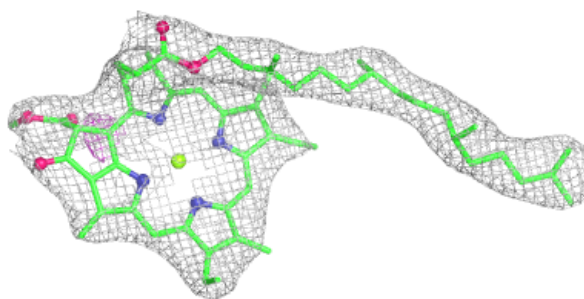
**Electron density around CLA C 503:**

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

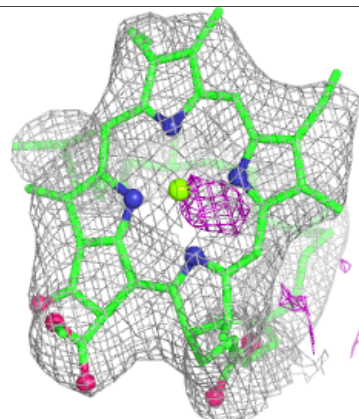
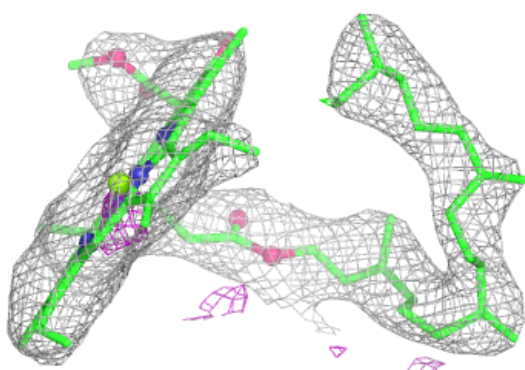
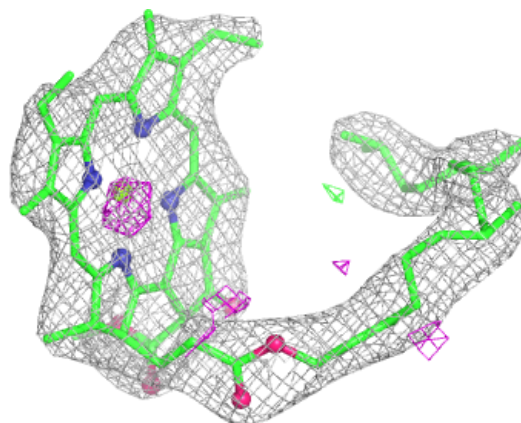


Electron density around CLA c 501:

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

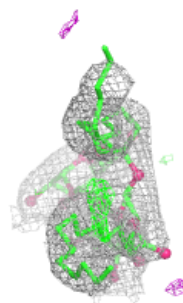
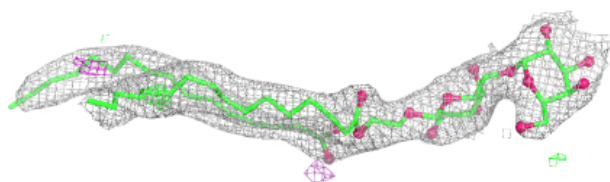
**Electron density around CLA C 504:**

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

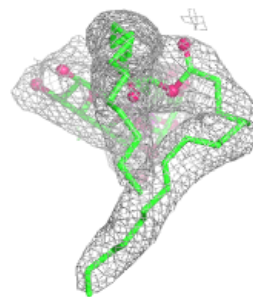
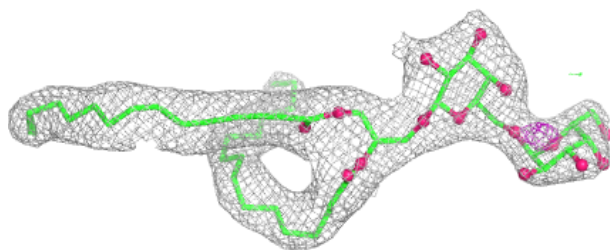
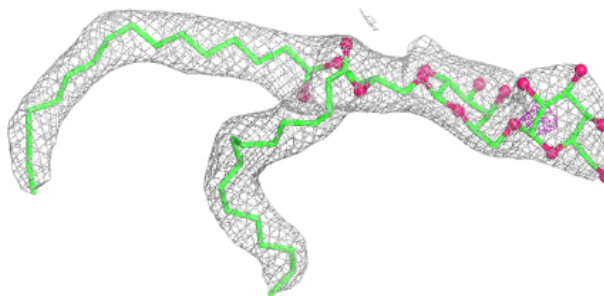


Electron density around DGD C 519:

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

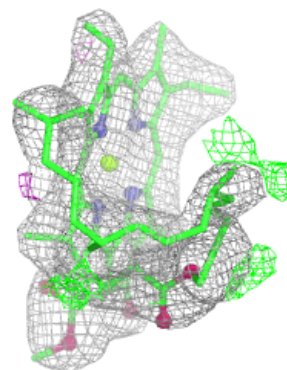
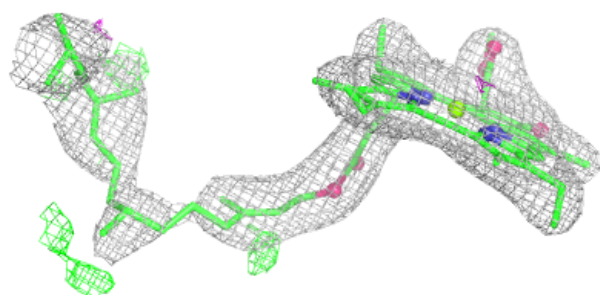
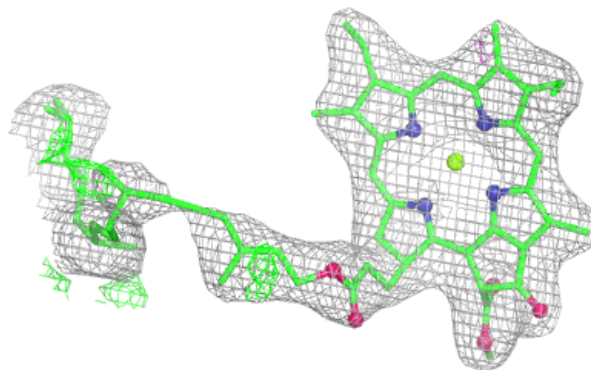
**Electron density around DGD H 102:**

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

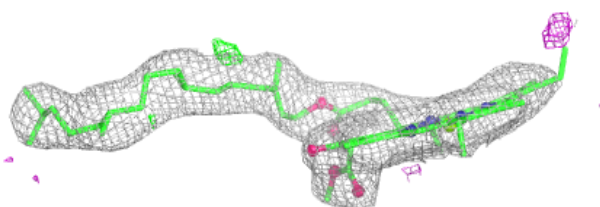
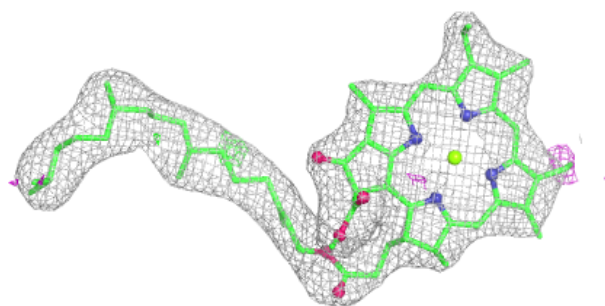


Electron density around CLA A 407:

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

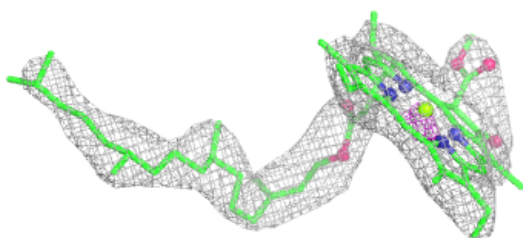
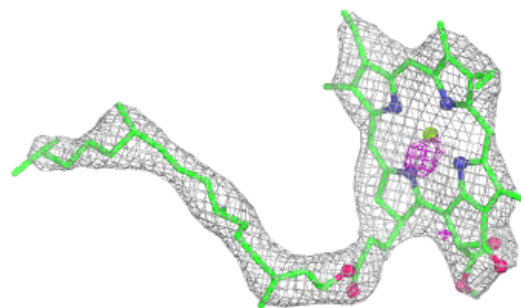
**Electron density around CLA B 603:**

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

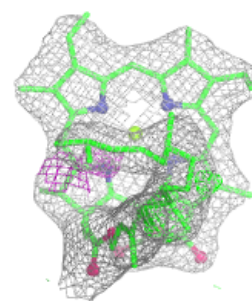
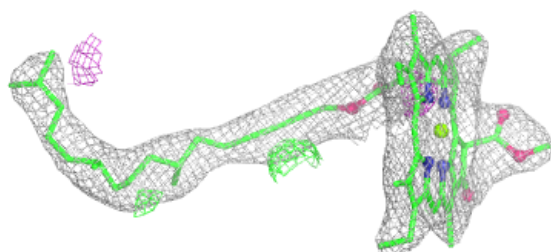
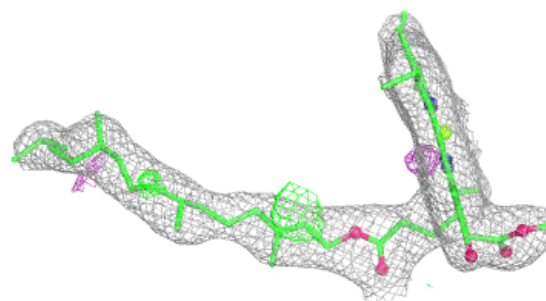


Electron density around CLA c 511:

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

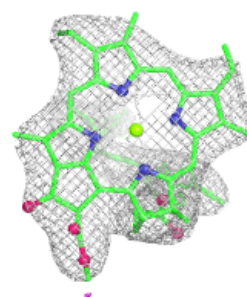
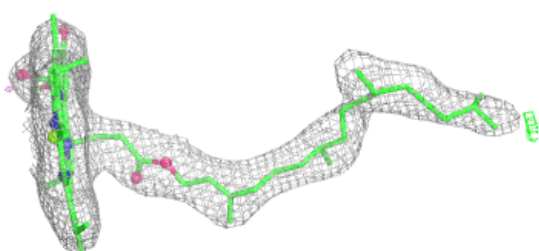
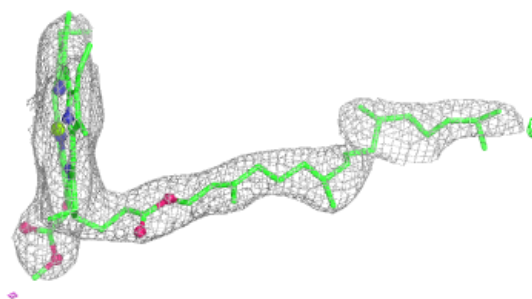
**Electron density around CLA b 605:**

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

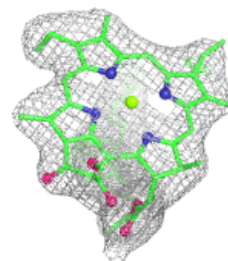
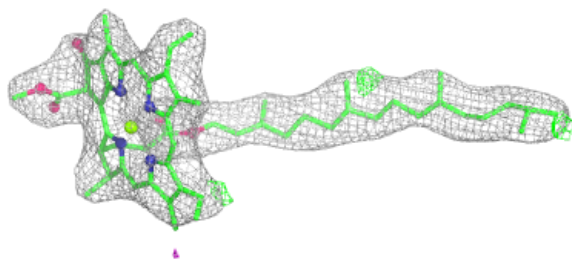
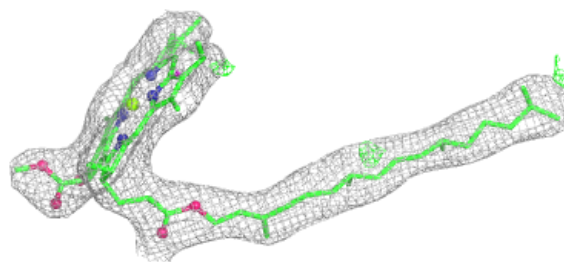


Electron density around CLA b 606:

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

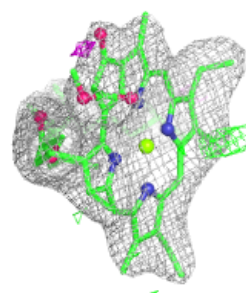
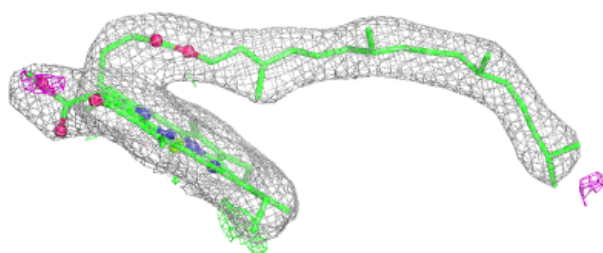
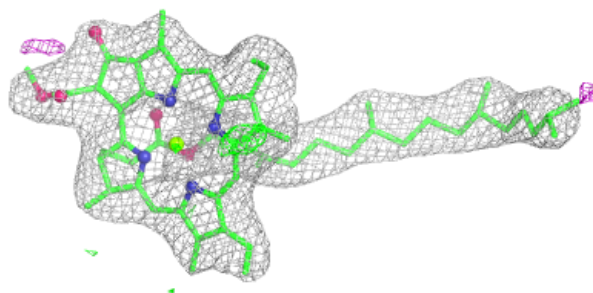
**Electron density around CLA b 607:**

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

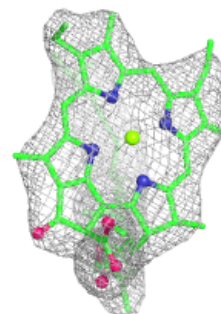
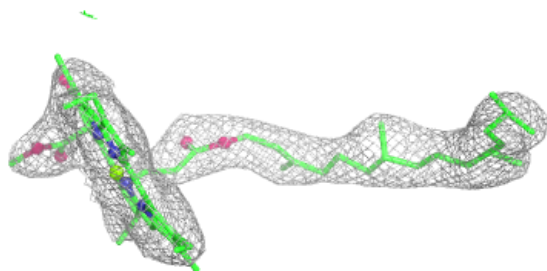
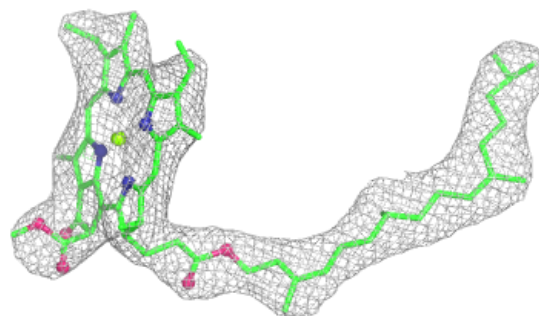


Electron density around CLA b 608:

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

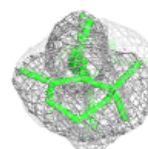
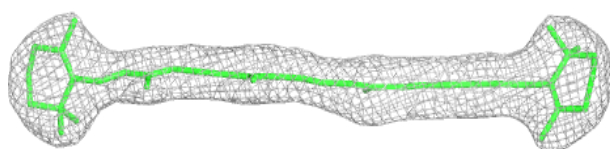
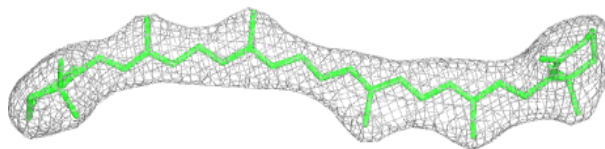
**Electron density around CLA b 609:**

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

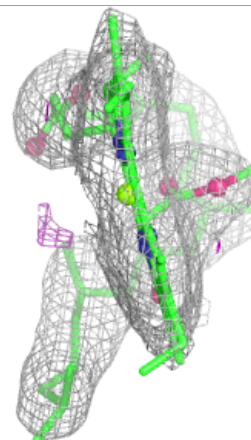
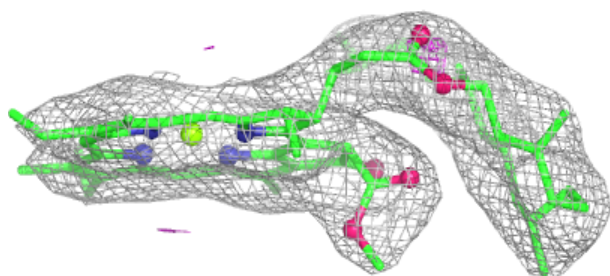
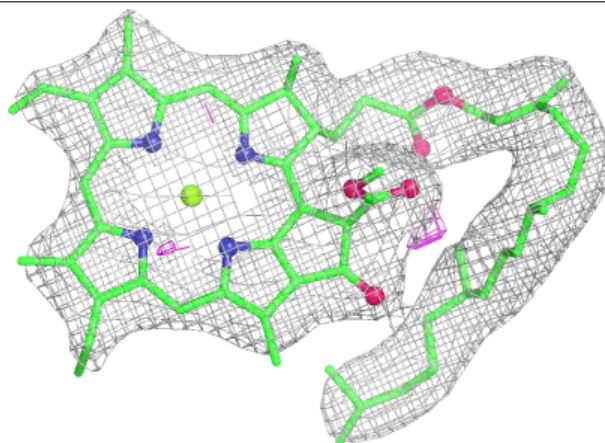


Electron density around BCR a 410:

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

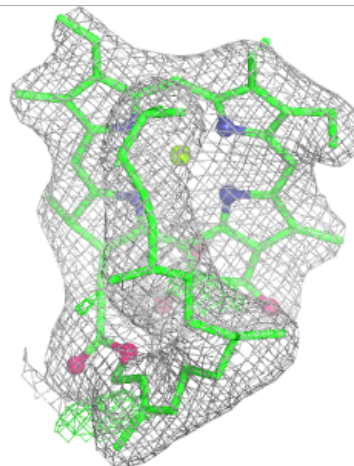
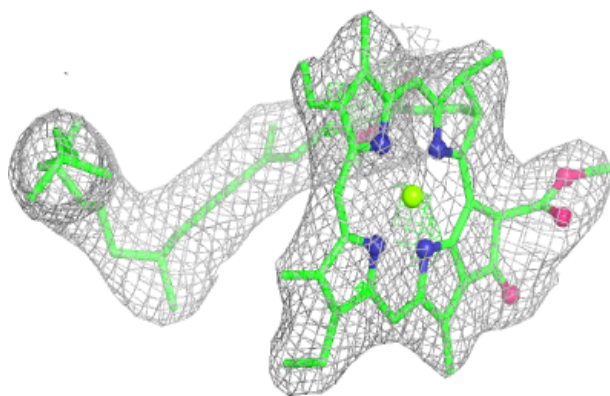
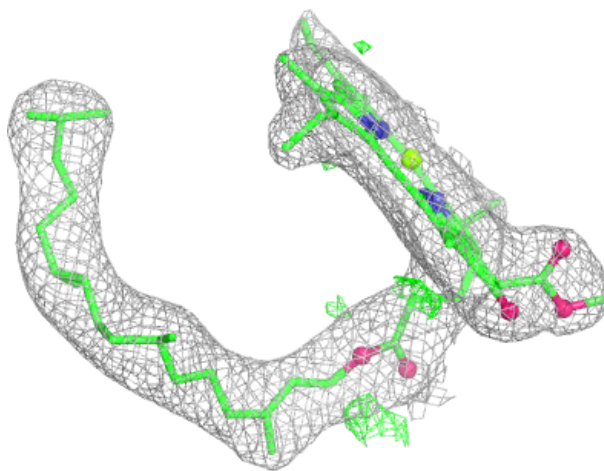
**Electron density around CLA b 610:**

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



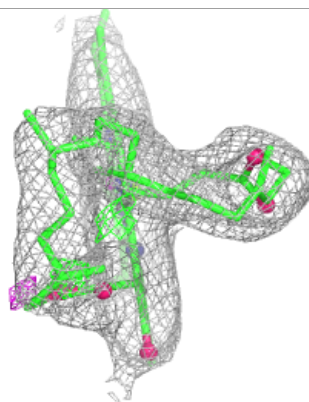
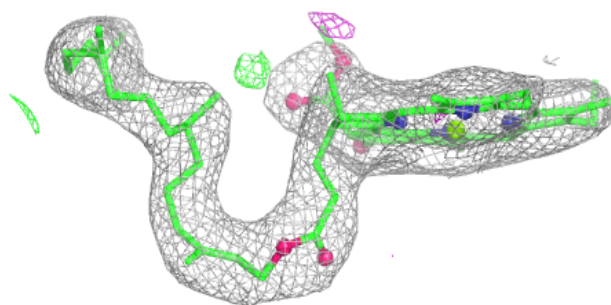
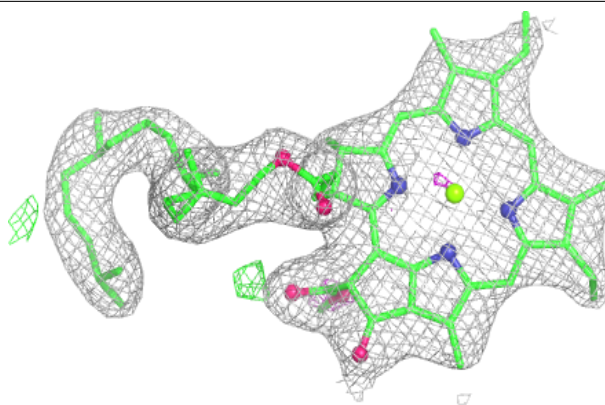
Electron density around CLA b 611:

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



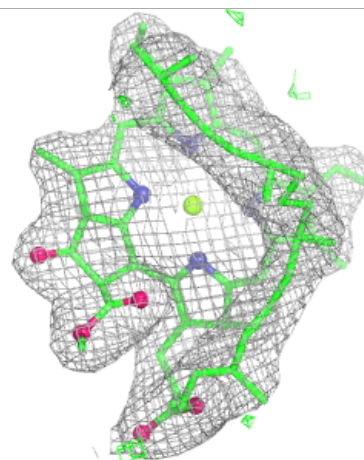
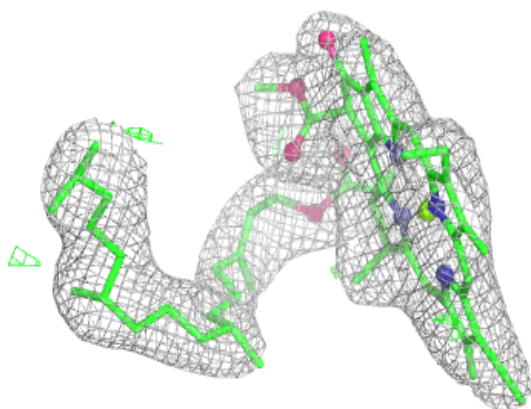
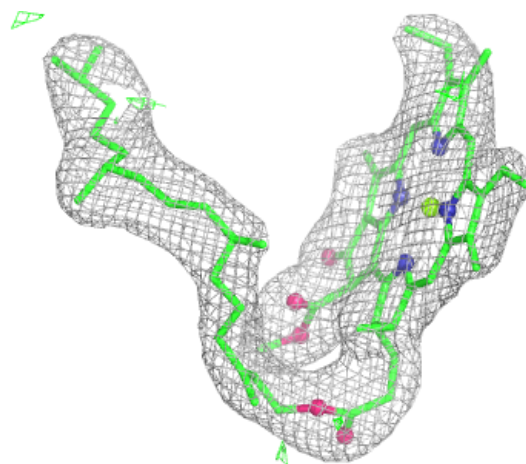
Electron density around CLA b 612:

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



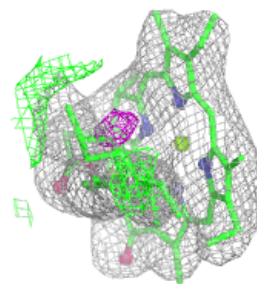
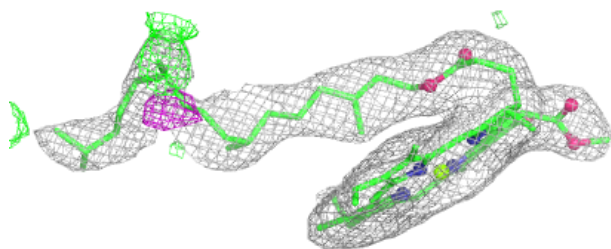
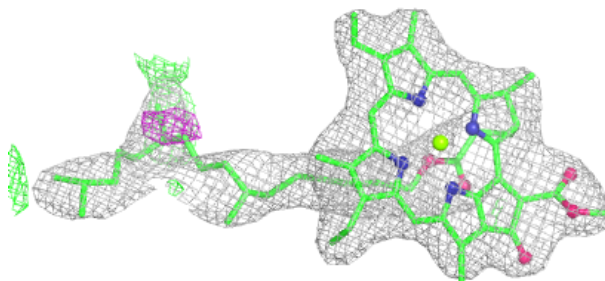
Electron density around CLA b 613:

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



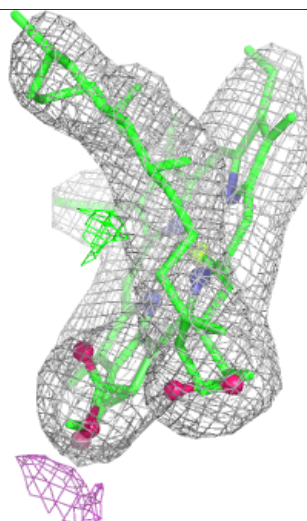
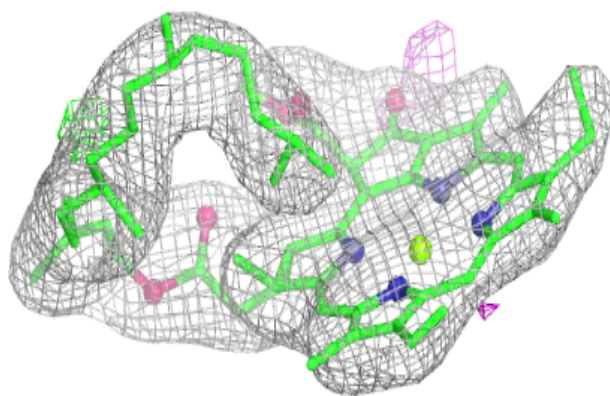
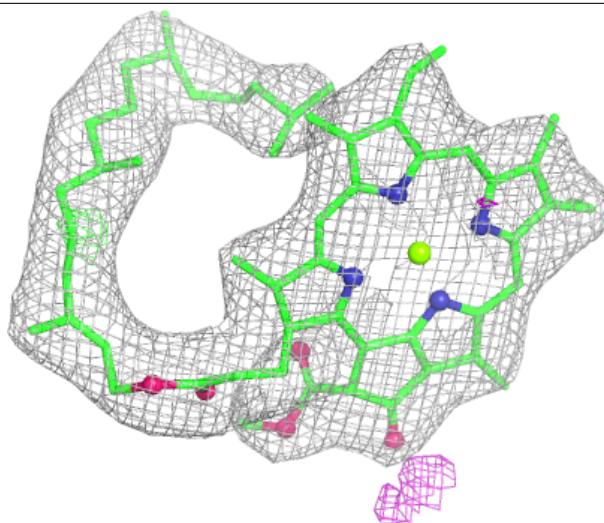
Electron density around CLA b 614:

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



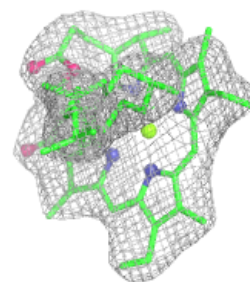
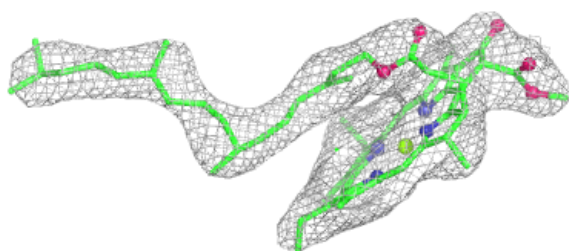
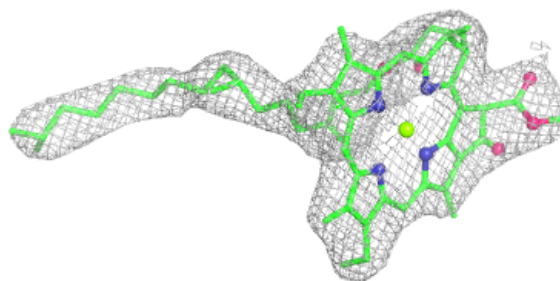
Electron density around CLA b 615:

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

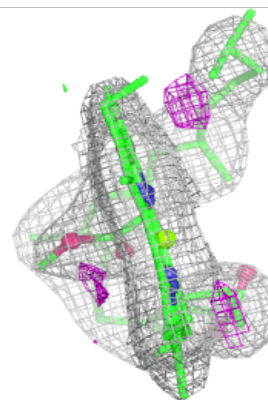
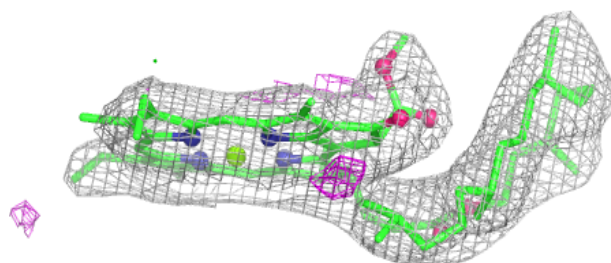
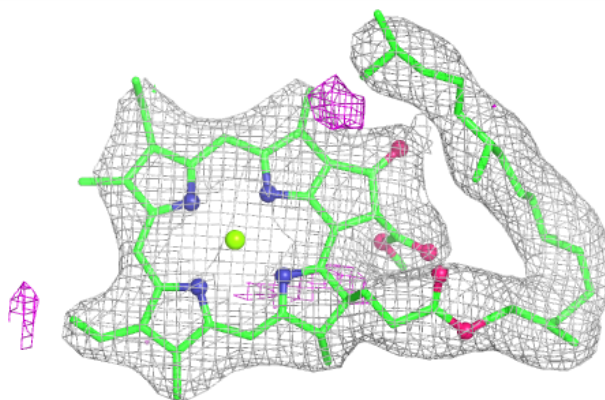


Electron density around CLA C 506:

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

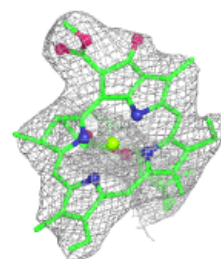
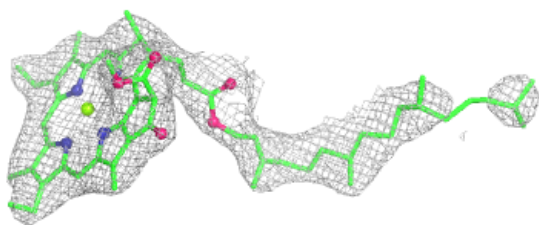
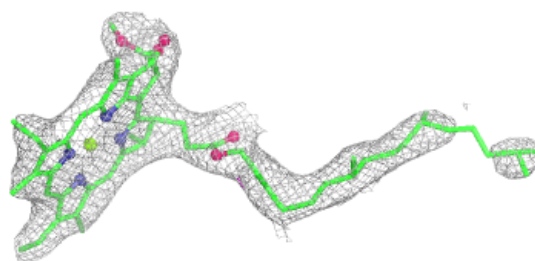
**Electron density around CLA B 611:**

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

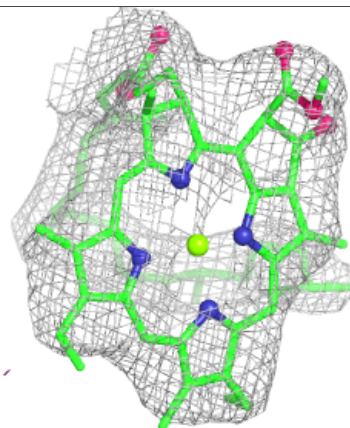
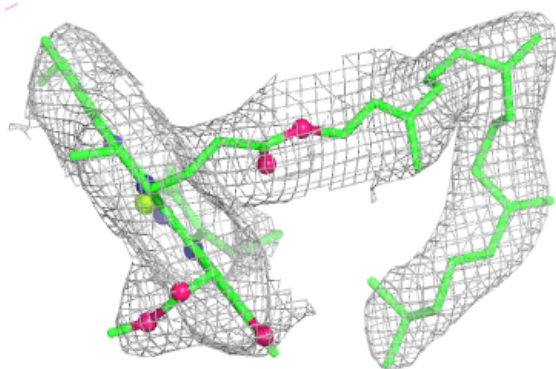
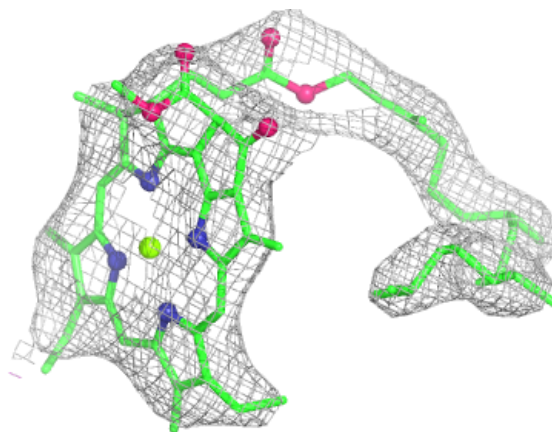


Electron density around CLA c 502:

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

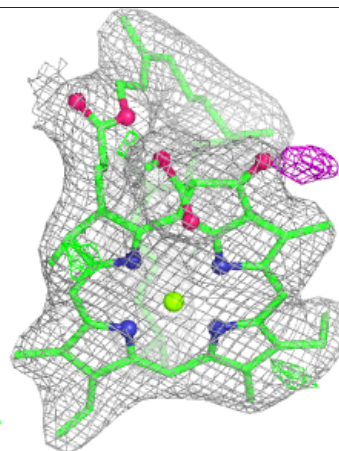
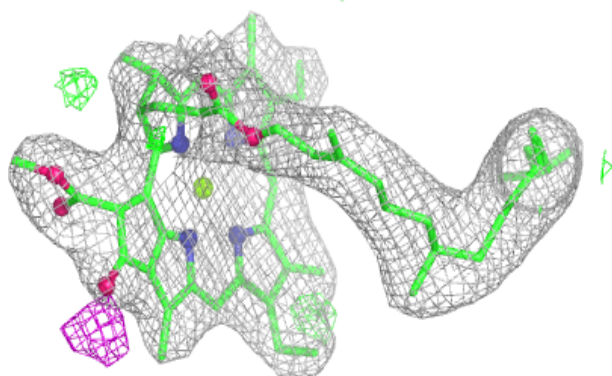
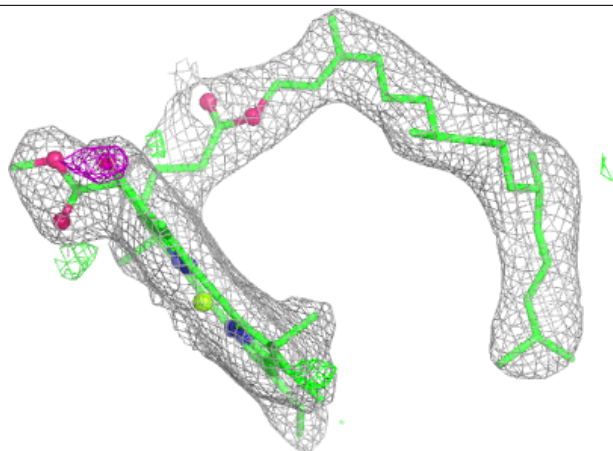
**Electron density around CLA c 503:**

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



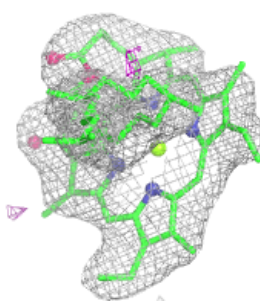
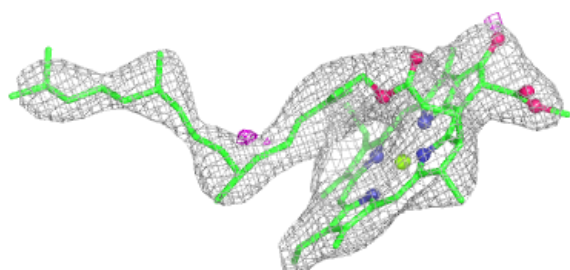
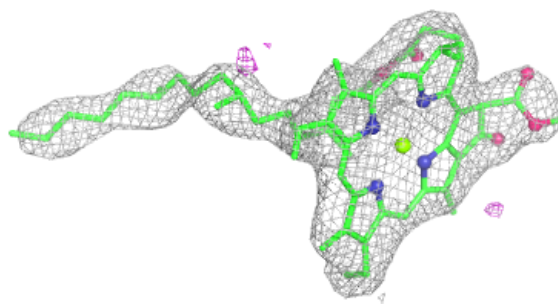
Electron density around CLA B 612:

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

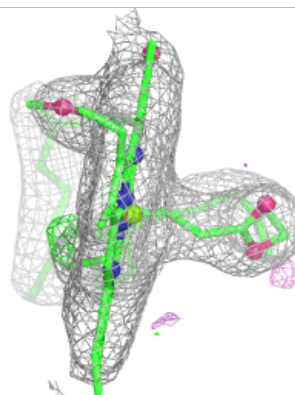
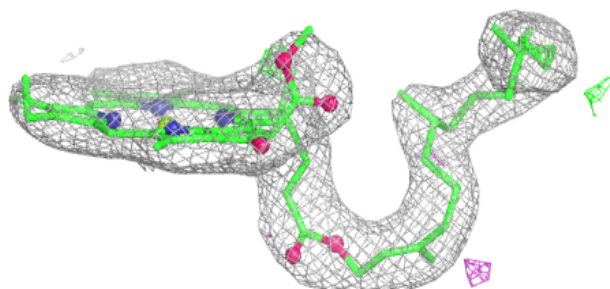
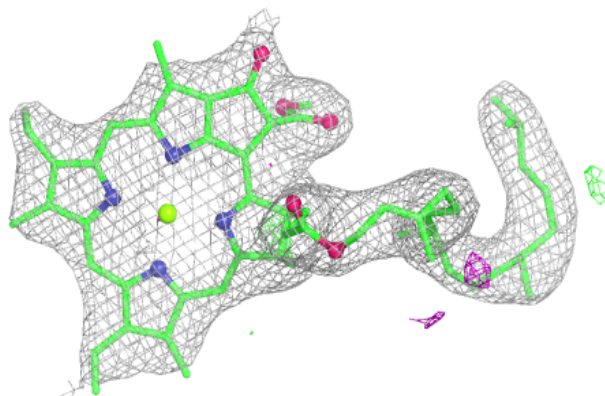


Electron density around CLA c 505:

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

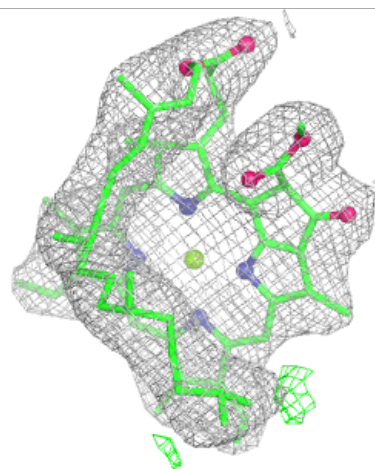
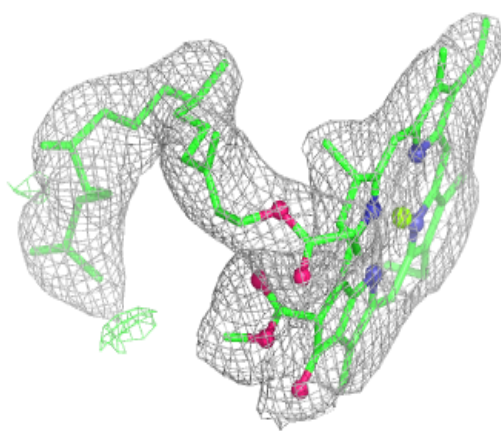
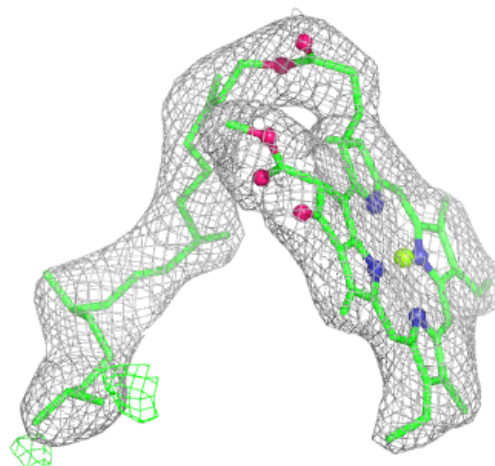
**Electron density around CLA B 613:**

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



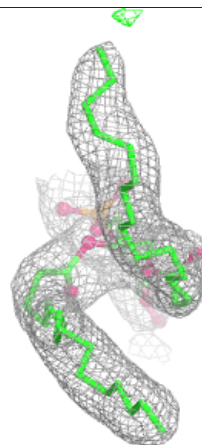
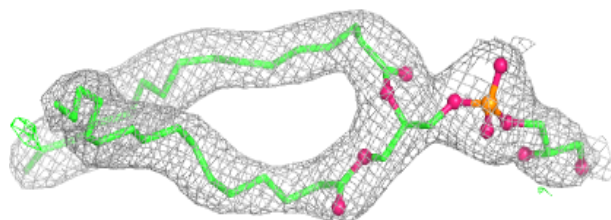
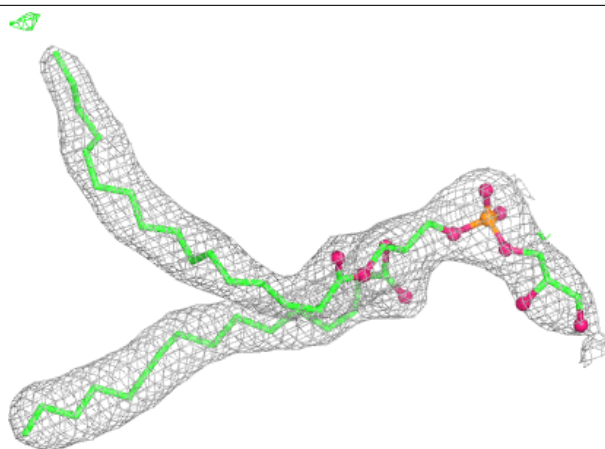
Electron density around CLA B 614:

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



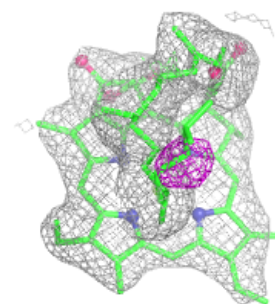
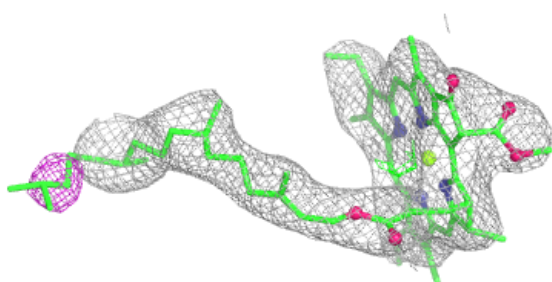
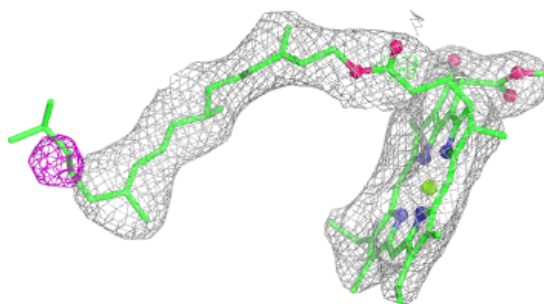
Electron density around LHG D 408:

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

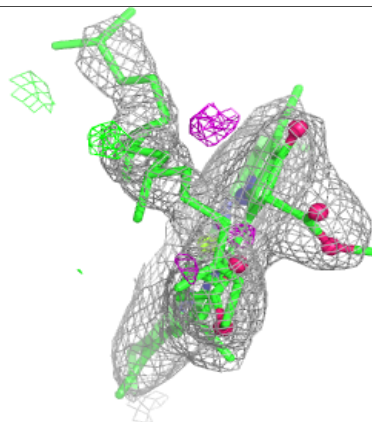
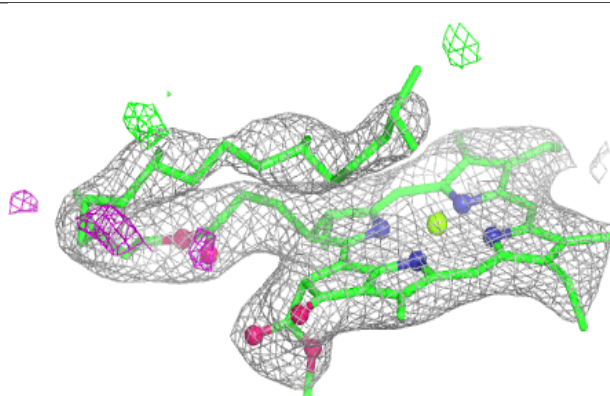
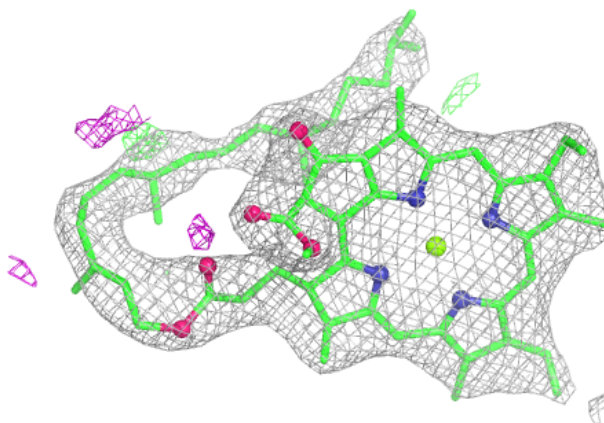


Electron density around CLA c 508:

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

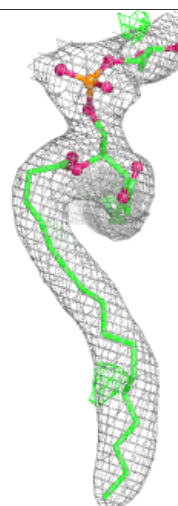
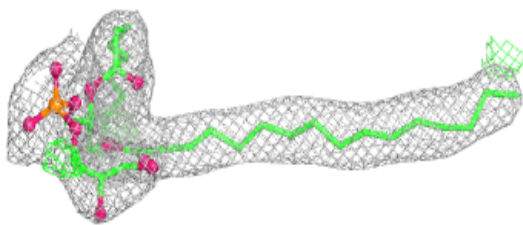
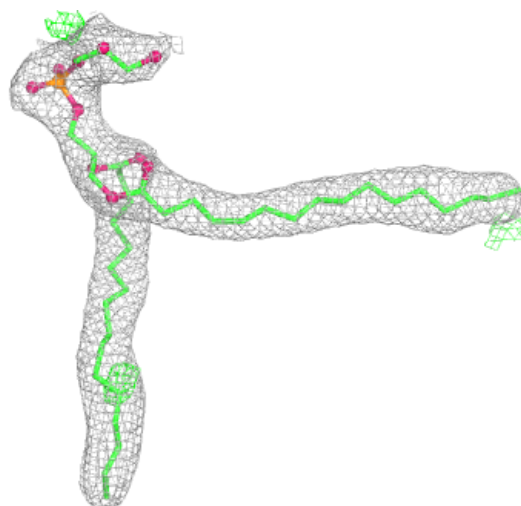
**Electron density around CLA c 509:**

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



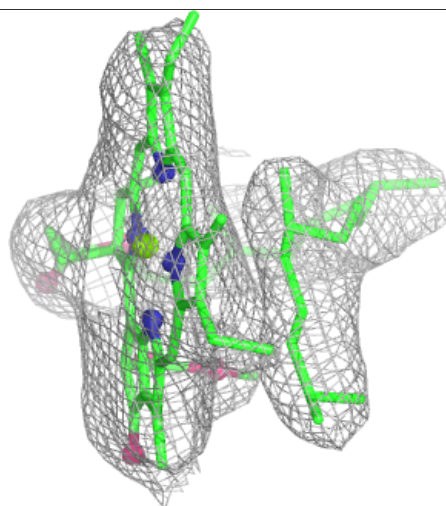
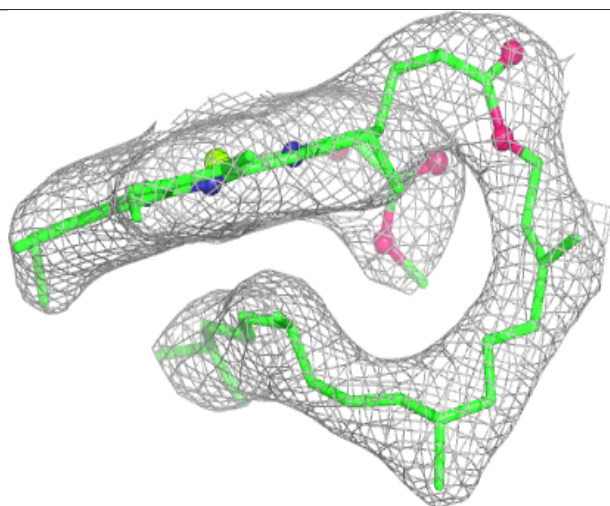
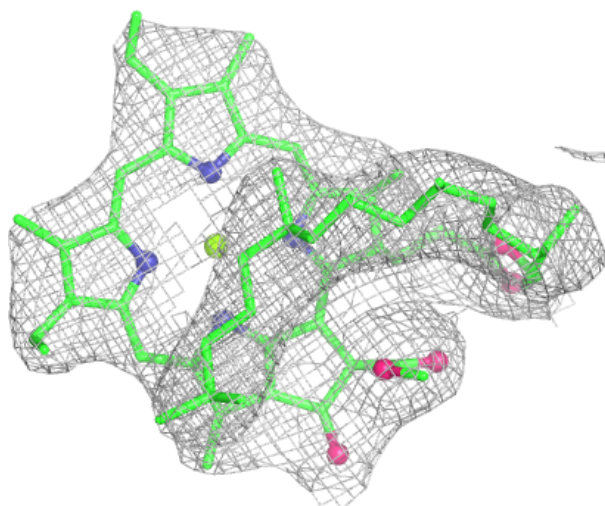
Electron density around LHG L 101:

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



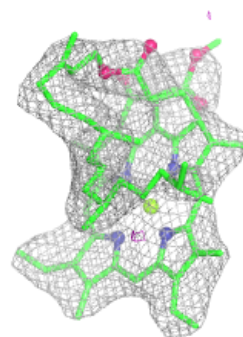
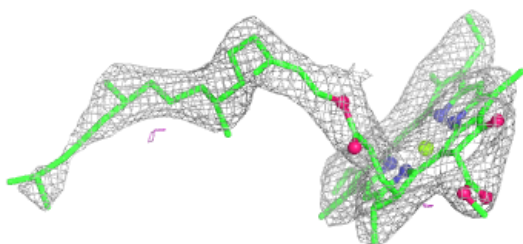
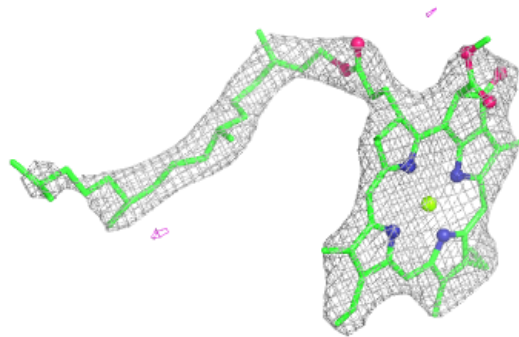
Electron density around CLA c 510:

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

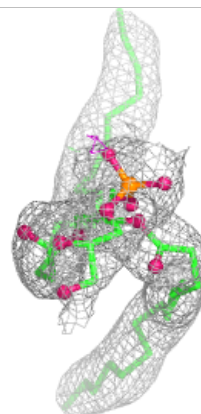
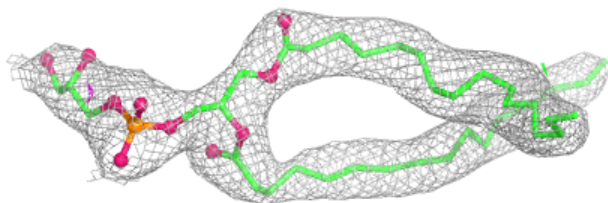
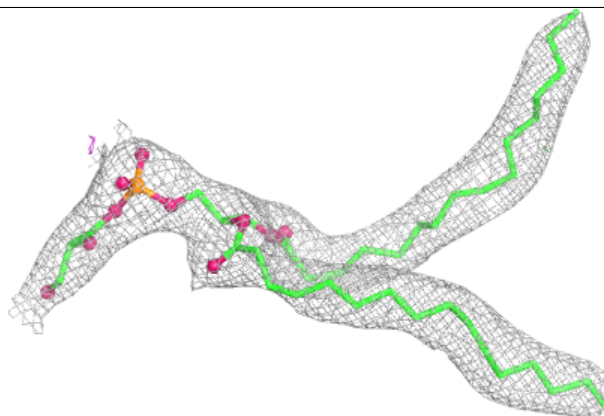


Electron density around CLA C 512:

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

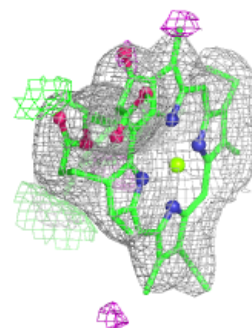
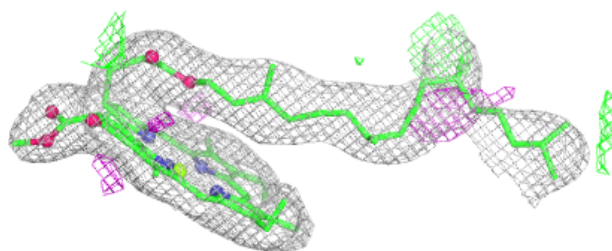
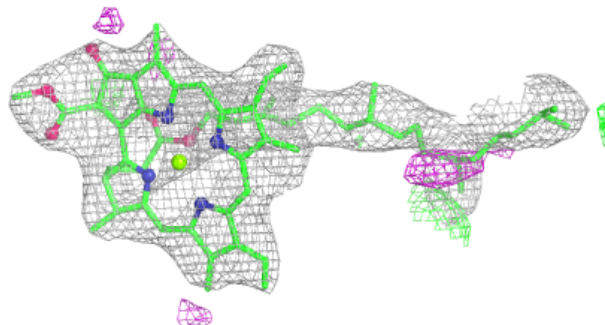
**Electron density around LHG d 407:**

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

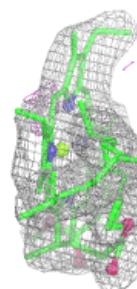
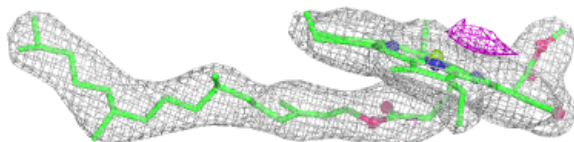
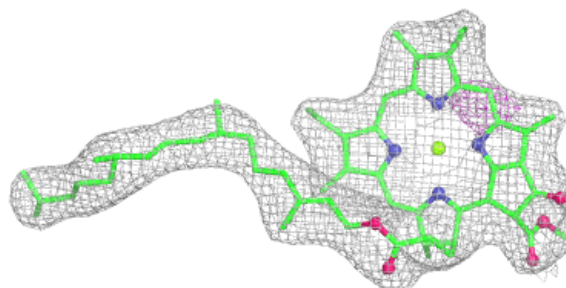


Electron density around CLA B 615:

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

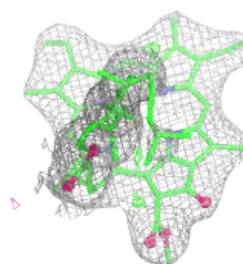
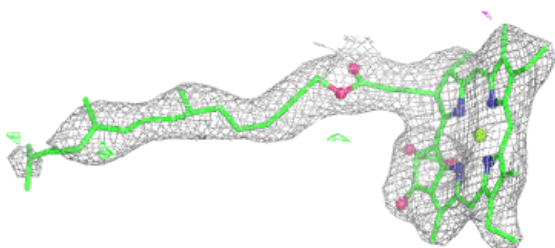
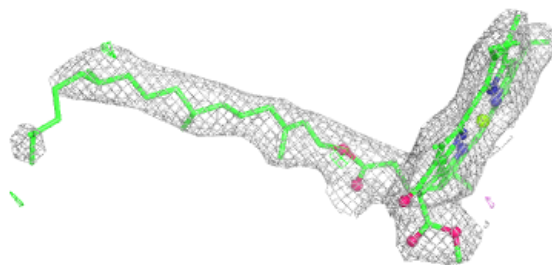
**Electron density around CLA B 604:**

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



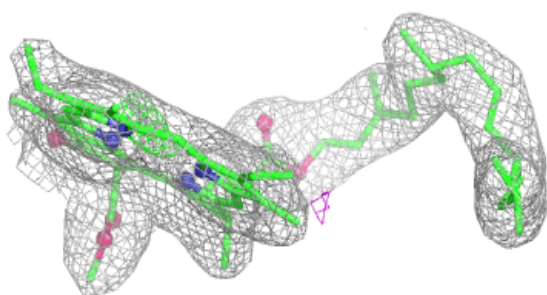
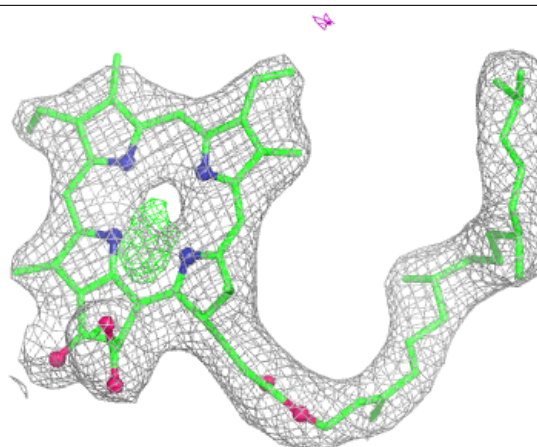
Electron density around CLA B 605:

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



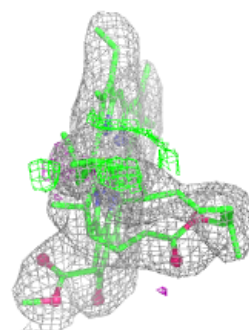
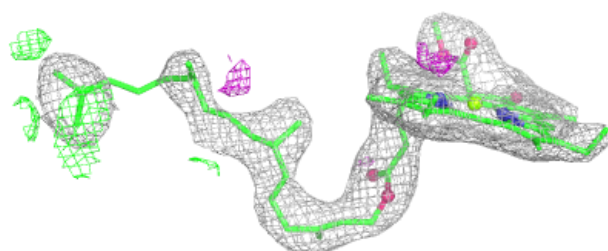
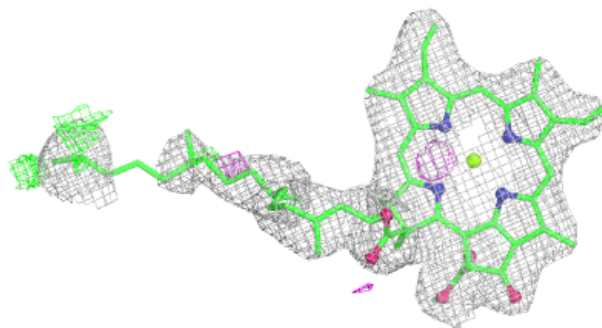
Electron density around PHO D 402:

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

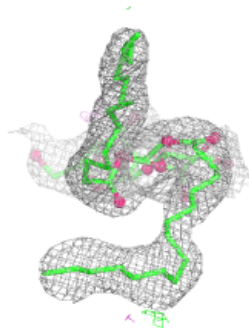
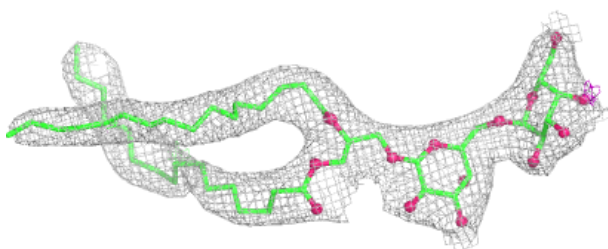
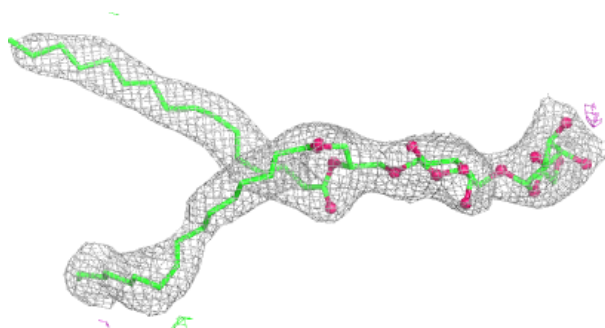


Electron density around CLA a 406:

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

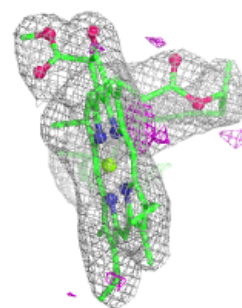
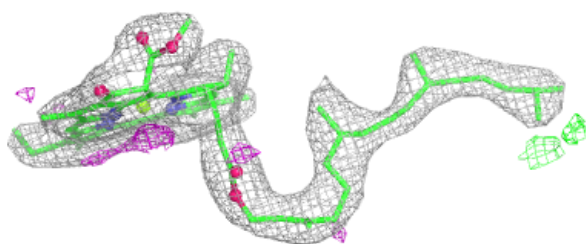
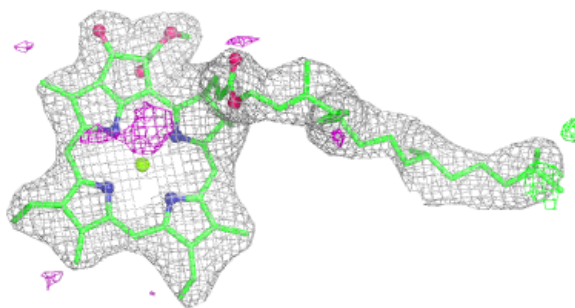
**Electron density around DGD C 517:**

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

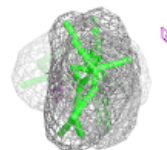
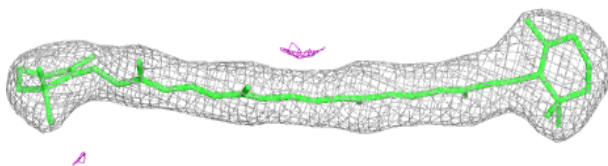
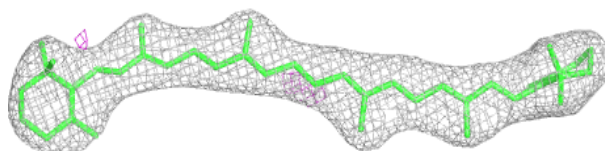


Electron density around CLA A 405:

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

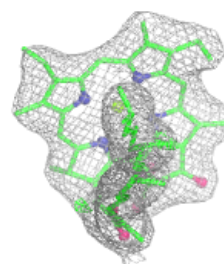
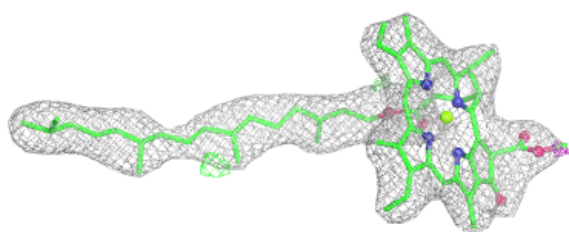
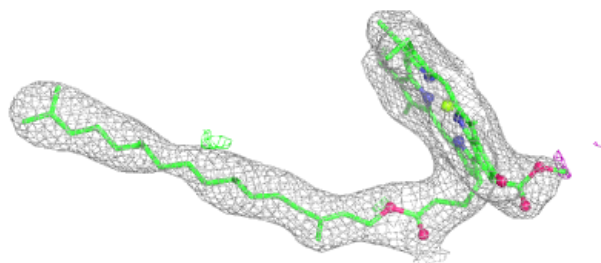
**Electron density around BCR B 618:**

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

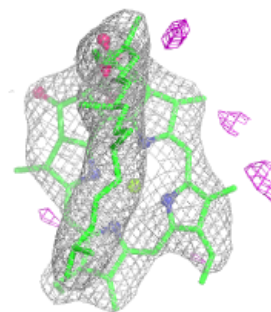
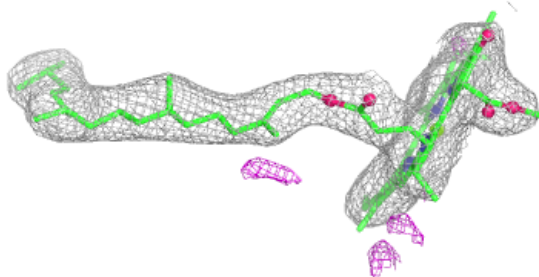
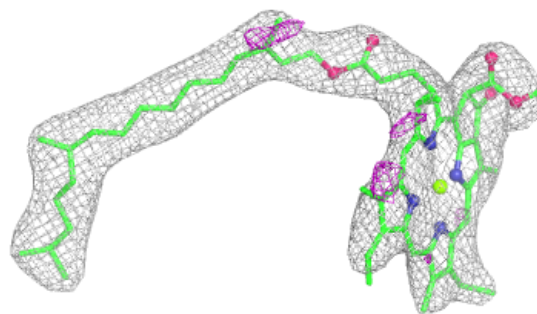


Electron density around CLA B 608:

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

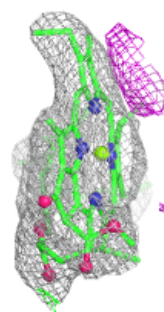
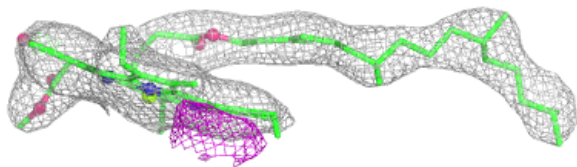
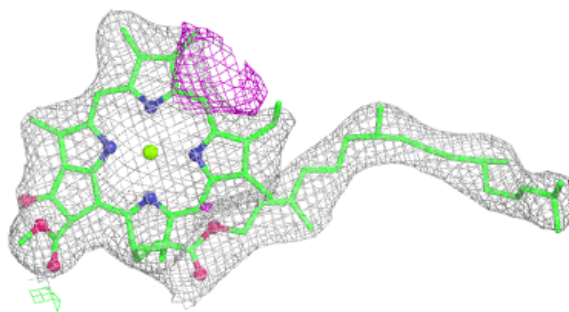
**Electron density around CLA B 610:**

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

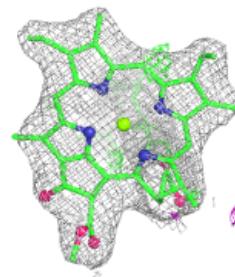
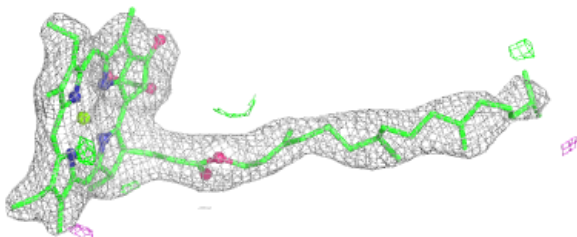
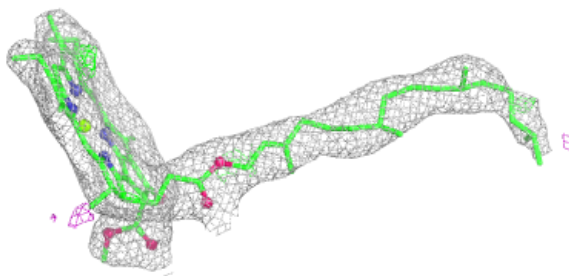


Electron density around CLA b 603:

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

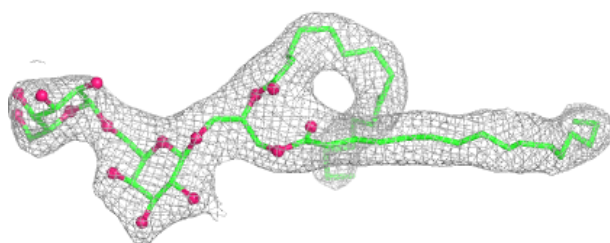
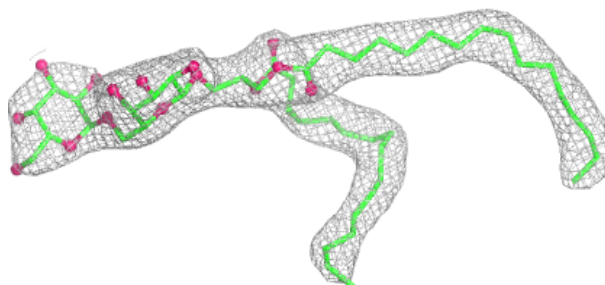
**Electron density around CLA b 604:**

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

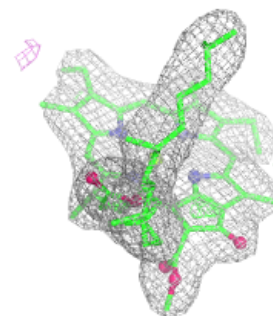
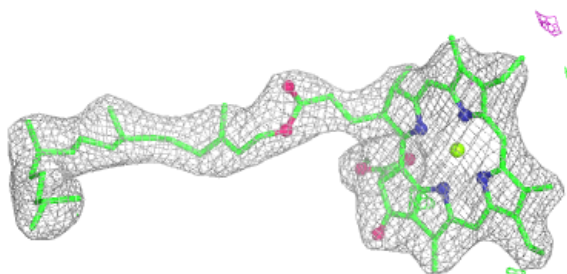
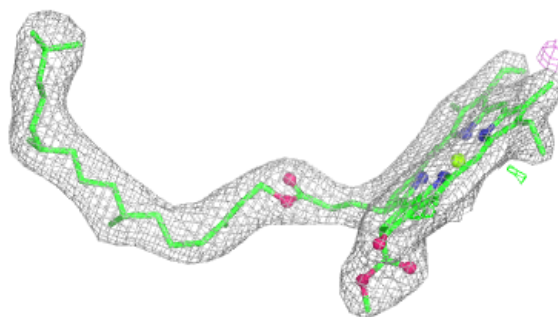


Electron density around DGD h 103:

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

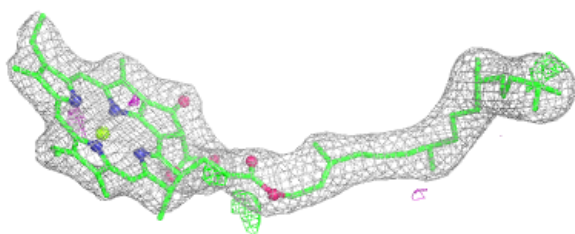
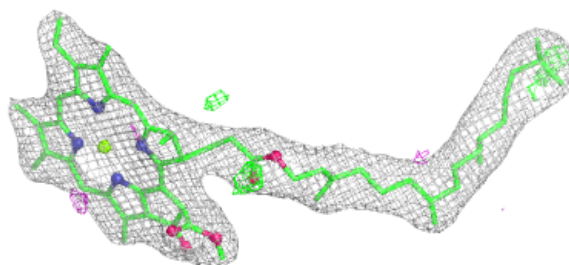
**Electron density around CLA D 404:**

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

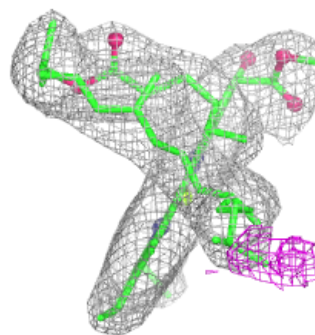
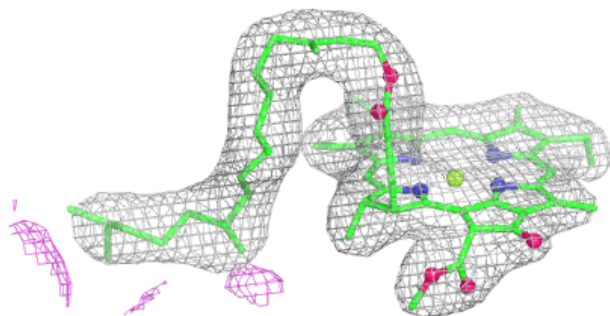
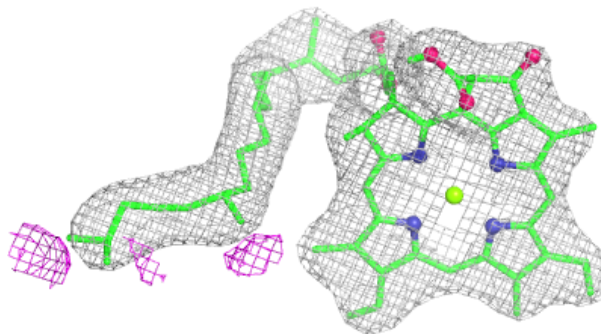


Electron density around CLA a 404:

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

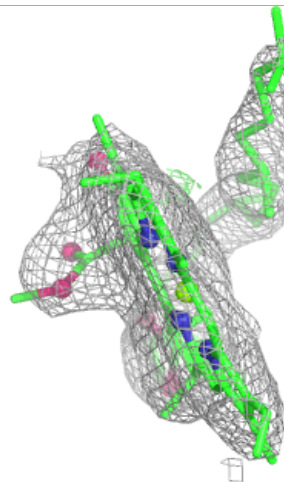
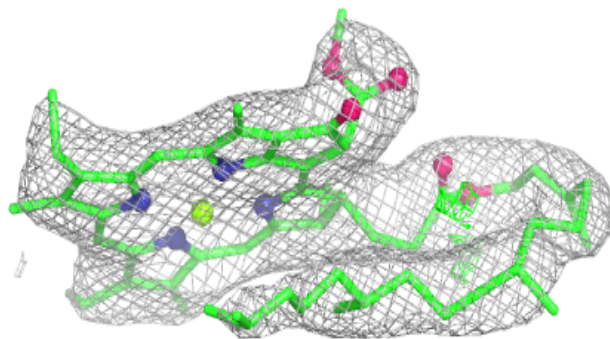
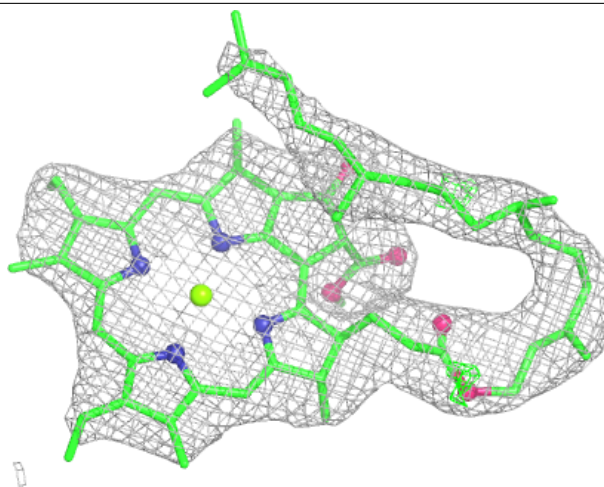
**Electron density around CLA a 405:**

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



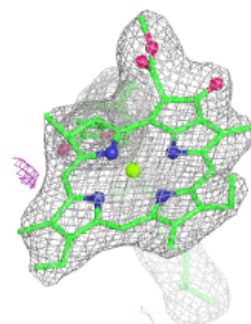
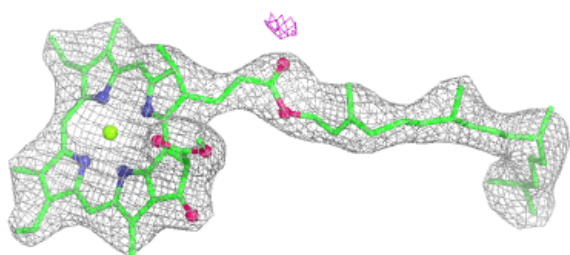
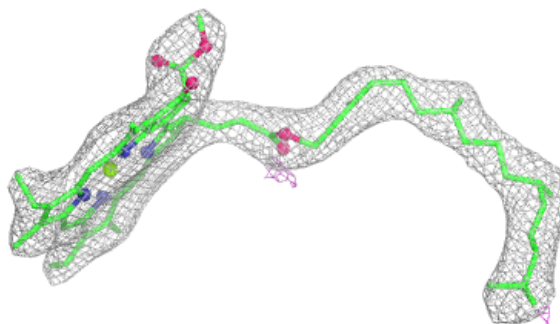
Electron density around CLA C 510:

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



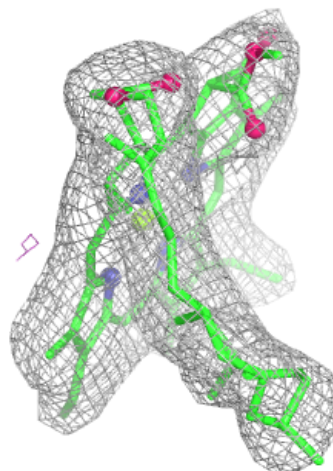
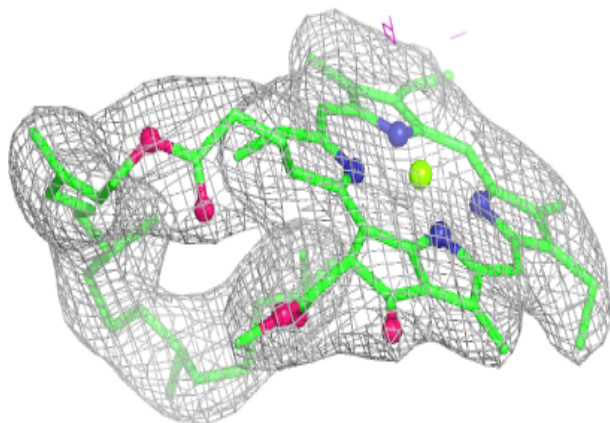
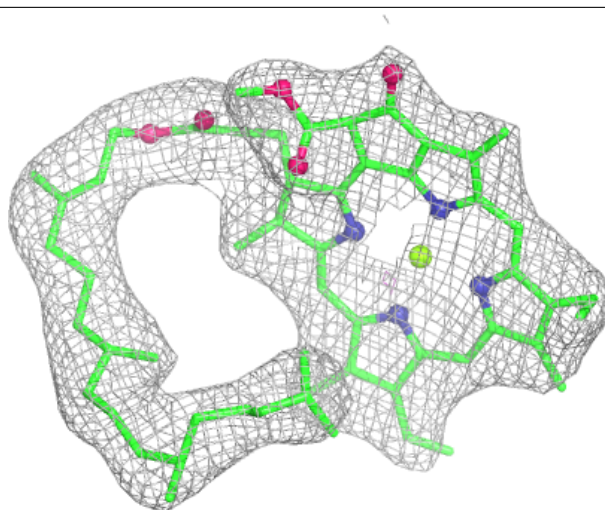
Electron density around CLA d 402:

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



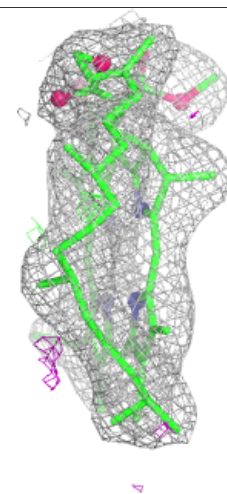
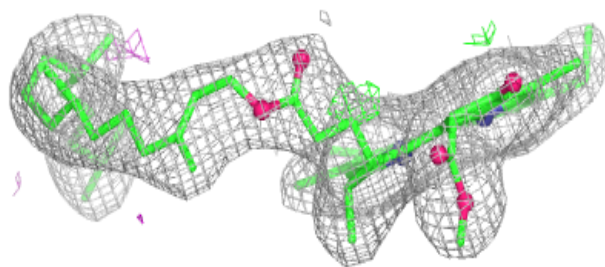
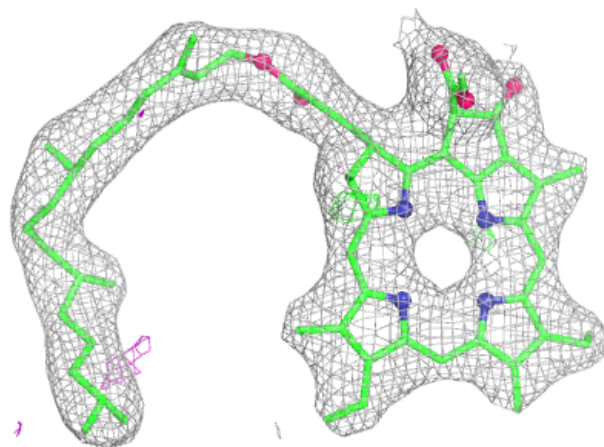
Electron density around CLA B 616:

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



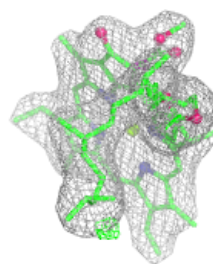
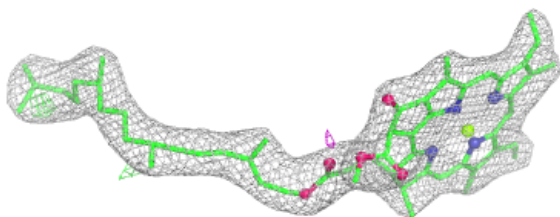
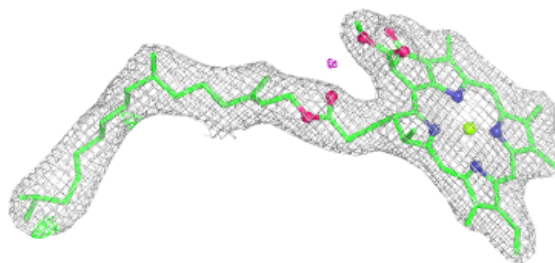
Electron density around PHO A 406:

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



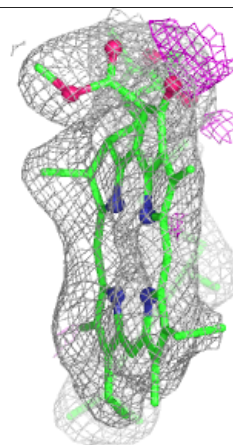
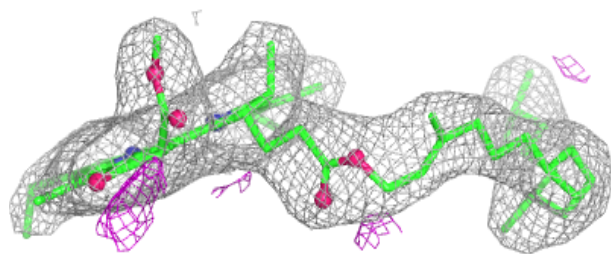
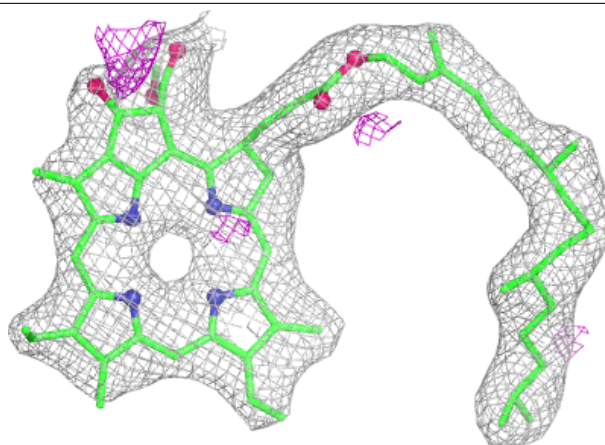
Electron density around CLA A 404:

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



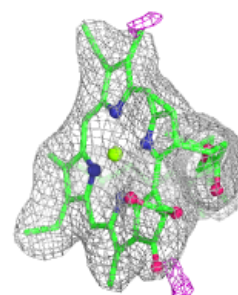
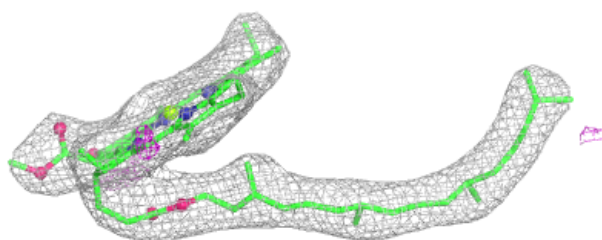
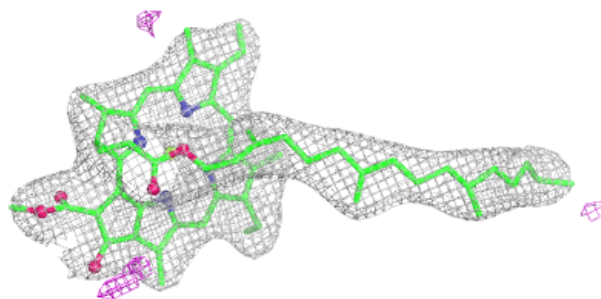
Electron density around PHO a 407:

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

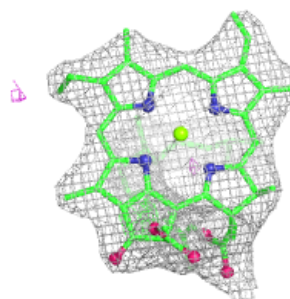
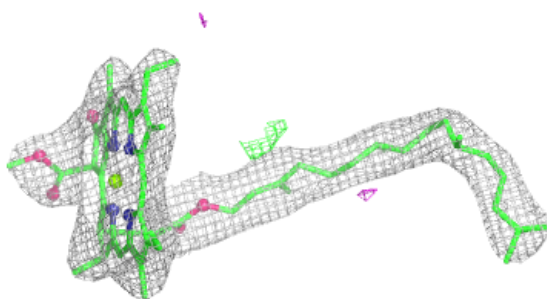
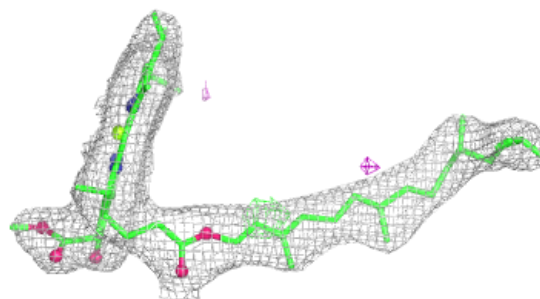


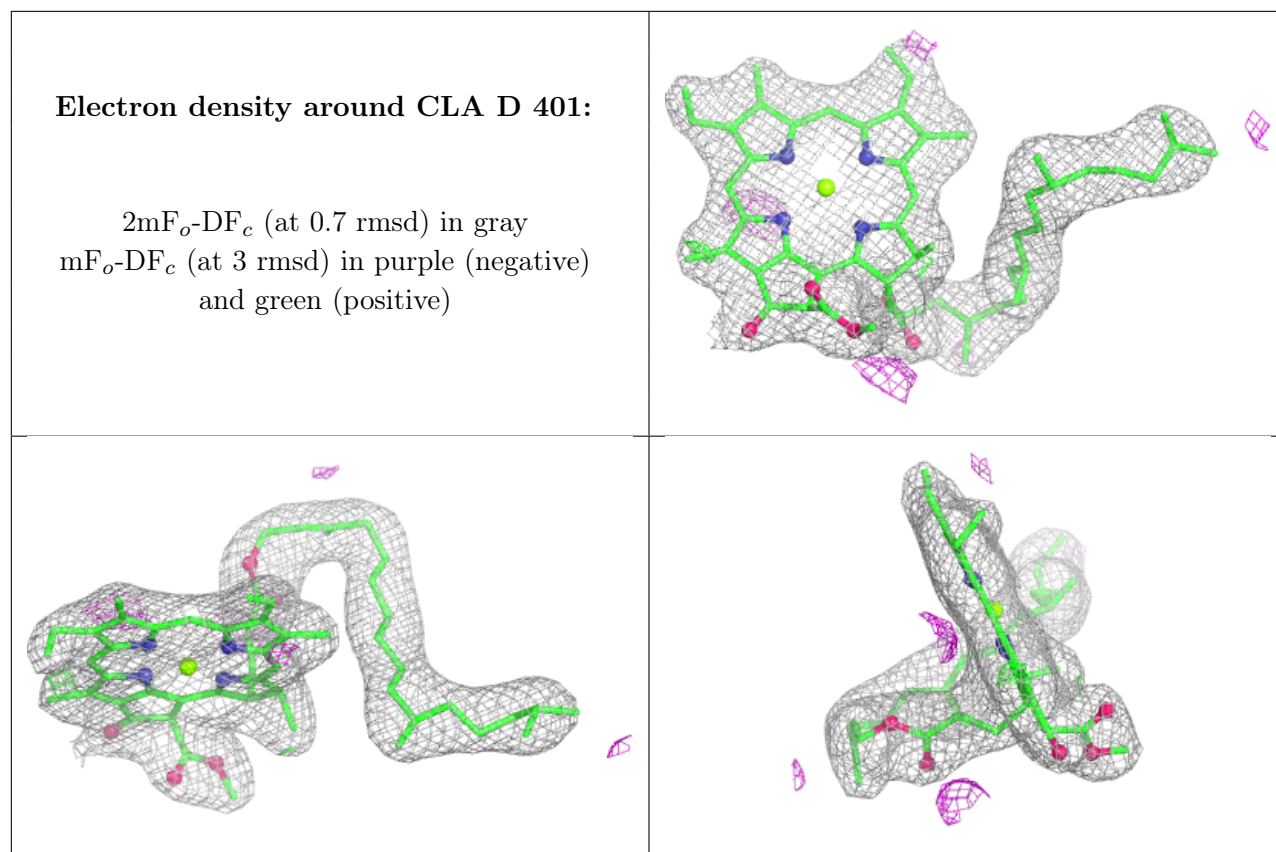
Electron density around CLA B 609:

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

**Electron density around CLA B 606:**

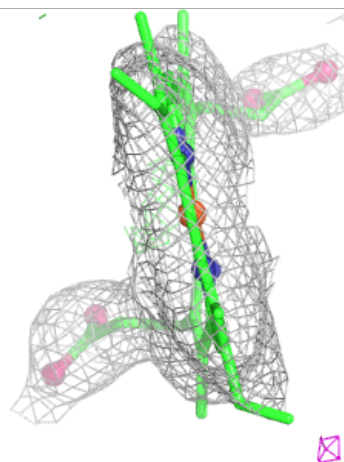
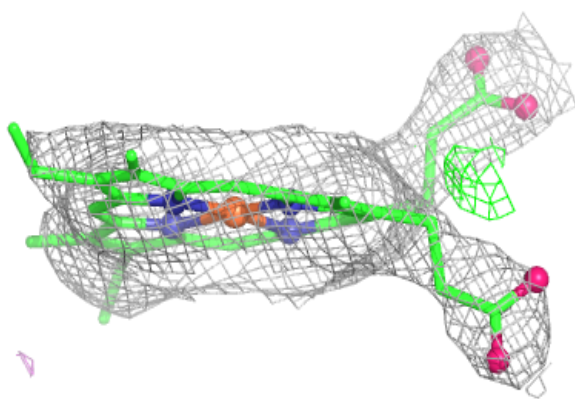
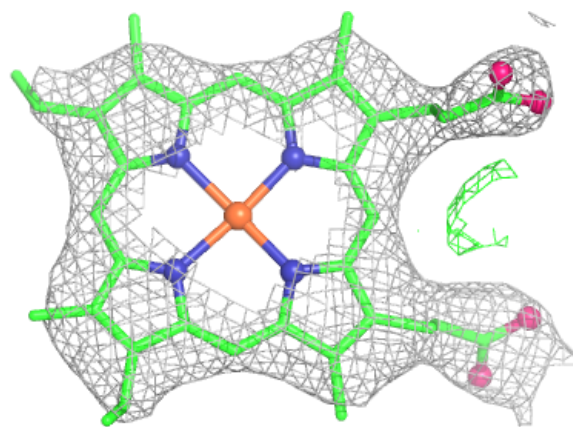
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





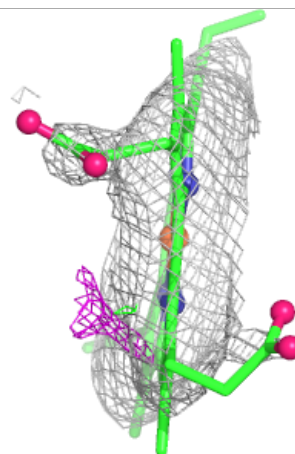
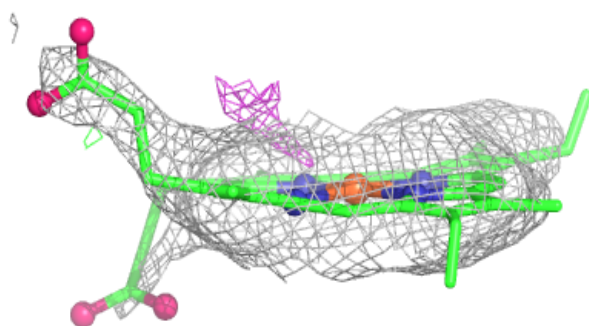
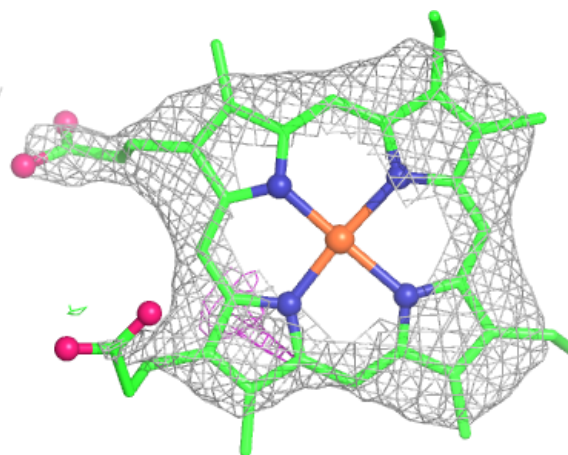
Electron density around HEM E 103:

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



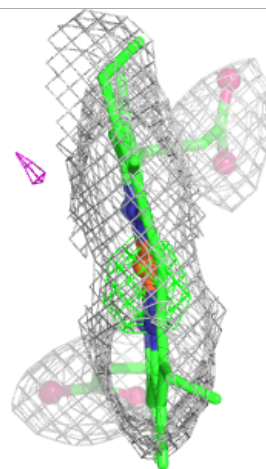
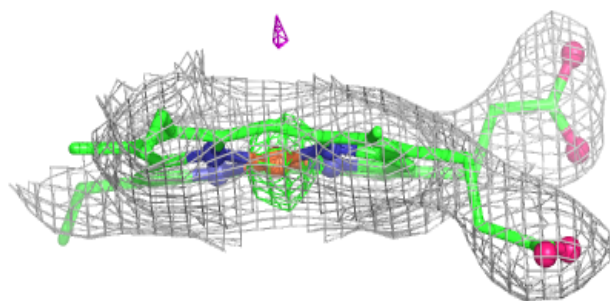
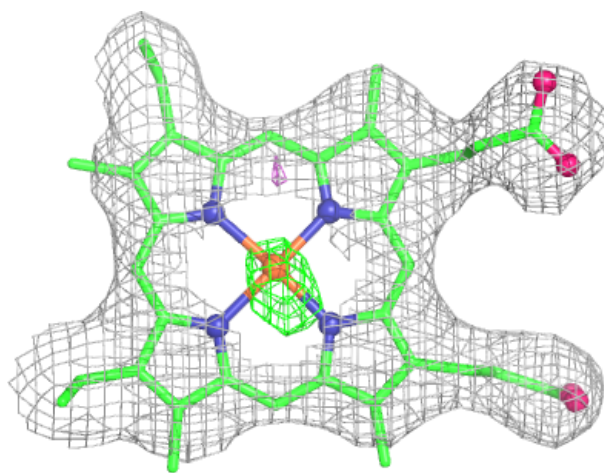
Electron density around HEM e 103:

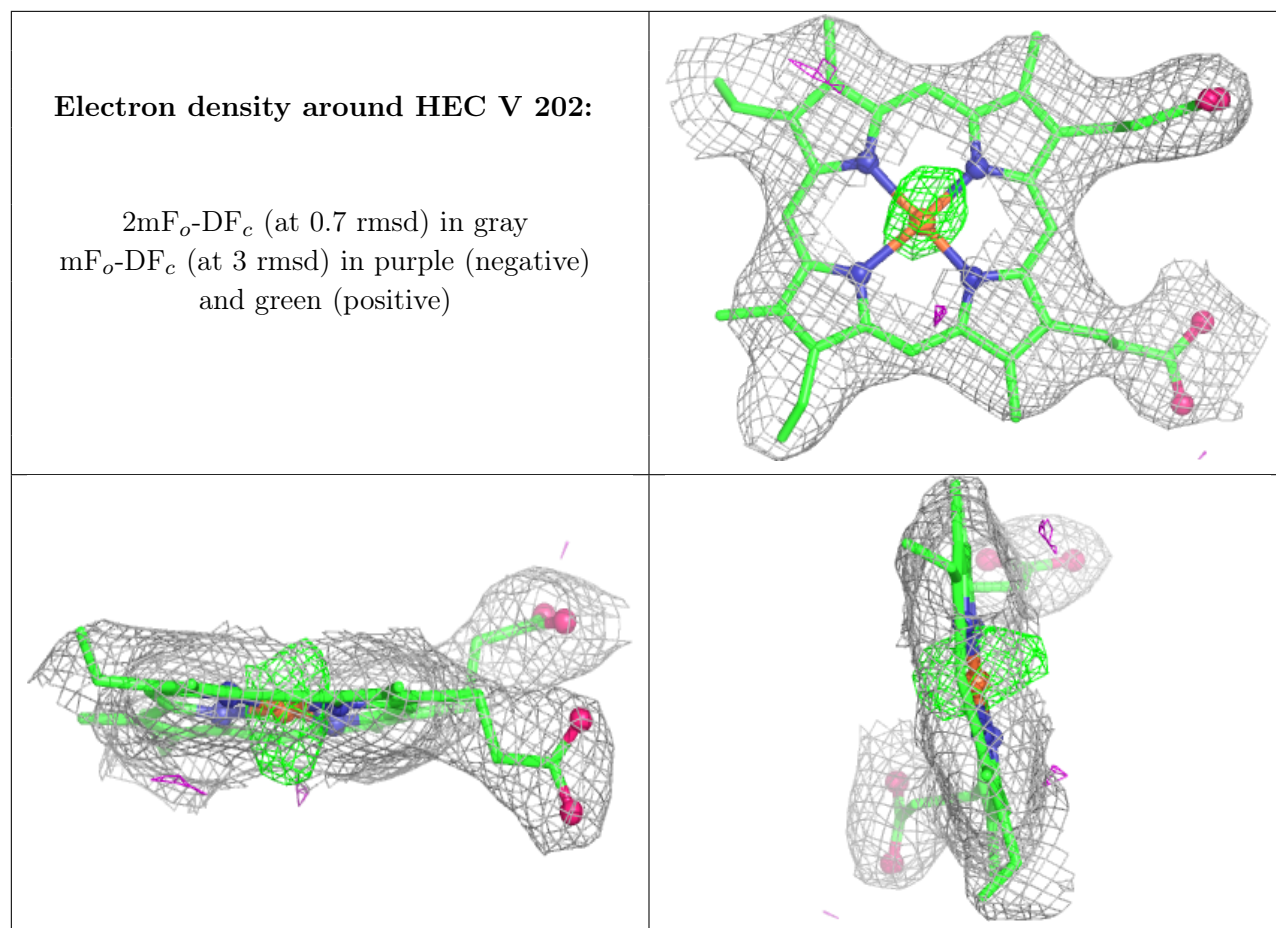
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.