



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 13, 2026 – 06:56 PM JST

PDB ID : 8IRH / pdb_00008irh
Title : XFEL structure of cyanobacterial photosystem II following two flashes (2F)
with a 200-microsecond delay
Authors : Li, H.; Suga, M.; Shen, J.R.
Deposited on : 2023-03-17
Resolution : 2.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

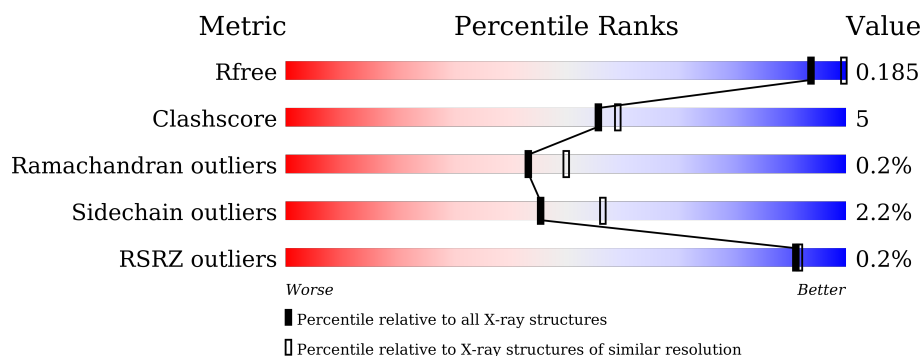
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	344	90% 7% .
1	a	344	87% 10% .
2	B	505	93% 7%
2	b	505	91% 8% .
3	C	455	91% 8% .
3	c	455	93% 6%

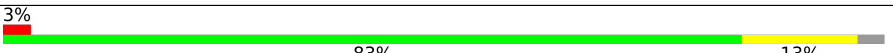
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Mol	Chain	Length	Quality of chain
4	D	342	
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V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

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Mol	Chain	Length	Quality of chain
16	v	137	 91% 9%
17	X	40	 85% 10% 5%
17	x	40	 82% 12% 5%
18	Y	30	 3% 83% 13% .
18	y	30	 73% 23% .
19	Z	62	 85% 13% .
19	z	62	 84% 15% .
20	R	34	 3% 74% 26%

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
28	GOL	a	419	-	-	X	-
41	HEC	V	201	X	-	-	-
41	HEC	v	201	X	-	-	-

2 Entry composition

There are 42 unique types of molecules in this entry. The entry contains 62605 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	222	0
			4338	2836	717	760	25			
1	a	334	Total	C	N	O	S	0	221	0
			4330	2830	716	759	25			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	20	0
			4146	2721	692	720	13			
2	b	504	Total	C	N	O	S	0	19	0
			4134	2718	687	716	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	97	0
			4260	2788	713	741	18			
3	c	455	Total	C	N	O	S	0	100	0
			4308	2821	719	750	18			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	expression tag	UNP D0VWR7
C	20	SER	-	expression tag	UNP D0VWR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	expression tag	UNP D0VWR7
C	22	PHE	-	expression tag	UNP D0VWR7
c	19	ASN	-	expression tag	UNP D0VWR7
c	20	SER	-	expression tag	UNP D0VWR7
c	21	ILE	-	expression tag	UNP D0VWR7
c	22	PHE	-	expression tag	UNP D0VWR7

- 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	114	0
			3620	2387	596	622	15			
4	d	341	Total	C	N	O	S	0	116	0
			3628	2391	599	623	15			

- 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	2	0
			670	439	110	121				

- 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	1	0
			261	179	43	38	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	64	Total	C	N	O	S	0	1	0
			517	345	85	85	2			

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	36	Total	C	N	O	0	2	0
			311	207	49	55			
11	l	36	Total	C	N	O	0	2	0
			311	207	49	55			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			268	179	39	49	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	2	0
			286	190	43	52	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	conflict	UNP P12312
m	8	LEU	PHE	conflict	UNP P12312

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	10	0
			1958	1221	335	398	4			
13	o	243	Total	C	N	O	S	0	8	0
			1933	1207	330	392	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	6	0
			311	213	48	48	2			
14	t	30	Total	C	N	O	S	0	5	0
			302	208	47	45	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	4	0
			800	508	133	159				
15	u	97	Total	C	N	O		0	4	0
			807	513	134	160				

- 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	6	0
			1120	711	185	220	4			
16	v	137	Total	C	N	O	S	0	6	0
			1117	712	185	216	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	1	0
			289	194	46	49			
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			

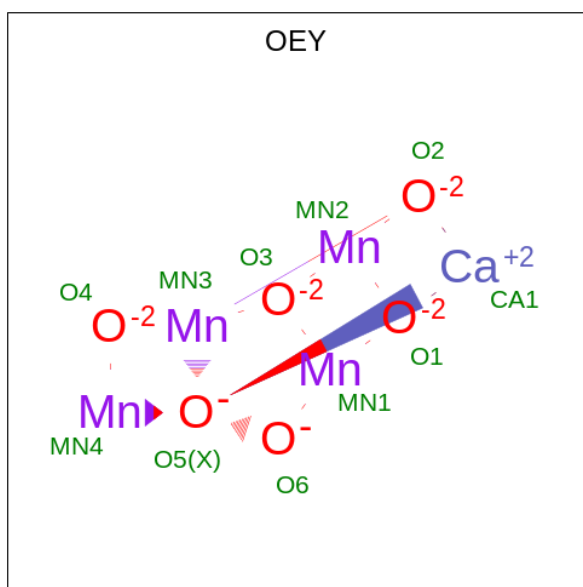
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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 CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: CaMn_4O_6).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	Ca	Mn	O	0	1
			11	1	4	6		
21	a	1	Total	Ca	Mn	O	0	1
			11	1	4	6		

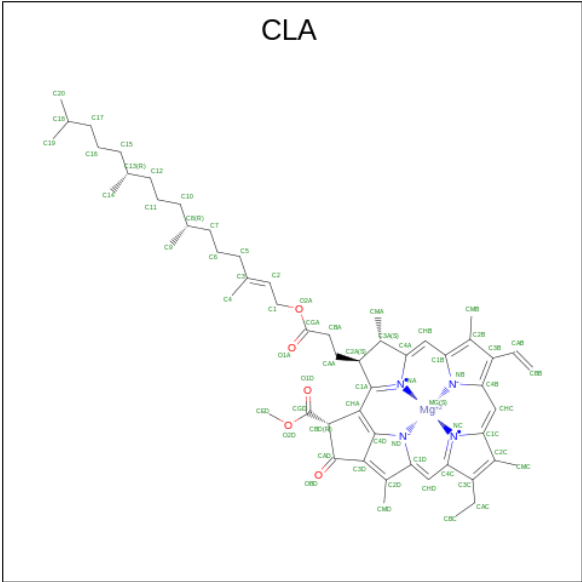
- Molecule 22 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 23 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	2	Total	Cl	0	2
			4	4		
23	a	2	Total	Cl	0	2
			4	4		

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	A	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
24	A	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
24	A	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
24	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	D	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
24	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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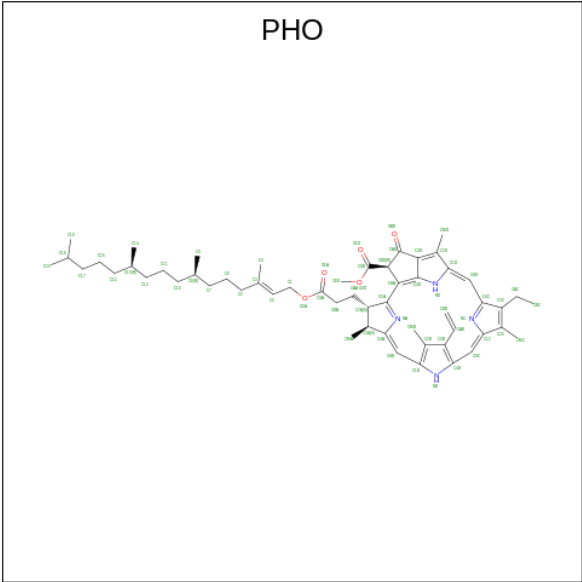
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
24	a	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
24	a	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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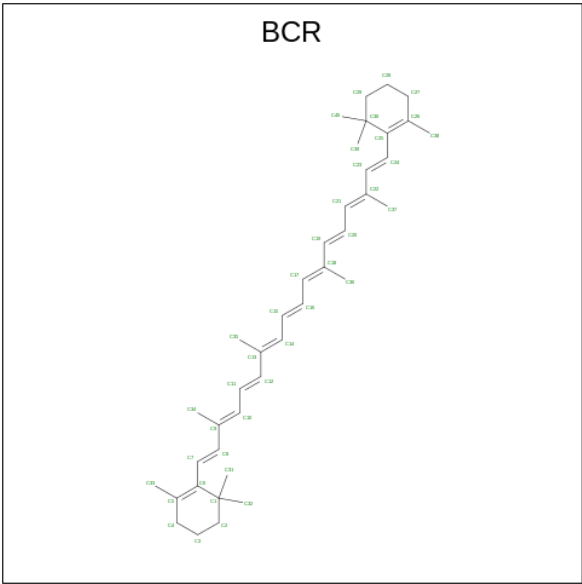
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	d	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
24	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



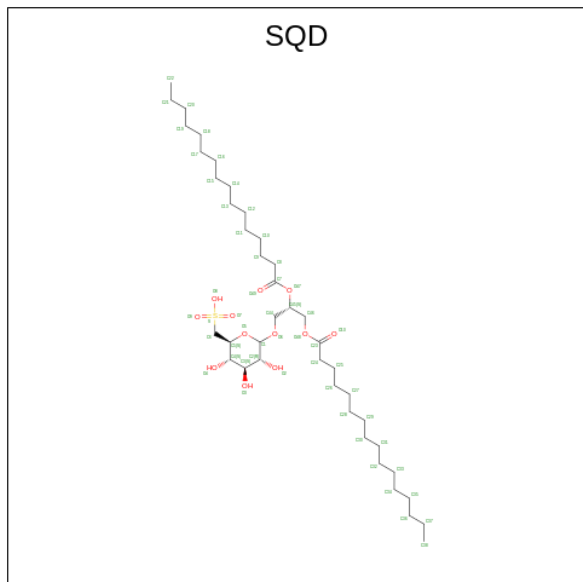
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	1
			128	110	8	10		
25	A	1	Total	C	N	O	0	1
			128	110	8	10		
25	a	1	Total	C	N	O	0	1
			128	110	8	10		
25	d	1	Total	C	N	O	0	1
			128	110	8	10		

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



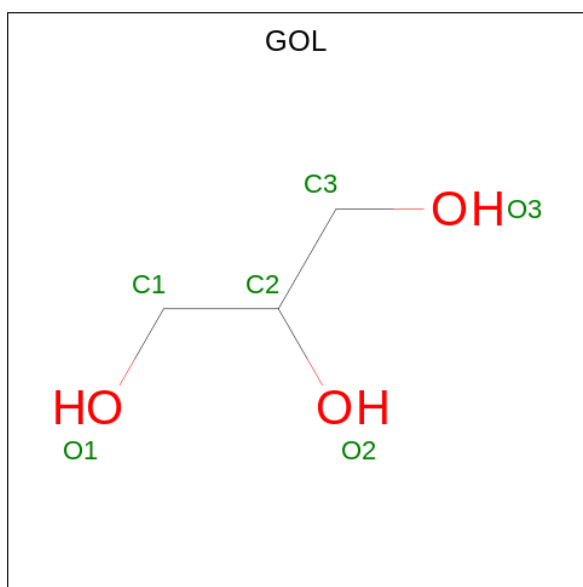
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Y	1	Total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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	S	0	1
			108	82	24	2		
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	B	1	Total	C	O	S	0	0
			54	41	12	1		
27	L	1	Total	C	O	S	0	0
			54	41	12	1		
27	X	1	Total	C	O	S	0	0
			43	30	12	1		
27	a	1	Total	C	O	S	0	1
			108	82	24	2		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	f	1	Total	C	O	S	0	0
			43	30	12	1		

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



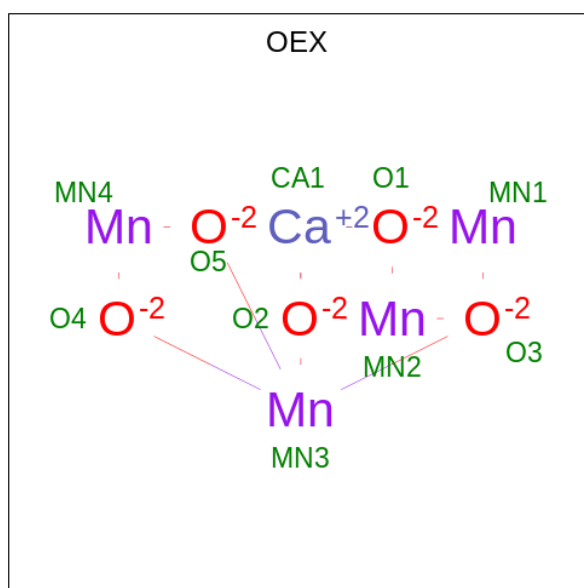
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			6	3	3		
28	A	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	C	1	Total	C	O	0	1
			12	6	6		
28	D	1	Total	C	O	0	0
			6	3	3		
28	O	1	Total	C	O	0	0
			6	3	3		
28	O	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	1
			12	6	6		
28	a	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	c	1	Total	C	O	0	1
			12	6	6		
28	c	1	Total	C	O	0	0
			6	3	3		
28	d	1	Total	C	O	0	0
			6	3	3		
28	l	1	Total	C	O	0	1
			12	6	6		
28	o	1	Total	C	O	0	0
			6	3	3		
28	o	1	Total	C	O	0	0
			6	3	3		
28	v	1	Total	C	O	0	1
			12	6	6		

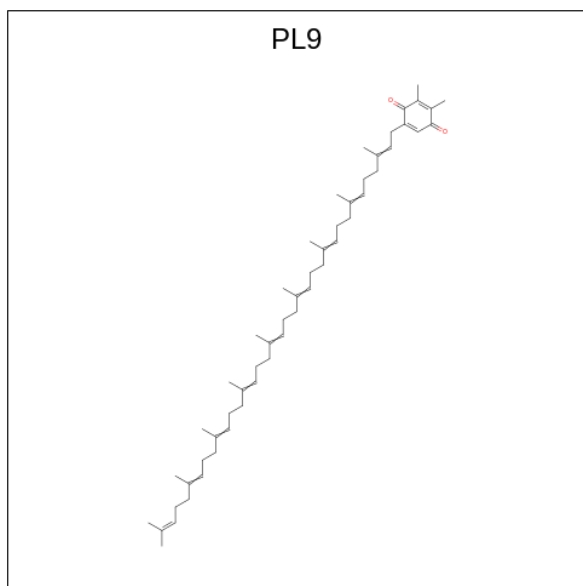
- Molecule 29 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 30 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: $\text{C}_{53}\text{H}_{80}\text{O}_2$)

(labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	1
			110	106	4		
30	D	1	Total	C	O	0	1
			110	106	4		
30	a	1	Total	C	O	0	1
			110	106	4		
30	d	1	Total	C	O	0	1
			110	106	4		

- Molecule 31 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

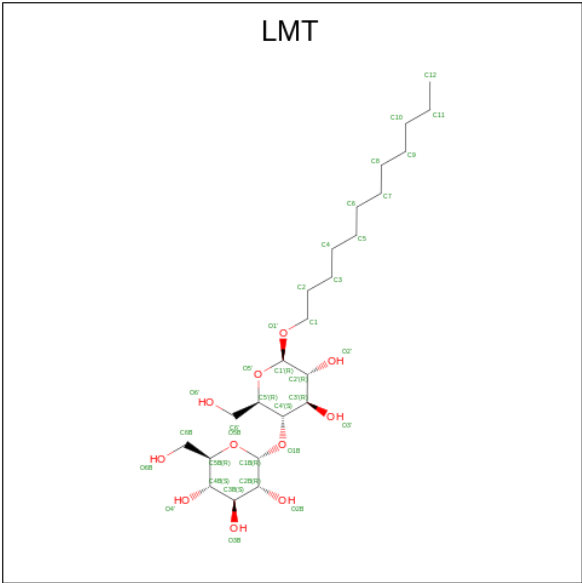
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			28	23	5		
31	B	2	Total	C	O	0	0
			73	63	10		
31	D	2	Total	C	O	0	0
			57	51	6		
31	I	1	Total	C	O	0	0
			40	35	5		
31	J	1	Total	C		0	0
			10	10			
31	K	1	Total	C	O	0	1
			68	58	10		
31	M	1	Total	C		0	0
			10	10			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	X	1	Total	C	O	0	0
			18	16	2		
31	a	1	Total	C	O	0	0
			30	25	5		
31	b	1	Total	C	O	0	0
			33	28	5		
31	c	1	Total	C	O	0	1
			64	54	10		
31	d	2	Total	C	O	0	0
			53	47	6		
31	j	1	Total	C		0	0
			10	10			
31	m	1	Total	C		0	0
			10	10			
31	x	1	Total	C	O	0	0
			18	16	2		

- Molecule 32 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



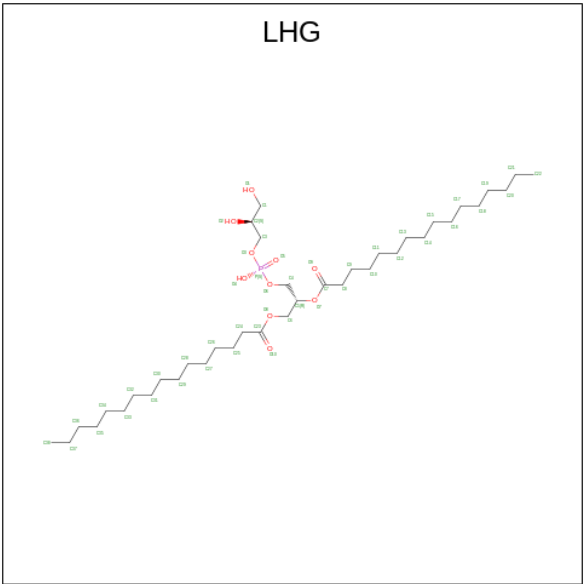
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			35	24	11		
32	A	1	Total	C	O	0	0
			35	24	11		
32	B	1	Total	C	O	0	0
			35	24	11		

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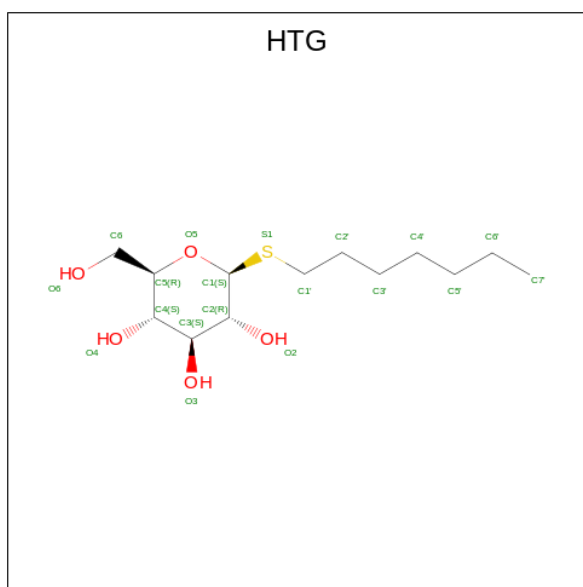
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	B	1	Total	C	O	0	0
			35	24	11		
32	B	1	Total	C	O	0	0
			25	19	6		
32	F	1	Total	C	O	0	0
			35	24	11		
32	M	1	Total	C	O	0	0
			35	24	11		
32	M	1	Total	C	O	0	0
			35	24	11		
32	b	1	Total	C	O	0	0
			25	19	6		
32	b	1	Total	C	O	0	0
			25	19	6		
32	c	1	Total	C	O	0	0
			35	24	11		
32	e	1	Total	C	O	0	0
			35	24	11		
32	m	1	Total	C	O	0	0
			35	24	11		
32	t	1	Total	C	O	0	0
			26	19	7		

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	A	1	Total	C	O	P	0	1
			98	76	20	2		
33	D	1	Total	C	O	P	0	1
			98	76	20	2		
33	D	1	Total	C	O	P	0	1
			98	76	20	2		
33	E	1	Total	C	O	P	0	1
			84	62	20	2		
33	L	1	Total	C	O	P	0	1
			98	76	20	2		
33	a	1	Total	C	O	P	0	1
			84	62	20	2		
33	b	1	Total	C	O	P	0	1
			98	76	20	2		
33	d	1	Total	C	O	P	0	1
			98	76	20	2		
33	d	1	Total	C	O	P	0	1
			98	76	20	2		
33	d	1	Total	C	O	P	0	1
			98	76	20	2		

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



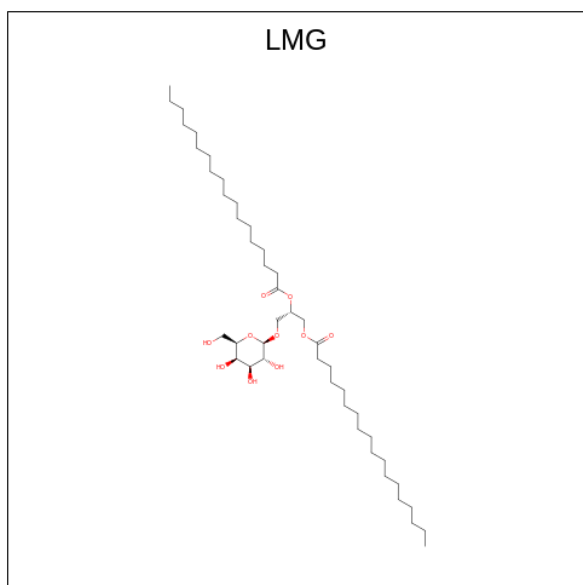
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		

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

- Molecule 35 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



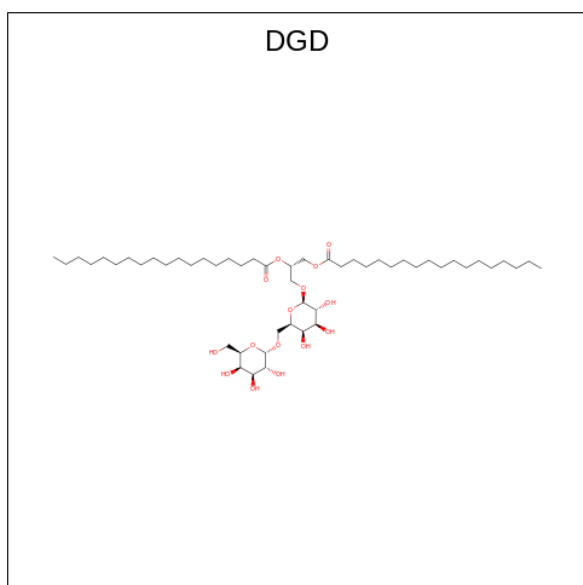
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	C	1	Total	C	O	0	0
			51	41	10		
35	C	1	Total	C	O	0	0
			51	41	10		

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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	C	1	Total	C	O	0	1
			124	94	30		

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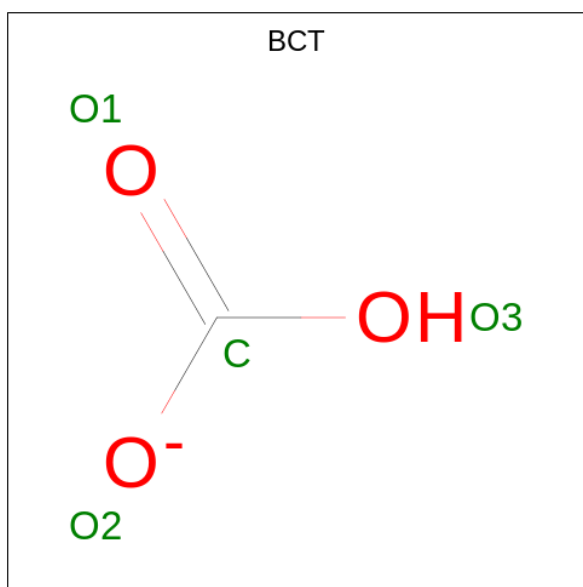
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	C	1	Total	C	O	0	1
			124	94	30		
36	C	1	Total	C	O	0	0
			62	47	15		
36	H	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	1
			124	94	30		
36	c	1	Total	C	O	0	1
			124	94	30		
36	c	1	Total	C	O	0	0
			62	47	15		
36	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 37 is CALCIUM ION (CCD ID: CA) (formula: Ca).

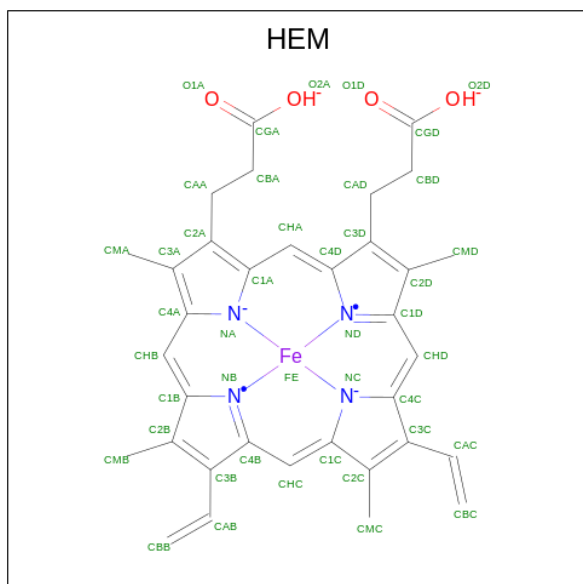
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	C	1	Total	Ca	0	0
			1	1		
37	F	1	Total	Ca	0	0
			1	1		
37	O	1	Total	Ca	0	0
			1	1		
37	c	2	Total	Ca	0	0
			2	2		
37	f	1	Total	Ca	0	0
			1	1		
37	o	1	Total	Ca	0	0
			1	1		

- Molecule 38 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	D	1	Total C O 8 2 6	0	1
38	d	1	Total C O 8 2 6	0	1

- Molecule 39 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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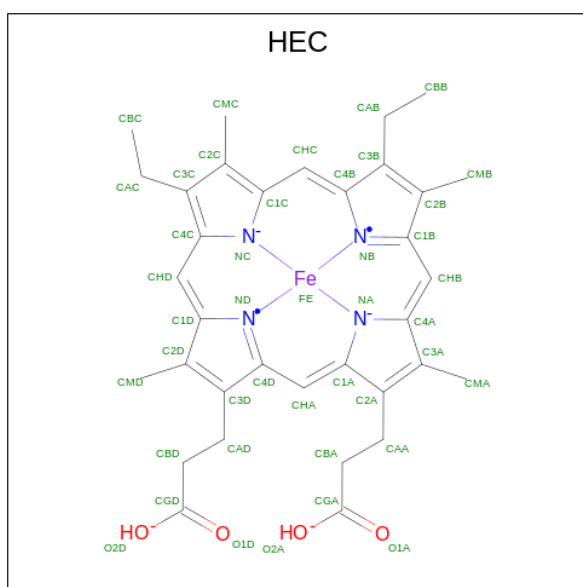
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
39	e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 40 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 41 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₆FeN₄O₄).



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

- Molecule 42 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	A	137	Total	O	0	84
			218	218		
42	B	183	Total	O	0	3
			186	186		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	C	166	Total 203	O 203	0	37
42	D	123	Total 158	O 158	0	35
42	E	16	Total 16	O 16	0	0
42	F	5	Total 5	O 5	0	0
42	H	24	Total 24	O 24	0	0
42	I	7	Total 7	O 7	0	0
42	J	7	Total 7	O 7	0	0
42	K	5	Total 5	O 5	0	0
42	L	9	Total 10	O 10	0	1
42	M	10	Total 10	O 10	0	0
42	O	101	Total 105	O 105	0	4
42	T	10	Total 13	O 13	0	3
42	U	46	Total 49	O 49	0	3
42	V	82	Total 84	O 84	0	2
42	X	8	Total 8	O 8	0	0
42	a	130	Total 208	O 208	0	80
42	b	203	Total 206	O 206	0	3
42	c	158	Total 191	O 191	0	33
42	d	118	Total 151	O 151	0	33
42	e	8	Total 8	O 8	0	0
42	f	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	h	18	Total 18	O 18	0	0
42	i	3	Total 3	O 3	0	0
42	j	2	Total 2	O 2	0	0
42	k	3	Total 3	O 3	0	0
42	l	8	Total 9	O 9	0	1
42	m	9	Total 9	O 9	0	0
42	o	97	Total 102	O 102	0	5
42	t	8	Total 11	O 11	0	3
42	u	50	Total 51	O 51	0	1
42	v	59	Total 62	O 62	0	3
42	x	8	Total 8	O 8	0	0
42	y	2	Total 2	O 2	0	0

3 Residue-property plots

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

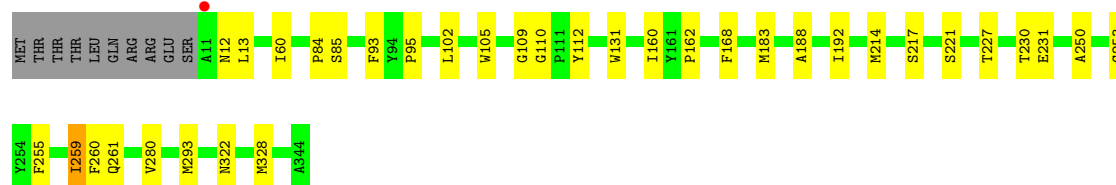
- Molecule 1: Photosystem II protein D1

Chain A: 



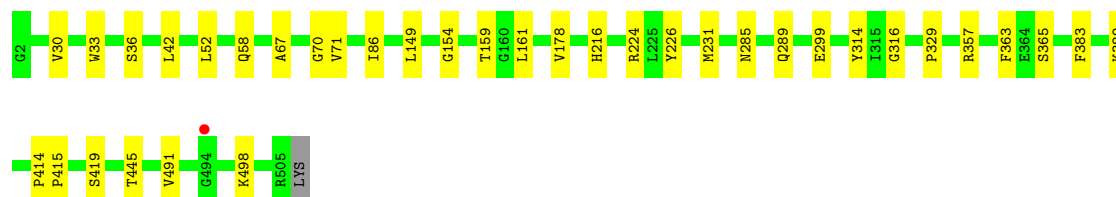
- Molecule 1: Photosystem II protein D1

Chain a: 



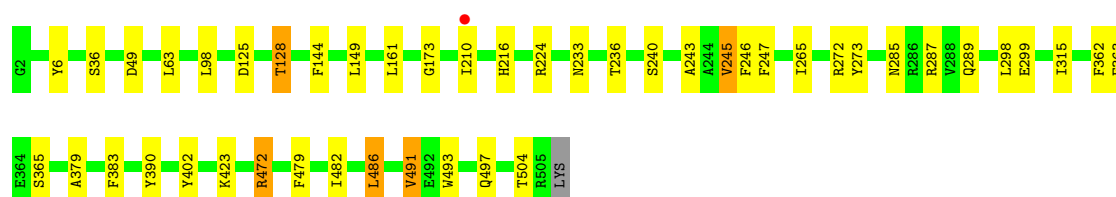
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B: 

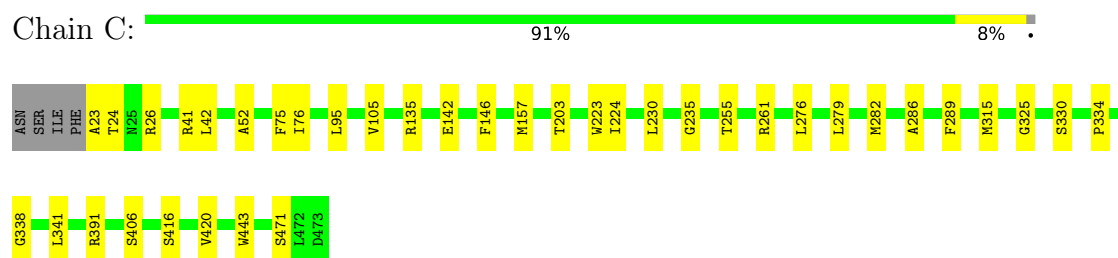


- Molecule 2: Photosystem II CP47 reaction center protein

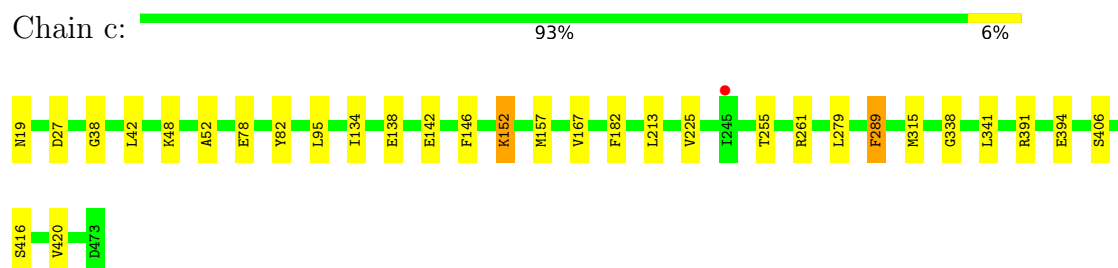
Chain b: 



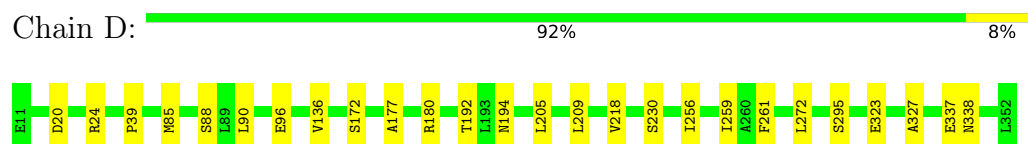
- Molecule 3: Photosystem II CP43 reaction center protein



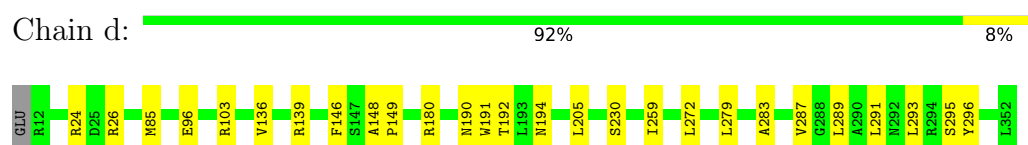
- Molecule 3: Photosystem II CP43 reaction center protein



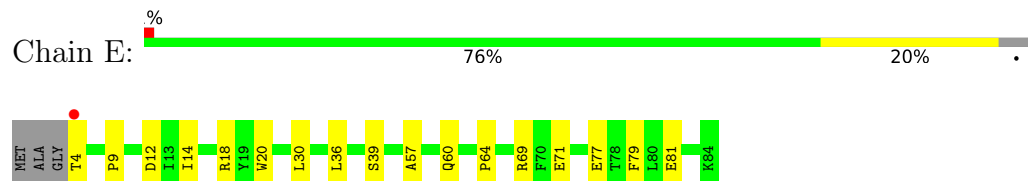
- Molecule 4: Photosystem II D2 protein



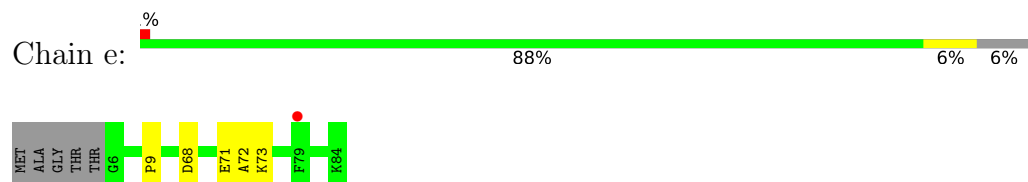
- Molecule 4: Photosystem II D2 protein



- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha



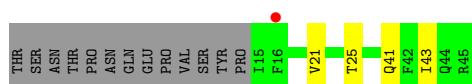
- Molecule 6: Cytochrome b559 subunit beta

Chain F:  64% 14% 23%

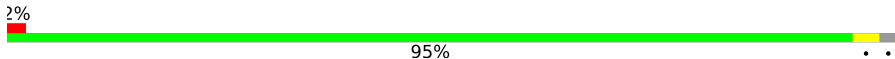


- Molecule 6: Cytochrome b559 subunit beta

Chain f:  2% 61% 9% 30%



- Molecule 7: Photosystem II reaction center protein H

Chain H:  2% 95% . .



- Molecule 7: Photosystem II reaction center protein H

Chain h:  2% 83% 15% .



- Molecule 8: Photosystem II reaction center protein I

Chain I:  76% 21% .



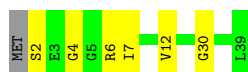
- Molecule 8: Photosystem II reaction center protein I

Chain i:  3% 76% 21% .



- Molecule 9: Photosystem II reaction center protein J

Chain J:  82% 15% .



- Molecule 9: Photosystem II reaction center protein J

Chain j:  87% 13%



- Molecule 10: Photosystem II reaction center protein K

Chain K:  73% 22% 5%



- Molecule 10: Photosystem II reaction center protein K

Chain k:  76% 19% 5%



- Molecule 11: Photosystem II reaction center protein L

Chain L:  95% . .



- Molecule 11: Photosystem II reaction center protein L

Chain l:  89% 8% .



- Molecule 12: Photosystem II reaction center protein M

Chain M:  78% 6% 8% 8%



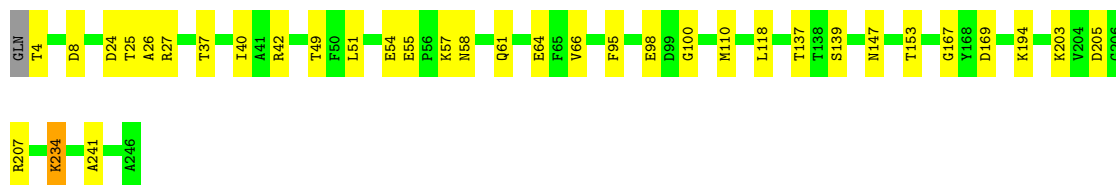
- Molecule 12: Photosystem II reaction center protein M

Chain m:  78% 14% . 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  85% 14%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  89% 10%



- Molecule 14: Photosystem II reaction center protein T

Chain T:  78% 16% 6%



- Molecule 14: Photosystem II reaction center protein T

Chain t:  78% 16% 6%



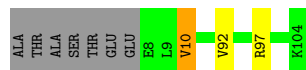
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  85% 8% 8%

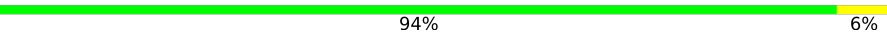


- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  90% 7%



- Molecule 16: Cytochrome c-550

Chain V:  94% 6%



- Molecule 16: Cytochrome c-550

Chain v:  91% 9%



- Molecule 17: Photosystem II reaction center protein X

Chain X:  85% 10% 5%



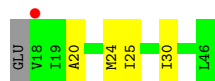
- Molecule 17: Photosystem II reaction center protein X

Chain x:  82% 12% 5%



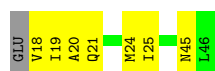
- Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:  3% 83% 13% .



- Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:  73% 23% .



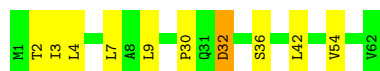
- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  85% 13% .



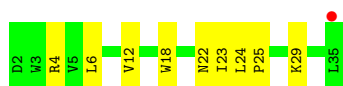
- Molecule 19: Photosystem II reaction center protein Z

Chain z:  84% 15% .



- Molecule 20: Photosystem II protein Y

Chain R:  3% 74% 26%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	125.77Å 231.76Å 288.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.25 19.99 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.25) 99.8 (19.99-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.26Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.143 , 0.183 0.144 , 0.185	Depositor DCC
R_{free} test set	19914 reflections (2.44%)	wwPDB-VP
Wilson B-factor (Å ²)	51.6	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 75.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	62605	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% 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: FE2, UNL, HEC, CL, DGD, HEM, MG, FME, OEY, PHO, SQD, LHG, GOL, HTG, OEX, LMG, CLA, BCR, CA, LMT, BCT, PL9

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	0.27	0/4478	0.43	0/6098
1	a	0.25	0/4470	0.40	0/6087
2	B	0.37	0/4293	0.50	0/5851
2	b	0.34	0/4285	0.49	0/5841
3	C	0.29	0/4404	0.43	0/5997
3	c	0.28	0/4459	0.43	0/6071
4	D	0.34	0/3741	0.46	0/5095
4	d	0.32	0/3749	0.45	0/5106
5	E	0.33	0/681	0.51	0/928
5	e	0.29	0/690	0.47	0/939
6	F	0.31	0/284	0.46	0/387
6	f	0.28	0/269	0.42	0/365
7	H	0.33	0/519	0.48	0/708
7	h	0.31	0/530	0.49	0/722
8	I	0.30	0/311	0.43	0/419
8	i	0.33	0/311	0.53	0/419
9	J	0.30	0/278	0.38	0/376
9	j	0.29	0/283	0.40	0/383
10	K	0.33	0/303	0.49	0/416
10	k	0.34	0/303	0.46	0/416
11	L	0.39	0/318	0.48	0/433
11	l	0.39	0/318	0.49	0/433
12	M	0.40	0/261	0.54	0/357
12	m	0.35	0/279	0.49	0/380
13	O	0.35	0/1991	0.52	0/2698
13	o	0.33	0/1966	0.51	0/2665
14	T	0.35	0/310	0.42	0/419
14	t	0.33	0/301	0.43	0/406
15	U	0.37	0/811	0.52	0/1095
15	u	0.36	0/818	0.53	0/1105
16	V	0.36	0/1142	0.50	0/1545

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.30	0/1139	0.48	0/1542
17	X	0.24	0/292	0.35	0/395
17	x	0.24	0/284	0.38	0/384
18	Y	0.25	0/216	0.43	0/289
18	y	0.24	0/216	0.38	0/289
19	Z	0.22	0/490	0.39	0/669
19	z	0.21	0/490	0.34	0/669
20	R	0.22	0/279	0.32	0/383
All	All	0.31	0/50562	0.46	0/68780

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4338	0	4142	19	0
1	a	4330	0	4132	35	0
2	B	4146	0	3983	27	0
2	b	4134	0	3976	37	0
3	C	4260	0	4123	25	0
3	c	4308	0	4172	23	0
4	D	3620	0	3484	28	0
4	d	3628	0	3490	19	0
5	E	662	0	648	12	0
5	e	670	0	655	4	0
6	F	275	0	282	5	0
6	f	261	0	269	4	0
7	H	506	0	529	2	0
7	h	517	0	541	7	0
8	I	314	0	328	6	0
8	i	314	0	328	5	0
9	J	272	0	279	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	277	0	284	3	0
10	K	293	0	305	6	0
10	k	293	0	305	7	0
11	L	311	0	320	1	0
11	l	311	0	320	4	0
12	M	268	0	285	4	0
12	m	286	0	305	8	0
13	O	1958	0	1920	19	0
13	o	1933	0	1900	12	0
14	T	311	0	318	2	0
14	t	302	0	311	5	0
15	U	800	0	796	4	0
15	u	807	0	805	2	0
16	V	1120	0	1122	4	0
16	v	1117	0	1131	9	0
17	X	289	0	322	3	0
17	x	281	0	312	4	0
18	Y	215	0	246	2	0
18	y	215	0	246	4	0
19	Z	479	0	516	6	0
19	z	479	0	516	2	0
20	R	273	0	305	4	0
21	A	11	0	0	1	0
21	a	11	0	0	1	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0
23	A	4	0	0	0	0
23	a	4	0	0	0	0
24	A	455	0	504	14	0
24	B	1040	0	1152	26	0
24	C	845	0	936	27	0
24	D	195	0	216	6	0
24	a	455	0	504	19	0
24	b	1040	0	1152	23	0
24	c	845	0	936	39	0
24	d	195	0	216	7	0
25	A	256	0	296	5	0
25	a	128	0	148	2	0
25	d	128	0	148	1	0
26	A	40	0	56	2	0
26	B	120	0	168	6	0
26	C	80	0	112	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	D	40	0	56	1	0
26	H	40	0	56	2	0
26	K	40	0	56	0	0
26	T	40	0	56	6	0
26	Y	40	0	56	1	0
26	a	40	0	56	1	0
26	b	120	0	168	7	0
26	c	80	0	112	3	0
26	d	40	0	56	3	0
26	h	40	0	56	3	0
26	k	40	0	56	2	0
26	t	40	0	56	6	0
26	y	40	0	56	1	0
27	A	162	0	233	3	0
27	B	54	0	78	1	0
27	L	54	0	78	1	0
27	X	43	0	53	2	0
27	a	162	0	232	10	0
27	f	43	0	53	0	0
28	A	12	0	15	3	0
28	B	12	0	16	2	0
28	C	12	0	16	0	0
28	D	6	0	7	3	0
28	O	12	0	16	3	0
28	V	12	0	16	0	0
28	a	18	0	24	6	0
28	b	12	0	16	3	0
28	c	18	0	24	0	0
28	d	6	0	8	0	0
28	l	12	0	16	2	0
28	o	12	0	16	0	0
28	v	12	0	16	3	0
29	A	10	0	0	0	0
29	a	10	0	0	0	0
30	A	110	0	160	19	0
30	D	110	0	160	1	0
30	a	110	0	160	8	0
30	d	110	0	160	0	0
31	A	28	0	0	0	0
31	B	73	0	0	0	0
31	D	57	0	0	0	0
31	I	40	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	J	10	0	0	0	0
31	K	68	0	0	0	0
31	M	10	0	0	0	0
31	X	18	0	0	0	0
31	a	30	0	0	0	0
31	b	33	0	0	0	0
31	c	64	0	0	0	0
31	d	53	0	0	0	0
31	j	10	0	0	0	0
31	m	10	0	0	0	0
31	x	18	0	0	0	0
32	A	70	0	92	1	0
32	B	95	0	127	4	0
32	F	35	0	46	0	0
32	M	70	0	90	2	0
32	b	50	0	70	1	0
32	c	35	0	46	0	0
32	e	35	0	46	1	0
32	m	35	0	46	0	0
32	t	26	0	35	1	0
33	A	98	0	148	3	0
33	D	196	0	296	10	0
33	E	84	0	114	6	0
33	L	98	0	148	0	0
33	a	84	0	114	8	0
33	b	98	0	148	1	0
33	d	294	0	444	23	0
34	B	57	0	78	2	0
34	C	19	0	26	0	0
34	D	16	0	17	0	0
34	V	11	0	10	0	0
34	b	57	0	78	3	0
34	c	19	0	26	1	0
34	d	16	0	17	0	0
35	C	153	0	216	3	0
35	D	51	0	72	0	0
35	M	51	0	72	1	0
35	Z	37	0	44	2	0
35	a	51	0	72	1	0
35	b	51	0	72	1	0
35	c	102	0	144	3	0
35	d	51	0	72	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	z	39	0	48	2	0
36	C	310	0	410	7	0
36	H	62	0	82	0	0
36	c	310	0	410	9	0
36	h	62	0	82	1	0
37	C	1	0	0	0	0
37	F	1	0	0	0	0
37	O	1	0	0	0	0
37	c	2	0	0	0	0
37	f	1	0	0	0	0
37	o	1	0	0	0	0
38	D	8	0	0	0	0
38	d	8	0	0	0	0
39	F	43	0	30	1	0
39	e	43	0	30	0	0
40	J	1	0	0	0	0
40	j	1	0	0	0	0
41	V	43	0	30	0	0
41	v	43	0	30	0	0
42	A	218	0	0	1	0
42	B	186	0	0	1	0
42	C	203	0	0	2	0
42	D	158	0	0	2	0
42	E	16	0	0	0	0
42	F	5	0	0	0	0
42	H	24	0	0	0	0
42	I	7	0	0	0	0
42	J	7	0	0	1	0
42	K	5	0	0	1	0
42	L	10	0	0	0	0
42	M	10	0	0	0	0
42	O	105	0	0	1	0
42	T	13	0	0	0	0
42	U	49	0	0	0	0
42	V	84	0	0	0	0
42	X	8	0	0	0	0
42	a	208	0	0	2	0
42	b	206	0	0	0	0
42	c	191	0	0	4	0
42	d	151	0	0	1	0
42	e	8	0	0	0	0
42	f	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	h	18	0	0	0	0
42	i	3	0	0	0	0
42	j	2	0	0	0	0
42	k	3	0	0	0	0
42	l	9	0	0	0	0
42	m	9	0	0	0	0
42	o	102	0	0	0	0
42	t	11	0	0	0	0
42	u	51	0	0	1	0
42	v	62	0	0	1	0
42	x	8	0	0	0	0
42	y	2	0	0	0	0
All	All	62605	0	61442	568	0

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

The worst 5 of 568 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)
28:A:419:GOL:H11	12:M:1:FME:HG2	1.44	1.00
1:a:250[B]:ALA:HA	2:b:491[B]:VAL:HG11	1.49	0.94
1:a:250[A]:ALA:HA	2:b:491[A]:VAL:HG11	1.51	0.93
21:A:401[B]:OEY:O6	21:A:401[B]:OEY:O5	1.89	0.91
21:a:401[B]:OEY:O6	21:a:401[B]:OEY:O5	1.88	0.90

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	553/344 (161%)	542 (98%)	9 (2%)	2 (0%)	30	31
1	a	552/344 (160%)	544 (99%)	6 (1%)	2 (0%)	30	31
2	B	522/505 (103%)	516 (99%)	6 (1%)	0	100	100
2	b	521/505 (103%)	510 (98%)	11 (2%)	0	100	100
3	C	546/455 (120%)	535 (98%)	10 (2%)	1 (0%)	43	50
3	c	553/455 (122%)	544 (98%)	8 (1%)	1 (0%)	43	50
4	D	453/342 (132%)	438 (97%)	15 (3%)	0	100	100
4	d	454/342 (133%)	444 (98%)	10 (2%)	0	100	100
5	E	79/84 (94%)	78 (99%)	1 (1%)	0	100	100
5	e	79/84 (94%)	79 (100%)	0	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
7	h	63/65 (97%)	58 (92%)	4 (6%)	1 (2%)	7	4
8	I	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	4	2
8	i	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	37 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	34/36 (94%)	34 (100%)	0	0	100	100
13	O	251/244 (103%)	243 (97%)	7 (3%)	1 (0%)	30	31
13	o	249/244 (102%)	244 (98%)	5 (2%)	0	100	100
14	T	33/32 (103%)	33 (100%)	0	0	100	100
14	t	32/32 (100%)	32 (100%)	0	0	100	100
15	U	97/104 (93%)	92 (95%)	5 (5%)	0	100	100
15	u	98/104 (94%)	94 (96%)	4 (4%)	0	100	100
16	V	140/137 (102%)	136 (97%)	4 (3%)	0	100	100
16	v	140/137 (102%)	134 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
17	x	36/40 (90%)	36 (100%)	0	0	100	100
18	Y	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
18	y	27/30 (90%)	27 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	3
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	7	3
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	6171/5384 (115%)	6037 (98%)	123 (2%)	11 (0%)	43	50

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
8	I	36	ASP
19	Z	31	GLN
3	c	416	SER
19	z	30	PRO

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	444/279 (159%)	439 (99%)	5 (1%)	65	75
1	a	443/279 (159%)	441 (100%)	2 (0%)	81	87
2	B	421/403 (104%)	417 (99%)	4 (1%)	68	77
2	b	420/403 (104%)	407 (97%)	13 (3%)	35	44
3	C	430/356 (121%)	422 (98%)	8 (2%)	50	61
3	c	436/356 (122%)	429 (98%)	7 (2%)	55	66
4	D	368/277 (133%)	365 (99%)	3 (1%)	73	80
4	d	369/277 (133%)	362 (98%)	7 (2%)	50	61
5	E	72/73 (99%)	70 (97%)	2 (3%)	38	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	e	72/73 (99%)	71 (99%)	1 (1%)	59	70
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	26/38 (68%)	26 (100%)	0	100	100
7	H	54/54 (100%)	53 (98%)	1 (2%)	50	61
7	h	55/54 (102%)	55 (100%)	0	100	100
8	I	34/34 (100%)	34 (100%)	0	100	100
8	i	34/34 (100%)	33 (97%)	1 (3%)	37	47
9	J	26/27 (96%)	25 (96%)	1 (4%)	29	36
9	j	26/27 (96%)	25 (96%)	1 (4%)	29	36
10	K	30/30 (100%)	26 (87%)	4 (13%)	4	2
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	5
11	L	36/35 (103%)	36 (100%)	0	100	100
11	l	36/35 (103%)	36 (100%)	0	100	100
12	M	30/32 (94%)	27 (90%)	3 (10%)	7	5
12	m	32/32 (100%)	30 (94%)	2 (6%)	16	16
13	O	216/207 (104%)	208 (96%)	8 (4%)	30	37
13	o	213/207 (103%)	205 (96%)	8 (4%)	29	36
14	T	32/28 (114%)	28 (88%)	4 (12%)	4	3
14	t	31/28 (111%)	31 (100%)	0	100	100
15	U	86/89 (97%)	84 (98%)	2 (2%)	44	55
15	u	87/89 (98%)	85 (98%)	2 (2%)	44	55
16	V	123/117 (105%)	122 (99%)	1 (1%)	73	80
16	v	123/117 (105%)	120 (98%)	3 (2%)	43	54
17	X	32/33 (97%)	32 (100%)	0	100	100
17	x	31/33 (94%)	30 (97%)	1 (3%)	34	43
18	Y	22/23 (96%)	21 (96%)	1 (4%)	24	29
18	y	22/23 (96%)	19 (86%)	3 (14%)	3	2
19	Z	52/52 (100%)	49 (94%)	3 (6%)	18	19
19	z	52/52 (100%)	46 (88%)	6 (12%)	5	3
20	R	29/29 (100%)	26 (90%)	3 (10%)	7	5
All	All	5103/4403 (116%)	4990 (98%)	113 (2%)	45	56

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	472	ARG
19	z	7	LEU
4	d	230[B]	SER
19	z	4	LEU
18	y	19	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	331	ASN
3	c	19	ASN
15	u	78	ASN
11	l	8	GLN
5	E	60	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	0.62	0	7,9,11	1.05	1 (14%)
8	FME	I	1	8	8,9,10	0.62	0	7,9,11	1.18	1 (14%)
12	FME	M	1	12	8,9,10	0.60	0	7,9,11	1.35	1 (14%)
12	FME	m	1	12	8,9,10	0.52	0	7,9,11	1.47	2 (28%)
14	FME	t	1	14	8,9,10	0.65	0	7,9,11	1.39	1 (14%)
14	FME	T	1	14	8,9,10	0.60	0	7,9,11	1.71	3 (42%)

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

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	CA-N-CN	2.40	126.52	122.82
12	m	1	FME	O1-CN-N	-2.39	118.98	125.27
12	M	1	FME	O-C-CA	-2.34	118.66	124.78
14	t	1	FME	O-C-CA	-2.26	118.85	124.78
14	T	1	FME	C-CA-N	2.22	113.75	109.73

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O-C-CA-CB
14	T	1	FME	O1-CN-N-CA
8	i	1	FME	CA-CB-CG-SD
14	T	1	FME	N-CA-CB-CG
14	T	1	FME	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	M	1	FME	1	0
12	m	1	FME	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 274 ligands modelled in this entry, 21 are monoatomic and 20 are unknown - leaving 233 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
33	LHG	d	407[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.04	4 (7%)
28	GOL	A	419	-	5,5,5	1.40	1 (20%)	5,5,5	0.82	0
36	DGD	C	518[B]	-	63,63,67	0.86	2 (3%)	77,77,81	1.04	6 (7%)
24	CLA	C	511	3	69,73,73	2.01	20 (28%)	83,113,113	2.98	34 (40%)
28	GOL	B	623	-	5,5,5	0.92	0	5,5,5	1.11	1 (20%)
27	SQD	f	101	-	42,43,54	1.19	3 (7%)	51,54,65	1.41	9 (17%)
28	GOL	O	303	-	5,5,5	1.02	0	5,5,5	1.00	0
30	PL9	a	415[A]	-	55,55,55	0.65	2 (3%)	68,69,69	2.01	22 (32%)
38	BCT	d	401[B]	22	2,3,3	0.63	0	2,3,3	0.87	0
28	GOL	a	418	-	5,5,5	1.09	0	5,5,5	0.96	0
28	GOL	C	523[A]	-	5,5,5	1.11	0	5,5,5	0.88	0
28	GOL	v	202[B]	-	5,5,5	1.10	0	5,5,5	0.85	0
29	OEX	a	414[A]	42,3,1	0,14,14	-	-	-	-	-
28	GOL	d	413	-	5,5,5	1.06	0	5,5,5	1.08	0
34	HTG	C	522	-	19,19,19	0.87	1 (5%)	23,24,24	1.39	2 (8%)
24	CLA	B	602	2	69,73,73	2.04	20 (28%)	83,113,113	2.83	34 (40%)
33	LHG	a	420[A]	-	41,41,48	1.06	2 (4%)	44,47,54	0.92	2 (4%)
24	CLA	A	406[A]	42	69,73,73	2.02	18 (26%)	83,113,113	2.85	33 (39%)
33	LHG	d	408[A]	-	48,48,48	0.92	2 (4%)	51,54,54	1.01	3 (5%)
26	BCR	h	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.46	10 (17%)
24	CLA	B	608	2	69,73,73	1.92	19 (27%)	83,113,113	2.82	33 (39%)
24	CLA	A	409	1	69,73,73	1.97	20 (28%)	83,113,113	3.00	33 (39%)
24	CLA	c	511	3	69,73,73	2.01	20 (28%)	83,113,113	2.80	31 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	GOL	B	626	-	5,5,5	1.02	0	5,5,5	0.96	0
32	LMT	t	101	-	26,26,36	0.90	2 (7%)	31,31,47	1.28	2 (6%)
34	HTG	B	622	-	19,19,19	0.82	1 (5%)	23,24,24	1.55	2 (8%)
34	HTG	c	522	-	19,19,19	0.93	1 (5%)	23,24,24	1.59	3 (13%)
38	BCT	D	401[B]	22	2,3,3	0.64	0	2,3,3	0.97	0
24	CLA	B	601	42	69,73,73	2.07	21 (30%)	83,113,113	2.84	28 (33%)
24	CLA	A	407[B]	42	69,73,73	2.07	20 (28%)	83,113,113	2.85	32 (38%)
27	SQD	X	101	-	42,43,54	1.21	4 (9%)	51,54,65	2.08	14 (27%)
24	CLA	D	402[B]	4	69,73,73	2.04	19 (27%)	83,113,113	2.83	27 (32%)
27	SQD	a	411[B]	-	53,54,54	0.98	3 (5%)	62,65,65	1.57	13 (20%)
33	LHG	A	420[B]	-	48,48,48	0.88	2 (4%)	51,54,54	1.17	6 (11%)
38	BCT	d	401[A]	22	2,3,3	0.59	0	2,3,3	1.49	0
30	PL9	A	415[A]	-	55,55,55	0.69	2 (3%)	68,69,69	2.01	24 (35%)
33	LHG	d	407[B]	-	48,48,48	0.88	2 (4%)	51,54,54	1.03	4 (7%)
24	CLA	B	613	2	69,73,73	2.00	19 (27%)	83,113,113	2.80	30 (36%)
28	GOL	v	202[A]	-	5,5,5	1.20	0	5,5,5	0.82	0
24	CLA	c	510	3	69,73,73	2.03	20 (28%)	83,113,113	2.90	34 (40%)
24	CLA	b	611	2	69,73,73	1.99	21 (30%)	83,113,113	2.96	30 (36%)
25	PHO	d	402[A]	-	58,69,69	2.77	13 (22%)	56,99,99	2.94	17 (30%)
30	PL9	a	415[B]	-	55,55,55	0.63	2 (3%)	68,69,69	1.87	21 (30%)
24	CLA	B	609	2	69,73,73	2.05	18 (26%)	83,113,113	2.74	30 (36%)
35	LMG	D	411	40	51,51,55	0.86	2 (3%)	59,59,63	0.99	4 (6%)
24	CLA	a	407[B]	42	69,73,73	2.06	19 (27%)	83,113,113	2.95	34 (40%)
21	OEY	a	401[B]	42,3,1	0,16,16	-	-	-	-	-
24	CLA	c	504	3	69,73,73	2.03	19 (27%)	83,113,113	2.84	30 (36%)
24	CLA	b	604	2	69,73,73	2.01	21 (30%)	83,113,113	2.73	27 (32%)
24	CLA	b	602	2	69,73,73	2.08	20 (28%)	83,113,113	2.87	35 (42%)
24	CLA	C	504	3	69,73,73	1.93	19 (27%)	83,113,113	2.87	26 (31%)
39	HEM	F	102	6,5	50,50,50	1.54	7 (14%)	66,82,82	1.92	17 (25%)
32	LMT	b	620	-	25,25,36	0.98	1 (4%)	30,30,47	1.15	2 (6%)
41	HEC	v	201	16	50,50,50	1.77	7 (14%)	68,82,82	1.38	9 (13%)
28	GOL	b	627	-	5,5,5	0.65	0	5,5,5	1.28	1 (20%)
24	CLA	A	406[B]	42	69,73,73	2.02	18 (26%)	83,113,113	2.87	33 (39%)
24	CLA	c	513	3	69,73,73	2.07	19 (27%)	83,113,113	2.88	33 (39%)
24	CLA	b	608	2	69,73,73	2.00	21 (30%)	83,113,113	2.78	32 (38%)
28	GOL	V	203[A]	-	5,5,5	1.34	0	5,5,5	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LMT	A	418	-	36,36,36	0.93	0	47,47,47	1.11	2 (4%)
33	LHG	E	101[A]	-	41,41,48	1.08	2 (4%)	44,47,54	1.10	3 (6%)
33	LHG	a	420[B]	-	41,41,48	1.04	2 (4%)	44,47,54	0.92	2 (4%)
33	LHG	b	628[A]	-	48,48,48	0.83	2 (4%)	51,54,54	1.04	4 (7%)
33	LHG	d	408[B]	-	48,48,48	0.91	2 (4%)	51,54,54	0.99	3 (5%)
34	HTG	b	622	-	19,19,19	0.99	1 (5%)	23,24,24	1.78	3 (13%)
32	LMT	F	101	-	36,36,36	1.04	1 (2%)	47,47,47	1.02	2 (4%)
24	CLA	C	510	3	69,73,73	2.02	19 (27%)	83,113,113	2.86	31 (37%)
26	BCR	b	619	-	41,41,41	1.04	1 (2%)	56,56,56	1.32	7 (12%)
26	BCR	B	619	-	41,41,41	1.10	2 (4%)	56,56,56	1.23	6 (10%)
24	CLA	B	615	2	69,73,73	2.01	17 (24%)	83,113,113	2.89	28 (33%)
26	BCR	A	410	-	41,41,41	1.07	1 (2%)	56,56,56	1.40	6 (10%)
35	LMG	b	629	-	51,51,55	0.85	2 (3%)	59,59,63	1.37	8 (13%)
36	DGD	c	517[A]	-	63,63,67	0.85	2 (3%)	77,77,81	1.10	7 (9%)
24	CLA	c	514	3	69,73,73	2.09	20 (28%)	83,113,113	2.87	31 (37%)
24	CLA	a	407[A]	42	69,73,73	1.98	19 (27%)	83,113,113	2.83	30 (36%)
30	PL9	A	415[B]	-	55,55,55	0.63	1 (1%)	68,69,69	1.95	22 (32%)
36	DGD	c	518[B]	-	63,63,67	0.86	2 (3%)	77,77,81	1.04	7 (9%)
24	CLA	C	502	3	69,73,73	2.01	19 (27%)	83,113,113	2.89	33 (39%)
21	OEY	A	401[B]	42,3,1	0,16,16	-	-	-	-	-
27	SQD	L	102	-	53,54,54	1.05	3 (5%)	62,65,65	1.72	10 (16%)
35	LMG	C	520	-	51,51,55	1.00	2 (3%)	59,59,63	1.11	4 (6%)
24	CLA	a	405[A]	1	69,73,73	1.99	20 (28%)	83,113,113	2.87	33 (39%)
26	BCR	T	101	-	41,41,41	1.10	1 (2%)	56,56,56	1.51	15 (26%)
32	LMT	B	628	-	36,36,36	1.00	3 (8%)	47,47,47	1.20	4 (8%)
26	BCR	D	404	-	41,41,41	1.11	1 (2%)	56,56,56	1.80	12 (21%)
32	LMT	c	501	-	36,36,36	1.01	1 (2%)	47,47,47	1.05	3 (6%)
26	BCR	y	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.60	13 (23%)
25	PHO	d	402[B]	-	58,69,69	2.80	12 (20%)	56,99,99	2.83	16 (28%)
24	CLA	b	609	2	69,73,73	2.04	19 (27%)	83,113,113	2.75	33 (39%)
34	HTG	D	410	-	16,16,19	1.00	1 (6%)	20,21,24	1.56	1 (5%)
26	BCR	d	405	-	41,41,41	1.14	1 (2%)	56,56,56	1.93	13 (23%)
24	CLA	b	613	2	69,73,73	1.97	18 (26%)	83,113,113	2.81	31 (37%)
24	CLA	C	507	3	69,73,73	1.97	20 (28%)	83,113,113	2.87	31 (37%)
28	GOL	O	302	-	5,5,5	0.88	0	5,5,5	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LMT	e	102	-	36,36,36	1.03	3 (8%)	47,47,47	0.94	1 (2%)
33	LHG	d	414[A]	-	48,48,48	0.89	2 (4%)	51,54,54	1.11	4 (7%)
24	CLA	c	509	3	69,73,73	2.09	20 (28%)	83,113,113	2.84	30 (36%)
24	CLA	d	404	4	69,73,73	2.07	20 (28%)	83,113,113	2.85	30 (36%)
34	HTG	d	411	-	16,16,19	0.97	1 (6%)	20,21,24	1.59	2 (10%)
33	LHG	E	101[B]	-	41,41,48	1.05	2 (4%)	44,47,54	1.11	3 (6%)
28	GOL	V	203[B]	-	5,5,5	1.10	0	5,5,5	0.86	0
27	SQD	A	411[A]	-	53,54,54	0.93	3 (5%)	62,65,65	1.88	10 (16%)
35	LMG	C	501	-	51,51,55	0.93	2 (3%)	59,59,63	1.57	9 (15%)
33	LHG	b	628[B]	-	48,48,48	0.89	2 (4%)	51,54,54	1.09	4 (7%)
24	CLA	C	506	3	69,73,73	2.02	19 (27%)	83,113,113	2.87	30 (36%)
41	HEC	V	201	16	50,50,50	1.79	8 (16%)	68,82,82	1.58	12 (17%)
26	BCR	c	516	-	41,41,41	1.03	1 (2%)	56,56,56	1.46	12 (21%)
28	GOL	c	527	-	5,5,5	1.13	0	5,5,5	0.90	0
36	DGD	c	518[A]	-	63,63,67	0.85	3 (4%)	77,77,81	0.97	3 (3%)
29	OEX	A	414[A]	42,3,1	0,14,14	-	-	-	-	-
24	CLA	b	606	2	69,73,73	2.00	20 (28%)	83,113,113	2.90	31 (37%)
27	SQD	a	411[A]	-	53,54,54	0.96	3 (5%)	62,65,65	1.83	13 (20%)
24	CLA	c	507	3	69,73,73	2.01	20 (28%)	83,113,113	2.82	30 (36%)
24	CLA	B	611	2	69,73,73	2.56	22 (31%)	83,113,113	4.02	31 (37%)
35	LMG	z	101	-	39,39,55	1.11	2 (5%)	47,47,63	1.11	5 (10%)
36	DGD	c	517[B]	-	63,63,67	0.86	2 (3%)	77,77,81	1.09	5 (6%)
24	CLA	c	503	3	69,73,73	1.98	18 (26%)	83,113,113	2.75	29 (34%)
26	BCR	b	617	-	41,41,41	1.05	1 (2%)	56,56,56	1.36	5 (8%)
32	LMT	m	102	-	36,36,36	1.02	3 (8%)	47,47,47	1.10	3 (6%)
28	GOL	o	302	-	5,5,5	0.99	0	5,5,5	0.93	0
30	PL9	D	405[A]	-	55,55,55	0.63	1 (1%)	68,69,69	1.61	17 (25%)
24	CLA	a	405[B]	1	69,73,73	2.03	20 (28%)	83,113,113	2.88	32 (38%)
36	DGD	C	517[B]	-	63,63,67	0.83	2 (3%)	77,77,81	1.07	5 (6%)
24	CLA	B	606	2	69,73,73	1.97	21 (30%)	83,113,113	2.96	31 (37%)
24	CLA	b	605	2	69,73,73	1.94	20 (28%)	83,113,113	3.02	33 (39%)
24	CLA	b	612	2	69,73,73	2.02	19 (27%)	83,113,113	2.79	27 (32%)
28	GOL	c	526[B]	-	5,5,5	1.04	0	5,5,5	0.92	0
24	CLA	b	607	42	69,73,73	1.96	20 (28%)	83,113,113	2.80	30 (36%)
28	GOL	A	412	-	5,5,5	1.25	0	5,5,5	0.62	0
24	CLA	B	614	2	69,73,73	2.01	19 (27%)	83,113,113	2.99	32 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	HTG	B	621	-	19,19,19	1.03	2 (10%)	23,24,24	1.55	5 (21%)
27	SQD	B	620	-	53,54,54	1.08	4 (7%)	62,65,65	1.78	12 (19%)
35	LMG	M	101	-	51,51,55	0.91	2 (3%)	59,59,63	1.26	3 (5%)
36	DGD	H	102	-	63,63,67	0.83	3 (4%)	77,77,81	1.13	8 (10%)
24	CLA	c	502	3	69,73,73	2.01	19 (27%)	83,113,113	2.83	29 (34%)
24	CLA	A	405[A]	1	69,73,73	2.00	20 (28%)	83,113,113	2.87	30 (36%)
33	LHG	d	414[B]	-	48,48,48	0.91	2 (4%)	51,54,54	1.01	3 (5%)
24	CLA	c	508	42	69,73,73	2.01	19 (27%)	83,113,113	2.83	30 (36%)
26	BCR	k	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.45	9 (16%)
27	SQD	A	411[B]	-	53,54,54	0.93	3 (5%)	62,65,65	1.70	9 (14%)
30	PL9	d	406[A]	-	55,55,55	0.70	1 (1%)	68,69,69	1.63	18 (26%)
24	CLA	b	603	2	69,73,73	1.96	20 (28%)	83,113,113	2.80	30 (36%)
24	CLA	B	605	2	69,73,73	2.01	19 (27%)	83,113,113	2.98	32 (38%)
32	LMT	b	626	-	25,25,36	0.88	1 (4%)	30,30,47	1.15	3 (10%)
24	CLA	b	610	42	69,73,73	2.04	20 (28%)	83,113,113	2.80	31 (37%)
24	CLA	c	505	42	69,73,73	2.11	21 (30%)	83,113,113	2.88	31 (37%)
24	CLA	B	612	2	69,73,73	2.04	21 (30%)	83,113,113	2.81	29 (34%)
26	BCR	b	618	-	41,41,41	1.00	1 (2%)	56,56,56	1.31	9 (16%)
36	DGD	C	517[A]	-	63,63,67	0.83	2 (3%)	77,77,81	1.20	8 (10%)
24	CLA	C	514	3	69,73,73	2.04	20 (28%)	83,113,113	2.84	31 (37%)
28	GOL	c	526[A]	-	5,5,5	1.00	0	5,5,5	0.98	0
28	GOL	a	419	-	5,5,5	1.16	1 (20%)	5,5,5	0.94	0
25	PHO	A	417[A]	-	58,69,69	2.79	15 (25%)	56,99,99	2.85	15 (26%)
39	HEM	e	101	6,5	50,50,50	1.49	6 (12%)	66,82,82	1.79	15 (22%)
26	BCR	a	410	-	41,41,41	1.08	2 (4%)	56,56,56	1.29	6 (10%)
24	CLA	c	506	3	69,73,73	2.05	17 (24%)	83,113,113	2.72	29 (34%)
28	GOL	o	303	-	5,5,5	1.36	1 (20%)	5,5,5	1.00	0
30	PL9	D	405[B]	-	55,55,55	0.61	1 (1%)	68,69,69	1.62	16 (23%)
35	LMG	d	412	40	51,51,55	0.89	2 (3%)	59,59,63	1.08	5 (8%)
24	CLA	b	616	2	69,73,73	2.02	19 (27%)	83,113,113	2.91	30 (36%)
26	BCR	B	618	-	41,41,41	0.97	1 (2%)	56,56,56	1.45	11 (19%)
24	CLA	d	403[B]	4	69,73,73	2.01	20 (28%)	83,113,113	2.87	31 (37%)
32	LMT	M	102	-	36,36,36	1.17	3 (8%)	47,47,47	1.17	3 (6%)
32	LMT	B	630	-	25,25,36	0.89	2 (8%)	30,30,47	1.13	3 (10%)
24	CLA	C	509	3	69,73,73	2.05	20 (28%)	83,113,113	2.69	28 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	GOL	D	412	-	5,5,5	1.43	1 (20%)	5,5,5	0.74	0
24	CLA	A	405[B]	1	69,73,73	2.13	20 (28%)	83,113,113	2.83	34 (40%)
35	LMG	c	521	-	51,51,55	1.01	2 (3%)	59,59,63	1.33	6 (10%)
35	LMG	c	520	-	51,51,55	0.91	2 (3%)	59,59,63	1.11	6 (10%)
24	CLA	B	616	2	69,73,73	1.98	21 (30%)	83,113,113	2.87	28 (33%)
33	LHG	D	407[A]	-	48,48,48	0.93	2 (4%)	51,54,54	1.02	3 (5%)
35	LMG	C	521	-	51,51,55	1.09	3 (5%)	59,59,63	1.34	6 (10%)
30	PL9	d	406[B]	-	55,55,55	0.64	2 (3%)	68,69,69	1.65	18 (26%)
36	DGD	C	519	-	63,63,67	0.86	3 (4%)	77,77,81	1.07	5 (6%)
26	BCR	C	515	-	41,41,41	1.03	1 (2%)	56,56,56	1.34	7 (12%)
34	HTG	b	624	-	19,19,19	1.02	2 (10%)	23,24,24	1.56	3 (13%)
25	PHO	a	408[A]	-	58,69,69	2.74	13 (22%)	56,99,99	2.81	14 (25%)
26	BCR	K	102	-	41,41,41	1.07	1 (2%)	56,56,56	1.50	12 (21%)
33	LHG	L	101[A]	-	48,48,48	0.88	2 (4%)	51,54,54	1.15	4 (7%)
24	CLA	B	603	2	69,73,73	1.99	20 (28%)	83,113,113	2.85	30 (36%)
24	CLA	C	503	3	69,73,73	2.03	20 (28%)	83,113,113	2.76	29 (34%)
24	CLA	b	615	2	69,73,73	2.03	18 (26%)	83,113,113	2.83	31 (37%)
24	CLA	d	403[A]	4	69,73,73	1.95	20 (28%)	83,113,113	2.76	32 (38%)
25	PHO	A	408[A]	-	58,69,69	2.66	12 (20%)	56,99,99	2.81	14 (25%)
24	CLA	B	607	42	69,73,73	2.00	20 (28%)	83,113,113	2.90	31 (37%)
24	CLA	b	601	42	69,73,73	2.09	19 (27%)	83,113,113	2.83	29 (34%)
25	PHO	A	417[B]	-	58,69,69	2.79	14 (24%)	56,99,99	2.82	15 (26%)
27	SQD	a	413	-	53,54,54	1.05	4 (7%)	62,65,65	1.23	8 (12%)
35	LMG	a	417	-	51,51,55	0.92	2 (3%)	59,59,63	1.23	4 (6%)
36	DGD	h	102	-	63,63,67	0.87	3 (4%)	77,77,81	1.21	7 (9%)
24	CLA	a	406[A]	42	69,73,73	2.04	17 (24%)	83,113,113	2.86	32 (38%)
24	CLA	c	512	3	69,73,73	2.09	21 (30%)	83,113,113	2.77	31 (37%)
26	BCR	c	515	-	41,41,41	1.00	1 (2%)	56,56,56	1.58	14 (25%)
34	HTG	B	624	-	19,19,19	1.17	2 (10%)	23,24,24	1.14	2 (8%)
35	LMG	Z	101	-	37,37,55	1.01	2 (5%)	45,45,63	1.44	6 (13%)
26	BCR	Y	101	-	41,41,41	0.96	1 (2%)	56,56,56	1.74	14 (25%)
28	GOL	l	801[A]	-	5,5,5	0.93	0	5,5,5	0.98	0
33	LHG	D	406[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.01	3 (5%)
24	CLA	C	508	42	69,73,73	1.97	19 (27%)	83,113,113	2.77	30 (36%)
36	DGD	C	518[A]	-	63,63,67	0.90	3 (4%)	77,77,81	1.03	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	SQD	A	413	-	53,54,54	1.03	3 (5%)	62,65,65	1.35	8 (12%)
33	LHG	D	407[B]	-	48,48,48	0.92	2 (4%)	51,54,54	0.99	3 (5%)
26	BCR	H	101	-	41,41,41	0.99	1 (2%)	56,56,56	1.52	9 (16%)
26	BCR	C	516	-	41,41,41	0.99	1 (2%)	56,56,56	1.35	7 (12%)
26	BCR	t	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.65	11 (19%)
24	CLA	B	610	42	69,73,73	2.03	19 (27%)	83,113,113	2.88	31 (37%)
24	CLA	C	505	42	69,73,73	1.95	19 (27%)	83,113,113	2.79	28 (33%)
24	CLA	a	409	1	69,73,73	2.03	18 (26%)	83,113,113	3.00	31 (37%)
28	GOL	a	412	-	5,5,5	0.96	0	5,5,5	0.96	0
25	PHO	a	408[B]	-	58,69,69	2.70	13 (22%)	56,99,99	2.84	18 (32%)
34	HTG	V	202	-	11,11,19	0.32	0	15,15,24	1.10	1 (6%)
24	CLA	D	403	4	69,73,73	2.10	18 (26%)	83,113,113	2.75	31 (37%)
24	CLA	C	512	3	69,73,73	2.03	21 (30%)	83,113,113	2.75	29 (34%)
36	DGD	c	519	-	63,63,67	0.88	3 (4%)	77,77,81	1.09	5 (6%)
33	LHG	L	101[B]	-	48,48,48	0.93	2 (4%)	51,54,54	1.14	5 (9%)
25	PHO	A	408[B]	-	58,69,69	2.74	15 (25%)	56,99,99	2.77	16 (28%)
32	LMT	B	627	-	36,36,36	1.15	4 (11%)	47,47,47	1.30	5 (10%)
32	LMT	A	421	-	36,36,36	1.05	2 (5%)	47,47,47	1.16	4 (8%)
26	BCR	B	617	-	41,41,41	1.05	1 (2%)	56,56,56	1.38	9 (16%)
28	GOL	C	523[B]	-	5,5,5	1.18	0	5,5,5	0.85	0
24	CLA	b	614	2	69,73,73	2.01	19 (27%)	83,113,113	2.97	30 (36%)
38	BCT	D	401[A]	22	2,3,3	0.64	0	2,3,3	1.30	0
32	LMT	M	104	-	36,36,36	1.06	3 (8%)	47,47,47	1.08	2 (4%)
34	HTG	b	621	-	19,19,19	1.26	2 (10%)	23,24,24	2.09	7 (30%)
24	CLA	C	513	3	69,73,73	2.04	20 (28%)	83,113,113	2.91	33 (39%)
24	CLA	B	604	2	69,73,73	2.00	22 (31%)	83,113,113	2.63	31 (37%)
24	CLA	a	406[B]	42	69,73,73	2.04	17 (24%)	83,113,113	2.79	30 (36%)
24	CLA	A	407[A]	42	69,73,73	2.04	19 (27%)	83,113,113	2.85	32 (38%)
28	GOL	b	623	-	5,5,5	1.20	1 (20%)	5,5,5	0.84	0
24	CLA	D	402[A]	4	69,73,73	2.00	20 (28%)	83,113,113	2.86	32 (38%)
28	GOL	l	801[B]	-	5,5,5	0.88	0	5,5,5	0.96	0
33	LHG	A	420[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.27	6 (11%)
33	LHG	D	406[B]	-	48,48,48	0.89	2 (4%)	51,54,54	0.99	3 (5%)

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
33	LHG	d	407[A]	-	-	13/53/53/53	-
28	GOL	A	419	-	-	0/4/4/4	-
36	DGD	C	518[B]	-	-	14/51/91/95	0/2/2/2
24	CLA	C	511	3	-	14/39/115/115	-
28	GOL	B	623	-	-	4/4/4/4	-
27	SQD	f	101	-	-	11/38/58/69	0/1/1/1
28	GOL	O	303	-	-	1/4/4/4	-
30	PL9	a	415[A]	-	-	14/53/73/73	0/1/1/1
28	GOL	a	418	-	-	2/4/4/4	-
28	GOL	C	523[A]	-	-	0/4/4/4	-
28	GOL	v	202[B]	-	-	2/4/4/4	-
28	GOL	d	413	-	-	2/4/4/4	-
34	HTG	C	522	-	-	0/10/30/30	0/1/1/1
24	CLA	B	602	2	-	7/39/115/115	-
33	LHG	a	420[A]	-	-	16/46/46/53	-
24	CLA	A	406[A]	42	-	3/39/115/115	-
33	LHG	d	408[A]	-	-	13/53/53/53	-
26	BCR	h	101	-	-	2/29/63/63	0/2/2/2
24	CLA	B	608	2	-	4/39/115/115	-
24	CLA	A	409	1	-	8/39/115/115	-
24	CLA	c	511	3	-	11/39/115/115	-
28	GOL	B	626	-	-	2/4/4/4	-
32	LMT	t	101	-	-	9/17/38/61	0/1/1/2
34	HTG	B	622	-	-	3/10/30/30	0/1/1/1
34	HTG	c	522	-	-	2/10/30/30	0/1/1/1
24	CLA	B	601	42	-	11/39/115/115	-
24	CLA	A	407[B]	42	-	6/39/115/115	-
27	SQD	X	101	-	-	15/38/58/69	0/1/1/1
24	CLA	D	402[B]	4	-	2/39/115/115	-
27	SQD	a	411[B]	-	-	11/49/69/69	0/1/1/1
33	LHG	A	420[B]	-	-	12/53/53/53	-
30	PL9	A	415[A]	-	-	15/53/73/73	0/1/1/1
33	LHG	d	407[B]	-	-	17/53/53/53	-
24	CLA	B	613	2	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	v	202[A]	-	-	2/4/4/4	-
24	CLA	c	510	3	-	15/39/115/115	-
24	CLA	b	611	2	-	2/39/115/115	-
25	PHO	d	402[A]	-	-	1/37/103/103	0/5/6/6
30	PL9	a	415[B]	-	-	14/53/73/73	0/1/1/1
24	CLA	B	609	2	-	1/39/115/115	-
35	LMG	D	411	40	-	10/46/66/70	0/1/1/1
24	CLA	a	407[B]	42	-	8/39/115/115	-
24	CLA	c	504	3	-	3/39/115/115	-
24	CLA	b	604	2	-	11/39/115/115	-
24	CLA	b	602	2	-	4/39/115/115	-
24	CLA	C	504	3	-	2/39/115/115	-
39	HEM	F	102	6,5	-	4/14/54/54	-
41	HEC	v	201	16	1/1/3/7	6/14/54/54	-
32	LMT	b	620	-	-	8/17/37/61	0/1/1/2
28	GOL	b	627	-	-	0/4/4/4	-
24	CLA	A	406[B]	42	-	4/39/115/115	-
24	CLA	c	513	3	-	13/39/115/115	-
24	CLA	b	608	2	-	7/39/115/115	-
28	GOL	V	203[A]	-	-	2/4/4/4	-
32	LMT	A	418	-	-	7/21/61/61	0/2/2/2
33	LHG	E	101[A]	-	-	22/46/46/53	-
33	LHG	a	420[B]	-	-	16/46/46/53	-
33	LHG	b	628[A]	-	-	14/53/53/53	-
33	LHG	d	408[B]	-	-	12/53/53/53	-
34	HTG	b	622	-	-	3/10/30/30	0/1/1/1
32	LMT	F	101	-	-	8/21/61/61	0/2/2/2
24	CLA	C	510	3	-	7/39/115/115	-
26	BCR	b	619	-	-	5/29/63/63	0/2/2/2
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
24	CLA	B	615	2	-	6/39/115/115	-
26	BCR	A	410	-	-	0/29/63/63	0/2/2/2
35	LMG	b	629	-	-	10/46/66/70	0/1/1/1
36	DGD	c	517[A]	-	-	18/51/91/95	0/2/2/2
24	CLA	c	514	3	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	a	407[A]	42	-	8/39/115/115	-
30	PL9	A	415[B]	-	-	14/53/73/73	0/1/1/1
36	DGD	c	518[B]	-	-	15/51/91/95	0/2/2/2
24	CLA	C	502	3	-	6/39/115/115	-
27	SQD	L	102	-	-	19/49/69/69	0/1/1/1
35	LMG	C	520	-	-	10/46/66/70	0/1/1/1
24	CLA	a	405[A]	1	-	4/39/115/115	-
26	BCR	T	101	-	-	1/29/63/63	0/2/2/2
32	LMT	B	628	-	-	13/21/61/61	0/2/2/2
26	BCR	D	404	-	-	4/29/63/63	0/2/2/2
32	LMT	c	501	-	-	11/21/61/61	0/2/2/2
26	BCR	y	101	-	-	3/29/63/63	0/2/2/2
25	PHO	d	402[B]	-	-	1/37/103/103	0/5/6/6
24	CLA	b	609	2	-	2/39/115/115	-
34	HTG	D	410	-	-	3/7/27/30	0/1/1/1
26	BCR	d	405	-	-	5/29/63/63	0/2/2/2
24	CLA	b	613	2	-	5/39/115/115	-
24	CLA	C	507	3	-	11/39/115/115	-
28	GOL	O	302	-	-	2/4/4/4	-
32	LMT	e	102	-	-	14/21/61/61	0/2/2/2
33	LHG	d	414[A]	-	-	17/53/53/53	-
24	CLA	c	509	3	-	6/39/115/115	-
24	CLA	d	404	4	-	8/39/115/115	-
34	HTG	d	411	-	-	1/7/27/30	0/1/1/1
33	LHG	E	101[B]	-	-	19/46/46/53	-
28	GOL	V	203[B]	-	-	4/4/4/4	-
27	SQD	A	411[A]	-	-	12/49/69/69	0/1/1/1
35	LMG	C	501	-	-	17/46/66/70	0/1/1/1
33	LHG	b	628[B]	-	-	18/53/53/53	-
24	CLA	C	506	3	-	8/39/115/115	-
41	HEC	V	201	16	1/1/3/7	6/14/54/54	-
26	BCR	c	516	-	-	0/29/63/63	0/2/2/2
28	GOL	c	527	-	-	3/4/4/4	-
36	DGD	c	518[A]	-	-	16/51/91/95	0/2/2/2
24	CLA	b	606	2	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SQD	a	411[A]	-	-	9/49/69/69	0/1/1/1
24	CLA	c	507	3	-	9/39/115/115	-
24	CLA	B	611	2	-	4/39/115/115	-
35	LMG	z	101	-	-	8/34/54/70	0/1/1/1
36	DGD	c	517[B]	-	-	16/51/91/95	0/2/2/2
24	CLA	c	503	3	-	8/39/115/115	-
26	BCR	b	617	-	-	2/29/63/63	0/2/2/2
32	LMT	m	102	-	-	6/21/61/61	0/2/2/2
28	GOL	o	302	-	-	4/4/4/4	-
30	PL9	D	405[A]	-	-	6/53/73/73	0/1/1/1
24	CLA	a	405[B]	1	-	5/39/115/115	-
36	DGD	C	517[B]	-	-	17/51/91/95	0/2/2/2
24	CLA	B	606	2	-	6/39/115/115	-
24	CLA	b	605	2	-	10/39/115/115	-
24	CLA	b	612	2	-	5/39/115/115	-
28	GOL	c	526[B]	-	-	0/4/4/4	-
24	CLA	b	607	42	-	3/39/115/115	-
28	GOL	A	412	-	-	2/4/4/4	-
24	CLA	B	614	2	-	14/39/115/115	-
34	HTG	B	621	-	-	4/10/30/30	0/1/1/1
27	SQD	B	620	-	-	14/49/69/69	0/1/1/1
35	LMG	M	101	-	-	18/46/66/70	0/1/1/1
36	DGD	H	102	-	-	10/51/91/95	0/2/2/2
24	CLA	c	502	3	-	4/39/115/115	-
24	CLA	A	405[A]	1	-	3/39/115/115	-
33	LHG	d	414[B]	-	-	10/53/53/53	-
24	CLA	c	508	42	-	8/39/115/115	-
26	BCR	k	101	-	-	1/29/63/63	0/2/2/2
27	SQD	A	411[B]	-	-	11/49/69/69	0/1/1/1
30	PL9	d	406[A]	-	-	7/53/73/73	0/1/1/1
24	CLA	b	603	2	-	9/39/115/115	-
24	CLA	B	605	2	-	7/39/115/115	-
32	LMT	b	626	-	-	11/17/37/61	0/1/1/2
24	CLA	b	610	42	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	505	42	-	6/39/115/115	-
24	CLA	B	612	2	-	4/39/115/115	-
26	BCR	b	618	-	-	0/29/63/63	0/2/2/2
36	DGD	C	517[A]	-	-	14/51/91/95	0/2/2/2
24	CLA	C	514	3	-	6/39/115/115	-
28	GOL	c	526[A]	-	-	0/4/4/4	-
28	GOL	a	419	-	-	2/4/4/4	-
25	PHO	A	417[A]	-	-	1/37/103/103	0/5/6/6
39	HEM	e	101	6,5	-	6/14/54/54	-
26	BCR	a	410	-	-	3/29/63/63	0/2/2/2
24	CLA	c	506	3	-	6/39/115/115	-
28	GOL	o	303	-	-	2/4/4/4	-
30	PL9	D	405[B]	-	-	7/53/73/73	0/1/1/1
35	LMG	d	412	40	-	12/46/66/70	0/1/1/1
24	CLA	b	616	2	-	9/39/115/115	-
26	BCR	B	618	-	-	0/29/63/63	0/2/2/2
24	CLA	d	403[B]	4	-	4/39/115/115	-
32	LMT	M	102	-	-	4/21/61/61	0/2/2/2
32	LMT	B	630	-	-	11/17/37/61	0/1/1/2
24	CLA	C	509	3	-	5/39/115/115	-
28	GOL	D	412	-	-	4/4/4/4	-
24	CLA	A	405[B]	1	-	5/39/115/115	-
35	LMG	c	521	-	-	11/46/66/70	0/1/1/1
35	LMG	c	520	-	-	12/46/66/70	0/1/1/1
24	CLA	B	616	2	-	5/39/115/115	-
33	LHG	D	407[A]	-	-	14/53/53/53	-
35	LMG	C	521	-	-	11/46/66/70	0/1/1/1
30	PL9	d	406[B]	-	-	8/53/73/73	0/1/1/1
36	DGD	C	519	-	-	17/51/91/95	0/2/2/2
26	BCR	C	515	-	-	0/29/63/63	0/2/2/2
34	HTG	b	624	-	-	4/10/30/30	0/1/1/1
25	PHO	a	408[A]	-	-	6/37/103/103	0/5/6/6
26	BCR	K	102	-	-	2/29/63/63	0/2/2/2
33	LHG	L	101[A]	-	-	20/53/53/53	-
24	CLA	B	603	2	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	503	3	-	7/39/115/115	-
24	CLA	b	615	2	-	8/39/115/115	-
24	CLA	d	403[A]	4	-	4/39/115/115	-
25	PHO	A	408[A]	-	-	3/37/103/103	0/5/6/6
24	CLA	B	607	42	-	3/39/115/115	-
24	CLA	b	601	42	-	19/39/115/115	-
25	PHO	A	417[B]	-	-	4/37/103/103	0/5/6/6
27	SQD	a	413	-	-	14/49/69/69	0/1/1/1
35	LMG	a	417	-	-	14/46/66/70	0/1/1/1
36	DGD	h	102	-	-	16/51/91/95	0/2/2/2
24	CLA	a	406[A]	42	-	8/39/115/115	-
24	CLA	c	512	3	-	6/39/115/115	-
26	BCR	c	515	-	-	1/29/63/63	0/2/2/2
34	HTG	B	624	-	-	4/10/30/30	0/1/1/1
35	LMG	Z	101	-	-	10/31/51/70	0/1/1/1
26	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
28	GOL	l	801[A]	-	-	1/4/4/4	-
33	LHG	D	406[A]	-	-	17/53/53/53	-
24	CLA	C	508	42	-	6/39/115/115	-
36	DGD	C	518[A]	-	-	13/51/91/95	0/2/2/2
27	SQD	A	413	-	-	12/49/69/69	0/1/1/1
33	LHG	D	407[B]	-	-	14/53/53/53	-
26	BCR	H	101	-	-	2/29/63/63	0/2/2/2
26	BCR	C	516	-	-	0/29/63/63	0/2/2/2
26	BCR	t	102	-	-	0/29/63/63	0/2/2/2
24	CLA	B	610	42	-	11/39/115/115	-
24	CLA	C	505	42	-	7/39/115/115	-
24	CLA	a	409	1	-	13/39/115/115	-
28	GOL	a	412	-	-	4/4/4/4	-
25	PHO	a	408[B]	-	-	4/37/103/103	0/5/6/6
34	HTG	V	202	-	-	0/2/19/30	0/1/1/1
24	CLA	D	403	4	-	16/39/115/115	-
24	CLA	C	512	3	-	3/39/115/115	-
36	DGD	c	519	-	-	9/51/91/95	0/2/2/2
33	LHG	L	101[B]	-	-	16/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PHO	A	408[B]	-	-	6/37/103/103	0/5/6/6
32	LMT	B	627	-	-	10/21/61/61	0/2/2/2
32	LMT	A	421	-	-	16/21/61/61	0/2/2/2
26	BCR	B	617	-	-	2/29/63/63	0/2/2/2
28	GOL	C	523[B]	-	-	0/4/4/4	-
24	CLA	b	614	2	-	14/39/115/115	-
32	LMT	M	104	-	-	6/21/61/61	0/2/2/2
34	HTG	b	621	-	-	3/10/30/30	0/1/1/1
24	CLA	C	513	3	-	11/39/115/115	-
24	CLA	B	604	2	-	4/39/115/115	-
24	CLA	a	406[B]	42	-	6/39/115/115	-
24	CLA	A	407[A]	42	-	5/39/115/115	-
28	GOL	b	623	-	-	2/4/4/4	-
24	CLA	D	402[A]	4	-	2/39/115/115	-
28	GOL	l	801[B]	-	-	1/4/4/4	-
33	LHG	A	420[A]	-	-	14/53/53/53	-
33	LHG	D	406[B]	-	-	15/53/53/53	-

The worst 5 of 1869 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	408[A]	PHO	C1B-C2B	9.21	1.49	1.39
25	d	402[B]	PHO	C1D-C2D	9.05	1.49	1.39
25	A	408[B]	PHO	C1B-C2B	9.03	1.49	1.39
25	A	408[B]	PHO	C1D-C2D	8.95	1.49	1.39
25	A	408[A]	PHO	C1D-C2D	8.89	1.49	1.39

The worst 5 of 3342 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	611	CLA	C2B-C1B-NB	16.44	121.25	110.23
24	B	611	CLA	C3B-C2B-C1B	-13.57	90.78	107.16
25	A	408[A]	PHO	C2D-C1D-ND	11.89	117.73	109.53
24	B	611	CLA	C1D-ND-C4D	-11.73	98.00	106.33
25	A	417[B]	PHO	C2D-C1D-ND	11.48	117.45	109.53

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
41	V	201	HEC	NA
41	v	201	HEC	NA

5 of 1687 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	405[B]	CLA	C2B-C3B-CAB-CBB
24	A	405[B]	CLA	C4B-C3B-CAB-CBB
24	B	614	CLA	CHA-CBD-CGD-O1D
24	B	614	CLA	CHA-CBD-CGD-O2D
24	B	614	CLA	CAD-CBD-CGD-O1D

There are no ring outliers.

169 monomers are involved in 335 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	d	407[A]	LHG	2	0
28	A	419	GOL	3	0
36	C	518[B]	DGD	2	0
24	C	511	CLA	3	0
28	B	623	GOL	2	0
28	O	303	GOL	2	0
30	a	415[A]	PL9	4	0
28	a	418	GOL	1	0
28	v	202[B]	GOL	2	0
33	a	420[A]	LHG	5	0
24	A	406[A]	CLA	1	0
33	d	408[A]	LHG	11	0
26	h	101	BCR	3	0
24	A	409	CLA	2	0
32	t	101	LMT	1	0
34	c	522	HTG	1	0
24	B	601	CLA	3	0
24	A	407[B]	CLA	2	0
27	X	101	SQD	2	0
24	D	402[B]	CLA	3	0
27	a	411[B]	SQD	5	0
33	A	420[B]	LHG	1	0
30	A	415[A]	PL9	11	0
33	d	407[B]	LHG	1	0
24	B	613	CLA	5	0
28	v	202[A]	GOL	1	0
24	c	510	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	d	402[A]	PHO	1	0
30	a	415[B]	PL9	4	0
24	B	609	CLA	2	0
24	a	407[B]	CLA	2	0
21	a	401[B]	OEY	1	0
24	c	504	CLA	3	0
24	b	604	CLA	3	0
24	C	504	CLA	3	0
39	F	102	HEM	1	0
32	b	620	LMT	1	0
28	b	627	GOL	3	0
24	A	406[B]	CLA	5	0
24	c	513	CLA	8	0
24	b	608	CLA	1	0
33	E	101[A]	LHG	4	0
33	a	420[B]	LHG	3	0
33	d	408[B]	LHG	9	0
24	C	510	CLA	2	0
26	b	619	BCR	4	0
26	B	619	BCR	1	0
24	B	615	CLA	5	0
26	A	410	BCR	2	0
35	b	629	LMG	1	0
36	c	517[A]	DGD	1	0
24	c	514	CLA	3	0
24	a	407[A]	CLA	2	0
30	A	415[B]	PL9	8	0
36	c	518[B]	DGD	2	0
24	C	502	CLA	4	0
21	A	401[B]	OEY	1	0
27	L	102	SQD	1	0
24	a	405[A]	CLA	2	0
26	T	101	BCR	6	0
32	B	628	LMT	2	0
26	D	404	BCR	1	0
26	y	101	BCR	1	0
24	b	609	CLA	3	0
26	d	405	BCR	3	0
24	b	613	CLA	1	0
24	C	507	CLA	5	0
28	O	302	GOL	1	0
32	e	102	LMT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	c	509	CLA	7	0
24	d	404	CLA	3	0
33	E	101[B]	LHG	2	0
27	A	411[A]	SQD	1	0
35	C	501	LMG	1	0
33	b	628[B]	LHG	1	0
24	C	506	CLA	3	0
26	c	516	BCR	1	0
36	c	518[A]	DGD	2	0
24	b	606	CLA	2	0
27	a	411[A]	SQD	5	0
24	c	507	CLA	3	0
35	z	101	LMG	2	0
36	c	517[B]	DGD	2	0
24	c	503	CLA	1	0
30	D	405[A]	PL9	1	0
24	a	405[B]	CLA	4	0
36	C	517[B]	DGD	3	0
24	B	606	CLA	1	0
24	b	605	CLA	4	0
24	b	612	CLA	2	0
24	b	607	CLA	1	0
24	B	614	CLA	3	0
34	B	621	HTG	1	0
27	B	620	SQD	1	0
35	M	101	LMG	1	0
24	c	502	CLA	3	0
24	A	405[A]	CLA	2	0
24	c	508	CLA	2	0
26	k	101	BCR	2	0
27	A	411[B]	SQD	1	0
24	b	603	CLA	1	0
24	B	605	CLA	4	0
24	b	610	CLA	1	0
26	b	618	BCR	3	0
36	C	517[A]	DGD	1	0
24	C	514	CLA	1	0
28	a	419	GOL	5	0
25	A	417[A]	PHO	1	0
26	a	410	BCR	1	0
24	c	506	CLA	7	0
35	d	412	LMG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	B	618	BCR	4	0
24	d	403[B]	CLA	3	0
32	M	102	LMT	2	0
32	B	630	LMT	1	0
24	C	509	CLA	3	0
28	D	412	GOL	3	0
24	A	405[B]	CLA	4	0
35	c	521	LMG	2	0
35	c	520	LMG	1	0
24	B	616	CLA	4	0
33	D	407[A]	LHG	3	0
35	C	521	LMG	2	0
26	C	515	BCR	1	0
34	b	624	HTG	1	0
24	B	603	CLA	1	0
24	C	503	CLA	1	0
24	b	615	CLA	3	0
24	d	403[A]	CLA	1	0
25	A	408[A]	PHO	1	0
24	b	601	CLA	1	0
25	A	417[B]	PHO	2	0
35	a	417	LMG	1	0
36	h	102	DGD	1	0
24	a	406[A]	CLA	3	0
24	c	512	CLA	6	0
26	c	515	BCR	2	0
34	B	624	HTG	1	0
35	Z	101	LMG	2	0
26	Y	101	BCR	1	0
28	l	801[A]	GOL	1	0
33	D	406[A]	LHG	2	0
24	C	508	CLA	2	0
36	C	518[A]	DGD	1	0
27	A	413	SQD	1	0
33	D	407[B]	LHG	4	0
26	H	101	BCR	2	0
26	C	516	BCR	1	0
26	t	102	BCR	6	0
24	B	610	CLA	1	0
24	C	505	CLA	1	0
24	a	409	CLA	3	0
25	a	408[B]	PHO	2	0

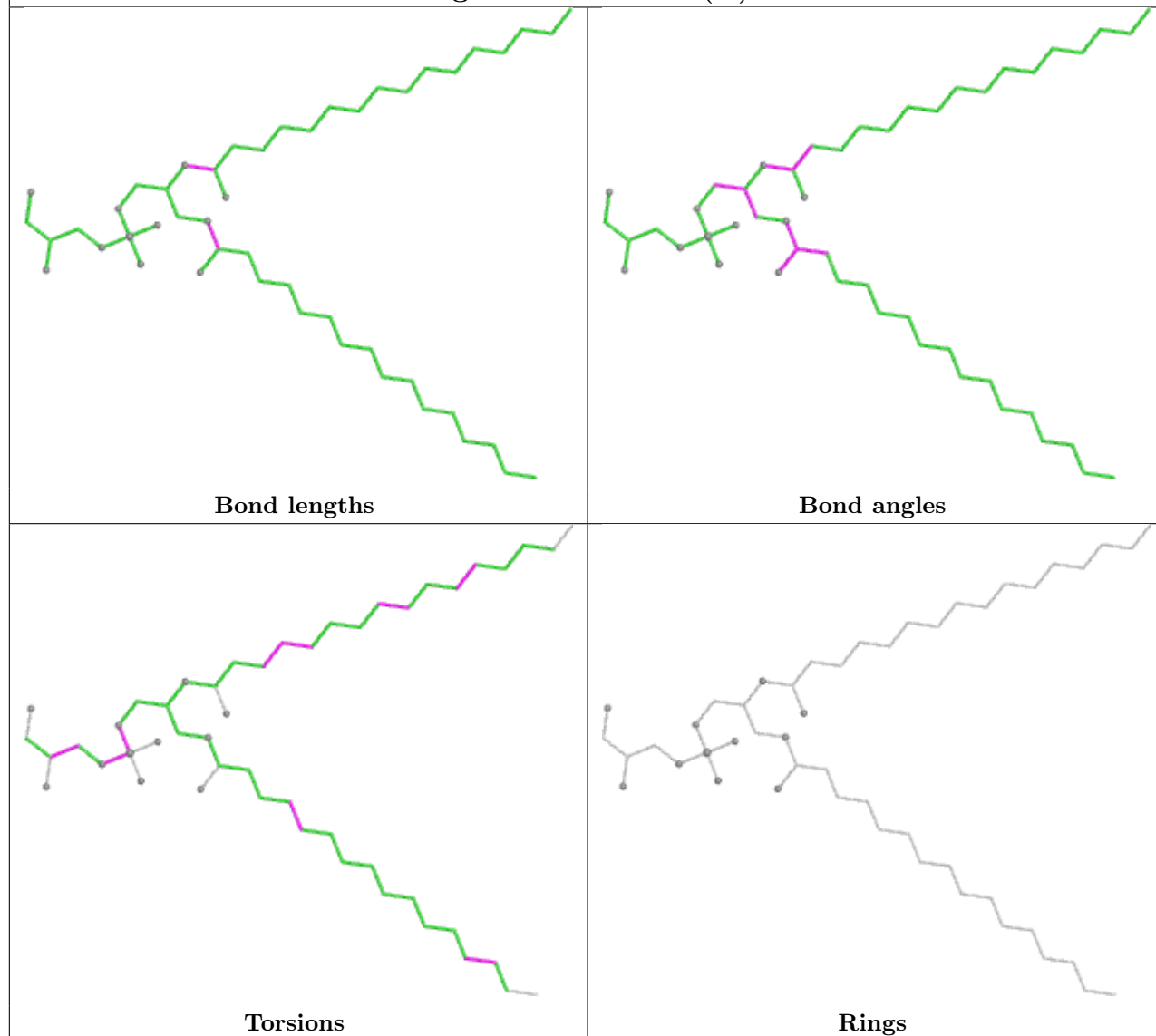
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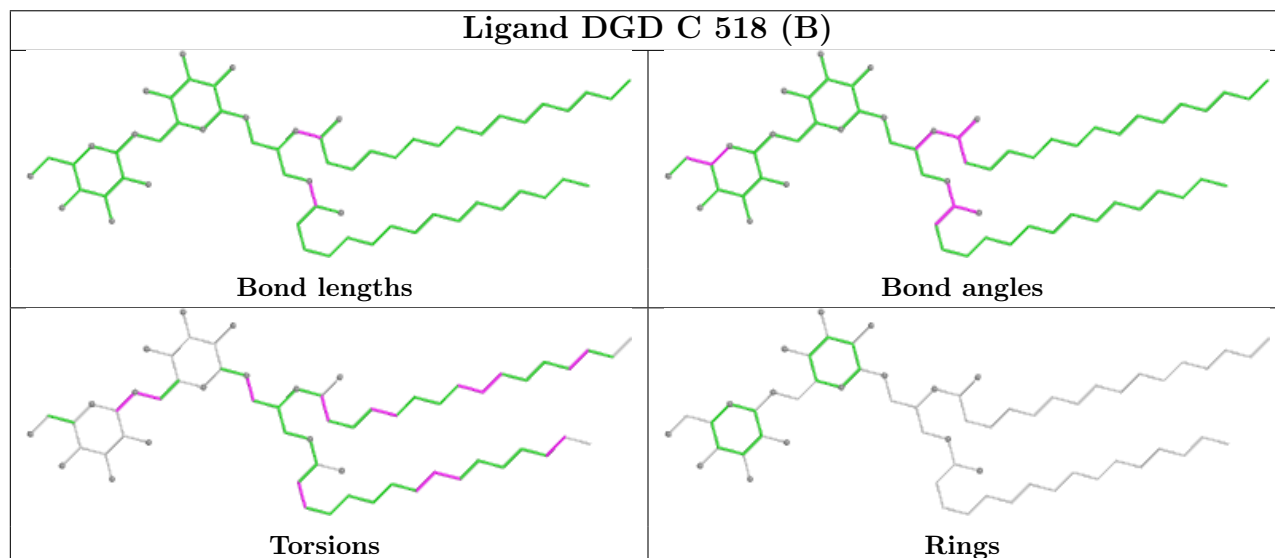
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	512	CLA	3	0
36	c	519	DGD	2	0
25	A	408[B]	PHO	1	0
32	B	627	LMT	1	0
32	A	421	LMT	1	0
26	B	617	BCR	1	0
24	b	614	CLA	2	0
34	b	621	HTG	2	0
24	C	513	CLA	2	0
24	B	604	CLA	2	0
24	a	406[B]	CLA	3	0
24	A	407[A]	CLA	1	0
24	D	402[A]	CLA	3	0
28	l	801[B]	GOL	1	0
33	A	420[A]	LHG	2	0
33	D	406[B]	LHG	1	0

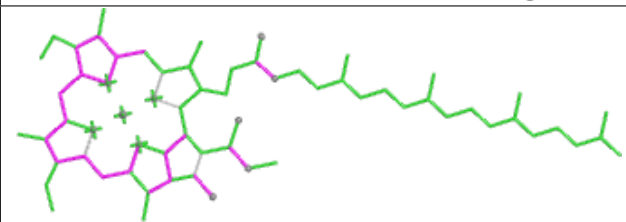
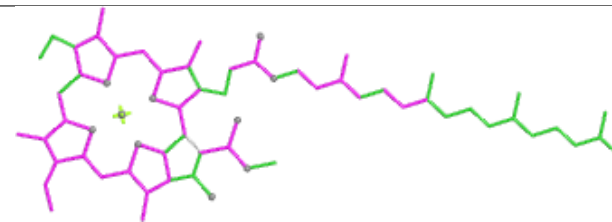
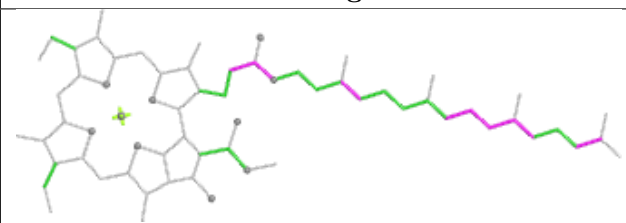
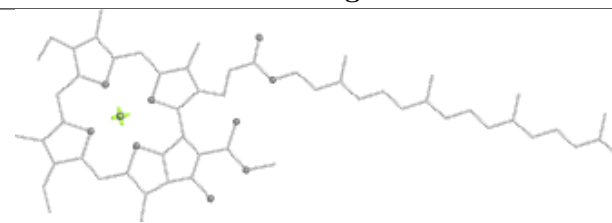
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

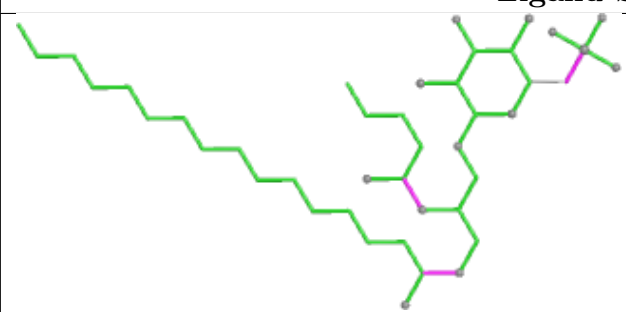
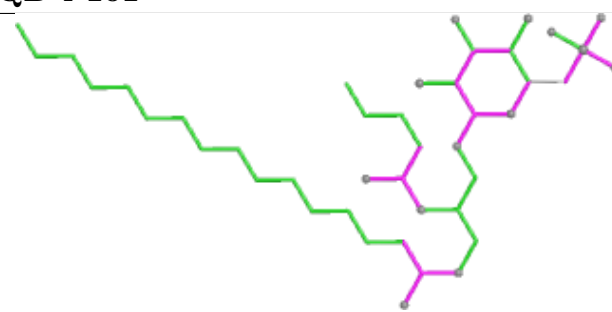
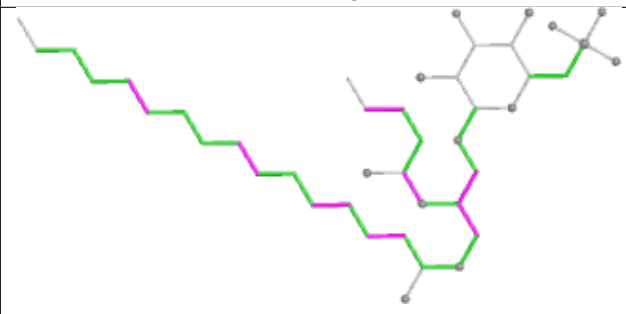
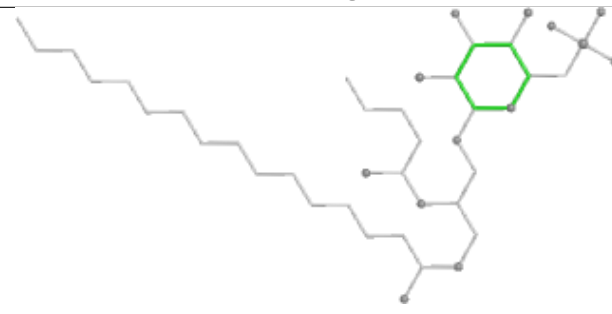
Ligand LHG d 407 (A)

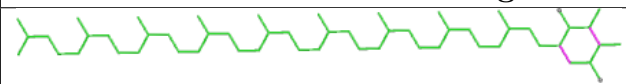
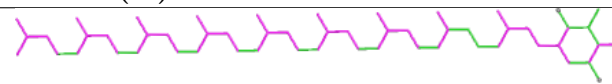
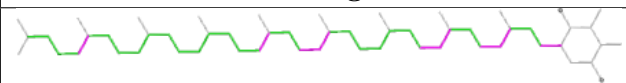
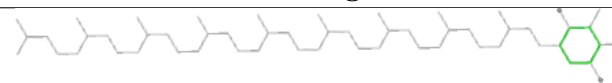


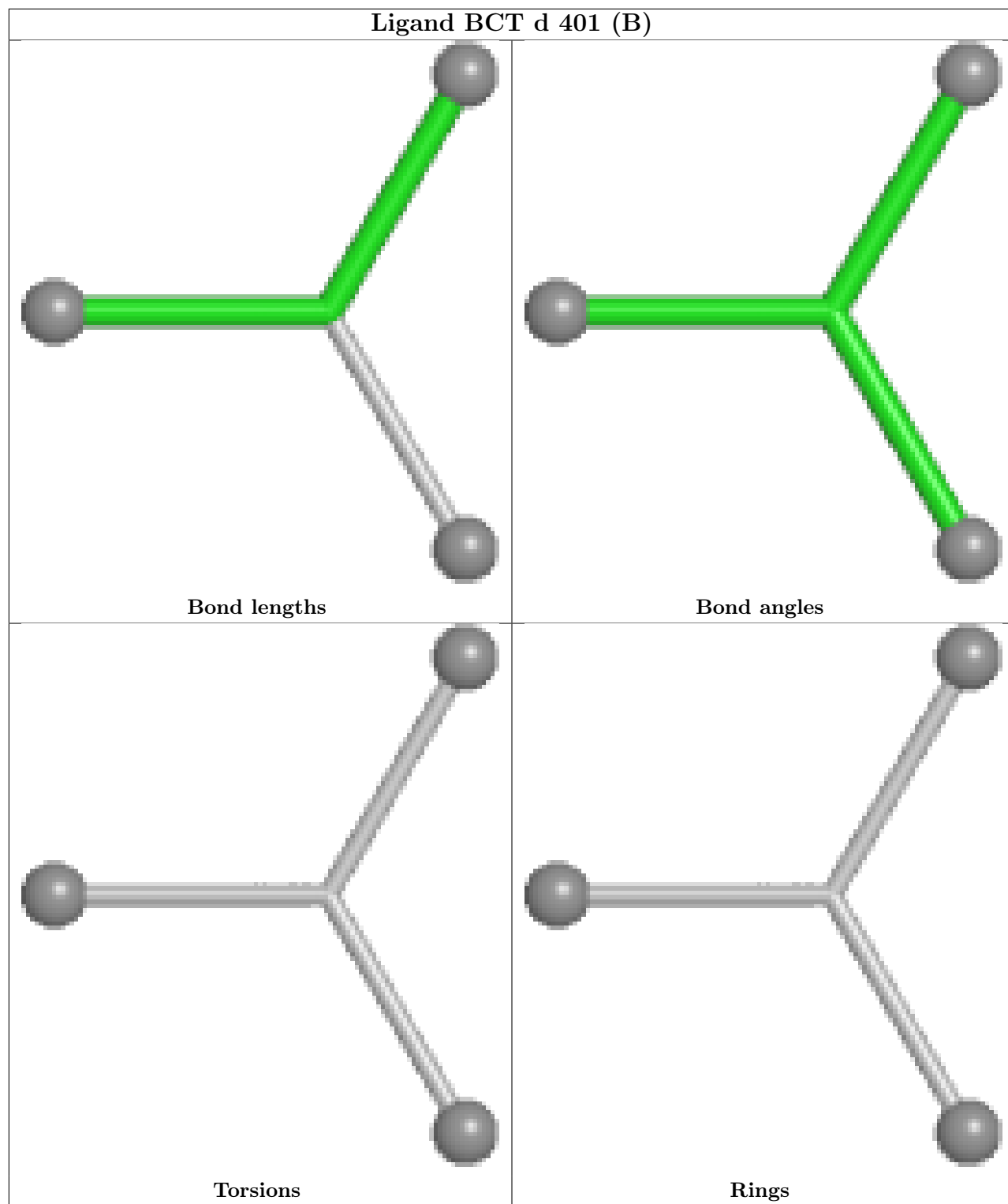
Ligand DGD C 518 (B)



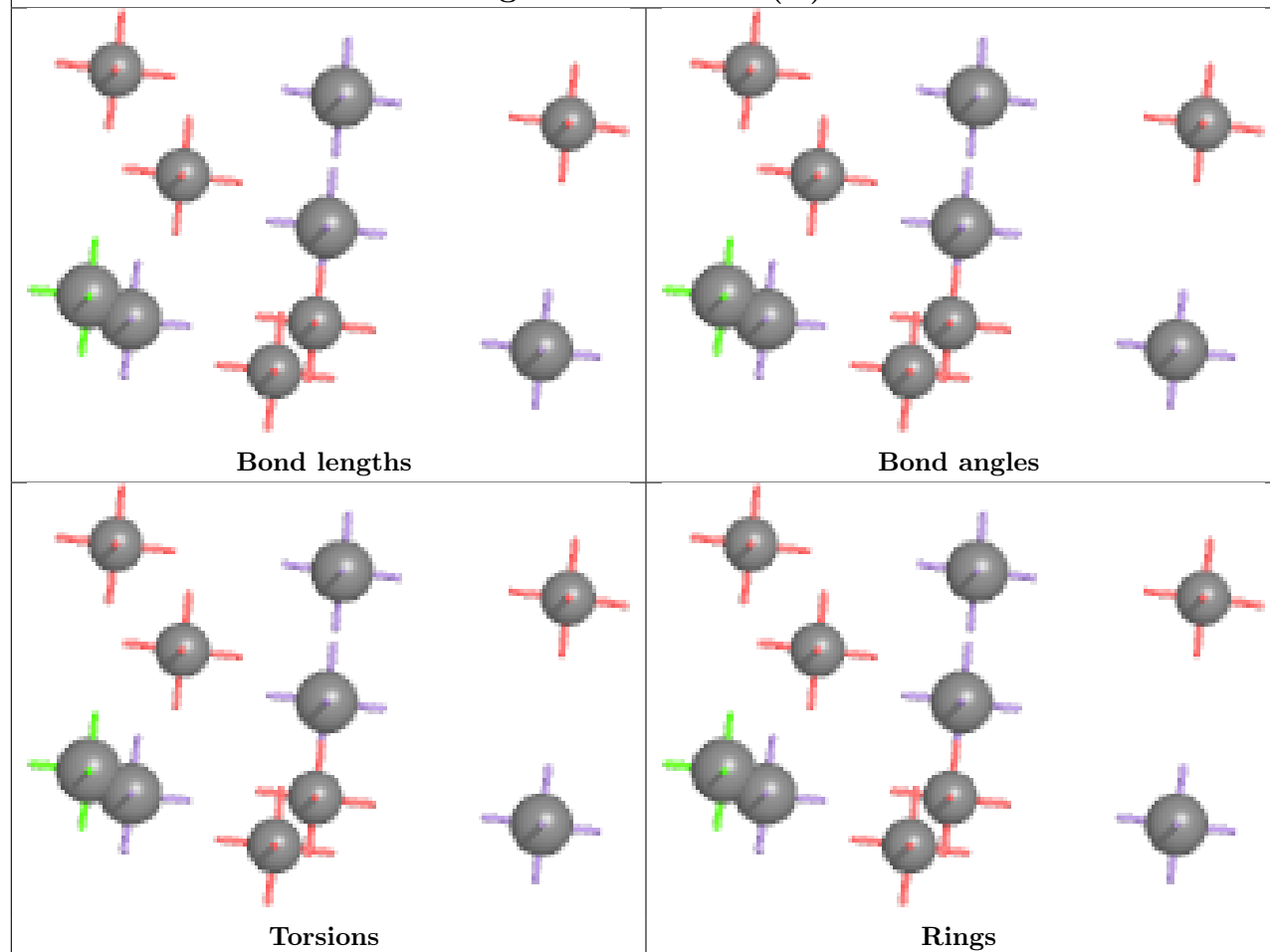
Ligand CLA C 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand SQD f 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

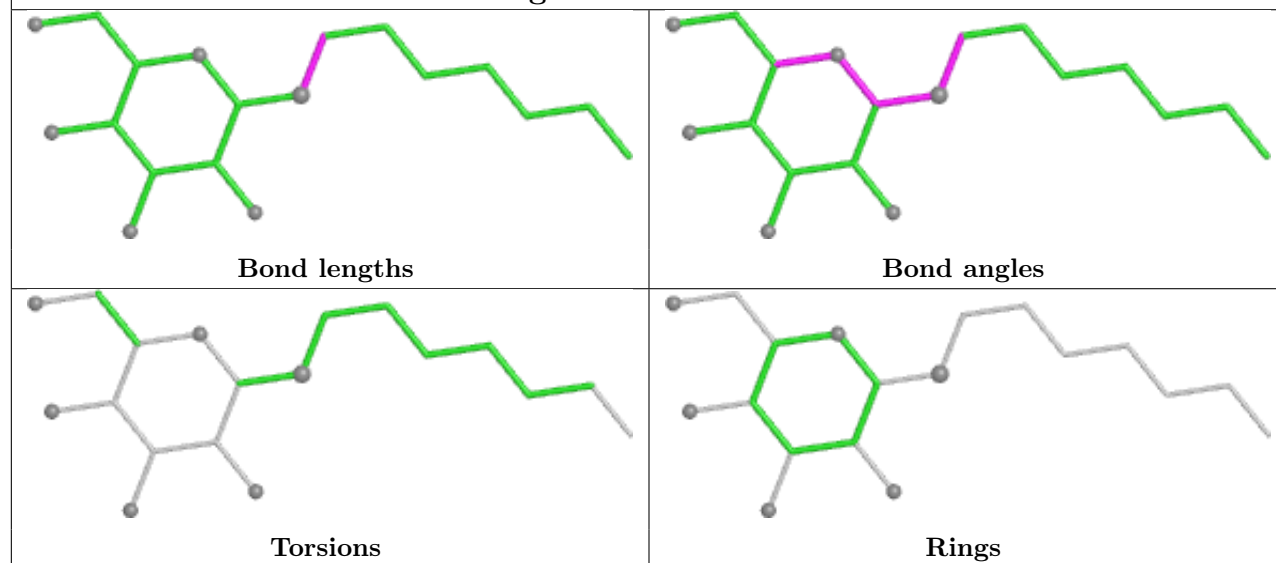
Ligand PL9 a 415 (A)	
	
Bond lengths	Bond angles
	
Torsions	Rings

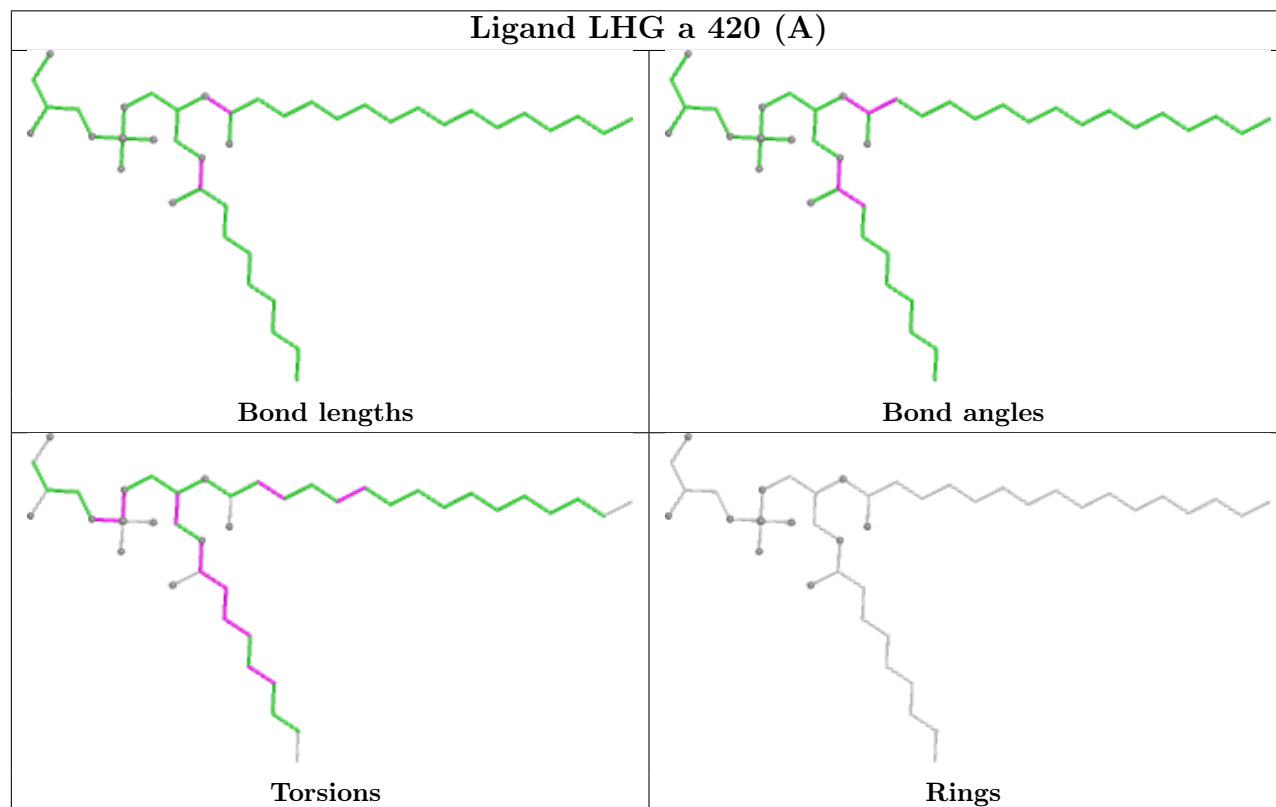
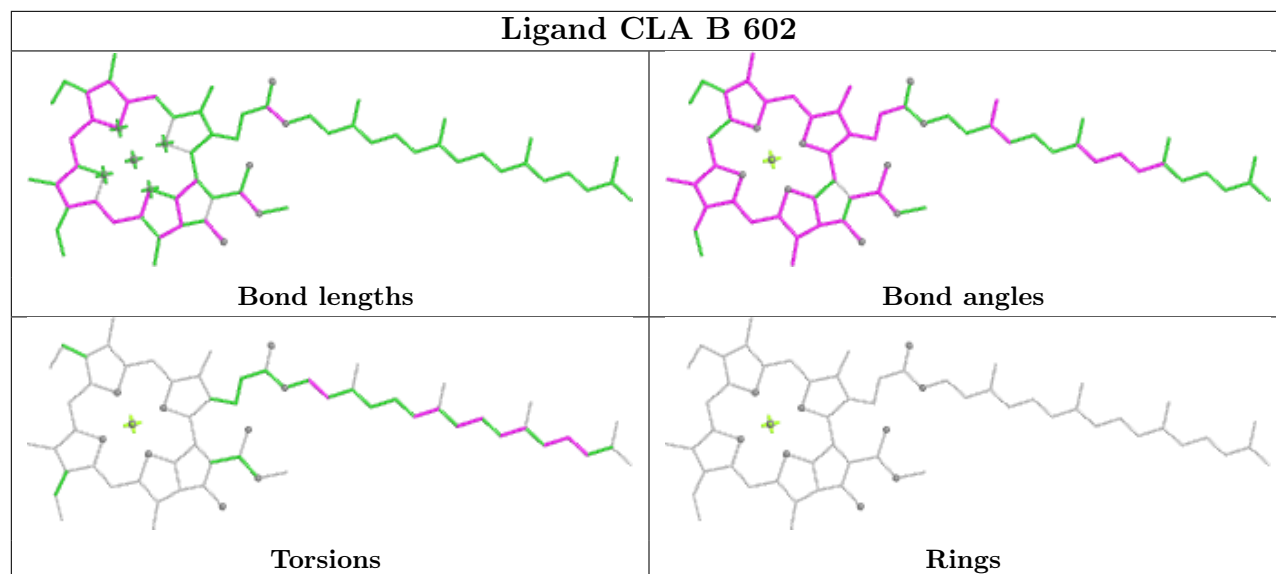


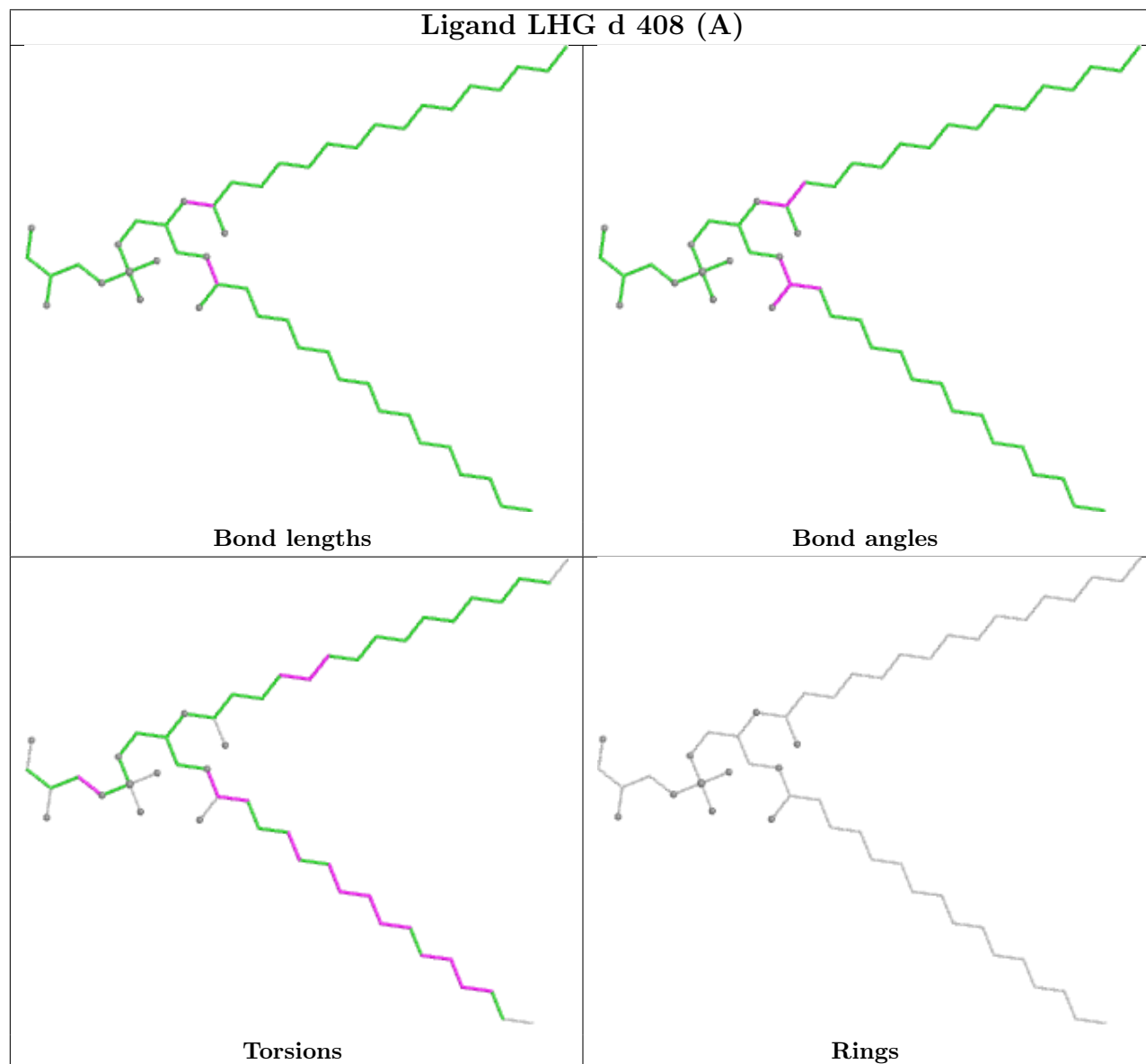
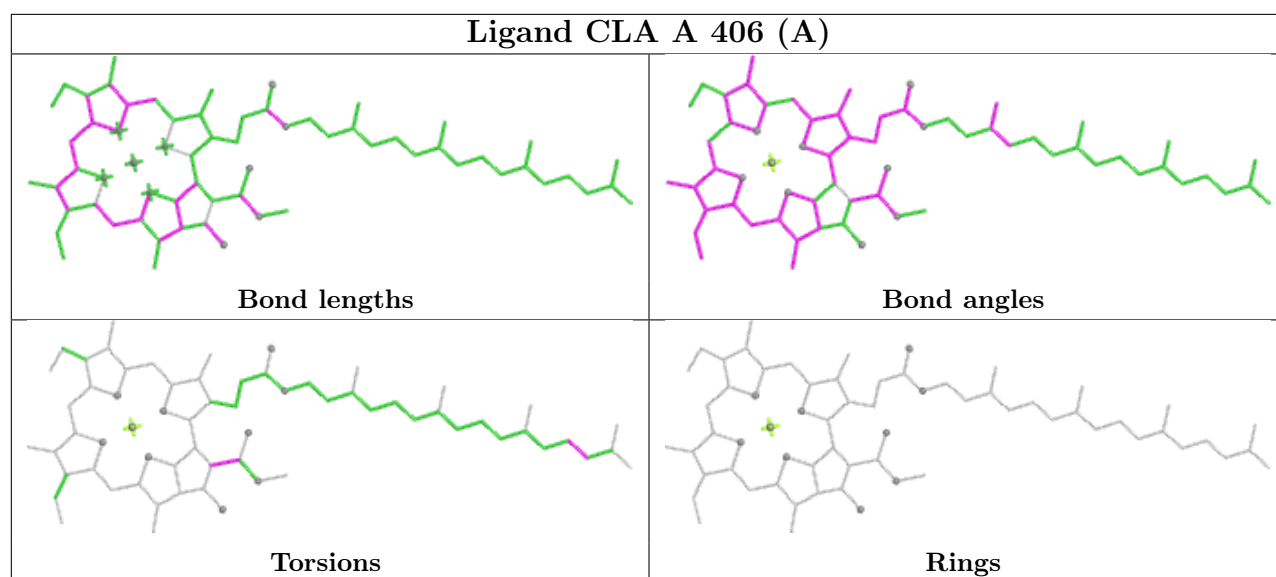
Ligand OEX a 414 (A)

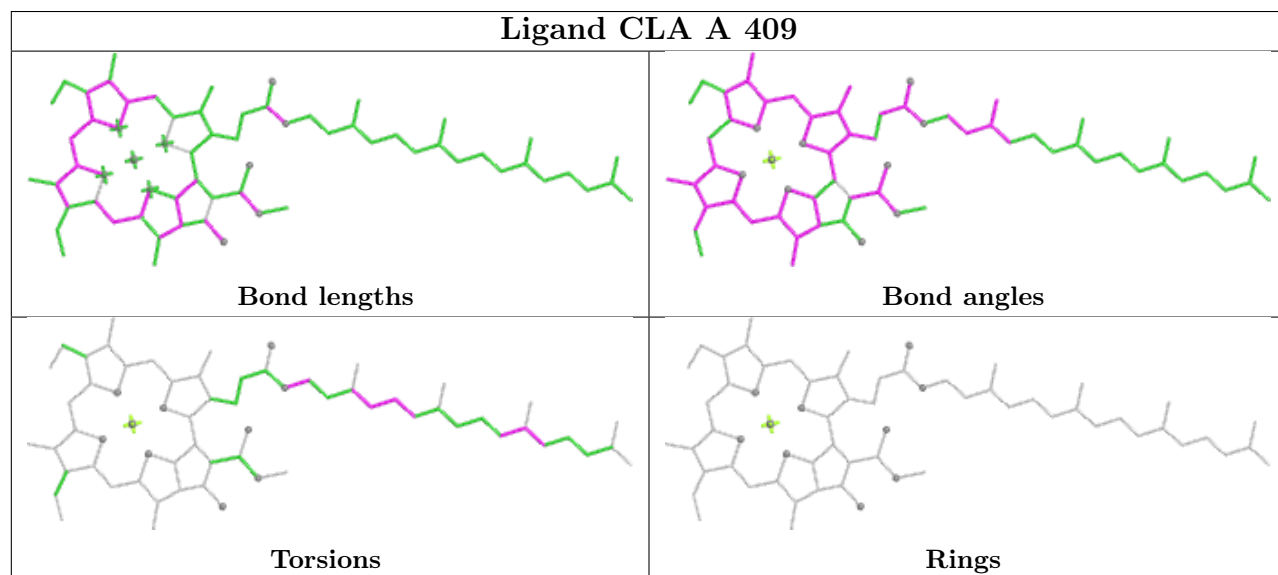
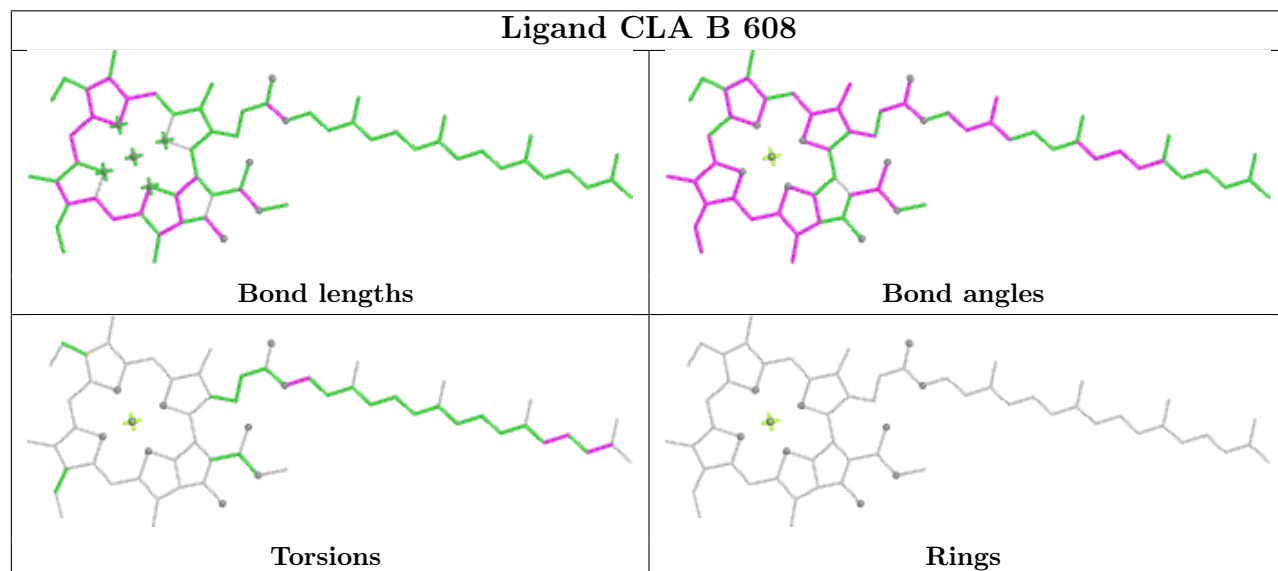
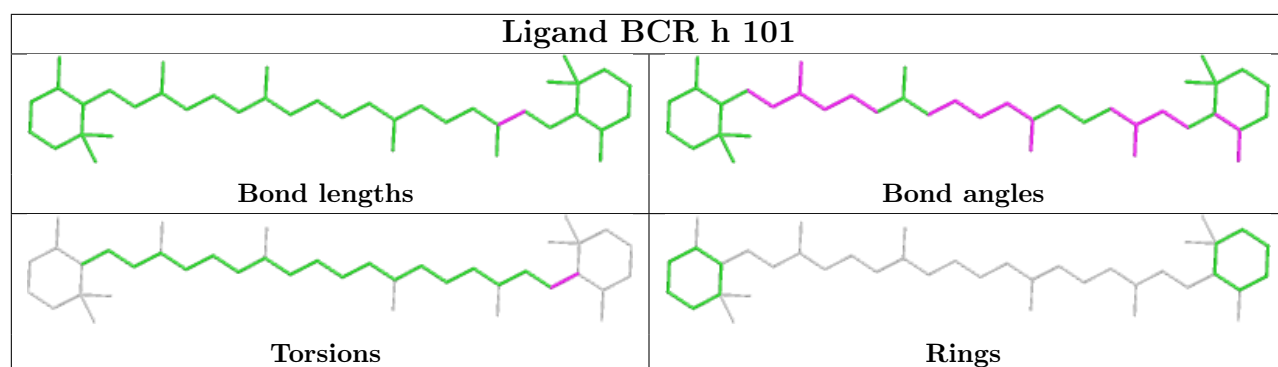


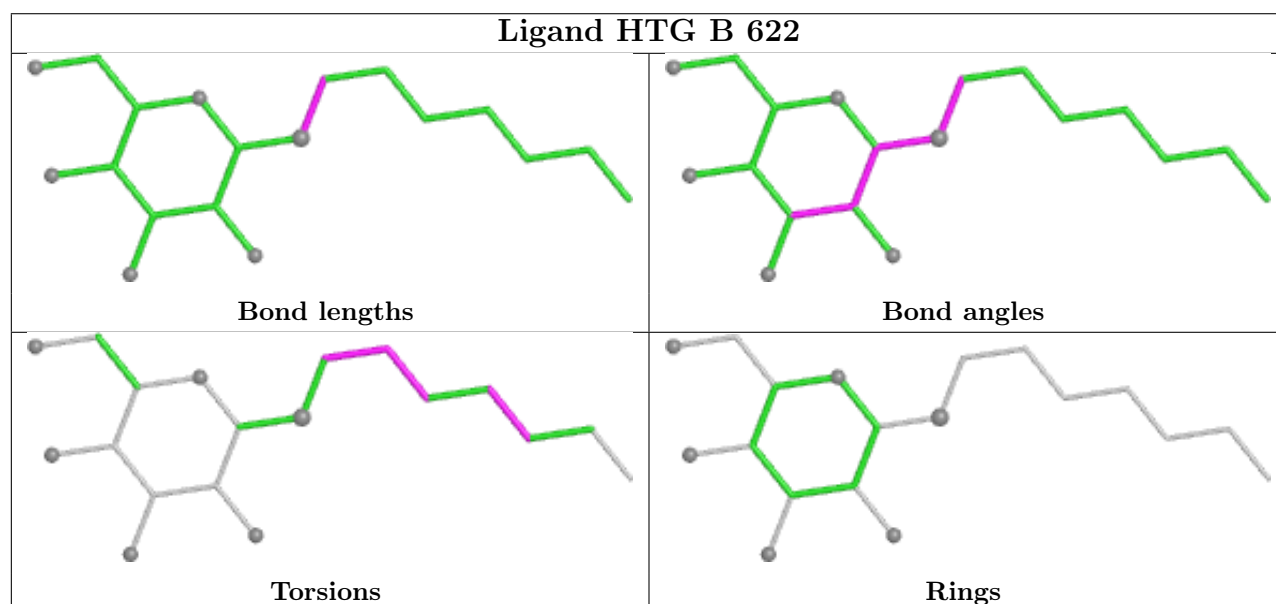
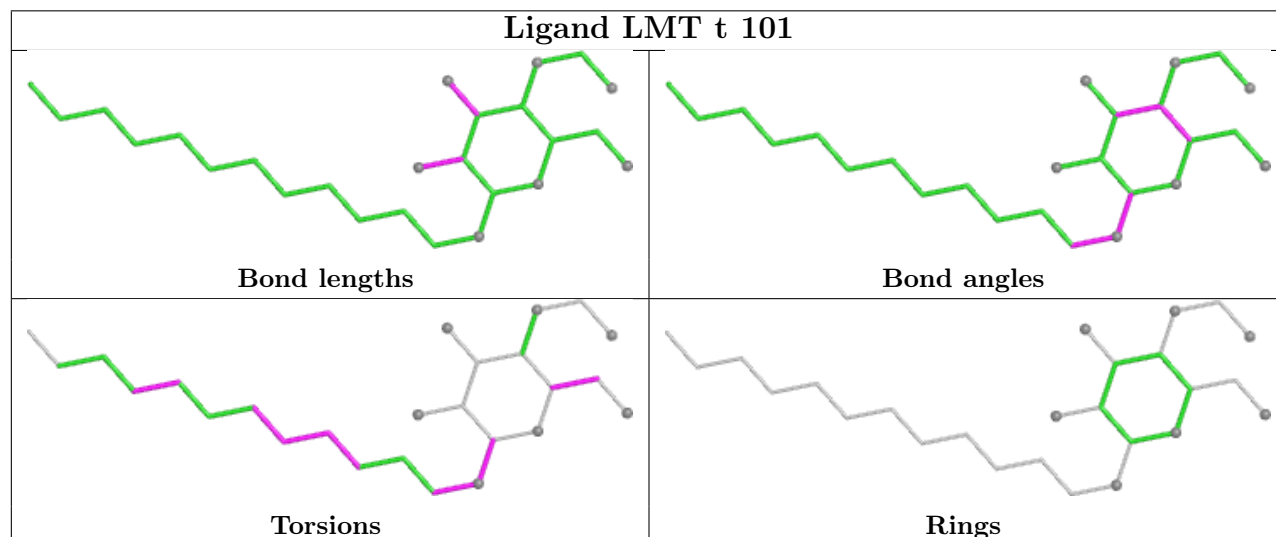
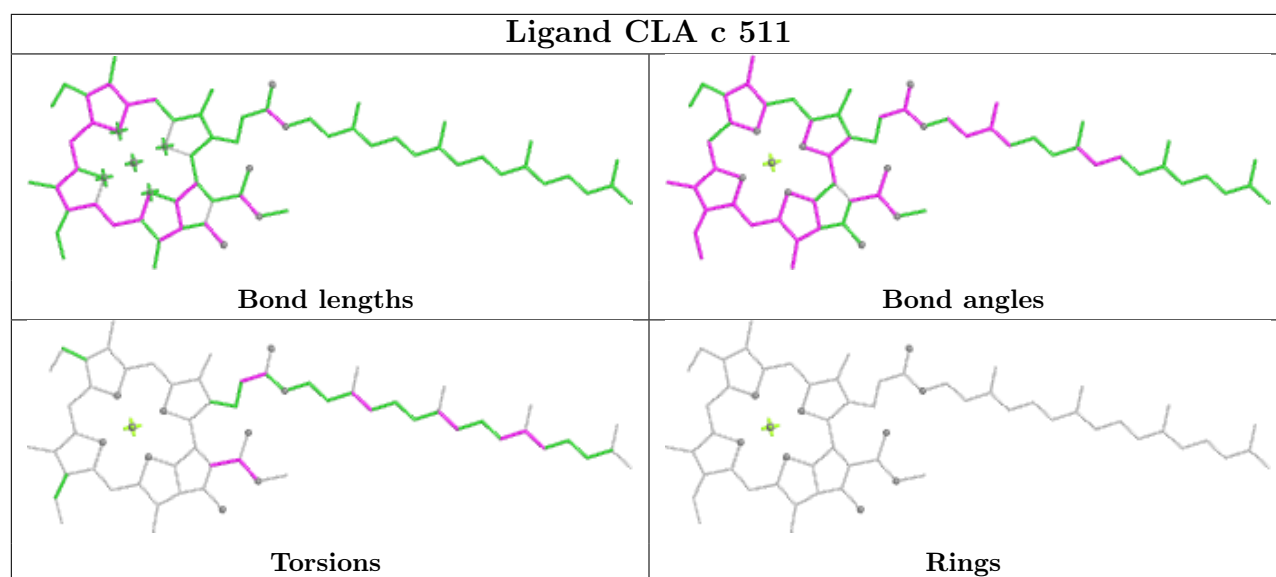
Ligand HTG C 522

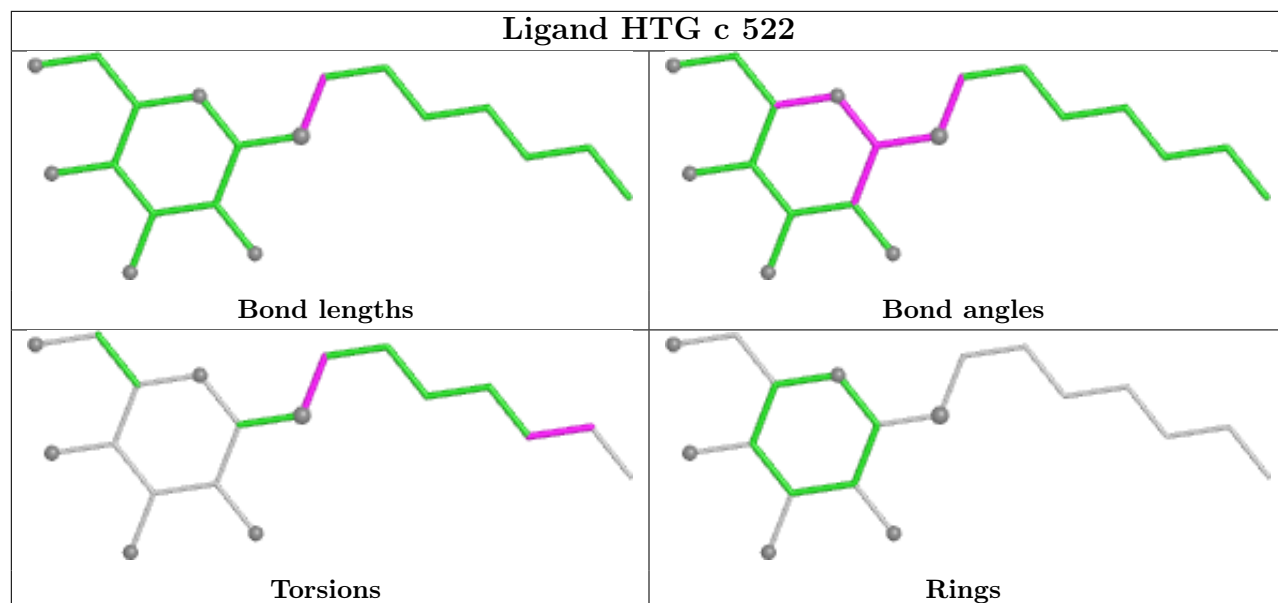


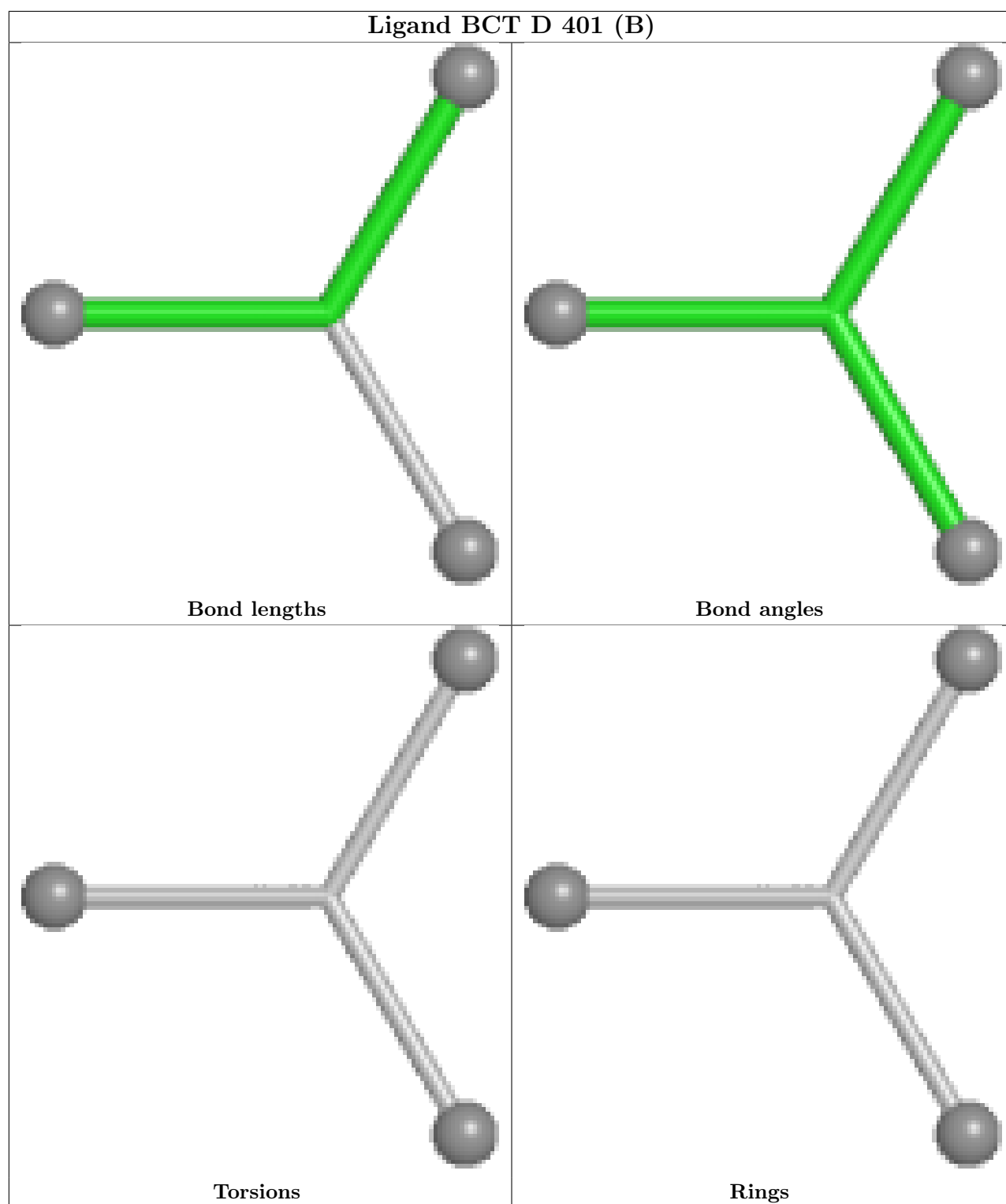


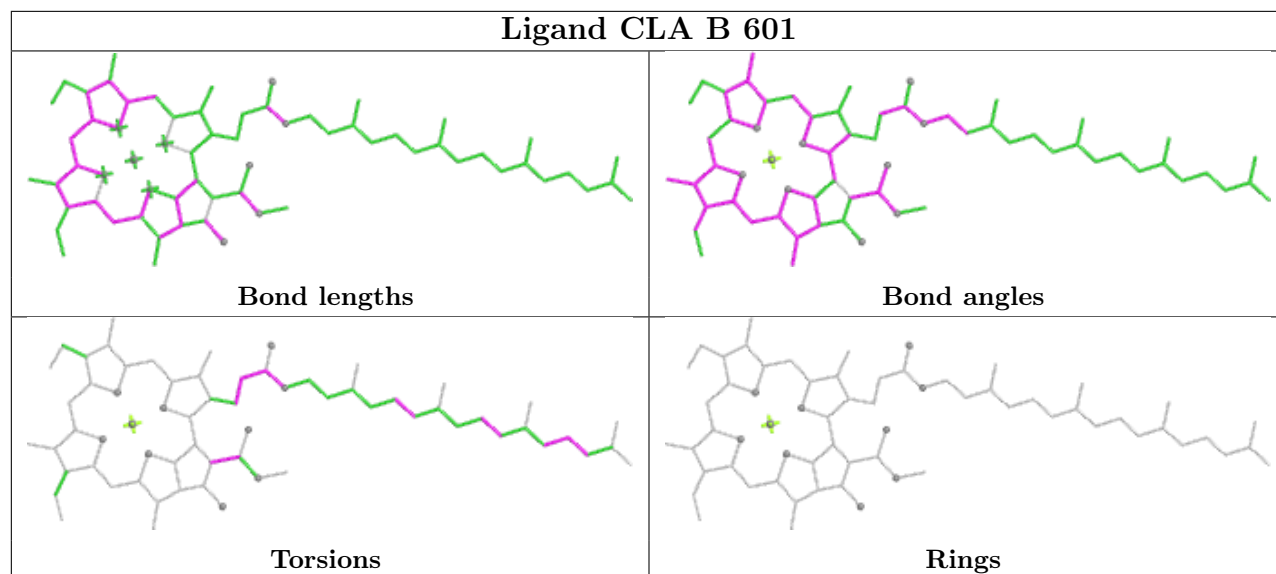
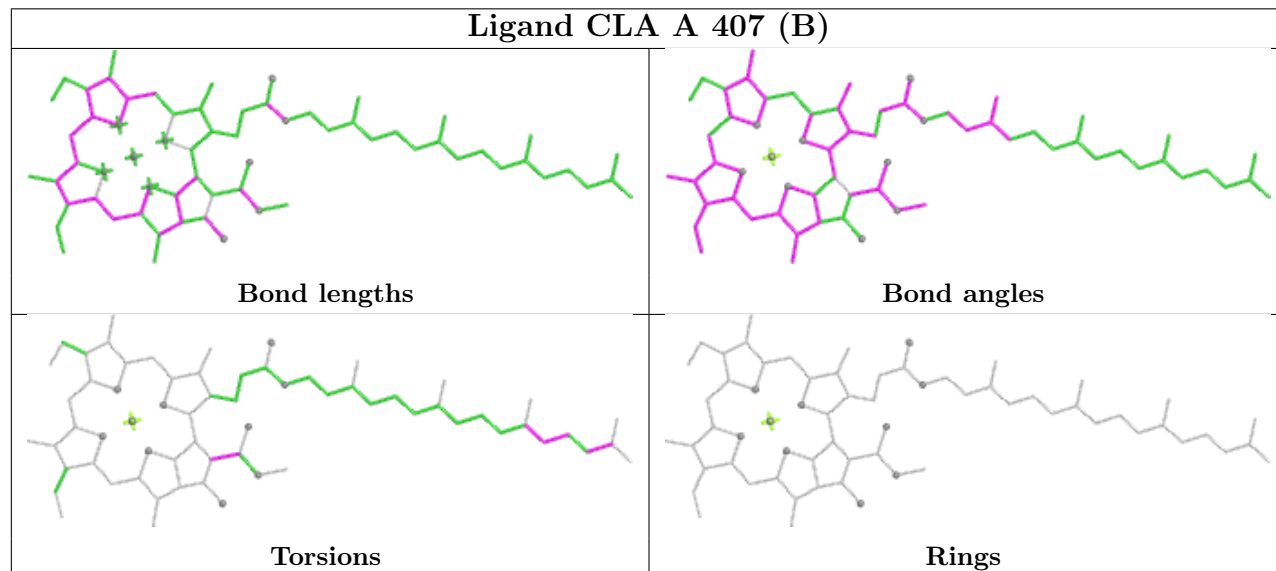


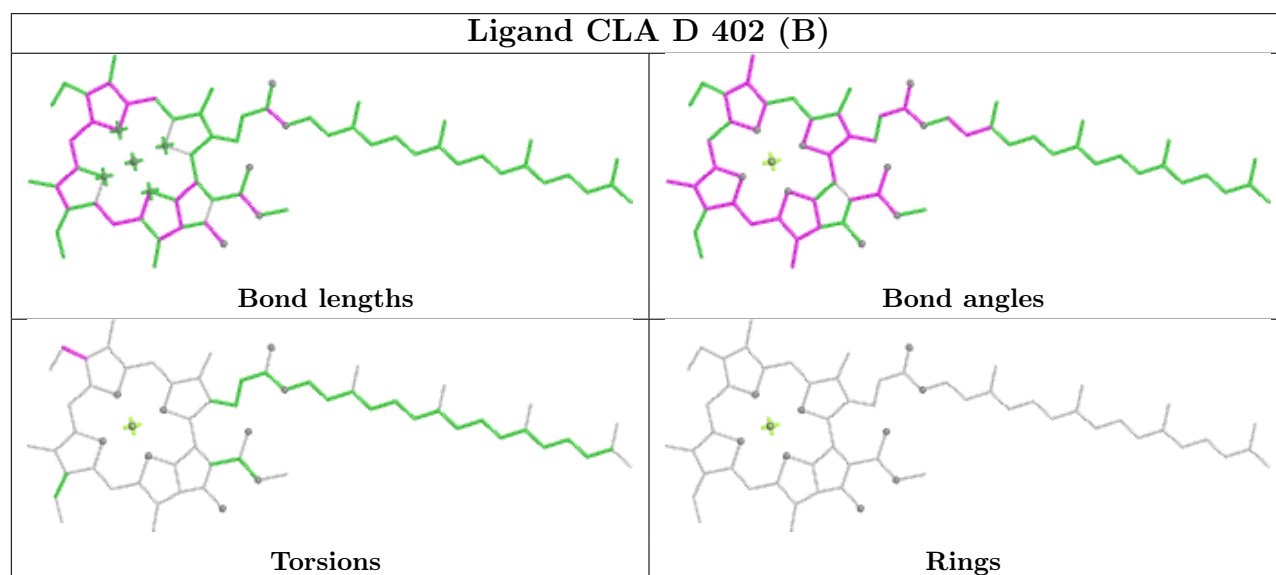
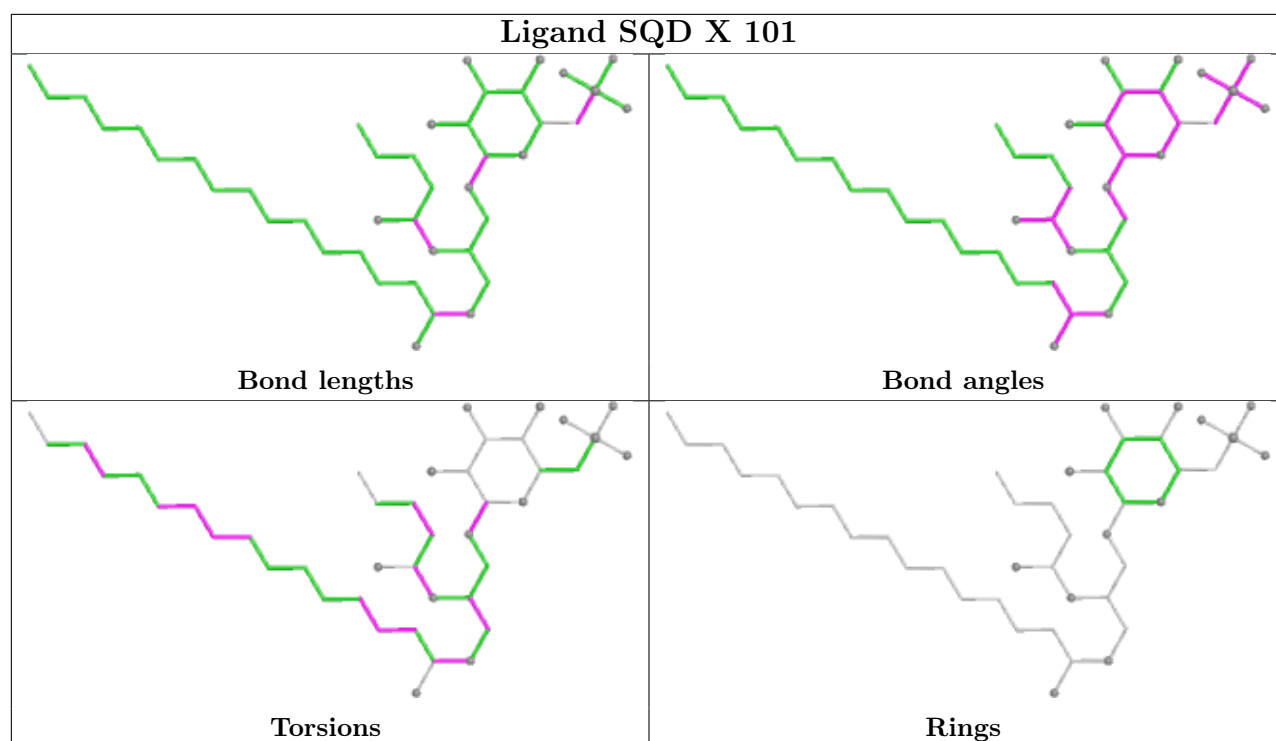


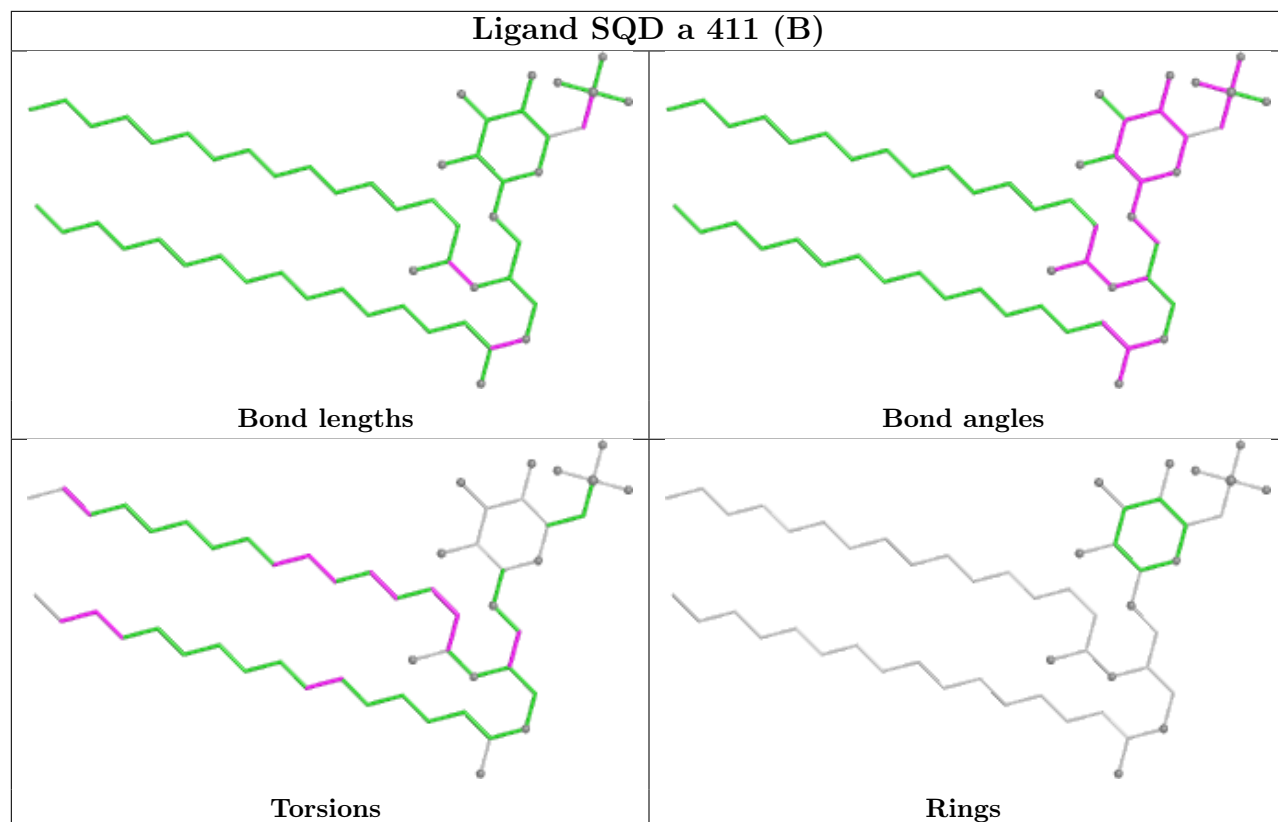


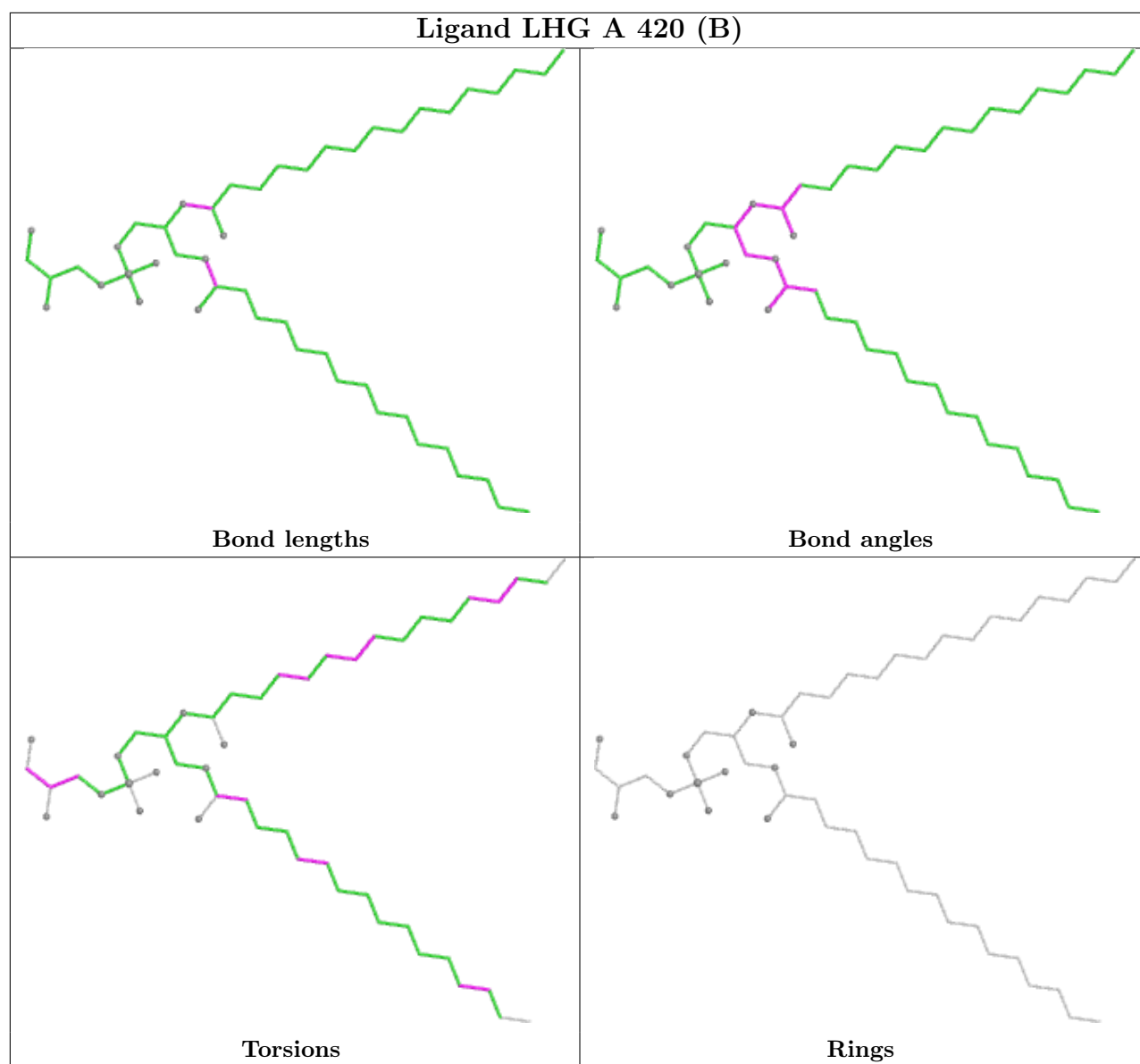


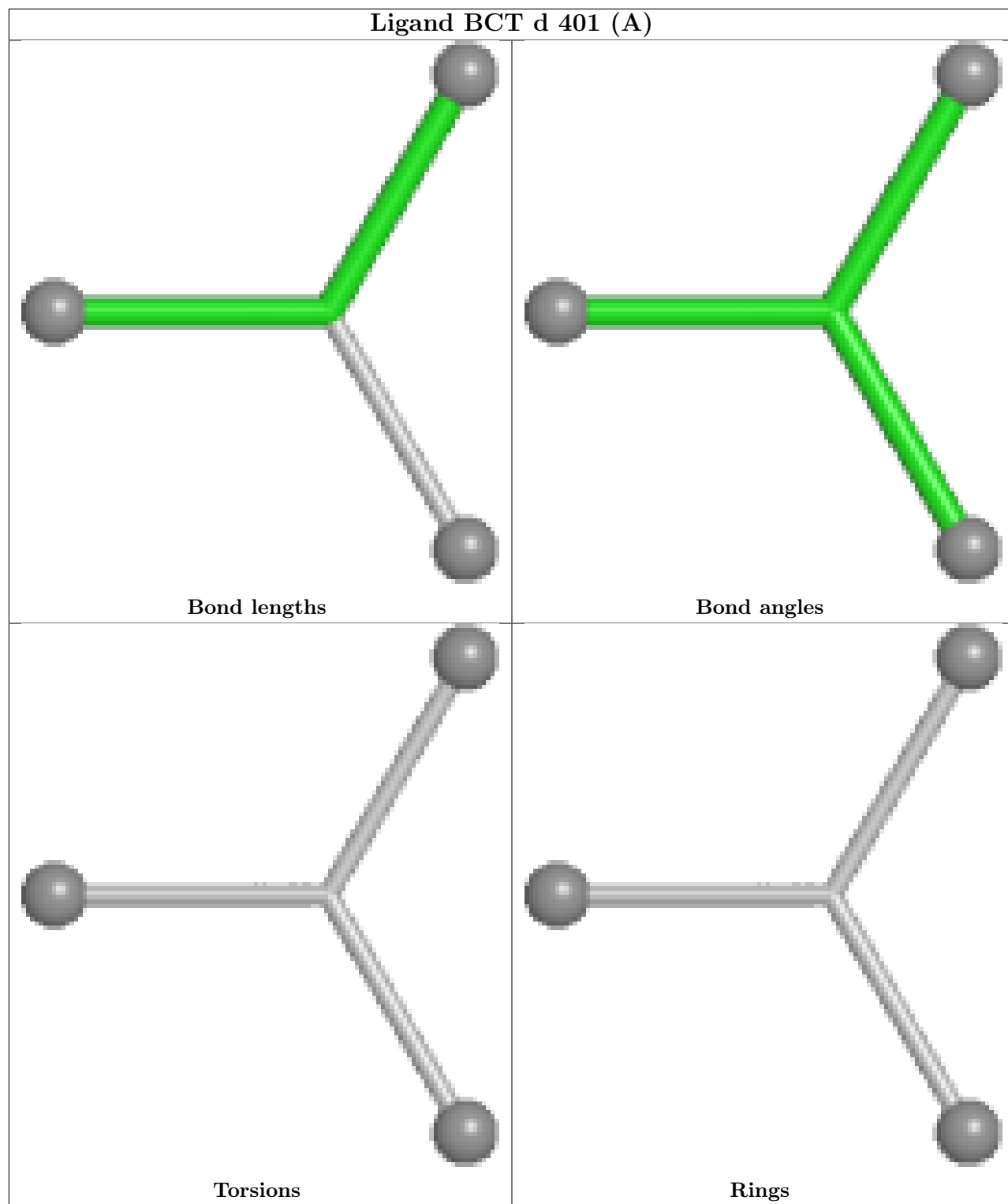


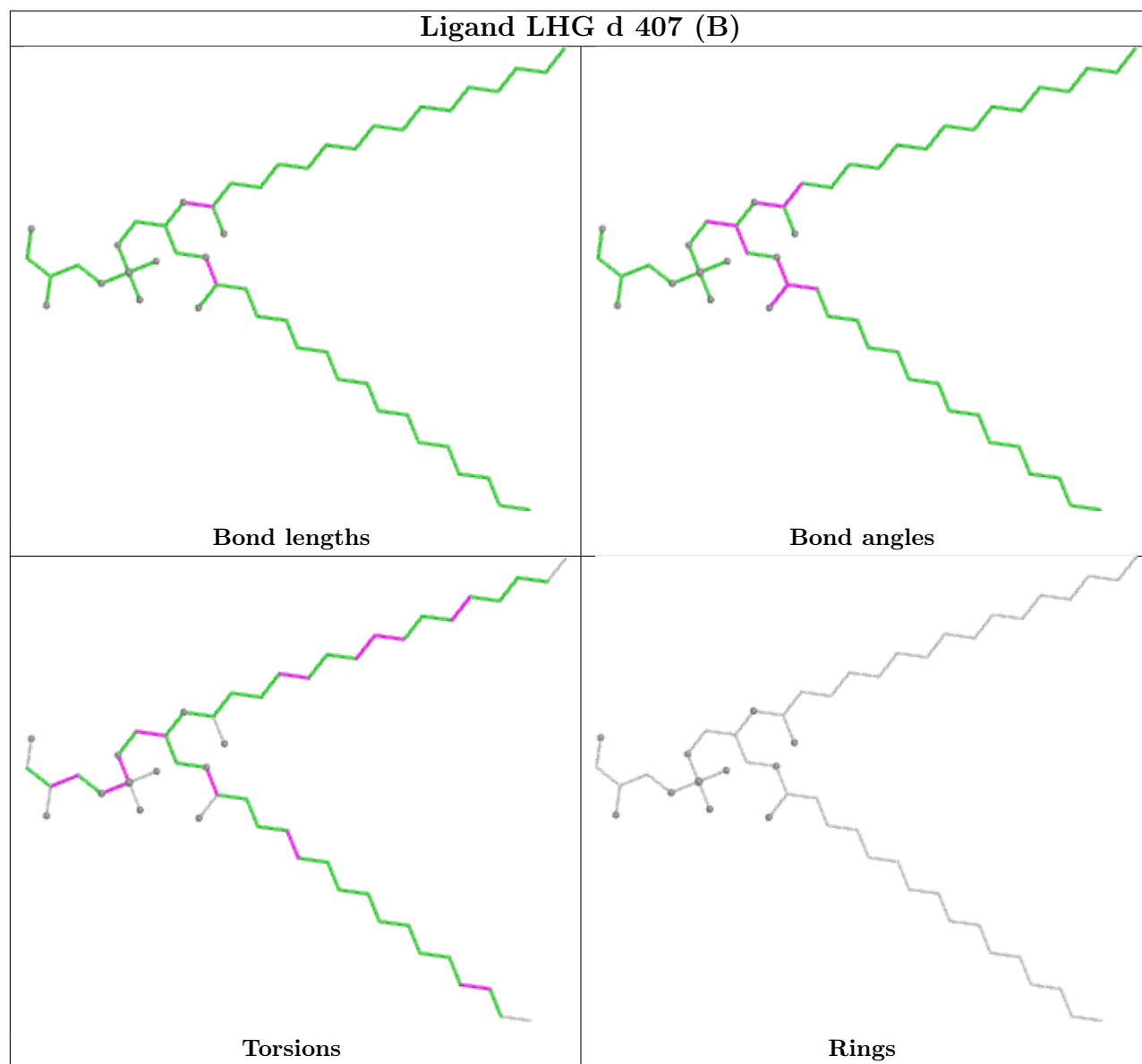
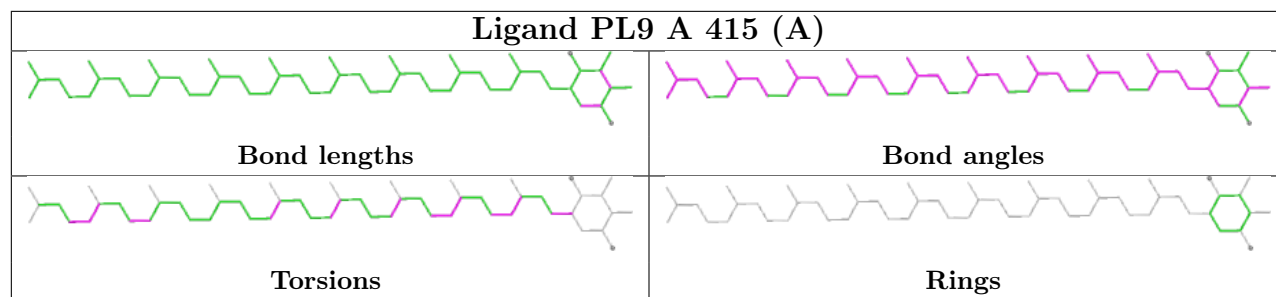
Ligand CLA B 601**Ligand CLA A 407 (B)**

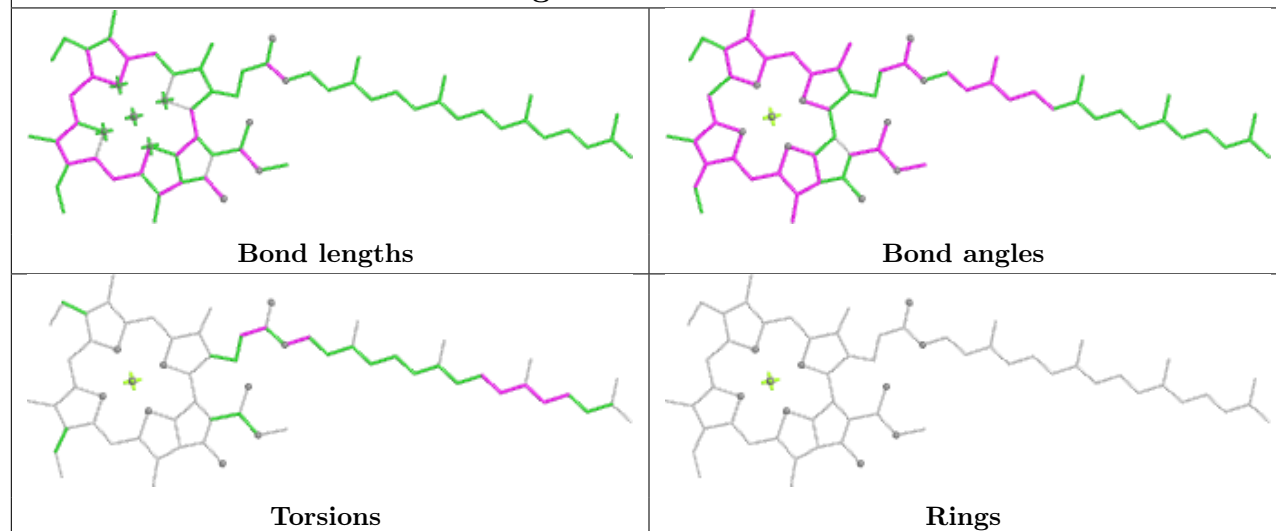
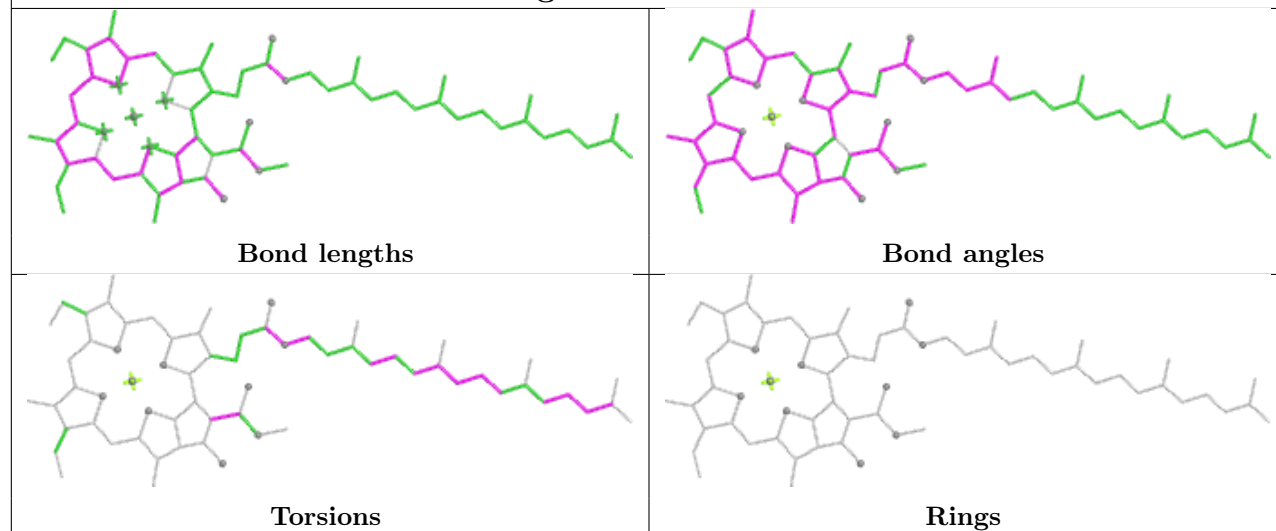
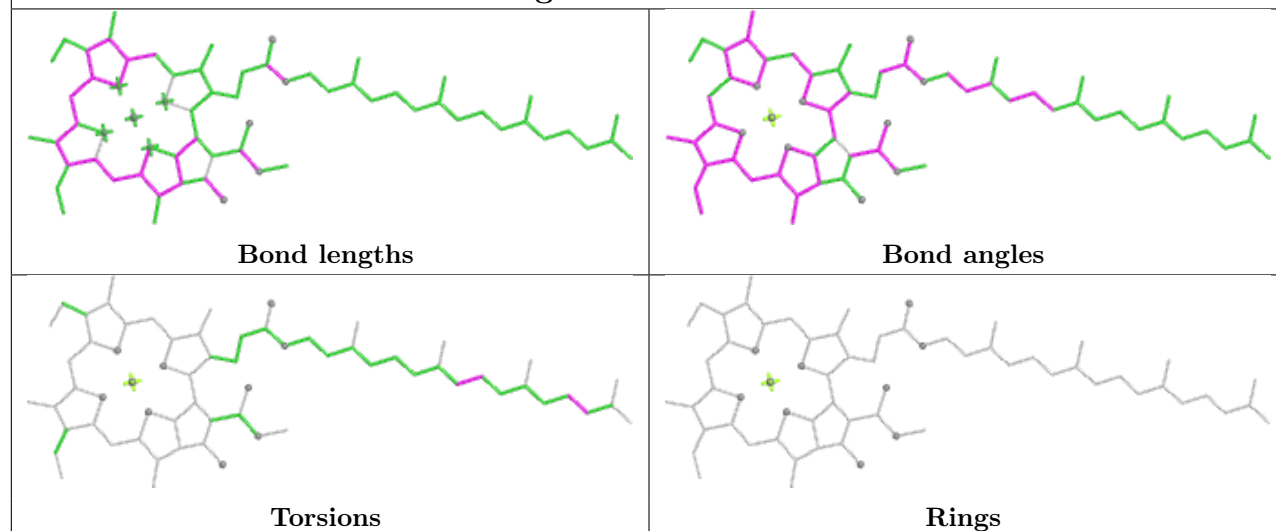


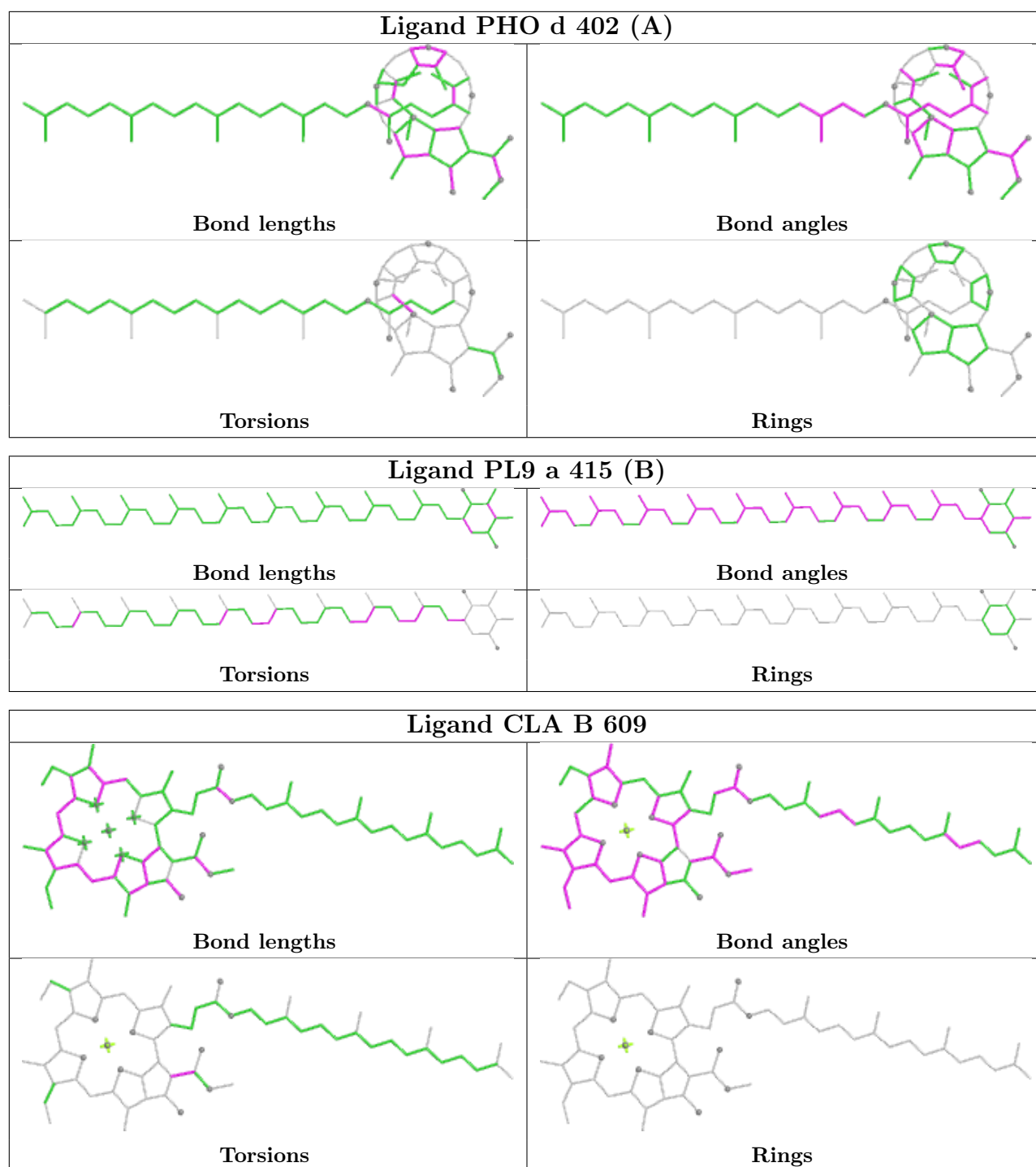


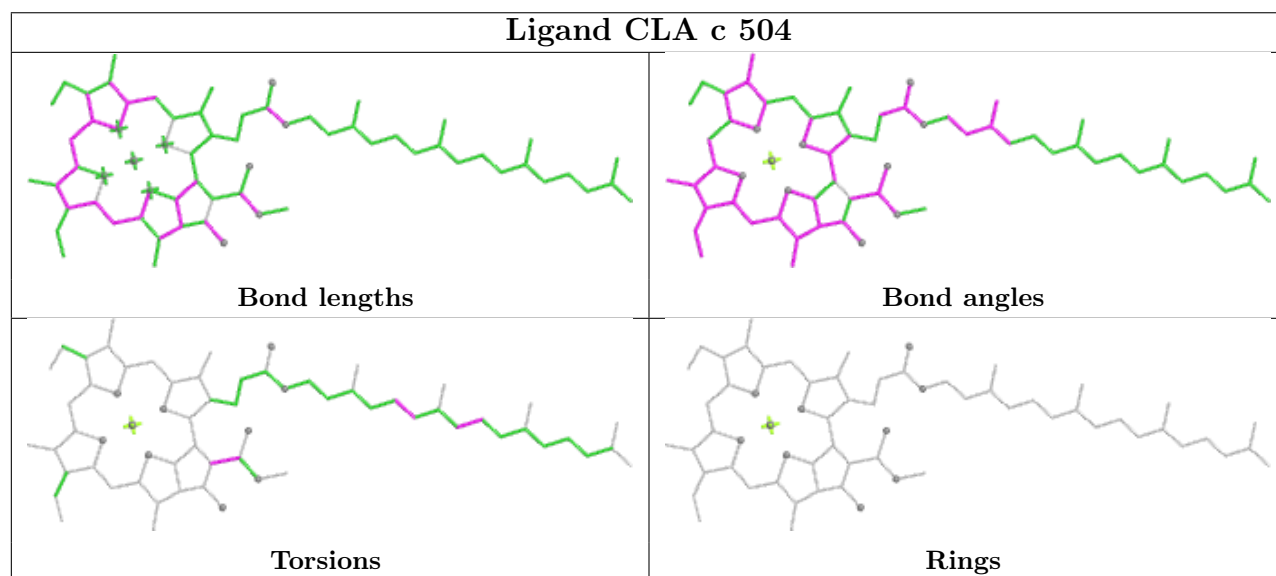
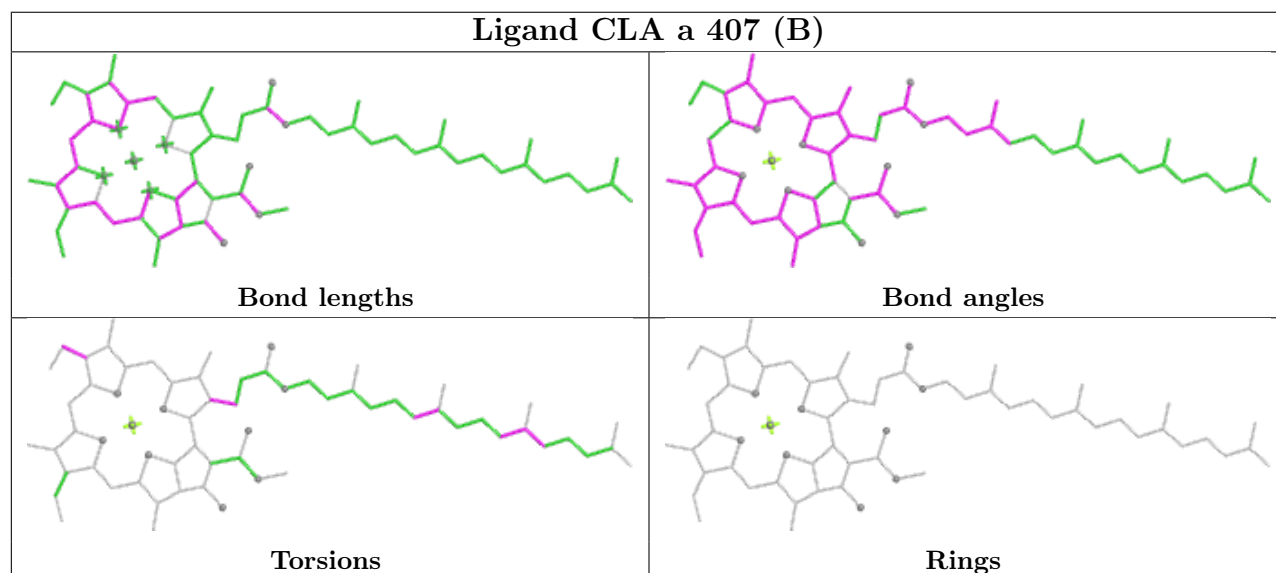
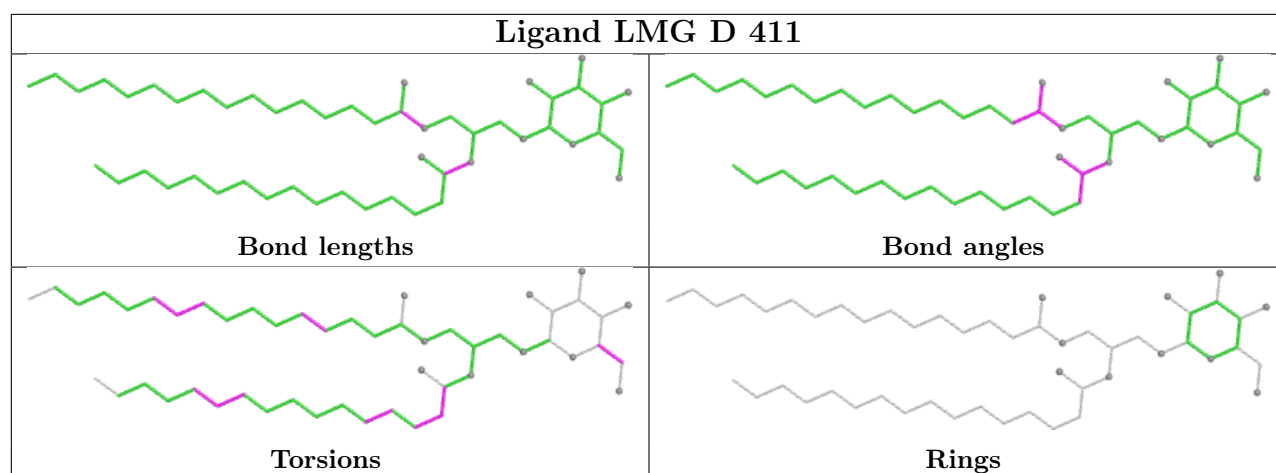


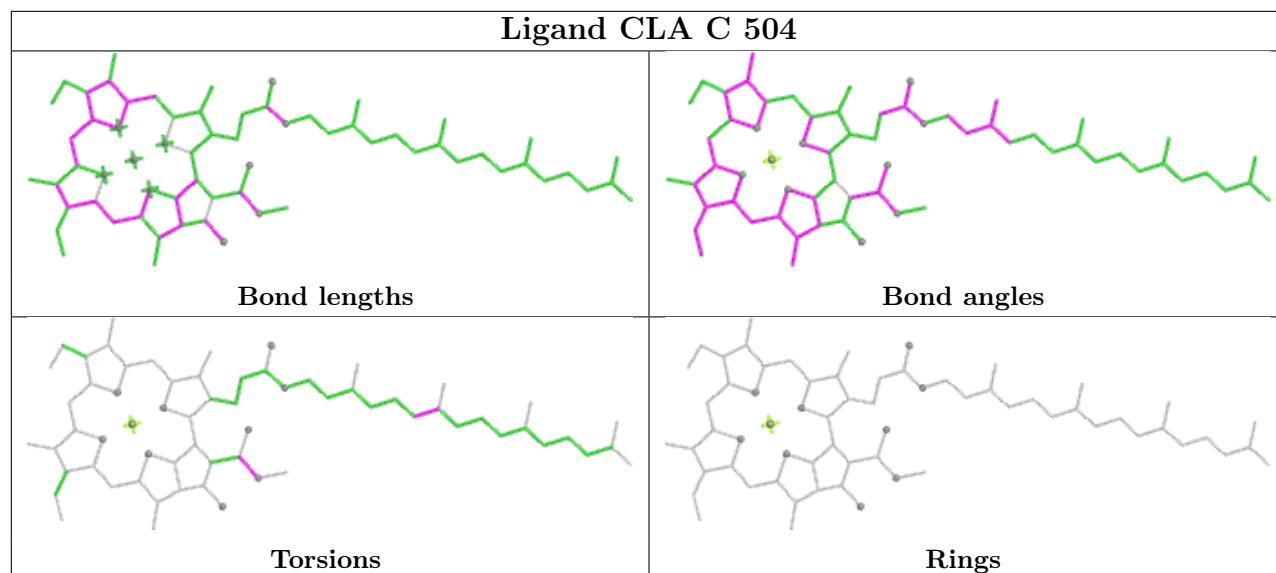
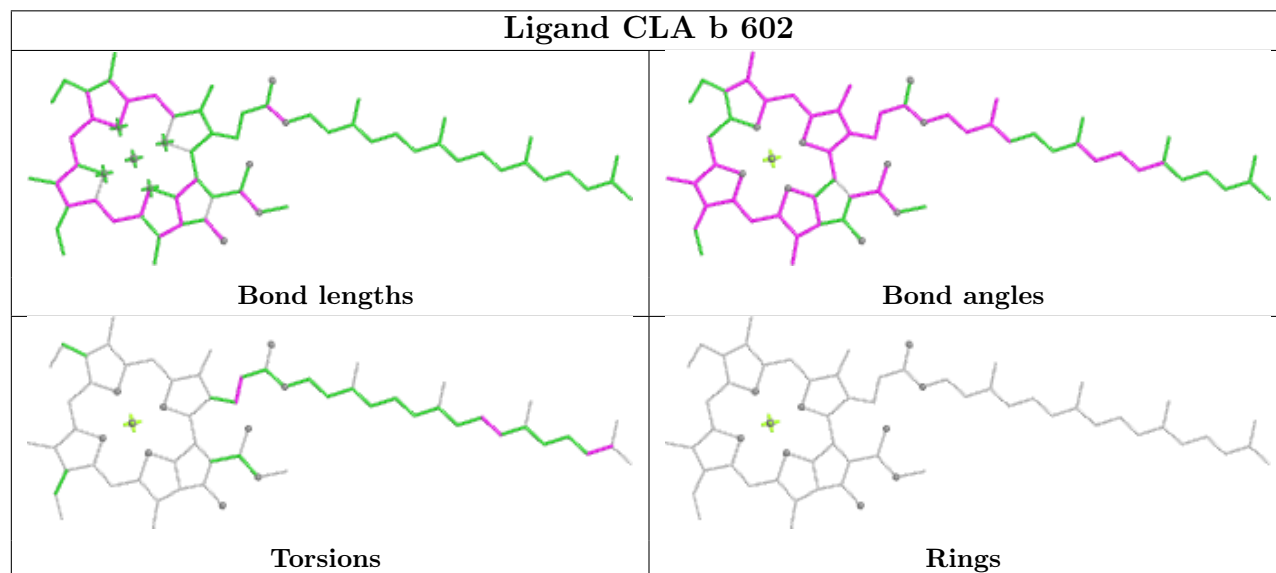
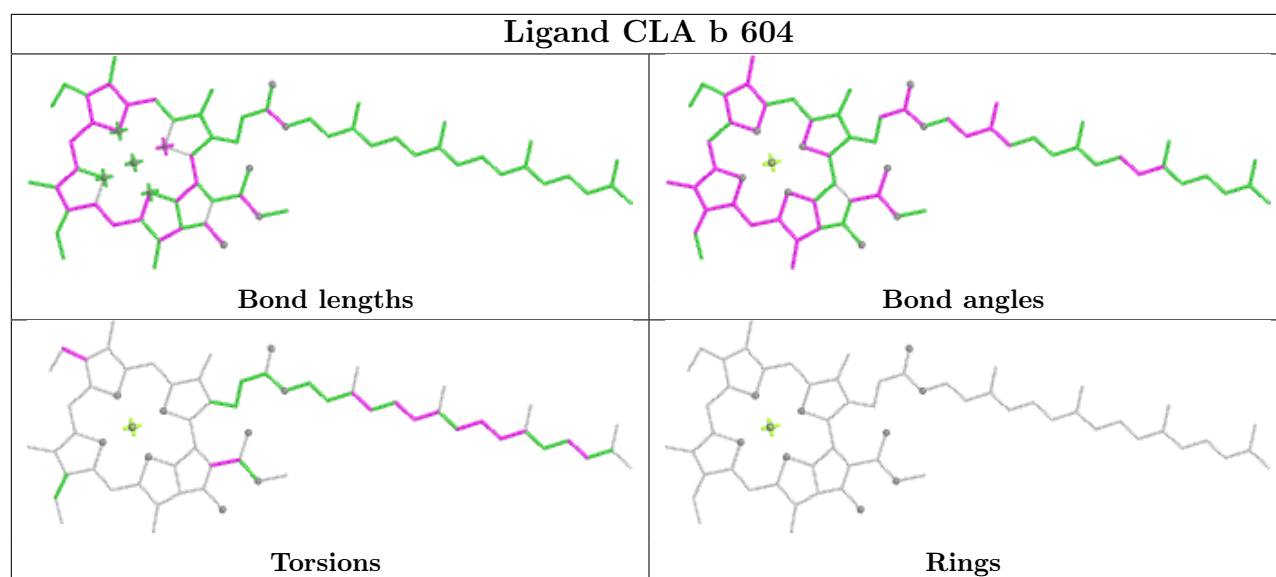


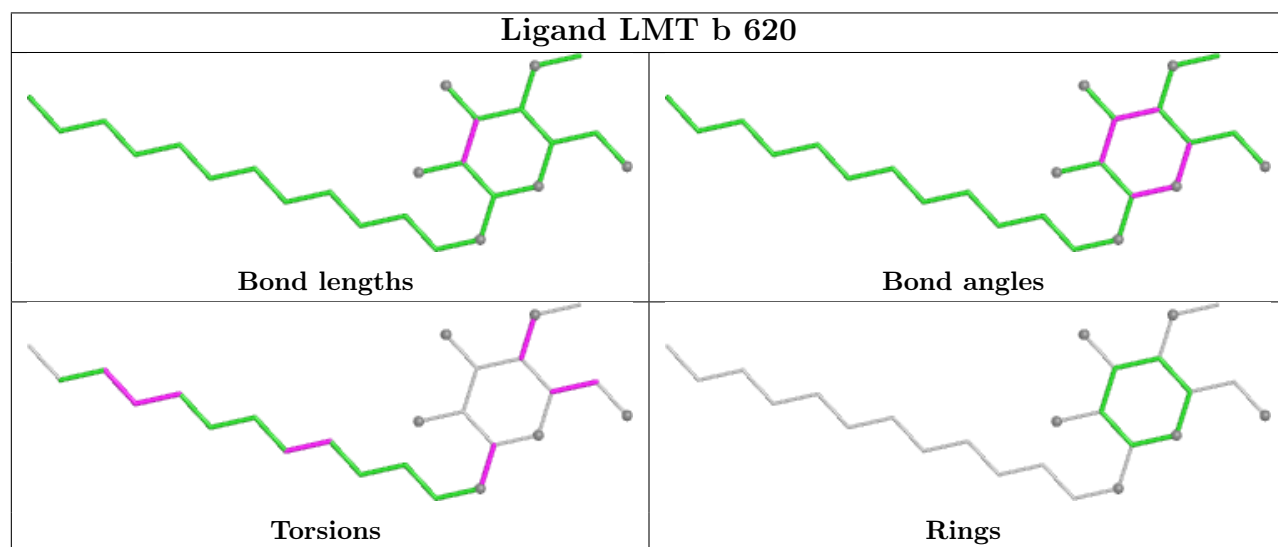
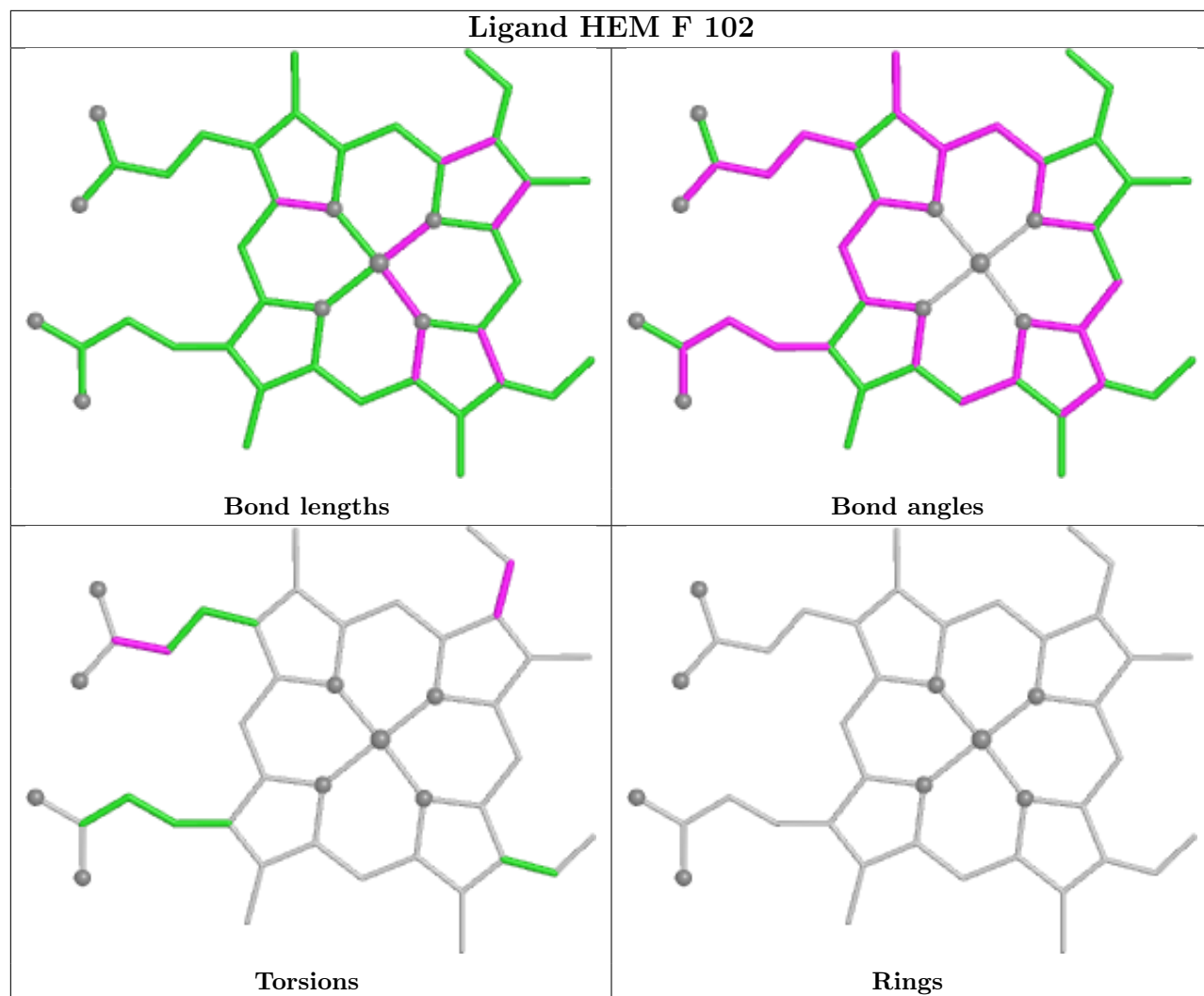


Ligand CLA B 613**Ligand CLA c 510****Ligand CLA b 611**

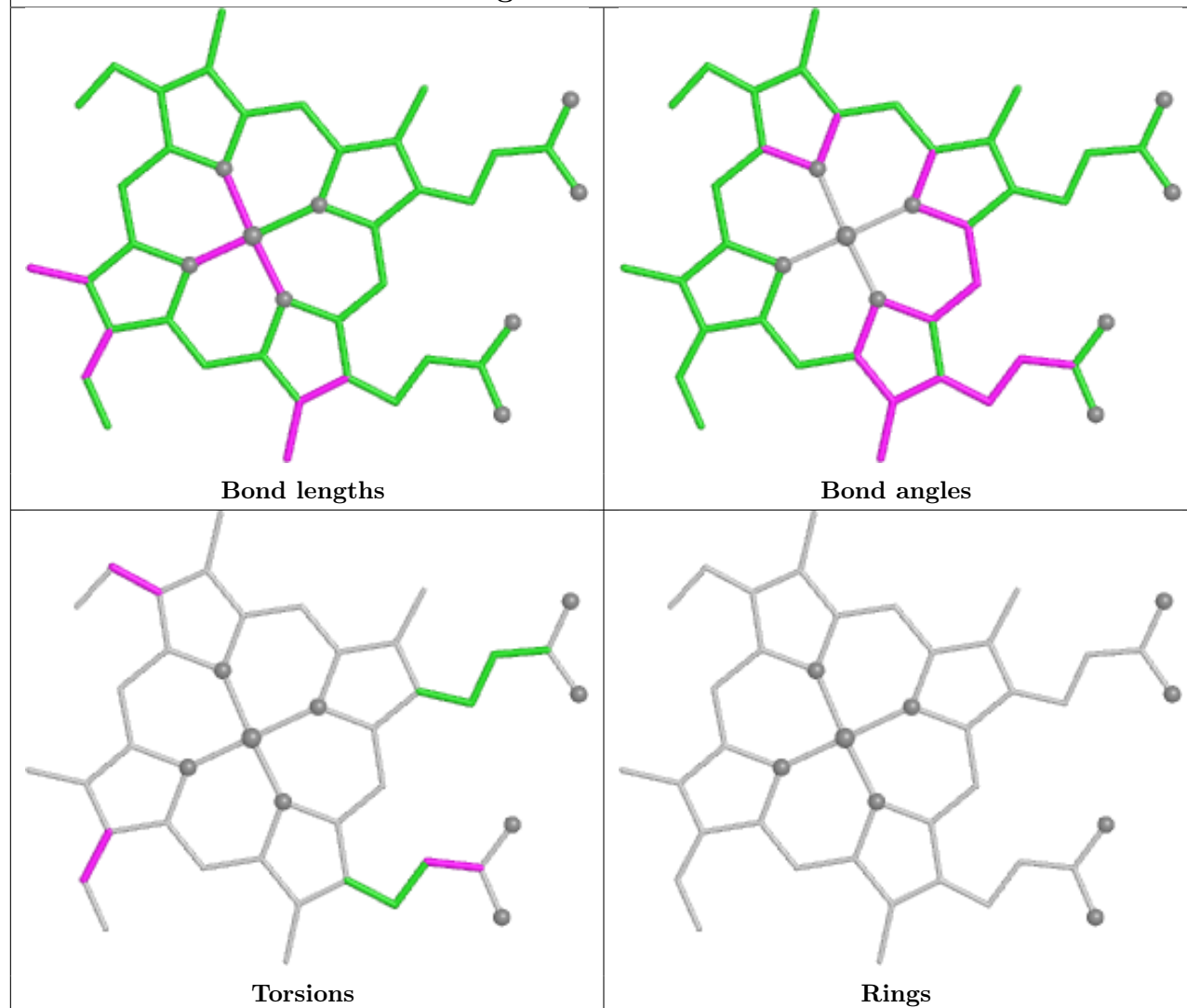




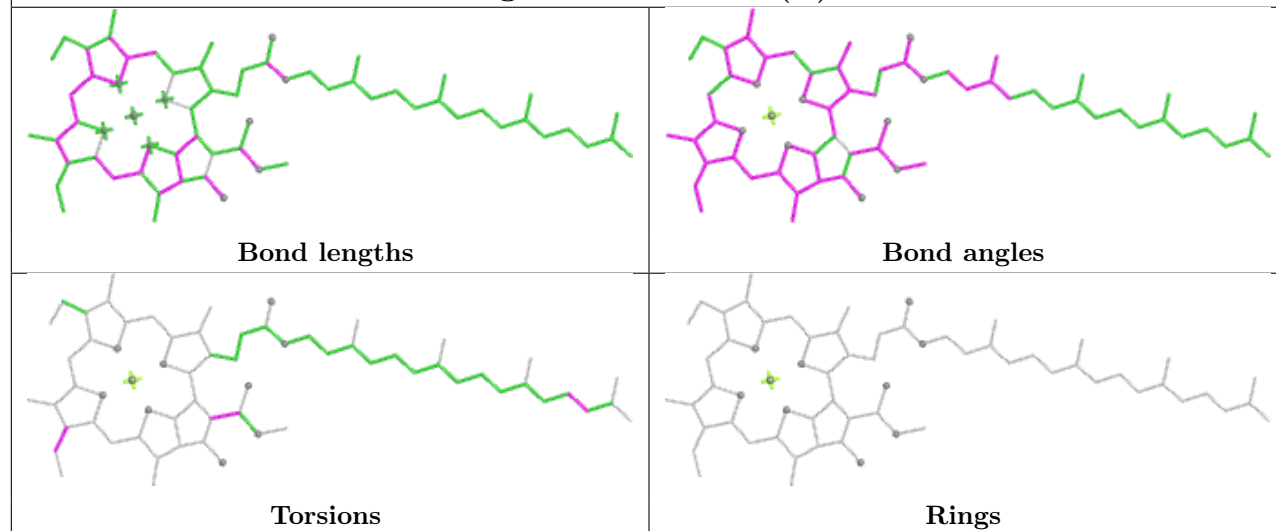


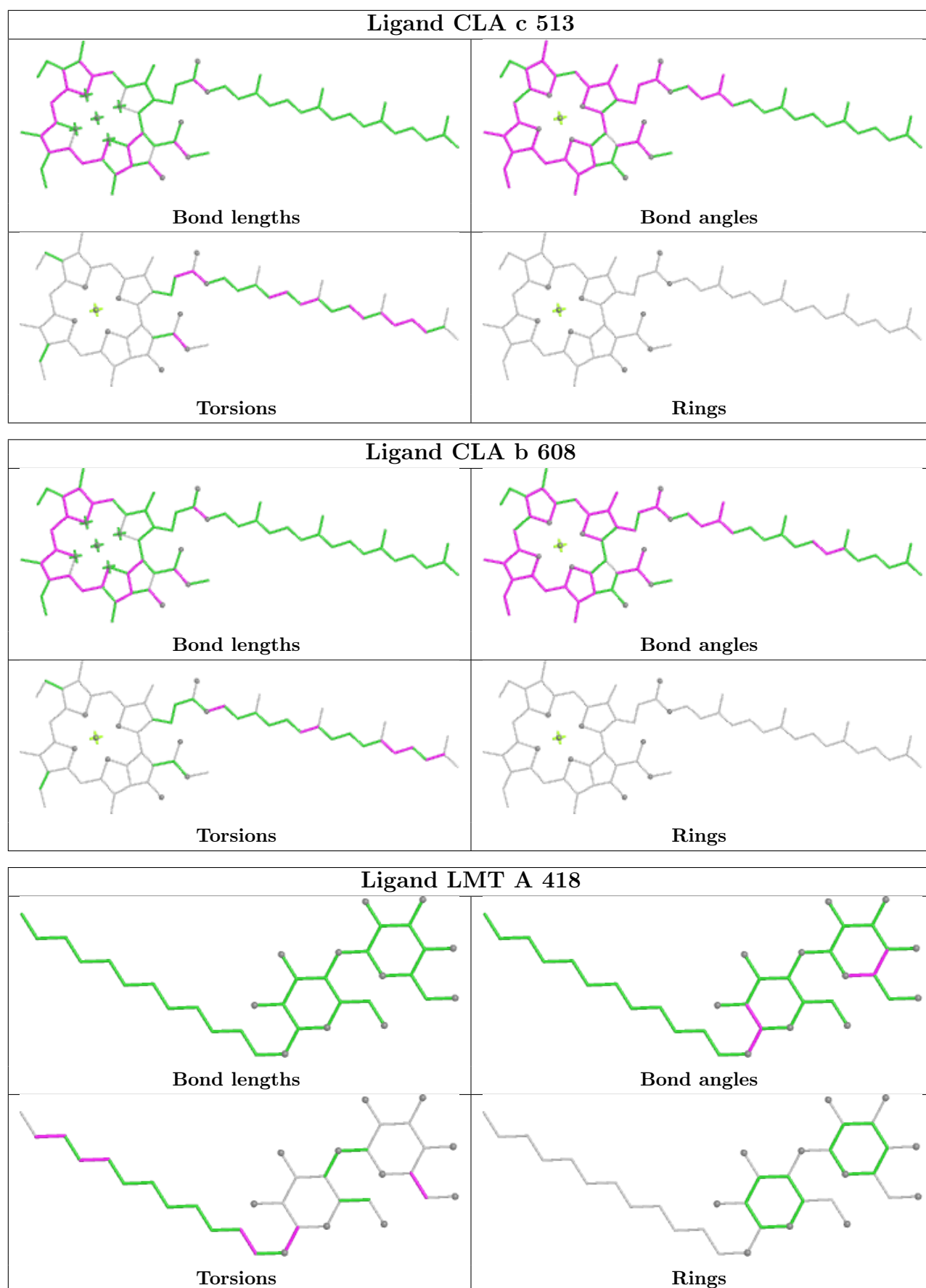


Ligand HEC v 201

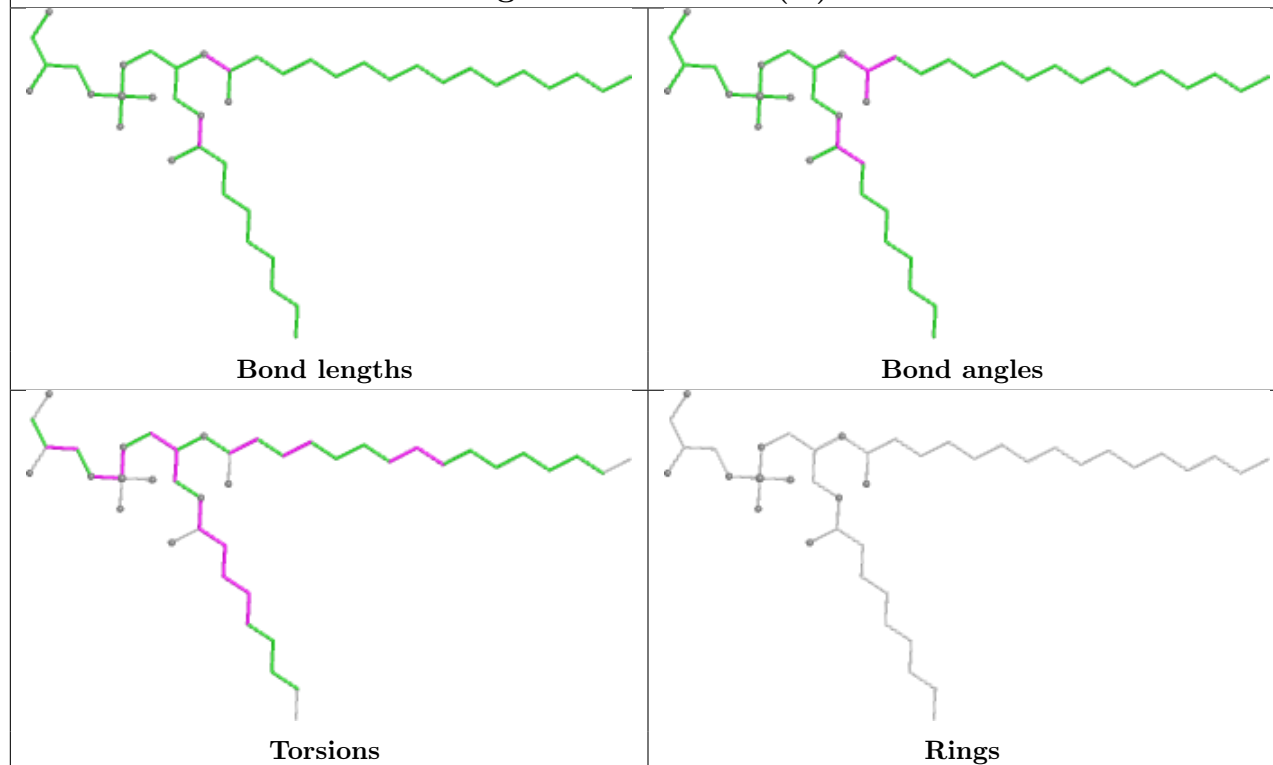


Ligand CLA A 406 (B)

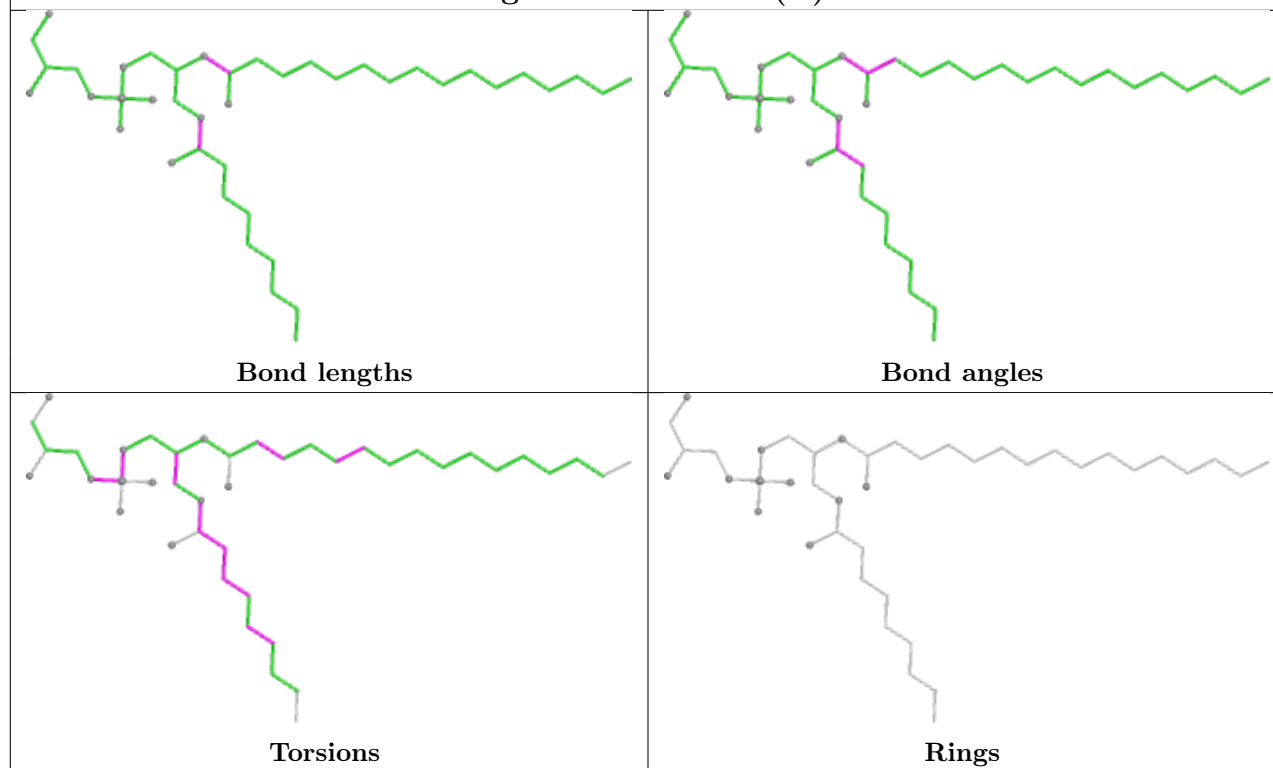


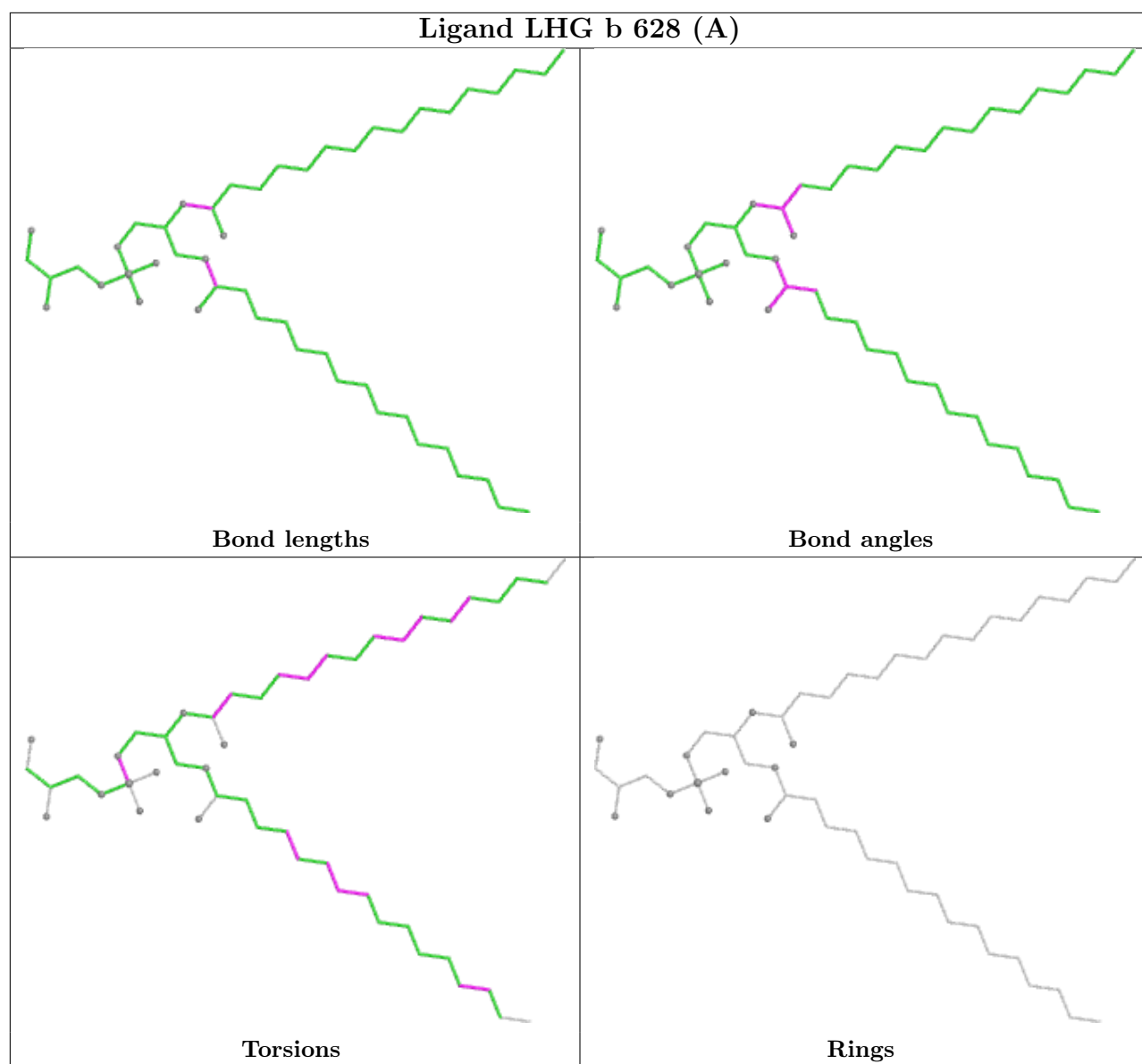


Ligand LHG E 101 (A)

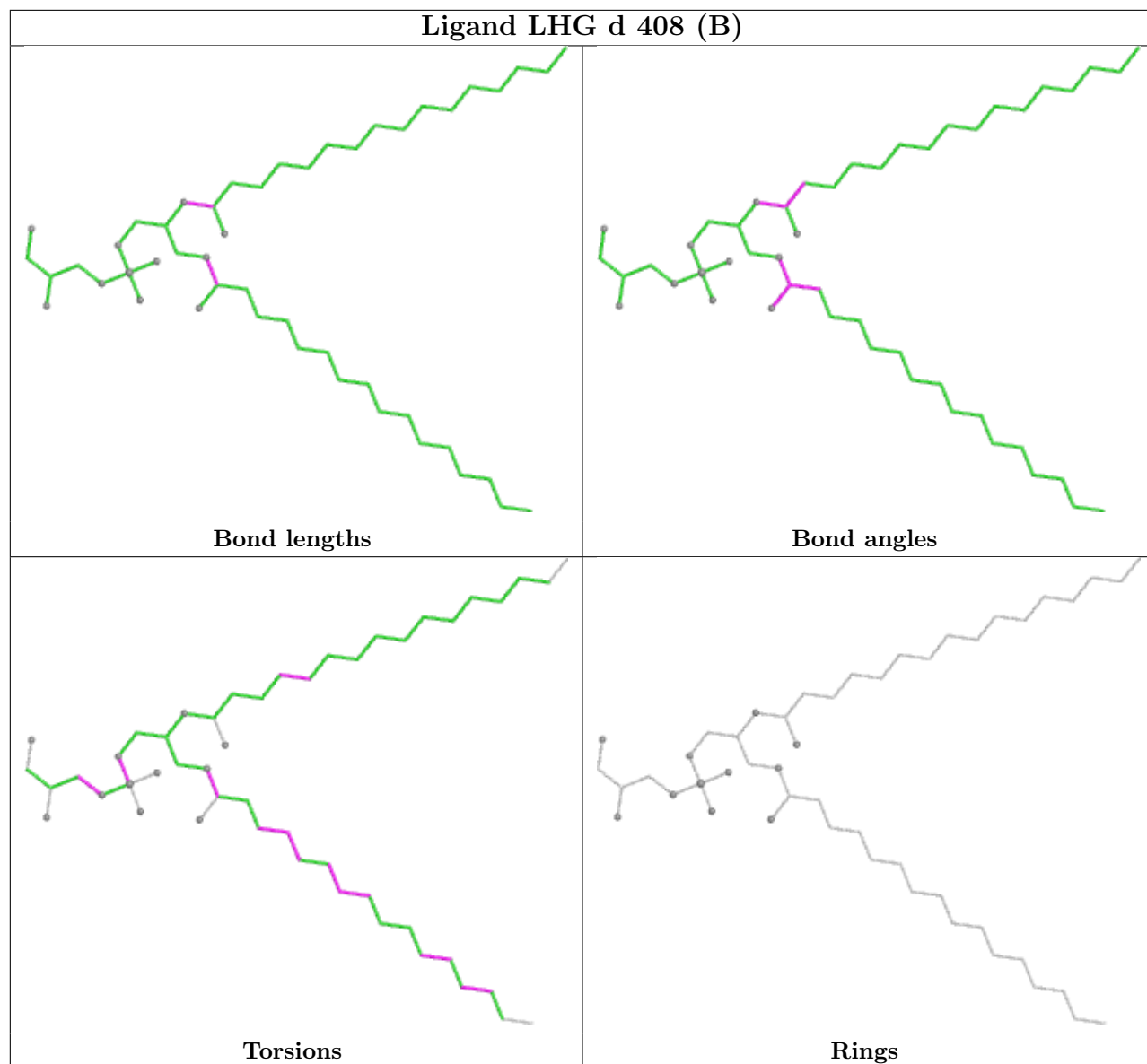


Ligand LHG a 420 (B)

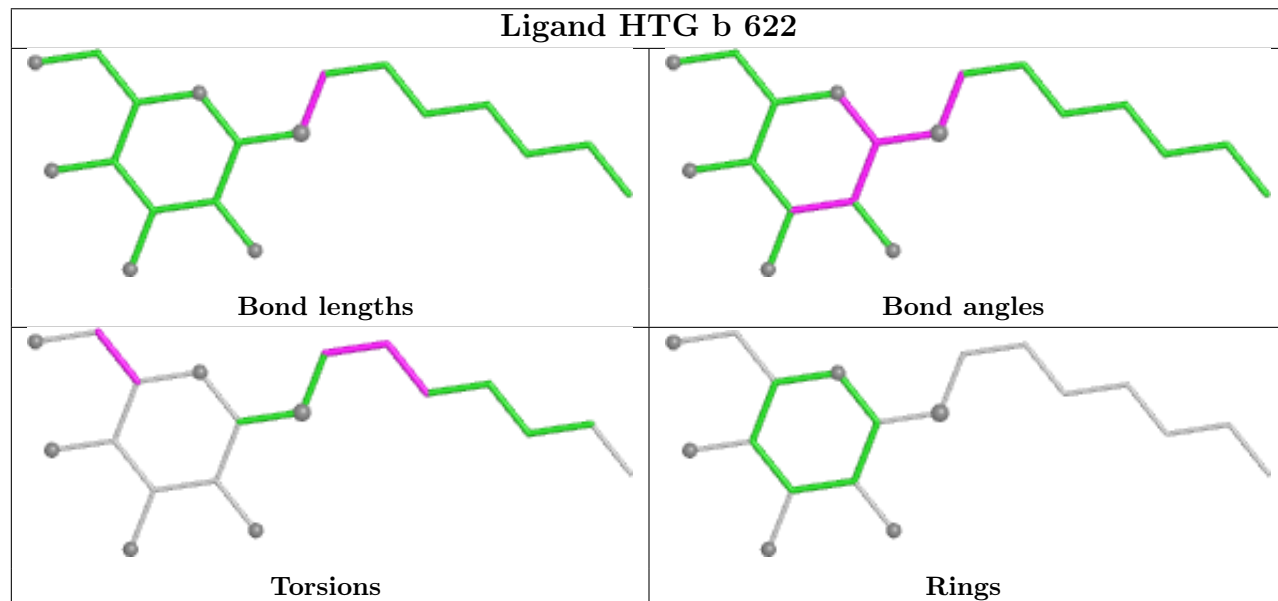


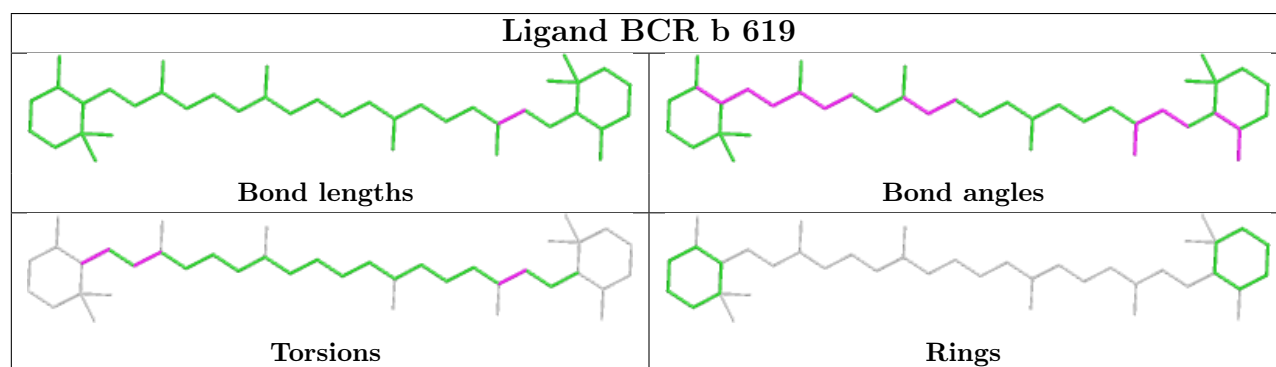
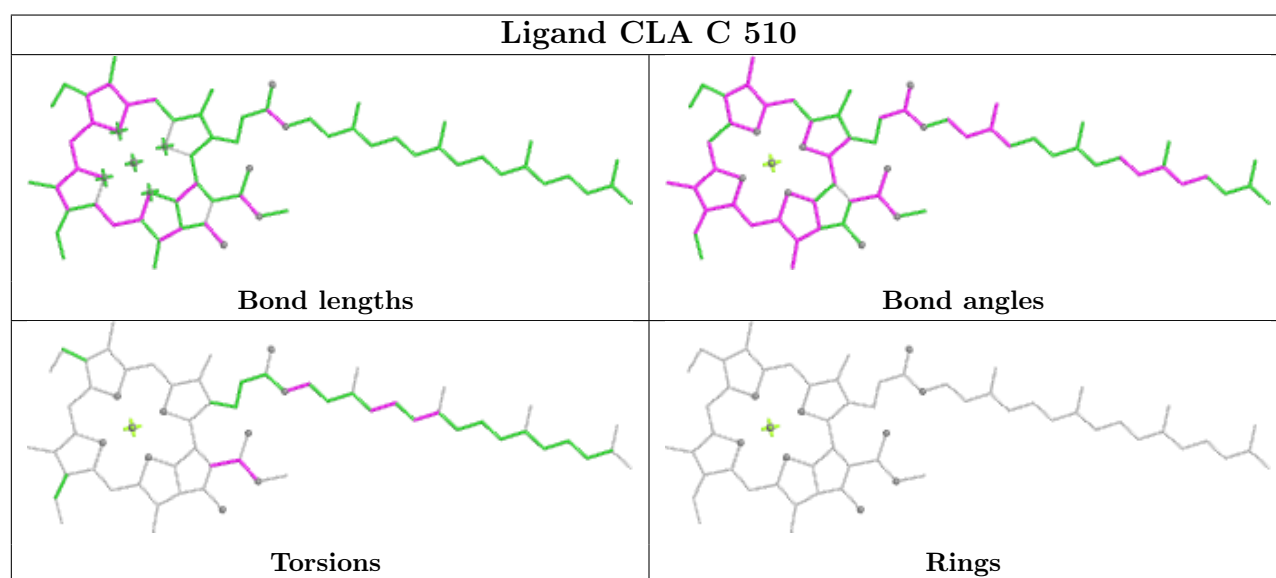
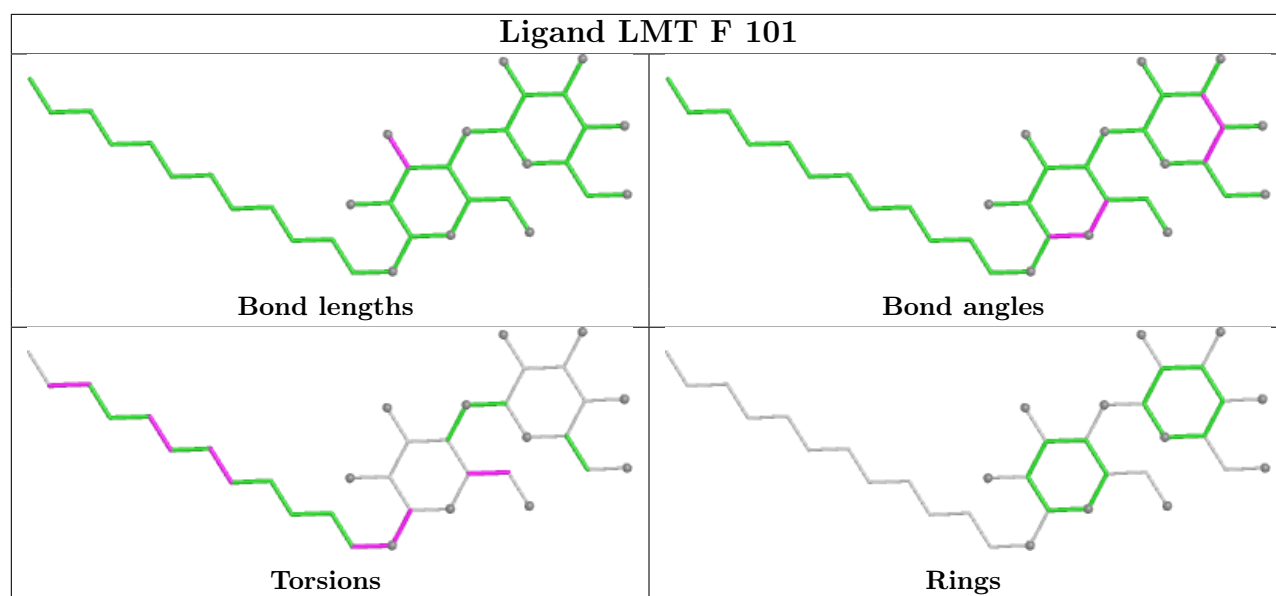


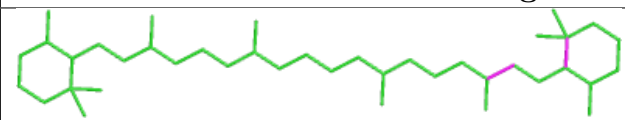
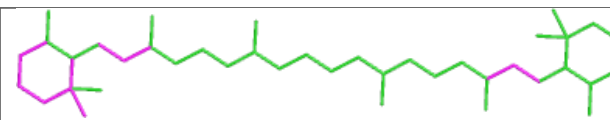
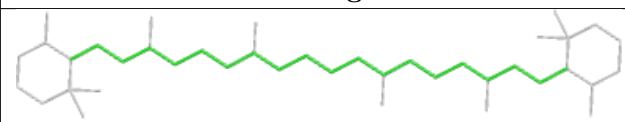
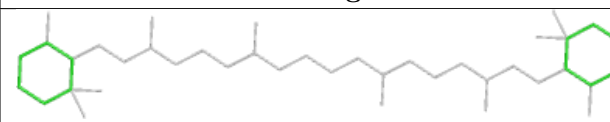
Ligand LHG d 408 (B)

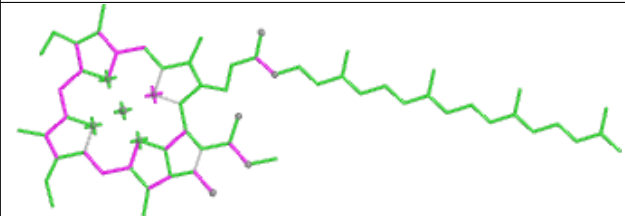
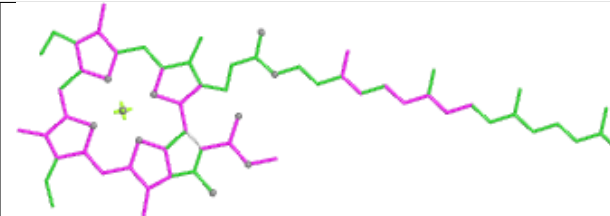
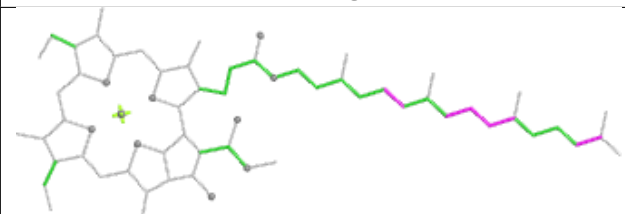
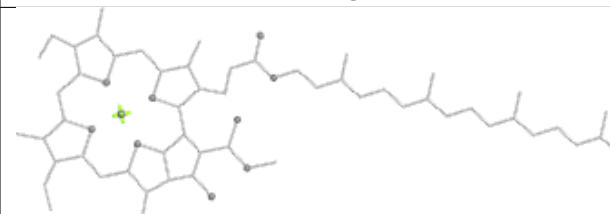


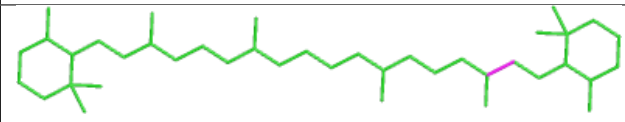
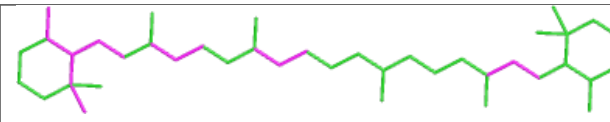
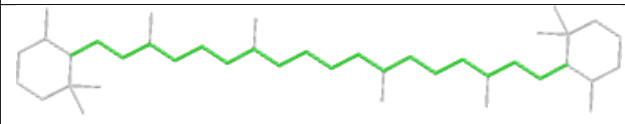
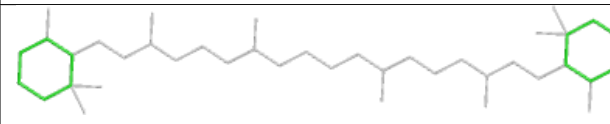
Ligand HTG b 622

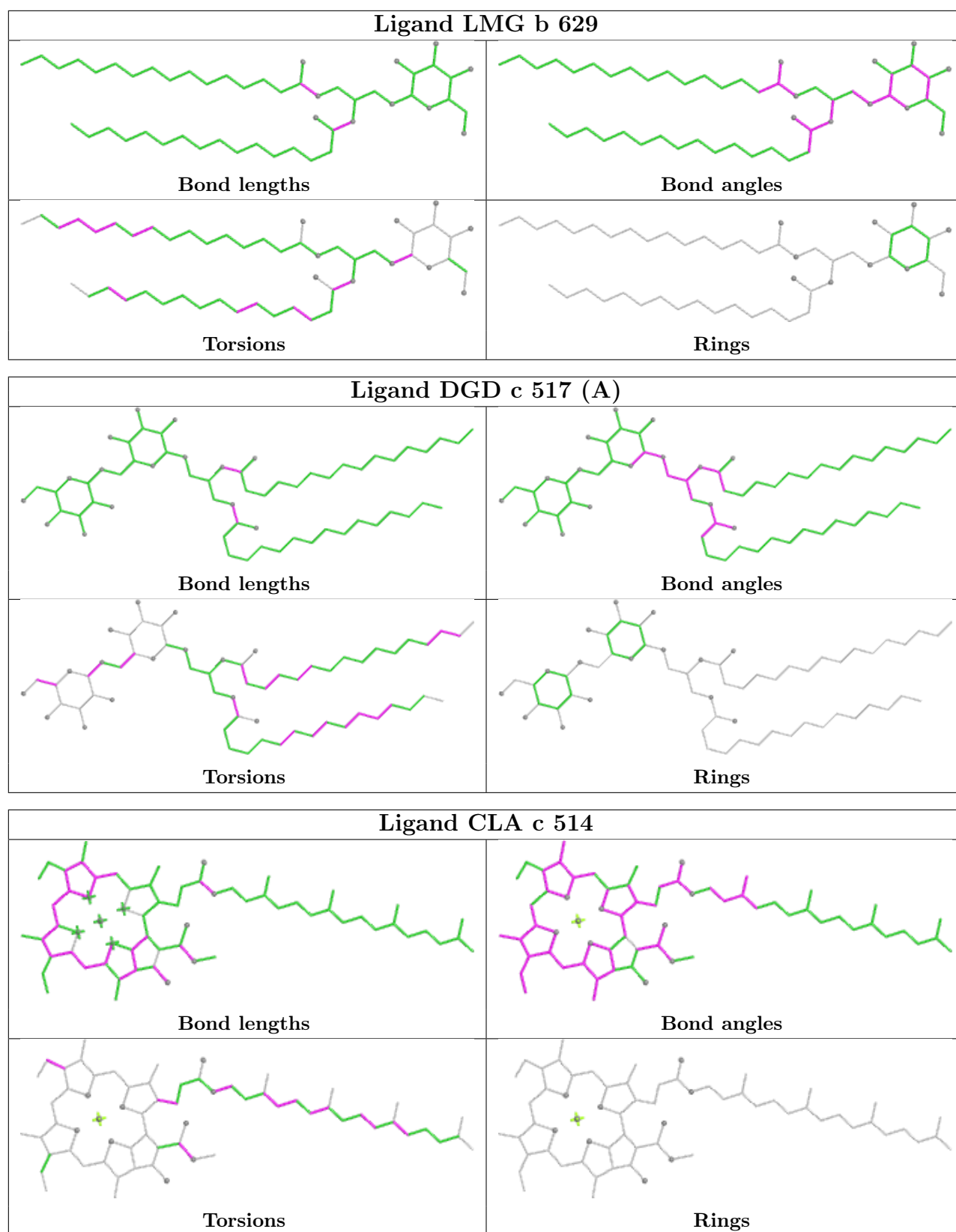


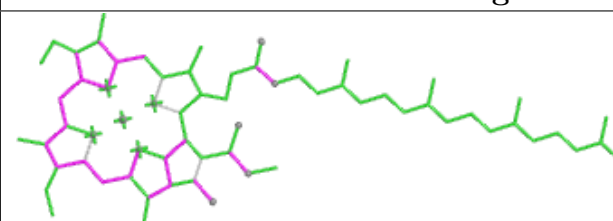
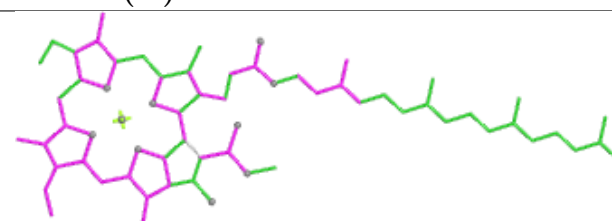
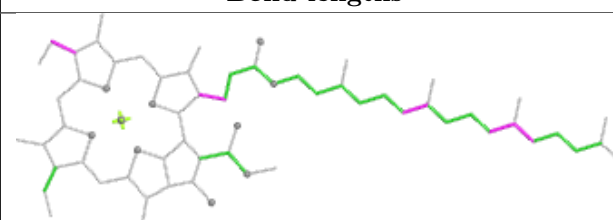
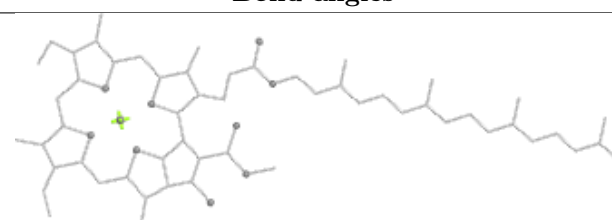
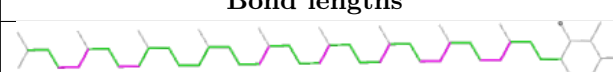
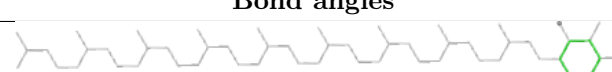
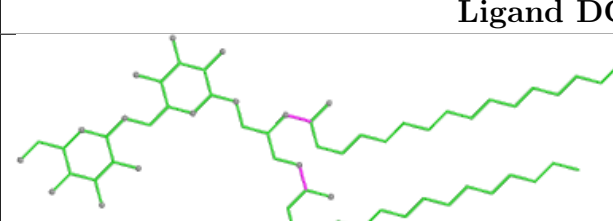
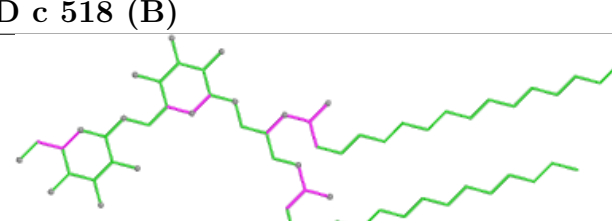
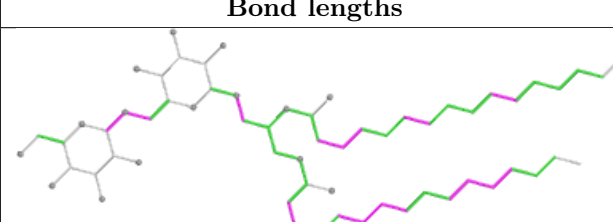
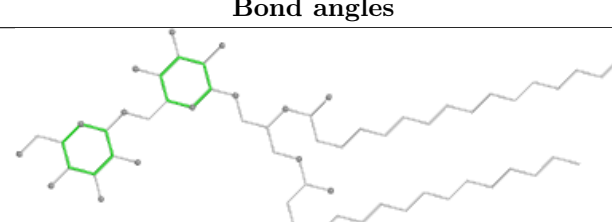


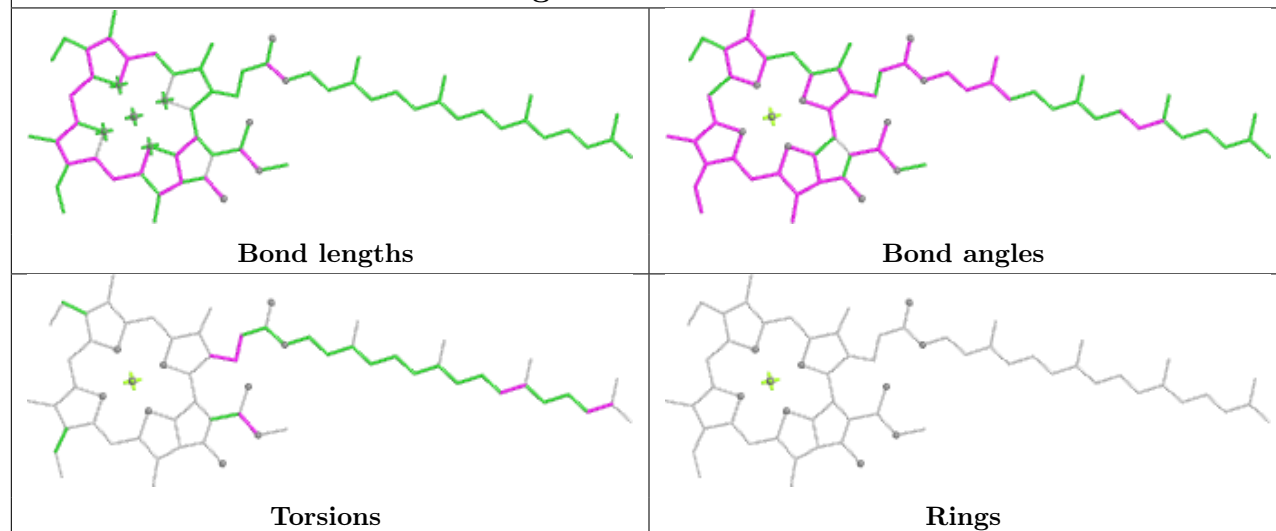
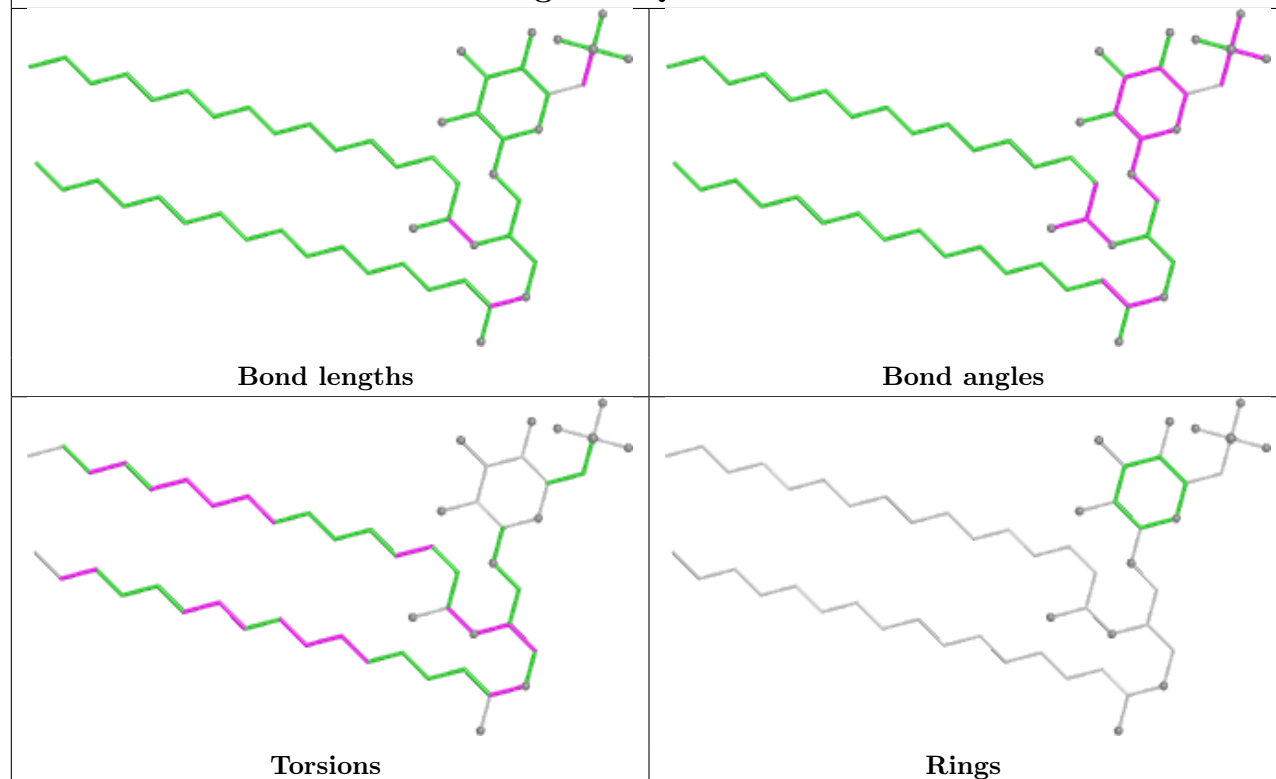
Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

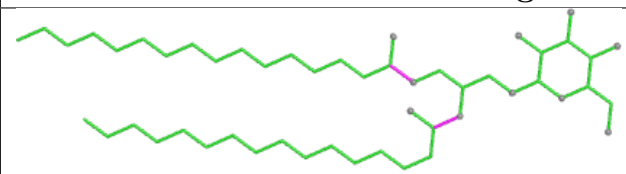
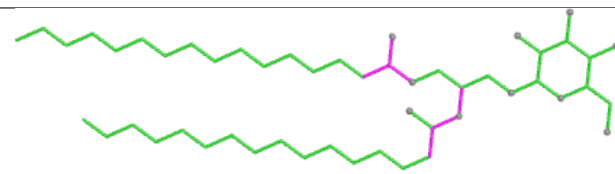
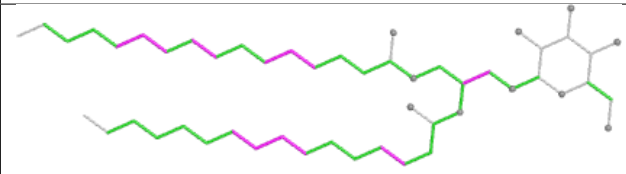
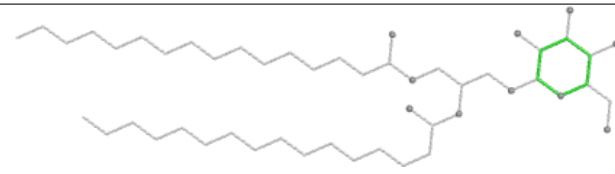
Ligand CLA B 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

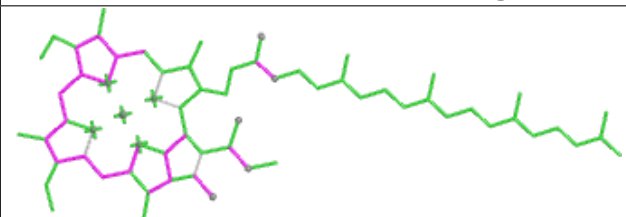
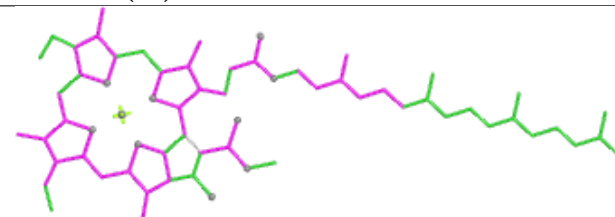
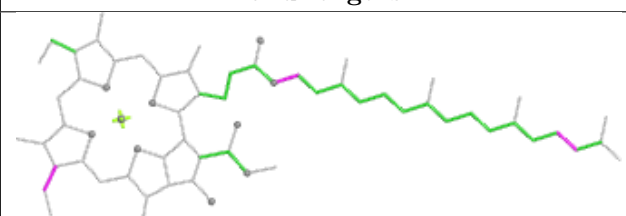
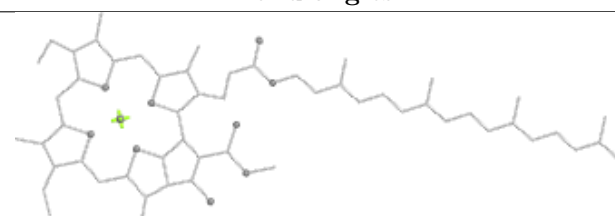
Ligand BCR A 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

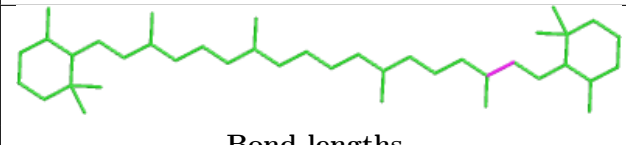
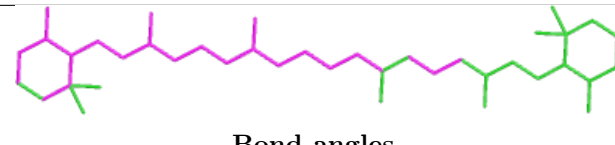
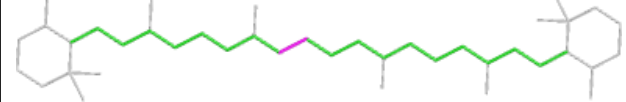
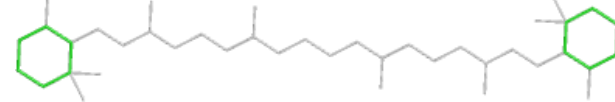


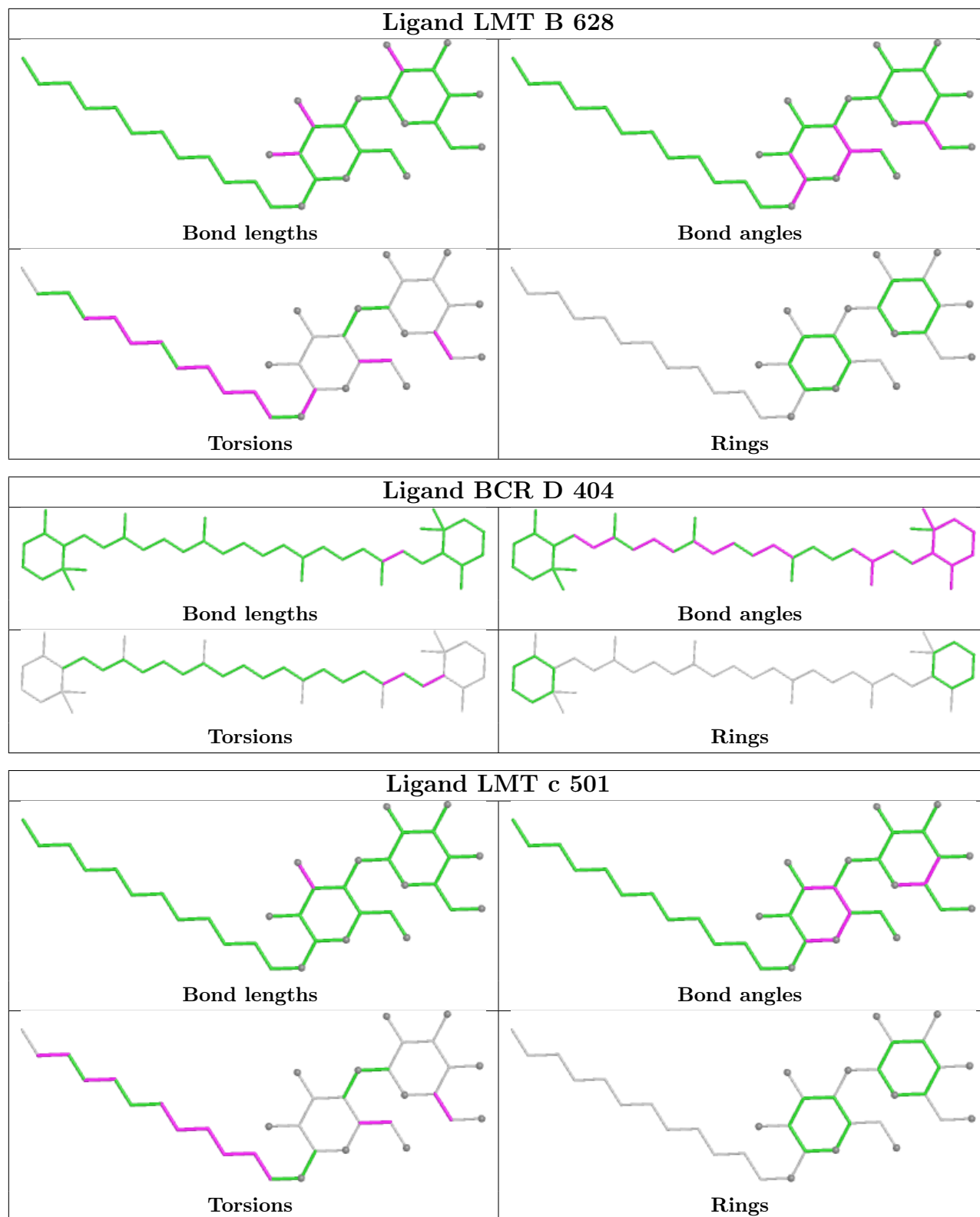
Ligand CLA a 407 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 A 415 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand DGD c 518 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings

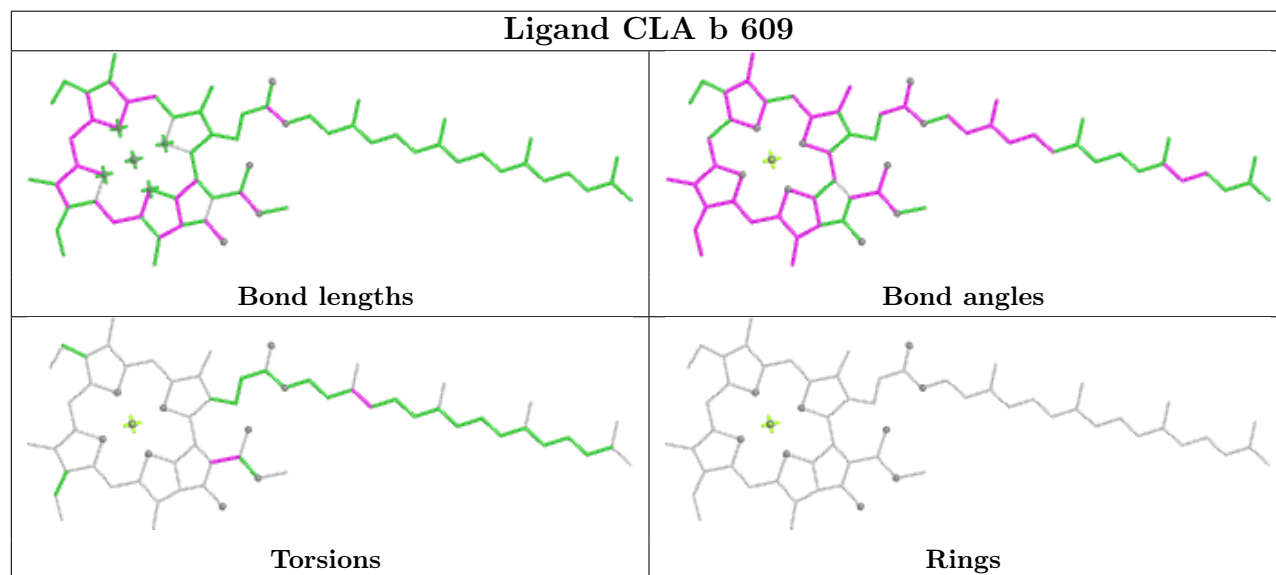
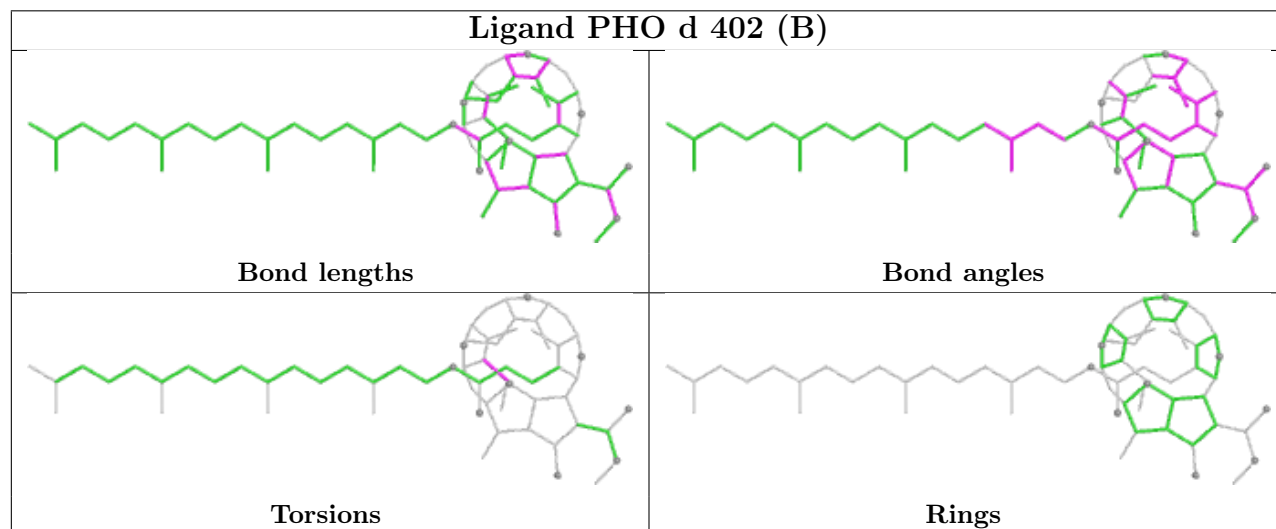
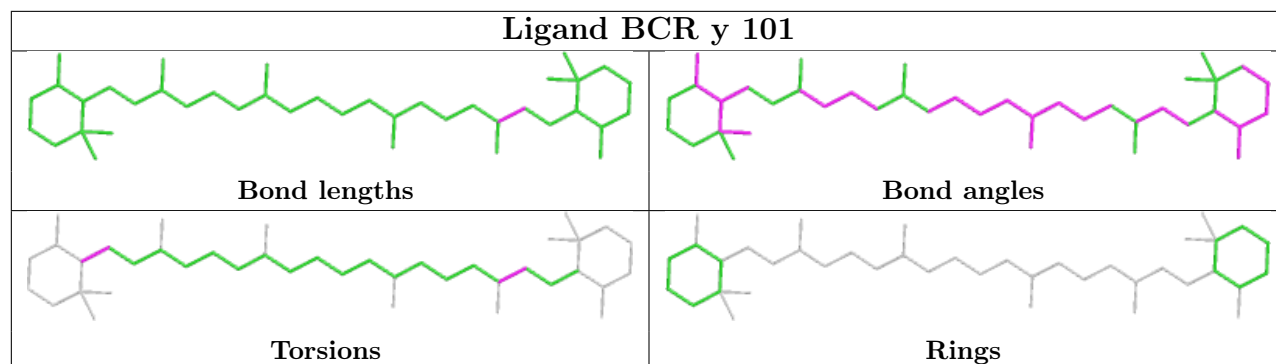
Ligand CLA C 502**Ligand SQD L 102**

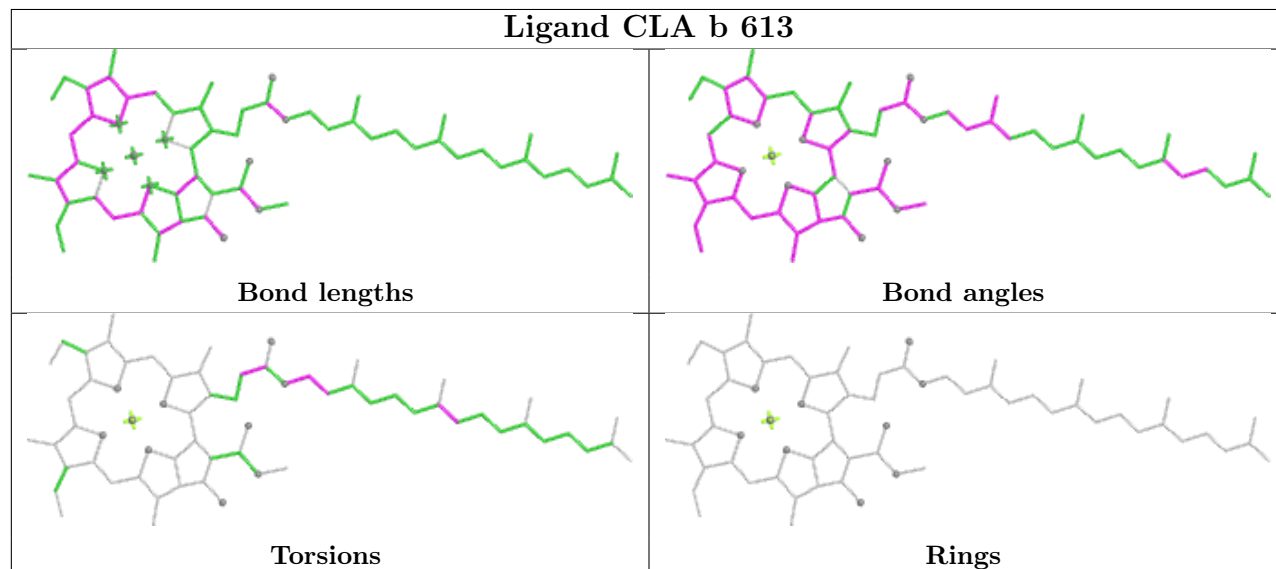
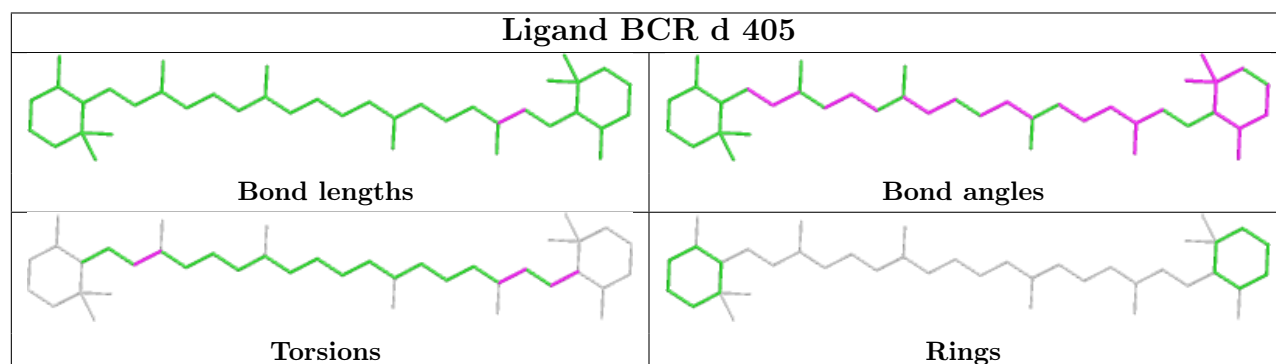
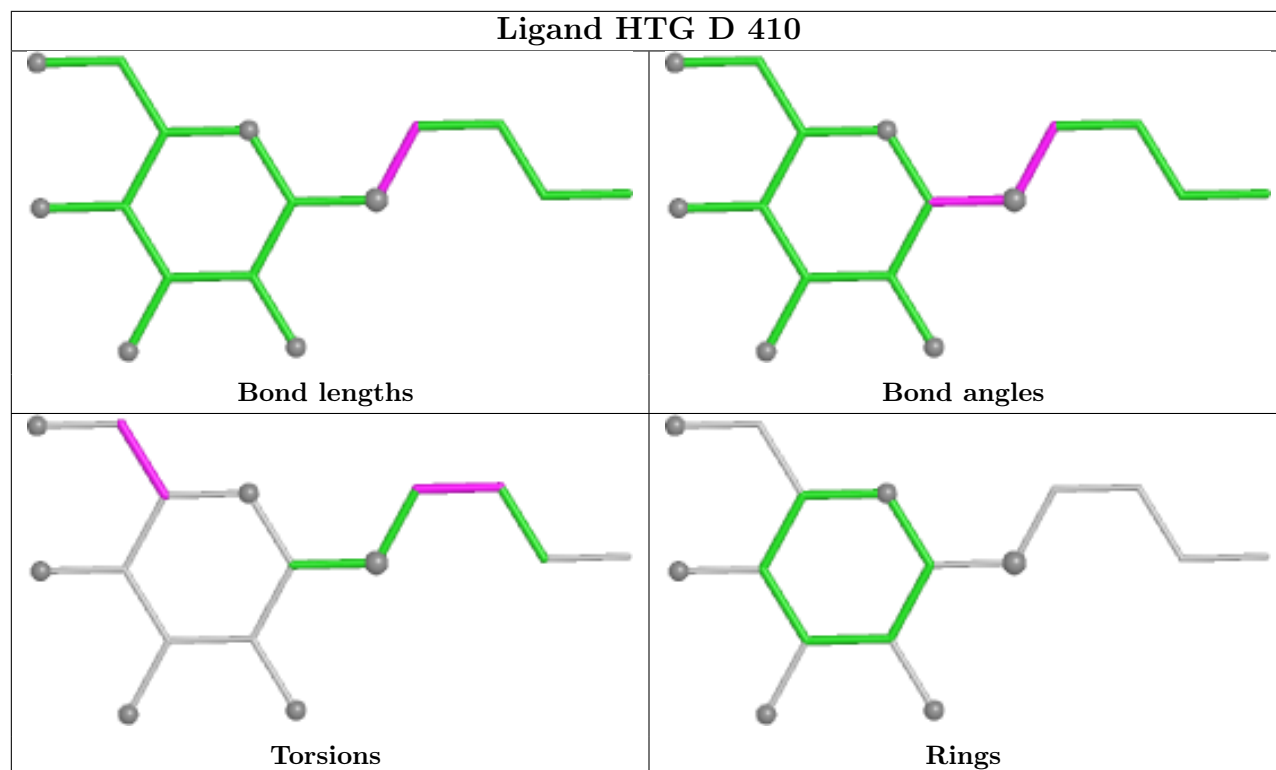
Ligand LMG C 520	
	
Bond lengths	Bond angles
	
Torsions	Rings

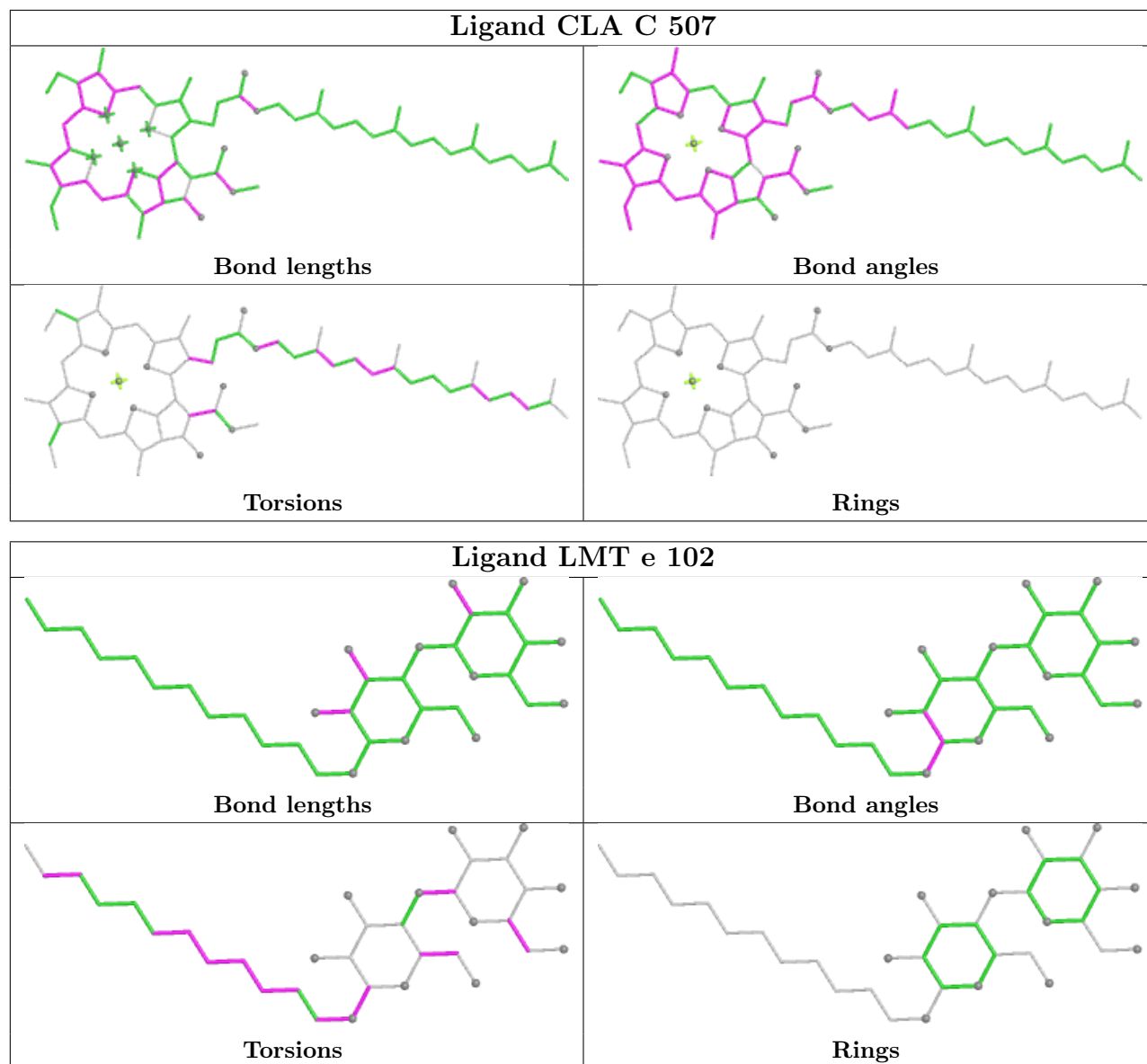
Ligand CLA a 405 (A)	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR T 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

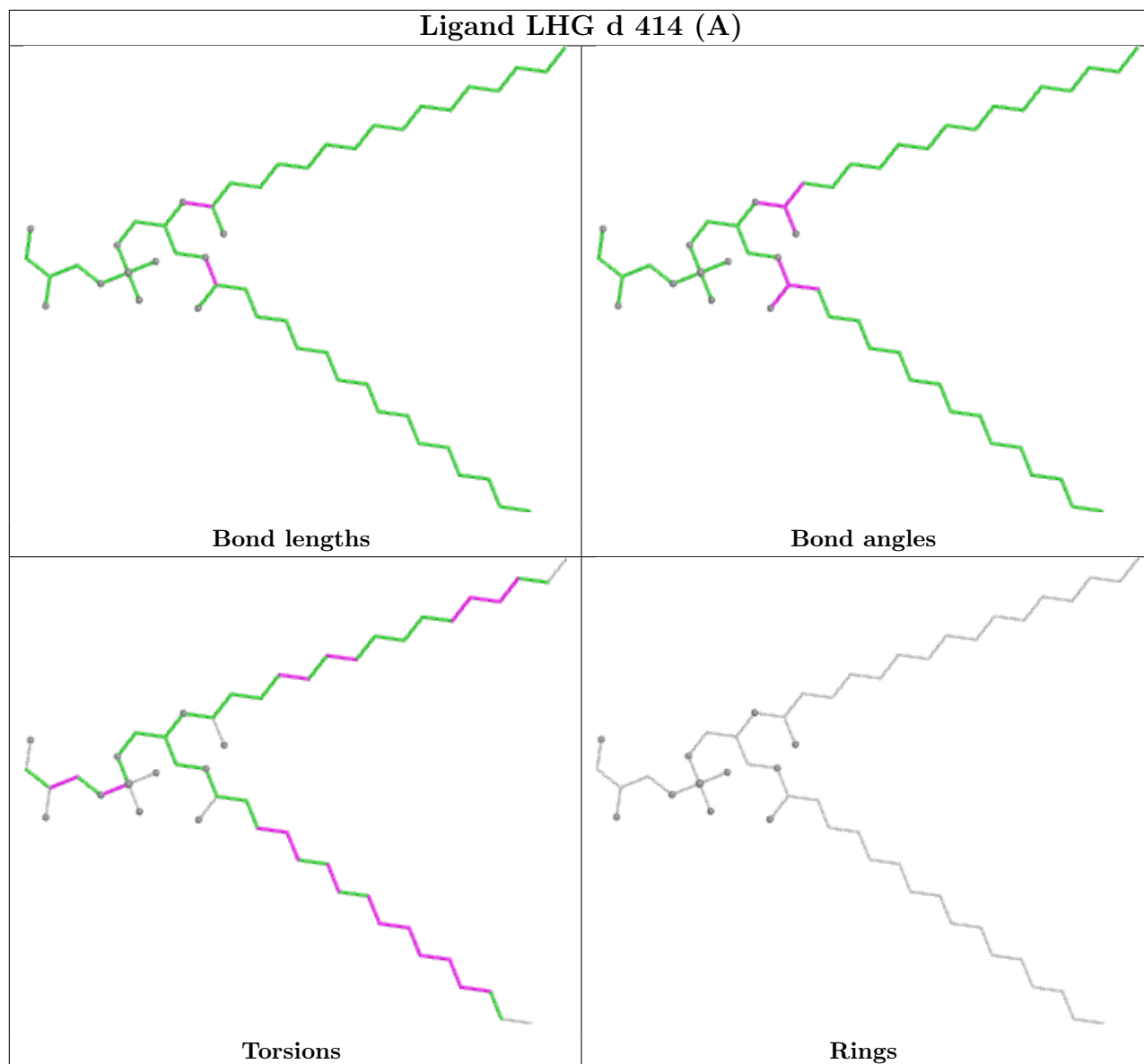




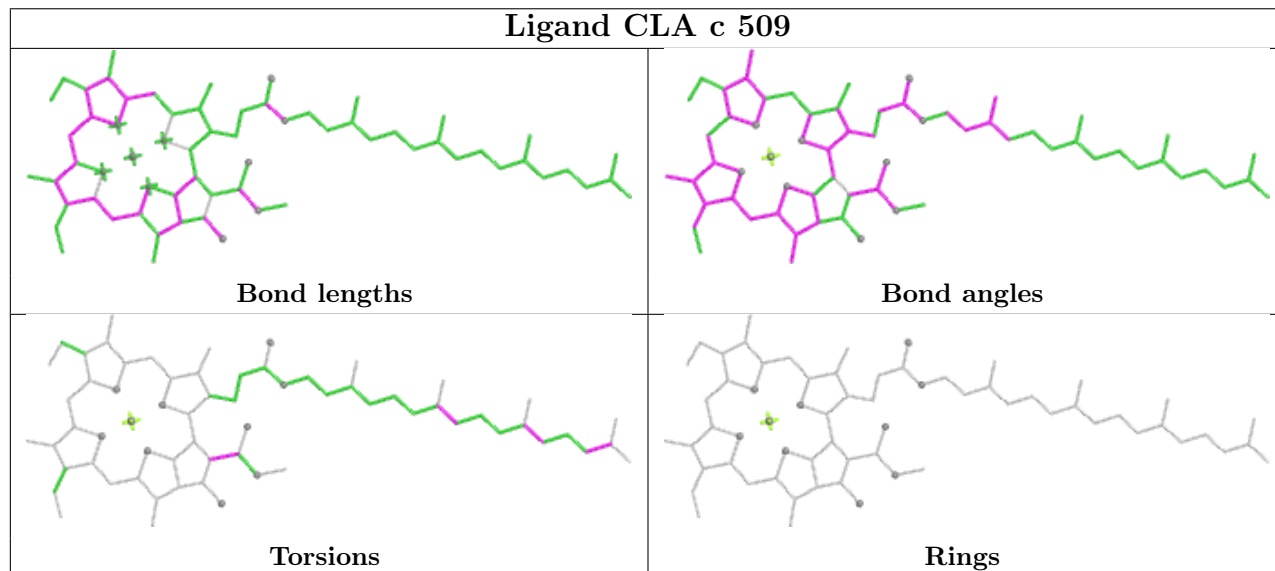


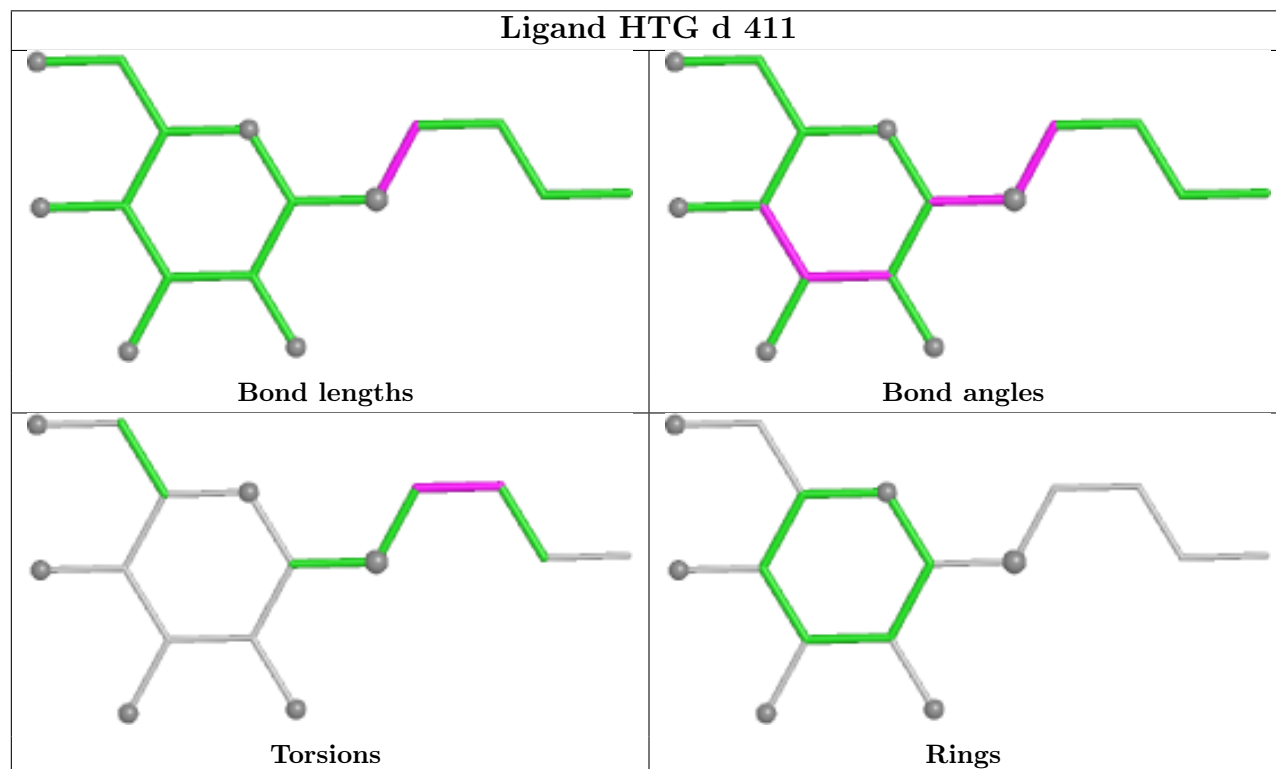
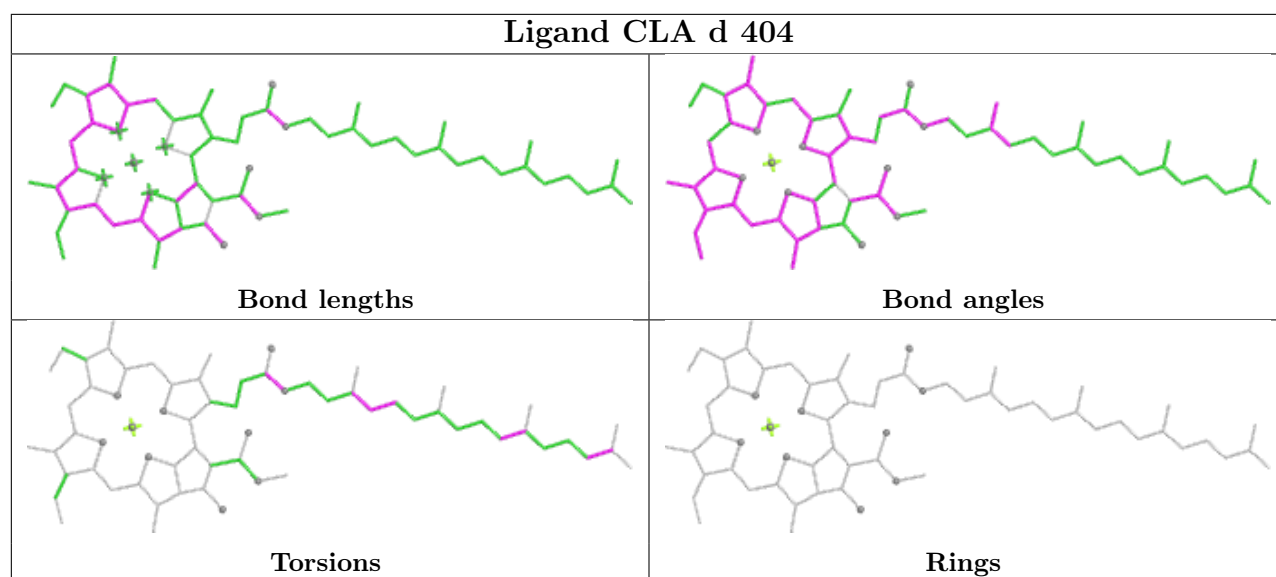


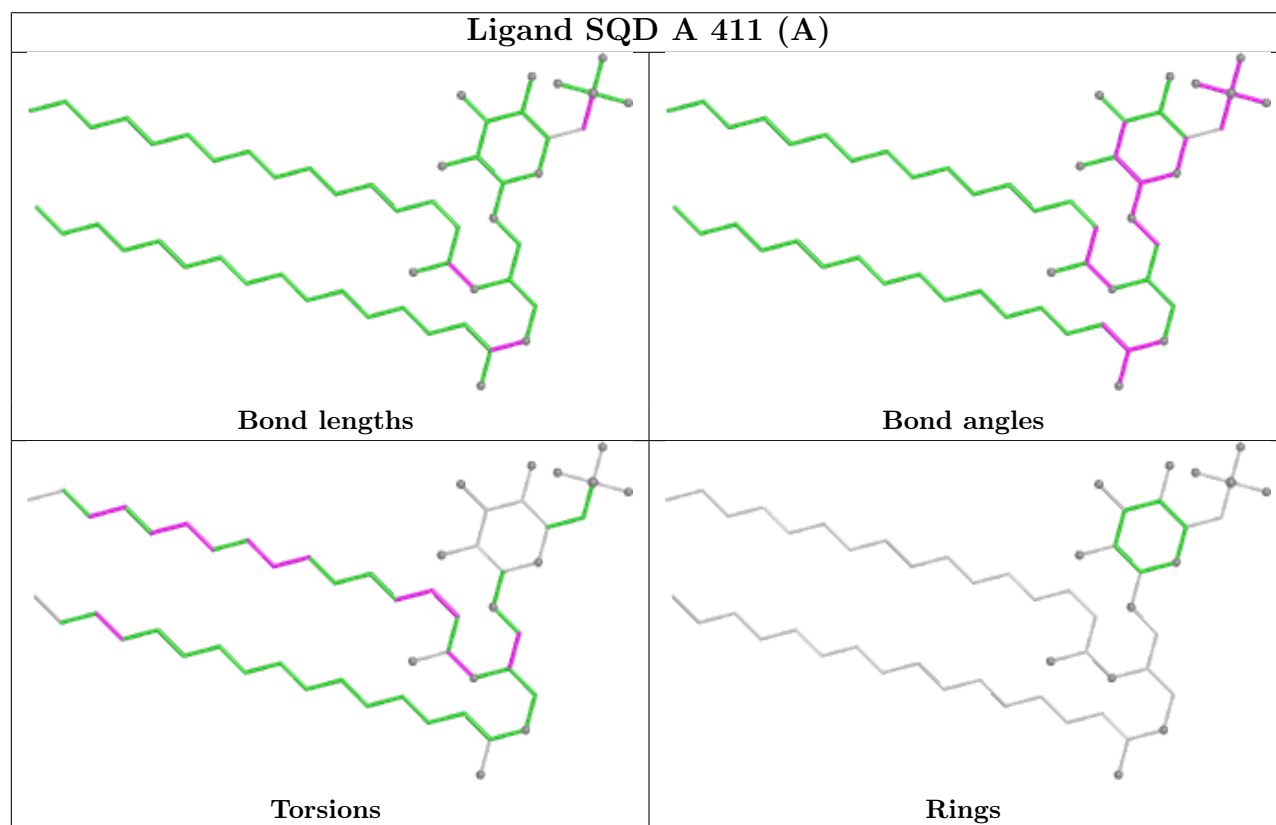
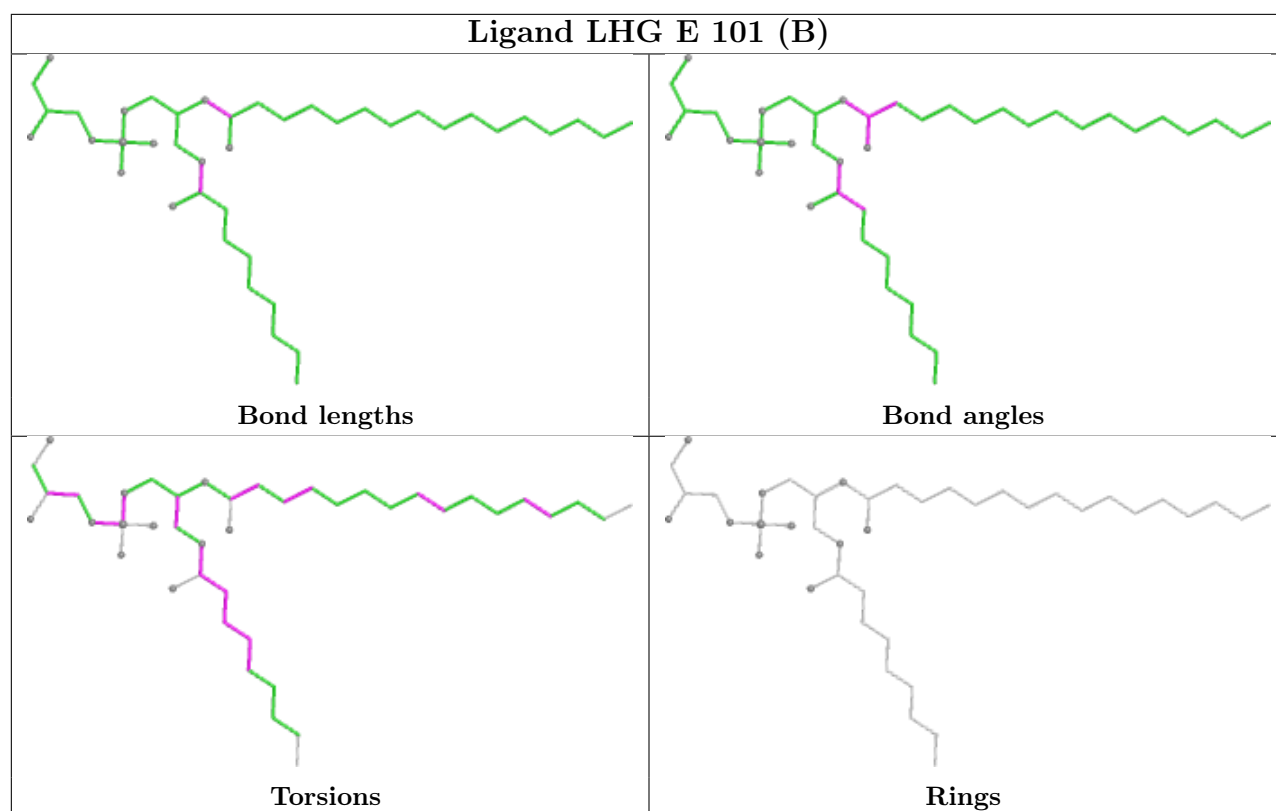
Ligand LHG d 414 (A)

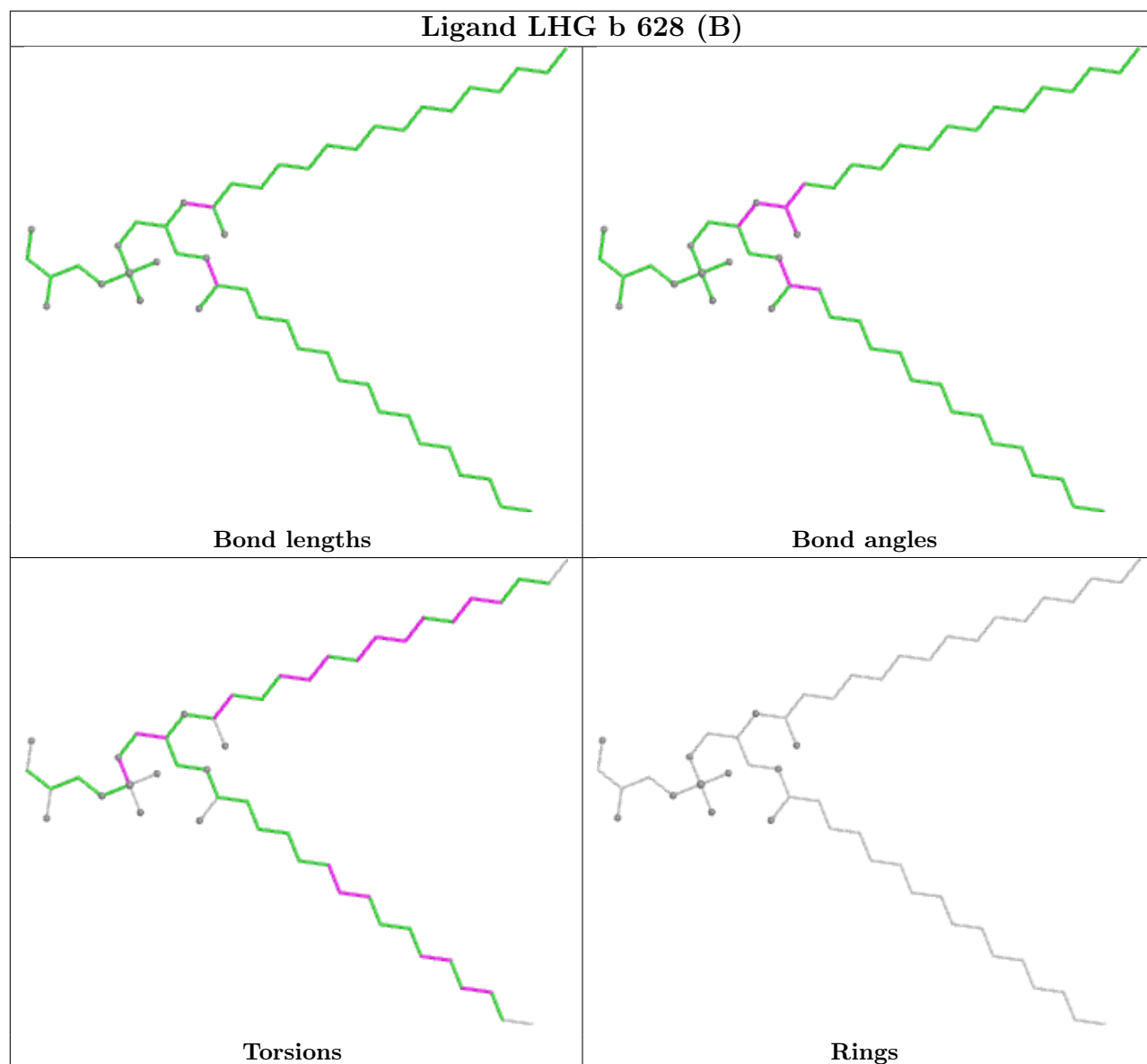
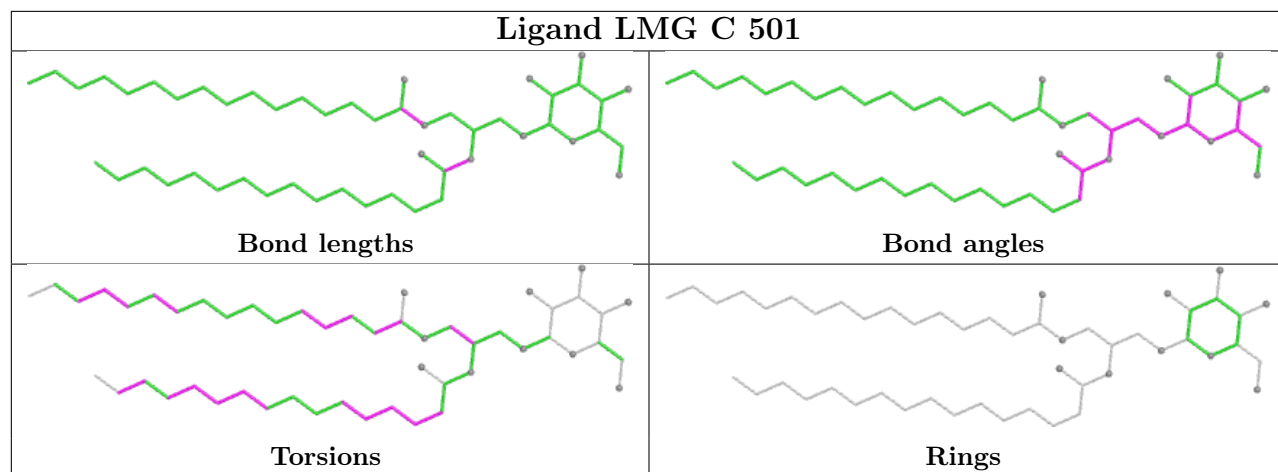


Ligand CLA c 509

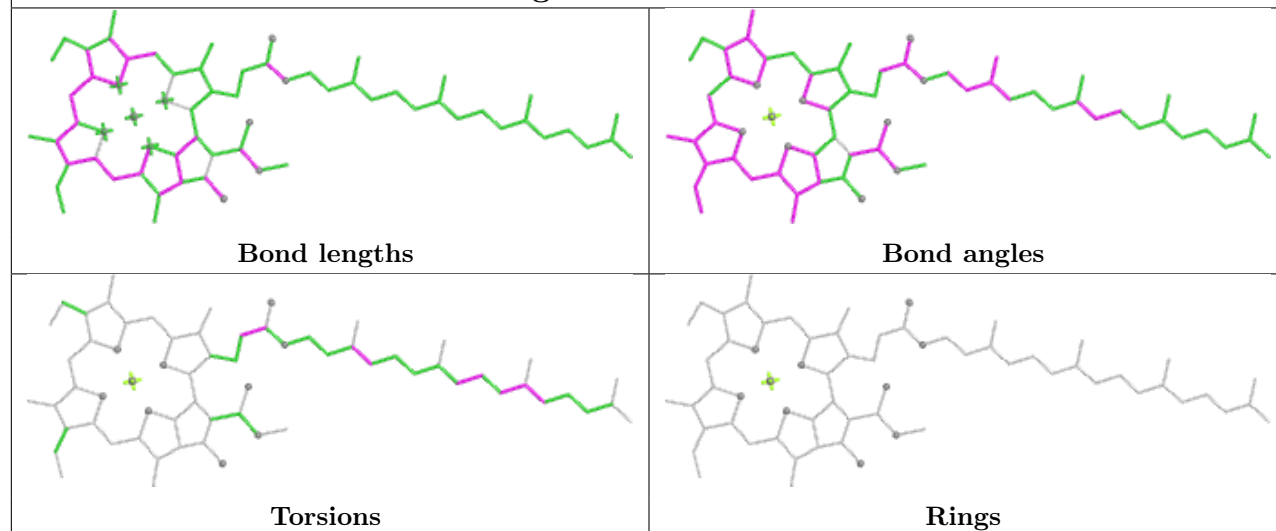




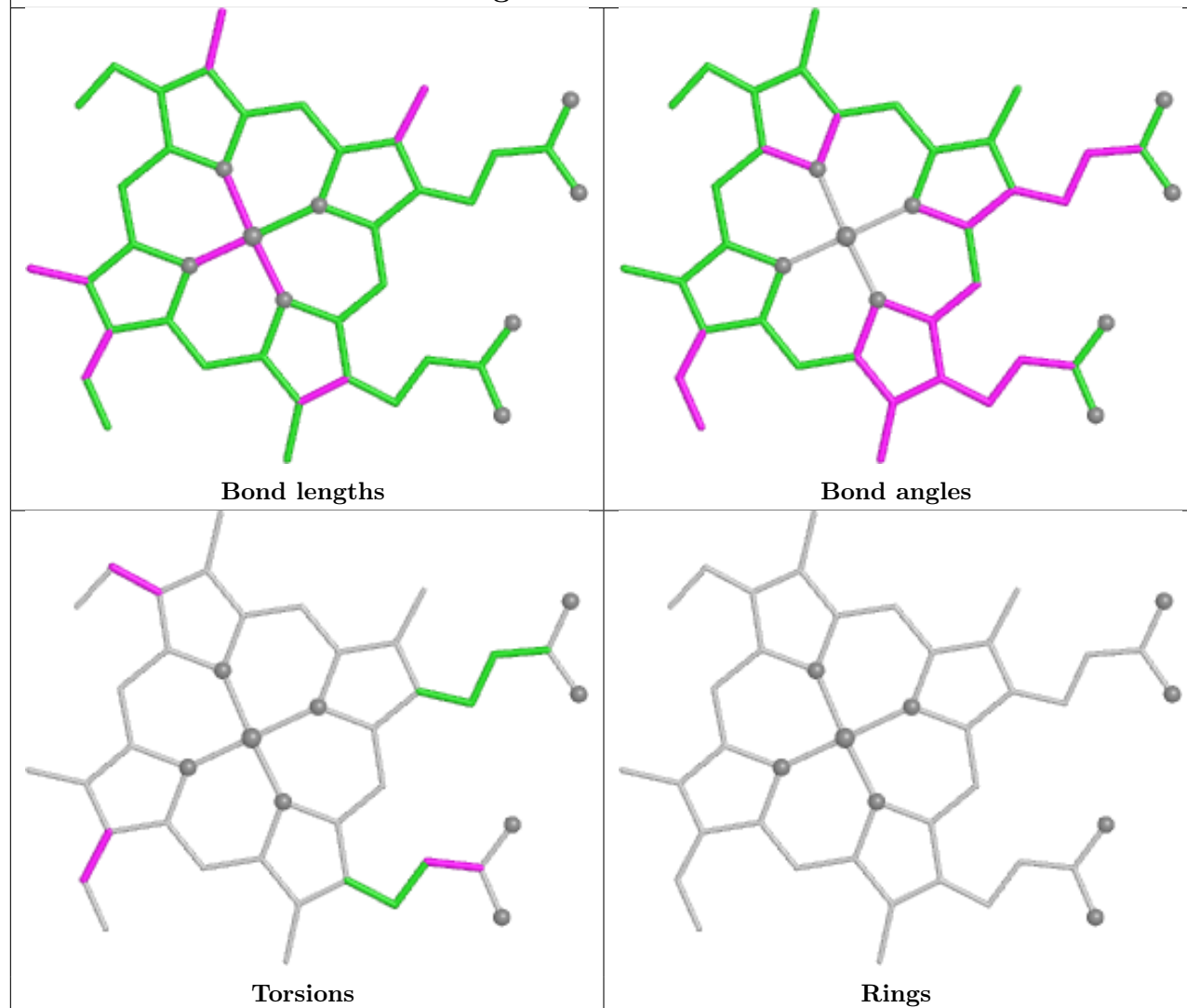


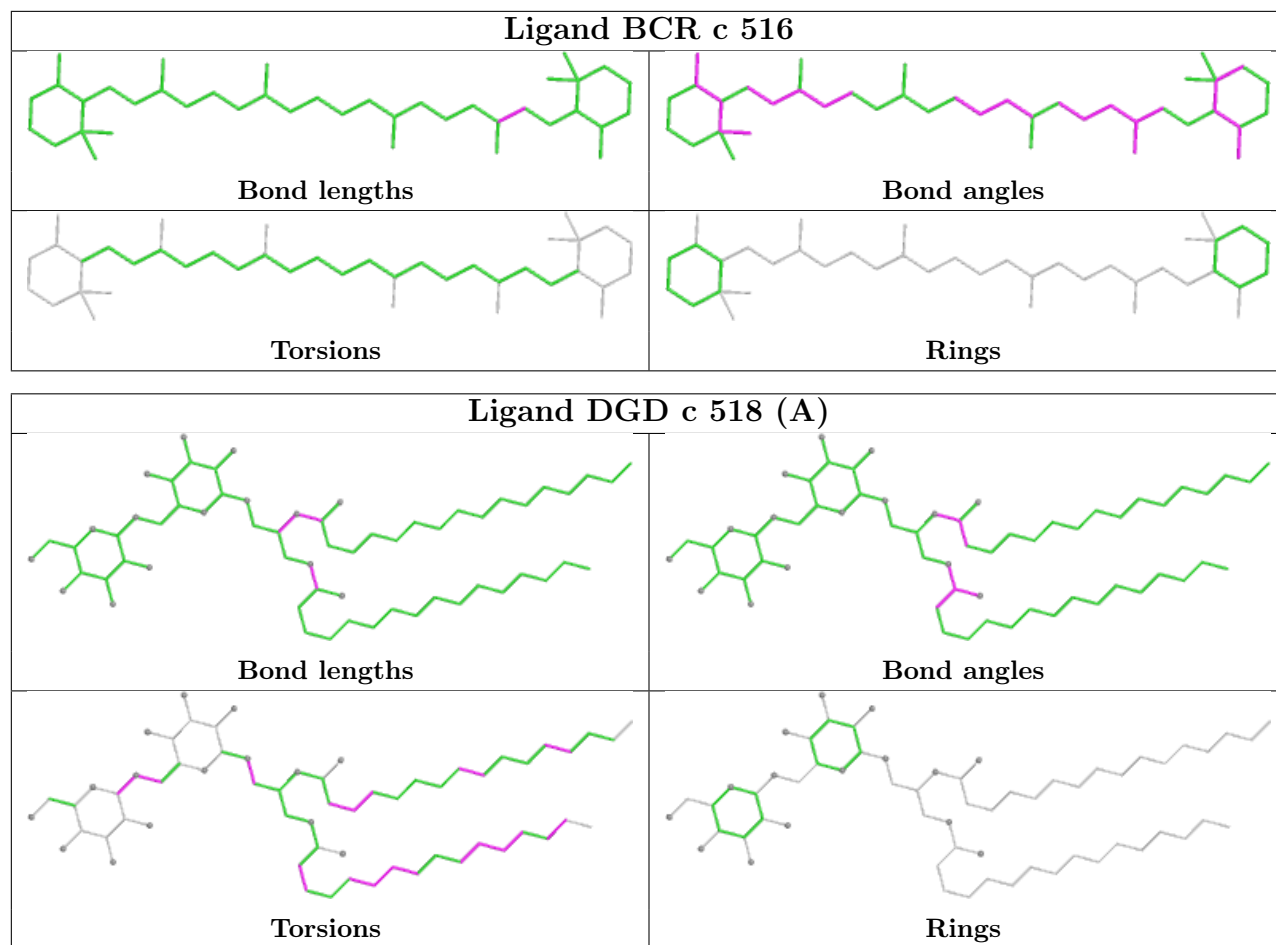


Ligand CLA C 506

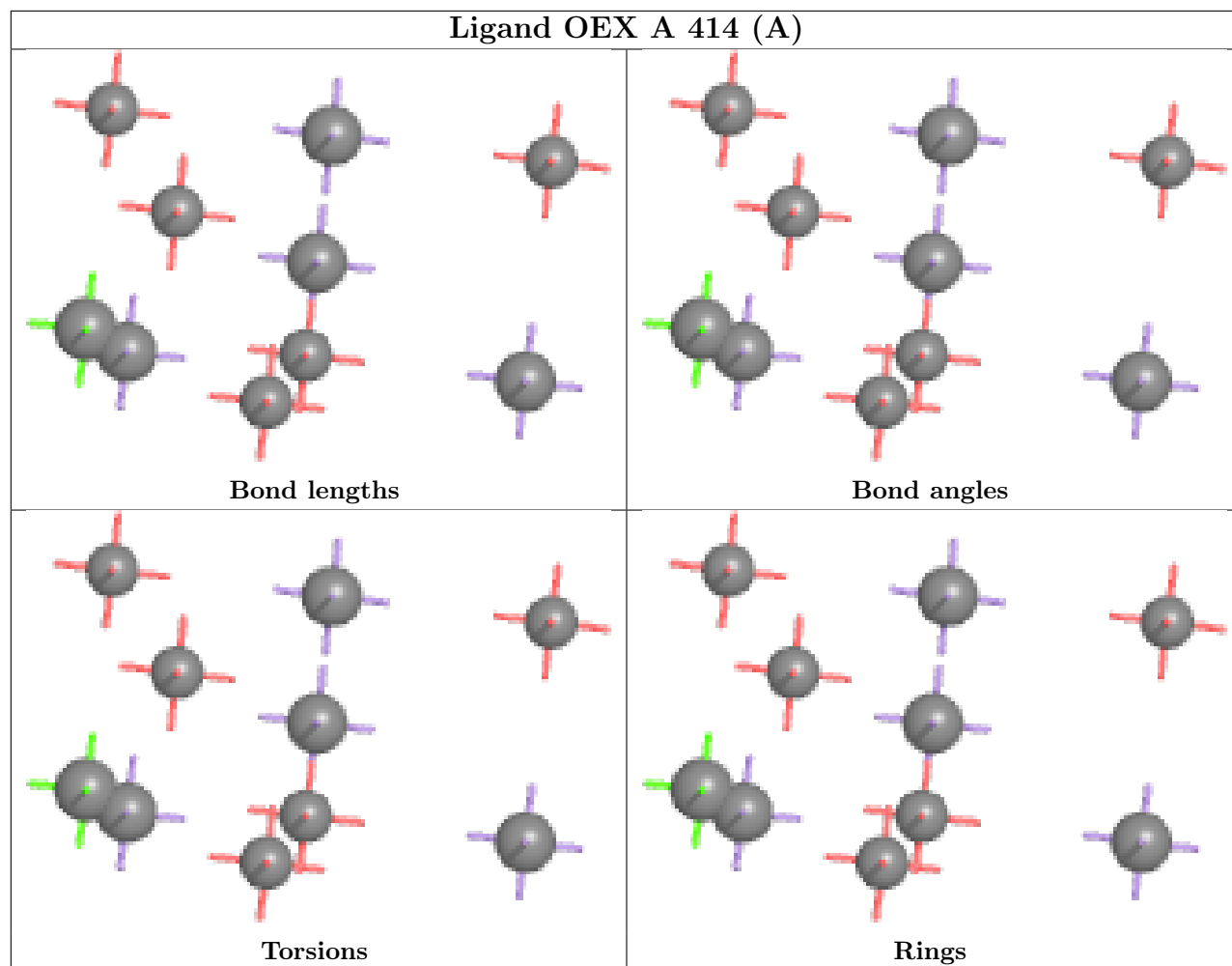


Ligand HEC V 201

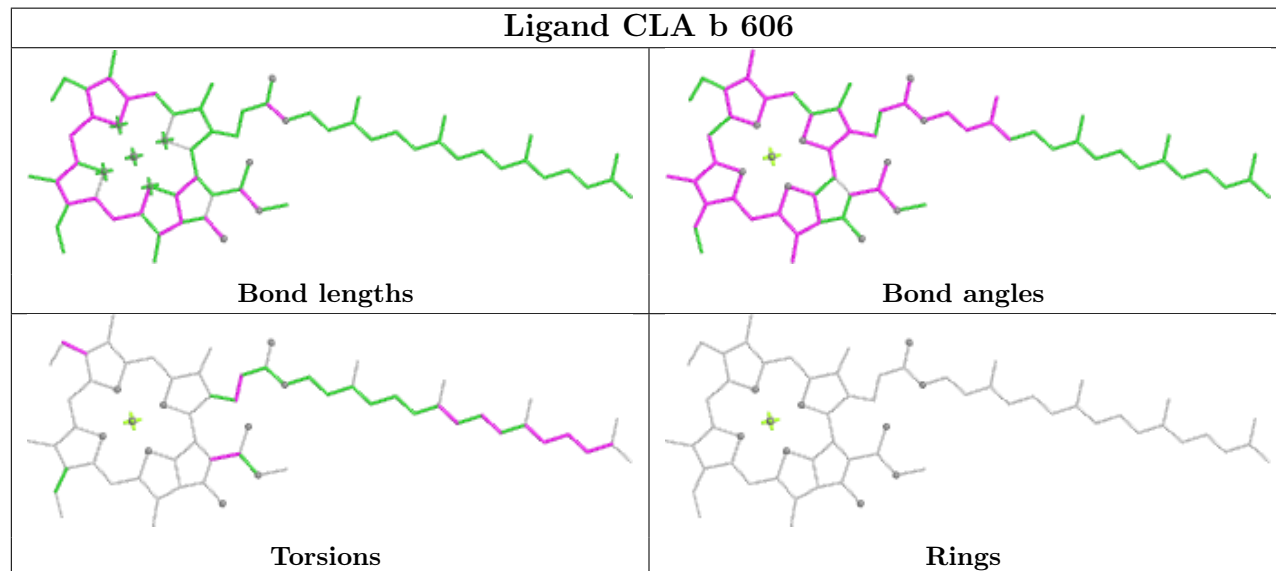


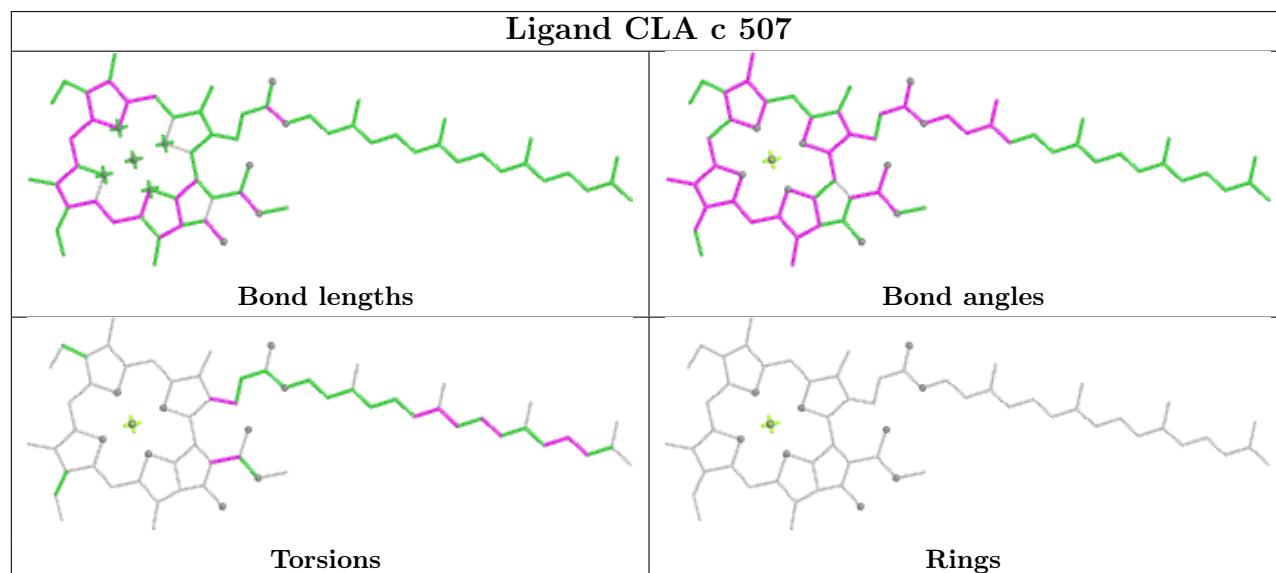
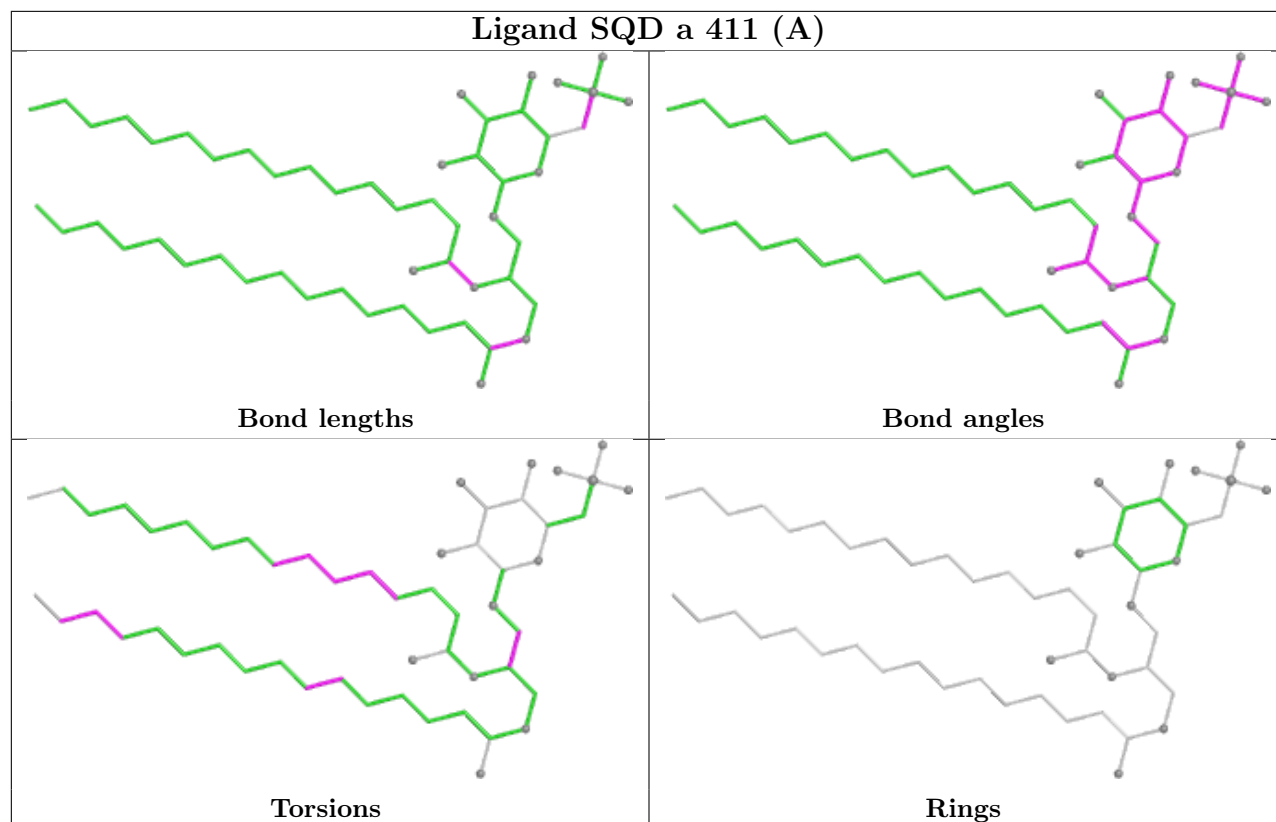


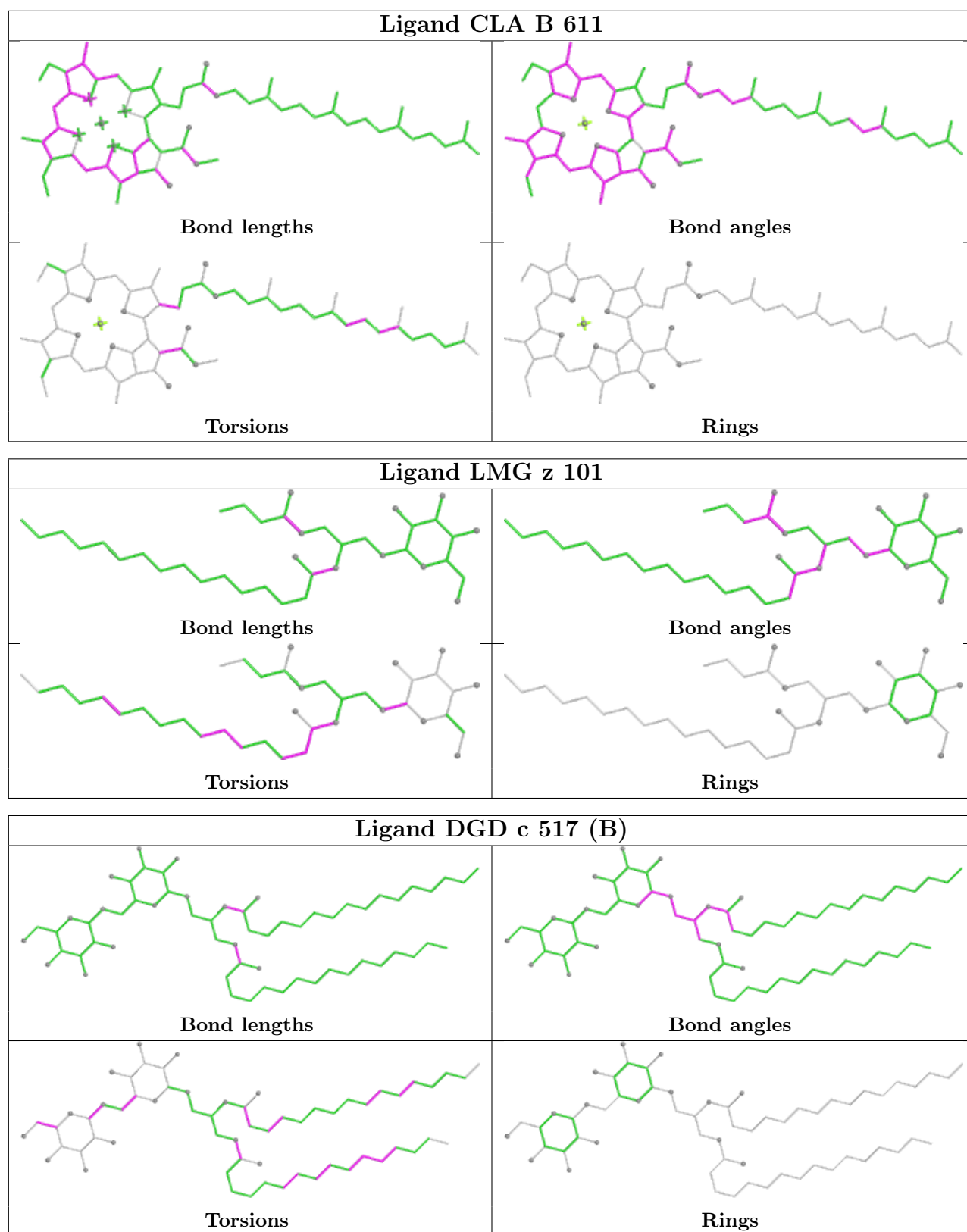
Ligand OEX A 414 (A)

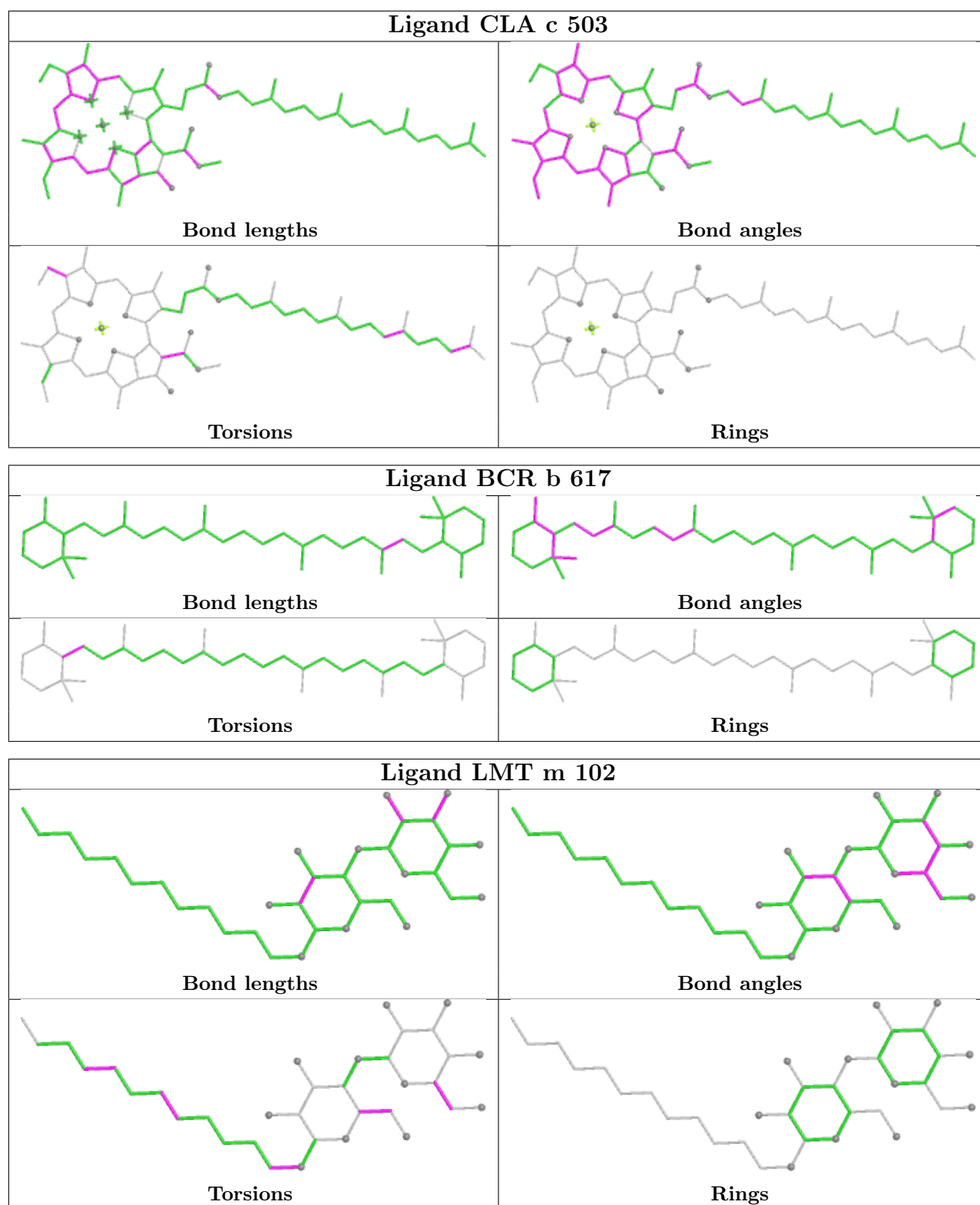


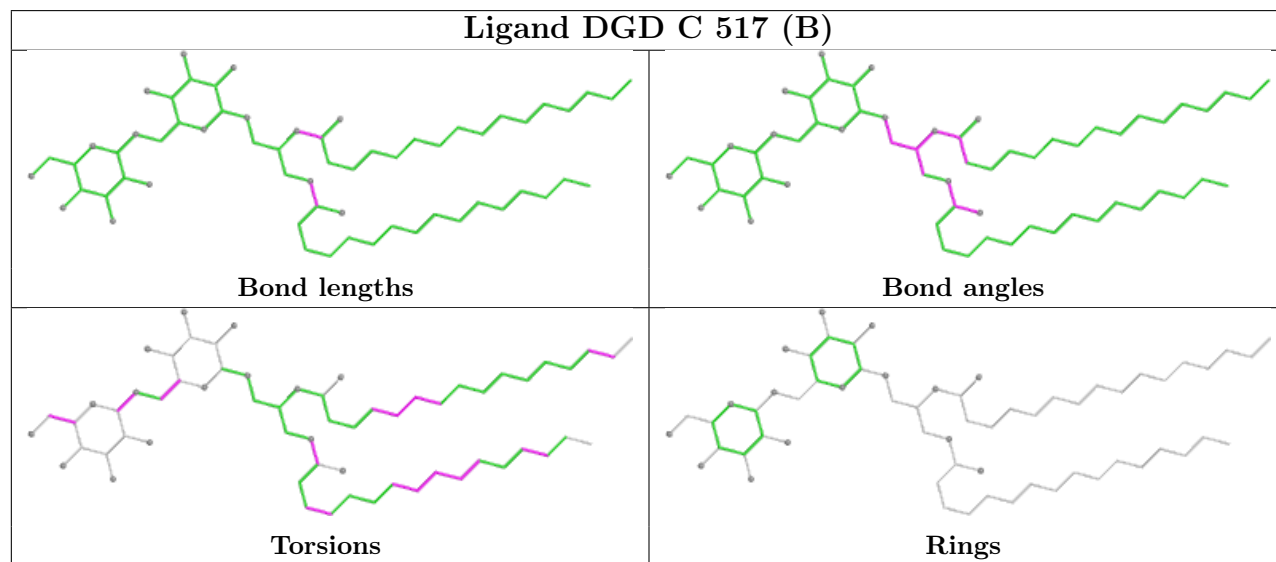
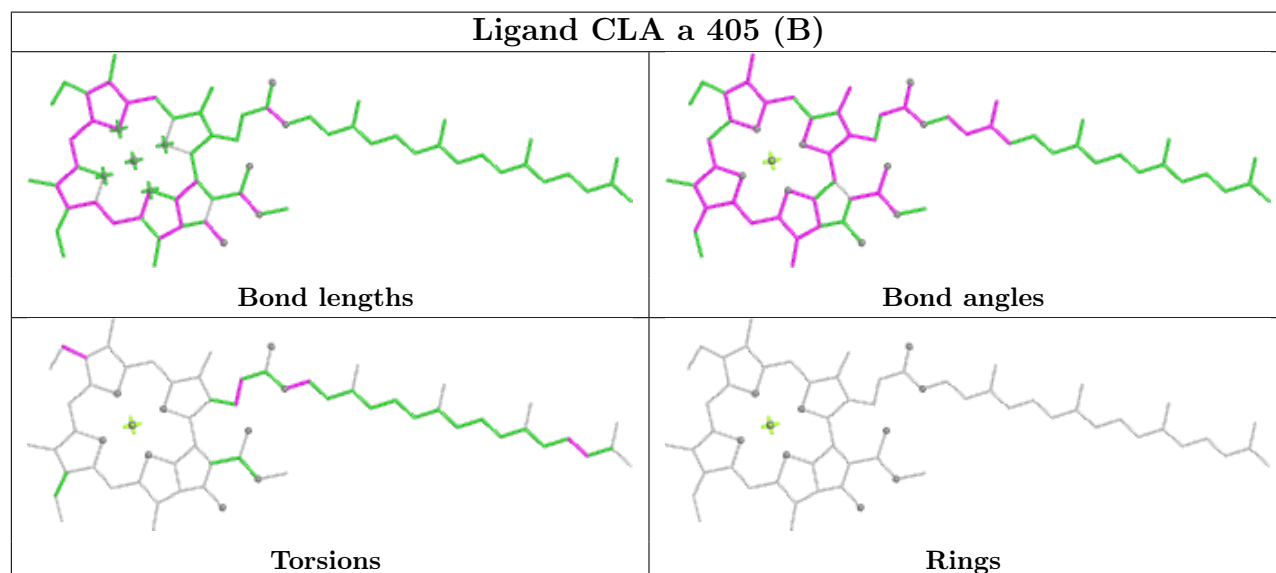
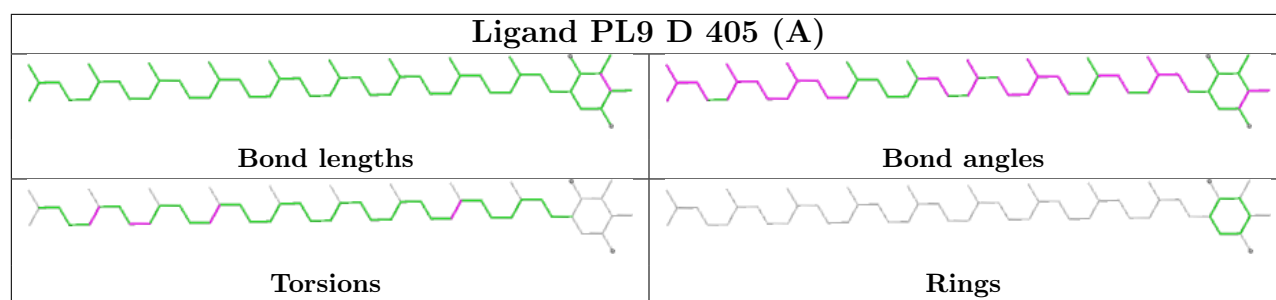
Ligand CLA b 606

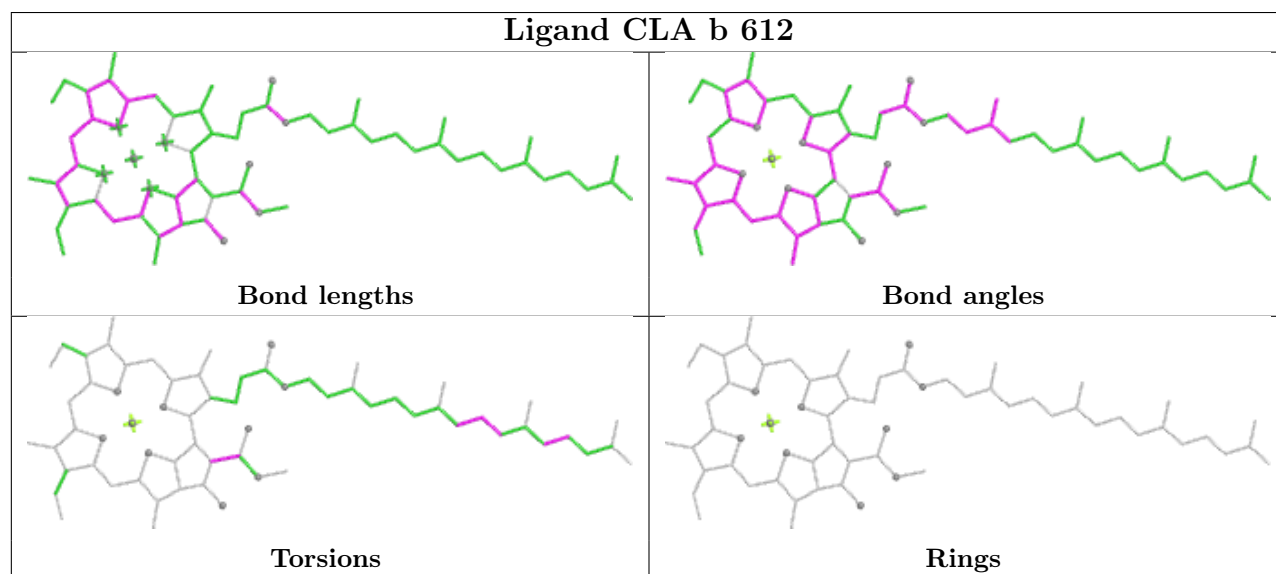
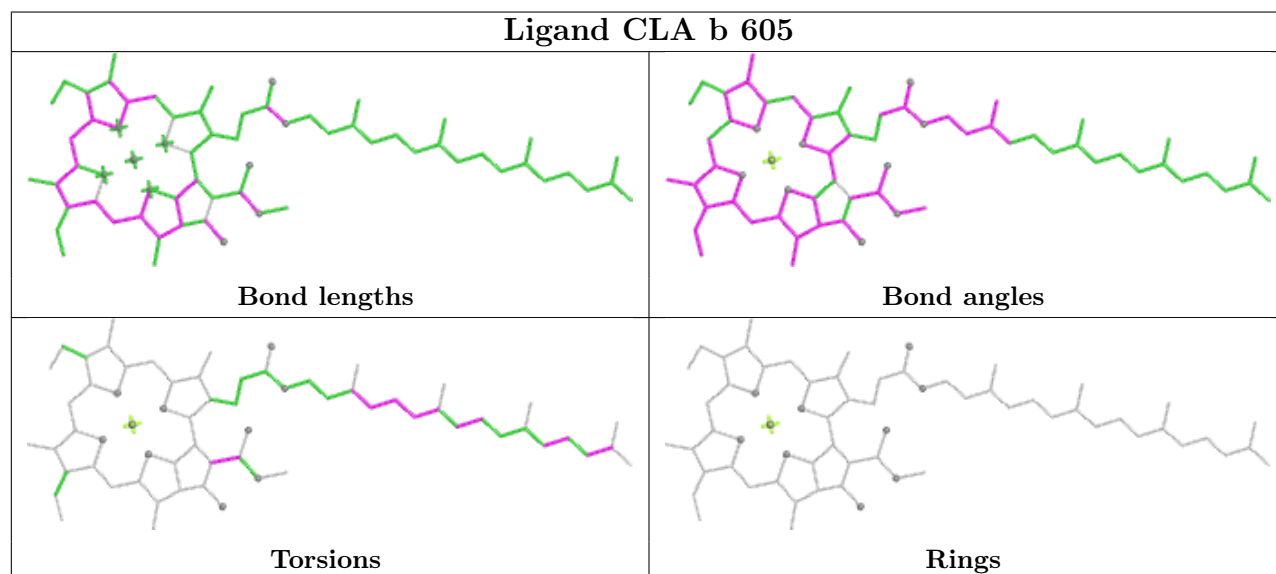
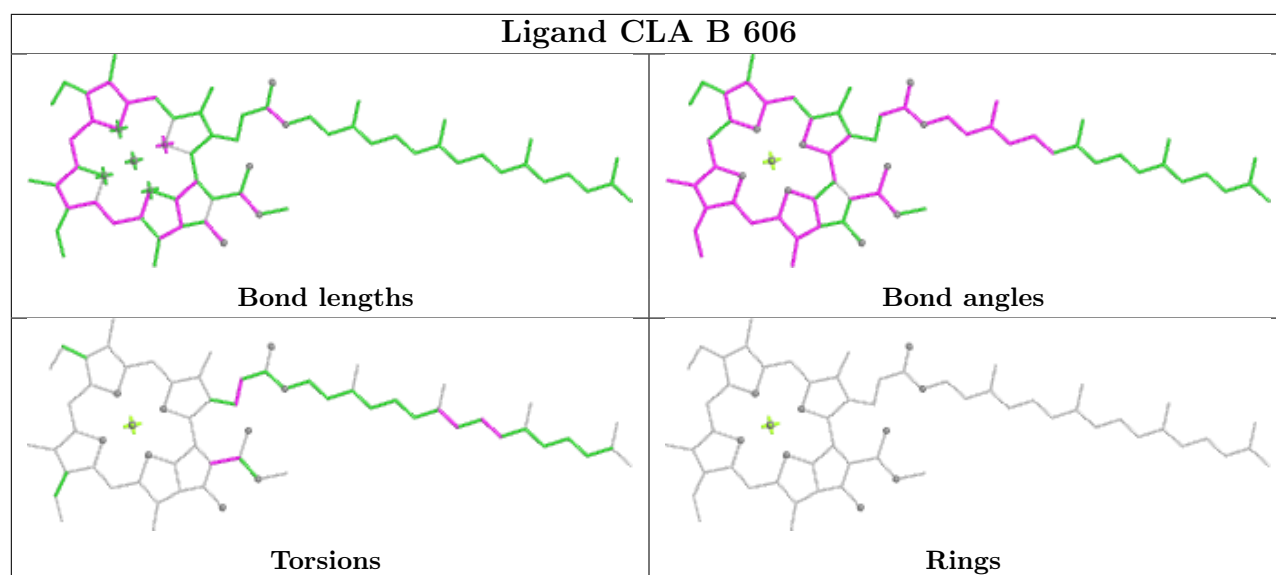




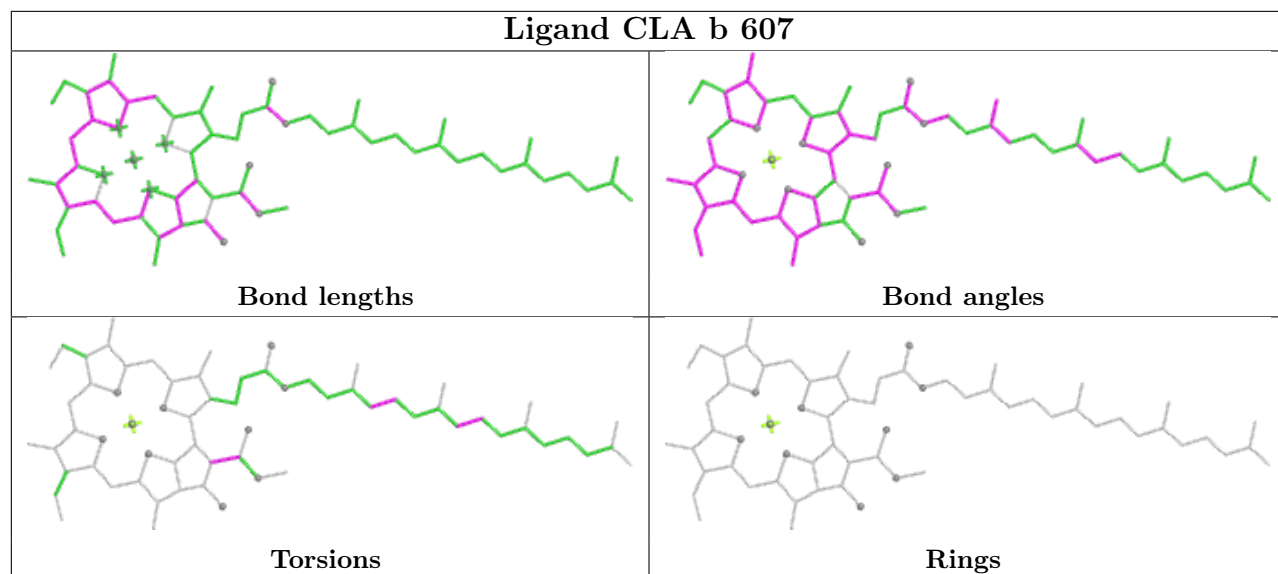




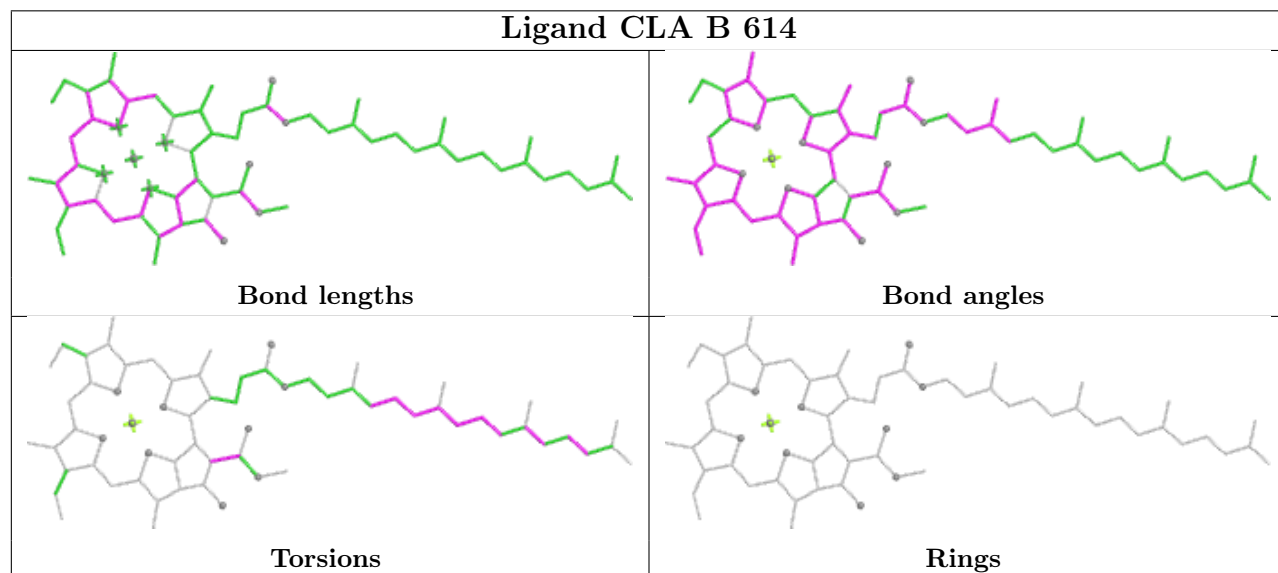




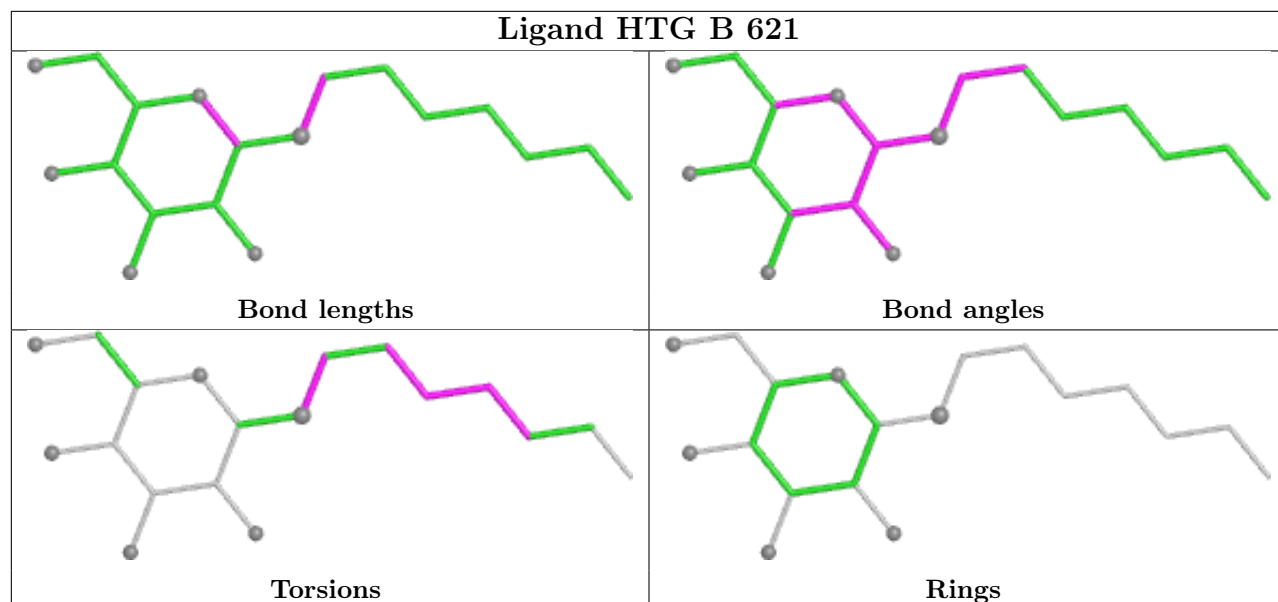
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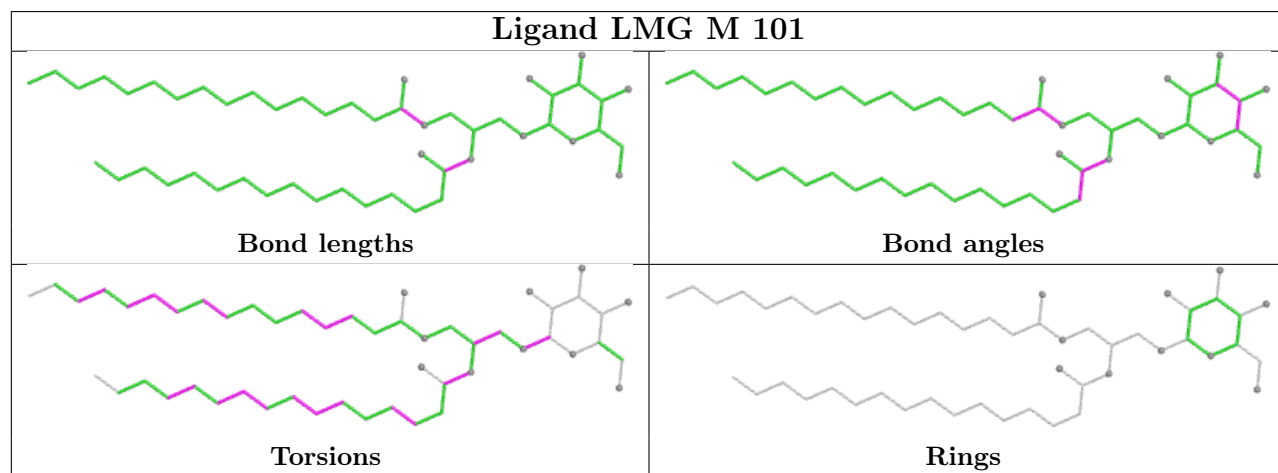
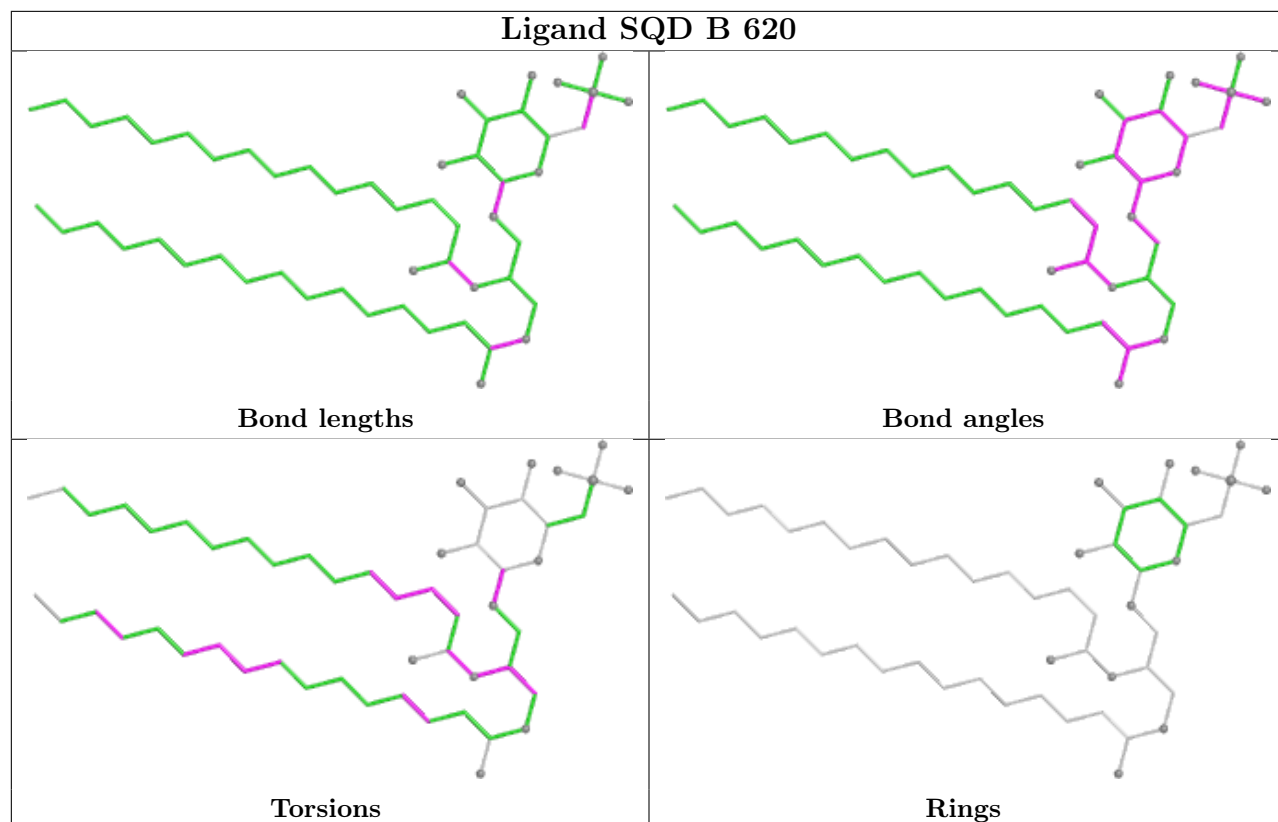


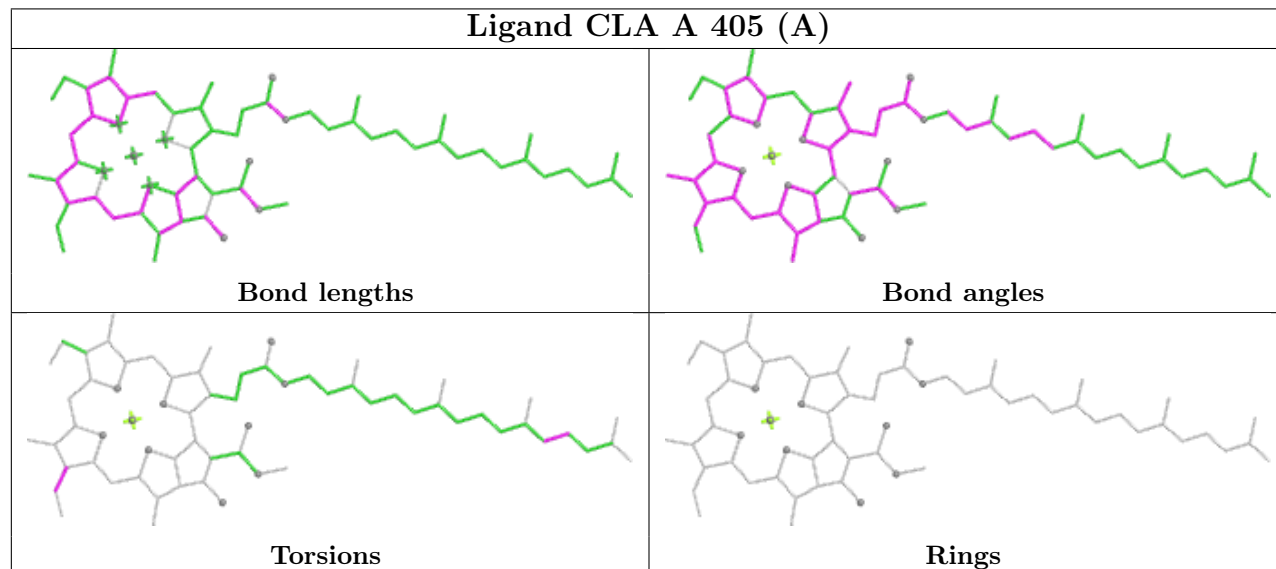
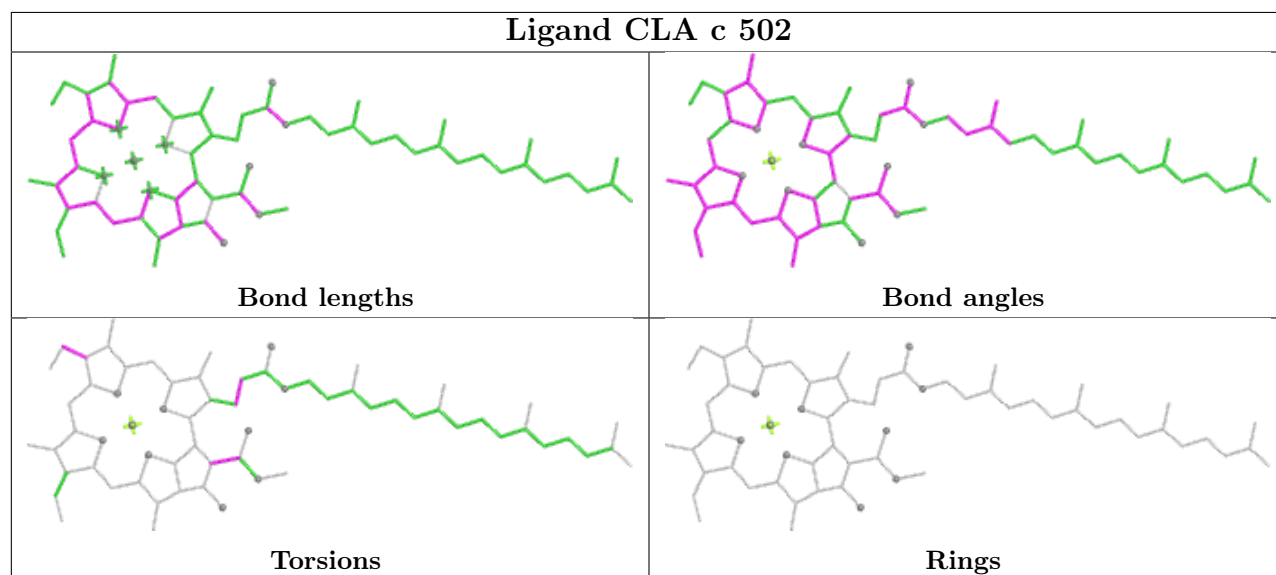
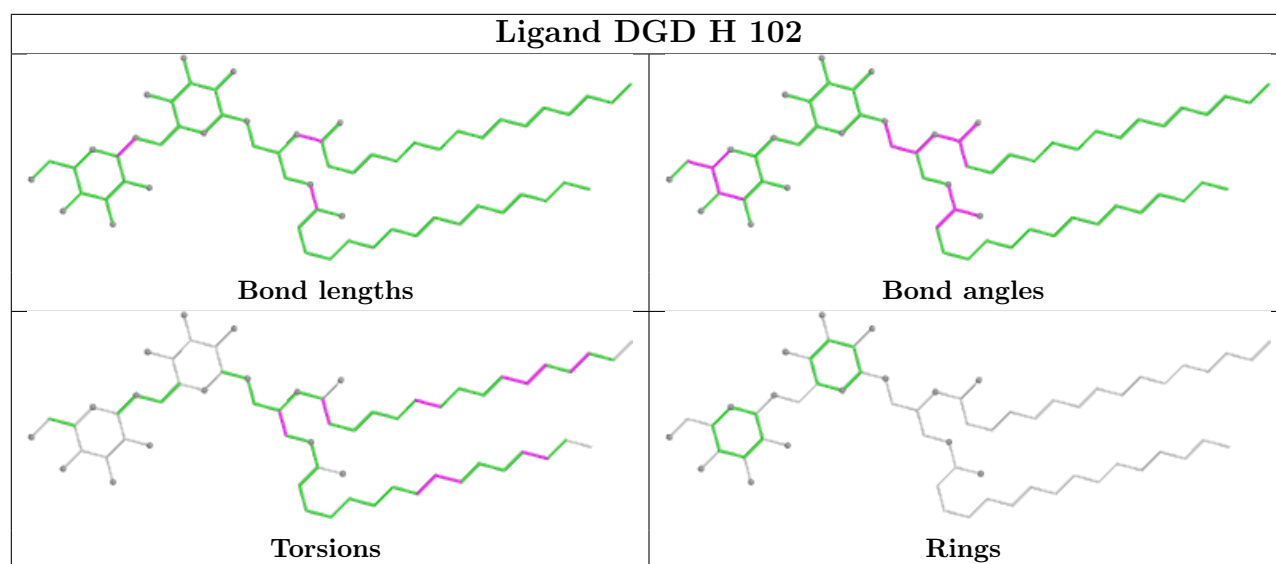
Ligand CLA B 614



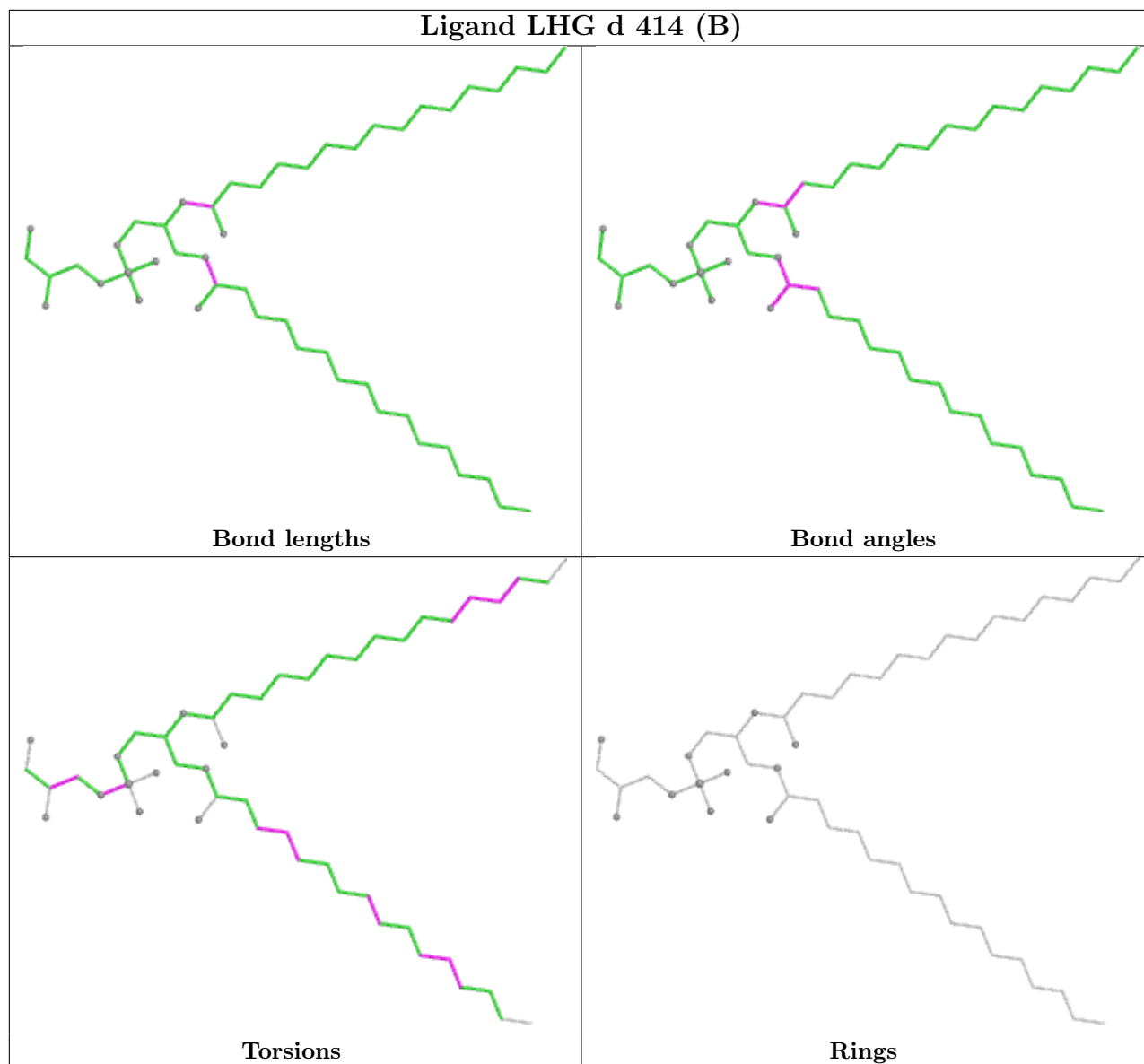
Ligand HTG B 621



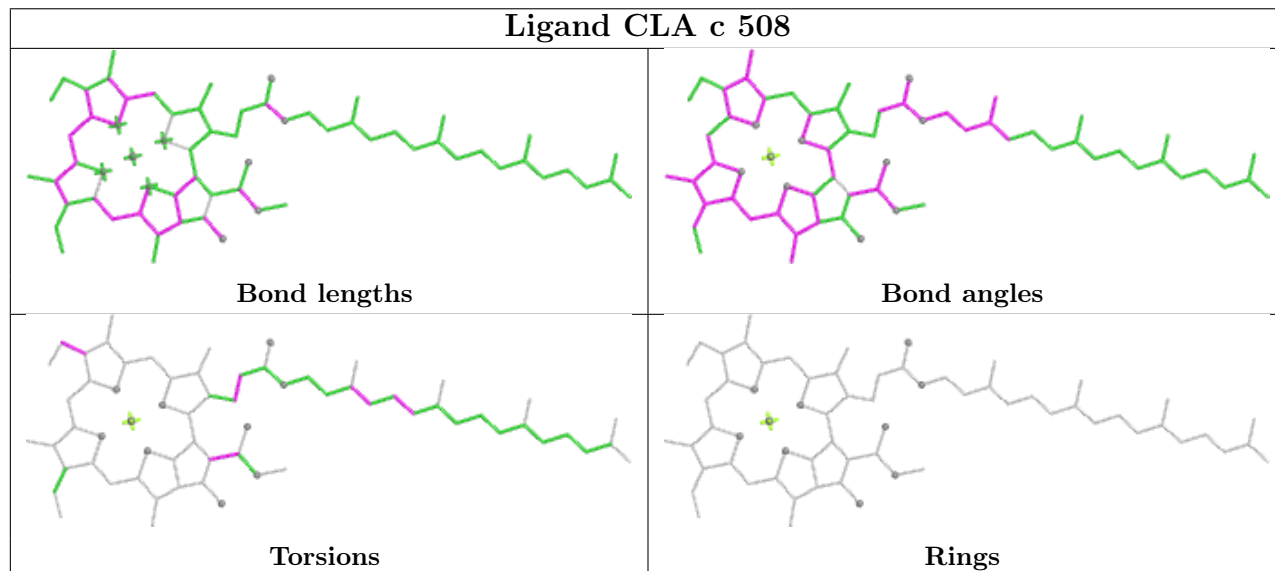


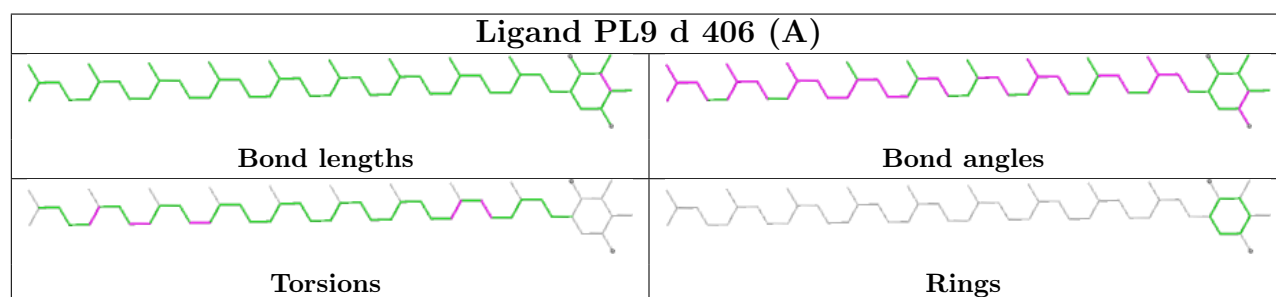
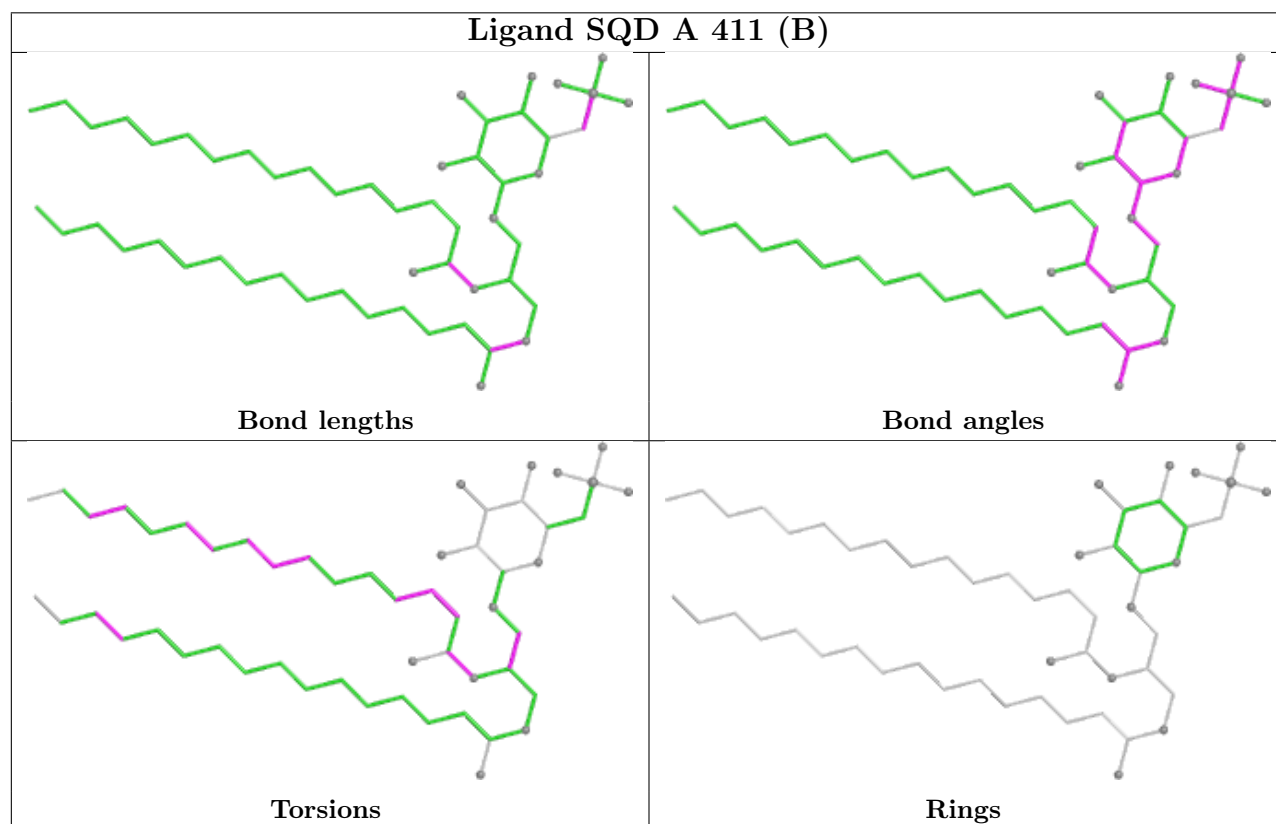
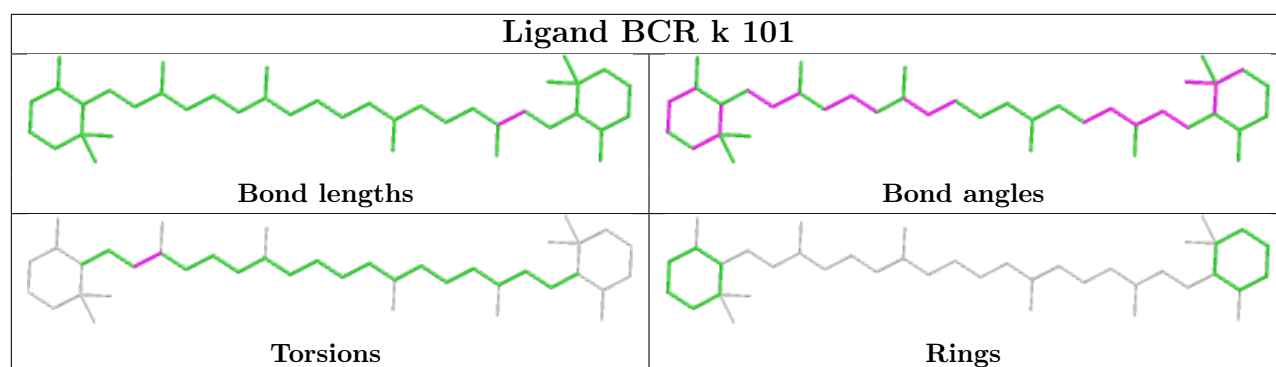


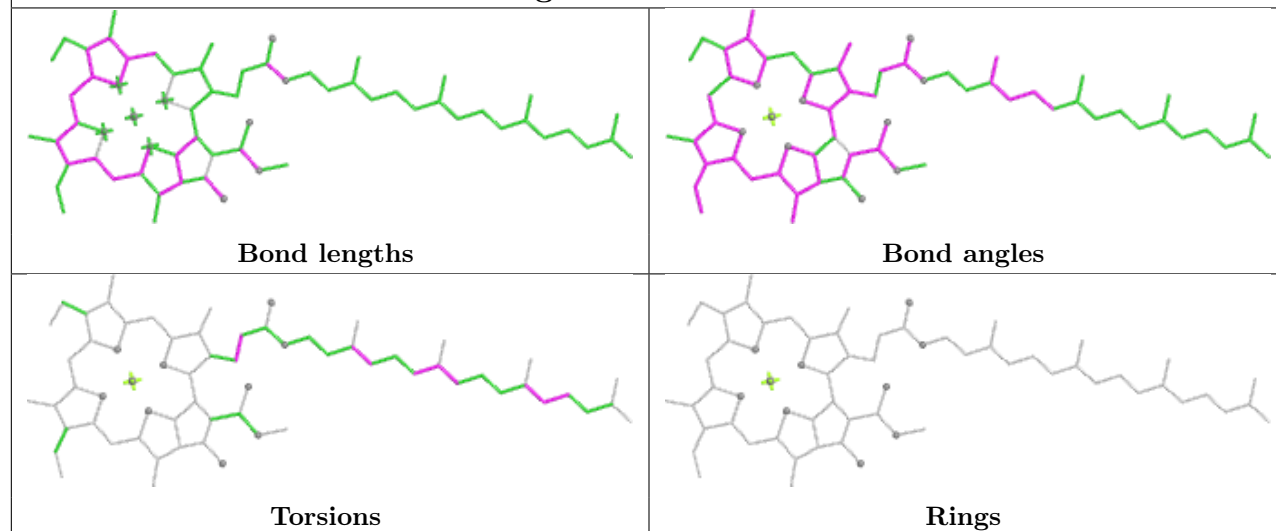
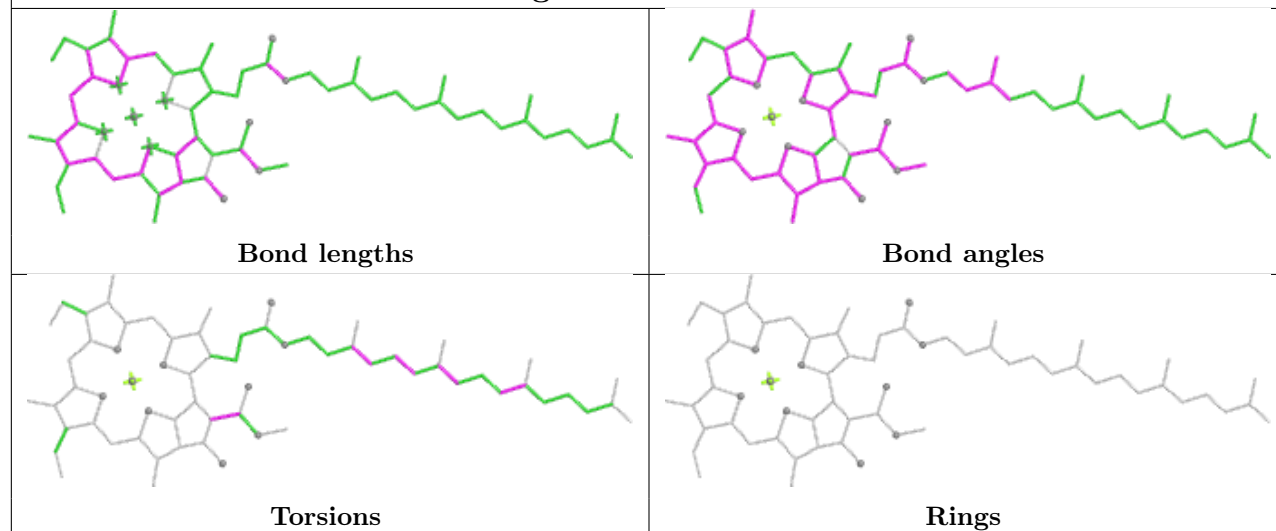
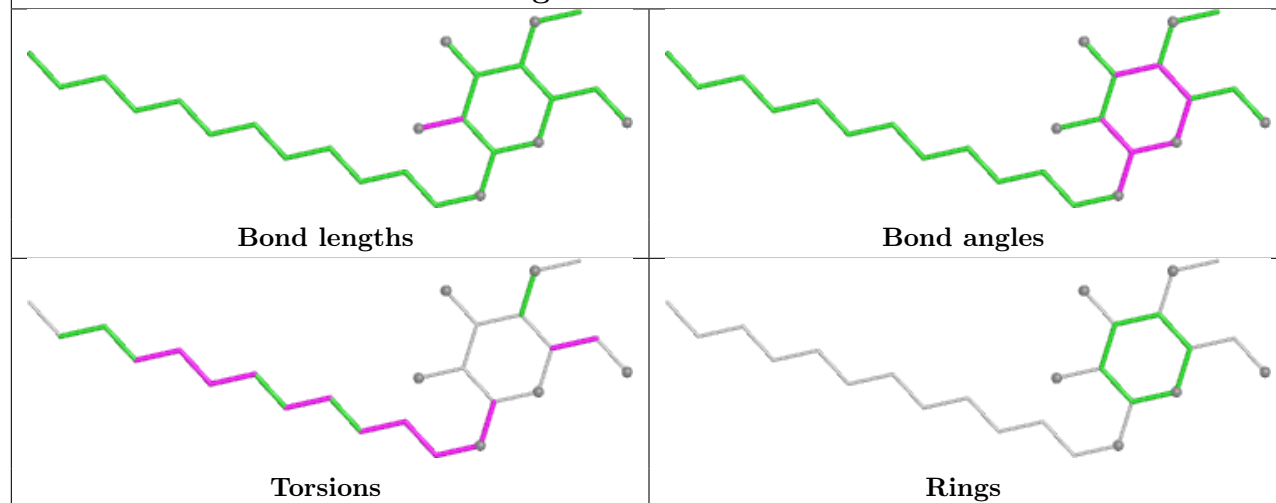
Ligand LHG d 414 (B)

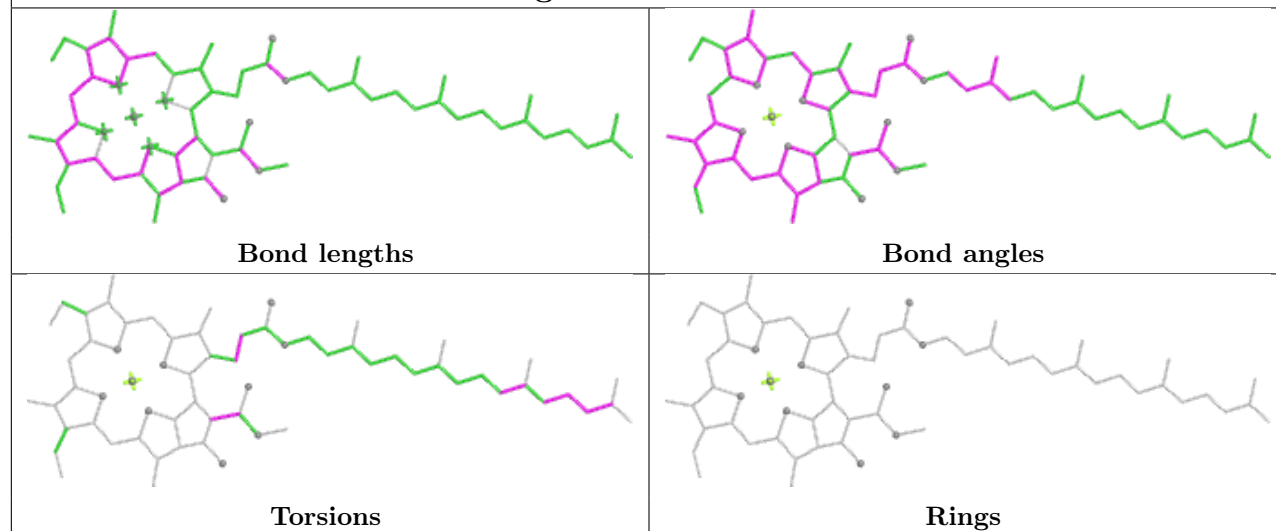
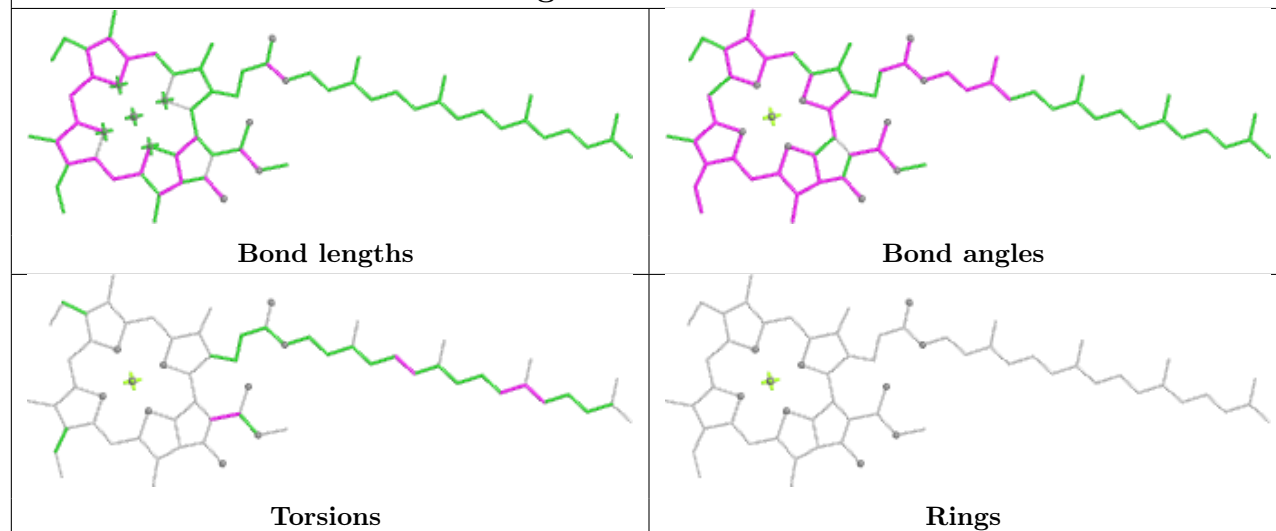
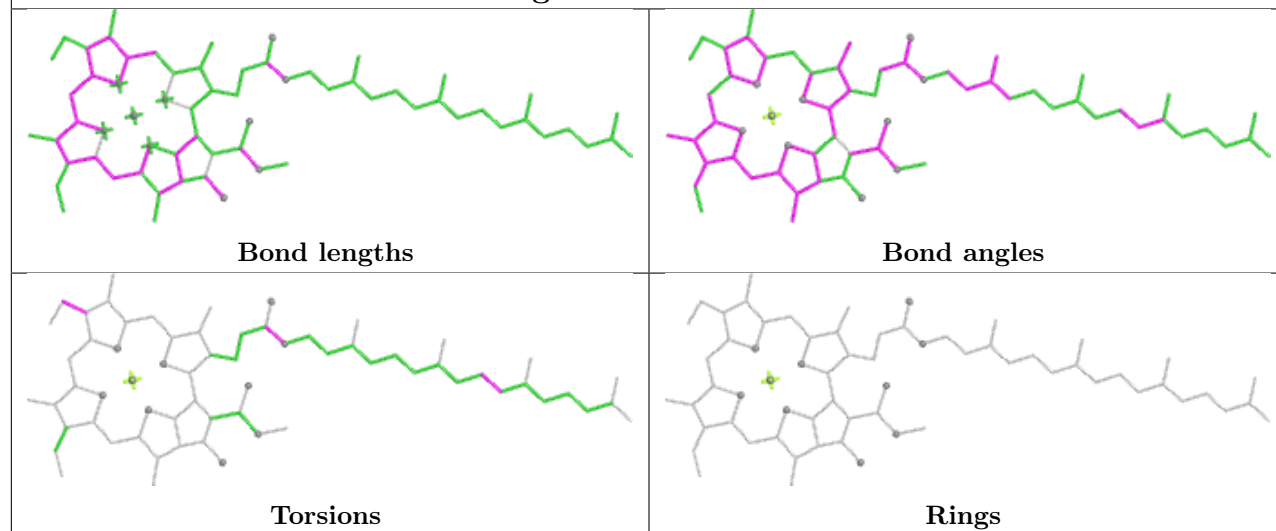


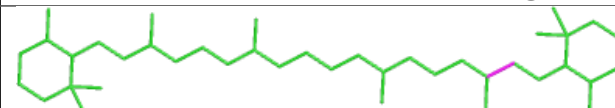
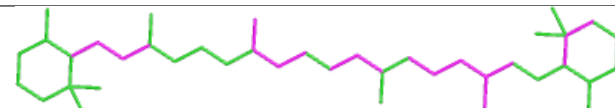
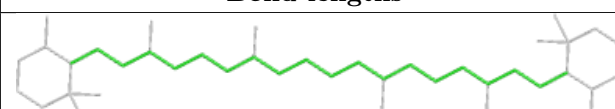
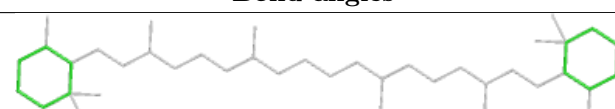
Ligand CLA c 508

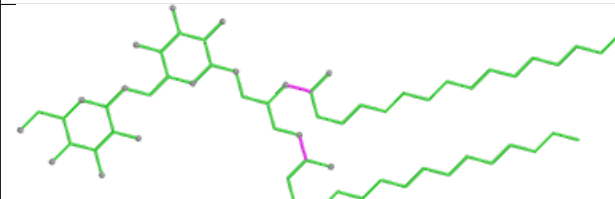
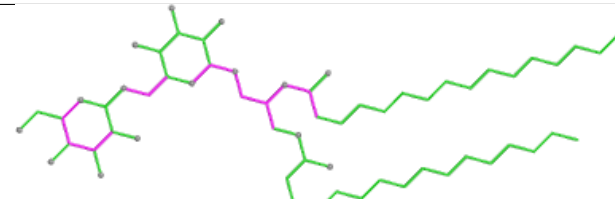
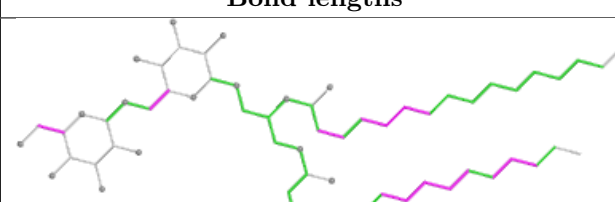
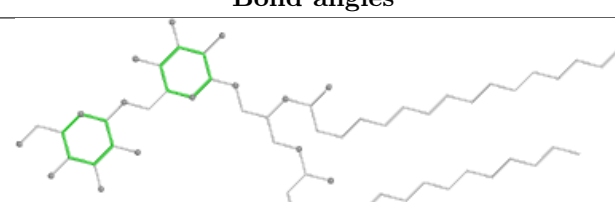


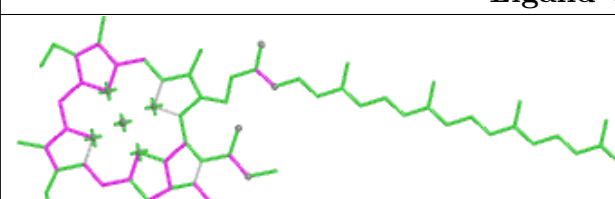
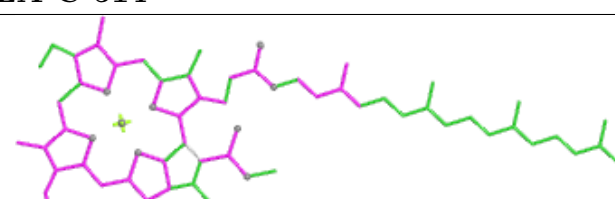
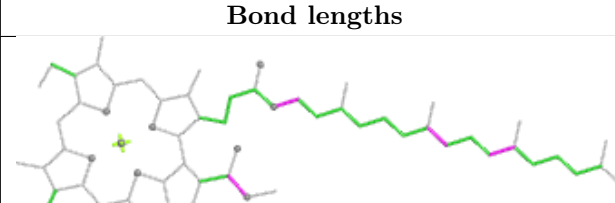
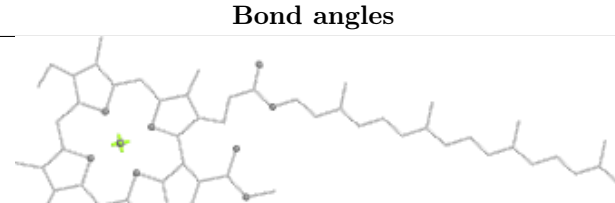


Ligand CLA b 603**Ligand CLA B 605****Ligand LMT b 626**

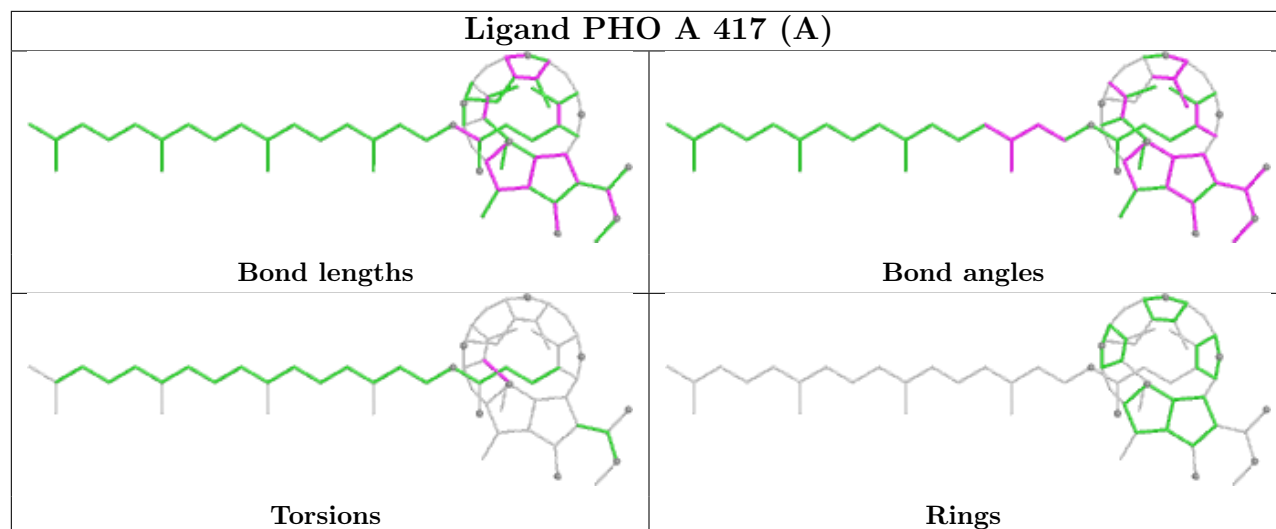
Ligand CLA b 610**Ligand CLA c 505****Ligand CLA B 612**

Ligand BCR b 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

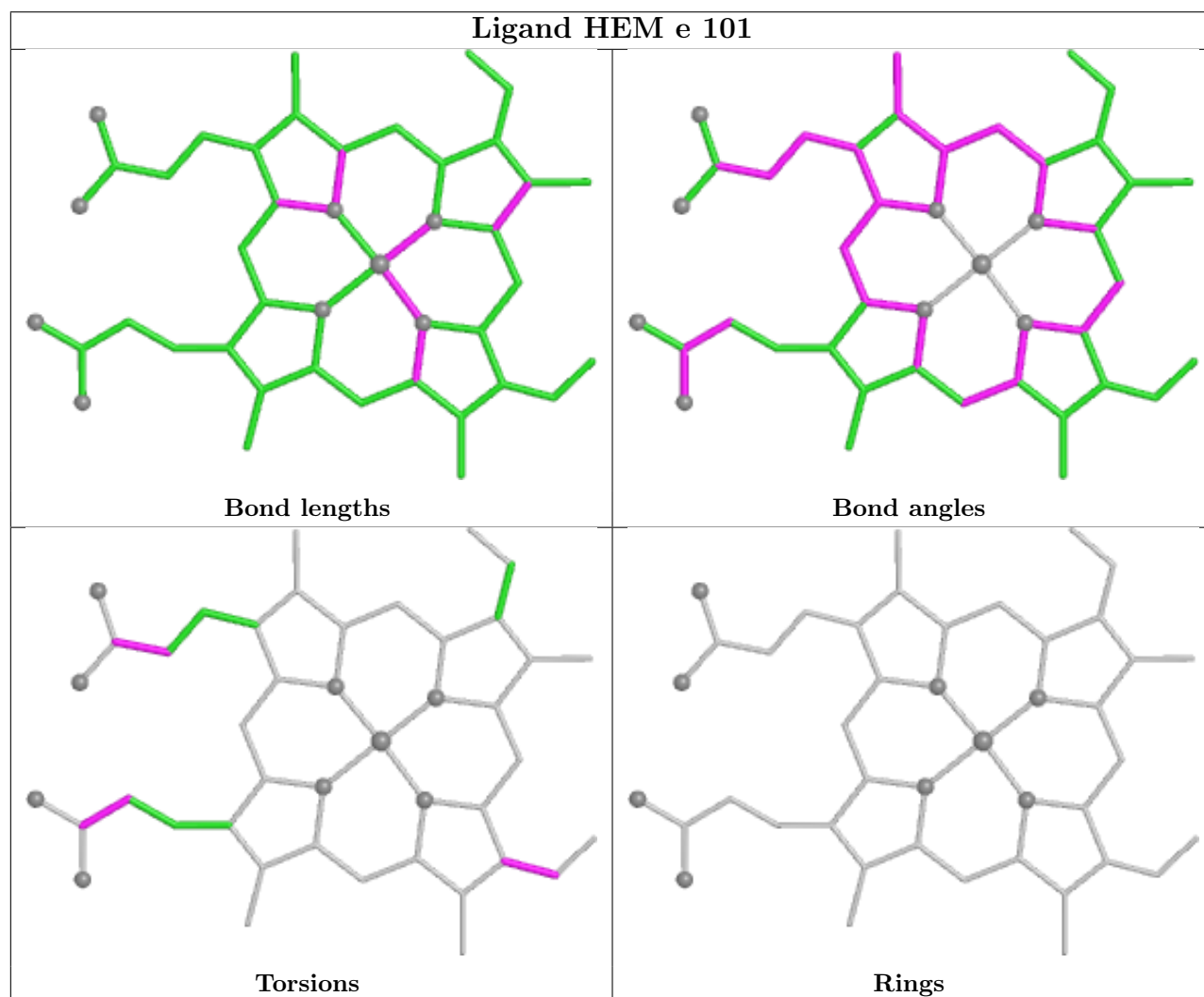
Ligand DGD C 517 (A)	
	
Bond lengths	Bond angles
	
Torsions	Rings

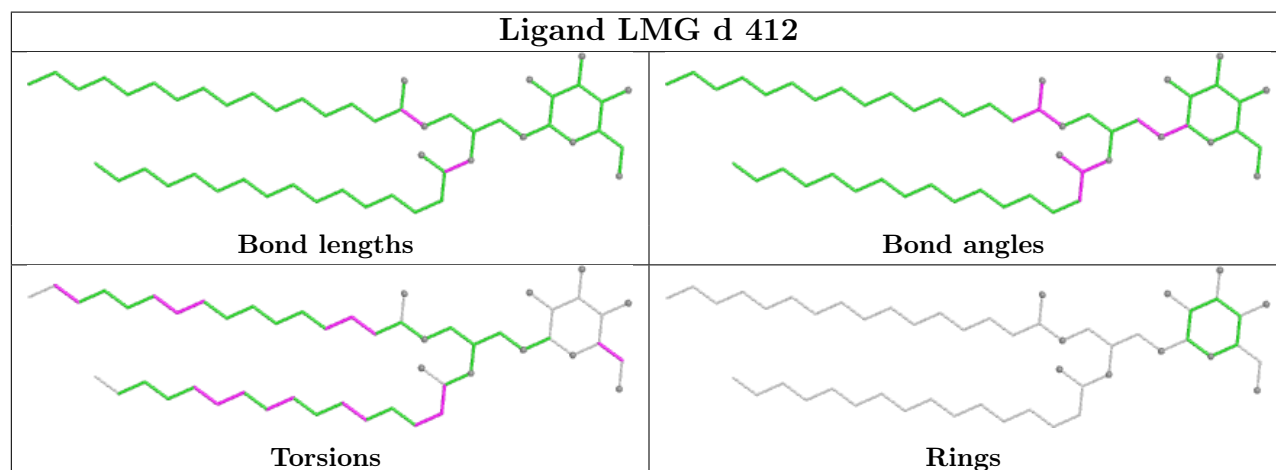
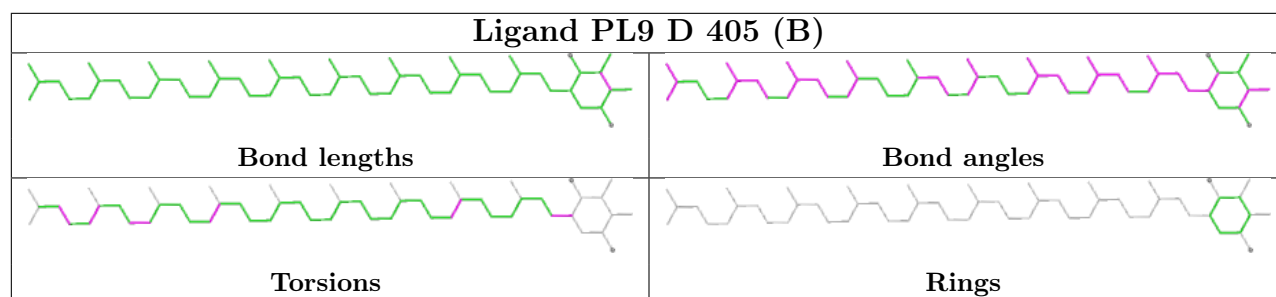
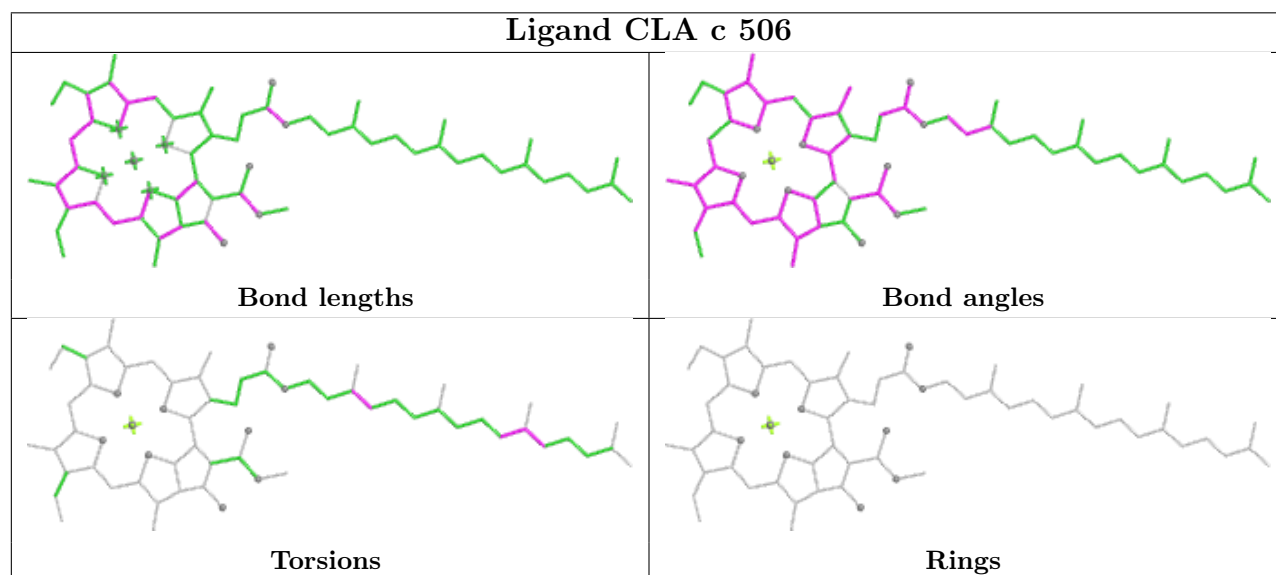
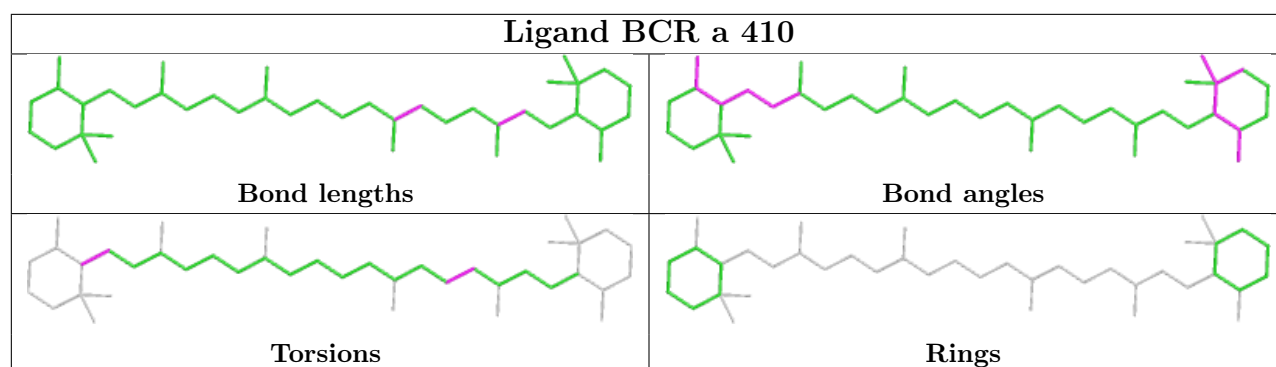
Ligand CLA C 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

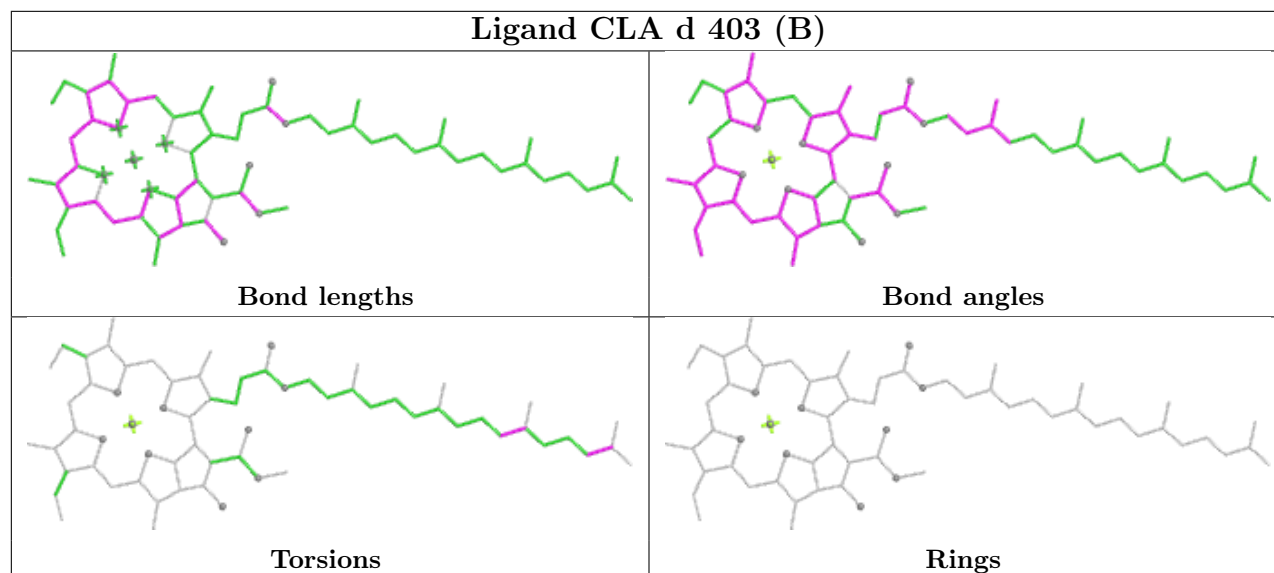
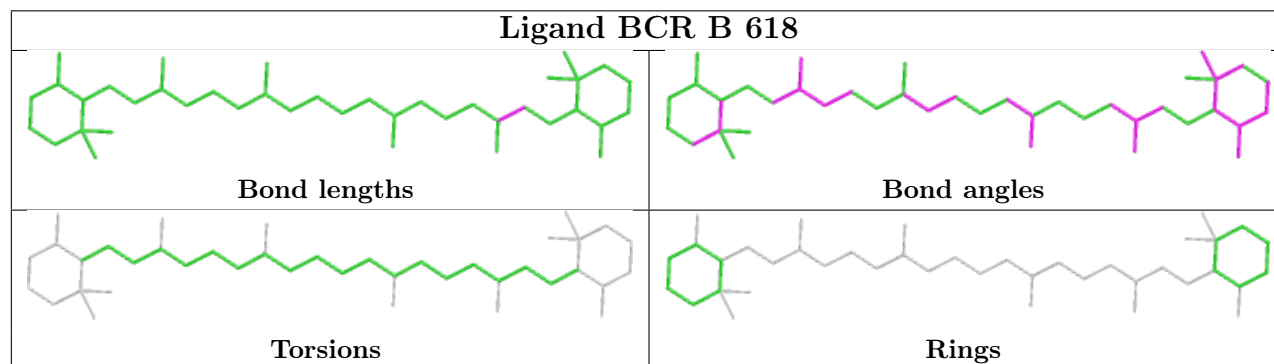
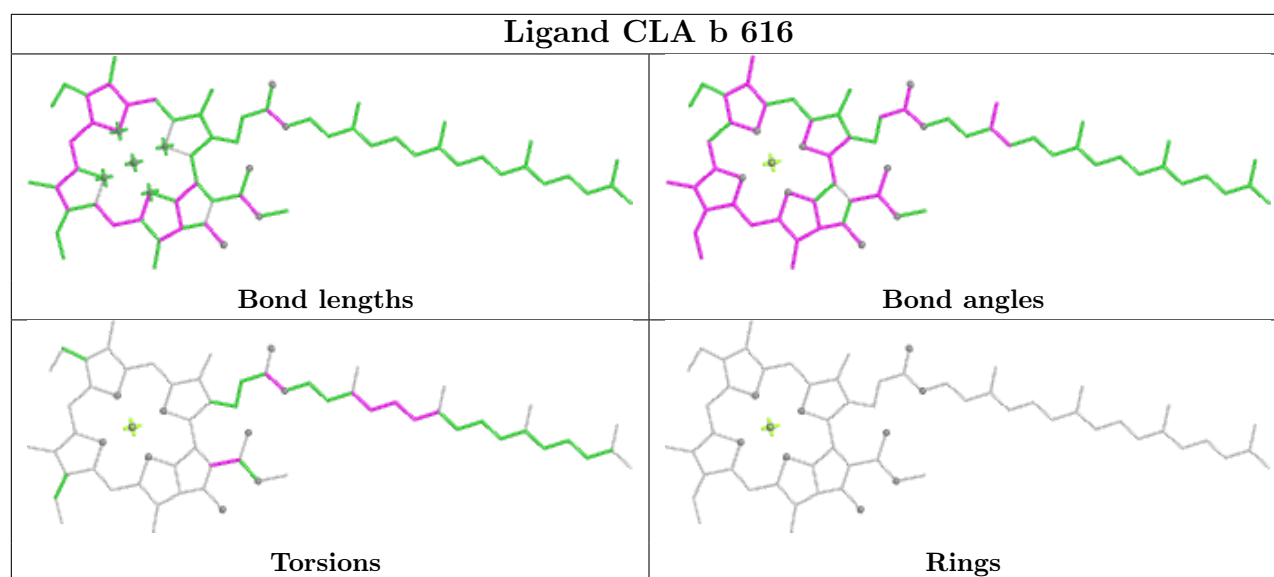
Ligand PHO A 417 (A)

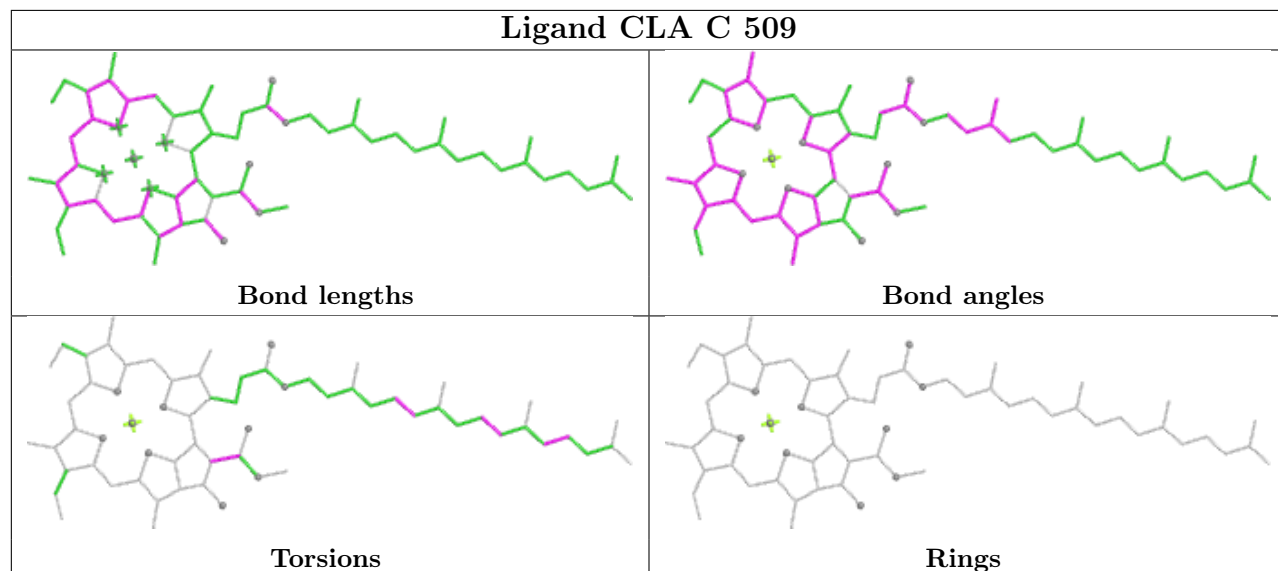
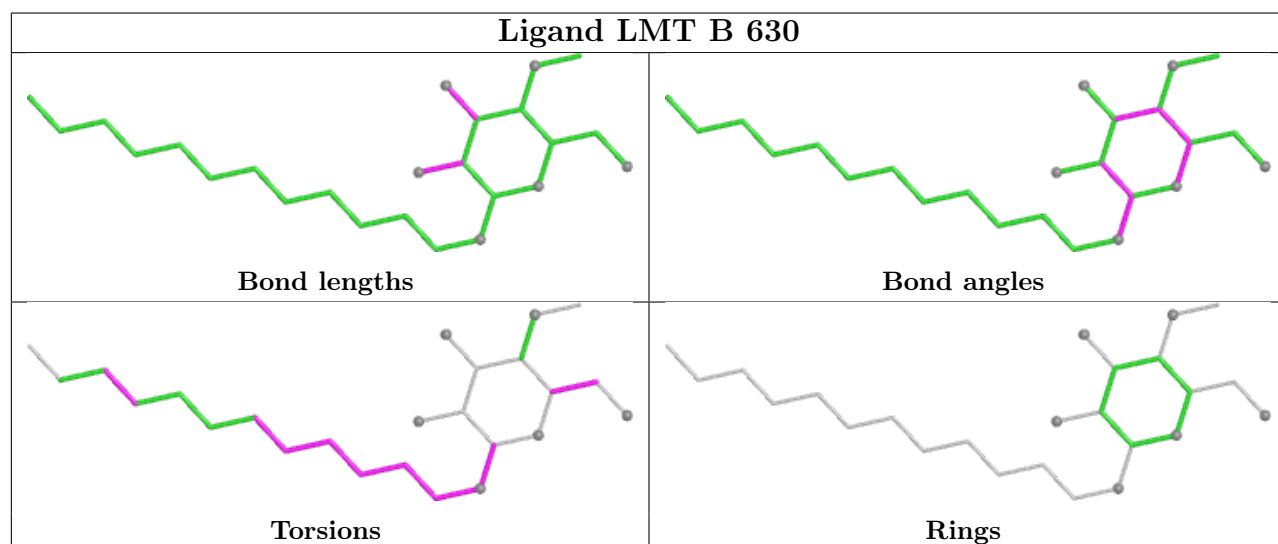
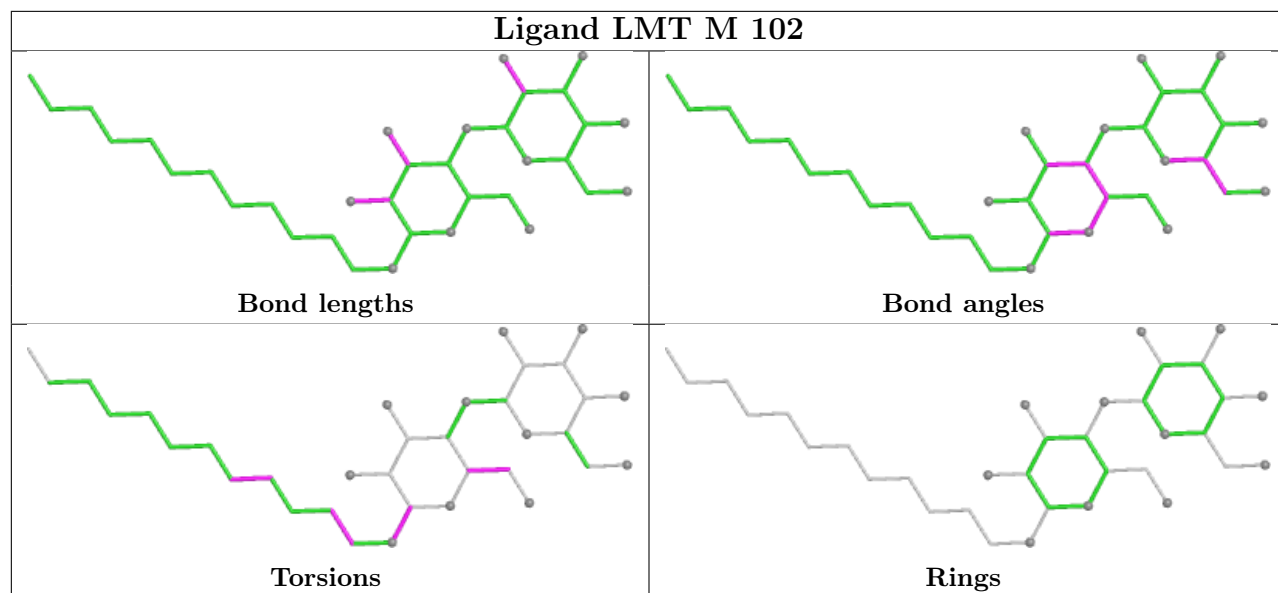


Ligand HEM e 101

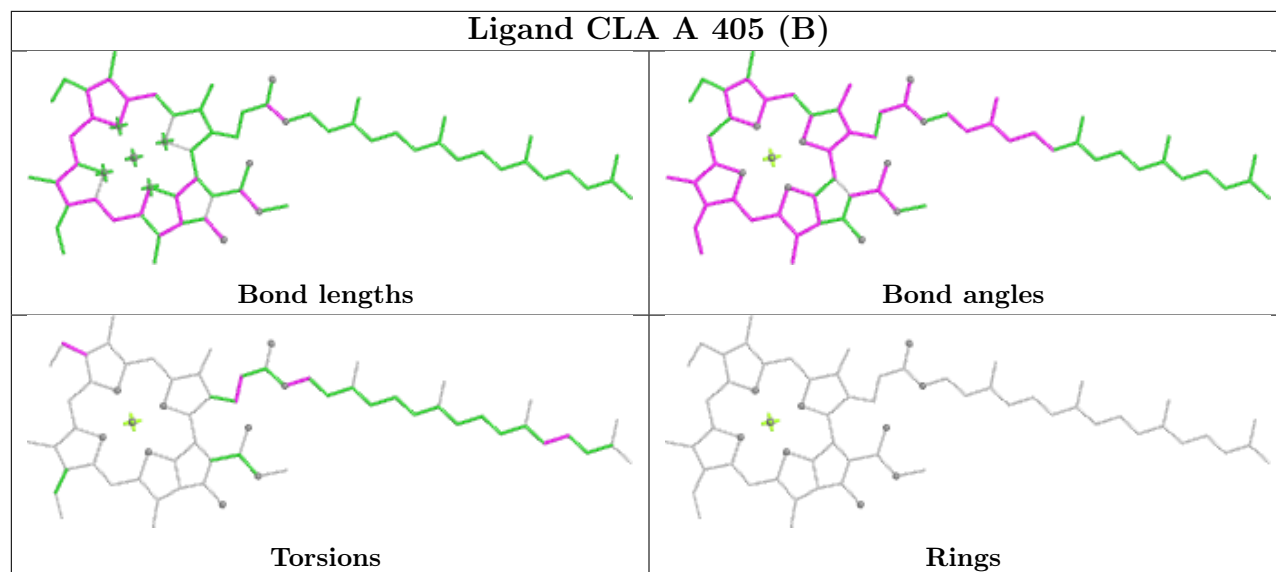




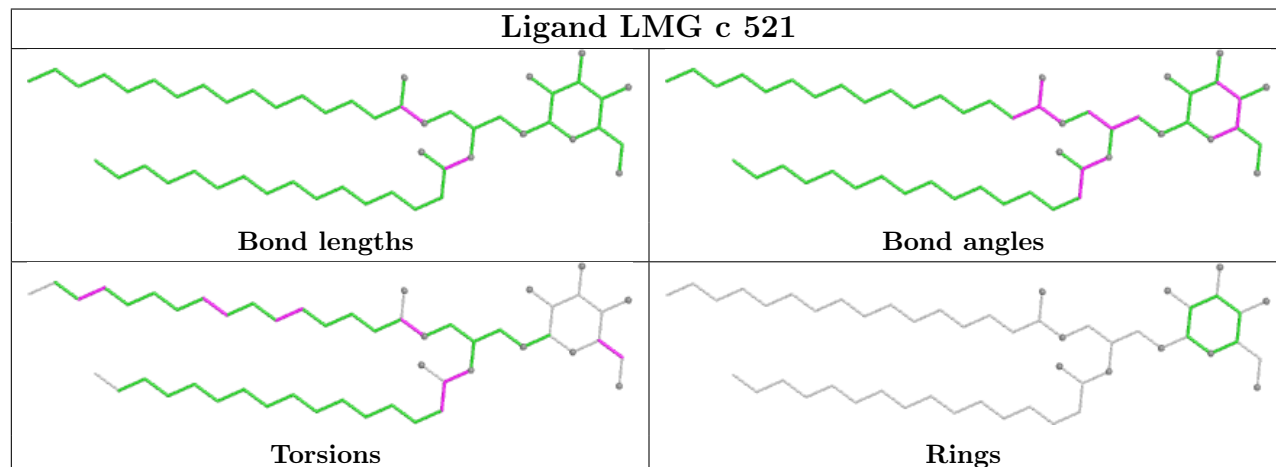




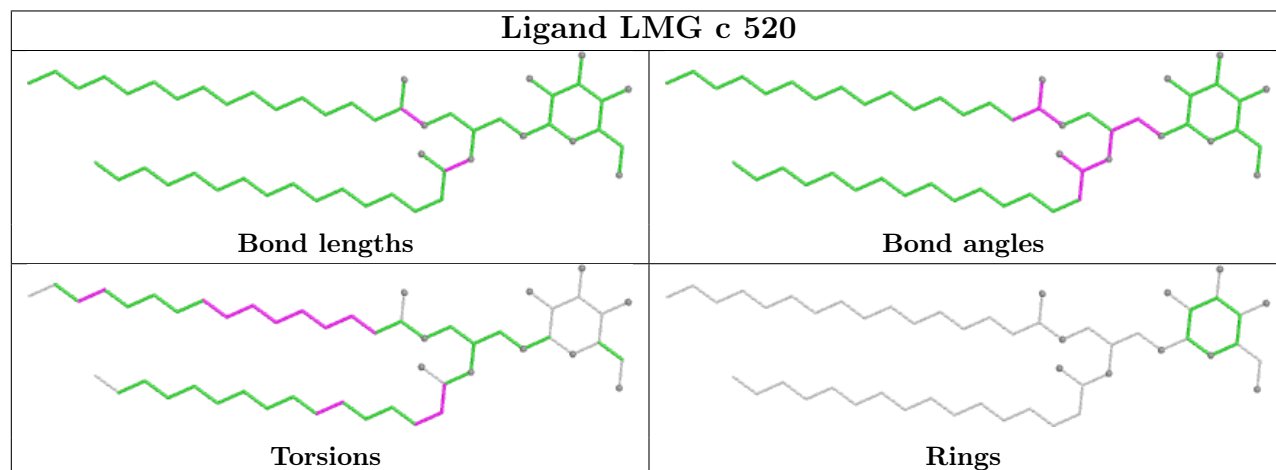
Ligand CLA A 405 (B)

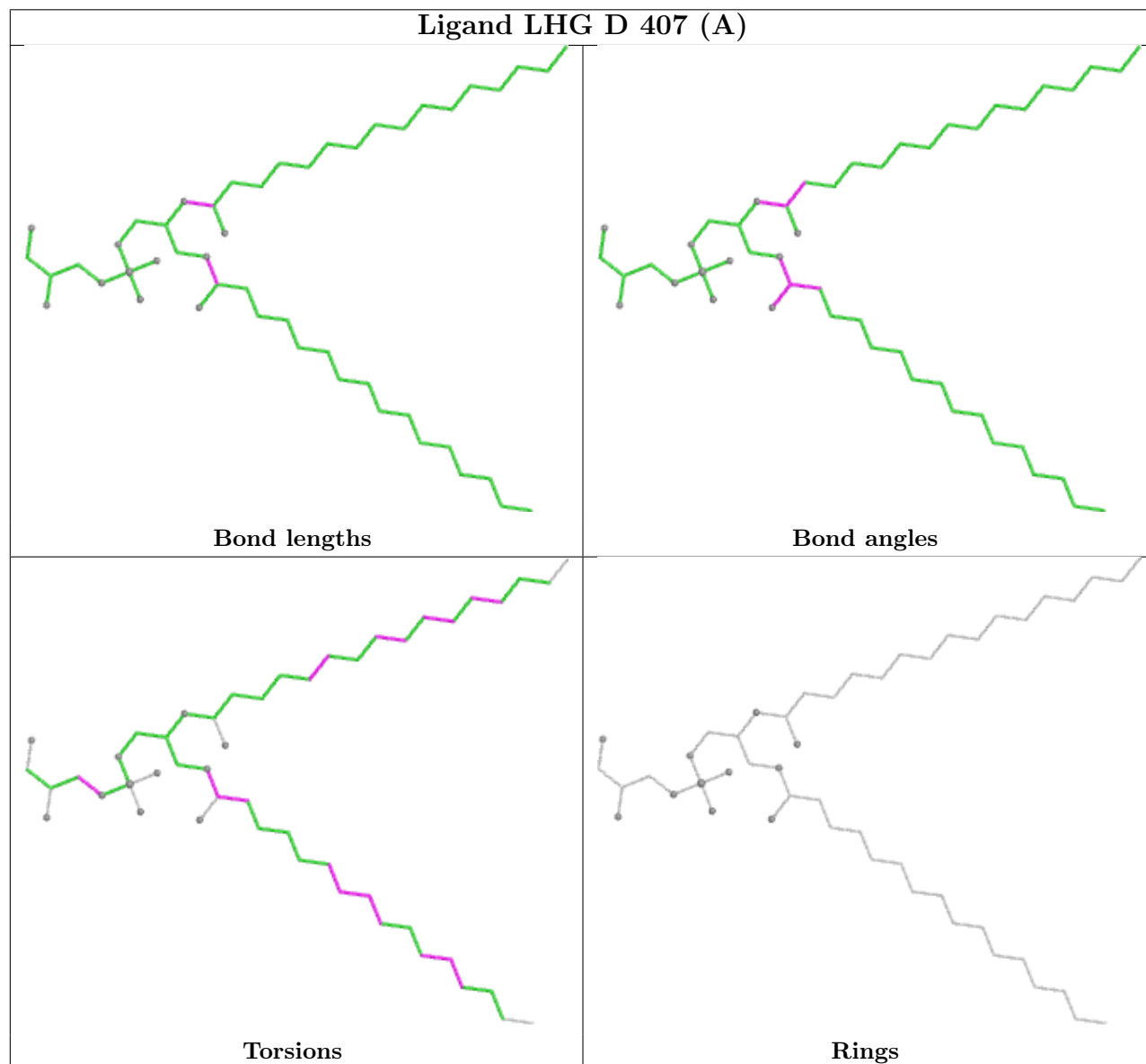
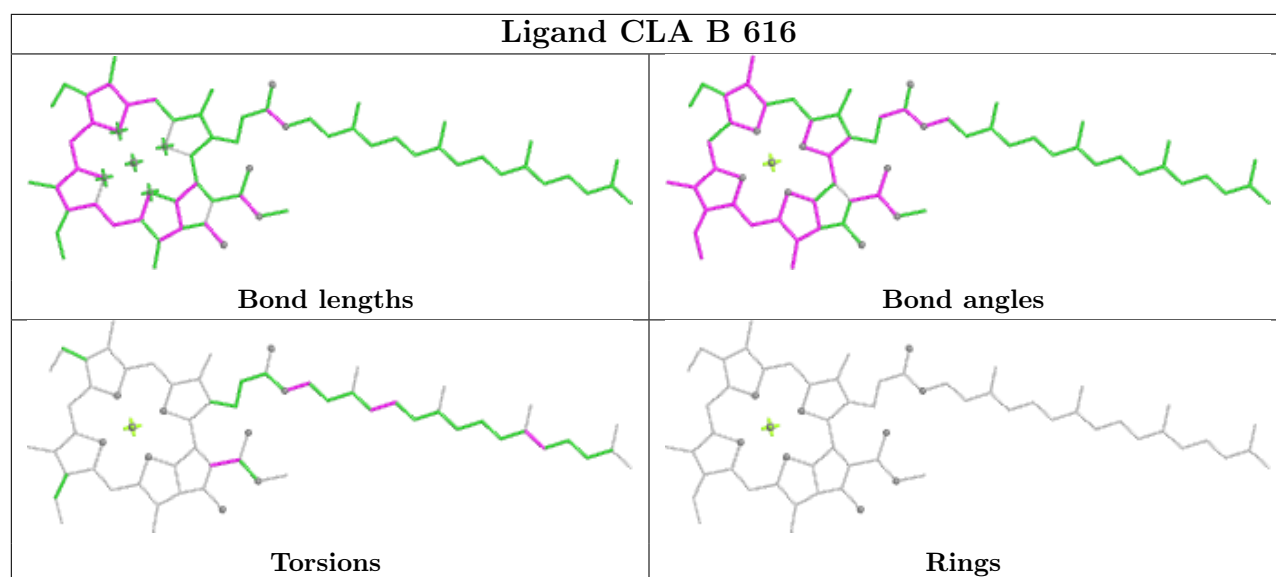


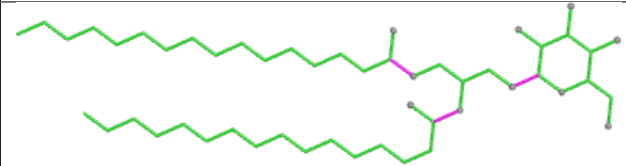
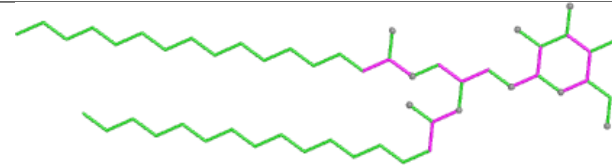
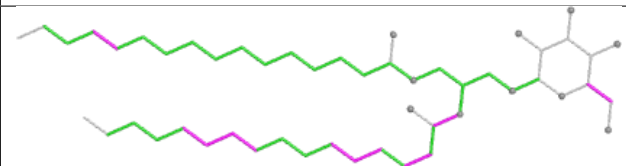
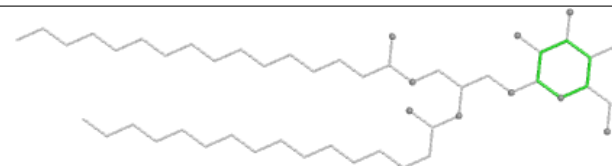
Ligand LMG c 521

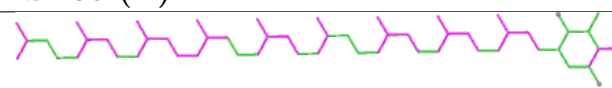
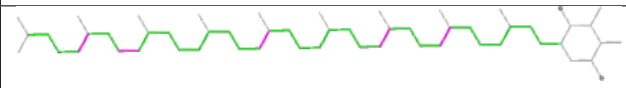
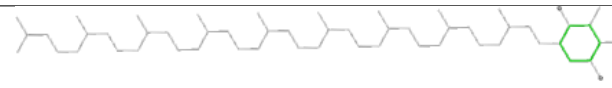


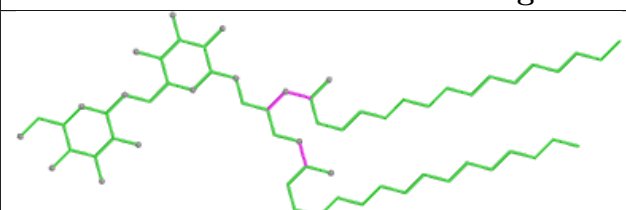
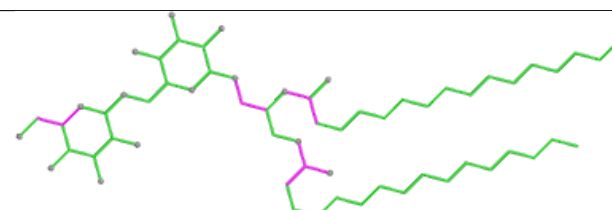
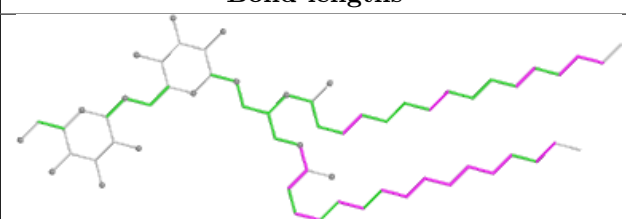
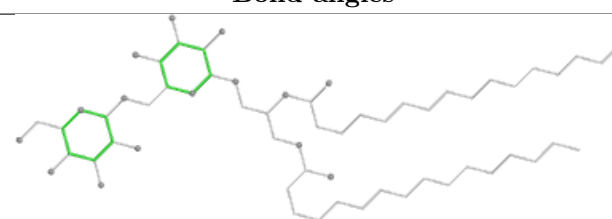
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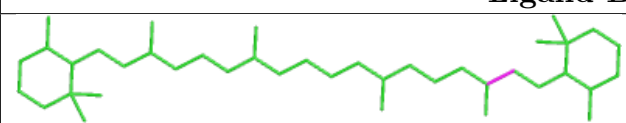
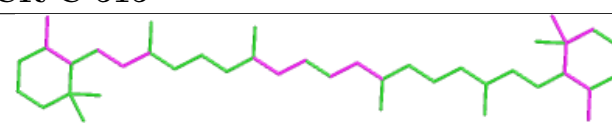
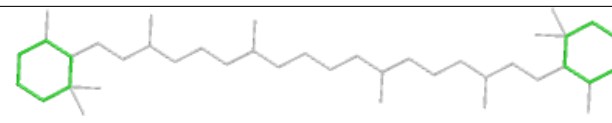


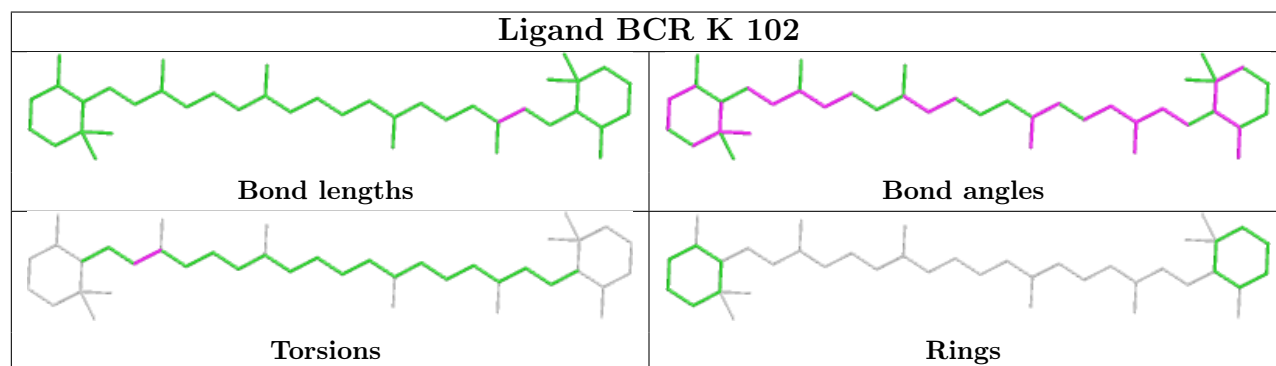
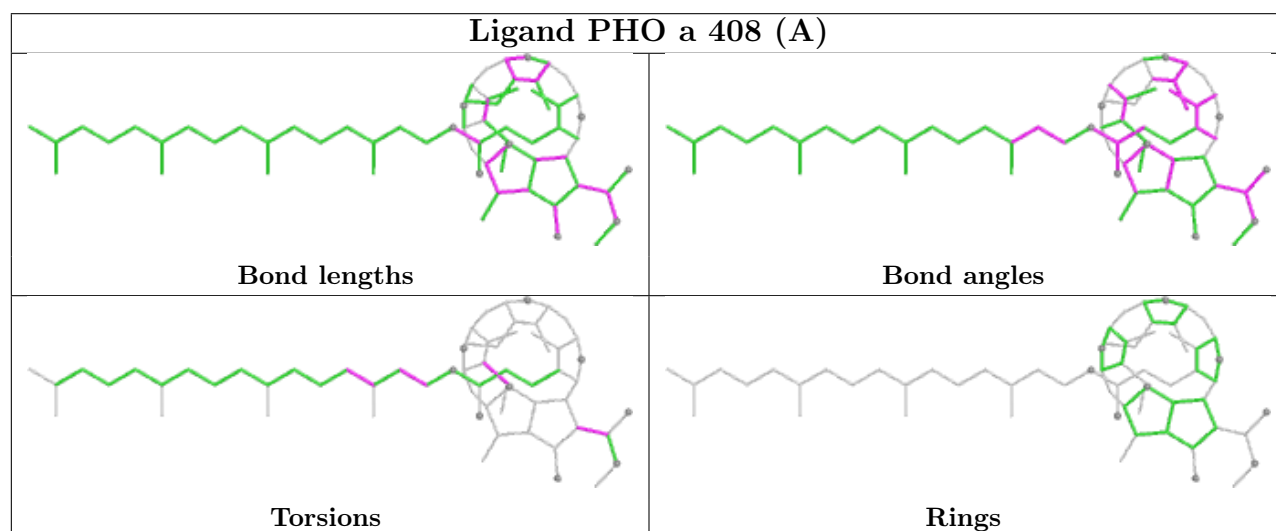
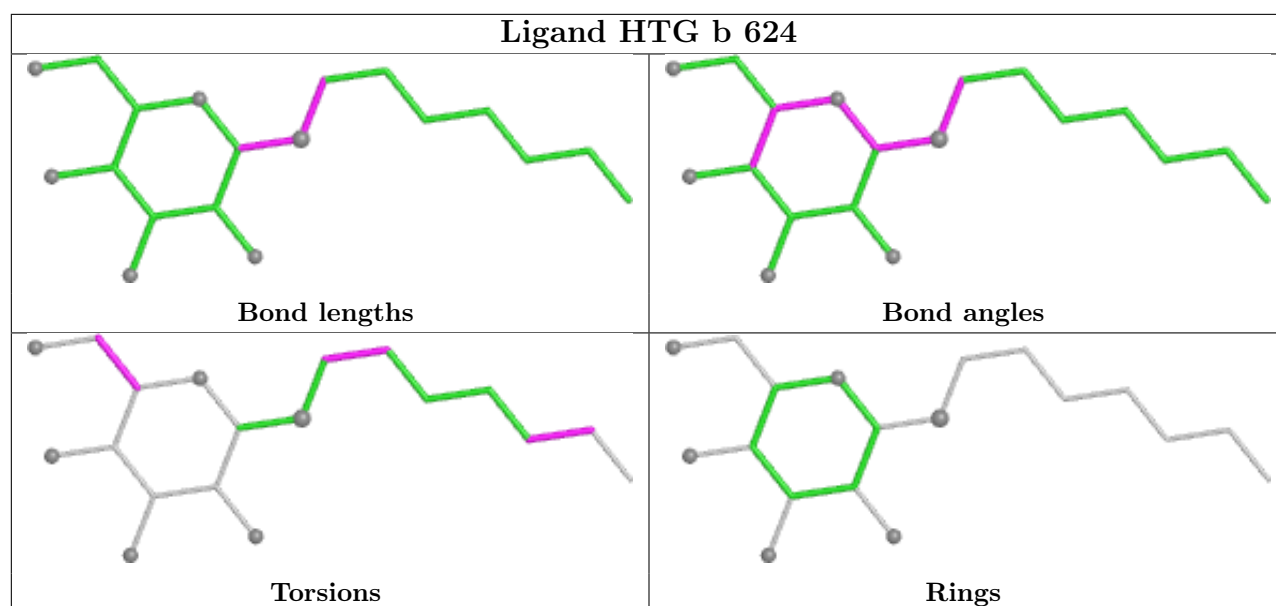


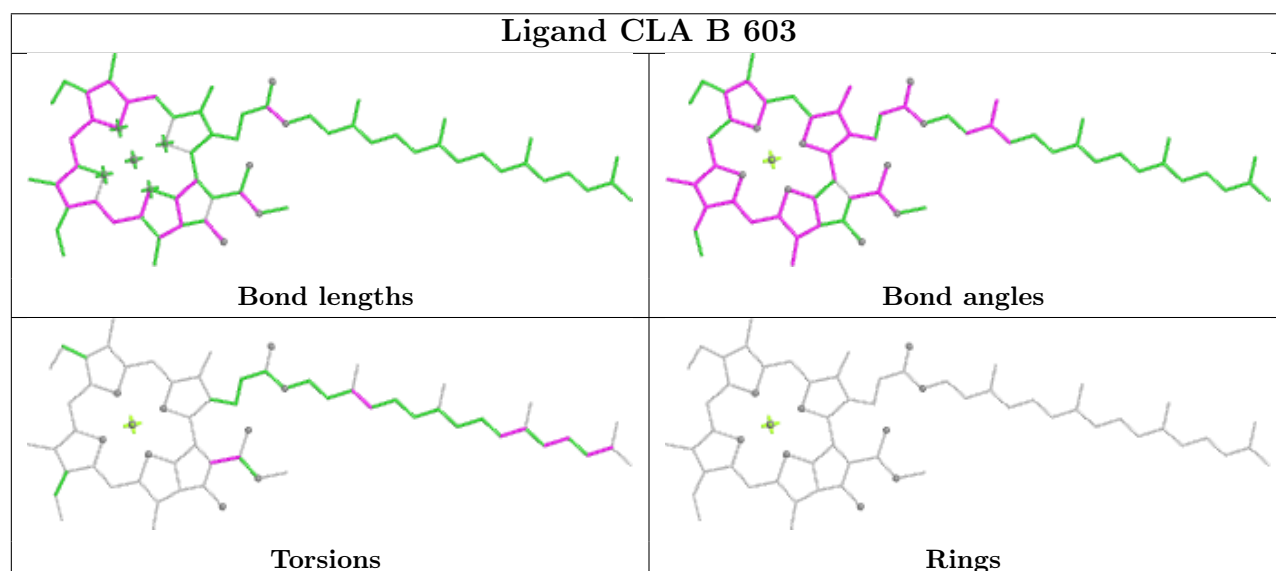
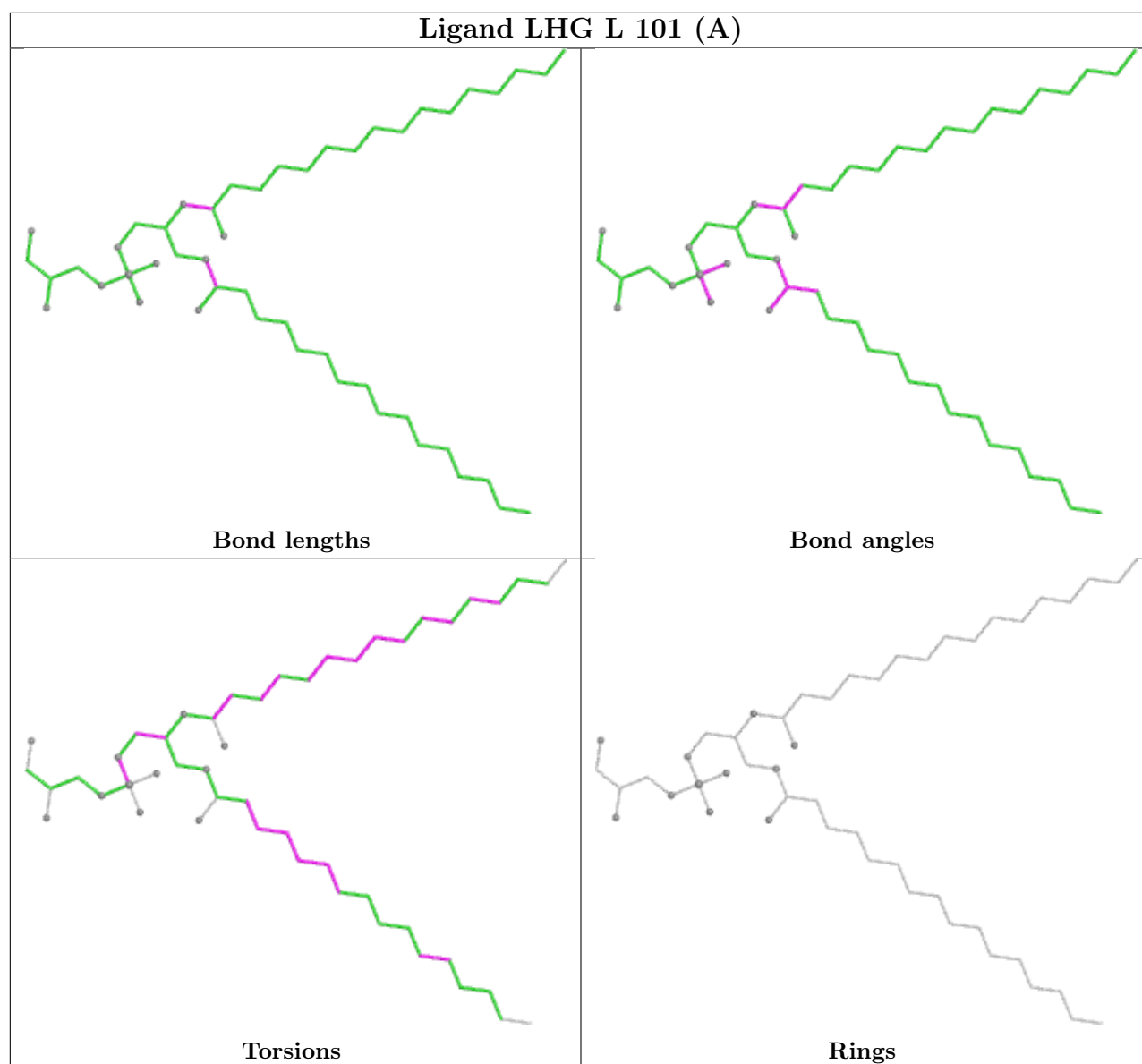
Ligand LMG C 521	
	
Bond lengths	Bond angles
	
Torsions	Rings

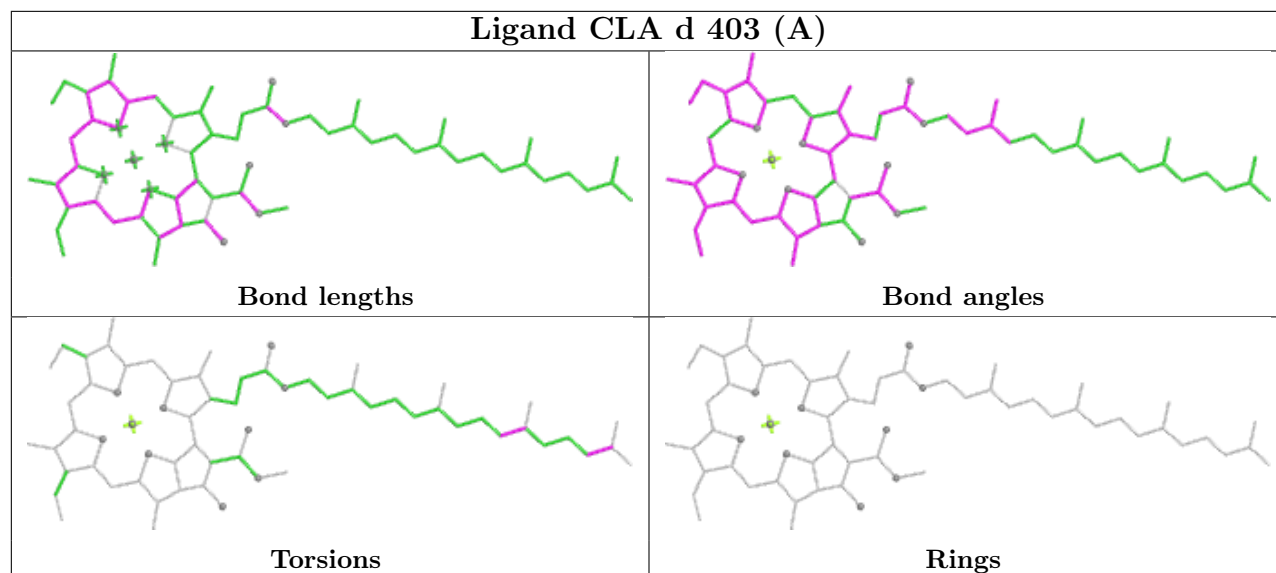
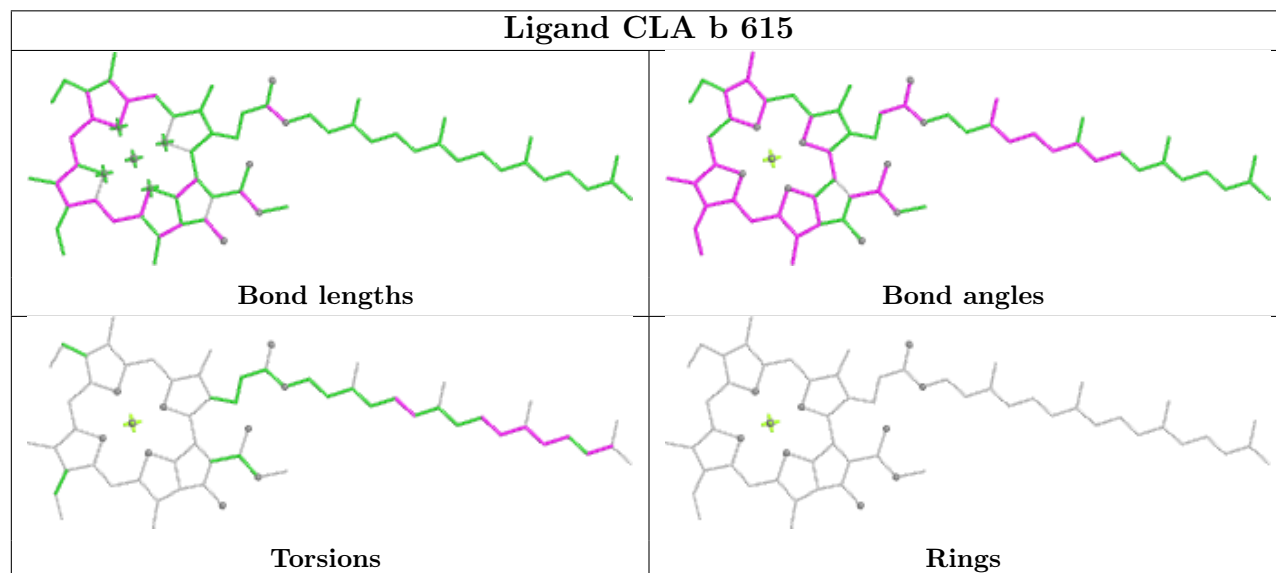
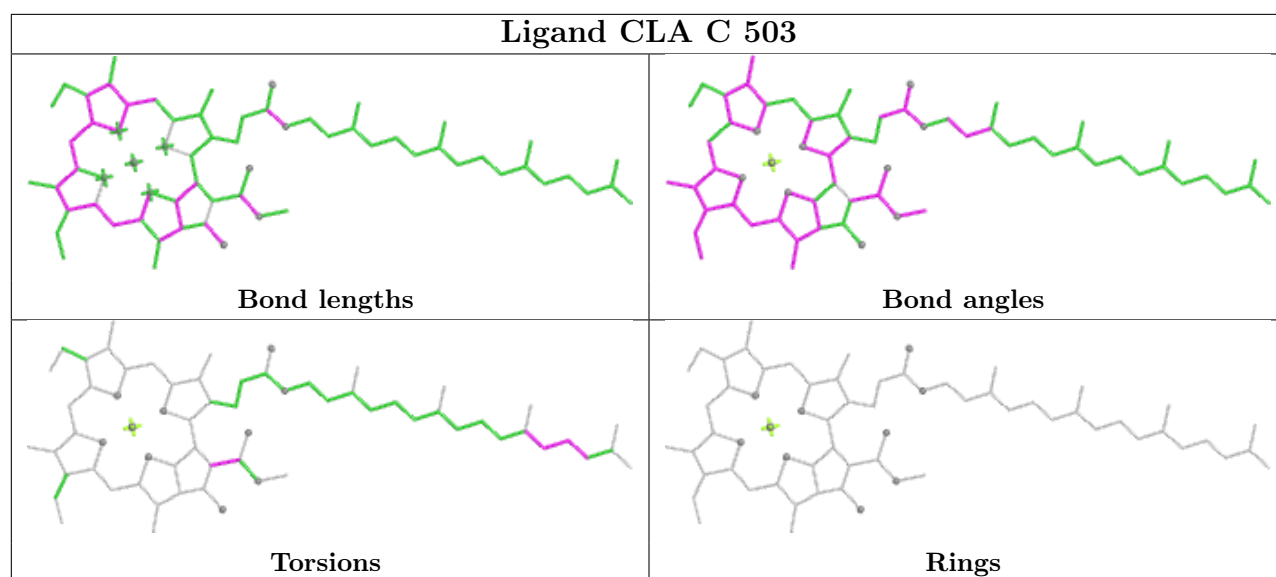
Ligand PL9 d 406 (B)	
	
Bond lengths	Bond angles
	
Torsions	Rings

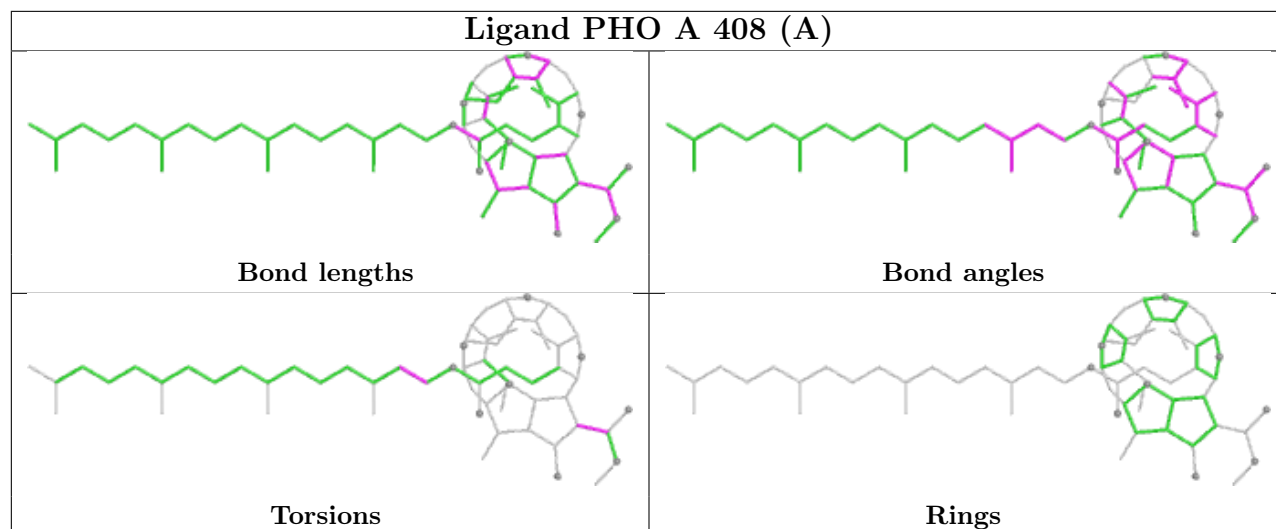
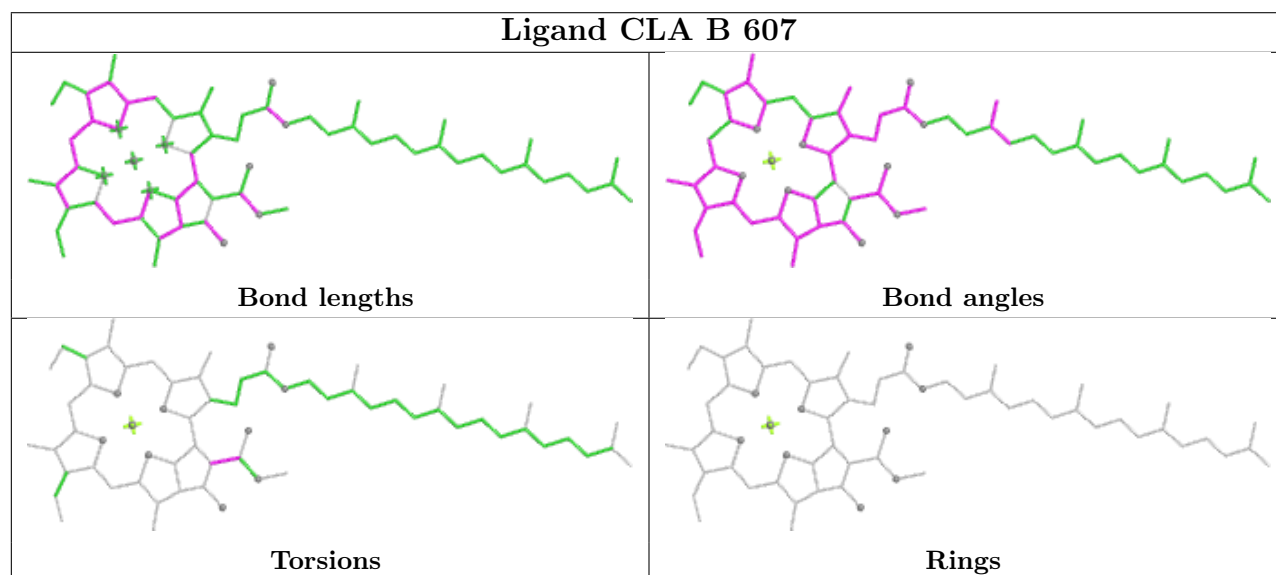
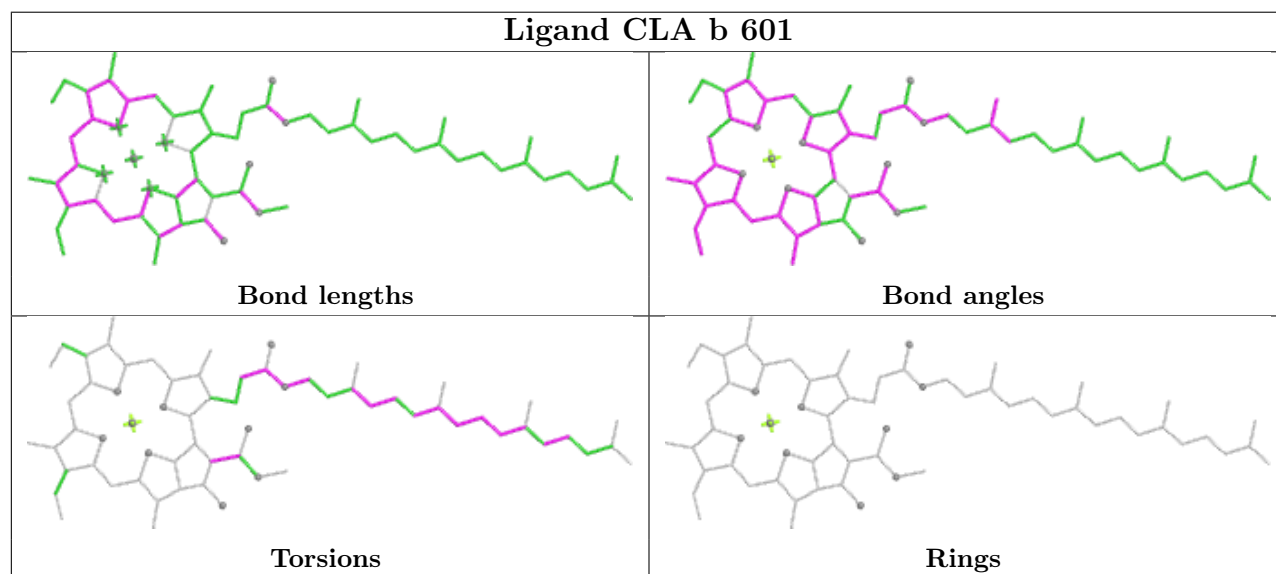
Ligand DGD C 519	
	
Bond lengths	Bond angles
	
Torsions	Rings

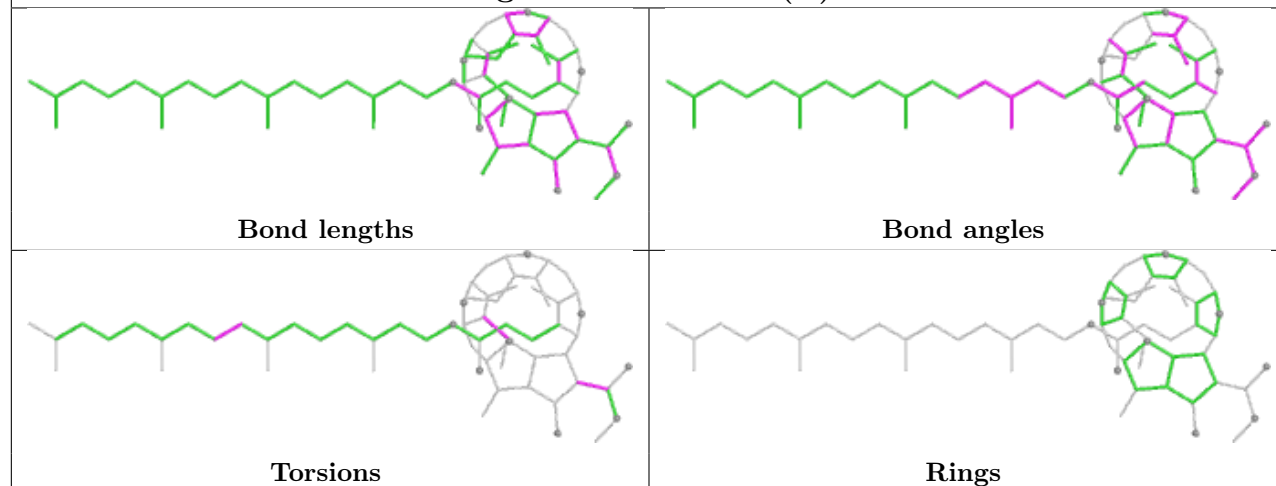
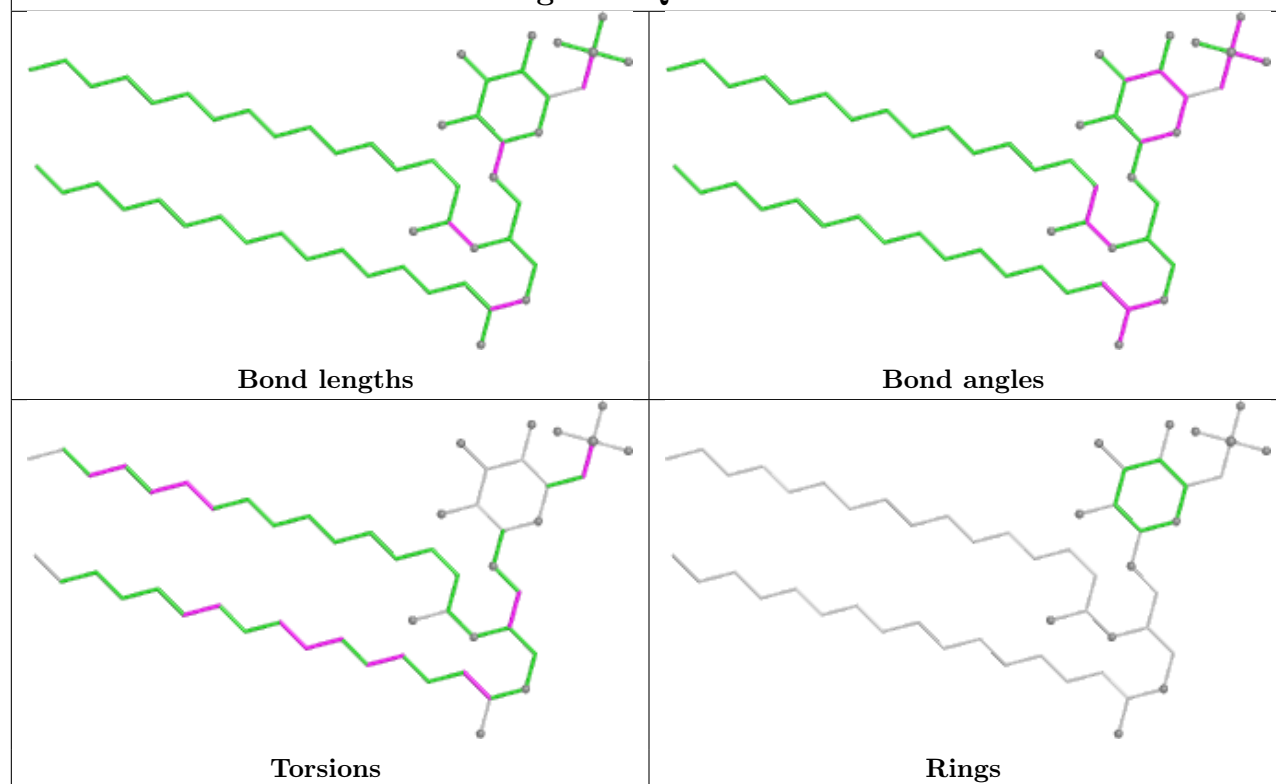
Ligand BCR C 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

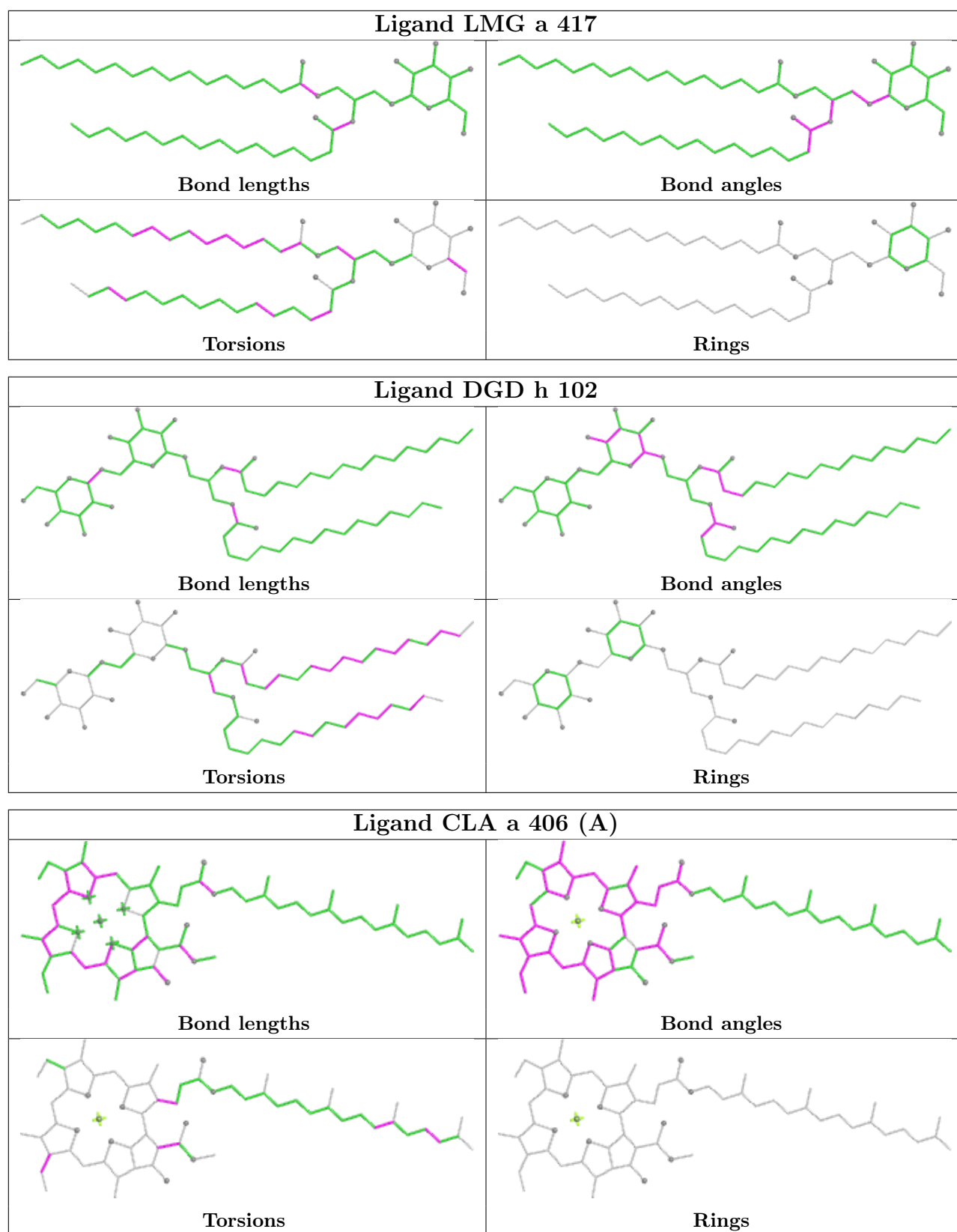


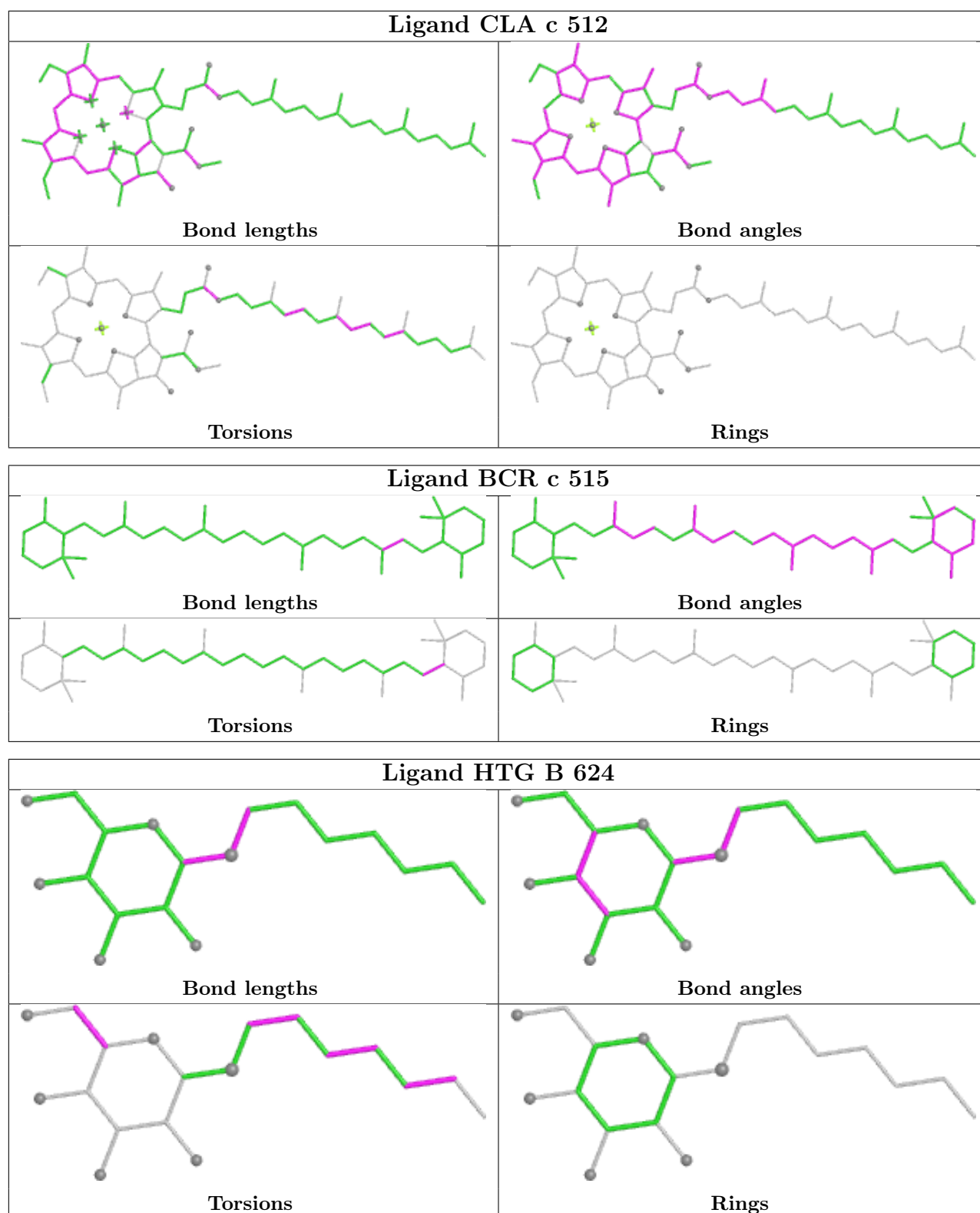


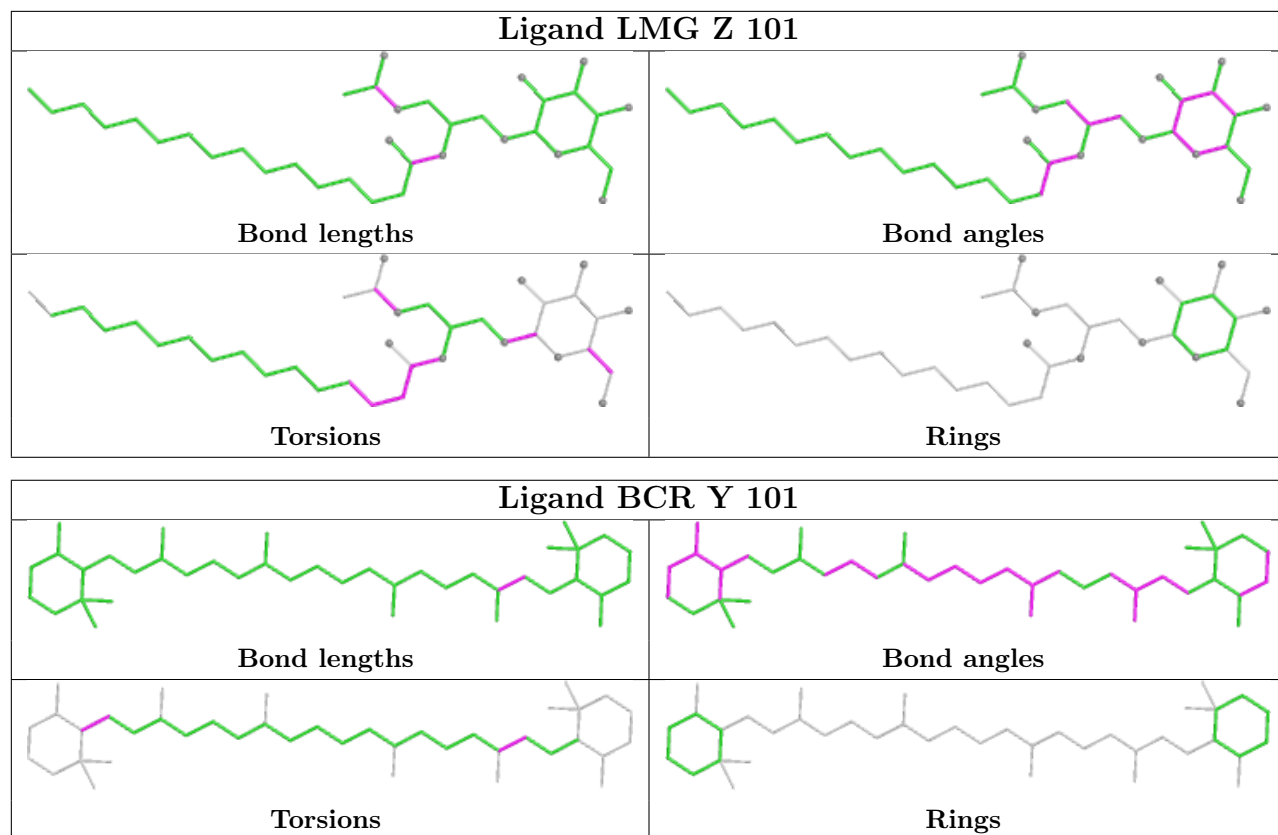


Ligand PHO A 408 (A)**Ligand CLA B 607****Ligand CLA b 601**

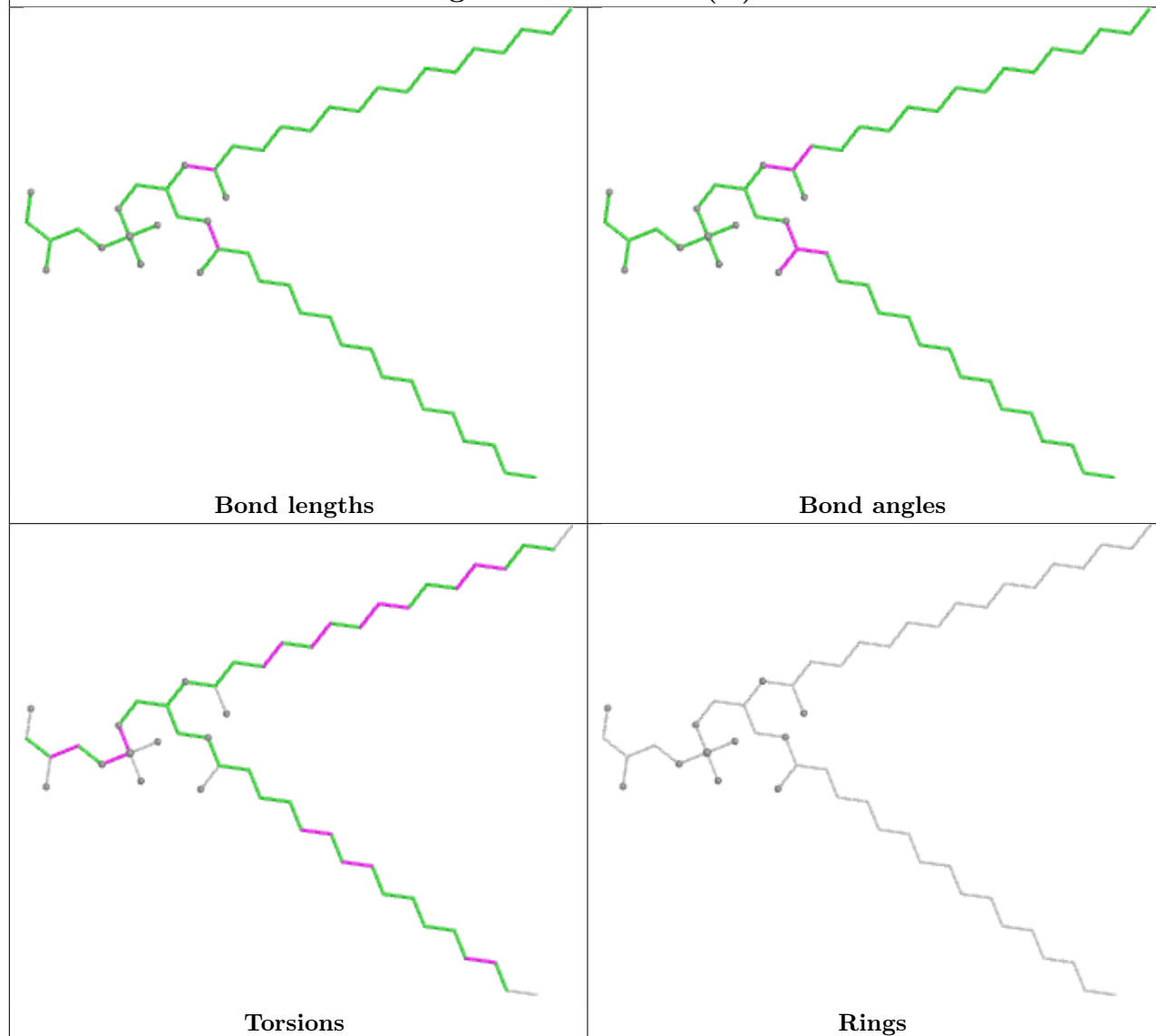
Ligand PHO A 417 (B)**Ligand SQD a 413**



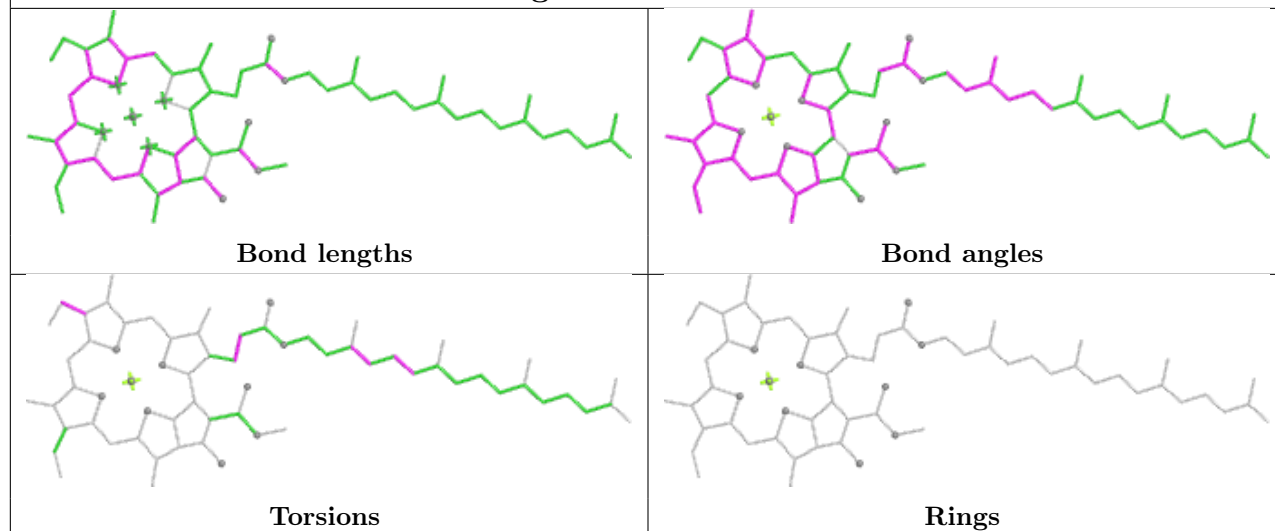


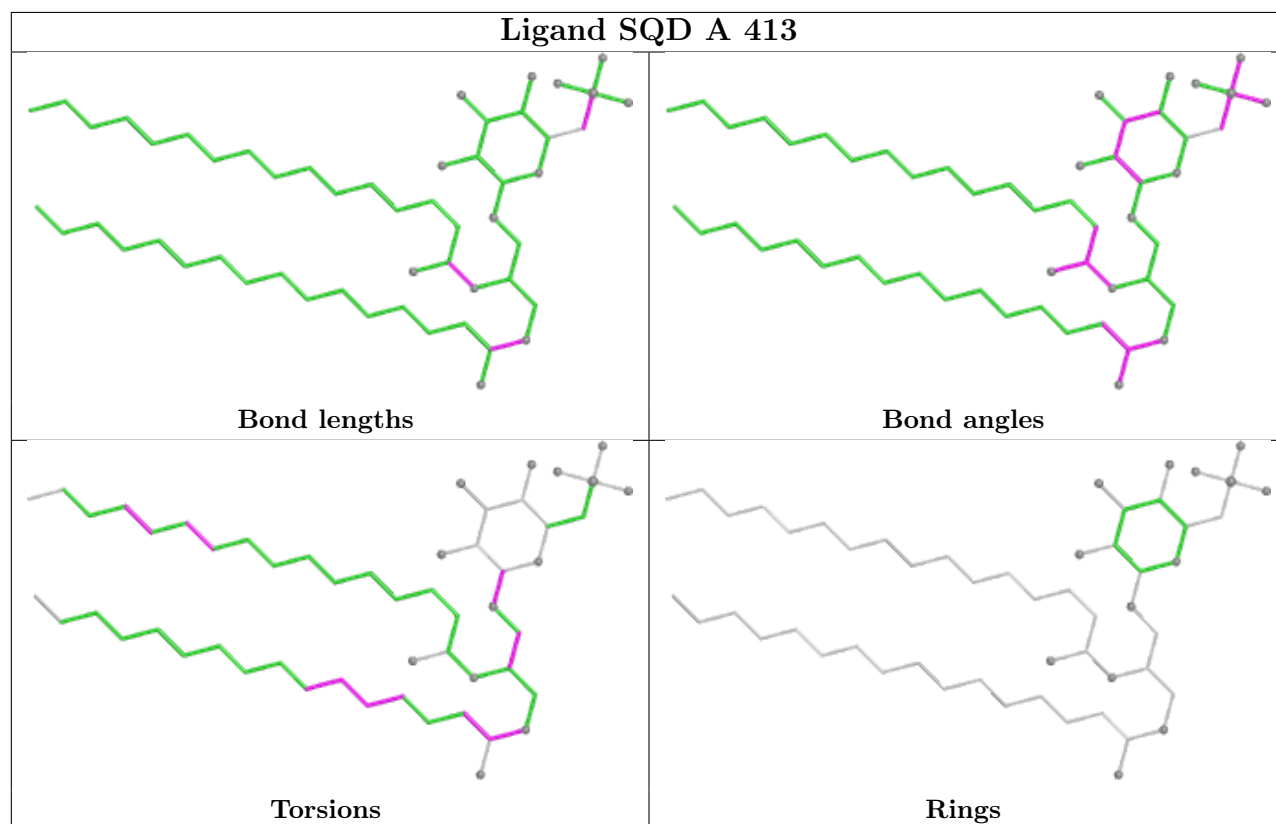
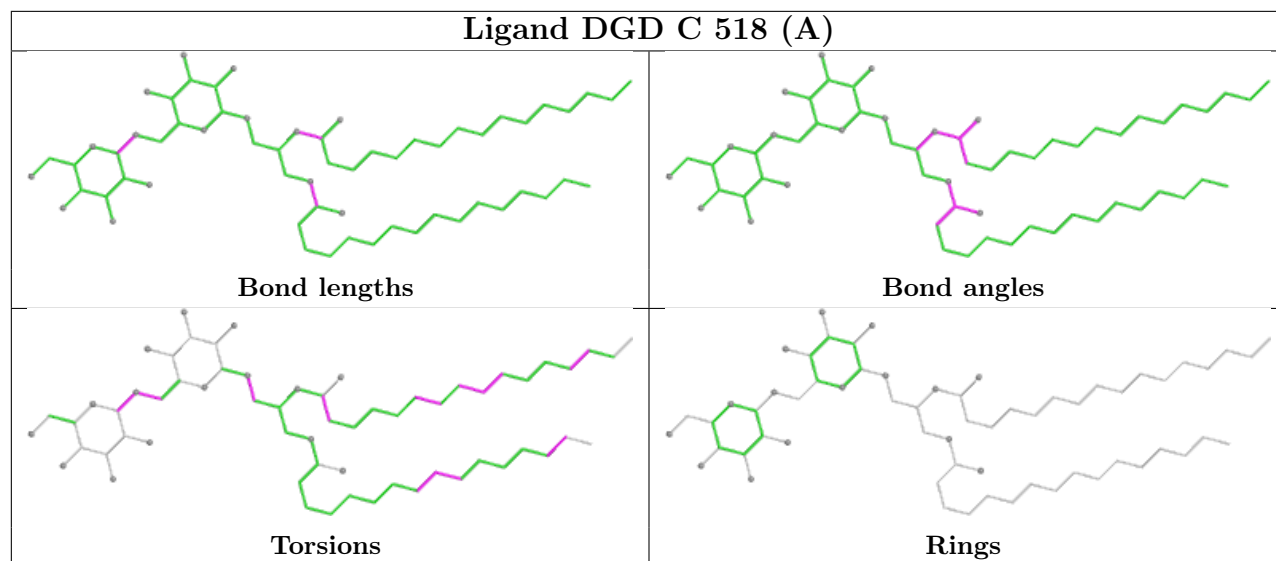


Ligand LHG D 406 (A)

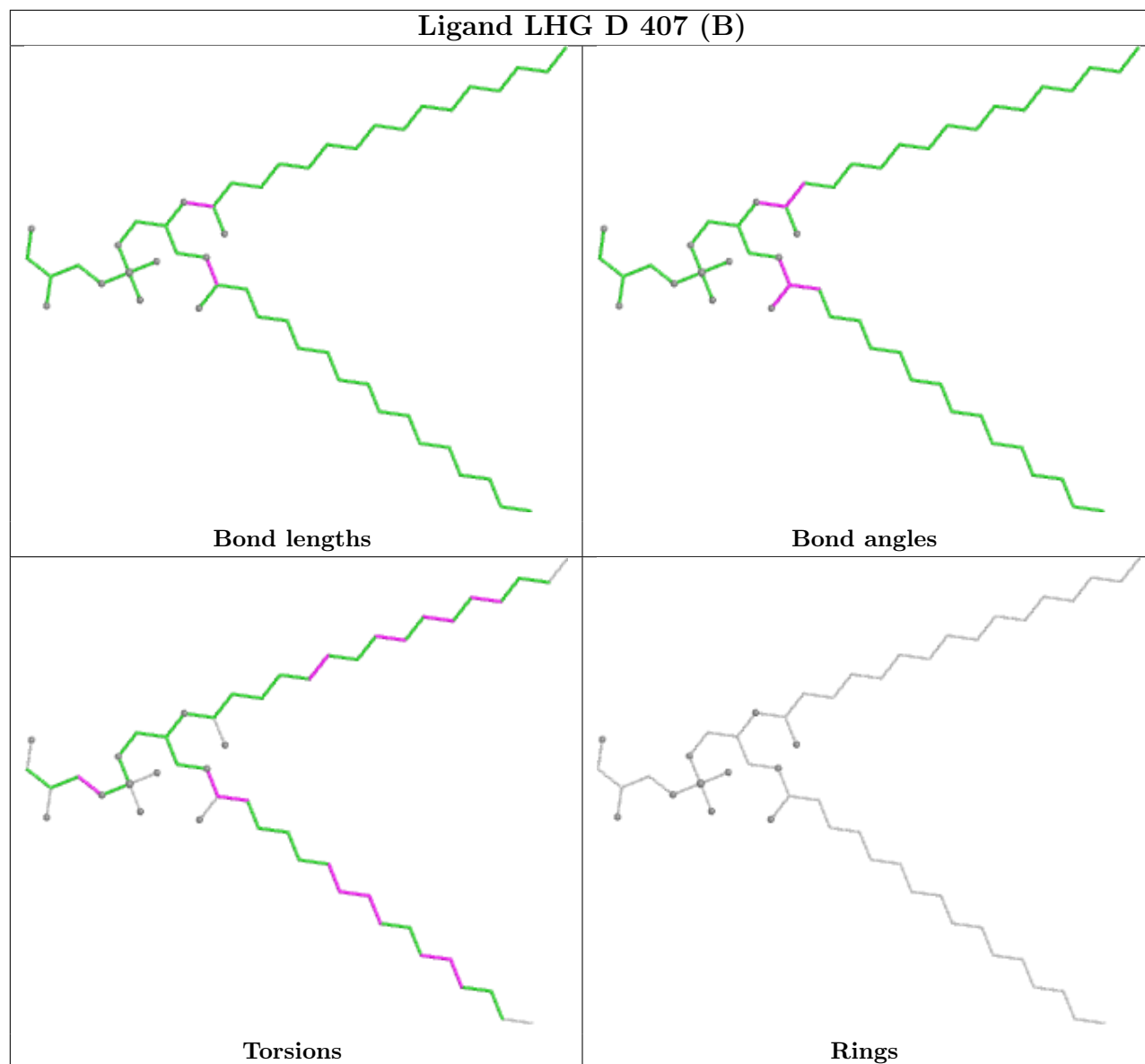


Ligand CLA C 508

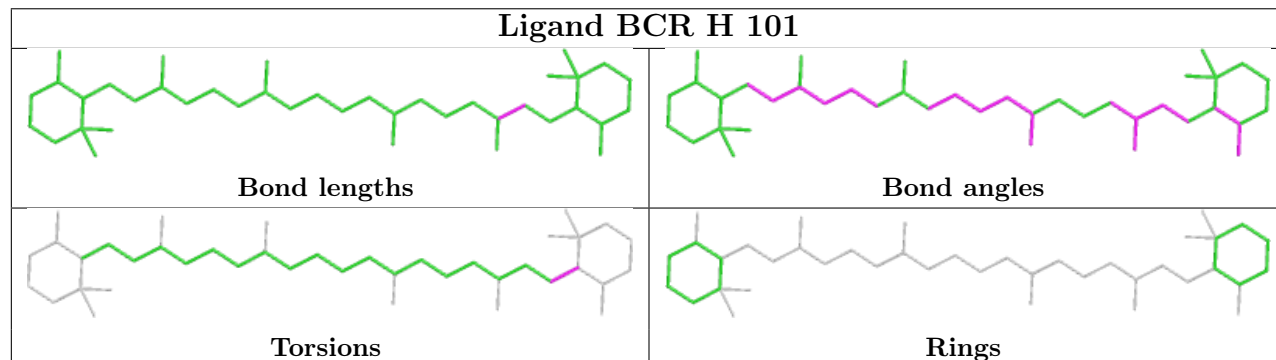


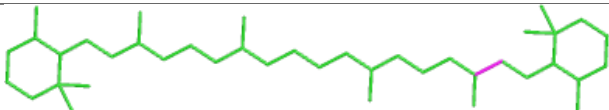
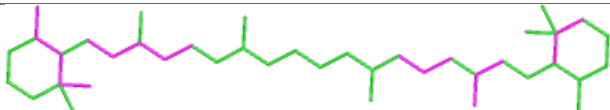
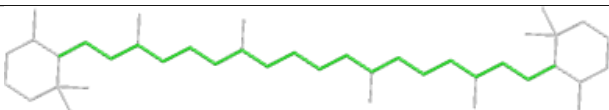
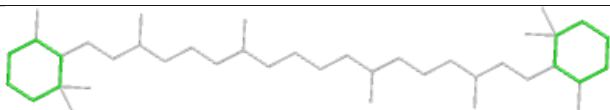


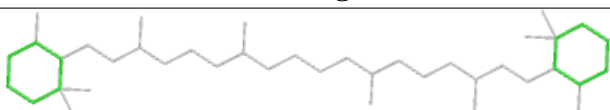
Ligand LHG D 407 (B)

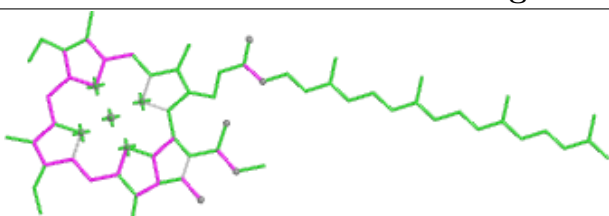
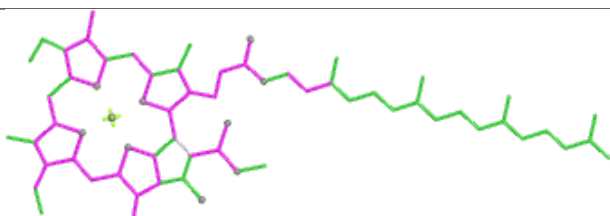
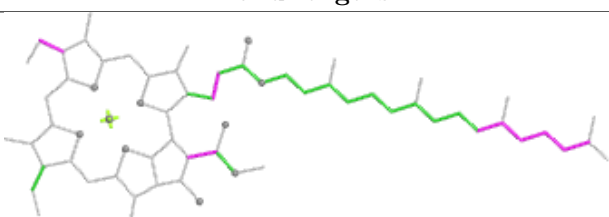
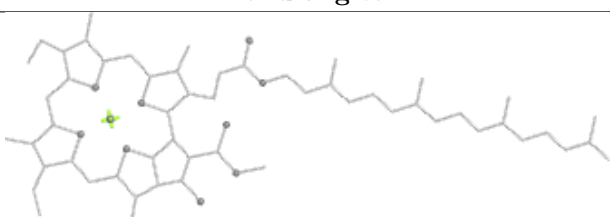


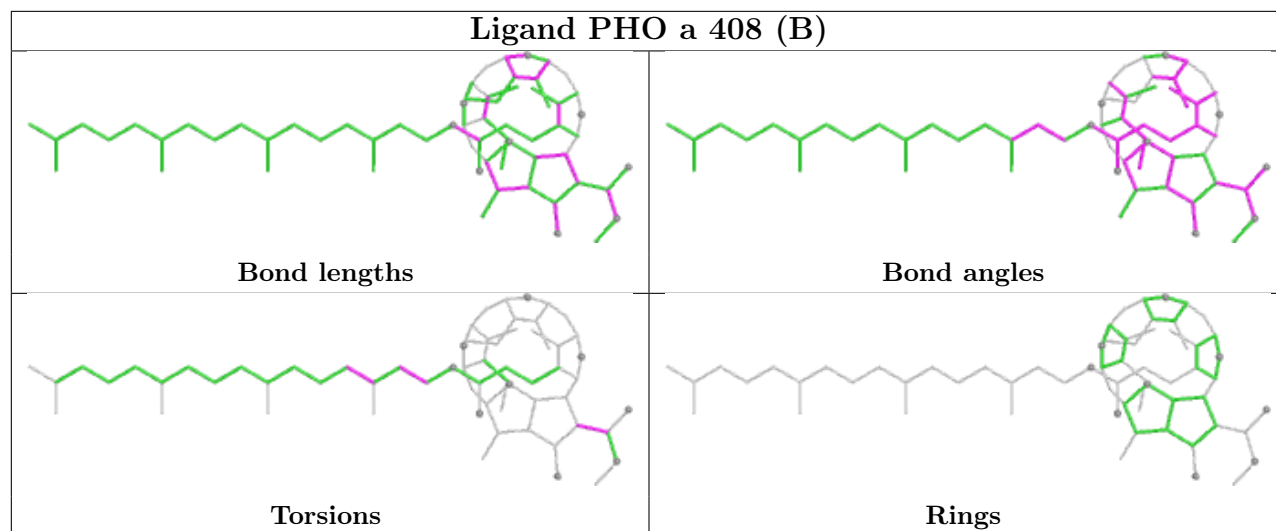
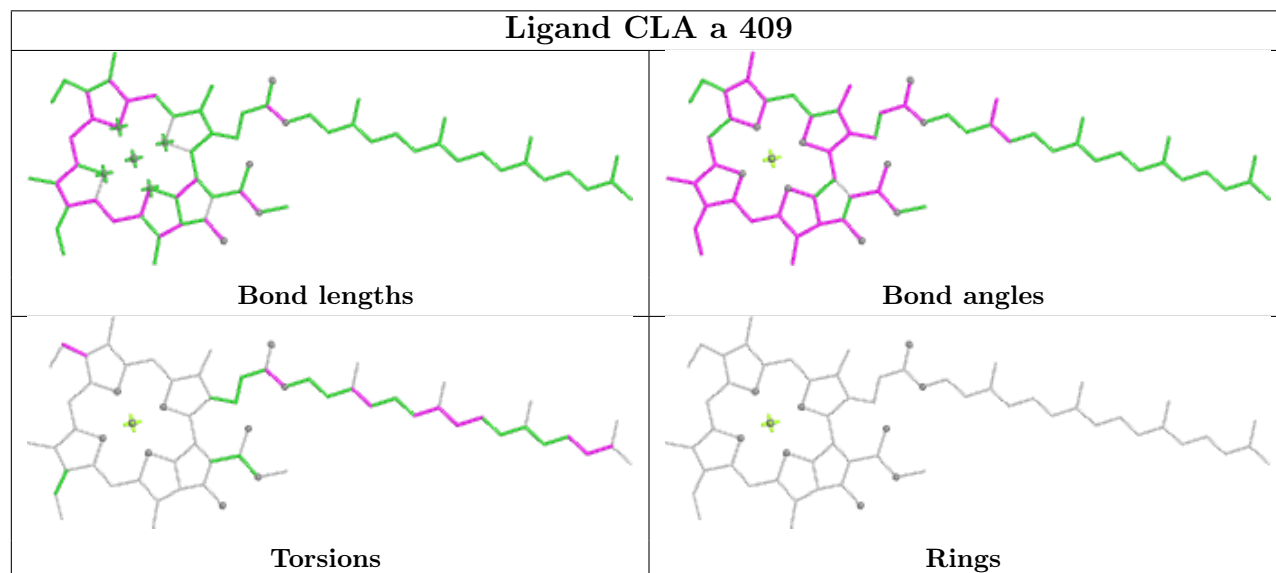
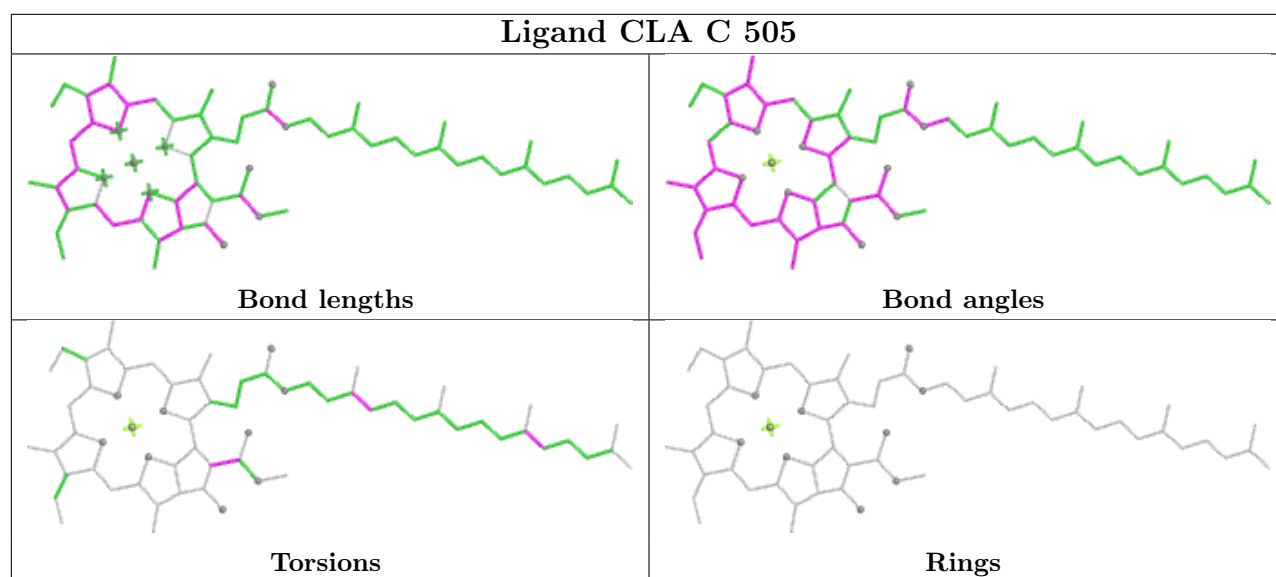
Ligand BCR H 101

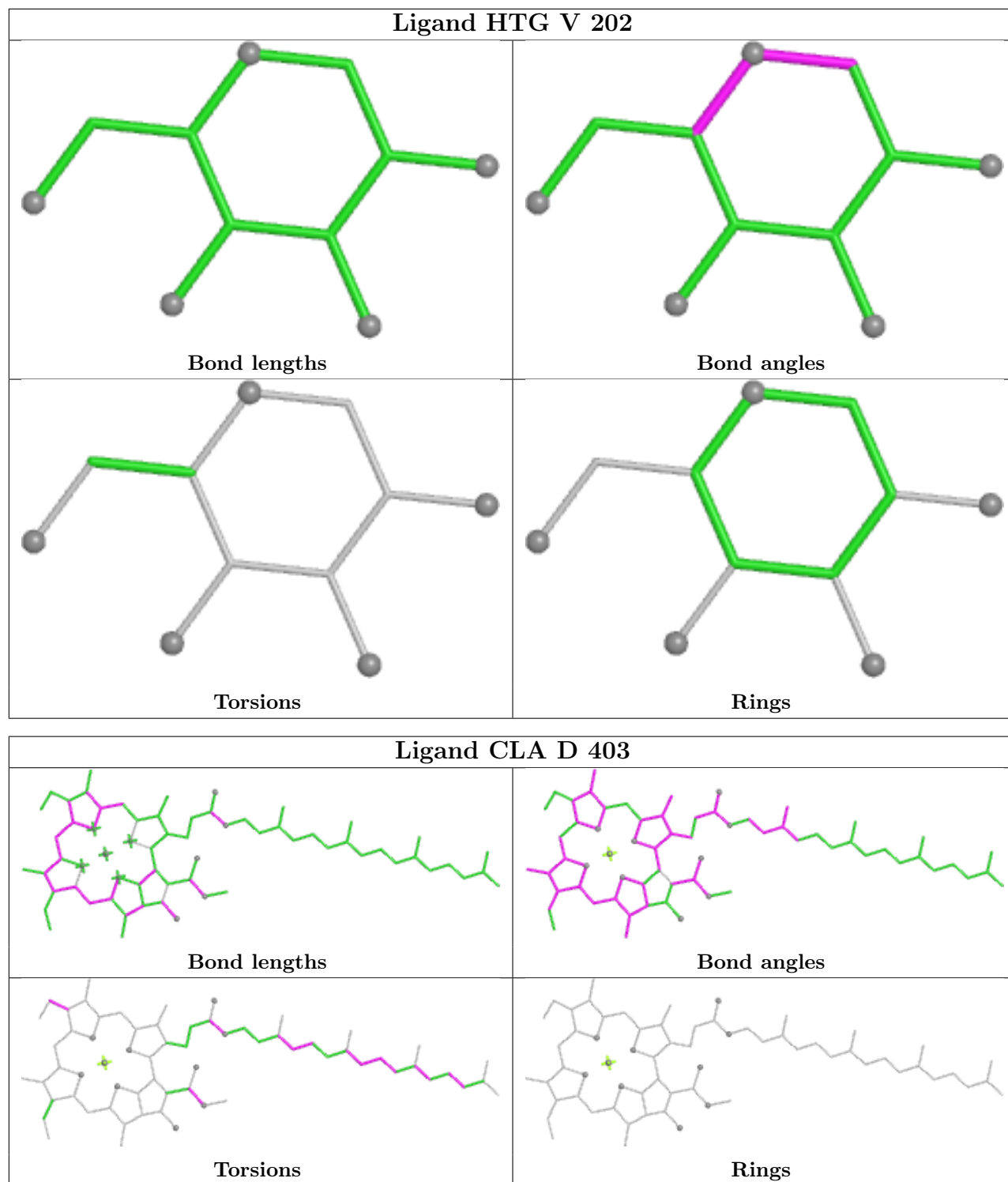


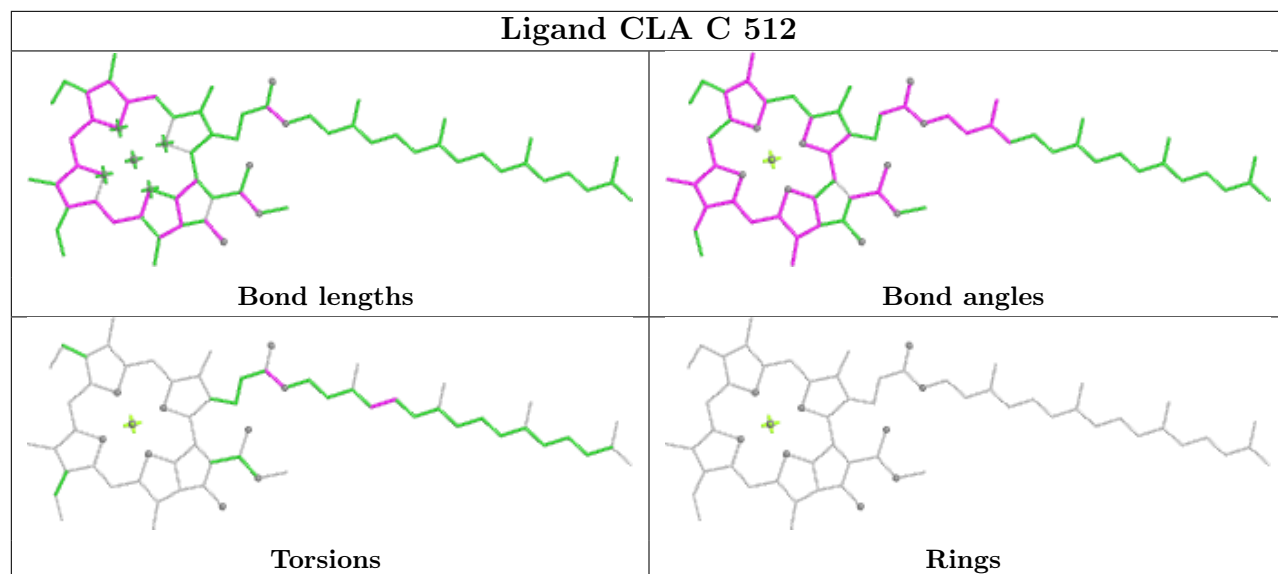
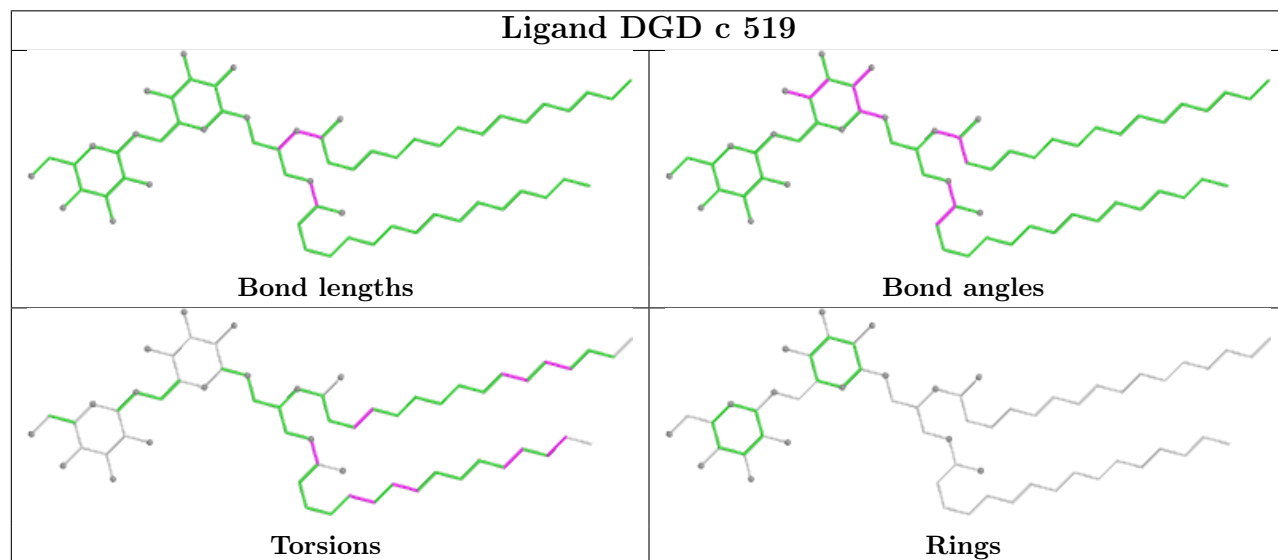
Ligand BCR C 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR t 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

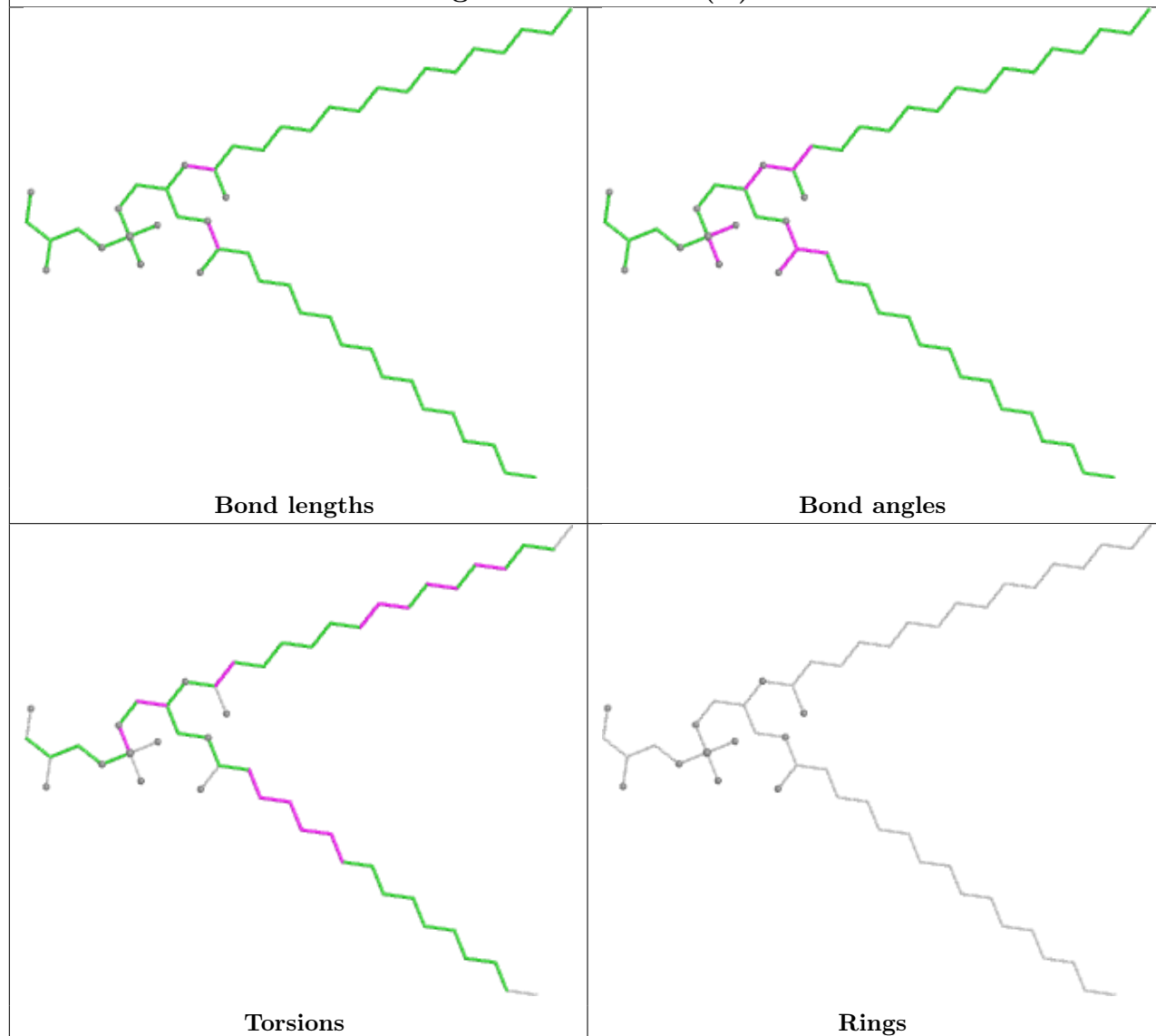
Ligand CLA B 610	
	
Bond lengths	Bond angles
	
Torsions	Rings



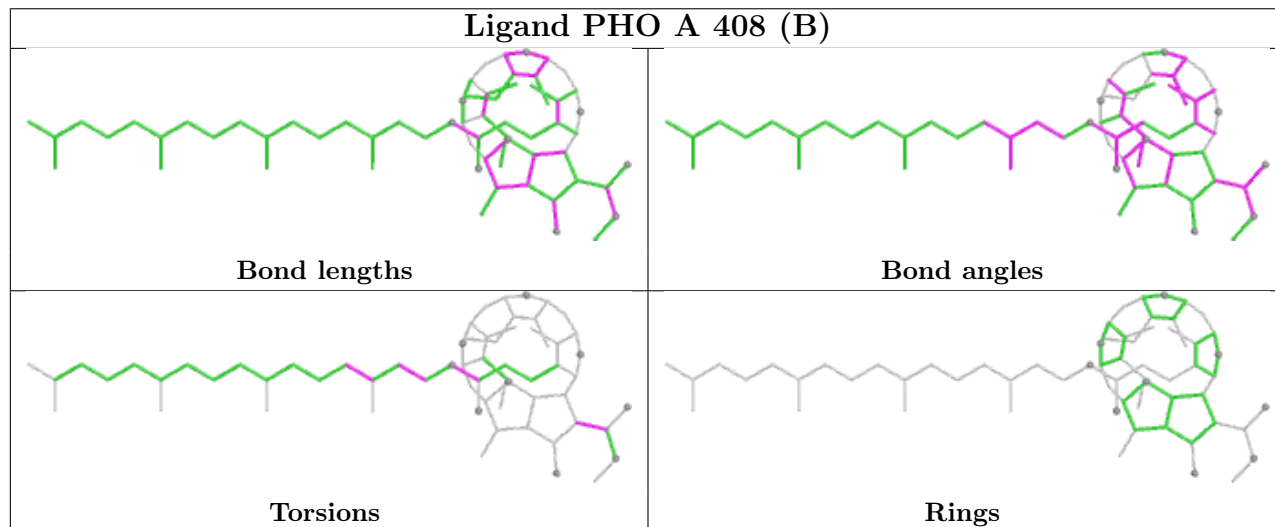


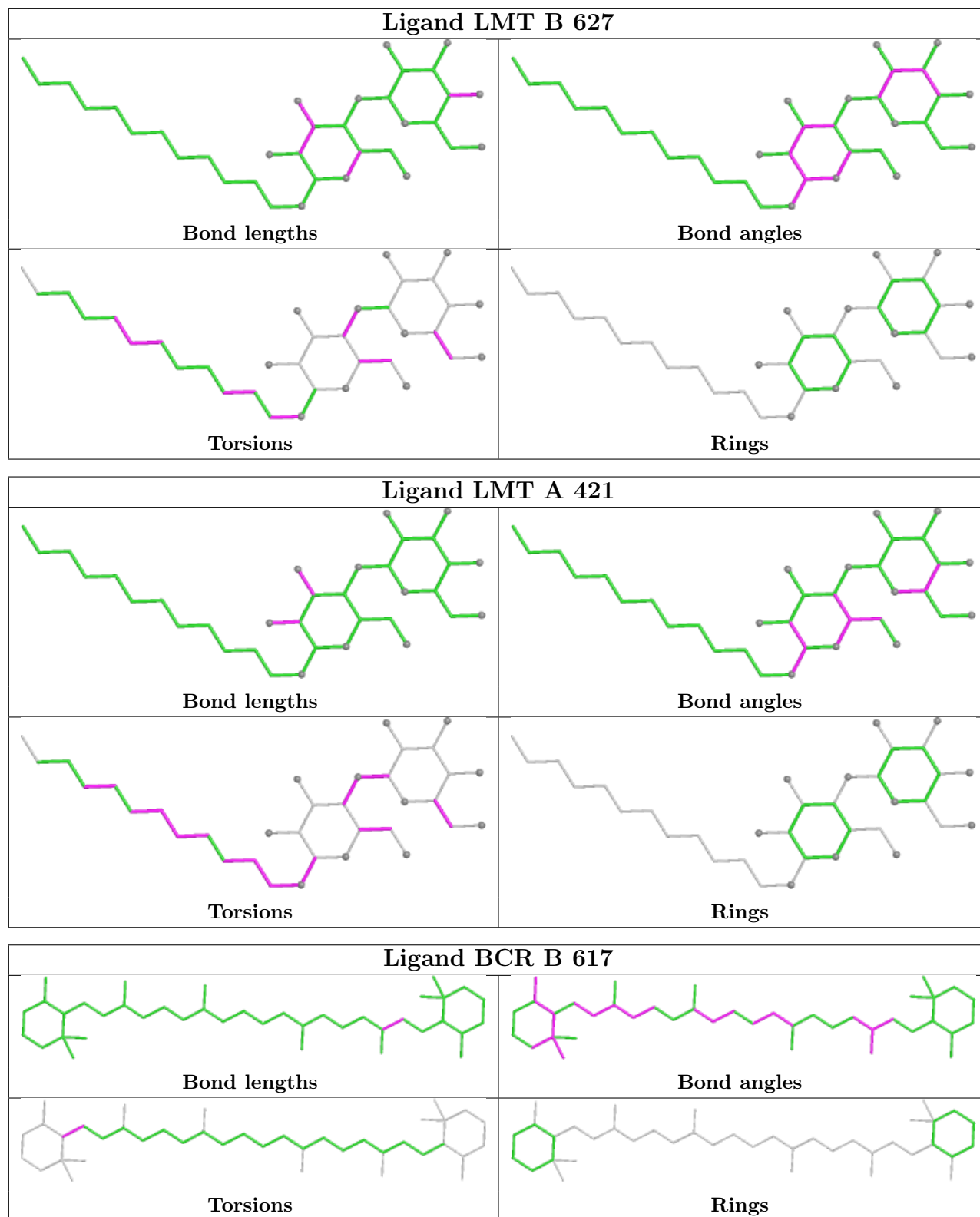
Ligand CLA C 512**Ligand DGD c 519**

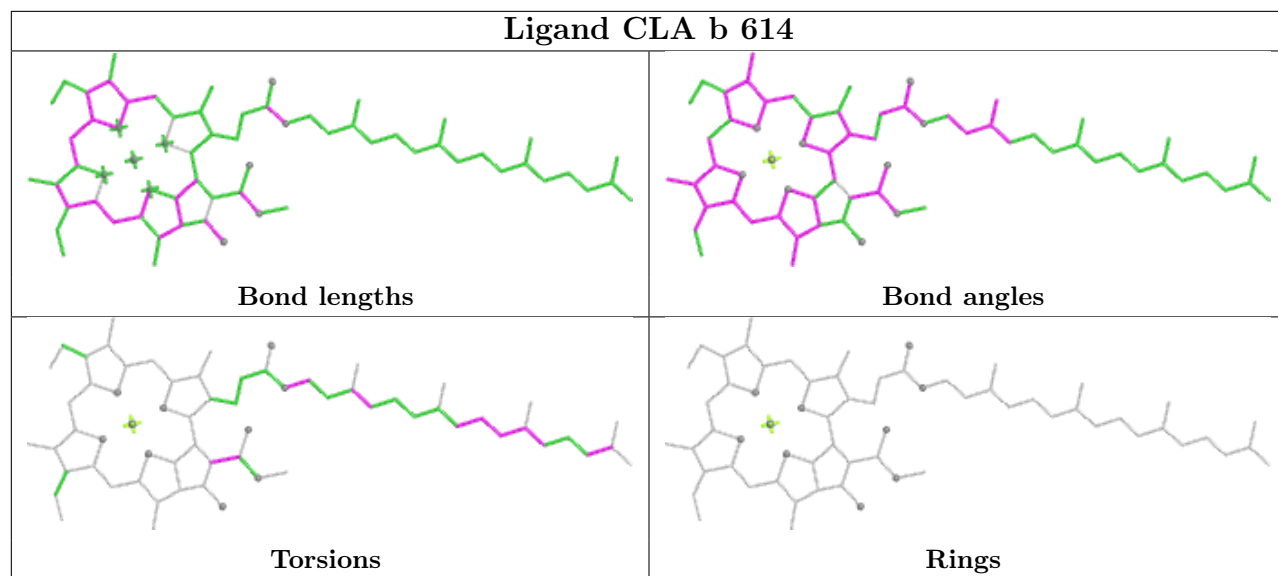
Ligand LHG L 101 (B)



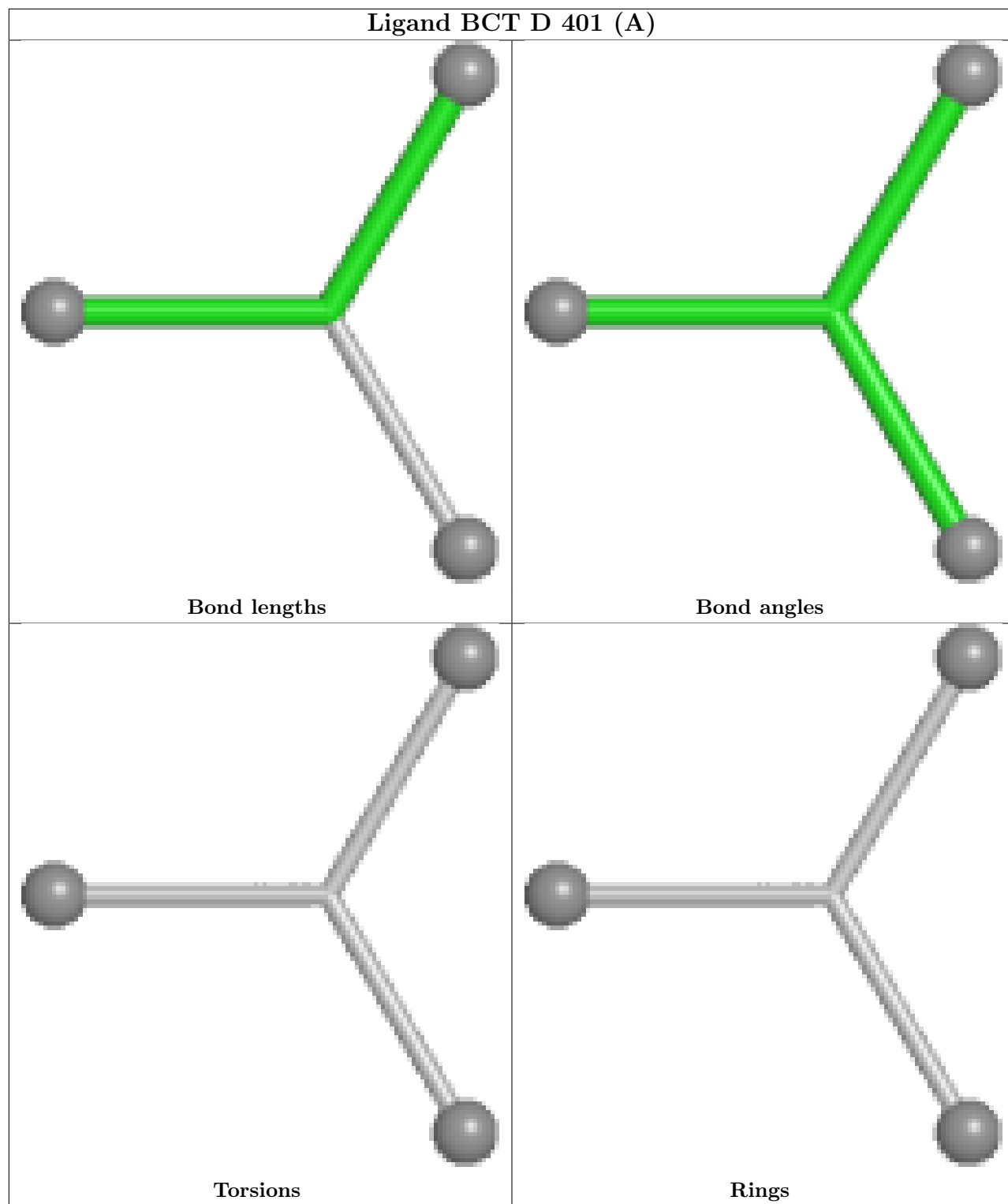
Ligand PHO A 408 (B)

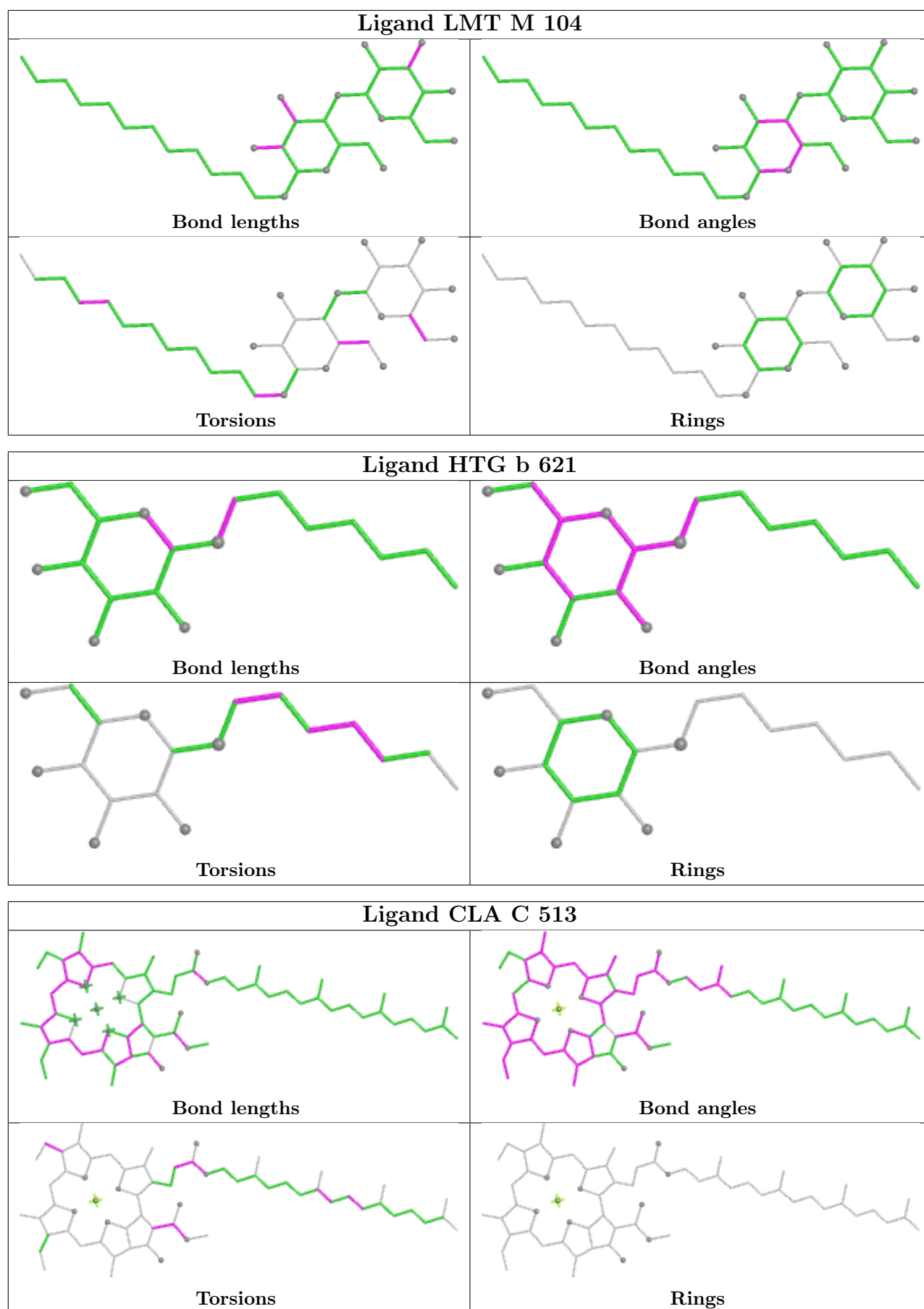


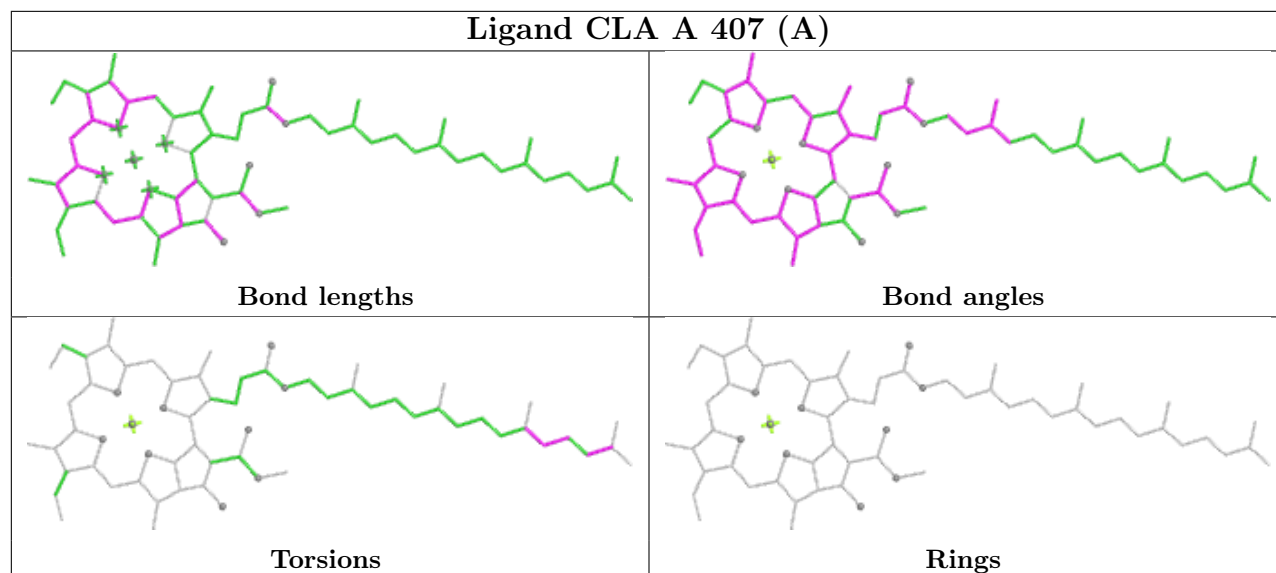
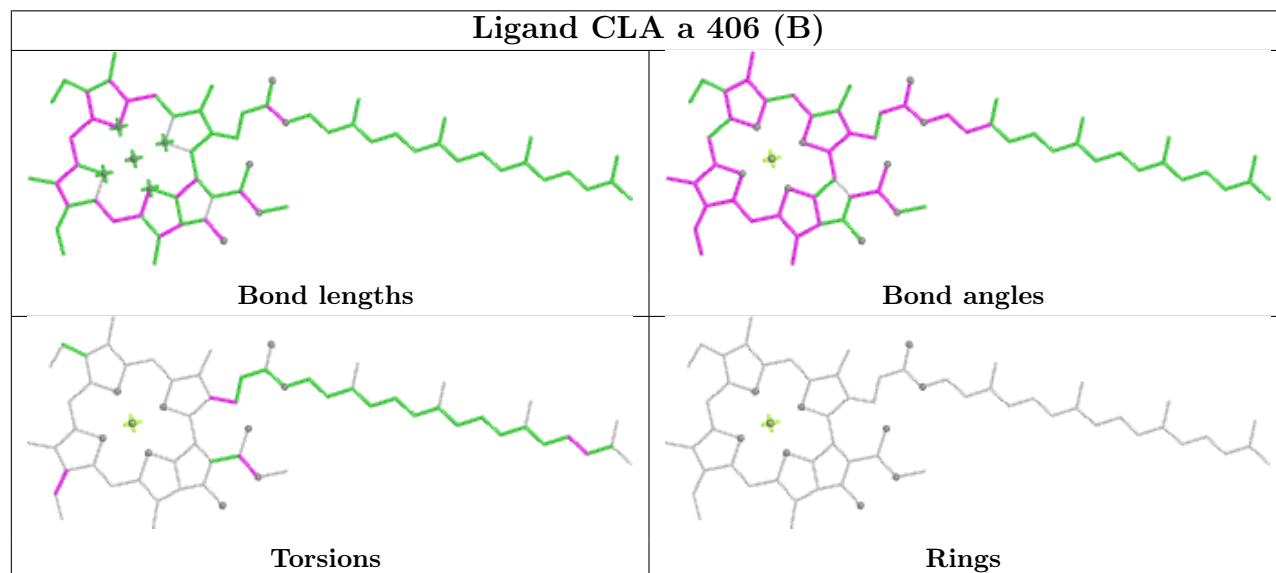
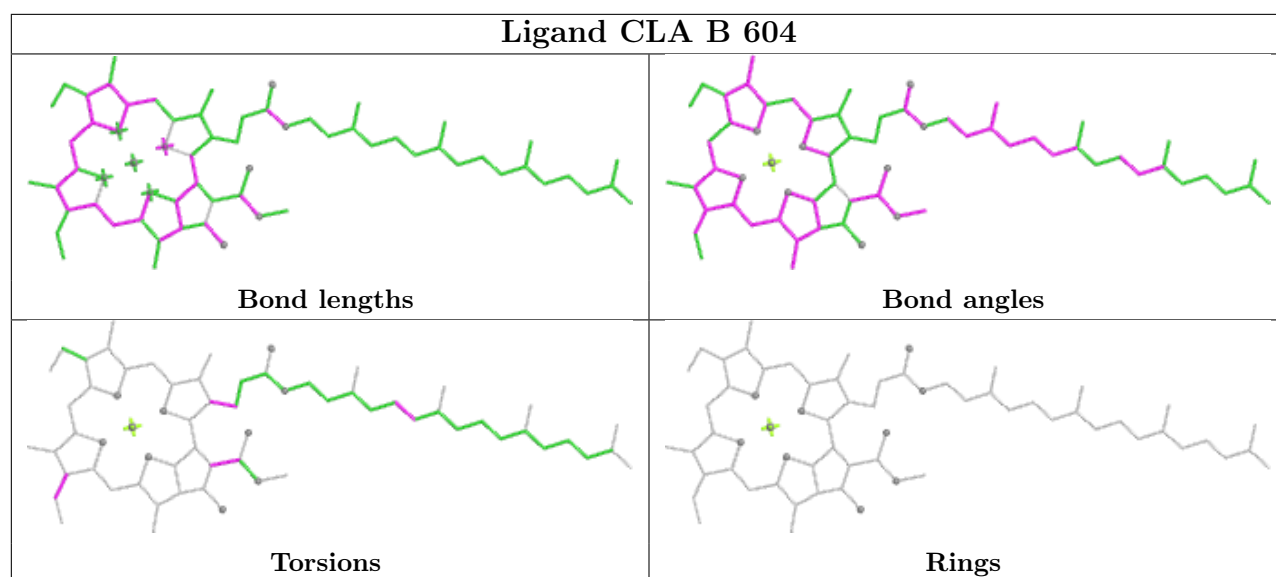


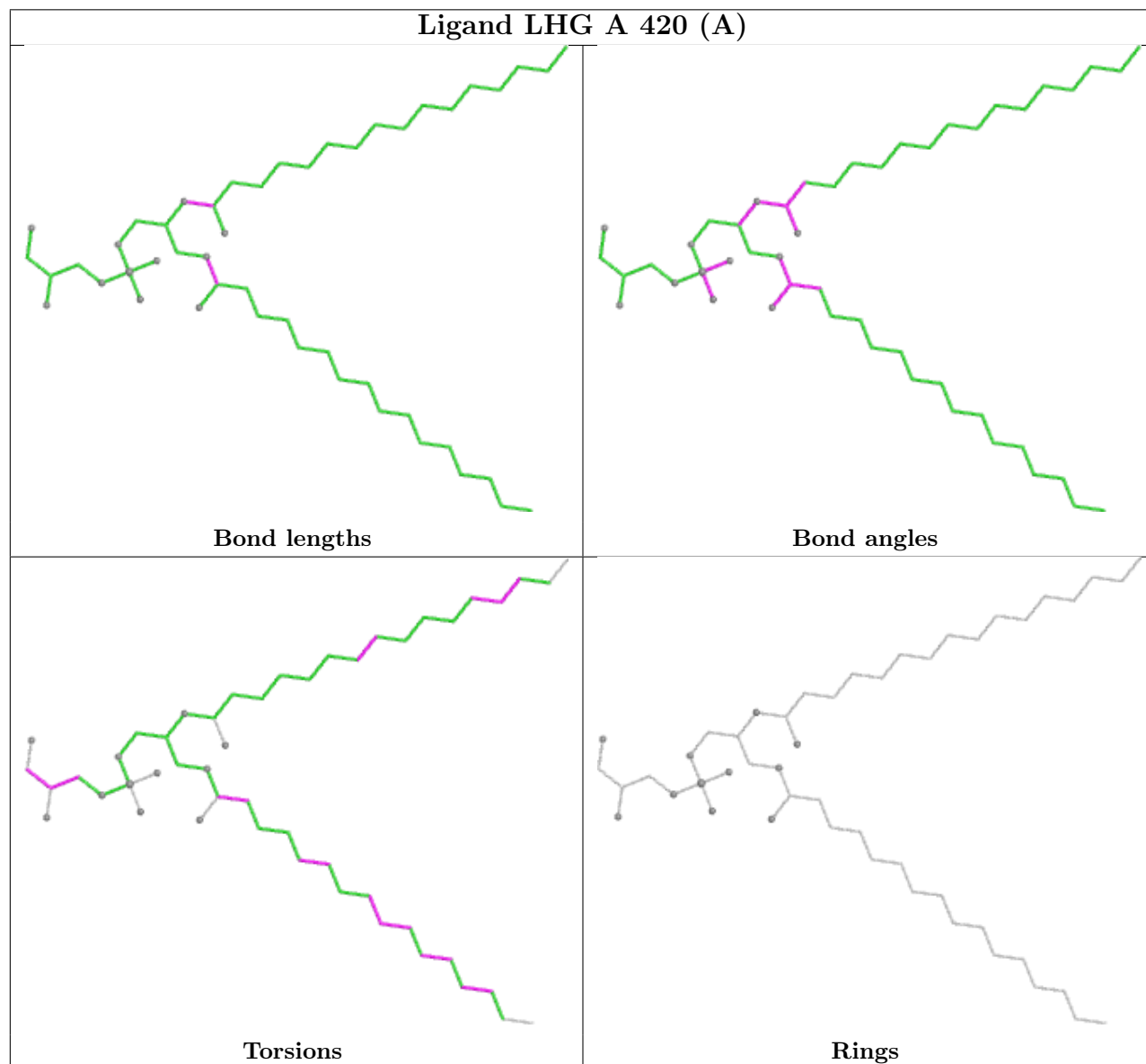
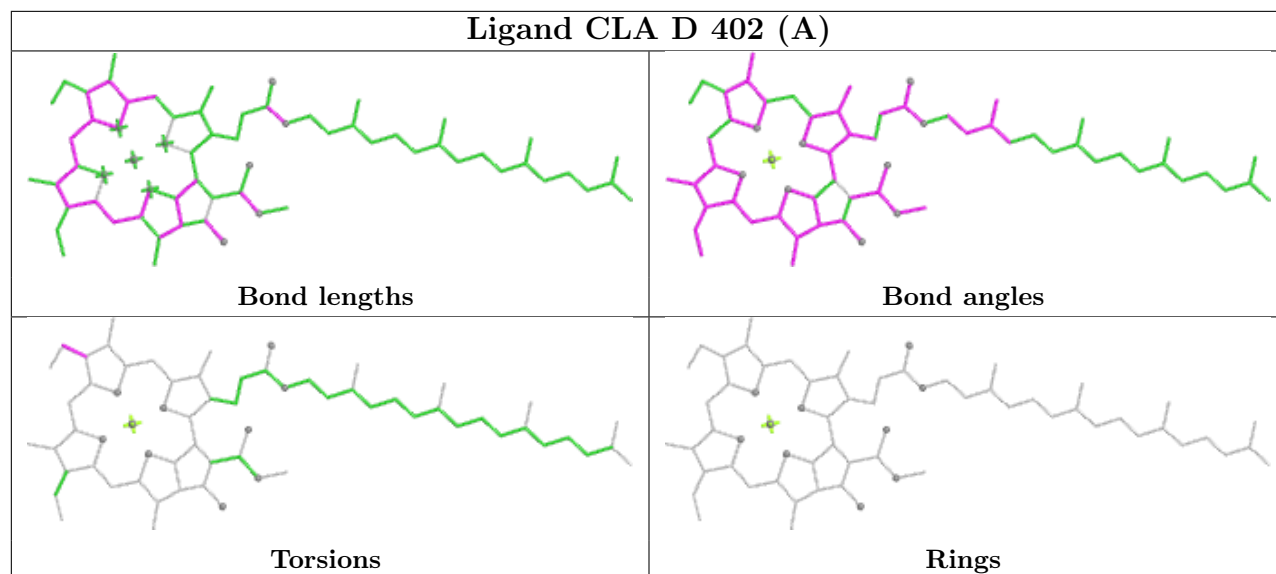


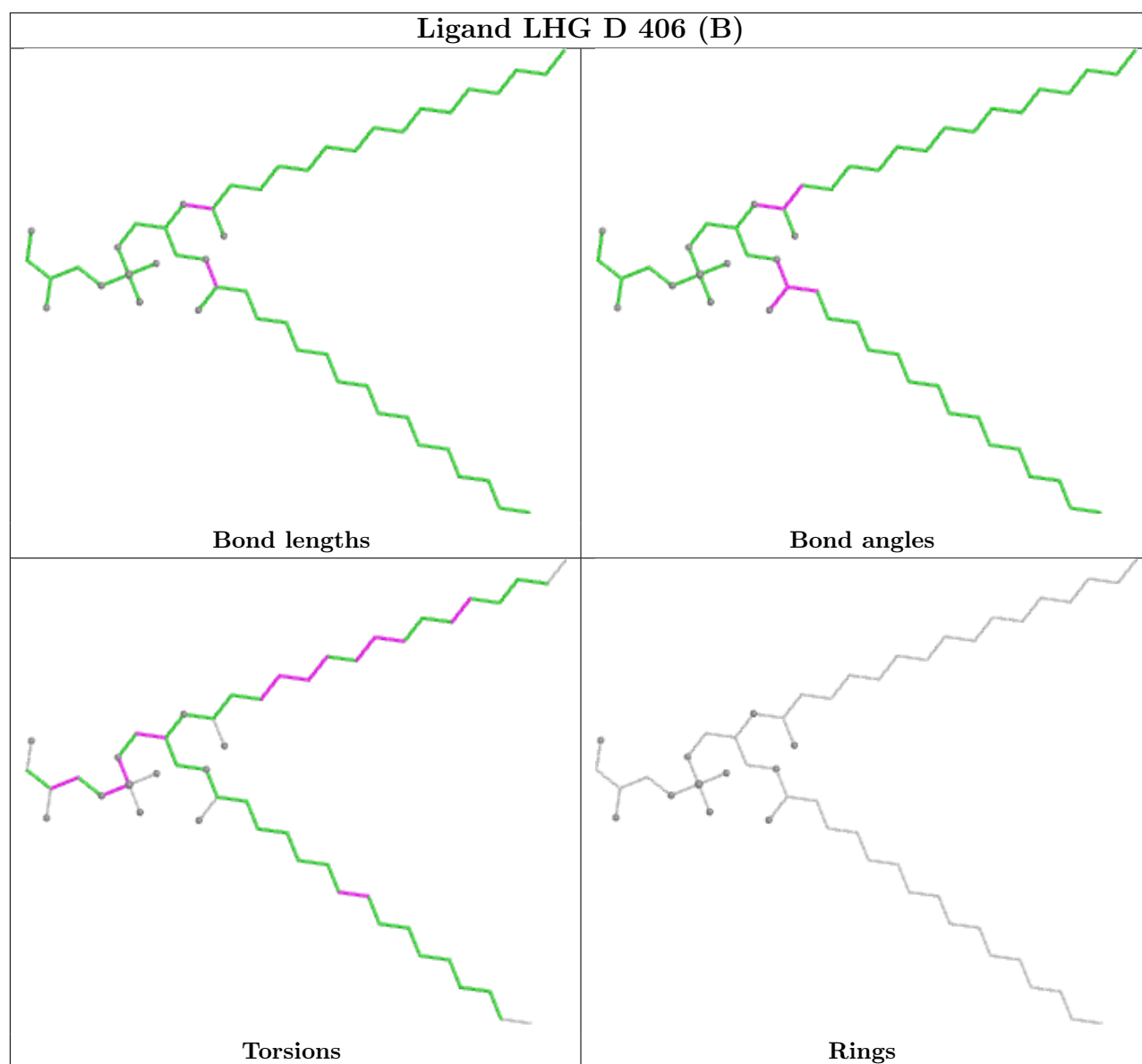
Ligand BCT D 401 (A)











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.71	1 (0%) 90 90	19, 26, 61, 124	222 (66%)
1	a	334/344 (97%)	-0.65	1 (0%) 90 90	20, 28, 64, 132	221 (66%)
2	B	504/505 (99%)	-0.61	1 (0%) 91 92	22, 53, 82, 114	20 (3%)
2	b	504/505 (99%)	-0.51	1 (0%) 91 92	24, 57, 96, 152	19 (3%)
3	C	451/455 (99%)	-0.59	0 100 100	21, 58, 84, 137	97 (21%)
3	c	455/455 (100%)	-0.50	1 (0%) 91 92	24, 65, 87, 125	100 (21%)
4	D	342/342 (100%)	-0.74	0 100 100	18, 44, 63, 132	114 (33%)
4	d	341/342 (99%)	-0.73	0 100 100	21, 49, 74, 130	116 (34%)
5	E	81/84 (96%)	-0.35	1 (1%) 76 77	52, 69, 101, 148	0
5	e	79/84 (94%)	-0.34	1 (1%) 75 76	33, 75, 119, 146	2 (2%)
6	F	34/44 (77%)	-0.57	0 100 100	51, 60, 89, 113	0
6	f	31/44 (70%)	-0.30	1 (3%) 50 50	55, 68, 95, 139	1 (3%)
7	H	64/65 (98%)	-0.32	1 (1%) 70 71	52, 63, 87, 106	0
7	h	64/65 (98%)	-0.32	1 (1%) 70 71	40, 72, 93, 104	1 (1%)
8	I	37/38 (97%)	-0.24	0 100 100	56, 65, 119, 143	0
8	i	37/38 (97%)	-0.26	1 (2%) 56 57	54, 64, 113, 135	0
9	J	38/39 (97%)	-0.41	0 100 100	48, 68, 115, 157	0
9	j	39/39 (100%)	-0.17	0 100 100	57, 76, 125, 156	0
10	K	37/37 (100%)	-0.68	0 100 100	57, 67, 82, 105	0
10	k	37/37 (100%)	-0.46	0 100 100	66, 74, 96, 112	0
11	L	36/37 (97%)	-0.71	0 100 100	22, 44, 113, 129	2 (5%)
11	l	36/37 (97%)	-0.66	0 100 100	23, 45, 102, 114	2 (5%)
12	M	32/36 (88%)	-0.62	0 100 100	26, 47, 73, 127	1 (3%)
12	m	33/36 (91%)	-0.69	0 100 100	24, 47, 70, 135	2 (6%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.51	0 100 100	21, 65, 120, 164	10 (4%)
13	o	243/244 (99%)	-0.46	0 100 100	22, 68, 122, 155	8 (3%)
14	T	29/32 (90%)	-0.73	0 100 100	26, 47, 54, 65	6 (20%)
14	t	29/32 (90%)	-0.71	0 100 100	27, 47, 58, 70	5 (17%)
15	U	96/104 (92%)	-0.63	0 100 100	25, 57, 90, 100	4 (4%)
15	u	97/104 (93%)	-0.66	0 100 100	28, 61, 83, 122	4 (4%)
16	V	137/137 (100%)	-0.71	0 100 100	23, 56, 83, 106	6 (4%)
16	v	137/137 (100%)	-0.54	0 100 100	26, 71, 102, 131	6 (4%)
17	X	38/40 (95%)	-0.19	0 100 100	35, 71, 93, 113	1 (2%)
17	x	38/40 (95%)	-0.05	0 100 100	67, 80, 124, 157	0
18	Y	29/30 (96%)	-0.12	1 (3%) 48 48	64, 84, 117, 122	0
18	y	29/30 (96%)	-0.14	0 100 100	76, 88, 109, 113	0
19	Z	62/62 (100%)	-0.31	0 100 100	67, 80, 133, 150	0
19	z	62/62 (100%)	0.17	0 100 100	79, 94, 141, 168	0
20	R	34/34 (100%)	0.54	1 (2%) 53 54	85, 109, 132, 142	0
All	All	5283/5384 (98%)	-0.55	13 (0%) 91 92	18, 57, 100, 168	970 (18%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	3.8
5	e	79[A]	PHE	3.7
6	f	16[A]	PHE	3.1
2	B	494	GLY	2.7
1	A	11	ALA	2.5

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	FME	I	1	10/11	0.95	0.07	59,70,76,78	0
14	FME	T	1	10/11	0.95	0.07	39,57,65,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	FME	t	1	10/11	0.96	0.07	43,47,56,74	0
8	FME	i	1	10/11	0.97	0.07	55,69,77,80	0
12	FME	m	1	10/11	0.97	0.06	50,63,91,114	0
12	FME	M	1	10/11	0.97	0.07	51,57,96,104	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
31	UNL	a	416	30/-	0.66	0.14	86,111,131,146	0
28	GOL	a	418	6/6	0.67	0.17	78,93,107,112	0
32	LMT	B	628	35/35	0.68	0.15	68,115,140,152	0
32	LMT	F	101	35/35	0.68	0.15	85,132,174,181	0
32	LMT	A	418	35/35	0.70	0.13	64,110,132,141	0
31	UNL	A	416	28/-	0.70	0.14	84,108,124,146	0
31	UNL	m	101	10/-	0.70	0.19	67,74,93,102	0
32	LMT	e	102	35/35	0.71	0.14	104,138,183,189	0
31	UNL	j	101	10/-	0.72	0.17	72,85,101,102	0
31	UNL	K	101[A]	34/-	0.73	0.14	77,101,118,120	34
31	UNL	K	101[B]	34/-	0.73	0.14	77,101,118,120	34
27	SQD	f	101	43/54	0.73	0.13	91,128,167,188	0
34	HTG	C	522	19/19	0.74	0.13	93,127,138,138	0
28	GOL	A	412	6/6	0.75	0.16	54,78,80,83	0
31	UNL	I	101	40/-	0.75	0.14	72,99,151,161	0
32	LMT	c	501	35/35	0.75	0.13	101,129,154,159	0
31	UNL	J	101	10/-	0.75	0.22	69,80,89,96	0
32	LMT	A	421	35/35	0.75	0.12	81,126,151,163	0
33	LHG	a	420[B]	42/49	0.76	0.12	87,129,143,149	42
33	LHG	a	420[A]	42/49	0.76	0.12	87,129,143,148	42
31	UNL	M	103	10/-	0.79	0.15	63,75,93,94	0
28	GOL	o	302	6/6	0.79	0.17	83,103,105,112	0
31	UNL	c	525[A]	32/-	0.79	0.14	86,104,118,129	32
31	UNL	c	525[B]	32/-	0.79	0.14	86,104,118,129	32

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	GOL	d	413	6/6	0.79	0.22	50,69,83,83	0
31	UNL	B	629	40/-	0.80	0.13	71,106,143,163	0
31	UNL	D	409	40/-	0.80	0.13	61,88,138,153	0
31	UNL	b	625	33/-	0.80	0.12	68,99,153,163	0
34	HTG	B	622	19/19	0.80	0.14	63,92,112,114	0
28	GOL	B	626	6/6	0.80	0.13	69,85,107,119	0
34	HTG	D	410	16/19	0.80	0.12	85,106,134,143	0
28	GOL	o	303	6/6	0.81	0.14	79,83,97,100	0
31	UNL	d	410	36/-	0.81	0.12	68,92,130,142	0
28	GOL	O	303	6/6	0.81	0.14	78,86,96,98	0
34	HTG	c	522	19/19	0.81	0.10	100,121,139,142	0
37	CA	F	103	1/1	0.81	0.23	121,121,121,121	0
32	LMT	b	620	25/35	0.82	0.11	76,114,160,172	0
35	LMG	C	521	51/55	0.82	0.11	59,115,159,173	0
34	HTG	b	622	19/19	0.82	0.11	83,129,157,161	0
30	PL9	A	415[A]	55/55	0.83	0.12	59,84,101,112	55
30	PL9	A	415[B]	55/55	0.83	0.12	60,84,101,112	55
28	GOL	O	302	6/6	0.83	0.10	79,94,101,109	0
28	GOL	v	202[A]	6/6	0.83	0.12	65,78,80,80	6
32	LMT	t	101	26/35	0.83	0.12	71,97,145,155	0
32	LMT	B	627	35/35	0.83	0.11	69,105,140,151	0
28	GOL	v	202[B]	6/6	0.83	0.12	65,78,80,81	6
34	HTG	b	621	19/19	0.84	0.13	61,79,113,124	0
31	UNL	B	625	33/-	0.84	0.13	59,111,142,148	0
30	PL9	a	415[B]	55/55	0.84	0.14	67,98,108,115	55
32	LMT	M	104	35/35	0.84	0.10	69,121,170,178	0
30	PL9	a	415[A]	55/55	0.84	0.14	68,98,108,115	55
32	LMT	B	630	25/35	0.85	0.12	58,82,147,160	0
35	LMG	c	521	51/55	0.85	0.10	71,132,161,181	0
35	LMG	Z	101	37/55	0.85	0.13	68,117,154,166	0
35	LMG	z	101	39/55	0.85	0.12	66,129,151,172	0
34	HTG	d	411	16/19	0.85	0.10	86,121,141,151	0
27	SQD	a	413	54/54	0.86	0.10	67,94,142,152	0
34	HTG	B	621	19/19	0.86	0.12	60,85,115,119	0
32	LMT	m	102	35/35	0.87	0.10	61,92,107,116	0
28	GOL	l	801[A]	6/6	0.87	0.18	64,92,95,96	6
28	GOL	l	801[B]	6/6	0.87	0.18	65,93,95,96	6
27	SQD	A	413	54/54	0.87	0.10	60,85,124,145	0
28	GOL	a	419	6/6	0.87	0.24	54,73,83,85	0
32	LMT	b	626	25/35	0.87	0.12	51,93,149,157	0
28	GOL	c	527	6/6	0.87	0.16	96,103,107,107	0
28	GOL	a	412	6/6	0.87	0.12	74,76,83,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	HTG	V	202	11/19	0.87	0.09	81,117,124,129	0
28	GOL	b	623	6/6	0.88	0.14	82,99,106,111	0
27	SQD	X	101	43/54	0.88	0.11	66,104,129,144	0
32	LMT	M	102	35/35	0.89	0.10	57,93,123,126	0
28	GOL	c	526[A]	6/6	0.89	0.10	66,71,76,77	6
28	GOL	c	526[B]	6/6	0.89	0.10	66,70,76,77	6
33	LHG	E	101[A]	42/49	0.89	0.11	68,97,110,116	42
33	LHG	E	101[B]	42/49	0.89	0.11	68,97,110,116	42
27	SQD	L	102	54/54	0.89	0.09	59,96,124,133	0
24	CLA	b	601	65/65	0.89	0.10	59,85,128,155	0
37	CA	f	102	1/1	0.89	0.13	117,117,117,117	0
28	GOL	D	412	6/6	0.90	0.15	44,64,69,84	0
27	SQD	B	620	54/54	0.90	0.09	62,91,136,142	0
35	LMG	C	501	51/55	0.90	0.09	66,91,116,128	0
35	LMG	a	417	51/55	0.91	0.09	66,92,114,118	0
28	GOL	B	623	6/6	0.91	0.09	68,74,81,82	0
24	CLA	B	601	65/65	0.91	0.09	56,78,110,153	0
28	GOL	C	523[A]	6/6	0.91	0.10	58,60,68,72	6
28	GOL	C	523[B]	6/6	0.91	0.10	58,61,68,72	6
28	GOL	A	419	6/6	0.91	0.23	50,74,76,82	0
37	CA	o	301	1/1	0.91	0.08	114,114,114,114	0
35	LMG	c	520	51/55	0.92	0.09	61,91,130,153	0
31	UNL	D	408	17/-	0.92	0.10	59,74,102,119	0
34	HTG	B	624	19/19	0.92	0.08	65,78,104,105	0
31	UNL	d	409	17/-	0.92	0.10	66,81,110,112	0
35	LMG	M	101	51/55	0.92	0.08	53,70,89,116	0
24	CLA	c	514	65/65	0.92	0.09	69,95,124,148	0
35	LMG	b	629	51/55	0.92	0.09	52,73,97,113	0
35	LMG	D	411	51/55	0.93	0.09	48,64,118,133	0
33	LHG	A	420[A]	49/49	0.93	0.09	46,60,81,88	49
33	LHG	A	420[B]	49/49	0.93	0.09	46,60,81,88	49
24	CLA	C	514	65/65	0.93	0.09	58,86,112,123	0
27	SQD	a	411[A]	54/54	0.93	0.09	60,80,117,121	54
27	SQD	a	411[B]	54/54	0.93	0.09	60,80,117,121	54
35	LMG	d	412	51/55	0.93	0.09	53,71,120,150	0
26	BCR	D	404	40/40	0.93	0.09	42,59,101,108	0
28	GOL	V	203[A]	6/6	0.93	0.11	57,68,75,79	6
28	GOL	V	203[B]	6/6	0.93	0.11	57,69,75,79	6
35	LMG	C	520	51/55	0.93	0.09	51,83,113,127	0
26	BCR	d	405	40/40	0.93	0.09	48,63,109,111	0
24	CLA	d	404	65/65	0.94	0.09	54,67,121,150	0
26	BCR	A	410	40/40	0.94	0.07	42,51,65,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	BCR	C	515	40/40	0.94	0.08	57,77,89,91	0
34	HTG	b	624	19/19	0.94	0.07	63,77,94,110	0
24	CLA	B	614	65/65	0.94	0.07	37,50,102,127	0
26	BCR	H	101	40/40	0.94	0.08	51,66,91,92	0
26	BCR	T	101	40/40	0.94	0.06	41,58,71,79	0
26	BCR	Y	101	40/40	0.94	0.08	49,63,79,85	0
33	LHG	D	407[A]	49/49	0.94	0.09	45,58,108,111	49
33	LHG	D	407[B]	49/49	0.94	0.09	44,58,108,110	49
24	CLA	C	507	65/65	0.94	0.08	54,69,119,142	0
26	BCR	h	101	40/40	0.94	0.09	55,69,93,96	0
26	BCR	t	102	40/40	0.94	0.06	42,61,78,84	0
27	SQD	A	411[A]	54/54	0.94	0.08	58,78,114,121	54
33	LHG	d	414[A]	49/49	0.94	0.08	49,67,78,86	49
33	LHG	d	414[B]	49/49	0.94	0.08	50,67,82,86	49
27	SQD	A	411[B]	54/54	0.94	0.08	58,78,114,121	54
24	CLA	b	616	65/65	0.94	0.08	49,63,127,143	0
36	DGD	C	518[A]	62/66	0.94	0.08	46,62,115,120	62
36	DGD	C	518[B]	62/66	0.94	0.08	46,62,115,120	62
36	DGD	c	517[A]	62/66	0.94	0.08	48,64,101,107	62
36	DGD	c	517[B]	62/66	0.94	0.08	48,64,101,107	62
36	DGD	c	518[A]	62/66	0.94	0.07	53,66,117,133	62
36	DGD	c	518[B]	62/66	0.94	0.07	53,66,117,133	62
24	CLA	c	513	65/65	0.94	0.09	59,82,122,130	0
31	UNL	X	102	18/-	0.94	0.10	61,74,107,110	0
24	CLA	C	513	65/65	0.94	0.08	59,73,111,124	0
26	BCR	B	618	40/40	0.95	0.06	39,51,69,78	0
26	BCR	B	619	40/40	0.95	0.07	46,59,91,99	0
24	CLA	B	606	65/65	0.95	0.07	43,58,112,128	0
24	CLA	a	407[A]	65/65	0.95	0.07	40,51,123,132	65
24	CLA	a	407[B]	65/65	0.95	0.07	40,51,123,132	65
26	BCR	K	102	40/40	0.95	0.08	55,63,77,82	0
24	CLA	a	409	65/65	0.95	0.09	42,56,133,155	0
30	PL9	D	405[A]	55/55	0.95	0.06	39,47,58,69	55
30	PL9	D	405[B]	55/55	0.95	0.06	39,47,58,68	55
24	CLA	A	407[B]	65/65	0.95	0.06	35,46,104,120	65
26	BCR	a	410	40/40	0.95	0.07	44,54,64,65	0
30	PL9	d	406[A]	55/55	0.95	0.06	37,49,60,68	55
30	PL9	d	406[B]	55/55	0.95	0.06	37,50,60,69	55
26	BCR	b	619	40/40	0.95	0.07	48,63,86,91	0
26	BCR	c	515	40/40	0.95	0.08	67,81,93,97	0
24	CLA	b	606	65/65	0.95	0.08	46,61,117,130	0
24	CLA	b	614	65/65	0.95	0.06	41,50,102,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	BCR	k	101	40/40	0.95	0.09	57,74,83,88	0
24	CLA	B	616	65/65	0.95	0.08	47,58,136,145	0
26	BCR	y	101	40/40	0.95	0.07	56,69,85,103	0
24	CLA	c	505	65/65	0.95	0.07	49,62,106,138	0
24	CLA	c	507	65/65	0.95	0.08	53,68,119,143	0
28	GOL	b	627	6/6	0.95	0.09	80,85,86,90	0
24	CLA	c	508	65/65	0.95	0.09	49,69,84,91	0
24	CLA	C	505	65/65	0.95	0.07	41,55,102,133	0
36	DGD	C	519	62/66	0.95	0.07	43,57,101,112	0
36	DGD	H	102	62/66	0.95	0.08	43,60,77,85	0
24	CLA	A	409	65/65	0.95	0.08	39,52,130,147	0
33	LHG	b	628[A]	49/49	0.95	0.07	47,55,71,84	49
33	LHG	b	628[B]	49/49	0.95	0.07	47,55,72,84	49
33	LHG	d	408[A]	49/49	0.95	0.09	51,62,111,128	49
36	DGD	c	519	62/66	0.95	0.07	49,66,104,131	0
36	DGD	h	102	62/66	0.95	0.07	51,66,80,87	0
33	LHG	d	408[B]	49/49	0.95	0.09	51,63,111,128	49
37	CA	O	301	1/1	0.95	0.05	107,107,107,107	0
37	CA	c	523	1/1	0.95	0.06	79,79,79,79	0
24	CLA	C	509	65/65	0.95	0.07	45,55,114,143	0
24	CLA	A	407[A]	65/65	0.95	0.06	35,46,104,120	65
38	BCT	d	401[A]	4/4	0.95	0.07	53,57,64,73	4
38	BCT	d	401[B]	4/4	0.95	0.07	53,57,64,70	4
24	CLA	A	405[A]	65/65	0.96	0.06	35,41,55,69	65
25	PHO	d	402[A]	64/64	0.96	0.07	45,54,63,68	64
25	PHO	d	402[B]	64/64	0.96	0.07	45,54,63,68	64
24	CLA	b	602	65/65	0.96	0.07	48,60,82,95	0
33	LHG	D	406[A]	49/49	0.96	0.07	44,52,66,77	49
33	LHG	D	406[B]	49/49	0.96	0.07	43,53,66,78	49
26	BCR	B	617	40/40	0.96	0.05	41,52,62,64	0
24	CLA	C	508	65/65	0.96	0.08	52,63,83,93	0
24	CLA	b	607	65/65	0.96	0.06	37,46,80,88	0
24	CLA	b	609	65/65	0.96	0.06	50,65,80,94	0
26	BCR	C	516	40/40	0.96	0.06	53,64,79,83	0
24	CLA	b	612	65/65	0.96	0.07	42,53,68,78	0
24	CLA	B	609	65/65	0.96	0.07	46,59,73,85	0
36	DGD	C	517[A]	62/66	0.96	0.06	44,58,95,100	62
36	DGD	C	517[B]	62/66	0.96	0.06	44,58,95,100	62
24	CLA	B	611	65/65	0.96	0.06	33,45,69,78	0
33	LHG	d	407[A]	49/49	0.96	0.07	45,55,71,77	49
33	LHG	d	407[B]	49/49	0.96	0.07	45,55,71,77	49
24	CLA	c	502	65/65	0.96	0.07	54,68,79,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	UNL	x	101	18/-	0.96	0.09	67,76,128,139	0
24	CLA	c	504	65/65	0.96	0.06	52,70,83,97	0
24	CLA	A	405[B]	65/65	0.96	0.06	35,41,60,69	65
26	BCR	b	617	40/40	0.96	0.05	43,52,62,66	0
26	BCR	b	618	40/40	0.96	0.06	39,55,74,86	0
24	CLA	c	506	65/65	0.96	0.07	47,63,96,105	0
24	CLA	D	403	65/65	0.96	0.08	47,58,124,137	0
26	BCR	c	516	40/40	0.96	0.07	51,67,76,84	0
24	CLA	B	602	65/65	0.96	0.07	46,56,74,89	0
24	CLA	c	509	65/65	0.96	0.07	47,62,119,153	0
24	CLA	c	512	65/65	0.96	0.07	54,68,85,103	0
24	CLA	C	502	65/65	0.96	0.07	50,61,71,78	0
24	CLA	B	603	65/65	0.96	0.07	43,52,71,82	0
24	CLA	B	612	65/65	0.97	0.06	36,48,60,69	0
24	CLA	b	610	65/65	0.97	0.06	49,58,70,80	0
24	CLA	b	611	65/65	0.97	0.06	37,49,72,85	0
24	CLA	C	510	65/65	0.97	0.07	46,58,82,102	0
24	CLA	b	613	65/65	0.97	0.05	40,49,86,108	0
24	CLA	C	511	65/65	0.97	0.06	47,57,78,86	0
24	CLA	b	615	65/65	0.97	0.06	47,60,80,86	0
24	CLA	C	512	65/65	0.97	0.07	49,63,78,90	0
24	CLA	B	613	65/65	0.97	0.06	34,44,97,112	0
24	CLA	c	503	65/65	0.97	0.06	43,58,82,100	0
24	CLA	B	605	65/65	0.97	0.06	37,48,65,83	0
24	CLA	D	402[A]	65/65	0.97	0.06	33,42,65,73	65
24	CLA	D	402[B]	65/65	0.97	0.06	33,42,65,73	65
24	CLA	B	615	65/65	0.97	0.06	42,53,79,91	0
24	CLA	a	405[A]	65/65	0.97	0.06	37,45,64,74	65
24	CLA	a	405[B]	65/65	0.97	0.06	37,45,64,74	65
24	CLA	c	510	65/65	0.97	0.07	42,59,88,95	0
24	CLA	c	511	65/65	0.97	0.06	49,62,79,84	0
24	CLA	a	406[A]	65/65	0.97	0.05	37,43,60,71	65
24	CLA	a	406[B]	65/65	0.97	0.05	37,43,60,71	65
24	CLA	A	406[A]	65/65	0.97	0.05	34,42,55,70	65
24	CLA	d	403[A]	65/65	0.97	0.06	38,46,76,89	65
24	CLA	d	403[B]	65/65	0.97	0.06	38,46,75,89	65
24	CLA	B	607	65/65	0.97	0.05	35,46,71,90	0
25	PHO	A	408[A]	64/64	0.97	0.05	35,44,51,56	64
25	PHO	A	408[B]	64/64	0.97	0.05	35,44,52,56	64
33	LHG	L	101[A]	49/49	0.97	0.06	46,54,69,86	49
33	LHG	L	101[B]	49/49	0.97	0.06	46,54,70,86	49
25	PHO	A	417[A]	64/64	0.97	0.05	35,48,53,61	64

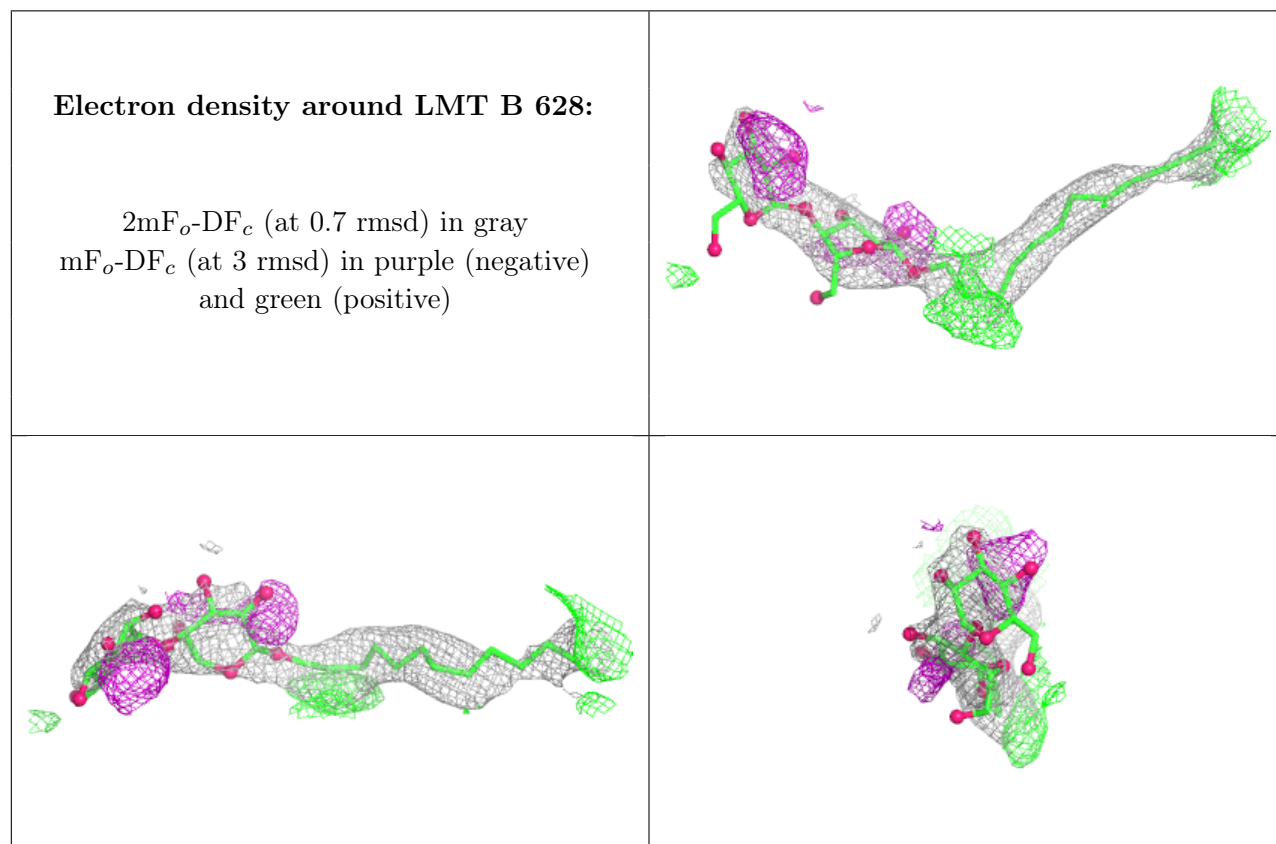
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	PHO	A	417[B]	64/64	0.97	0.05	35,48,53,61	64
25	PHO	a	408[A]	64/64	0.97	0.05	40,48,53,54	64
25	PHO	a	408[B]	64/64	0.97	0.05	40,48,52,54	64
24	CLA	C	504	65/65	0.97	0.06	47,61,72,87	0
24	CLA	A	406[B]	65/65	0.97	0.05	34,42,56,70	65
24	CLA	C	506	65/65	0.97	0.06	48,60,88,104	0
24	CLA	b	603	65/65	0.97	0.06	43,56,78,95	0
24	CLA	b	604	65/65	0.97	0.06	40,53,97,117	0
24	CLA	b	605	65/65	0.97	0.07	38,49,73,82	0
38	BCT	D	401[A]	4/4	0.97	0.06	52,56,60,66	4
38	BCT	D	401[B]	4/4	0.97	0.06	52,56,60,66	4
24	CLA	B	610	65/65	0.97	0.07	39,53,63,81	0
24	CLA	B	604	65/65	0.97	0.06	36,47,119,138	0
24	CLA	b	608	65/65	0.98	0.05	42,54,78,90	0
24	CLA	B	608	65/65	0.98	0.05	37,50,65,78	0
37	CA	C	524	1/1	0.98	0.05	78,78,78,78	0
24	CLA	C	503	65/65	0.98	0.06	43,55,78,90	0
39	HEM	F	102	43/43	0.98	0.06	55,68,81,89	0
39	HEM	e	101	43/43	0.98	0.08	62,82,110,130	0
41	HEC	v	201	43/43	0.98	0.07	51,62,70,75	0
23	CL	A	404[B]	1/1	0.99	0.04	47,47,47,47	1
23	CL	a	403[A]	1/1	0.99	0.05	49,49,49,49	1
29	OEX	A	414[A]	10/10	0.99	0.03	39,45,49,49	10
23	CL	a	403[B]	1/1	0.99	0.05	49,49,49,49	1
23	CL	a	404[A]	1/1	0.99	0.05	52,52,52,52	1
23	CL	a	404[B]	1/1	0.99	0.05	52,52,52,52	1
21	OEY	A	401[B]	11/11	0.99	0.03	38,44,49,51	11
23	CL	A	404[A]	1/1	0.99	0.04	47,47,47,47	1
40	MG	J	102	1/1	0.99	0.07	54,54,54,54	0
40	MG	j	102	1/1	0.99	0.04	63,63,63,63	0
41	HEC	V	201	43/43	0.99	0.05	42,50,56,60	0
37	CA	c	524	1/1	0.99	0.05	76,76,76,76	0
23	CL	A	403[B]	1/1	1.00	0.08	41,41,41,41	1
21	OEY	a	401[B]	11/11	1.00	0.02	46,48,51,53	11
22	FE2	A	402[A]	1/1	1.00	0.01	51,51,51,51	1
22	FE2	A	402[B]	1/1	1.00	0.01	51,51,51,51	1
22	FE2	a	402[A]	1/1	1.00	0.01	52,52,52,52	1
29	OEX	a	414[A]	10/10	1.00	0.02	46,47,50,53	10
22	FE2	a	402[B]	1/1	1.00	0.01	53,53,53,53	1
23	CL	A	403[A]	1/1	1.00	0.08	41,41,41,41	1

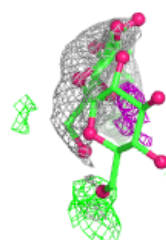
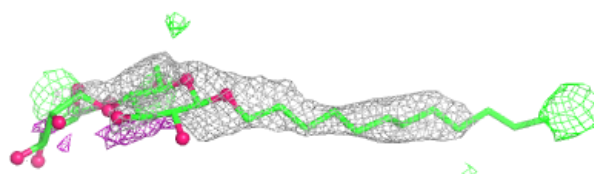
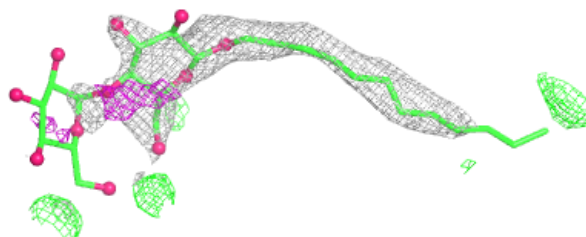
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

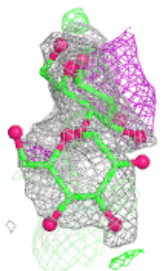
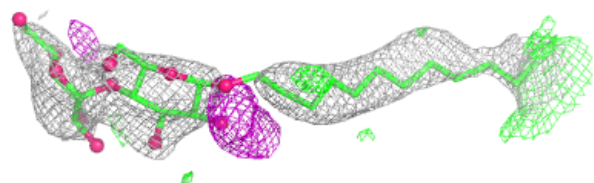
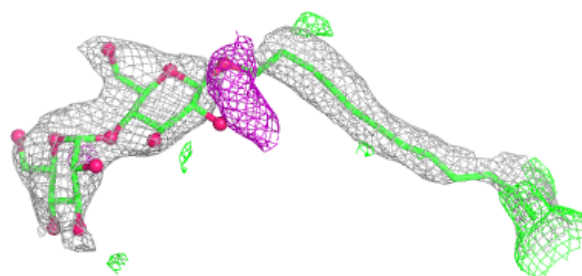


Electron density around LMT F 101:

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

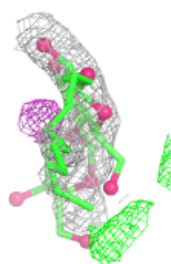
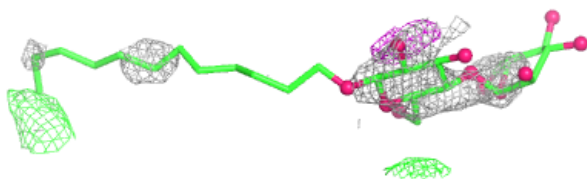
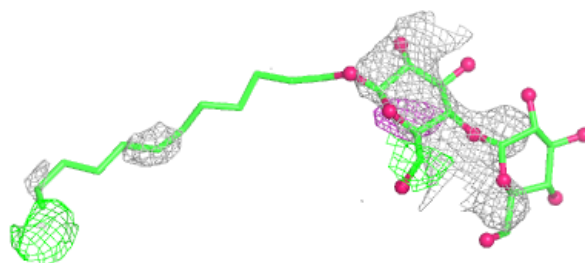
**Electron density around LMT A 418:**

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

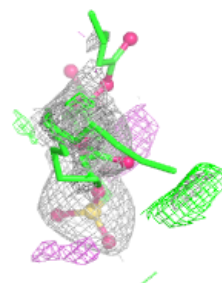
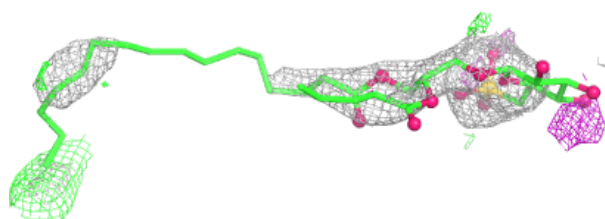
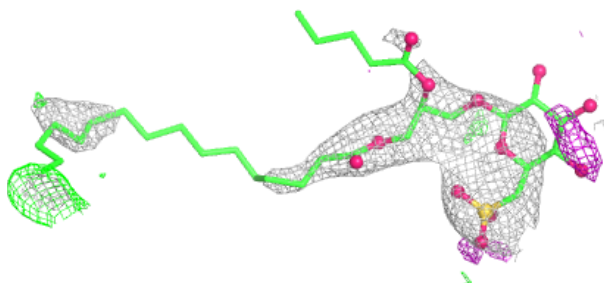


Electron density around LMT e 102:

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

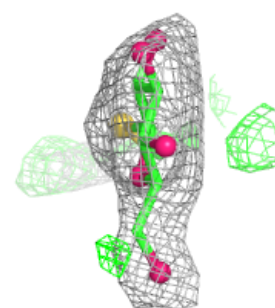
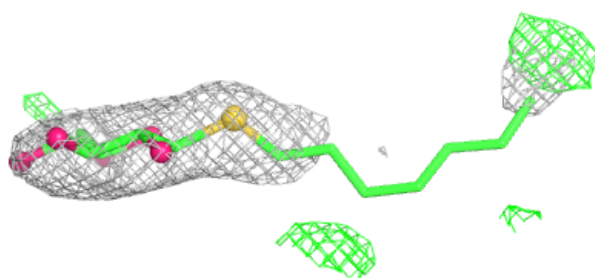
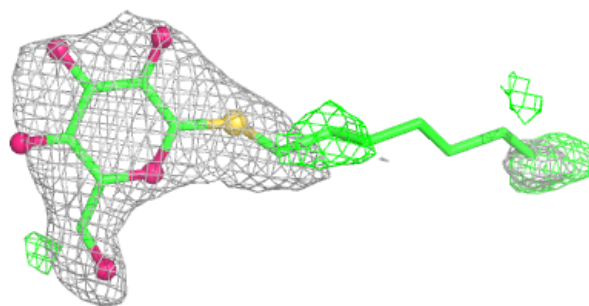
**Electron density around SQD f 101:**

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

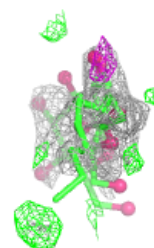
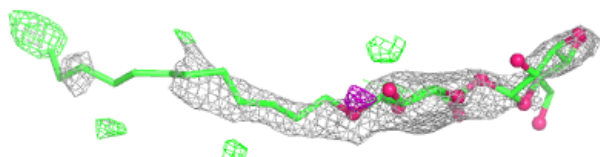
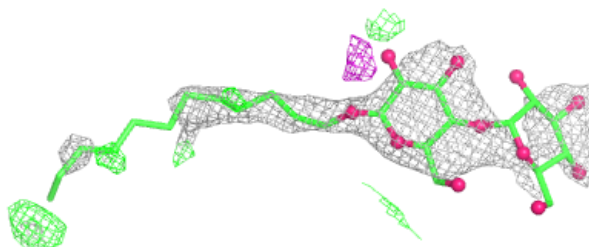


Electron density around HTG C 522:

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

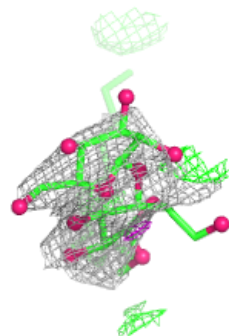
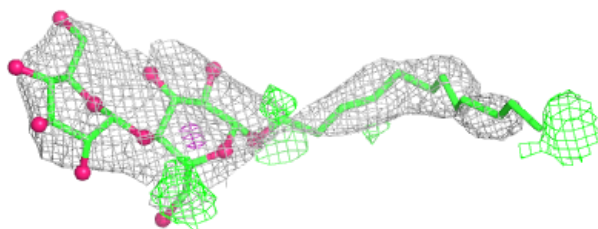
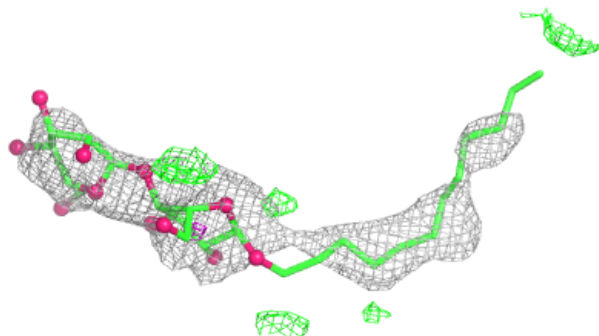
**Electron density around LMT c 501:**

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

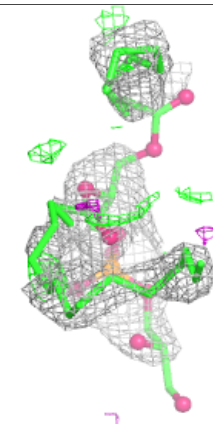
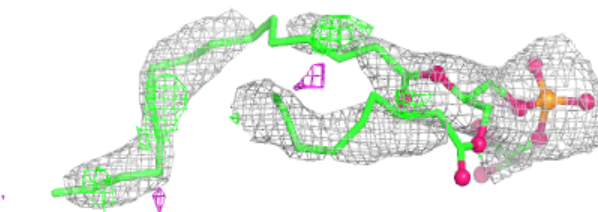
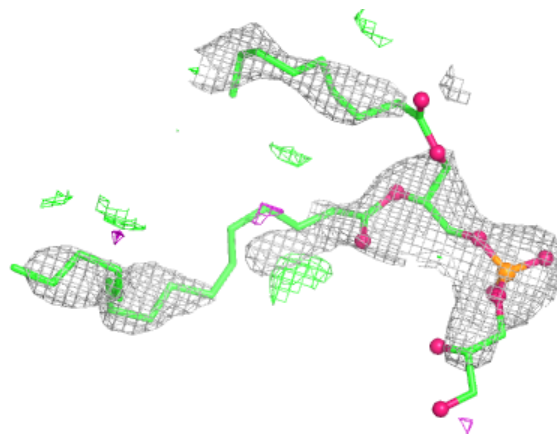


Electron density around LMT A 421:

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

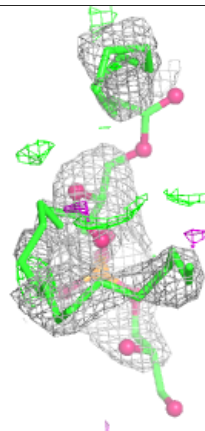
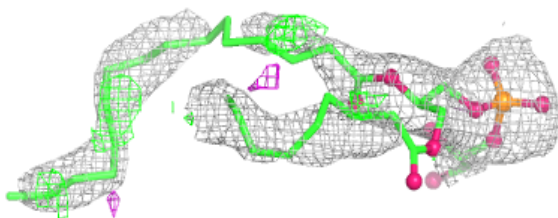
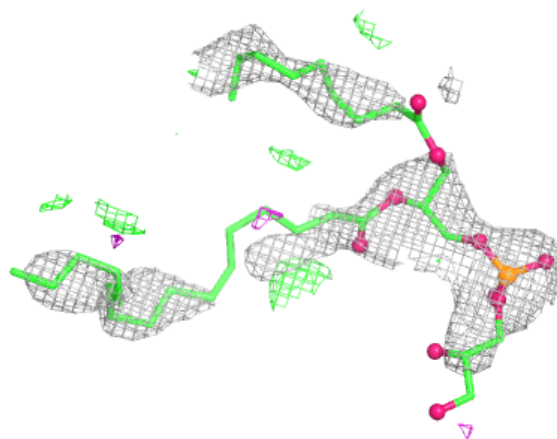
**Electron density around LHG a 420 (B):**

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



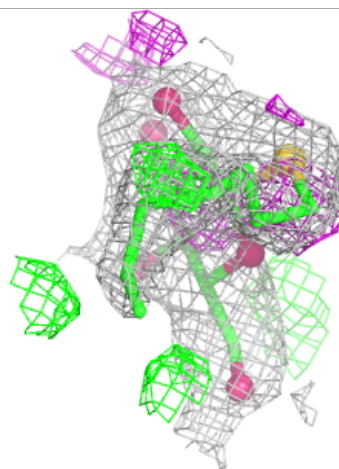
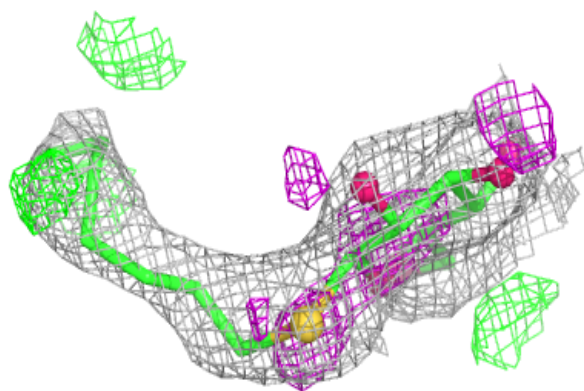
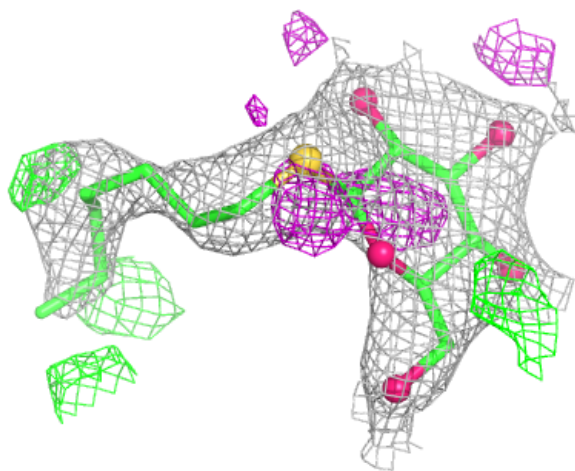
Electron density around LHG a 420 (A):

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



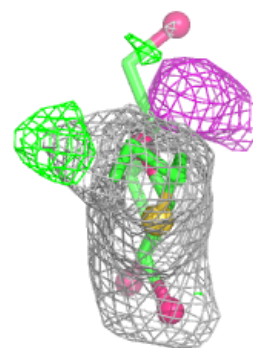
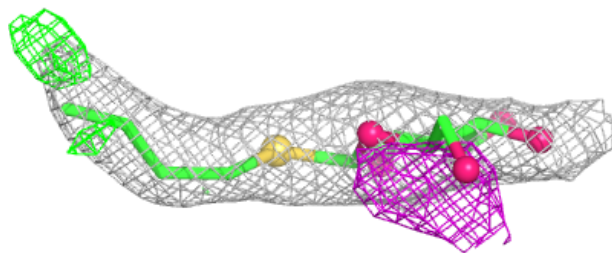
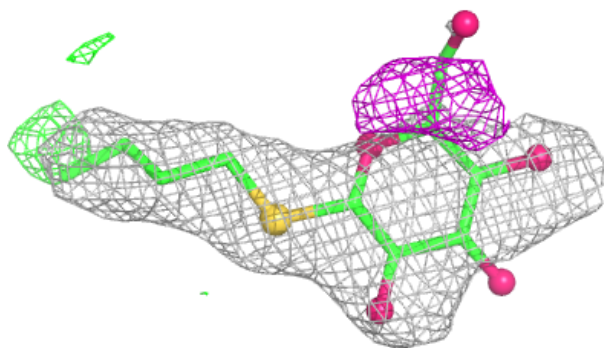
Electron density around HTG B 622:

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

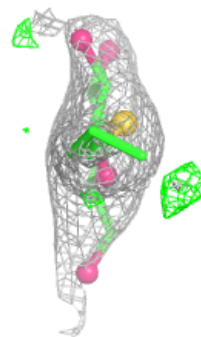
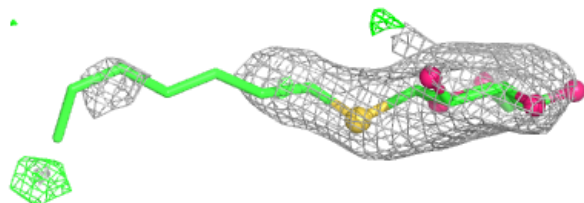
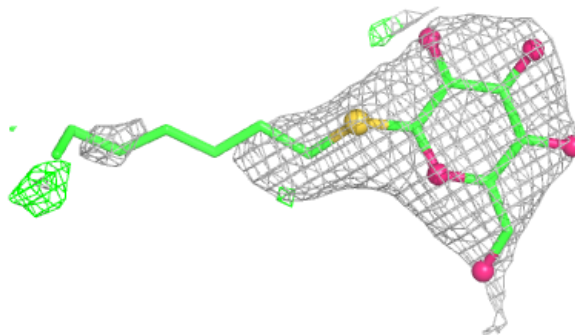


Electron density around HTG D 410:

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

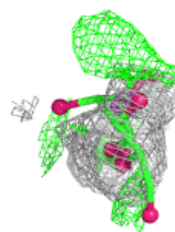
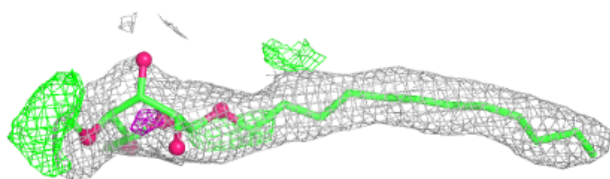
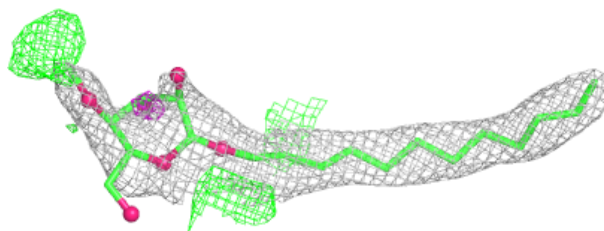
**Electron density around HTG c 522:**

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

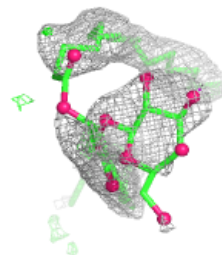
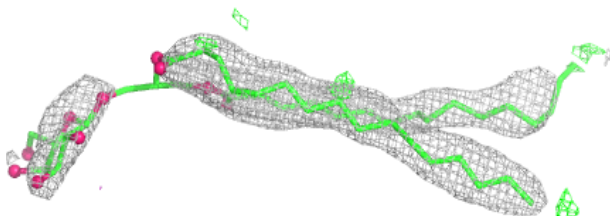
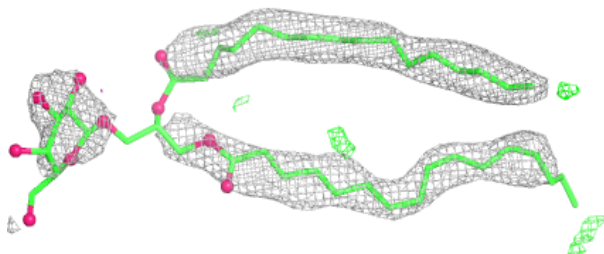


Electron density around LMT b 620:

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

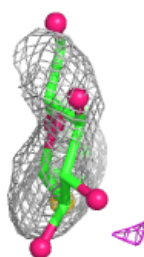
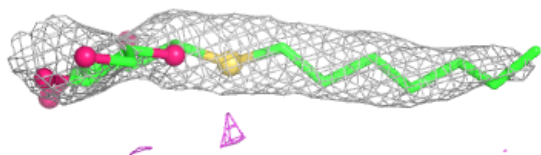
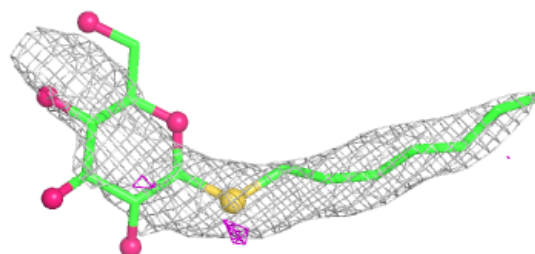
**Electron density around LMG C 521:**

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

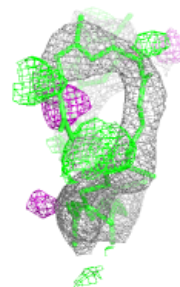
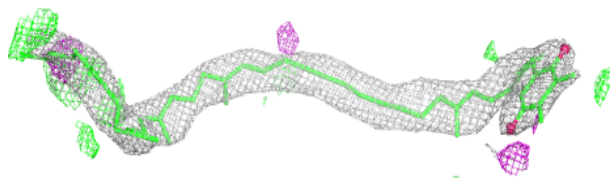
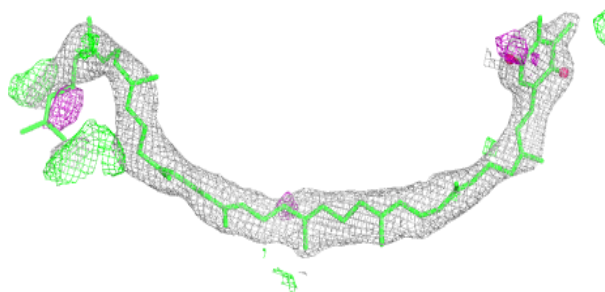


Electron density around HTG b 622:

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

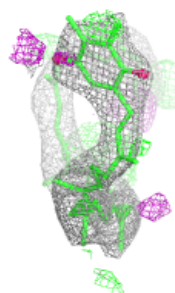
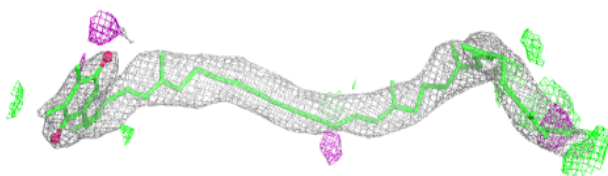
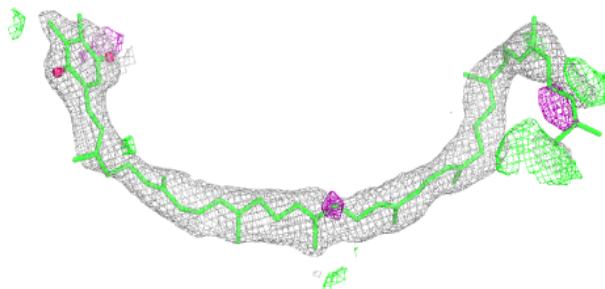
**Electron density around PL9 A 415 (A):**

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

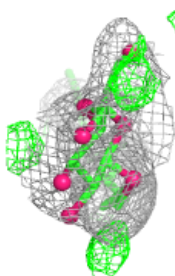
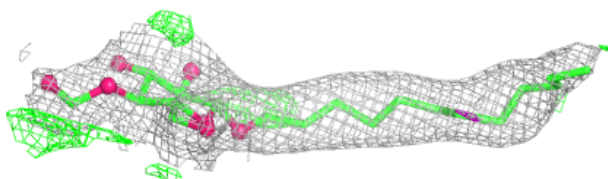
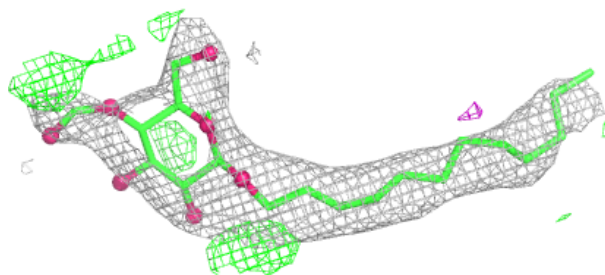


Electron density around PL9 A 415 (B):

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

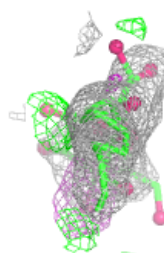
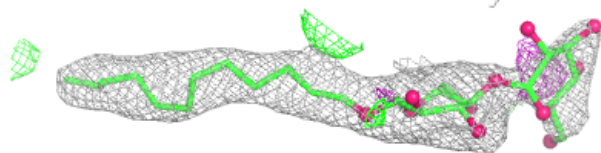
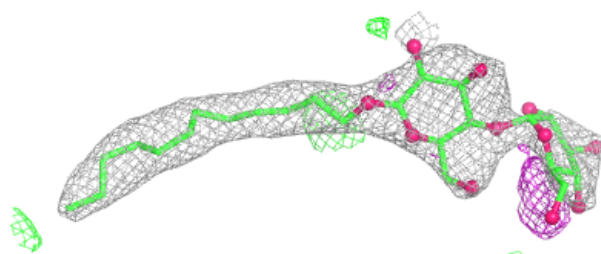
**Electron density around LMT t 101:**

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

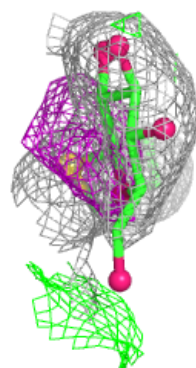
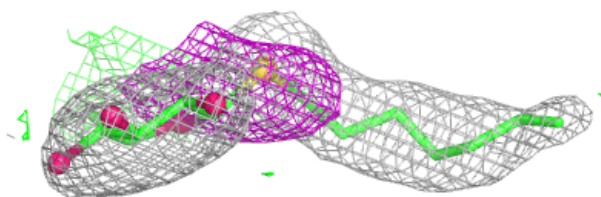
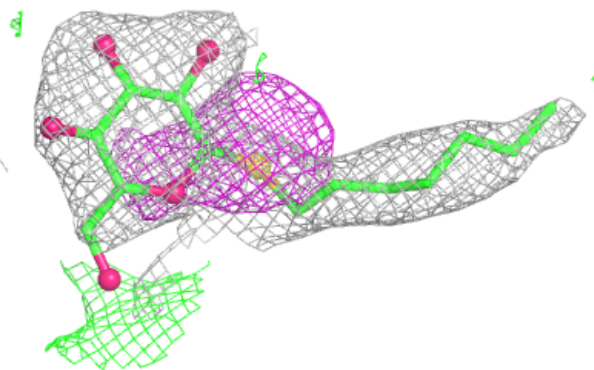


Electron density around LMT B 627:

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

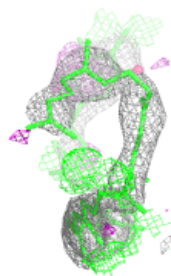
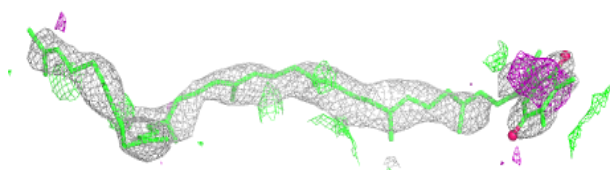
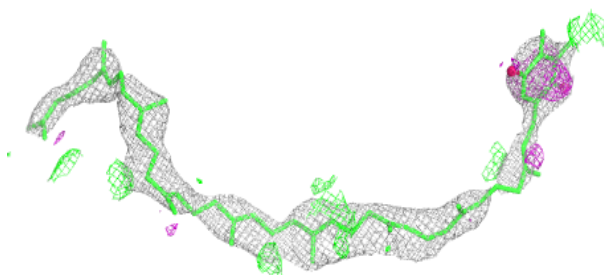
**Electron density around HTG b 621:**

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

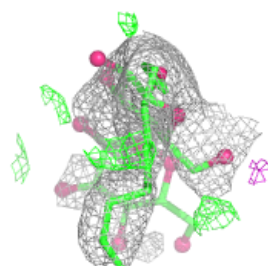
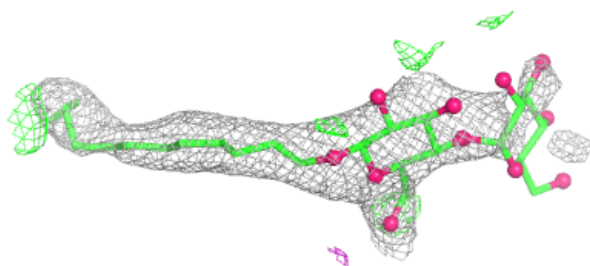
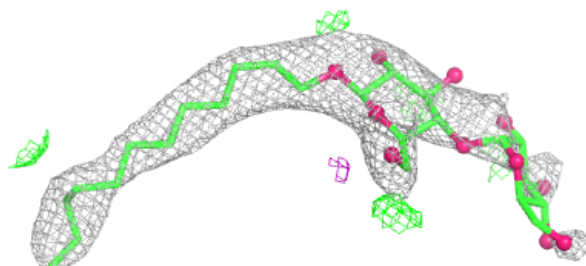


Electron density around PL9 a 415 (B):

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

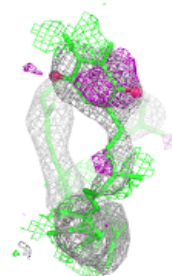
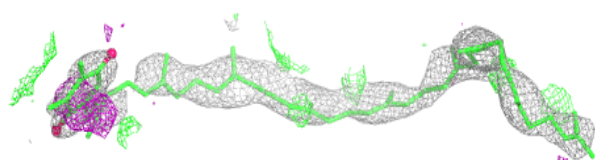
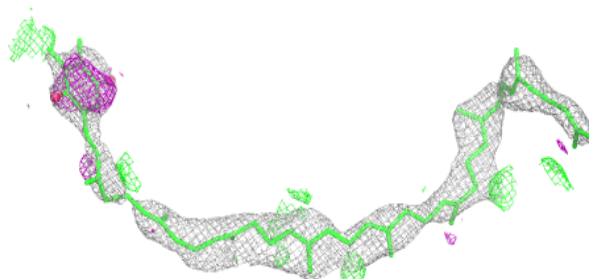
**Electron density around LMT M 104:**

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

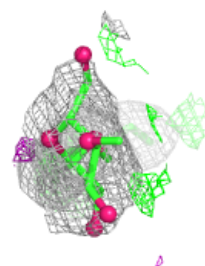
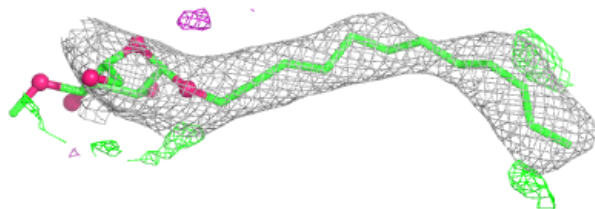
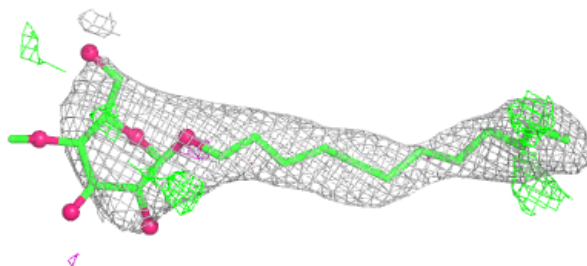


Electron density around PL9 a 415 (A):

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

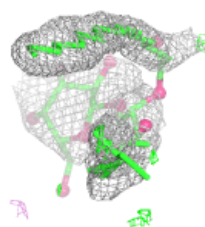
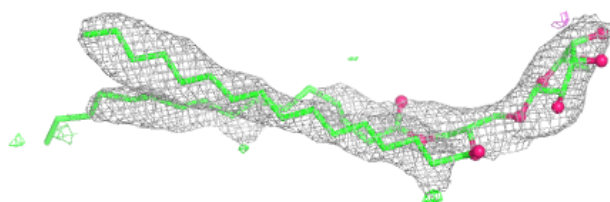
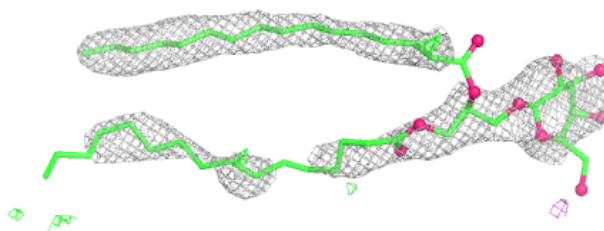
**Electron density around LMT B 630:**

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

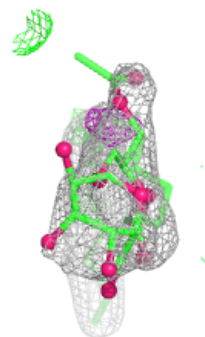
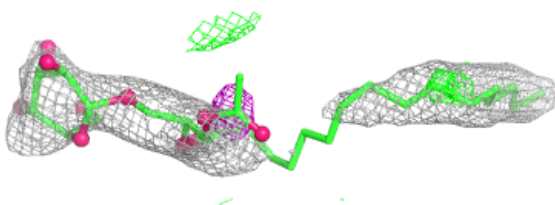
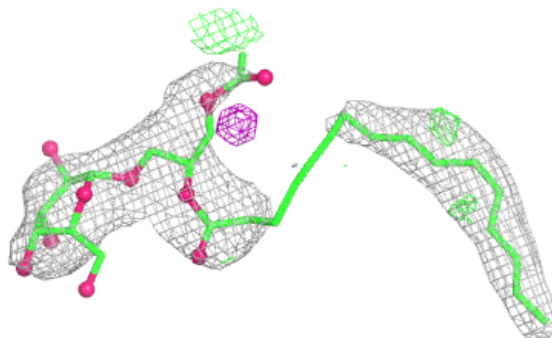


Electron density around LMG c 521:

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

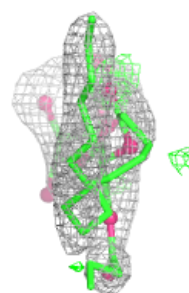
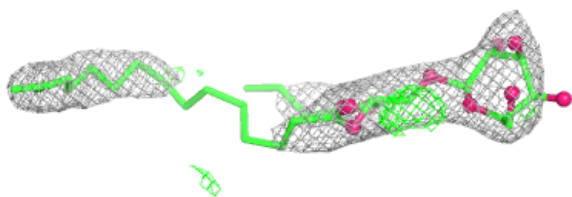
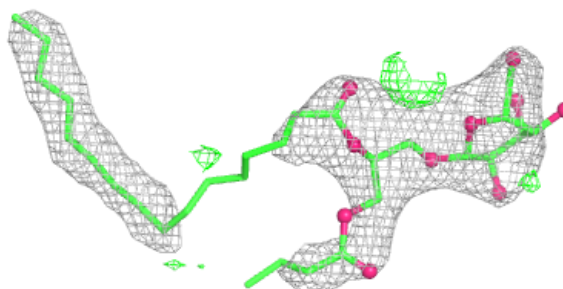
**Electron density around LMG Z 101:**

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

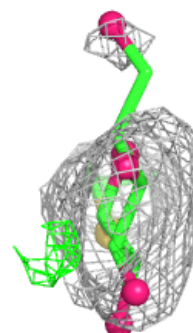
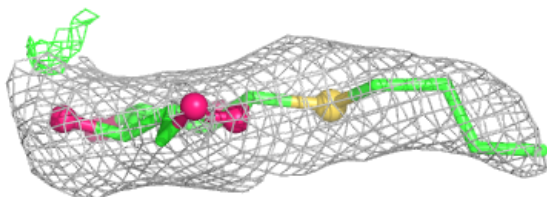
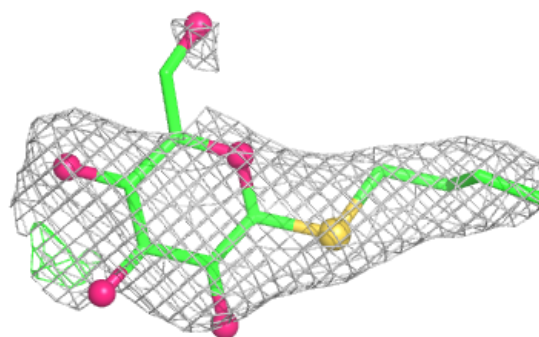


Electron density around LMG z 101:

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

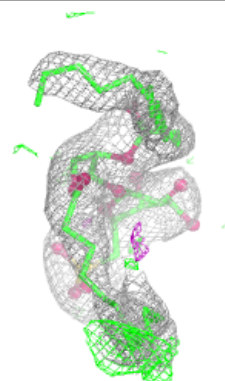
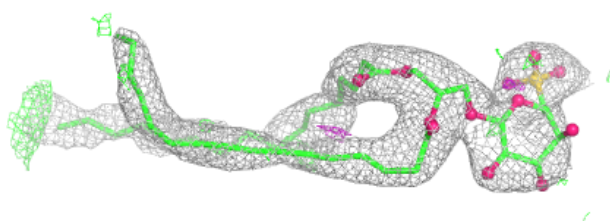
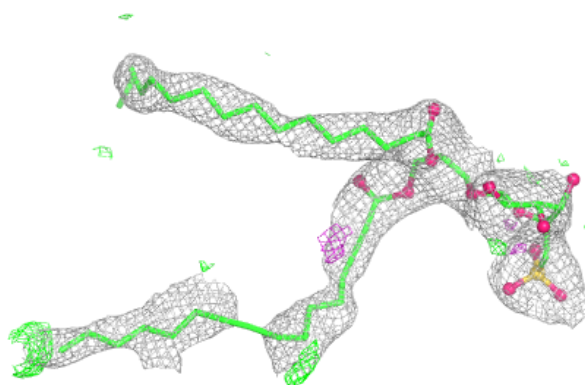
**Electron density around HTG d 411:**

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

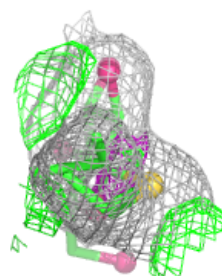
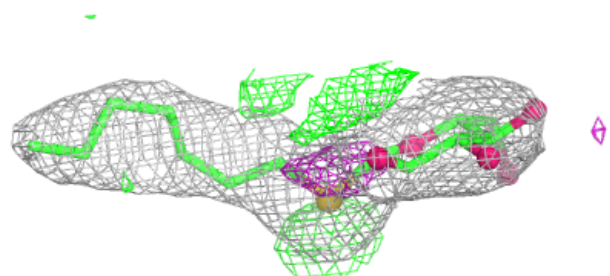
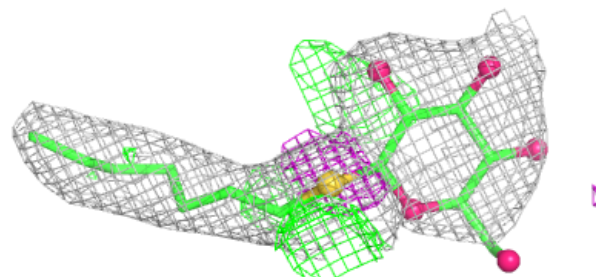


Electron density around SQD a 413:

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

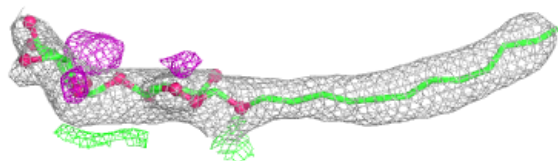
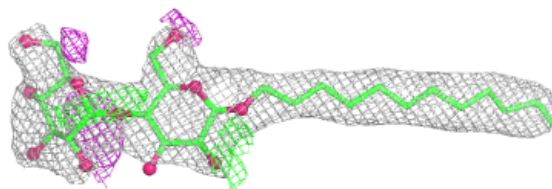
**Electron density around HTG B 621:**

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

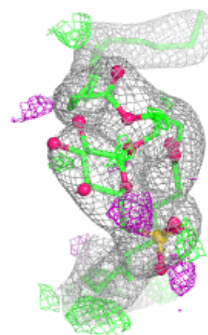
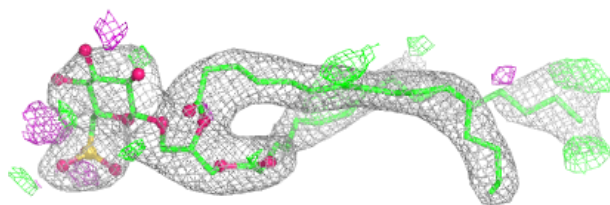
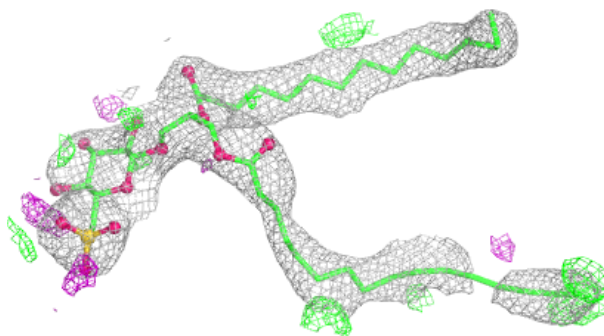


Electron density around LMT m 102:

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

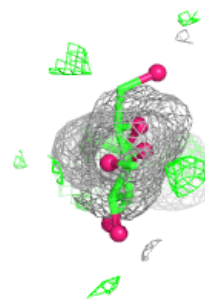
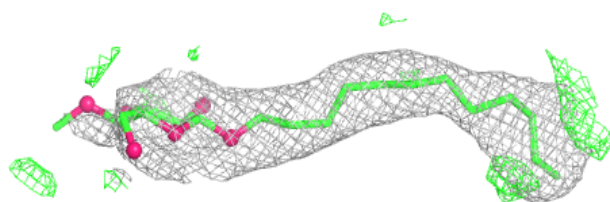
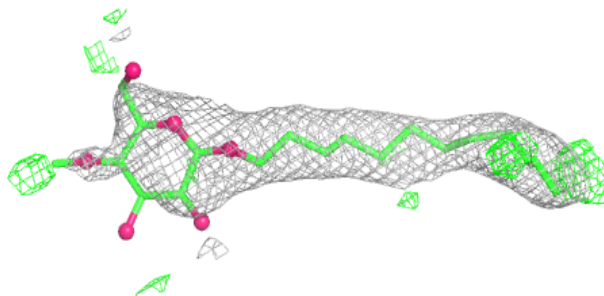
**Electron density around SQD A 413:**

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



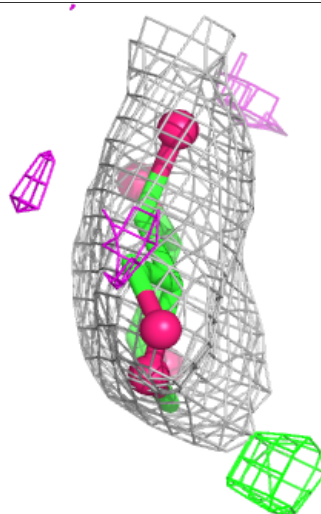
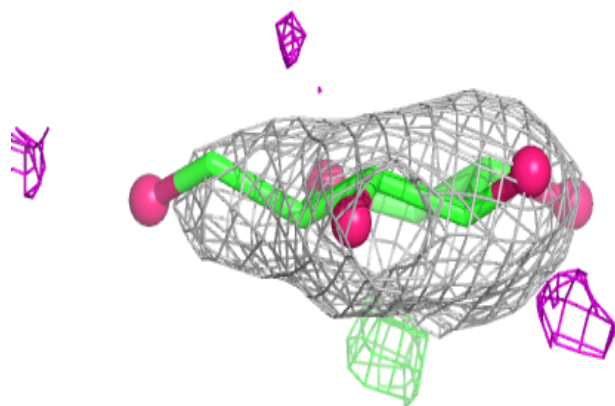
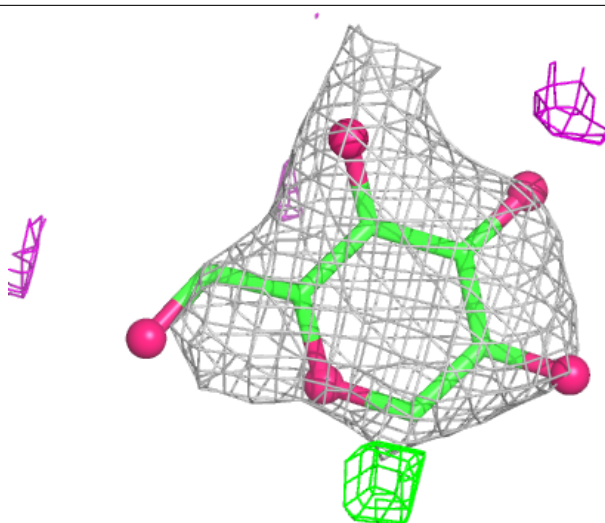
Electron density around LMT b 626:

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



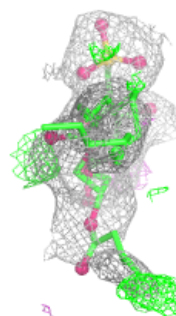
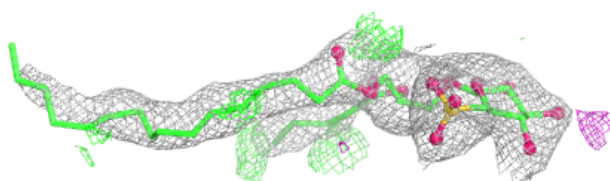
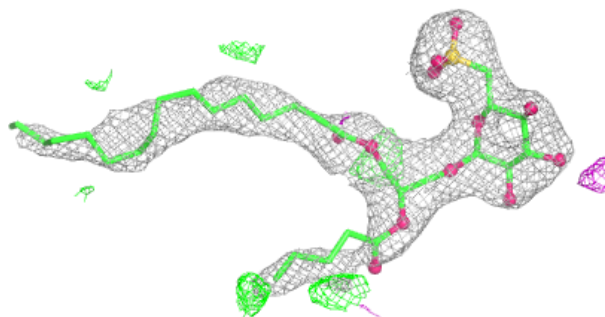
Electron density around HTG V 202:

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

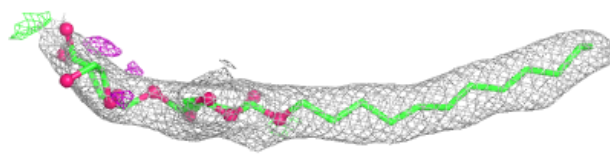
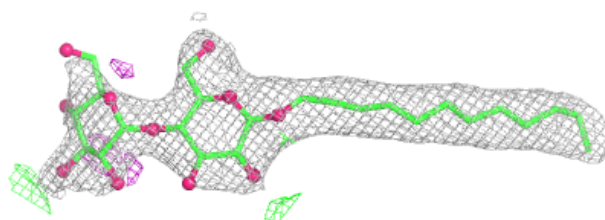


Electron density around SQD X 101:

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

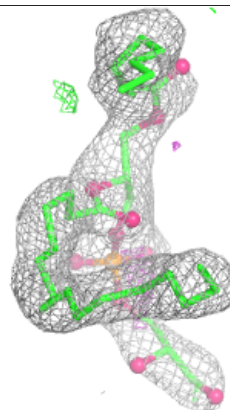
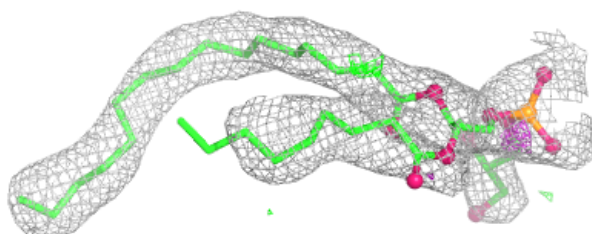
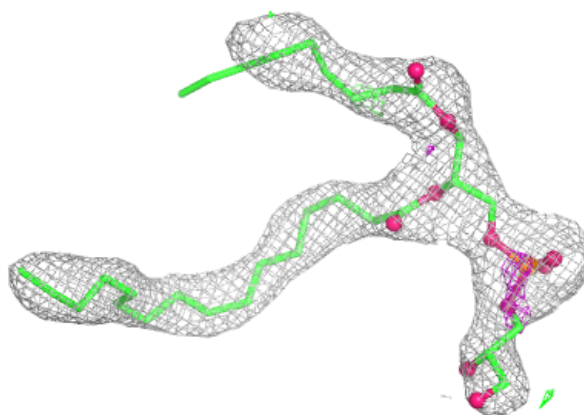
**Electron density around LMT M 102:**

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

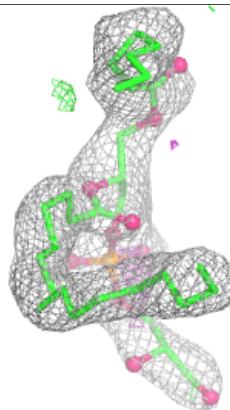
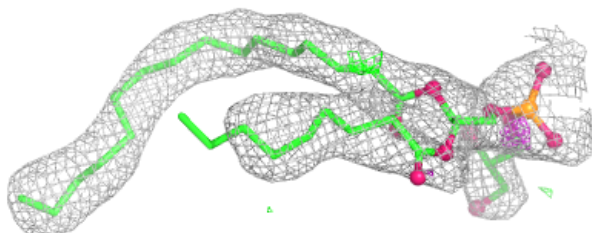
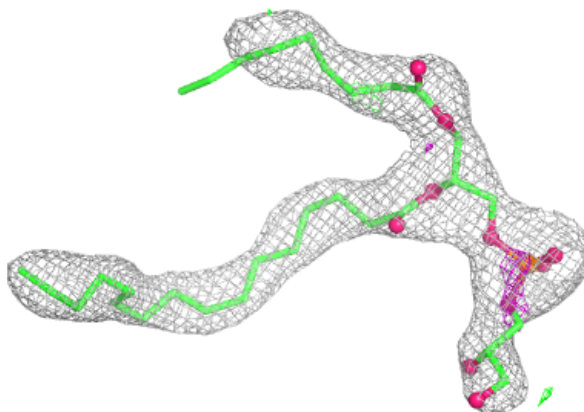


Electron density around LHG E 101 (A):

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

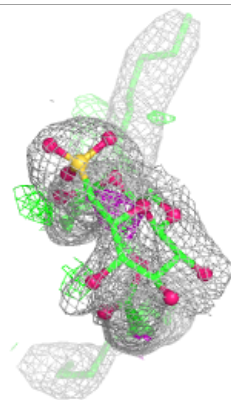
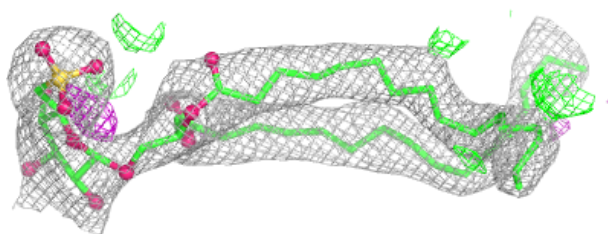
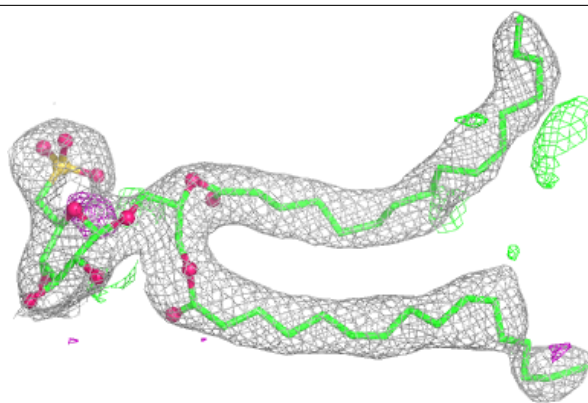
**Electron density around LHG E 101 (B):**

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



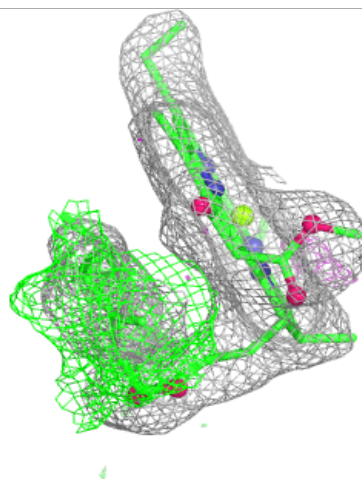
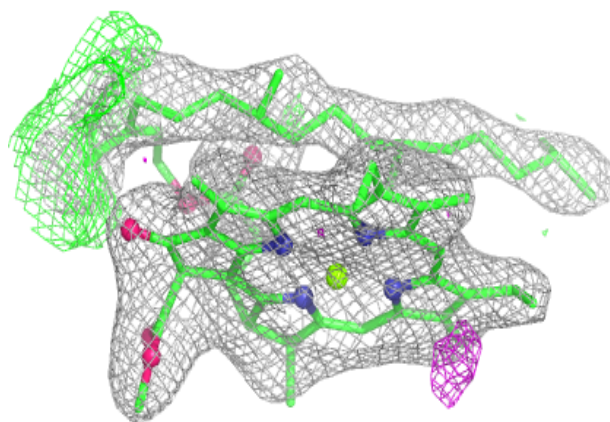
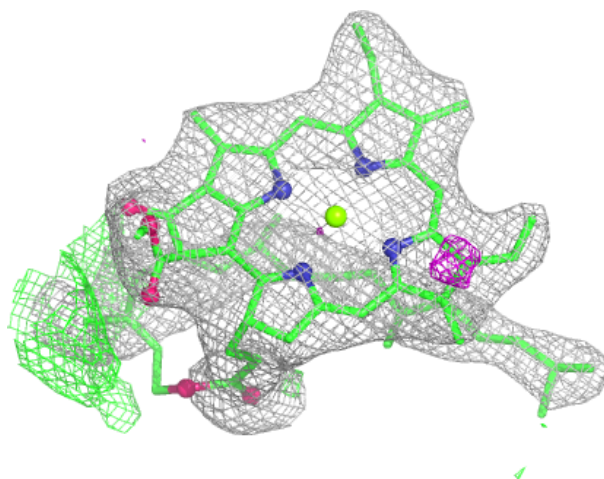
Electron density around SQD L 102:

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



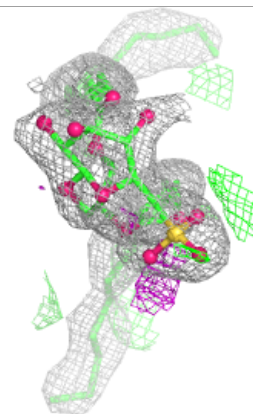
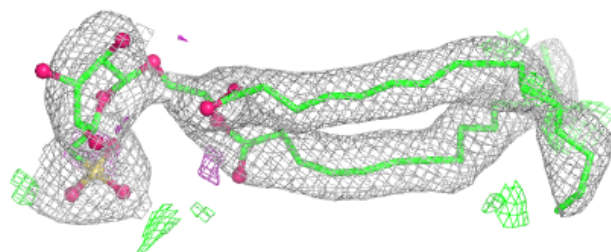
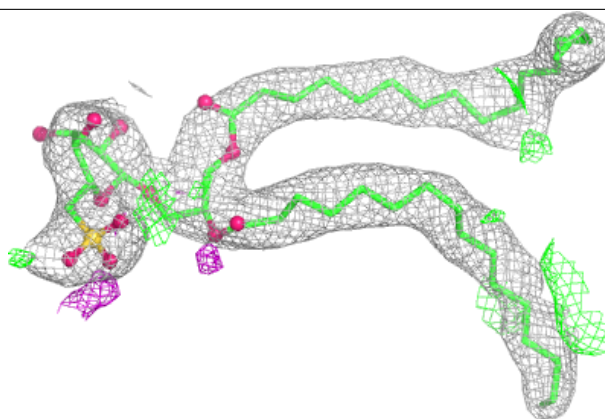
Electron density around CLA b 601:

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

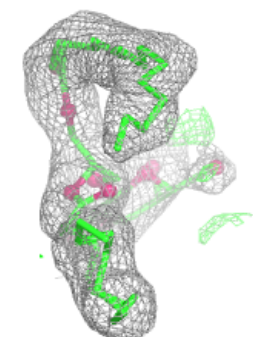
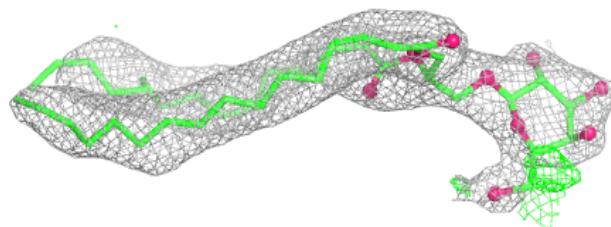
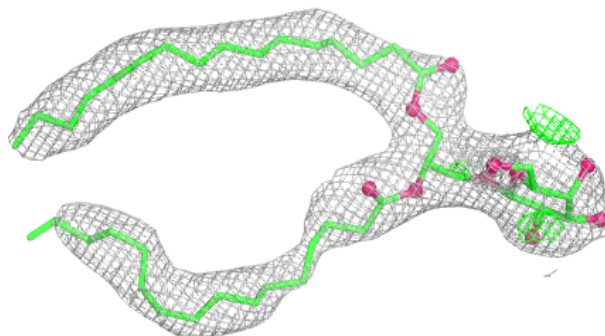


Electron density around SQD B 620:

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

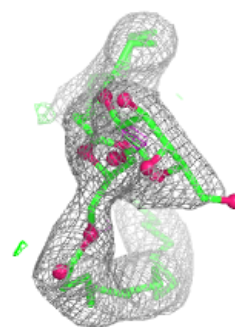
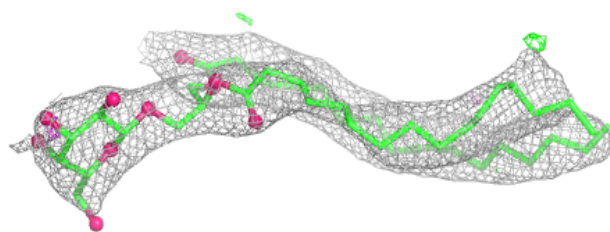
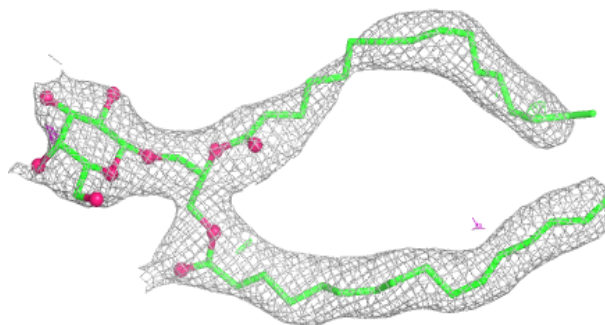
**Electron density around LMG C 501:**

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

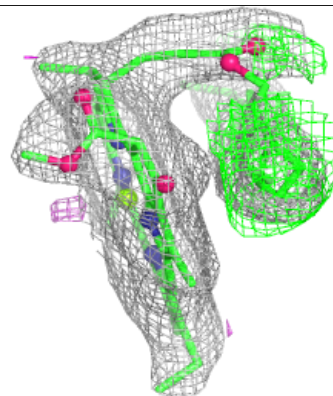
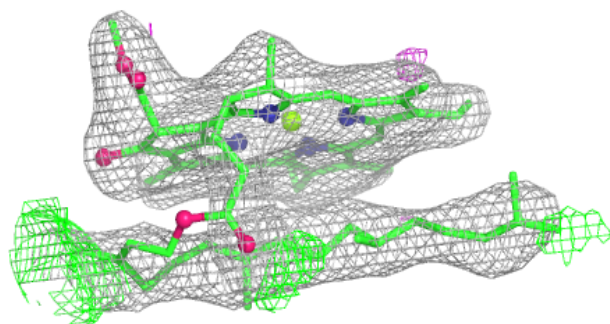
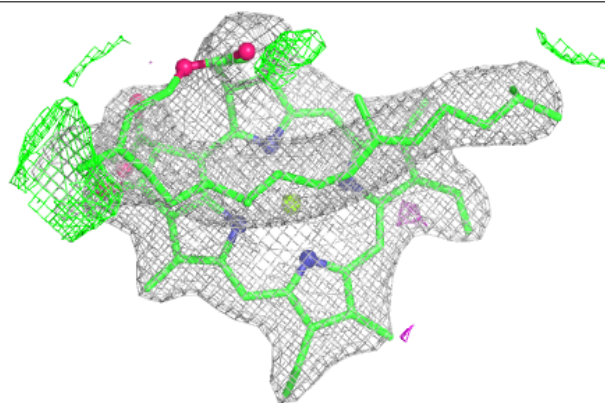


Electron density around LMG a 417:

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

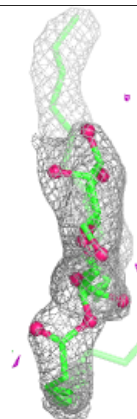
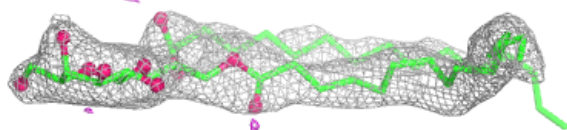
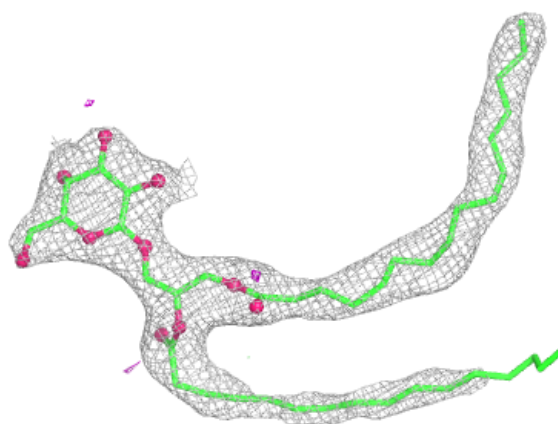
**Electron density around CLA B 601:**

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

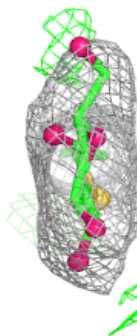
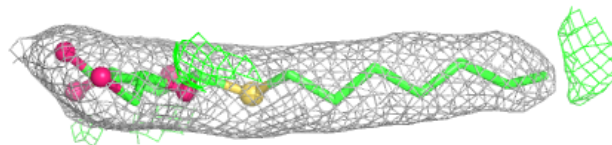
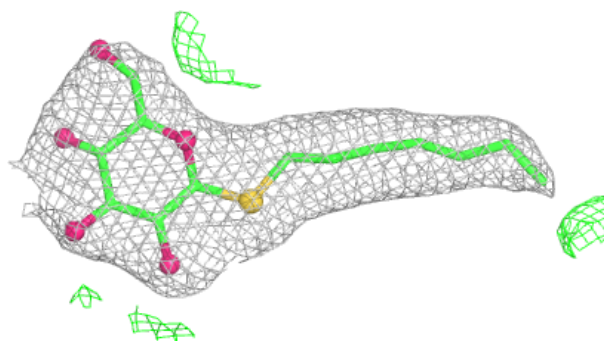


Electron density around LMG c 520:

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

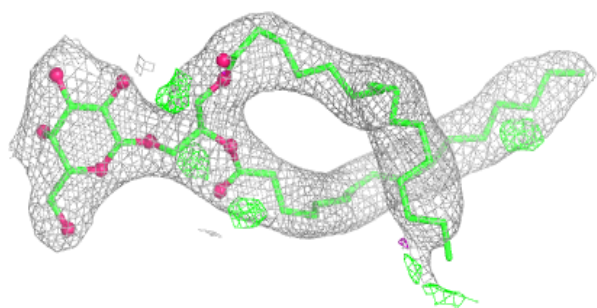
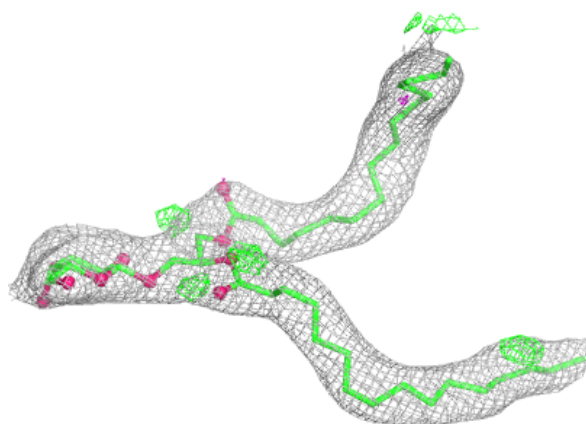
**Electron density around HTG B 624:**

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

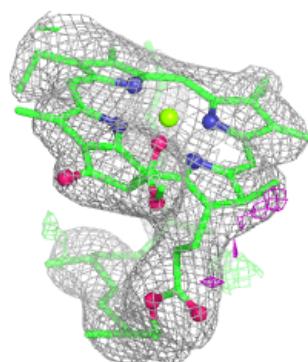
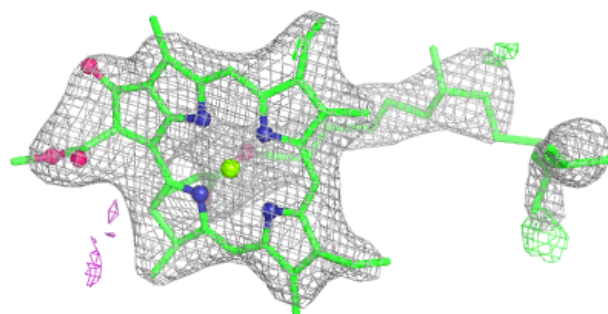
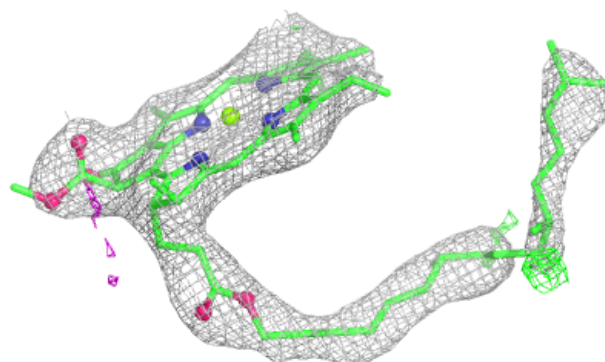


Electron density around LMG M 101:

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

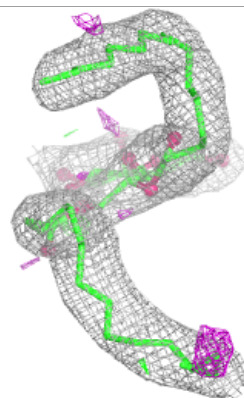
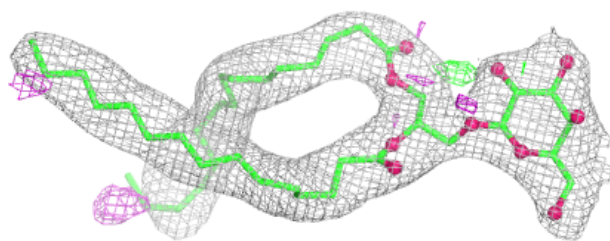
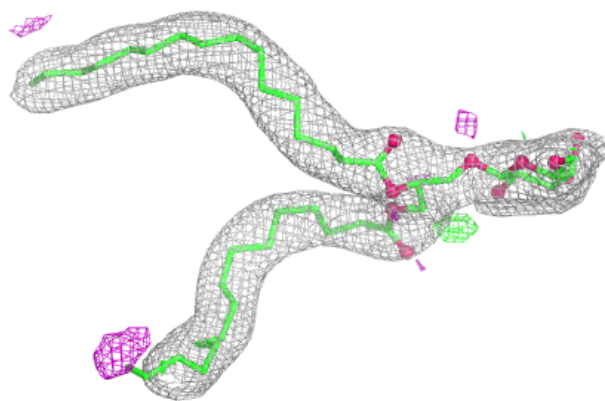
**Electron density around CLA c 514:**

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

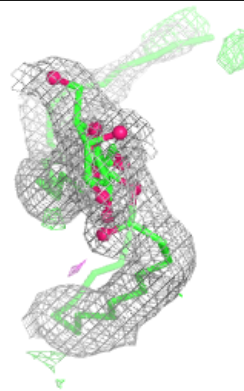
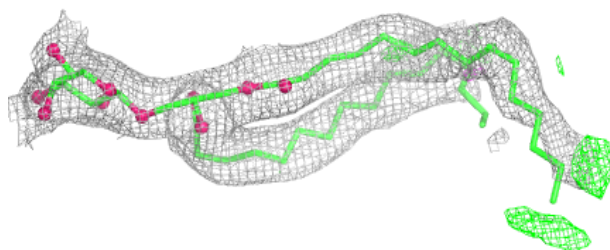
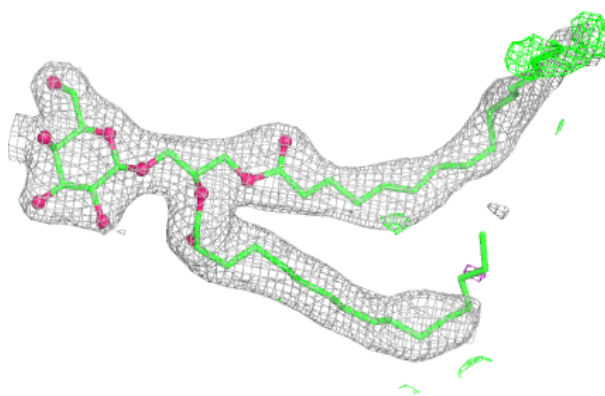


Electron density around LMG b 629:

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

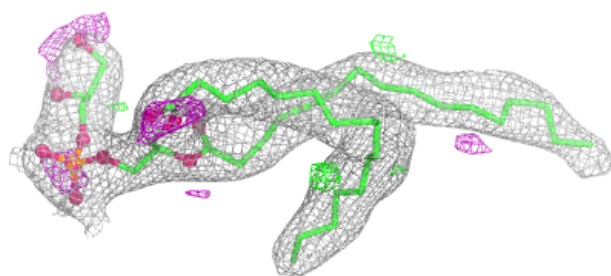
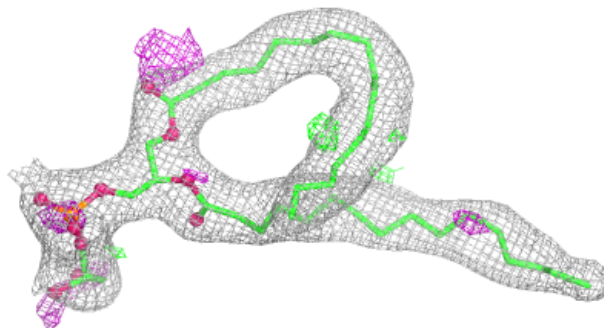
**Electron density around LMG D 411:**

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

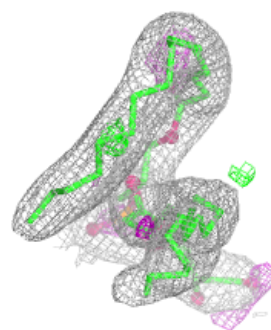
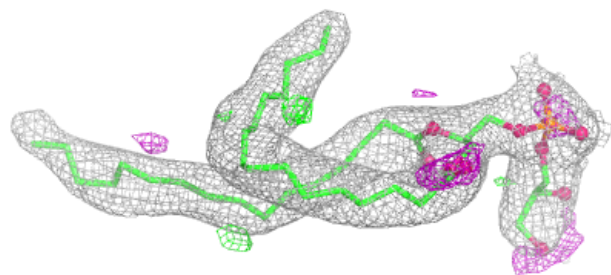
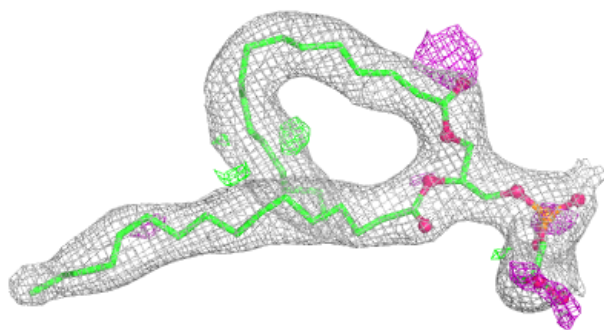


Electron density around LHG A 420 (A):

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

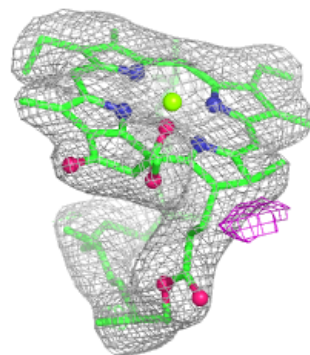
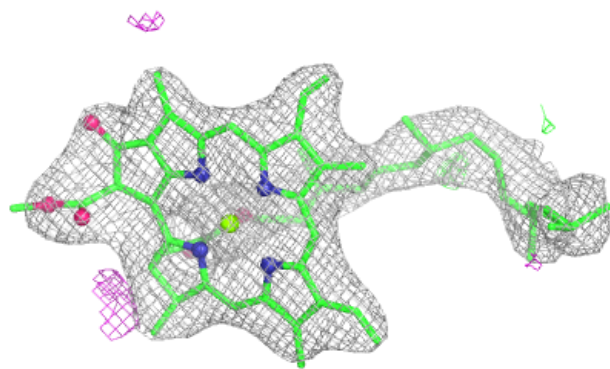
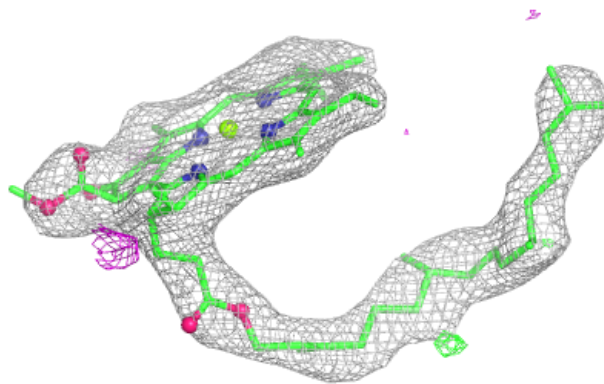
**Electron density around LHG A 420 (B):**

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



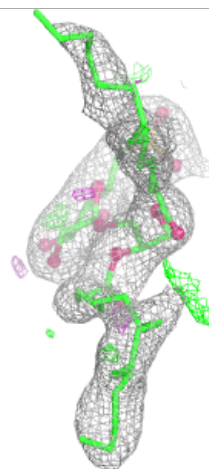
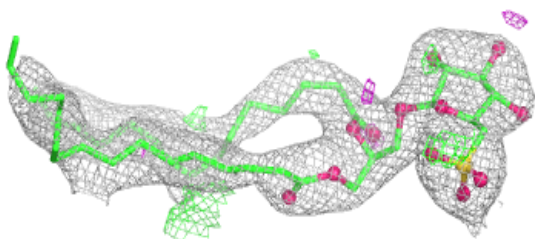
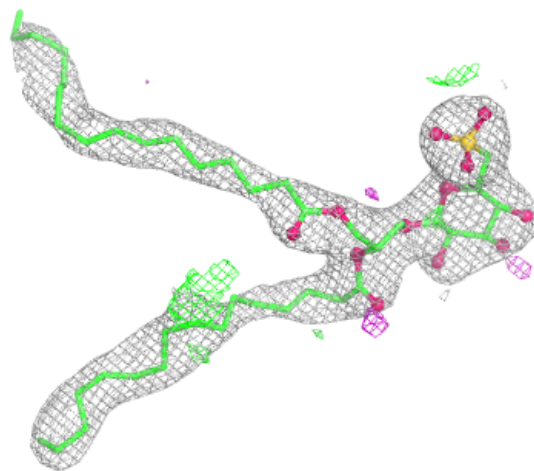
Electron density around CLA C 514:

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



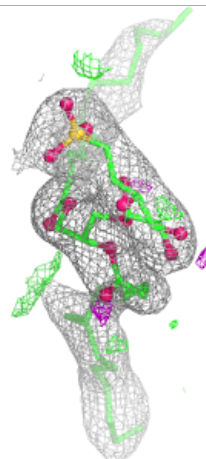
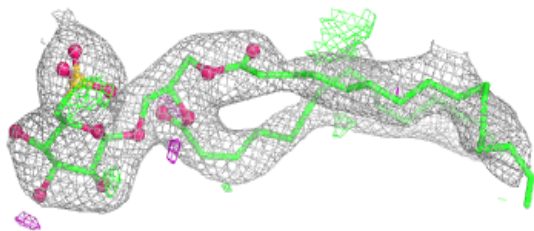
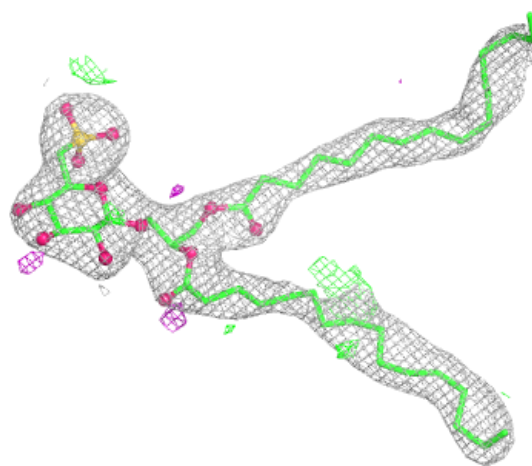
Electron density around SQD a 411 (A):

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



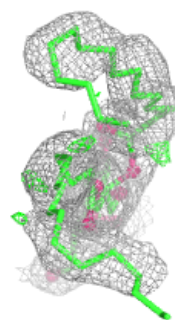
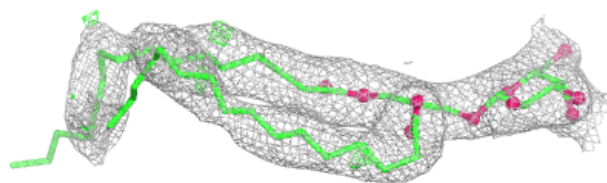
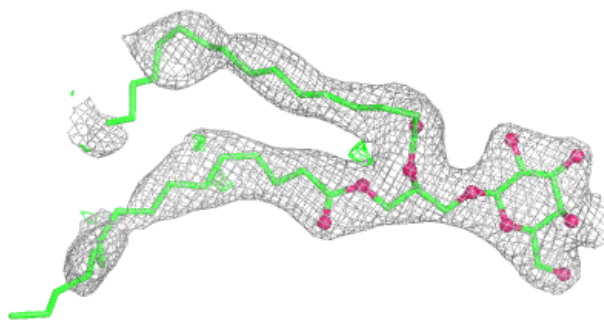
Electron density around SQD a 411 (B):

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

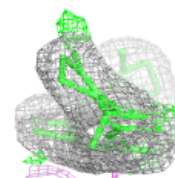
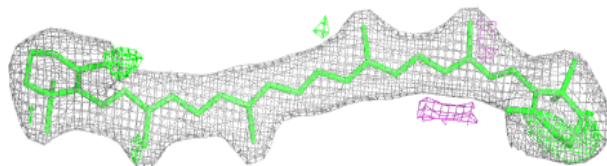
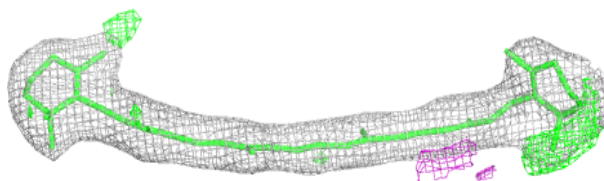


Electron density around LMG d 412:

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

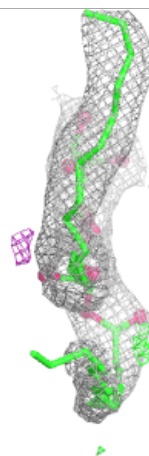
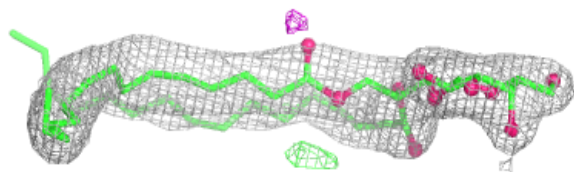
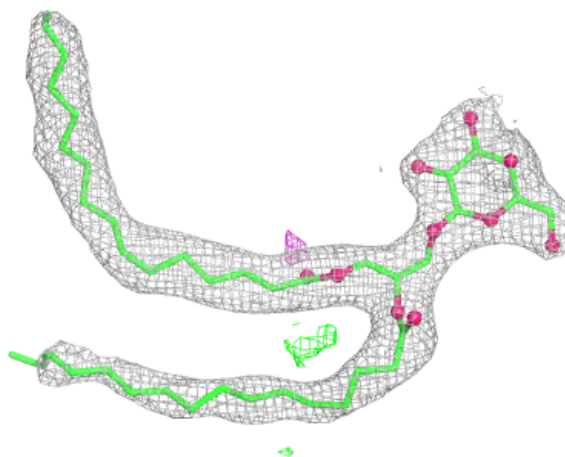
**Electron density around BCR D 404:**

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



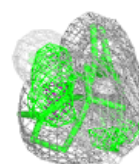
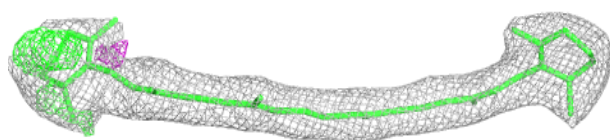
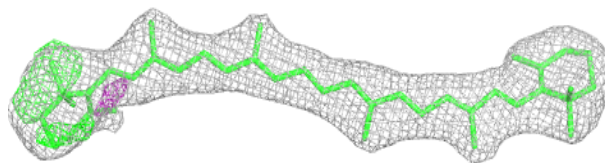
Electron density around LMG C 520:

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

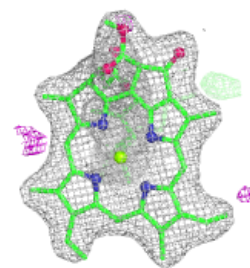
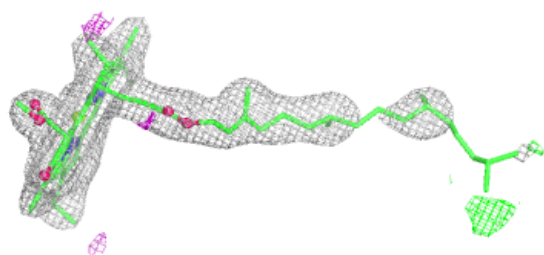
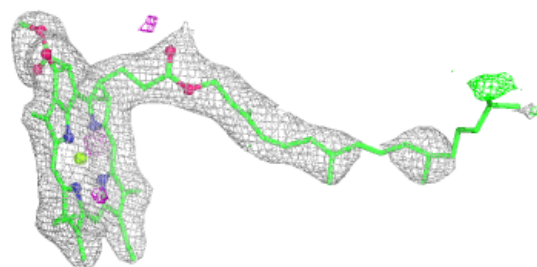


Electron density around BCR d 405:

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

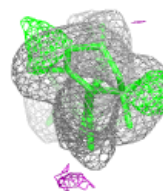
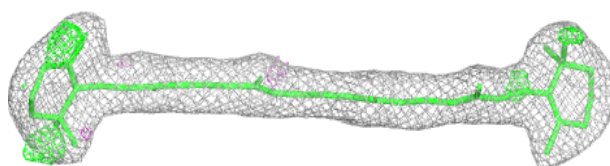
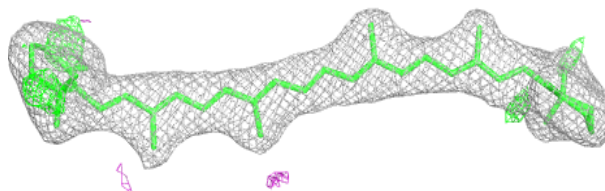
**Electron density around CLA d 404:**

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

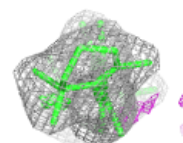
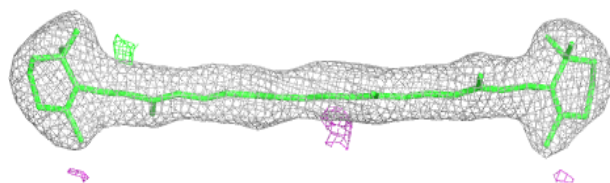
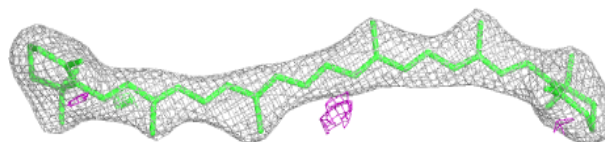


Electron density around BCR A 410:

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

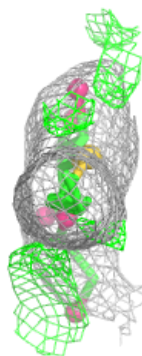
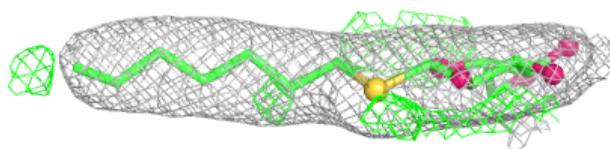
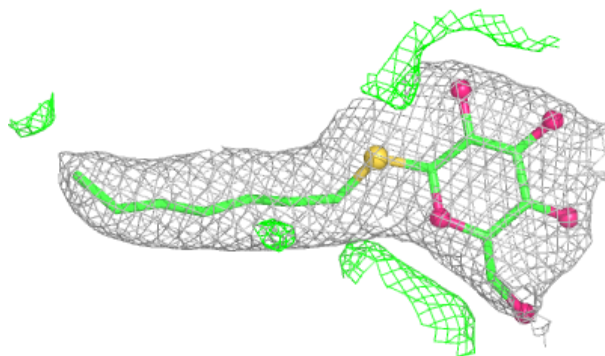
**Electron density around BCR C 515:**

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

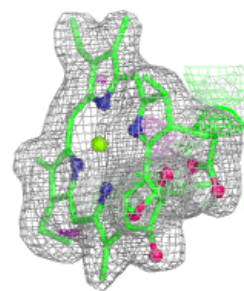
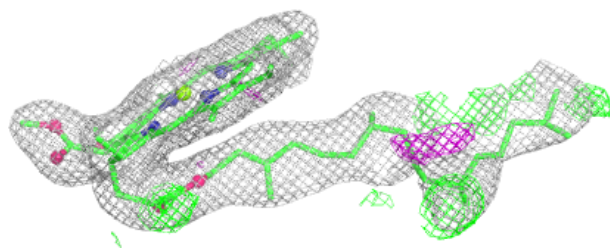
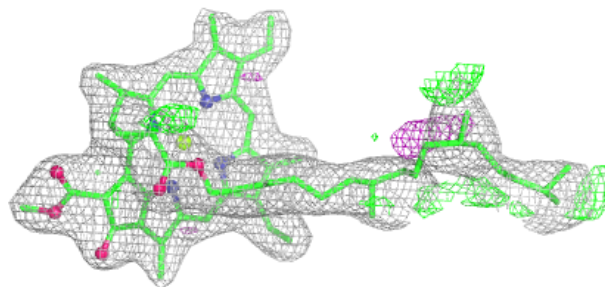


Electron density around HTG b 624:

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

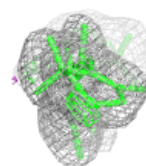
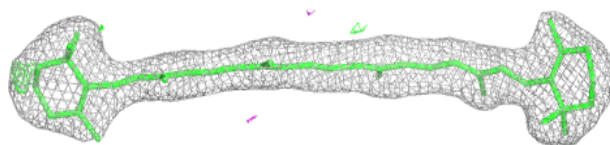
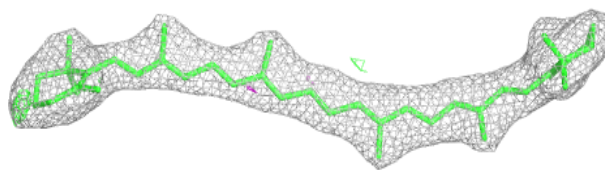
**Electron density around CLA B 614:**

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

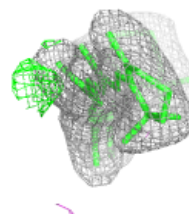
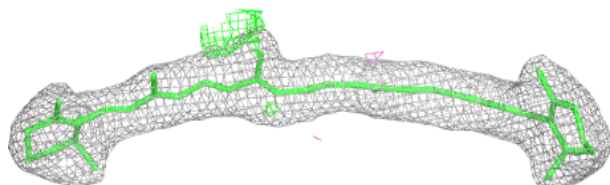
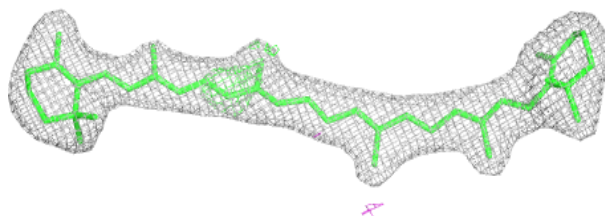


Electron density around BCR H 101:

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

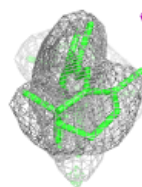
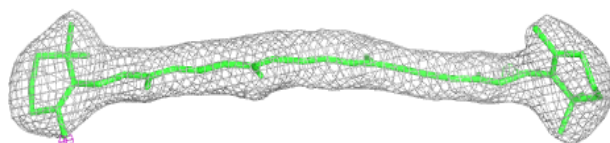
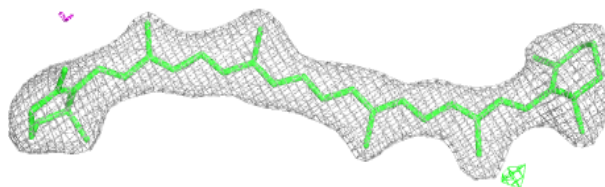
**Electron density around BCR T 101:**

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

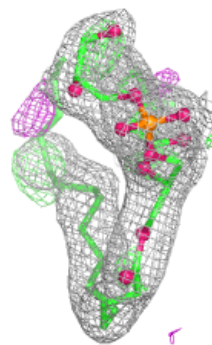
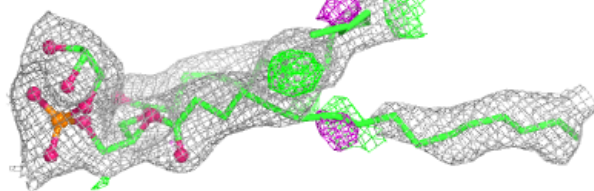
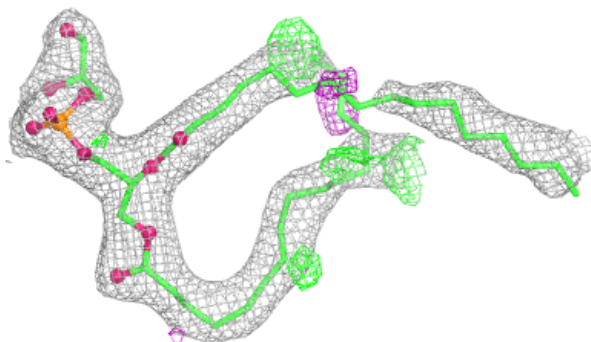


Electron density around BCR Y 101:

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

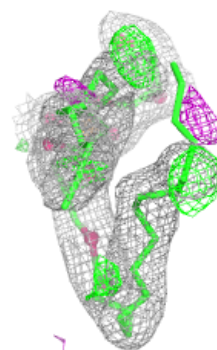
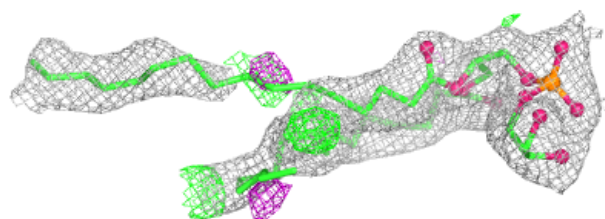
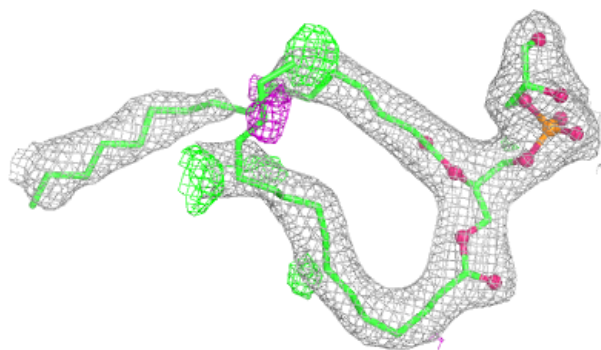
**Electron density around LHG D 407 (A):**

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

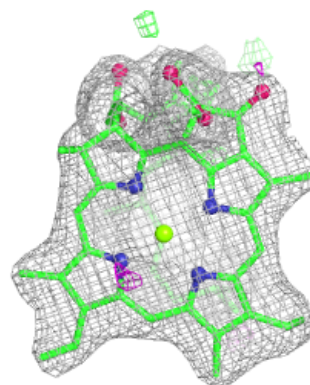
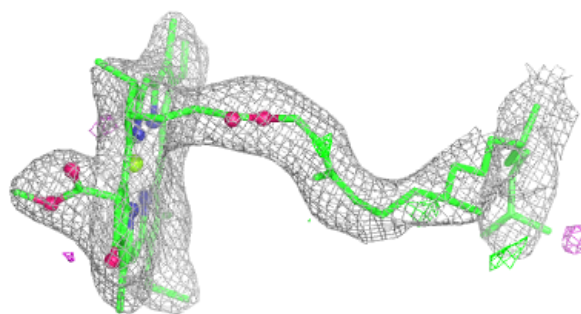
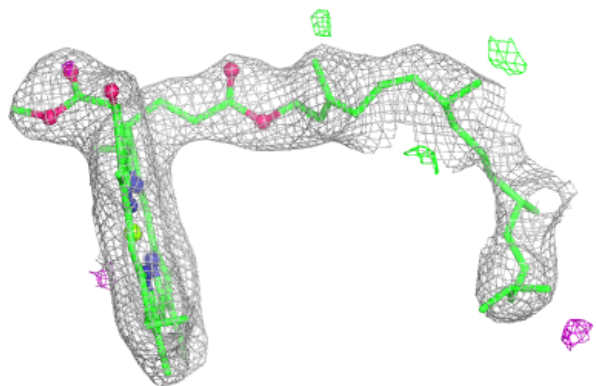


Electron density around LHG D 407 (B):

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

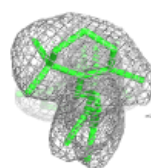
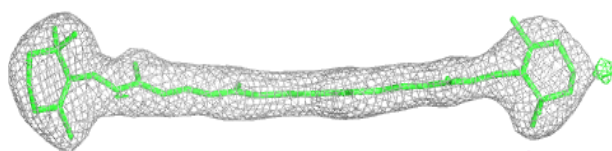
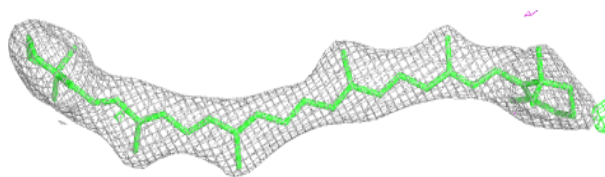
**Electron density around CLA C 507:**

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

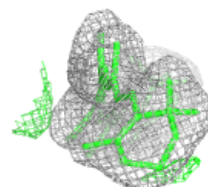
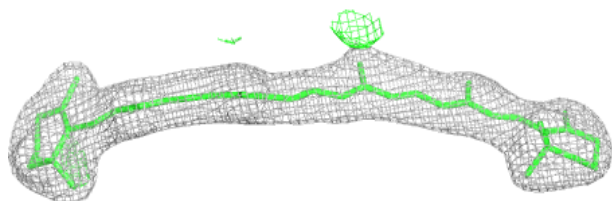
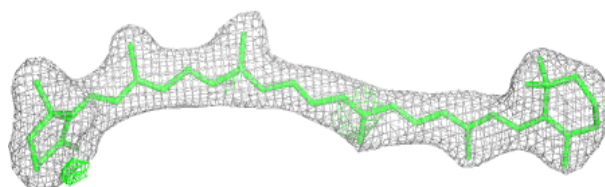


Electron density around BCR h 101:

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

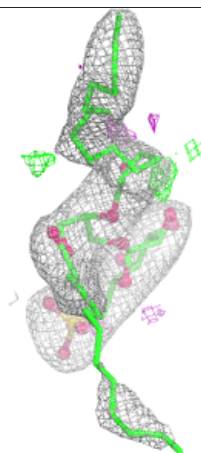
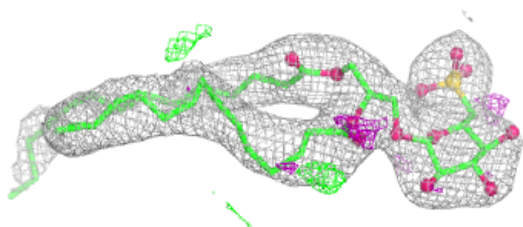
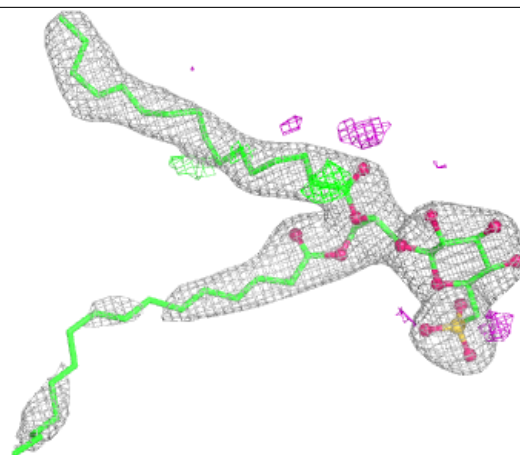
**Electron density around BCR t 102:**

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



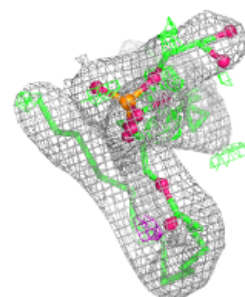
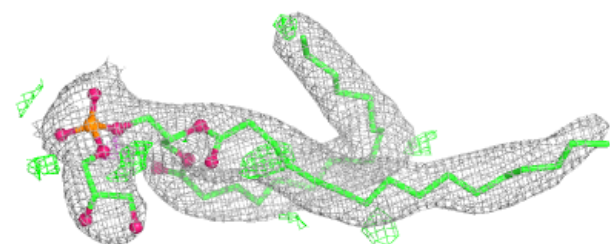
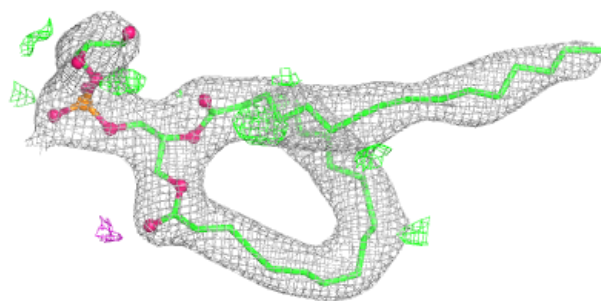
Electron density around SQD A 411 (A):

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

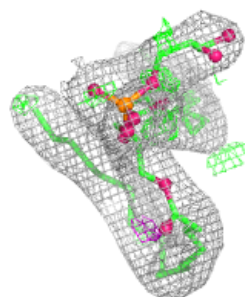
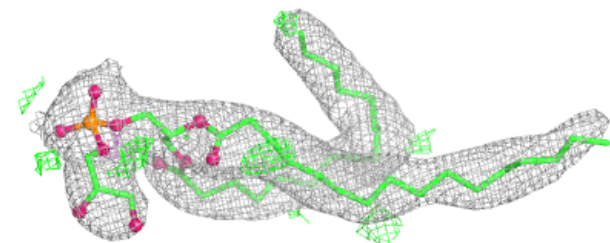
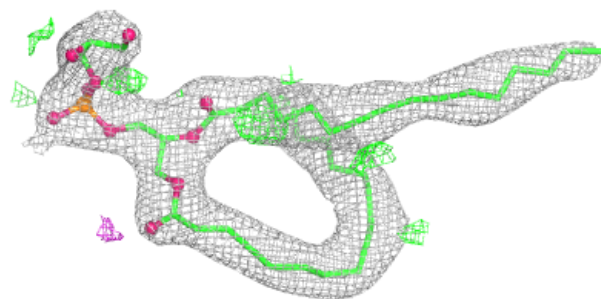


Electron density around LHG d 414 (A):

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

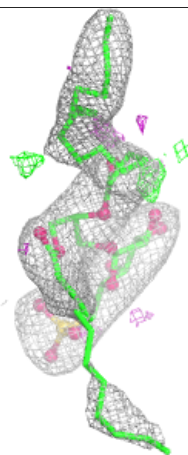
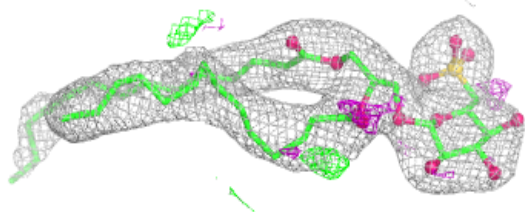
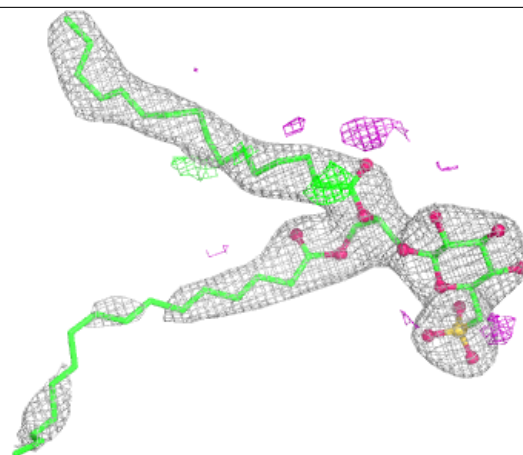
**Electron density around LHG d 414 (B):**

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



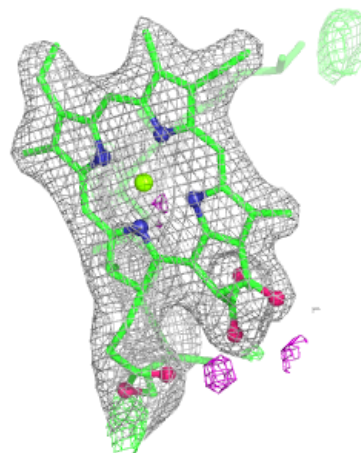
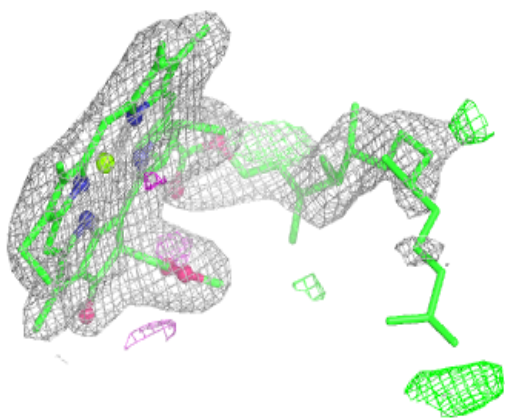
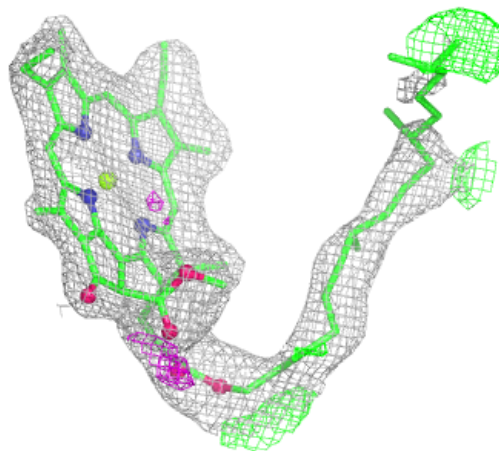
Electron density around SQD A 411 (B):

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



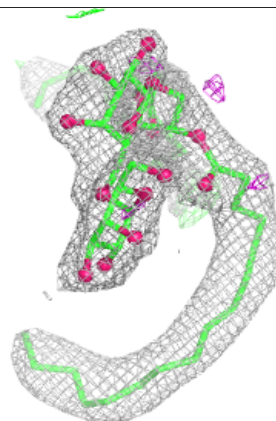
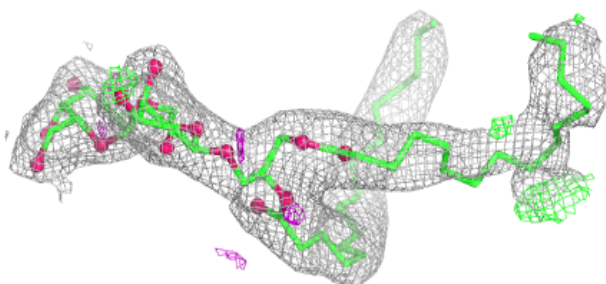
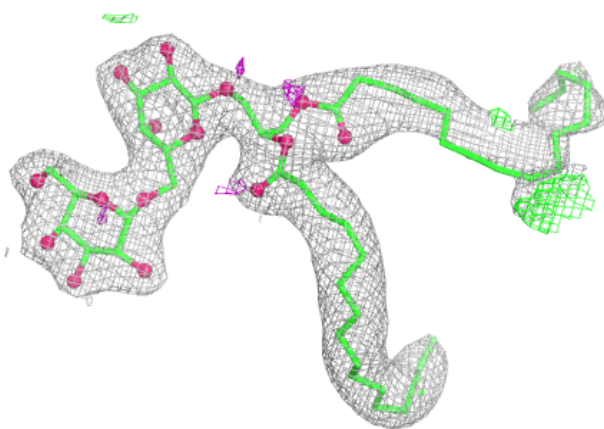
Electron density around CLA b 616:

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

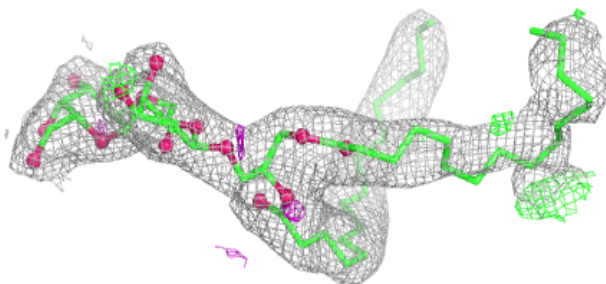
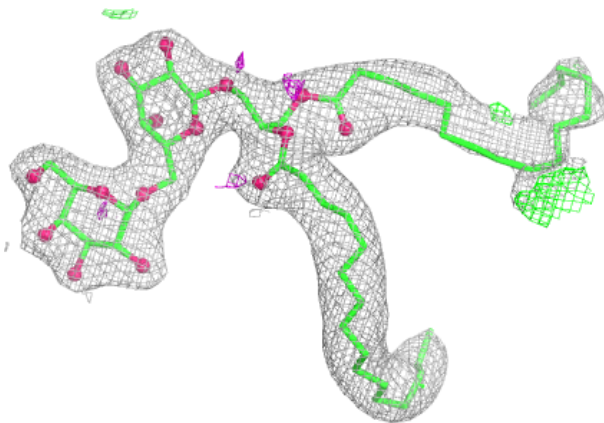


Electron density around DGD C 518 (A):

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

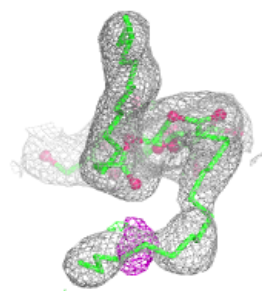
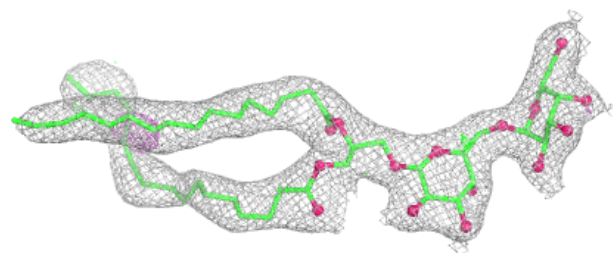
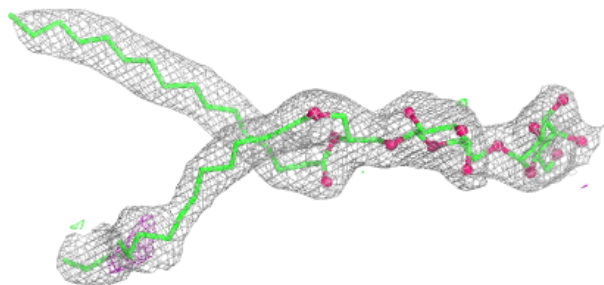
**Electron density around DGD C 518 (B):**

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

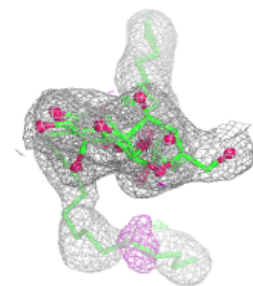
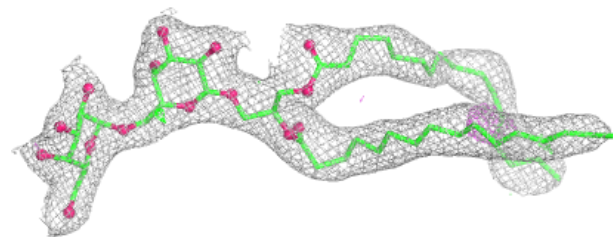
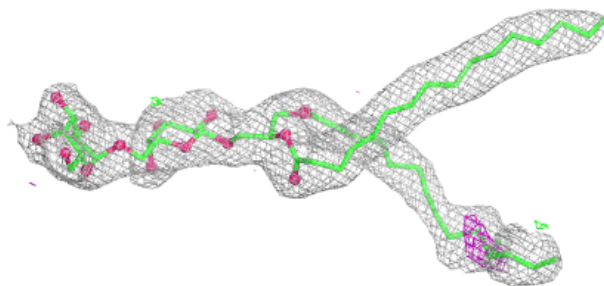


Electron density around DGD c 517 (A):

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

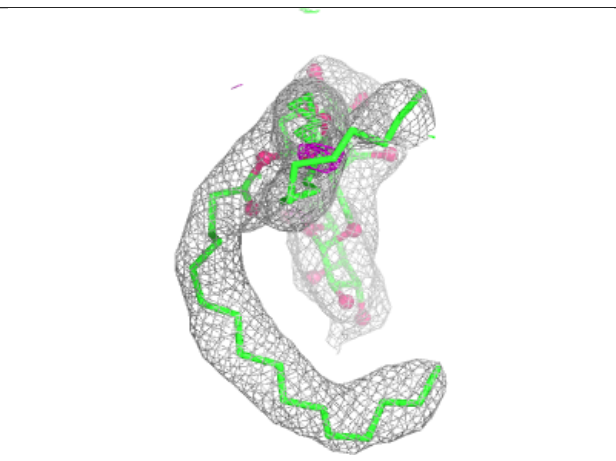
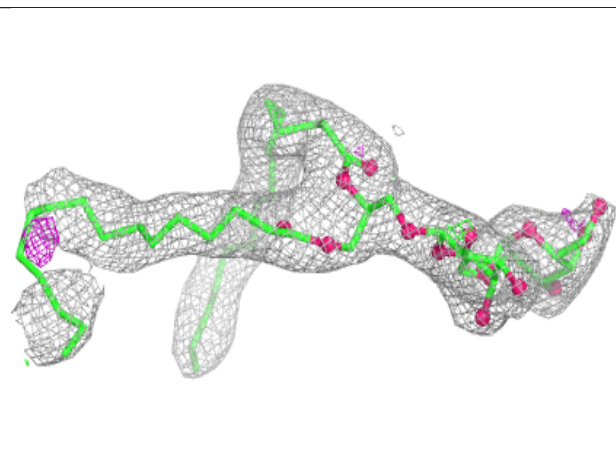
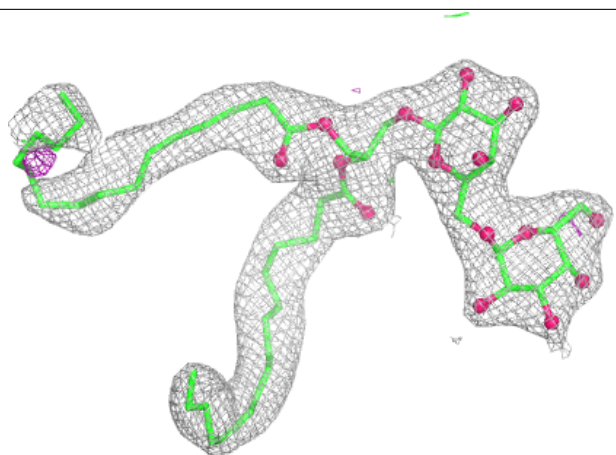
**Electron density around DGD c 517 (B):**

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



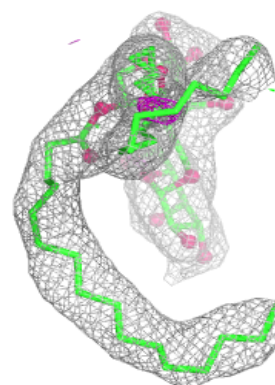
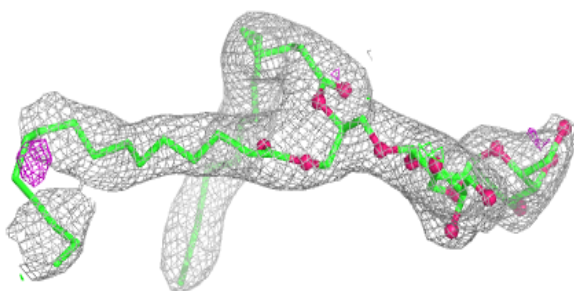
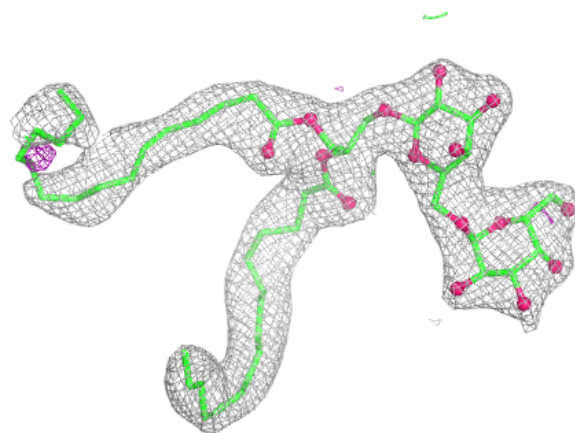
Electron density around DGD c 518 (A):

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



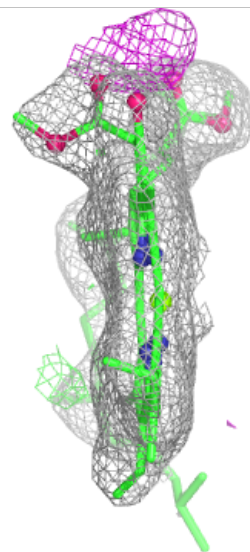
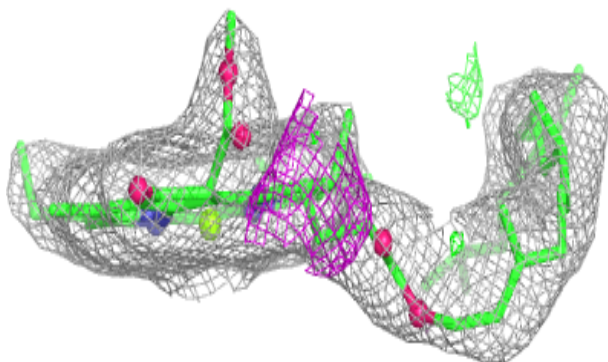
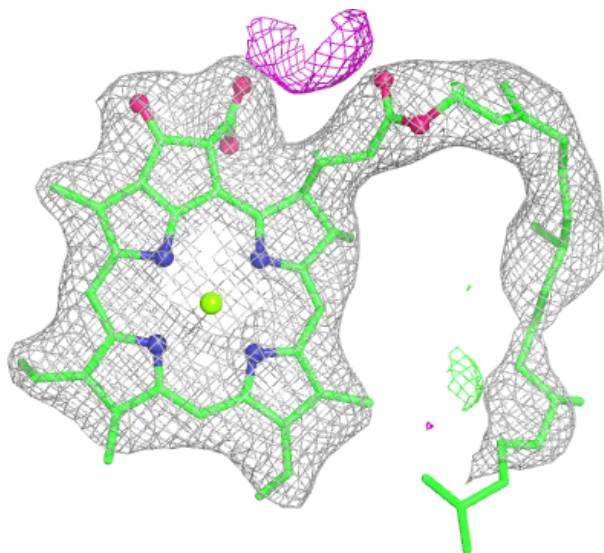
Electron density around DGD c 518 (B):

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



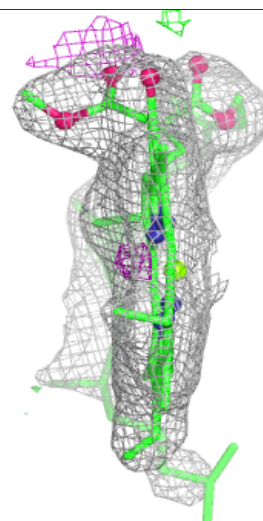
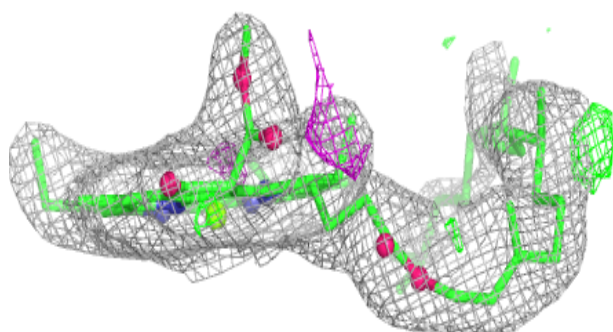
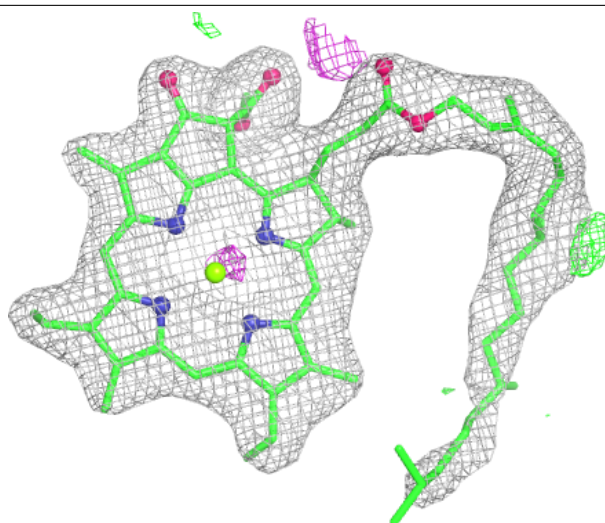
Electron density around CLA c 513:

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



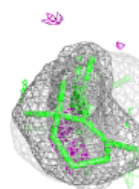
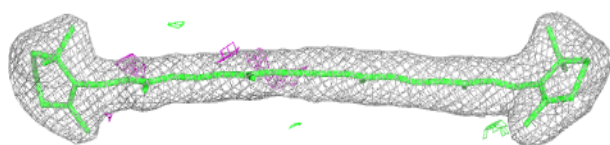
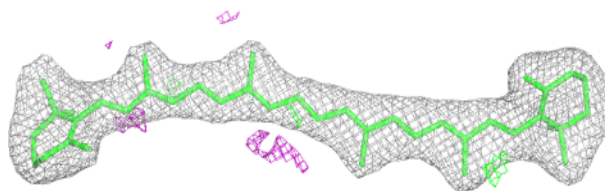
Electron density around CLA C 513:

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

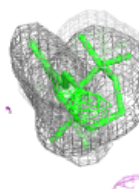
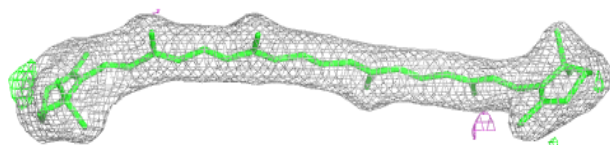
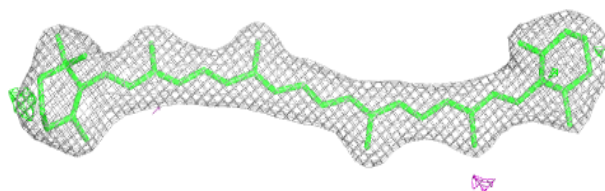


Electron density around BCR B 618:

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

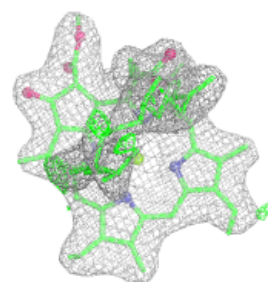
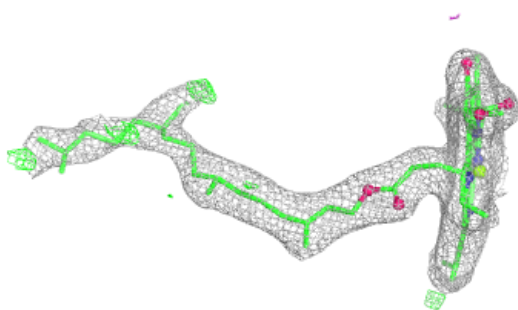
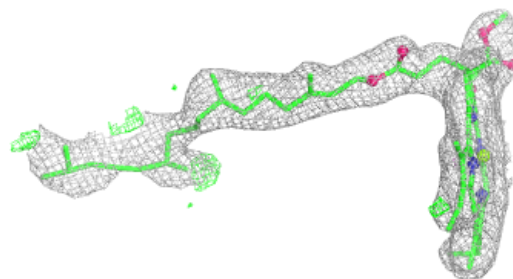
**Electron density around BCR B 619:**

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

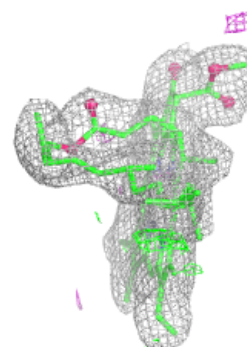
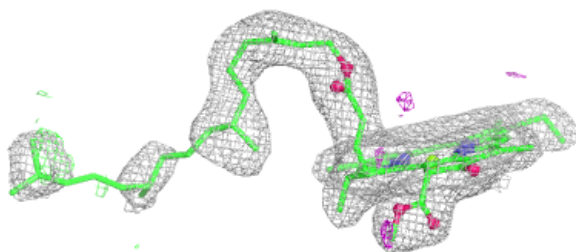
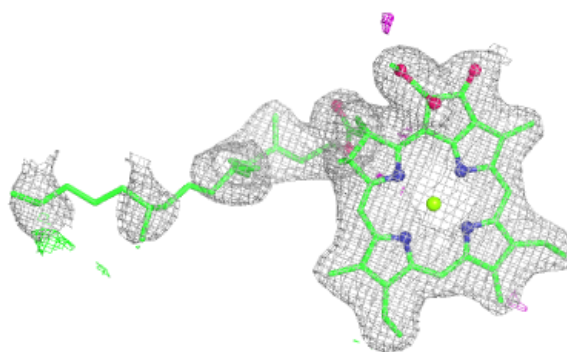


Electron density around CLA B 606:

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

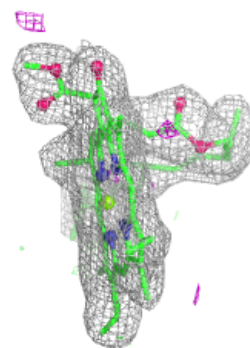
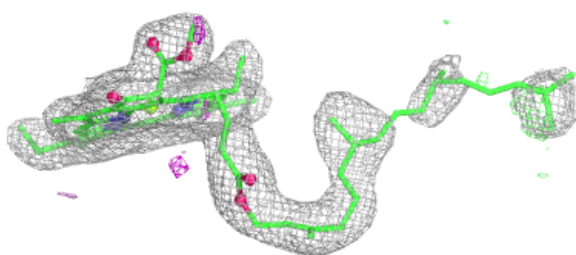
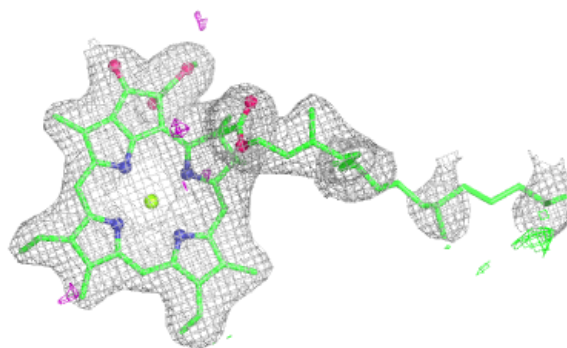
**Electron density around CLA a 407 (A):**

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

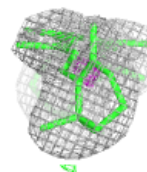
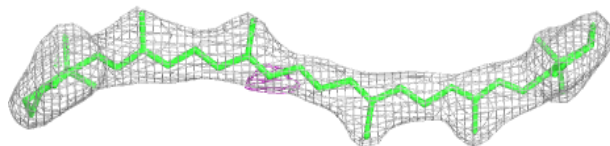
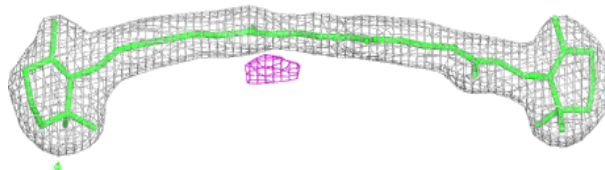


Electron density around CLA a 407 (B):

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

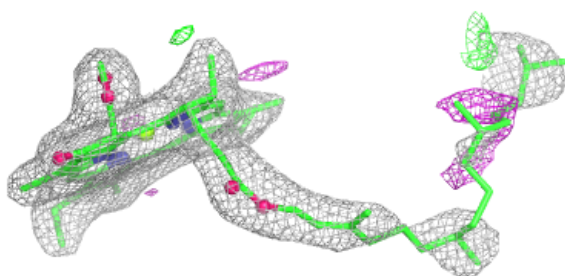
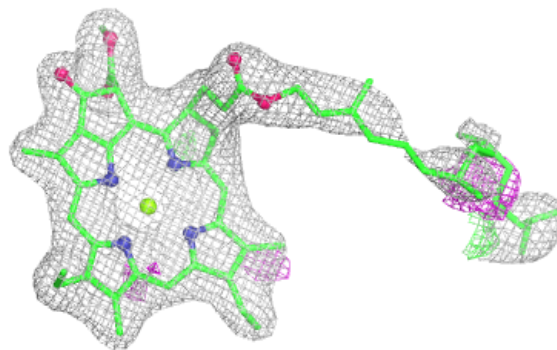
**Electron density around BCR K 102:**

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

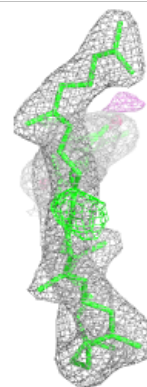
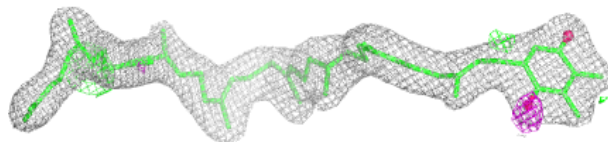
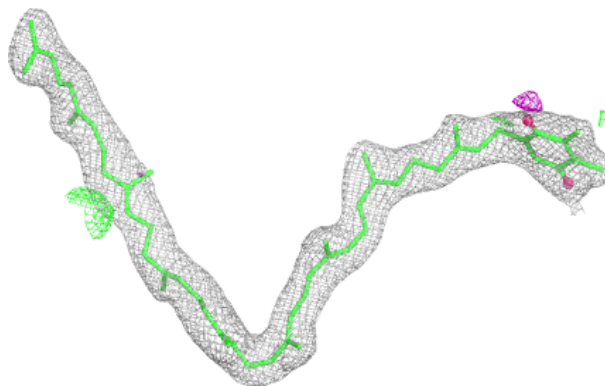


Electron density around CLA a 409:

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

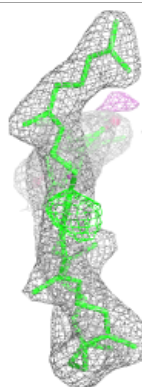
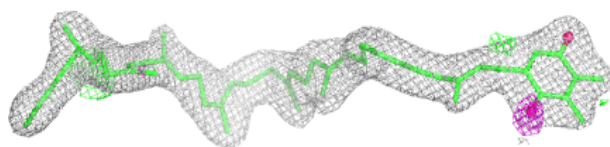
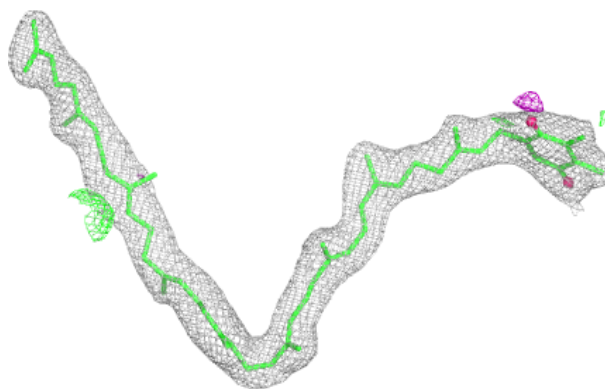
**Electron density around PL9 D 405 (A):**

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

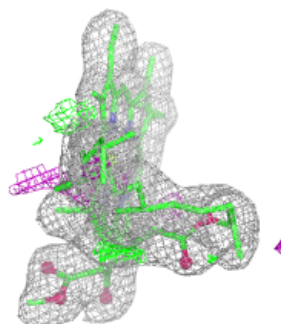
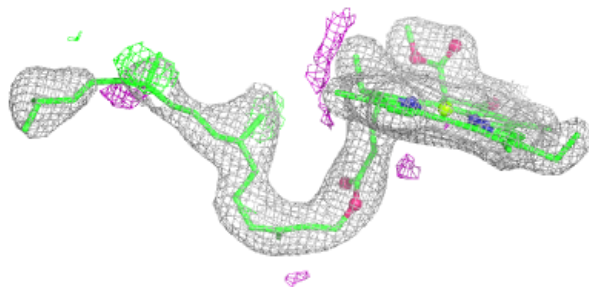
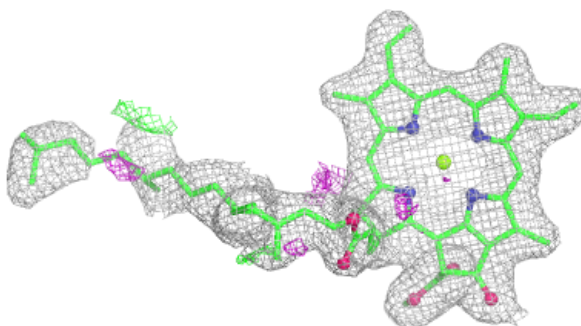


Electron density around PL9 D 405 (B):

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

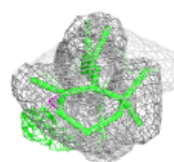
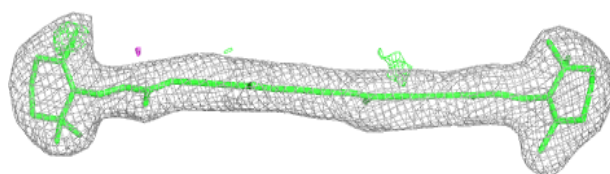
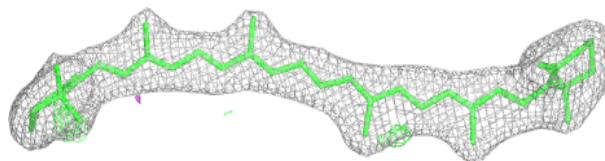
**Electron density around CLA A 407 (B):**

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

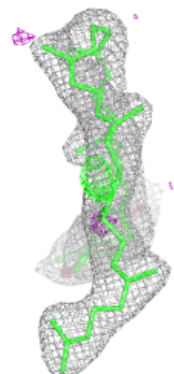
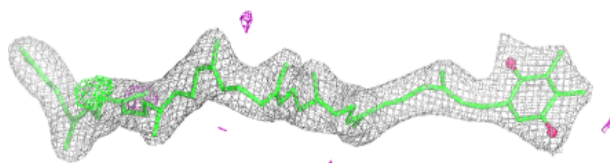
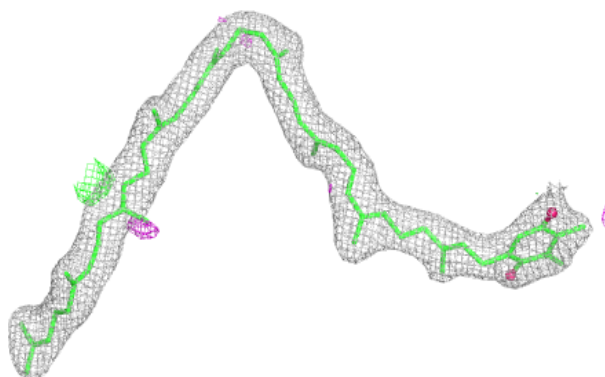


Electron density around BCR a 410:

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

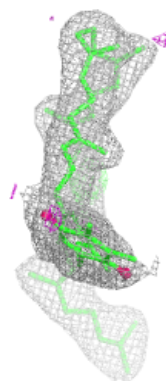
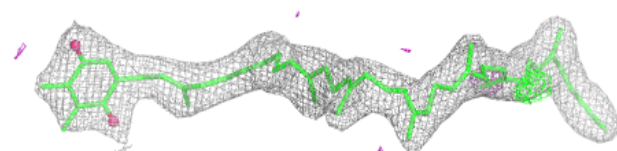
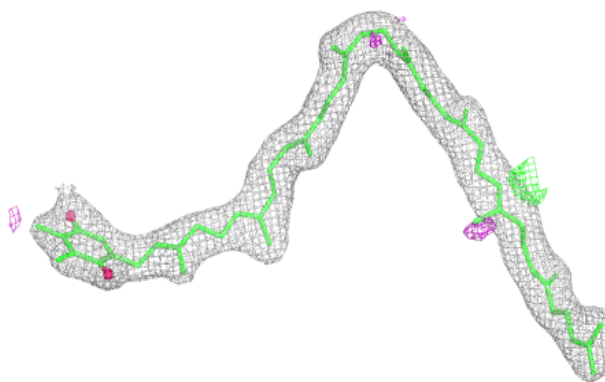
**Electron density around PL9 d 406 (A):**

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

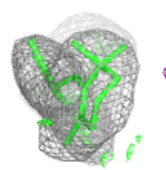
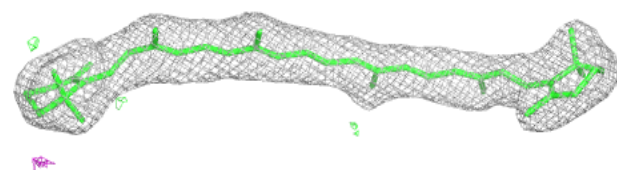
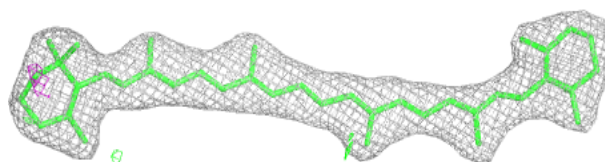


Electron density around PL9 d 406 (B):

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

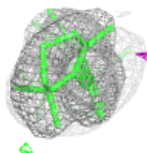
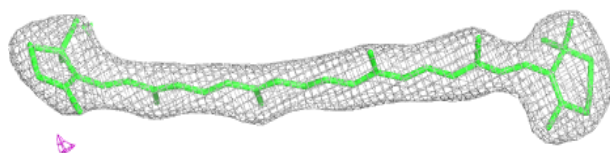
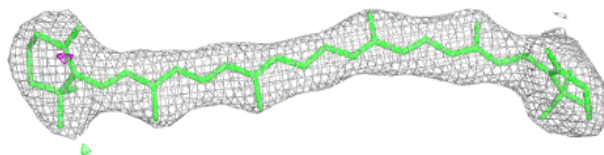
**Electron density around BCR b 619:**

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

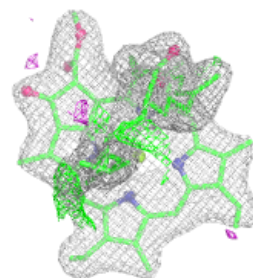
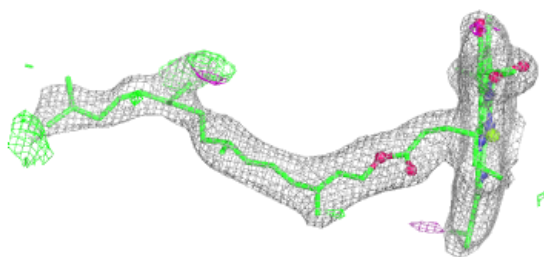
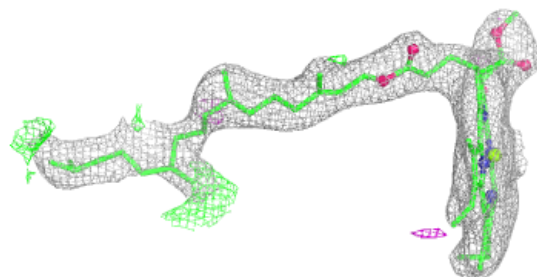


Electron density around BCR c 515:

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

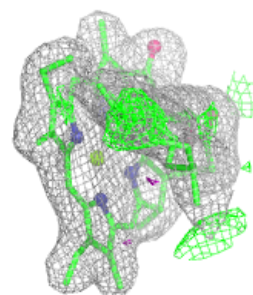
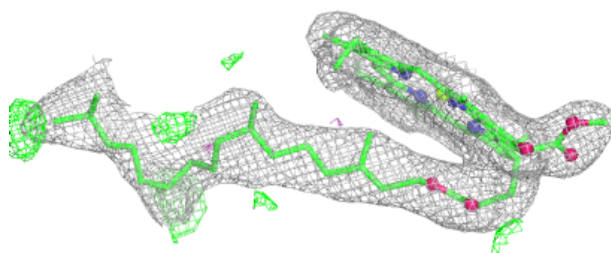
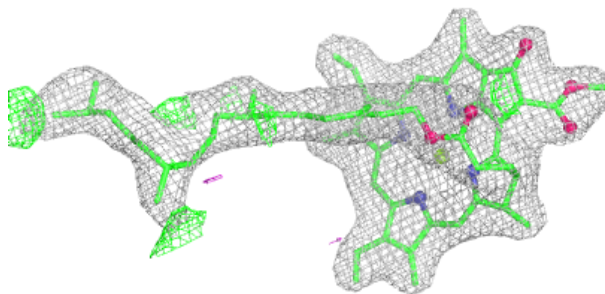
**Electron density around CLA b 606:**

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

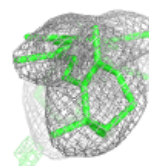
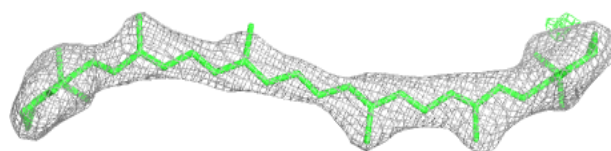
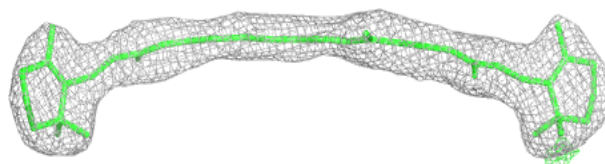


Electron density around CLA b 614:

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

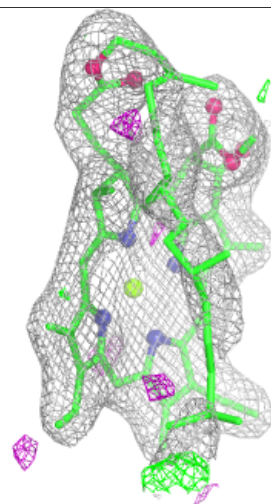
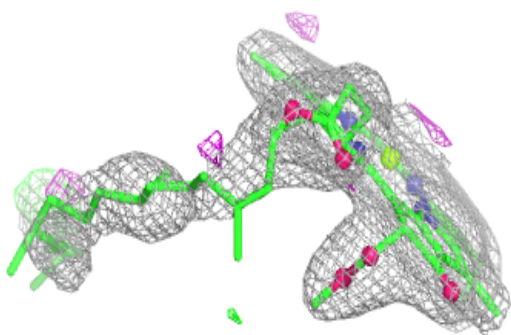
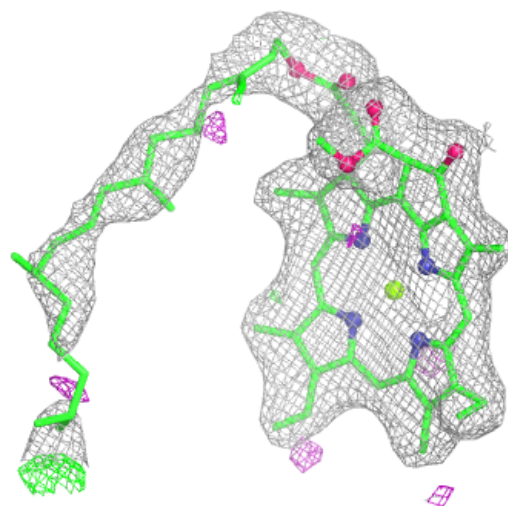
**Electron density around BCR k 101:**

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



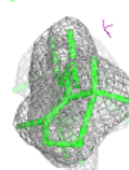
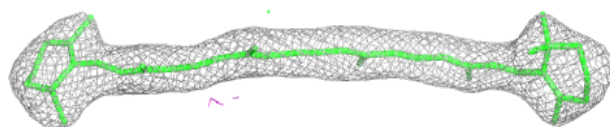
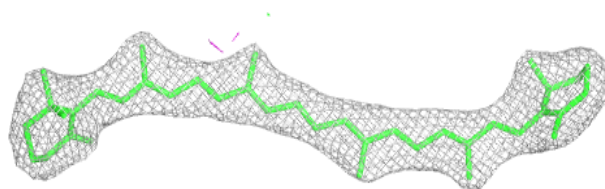
Electron density around CLA B 616:

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

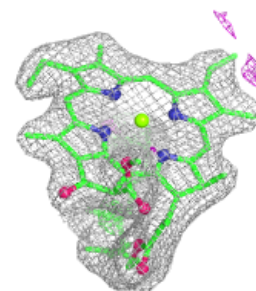
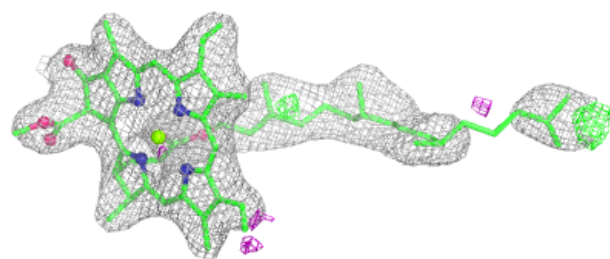
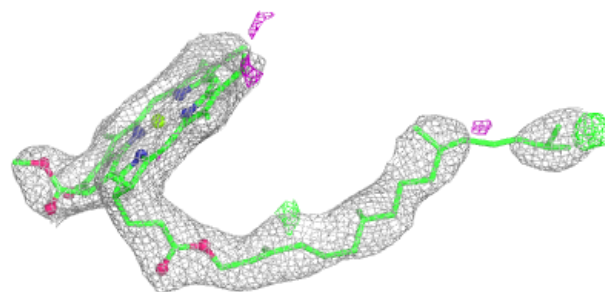


Electron density around BCR y 101:

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

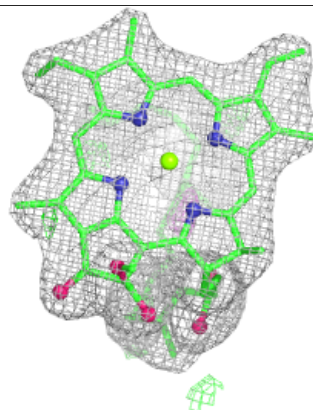
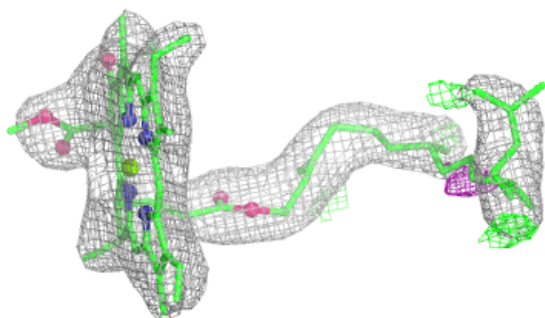
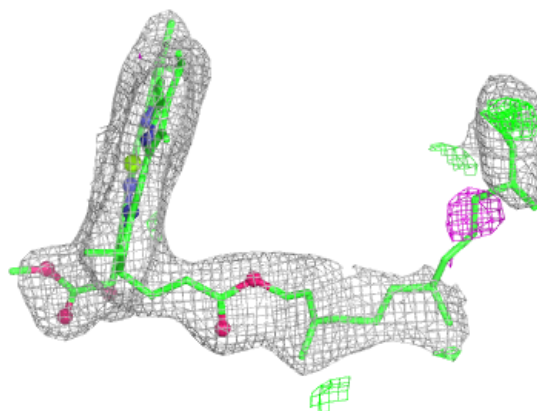
**Electron density around CLA c 505:**

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



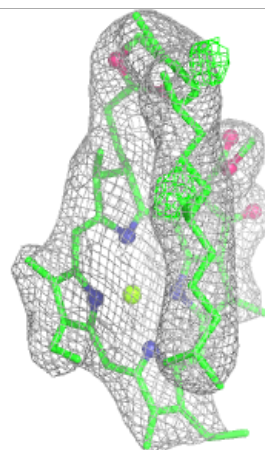
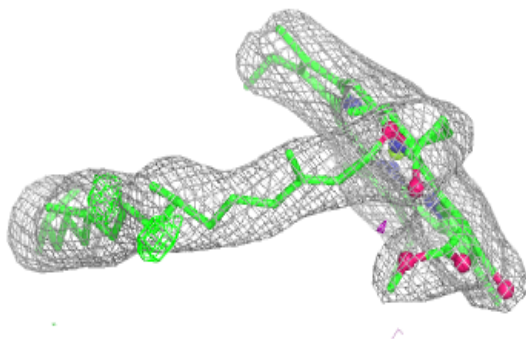
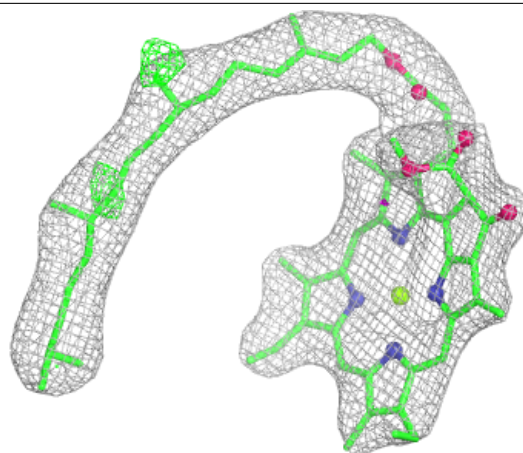
Electron density around CLA c 507:

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



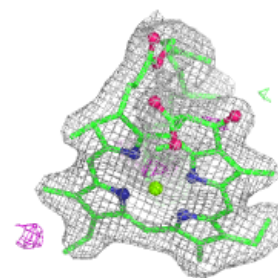
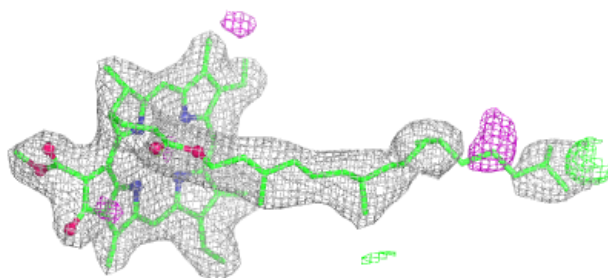
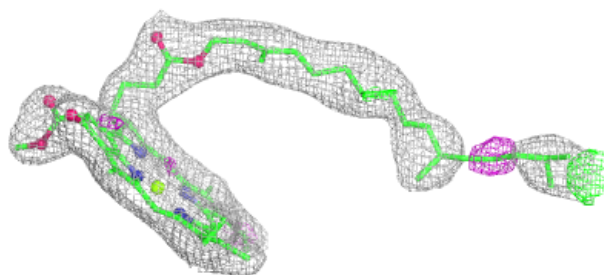
Electron density around CLA c 508:

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

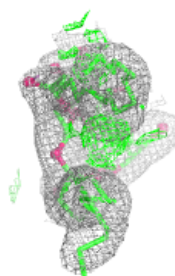
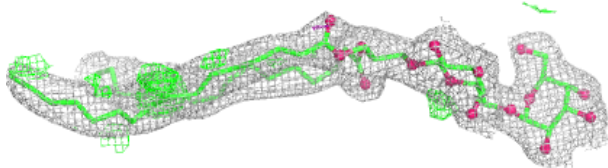
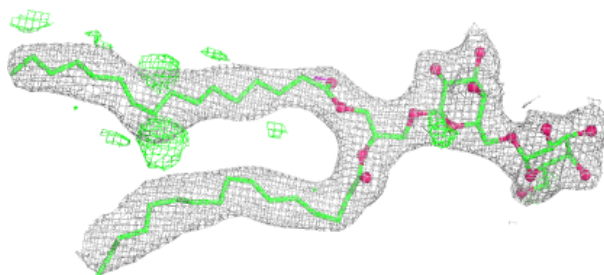


Electron density around CLA C 505:

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

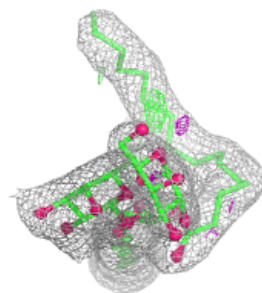
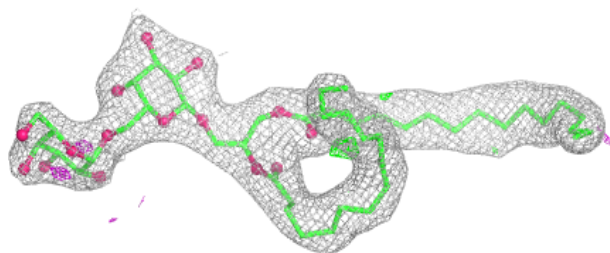
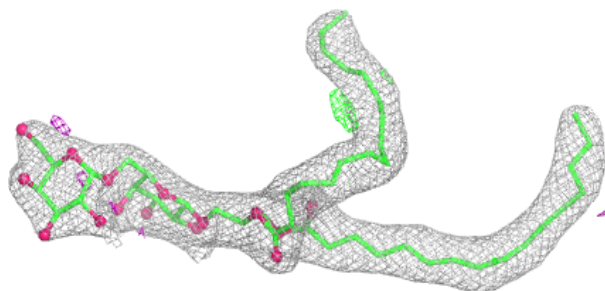
**Electron density around DGD C 519:**

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

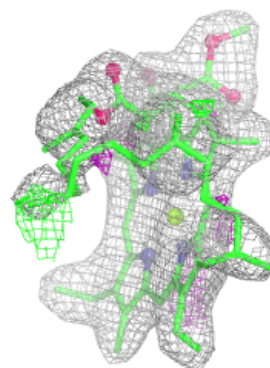
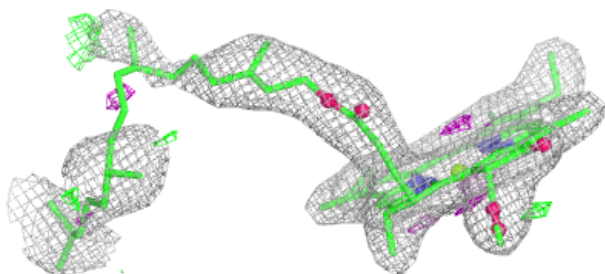
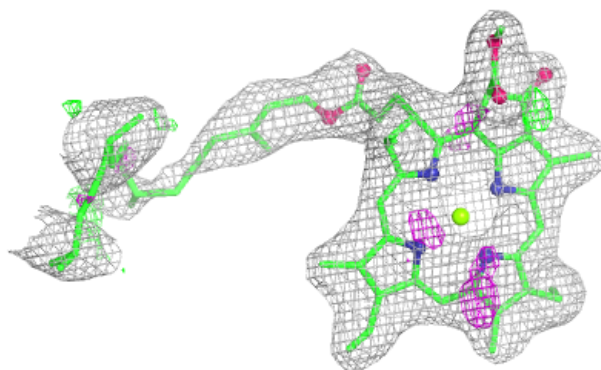


Electron density around DGD H 102:

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

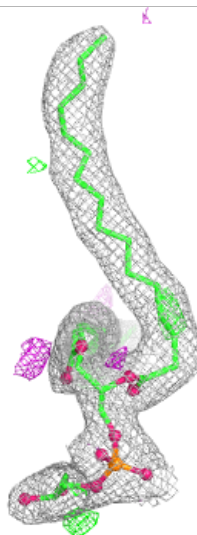
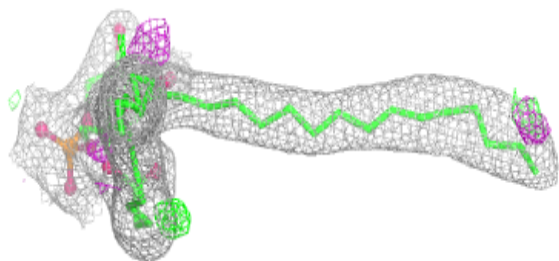
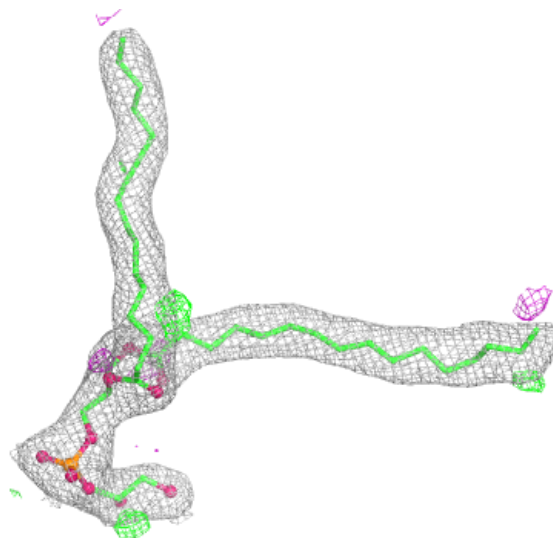
**Electron density around CLA A 409:**

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



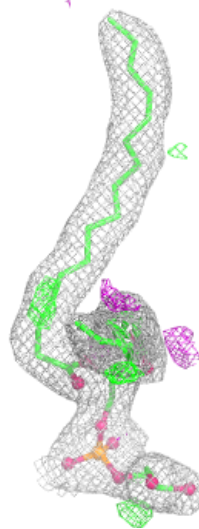
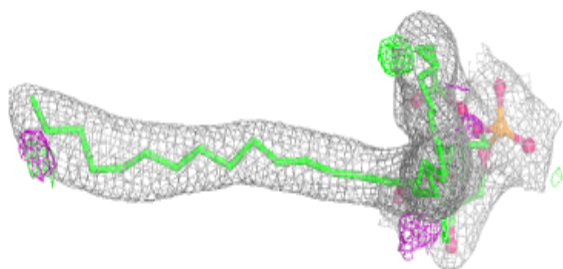
Electron density around LHG b 628 (A):

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



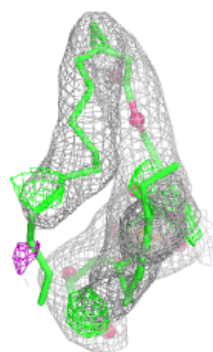
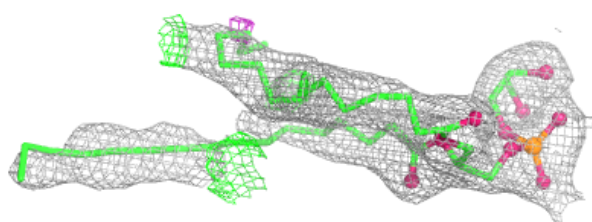
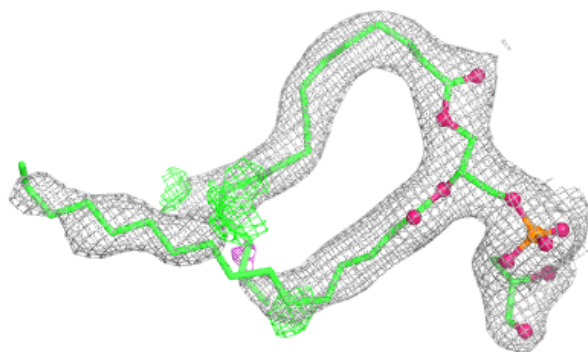
Electron density around LHG b 628 (B):

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

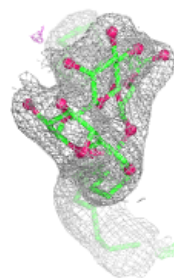
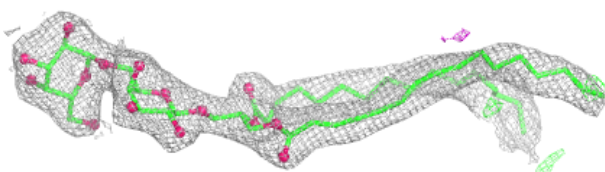
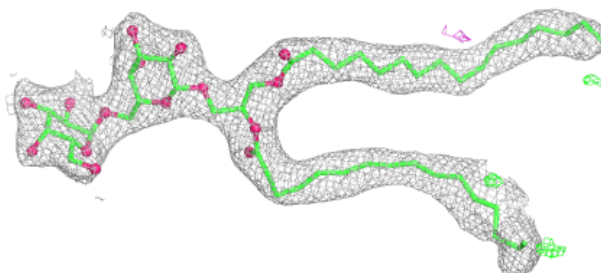


Electron density around LHG d 408 (A):

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

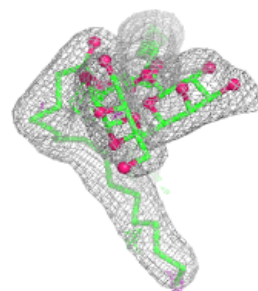
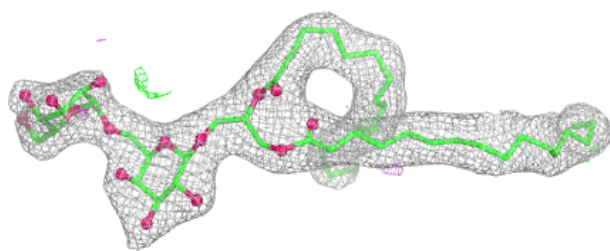
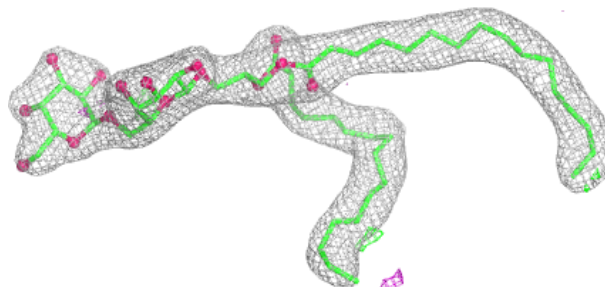
**Electron density around DGD c 519:**

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

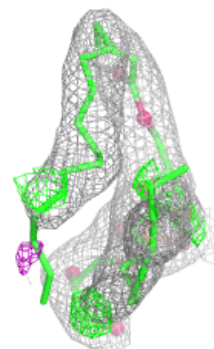
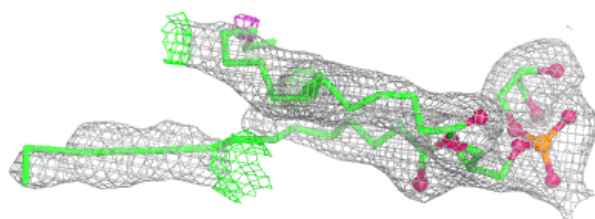
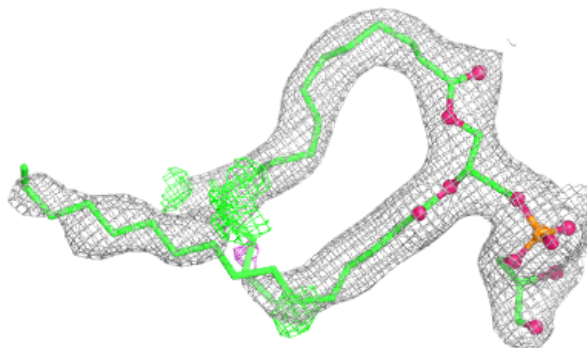


Electron density around DGD h 102:

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

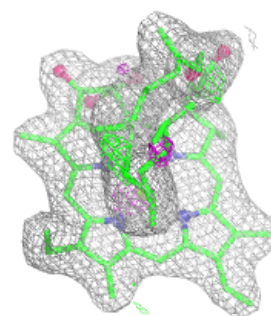
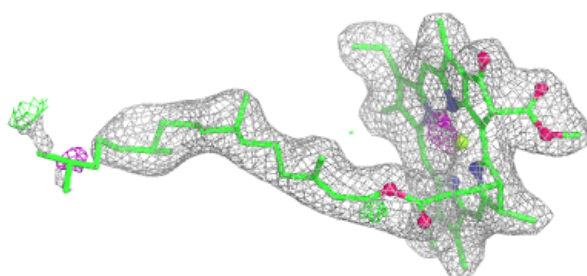
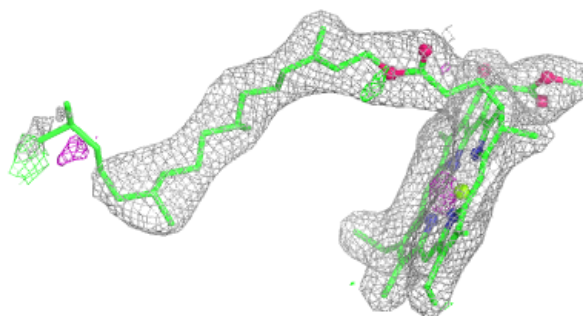
**Electron density around LHG d 408 (B):**

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

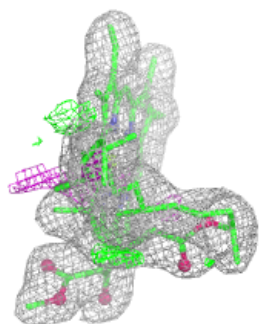
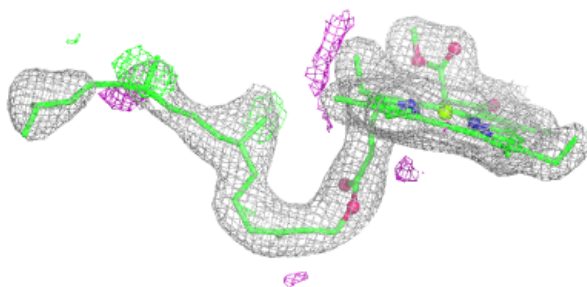
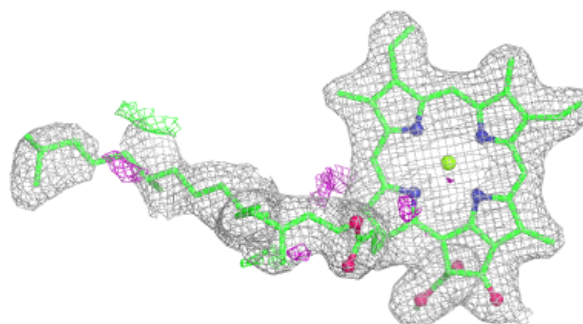


Electron density around CLA C 509:

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

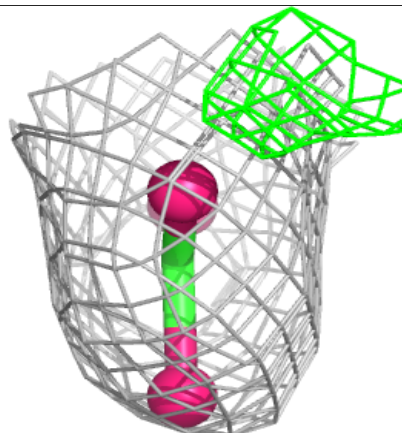
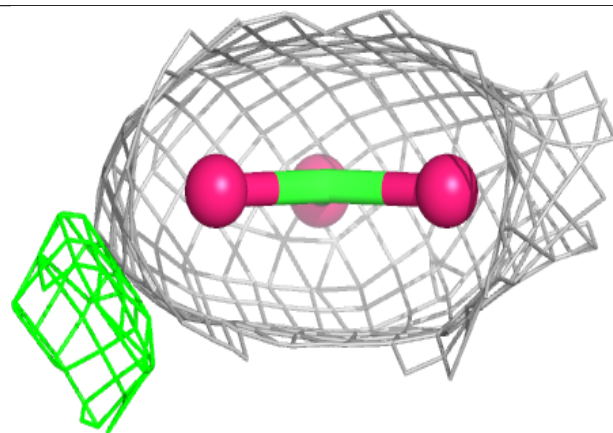
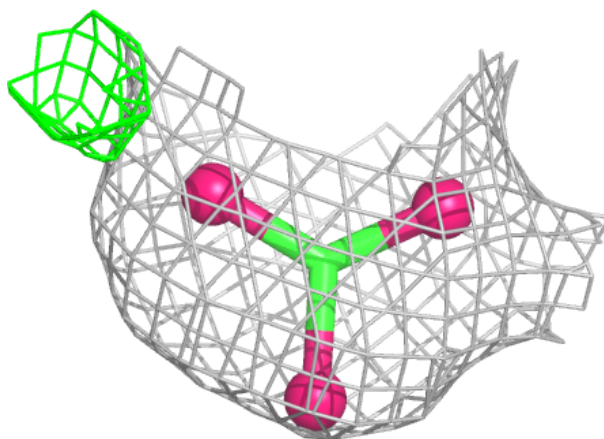
**Electron density around CLA A 407 (A):**

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



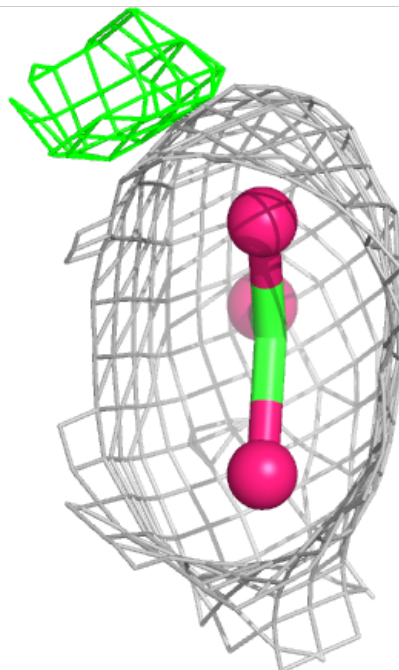
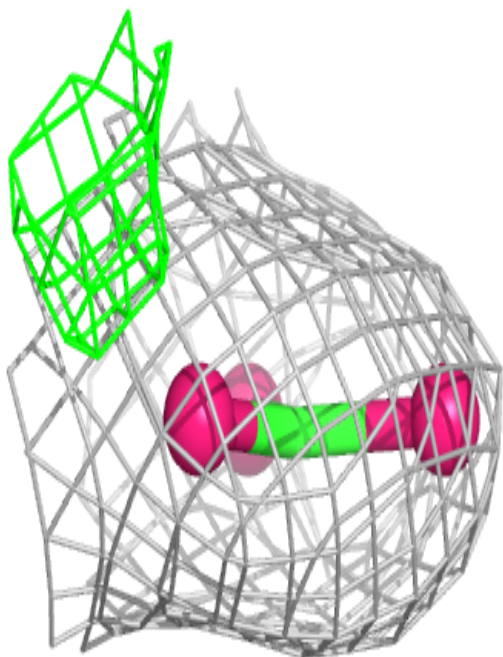
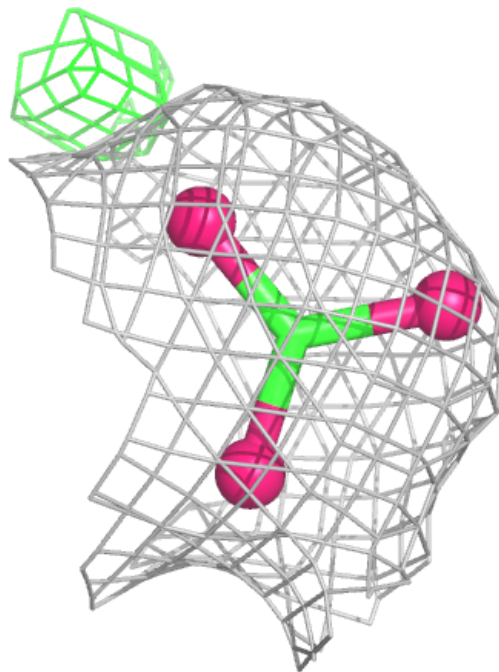
Electron density around BCT d 401 (A):

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



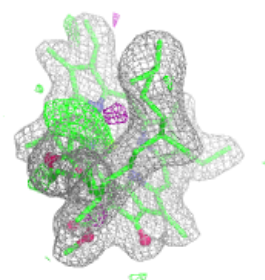
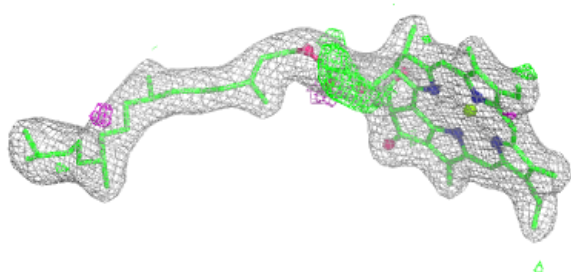
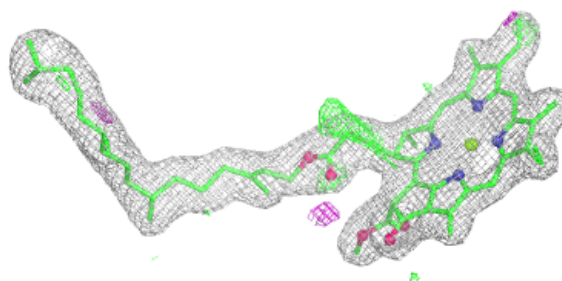
Electron density around BCT d 401 (B):

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



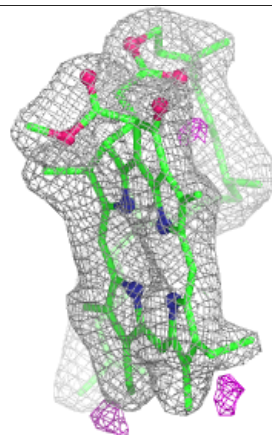
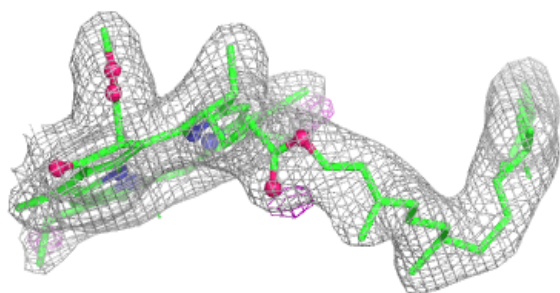
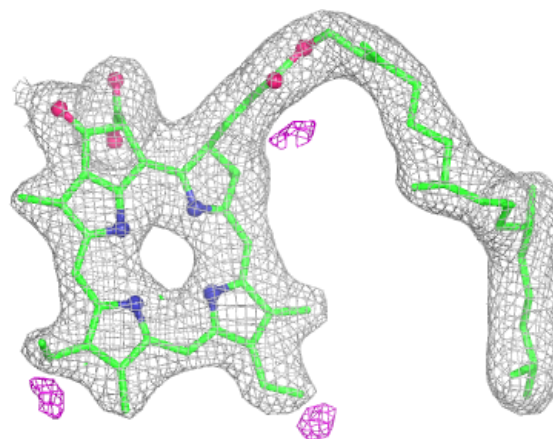
Electron density around CLA A 405 (A):

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



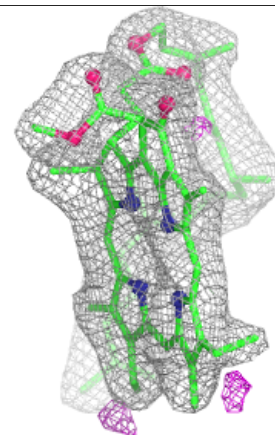
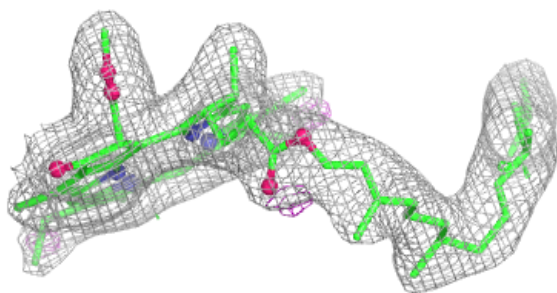
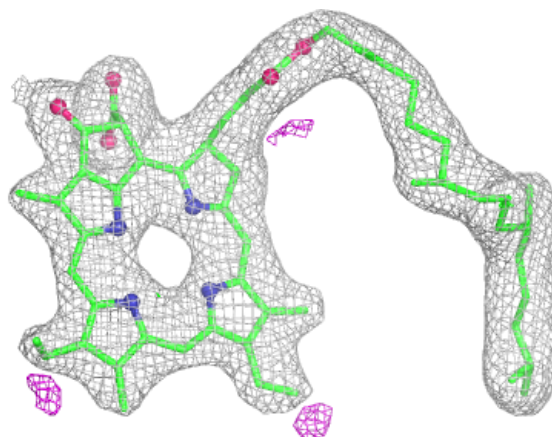
Electron density around PHO d 402 (A):

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

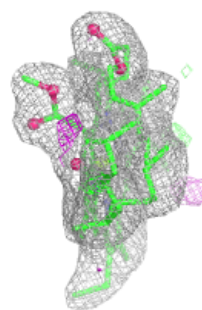
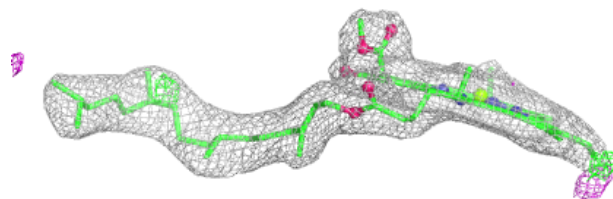
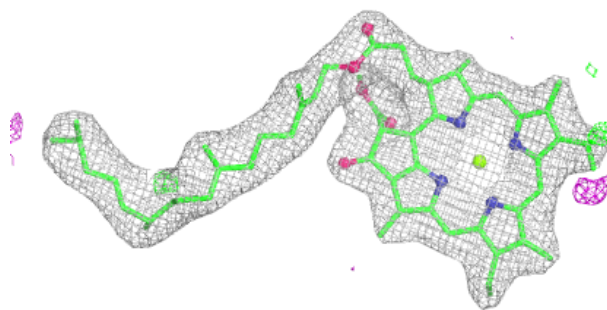


Electron density around PHO d 402 (B):

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

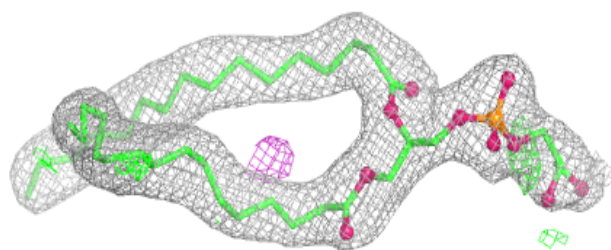
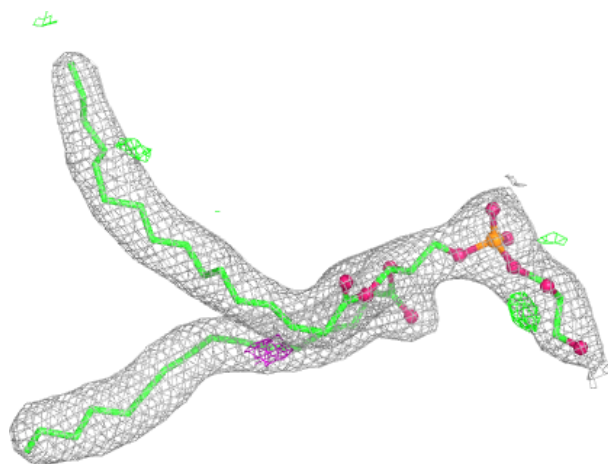
**Electron density around CLA b 602:**

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



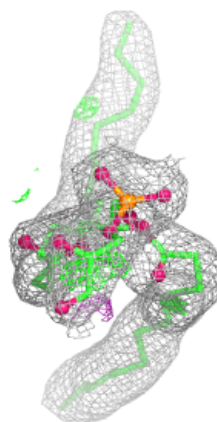
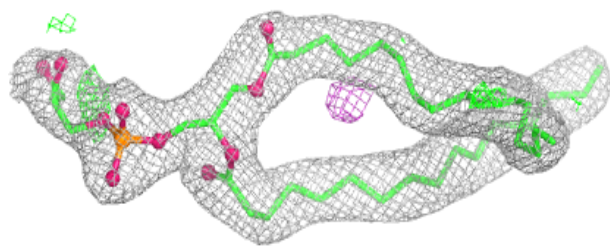
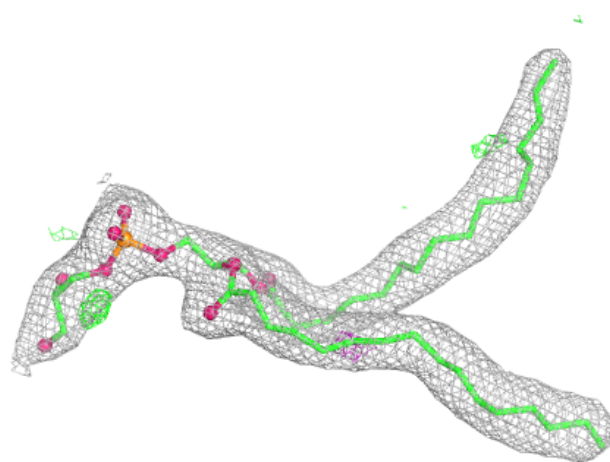
Electron density around LHG D 406 (A):

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



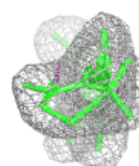
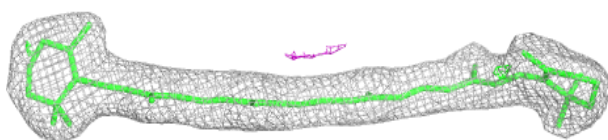
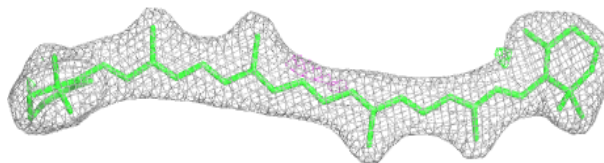
Electron density around LHG D 406 (B):

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

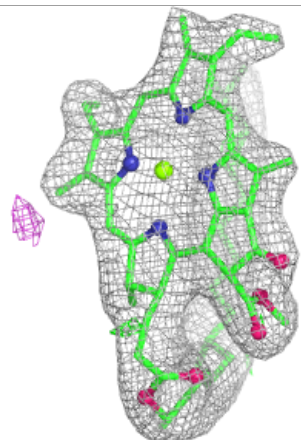
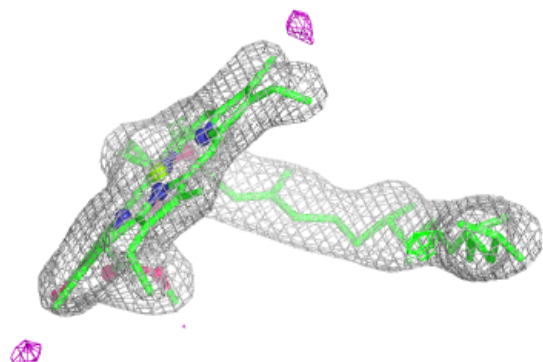
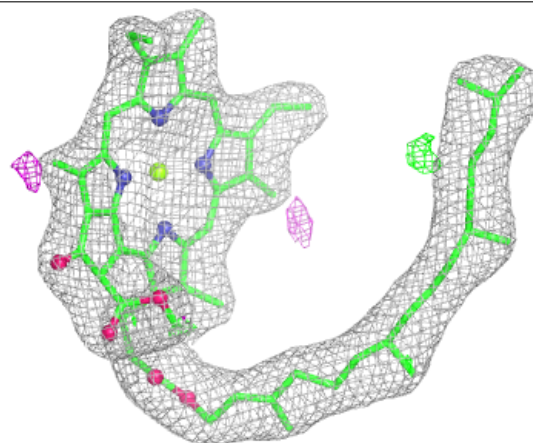


Electron density around BCR B 617:

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

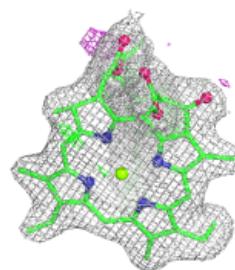
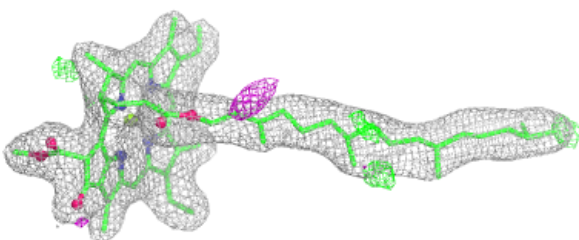
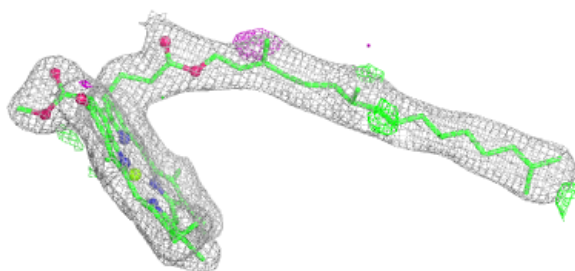
**Electron density around CLA C 508:**

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

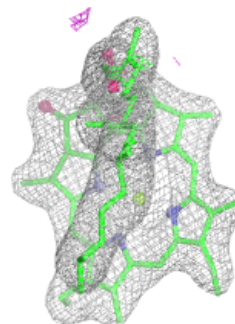
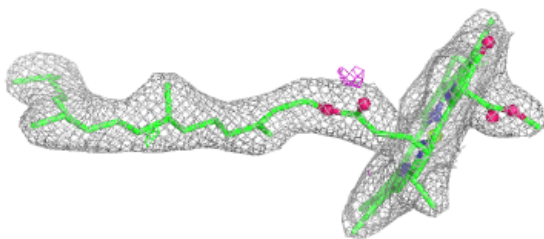
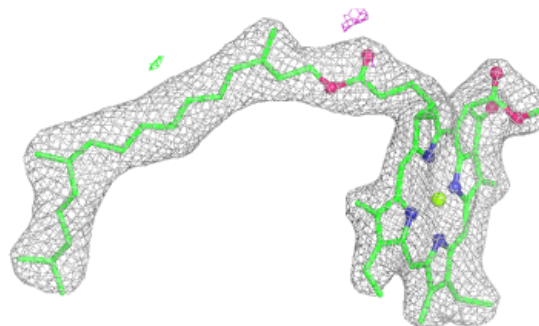


Electron density around CLA b 607:

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

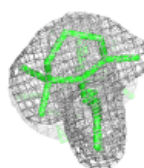
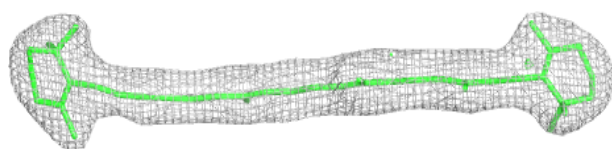
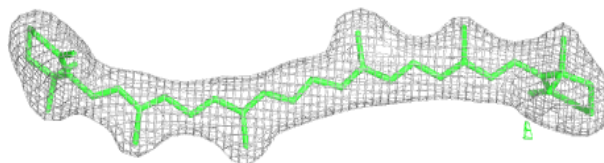
**Electron density around CLA b 609:**

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

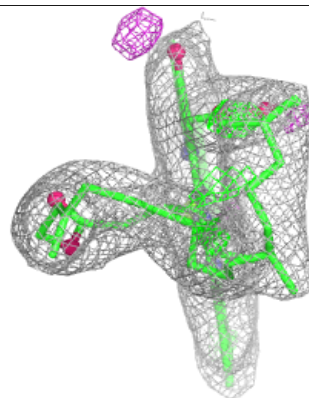
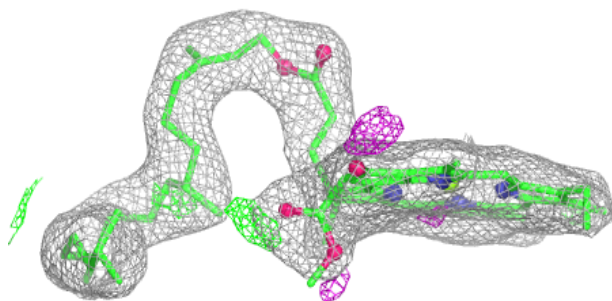
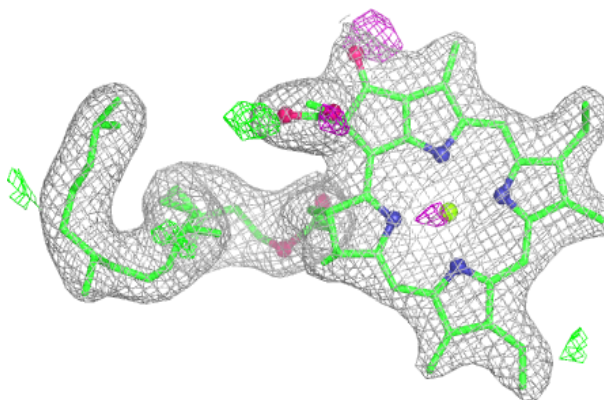


Electron density around BCR C 516:

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

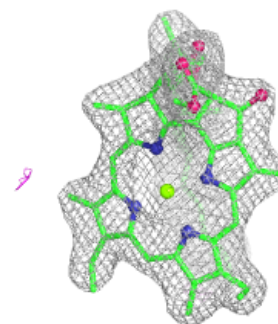
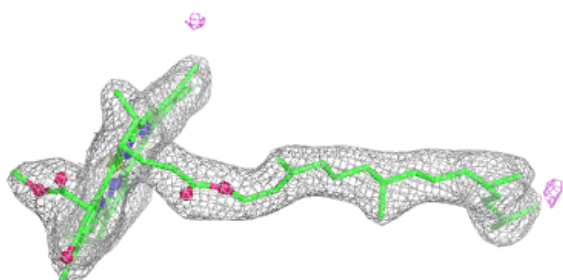
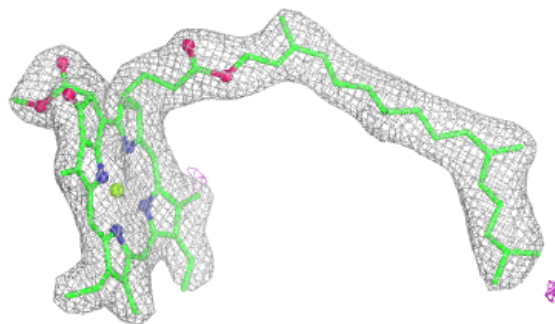
**Electron density around CLA b 612:**

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

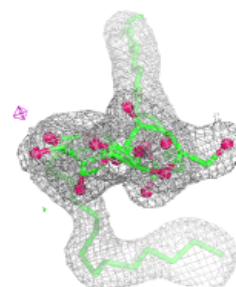
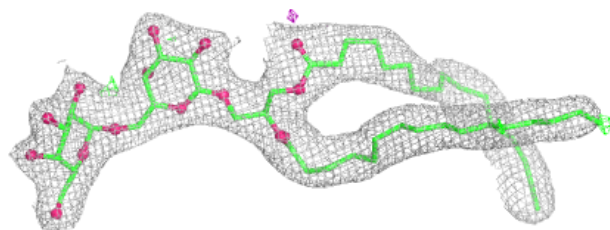
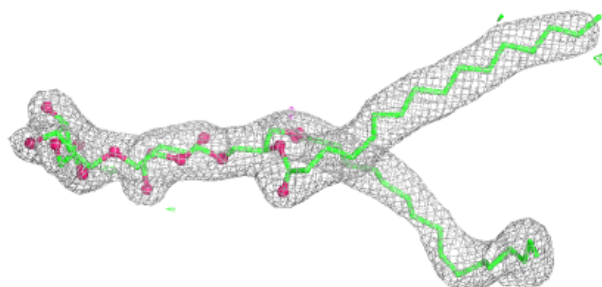


Electron density around CLA B 609:

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

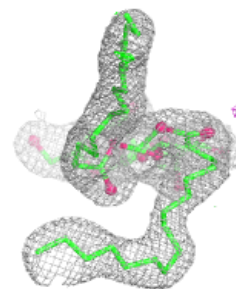
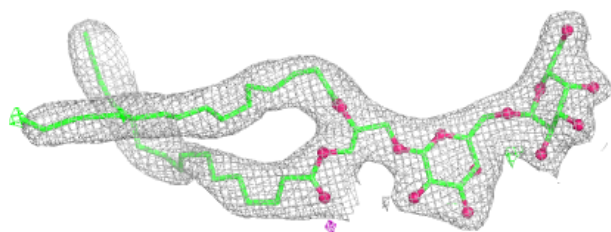
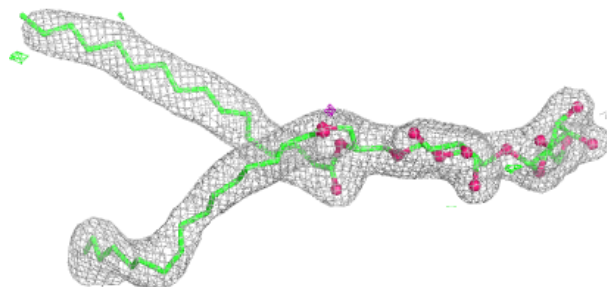
**Electron density around DGD C 517 (A):**

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



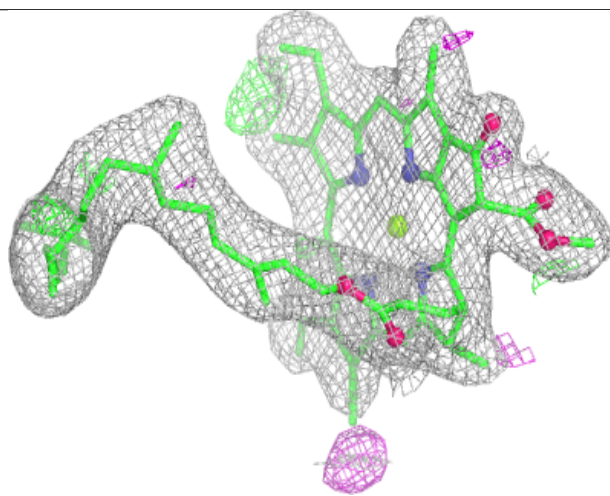
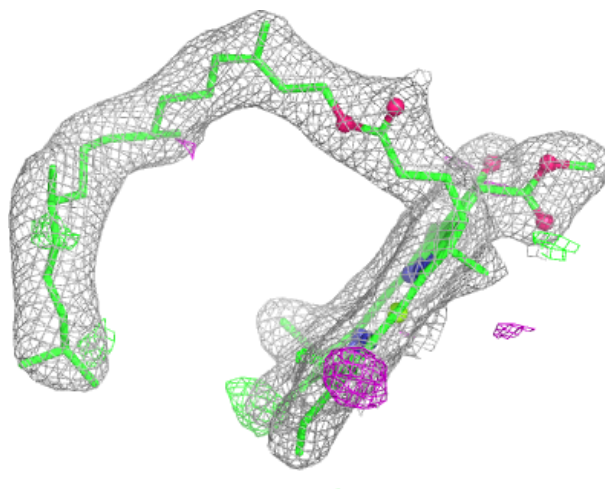
Electron density around DGD C 517 (B):

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



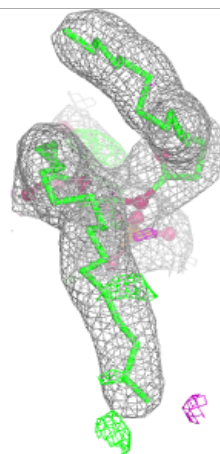
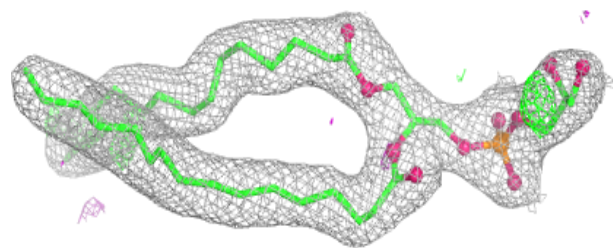
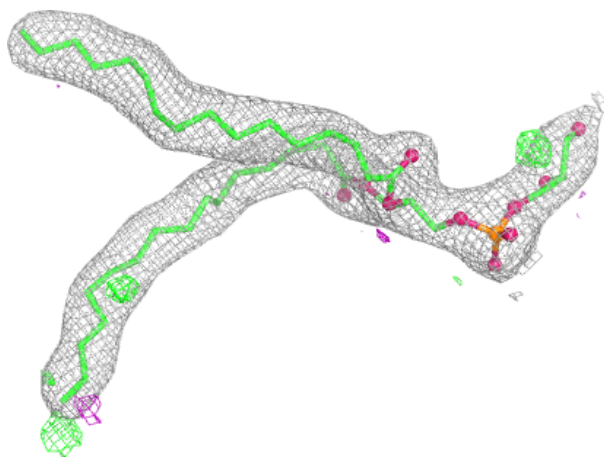
Electron density around CLA B 611:

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



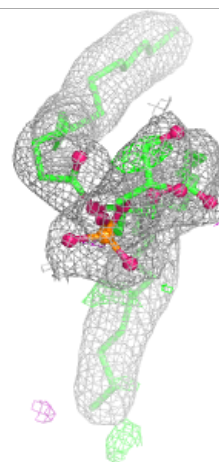
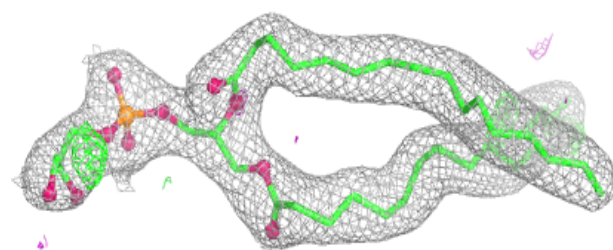
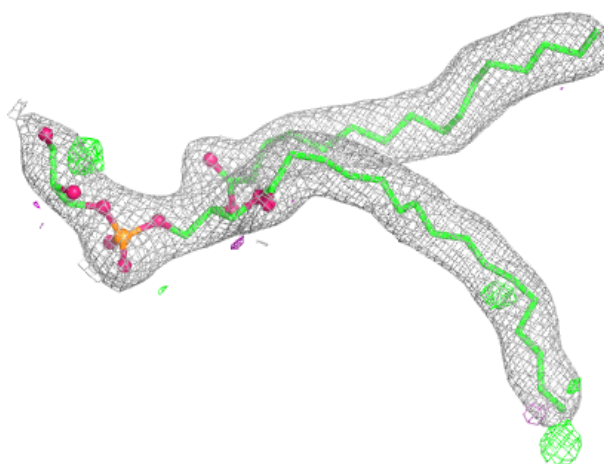
Electron density around LHG d 407 (A):

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



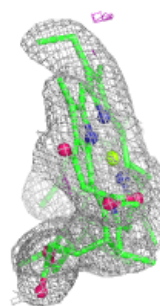
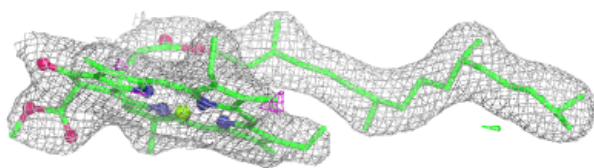
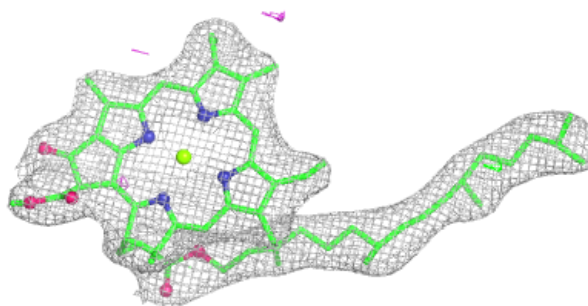
Electron density around LHG d 407 (B):

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



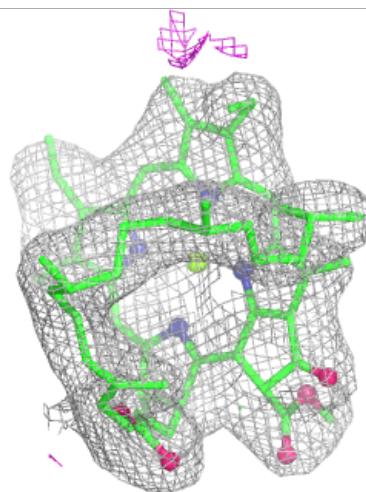
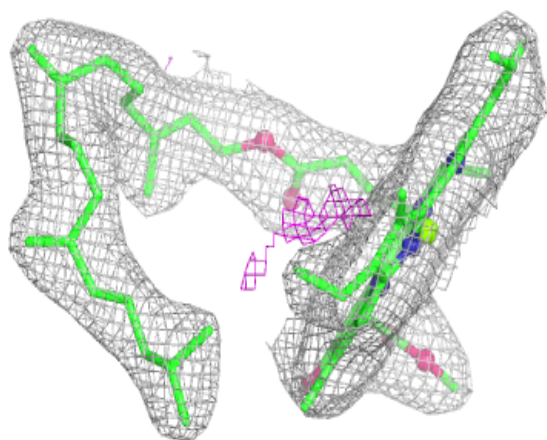
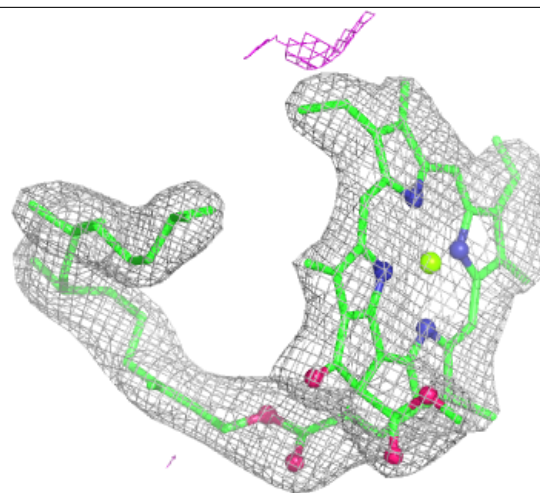
Electron density around CLA c 502:

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



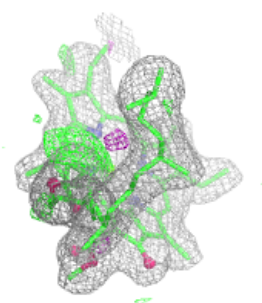
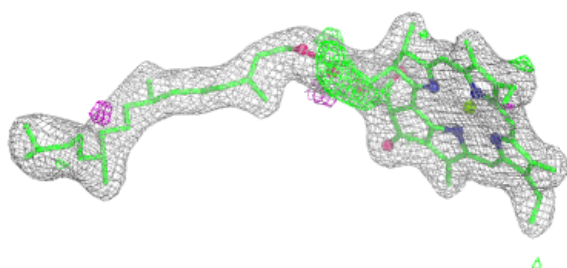
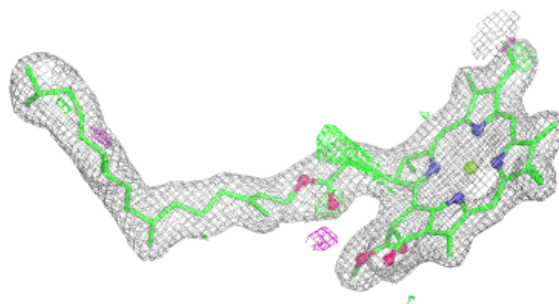
Electron density around CLA c 504:

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

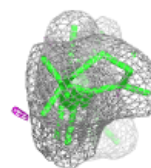
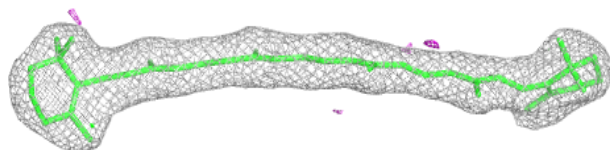
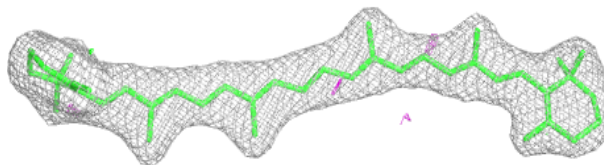


Electron density around CLA A 405 (B):

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

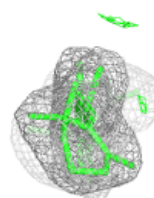
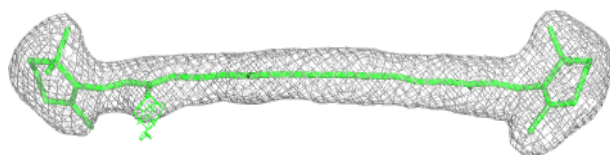
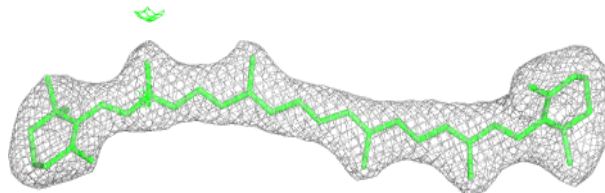
**Electron density around BCR b 617:**

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

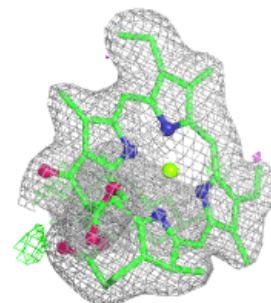
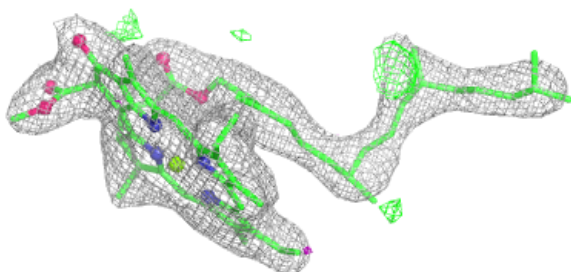
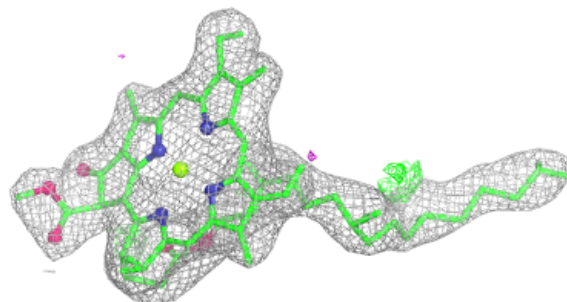


Electron density around BCR b 618:

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

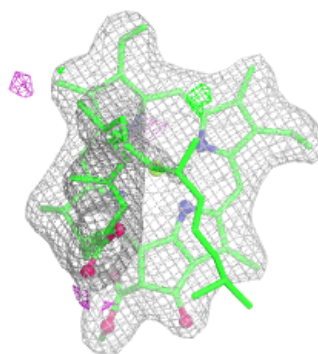
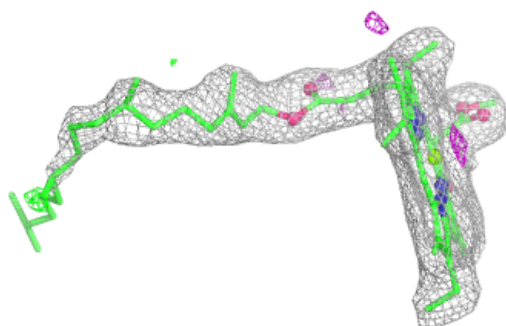
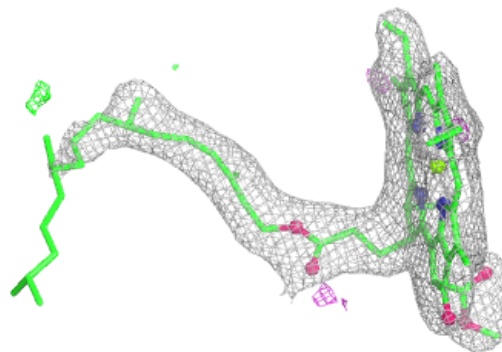
**Electron density around CLA c 506:**

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

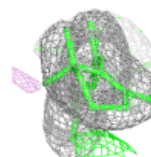
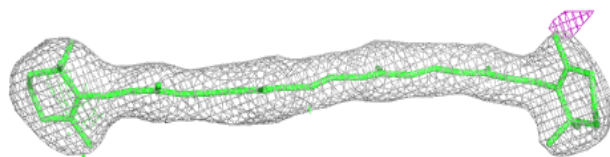
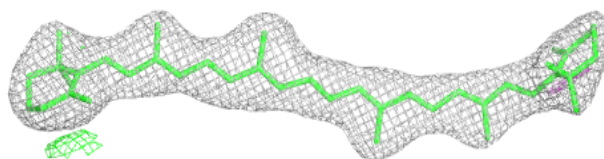


Electron density around CLA D 403:

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

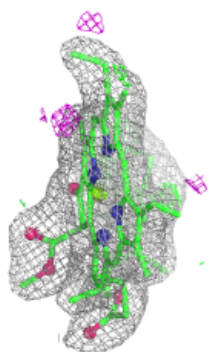
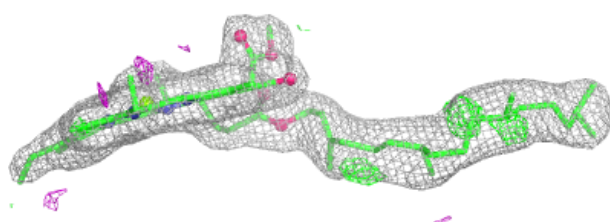
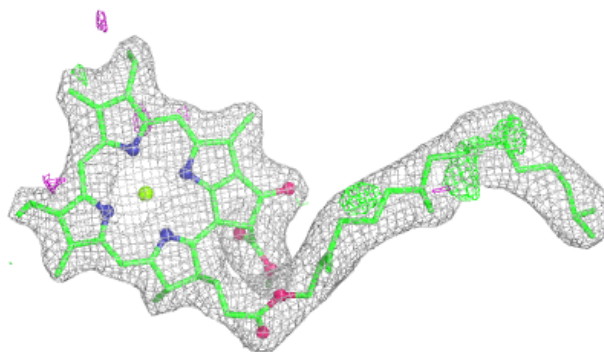
**Electron density around BCR c 516:**

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

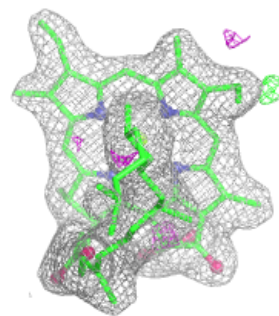
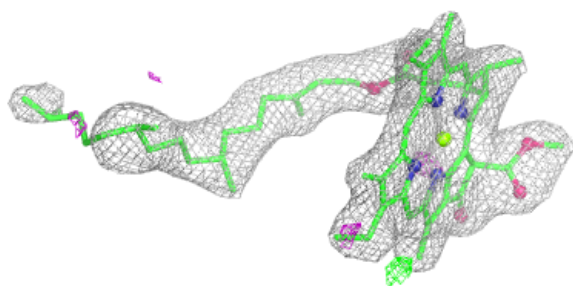
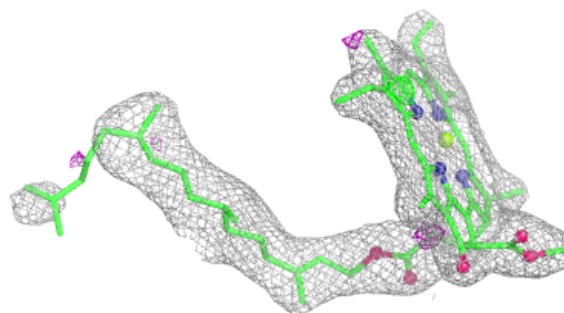


Electron density around CLA B 602:

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

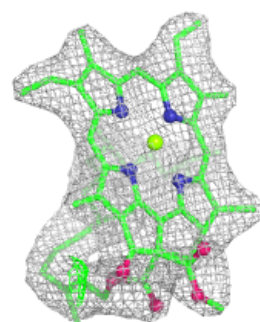
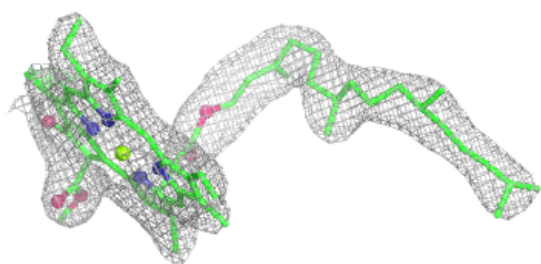
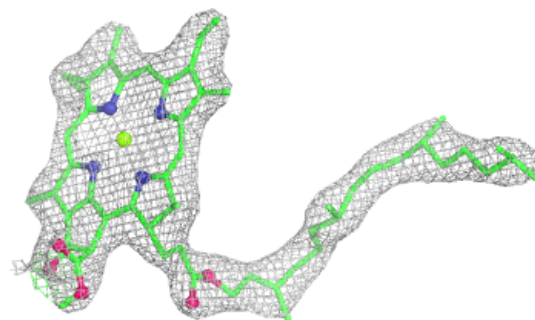
**Electron density around CLA c 509:**

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

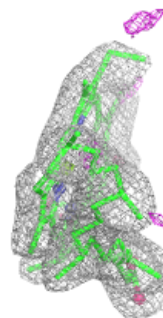
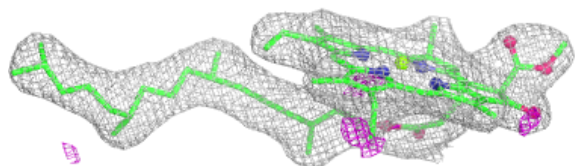
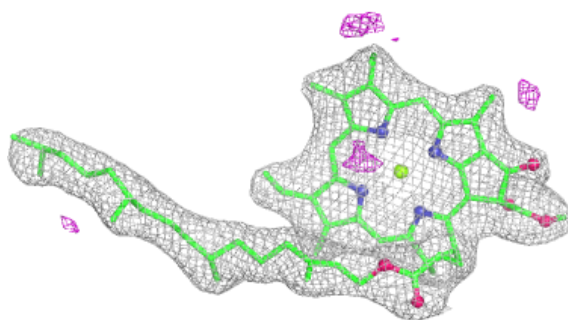


Electron density around CLA c 512:

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

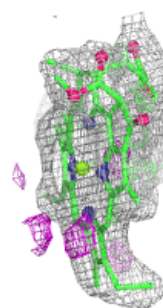
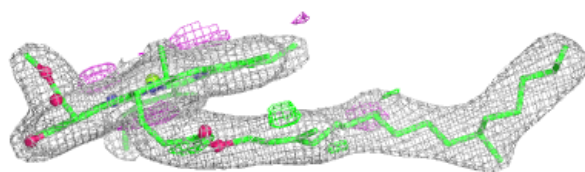
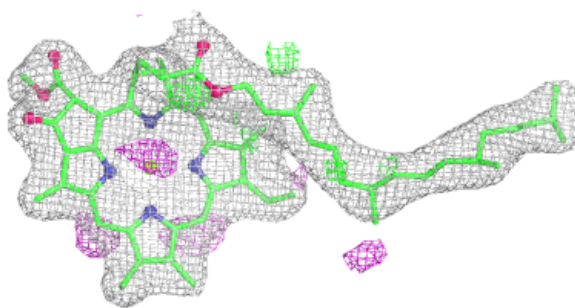
**Electron density around CLA C 502:**

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

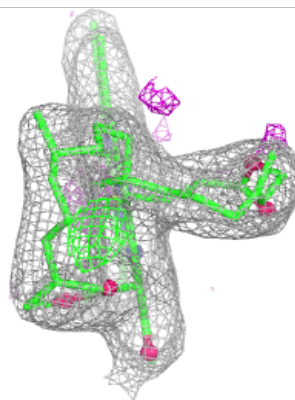
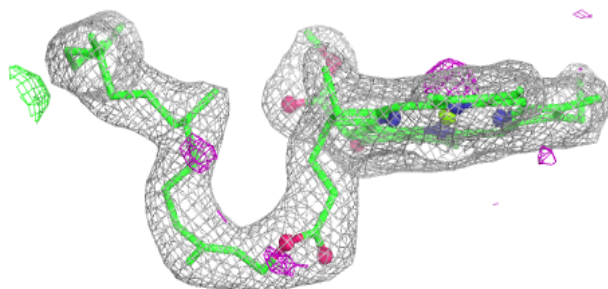
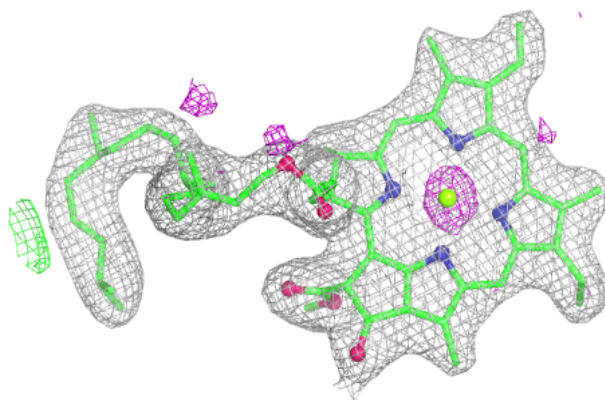


Electron density around CLA B 603:

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

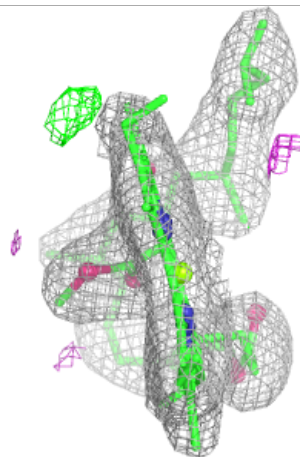
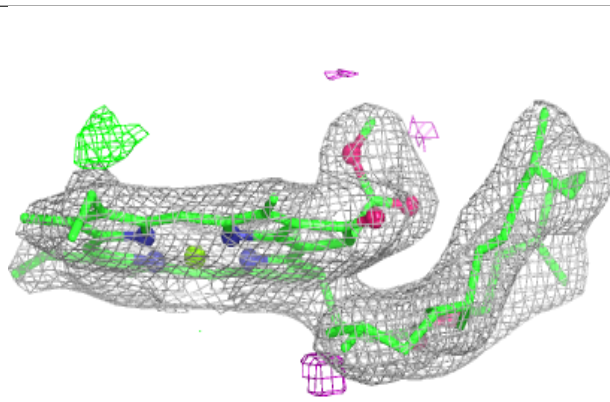
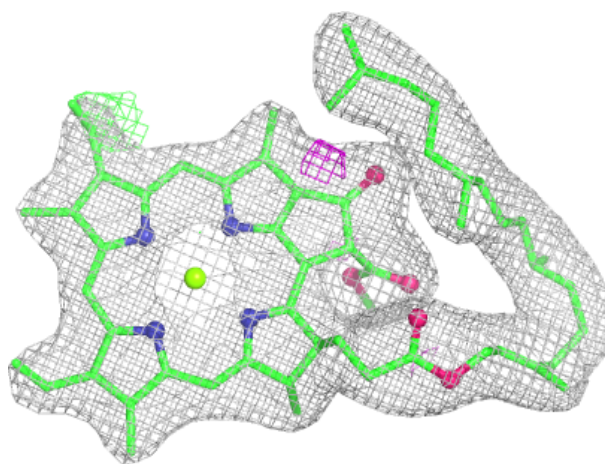
**Electron density around CLA B 612:**

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



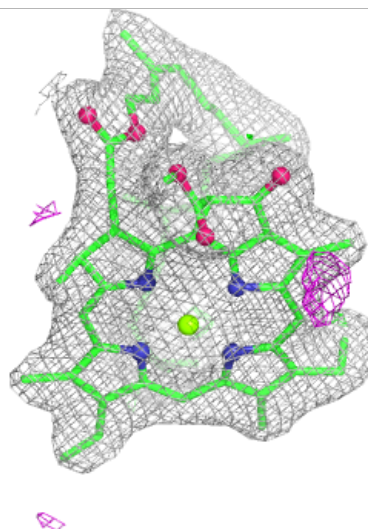
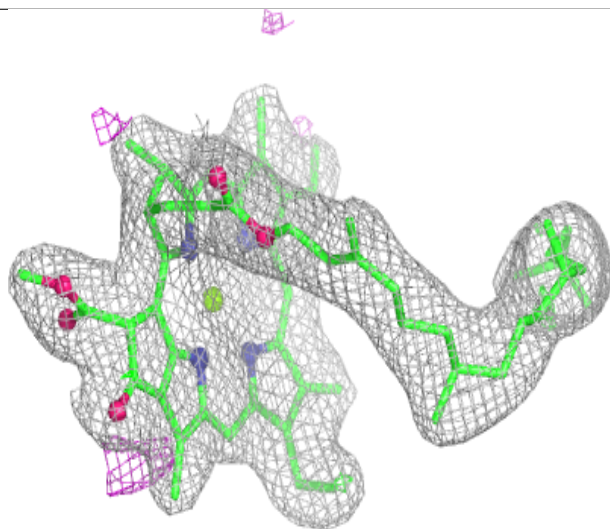
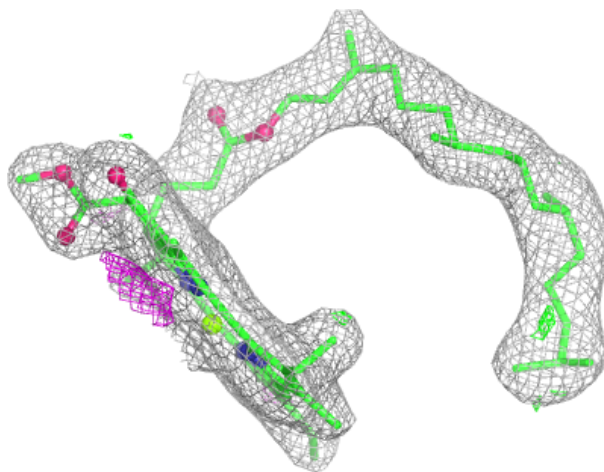
Electron density around CLA b 610:

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



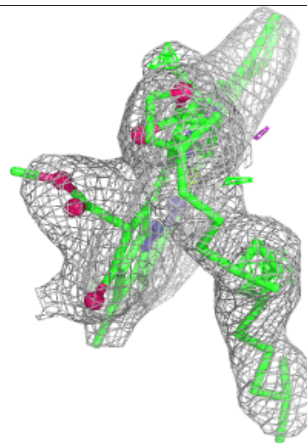
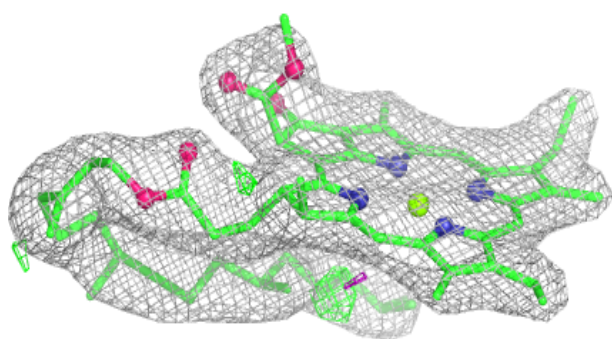
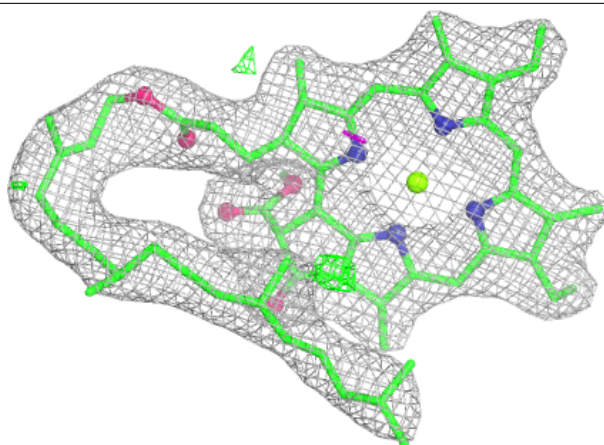
Electron density around CLA b 611:

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



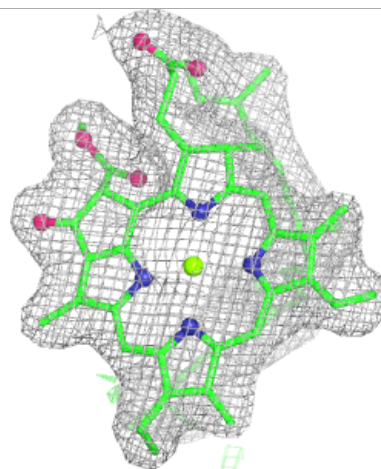
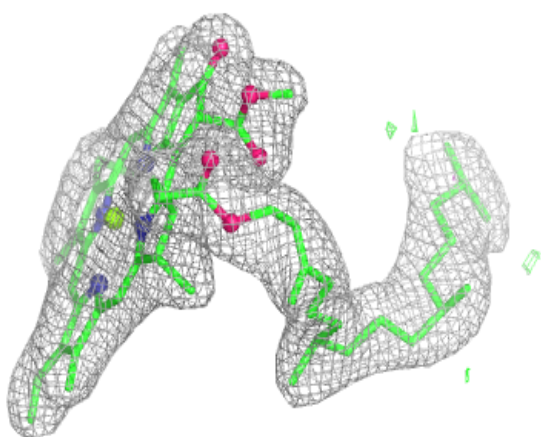
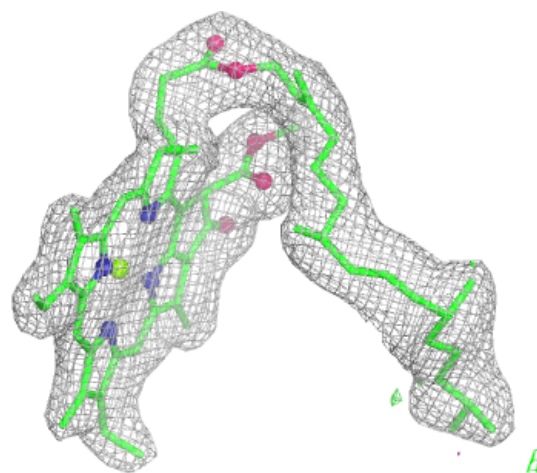
Electron density around CLA C 510:

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



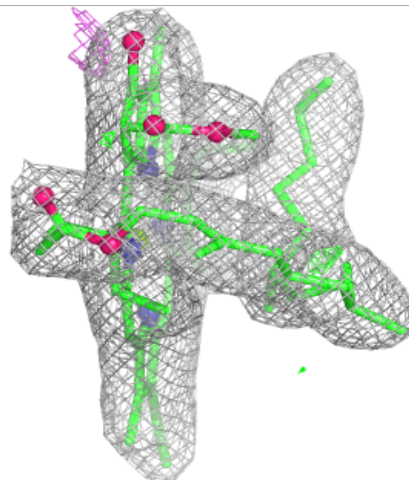
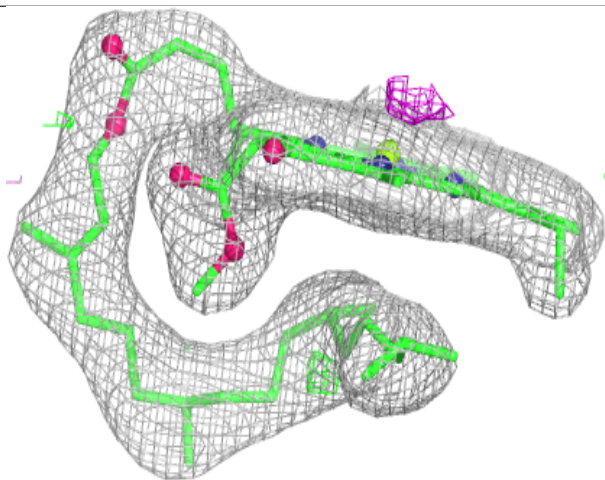
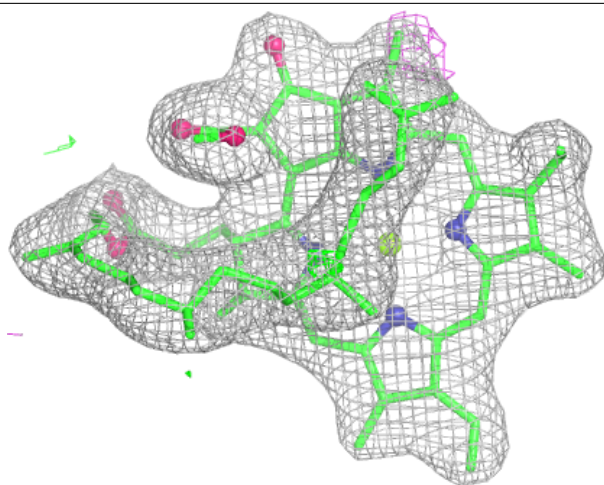
Electron density around CLA b 613:

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



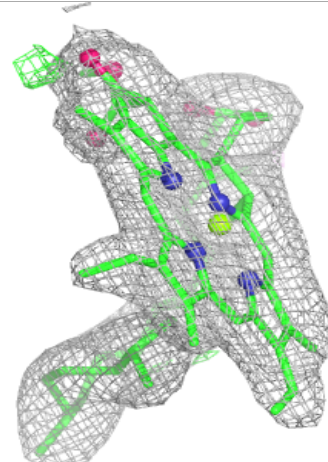
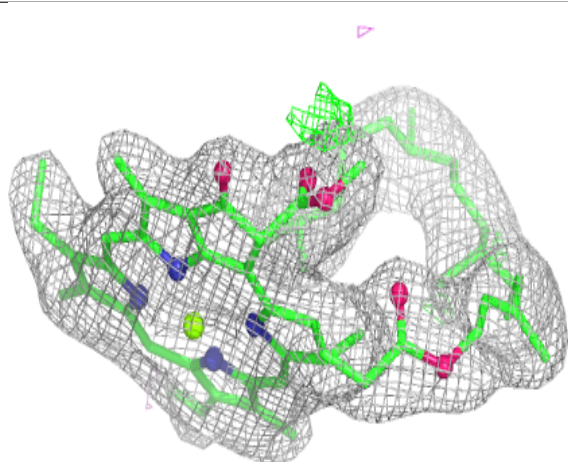
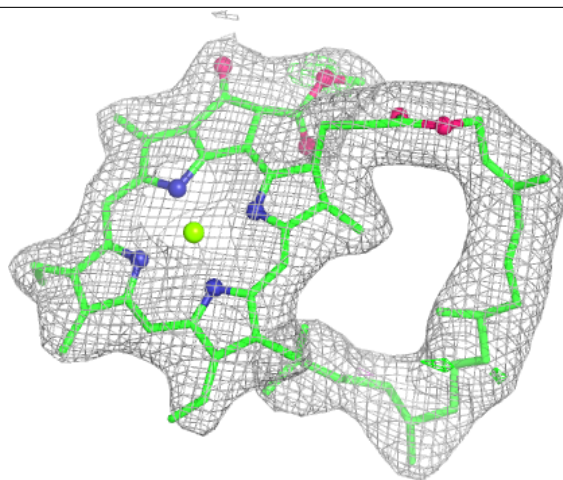
Electron density around CLA C 511:

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



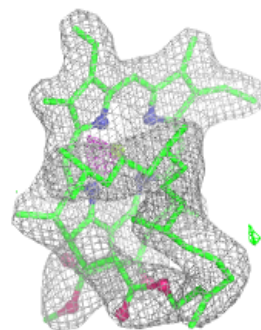
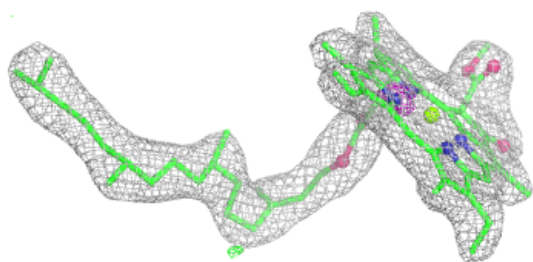
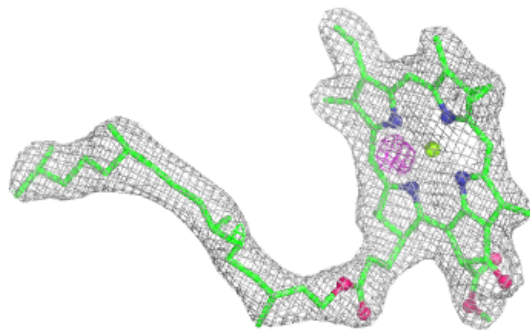
Electron density around CLA b 615:

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



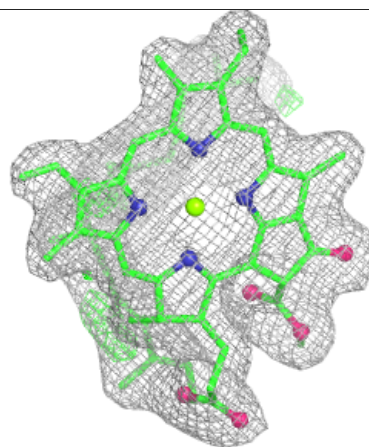
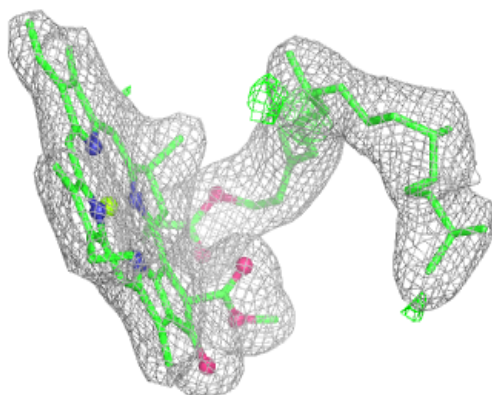
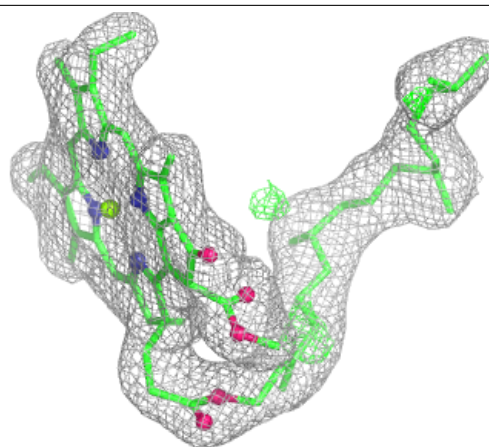
Electron density around CLA C 512:

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



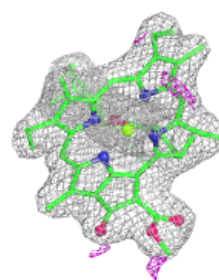
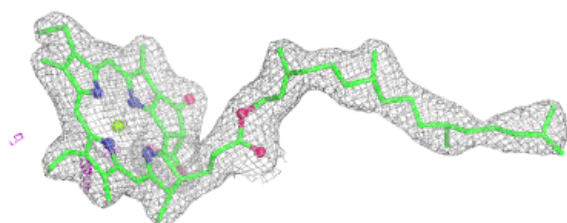
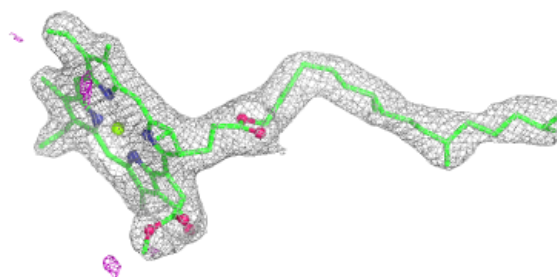
Electron density around CLA B 613:

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

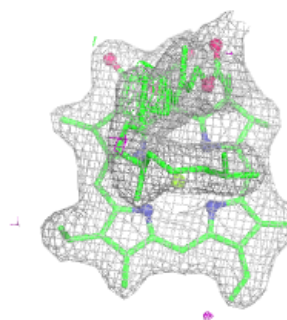
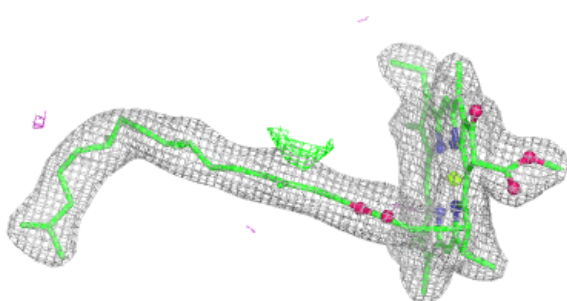
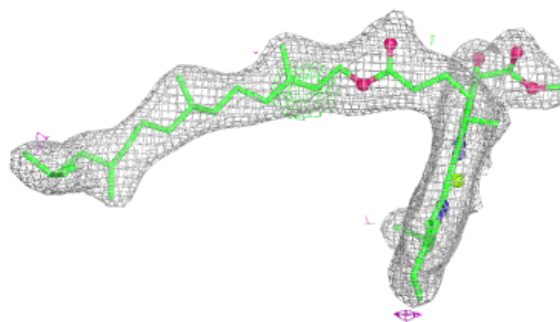


Electron density around CLA c 503:

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

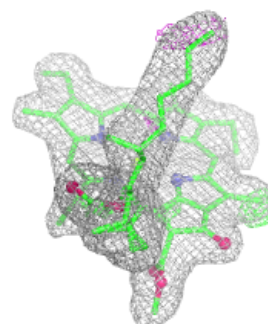
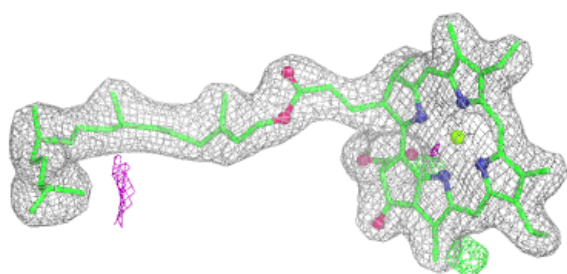
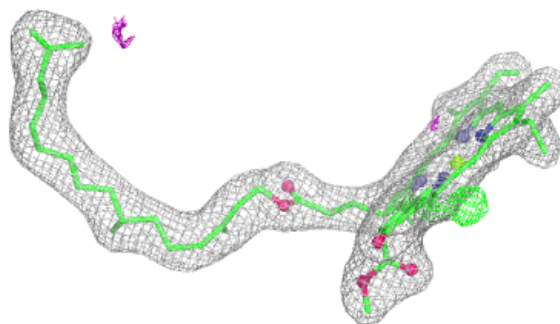
**Electron density around CLA B 605:**

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

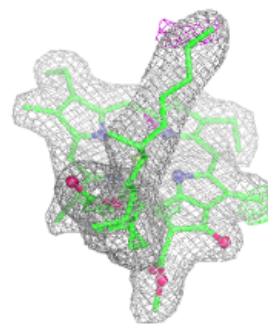
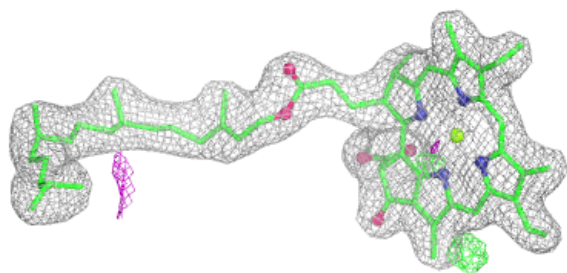
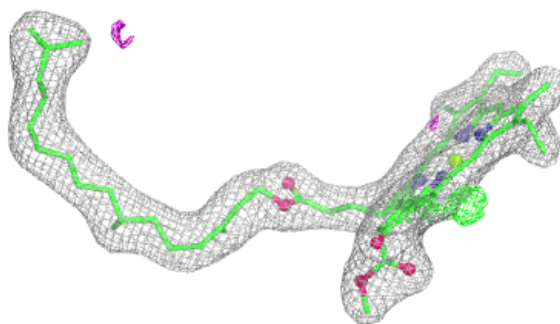


Electron density around CLA D 402 (A):

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

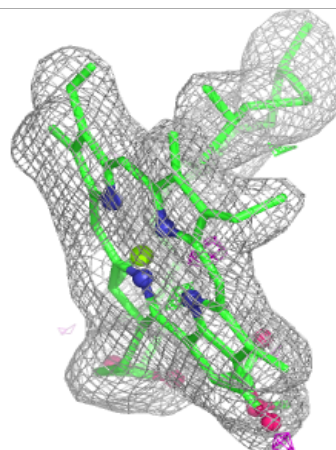
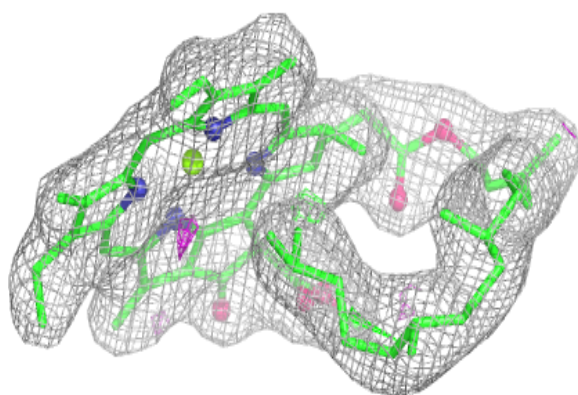
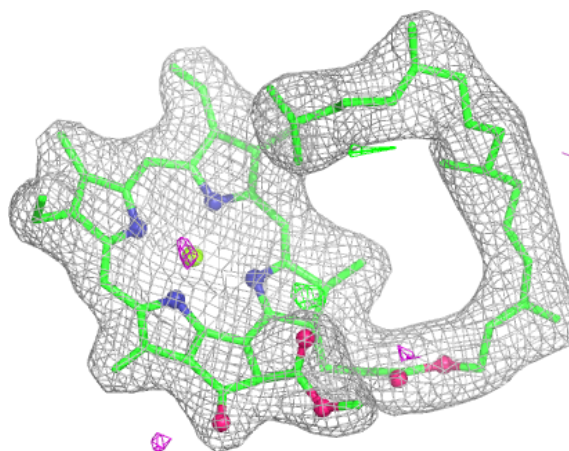
**Electron density around CLA D 402 (B):**

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



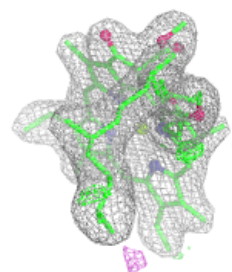
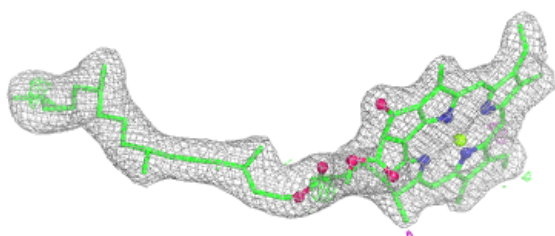
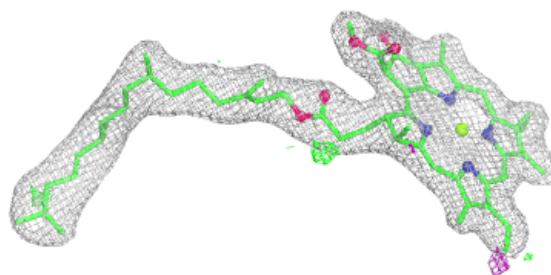
Electron density around CLA B 615:

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

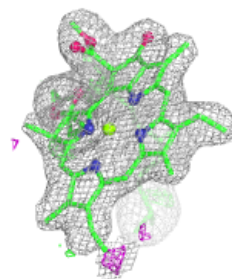
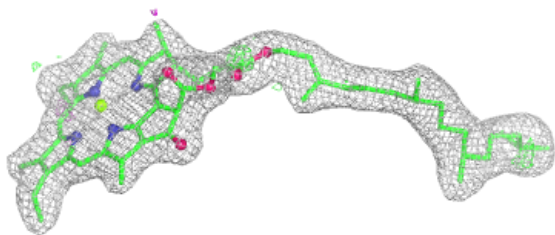
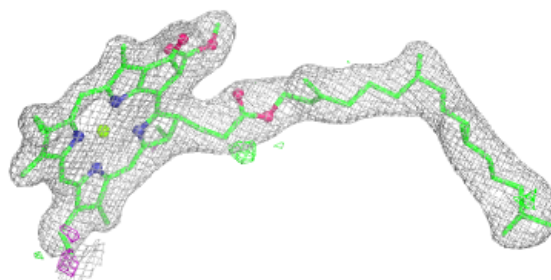


Electron density around CLA a 405 (A):

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

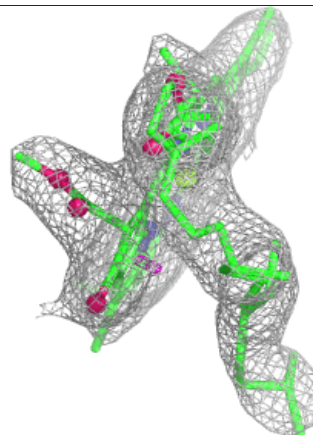
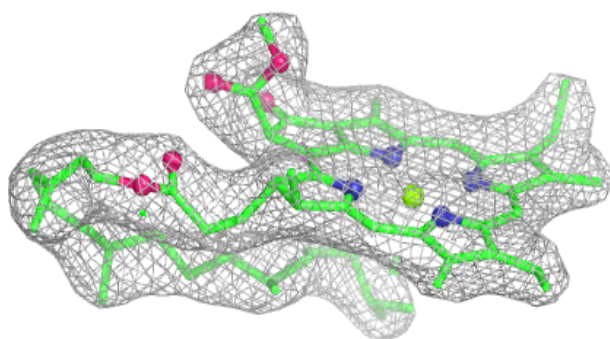
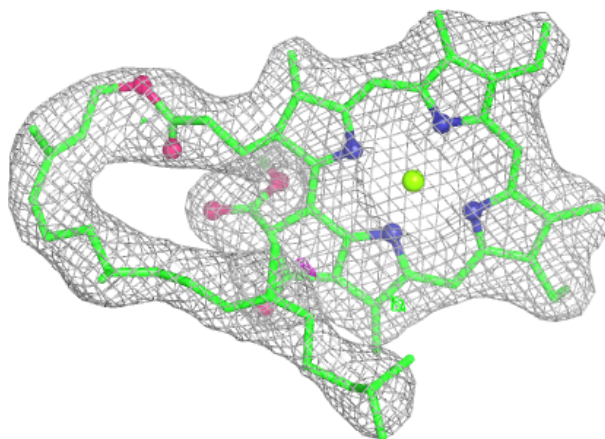
**Electron density around CLA a 405 (B):**

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



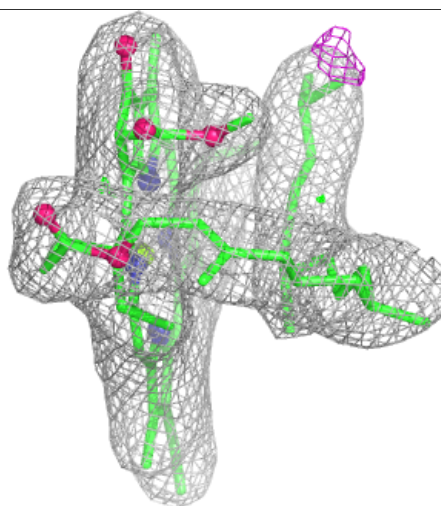
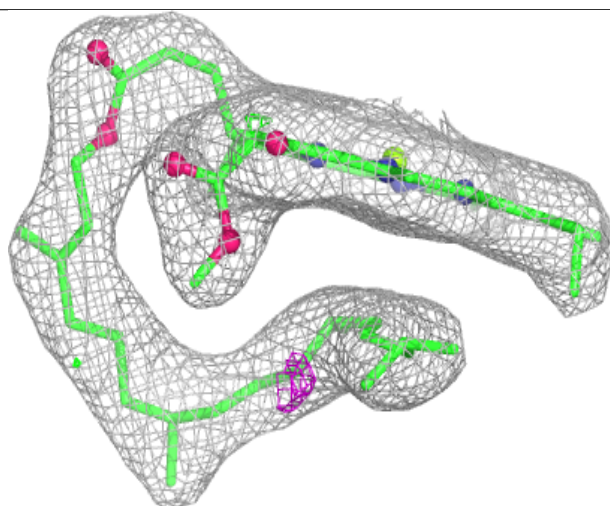
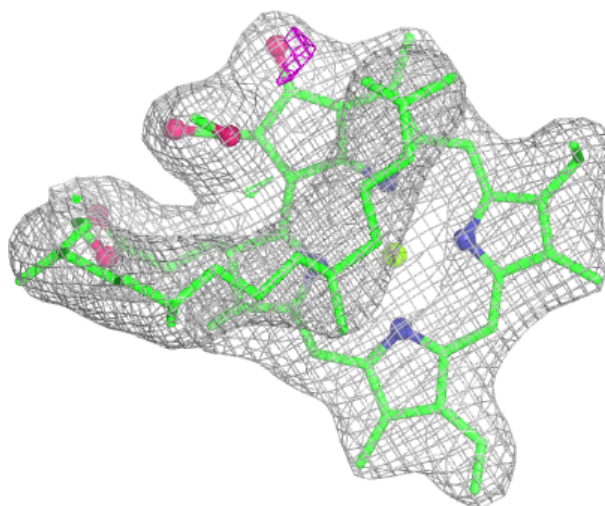
Electron density around CLA c 510:

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



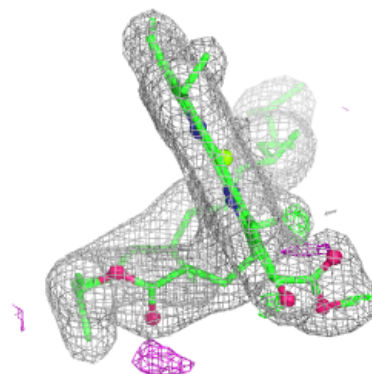
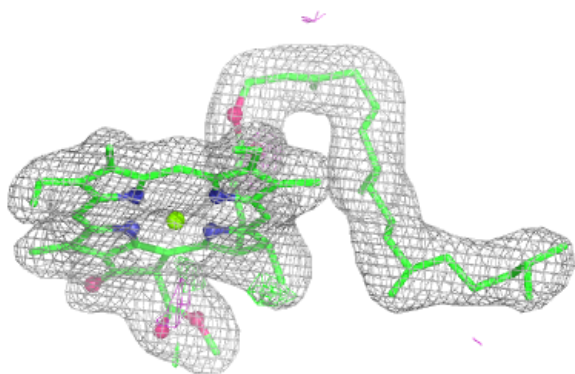
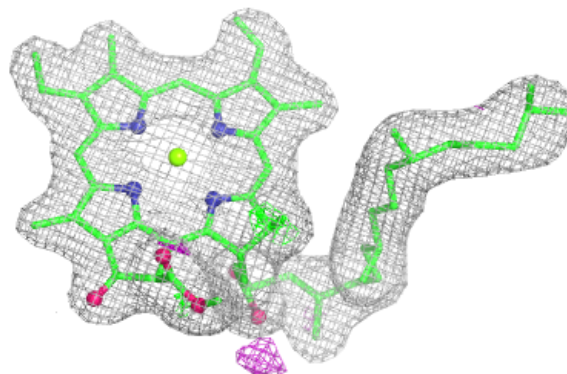
Electron density around CLA c 511:

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

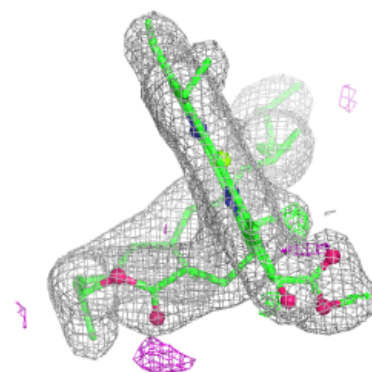
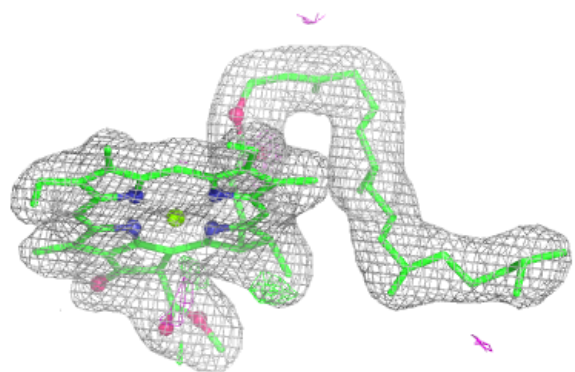
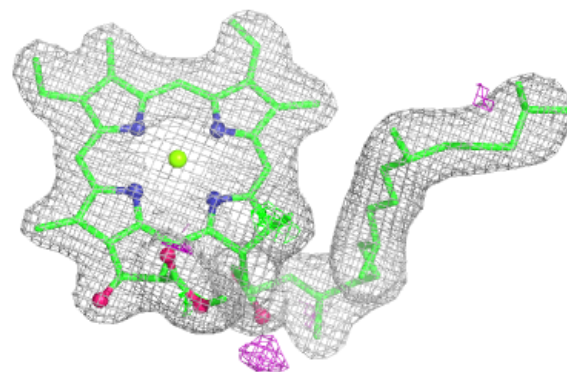


Electron density around CLA a 406 (A):

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

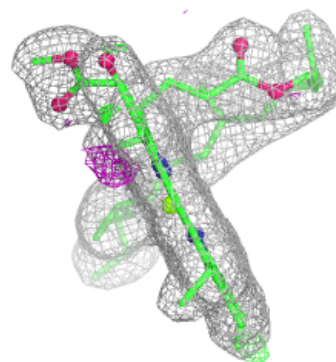
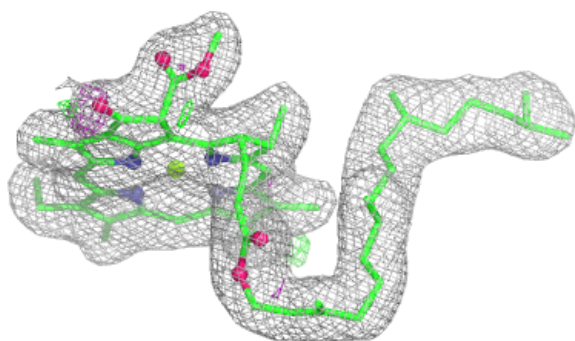
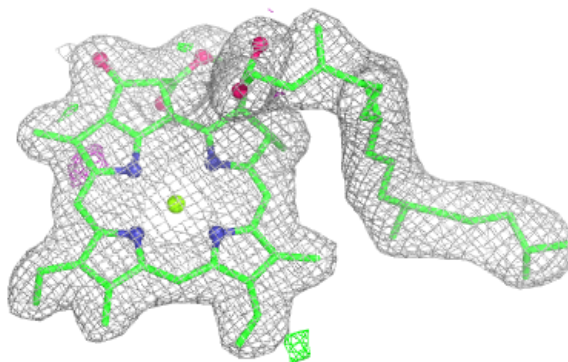
**Electron density around CLA a 406 (B):**

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

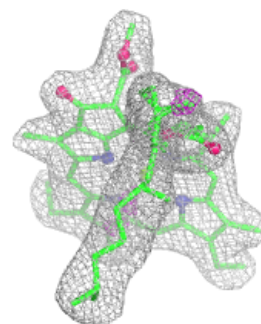
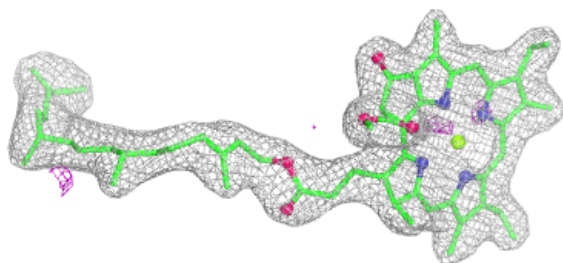
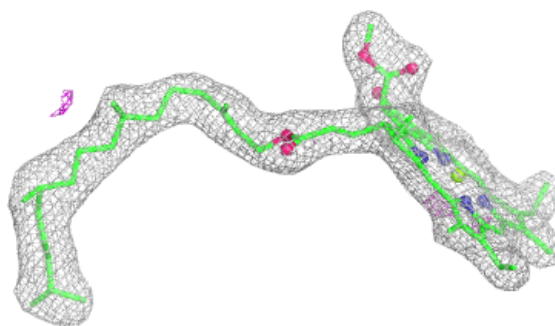


Electron density around CLA A 406 (A):

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

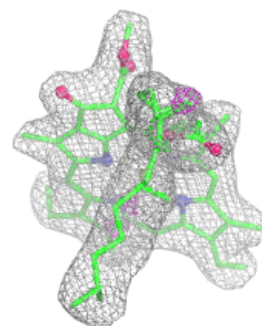
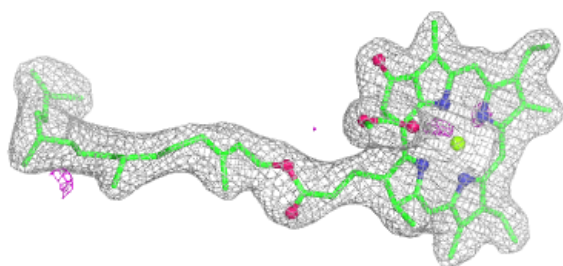
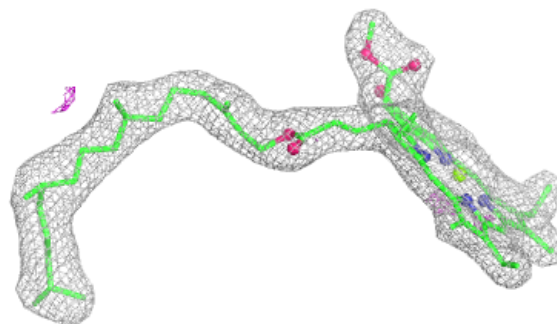
**Electron density around CLA d 403 (A):**

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

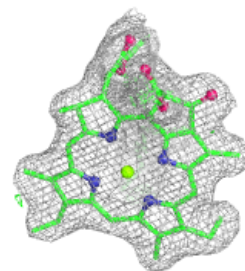
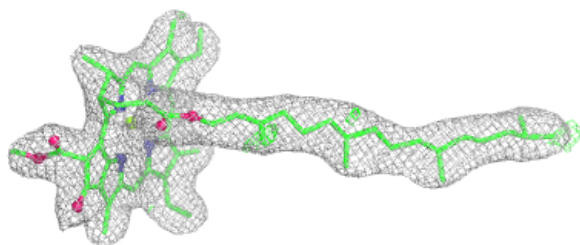
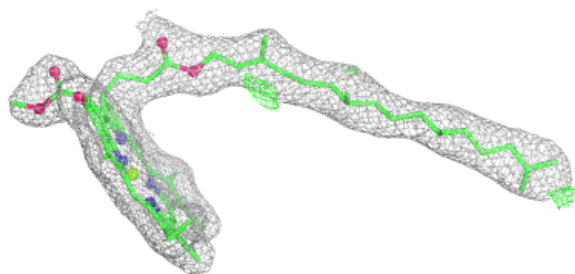


Electron density around CLA d 403 (B):

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

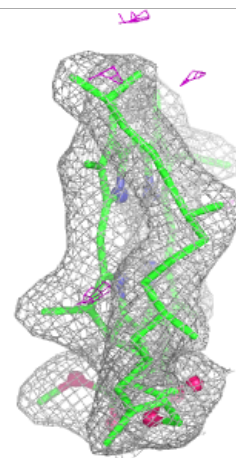
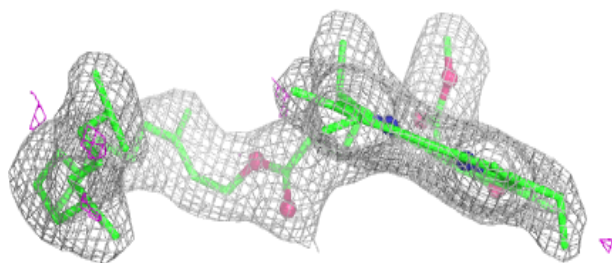
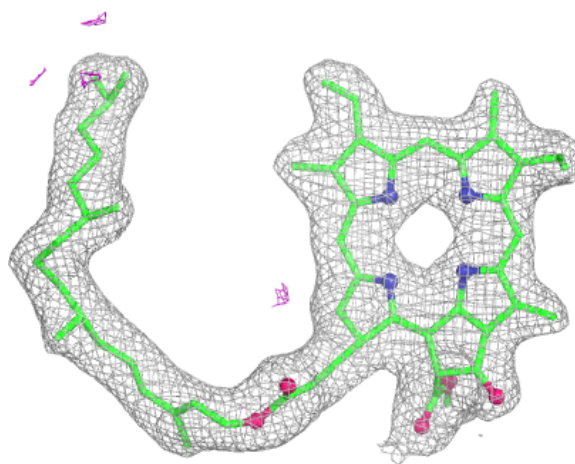
**Electron density around CLA B 607:**

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



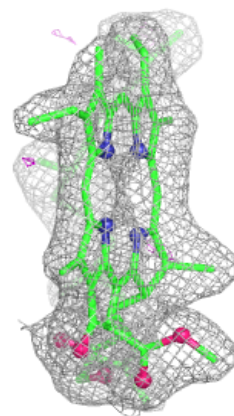
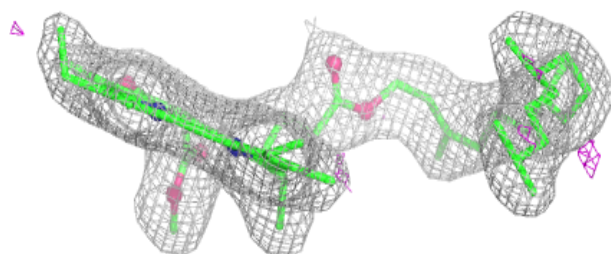
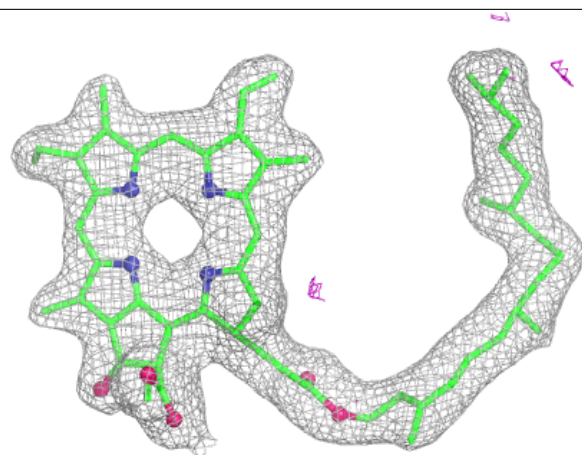
Electron density around PHO A 408 (A):

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



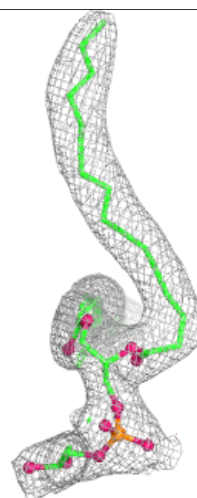
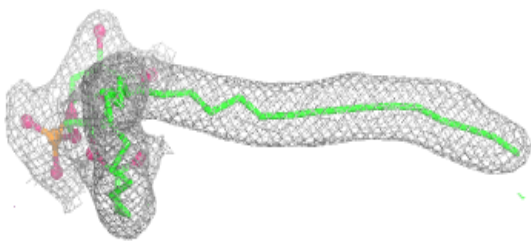
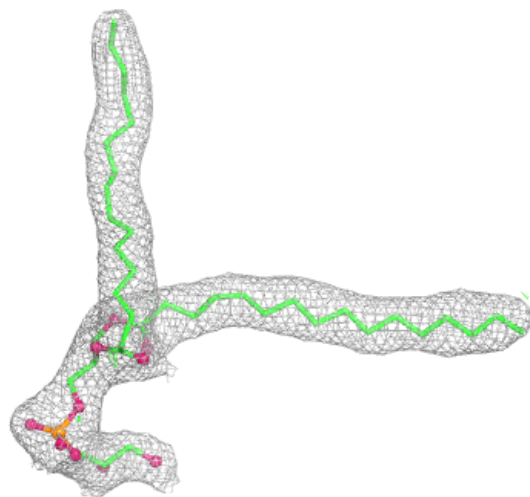
Electron density around PHO A 408 (B):

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



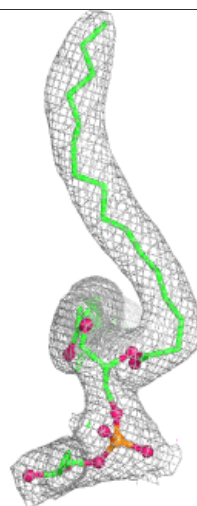
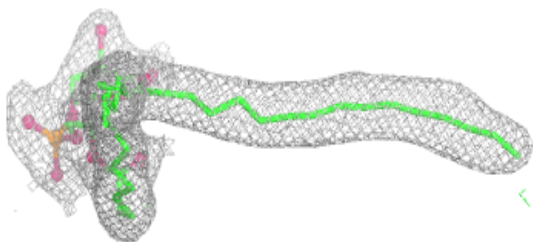
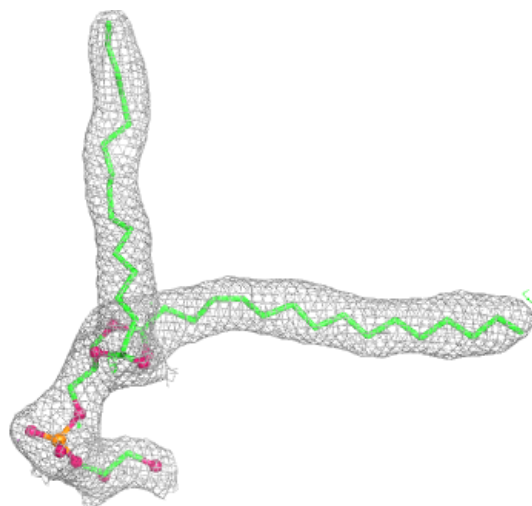
Electron density around LHG L 101 (A):

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



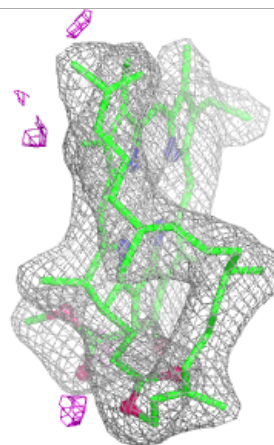
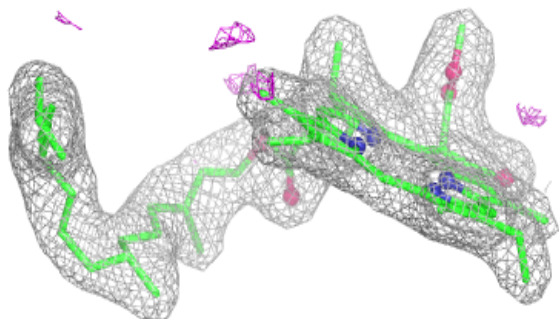
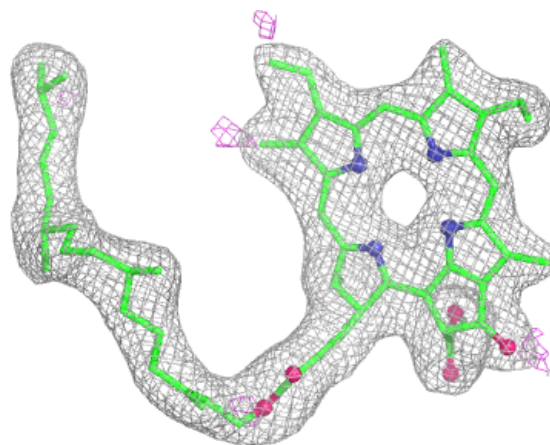
Electron density around LHG L 101 (B):

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



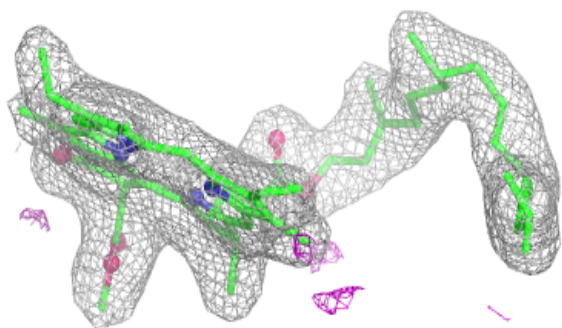
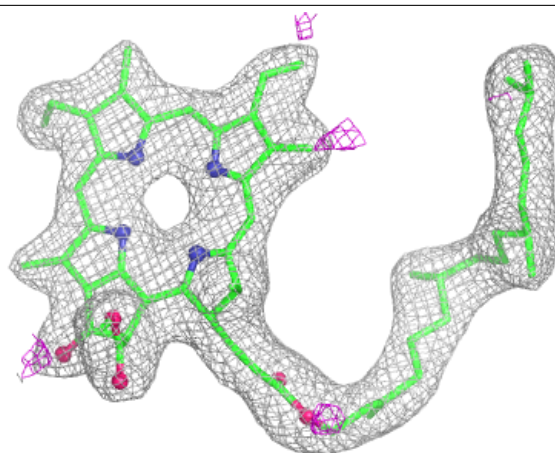
Electron density around PHO A 417 (A):

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



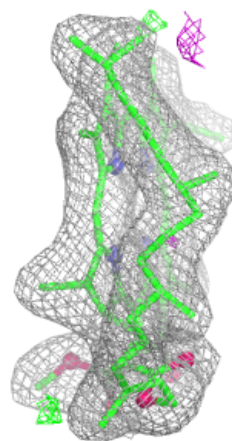
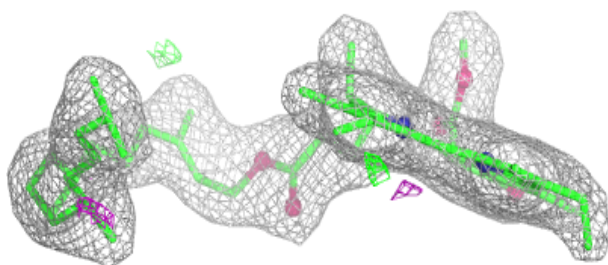
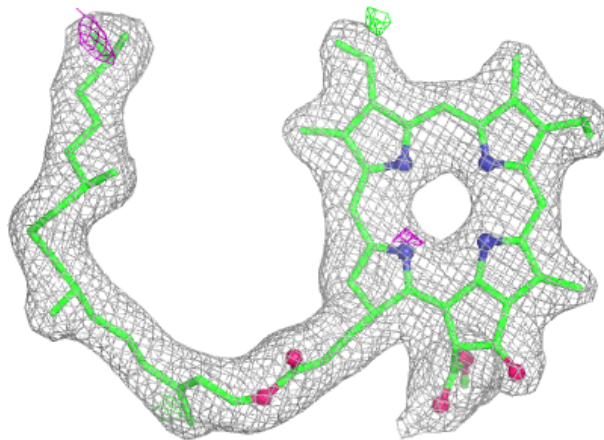
Electron density around PHO A 417 (B):

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



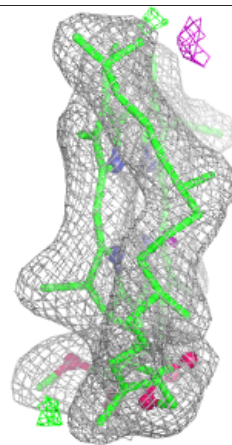
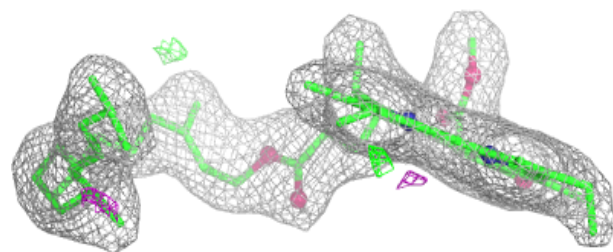
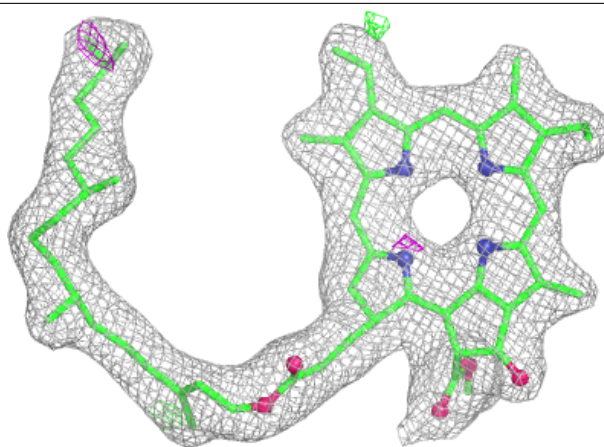
Electron density around PHO a 408 (A):

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



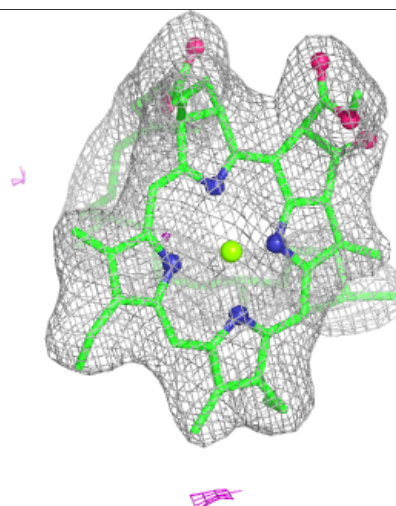
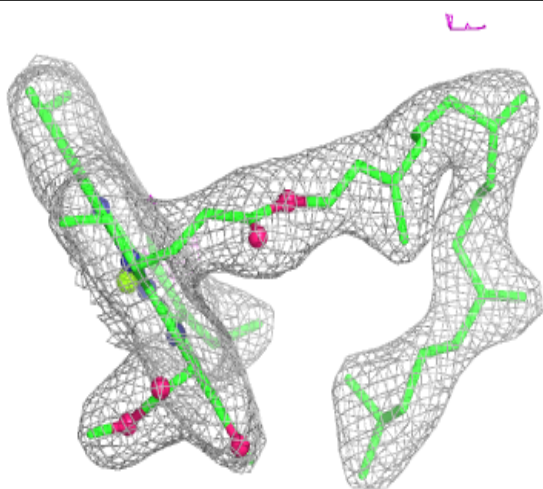
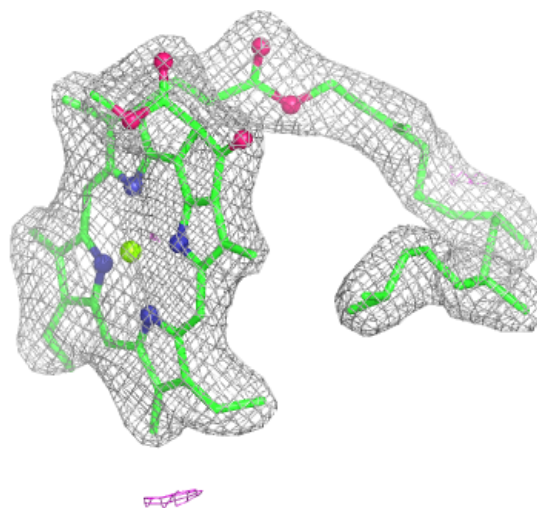
Electron density around PHO a 408 (B):

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



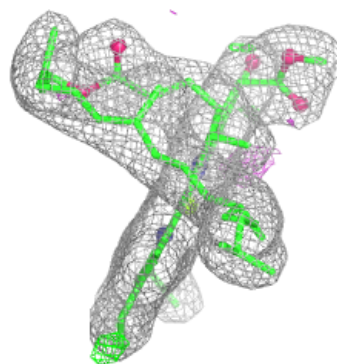
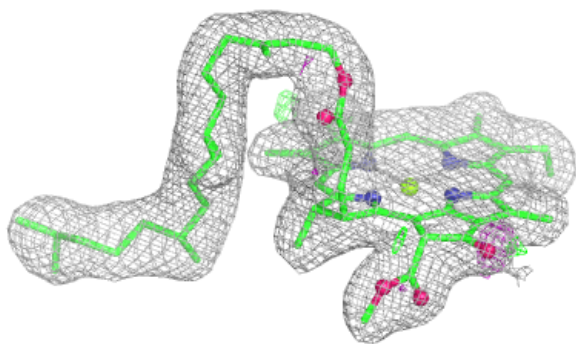
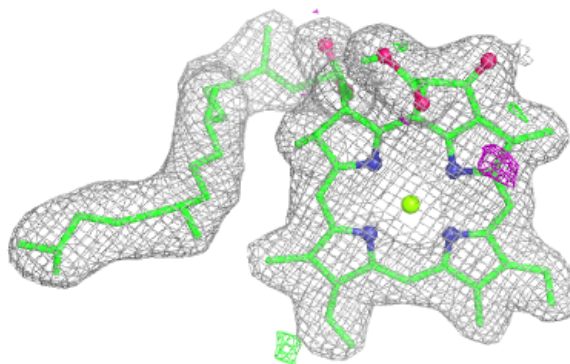
Electron density around CLA C 504:

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

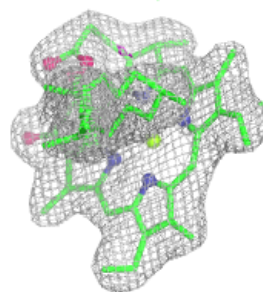
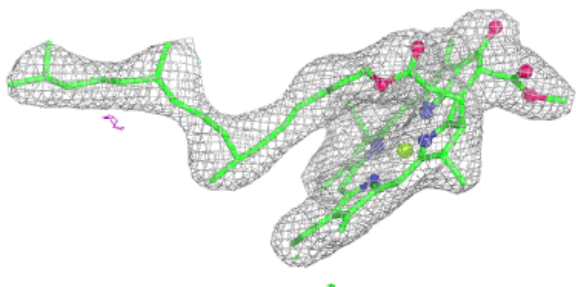
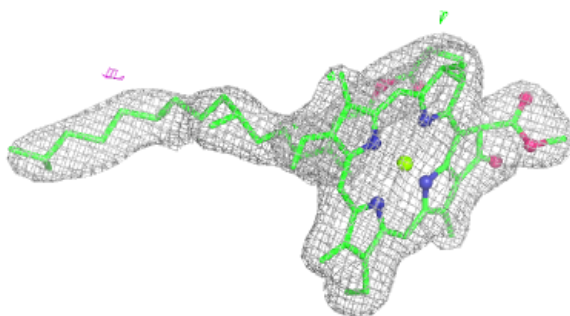


Electron density around CLA A 406 (B):

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

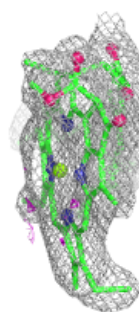
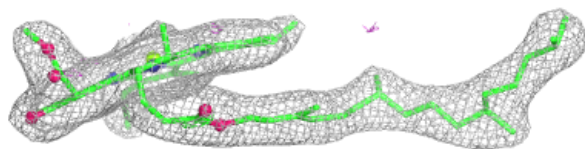
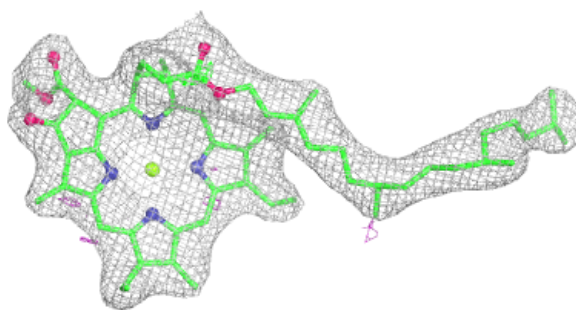
**Electron density around CLA C 506:**

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

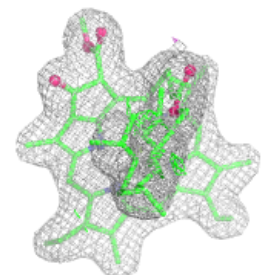
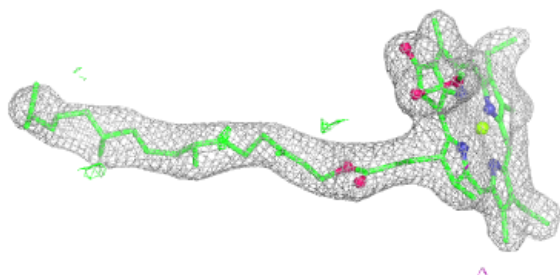
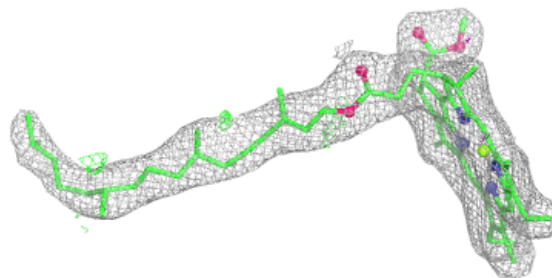


Electron density around CLA b 603:

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

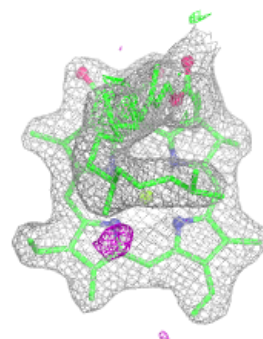
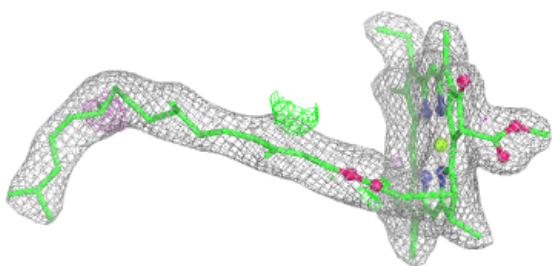
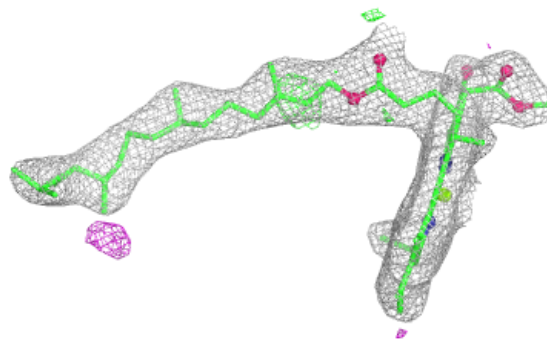
**Electron density around CLA b 604:**

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



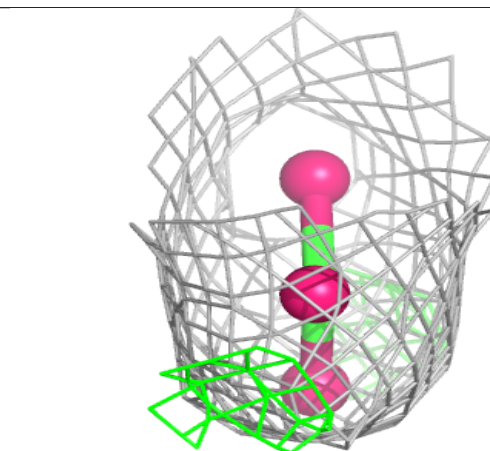
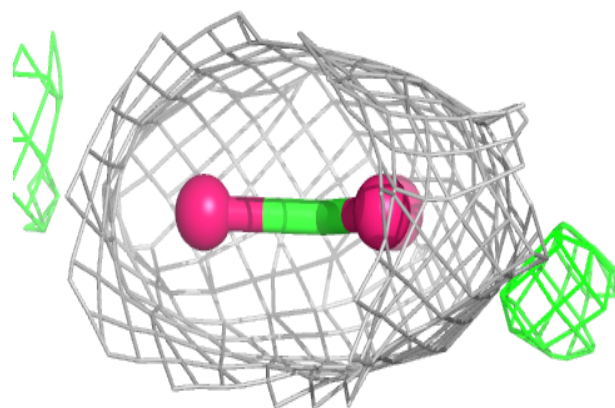
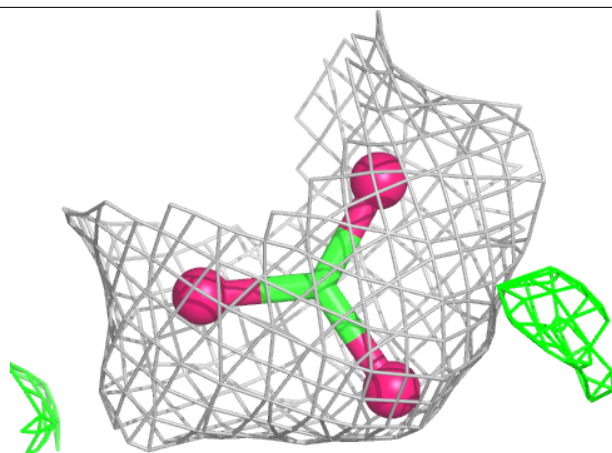
Electron density around CLA b 605:

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



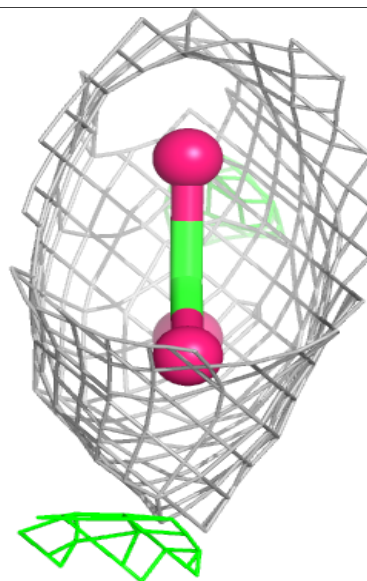
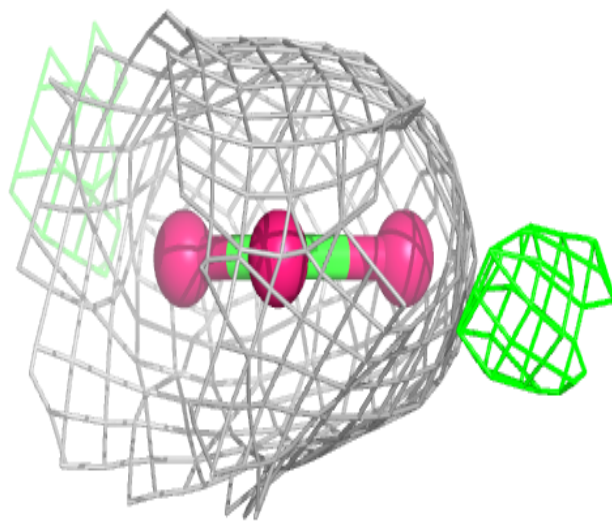
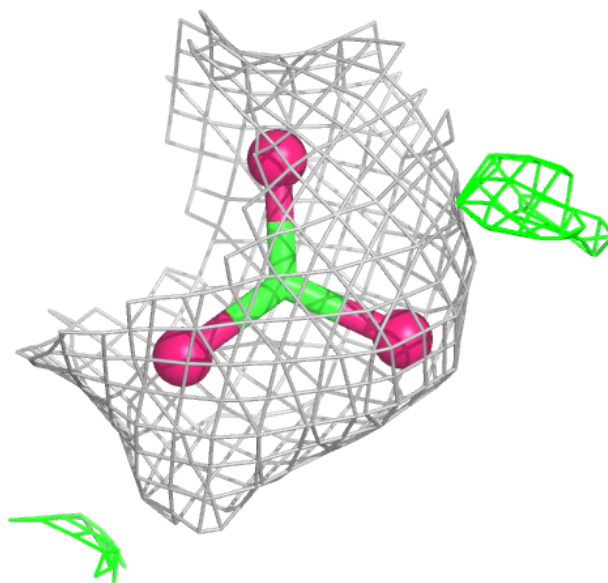
Electron density around BCT D 401 (A):

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



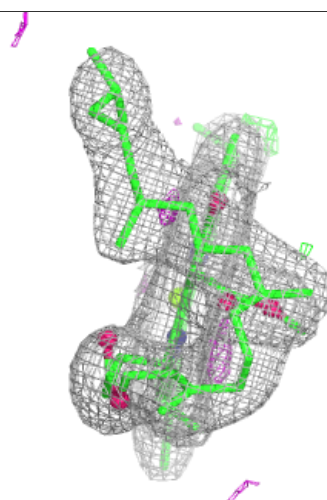
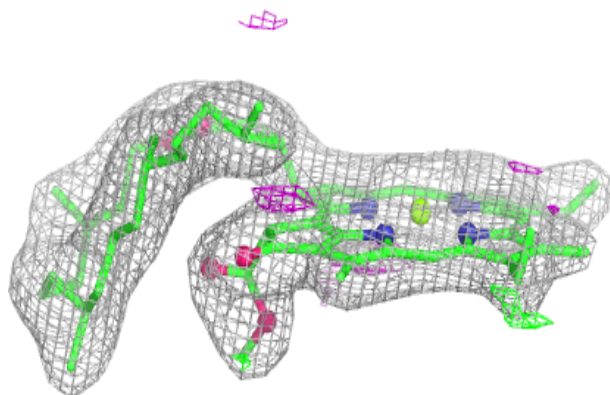
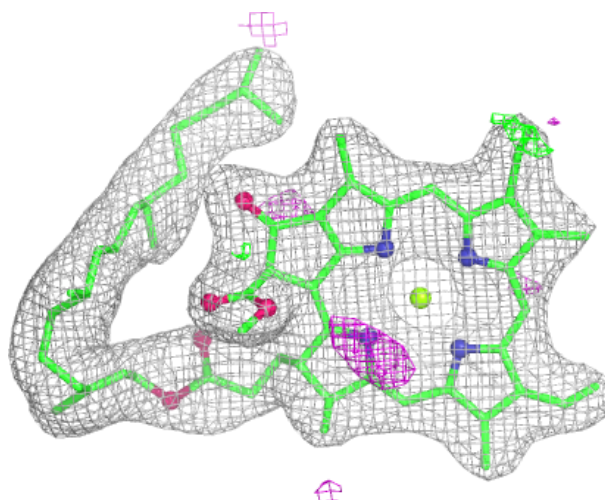
Electron density around BCT D 401 (B):

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



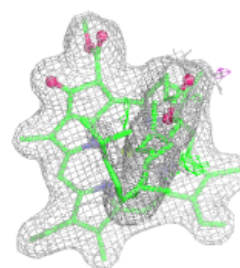
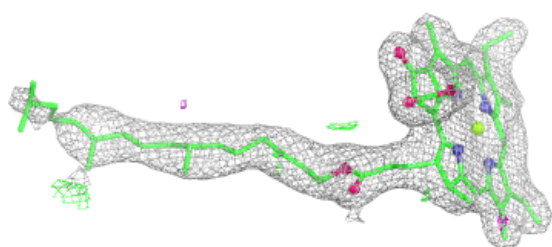
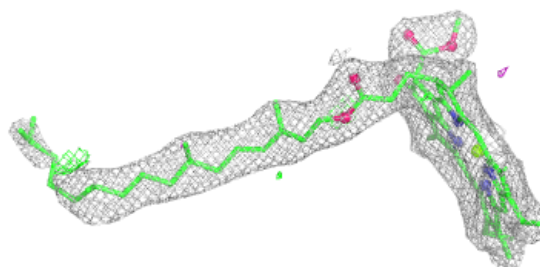
Electron density around CLA B 610:

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

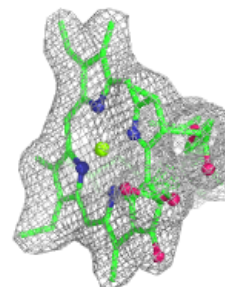
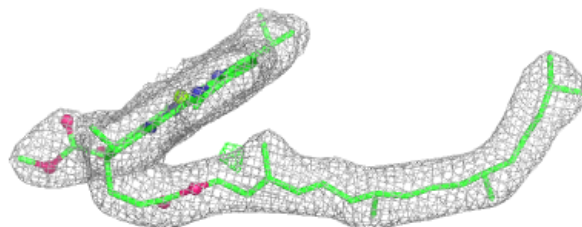
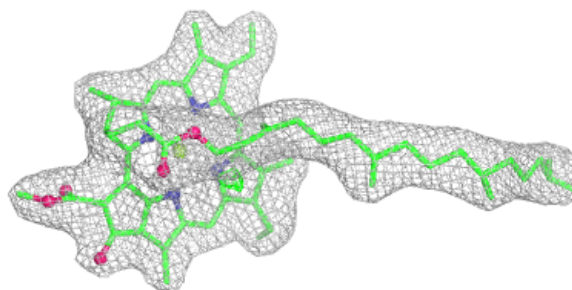


Electron density around CLA B 604:

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

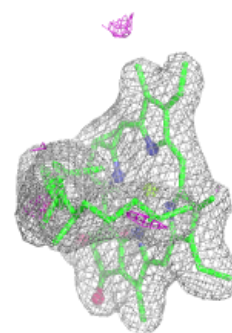
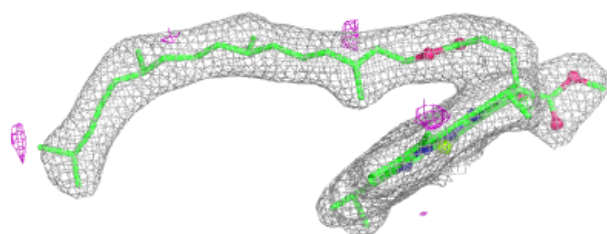
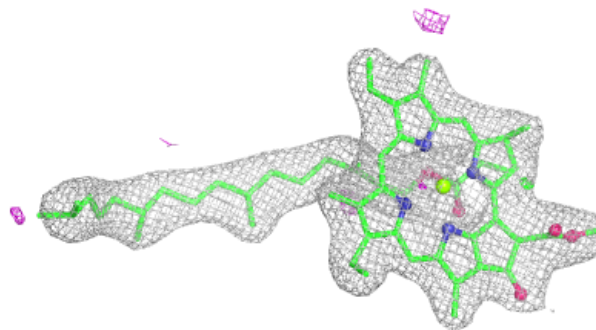
**Electron density around CLA b 608:**

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

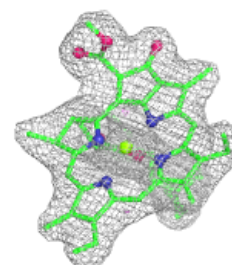
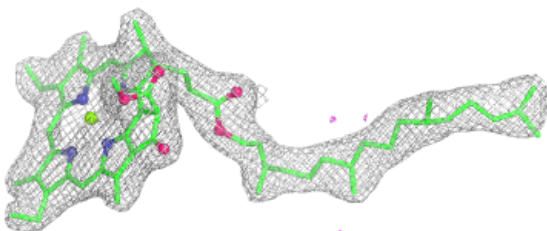
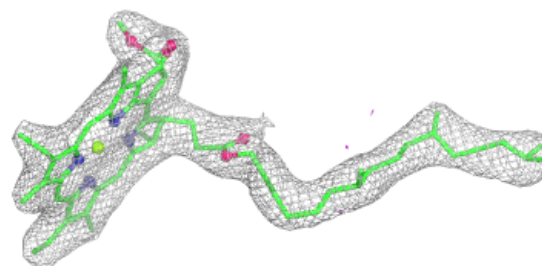


Electron density around CLA B 608:

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

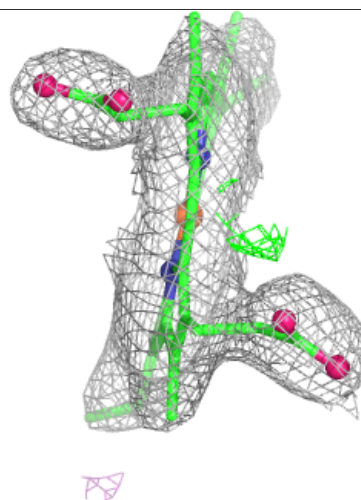
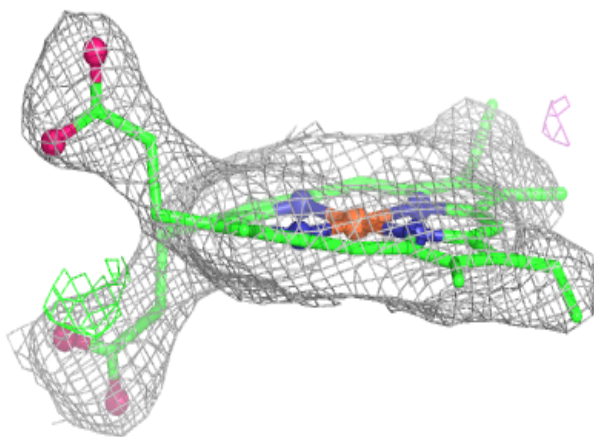
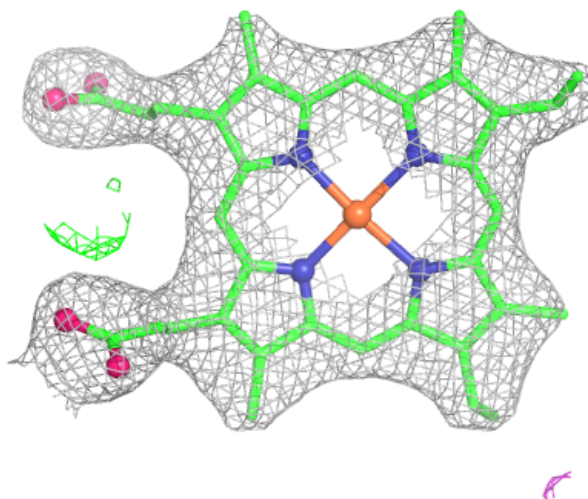
**Electron density around CLA C 503:**

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



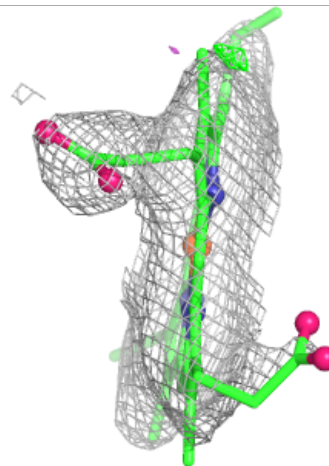
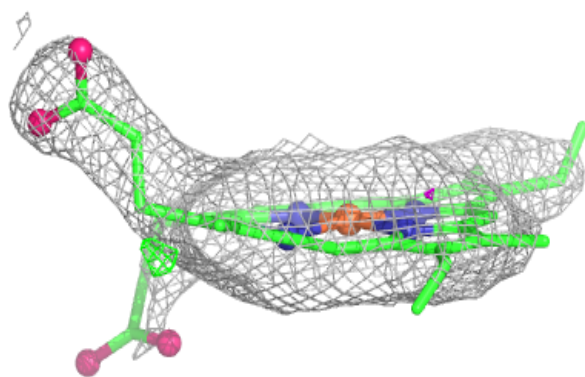
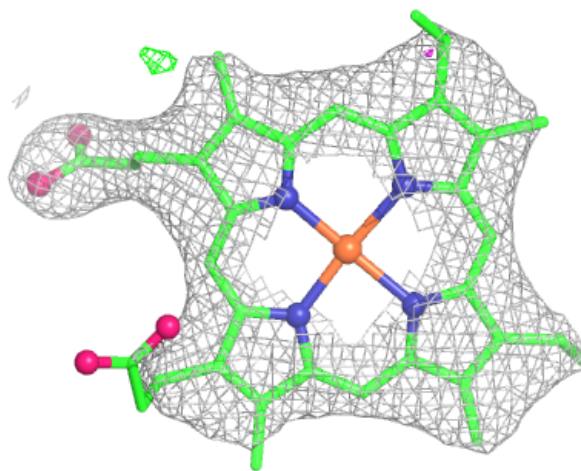
Electron density around HEM F 102:

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



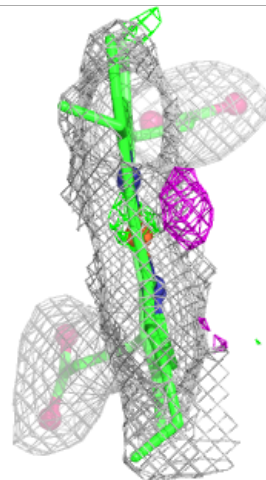
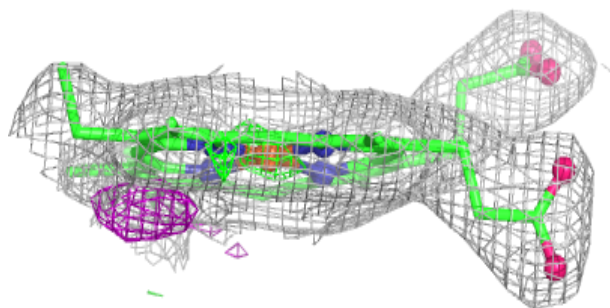
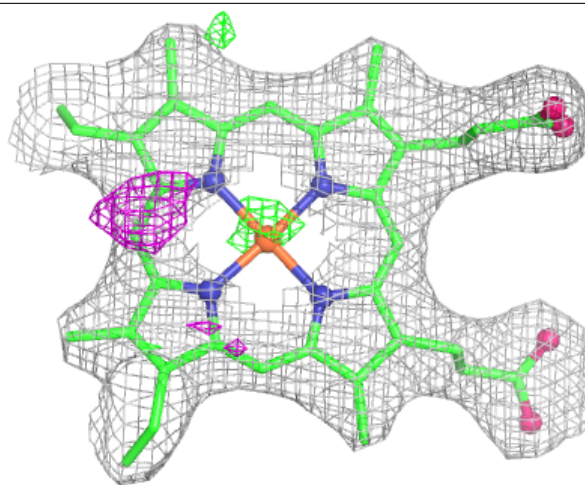
Electron density around HEM e 101:

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



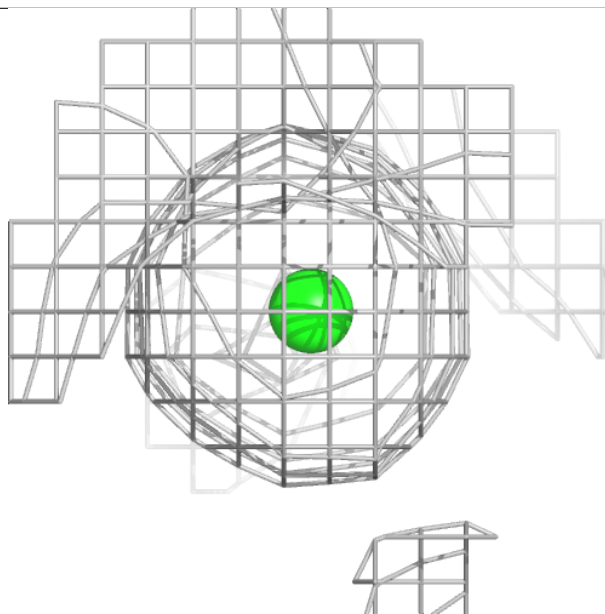
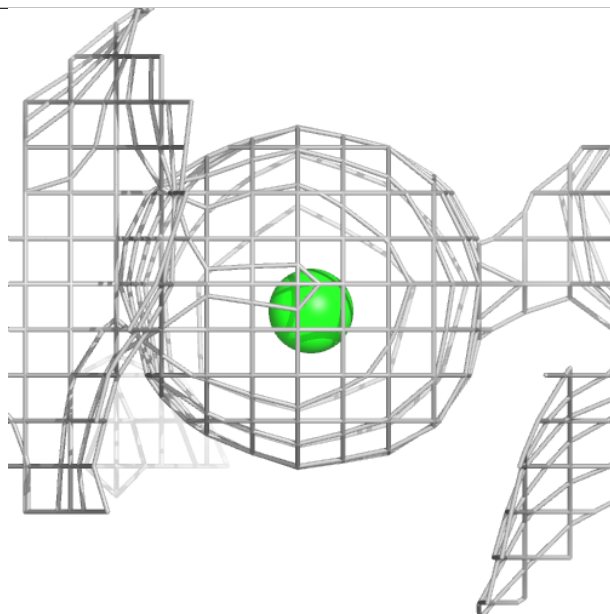
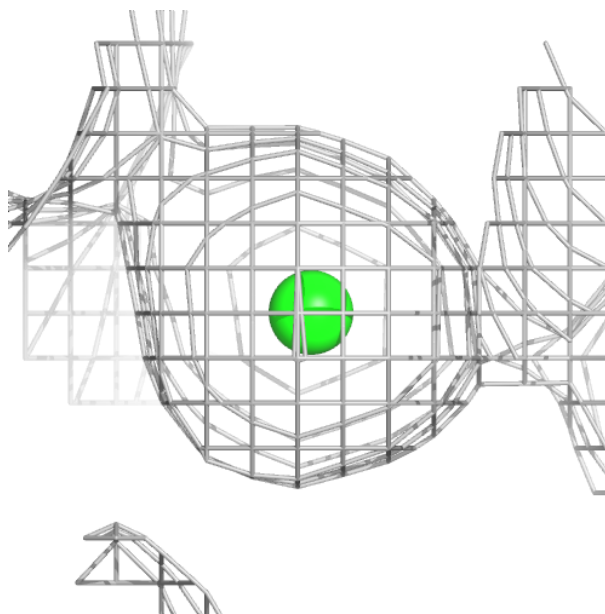
Electron density around HEC v 201:

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



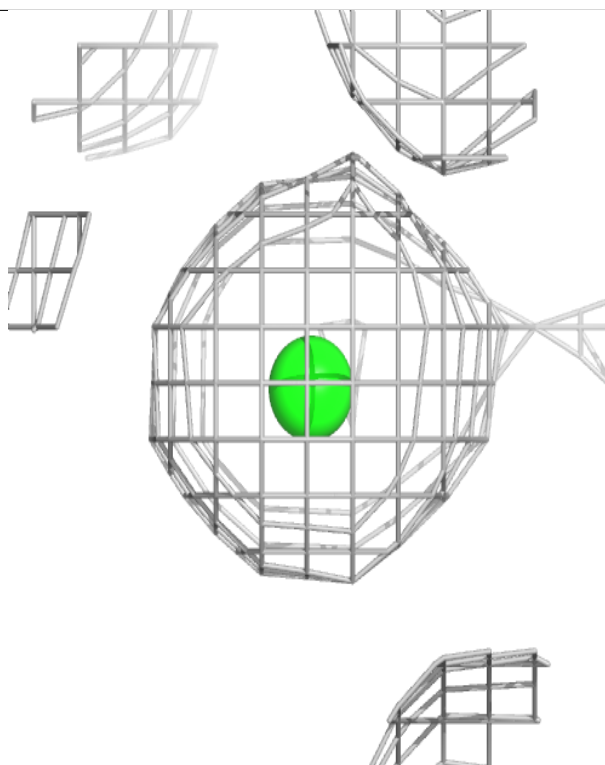
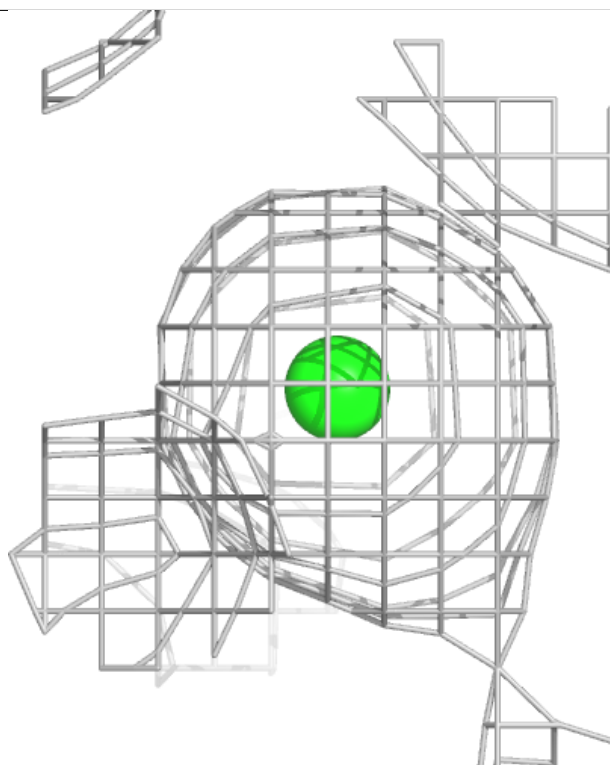
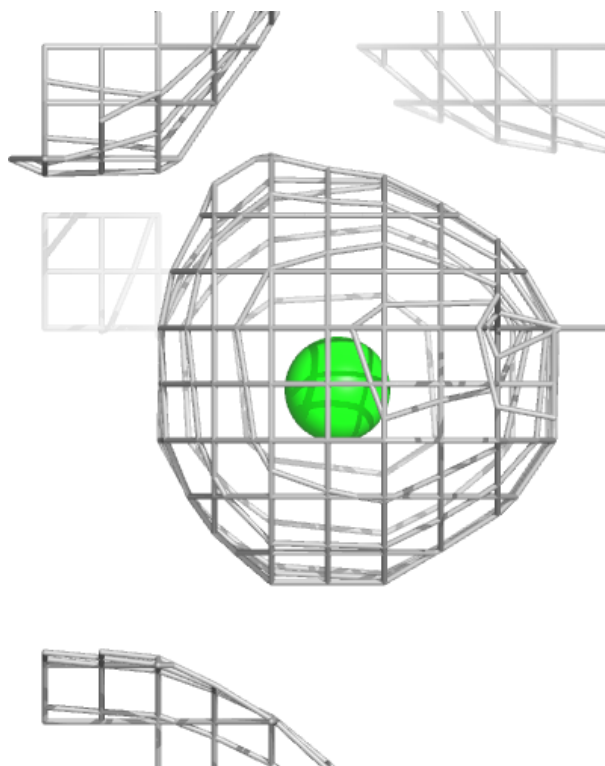
Electron density around CL A 404 (B):

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



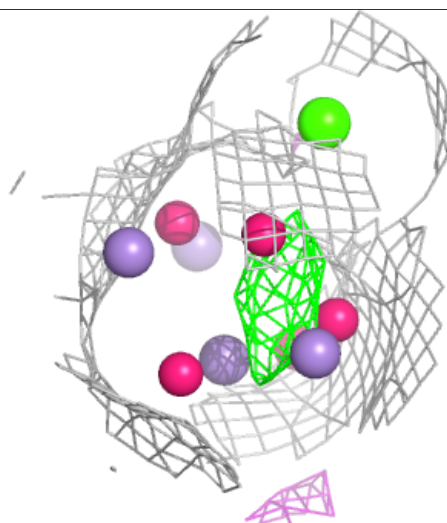
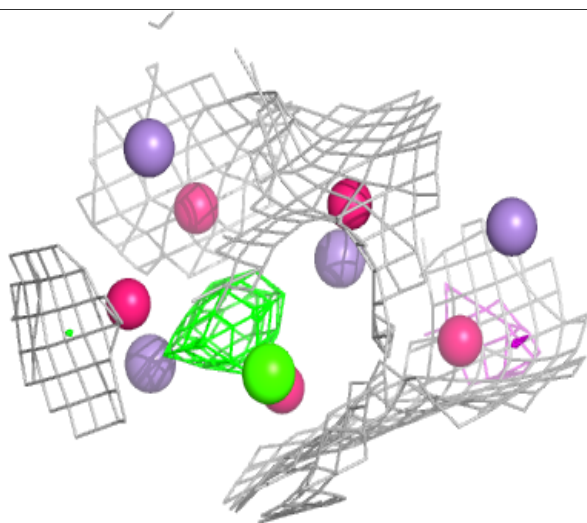
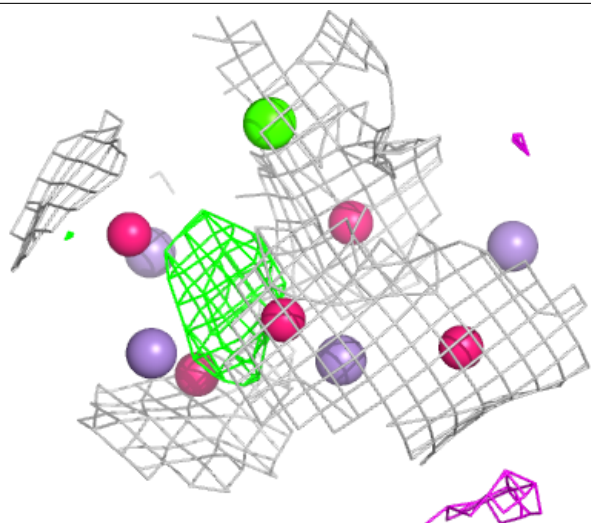
Electron density around CL a 403 (A):

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



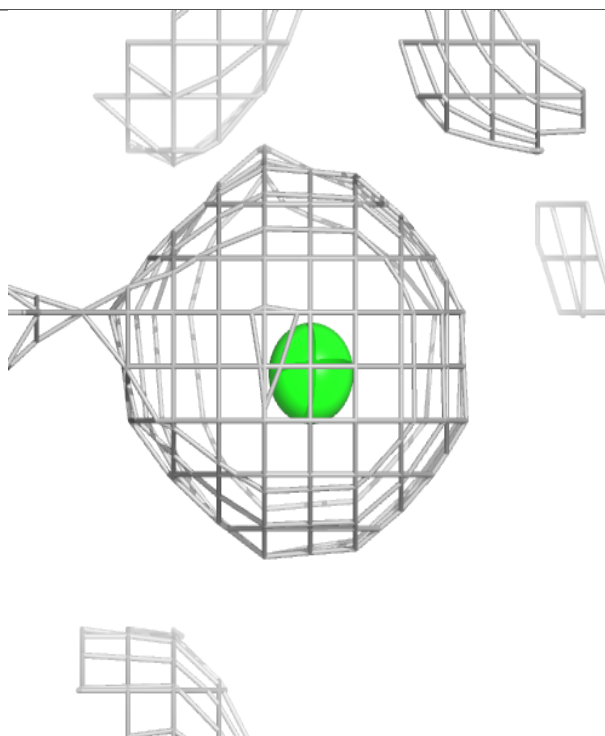
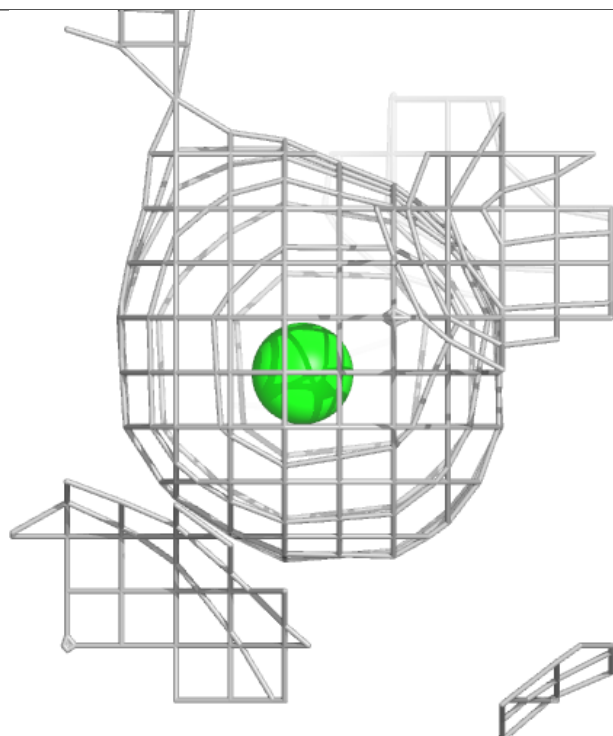
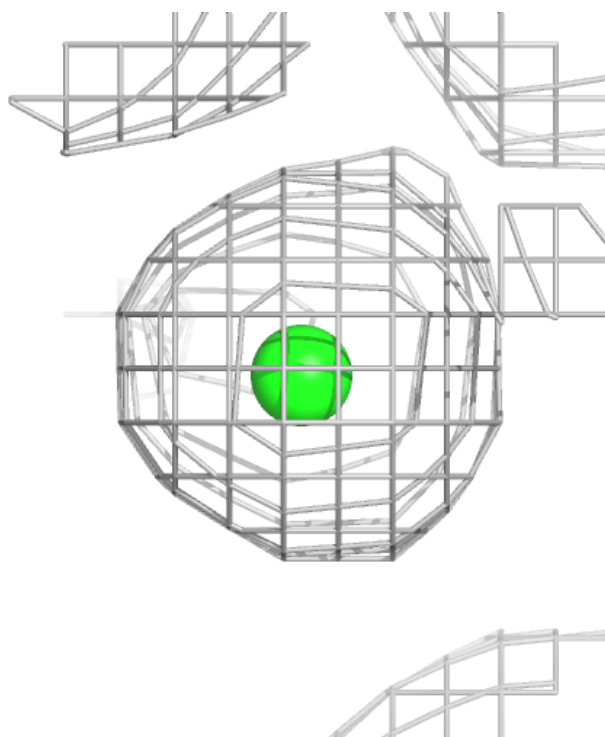
Electron density around OEX A 414 (A):

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



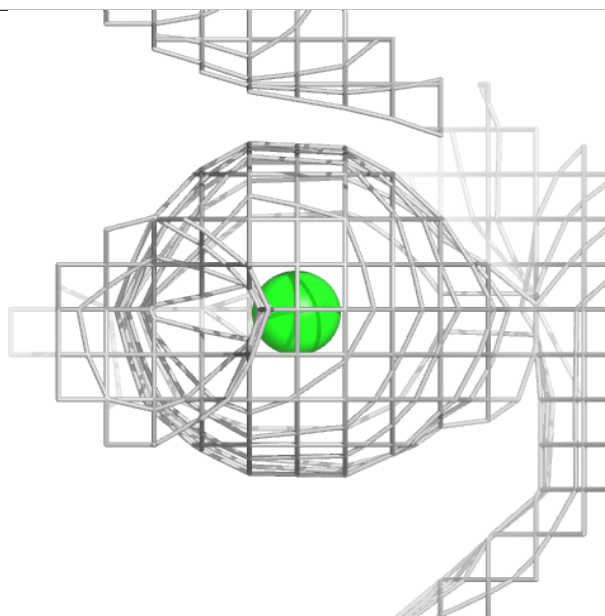
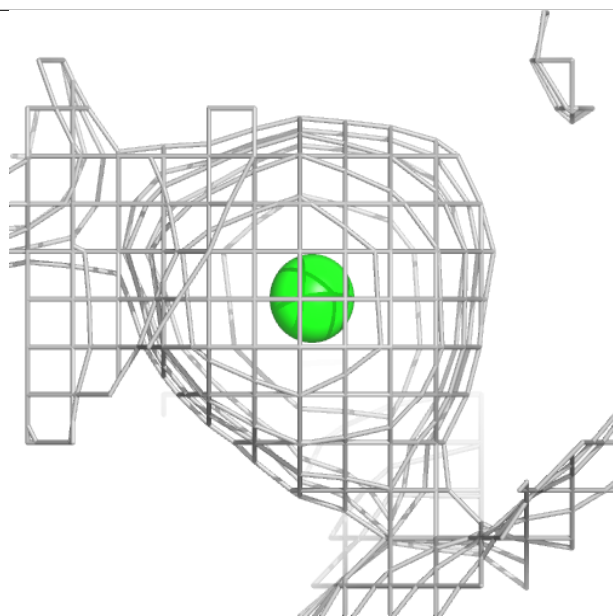
Electron density around CL a 403 (B):

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



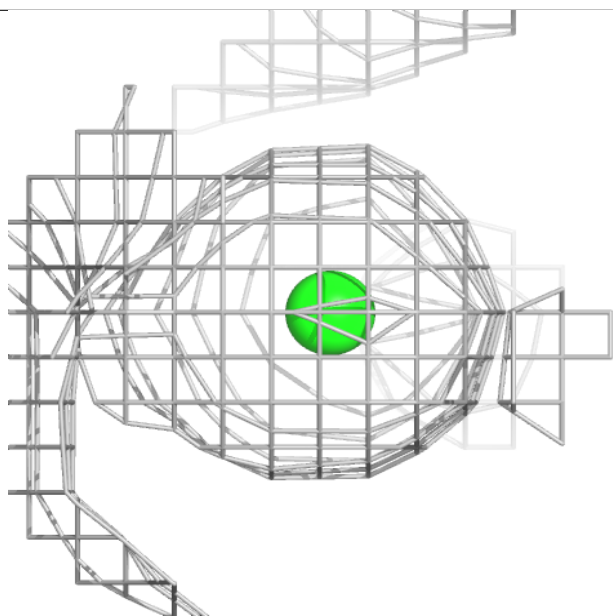
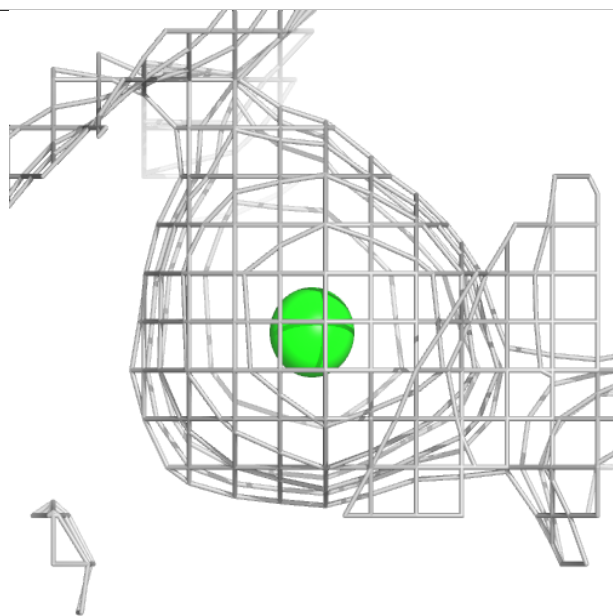
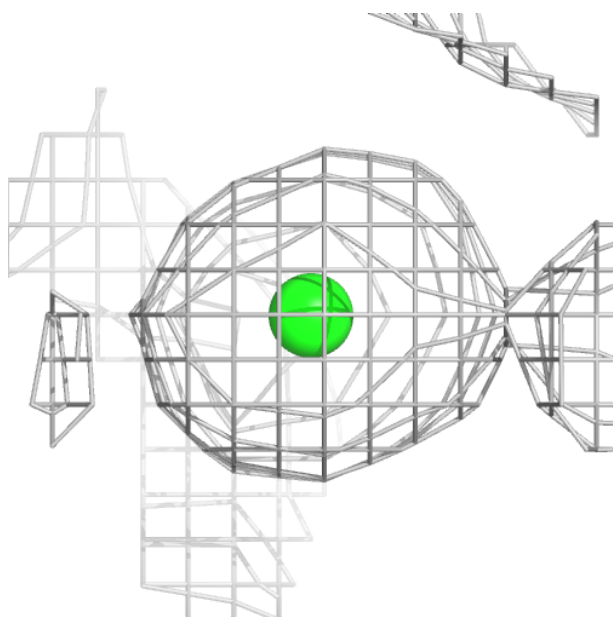
Electron density around CL a 404 (A):

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



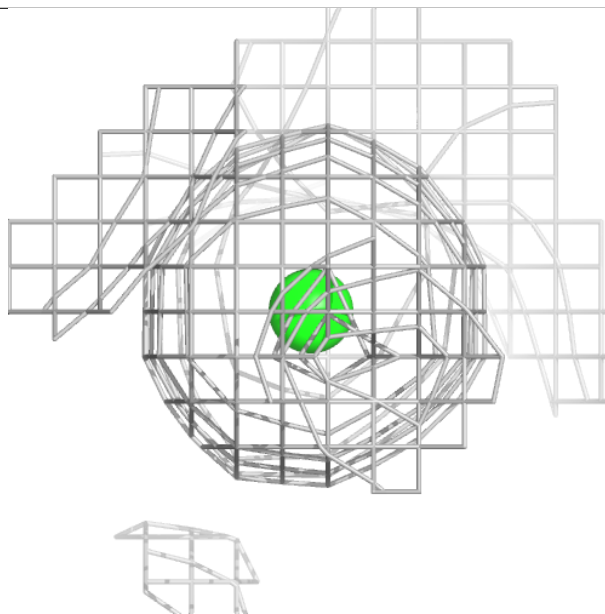
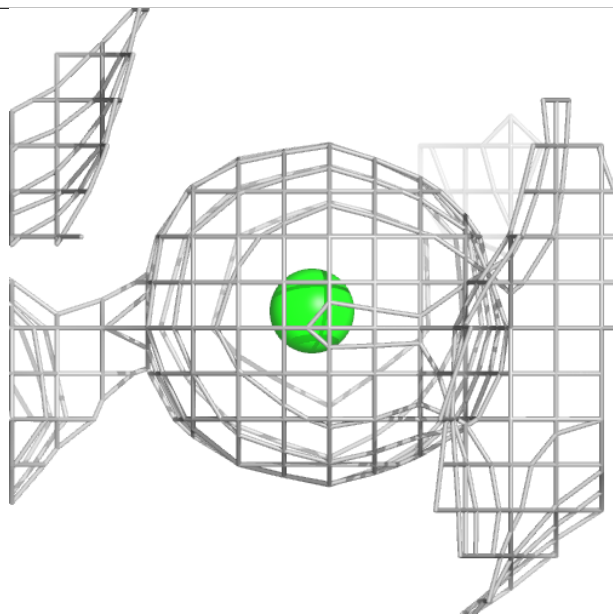
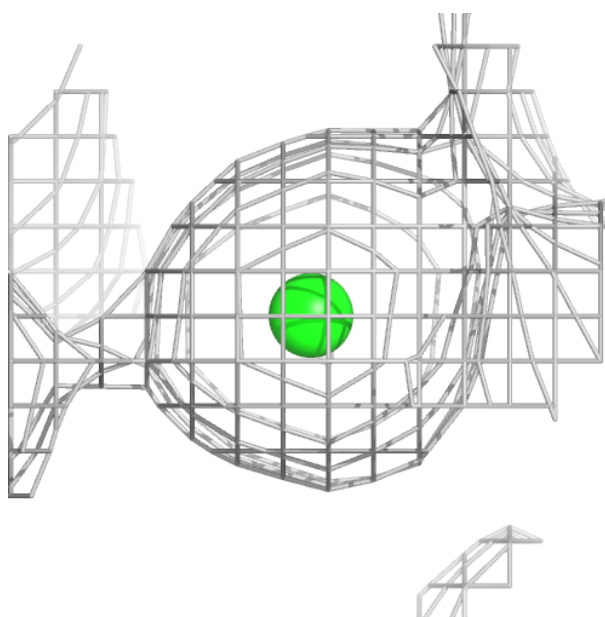
Electron density around CL a 404 (B):

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



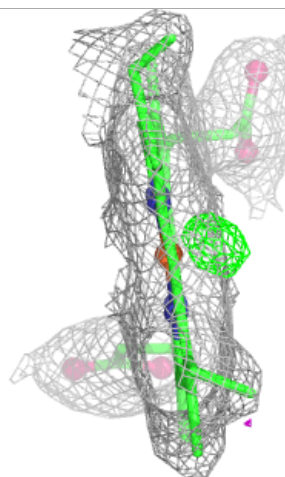
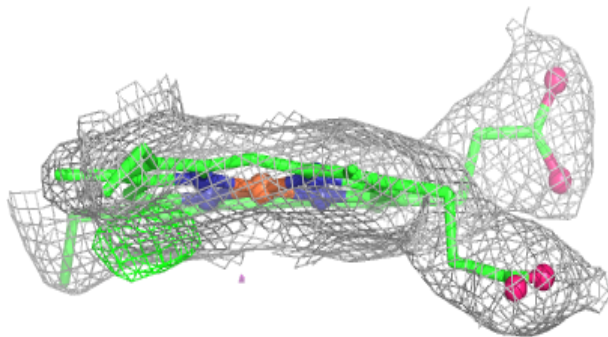
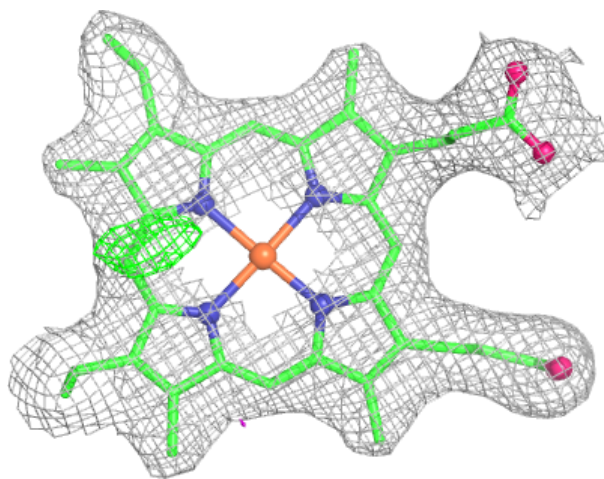
Electron density around CL A 404 (A):

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



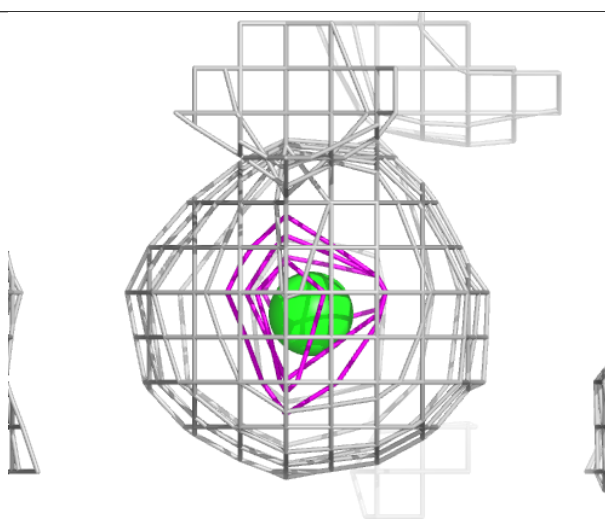
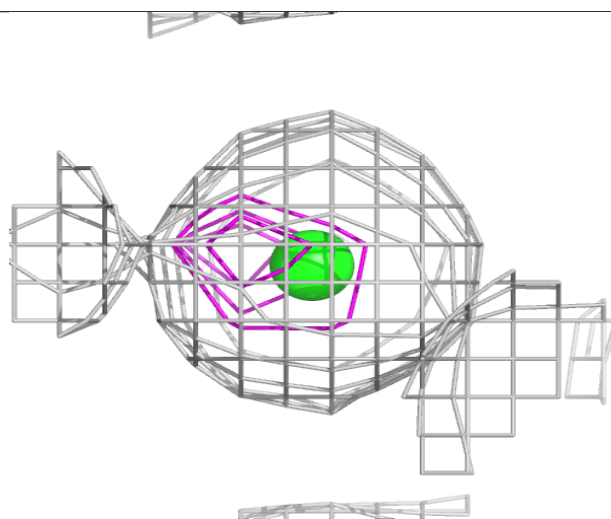
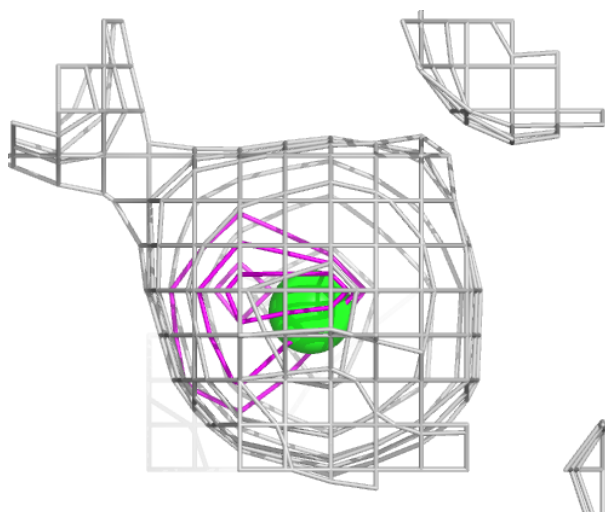
Electron density around HEC V 201:

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



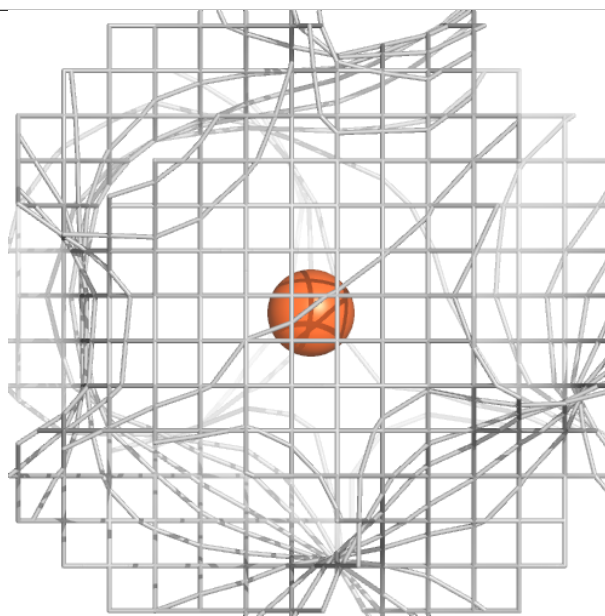
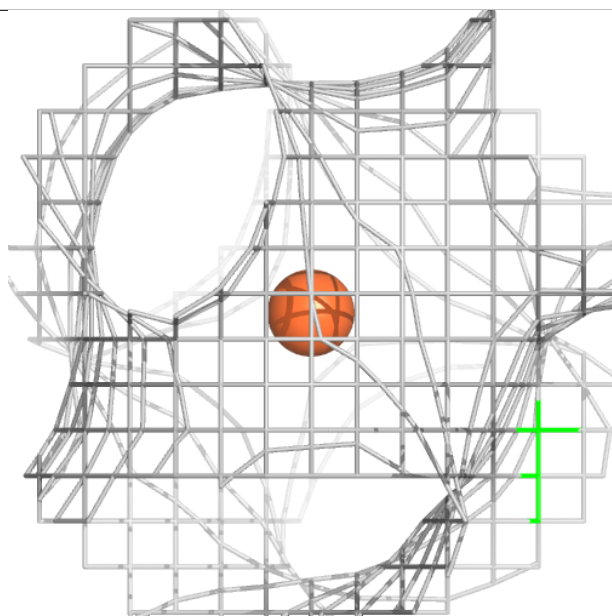
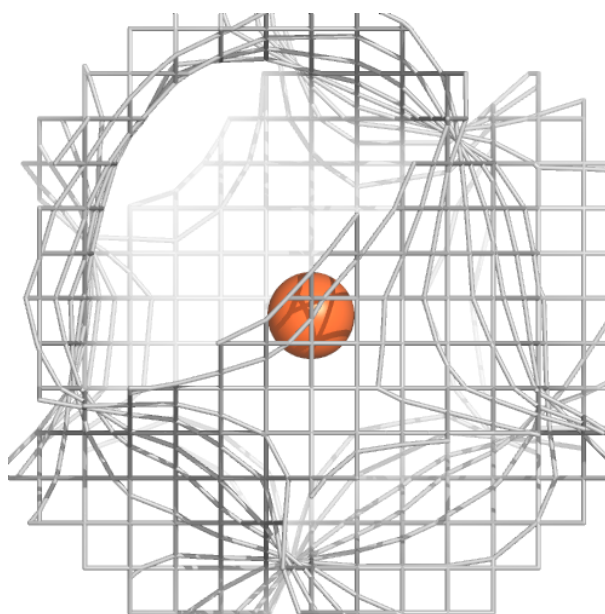
Electron density around CL A 403 (B):

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



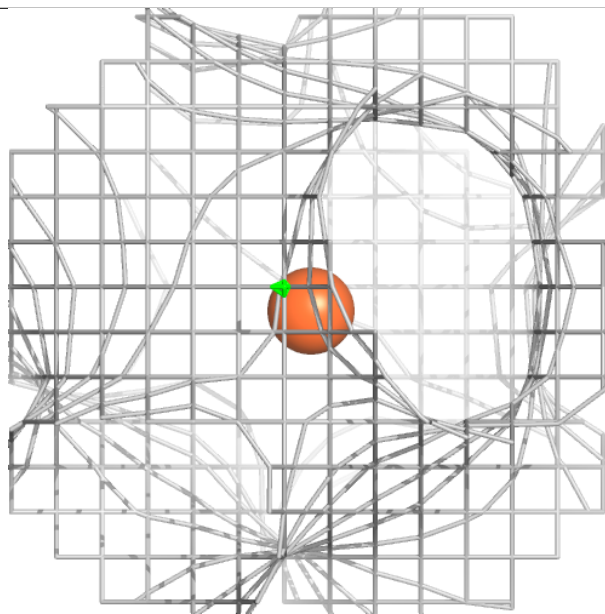
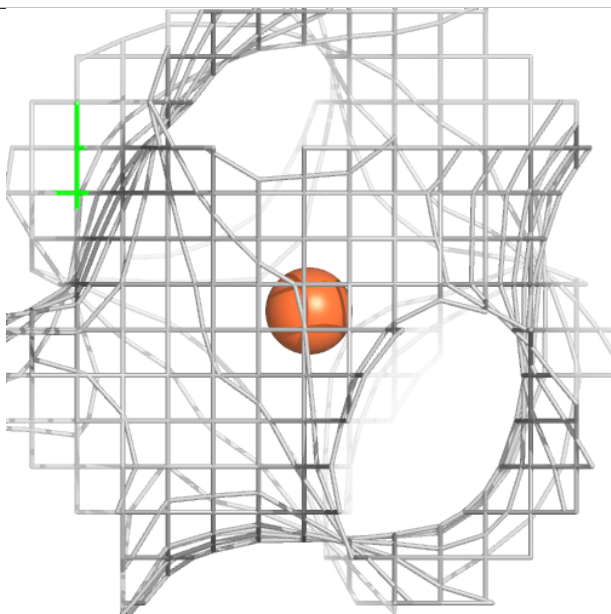
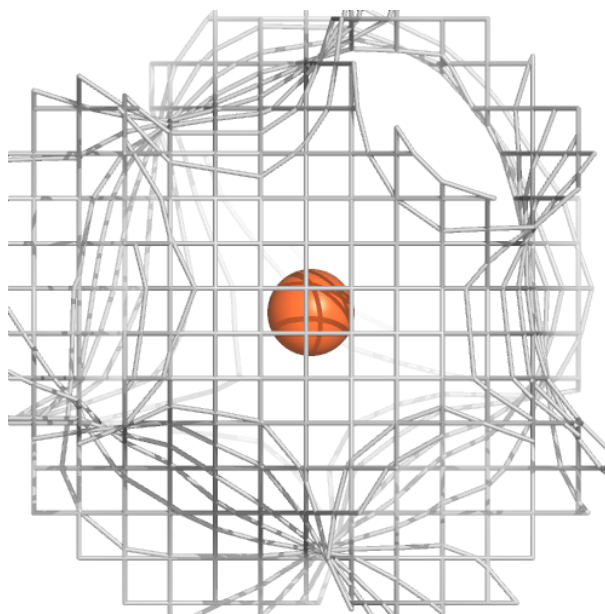
Electron density around FE2 A 402 (A):

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



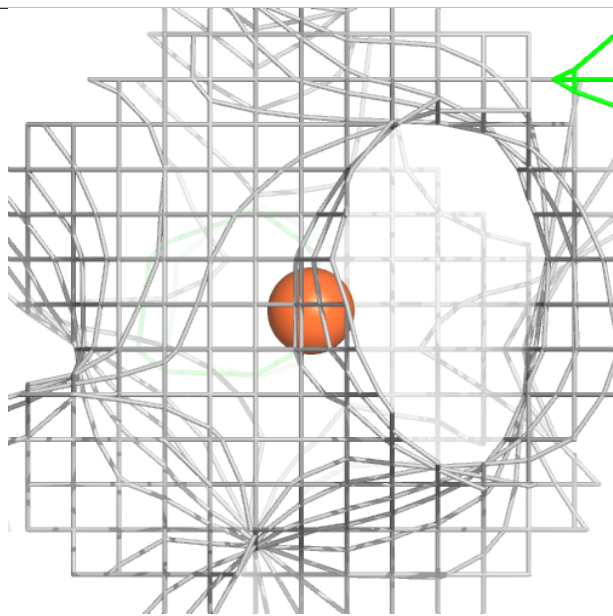
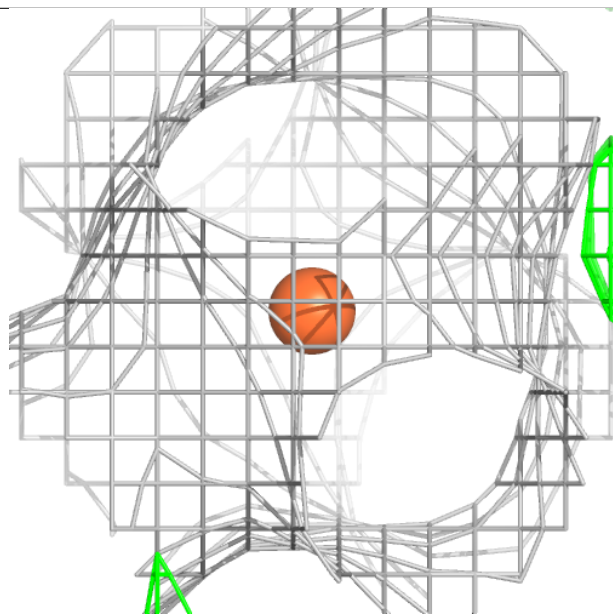
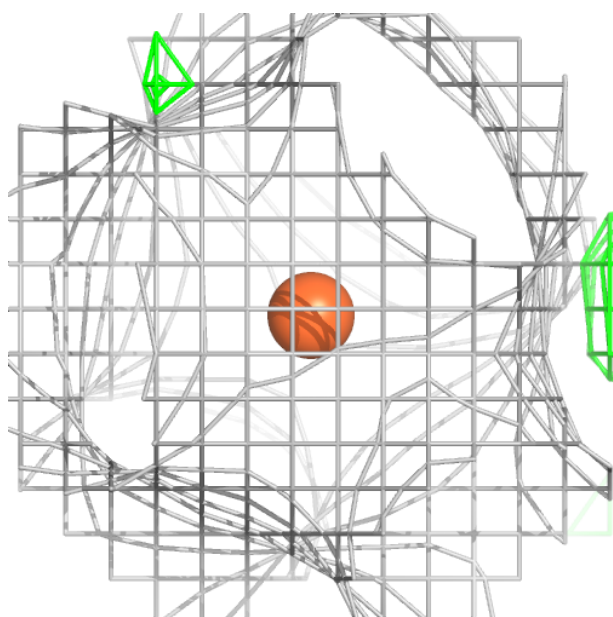
Electron density around FE2 A 402 (B):

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



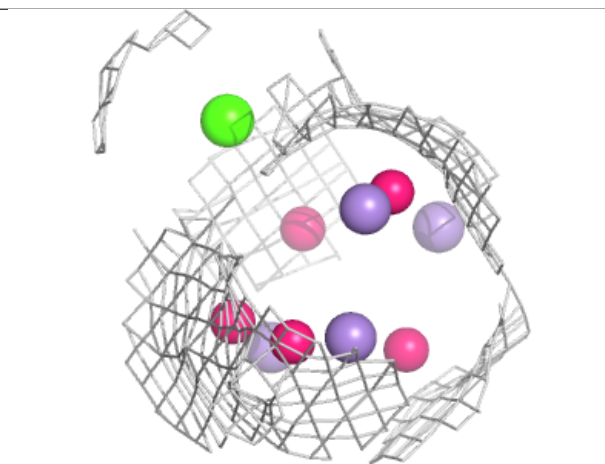
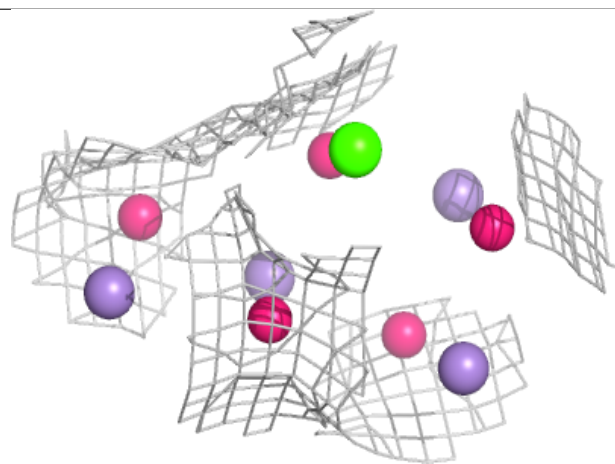
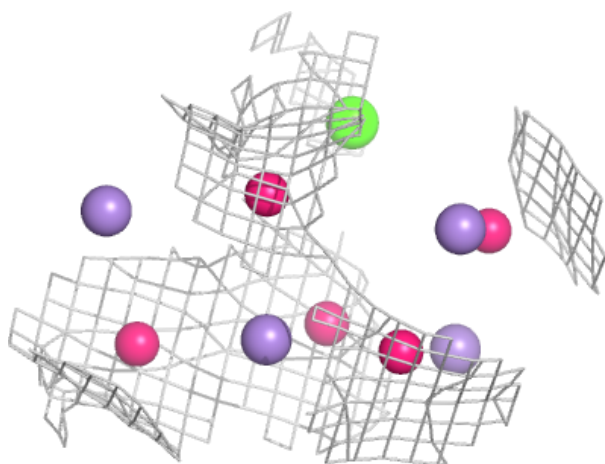
Electron density around FE2 a 402 (A):

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



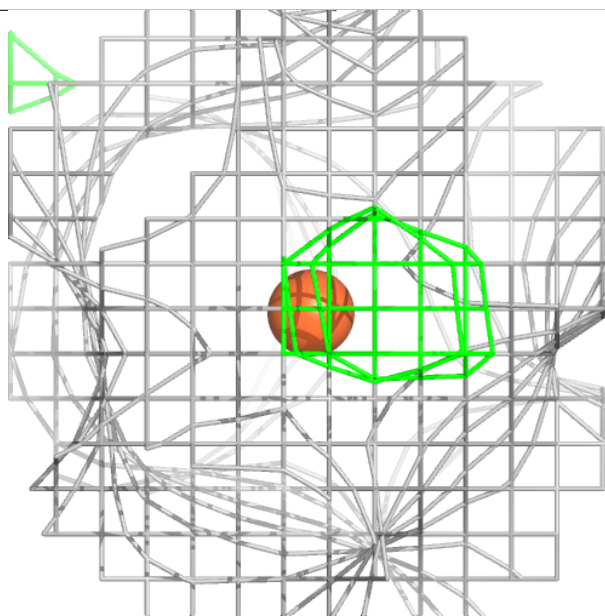
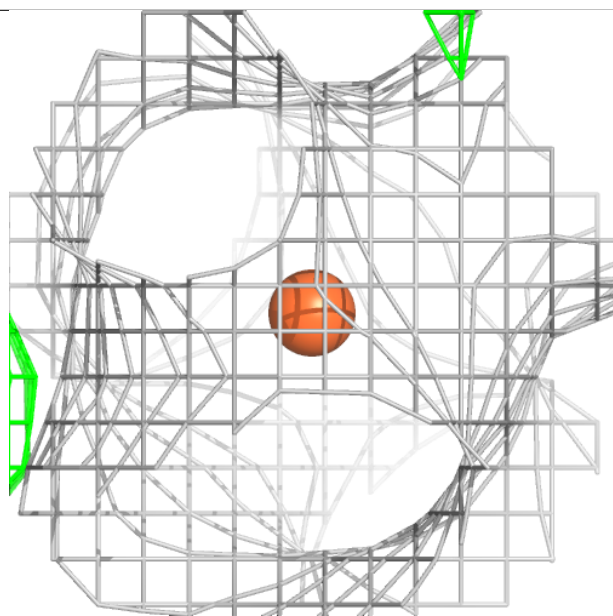
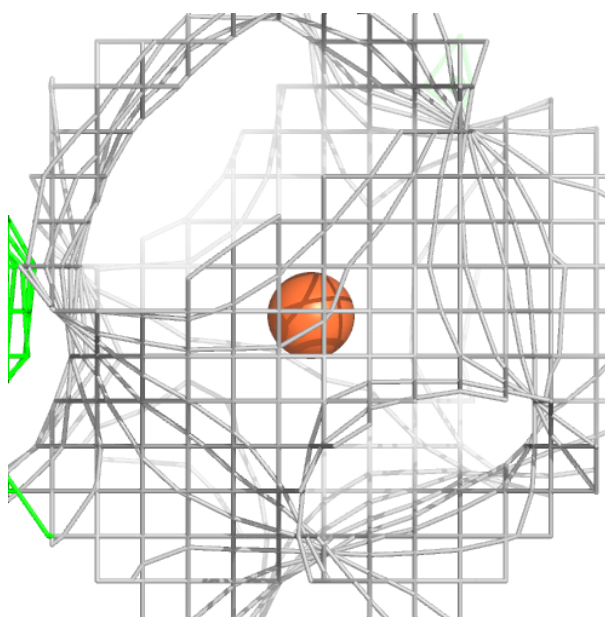
Electron density around OEX a 414 (A):

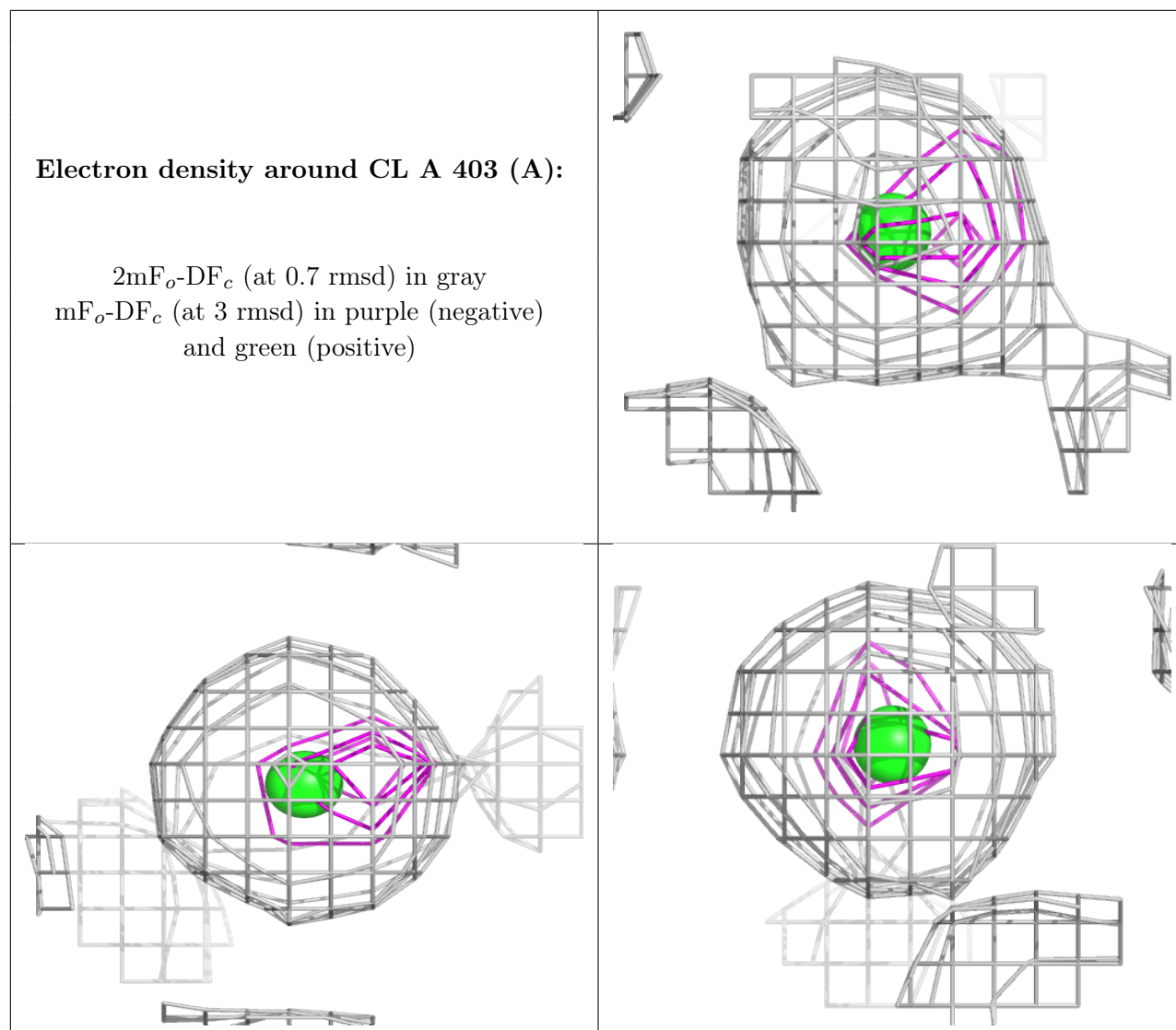
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE2 a 402 (B):

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





6.5 Other polymers [i](#)

There are no such residues in this entry.