



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 13, 2026 – 08:26 PM JST

PDB ID : 8IR7 / pdb_00008ir7
Title : XFEL structure of cyanobacterial photosystem II following one flash (1F) with a 200-nanosecond 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

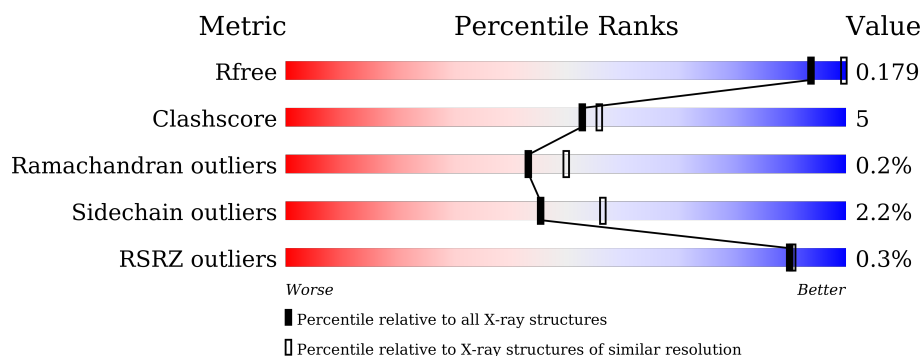
1 Overall quality at a glance

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.



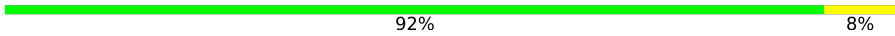
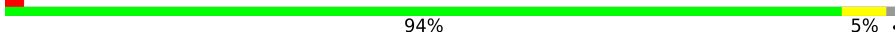
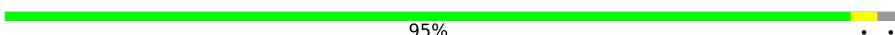
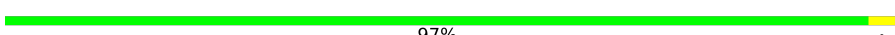
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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% 9% .
3	C	455	91% 7% .
3	c	455	92% 7% .

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

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Mol	Chain	Length	Quality of chain
16	v	137	 91% 8% .
17	X	40	 85% 10% 5%
17	x	40	 90% 5% 5%
18	Y	30	 3% 87% 10% .
18	y	30	 67% 30% .
19	Z	62	 90% 8% .
19	z	62	 74% 24% .
20	R	34	 9% 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
27	GOL	D	402	-	-	X	-
27	GOL	D	413	-	X	-	-
27	GOL	a	417	-	-	X	-
40	HEC	V	201	X	-	-	-
40	HEC	v	201	X	-	-	-

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 62674 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	220	0
			4318	2821	715	757	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	22	0
			4166	2735	694	724	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	99	0
			4272	2796	715	743	18			
3	c	455	Total	C	N	O	S	0	101	0
			4316	2827	720	751	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	115	0
			3625	2390	597	623	15			
4	d	341	Total	C	N	O	S	0	119	0
			3658	2412	605	626	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	5	0
			815	519	135	161				

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

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

- Molecule 22 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

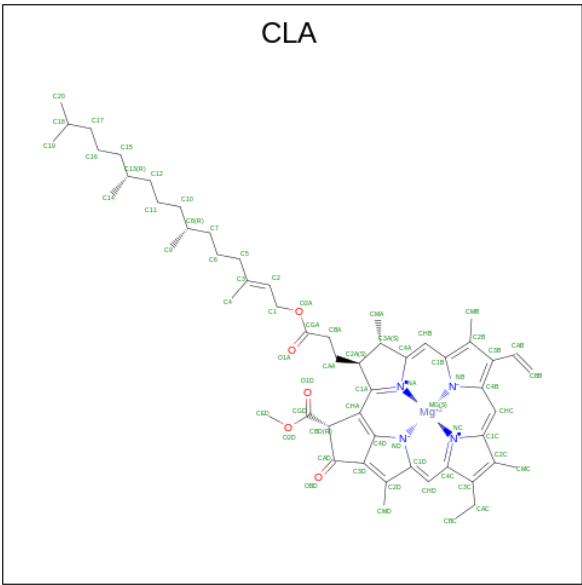
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	2
			4	4		

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

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



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

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

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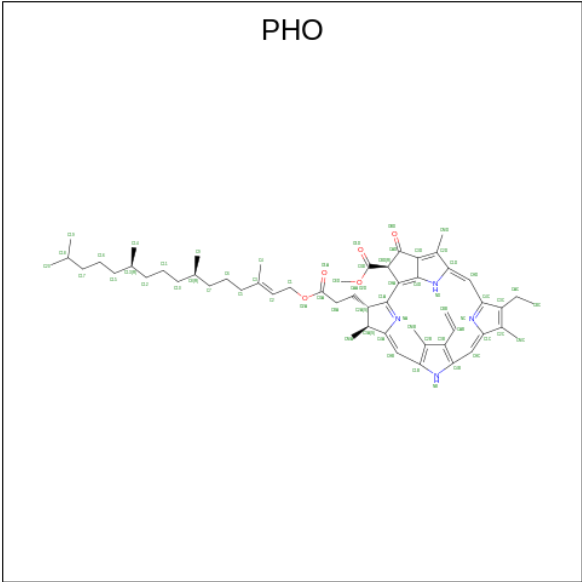
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	a	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	a	1	Total 65	C 55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

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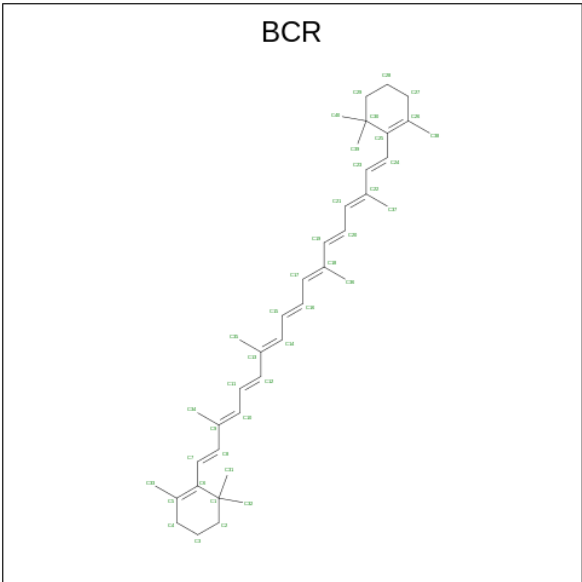
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 24 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



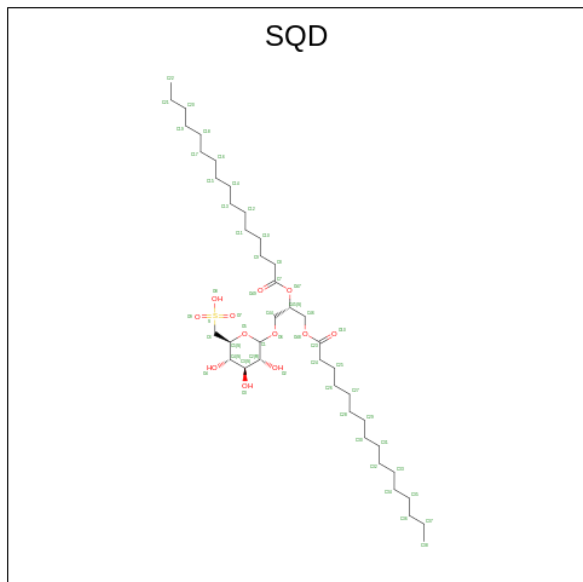
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	1
			128	110	8	10		
24	A	1	Total	C	N	O	0	1
			128	110	8	10		
24	a	1	Total	C	N	O	0	1
			128	110	8	10		
24	a	1	Total	C	N	O	0	1
			128	110	8	10		

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



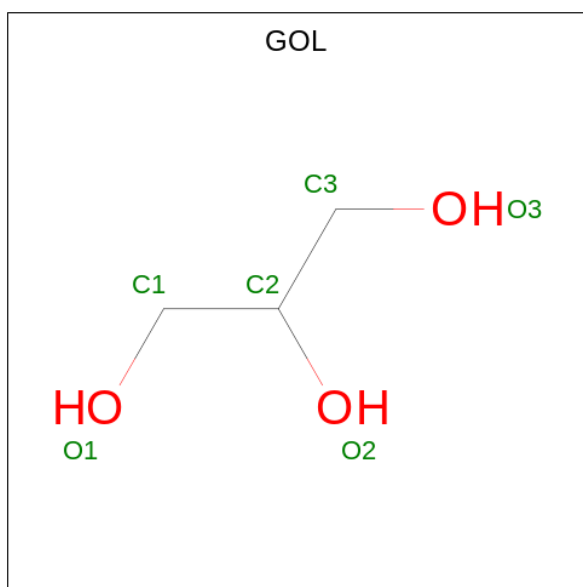
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total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

- Molecule 26 is 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
26	A	1	Total	C	O	S	0	1
			108	82	24	2		
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	B	1	Total	C	O	S	0	0
			54	41	12	1		
26	F	1	Total	C	O	S	0	0
			43	30	12	1		
26	a	1	Total	C	O	S	0	1
			108	82	24	2		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	b	1	Total	C	O	S	0	0
			54	41	12	1		
26	f	1	Total	C	O	S	0	0
			43	30	12	1		

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



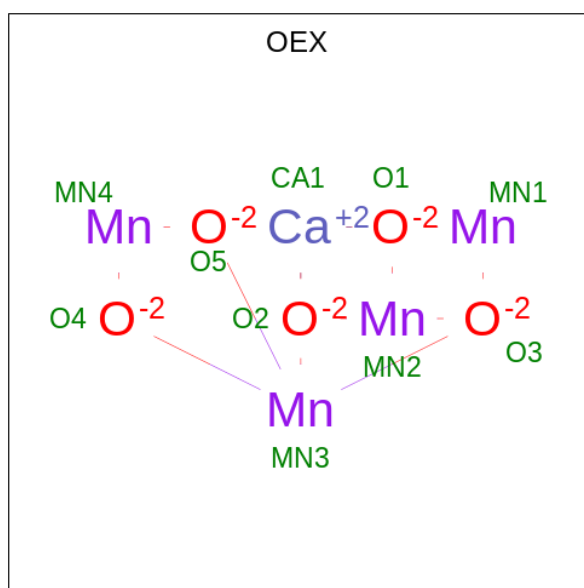
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	1
			12	6	6		
27	D	1	Total	C	O	0	0
			6	3	3		
27	D	1	Total	C	O	0	0
			6	3	3		
27	O	1	Total	C	O	0	0
			6	3	3		
27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

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

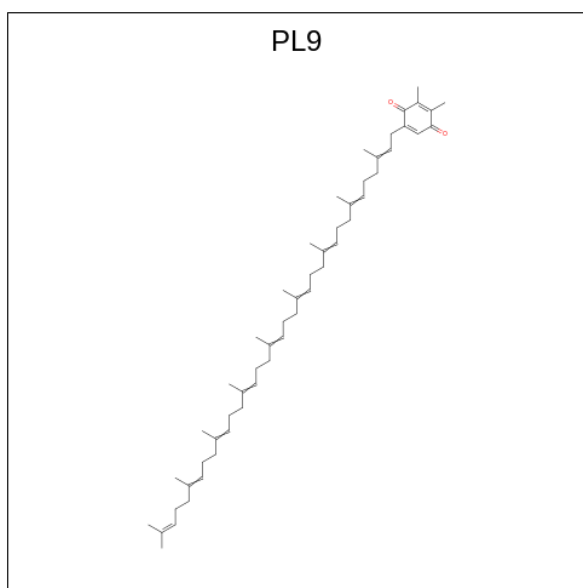
- Molecule 28 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	Ca	Mn	O	0	1
			20	2	8	10		
28	a	1	Total	Ca	Mn	O	0	1
			20	2	8	10		

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $\text{C}_{53}\text{H}_{80}\text{O}_2$)

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



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

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

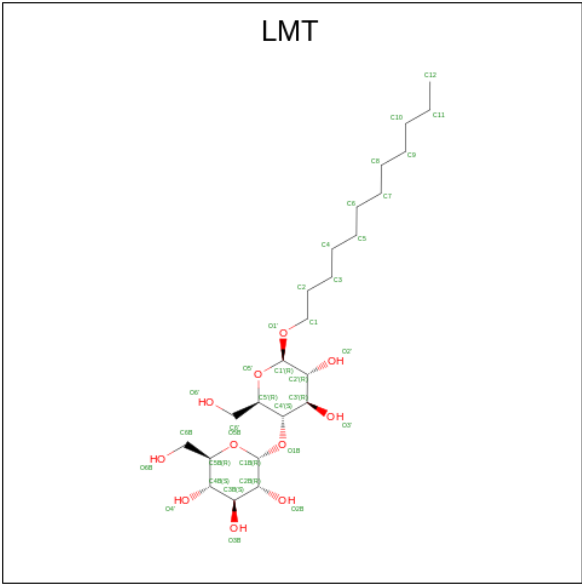
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			28	23	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	I	1	Total	C	O	0	0
			40	35	5		
30	J	1	Total	C		0	0
			10	10			
30	K	1	Total	C	O	0	1
			68	58	10		
30	X	1	Total	C	O	0	0
			18	16	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	a	1	Total	C	O	0	0
			30	25	5		
30	b	1	Total	C	O	0	0
			33	28	5		
30	c	1	Total	C	O	0	1
			64	54	10		
30	d	2	Total	C	O	0	0
			53	47	6		
30	i	1	Total	C	O	0	0
			40	35	5		
30	j	1	Total	C		0	0
			10	10			
30	l	1	Total	C		0	0
			10	10			
30	m	1	Total	C		0	0
			10	10			
30	x	1	Total	C	O	0	0
			18	16	2		

- Molecule 31 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



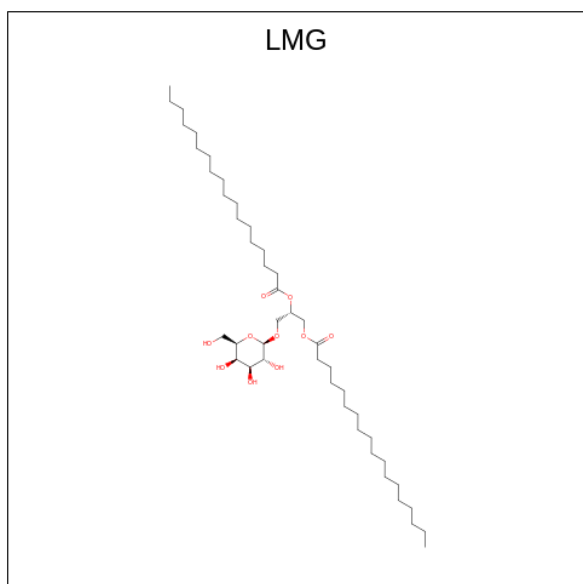
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			35	24	11		
31	A	1	Total	C	O	0	0
			35	24	11		

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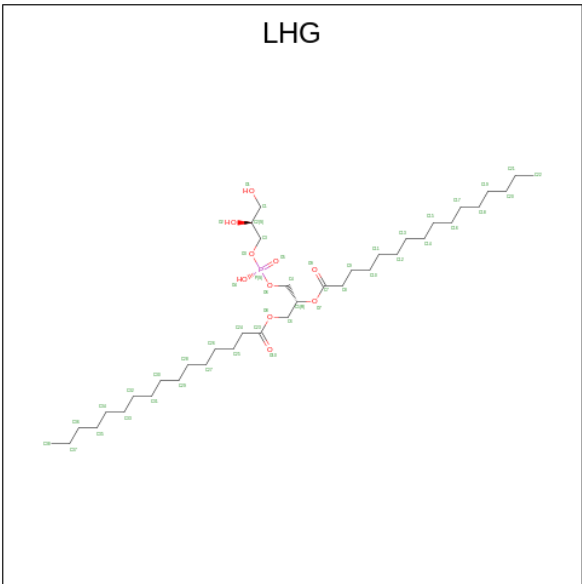
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			25	19	6		
31	F	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total	C	O	0	0
			35	24	11		
31	a	1	Total	C	O	0	0
			35	24	11		
31	b	1	Total	C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

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



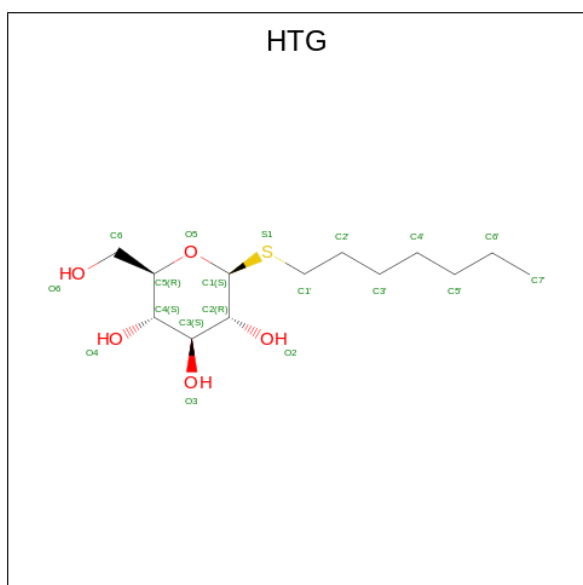
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total C O 51 41 10	0	0
32	B	1	Total C O 51 41 10	0	0
32	C	1	Total C O 51 41 10	0	0
32	C	1	Total C O 51 41 10	0	0
32	D	1	Total C O 51 41 10	0	0
32	c	1	Total C O 51 41 10	0	0
32	c	1	Total C O 51 41 10	0	0
32	c	1	Total C O 51 41 10	0	0
32	d	1	Total C O 51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

- 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).



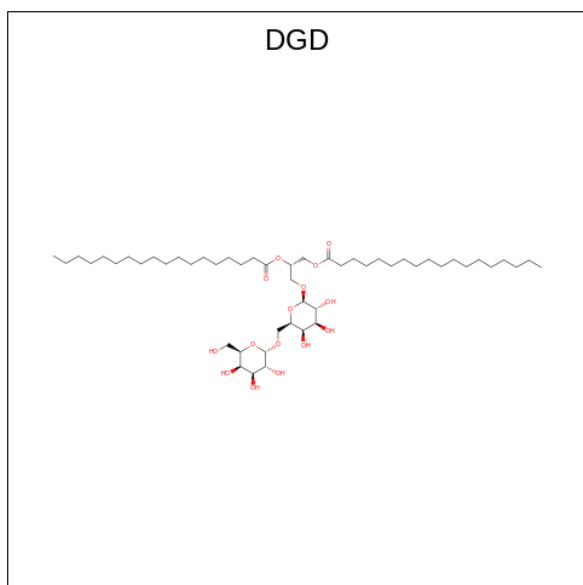
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		

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



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

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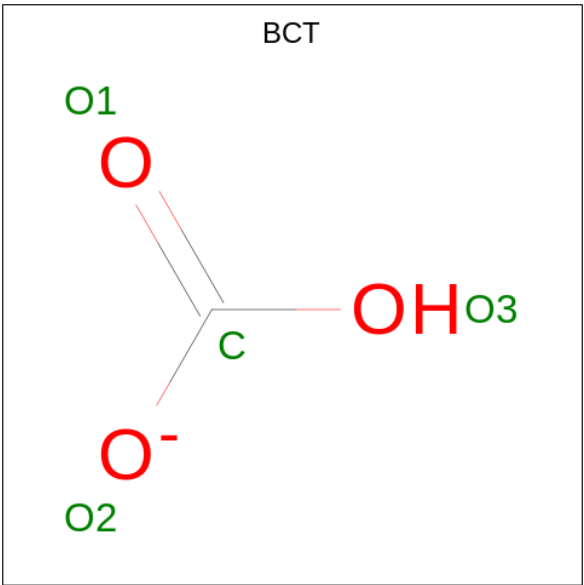
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	C	1	Total	C	O	0	0
			62	47	15		
35	H	1	Total	C	O	0	0
			62	47	15		
35	c	1	Total	C	O	0	1
			124	94	30		
35	c	1	Total	C	O	0	1
			124	94	30		
35	c	1	Total	C	O	0	0
			62	47	15		
35	h	1	Total	C	O	0	0
			62	47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

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

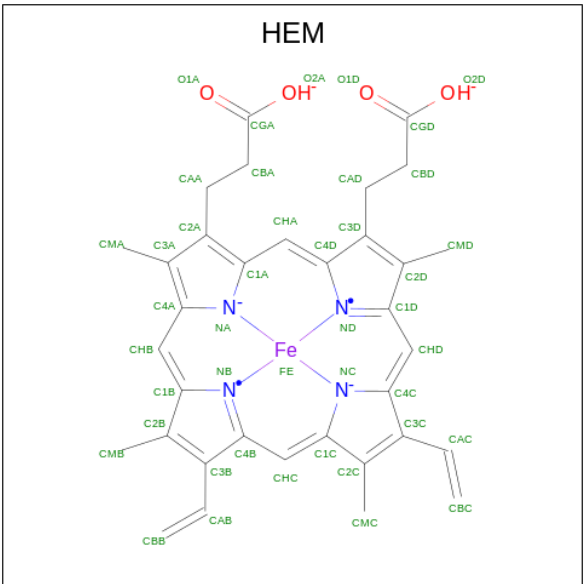
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	C	1	Total	Ca	0	0
			1	1		
36	F	1	Total	Ca	0	0
			1	1		
36	O	1	Total	Ca	0	0
			1	1		
36	c	2	Total	Ca	0	0
			2	2		
36	f	1	Total	Ca	0	0
			1	1		
36	o	1	Total	Ca	0	0
			1	1		

- Molecule 37 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



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

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



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

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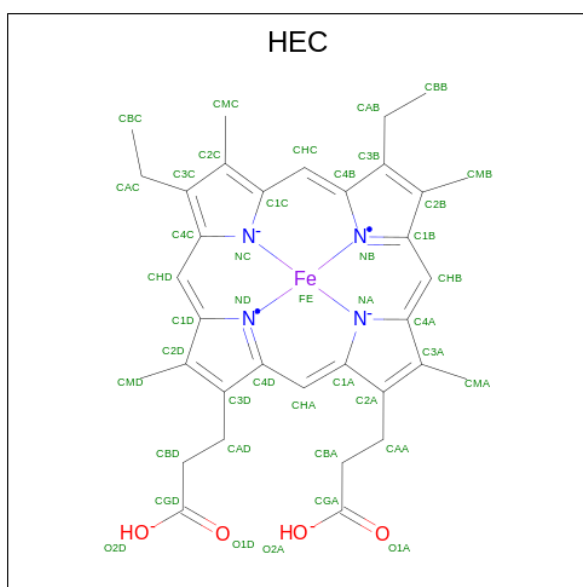
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	f	1	Total	C	Fe	N	O	
			43	34	1	4	4	
							0	0

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

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

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



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	136	Total	O		
			221	221	0	86
41	B	189	Total	O		
			191	191	0	2

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	C	169	Total 206	O 206	0	38
41	D	123	Total 157	O 157	0	34
41	E	15	Total 15	O 15	0	0
41	F	6	Total 6	O 6	0	0
41	H	23	Total 23	O 23	0	0
41	I	4	Total 4	O 4	0	0
41	J	7	Total 7	O 7	0	0
41	K	6	Total 6	O 6	0	0
41	L	9	Total 10	O 10	0	1
41	M	5	Total 5	O 5	0	0
41	O	106	Total 111	O 111	0	5
41	T	11	Total 14	O 14	0	3
41	U	42	Total 44	O 44	0	2
41	V	80	Total 81	O 81	0	1
41	X	7	Total 7	O 7	0	0
41	a	129	Total 209	O 209	0	81
41	b	199	Total 202	O 202	0	3
41	c	158	Total 191	O 191	0	34
41	d	121	Total 153	O 153	0	32
41	e	9	Total 9	O 9	0	0
41	f	3	Total 3	O 3	0	0

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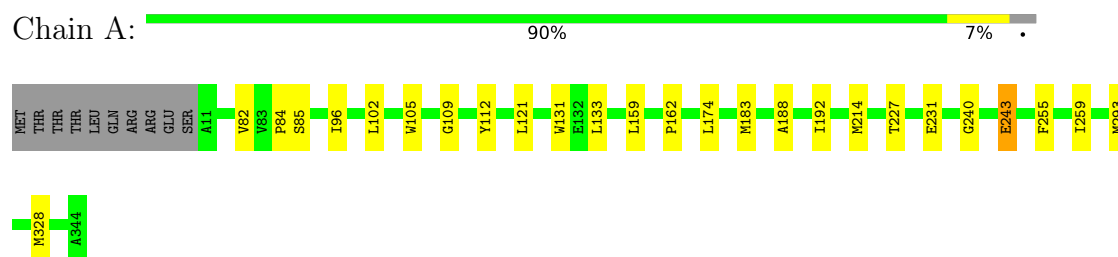
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	h	16	Total 16	O 16	0	0
41	i	2	Total 2	O 2	0	0
41	j	2	Total 2	O 2	0	0
41	k	3	Total 3	O 3	0	0
41	l	8	Total 10	O 10	0	2
41	m	13	Total 13	O 13	0	0
41	o	100	Total 104	O 104	0	4
41	t	7	Total 10	O 10	0	3
41	u	49	Total 50	O 50	0	1
41	v	59	Total 61	O 61	0	2
41	x	7	Total 7	O 7	0	0
41	y	2	Total 2	O 2	0	0

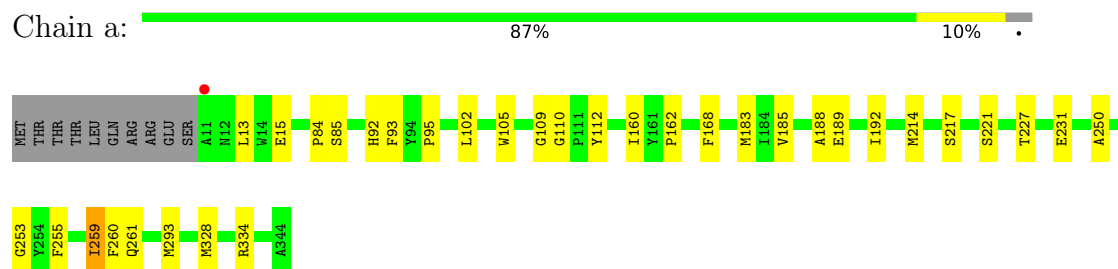
3 Residue-property plots

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.

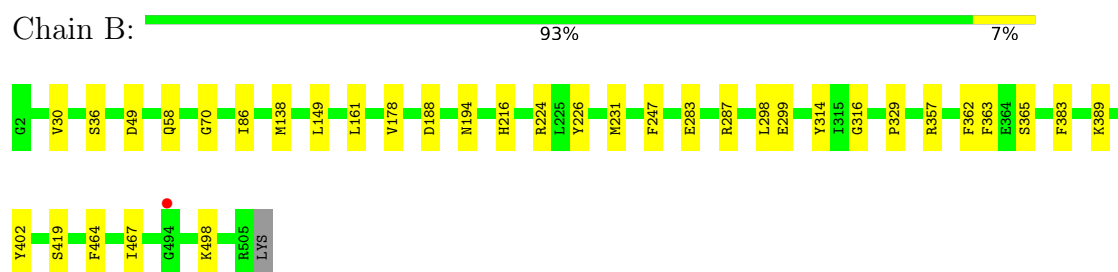
• Molecule 1: Photosystem II protein D1



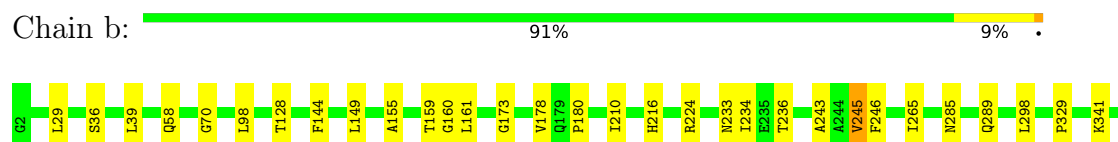
• Molecule 1: Photosystem II protein D1



• Molecule 2: Photosystem II CP47 reaction center protein



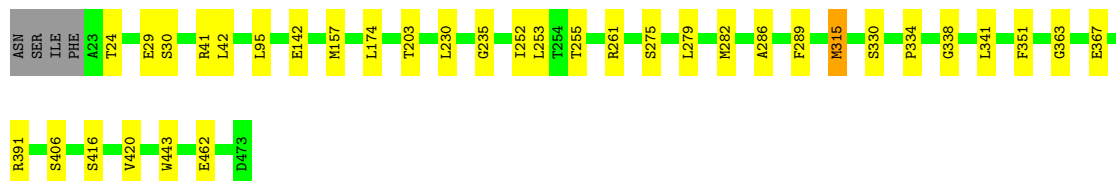
• Molecule 2: Photosystem II CP47 reaction center protein





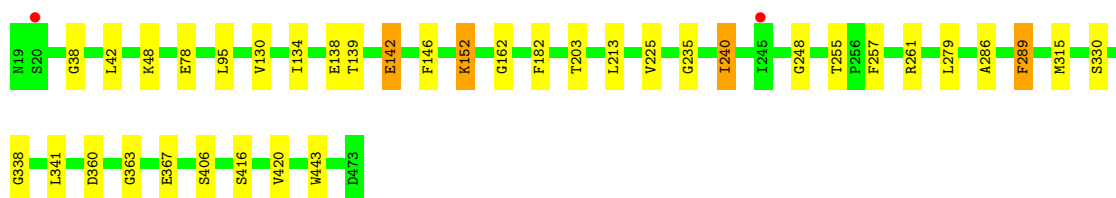
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 91% 7% .



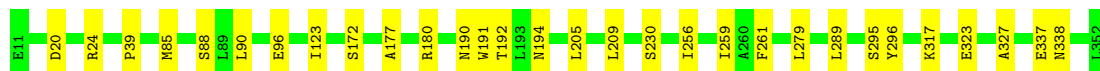
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 92% 7% .



- Molecule 4: Photosystem II D2 protein

Chain D: 91% 9%



- Molecule 4: Photosystem II D2 protein

Chain d: 92% 8%



- Molecule 5: Cytochrome b559 subunit alpha

Chain E: 77% 19% .



- Molecule 5: Cytochrome b559 subunit alpha

Chain e: 83% 11% 6%



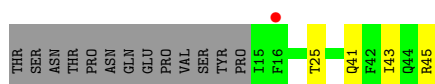
- Molecule 6: Cytochrome b559 subunit beta

Chain F: 66% 11% 23%



- Molecule 6: Cytochrome b559 subunit beta

Chain f: 2% 61% 9% 30%



- Molecule 7: Photosystem II reaction center protein H

Chain H: 2% 94% 5%



- Molecule 7: Photosystem II reaction center protein H

Chain h: 92% 6%



- Molecule 8: Photosystem II reaction center protein I

Chain I: 82% 11% 8%



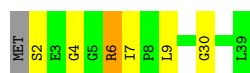
- Molecule 8: Photosystem II reaction center protein I

Chain i: 3% 87% 11%

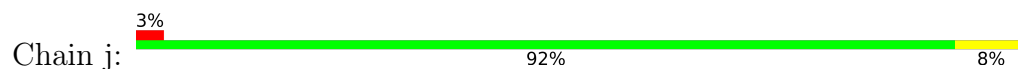


- Molecule 9: Photosystem II reaction center protein J

Chain J: 82% 13% 5%



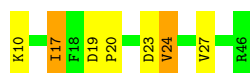
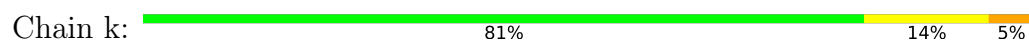
- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K



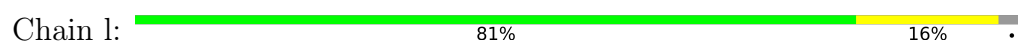
- Molecule 10: Photosystem II reaction center protein K



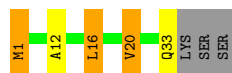
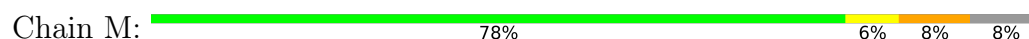
- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M



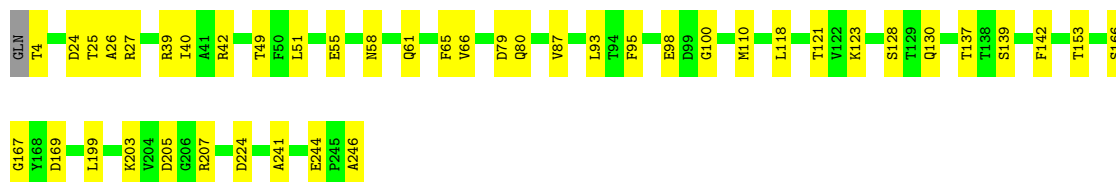
- Molecule 12: Photosystem II reaction center protein M





- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 82% 18%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 92% 7%



- Molecule 14: Photosystem II reaction center protein T

Chain T: 78% 16% 6%



- Molecule 14: Photosystem II reaction center protein T

Chain t: 3% 81% 12% 6%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 83% 10% 8%

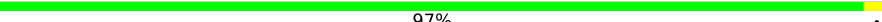


- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 88% 5% 7%



- Molecule 16: Cytochrome c-550

Chain V:  97% .



- Molecule 16: Cytochrome c-550

Chain v:  91% 8% .



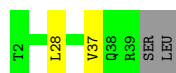
- Molecule 17: Photosystem II reaction center protein X

Chain X:  85% 10% 5%



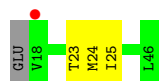
- Molecule 17: Photosystem II reaction center protein X

Chain x:  90% 5% 5%



- Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:  3% 87% 10% .



- Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:  67% 30% .



- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  90% 8% .

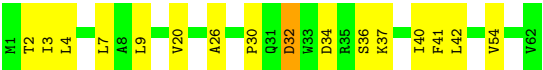


- Molecule 19: Photosystem II reaction center protein Z

Chain z:

74%

24%



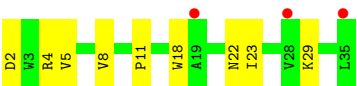
● Molecule 20: Photosystem II protein Y

Chain R:

9%

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	125.75Å 231.60Å 288.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.25 19.98 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.98-2.25) 99.7 (19.98-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.26Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.140 , 0.177 0.141 , 0.179	Depositor DCC
R_{free} test set	19865 reflections (2.44%)	wwPDB-VP
Wilson B-factor (Å ²)	50.3	Xtriage
Anisotropy	0.516	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 68.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	62674	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.71% 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: GOL, FE2, OEX, LMT, HTG, SQD, HEC, LMG, LHG, PHO, FME, BCR, CLA, DGD, CA, UNL, PL9, MG, CL, BCT, HEM

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	0.26	0/4478	0.44	0/6098
1	a	0.25	0/4457	0.41	0/6069
2	B	0.34	0/4314	0.49	0/5879
2	b	0.31	0/4285	0.48	0/5841
3	C	0.27	0/4416	0.43	0/6013
3	c	0.27	0/4467	0.42	0/6082
4	D	0.31	0/3746	0.47	0/5102
4	d	0.30	0/3780	0.44	0/5147
5	E	0.31	0/681	0.48	0/928
5	e	0.28	0/690	0.46	0/939
6	F	0.28	0/284	0.45	0/387
6	f	0.26	0/269	0.38	0/365
7	H	0.30	0/519	0.49	0/708
7	h	0.28	0/530	0.46	0/722
8	I	0.26	0/311	0.42	0/419
8	i	0.32	0/311	0.43	0/419
9	J	0.28	0/278	0.38	0/376
9	j	0.28	0/283	0.40	0/383
10	K	0.32	0/303	0.47	0/416
10	k	0.33	0/303	0.45	0/416
11	L	0.34	0/318	0.47	0/433
11	l	0.35	0/318	0.47	0/433
12	M	0.39	0/261	0.55	0/357
12	m	0.32	0/279	0.48	0/380
13	O	0.33	0/1991	0.50	0/2698
13	o	0.30	0/1966	0.49	0/2665
14	T	0.32	0/310	0.41	0/419
14	t	0.31	0/301	0.43	0/406
15	U	0.35	0/811	0.55	0/1095
15	u	0.35	0/826	0.54	0/1116
16	V	0.34	0/1142	0.49	0/1545

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.29	0/1139	0.44	0/1542
17	X	0.22	0/292	0.34	0/395
17	x	0.23	0/284	0.35	0/384
18	Y	0.23	0/216	0.43	0/289
18	y	0.23	0/216	0.38	0/289
19	Z	0.21	0/490	0.35	0/669
19	z	0.23	0/490	0.41	0/669
20	R	0.26	0/279	0.33	0/383
All	All	0.29	0/50634	0.45	0/68876

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	20	0
1	a	4318	0	4124	34	0
2	B	4166	0	3999	26	0
2	b	4134	0	3976	41	0
3	C	4272	0	4138	23	0
3	c	4316	0	4184	30	0
4	D	3625	0	3489	31	0
4	d	3658	0	3522	24	0
5	E	662	0	648	11	0
5	e	670	0	655	7	0
6	F	275	0	282	4	0
6	f	261	0	269	5	0
7	H	506	0	529	2	0
7	h	517	0	541	3	0
8	I	314	0	328	5	0
8	i	314	0	328	3	0
9	J	272	0	279	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	277	0	284	2	0
10	K	293	0	305	7	0
10	k	293	0	305	6	0
11	L	311	0	320	1	0
11	l	311	0	320	5	0
12	M	268	0	285	6	0
12	m	286	0	305	9	0
13	O	1958	0	1920	25	0
13	o	1933	0	1900	11	0
14	T	311	0	318	3	0
14	t	302	0	311	5	0
15	U	800	0	796	5	0
15	u	815	0	817	4	0
16	V	1120	0	1122	2	0
16	v	1117	0	1131	8	0
17	X	289	0	322	4	0
17	x	281	0	312	2	0
18	Y	215	0	246	2	0
18	y	215	0	246	5	0
19	Z	479	0	516	2	0
19	z	479	0	516	5	0
20	R	273	0	305	4	0
21	A	2	0	0	0	0
21	a	2	0	0	0	0
22	A	4	0	0	0	0
22	a	4	0	0	0	0
23	A	455	0	504	20	0
23	B	1040	0	1152	28	0
23	C	845	0	936	37	0
23	D	195	0	216	6	0
23	a	325	0	360	17	0
23	b	1040	0	1152	28	0
23	c	845	0	936	37	0
23	d	325	0	360	15	0
24	A	256	0	296	7	0
24	a	256	0	296	3	0
25	A	40	0	56	2	0
25	B	120	0	168	8	0
25	C	80	0	112	2	0
25	D	40	0	56	1	0
25	H	40	0	56	1	0
25	K	40	0	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	T	40	0	56	6	0
25	Y	40	0	56	2	0
25	a	40	0	56	1	0
25	b	120	0	168	9	0
25	c	80	0	112	3	0
25	d	40	0	56	2	0
25	h	40	0	56	3	0
25	k	40	0	56	2	0
25	t	40	0	56	6	0
25	y	40	0	56	2	0
26	A	162	0	232	4	0
26	B	54	0	78	1	0
26	F	43	0	53	2	0
26	a	162	0	232	9	0
26	b	54	0	78	4	0
26	f	43	0	53	0	0
27	A	6	0	8	0	0
27	B	18	0	24	1	0
27	C	12	0	16	0	0
27	D	12	0	15	8	0
27	O	12	0	16	4	0
27	V	12	0	16	0	0
27	a	12	0	16	6	0
27	b	12	0	16	1	0
27	c	18	0	24	0	0
27	d	6	0	8	0	0
27	l	12	0	16	2	0
27	o	12	0	16	0	0
27	v	12	0	16	3	0
28	A	20	0	0	0	0
28	a	20	0	0	0	0
29	A	110	0	160	19	0
29	D	110	0	160	0	0
29	a	110	0	160	8	0
29	d	110	0	160	0	0
30	A	28	0	0	0	0
30	B	33	0	0	0	0
30	D	57	0	0	0	0
30	I	40	0	0	0	0
30	J	10	0	0	0	0
30	K	68	0	0	0	0
30	X	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	a	30	0	0	0	0
30	b	33	0	0	0	0
30	c	64	0	0	0	0
30	d	53	0	0	0	0
30	i	40	0	0	0	0
30	j	10	0	0	0	0
30	l	10	0	0	0	0
30	m	10	0	0	0	0
30	x	18	0	0	0	0
31	A	70	0	92	2	0
31	B	95	0	126	2	0
31	F	35	0	46	0	0
31	M	70	0	91	3	0
31	a	35	0	46	1	0
31	b	50	0	70	1	0
31	e	35	0	46	1	0
31	m	35	0	46	0	0
31	t	26	0	34	2	0
32	A	51	0	72	0	0
32	B	51	0	72	1	0
32	C	102	0	144	2	0
32	D	51	0	72	0	0
32	Z	37	0	44	1	0
32	c	153	0	216	2	0
32	d	51	0	72	3	0
32	m	51	0	72	0	0
32	z	39	0	48	2	0
33	A	98	0	148	3	0
33	D	196	0	296	12	0
33	E	84	0	114	8	0
33	L	98	0	148	0	0
33	a	84	0	114	8	0
33	b	98	0	148	0	0
33	d	294	0	444	23	0
34	B	57	0	78	3	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	4	0
34	c	19	0	26	1	0
34	d	16	0	17	0	0
35	C	310	0	410	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	H	62	0	82	1	0
35	c	310	0	410	7	0
35	h	62	0	82	0	0
36	C	1	0	0	0	0
36	F	1	0	0	0	0
36	O	1	0	0	0	0
36	c	2	0	0	0	0
36	f	1	0	0	0	0
36	o	1	0	0	0	0
37	D	8	0	0	0	0
37	d	8	0	0	0	0
38	F	43	0	30	1	0
38	f	43	0	30	1	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	V	43	0	30	1	0
40	v	43	0	30	0	0
41	A	221	0	0	0	0
41	B	191	0	0	0	0
41	C	206	0	0	3	0
41	D	157	0	0	5	0
41	E	15	0	0	0	0
41	F	6	0	0	0	0
41	H	23	0	0	0	0
41	I	4	0	0	0	0
41	J	7	0	0	2	0
41	K	6	0	0	1	0
41	L	10	0	0	0	0
41	M	5	0	0	0	0
41	O	111	0	0	2	0
41	T	14	0	0	0	0
41	U	44	0	0	0	0
41	V	81	0	0	0	0
41	X	7	0	0	0	0
41	a	209	0	0	3	0
41	b	202	0	0	0	0
41	c	191	0	0	3	0
41	d	153	0	0	1	0
41	e	9	0	0	0	0
41	f	3	0	0	1	0
41	h	16	0	0	0	0
41	i	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	j	2	0	0	0	0
41	k	3	0	0	0	0
41	l	10	0	0	0	0
41	m	13	0	0	0	0
41	o	104	0	0	0	0
41	t	10	0	0	1	0
41	u	50	0	0	1	0
41	v	61	0	0	0	0
41	x	7	0	0	0	0
41	y	2	0	0	0	0
All	All	62674	0	61525	606	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 606 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)
27:D:402:GOL:H11	12:M:1:FME:HG2	1.44	1.00
23:B:604:CLA:H42	23:B:605:CLA:H2	1.45	0.98
1:a:250[B]:ALA:HA	2:b:491[B]:VAL:HG11	1.53	0.91
1:a:250[A]:ALA:HA	2:b:491[A]:VAL:HG11	1.53	0.88
23:c:504:CLA:HBB1	23:c:513:CLA:H41	1.61	0.83

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%)	544 (98%)	7 (1%)	2 (0%)	30	31
1	a	551/344 (160%)	539 (98%)	10 (2%)	2 (0%)	30	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	524/505 (104%)	516 (98%)	8 (2%)	0	100	100
2	b	521/505 (103%)	510 (98%)	11 (2%)	0	100	100
3	C	548/455 (120%)	537 (98%)	10 (2%)	1 (0%)	43	50
3	c	554/455 (122%)	543 (98%)	10 (2%)	1 (0%)	43	50
4	D	454/342 (133%)	440 (97%)	14 (3%)	0	100	100
4	d	457/342 (134%)	444 (97%)	13 (3%)	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%)	62 (100%)	0	0	100	100
7	h	63/65 (97%)	59 (94%)	3 (5%)	1 (2%)	7	4
8	I	36/38 (95%)	33 (92%)	2 (6%)	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%)	34 (97%)	1 (3%)	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%)	242 (96%)	8 (3%)	1 (0%)	30	31
13	o	249/244 (102%)	243 (98%)	6 (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%)	93 (96%)	4 (4%)	0	100	100
15	u	99/104 (95%)	95 (96%)	4 (4%)	0	100	100
16	V	140/137 (102%)	137 (98%)	3 (2%)	0	100	100
16	v	140/137 (102%)	134 (96%)	6 (4%)	0	100	100
17	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	x	36/40 (90%)	36 (100%)	0	0	100	100
18	Y	27/30 (90%)	24 (89%)	3 (11%)	0	100	100
18	y	27/30 (90%)	26 (96%)	1 (4%)	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	6180/5384 (115%)	6036 (98%)	133 (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
3	c	416	SER
19	Z	31	GLN
13	O	26	ALA

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%)	441 (99%)	3 (1%)	76	82
1	a	442/279 (158%)	441 (100%)	1 (0%)	87	92
2	B	423/403 (105%)	418 (99%)	5 (1%)	63	74
2	b	420/403 (104%)	411 (98%)	9 (2%)	47	58
3	C	431/356 (121%)	422 (98%)	9 (2%)	47	58
3	c	437/356 (123%)	430 (98%)	7 (2%)	55	66
4	D	368/277 (133%)	365 (99%)	3 (1%)	73	80
4	d	372/277 (134%)	368 (99%)	4 (1%)	65	75
5	E	72/73 (99%)	70 (97%)	2 (3%)	38	48
5	e	72/73 (99%)	71 (99%)	1 (1%)	59	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	52 (96%)	2 (4%)	30	37
7	h	55/54 (102%)	55 (100%)	0	100	100
8	I	34/34 (100%)	32 (94%)	2 (6%)	18	18
8	i	34/34 (100%)	33 (97%)	1 (3%)	37	47
9	J	26/27 (96%)	24 (92%)	2 (8%)	12	10
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%)	35 (97%)	1 (3%)	38	48
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%)	209 (97%)	7 (3%)	34	43
13	o	213/207 (103%)	207 (97%)	6 (3%)	38	48
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	88/89 (99%)	86 (98%)	2 (2%)	44	55
16	V	123/117 (105%)	122 (99%)	1 (1%)	73	80
16	v	123/117 (105%)	119 (97%)	4 (3%)	33	42
17	X	32/33 (97%)	32 (100%)	0	100	100
17	x	31/33 (94%)	31 (100%)	0	100	100
18	Y	22/23 (96%)	22 (100%)	0	100	100
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%)	44 (85%)	8 (15%)	2	1
20	R	29/29 (100%)	27 (93%)	2 (7%)	14	13
All	All	5110/4403 (116%)	5003 (98%)	107 (2%)	45	58

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	491[A]	VAL
8	i	33	LYS
19	z	2	THR
3	c	142	GLU
3	c	315[B]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
3	c	415	ASN
11	l	8	GLN
19	Z	31	GLN
16	v	86	GLN
18	y	45	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	FME	m	1	12	8,9,10	0.53	0	7,9,11	1.44	2 (28%)
12	FME	M	1	12	8,9,10	0.61	0	7,9,11	1.13	1 (14%)
8	FME	i	1	8	8,9,10	0.65	0	7,9,11	1.24	0
8	FME	I	1	8	8,9,10	0.59	0	7,9,11	1.32	2 (28%)
14	FME	t	1	14	8,9,10	0.73	0	7,9,11	1.39	1 (14%)
14	FME	T	1	14	8,9,10	0.72	0	7,9,11	1.64	1 (14%)

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

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

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

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	O-C-CA	-2.74	117.60	124.78
14	T	1	FME	CG-CB-CA	2.53	119.98	112.95
12	m	1	FME	O1-CN-N	-2.45	118.81	125.27
8	I	1	FME	O-C-CA	-2.28	118.80	124.78
12	M	1	FME	O-C-CA	-2.19	119.05	124.78

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
12	m	1	FME	O1-CN-N-CA
12	m	1	FME	O-C-CA-CB
14	T	1	FME	C-CA-CB-CG
8	I	1	FME	O1-CN-N-CA

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	m	1	FME	3	0
12	M	1	FME	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
23	CLA	B	612	2	69,73,73	1.98	19 (27%)	83,113,113	2.89	29 (34%)
23	CLA	d	403[B]	4	69,73,73	1.95	20 (28%)	83,113,113	2.82	30 (36%)
32	LMG	D	412	39	51,51,55	0.84	2 (3%)	59,59,63	1.11	4 (6%)
24	PHO	a	414[A]	-	58,69,69	2.75	14 (24%)	56,99,99	3.01	17 (30%)
23	CLA	B	603	2	69,73,73	2.03	19 (27%)	83,113,113	2.94	31 (37%)
23	CLA	b	603	2	69,73,73	1.99	20 (28%)	83,113,113	2.88	33 (39%)
35	DGD	C	517[B]	-	63,63,67	0.86	2 (3%)	77,77,81	0.96	5 (6%)
23	CLA	C	510	3	69,73,73	2.03	20 (28%)	83,113,113	2.99	33 (39%)
23	CLA	A	404[B]	1	69,73,73	2.04	20 (28%)	83,113,113	2.83	29 (34%)
23	CLA	c	513	3	69,73,73	2.07	19 (27%)	83,113,113	2.85	31 (37%)
29	PL9	a	412[B]	-	55,55,55	0.64	2 (3%)	68,69,69	1.97	22 (32%)
23	CLA	d	404	4	69,73,73	2.03	20 (28%)	83,113,113	2.92	30 (36%)
27	GOL	o	302	-	5,5,5	0.95	0	5,5,5	0.99	0
25	BCR	c	516	-	41,41,41	1.04	1 (2%)	56,56,56	1.44	12 (21%)
32	LMG	d	412	39	51,51,55	0.89	2 (3%)	59,59,63	1.11	4 (6%)
38	HEM	f	101	6,5	50,50,50	1.48	6 (12%)	66,82,82	1.75	13 (19%)
23	CLA	b	615	2	69,73,73	2.01	19 (27%)	83,113,113	2.81	33 (39%)
23	CLA	B	604	2	69,73,73	2.00	21 (30%)	83,113,113	2.71	30 (36%)
24	PHO	a	414[B]	-	58,69,69	2.78	13 (22%)	56,99,99	2.91	16 (28%)
33	LHG	a	418[A]	-	41,41,48	1.04	2 (4%)	44,47,54	0.92	2 (4%)
32	LMG	c	501	-	51,51,55	0.92	2 (3%)	59,59,63	1.17	4 (6%)
33	LHG	A	419[B]	-	48,48,48	0.86	2 (4%)	51,54,54	1.22	6 (11%)
23	CLA	C	504	41	69,73,73	1.96	19 (27%)	83,113,113	2.79	29 (34%)
23	CLA	B	608	2	69,73,73	1.91	21 (30%)	83,113,113	2.91	33 (39%)
27	GOL	c	527	-	5,5,5	1.12	0	5,5,5	0.97	0
28	OEX	a	411[A]	41,3,1	0,14,14	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	508	41	69,73,73	2.03	19 (27%)	83,113,113	2.88	29 (34%)
24	PHO	A	416[A]	-	58,69,69	2.74	15 (25%)	56,99,99	2.87	17 (30%)
31	LMT	M	101	-	36,36,36	1.13	4 (11%)	47,47,47	1.22	4 (8%)
33	LHG	d	414[A]	-	48,48,48	0.89	2 (4%)	51,54,54	1.12	4 (7%)
23	CLA	B	609	2	69,73,73	2.01	18 (26%)	83,113,113	2.80	29 (34%)
34	HTG	B	623	-	19,19,19	0.83	2 (10%)	23,24,24	1.46	1 (4%)
31	LMT	B	630	-	36,36,36	1.04	3 (8%)	47,47,47	1.14	4 (8%)
32	LMG	Z	101	-	37,37,55	1.00	2 (5%)	45,45,63	1.46	8 (17%)
27	GOL	A	411	-	5,5,5	1.09	0	5,5,5	0.77	0
33	LHG	a	418[B]	-	41,41,48	1.04	2 (4%)	44,47,54	0.93	2 (4%)
25	BCR	A	409	-	41,41,41	1.04	1 (2%)	56,56,56	1.29	7 (12%)
25	BCR	k	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.46	12 (21%)
31	LMT	t	101	-	26,26,36	0.94	2 (7%)	31,31,47	1.30	2 (6%)
23	CLA	B	610	41	69,73,73	2.06	19 (27%)	83,113,113	2.88	33 (39%)
27	GOL	d	413	-	5,5,5	1.07	0	5,5,5	0.92	0
35	DGD	C	517[A]	-	63,63,67	0.89	3 (4%)	77,77,81	1.02	5 (6%)
35	DGD	c	519	-	63,63,67	0.89	4 (6%)	77,77,81	1.06	4 (5%)
32	LMG	A	418	-	51,51,55	0.91	2 (3%)	59,59,63	1.49	8 (13%)
23	CLA	b	611	2	69,73,73	1.95	21 (30%)	83,113,113	2.94	29 (34%)
24	PHO	A	407[B]	-	58,69,69	2.72	14 (24%)	56,99,99	2.68	16 (28%)
31	LMT	A	417	-	36,36,36	0.93	2 (5%)	47,47,47	1.01	1 (2%)
24	PHO	A	416[B]	-	58,69,69	2.74	15 (25%)	56,99,99	2.88	16 (28%)
31	LMT	b	627	-	25,25,36	0.88	1 (4%)	30,30,47	1.13	1 (3%)
35	DGD	h	102	-	63,63,67	0.87	3 (4%)	77,77,81	1.08	5 (6%)
23	CLA	c	510	3	69,73,73	2.05	20 (28%)	83,113,113	2.84	31 (37%)
23	CLA	C	513	3	69,73,73	2.04	19 (27%)	83,113,113	2.85	31 (37%)
40	HEC	V	201	16	50,50,50	1.77	6 (12%)	68,82,82	1.47	9 (13%)
23	CLA	A	406[A]	41	69,73,73	1.99	18 (26%)	83,113,113	2.86	32 (38%)
26	SQD	a	410	-	53,54,54	1.07	4 (7%)	62,65,65	1.25	8 (12%)
27	GOL	a	417	-	5,5,5	1.08	0	5,5,5	0.95	0
27	GOL	B	624	-	5,5,5	0.95	0	5,5,5	1.17	1 (20%)
23	CLA	a	404[A]	1	69,73,73	1.96	19 (27%)	83,113,113	2.88	33 (39%)
25	BCR	T	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.64	15 (26%)
28	OEX	A	413[A]	41,3,1	0,14,14	-	-	-	-	-
33	LHG	A	419[A]	-	48,48,48	0.84	2 (4%)	51,54,54	1.31	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	DGD	H	102	-	63,63,67	0.88	3 (4%)	77,77,81	1.07	6 (7%)
23	CLA	D	403[A]	4	69,73,73	1.98	19 (27%)	83,113,113	2.88	31 (37%)
29	PL9	D	406[A]	-	55,55,55	0.62	2 (3%)	68,69,69	1.64	18 (26%)
29	PL9	d	406[A]	-	55,55,55	0.65	1 (1%)	68,69,69	1.63	17 (25%)
31	LMT	B	631	-	25,25,36	0.88	1 (4%)	30,30,47	1.19	3 (10%)
23	CLA	C	505	3	69,73,73	1.99	19 (27%)	83,113,113	2.81	31 (37%)
23	CLA	A	406[B]	41	69,73,73	2.08	19 (27%)	83,113,113	2.84	32 (38%)
23	CLA	C	501	3	69,73,73	1.96	20 (28%)	83,113,113	2.87	32 (38%)
25	BCR	b	618	-	41,41,41	0.98	1 (2%)	56,56,56	1.27	7 (12%)
26	SQD	F	103	-	42,43,54	1.22	4 (9%)	51,54,65	2.18	14 (27%)
34	HTG	c	522	-	19,19,19	0.98	1 (5%)	23,24,24	1.54	1 (4%)
31	LMT	M	102	-	36,36,36	1.09	3 (8%)	47,47,47	1.07	2 (4%)
33	LHG	D	407[A]	-	48,48,48	0.86	2 (4%)	51,54,54	0.99	3 (5%)
23	CLA	c	507	3	69,73,73	2.02	20 (28%)	83,113,113	2.83	31 (37%)
25	BCR	C	515	-	41,41,41	1.05	1 (2%)	56,56,56	1.39	9 (16%)
23	CLA	a	404[B]	1	69,73,73	2.02	20 (28%)	83,113,113	2.91	32 (38%)
23	CLA	b	608	2	69,73,73	2.00	20 (28%)	83,113,113	2.82	33 (39%)
29	PL9	A	414[A]	-	55,55,55	0.68	2 (3%)	68,69,69	2.08	25 (36%)
28	OEX	A	413[B]	41,3,1	0,14,14	-	-	-	-	-
32	LMG	m	101	-	51,51,55	0.89	2 (3%)	59,59,63	1.23	4 (6%)
23	CLA	C	506	3	69,73,73	2.03	21 (30%)	83,113,113	2.84	31 (37%)
33	LHG	b	629[A]	-	48,48,48	0.85	3 (6%)	51,54,54	1.03	4 (7%)
23	CLA	D	403[B]	4	69,73,73	2.01	19 (27%)	83,113,113	2.83	31 (37%)
29	PL9	D	406[B]	-	55,55,55	0.61	1 (1%)	68,69,69	1.68	15 (22%)
29	PL9	d	406[B]	-	55,55,55	0.68	1 (1%)	68,69,69	1.60	19 (27%)
23	CLA	b	604	2	69,73,73	1.99	20 (28%)	83,113,113	2.83	30 (36%)
37	BCT	d	401[A]	21	2,3,3	0.57	0	2,3,3	1.58	1 (50%)
40	HEC	v	201	16	50,50,50	1.77	6 (12%)	68,82,82	1.35	5 (7%)
24	PHO	A	407[A]	-	58,69,69	2.69	14 (24%)	56,99,99	2.78	15 (26%)
23	CLA	B	616	2	69,73,73	1.98	20 (28%)	83,113,113	2.92	27 (32%)
23	CLA	c	503	3	69,73,73	2.00	18 (26%)	83,113,113	2.69	28 (33%)
25	BCR	Y	101	-	41,41,41	0.99	1 (2%)	56,56,56	1.66	10 (17%)
33	LHG	D	407[B]	-	48,48,48	0.89	2 (4%)	51,54,54	0.98	3 (5%)
34	HTG	B	622	-	19,19,19	1.05	2 (10%)	23,24,24	1.56	5 (21%)
31	LMT	F	101	-	36,36,36	1.07	1 (2%)	47,47,47	1.05	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	HTG	b	622	-	19,19,19	1.22	2 (10%)	23,24,24	1.98	7 (30%)
23	CLA	B	614	2	69,73,73	2.05	20 (28%)	83,113,113	3.01	31 (37%)
23	CLA	a	407	1	69,73,73	1.96	20 (28%)	83,113,113	2.89	31 (37%)
27	GOL	B	629	-	5,5,5	0.99	0	5,5,5	0.96	0
26	SQD	a	409[A]	-	53,54,54	0.95	3 (5%)	62,65,65	1.77	13 (20%)
23	CLA	c	505	41	69,73,73	2.07	20 (28%)	83,113,113	2.80	30 (36%)
23	CLA	B	605	2	69,73,73	2.03	19 (27%)	83,113,113	2.90	30 (36%)
27	GOL	O	303	-	5,5,5	0.82	0	5,5,5	1.14	1 (20%)
29	PL9	A	414[B]	-	55,55,55	0.65	2 (3%)	68,69,69	1.98	24 (35%)
33	LHG	b	629[B]	-	48,48,48	0.87	2 (4%)	51,54,54	1.03	4 (7%)
25	BCR	B	619	-	41,41,41	1.11	2 (4%)	56,56,56	1.37	12 (21%)
33	LHG	L	101[A]	-	48,48,48	0.89	2 (4%)	51,54,54	1.15	3 (5%)
25	BCR	b	619	-	41,41,41	1.07	1 (2%)	56,56,56	1.42	8 (14%)
23	CLA	C	503	3	69,73,73	2.00	19 (27%)	83,113,113	2.85	29 (34%)
33	LHG	D	408[A]	-	48,48,48	0.92	2 (4%)	51,54,54	0.99	4 (7%)
33	LHG	d	408[A]	-	48,48,48	0.92	2 (4%)	51,54,54	0.99	3 (5%)
34	HTG	C	521	-	19,19,19	0.86	1 (5%)	23,24,24	1.37	2 (8%)
31	LMT	A	420	-	36,36,36	1.06	2 (5%)	47,47,47	1.15	4 (8%)
23	CLA	B	602	2	69,73,73	2.00	20 (28%)	83,113,113	2.84	28 (33%)
34	HTG	b	625	-	19,19,19	0.97	2 (10%)	23,24,24	1.50	3 (13%)
37	BCT	D	401[B]	21	2,3,3	0.65	0	2,3,3	1.24	0
23	CLA	C	508	3	69,73,73	2.05	21 (30%)	83,113,113	2.81	26 (31%)
37	BCT	d	401[B]	21	2,3,3	0.64	0	2,3,3	1.22	0
38	HEM	F	102	6,5	50,50,50	1.54	7 (14%)	66,82,82	1.91	15 (22%)
23	CLA	b	612	2	69,73,73	2.01	20 (28%)	83,113,113	2.75	29 (34%)
23	CLA	A	405[A]	41	69,73,73	1.93	18 (26%)	83,113,113	2.88	33 (39%)
25	BCR	D	405	-	41,41,41	1.10	1 (2%)	56,56,56	1.84	16 (28%)
27	GOL	v	202[A]	-	5,5,5	1.27	0	5,5,5	0.72	0
23	CLA	b	616	2	69,73,73	2.00	19 (27%)	83,113,113	2.96	33 (39%)
31	LMT	a	415	-	36,36,36	1.01	1 (2%)	47,47,47	1.04	2 (4%)
26	SQD	a	409[B]	-	53,54,54	0.97	3 (5%)	62,65,65	1.64	11 (17%)
26	SQD	f	102	-	42,43,54	1.19	3 (7%)	51,54,65	1.52	11 (21%)
23	CLA	b	614	2	69,73,73	1.99	20 (28%)	83,113,113	2.95	31 (37%)
34	HTG	d	411	-	16,16,19	0.96	1 (6%)	20,21,24	1.64	1 (5%)
23	CLA	c	502	3	69,73,73	2.02	21 (30%)	83,113,113	2.87	29 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LHG	L	101[B]	-	48,48,48	0.92	2 (4%)	51,54,54	1.04	2 (3%)
23	CLA	B	613	2	69,73,73	2.02	20 (28%)	83,113,113	2.73	30 (36%)
33	LHG	D	408[B]	-	48,48,48	0.91	2 (4%)	51,54,54	0.98	3 (5%)
33	LHG	d	408[B]	-	48,48,48	0.92	2 (4%)	51,54,54	1.01	2 (3%)
25	BCR	c	515	-	41,41,41	0.99	1 (2%)	56,56,56	1.71	15 (26%)
23	CLA	c	504	3	69,73,73	2.05	19 (27%)	83,113,113	2.85	30 (36%)
35	DGD	C	518	-	63,63,67	0.88	3 (4%)	77,77,81	0.99	4 (5%)
23	CLA	c	512	3	69,73,73	2.05	21 (30%)	83,113,113	2.84	32 (38%)
23	CLA	A	405[B]	41	69,73,73	2.01	20 (28%)	83,113,113	2.88	32 (38%)
26	SQD	A	412	-	53,54,54	1.01	3 (5%)	62,65,65	1.21	7 (11%)
27	GOL	a	416	-	5,5,5	1.03	0	5,5,5	1.02	0
23	CLA	C	509	3	69,73,73	2.06	20 (28%)	83,113,113	2.89	32 (38%)
27	GOL	v	202[B]	-	5,5,5	1.05	0	5,5,5	0.88	0
23	CLA	C	502	3	69,73,73	2.03	20 (28%)	83,113,113	2.71	29 (34%)
27	GOL	l	102[A]	-	5,5,5	0.96	0	5,5,5	0.97	0
23	CLA	B	611	2	69,73,73	2.49	19 (27%)	83,113,113	4.11	32 (38%)
25	BCR	y	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.60	11 (19%)
25	BCR	h	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.46	10 (17%)
33	LHG	d	407[A]	-	48,48,48	0.86	2 (4%)	51,54,54	1.08	4 (7%)
23	CLA	A	408	1	69,73,73	1.93	19 (27%)	83,113,113	3.03	36 (43%)
25	BCR	H	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.49	9 (16%)
23	CLA	b	609	2	69,73,73	2.02	18 (26%)	83,113,113	2.84	31 (37%)
34	HTG	b	623	-	19,19,19	1.07	1 (5%)	23,24,24	1.87	2 (8%)
27	GOL	o	303	-	5,5,5	1.00	0	5,5,5	1.07	0
23	CLA	B	607	41	69,73,73	1.94	19 (27%)	83,113,113	2.88	30 (36%)
23	CLA	b	607	41	69,73,73	1.94	20 (28%)	83,113,113	2.77	28 (33%)
37	BCT	D	401[A]	21	2,3,3	0.54	0	2,3,3	1.81	1 (50%)
23	CLA	B	601	41	69,73,73	2.10	21 (30%)	83,113,113	2.89	30 (36%)
26	SQD	b	620	-	53,54,54	1.05	3 (5%)	62,65,65	1.69	12 (19%)
23	CLA	b	601	41	69,73,73	2.10	19 (27%)	83,113,113	2.82	29 (34%)
27	GOL	l	102[B]	-	5,5,5	0.84	0	5,5,5	1.02	0
27	GOL	C	522[A]	-	5,5,5	1.18	0	5,5,5	0.83	0
27	GOL	D	402	-	5,5,5	1.64	2 (40%)	5,5,5	1.01	1 (20%)
23	CLA	c	511	3	69,73,73	1.99	20 (28%)	83,113,113	2.84	34 (40%)
23	CLA	c	509	3	69,73,73	2.09	20 (28%)	83,113,113	2.80	26 (31%)
32	LMG	B	621	-	51,51,55	0.93	2 (3%)	59,59,63	1.31	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	610	41	69,73,73	2.03	20 (28%)	83,113,113	2.91	32 (38%)
23	CLA	a	405[B]	41	69,73,73	2.02	19 (27%)	83,113,113	2.90	31 (37%)
33	LHG	d	407[B]	-	48,48,48	0.88	2 (4%)	51,54,54	1.05	4 (7%)
23	CLA	b	613	2	69,73,73	1.95	19 (27%)	83,113,113	2.79	29 (34%)
27	GOL	V	203[A]	-	5,5,5	1.22	0	5,5,5	0.91	0
25	BCR	t	102	-	41,41,41	1.06	1 (2%)	56,56,56	1.59	10 (17%)
23	CLA	D	404	4	69,73,73	2.11	18 (26%)	83,113,113	2.74	30 (36%)
34	HTG	D	411	-	16,16,19	1.04	1 (6%)	20,21,24	1.54	1 (5%)
32	LMG	C	519	-	51,51,55	0.94	2 (3%)	59,59,63	1.11	4 (6%)
27	GOL	C	522[B]	-	5,5,5	1.08	0	5,5,5	0.86	0
32	LMG	c	520	-	51,51,55	0.90	2 (3%)	59,59,63	1.12	6 (10%)
23	CLA	C	511	3	69,73,73	2.03	20 (28%)	83,113,113	2.80	29 (34%)
27	GOL	b	624	-	5,5,5	1.20	1 (20%)	5,5,5	0.79	0
23	CLA	b	602	2	69,73,73	2.09	19 (27%)	83,113,113	2.99	36 (43%)
31	LMT	m	103	-	36,36,36	1.08	3 (8%)	47,47,47	1.08	3 (6%)
33	LHG	E	101[A]	-	41,41,48	1.06	2 (4%)	44,47,54	1.11	3 (6%)
32	LMG	C	520	-	51,51,55	1.06	3 (5%)	59,59,63	1.34	6 (10%)
23	CLA	B	615	2	69,73,73	2.03	18 (26%)	83,113,113	2.88	30 (36%)
27	GOL	B	627	-	5,5,5	0.89	0	5,5,5	1.04	1 (20%)
25	BCR	B	617	-	41,41,41	1.08	1 (2%)	56,56,56	1.28	7 (12%)
26	SQD	A	410[A]	-	53,54,54	0.93	3 (5%)	62,65,65	1.81	10 (16%)
27	GOL	c	526[A]	-	5,5,5	0.94	0	5,5,5	0.95	0
25	BCR	b	617	-	41,41,41	1.08	1 (2%)	56,56,56	1.34	6 (10%)
27	GOL	V	203[B]	-	5,5,5	1.06	0	5,5,5	0.85	0
23	CLA	C	507	41	69,73,73	1.98	19 (27%)	83,113,113	2.78	27 (32%)
25	BCR	B	618	-	41,41,41	0.98	1 (2%)	56,56,56	1.40	7 (12%)
23	CLA	b	606	2	69,73,73	1.98	19 (27%)	83,113,113	2.87	31 (37%)
23	CLA	B	606	2	69,73,73	1.95	19 (27%)	83,113,113	2.98	29 (34%)
23	CLA	C	512	3	69,73,73	2.04	19 (27%)	83,113,113	2.87	34 (40%)
27	GOL	O	302	-	5,5,5	0.96	0	5,5,5	0.89	0
33	LHG	E	101[B]	-	41,41,48	1.06	2 (4%)	44,47,54	1.10	4 (9%)
31	LMT	b	621	-	25,25,36	0.96	2 (8%)	30,30,47	1.19	3 (10%)
23	CLA	c	514	3	69,73,73	2.12	21 (30%)	83,113,113	2.87	31 (37%)
27	GOL	D	413	-	5,5,5	1.45	2 (40%)	5,5,5	0.81	0
27	GOL	c	526[B]	-	5,5,5	0.84	0	5,5,5	0.97	0
25	BCR	d	405	-	41,41,41	1.11	2 (4%)	56,56,56	2.03	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	SQD	A	410[B]	-	53,54,54	0.94	3 (5%)	62,65,65	1.76	11 (17%)
32	LMG	c	521	-	51,51,55	1.01	2 (3%)	59,59,63	1.36	7 (11%)
23	CLA	a	405[A]	41	69,73,73	1.96	19 (27%)	83,113,113	2.86	30 (36%)
23	CLA	d	402[A]	41	69,73,73	2.01	17 (24%)	83,113,113	2.80	29 (34%)
24	PHO	a	406[A]	-	58,69,69	2.72	12 (20%)	56,99,99	2.76	15 (26%)
31	LMT	B	628	-	36,36,36	1.17	4 (11%)	47,47,47	1.37	6 (12%)
35	DGD	c	517[A]	-	63,63,67	0.85	2 (3%)	77,77,81	1.12	6 (7%)
35	DGD	c	518[A]	-	63,63,67	0.84	2 (3%)	77,77,81	0.97	5 (6%)
35	DGD	C	516[A]	-	63,63,67	0.81	2 (3%)	77,77,81	1.21	8 (10%)
23	CLA	d	403[A]	4	69,73,73	1.94	20 (28%)	83,113,113	2.78	29 (34%)
26	SQD	B	620	-	53,54,54	1.07	4 (7%)	62,65,65	1.74	12 (19%)
34	HTG	V	202	-	11,11,19	0.26	0	15,15,24	1.20	1 (6%)
25	BCR	C	514	-	41,41,41	1.04	1 (2%)	56,56,56	1.46	6 (10%)
25	BCR	a	408	-	41,41,41	1.05	1 (2%)	56,56,56	1.40	6 (10%)
23	CLA	b	605	2	69,73,73	1.95	18 (26%)	83,113,113	2.97	31 (37%)
32	LMG	z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.06	3 (6%)
23	CLA	A	404[A]	1	69,73,73	1.98	20 (28%)	83,113,113	2.82	32 (38%)
29	PL9	a	412[A]	-	55,55,55	0.65	2 (3%)	68,69,69	2.00	22 (32%)
28	OEX	a	411[B]	41,3,1	0,14,14	-	-	-	-	-
23	CLA	d	402[B]	41	69,73,73	2.06	18 (26%)	83,113,113	2.93	32 (38%)
24	PHO	a	406[B]	-	58,69,69	2.75	13 (22%)	56,99,99	2.77	16 (28%)
27	GOL	b	628	-	5,5,5	0.50	0	5,5,5	1.34	1 (20%)
23	CLA	c	506	3	69,73,73	2.03	18 (26%)	83,113,113	2.80	29 (34%)
33	LHG	d	414[B]	-	48,48,48	0.90	2 (4%)	51,54,54	1.06	4 (7%)
25	BCR	K	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.40	10 (17%)
34	HTG	B	625	-	19,19,19	1.06	2 (10%)	23,24,24	1.21	3 (13%)
35	DGD	c	517[B]	-	63,63,67	0.86	2 (3%)	77,77,81	1.10	5 (6%)
35	DGD	c	518[B]	-	63,63,67	0.86	2 (3%)	77,77,81	0.95	5 (6%)
31	LMT	e	101	-	36,36,36	1.02	4 (11%)	47,47,47	1.02	1 (2%)
35	DGD	C	516[B]	-	63,63,67	0.84	2 (3%)	77,77,81	1.10	7 (9%)

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
23	CLA	B	612	2	-	4/39/115/115	-
23	CLA	d	403[B]	4	-	4/39/115/115	-
32	LMG	D	412	39	-	8/46/66/70	0/1/1/1
24	PHO	a	414[A]	-	-	1/37/103/103	0/5/6/6
23	CLA	B	603	2	-	6/39/115/115	-
23	CLA	b	603	2	-	6/39/115/115	-
35	DGD	C	517[B]	-	-	14/51/91/95	0/2/2/2
23	CLA	C	510	3	-	13/39/115/115	-
23	CLA	A	404[B]	1	-	7/39/115/115	-
23	CLA	c	513	3	-	14/39/115/115	-
29	PL9	a	412[B]	-	-	15/53/73/73	0/1/1/1
23	CLA	d	404	4	-	8/39/115/115	-
27	GOL	o	302	-	-	2/4/4/4	-
25	BCR	c	516	-	-	0/29/63/63	0/2/2/2
32	LMG	d	412	39	-	10/46/66/70	0/1/1/1
38	HEM	f	101	6,5	-	6/14/54/54	-
23	CLA	b	615	2	-	7/39/115/115	-
23	CLA	B	604	2	-	1/39/115/115	-
24	PHO	a	414[B]	-	-	1/37/103/103	0/5/6/6
33	LHG	a	418[A]	-	-	16/46/46/53	-
32	LMG	c	501	-	-	13/46/66/70	0/1/1/1
33	LHG	A	419[B]	-	-	14/53/53/53	-
23	CLA	C	504	41	-	8/39/115/115	-
23	CLA	B	608	2	-	3/39/115/115	-
27	GOL	c	527	-	-	3/4/4/4	-
23	CLA	c	508	41	-	9/39/115/115	-
24	PHO	A	416[A]	-	-	1/37/103/103	0/5/6/6
31	LMT	M	101	-	-	4/21/61/61	0/2/2/2
33	LHG	d	414[A]	-	-	13/53/53/53	-
23	CLA	B	609	2	-	1/39/115/115	-
34	HTG	B	623	-	-	2/10/30/30	0/1/1/1
31	LMT	B	630	-	-	10/21/61/61	0/2/2/2
32	LMG	Z	101	-	-	10/31/51/70	0/1/1/1
27	GOL	A	411	-	-	2/4/4/4	-
33	LHG	a	418[B]	-	-	16/46/46/53	-
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2
31	LMT	t	101	-	-	10/17/38/61	0/1/1/2
23	CLA	B	610	41	-	9/39/115/115	-
27	GOL	d	413	-	-	4/4/4/4	-
35	DGD	C	517[A]	-	-	15/51/91/95	0/2/2/2
35	DGD	c	519	-	-	12/51/91/95	0/2/2/2
32	LMG	A	418	-	-	14/46/66/70	0/1/1/1
23	CLA	b	611	2	-	3/39/115/115	-
24	PHO	A	407[B]	-	-	2/37/103/103	0/5/6/6
31	LMT	A	417	-	-	7/21/61/61	0/2/2/2
24	PHO	A	416[B]	-	-	3/37/103/103	0/5/6/6
31	LMT	b	627	-	-	11/17/37/61	0/1/1/2
35	DGD	h	102	-	-	15/51/91/95	0/2/2/2
23	CLA	c	510	3	-	15/39/115/115	-
23	CLA	C	513	3	-	7/39/115/115	-
40	HEC	V	201	16	1/1/3/7	6/14/54/54	-
23	CLA	A	406[A]	41	-	7/39/115/115	-
26	SQD	a	410	-	-	13/49/69/69	0/1/1/1
27	GOL	a	417	-	-	0/4/4/4	-
27	GOL	B	624	-	-	3/4/4/4	-
23	CLA	a	404[A]	1	-	3/39/115/115	-
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
33	LHG	A	419[A]	-	-	10/53/53/53	-
35	DGD	H	102	-	-	9/51/91/95	0/2/2/2
23	CLA	D	403[A]	4	-	0/39/115/115	-
29	PL9	D	406[A]	-	-	8/53/73/73	0/1/1/1
29	PL9	d	406[A]	-	-	6/53/73/73	0/1/1/1
31	LMT	B	631	-	-	11/17/37/61	0/1/1/2
23	CLA	C	505	3	-	6/39/115/115	-
23	CLA	A	406[B]	41	-	4/39/115/115	-
23	CLA	C	501	3	-	5/39/115/115	-
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
26	SQD	F	103	-	-	14/38/58/69	0/1/1/1
34	HTG	c	522	-	-	2/10/30/30	0/1/1/1
31	LMT	M	102	-	-	6/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LHG	D	407[A]	-	-	16/53/53/53	-
23	CLA	c	507	3	-	6/39/115/115	-
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
23	CLA	a	404[B]	1	-	5/39/115/115	-
23	CLA	b	608	2	-	5/39/115/115	-
29	PL9	A	414[A]	-	-	15/53/73/73	0/1/1/1
32	LMG	m	101	-	-	11/46/66/70	0/1/1/1
23	CLA	C	506	3	-	12/39/115/115	-
33	LHG	b	629[A]	-	-	20/53/53/53	-
23	CLA	D	403[B]	4	-	4/39/115/115	-
29	PL9	D	406[B]	-	-	9/53/73/73	0/1/1/1
29	PL9	d	406[B]	-	-	6/53/73/73	0/1/1/1
40	HEC	v	201	16	1/1/3/7	6/14/54/54	-
23	CLA	b	604	2	-	10/39/115/115	-
24	PHO	A	407[A]	-	-	3/37/103/103	0/5/6/6
23	CLA	B	616	2	-	5/39/115/115	-
23	CLA	c	503	3	-	7/39/115/115	-
25	BCR	Y	101	-	-	2/29/63/63	0/2/2/2
33	LHG	D	407[B]	-	-	16/53/53/53	-
34	HTG	B	622	-	-	3/10/30/30	0/1/1/1
31	LMT	F	101	-	-	8/21/61/61	0/2/2/2
34	HTG	b	622	-	-	5/10/30/30	0/1/1/1
23	CLA	B	614	2	-	14/39/115/115	-
23	CLA	a	407	1	-	9/39/115/115	-
27	GOL	B	629	-	-	4/4/4/4	-
26	SQD	a	409[A]	-	-	10/49/69/69	0/1/1/1
23	CLA	c	505	41	-	6/39/115/115	-
23	CLA	B	605	2	-	5/39/115/115	-
27	GOL	O	303	-	-	2/4/4/4	-
29	PL9	A	414[B]	-	-	15/53/73/73	0/1/1/1
33	LHG	b	629[B]	-	-	19/53/53/53	-
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
33	LHG	L	101[A]	-	-	19/53/53/53	-
25	BCR	b	619	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	503	3	-	2/39/115/115	-
33	LHG	D	408[A]	-	-	14/53/53/53	-
33	LHG	d	408[A]	-	-	11/53/53/53	-
34	HTG	C	521	-	-	0/10/30/30	0/1/1/1
31	LMT	A	420	-	-	16/21/61/61	0/2/2/2
23	CLA	B	602	2	-	9/39/115/115	-
34	HTG	b	625	-	-	3/10/30/30	0/1/1/1
23	CLA	C	508	3	-	3/39/115/115	-
38	HEM	F	102	6,5	-	6/14/54/54	-
23	CLA	b	612	2	-	3/39/115/115	-
23	CLA	A	405[A]	41	-	4/39/115/115	-
25	BCR	D	405	-	-	4/29/63/63	0/2/2/2
27	GOL	v	202[A]	-	-	1/4/4/4	-
23	CLA	b	616	2	-	9/39/115/115	-
31	LMT	a	415	-	-	10/21/61/61	0/2/2/2
26	SQD	a	409[B]	-	-	10/49/69/69	0/1/1/1
26	SQD	f	102	-	-	13/38/58/69	0/1/1/1
23	CLA	b	614	2	-	15/39/115/115	-
34	HTG	d	411	-	-	1/7/27/30	0/1/1/1
23	CLA	c	502	3	-	2/39/115/115	-
33	LHG	L	101[B]	-	-	17/53/53/53	-
23	CLA	B	613	2	-	9/39/115/115	-
33	LHG	D	408[B]	-	-	13/53/53/53	-
33	LHG	d	408[B]	-	-	14/53/53/53	-
25	BCR	c	515	-	-	0/29/63/63	0/2/2/2
23	CLA	c	504	3	-	1/39/115/115	-
35	DGD	C	518	-	-	19/51/91/95	0/2/2/2
23	CLA	c	512	3	-	6/39/115/115	-
23	CLA	A	405[B]	41	-	3/39/115/115	-
26	SQD	A	412	-	-	16/49/69/69	0/1/1/1
27	GOL	a	416	-	-	2/4/4/4	-
23	CLA	C	509	3	-	9/39/115/115	-
27	GOL	v	202[B]	-	-	2/4/4/4	-
23	CLA	C	502	3	-	11/39/115/115	-
27	GOL	l	102[A]	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	611	2	-	1/39/115/115	-
25	BCR	y	101	-	-	4/29/63/63	0/2/2/2
25	BCR	h	101	-	-	1/29/63/63	0/2/2/2
33	LHG	d	407[A]	-	-	13/53/53/53	-
23	CLA	A	408	1	-	8/39/115/115	-
25	BCR	H	101	-	-	3/29/63/63	0/2/2/2
23	CLA	b	609	2	-	1/39/115/115	-
34	HTG	b	623	-	-	4/10/30/30	0/1/1/1
27	GOL	o	303	-	-	3/4/4/4	-
23	CLA	B	607	41	-	3/39/115/115	-
23	CLA	b	607	41	-	4/39/115/115	-
23	CLA	B	601	41	-	11/39/115/115	-
26	SQD	b	620	-	-	16/49/69/69	0/1/1/1
23	CLA	b	601	41	-	18/39/115/115	-
27	GOL	l	102[B]	-	-	1/4/4/4	-
27	GOL	C	522[A]	-	-	0/4/4/4	-
27	GOL	D	402	-	-	2/4/4/4	-
23	CLA	c	511	3	-	10/39/115/115	-
23	CLA	c	509	3	-	5/39/115/115	-
32	LMG	B	621	-	-	18/46/66/70	0/1/1/1
23	CLA	b	610	41	-	5/39/115/115	-
23	CLA	a	405[B]	41	-	5/39/115/115	-
33	LHG	d	407[B]	-	-	15/53/53/53	-
23	CLA	b	613	2	-	3/39/115/115	-
27	GOL	V	203[A]	-	-	2/4/4/4	-
25	BCR	t	102	-	-	5/29/63/63	0/2/2/2
23	CLA	D	404	4	-	12/39/115/115	-
34	HTG	D	411	-	-	3/7/27/30	0/1/1/1
32	LMG	C	519	-	-	10/46/66/70	0/1/1/1
27	GOL	C	522[B]	-	-	0/4/4/4	-
32	LMG	c	520	-	-	12/46/66/70	0/1/1/1
23	CLA	C	511	3	-	4/39/115/115	-
27	GOL	b	624	-	-	2/4/4/4	-
23	CLA	b	602	2	-	5/39/115/115	-
31	LMT	m	103	-	-	5/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LHG	E	101[A]	-	-	22/46/46/53	-
32	LMG	C	520	-	-	13/46/66/70	0/1/1/1
23	CLA	B	615	2	-	8/39/115/115	-
27	GOL	B	627	-	-	0/4/4/4	-
25	BCR	B	617	-	-	2/29/63/63	0/2/2/2
26	SQD	A	410[A]	-	-	12/49/69/69	0/1/1/1
27	GOL	c	526[A]	-	-	0/4/4/4	-
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
27	GOL	V	203[B]	-	-	2/4/4/4	-
23	CLA	C	507	41	-	7/39/115/115	-
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
23	CLA	b	606	2	-	13/39/115/115	-
23	CLA	B	606	2	-	9/39/115/115	-
23	CLA	C	512	3	-	11/39/115/115	-
27	GOL	O	302	-	-	2/4/4/4	-
33	LHG	E	101[B]	-	-	22/46/46/53	-
31	LMT	b	621	-	-	8/17/37/61	0/1/1/2
23	CLA	c	514	3	-	12/39/115/115	-
27	GOL	D	413	-	-	4/4/4/4	-
27	GOL	c	526[B]	-	-	0/4/4/4	-
25	BCR	d	405	-	-	5/29/63/63	0/2/2/2
26	SQD	A	410[B]	-	-	12/49/69/69	0/1/1/1
32	LMG	c	521	-	-	12/46/66/70	0/1/1/1
23	CLA	a	405[A]	41	-	7/39/115/115	-
23	CLA	d	402[A]	41	-	8/39/115/115	-
24	PHO	a	406[A]	-	-	5/37/103/103	0/5/6/6
31	LMT	B	628	-	-	12/21/61/61	0/2/2/2
35	DGD	c	517[A]	-	-	20/51/91/95	0/2/2/2
35	DGD	c	518[A]	-	-	17/51/91/95	0/2/2/2
35	DGD	C	516[A]	-	-	11/51/91/95	0/2/2/2
23	CLA	d	403[A]	4	-	2/39/115/115	-
26	SQD	B	620	-	-	14/49/69/69	0/1/1/1
34	HTG	V	202	-	-	0/2/19/30	0/1/1/1
25	BCR	C	514	-	-	1/29/63/63	0/2/2/2
25	BCR	a	408	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	605	2	-	7/39/115/115	-
32	LMG	z	101	-	-	9/34/54/70	0/1/1/1
23	CLA	A	404[A]	1	-	5/39/115/115	-
29	PL9	a	412[A]	-	-	14/53/73/73	0/1/1/1
23	CLA	d	402[B]	41	-	3/39/115/115	-
24	PHO	a	406[B]	-	-	5/37/103/103	0/5/6/6
27	GOL	b	628	-	-	0/4/4/4	-
23	CLA	c	506	3	-	7/39/115/115	-
33	LHG	d	414[B]	-	-	12/53/53/53	-
25	BCR	K	102	-	-	2/29/63/63	0/2/2/2
34	HTG	B	625	-	-	4/10/30/30	0/1/1/1
35	DGD	c	517[B]	-	-	19/51/91/95	0/2/2/2
35	DGD	c	518[B]	-	-	17/51/91/95	0/2/2/2
31	LMT	e	101	-	-	15/21/61/61	0/2/2/2
35	DGD	C	516[B]	-	-	14/51/91/95	0/2/2/2

The worst 5 of 1871 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407[B]	PHO	C1D-C2D	9.33	1.49	1.39
24	a	406[B]	PHO	C1B-C2B	9.13	1.49	1.39
24	A	407[A]	PHO	C1D-C2D	9.11	1.49	1.39
24	a	406[A]	PHO	C1B-C2B	8.96	1.49	1.39
24	a	414[B]	PHO	C1D-C2D	8.78	1.49	1.39

The worst 5 of 3321 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	C2B-C1B-NB	16.86	121.53	110.23
23	B	611	CLA	C3B-C2B-C1B	-13.43	90.94	107.16
23	B	611	CLA	C1D-ND-C4D	-12.14	97.71	106.33
24	a	414[A]	PHO	C2D-C1D-ND	11.91	117.75	109.53
24	A	407[A]	PHO	C2D-C1D-ND	11.43	117.42	109.53

All (2) chirality outliers are listed below:

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

5 of 1656 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	408	CLA	C4-C3-C5-C6
23	B	614	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D

There are no ring outliers.

170 monomers are involved in 371 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	612	CLA	1	0
23	d	403[B]	CLA	5	0
24	a	414[A]	PHO	2	0
35	C	517[B]	DGD	1	0
23	C	510	CLA	4	0
23	A	404[B]	CLA	4	0
23	c	513	CLA	5	0
29	a	412[B]	PL9	4	0
23	d	404	CLA	2	0
32	d	412	LMG	3	0
38	f	101	HEM	1	0
23	b	615	CLA	1	0
23	B	604	CLA	1	0
33	a	418[A]	LHG	4	0
33	A	419[B]	LHG	1	0
23	C	504	CLA	1	0
23	c	508	CLA	2	0
24	A	416[A]	PHO	1	0
31	M	101	LMT	2	0
23	B	609	CLA	2	0
31	B	630	LMT	1	0
32	Z	101	LMG	1	0
33	a	418[B]	LHG	4	0
25	A	409	BCR	2	0
25	k	101	BCR	2	0
31	t	101	LMT	2	0
35	C	517[A]	DGD	2	0
35	c	519	DGD	2	0
24	A	407[B]	PHO	1	0
31	A	417	LMT	1	0
24	A	416[B]	PHO	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	c	510	CLA	4	0
23	C	513	CLA	1	0
40	V	201	HEC	1	0
23	A	406[A]	CLA	1	0
26	a	410	SQD	2	0
27	a	417	GOL	4	0
27	B	624	GOL	1	0
23	a	404[A]	CLA	3	0
25	T	101	BCR	6	0
33	A	419[A]	LHG	2	0
35	H	102	DGD	1	0
23	D	403[A]	CLA	3	0
31	B	631	LMT	1	0
23	C	505	CLA	6	0
23	A	406[B]	CLA	1	0
23	C	501	CLA	5	0
25	b	618	BCR	4	0
26	F	103	SQD	2	0
34	c	522	HTG	1	0
31	M	102	LMT	1	0
33	D	407[A]	LHG	2	0
23	c	507	CLA	4	0
25	C	515	BCR	1	0
23	a	404[B]	CLA	4	0
29	A	414[A]	PL9	10	0
23	C	506	CLA	5	0
23	D	403[B]	CLA	3	0
23	b	604	CLA	4	0
24	A	407[A]	PHO	2	0
23	B	616	CLA	4	0
23	c	503	CLA	2	0
25	Y	101	BCR	2	0
33	D	407[B]	LHG	1	0
34	B	622	HTG	2	0
34	b	622	HTG	3	0
23	B	614	CLA	2	0
23	a	407	CLA	5	0
26	a	409[A]	SQD	4	0
23	c	505	CLA	2	0
23	B	605	CLA	4	0
27	O	303	GOL	3	0
29	A	414[B]	PL9	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	619	BCR	2	0
25	b	619	BCR	4	0
23	C	503	CLA	6	0
33	D	408[A]	LHG	6	0
33	d	408[A]	LHG	9	0
31	A	420	LMT	1	0
23	B	602	CLA	2	0
34	b	625	HTG	1	0
23	C	508	CLA	5	0
38	F	102	HEM	1	0
23	b	612	CLA	1	0
23	A	405[A]	CLA	4	0
25	D	405	BCR	1	0
27	v	202[A]	GOL	1	0
23	b	616	CLA	1	0
31	a	415	LMT	1	0
26	a	409[B]	SQD	3	0
23	b	614	CLA	3	0
23	c	502	CLA	3	0
23	B	613	CLA	5	0
33	D	408[B]	LHG	3	0
33	d	408[B]	LHG	7	0
25	c	515	BCR	3	0
23	c	504	CLA	3	0
35	C	518	DGD	3	0
23	c	512	CLA	5	0
23	A	405[B]	CLA	6	0
26	A	412	SQD	1	0
27	a	416	GOL	2	0
23	C	509	CLA	2	0
27	v	202[B]	GOL	2	0
23	C	502	CLA	3	0
27	l	102[A]	GOL	1	0
25	y	101	BCR	2	0
25	h	101	BCR	3	0
33	d	407[A]	LHG	3	0
23	A	408	CLA	3	0
25	H	101	BCR	1	0
23	b	609	CLA	4	0
23	b	607	CLA	3	0
23	B	601	CLA	3	0
26	b	620	SQD	4	0

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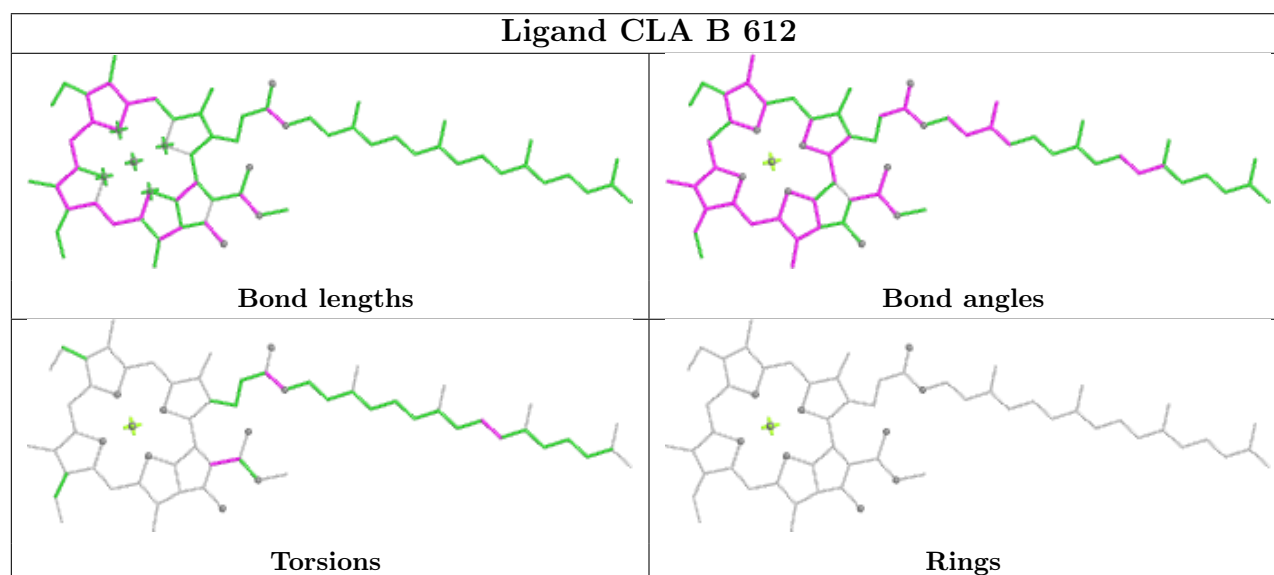
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	b	601	CLA	2	0
27	l	102[B]	GOL	1	0
27	D	402	GOL	5	0
23	c	511	CLA	1	0
23	c	509	CLA	9	0
32	B	621	LMG	1	0
23	a	405[B]	CLA	3	0
33	d	407[B]	LHG	3	0
23	b	613	CLA	4	0
25	t	102	BCR	6	0
32	c	520	LMG	1	0
23	C	511	CLA	3	0
27	b	624	GOL	1	0
33	E	101[A]	LHG	5	0
32	C	520	LMG	2	0
23	B	615	CLA	6	0
25	B	617	BCR	2	0
26	A	410[A]	SQD	2	0
25	b	617	BCR	1	0
23	C	507	CLA	2	0
25	B	618	BCR	4	0
23	b	606	CLA	3	0
23	B	606	CLA	2	0
23	C	512	CLA	2	0
27	O	302	GOL	1	0
33	E	101[B]	LHG	3	0
31	b	621	LMT	1	0
23	c	514	CLA	2	0
27	D	413	GOL	3	0
25	d	405	BCR	2	0
26	A	410[B]	SQD	1	0
32	c	521	LMG	1	0
23	a	405[A]	CLA	2	0
23	d	402[A]	CLA	2	0
35	c	517[A]	DGD	2	0
35	c	518[A]	DGD	1	0
35	C	516[A]	DGD	2	0
23	d	403[A]	CLA	2	0
26	B	620	SQD	1	0
25	C	514	BCR	1	0
25	a	408	BCR	1	0
23	b	605	CLA	5	0

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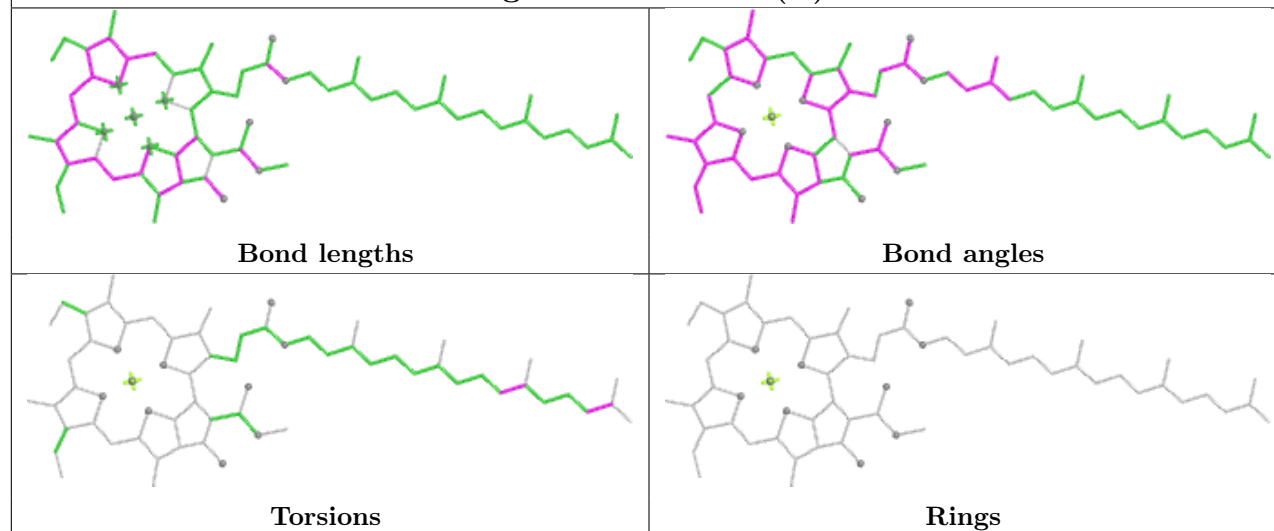
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	z	101	LMG	2	0
23	A	404[A]	CLA	5	0
29	a	412[A]	PL9	4	0
23	d	402[B]	CLA	4	0
24	a	406[B]	PHO	1	0
23	c	506	CLA	4	0
33	d	414[B]	LHG	1	0
25	K	102	BCR	1	0
34	B	625	HTG	1	0
35	c	517[B]	DGD	1	0
35	c	518[B]	DGD	1	0
31	e	101	LMT	1	0
35	C	516[B]	DGD	3	0

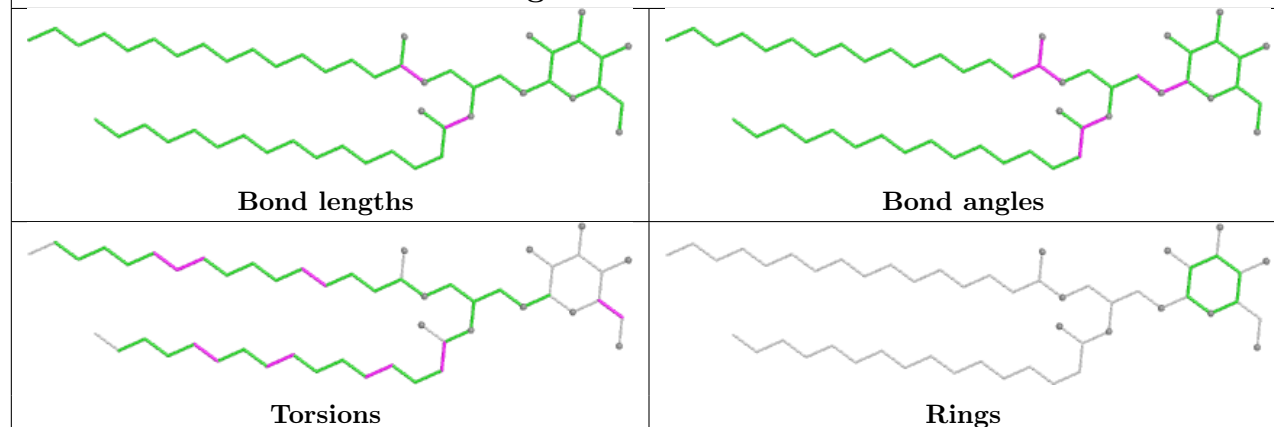
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



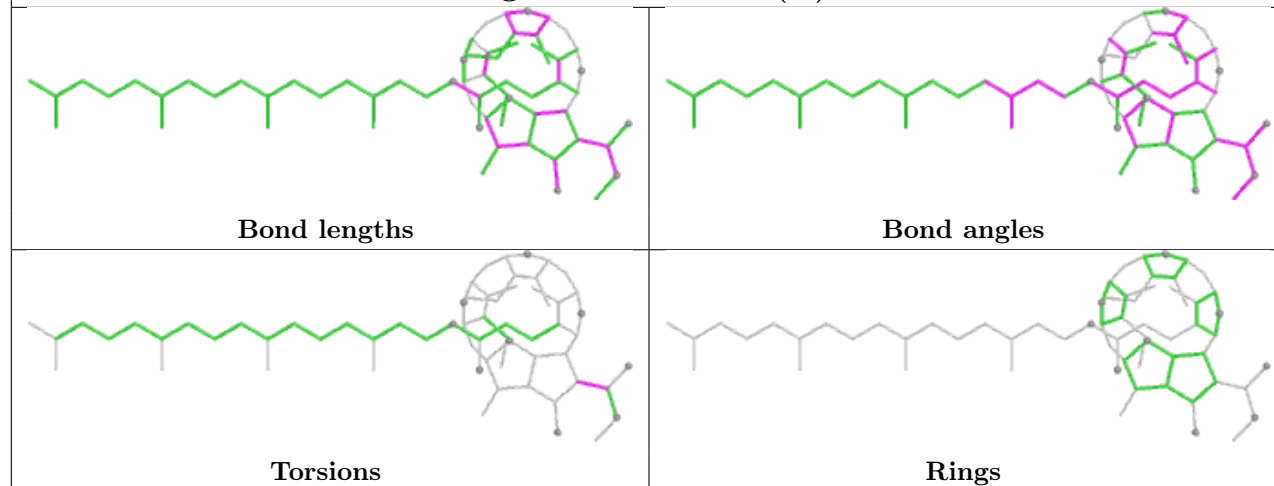
Ligand CLA d 403 (B)

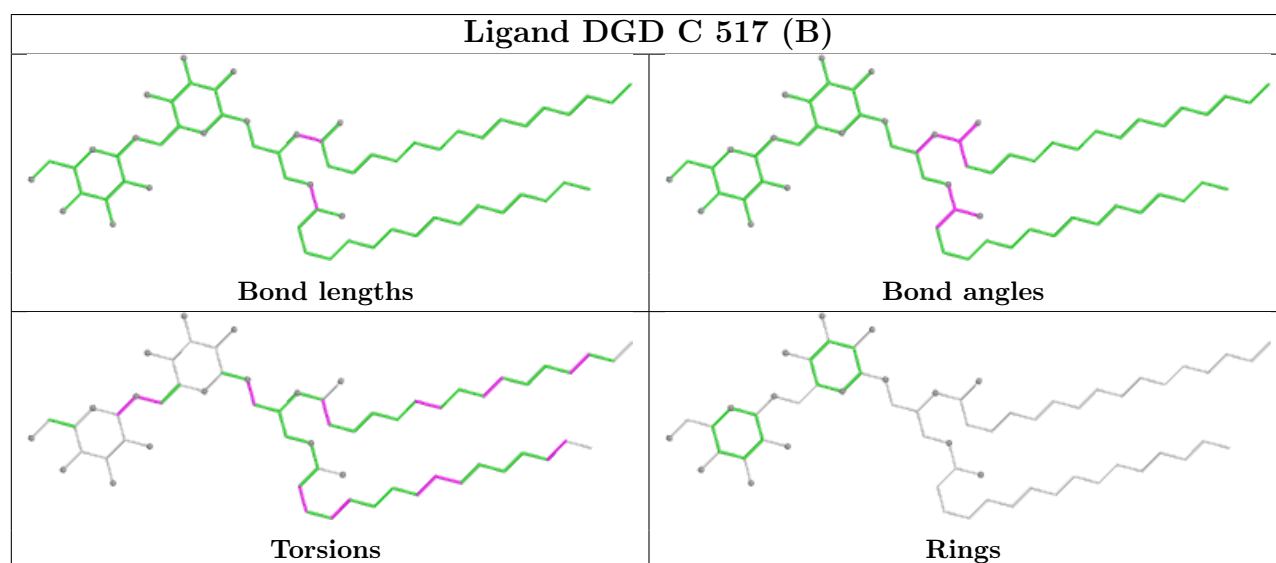
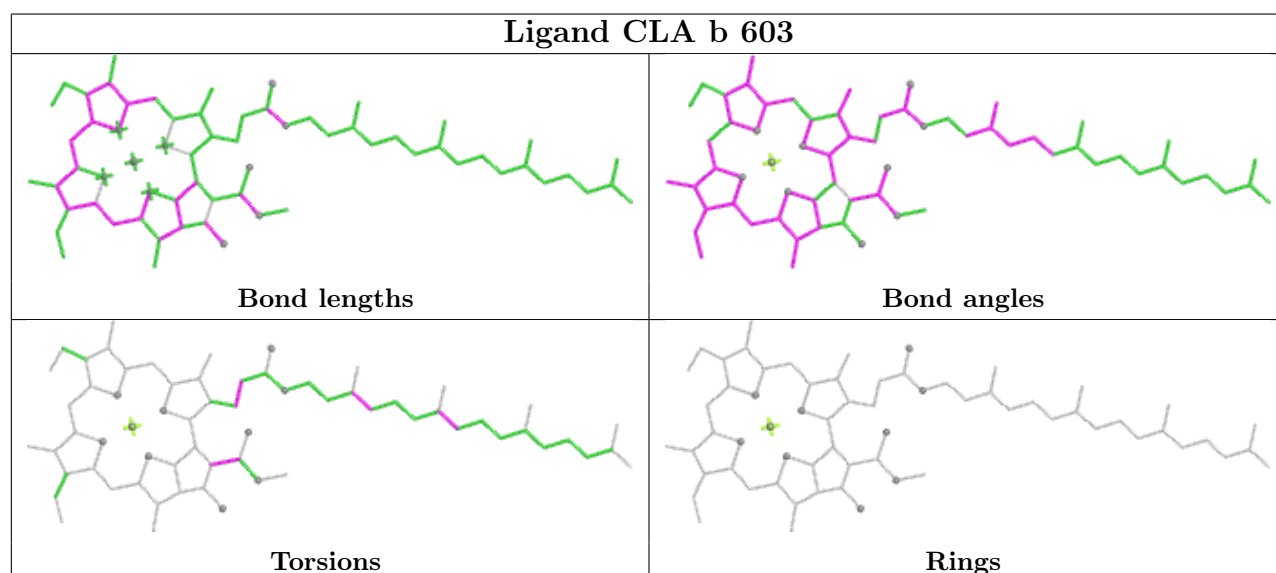
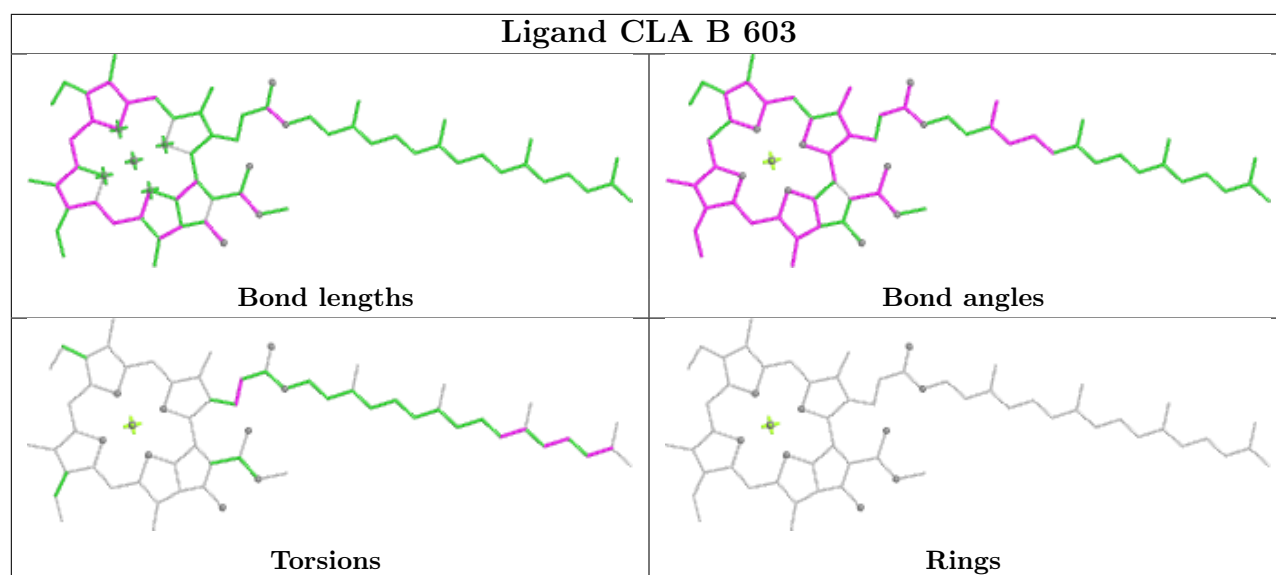


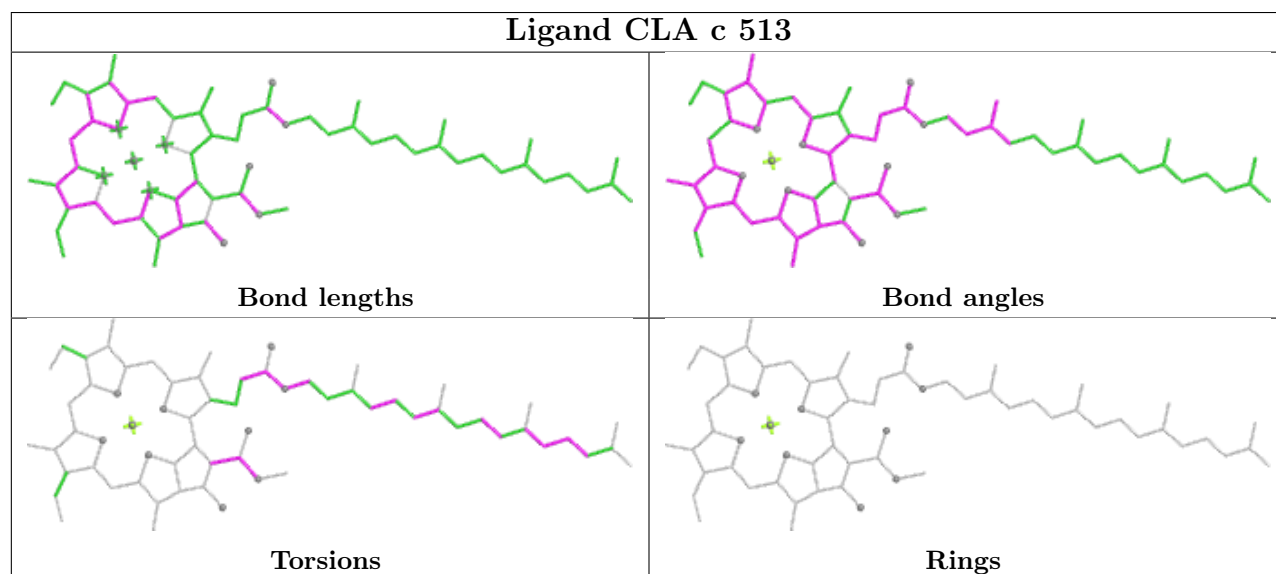
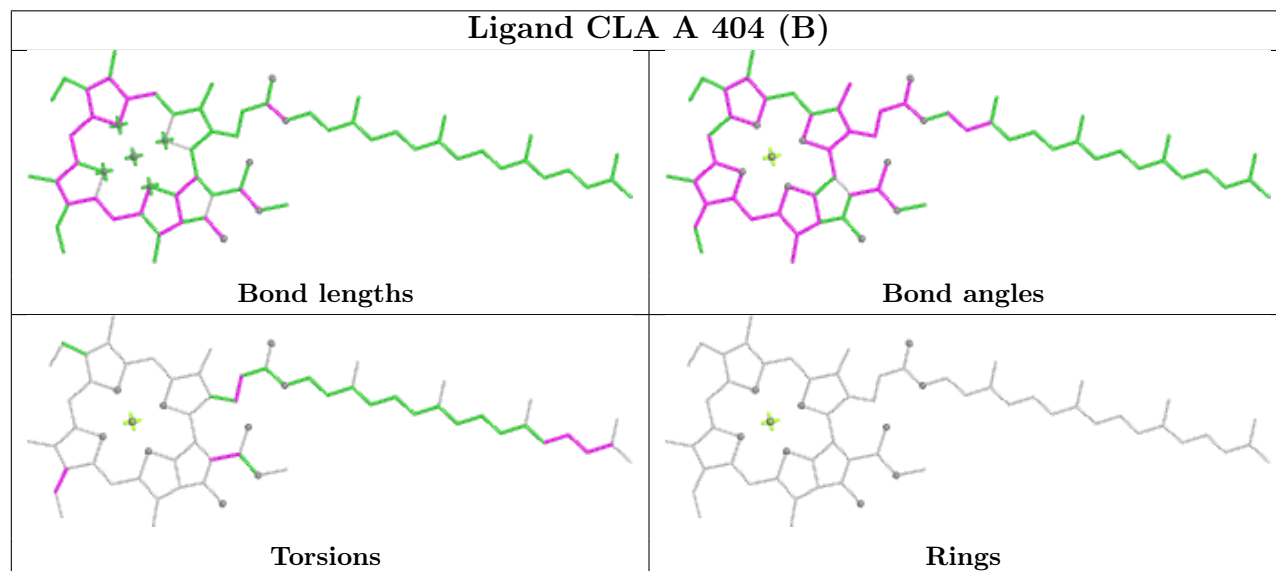
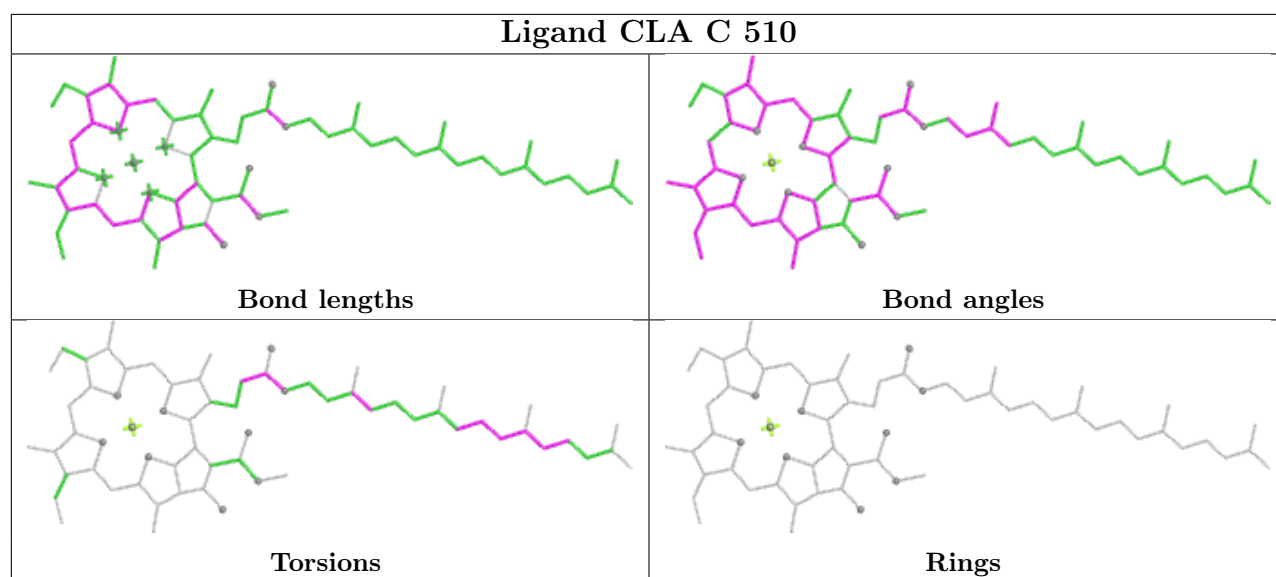
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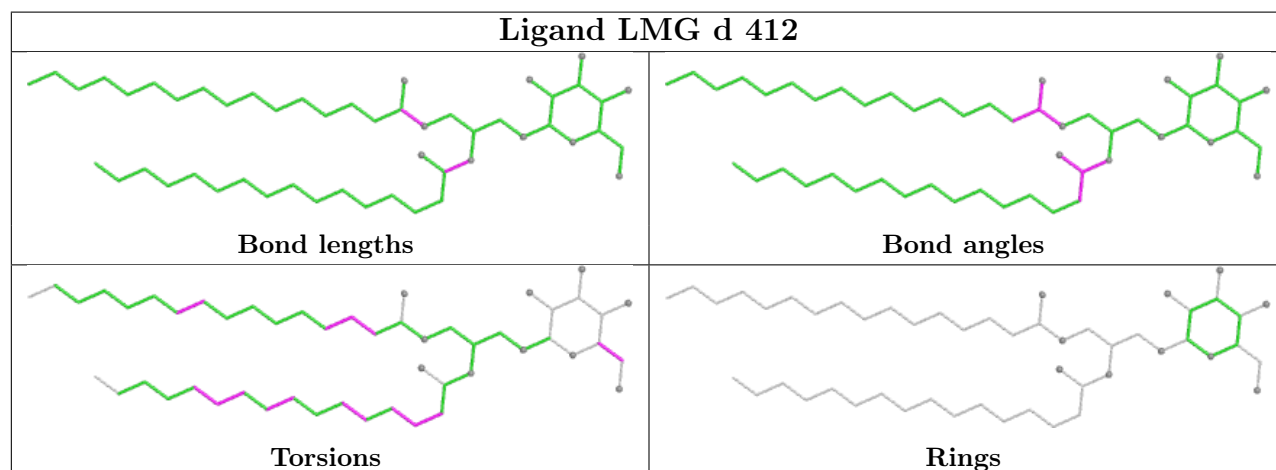
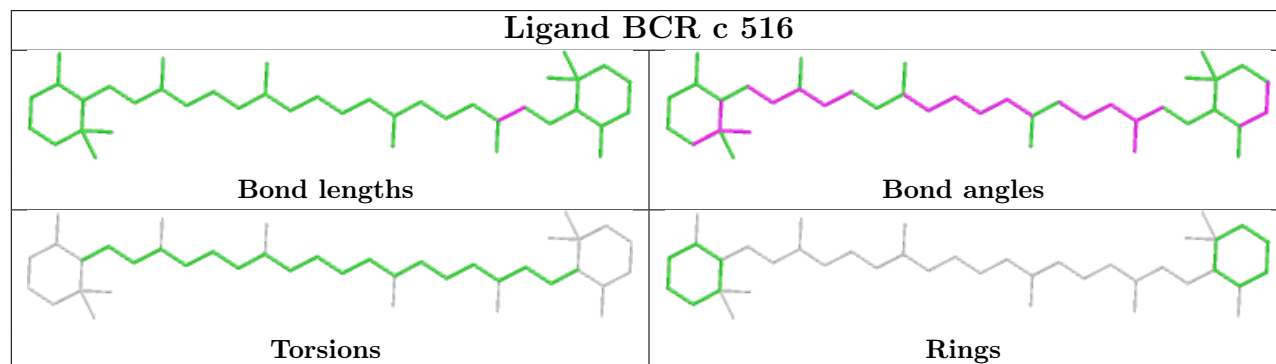
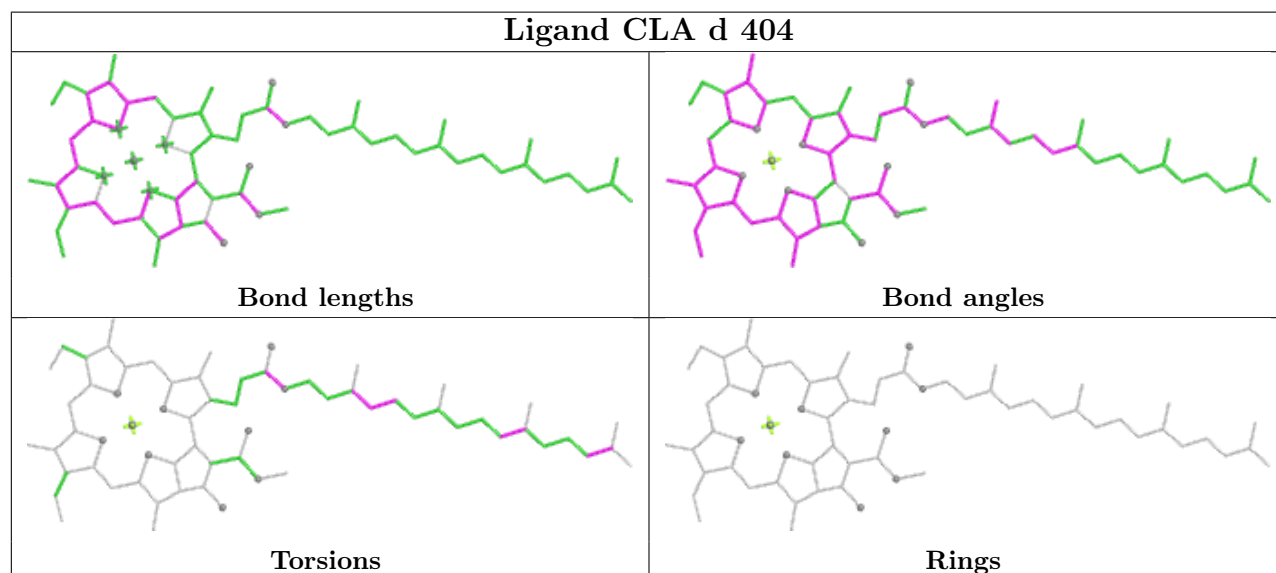
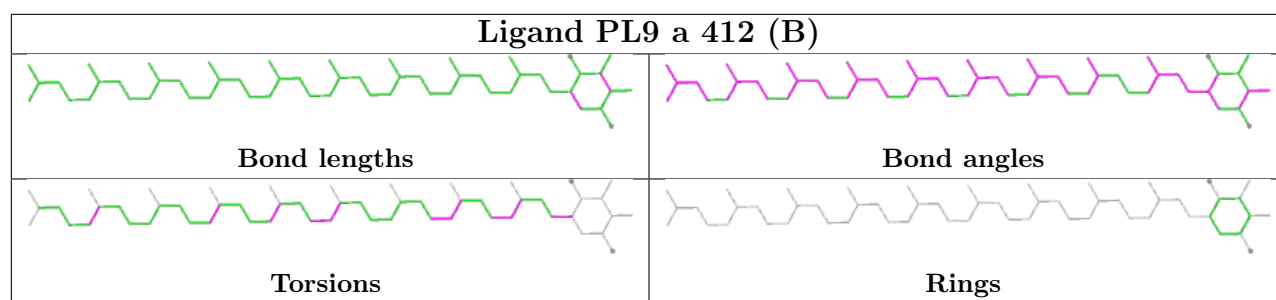


Ligand PHO a 414 (A)

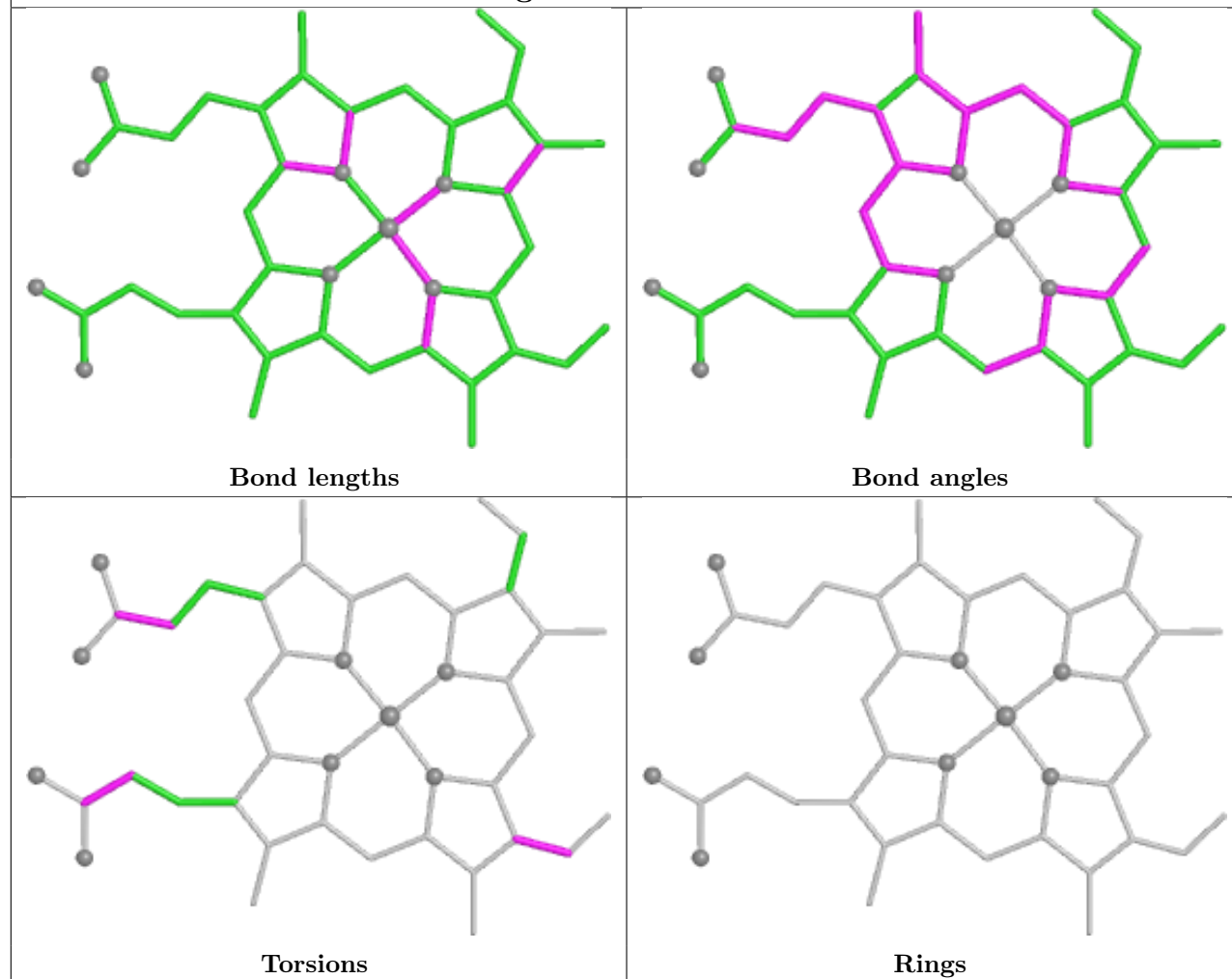




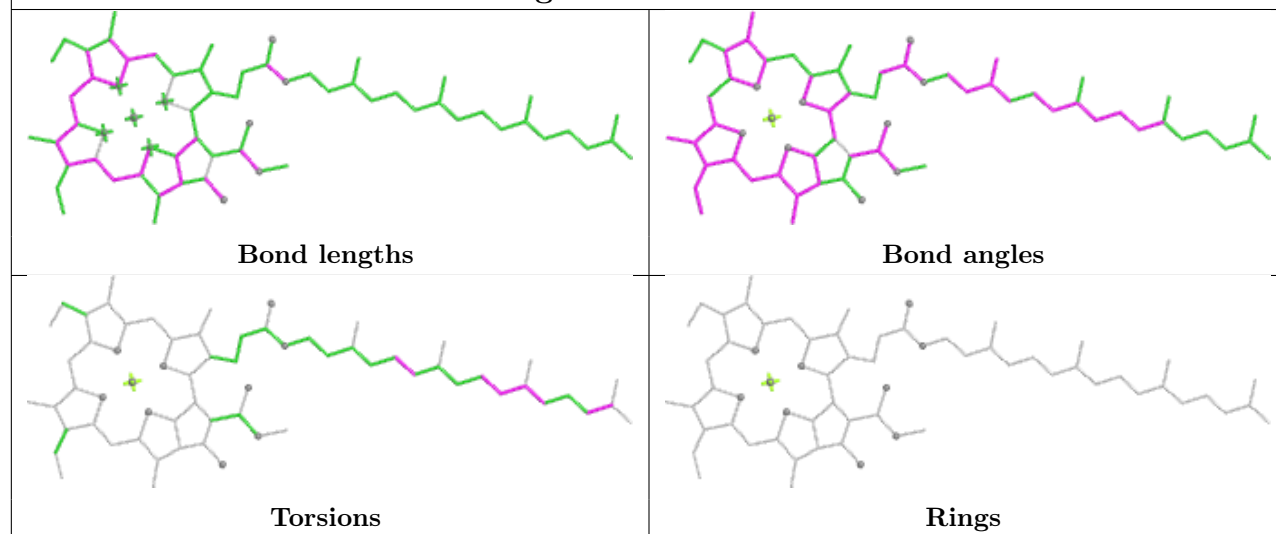


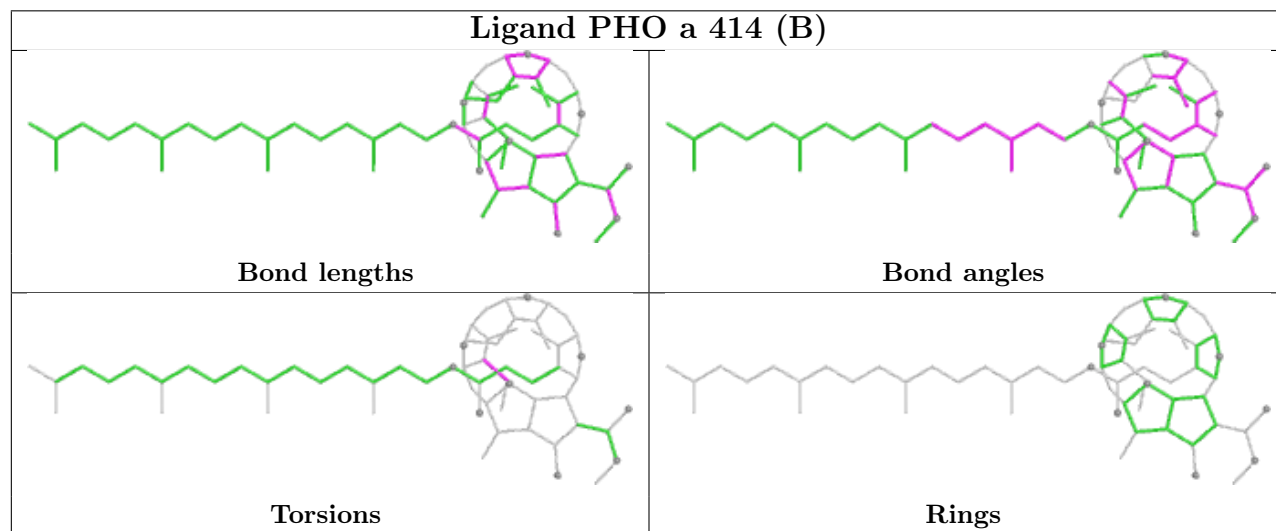
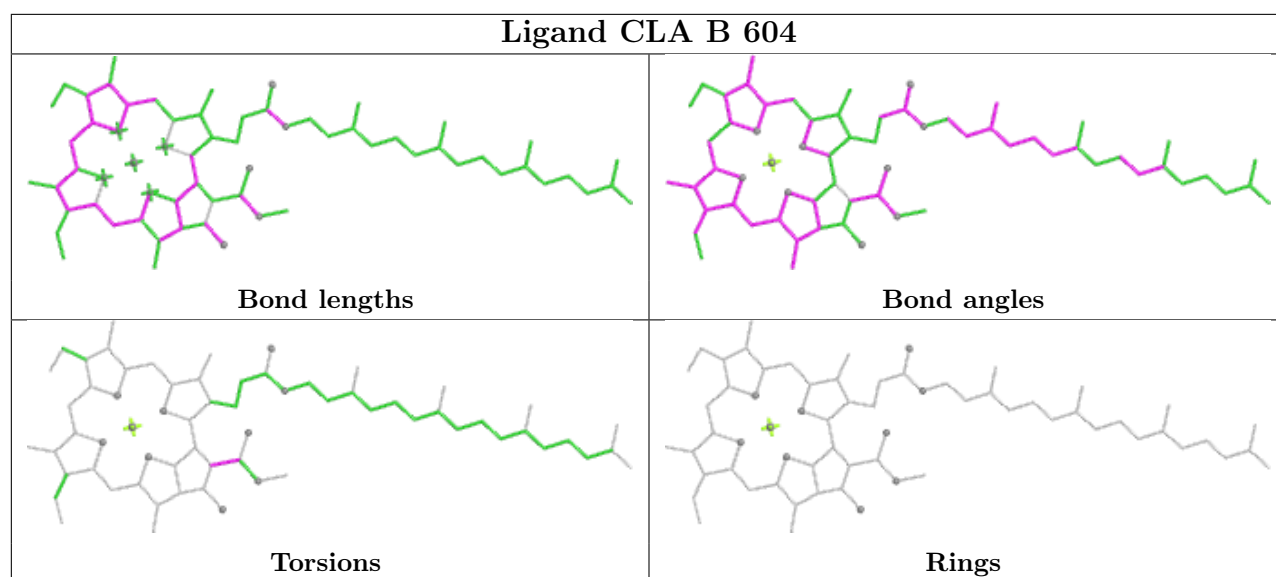


Ligand HEM f 101

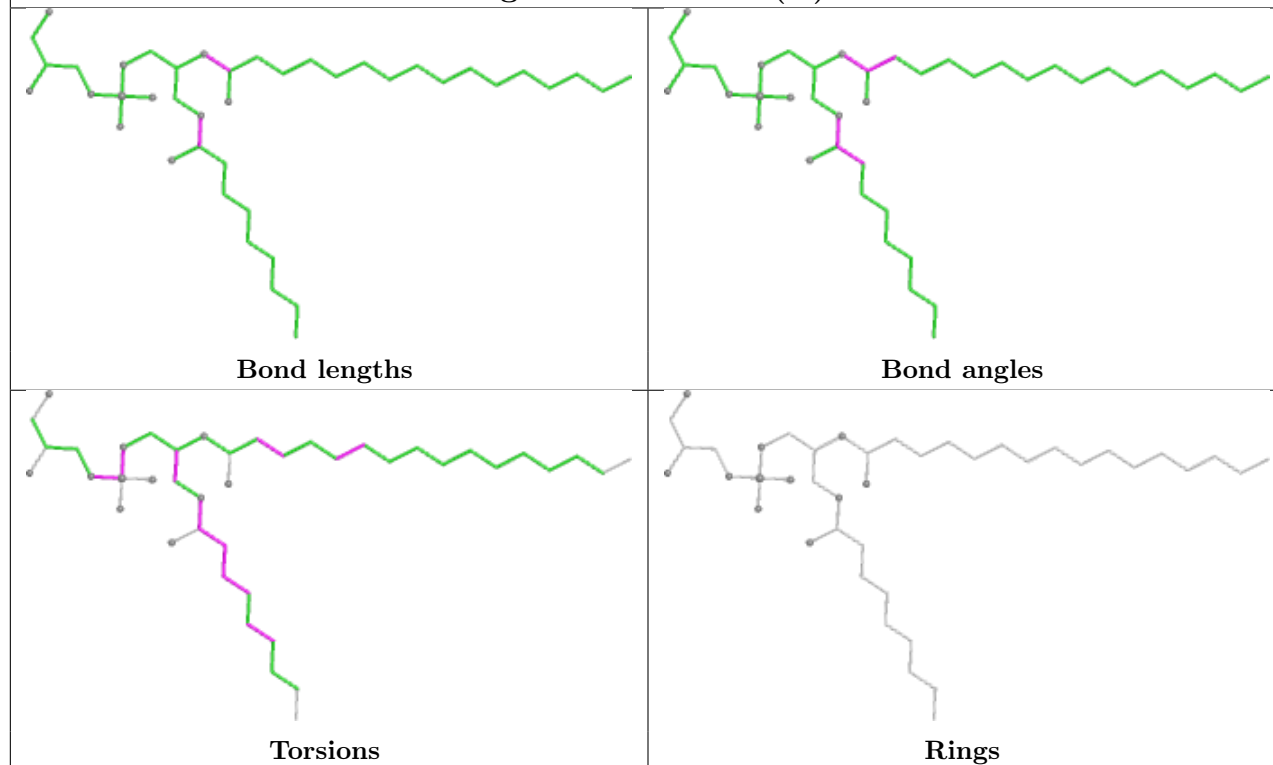


Ligand CLA b 615

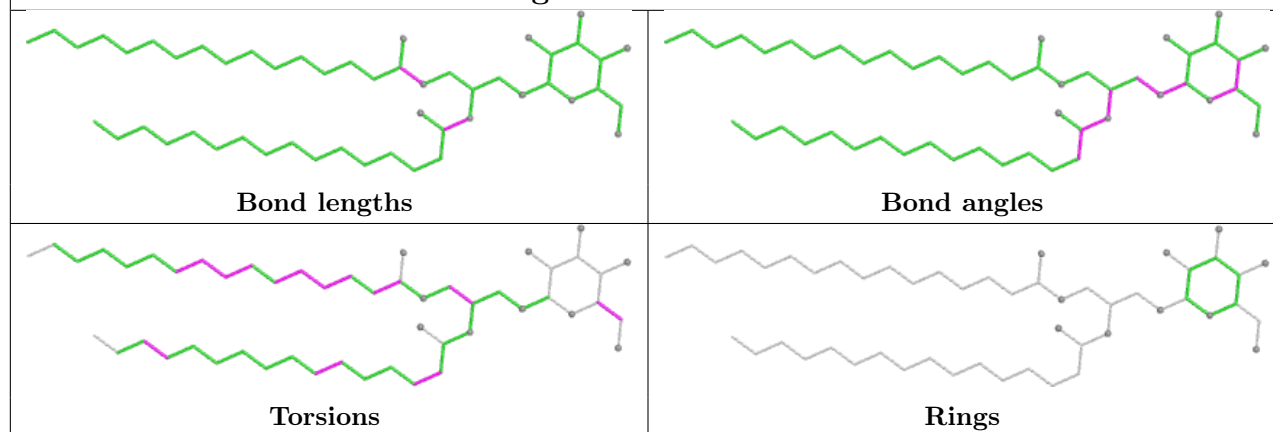




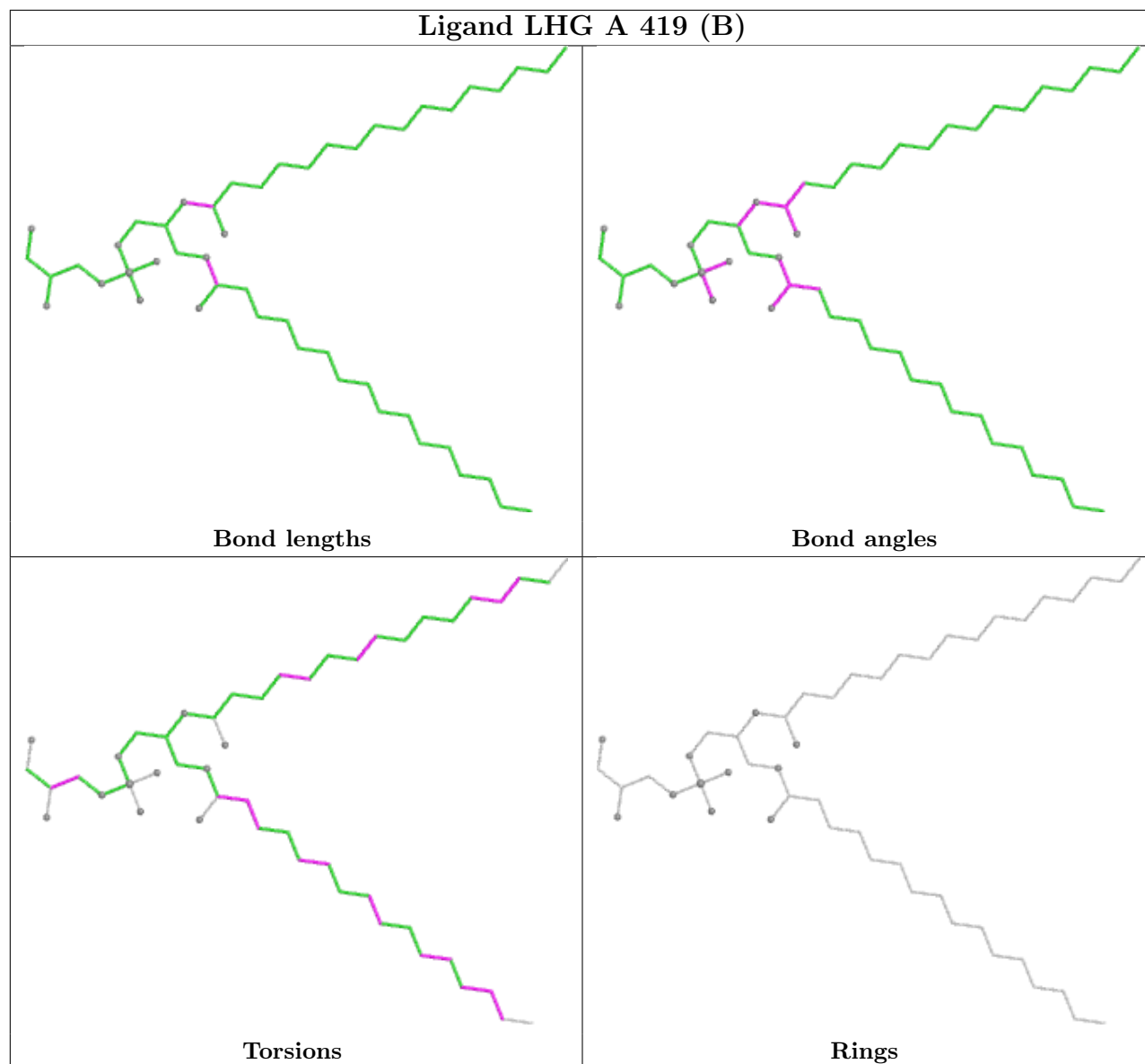
Ligand LHG a 418 (A)



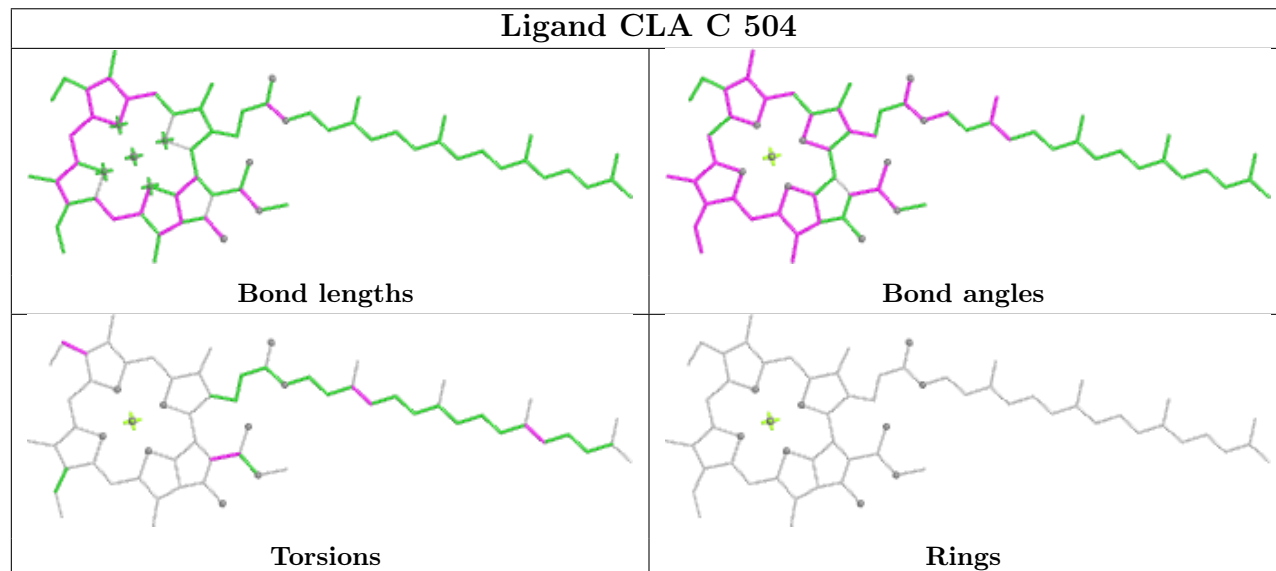
Ligand LMG c 501

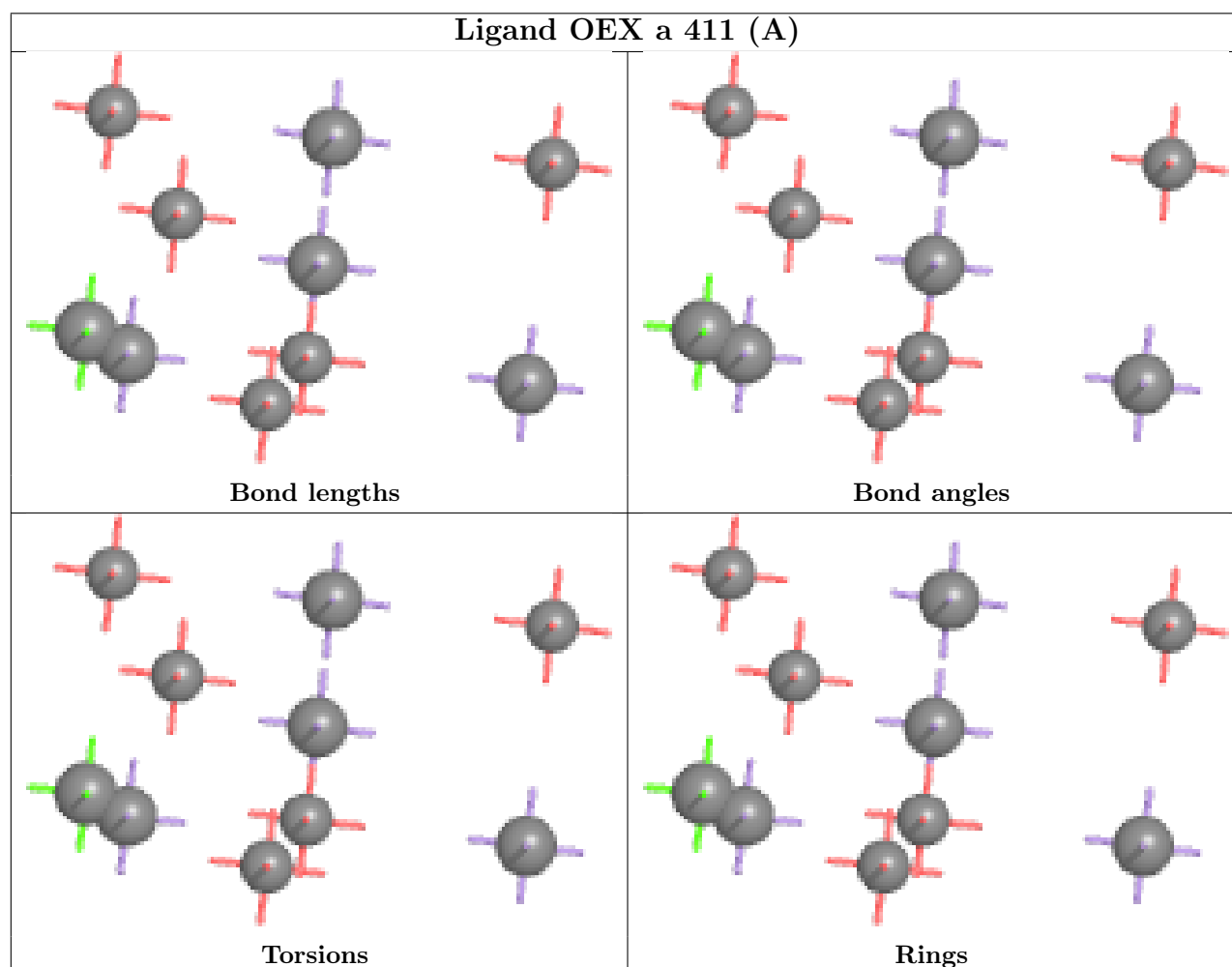
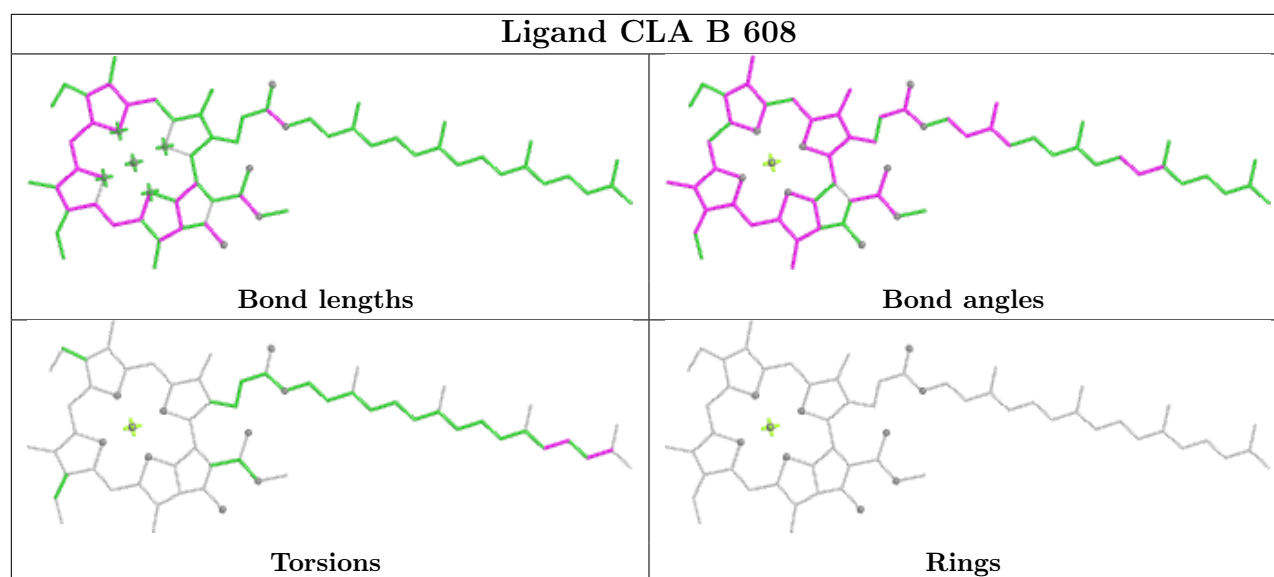


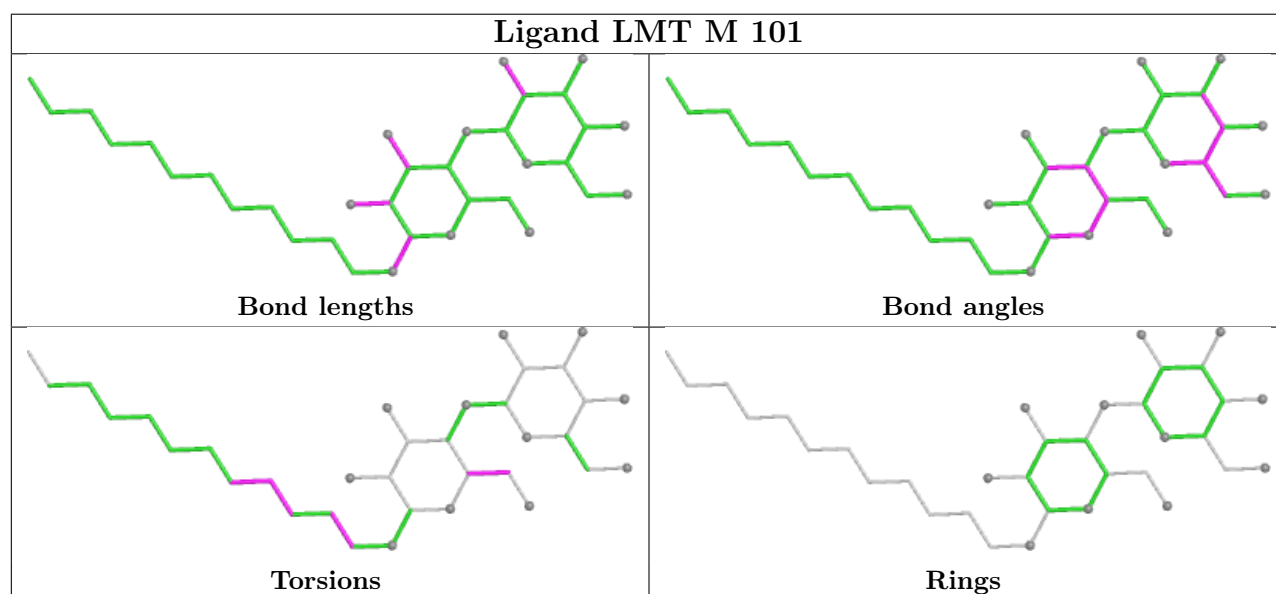
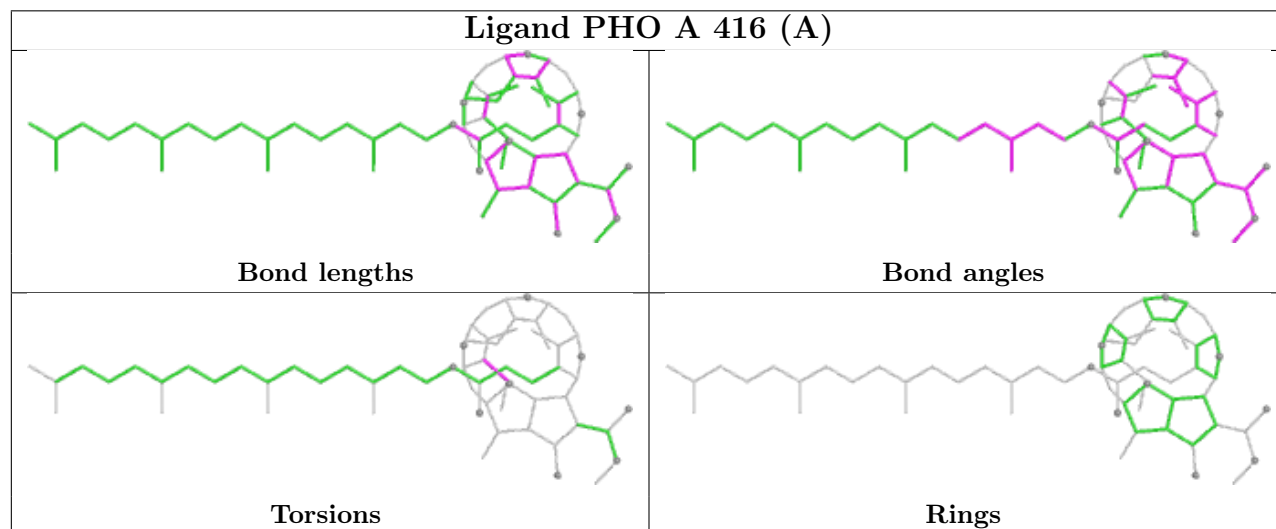
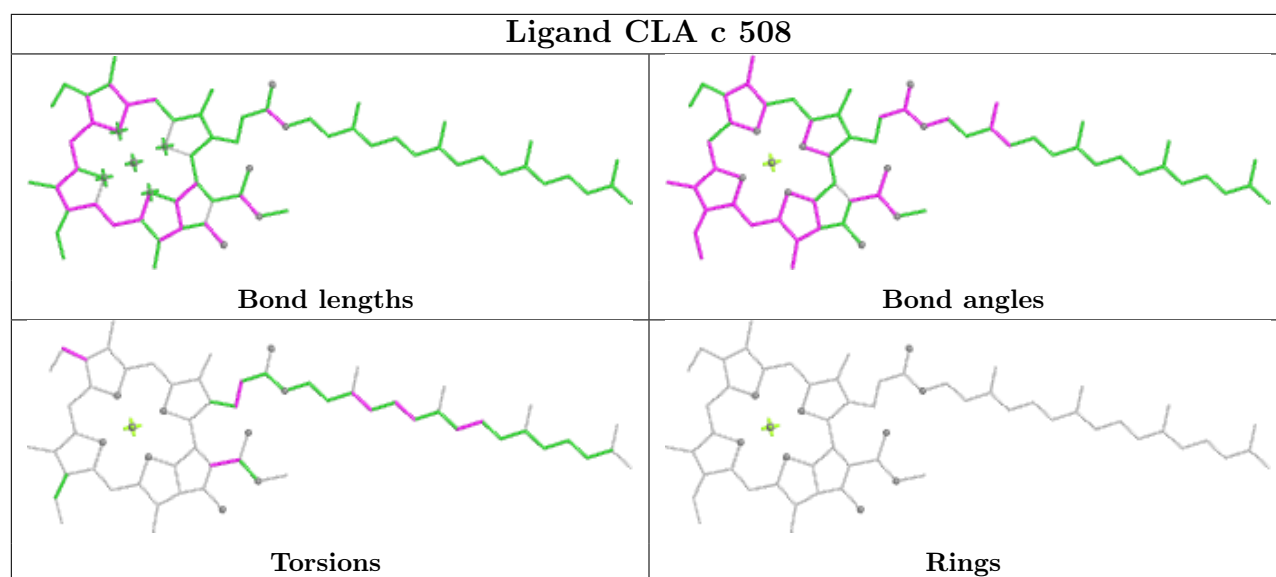
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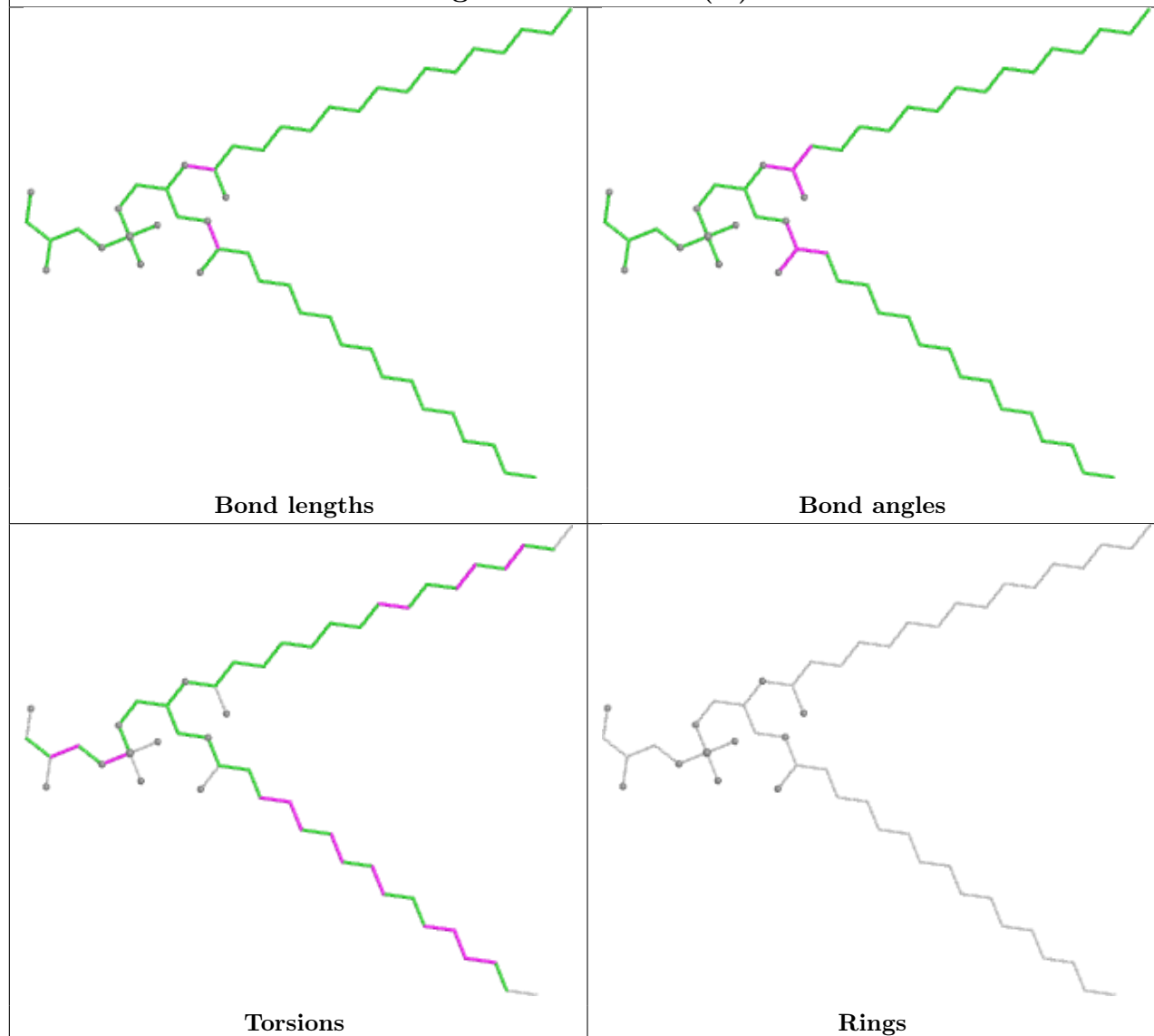
Ligand CLA C 504



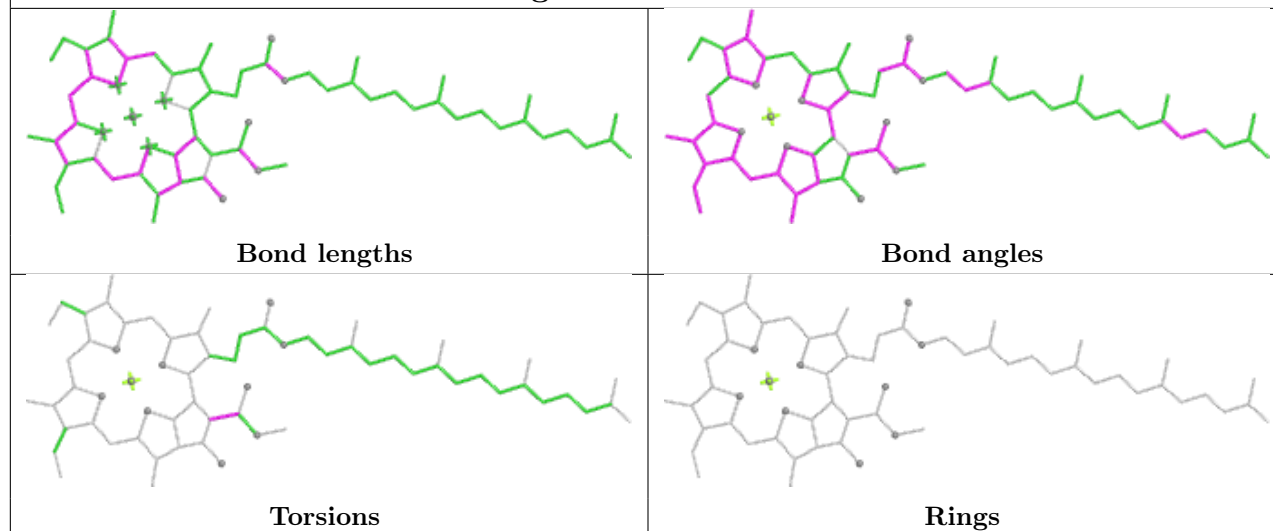


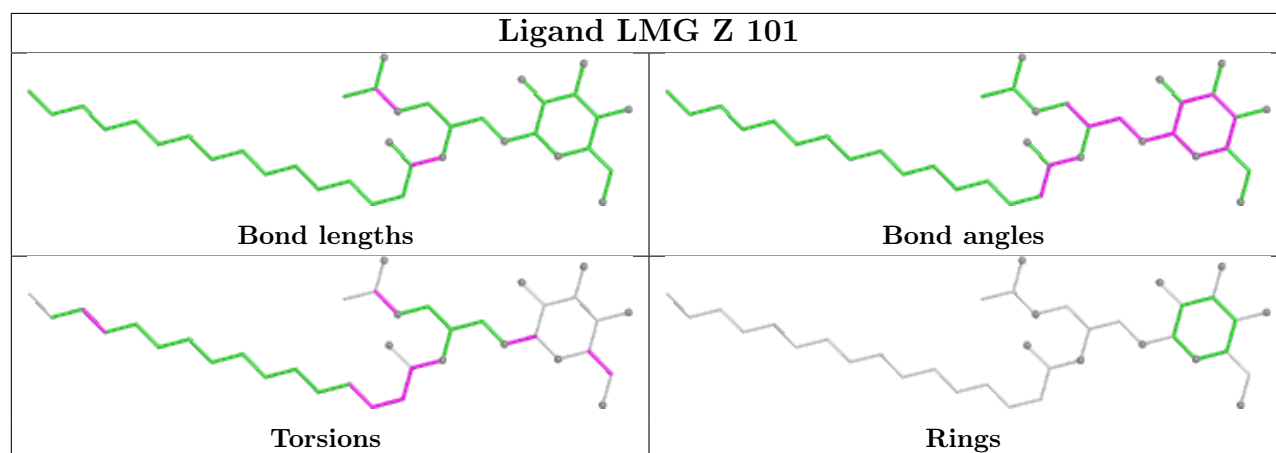
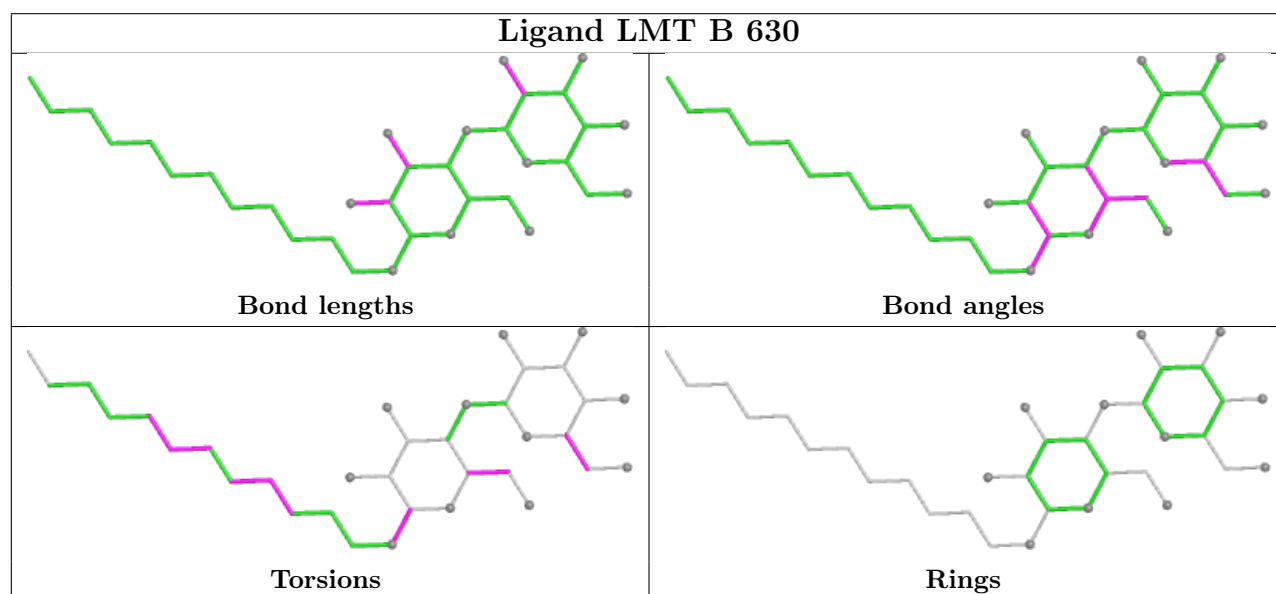
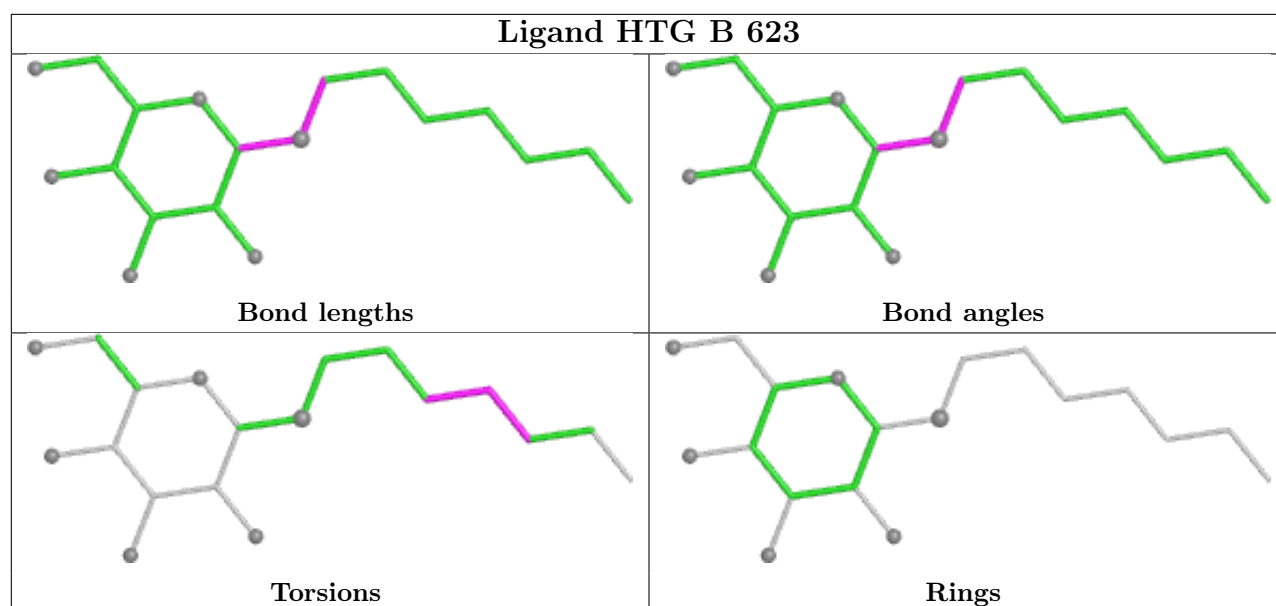


Ligand LHG d 414 (A)

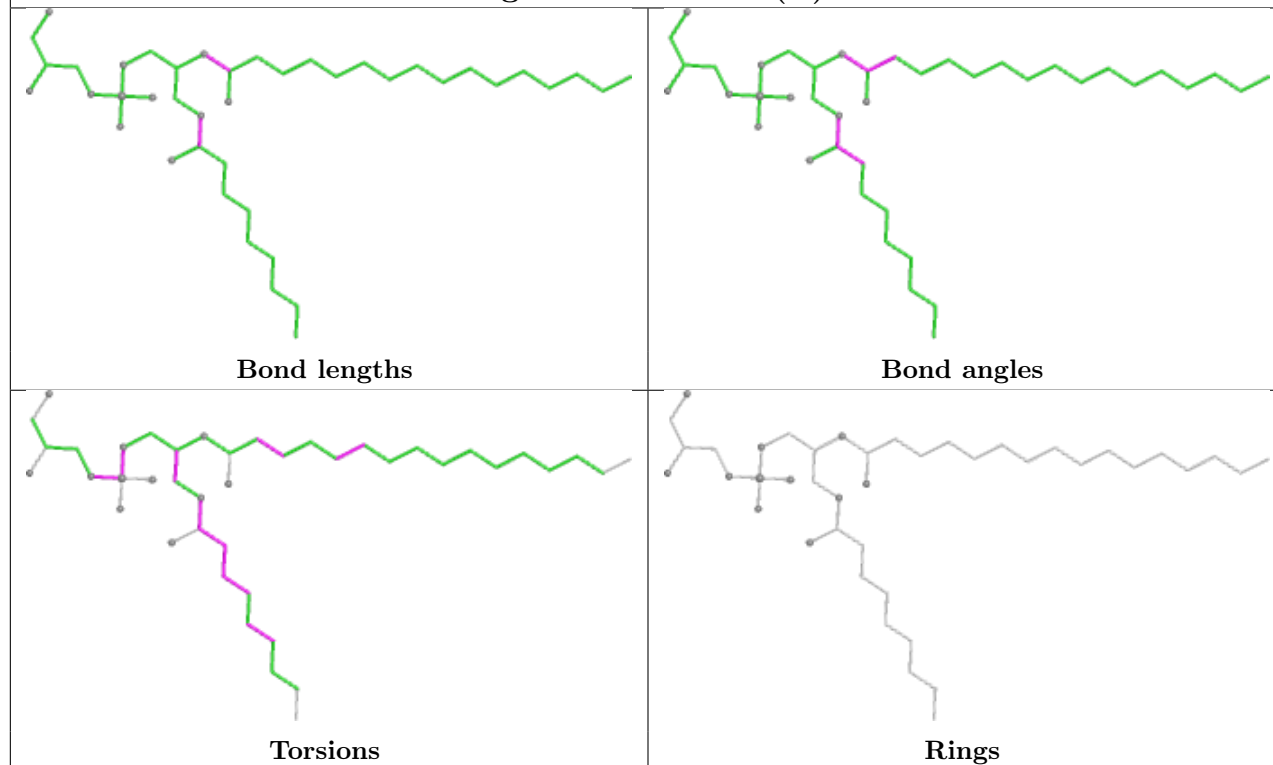


Ligand CLA B 609

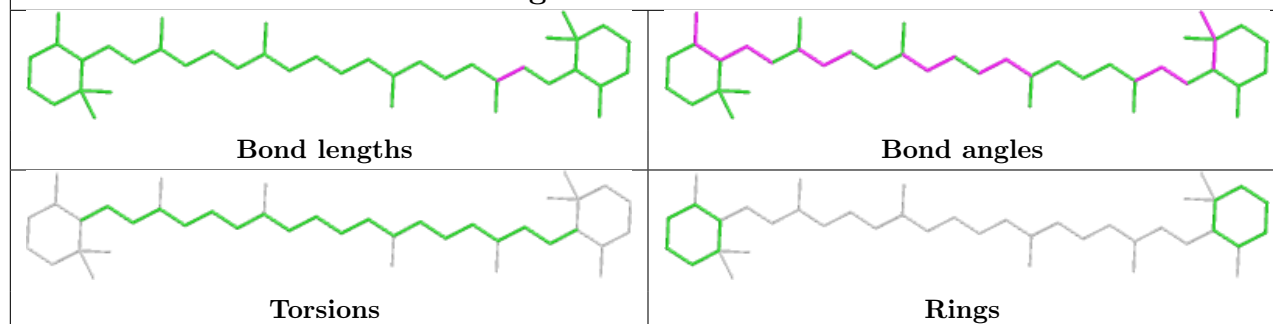




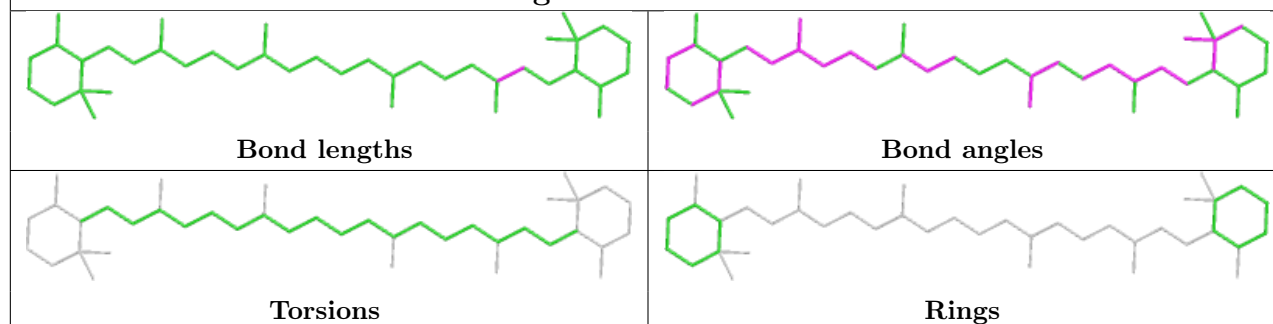
Ligand LHG a 418 (B)

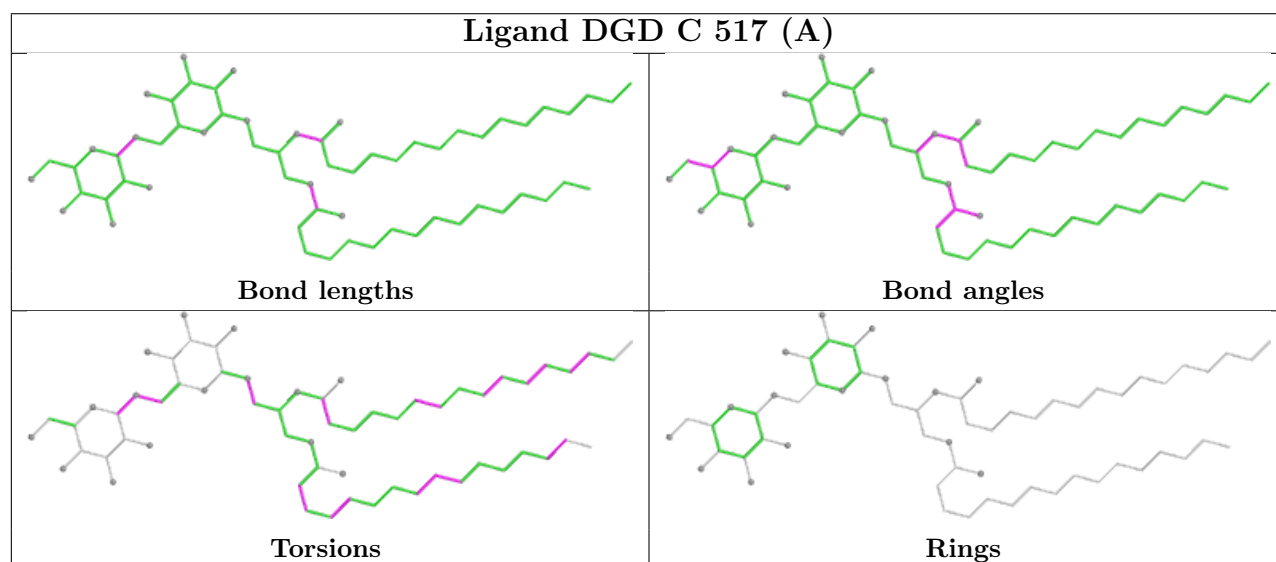
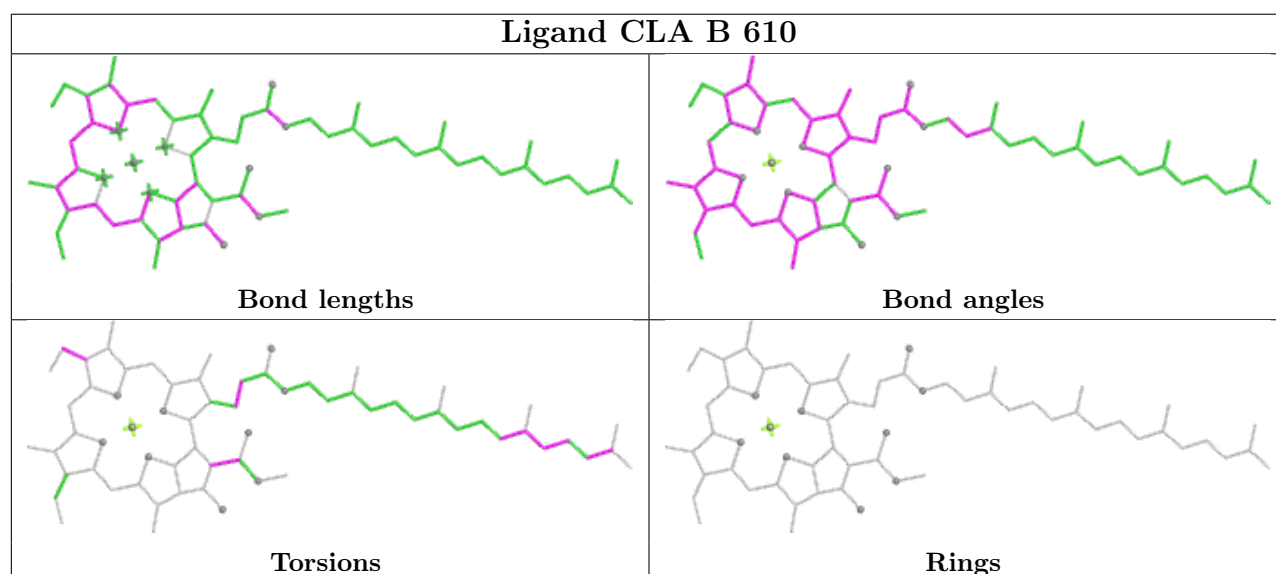
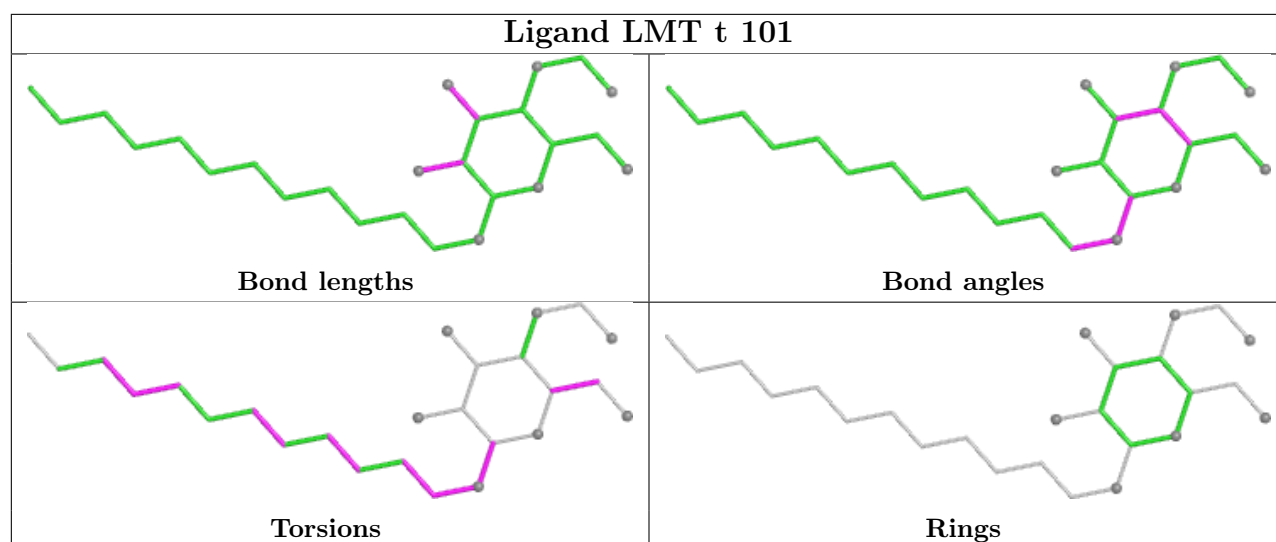


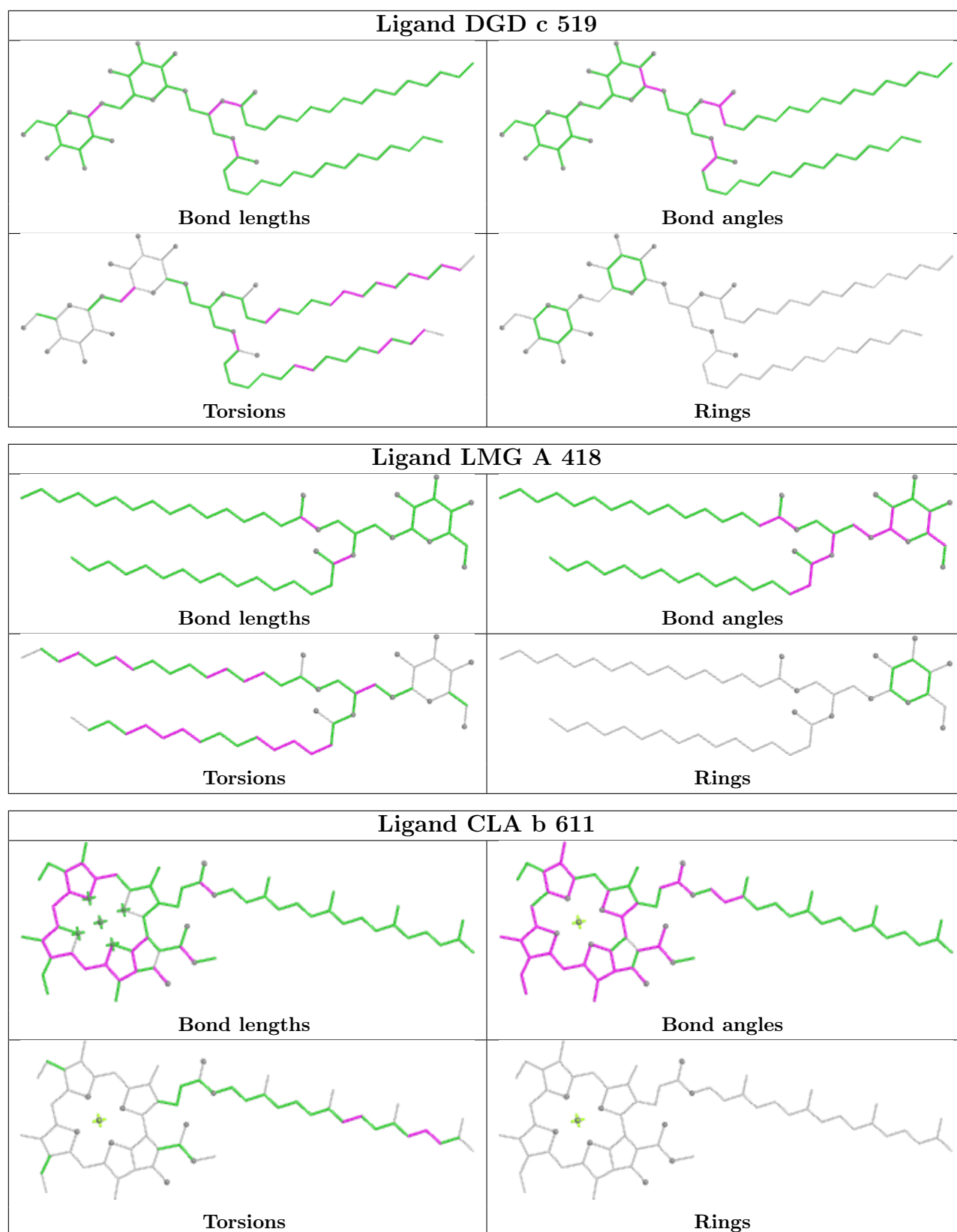
Ligand BCR A 409



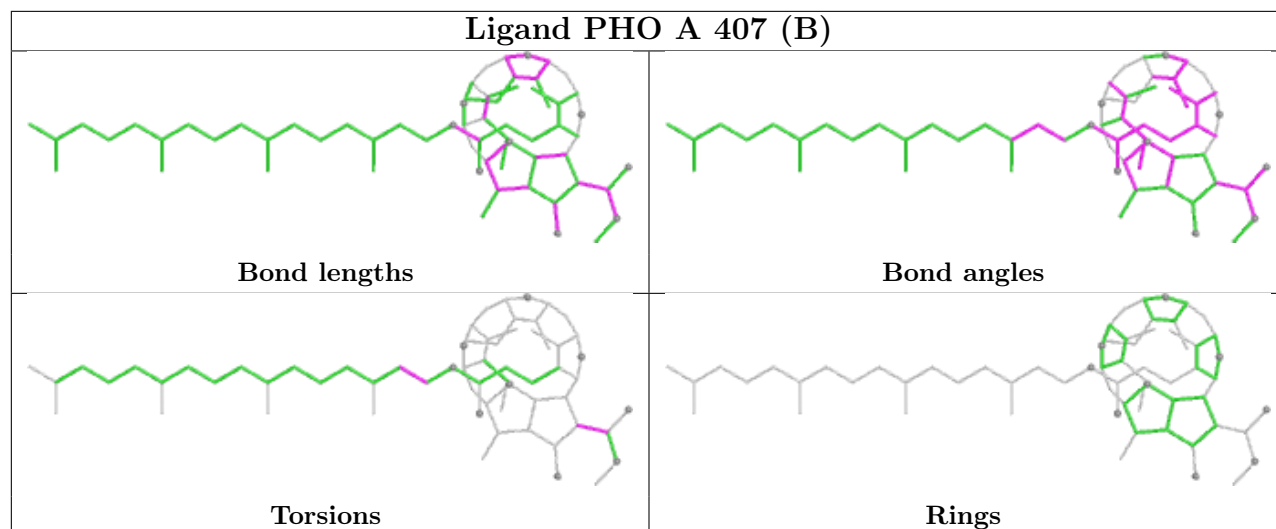
Ligand BCR k 101



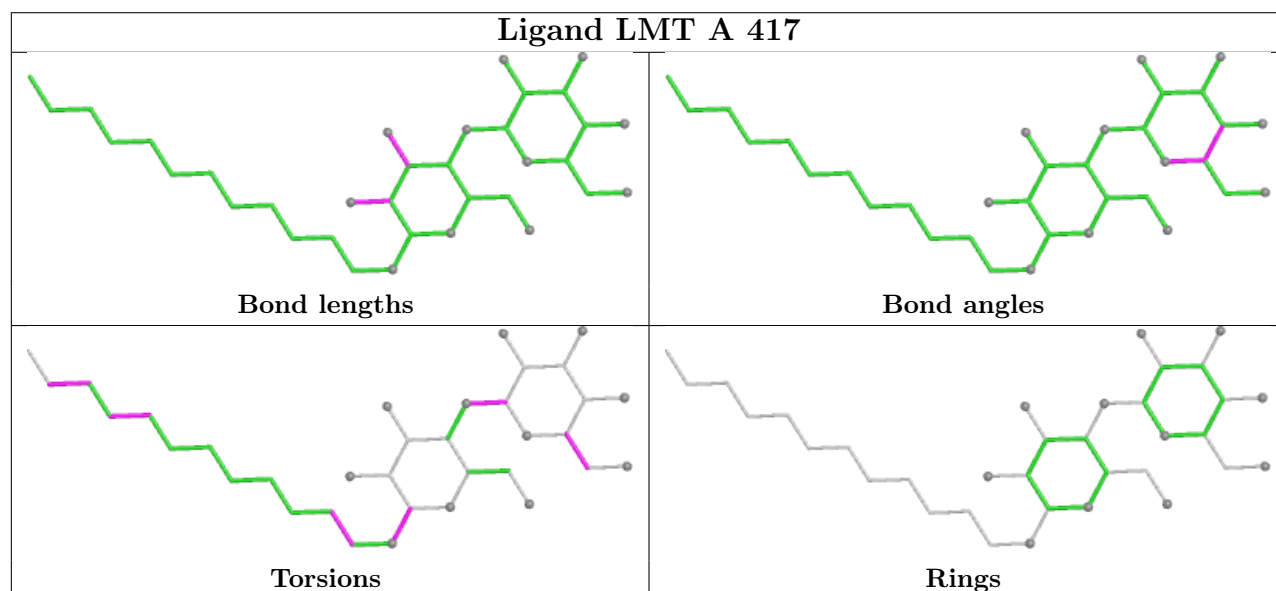




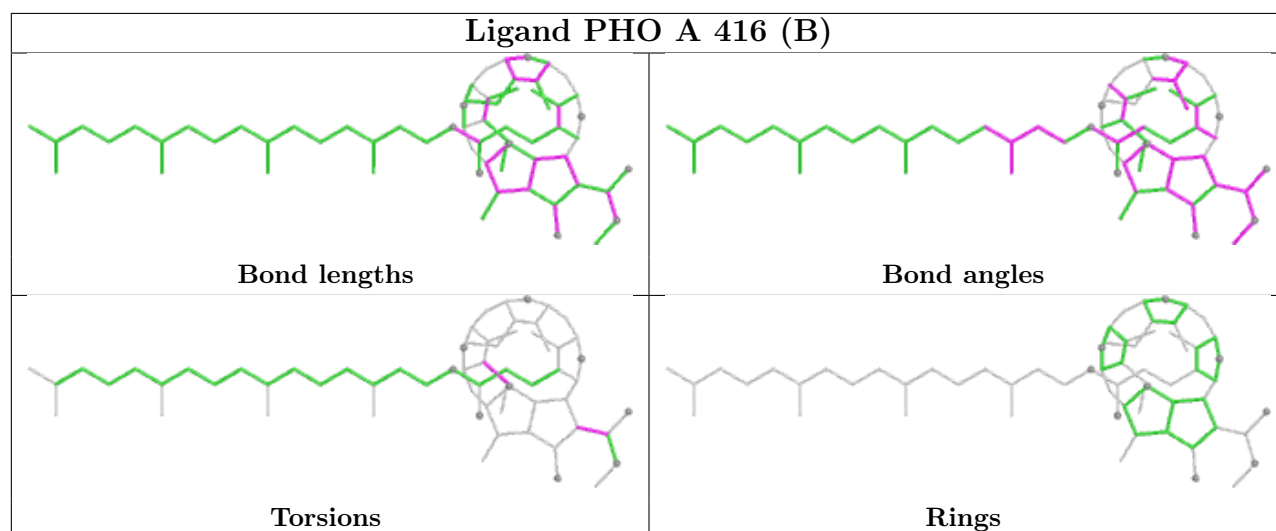
Ligand PHO A 407 (B)

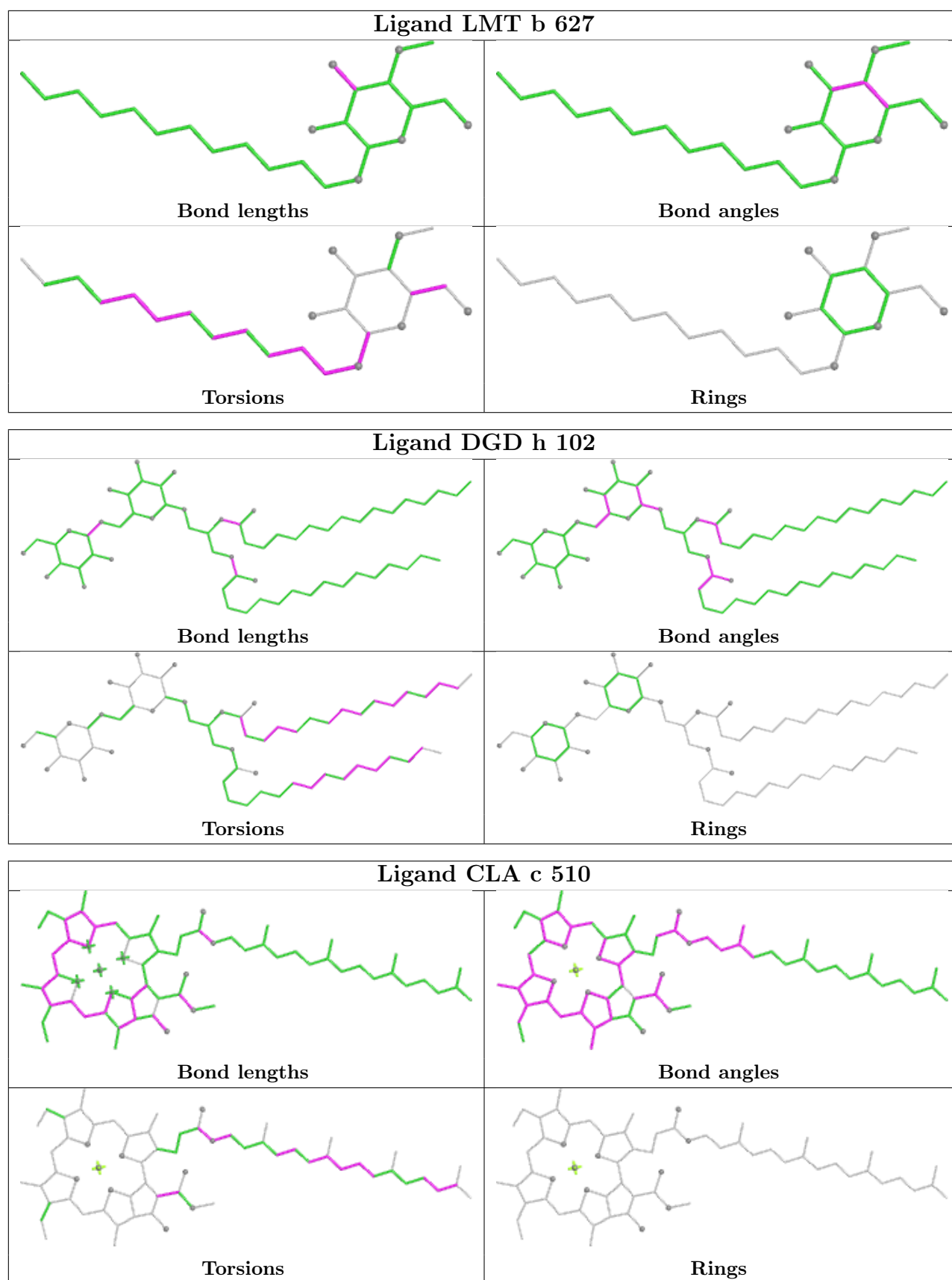


Ligand LMT A 417

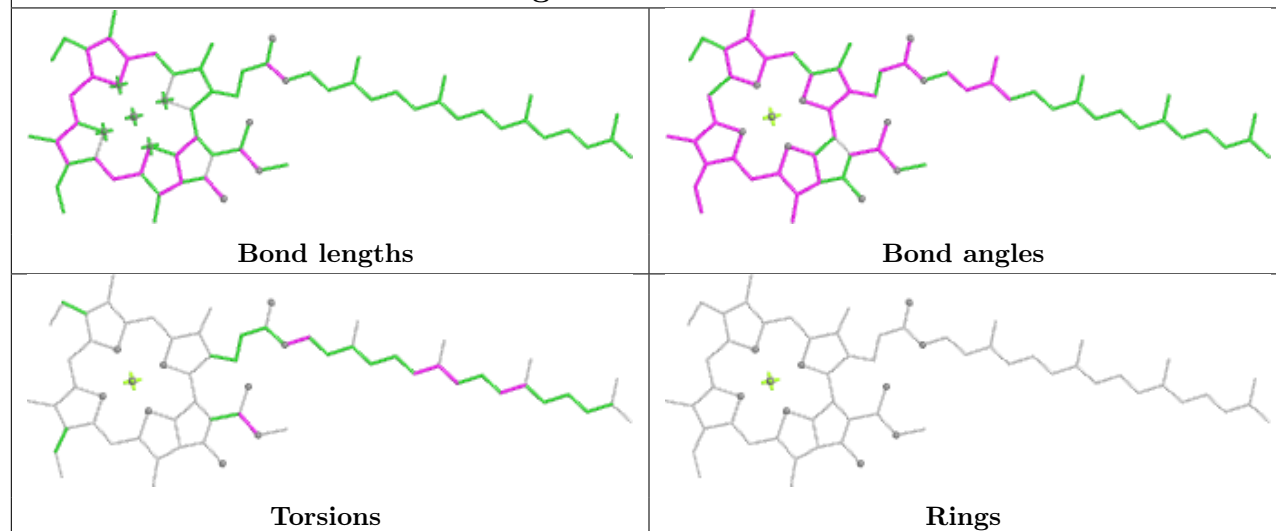


Ligand PHO A 416 (B)

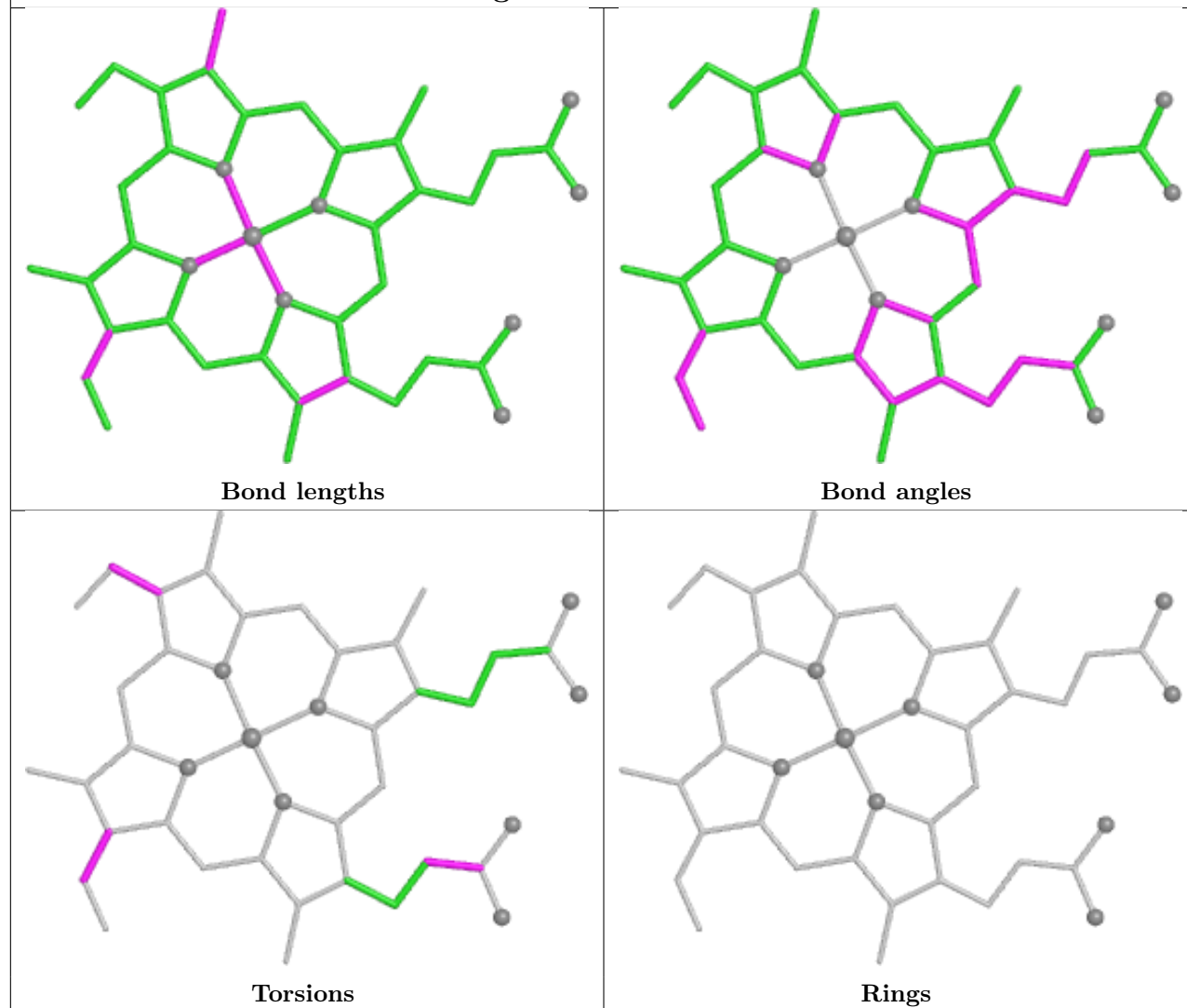


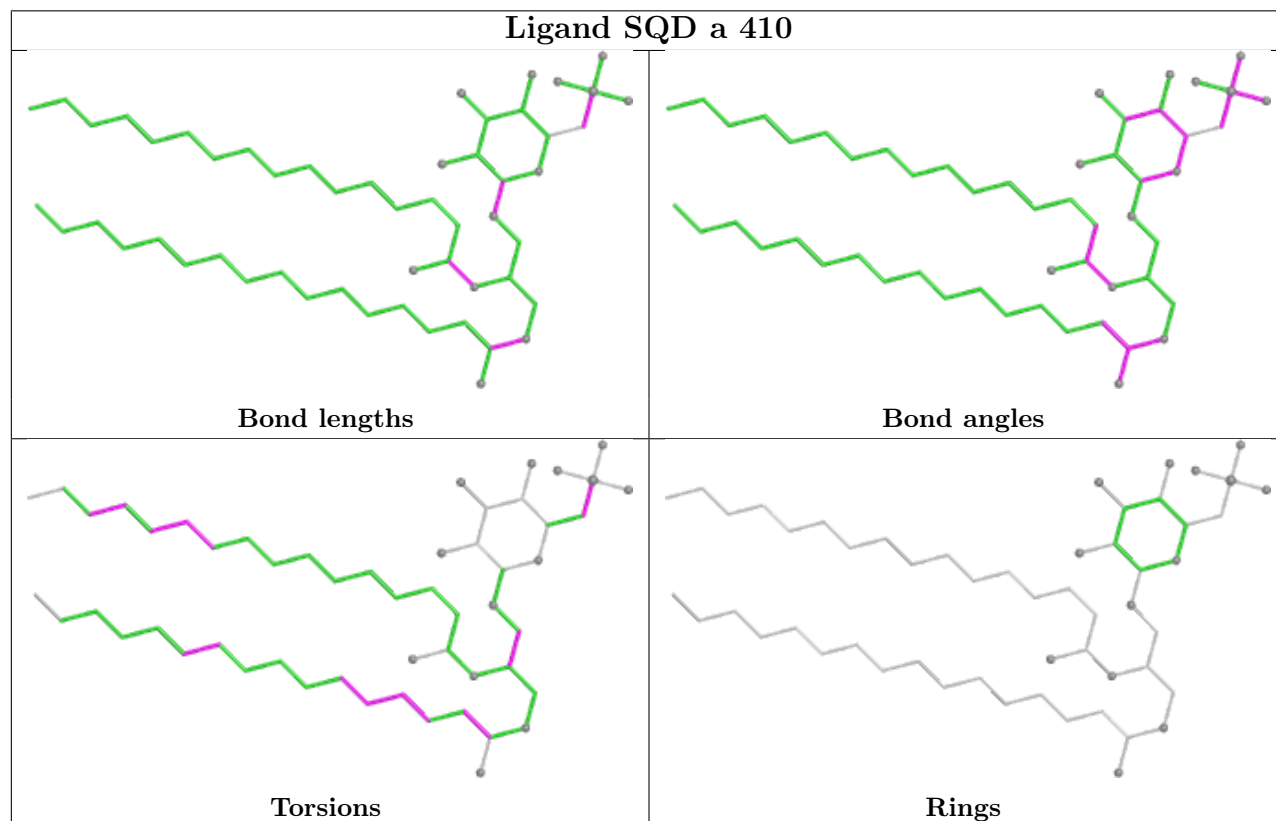
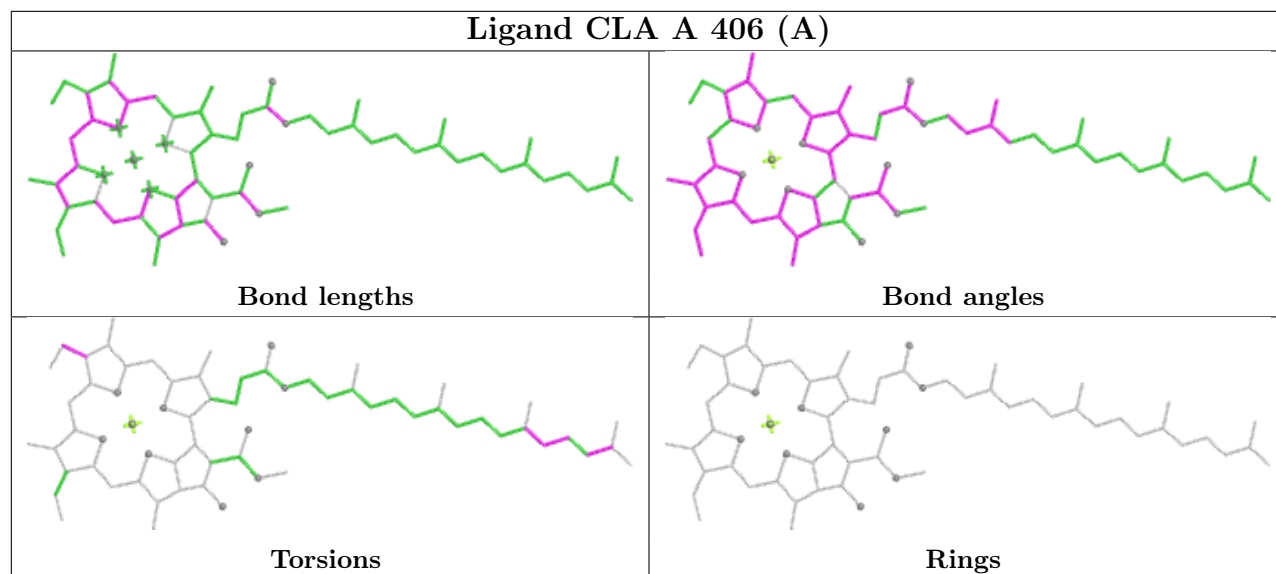


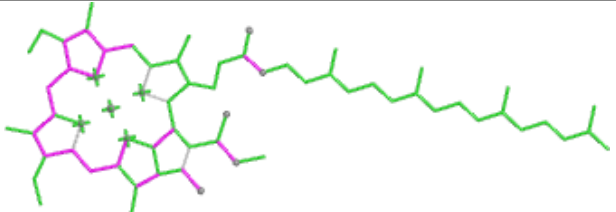
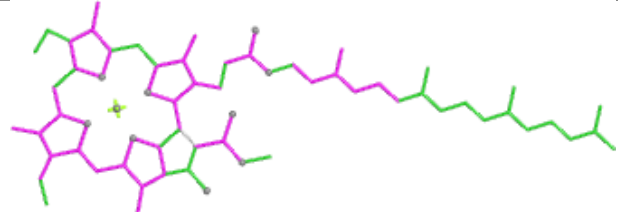
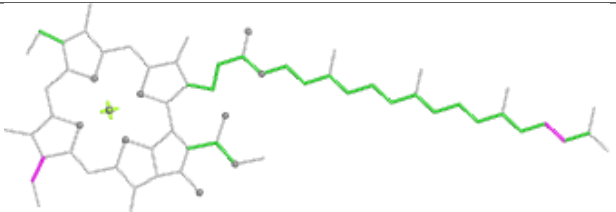
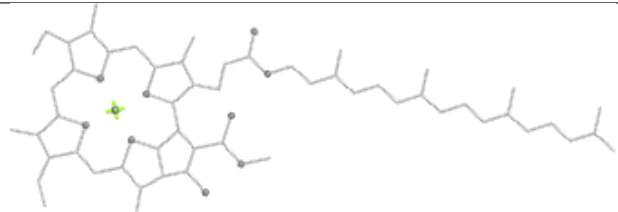
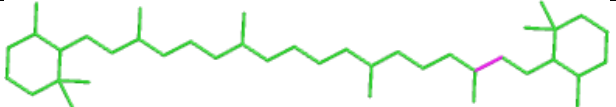
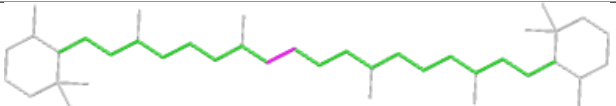
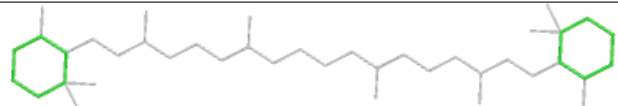
Ligand CLA C 513

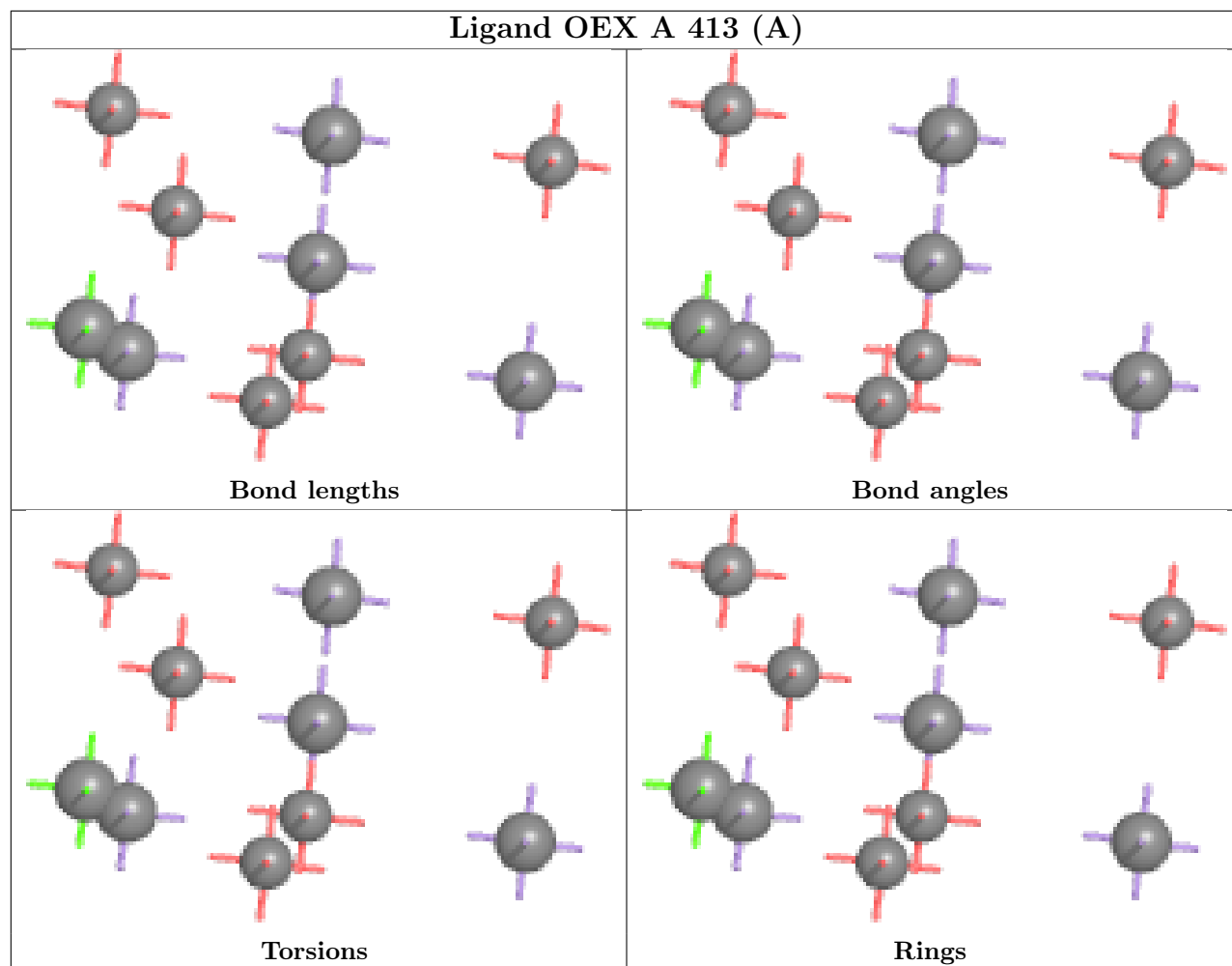


Ligand HEC V 201

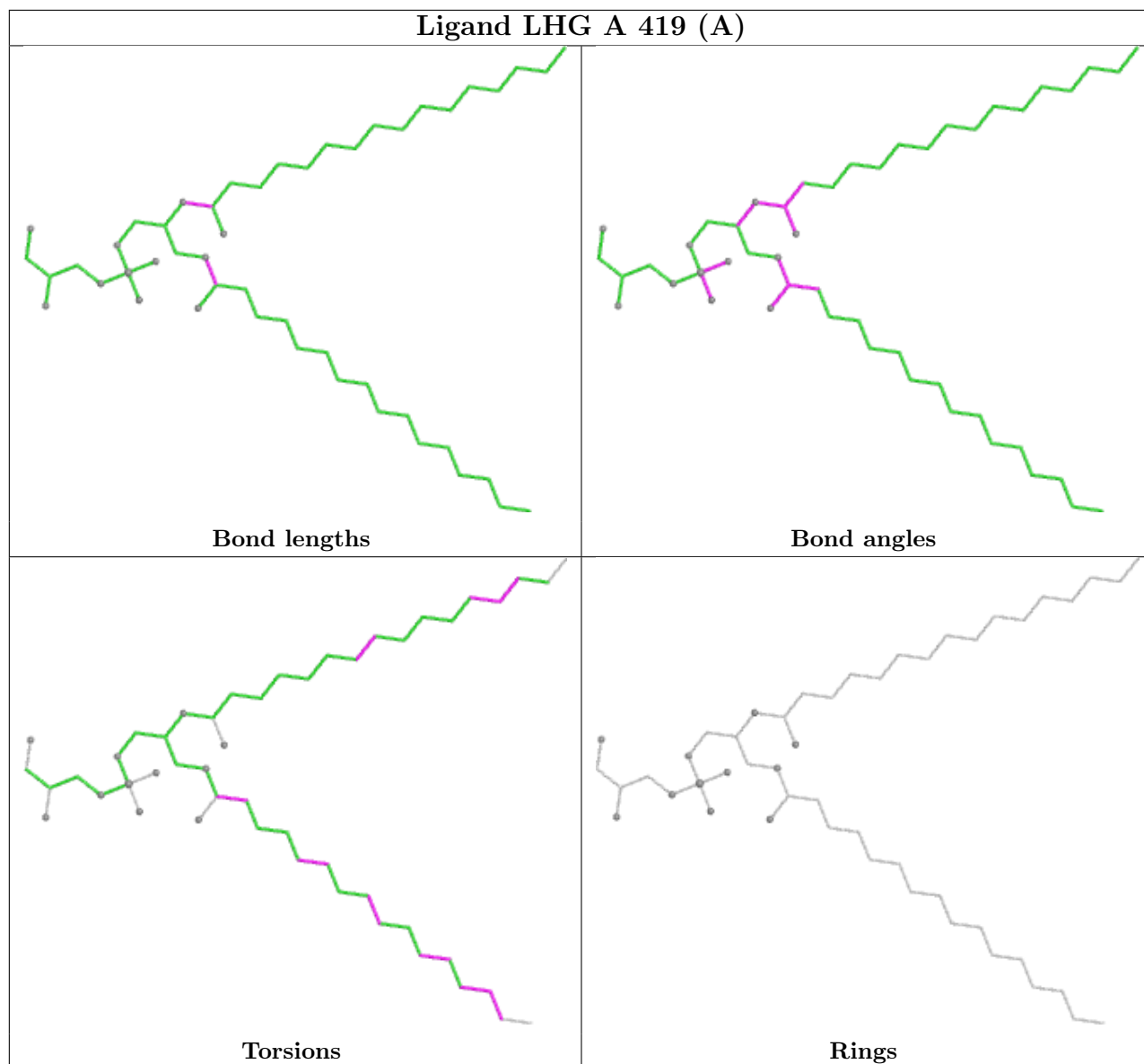




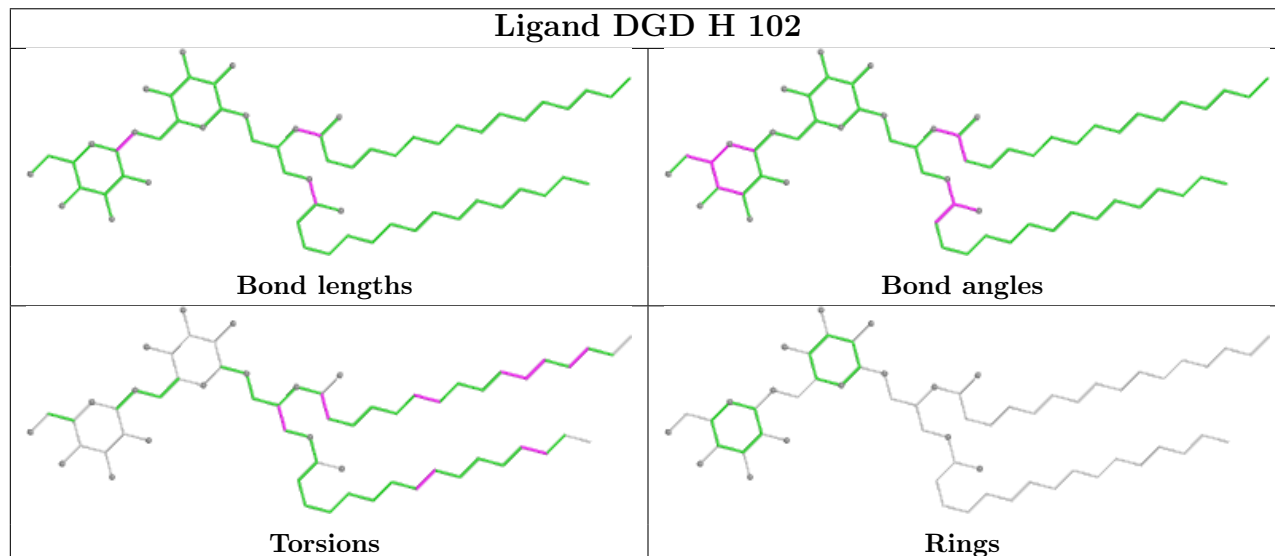
Ligand CLA a 404 (A)	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR T 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

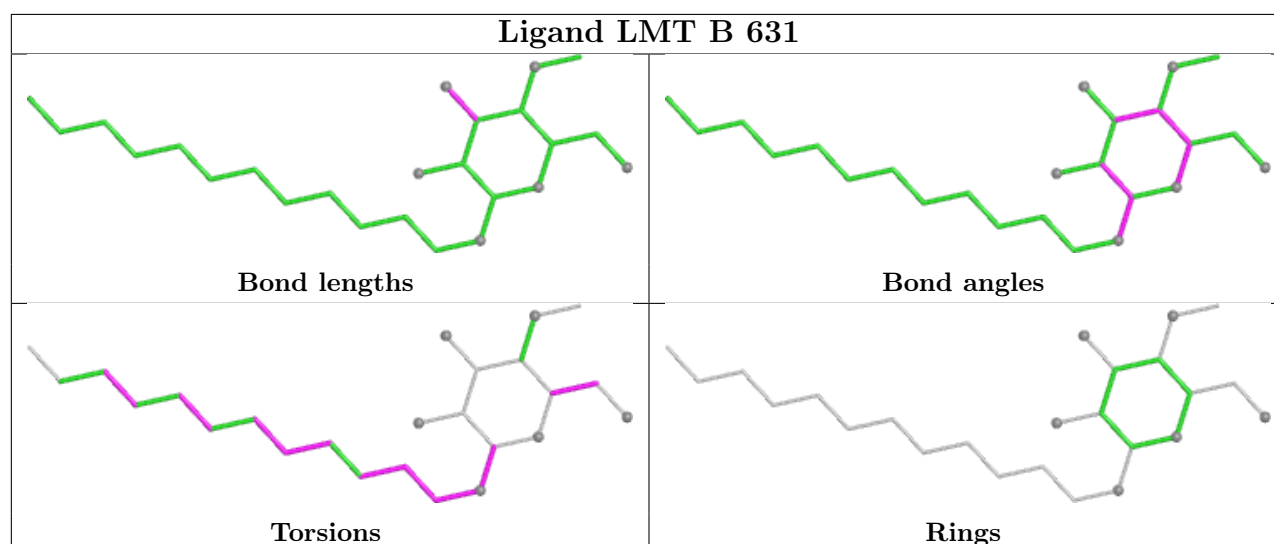
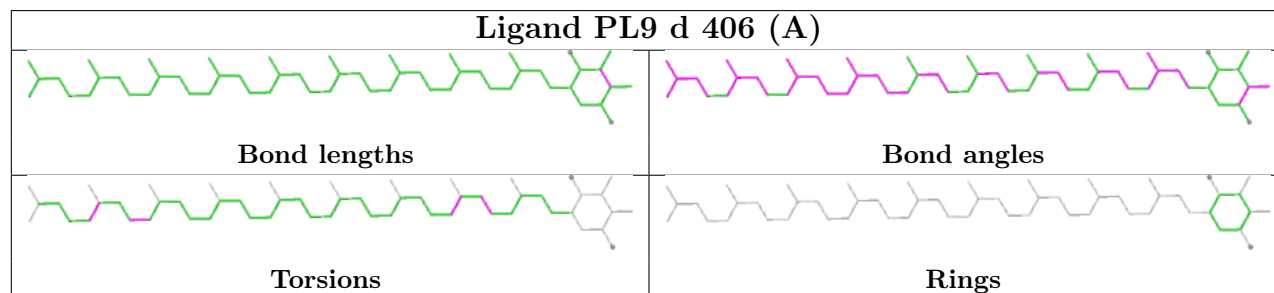
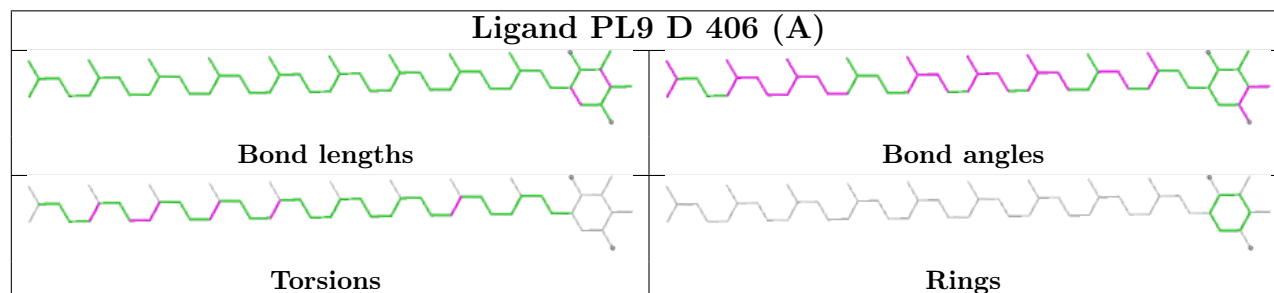
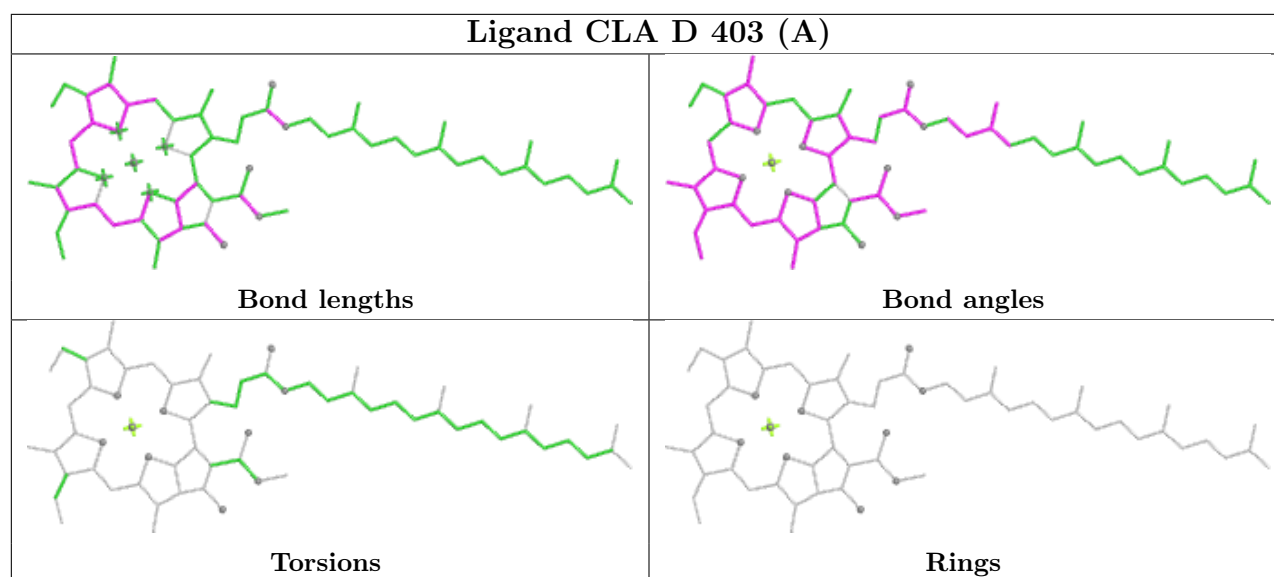


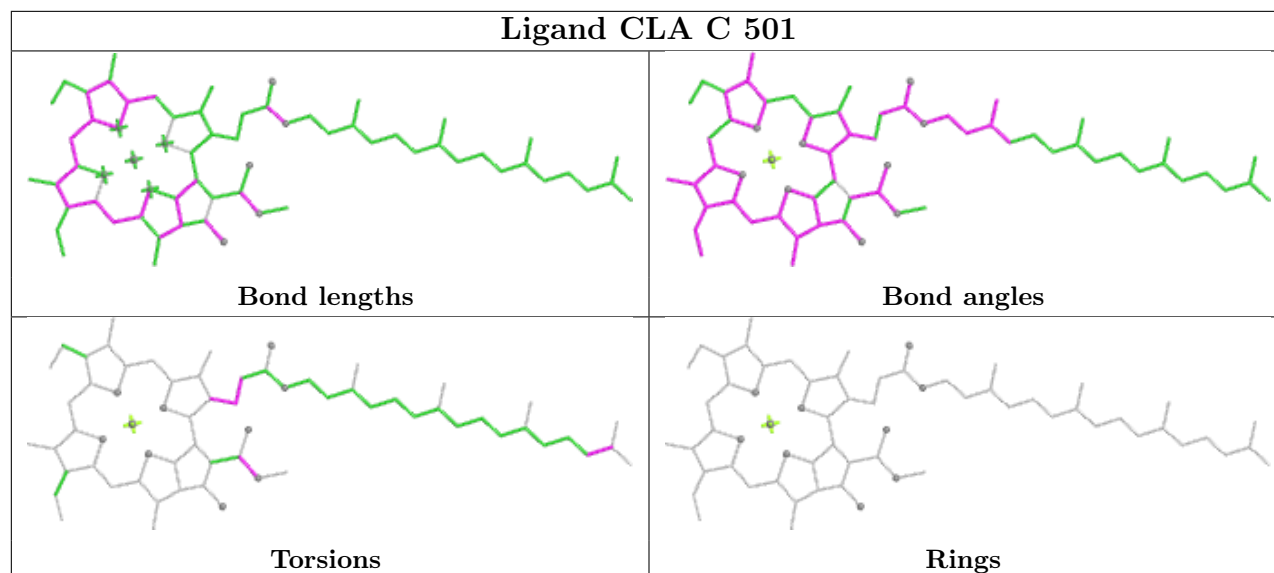
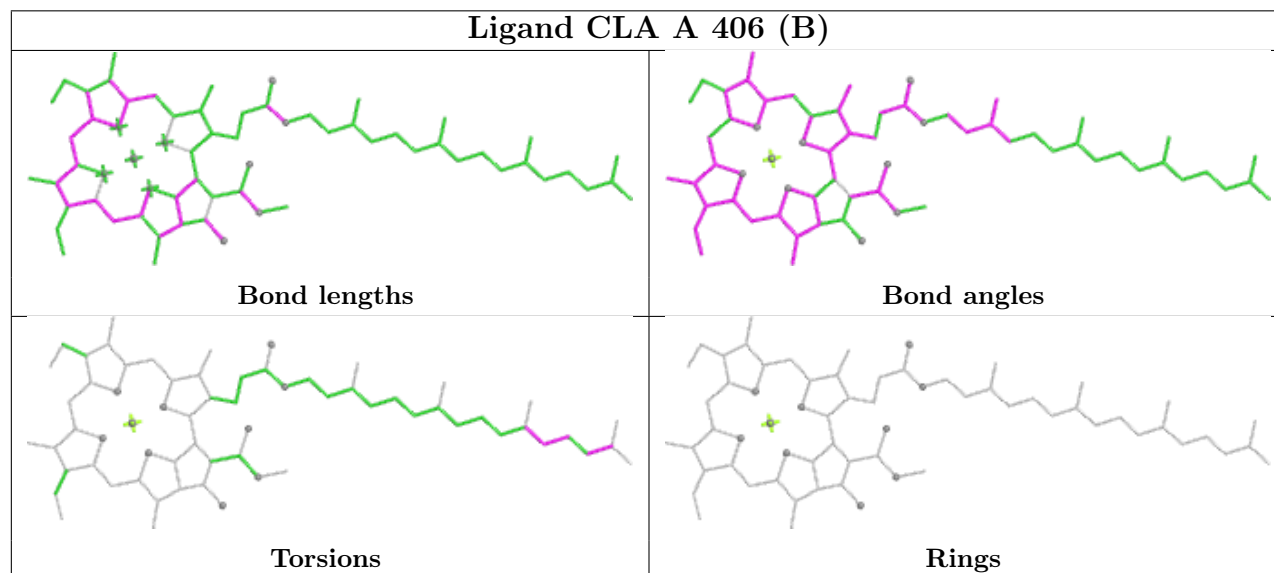
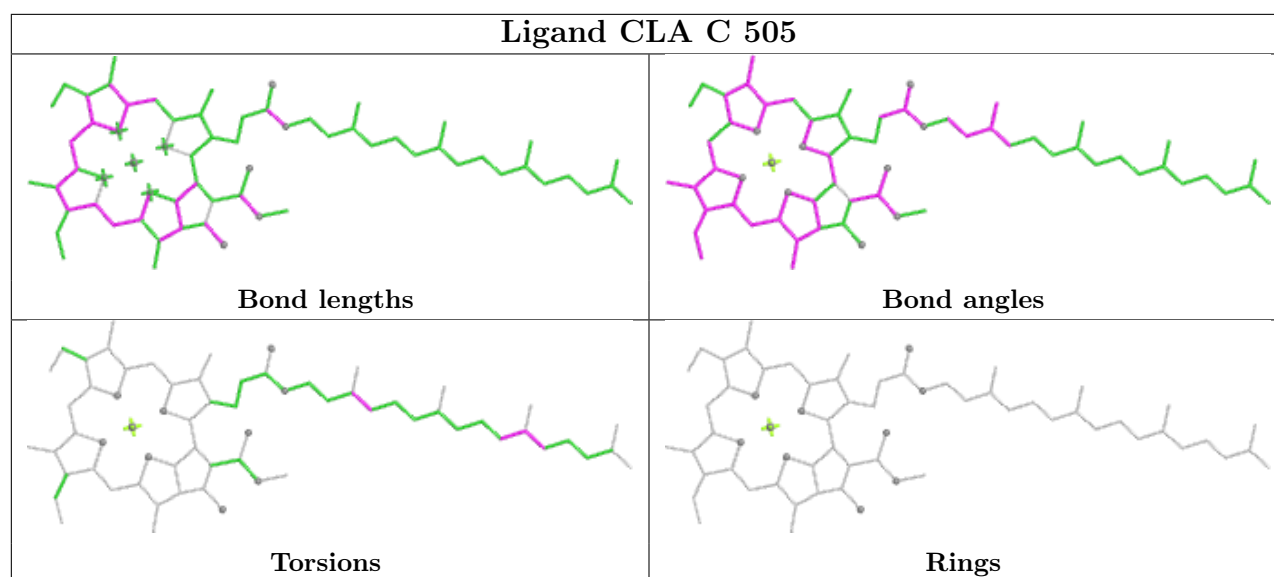
Ligand LHG A 419 (A)

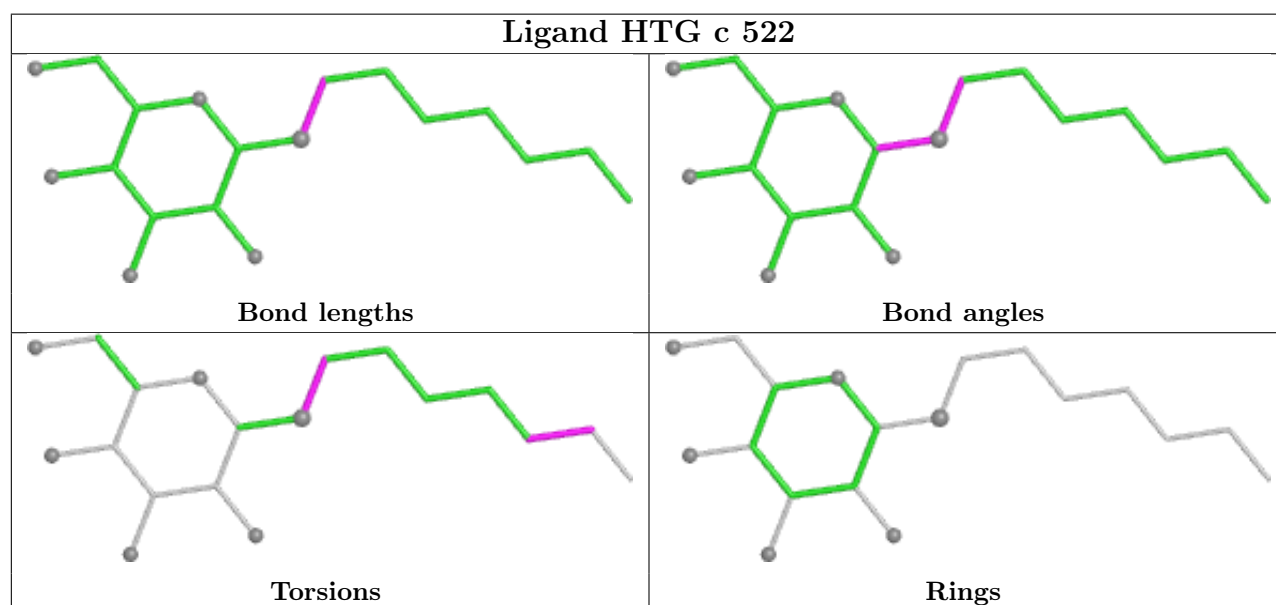
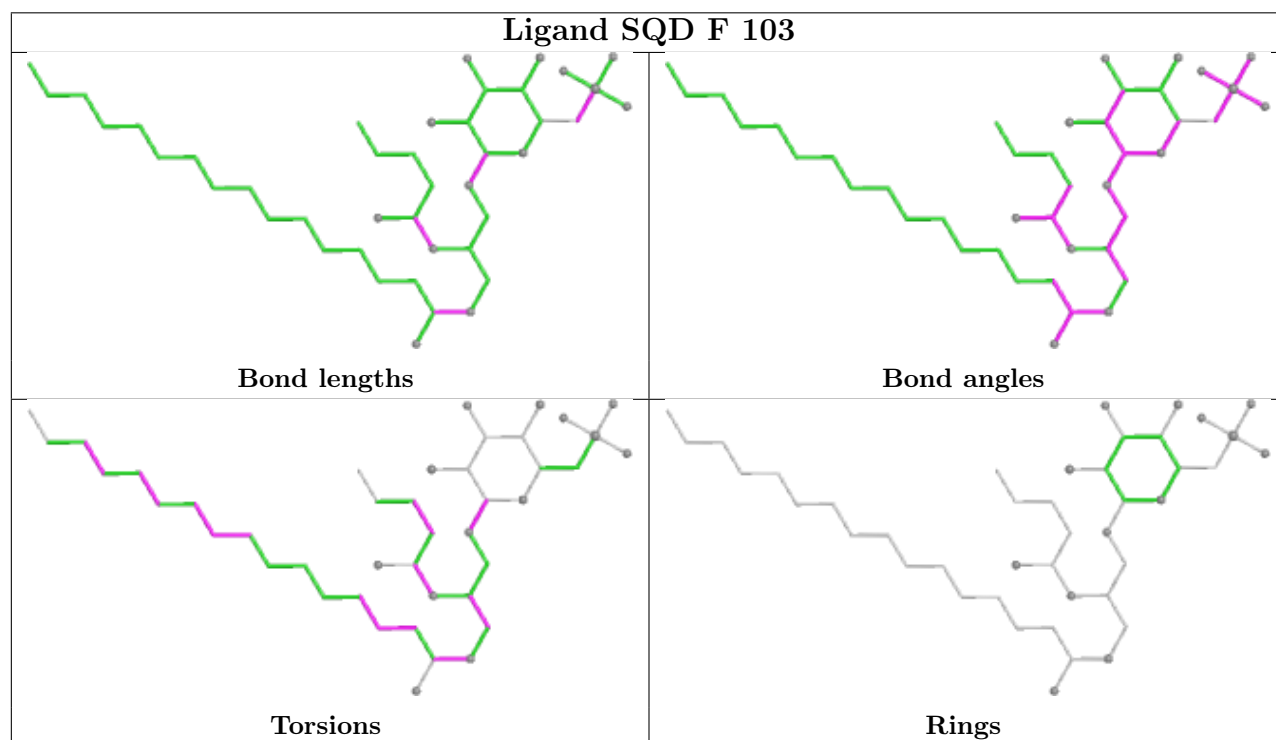
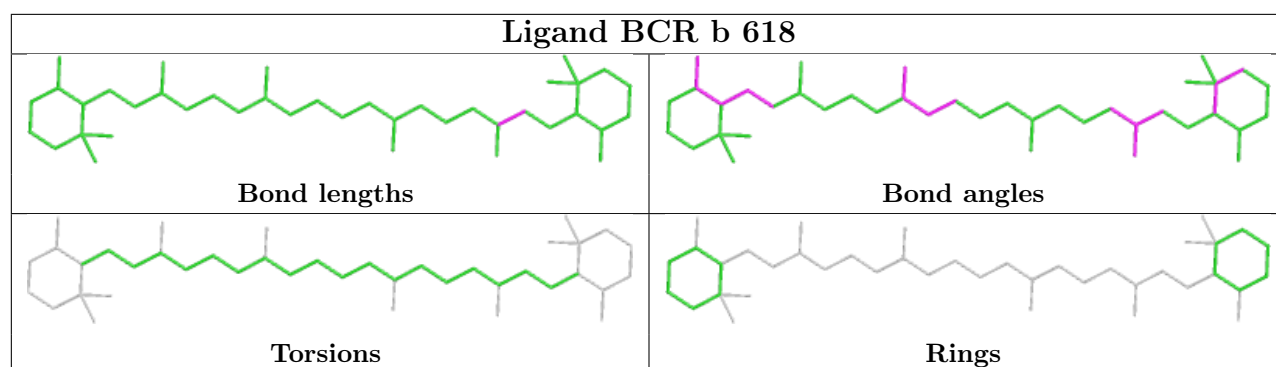


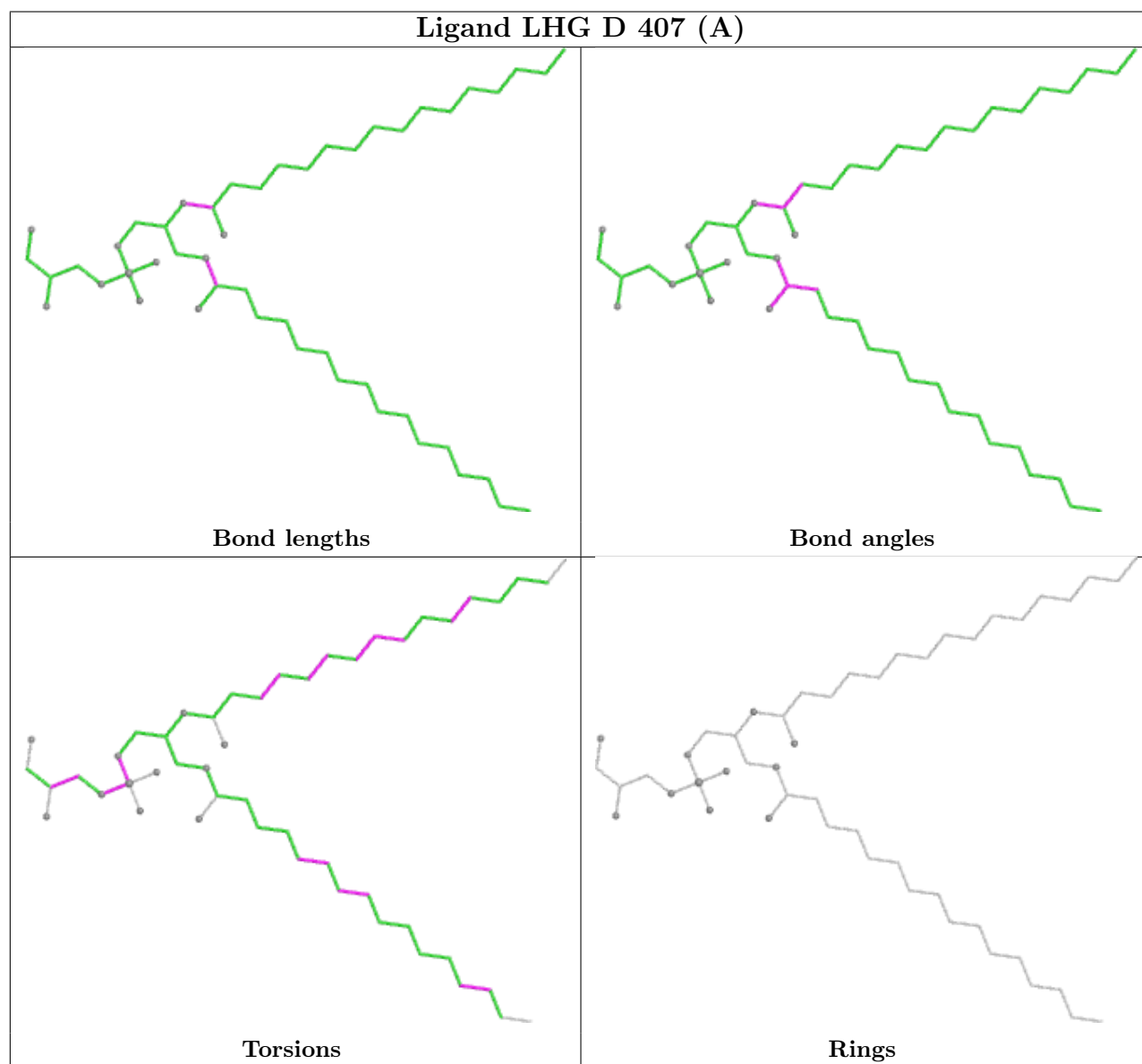
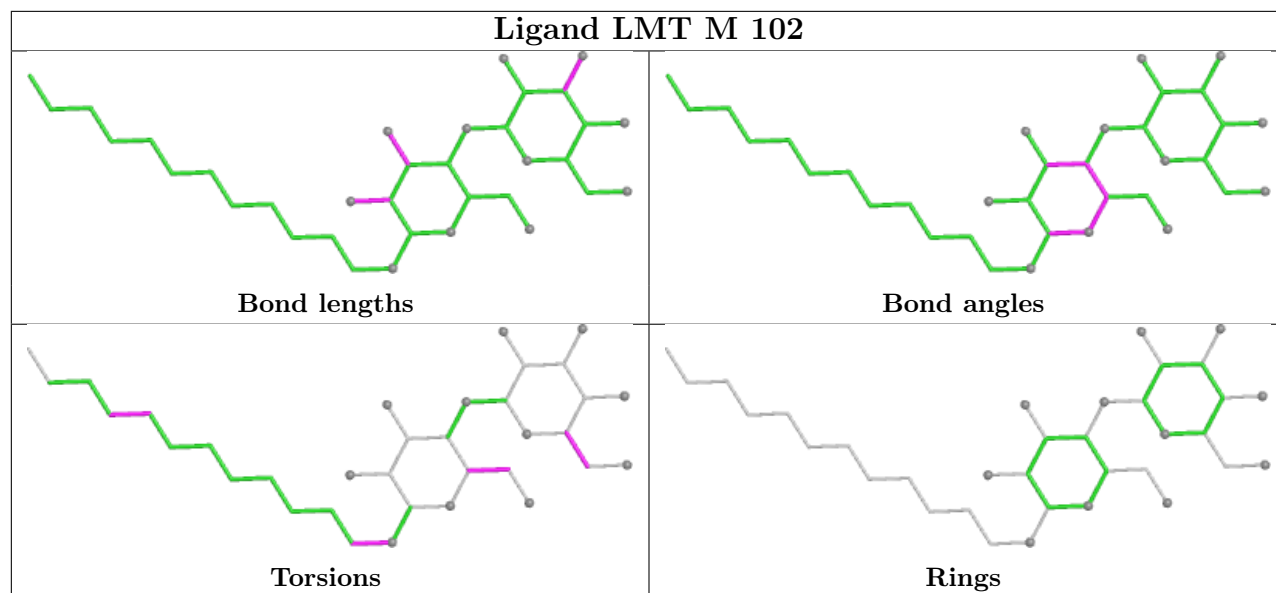
Ligand DGD H 102

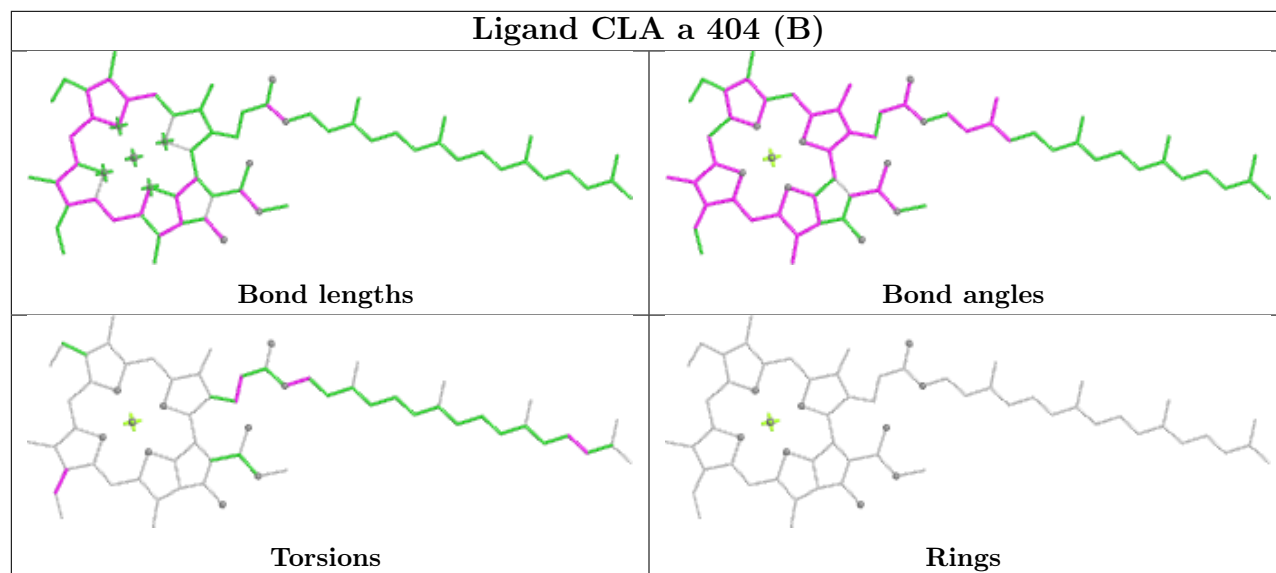
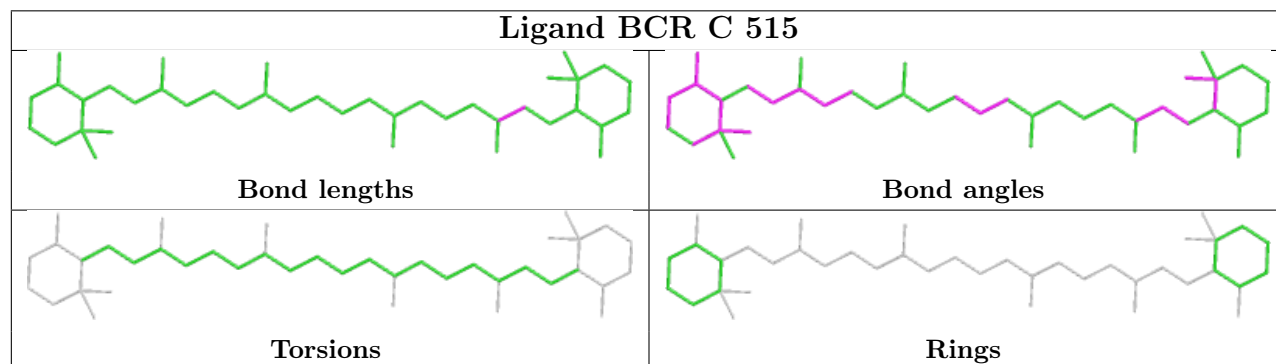
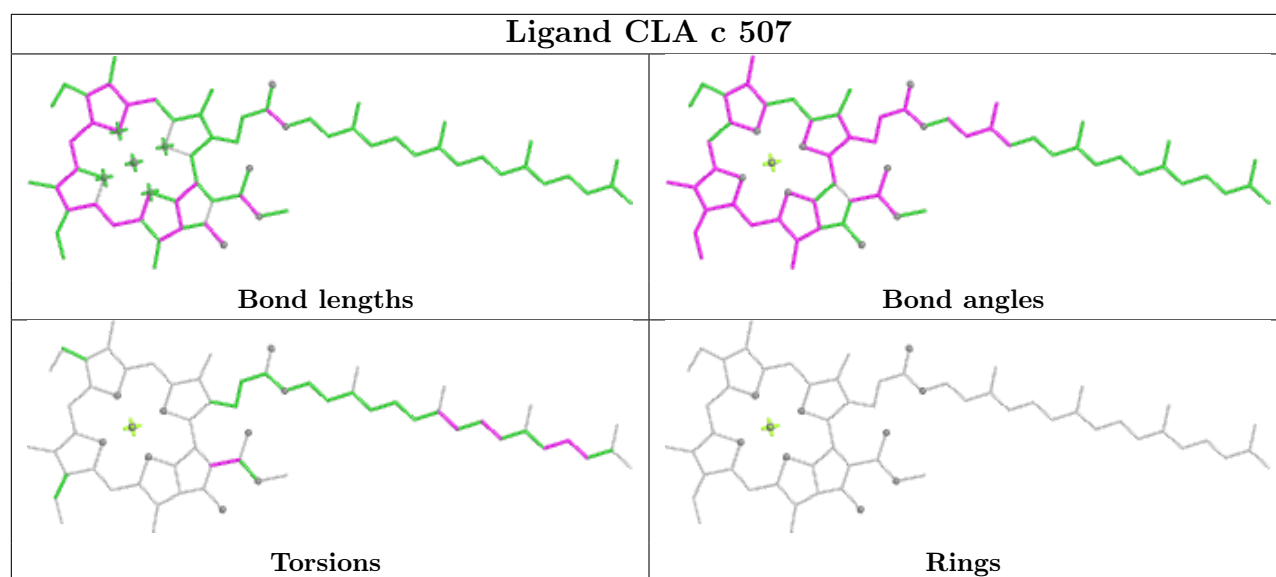


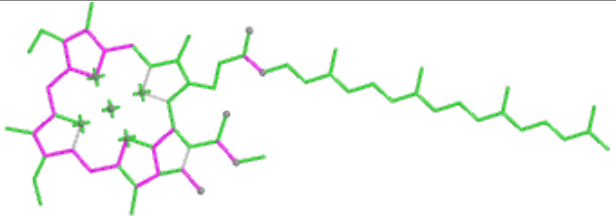
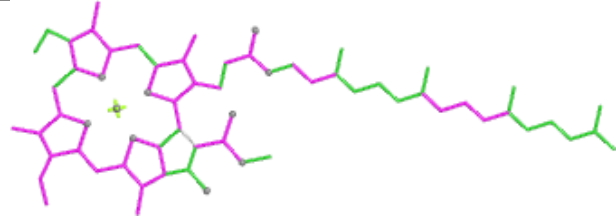
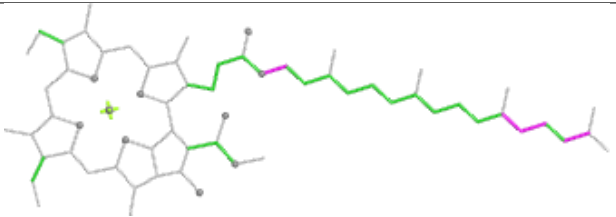
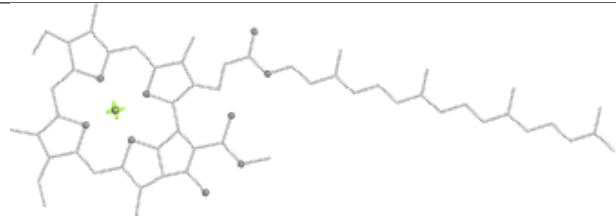


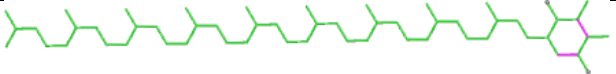
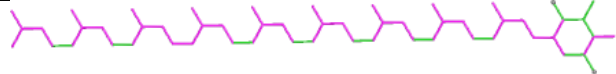
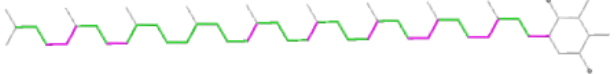
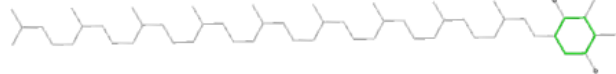


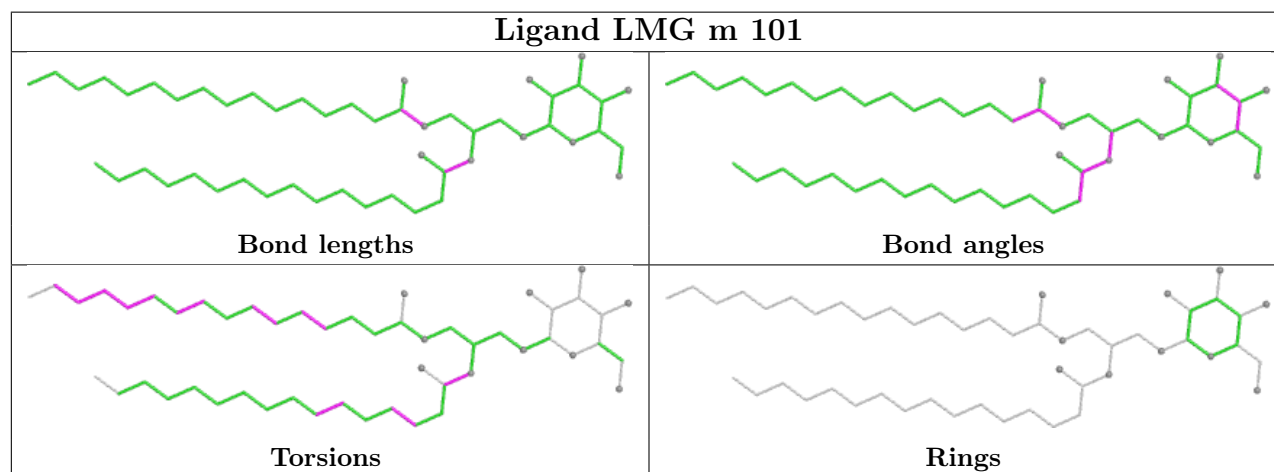
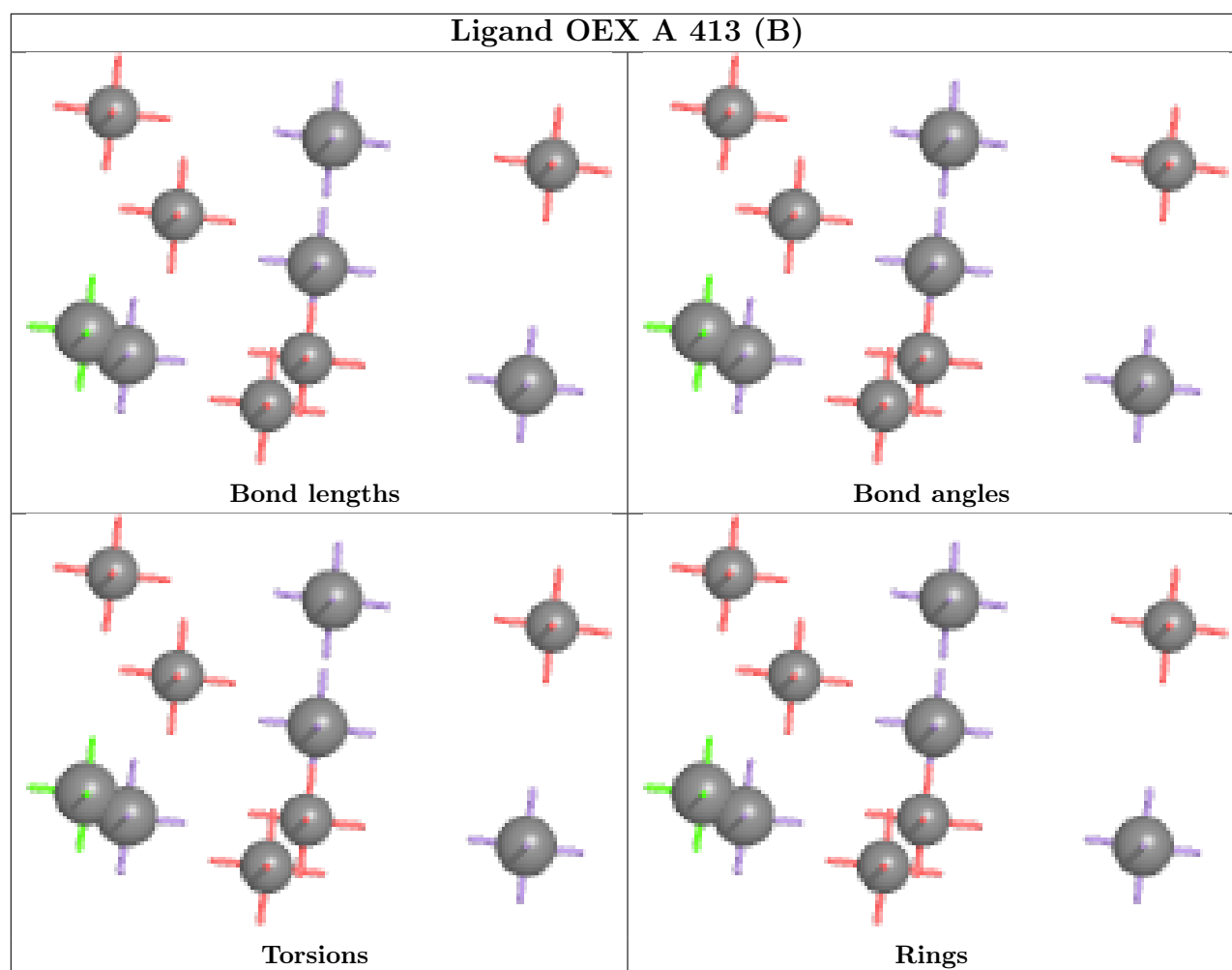


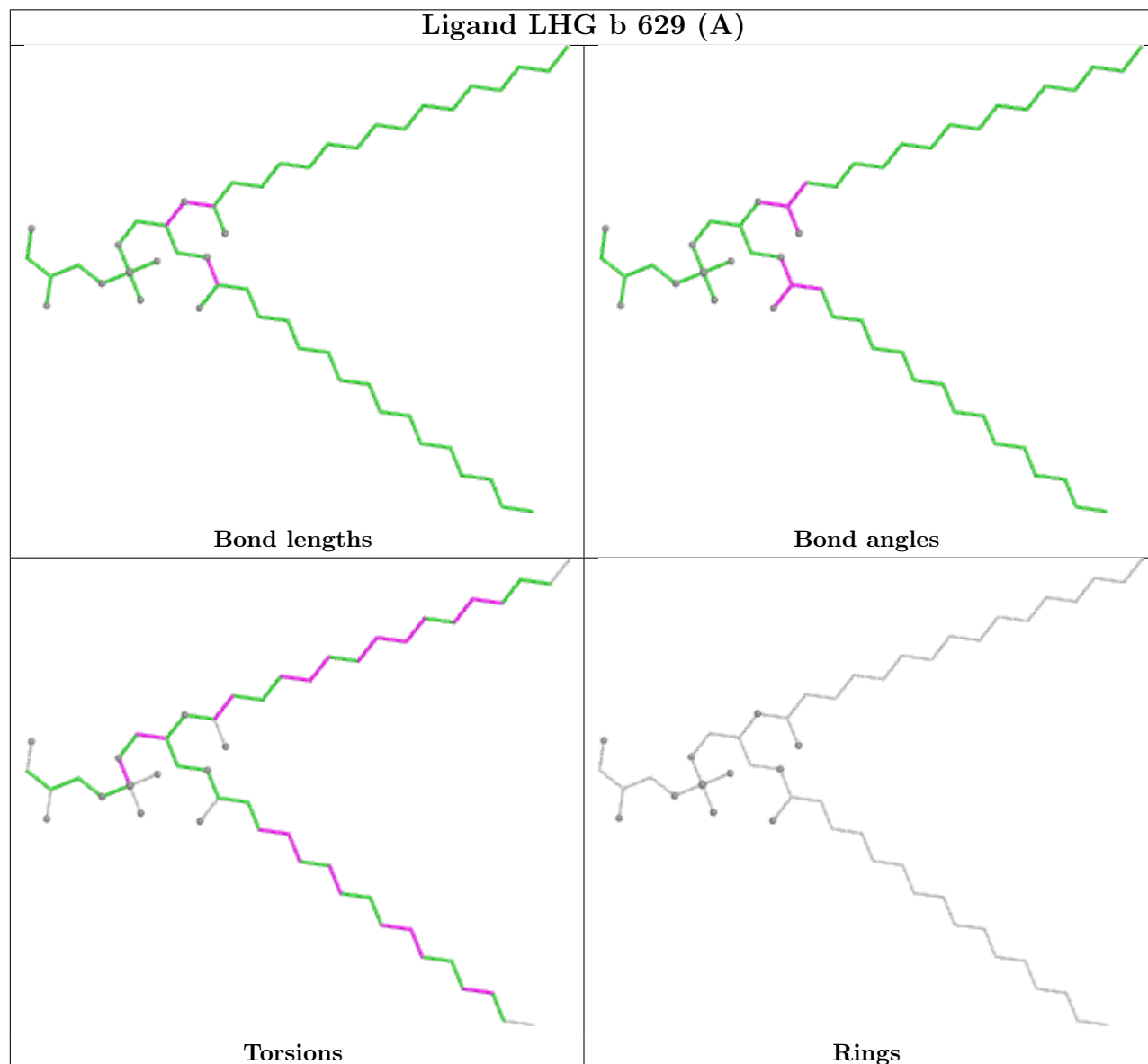
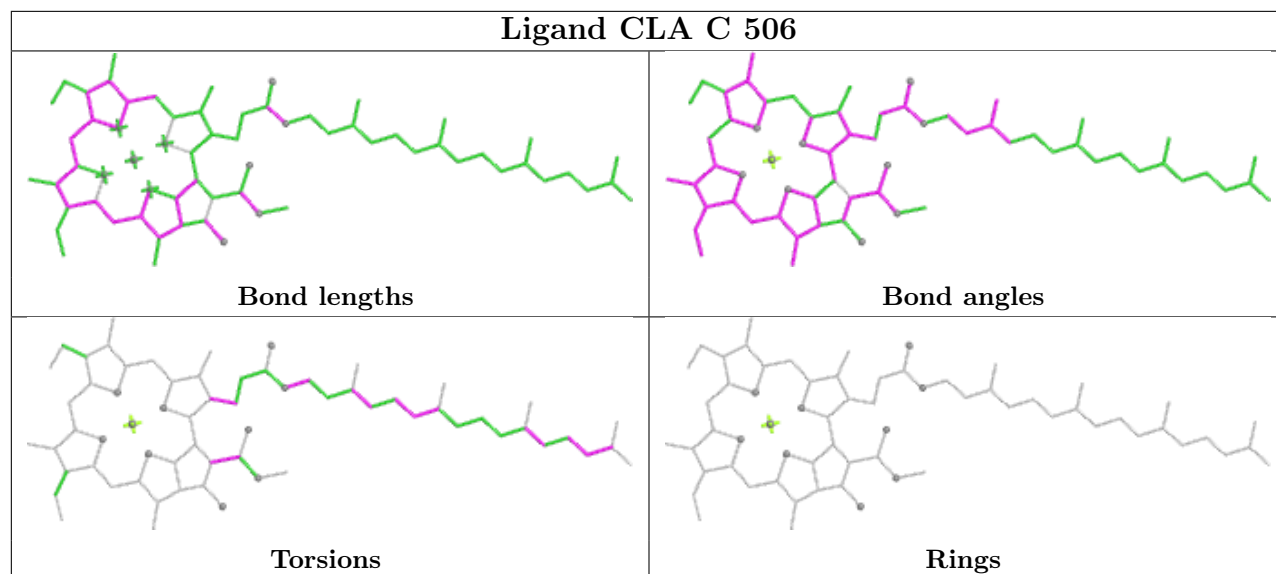


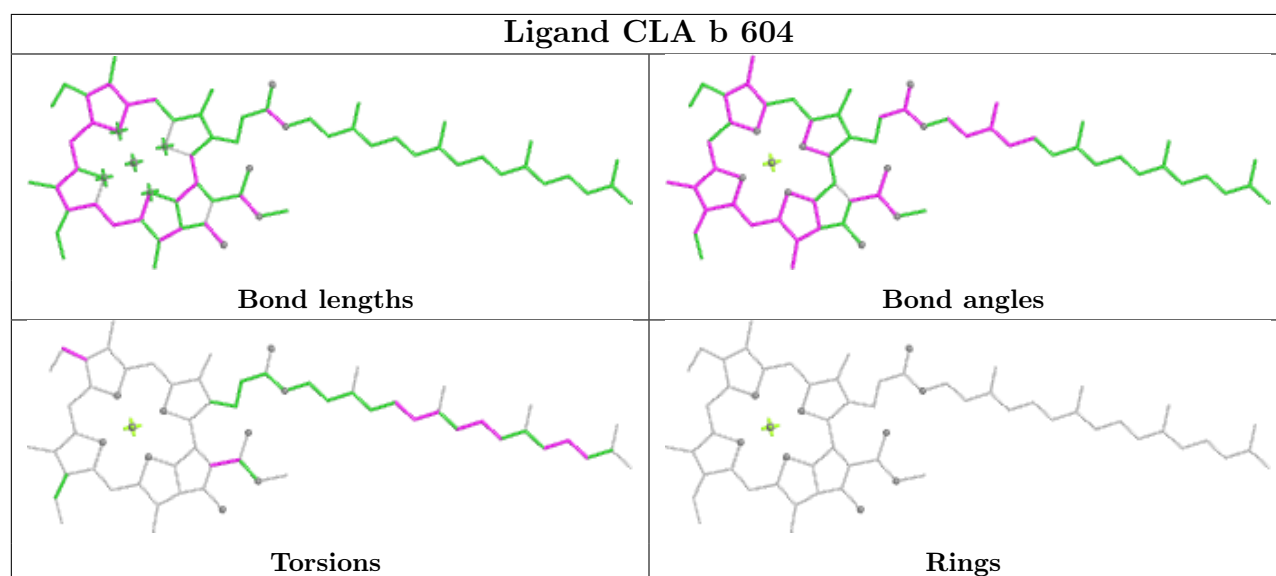
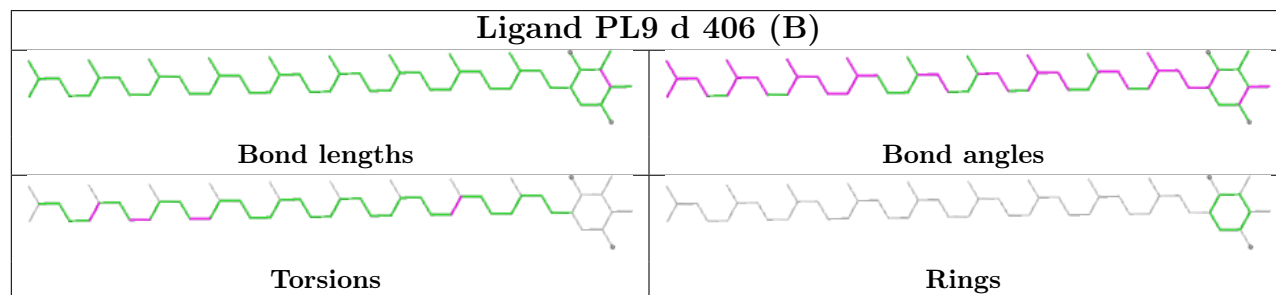
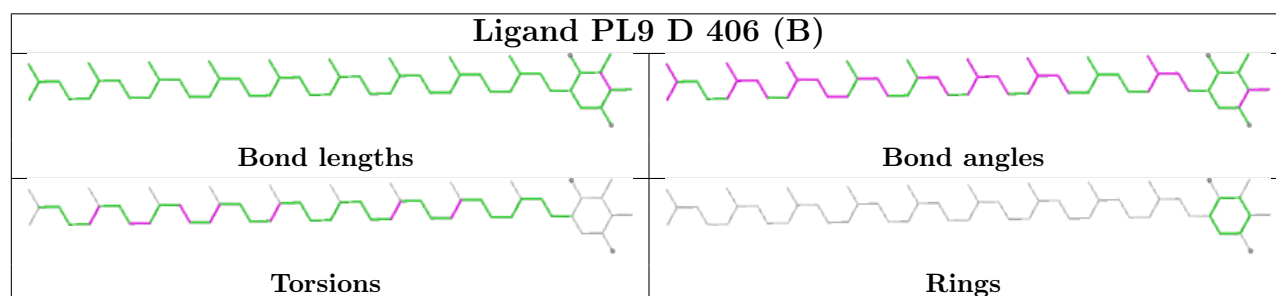
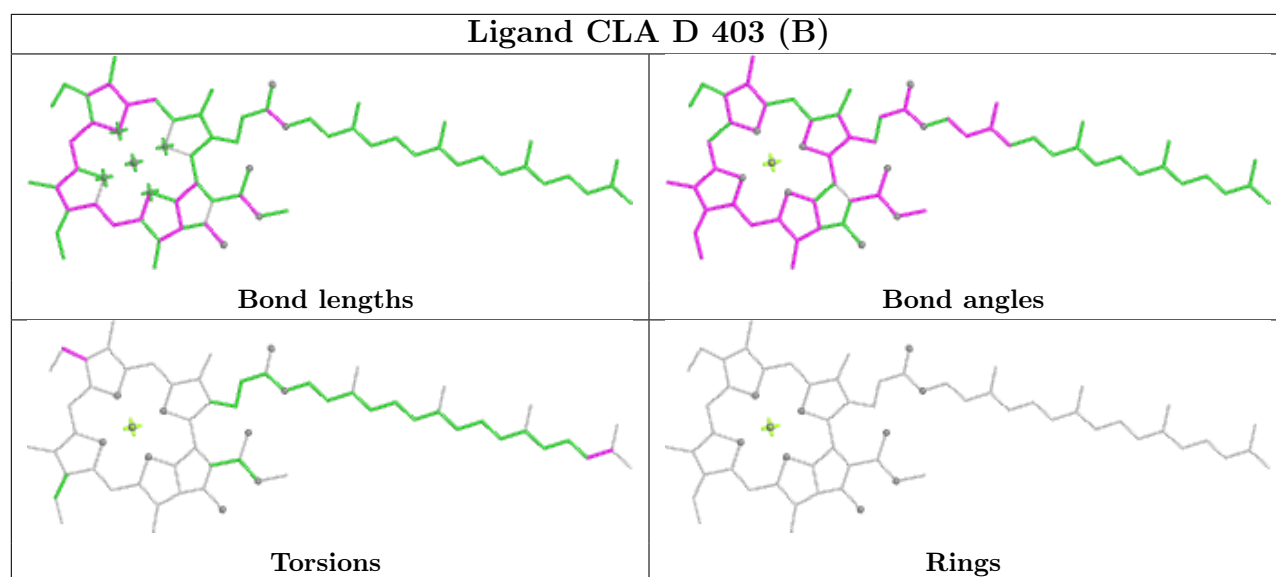


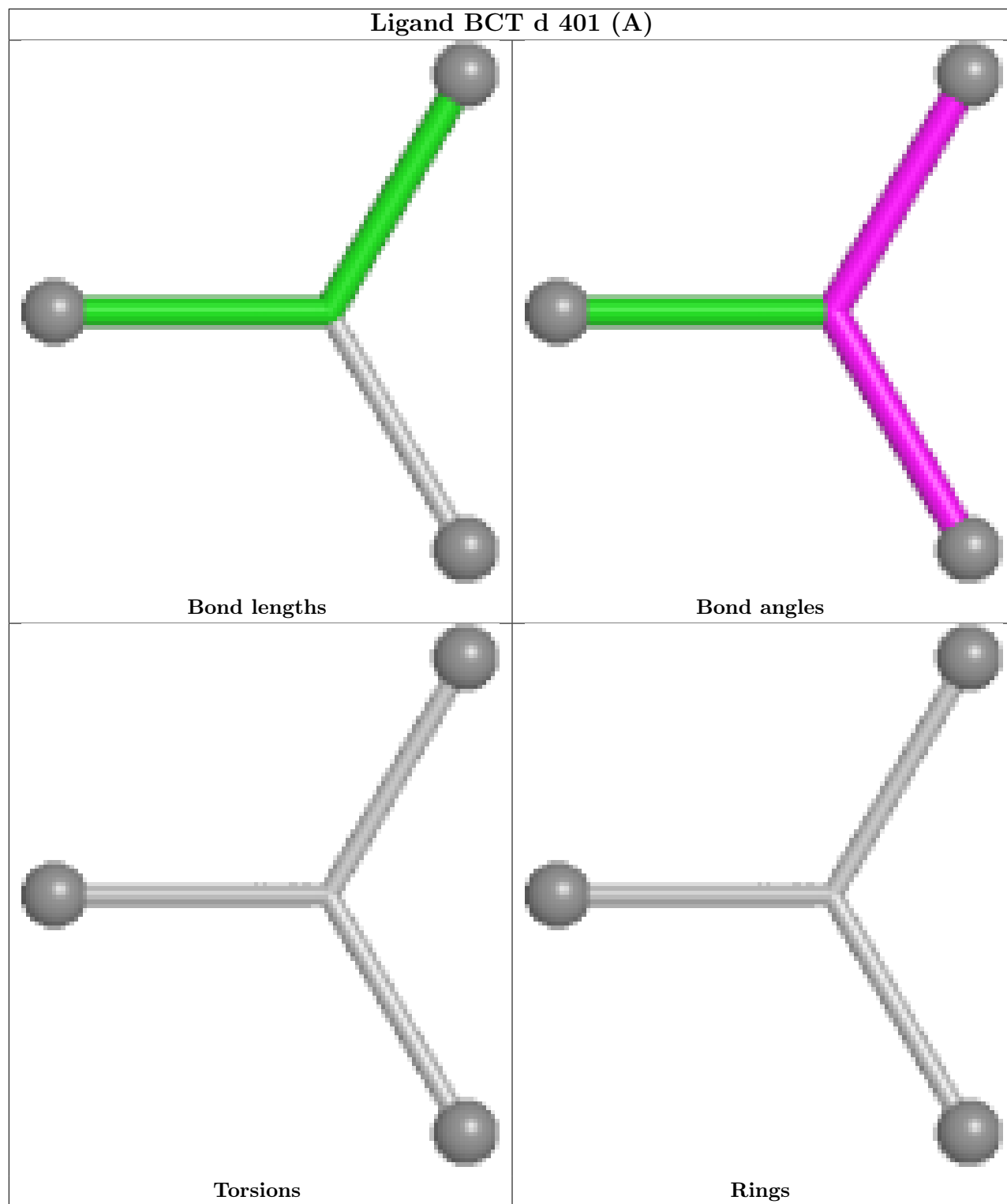
Ligand CLA b 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 A 414 (A)	
	
Bond lengths	Bond angles
	
Torsions	Rings

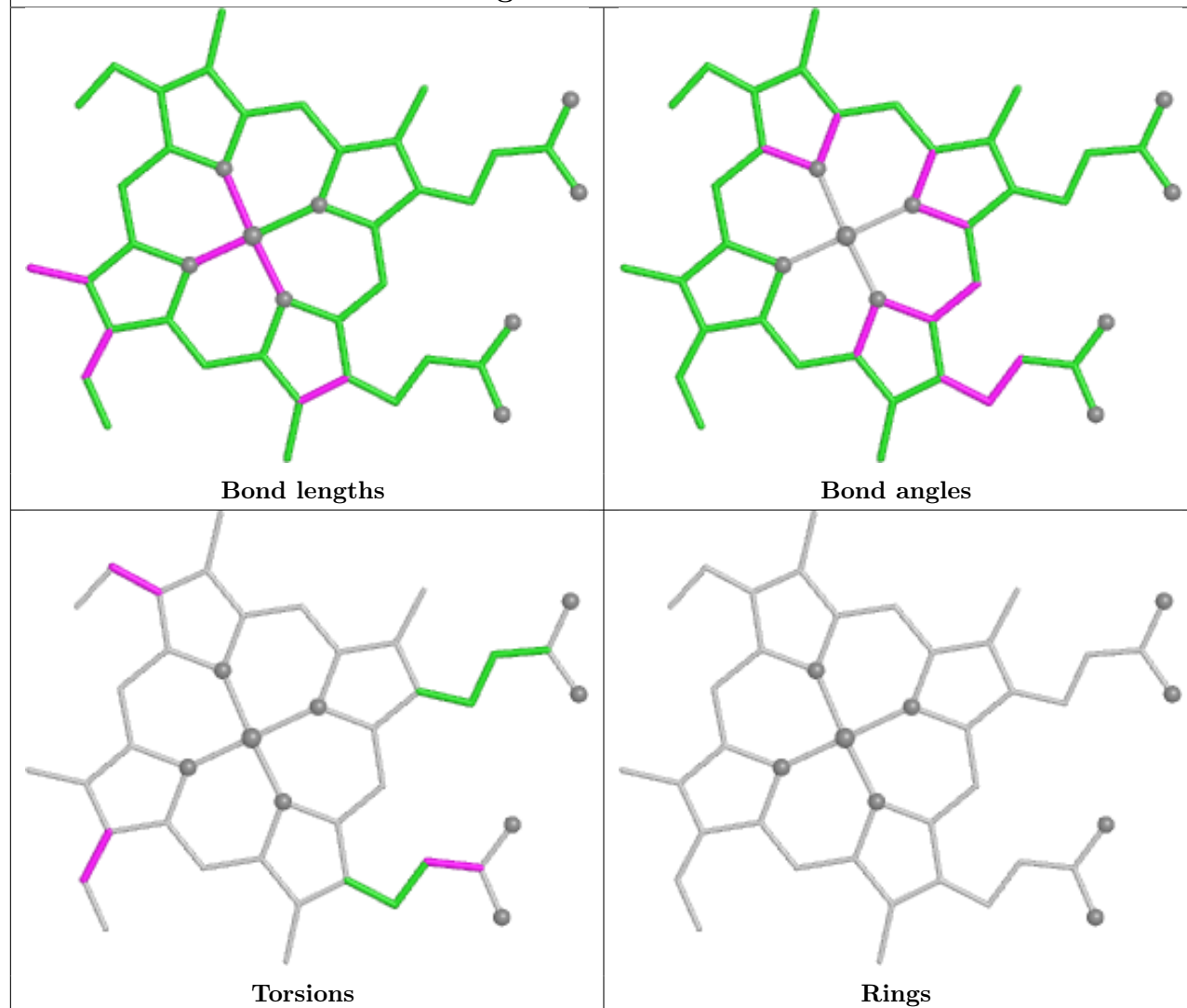




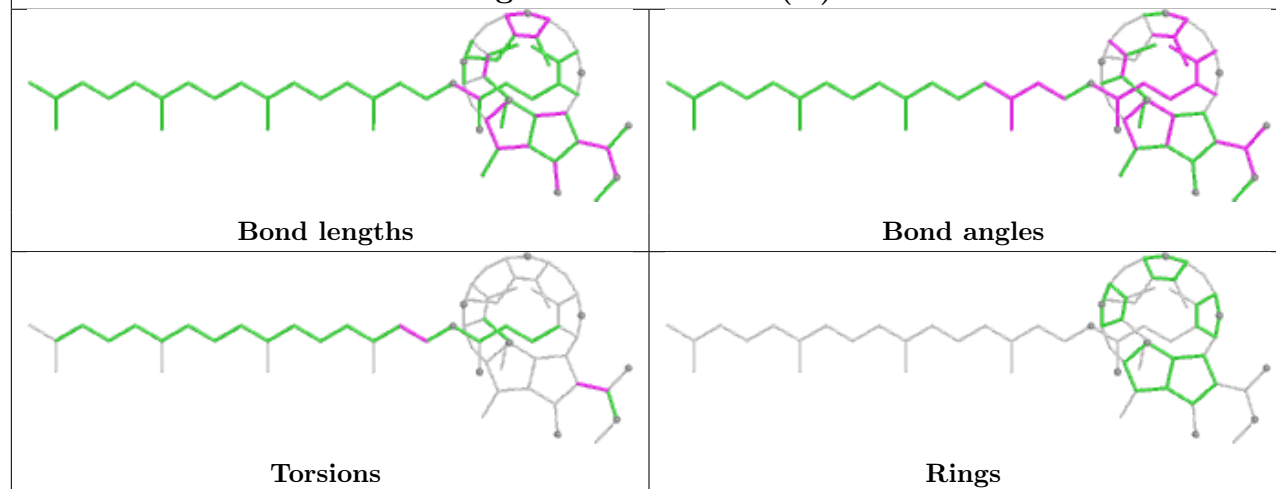


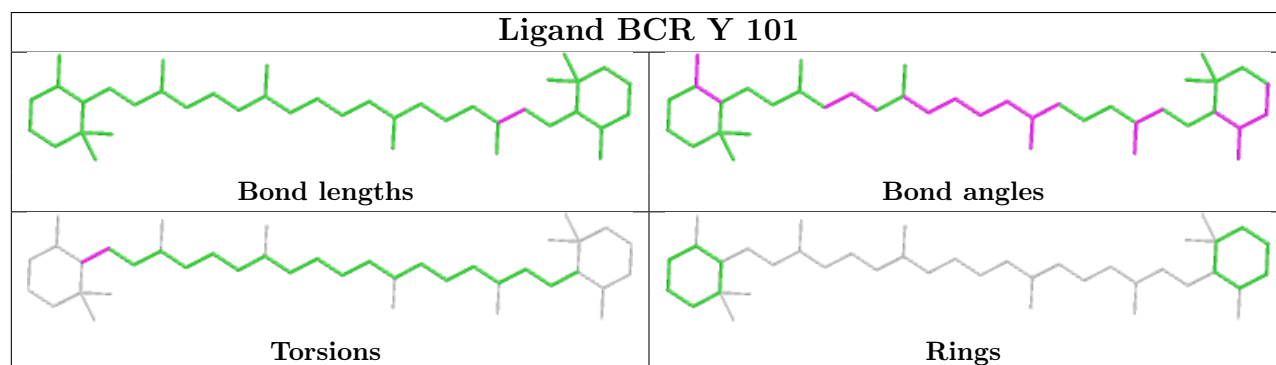
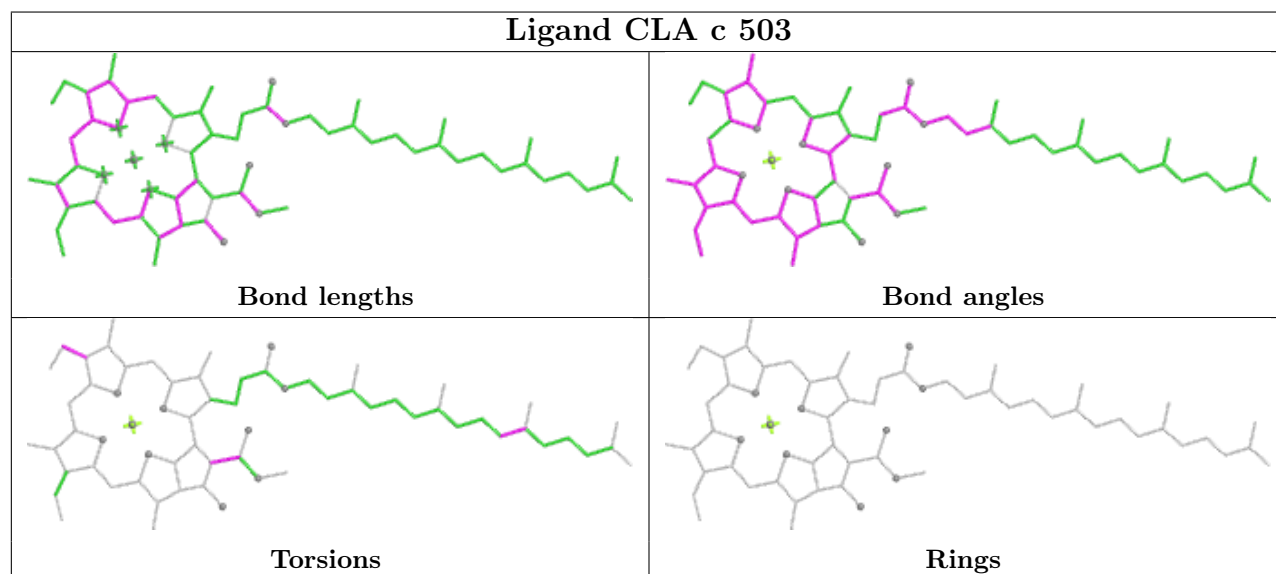
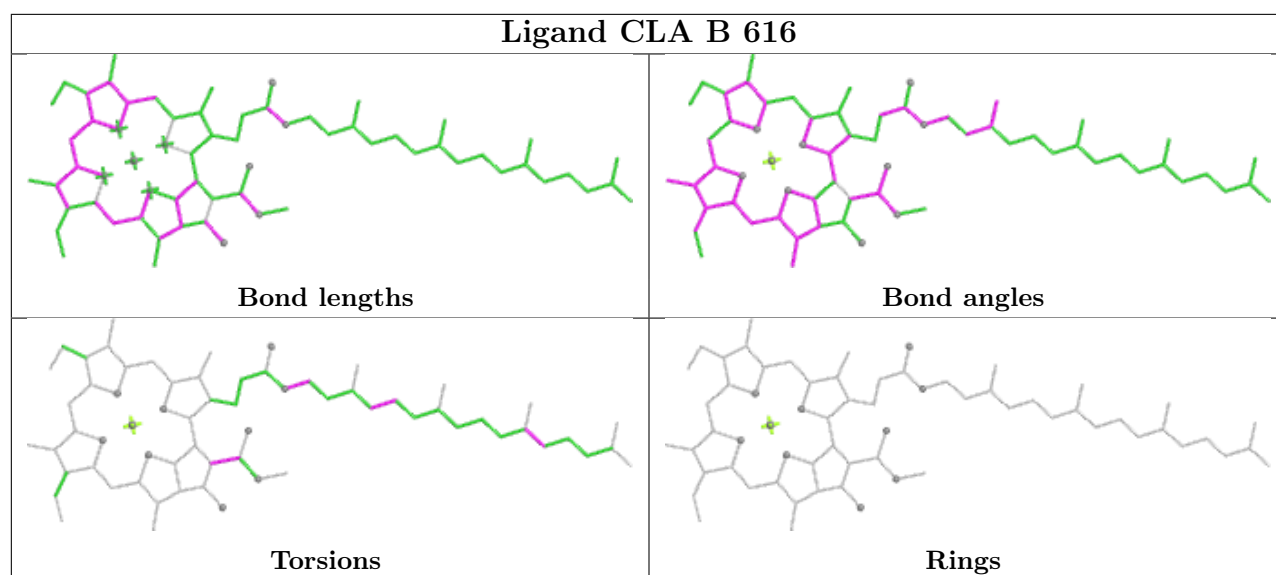


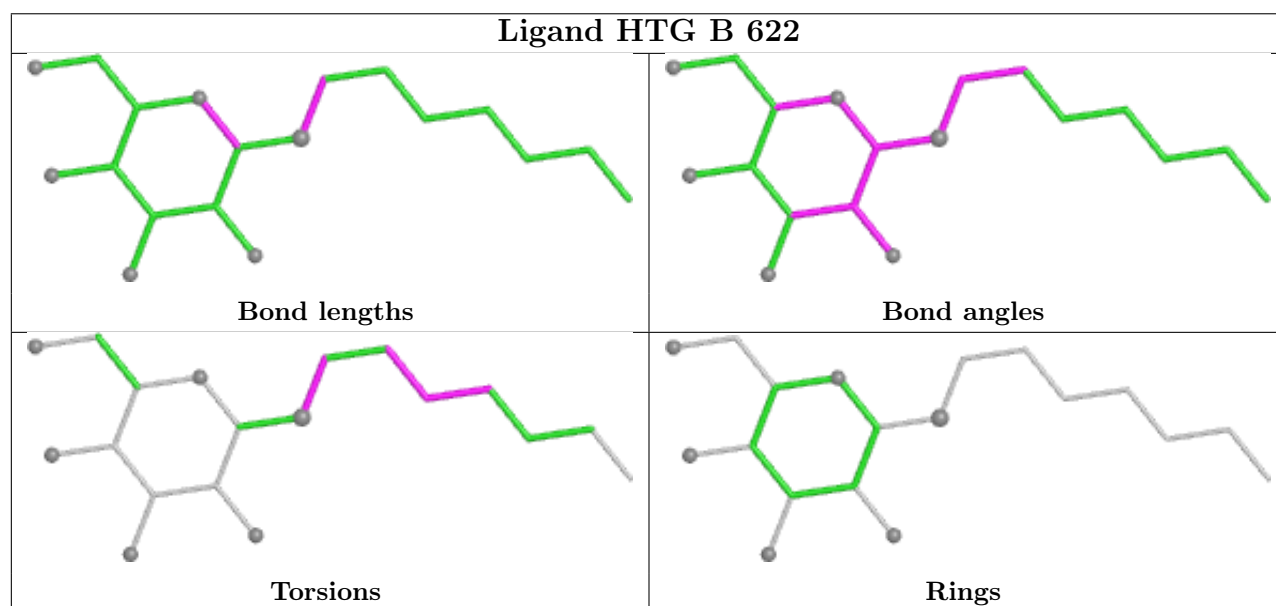
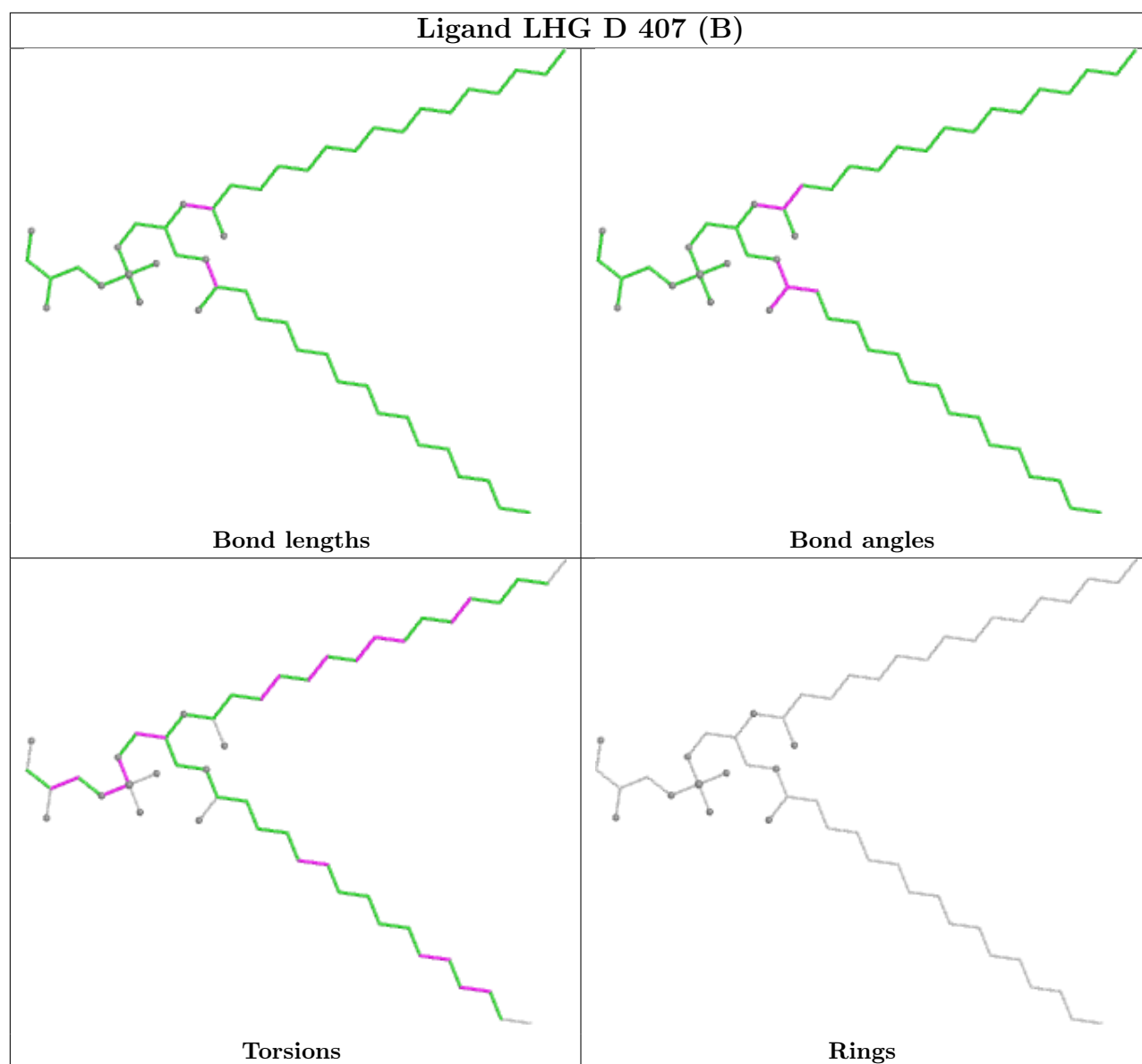
Ligand HEC v 201

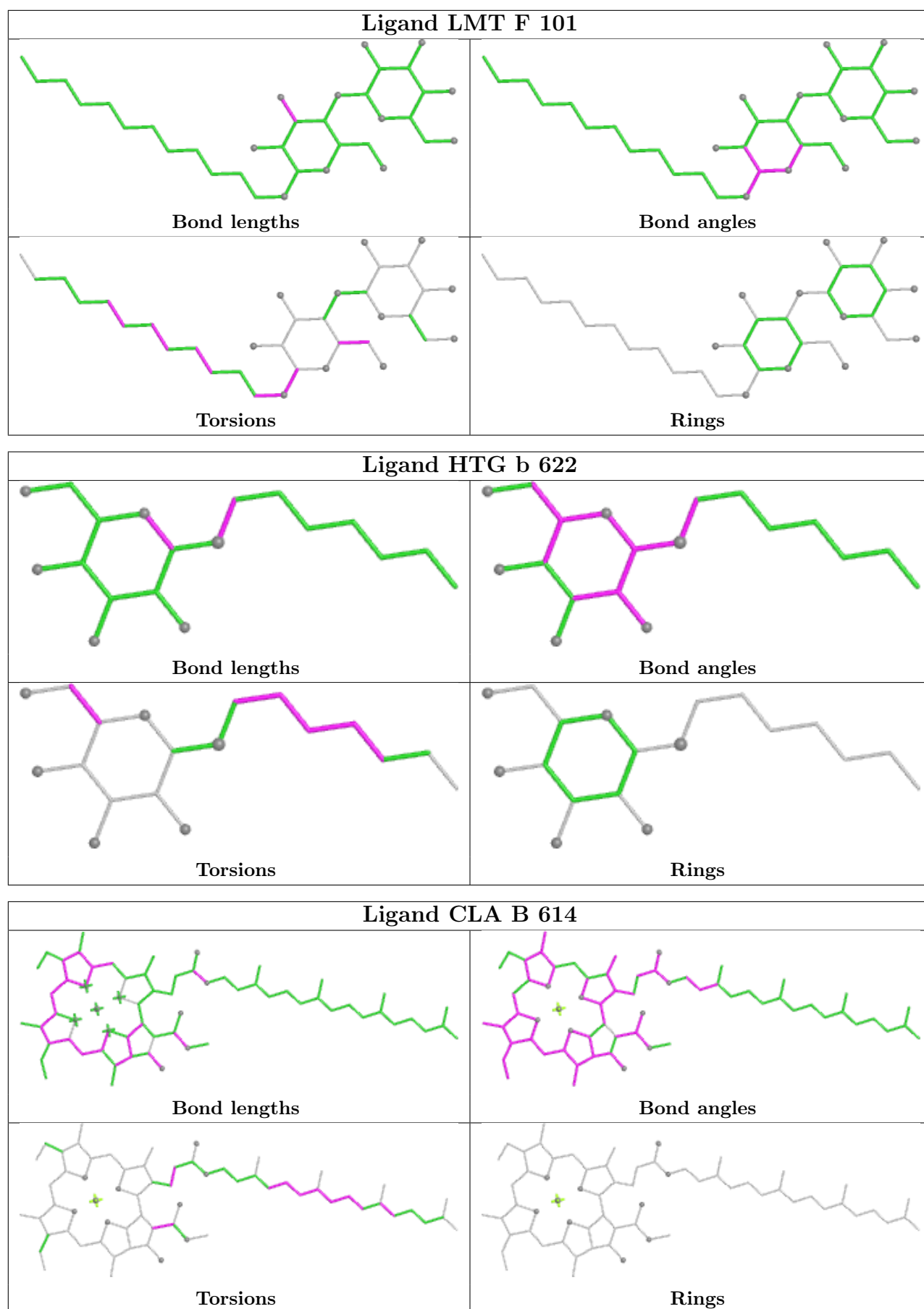


Ligand PHO A 407 (A)

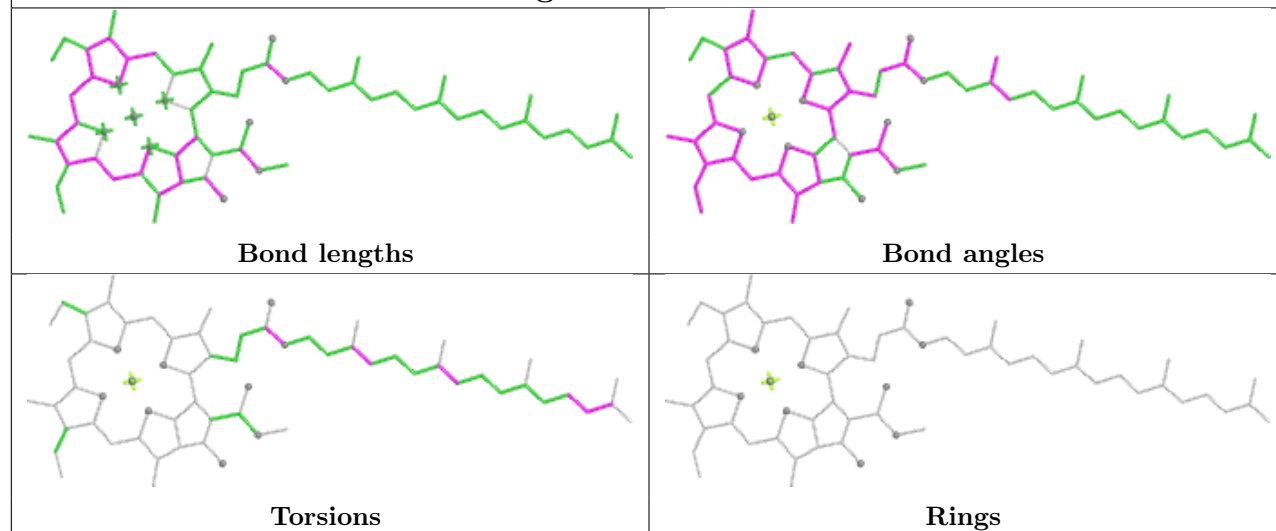




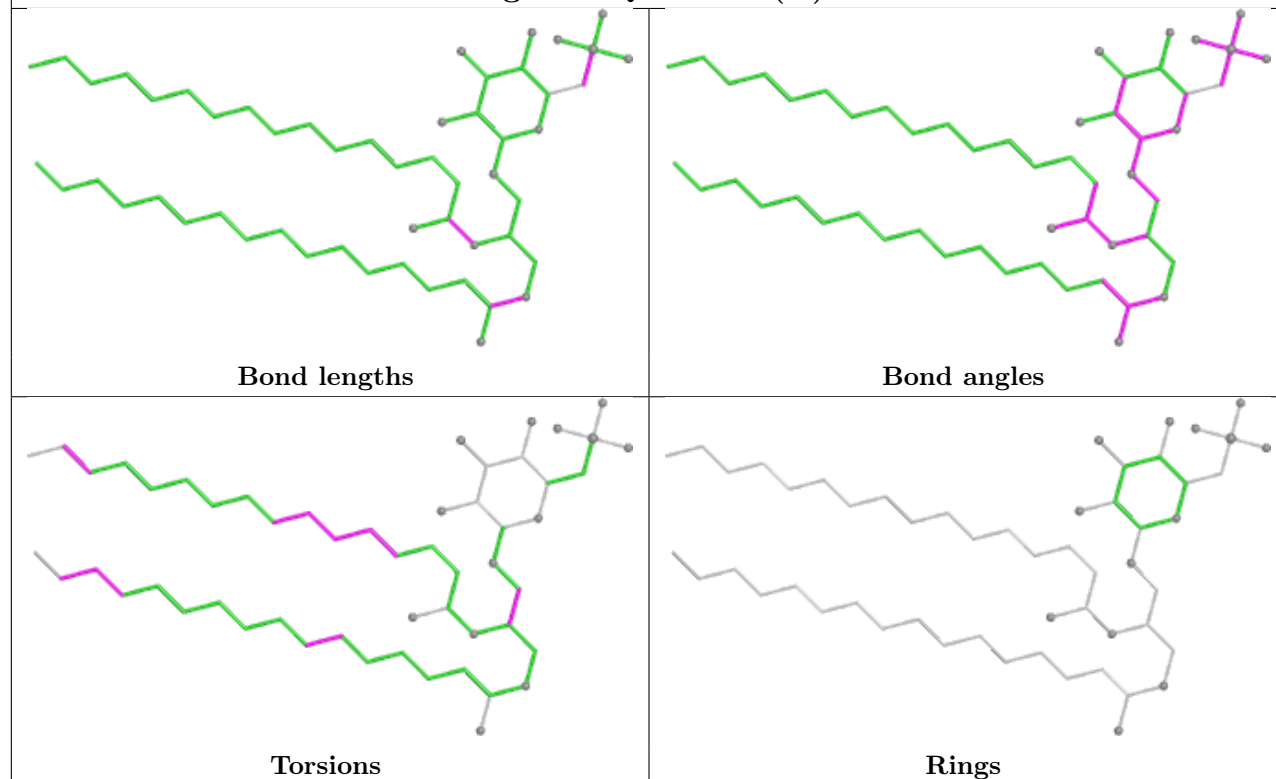


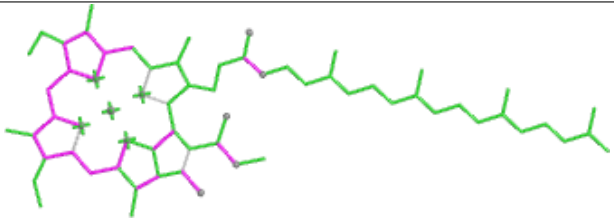
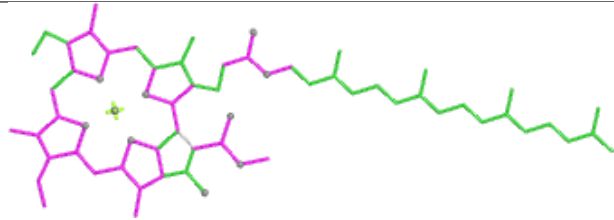
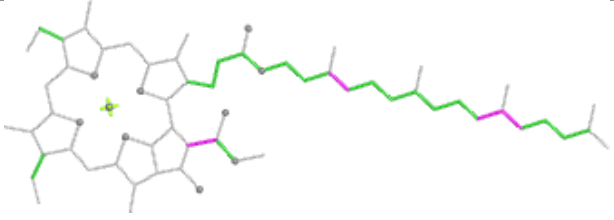
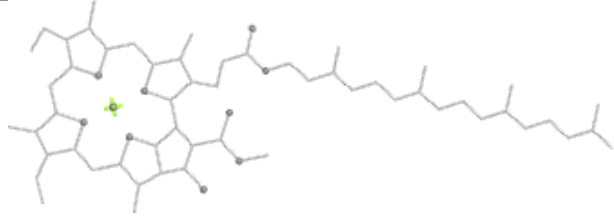


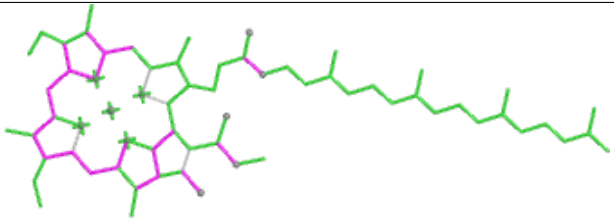
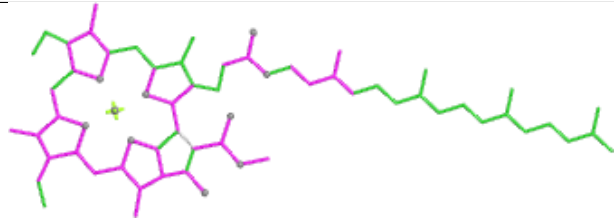
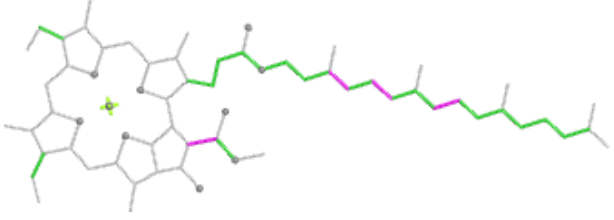
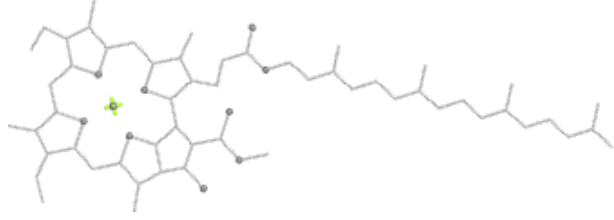
Ligand CLA a 407

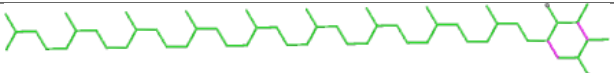
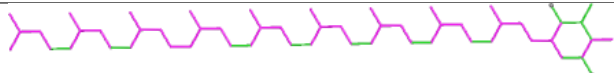
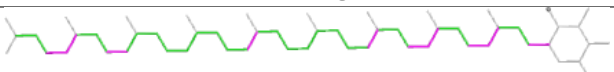
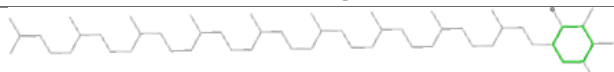


Ligand SQD a 409 (A)

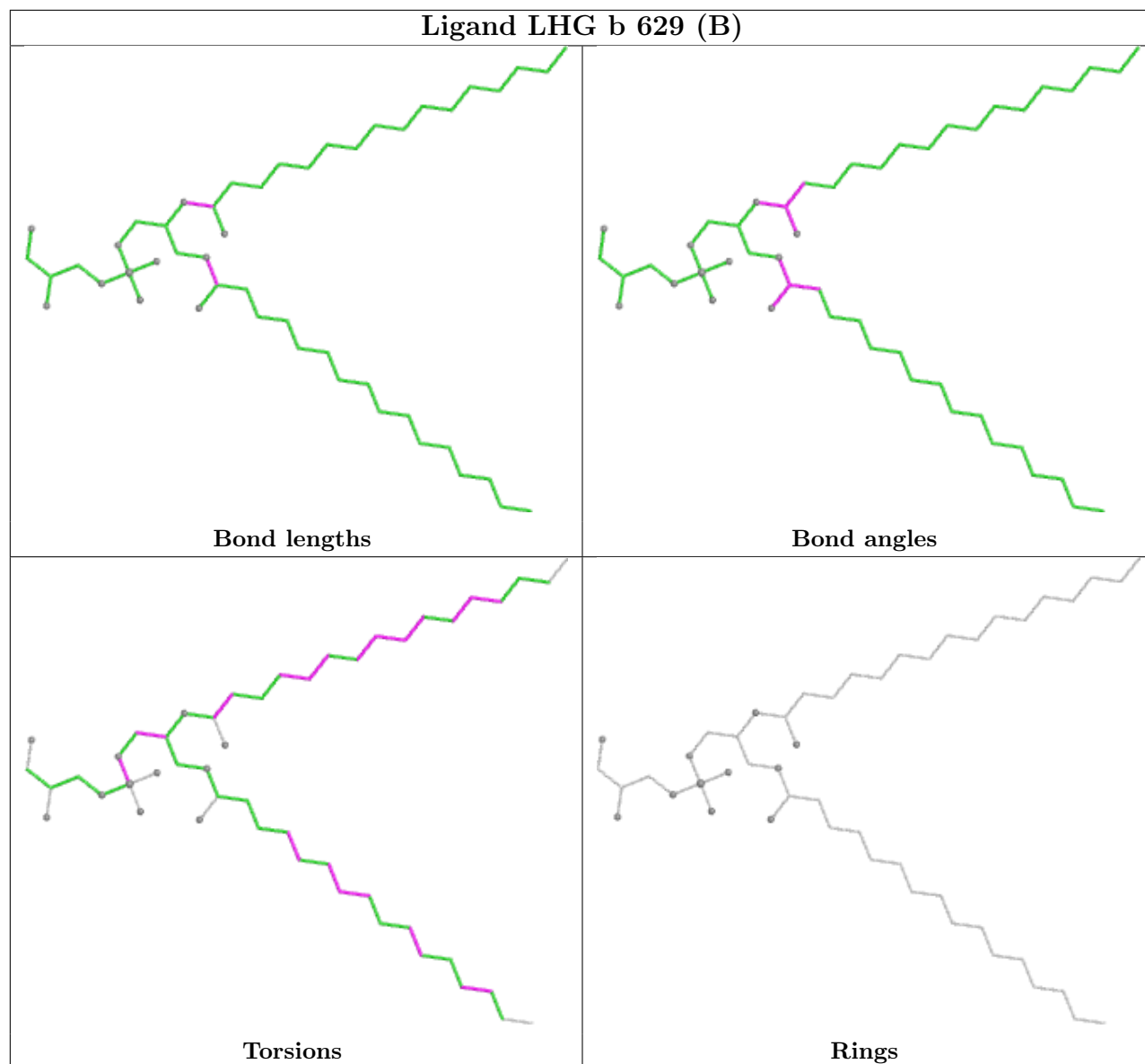


Ligand CLA c 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

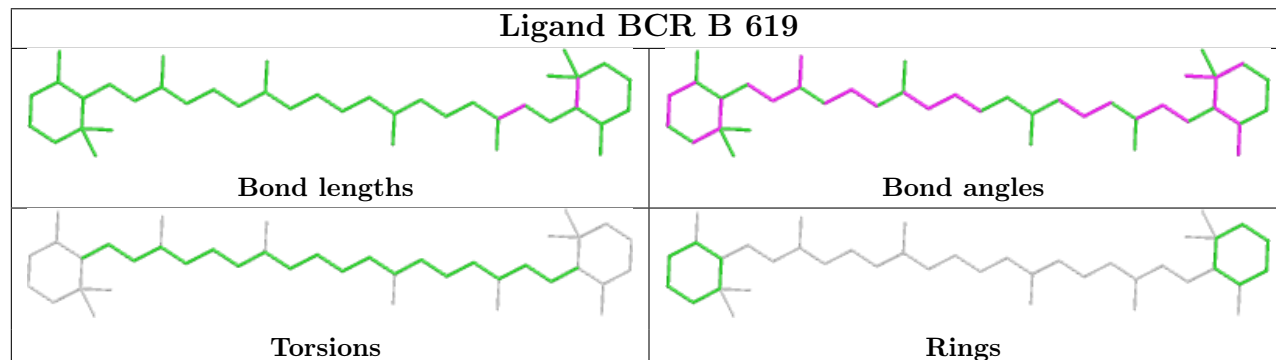
Ligand CLA B 605	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 A 414 (B)	
	
Bond lengths	Bond angles
	
Torsions	Rings

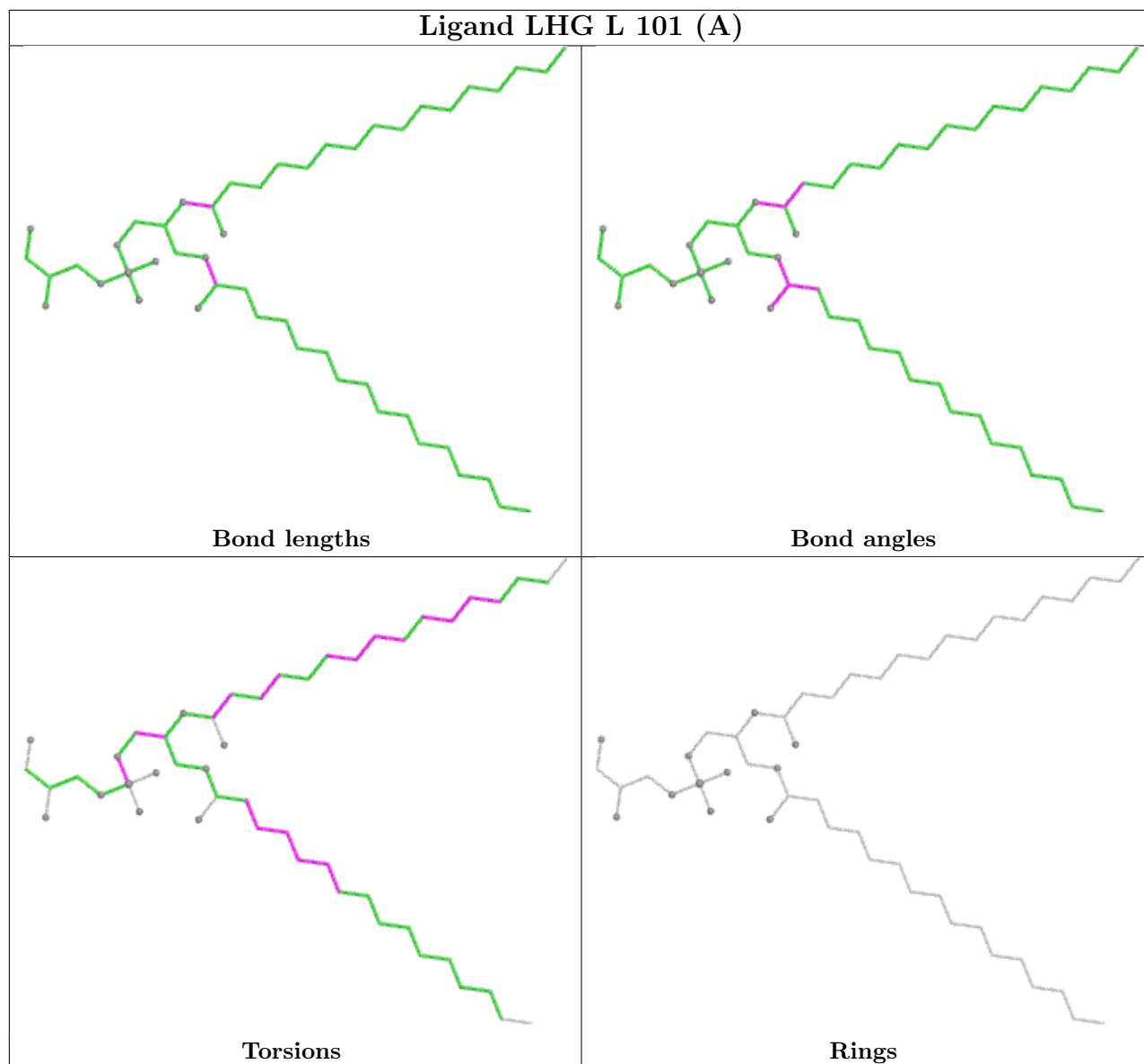
Ligand LHG b 629 (B)



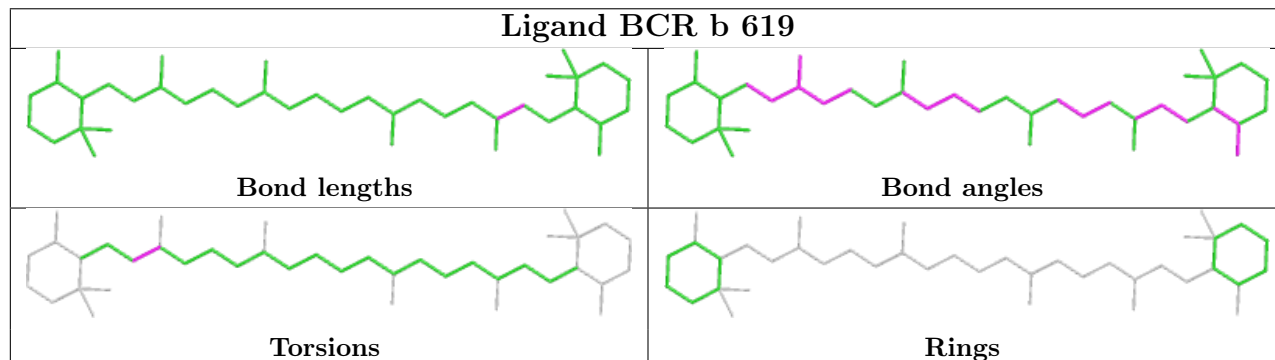
Ligand BCR B 619

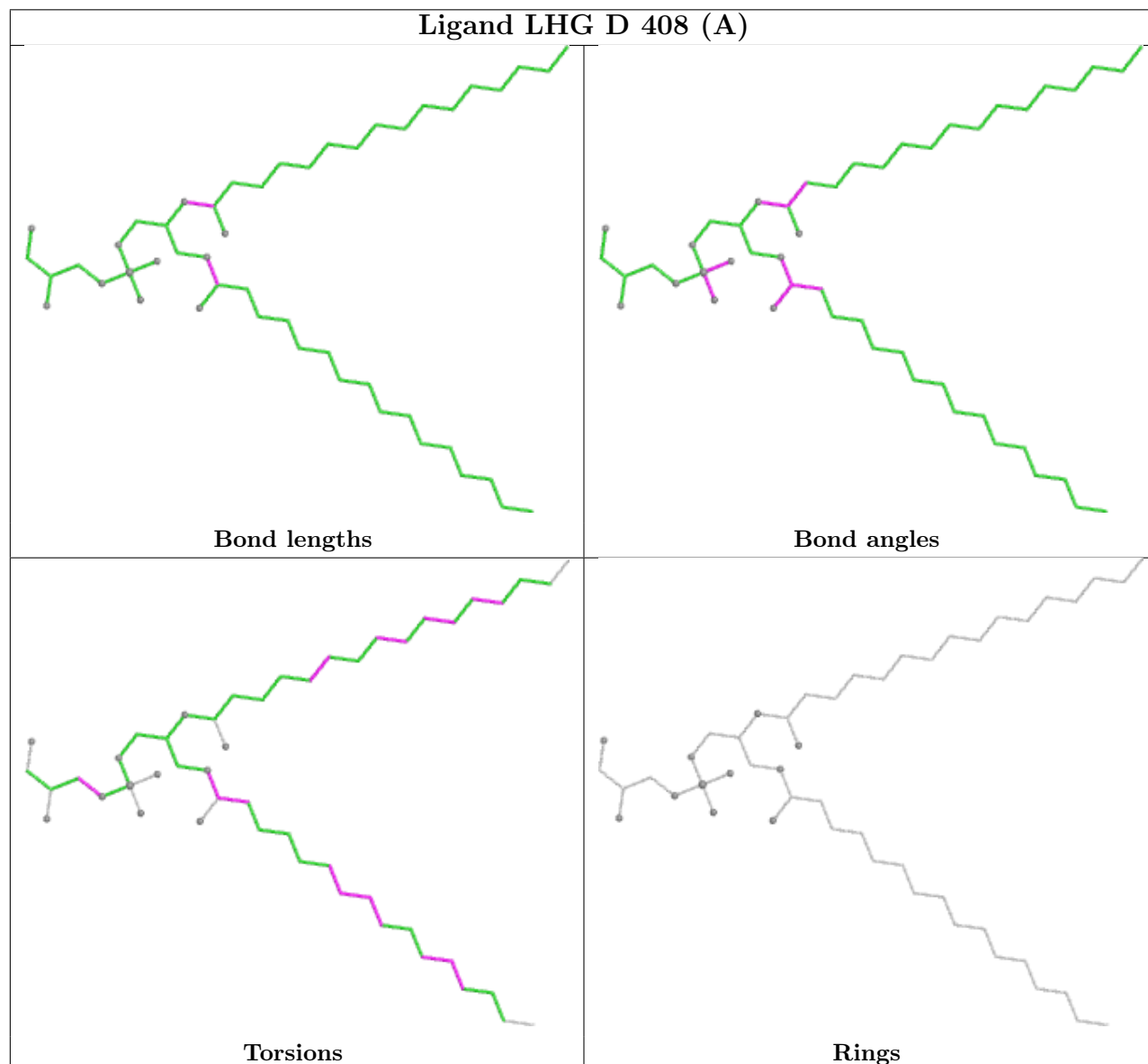
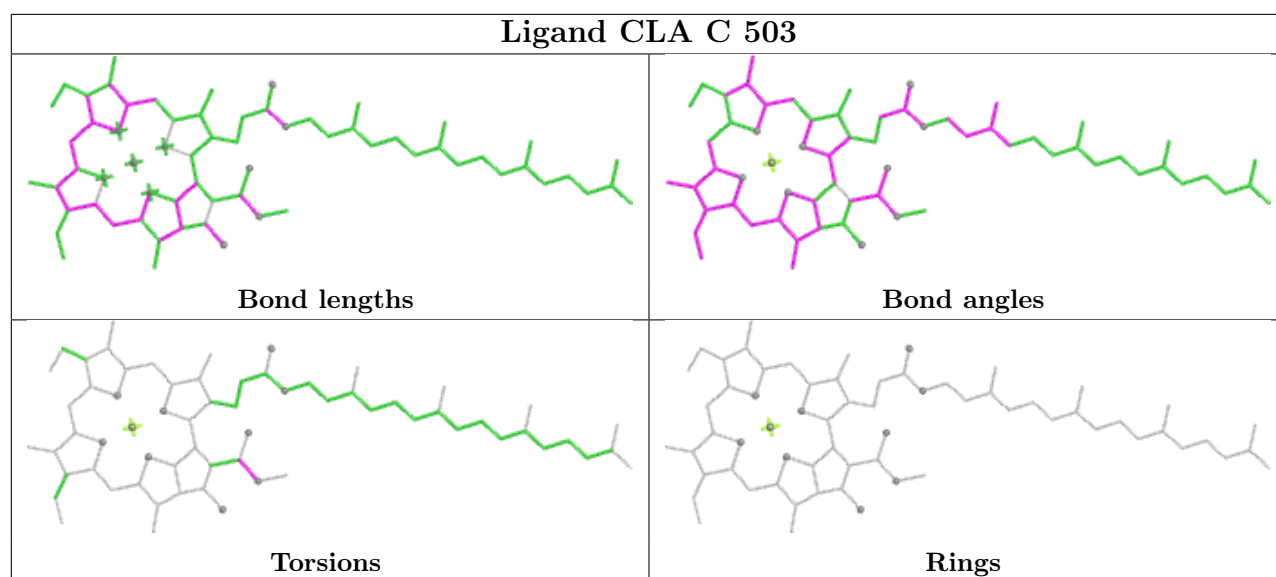


Ligand LHG L 101 (A)

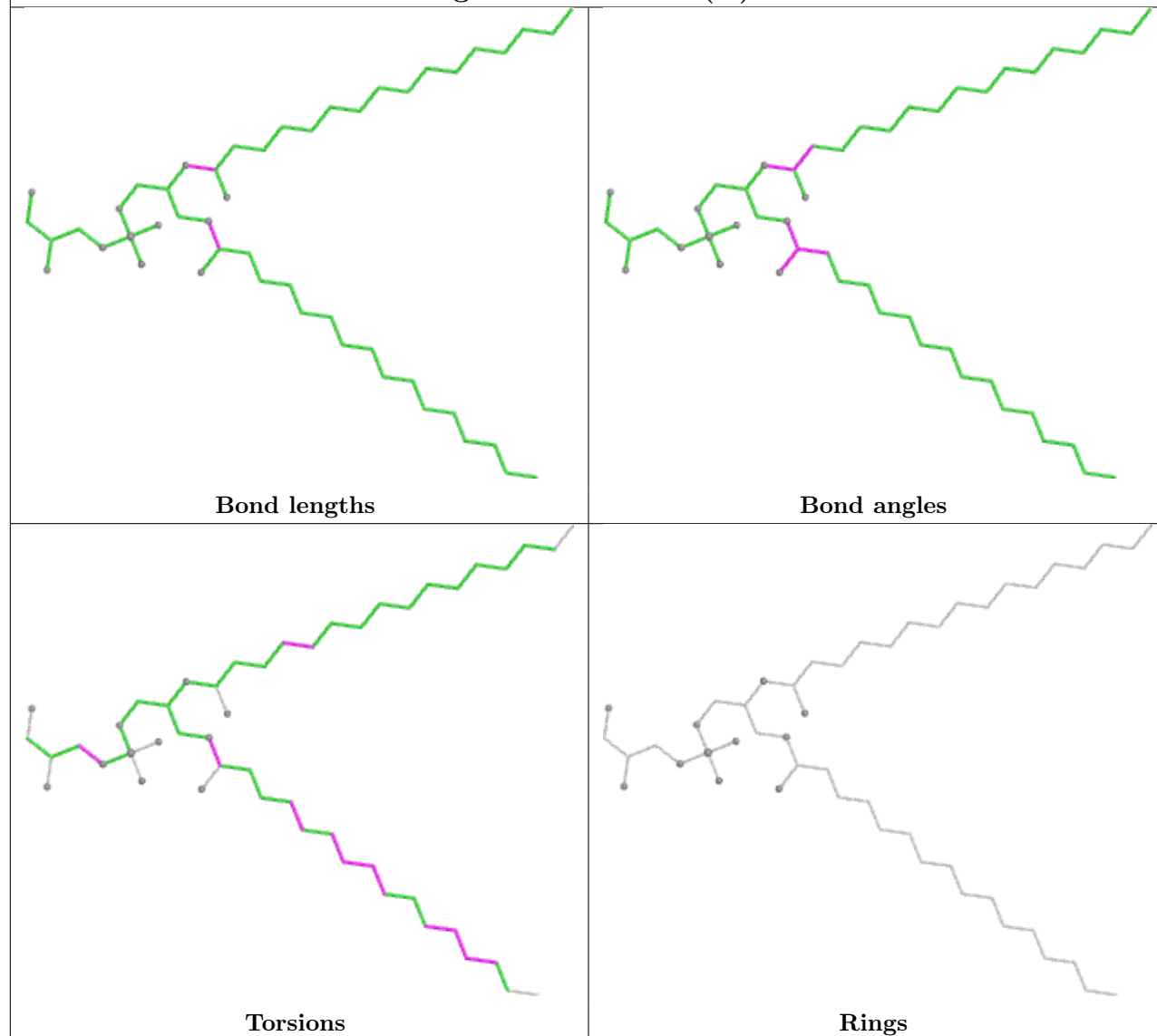


Ligand BCR b 619

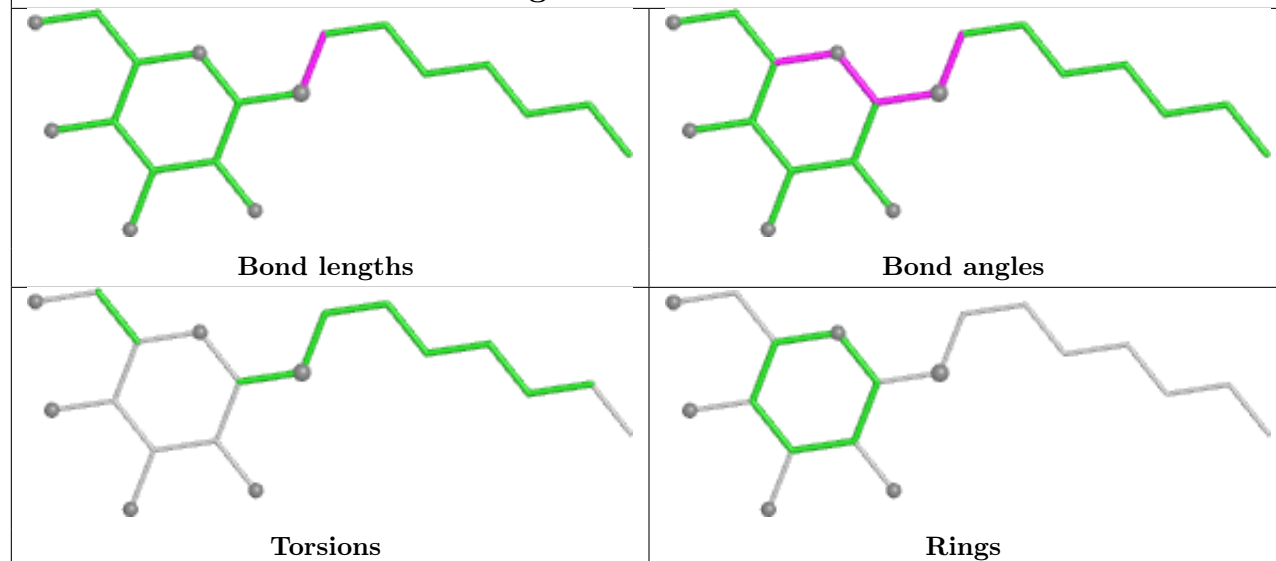


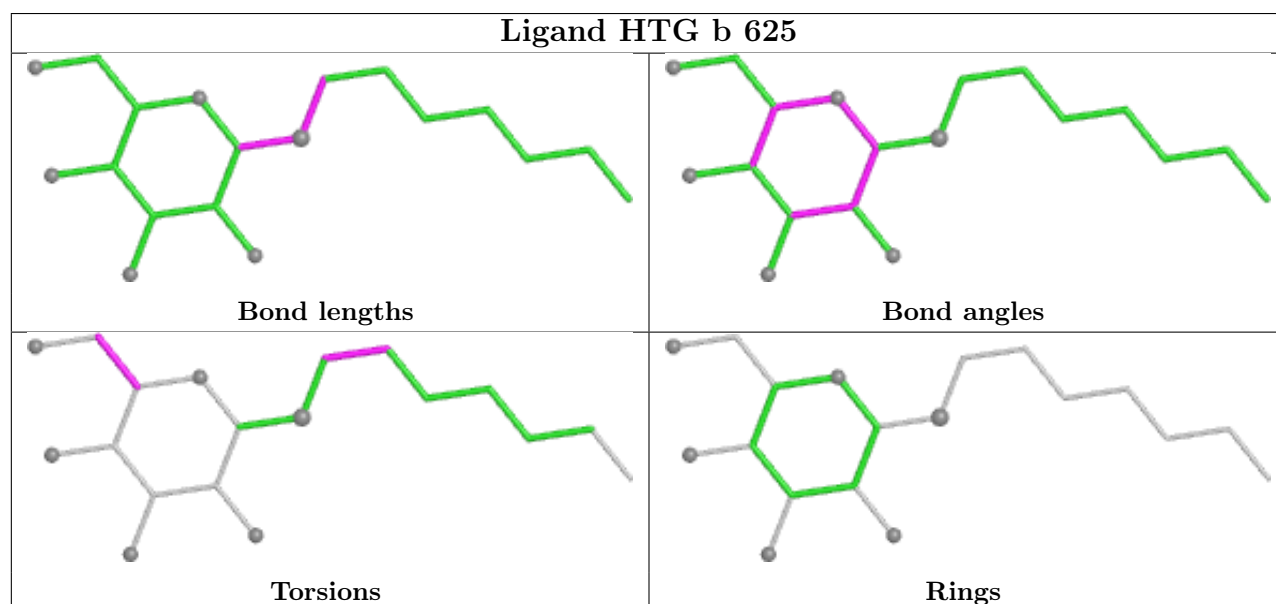
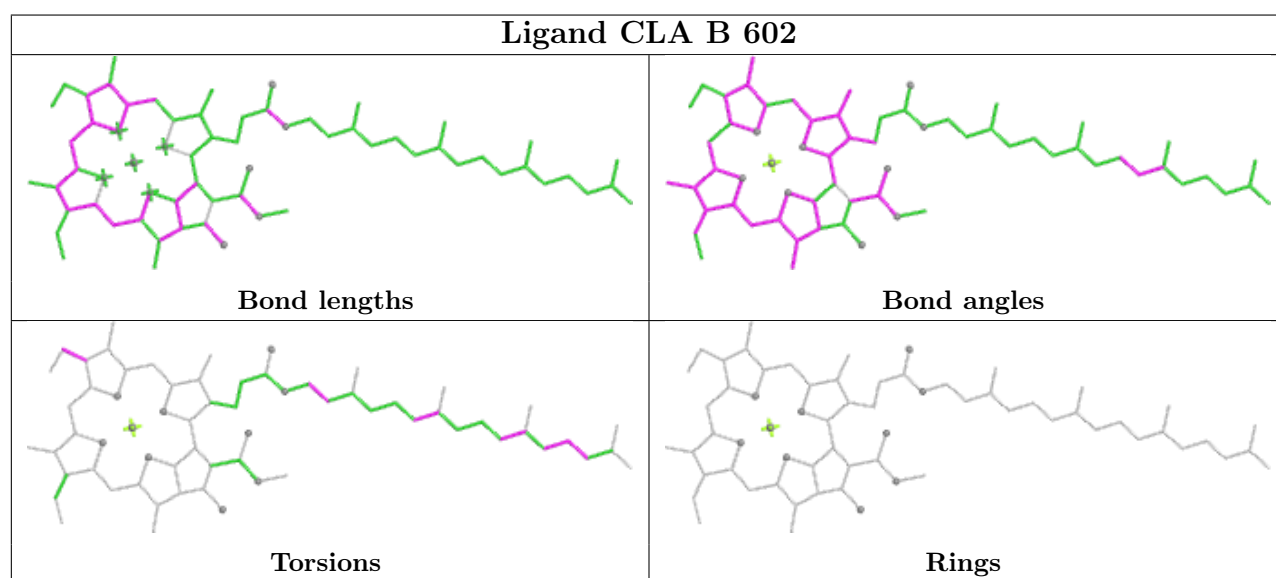
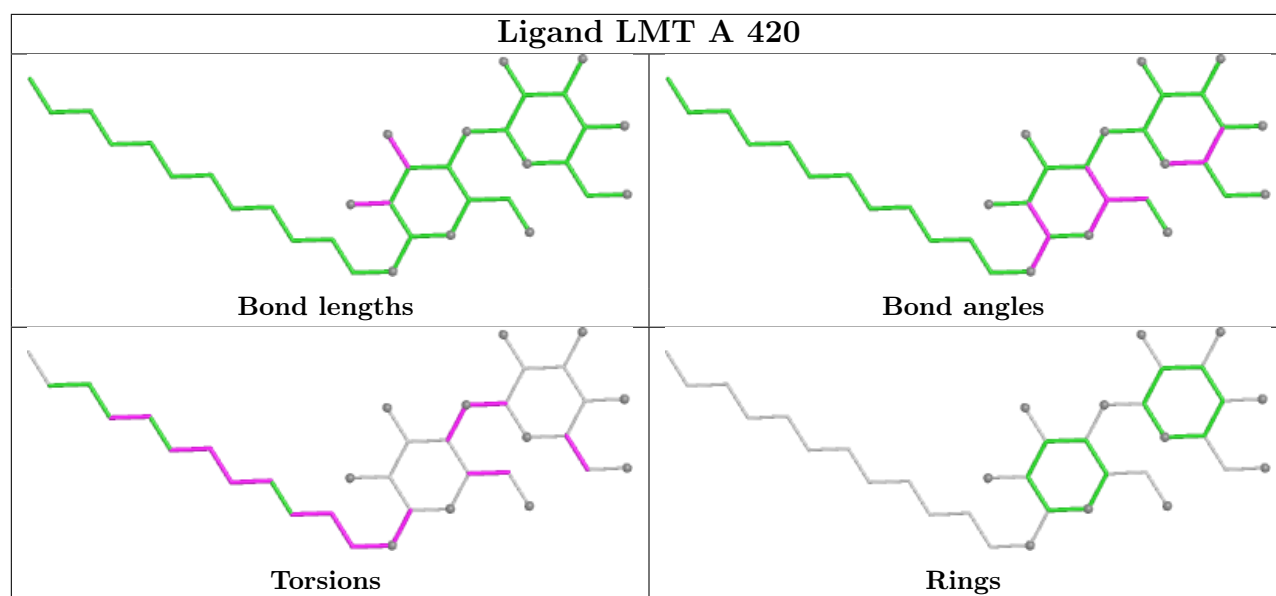


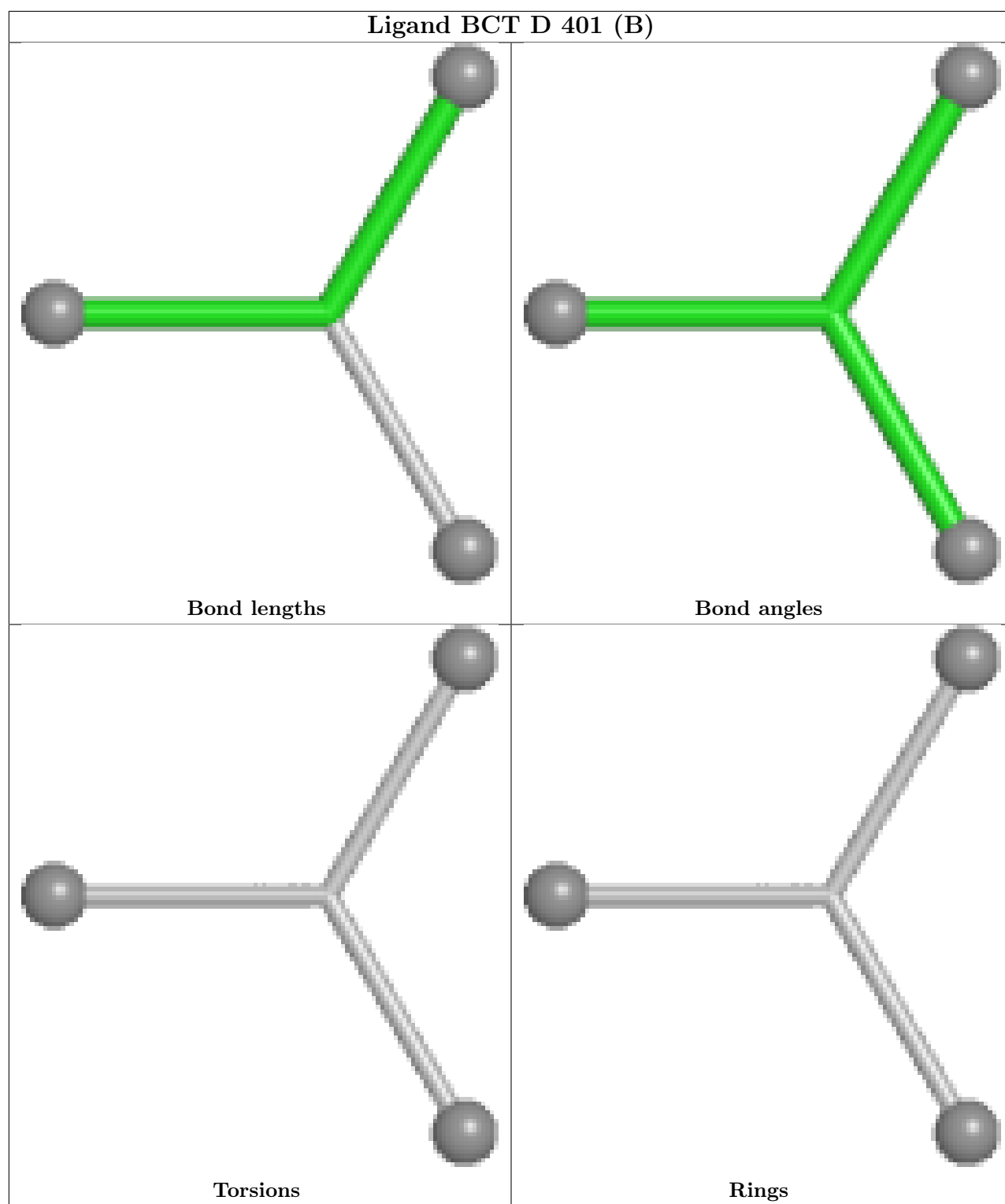
Ligand LHG d 408 (A)

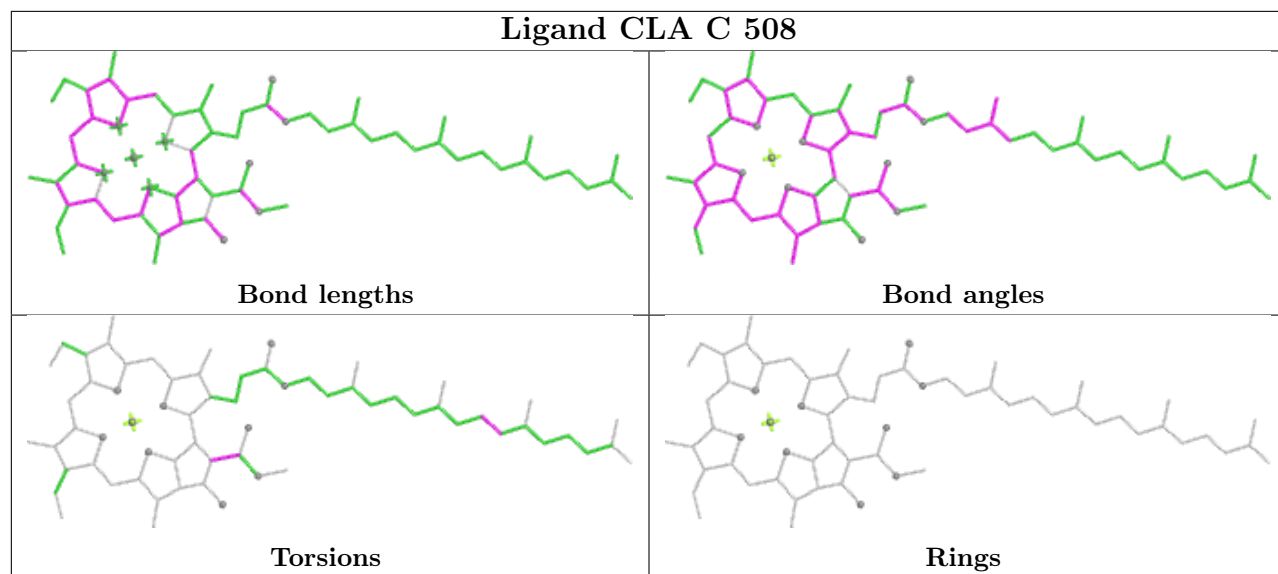


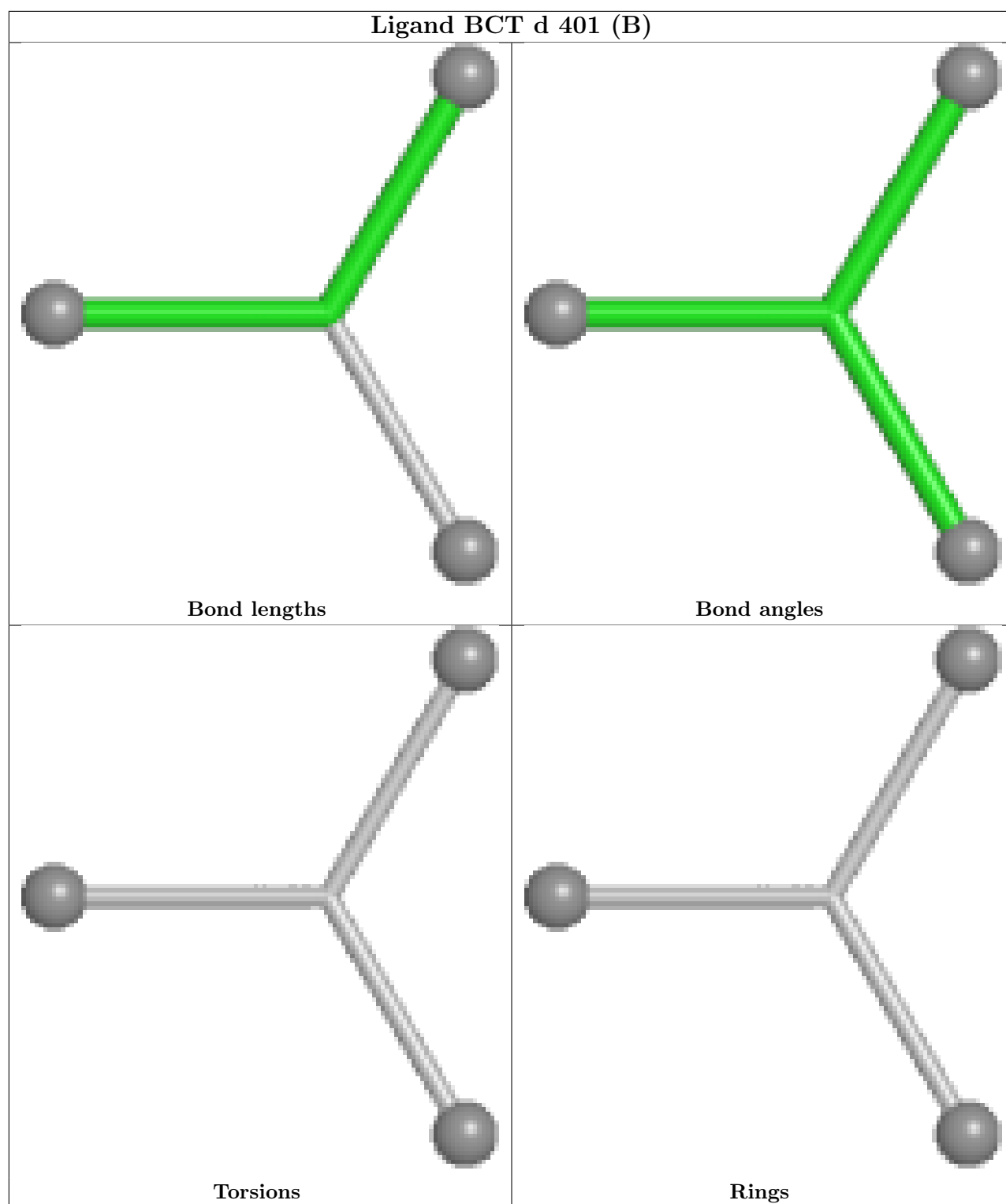
Ligand HTG C 521

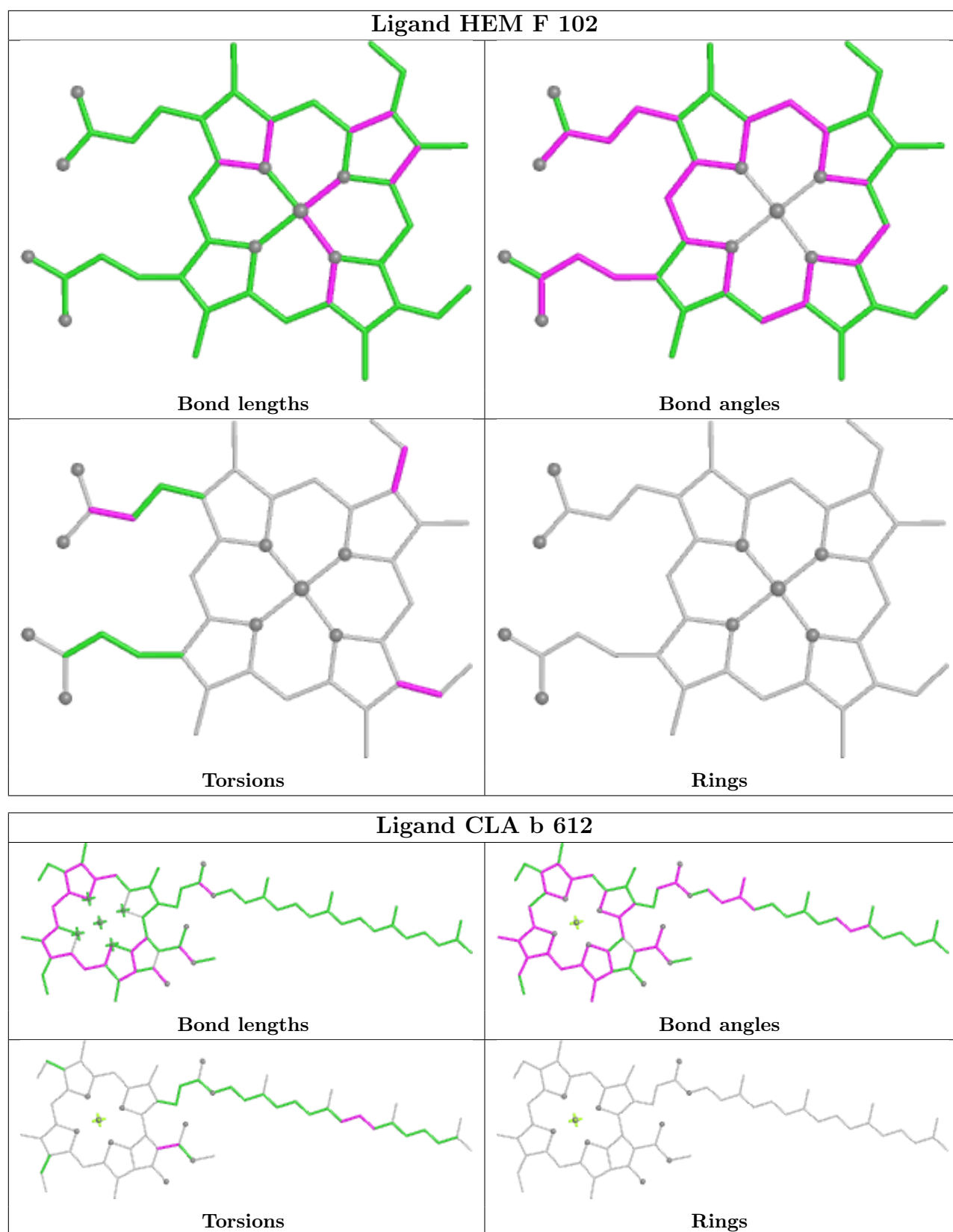


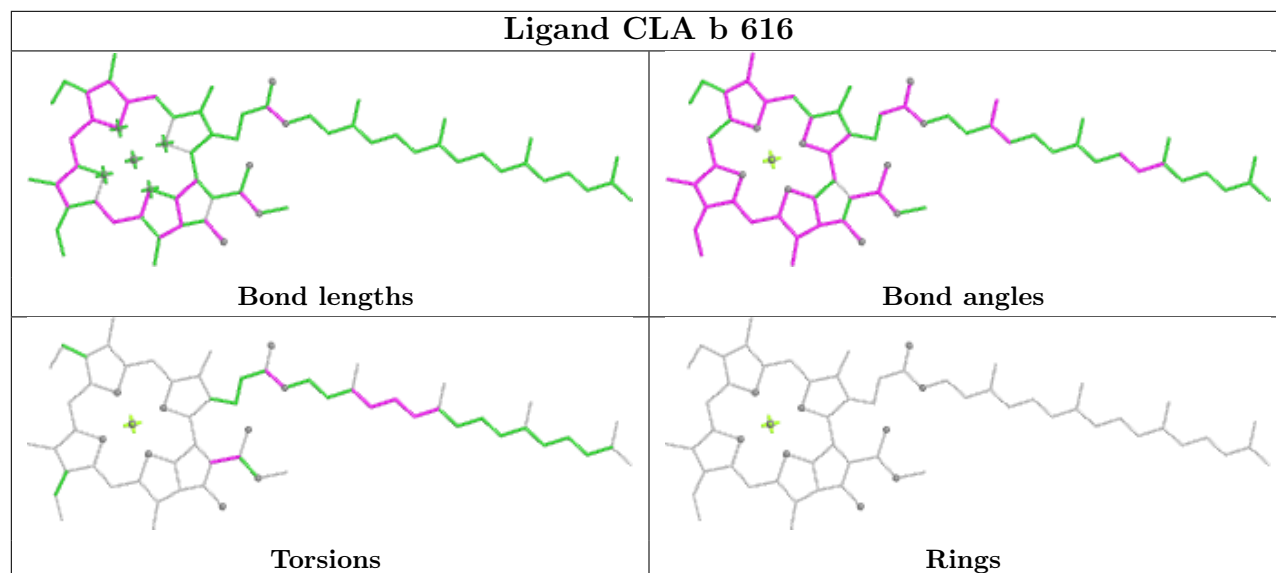
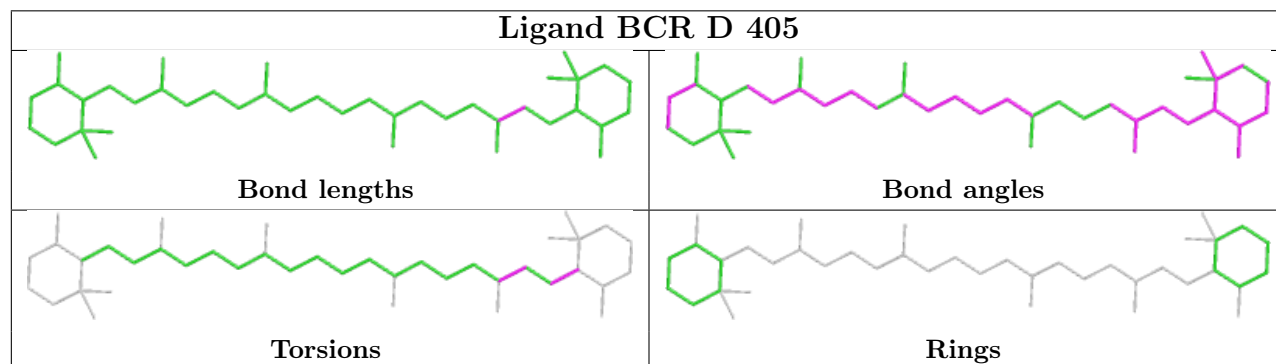
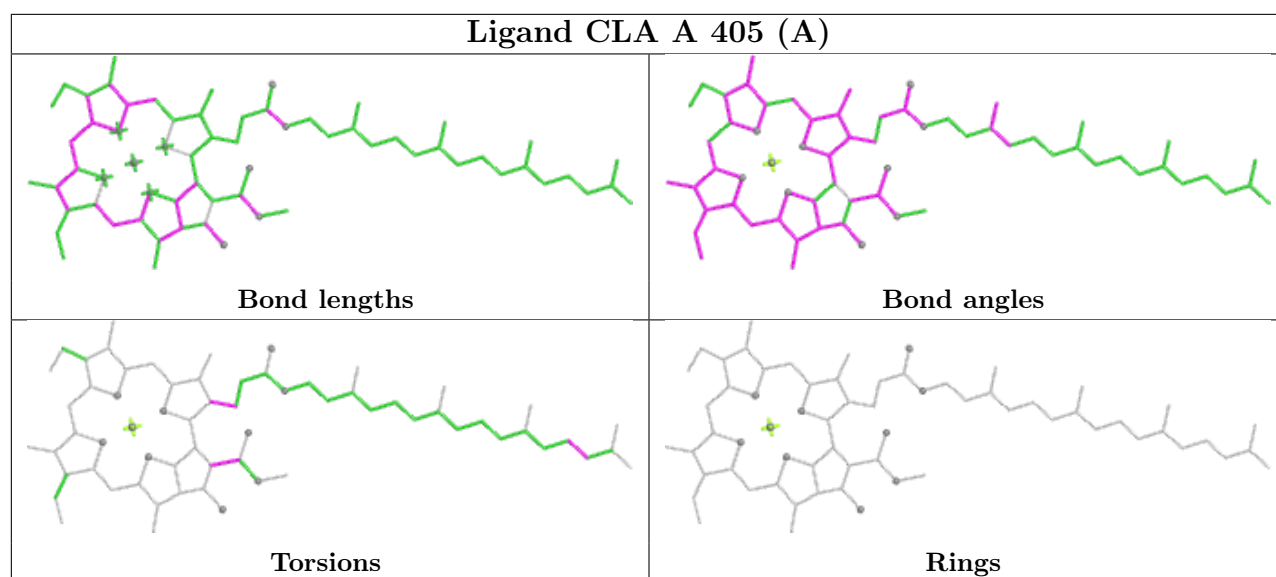


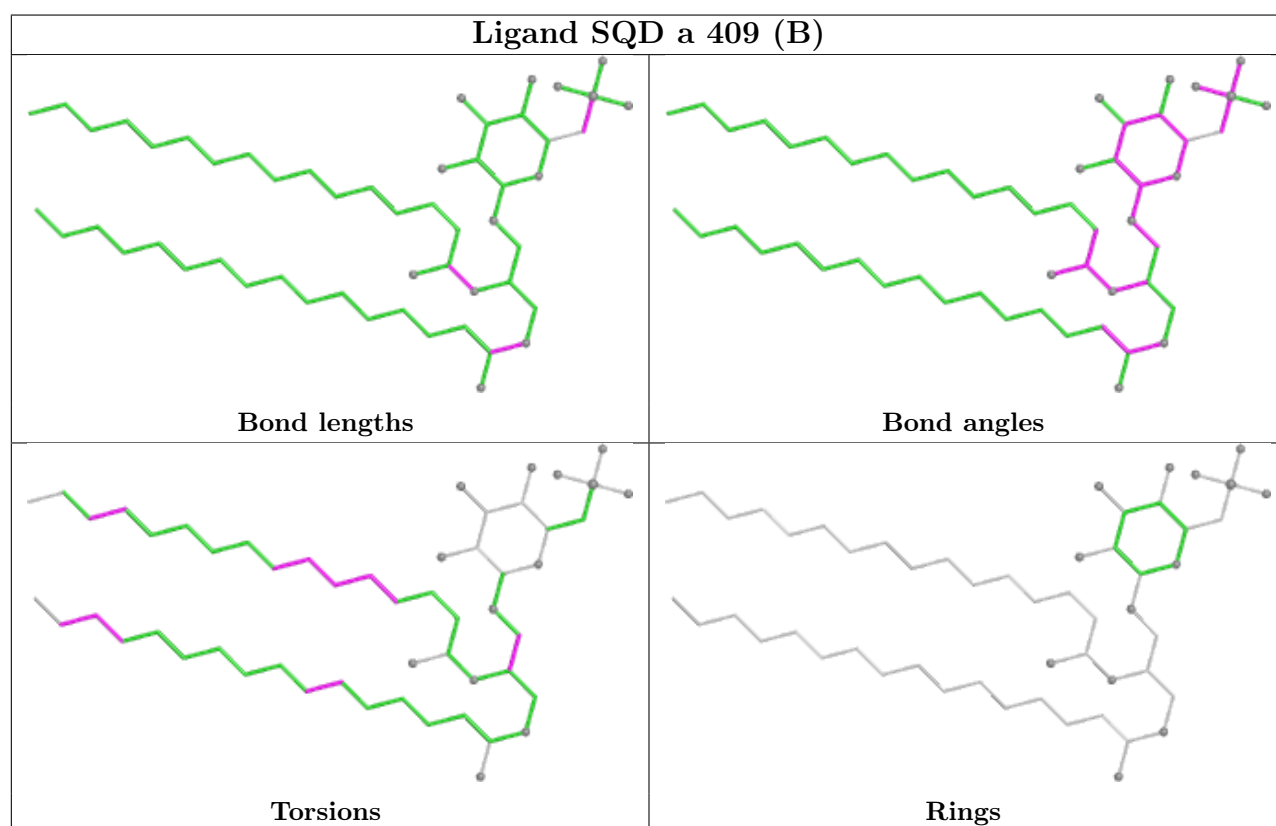
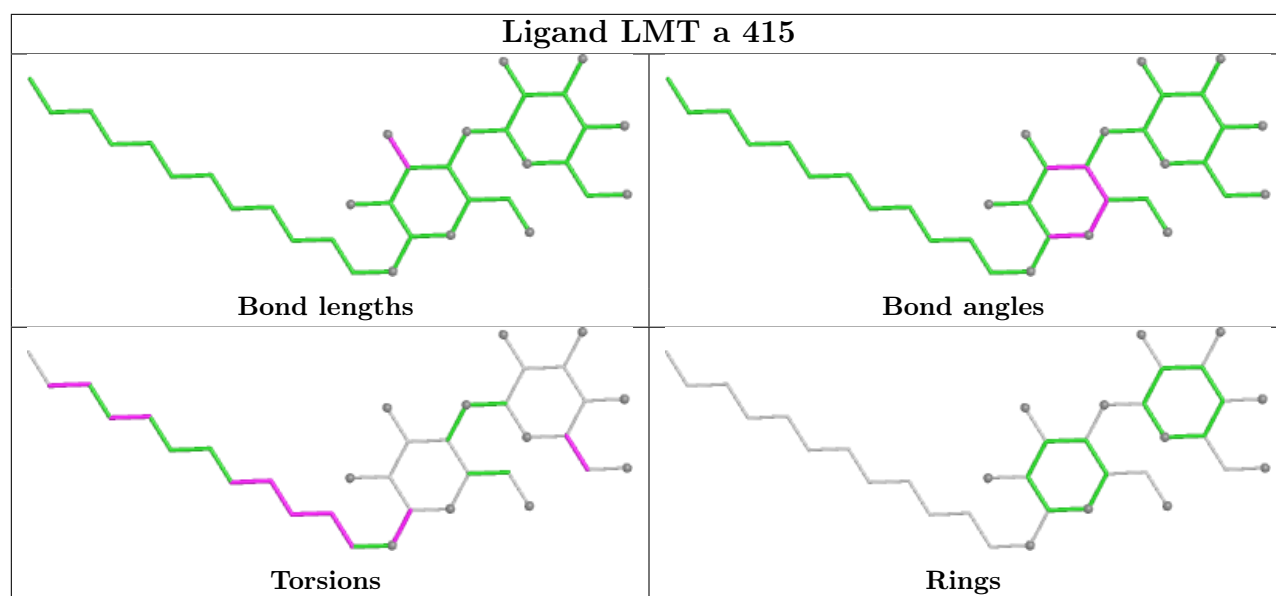


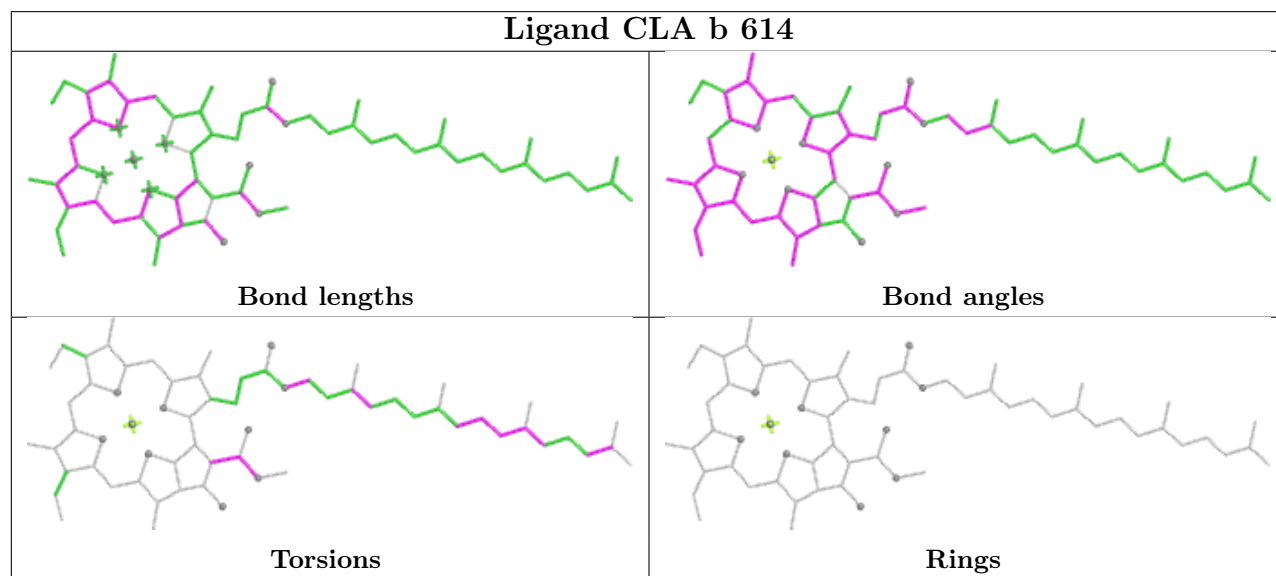
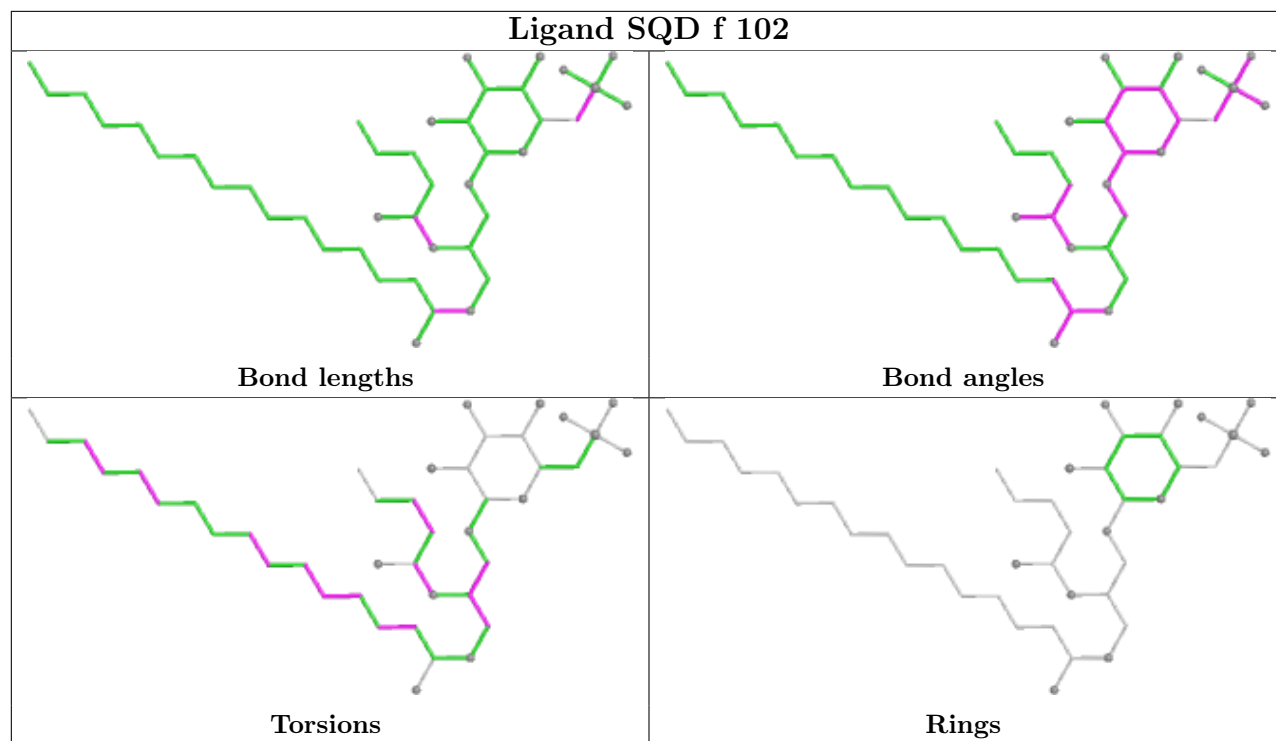


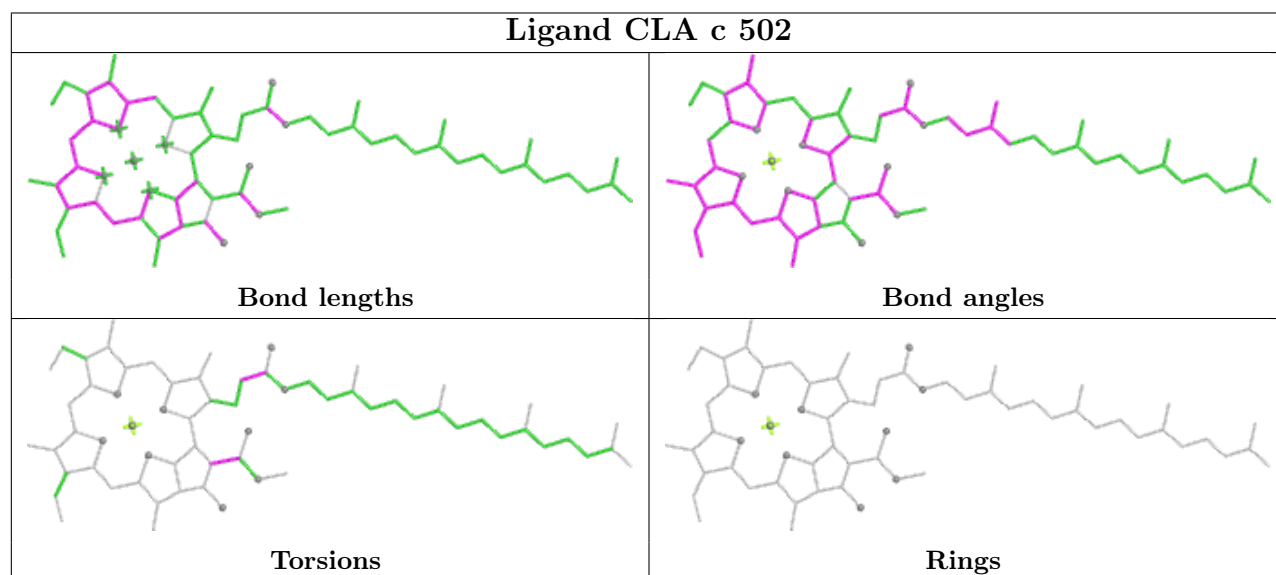
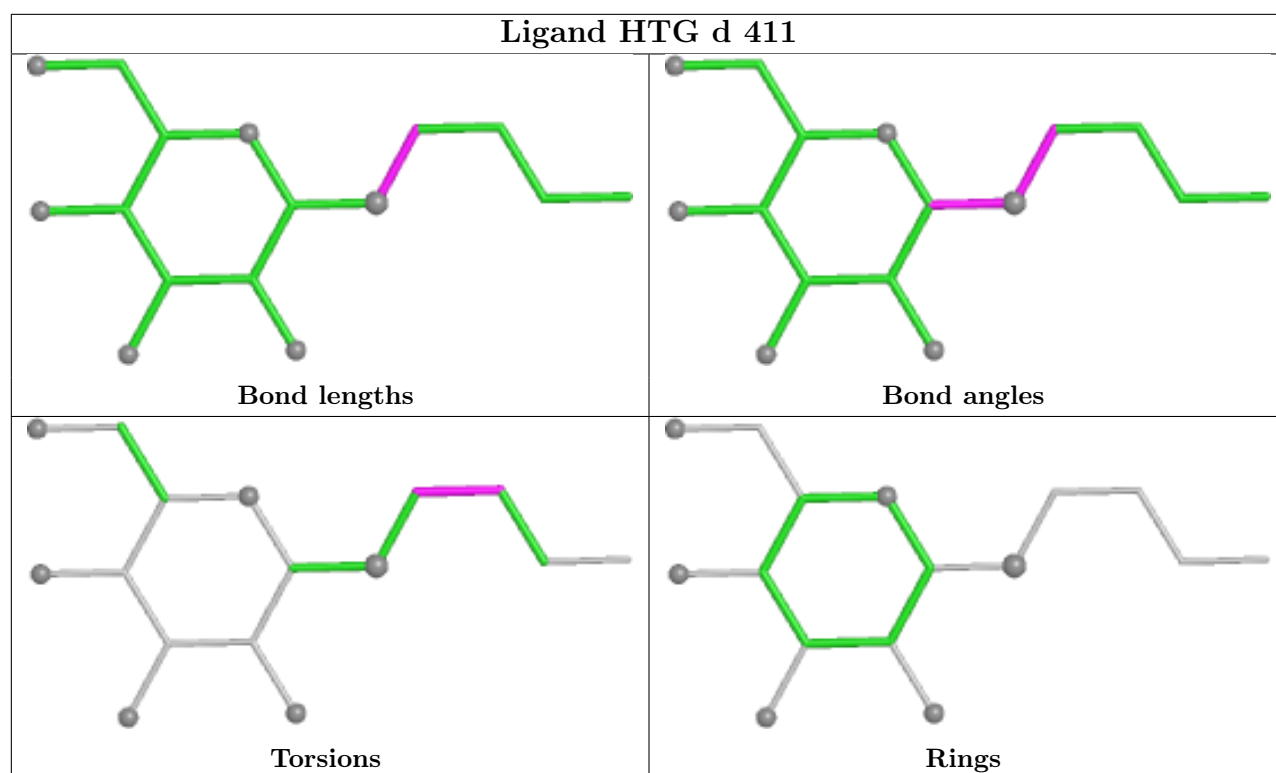




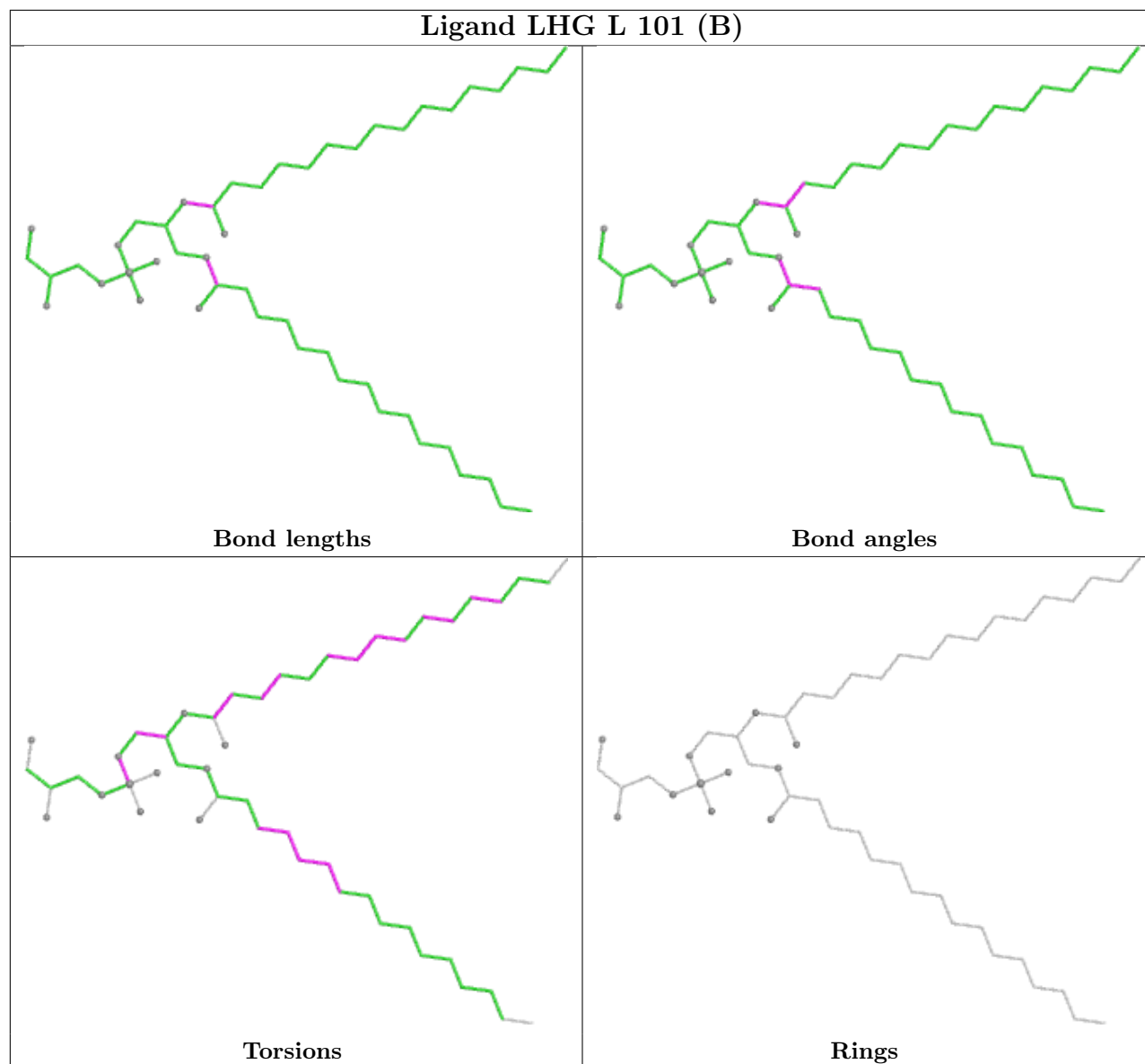




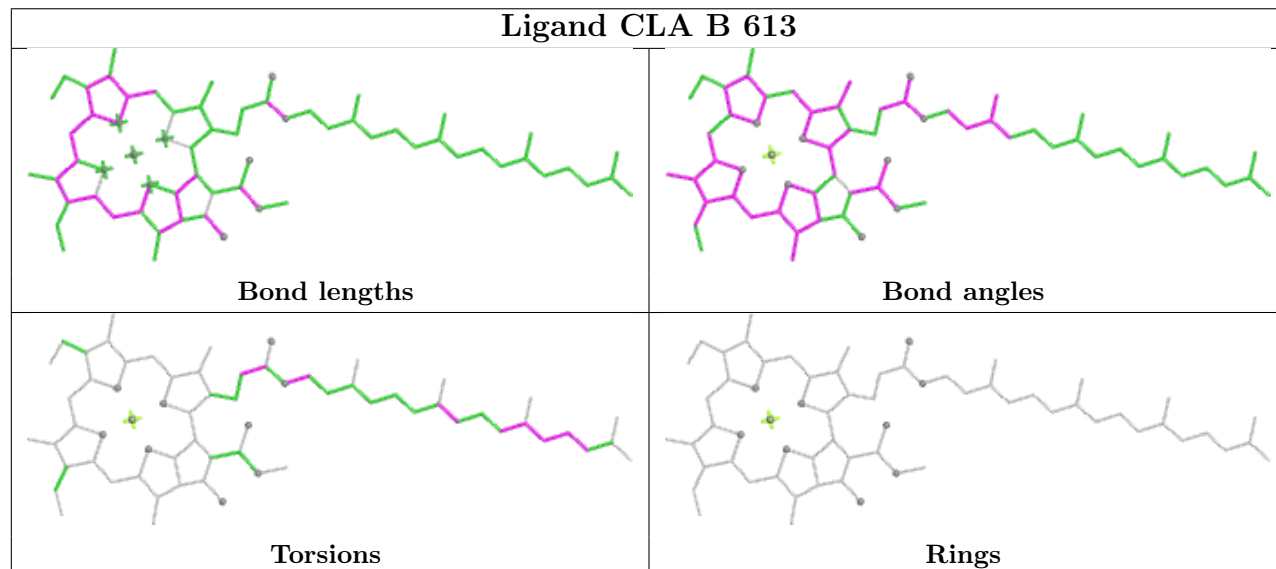


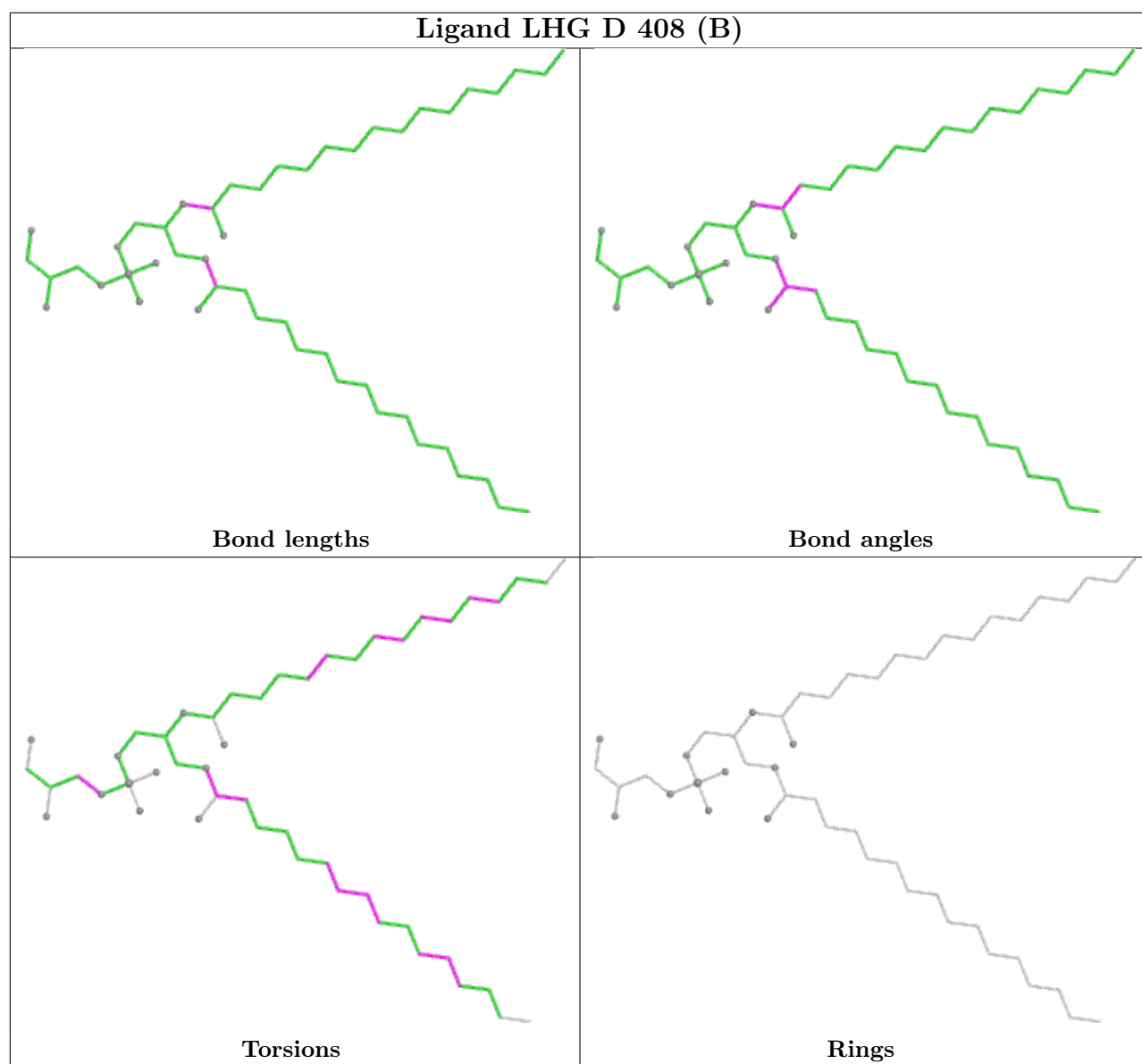


Ligand LHG L 101 (B)

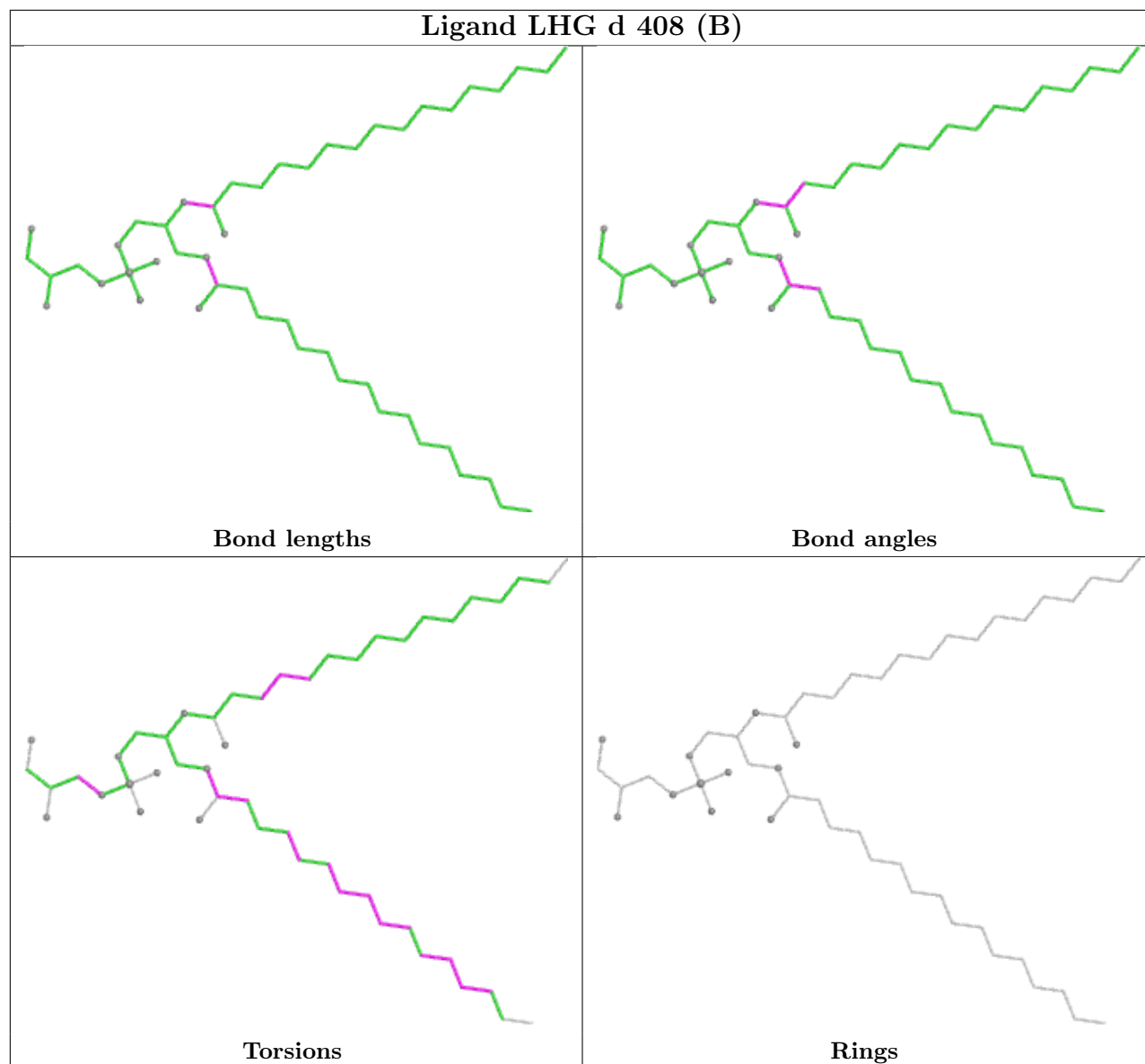


Ligand CLA B 613

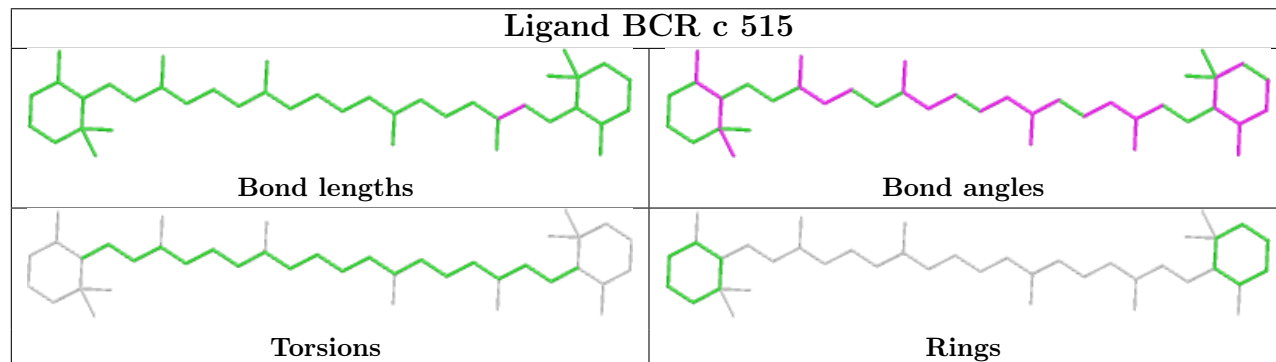




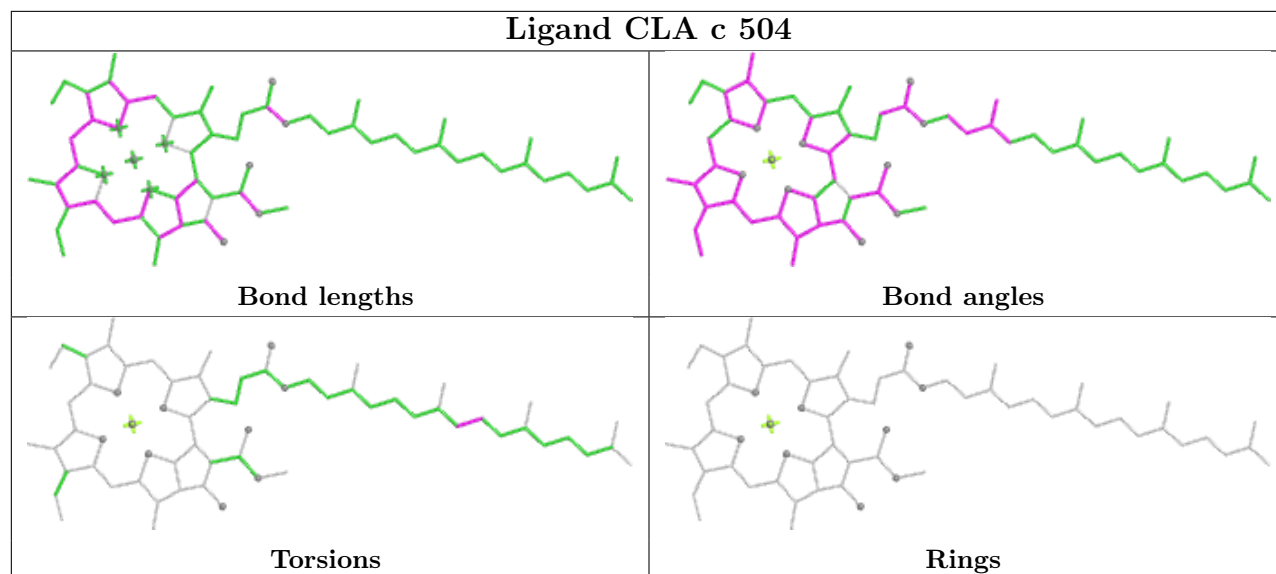
Ligand LHG d 408 (B)



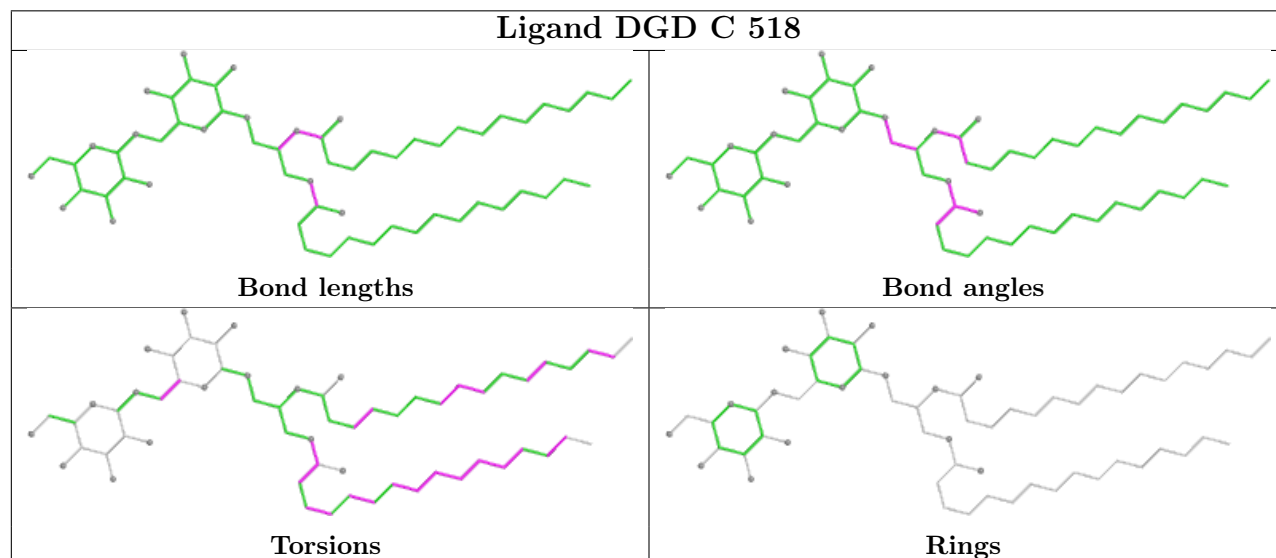
Ligand BCR c 515



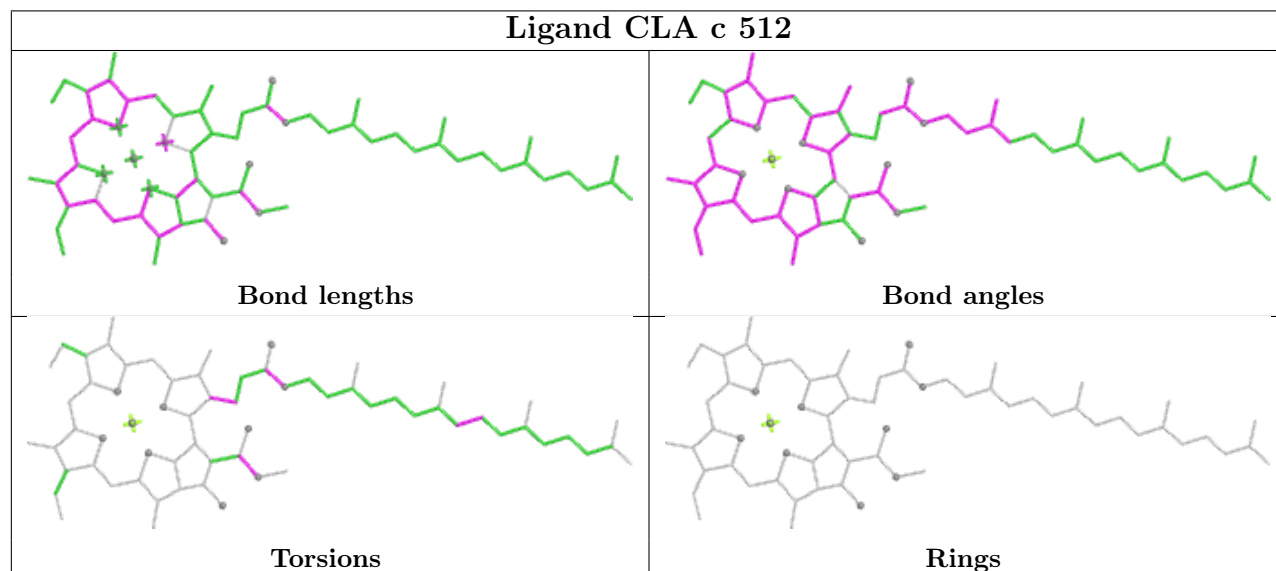
Ligand CLA c 504



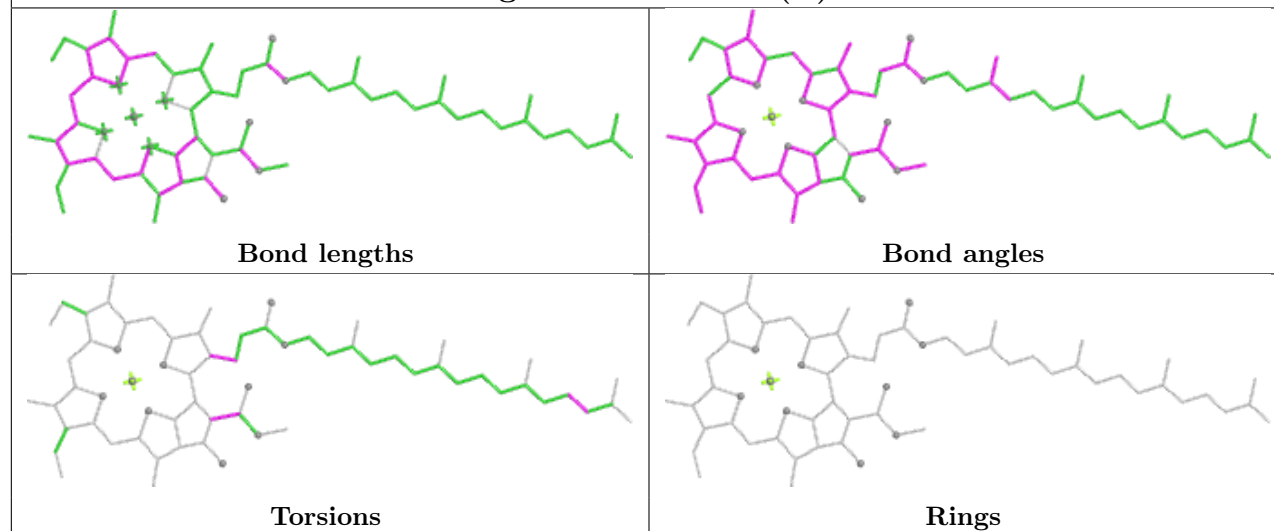
Ligand DGD C 518



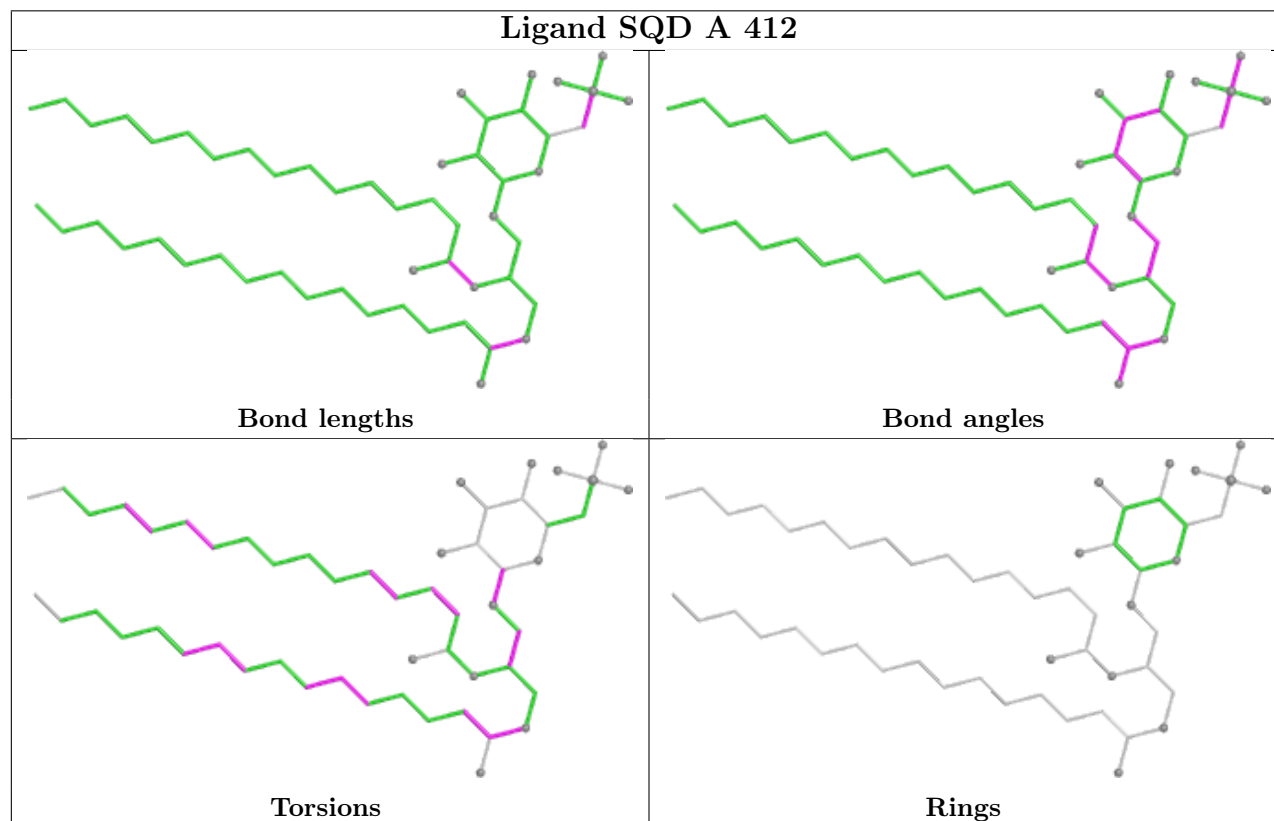
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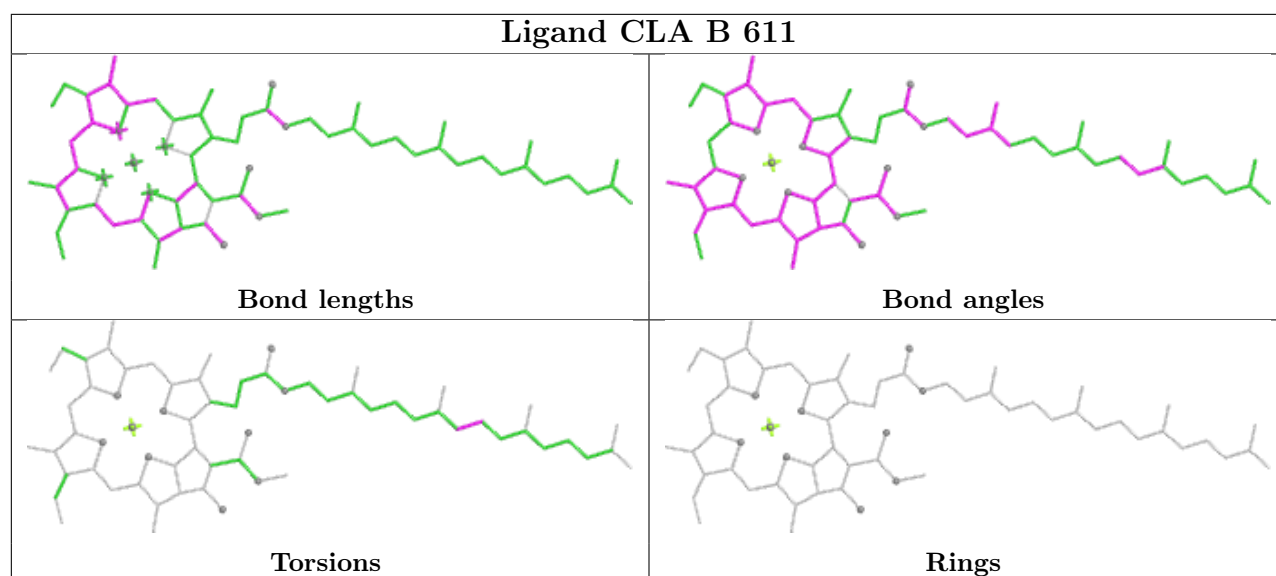
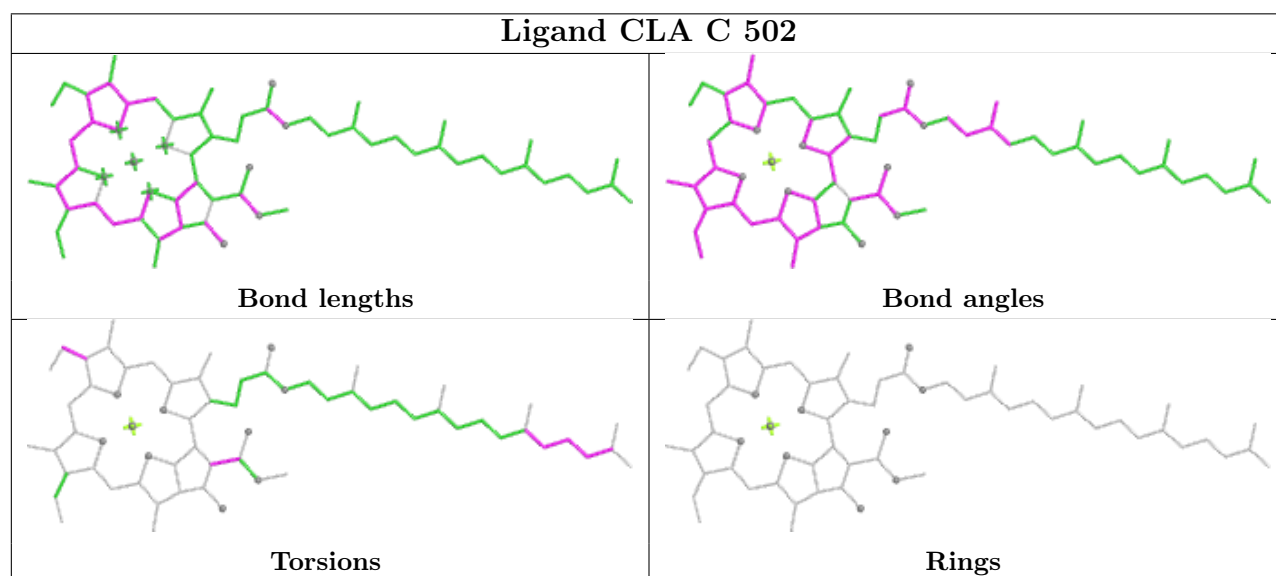
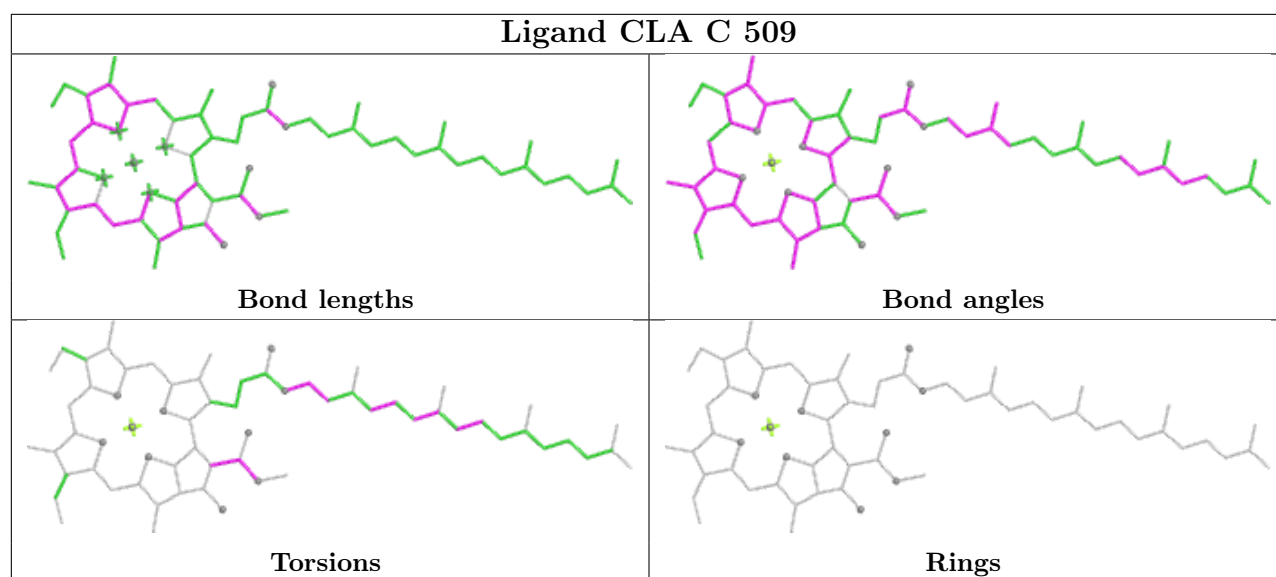


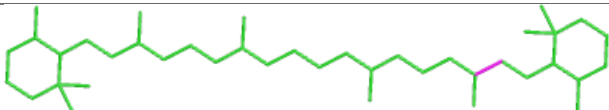
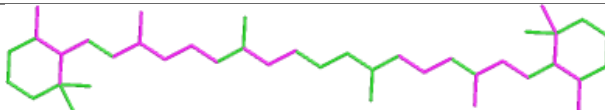
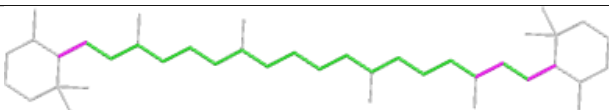
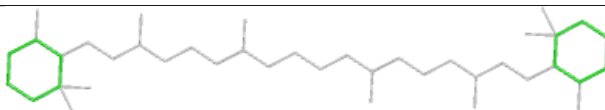
Ligand CLA A 405 (B)

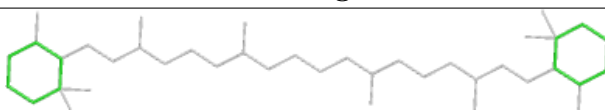


Ligand SQD A 412

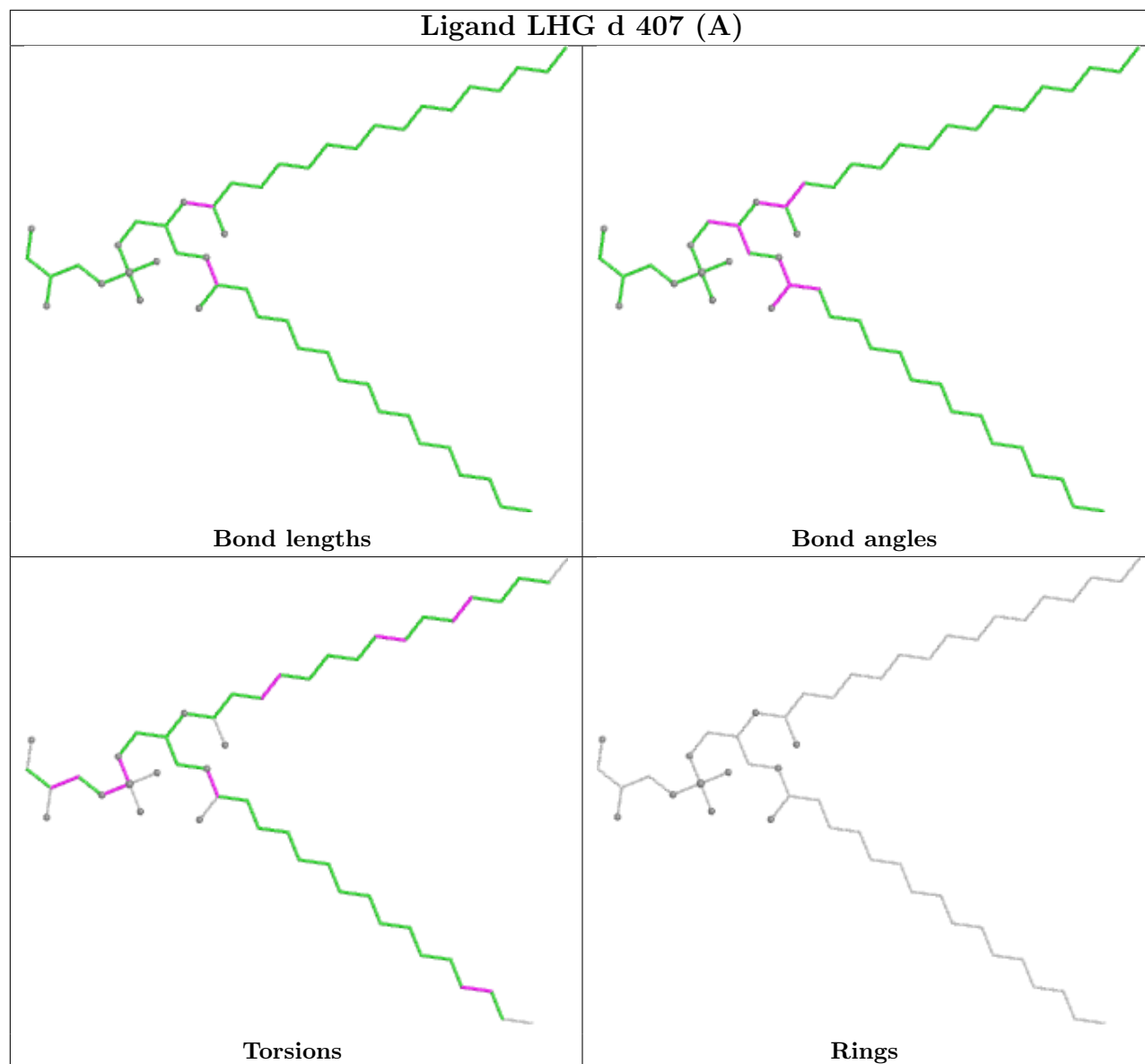




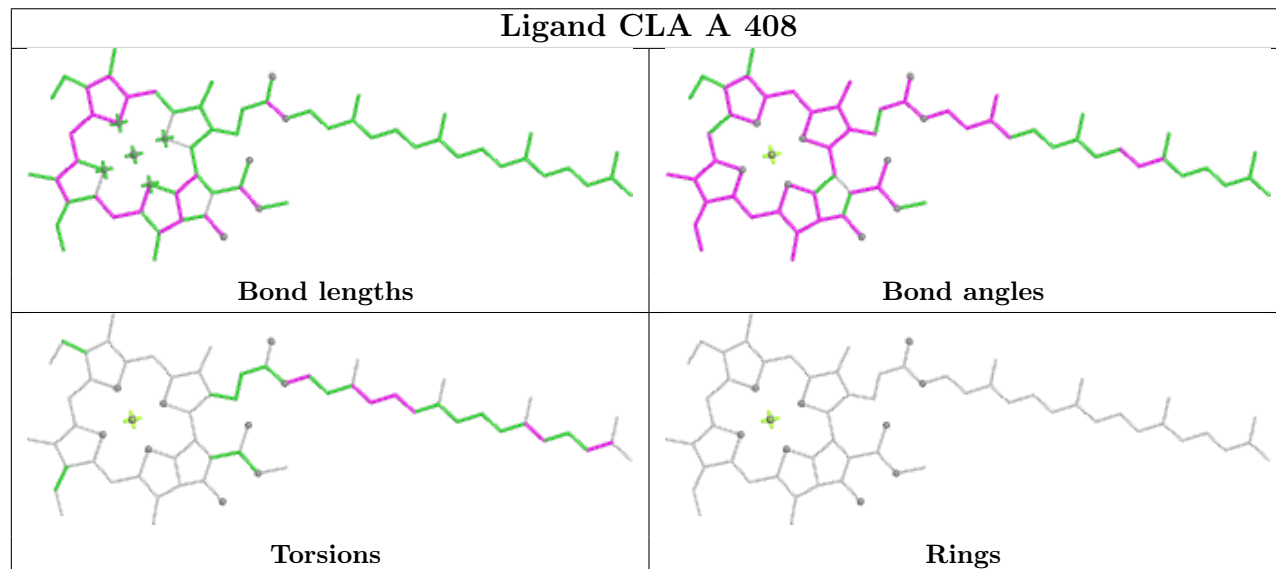
Ligand BCR y 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

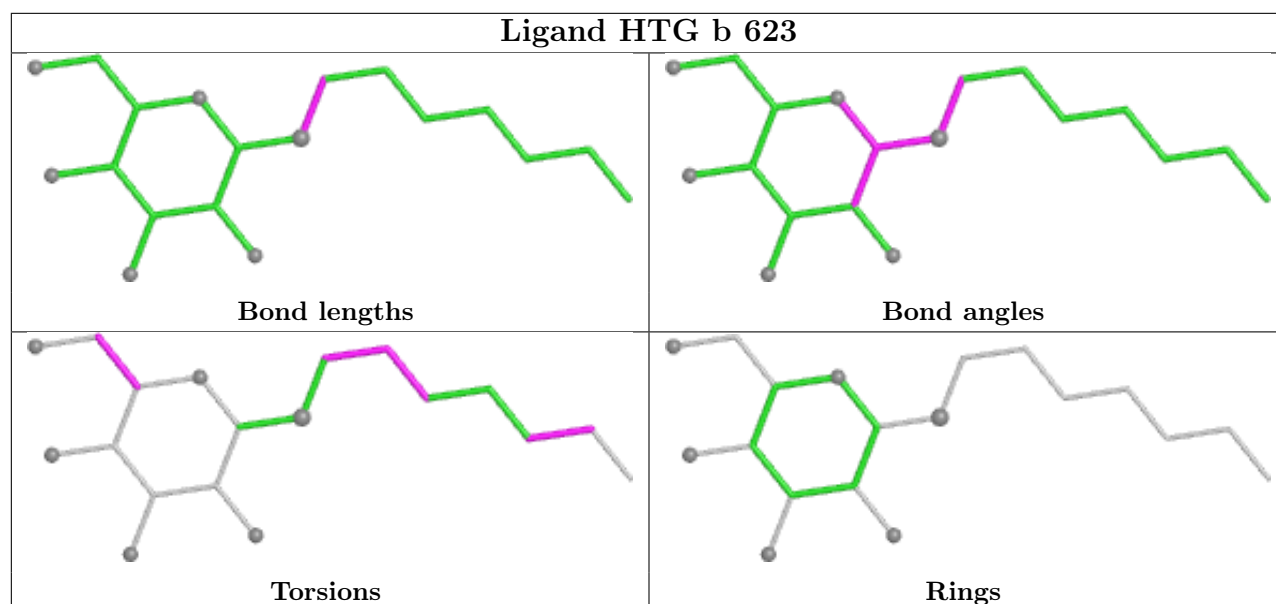
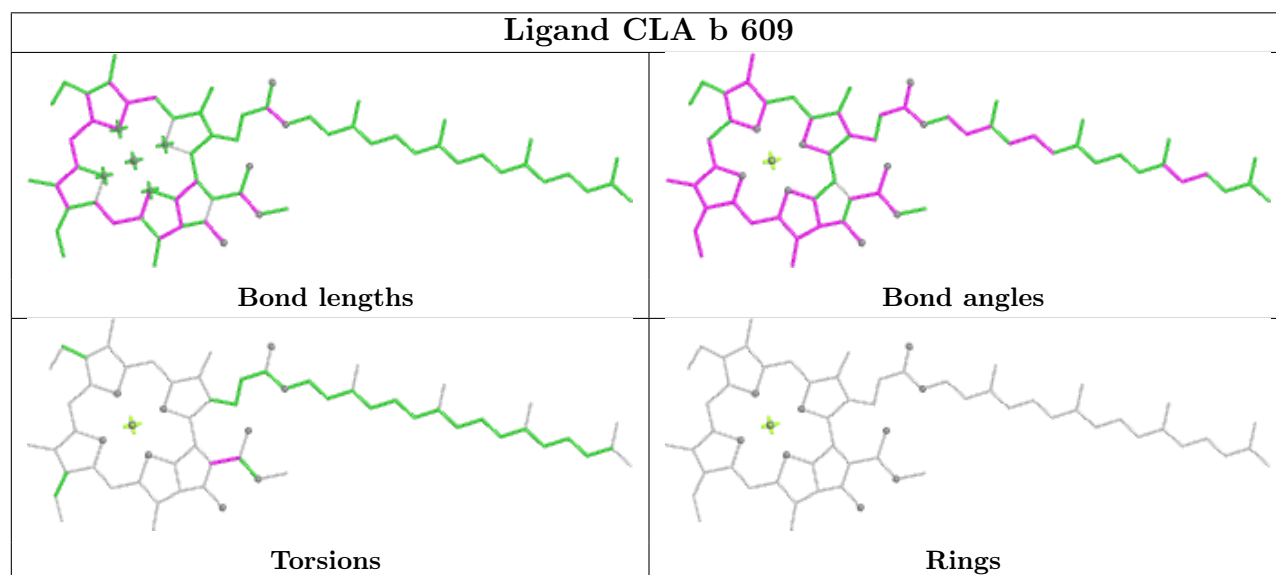
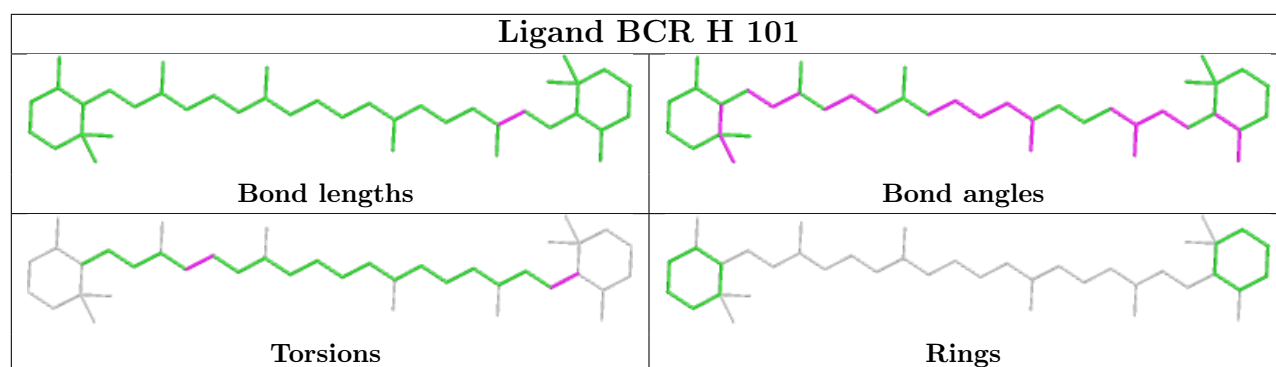
Ligand BCR h 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

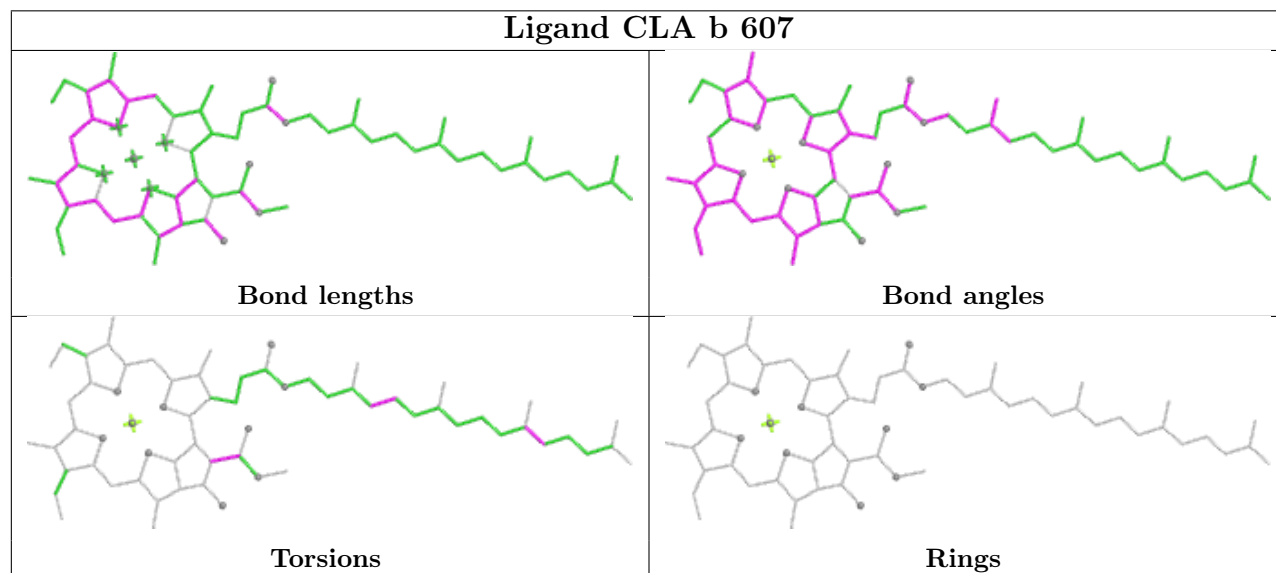
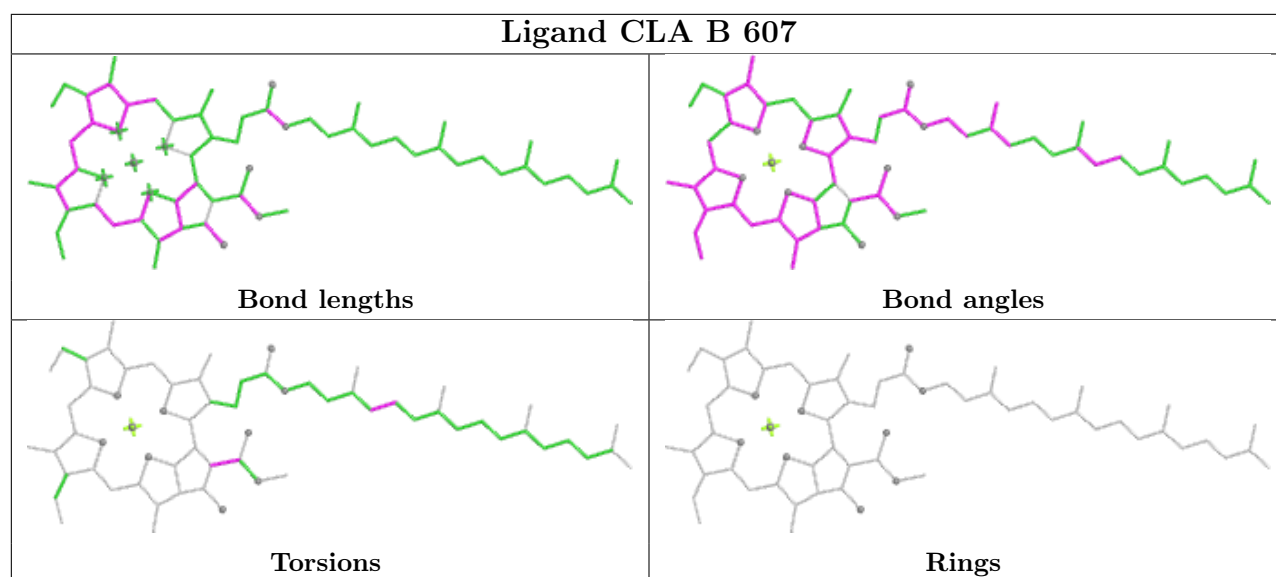
Ligand LHG d 407 (A)

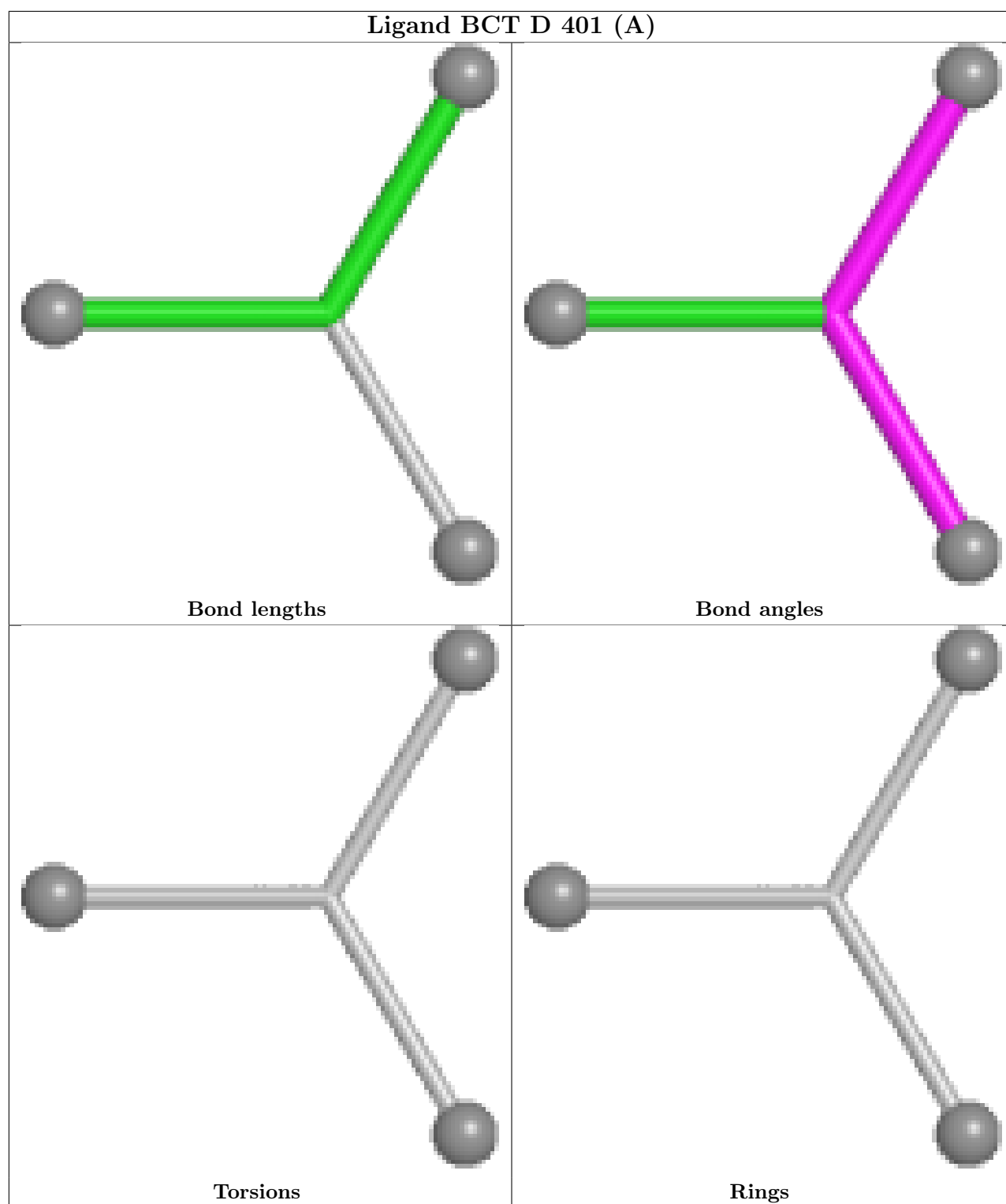


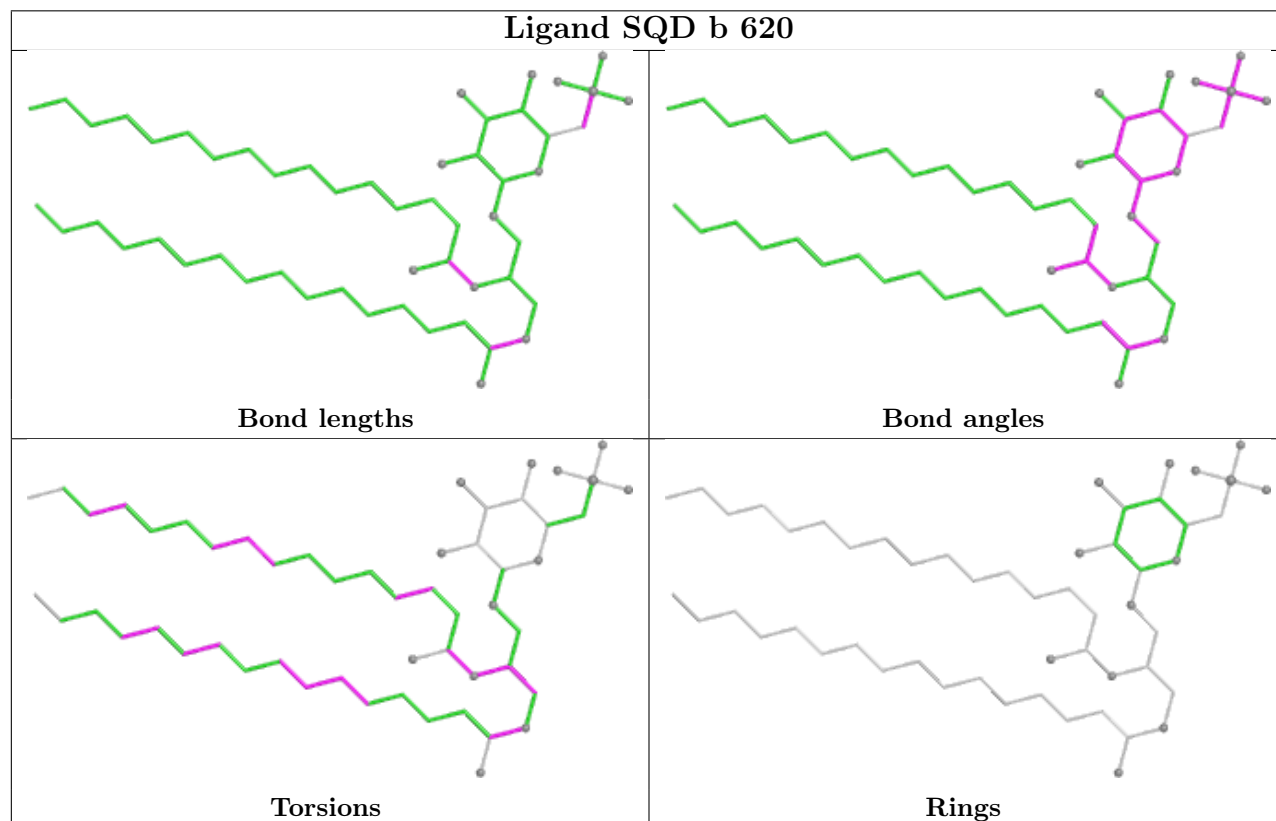
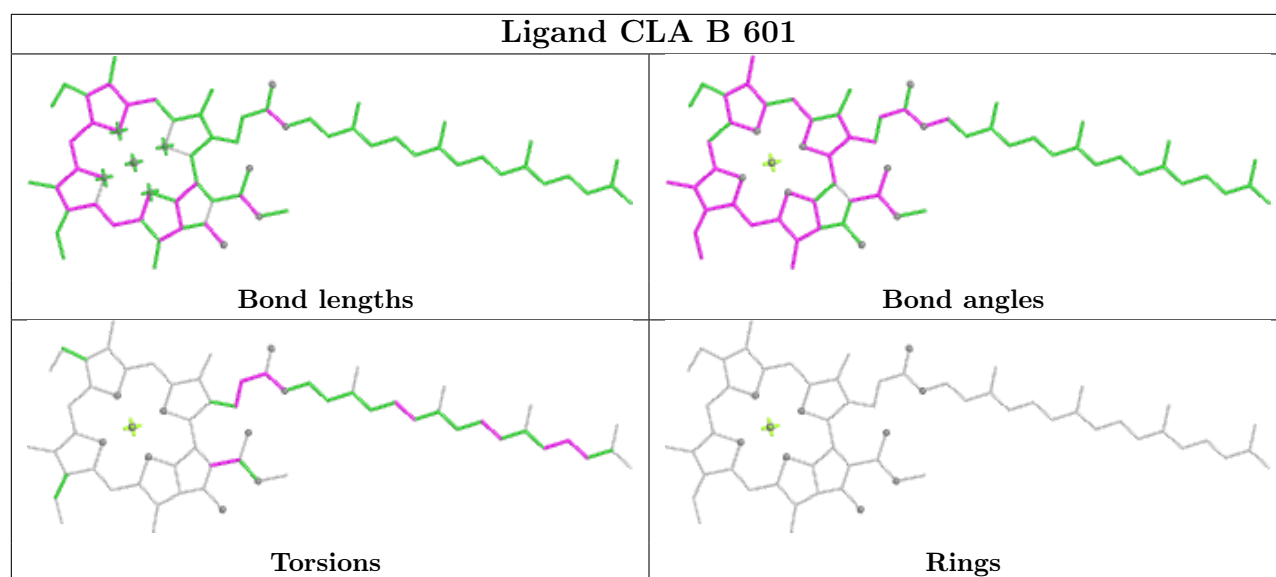
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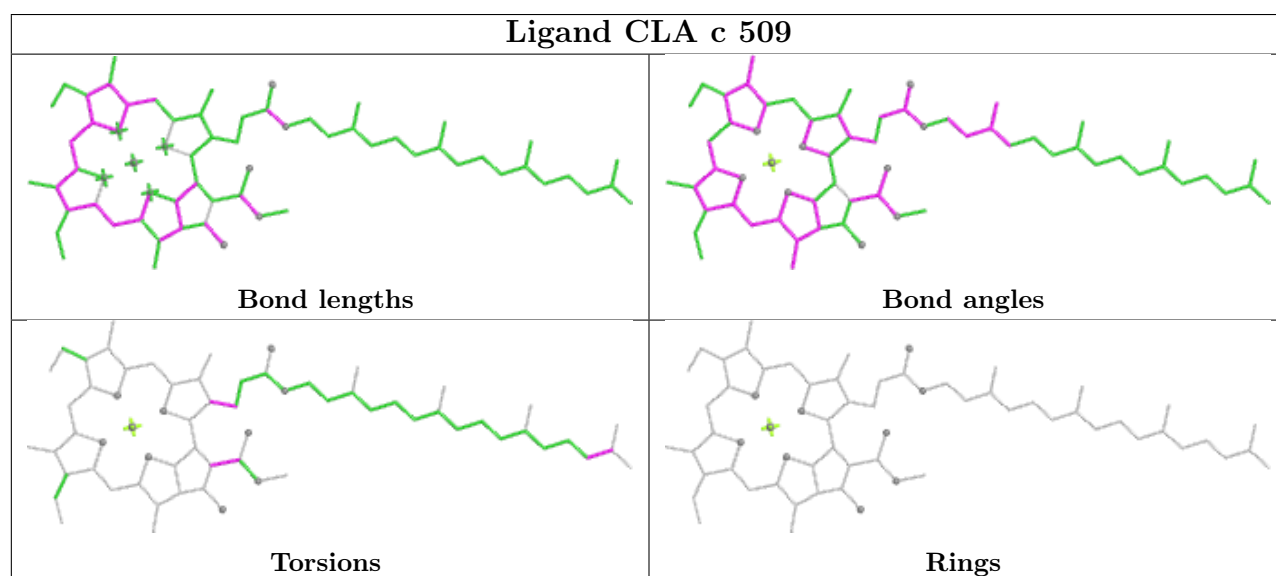
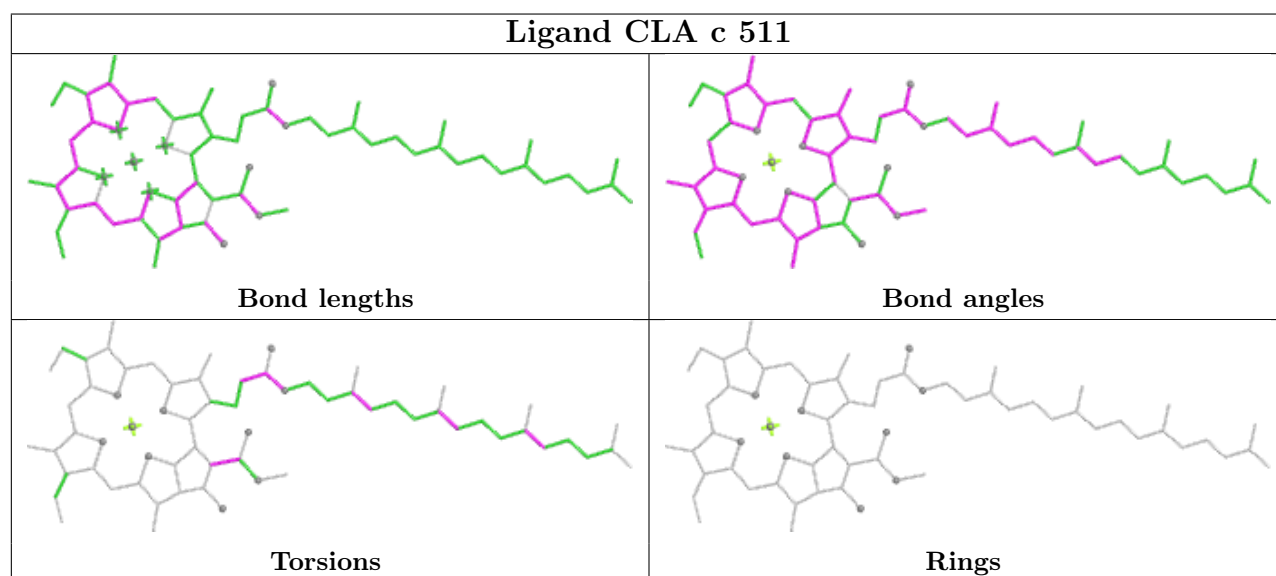
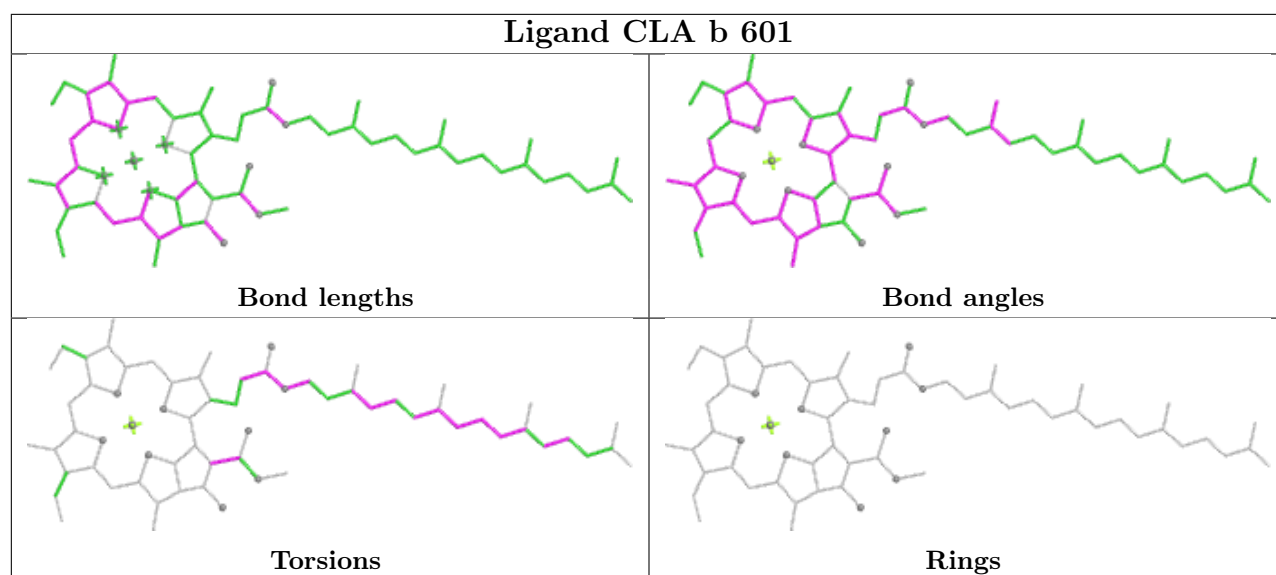


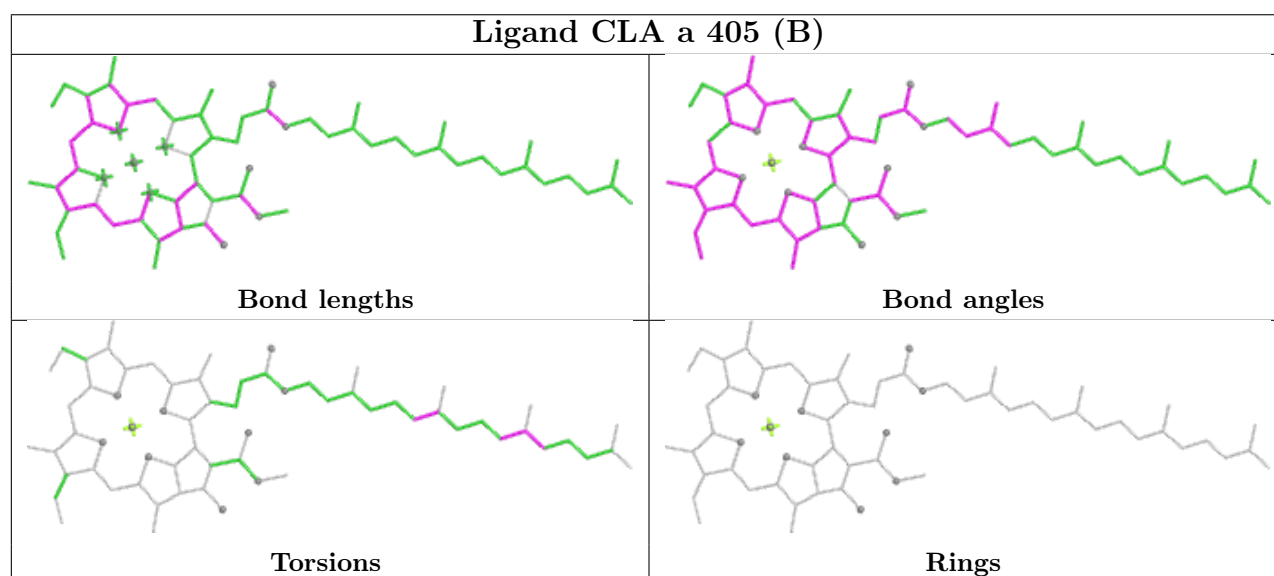
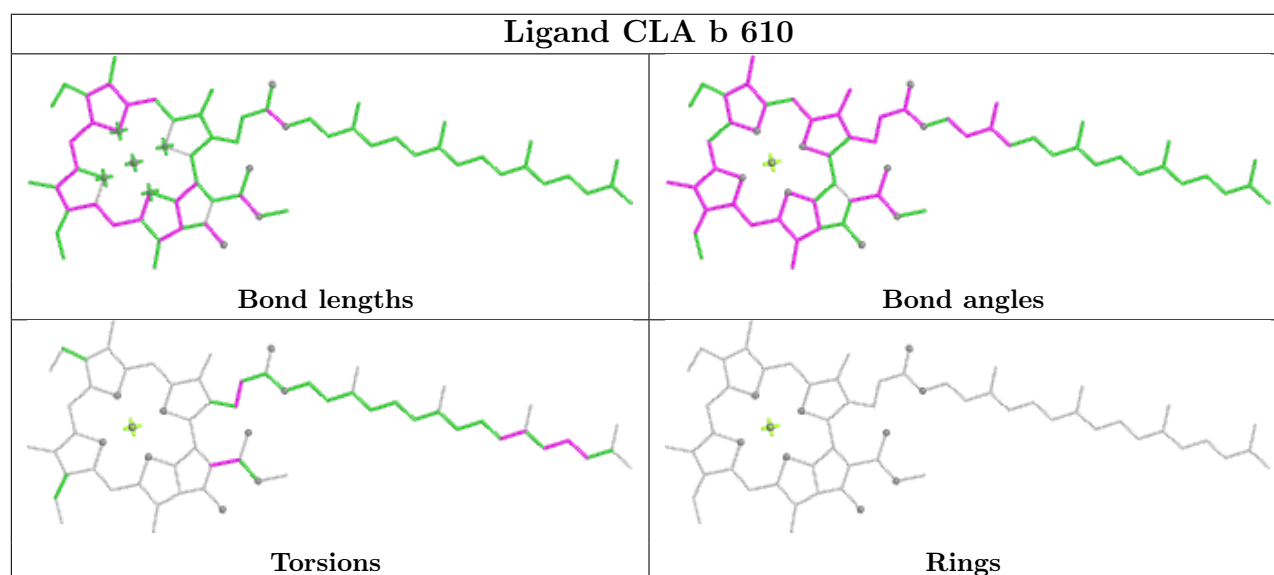
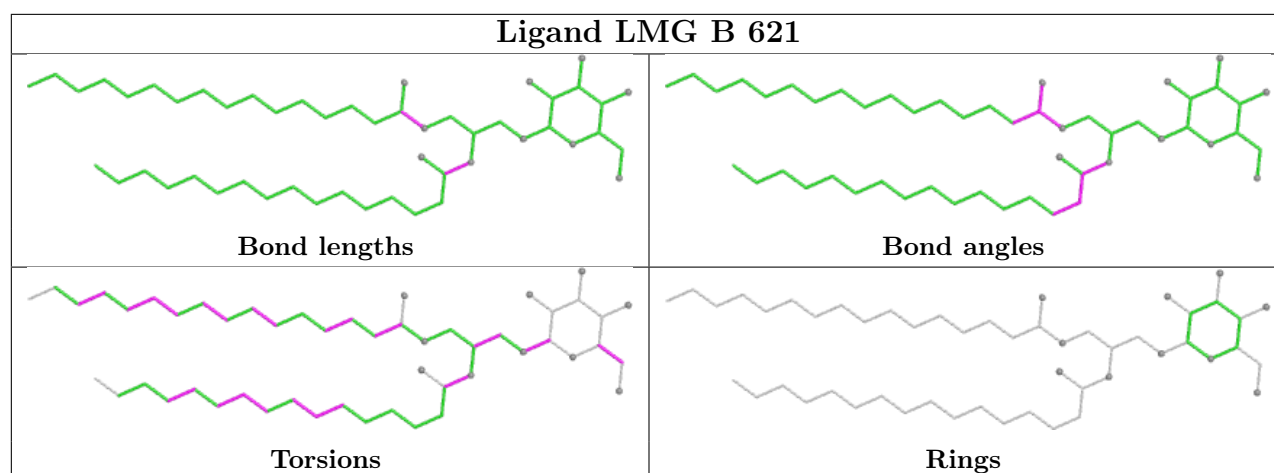




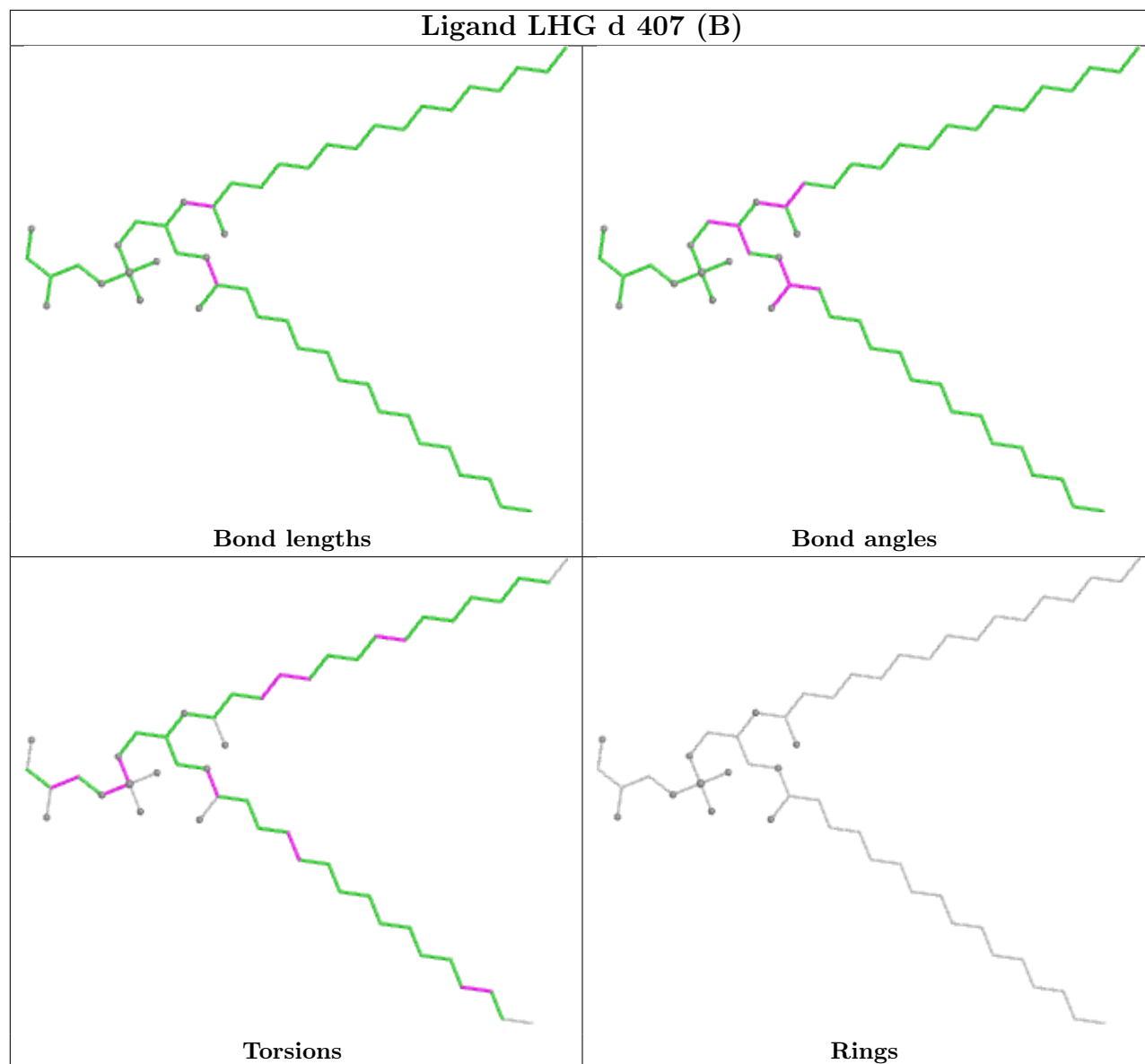




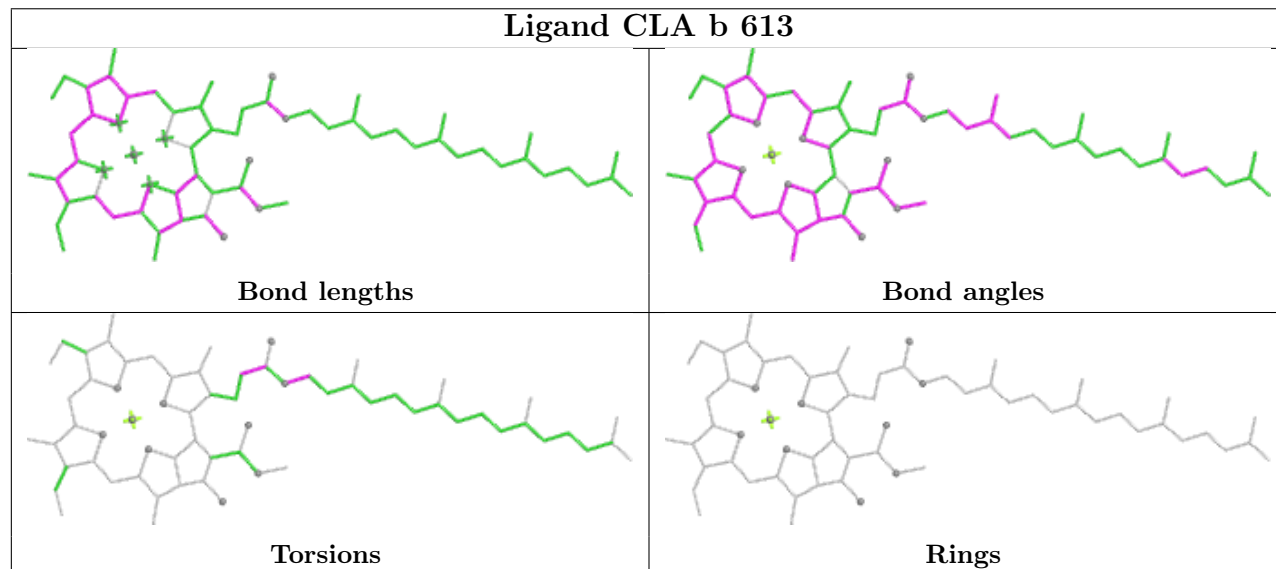




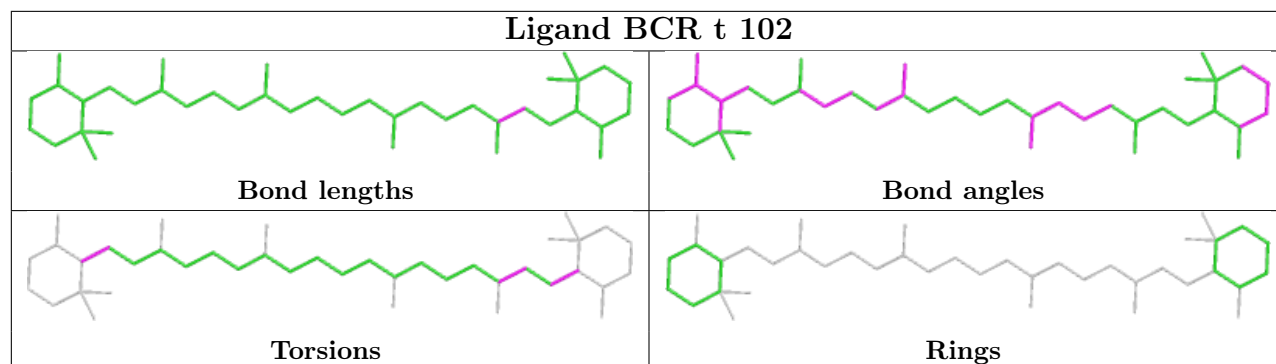
Ligand LHG d 407 (B)



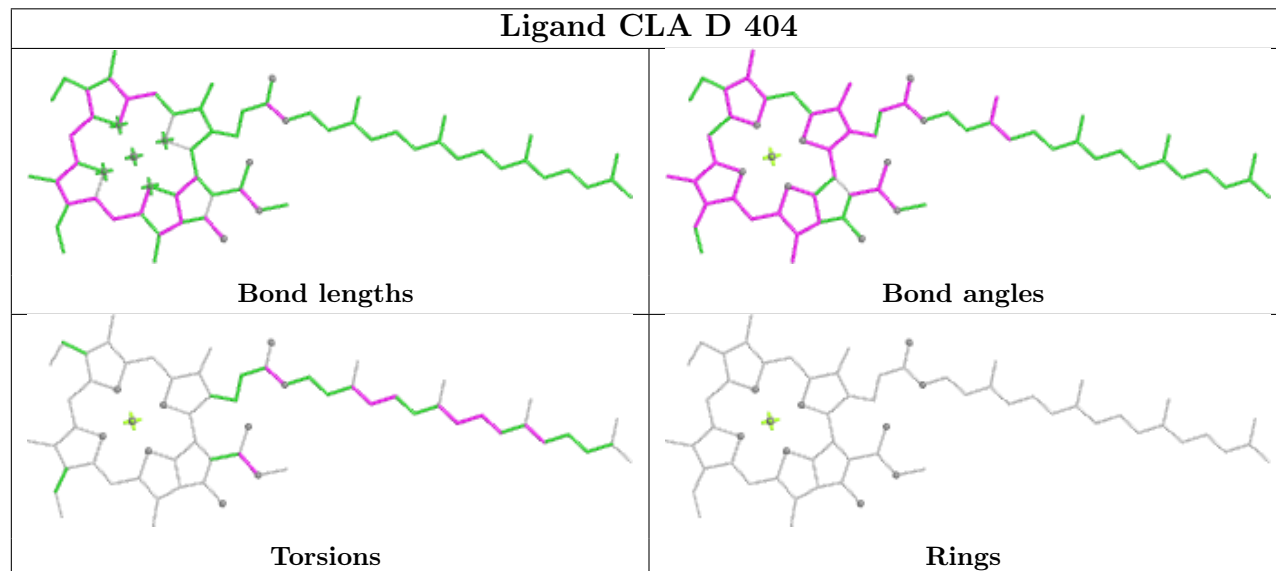
Ligand CLA b 613



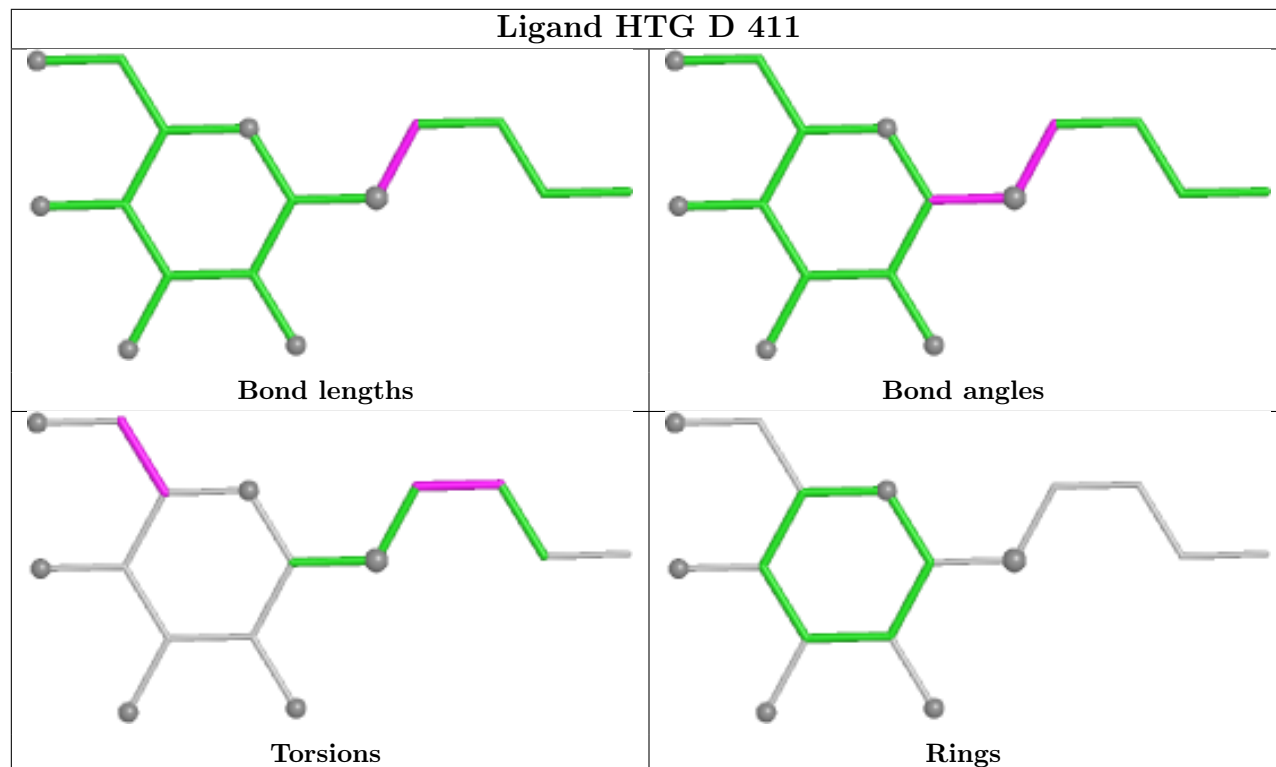
Ligand BCR t 102

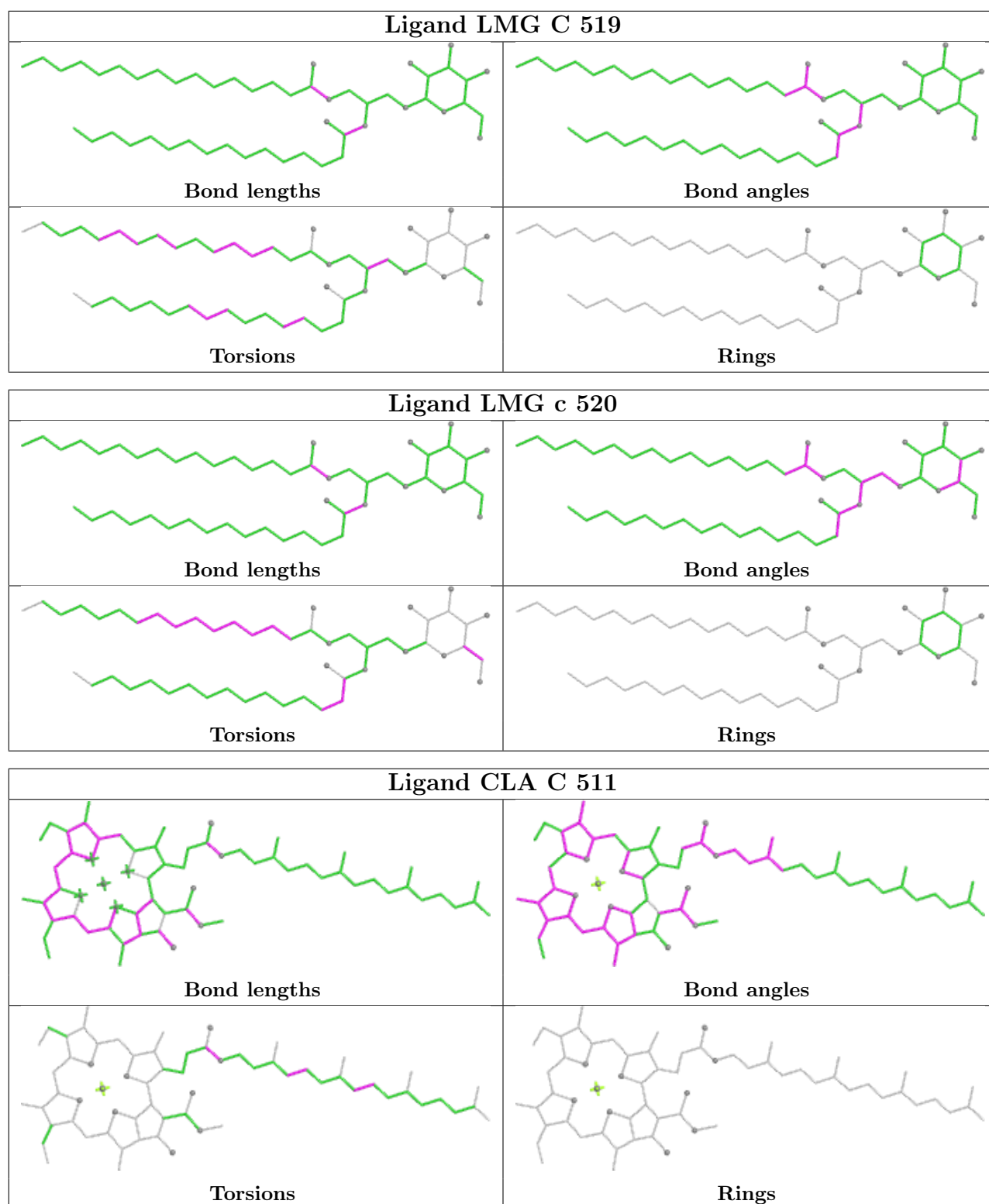


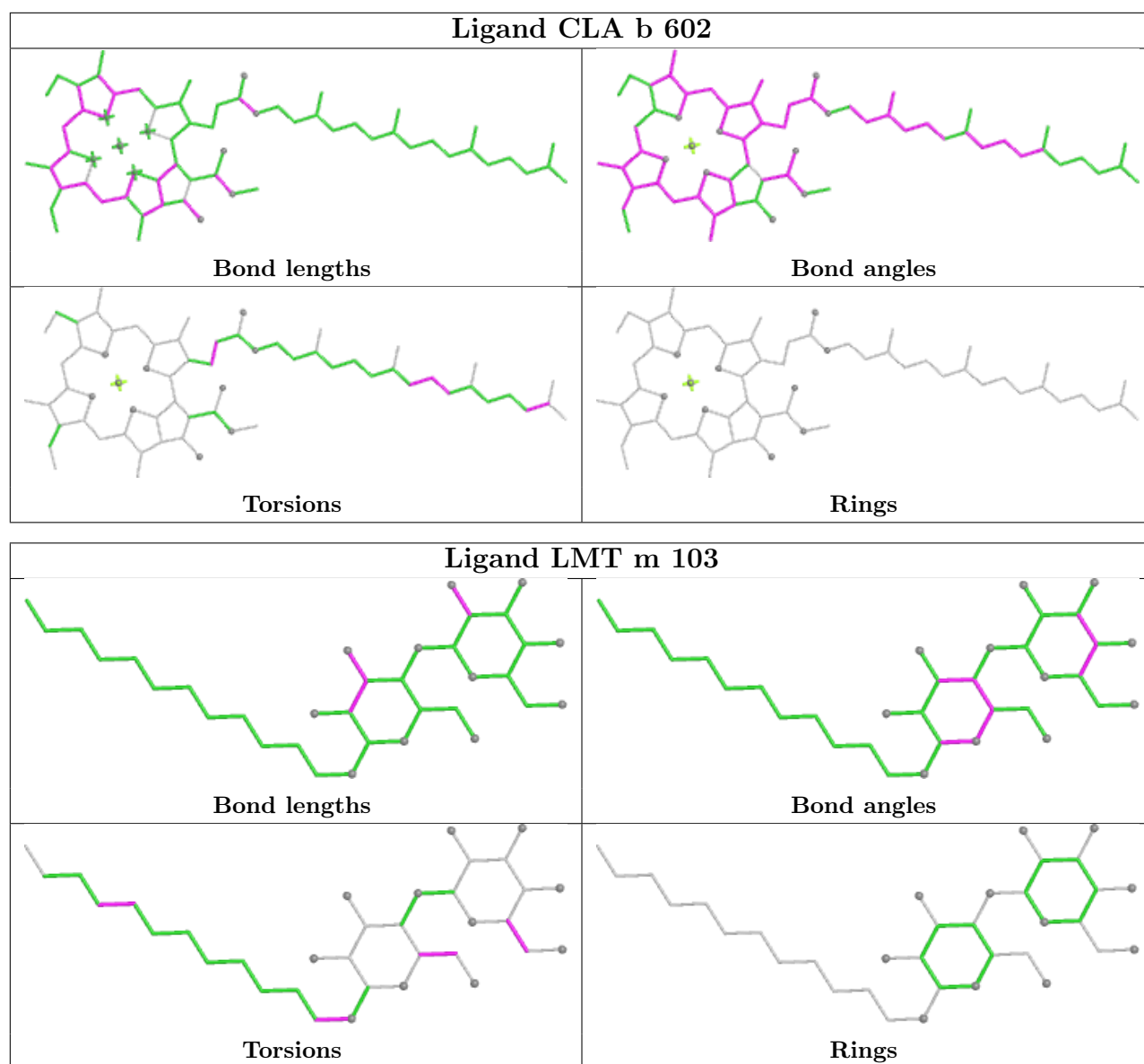
Ligand CLA D 404



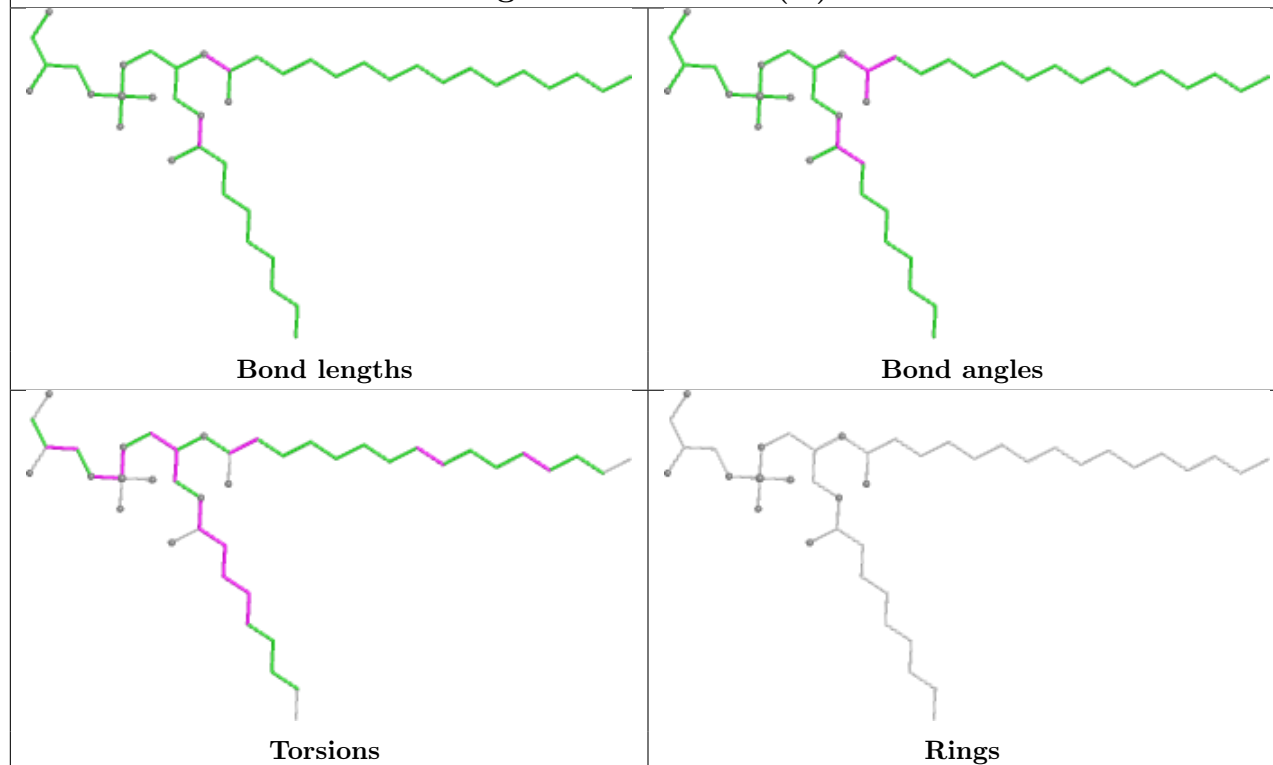
Ligand HTG D 411



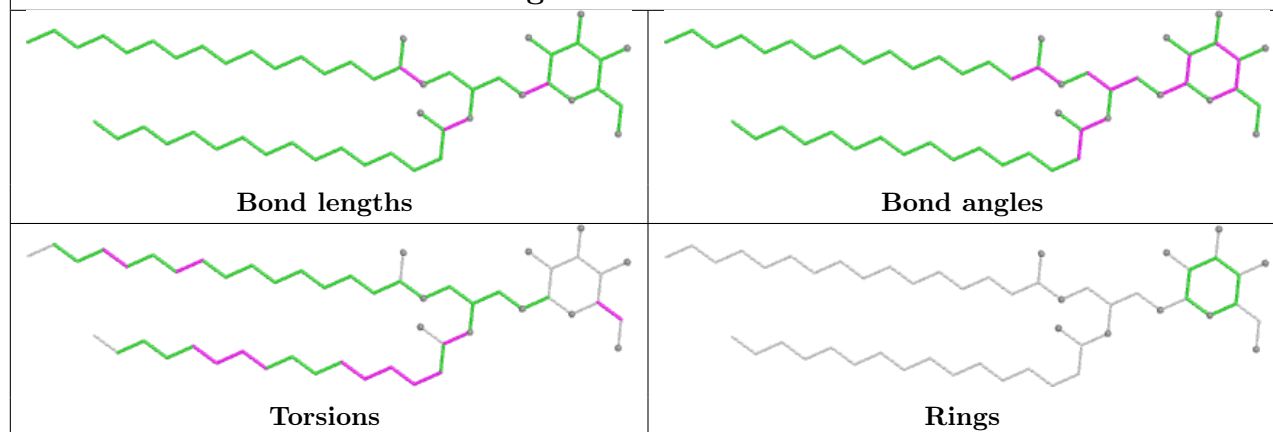


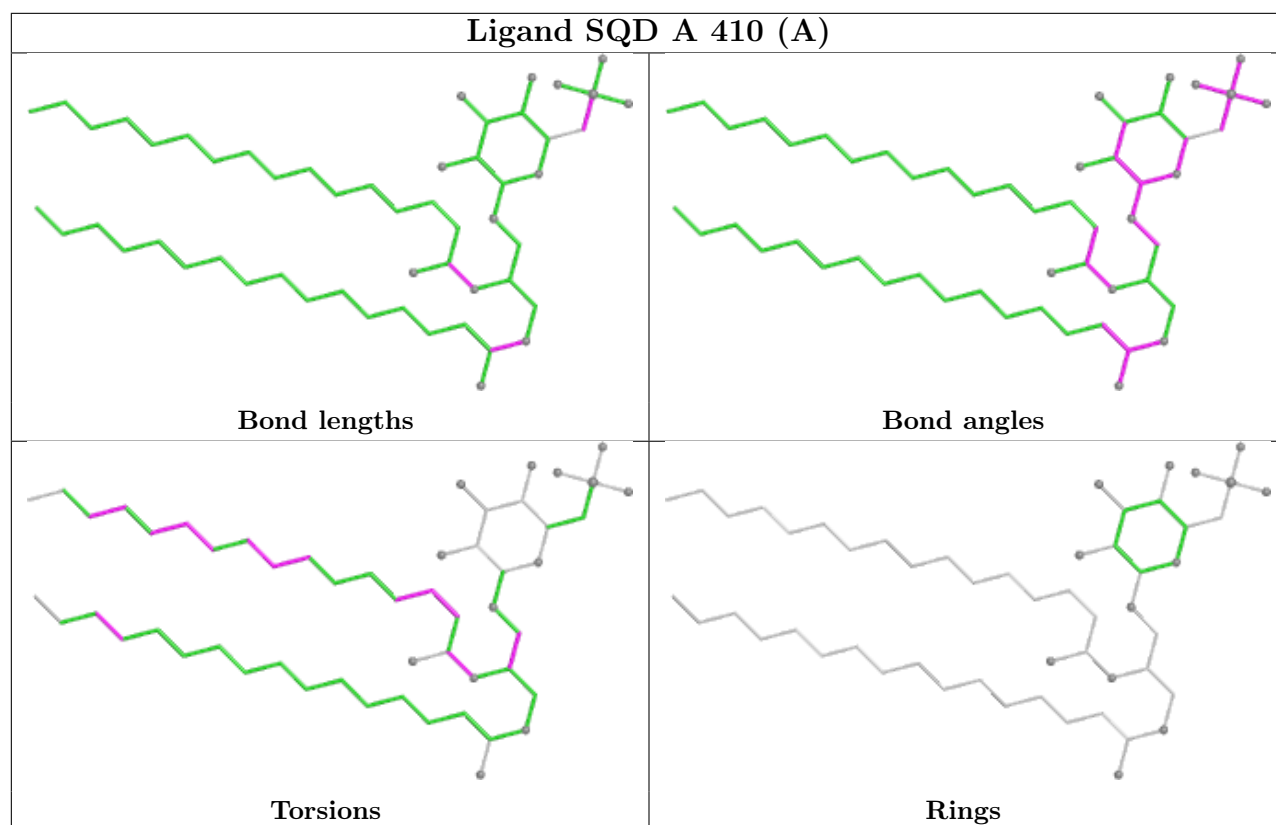
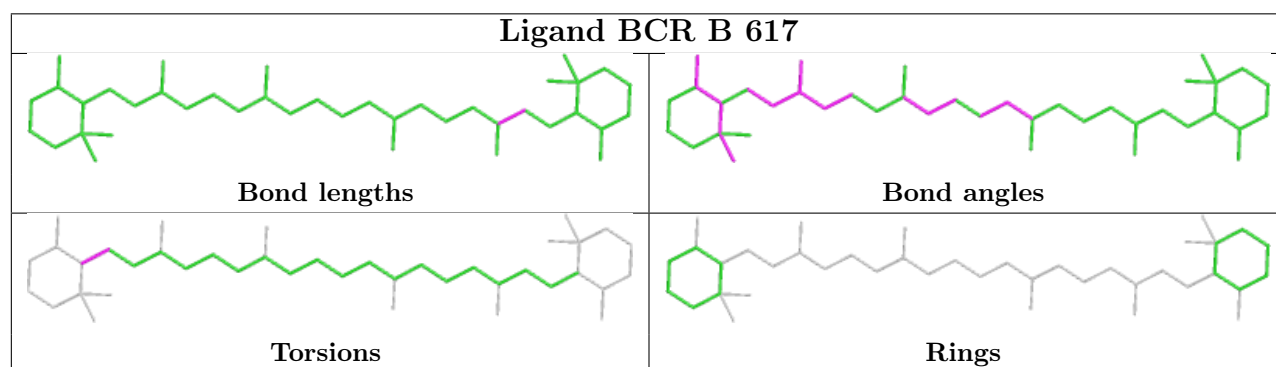
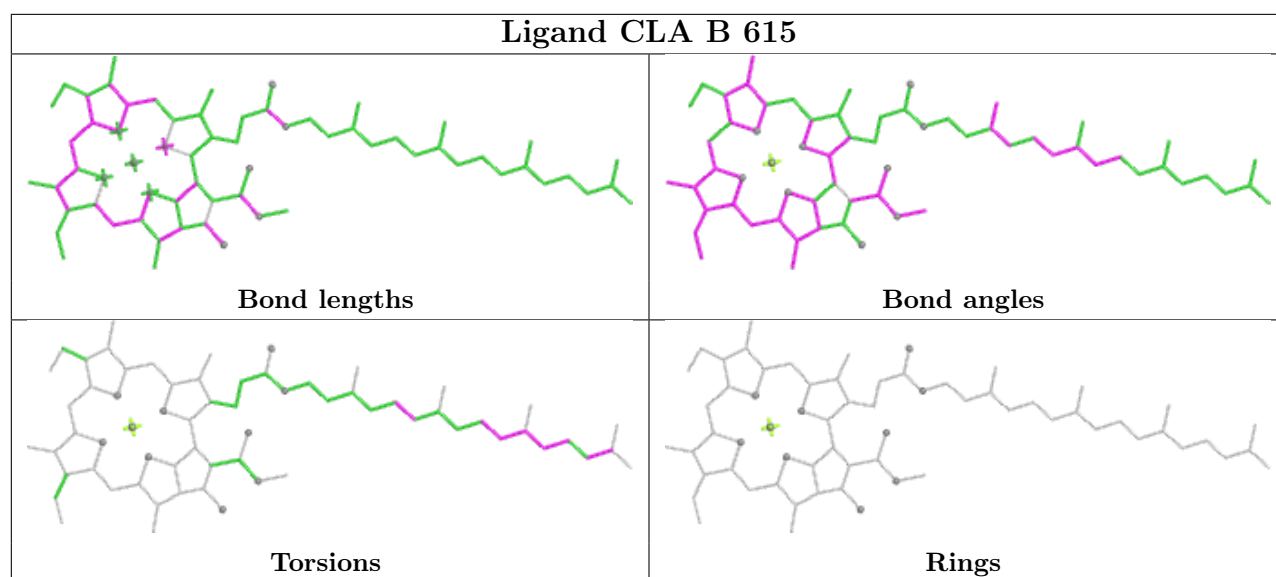


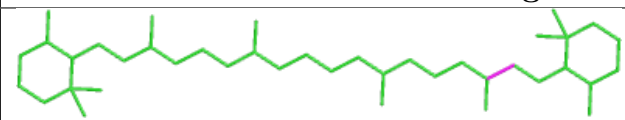
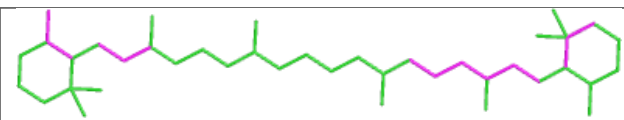
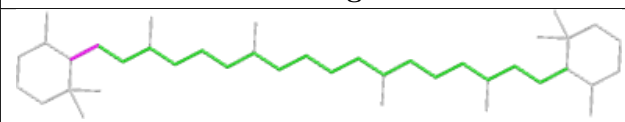
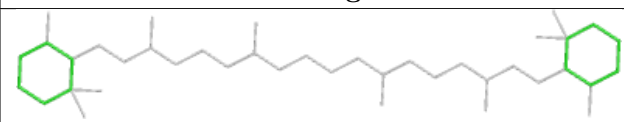
Ligand LHG E 101 (A)

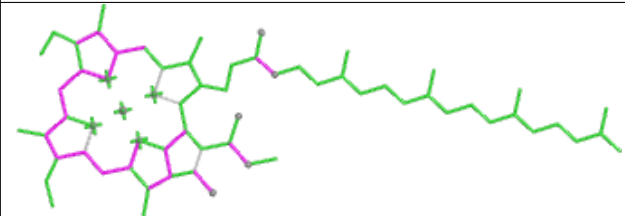
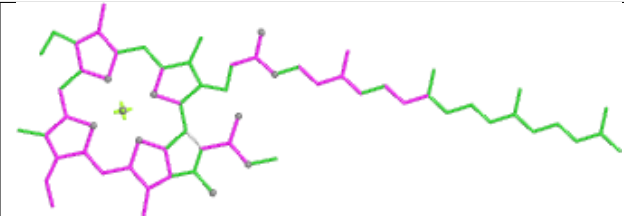
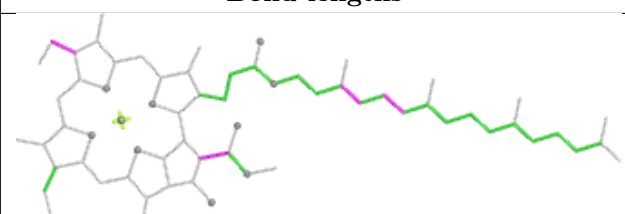
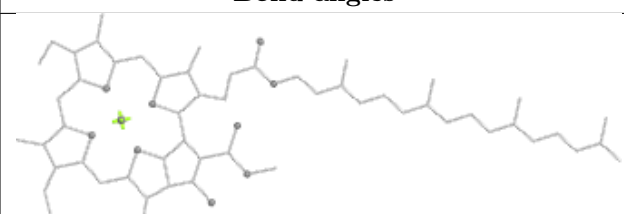


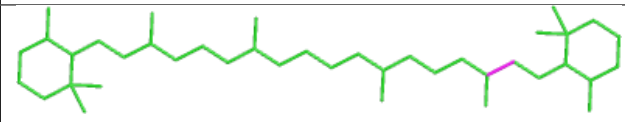
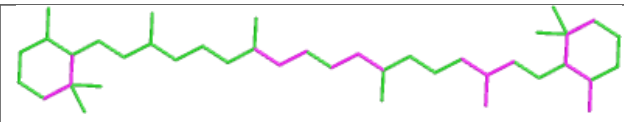
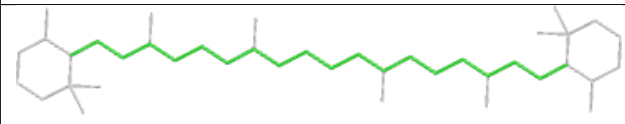
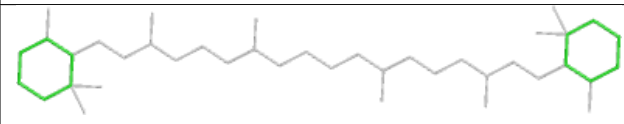
Ligand LMG C 520

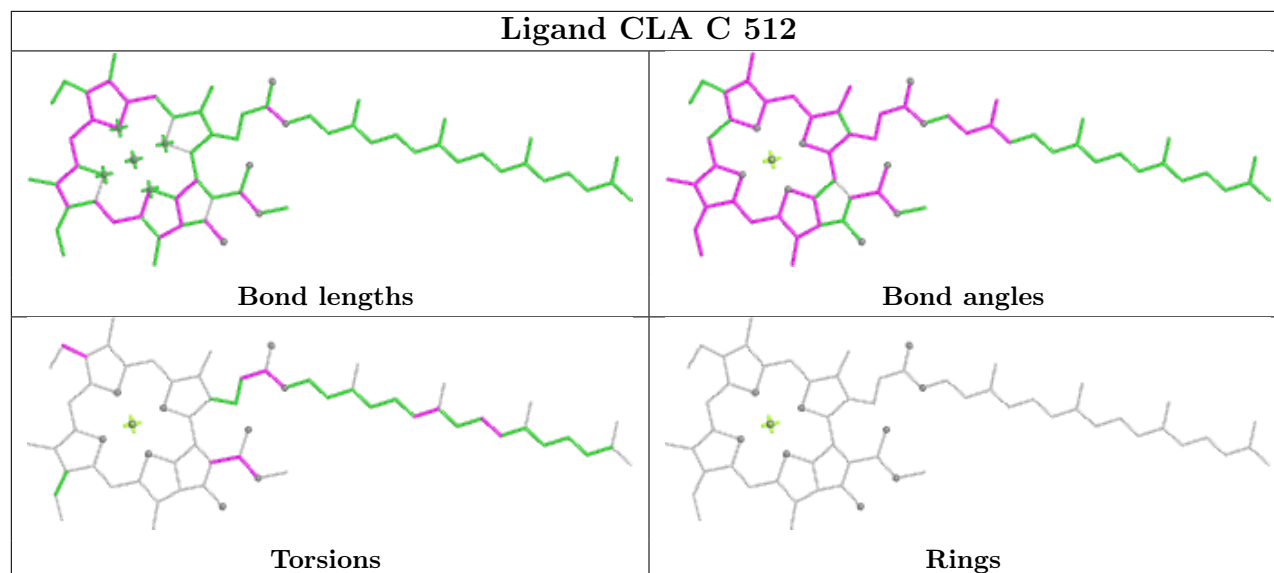
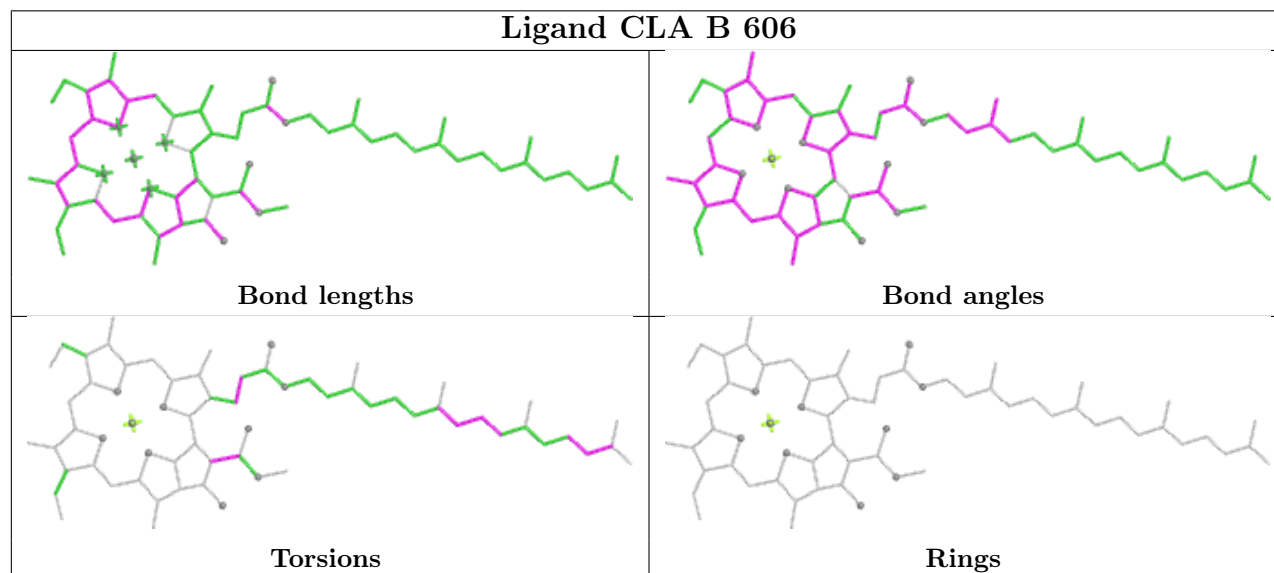
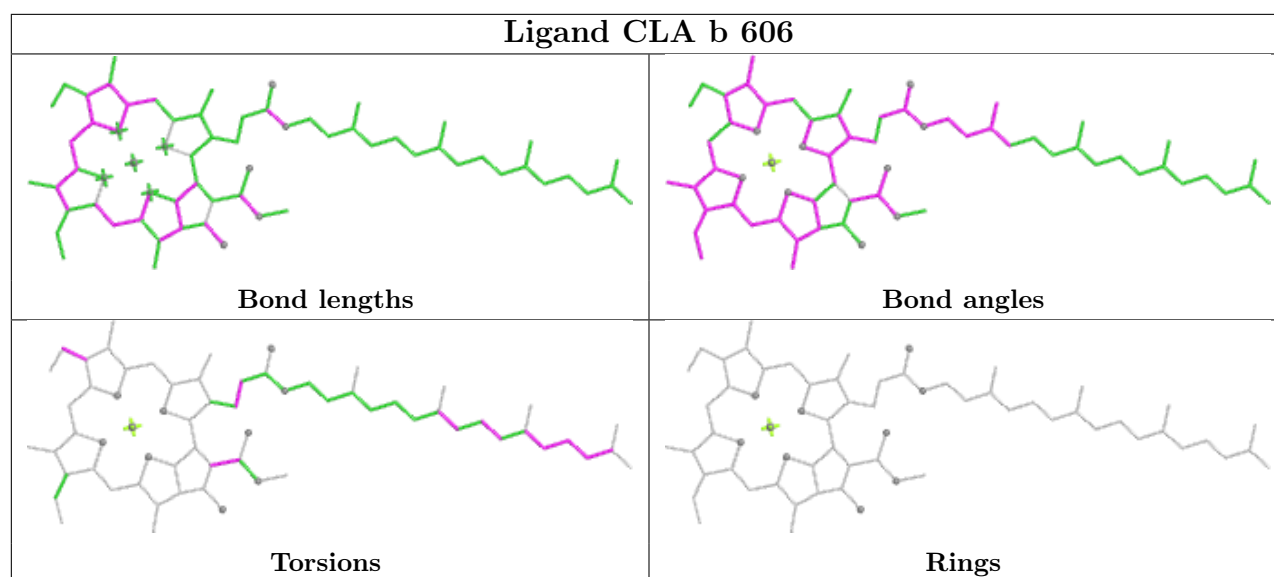




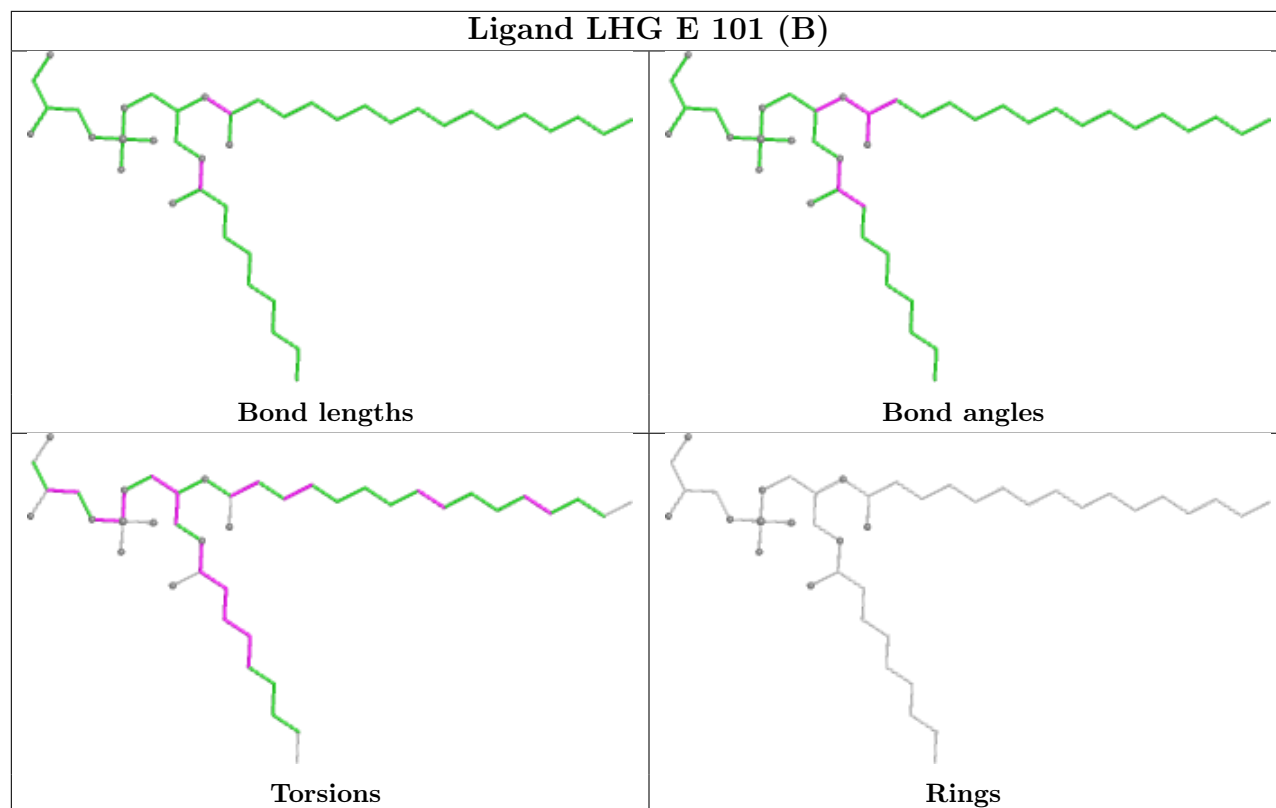
Ligand BCR b 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

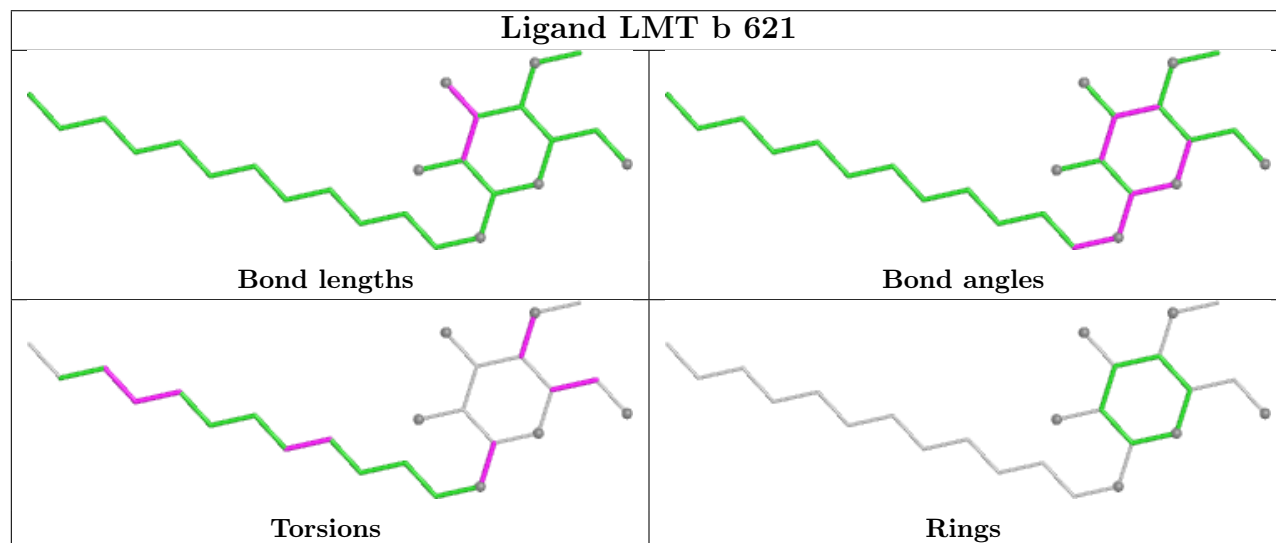
Ligand BCR B 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

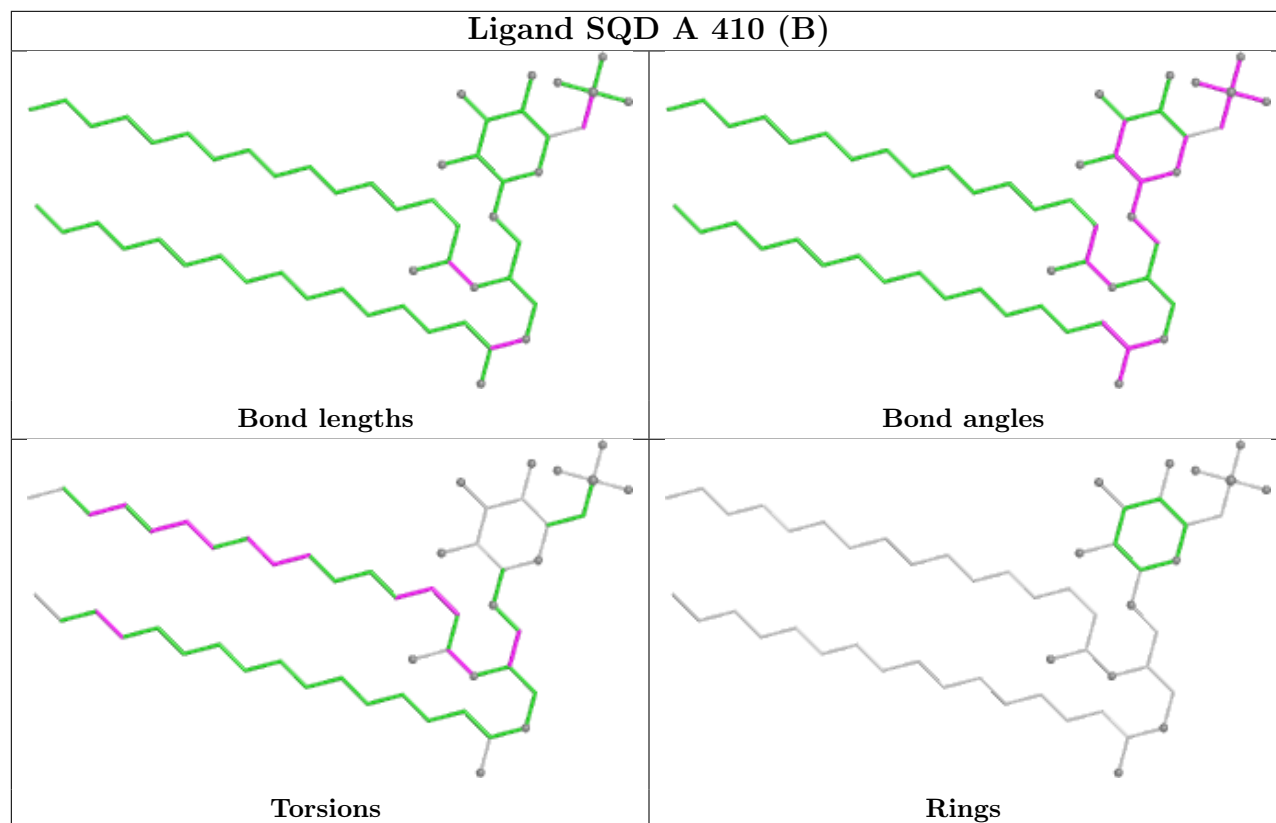
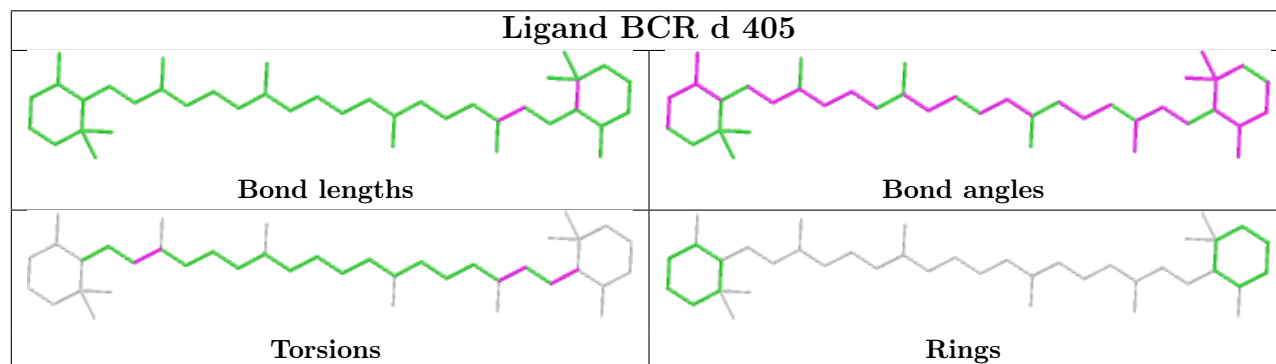
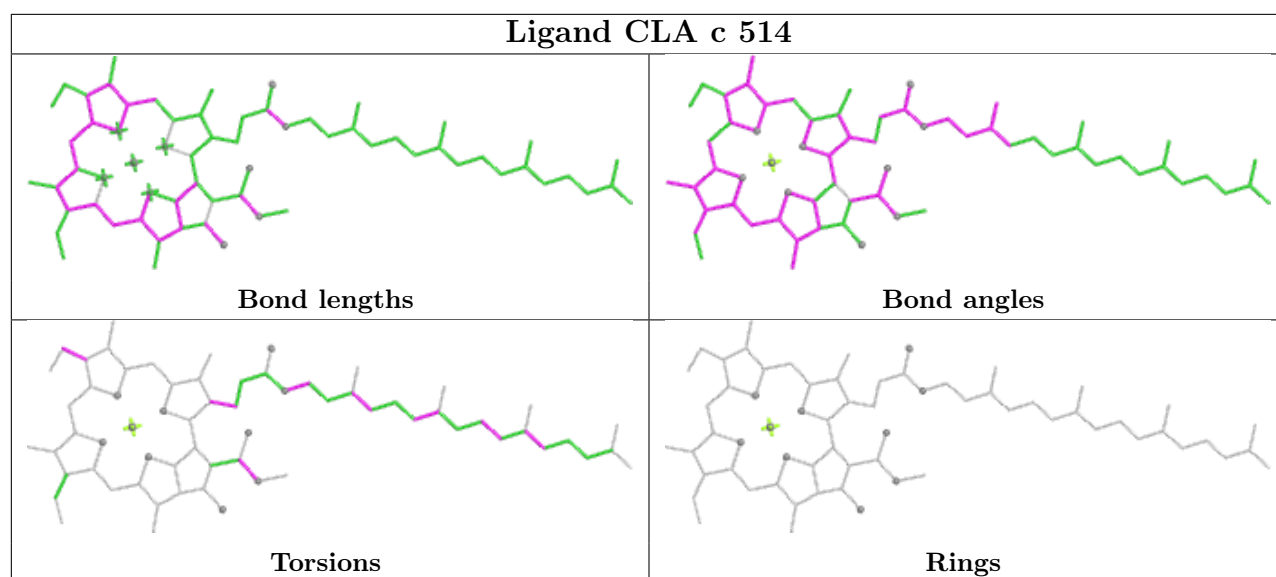


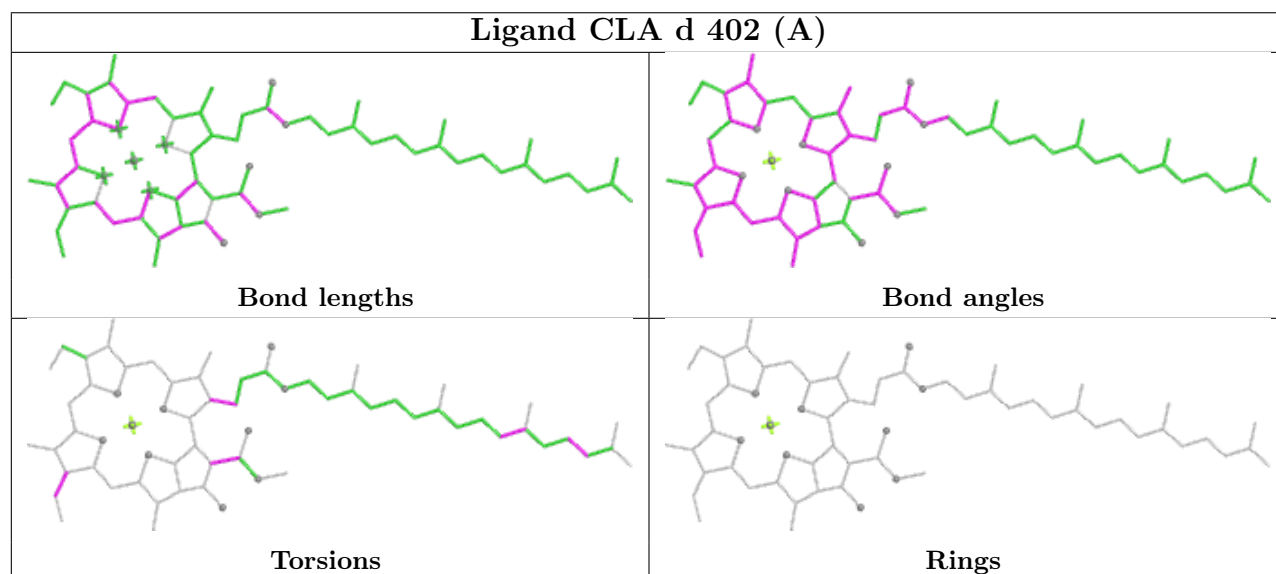
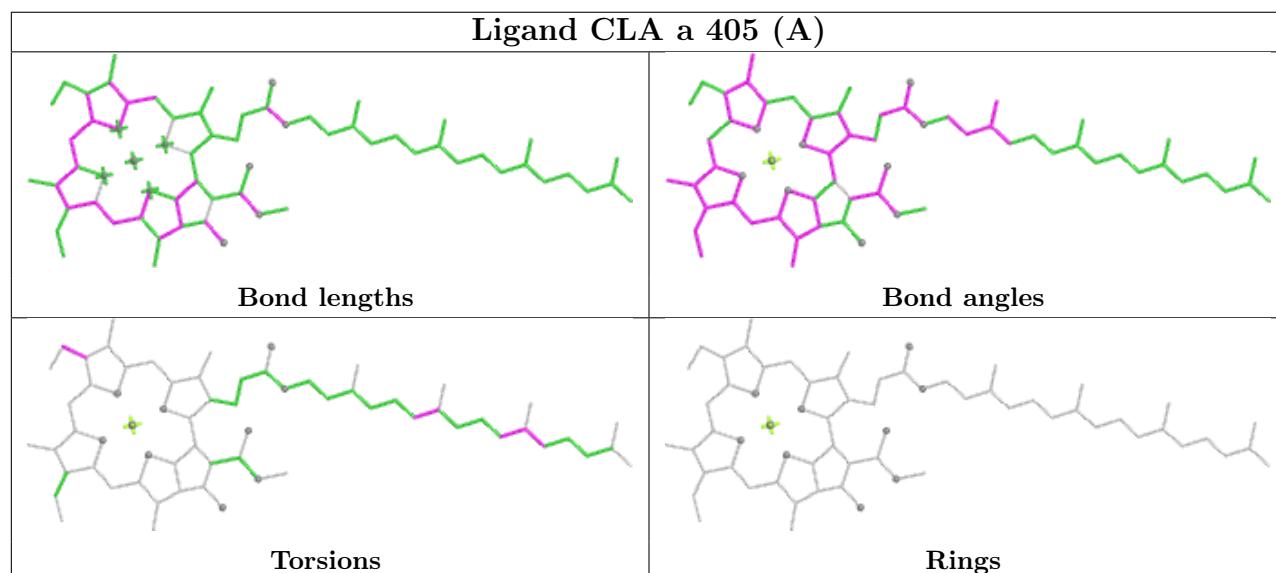
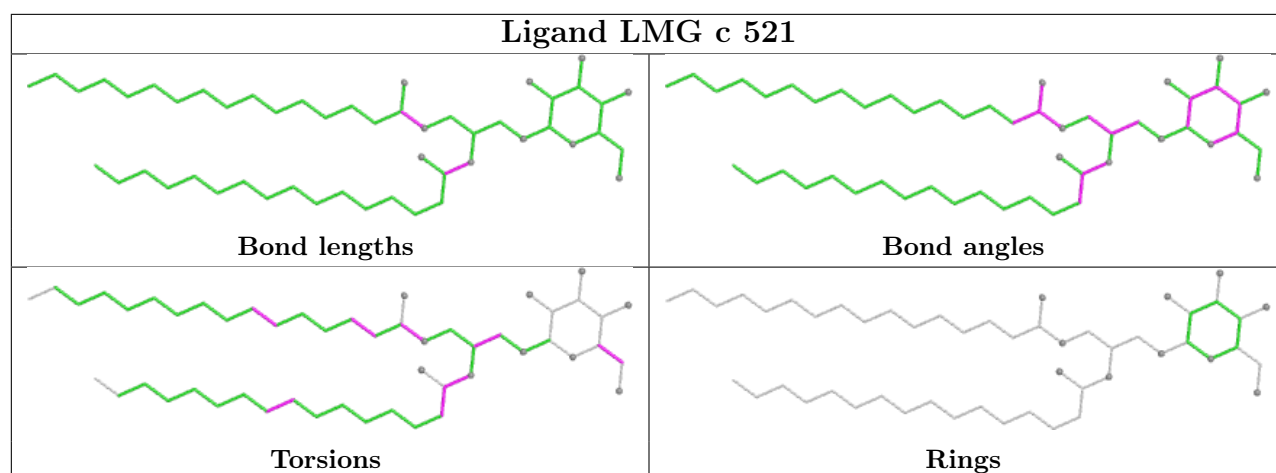
Ligand LHG E 101 (B)

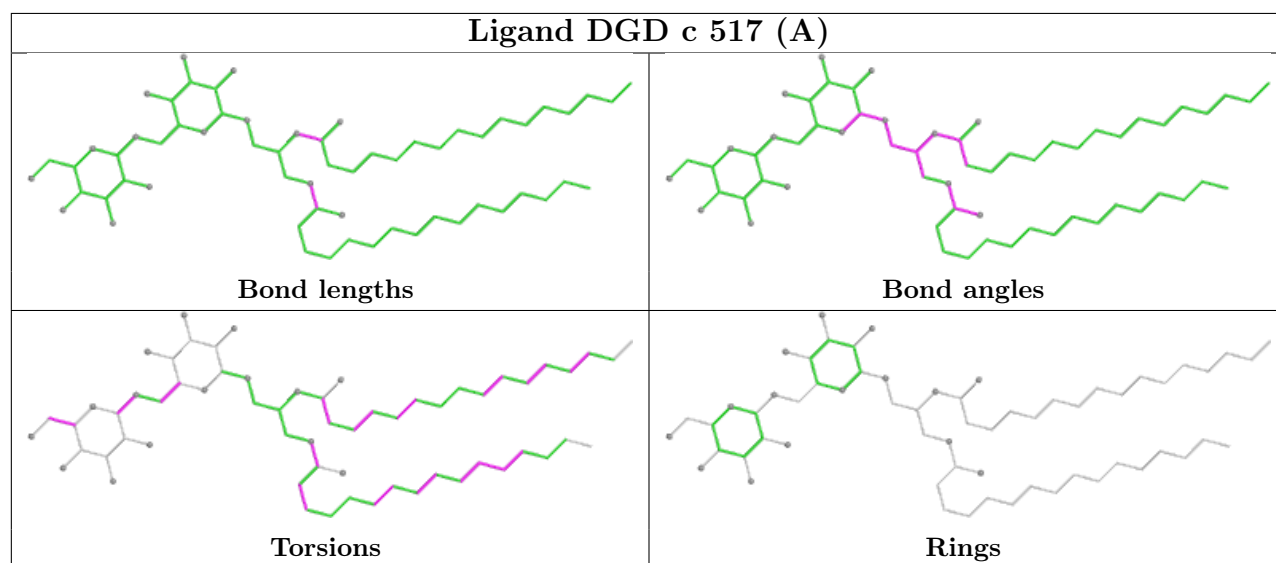
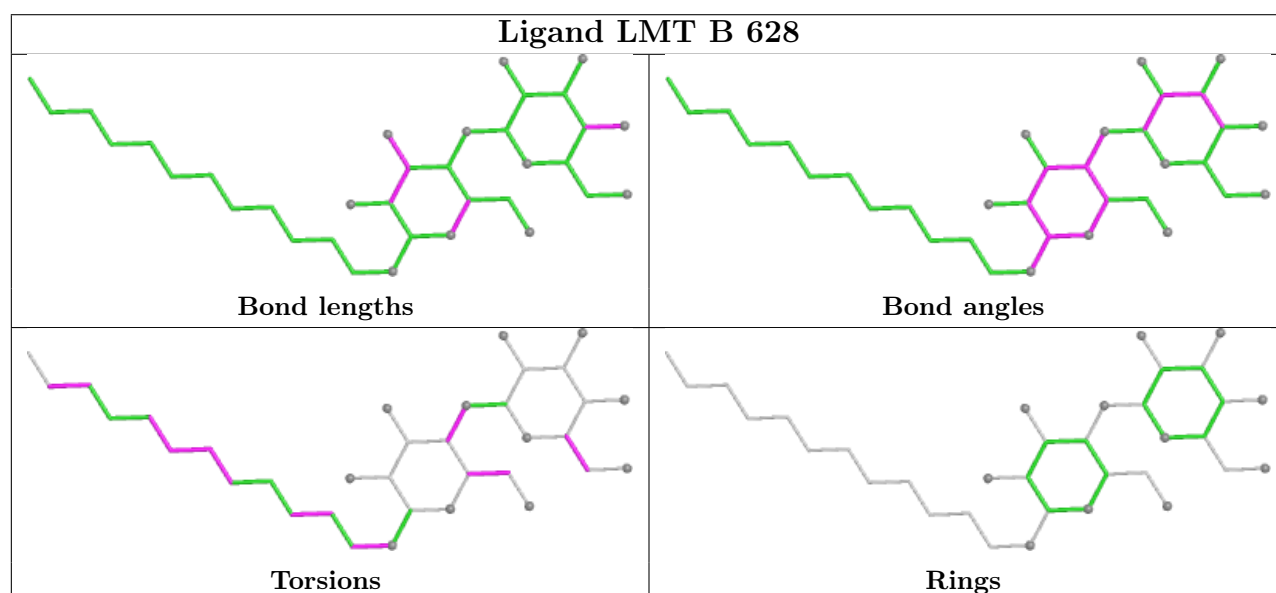
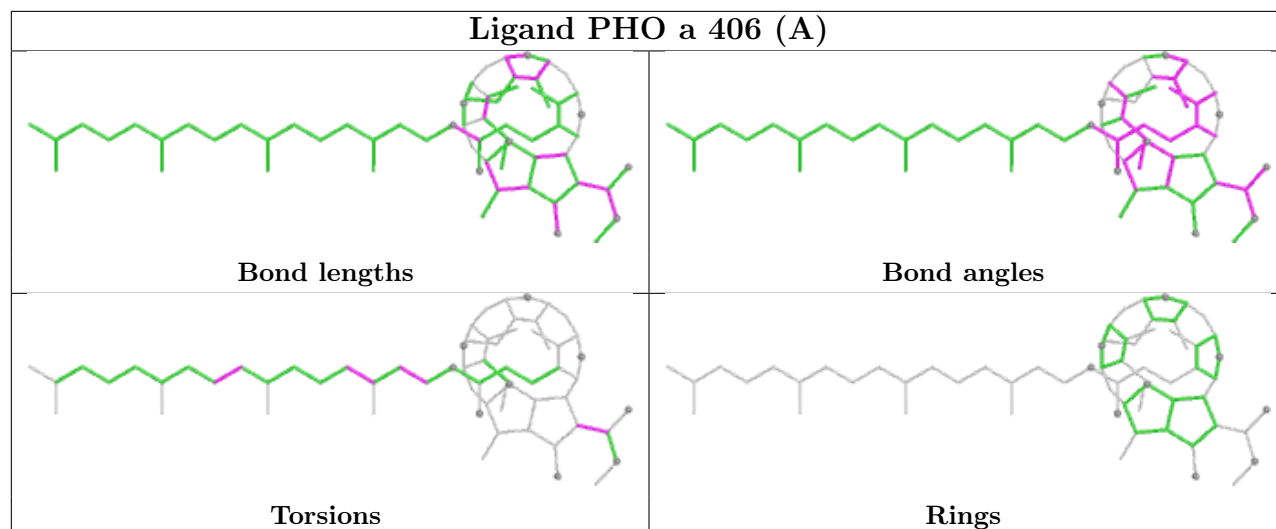


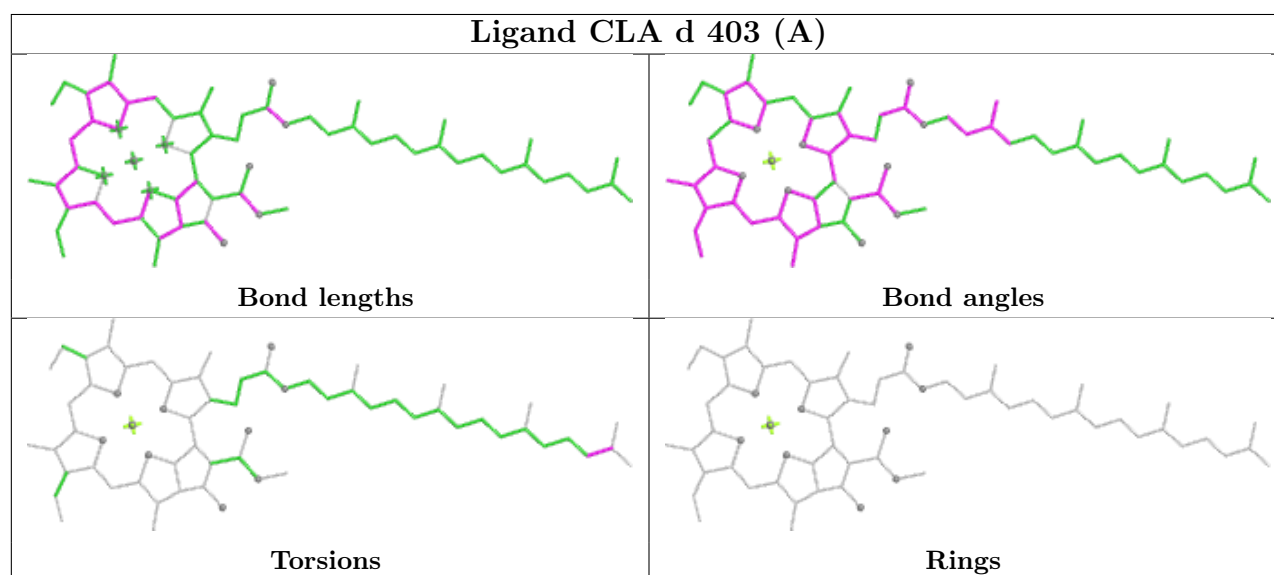
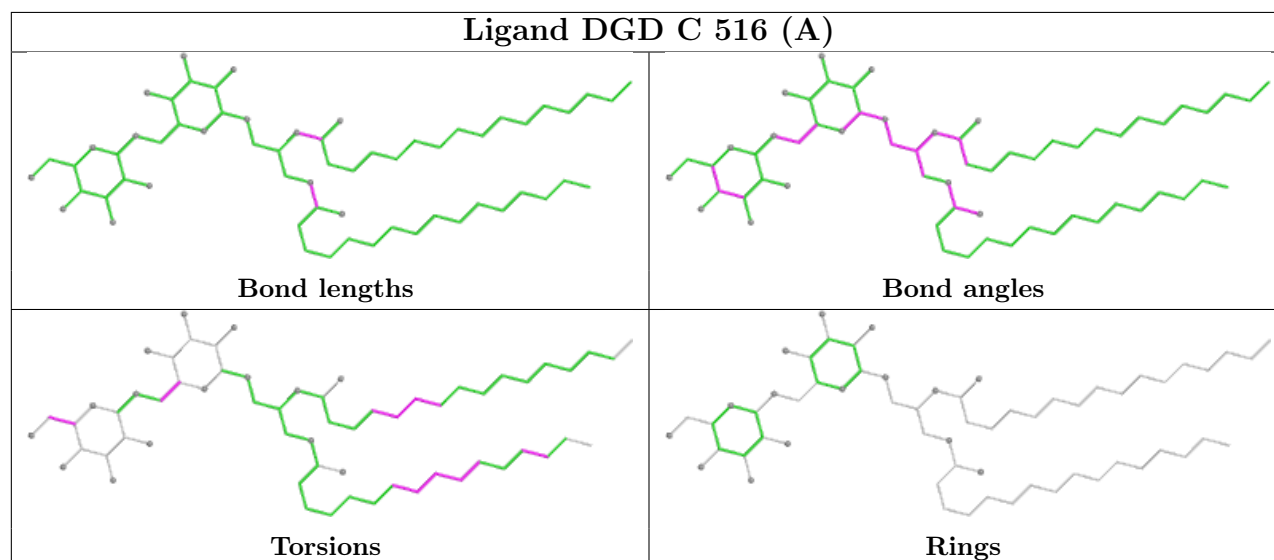
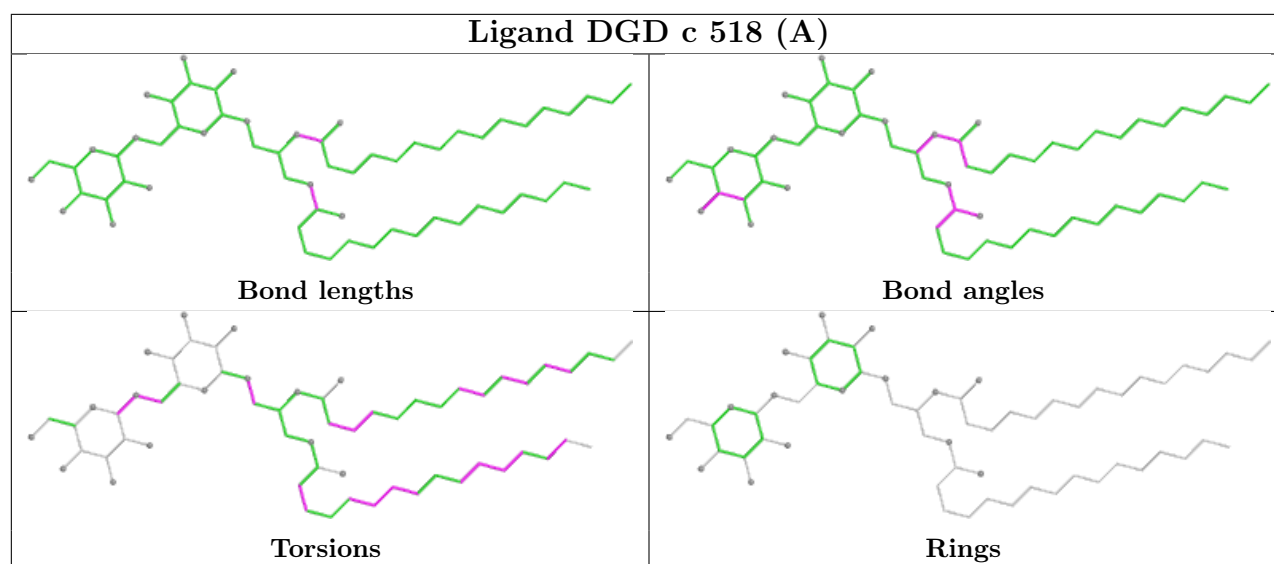
Ligand LMT b 621

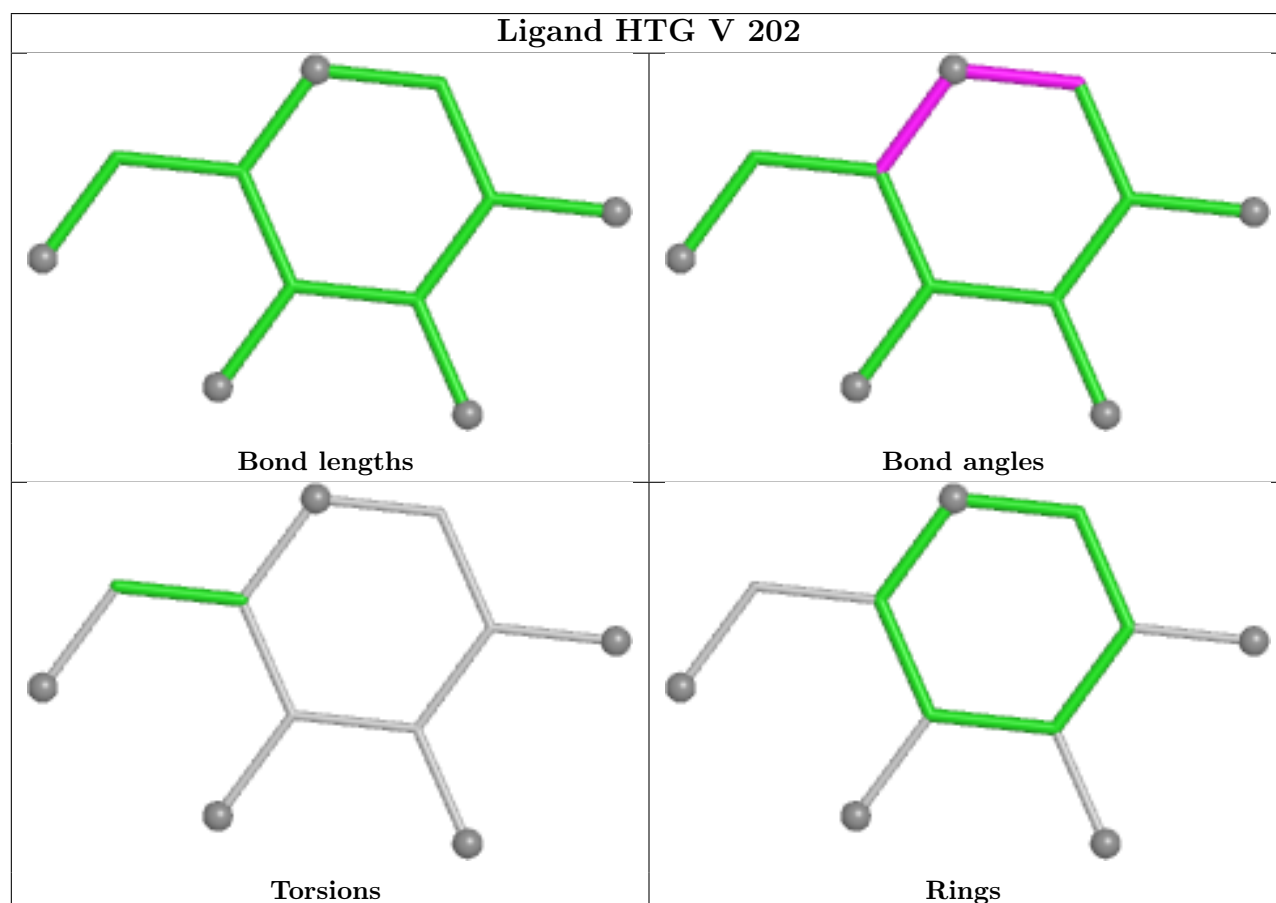
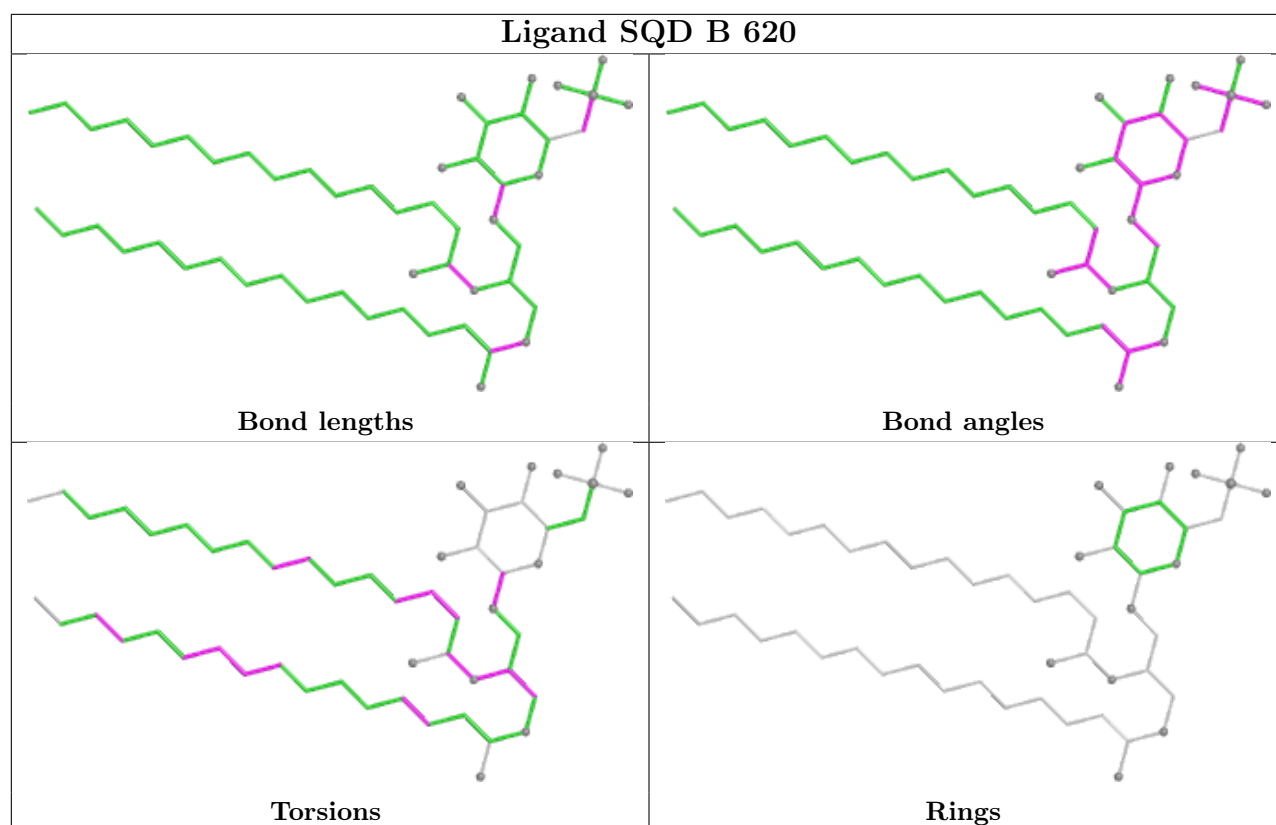


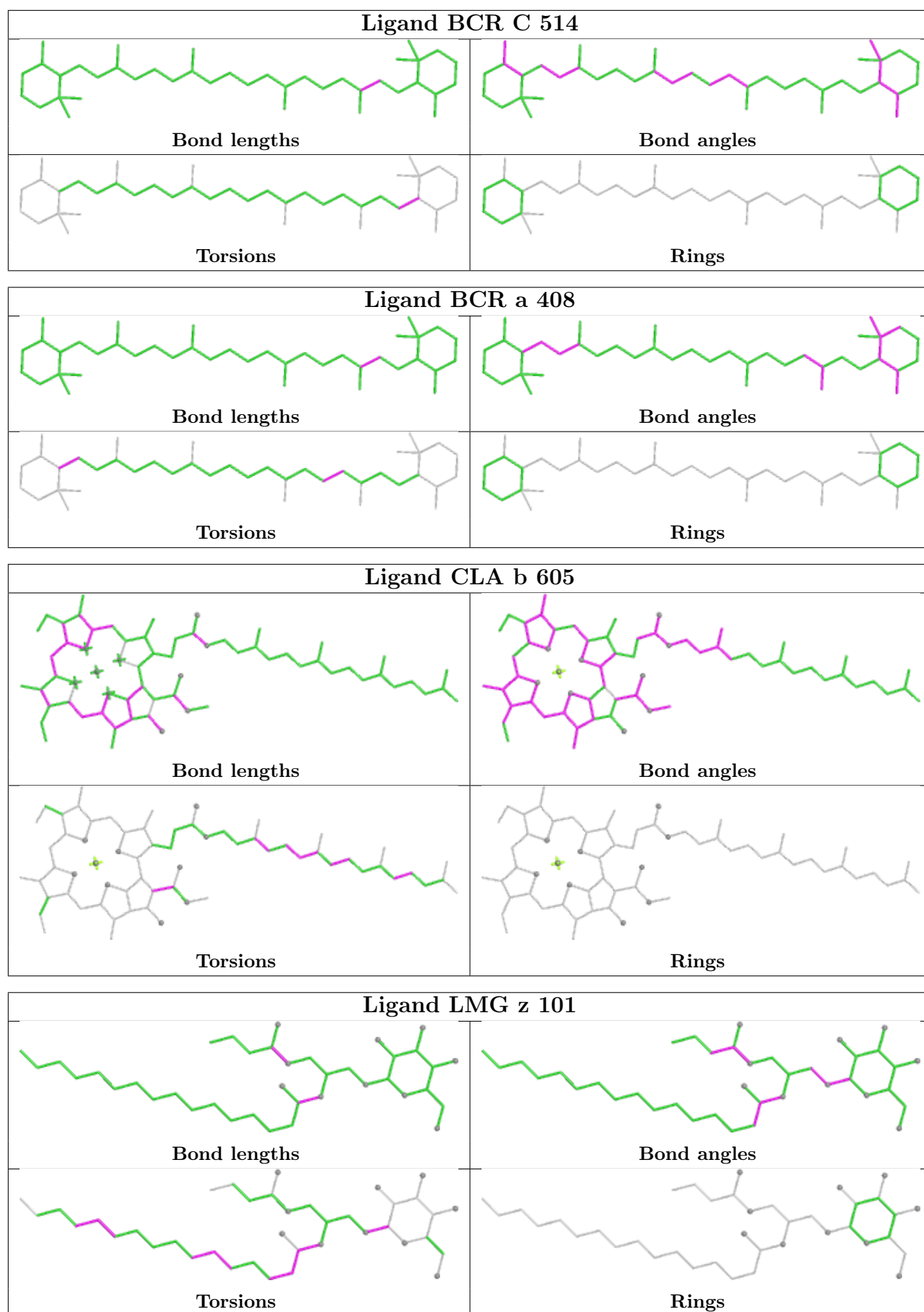


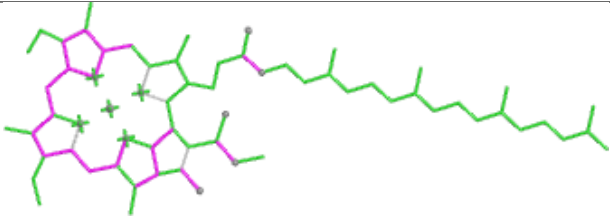
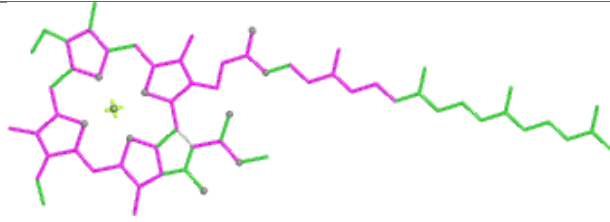
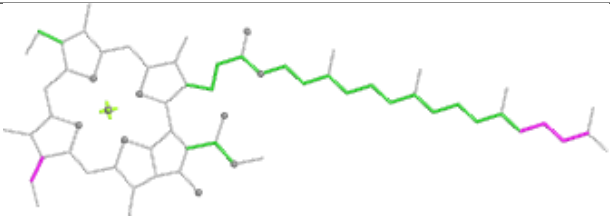
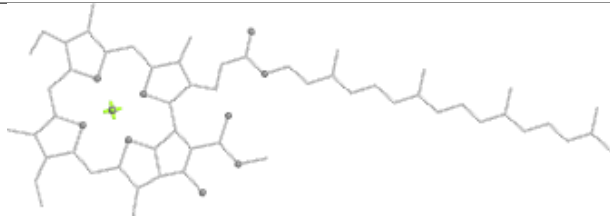
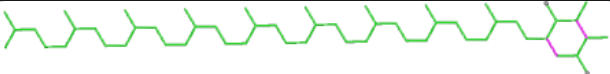
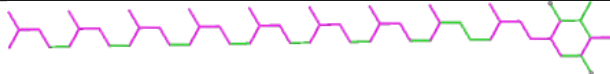
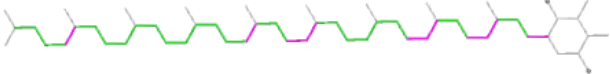
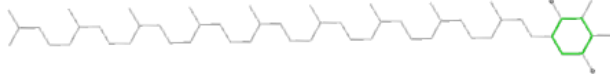




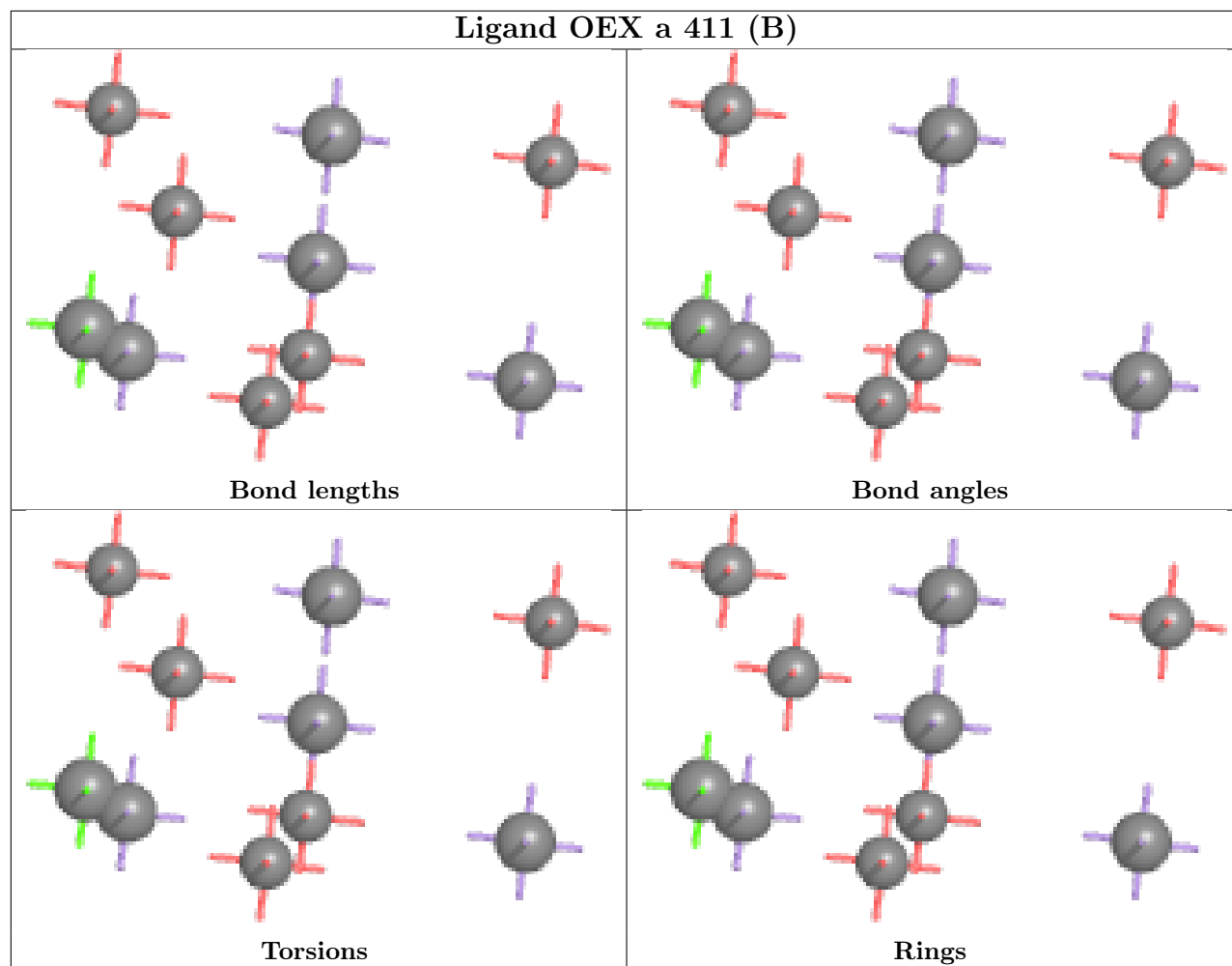




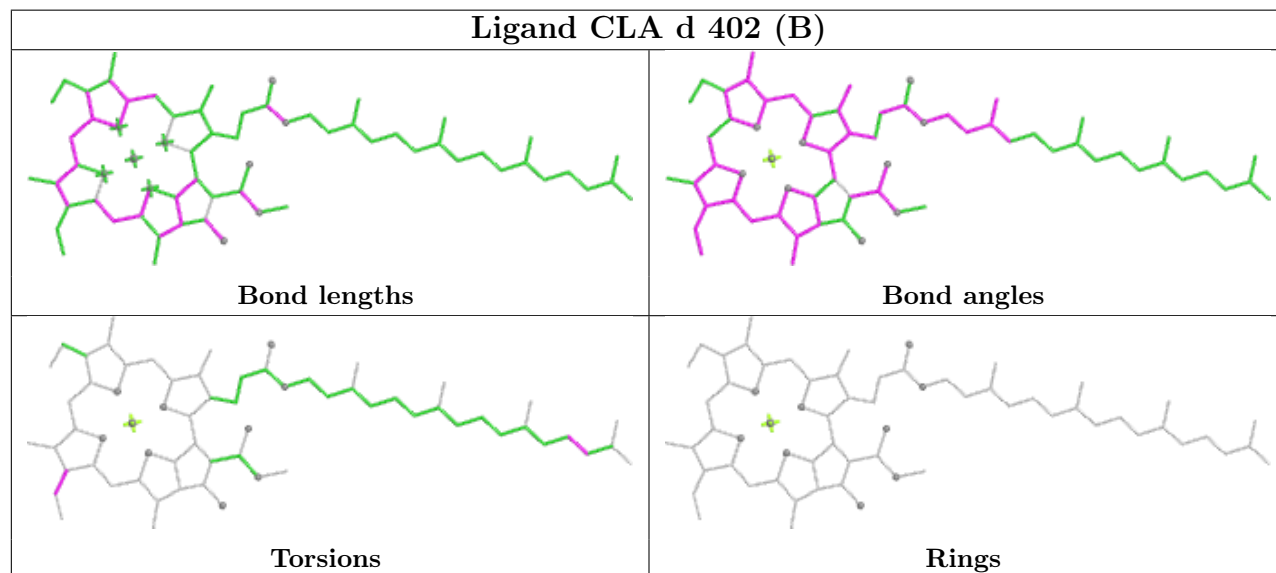


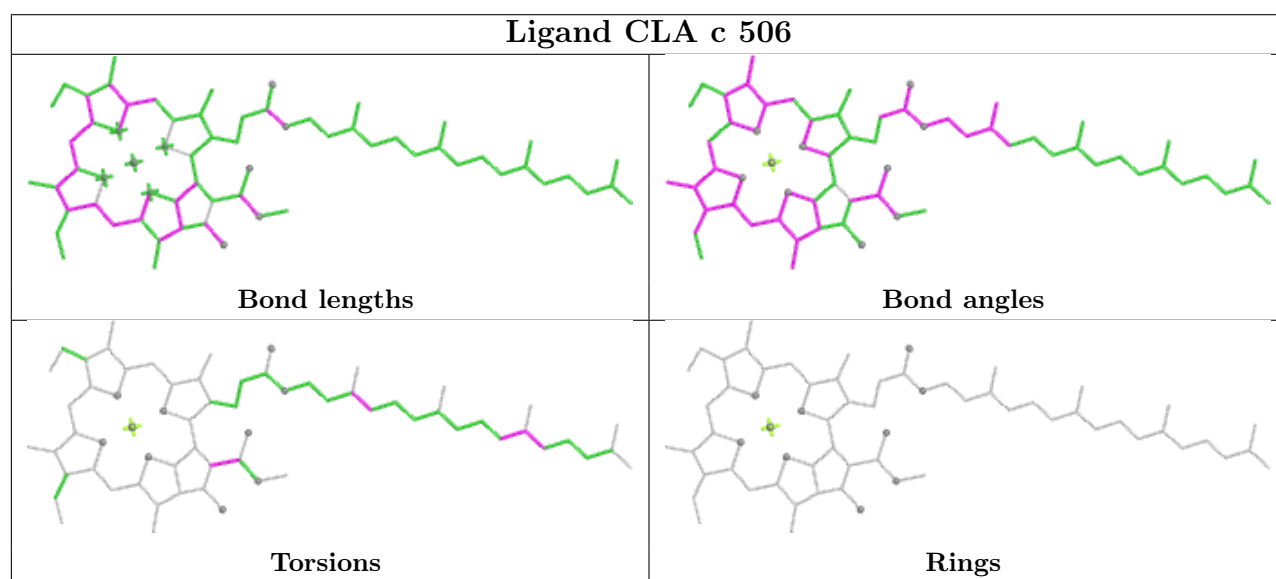
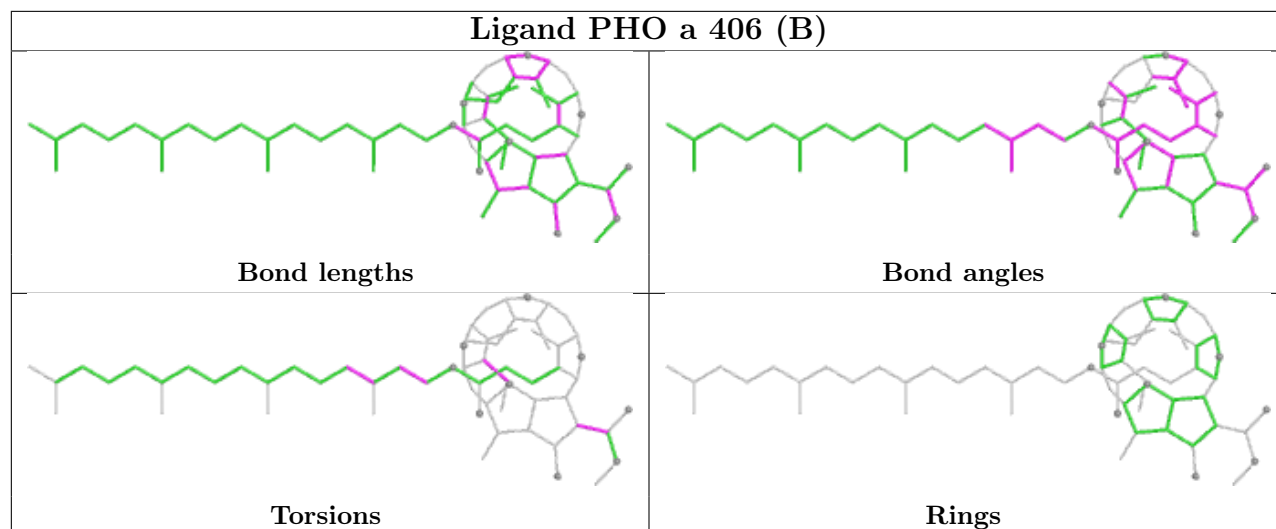
Ligand CLA A 404 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 a 412 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand OEX a 411 (B)

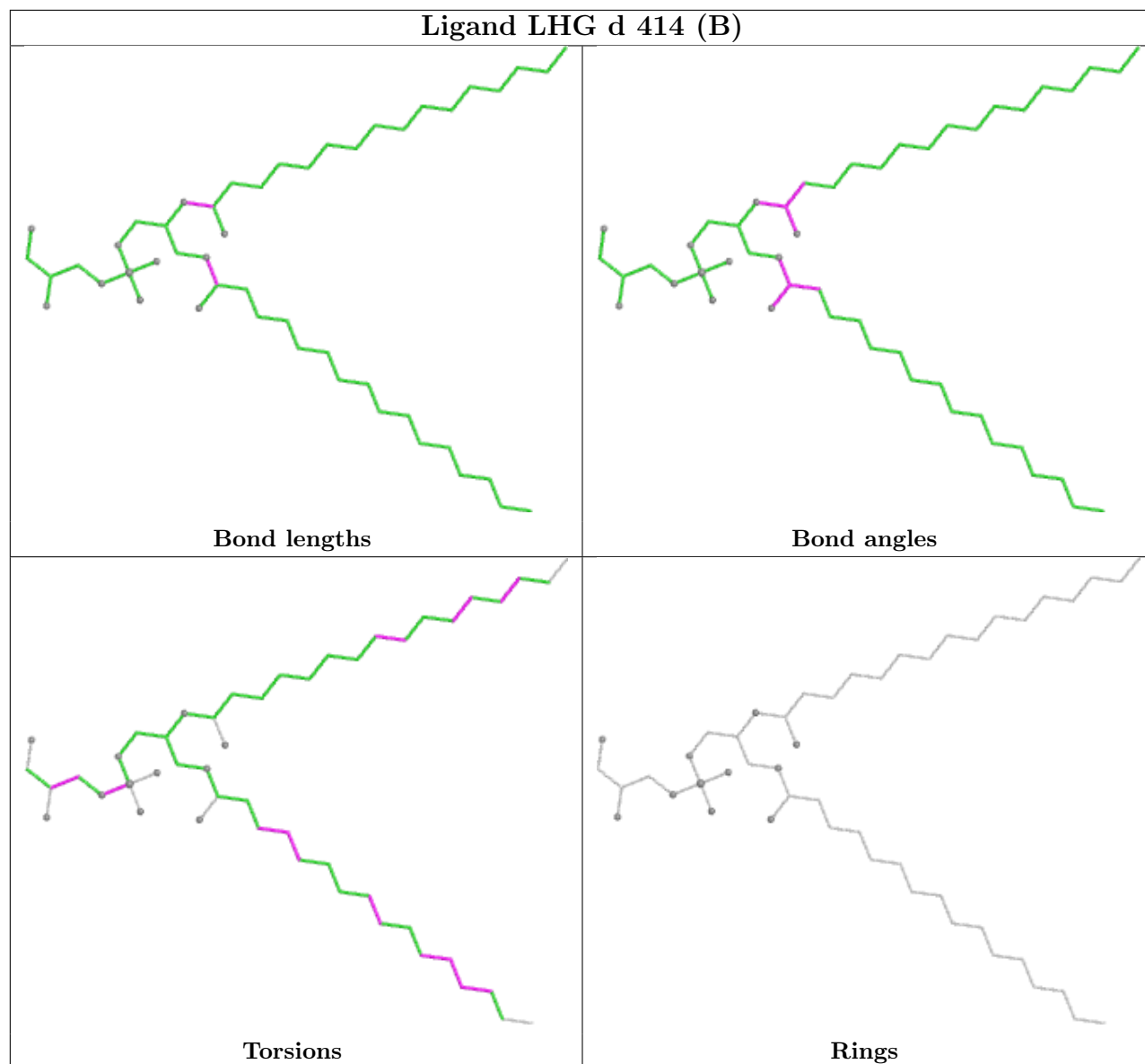


Ligand CLA d 402 (B)

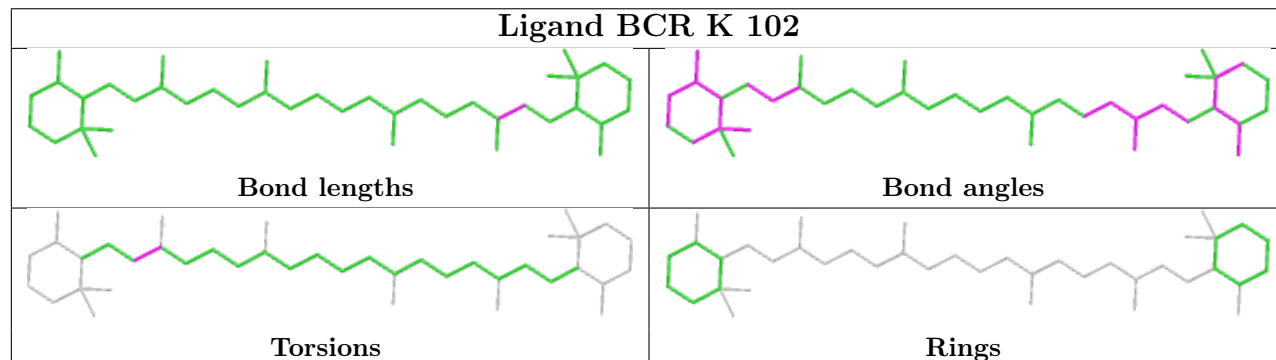


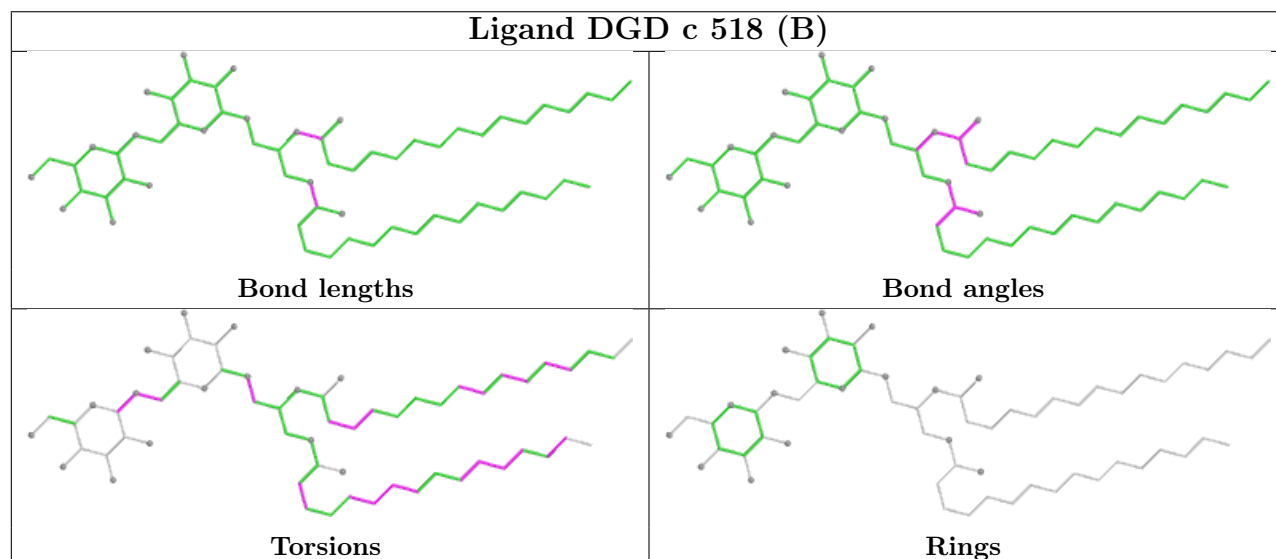
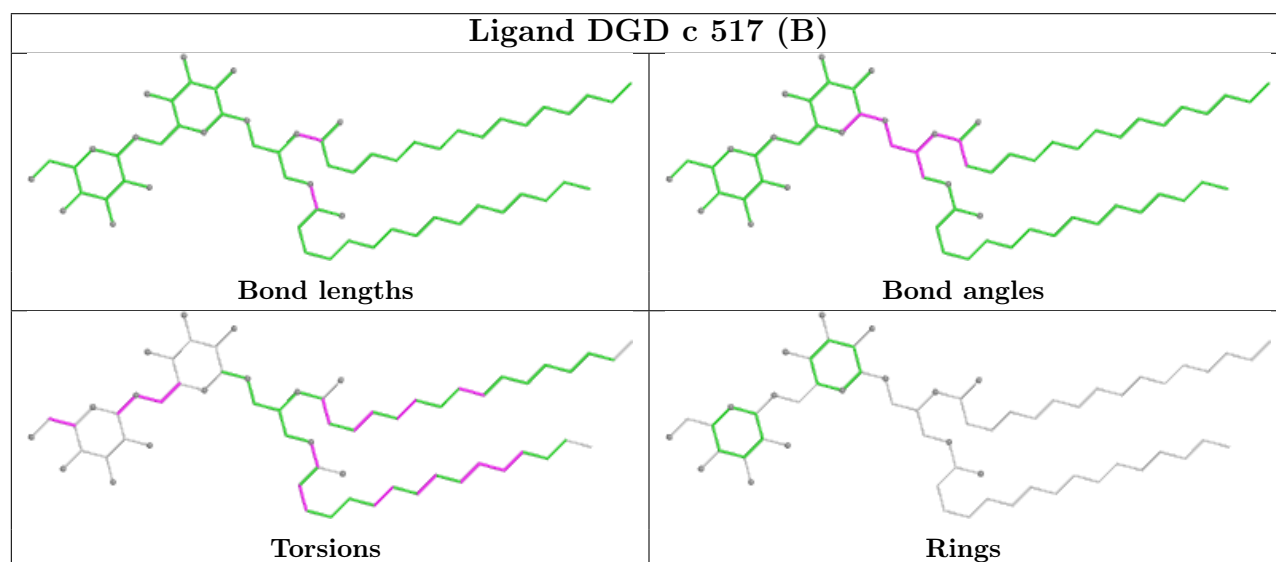
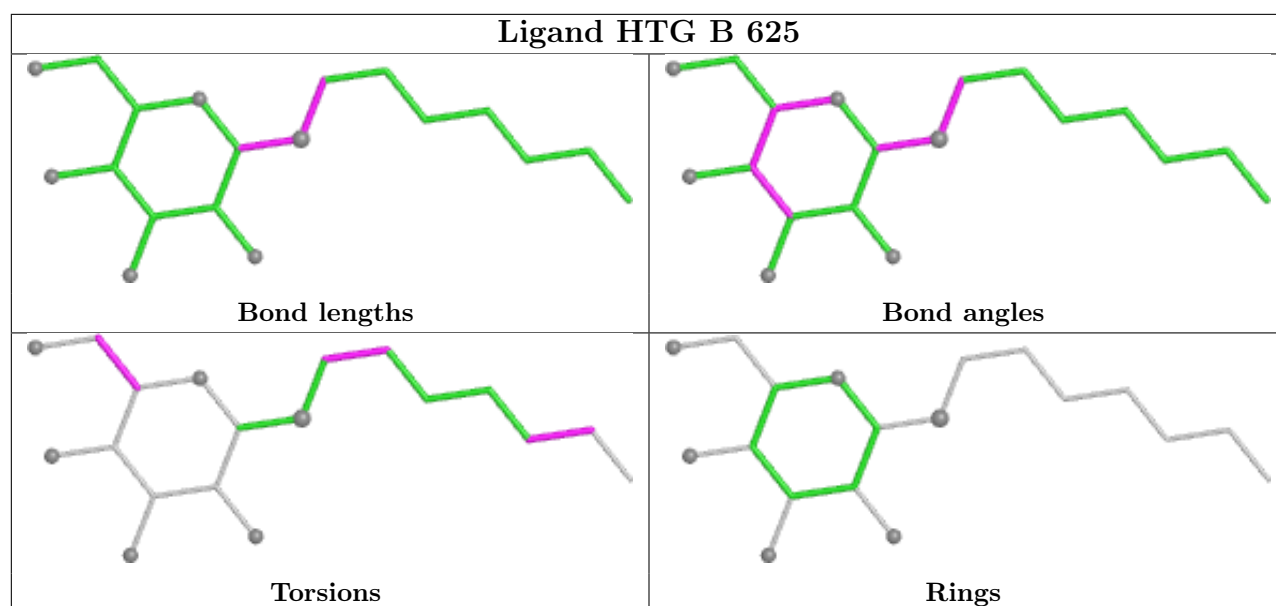


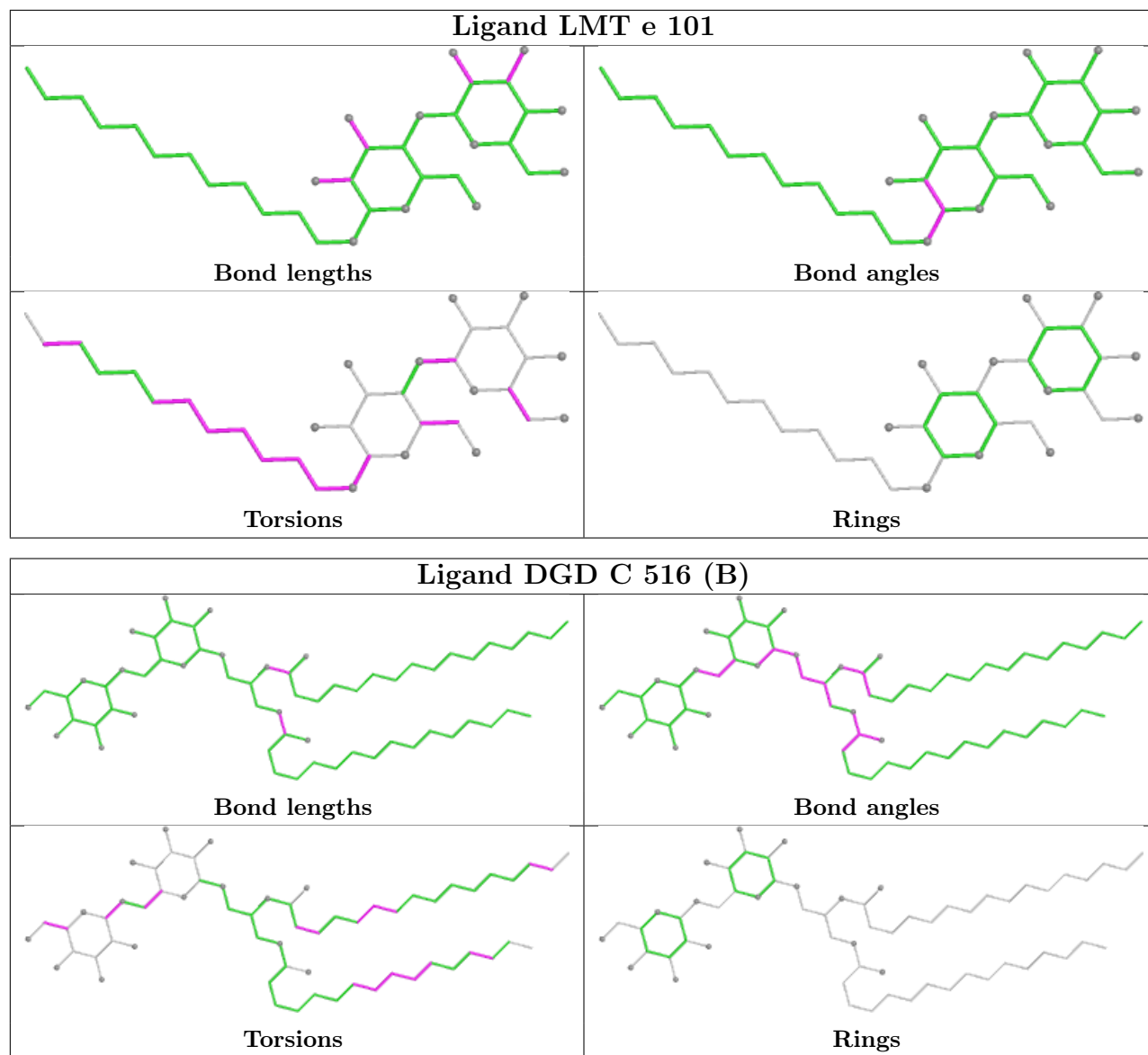
Ligand LHG d 414 (B)



Ligand BCR K 102







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%)	-0.58	0 100 100	21, 27, 60, 127	222 (66%)
1	a	334/344 (97%)	-0.56	1 (0%) 90 90	21, 29, 65, 127	220 (65%)
2	B	504/505 (99%)	-0.54	1 (0%) 91 92	22, 54, 83, 117	22 (4%)
2	b	504/505 (99%)	-0.46	2 (0%) 88 89	24, 58, 95, 162	19 (3%)
3	C	451/455 (99%)	-0.52	0 100 100	22, 59, 81, 158	99 (21%)
3	c	455/455 (100%)	-0.50	2 (0%) 88 89	24, 65, 86, 124	101 (22%)
4	D	342/342 (100%)	-0.60	0 100 100	21, 47, 65, 138	115 (33%)
4	d	341/342 (99%)	-0.60	0 100 100	22, 50, 72, 134	119 (34%)
5	E	81/84 (96%)	-0.38	1 (1%) 76 77	52, 71, 98, 166	0
5	e	79/84 (94%)	-0.38	1 (1%) 75 76	32, 76, 119, 150	2 (2%)
6	F	34/44 (77%)	-0.60	0 100 100	54, 62, 88, 115	0
6	f	31/44 (70%)	-0.39	1 (3%) 50 50	56, 67, 96, 152	1 (3%)
7	H	64/65 (98%)	-0.31	1 (1%) 70 71	51, 63, 84, 112	0
7	h	64/65 (98%)	-0.43	0 100 100	39, 69, 94, 111	1 (1%)
8	I	37/38 (97%)	-0.20	0 100 100	56, 63, 127, 163	0
8	i	37/38 (97%)	-0.34	1 (2%) 56 57	56, 63, 124, 148	0
9	J	38/39 (97%)	-0.33	0 100 100	53, 71, 122, 182	0
9	j	39/39 (100%)	-0.36	1 (2%) 57 58	60, 75, 131, 175	0
10	K	37/37 (100%)	-0.69	0 100 100	59, 69, 88, 110	0
10	k	37/37 (100%)	-0.55	0 100 100	69, 75, 98, 113	0
11	L	36/37 (97%)	-0.60	0 100 100	23, 47, 105, 144	2 (5%)
11	l	36/37 (97%)	-0.55	0 100 100	25, 48, 97, 125	2 (5%)
12	M	32/36 (88%)	-0.58	0 100 100	27, 49, 77, 140	1 (3%)
12	m	33/36 (91%)	-0.50	0 100 100	24, 50, 72, 153	2 (6%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.54	0 100 100	22, 64, 119, 185	10 (4%)
13	o	243/244 (99%)	-0.50	0 100 100	23, 67, 128, 169	8 (3%)
14	T	29/32 (90%)	-0.56	0 100 100	27, 48, 58, 66	6 (20%)
14	t	29/32 (90%)	-0.56	1 (3%) 48 48	28, 49, 64, 75	5 (17%)
15	U	96/104 (92%)	-0.59	0 100 100	26, 59, 92, 101	4 (4%)
15	u	97/104 (93%)	-0.63	0 100 100	29, 62, 83, 135	5 (5%)
16	V	137/137 (100%)	-0.67	0 100 100	24, 58, 82, 105	6 (4%)
16	v	137/137 (100%)	-0.60	0 100 100	27, 71, 104, 138	6 (4%)
17	X	38/40 (95%)	-0.31	0 100 100	35, 72, 94, 115	1 (2%)
17	x	38/40 (95%)	-0.14	0 100 100	65, 78, 119, 163	0
18	Y	29/30 (96%)	-0.06	1 (3%) 48 48	69, 85, 126, 135	0
18	y	29/30 (96%)	-0.34	0 100 100	77, 90, 111, 120	0
19	Z	62/62 (100%)	-0.33	0 100 100	67, 80, 140, 163	0
19	z	62/62 (100%)	0.05	0 100 100	80, 95, 144, 189	0
20	R	34/34 (100%)	0.56	3 (8%) 15 14	85, 109, 136, 155	0
All	All	5283/5384 (98%)	-0.51	17 (0%) 90 90	21, 58, 100, 189	979 (18%)

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	4.0
5	e	79[A]	PHE	3.6
6	f	16[A]	PHE	2.9
2	b	499	VAL	2.8
14	t	30[A]	THR	2.6

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	T	1	10/11	0.94	0.07	43,57,72,74	0
8	FME	I	1	10/11	0.96	0.07	61,69,76,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	FME	i	1	10/11	0.96	0.07	53,71,78,80	0
14	FME	t	1	10/11	0.96	0.07	46,50,59,77	0
12	FME	m	1	10/11	0.97	0.07	50,64,86,115	0
12	FME	M	1	10/11	0.97	0.06	48,60,93,98	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
27	GOL	a	416	6/6	0.61	0.15	77,99,109,115	0
31	LMT	F	101	35/35	0.69	0.15	101,134,184,188	0
30	UNL	j	101	10/-	0.70	0.19	75,91,107,111	0
30	UNL	A	415	28/-	0.71	0.14	89,114,133,157	0
31	LMT	B	630	35/35	0.71	0.14	65,119,149,170	0
30	UNL	a	413	30/-	0.71	0.12	91,122,144,152	0
30	UNL	J	101	10/-	0.72	0.26	74,84,93,99	0
30	UNL	m	102	10/-	0.72	0.20	72,78,95,98	0
30	UNL	I	101	40/-	0.73	0.15	72,105,157,164	0
31	LMT	A	417	35/35	0.74	0.13	67,117,141,143	0
30	UNL	K	101[A]	34/-	0.75	0.14	89,111,127,127	34
30	UNL	K	101[B]	34/-	0.75	0.14	89,111,127,127	34
31	LMT	a	415	35/35	0.75	0.13	108,136,150,161	0
30	UNL	l	101	10/-	0.76	0.17	72,84,95,97	0
36	CA	F	104	1/1	0.76	0.24	128,128,128,128	0
27	GOL	o	302	6/6	0.77	0.18	89,105,115,125	0
31	LMT	e	101	35/35	0.77	0.13	103,152,193,201	0
34	HTG	C	521	19/19	0.77	0.12	105,130,146,146	0
31	LMT	A	420	35/35	0.77	0.12	98,138,160,173	0
26	SQD	f	102	43/54	0.78	0.12	98,128,180,194	0
34	HTG	B	623	19/19	0.78	0.15	65,97,115,117	0
30	UNL	i	101	40/-	0.79	0.13	78,107,158,162	0
30	UNL	D	410	40/-	0.79	0.13	66,93,138,147	0
34	HTG	D	411	16/19	0.79	0.12	85,109,138,155	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	LMG	C	520	51/55	0.79	0.11	63,120,162,184	0
27	GOL	d	413	6/6	0.80	0.25	56,70,85,97	0
33	LHG	a	418[A]	42/49	0.80	0.11	99,142,159,169	42
33	LHG	a	418[B]	42/49	0.80	0.11	99,142,160,170	42
27	GOL	B	627	6/6	0.80	0.14	67,92,106,120	0
27	GOL	b	624	6/6	0.80	0.18	87,102,106,114	0
30	UNL	b	626	33/-	0.80	0.12	72,98,155,160	0
30	UNL	d	410	36/-	0.80	0.12	72,94,131,144	0
27	GOL	O	302	6/6	0.81	0.10	76,91,103,107	0
30	UNL	c	525[A]	32/-	0.81	0.14	97,116,129,140	32
30	UNL	c	525[B]	32/-	0.81	0.14	97,116,129,141	32
31	LMT	b	621	25/35	0.81	0.12	80,113,162,172	0
27	GOL	o	303	6/6	0.81	0.15	84,94,101,105	0
34	HTG	V	202	11/19	0.81	0.09	77,111,125,125	0
27	GOL	A	411	6/6	0.81	0.13	65,81,86,86	0
27	GOL	l	102[A]	6/6	0.82	0.18	70,103,107,112	6
34	HTG	c	522	19/19	0.82	0.09	111,129,143,150	0
27	GOL	l	102[B]	6/6	0.82	0.18	69,103,108,112	6
31	LMT	B	628	35/35	0.83	0.11	65,105,146,152	0
27	GOL	O	303	6/6	0.83	0.13	85,103,105,108	0
30	UNL	B	626	33/-	0.83	0.14	52,106,144,150	0
34	HTG	b	622	19/19	0.84	0.12	58,88,121,122	0
26	SQD	a	410	54/54	0.84	0.10	63,99,137,154	0
34	HTG	d	411	16/19	0.84	0.10	84,123,143,152	0
31	LMT	M	102	35/35	0.84	0.11	74,127,183,188	0
36	CA	f	103	1/1	0.84	0.13	124,124,124,124	0
31	LMT	B	631	25/35	0.85	0.12	62,89,154,167	0
34	HTG	b	623	19/19	0.85	0.10	86,126,163,167	0
29	PL9	A	414[B]	55/55	0.85	0.14	73,99,113,115	55
31	LMT	m	103	35/35	0.85	0.11	59,91,108,120	0
26	SQD	A	412	54/54	0.85	0.11	68,93,134,159	0
29	PL9	A	414[A]	55/55	0.85	0.14	73,99,113,114	55
31	LMT	b	627	25/35	0.86	0.12	60,99,146,162	0
31	LMT	t	101	26/35	0.86	0.11	72,104,148,156	0
27	GOL	c	527	6/6	0.86	0.18	106,114,129,130	0
32	LMG	Z	101	37/55	0.86	0.13	70,121,155,172	0
27	GOL	v	202[B]	6/6	0.87	0.13	67,80,85,87	6
32	LMG	z	101	39/55	0.87	0.12	76,128,154,167	0
27	GOL	B	629	6/6	0.87	0.13	75,77,89,98	0
27	GOL	v	202[A]	6/6	0.87	0.13	67,80,85,87	6
29	PL9	a	412[A]	55/55	0.87	0.15	89,110,123,125	55
29	PL9	a	412[B]	55/55	0.87	0.15	90,110,123,126	55

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
32	LMG	c	521	51/55	0.87	0.10	74,136,164,192	0
26	SQD	b	620	54/54	0.88	0.10	66,95,127,132	0
27	GOL	V	203[A]	6/6	0.88	0.12	56,66,76,77	6
27	GOL	V	203[B]	6/6	0.88	0.12	56,66,76,77	6
27	GOL	D	413	6/6	0.88	0.16	50,65,76,97	0
31	LMT	M	101	35/35	0.88	0.10	60,98,124,133	0
27	GOL	a	417	6/6	0.88	0.13	59,81,81,85	0
26	SQD	F	103	43/54	0.88	0.11	70,104,133,142	0
23	CLA	b	601	65/65	0.89	0.10	59,84,124,161	0
27	GOL	D	402	6/6	0.89	0.28	53,80,82,89	0
26	SQD	B	620	54/54	0.89	0.10	64,93,135,152	0
30	UNL	D	409	17/-	0.89	0.11	59,77,102,118	0
33	LHG	E	101[A]	42/49	0.90	0.11	76,106,119,123	42
33	LHG	E	101[B]	42/49	0.90	0.11	76,106,119,124	42
27	GOL	B	624	6/6	0.90	0.09	73,81,88,89	0
32	LMG	A	418	51/55	0.90	0.09	67,91,119,134	0
34	HTG	B	622	19/19	0.90	0.11	60,87,119,127	0
34	HTG	B	625	19/19	0.91	0.08	68,82,99,100	0
27	GOL	C	522[A]	6/6	0.91	0.09	58,61,63,72	6
27	GOL	C	522[B]	6/6	0.91	0.09	58,62,63,72	6
23	CLA	B	601	65/65	0.91	0.09	53,79,109,156	0
32	LMG	m	101	51/55	0.91	0.09	57,77,101,118	0
32	LMG	C	519	51/55	0.92	0.09	59,83,120,134	0
23	CLA	c	514	65/65	0.92	0.09	62,95,121,145	0
32	LMG	c	501	51/55	0.92	0.08	65,96,111,119	0
32	LMG	c	520	51/55	0.92	0.09	60,90,133,162	0
25	BCR	T	101	40/40	0.92	0.07	45,60,73,80	0
25	BCR	t	102	40/40	0.92	0.07	43,60,79,87	0
30	UNL	d	409	17/-	0.92	0.09	67,83,114,117	0
32	LMG	B	621	51/55	0.92	0.08	55,73,94,118	0
33	LHG	A	419[A]	49/49	0.93	0.09	50,65,85,89	49
33	LHG	A	419[B]	49/49	0.93	0.09	50,65,85,90	49
34	HTG	b	625	19/19	0.93	0.07	65,80,96,103	0
32	LMG	d	412	51/55	0.93	0.08	55,71,117,152	0
23	CLA	C	513	65/65	0.93	0.08	60,86,109,119	0
35	DGD	C	517[A]	62/66	0.93	0.08	51,65,110,116	62
35	DGD	C	517[B]	62/66	0.93	0.08	51,65,110,116	62
25	BCR	d	405	40/40	0.93	0.08	51,65,107,114	0
32	LMG	D	412	51/55	0.93	0.09	51,66,122,146	0
23	CLA	b	616	65/65	0.94	0.08	48,64,125,141	0
26	SQD	A	410[A]	54/54	0.94	0.08	56,80,112,118	54
26	SQD	A	410[B]	54/54	0.94	0.08	56,80,112,119	54

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	LHG	D	408[A]	49/49	0.94	0.09	49,62,111,112	49
33	LHG	D	408[B]	49/49	0.94	0.09	49,62,111,113	49
23	CLA	c	505	65/65	0.94	0.07	50,65,107,140	0
23	CLA	c	507	65/65	0.94	0.08	55,72,124,142	0
23	CLA	c	513	65/65	0.94	0.09	62,82,129,135	0
26	SQD	a	409[A]	54/54	0.94	0.09	58,83,118,125	54
26	SQD	a	409[B]	54/54	0.94	0.09	58,83,119,125	54
30	UNL	X	101	18/-	0.94	0.11	63,74,107,110	0
23	CLA	C	504	65/65	0.94	0.08	39,58,107,136	0
23	CLA	d	404	65/65	0.94	0.09	50,67,120,154	0
25	BCR	B	619	40/40	0.94	0.08	48,60,92,98	0
25	BCR	C	514	40/40	0.94	0.07	55,76,88,94	0
25	BCR	D	405	40/40	0.94	0.08	46,62,103,107	0
25	BCR	H	101	40/40	0.94	0.08	49,66,82,87	0
25	BCR	K	102	40/40	0.94	0.09	58,67,79,84	0
23	CLA	C	506	65/65	0.94	0.08	57,71,122,143	0
25	BCR	Y	101	40/40	0.94	0.08	53,66,81,88	0
29	PL9	D	406[A]	55/55	0.94	0.07	39,50,60,73	55
29	PL9	D	406[B]	55/55	0.94	0.07	39,50,60,73	55
35	DGD	c	517[A]	62/66	0.94	0.07	50,65,99,107	62
35	DGD	c	517[B]	62/66	0.94	0.07	50,65,100,107	62
35	DGD	c	518[A]	62/66	0.94	0.07	53,68,119,132	62
35	DGD	c	518[B]	62/66	0.94	0.07	53,68,119,133	62
35	DGD	c	519	62/66	0.94	0.07	51,68,101,132	0
25	BCR	c	515	40/40	0.94	0.08	68,80,93,96	0
23	CLA	b	614	65/65	0.94	0.07	42,51,101,119	0
36	CA	o	301	1/1	0.94	0.05	104,104,104,104	0
25	BCR	A	409	40/40	0.95	0.07	40,52,65,71	0
25	BCR	B	618	40/40	0.95	0.06	44,57,74,83	0
23	CLA	B	606	65/65	0.95	0.08	44,59,106,130	0
23	CLA	D	404	65/65	0.95	0.08	48,60,122,143	0
23	CLA	a	405[A]	65/65	0.95	0.07	42,54,121,135	65
23	CLA	a	405[B]	65/65	0.95	0.07	42,54,121,135	65
23	CLA	a	407	65/65	0.95	0.10	45,58,147,168	0
33	LHG	b	629[A]	49/49	0.95	0.08	50,59,71,93	49
33	LHG	b	629[B]	49/49	0.95	0.08	50,59,71,94	49
33	LHG	d	408[A]	49/49	0.95	0.08	52,65,110,124	49
33	LHG	d	408[B]	49/49	0.95	0.08	52,65,110,124	49
33	LHG	d	414[A]	49/49	0.95	0.09	55,68,80,91	49
33	LHG	d	414[B]	49/49	0.95	0.09	55,69,80,91	49
23	CLA	B	611	65/65	0.95	0.07	38,47,67,77	0
29	PL9	d	406[A]	55/55	0.95	0.07	42,52,62,71	55

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	PL9	d	406[B]	55/55	0.95	0.07	42,53,62,71	55
23	CLA	b	606	65/65	0.95	0.07	45,60,112,121	0
25	BCR	a	408	40/40	0.95	0.06	46,55,66,71	0
25	BCR	b	618	40/40	0.95	0.06	45,58,78,85	0
25	BCR	b	619	40/40	0.95	0.07	50,66,88,92	0
23	CLA	b	612	65/65	0.95	0.08	42,54,66,75	0
23	CLA	B	614	65/65	0.95	0.07	41,50,106,118	0
25	BCR	h	101	40/40	0.95	0.08	57,70,91,98	0
23	CLA	B	616	65/65	0.95	0.09	46,60,132,143	0
35	DGD	C	516[A]	62/66	0.95	0.07	48,59,99,107	62
35	DGD	C	516[B]	62/66	0.95	0.07	48,59,99,107	62
25	BCR	y	101	40/40	0.95	0.07	59,71,85,102	0
23	CLA	C	501	65/65	0.95	0.07	49,61,72,80	0
35	DGD	C	518	62/66	0.95	0.07	46,62,94,114	0
35	DGD	H	102	62/66	0.95	0.09	46,61,80,94	0
27	GOL	c	526[A]	6/6	0.95	0.08	66,69,73,74	6
27	GOL	c	526[B]	6/6	0.95	0.08	66,69,73,74	6
23	CLA	A	408	65/65	0.95	0.08	43,53,132,147	0
23	CLA	c	508	65/65	0.95	0.08	54,69,86,92	0
23	CLA	c	509	65/65	0.95	0.07	47,63,123,148	0
35	DGD	h	102	62/66	0.95	0.08	52,66,82,87	0
23	CLA	B	603	65/65	0.95	0.08	45,53,72,83	0
23	CLA	C	508	65/65	0.95	0.07	47,56,111,146	0
23	CLA	C	512	65/65	0.95	0.08	57,74,115,133	0
37	BCT	d	401[A]	4/4	0.95	0.07	59,63,67,79	4
37	BCT	d	401[B]	4/4	0.95	0.07	59,64,67,80	4
33	LHG	L	101[A]	49/49	0.96	0.07	50,58,71,92	49
33	LHG	L	101[B]	49/49	0.96	0.07	49,58,71,92	49
27	GOL	b	628	6/6	0.96	0.07	78,86,89,89	0
23	CLA	b	611	65/65	0.96	0.06	39,50,72,82	0
23	CLA	C	503	65/65	0.96	0.06	51,61,72,78	0
30	UNL	x	101	18/-	0.96	0.10	72,82,136,137	0
33	LHG	d	407[A]	49/49	0.96	0.07	49,57,71,77	49
33	LHG	d	407[B]	49/49	0.96	0.07	49,57,72,78	49
23	CLA	B	602	65/65	0.96	0.07	45,57,73,89	0
25	BCR	c	516	40/40	0.96	0.07	55,67,77,93	0
23	CLA	C	505	65/65	0.96	0.07	48,60,89,106	0
23	CLA	c	502	65/65	0.96	0.07	56,68,81,89	0
25	BCR	k	101	40/40	0.96	0.08	56,74,87,91	0
23	CLA	c	504	65/65	0.96	0.06	51,71,84,98	0
23	CLA	A	405[A]	65/65	0.96	0.06	38,45,56,70	65
23	CLA	c	506	65/65	0.96	0.07	49,65,91,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	C	507	65/65	0.96	0.07	49,64,82,96	0
23	CLA	A	405[B]	65/65	0.96	0.06	37,45,56,70	65
23	CLA	C	509	65/65	0.96	0.08	46,60,85,93	0
23	CLA	c	512	65/65	0.96	0.07	57,68,88,104	0
23	CLA	B	607	65/65	0.96	0.06	36,49,73,84	0
23	CLA	B	609	65/65	0.96	0.07	43,59,71,80	0
23	CLA	B	610	65/65	0.96	0.08	43,56,67,85	0
24	PHO	A	416[A]	64/64	0.96	0.06	39,51,57,64	64
24	PHO	A	416[B]	64/64	0.96	0.06	38,51,57,65	64
24	PHO	a	414[A]	64/64	0.96	0.06	45,55,62,67	64
24	PHO	a	414[B]	64/64	0.96	0.06	45,55,62,67	64
23	CLA	A	406[A]	65/65	0.96	0.06	41,48,114,126	65
25	BCR	B	617	40/40	0.96	0.06	42,53,64,66	0
23	CLA	B	613	65/65	0.96	0.06	40,47,94,117	0
23	CLA	A	406[B]	65/65	0.96	0.06	41,48,114,126	65
23	CLA	A	404[A]	65/65	0.96	0.06	37,44,62,70	65
25	BCR	C	515	40/40	0.96	0.06	50,65,76,85	0
23	CLA	b	602	65/65	0.96	0.07	48,60,80,86	0
23	CLA	b	603	65/65	0.96	0.06	45,57,81,98	0
23	CLA	b	604	65/65	0.96	0.07	39,52,101,120	0
36	CA	c	523	1/1	0.96	0.07	75,75,75,75	0
23	CLA	A	404[B]	65/65	0.96	0.06	37,44,63,70	65
23	CLA	b	607	65/65	0.96	0.07	38,49,81,92	0
23	CLA	b	609	65/65	0.96	0.06	47,65,78,89	0
25	BCR	b	617	40/40	0.96	0.06	46,55,65,68	0
23	CLA	d	402[A]	65/65	0.97	0.05	40,45,63,73	65
23	CLA	d	402[B]	65/65	0.97	0.05	40,45,64,73	65
23	CLA	d	403[A]	65/65	0.97	0.06	39,47,77,91	65
23	CLA	d	403[B]	65/65	0.97	0.06	39,47,77,91	65
22	CL	A	403[A]	1/1	0.97	0.03	47,47,47,47	1
24	PHO	A	407[A]	64/64	0.97	0.05	38,47,55,57	64
24	PHO	A	407[B]	64/64	0.97	0.05	38,47,55,57	64
23	CLA	b	605	65/65	0.97	0.07	39,51,72,81	0
23	CLA	B	612	65/65	0.97	0.06	37,50,64,71	0
24	PHO	a	406[A]	64/64	0.97	0.05	44,50,54,57	64
24	PHO	a	406[B]	64/64	0.97	0.05	44,50,54,58	64
22	CL	A	403[B]	1/1	0.97	0.03	47,47,47,47	1
23	CLA	b	608	65/65	0.97	0.05	43,57,78,91	0
23	CLA	C	510	65/65	0.97	0.06	46,60,82,88	0
23	CLA	b	610	65/65	0.97	0.07	49,58,69,74	0
23	CLA	C	511	65/65	0.97	0.07	49,65,83,87	0
23	CLA	B	604	65/65	0.97	0.06	38,48,111,141	0

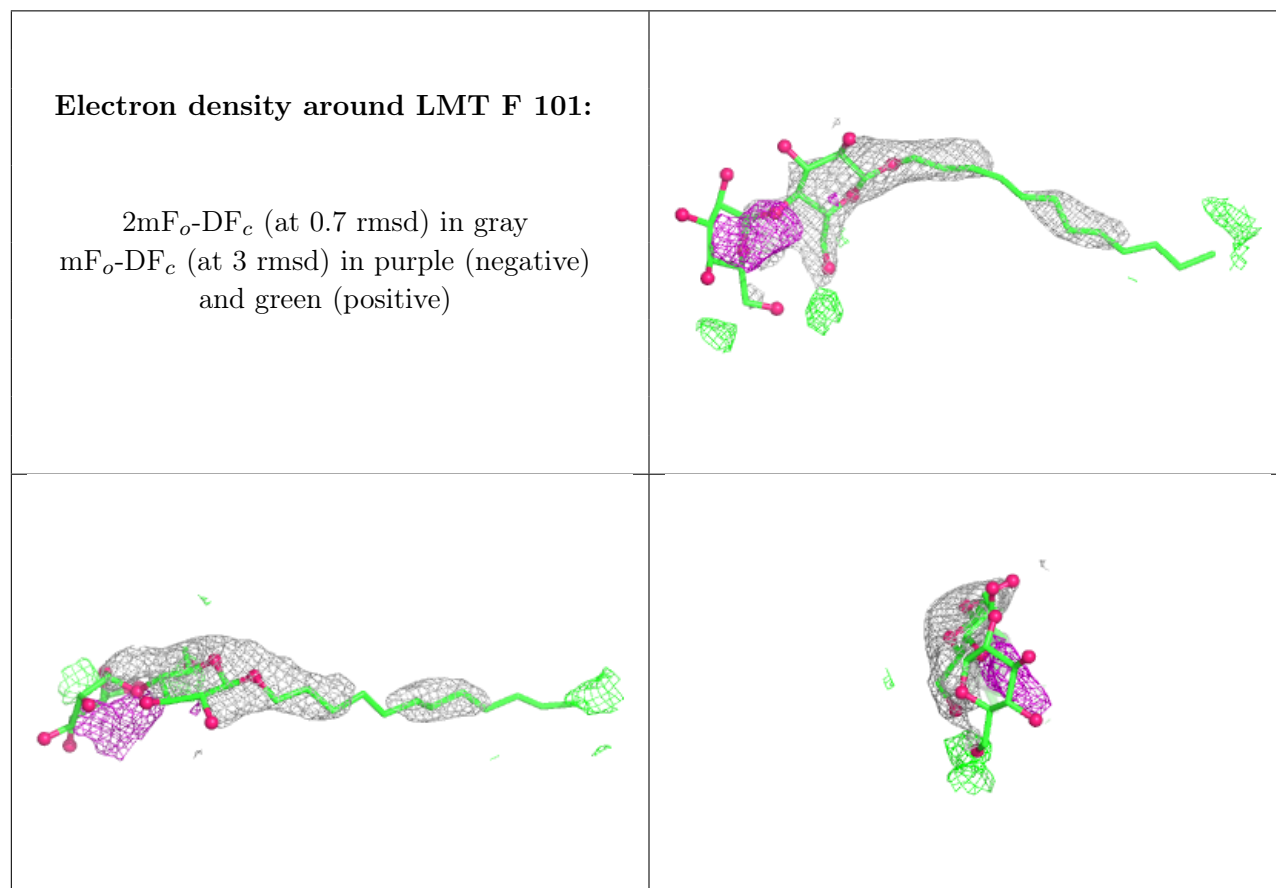
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	b	613	65/65	0.97	0.06	42,50,90,102	0
23	CLA	B	615	65/65	0.97	0.06	43,54,80,90	0
23	CLA	b	615	65/65	0.97	0.06	46,59,79,92	0
23	CLA	D	403[A]	65/65	0.97	0.06	34,44,71,78	65
23	CLA	D	403[B]	65/65	0.97	0.06	34,44,72,79	65
23	CLA	c	503	65/65	0.97	0.06	44,59,89,106	0
23	CLA	B	605	65/65	0.97	0.06	40,49,66,84	0
23	CLA	a	404[A]	65/65	0.97	0.06	39,48,64,75	65
33	LHG	D	407[A]	49/49	0.97	0.07	48,56,68,81	49
33	LHG	D	407[B]	49/49	0.97	0.07	47,56,68,81	49
23	CLA	a	404[B]	65/65	0.97	0.06	39,48,65,75	65
22	CL	a	403[A]	1/1	0.97	0.08	52,52,52,52	1
23	CLA	C	502	65/65	0.97	0.06	45,56,83,92	0
36	CA	C	523	1/1	0.97	0.06	75,75,75,75	0
22	CL	a	403[B]	1/1	0.97	0.08	52,52,52,52	1
36	CA	O	301	1/1	0.97	0.04	105,105,105,105	0
23	CLA	c	510	65/65	0.97	0.07	47,63,88,100	0
23	CLA	c	511	65/65	0.97	0.06	51,65,80,93	0
23	CLA	B	608	65/65	0.97	0.05	43,51,71,83	0
37	BCT	D	401[A]	4/4	0.97	0.06	55,60,61,68	4
37	BCT	D	401[B]	4/4	0.97	0.06	55,57,62,72	4
22	CL	A	402[A]	1/1	0.97	0.06	44,44,44,44	1
22	CL	A	402[B]	1/1	0.97	0.06	44,44,44,44	1
22	CL	a	402[B]	1/1	0.98	0.05	50,50,50,50	1
22	CL	a	402[A]	1/1	0.98	0.05	50,50,50,50	1
38	HEM	f	101	43/43	0.98	0.08	61,82,118,133	0
39	MG	J	102	1/1	0.98	0.04	59,59,59,59	0
40	HEC	V	201	43/43	0.98	0.06	39,50,58,63	0
40	HEC	v	201	43/43	0.98	0.07	52,63,72,74	0
21	FE2	a	401[B]	1/1	0.99	0.02	55,55,55,55	1
38	HEM	F	102	43/43	0.99	0.06	55,69,84,89	0
28	OEX	A	413[A]	10/10	0.99	0.03	40,44,50,50	10
28	OEX	A	413[B]	10/10	0.99	0.03	40,44,50,51	10
39	MG	j	102	1/1	0.99	0.07	63,63,63,63	0
21	FE2	a	401[A]	1/1	0.99	0.02	55,55,55,55	1
36	CA	c	524	1/1	0.99	0.04	77,77,77,77	0
28	OEX	a	411[A]	10/10	1.00	0.02	46,49,51,56	10
28	OEX	a	411[B]	10/10	1.00	0.02	46,50,54,56	10
21	FE2	A	401[A]	1/1	1.00	0.01	52,52,52,52	1
21	FE2	A	401[B]	1/1	1.00	0.01	52,52,52,52	1

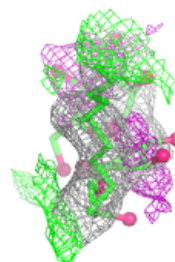
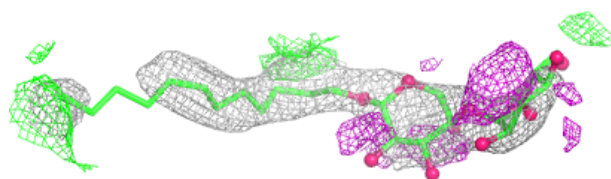
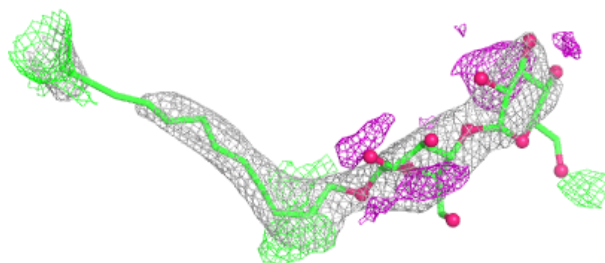
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

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

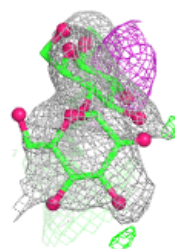
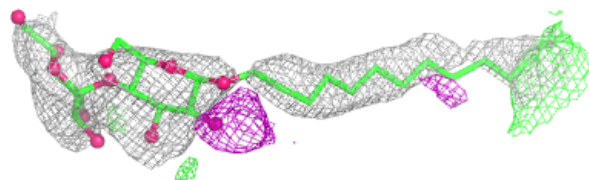
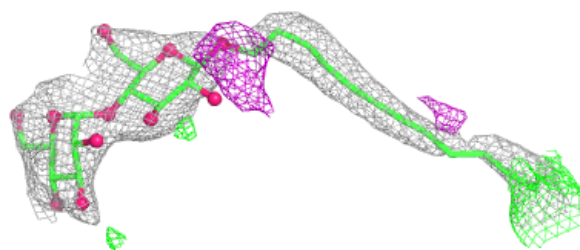


Electron density around LMT B 630:

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

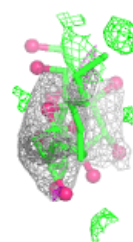
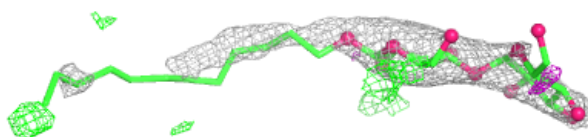
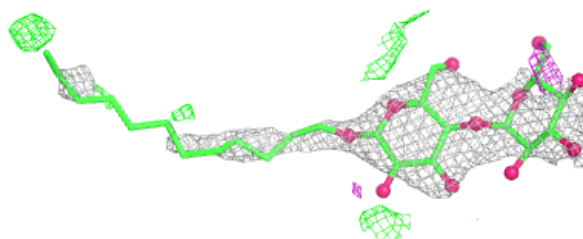
**Electron density around LMT A 417:**

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

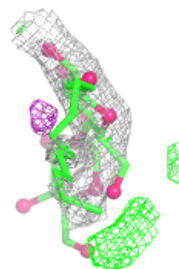
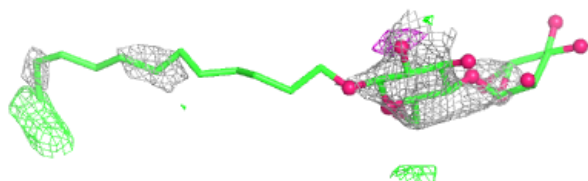
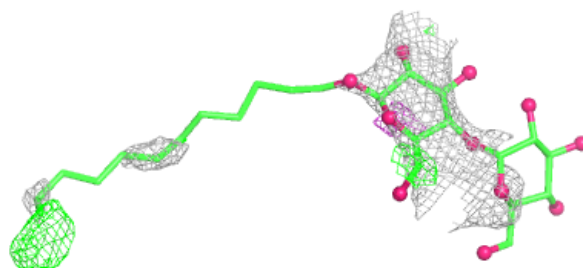


Electron density around LMT a 415:

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

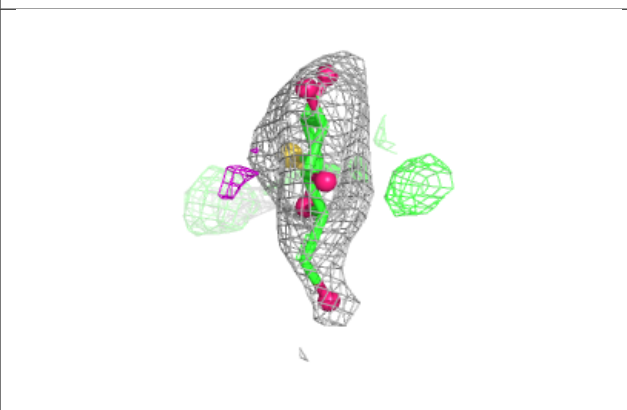
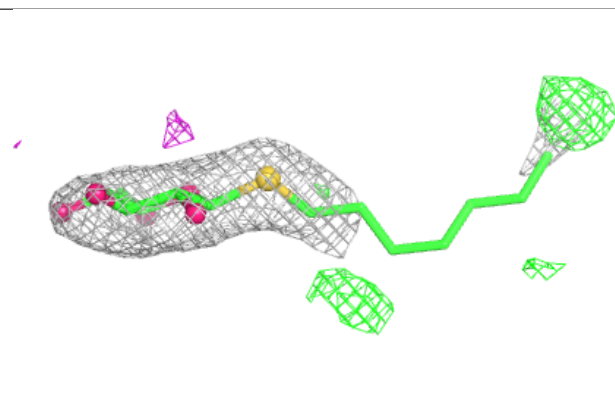
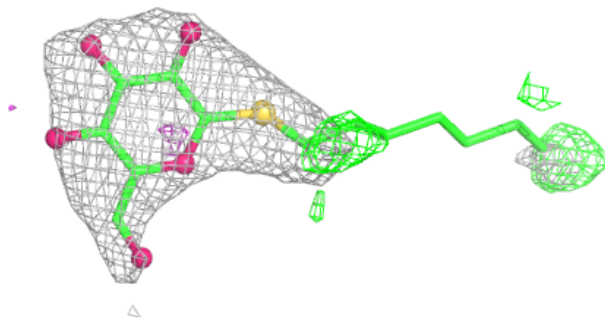
**Electron density around LMT e 101:**

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

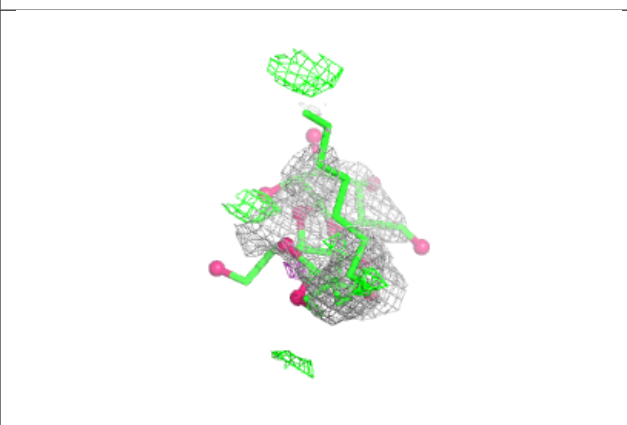
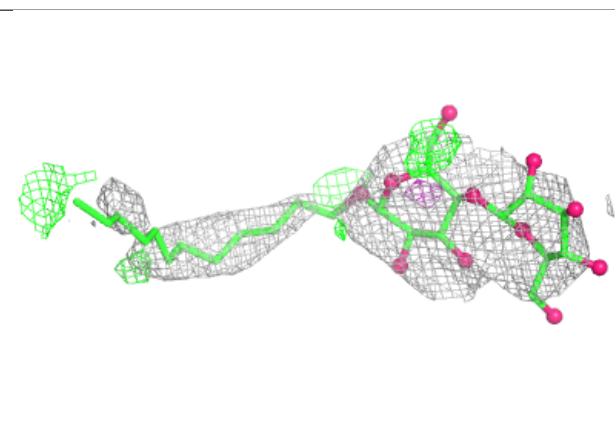
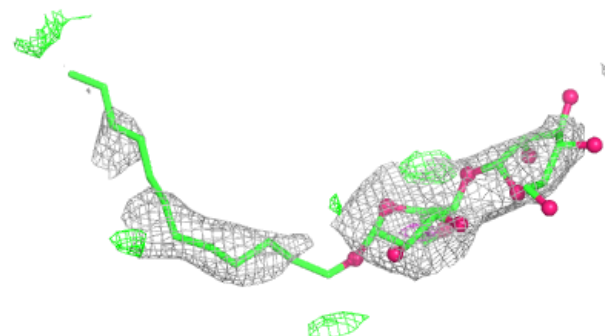


Electron density around HTG C 521:

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

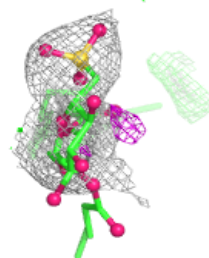
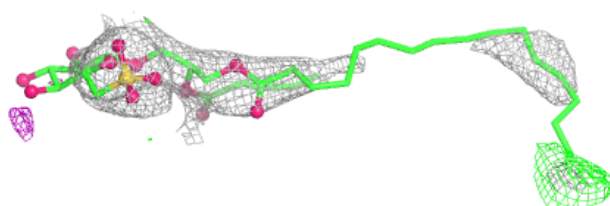
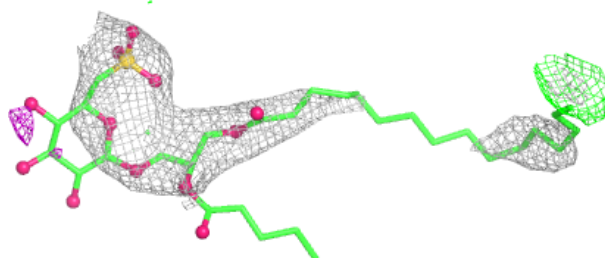
**Electron density around LMT A 420:**

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

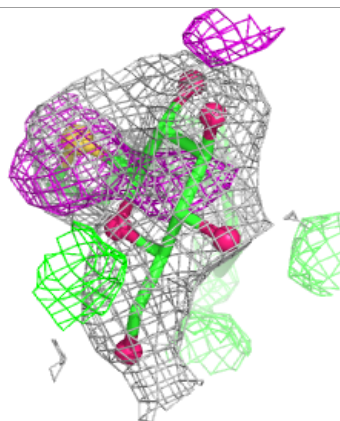
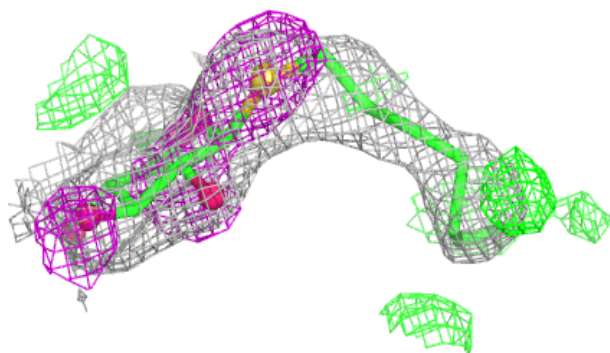
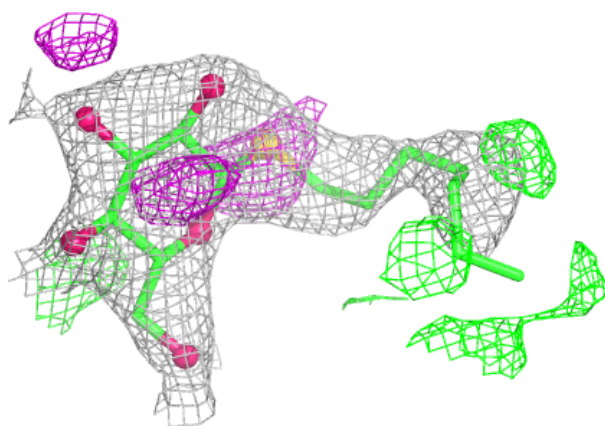


Electron density around SQD f 102:

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

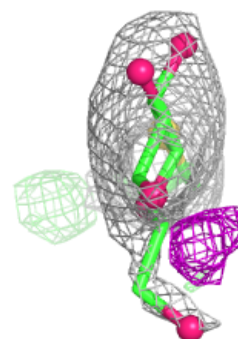
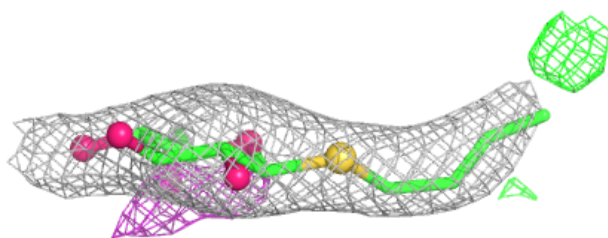
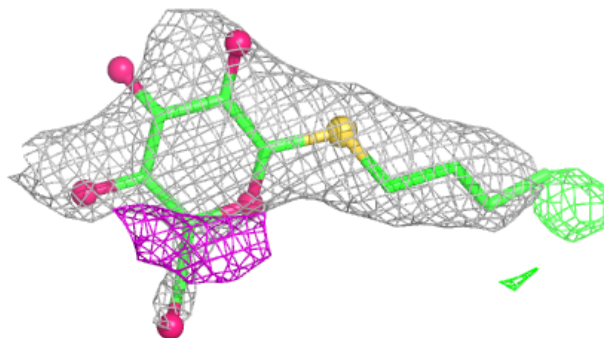
**Electron density around HTG B 623:**

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

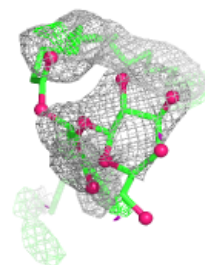
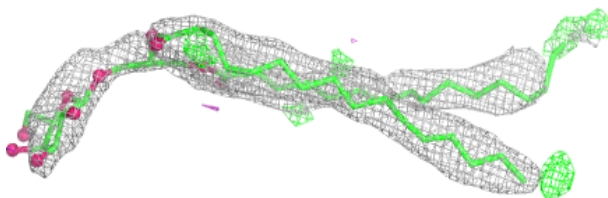
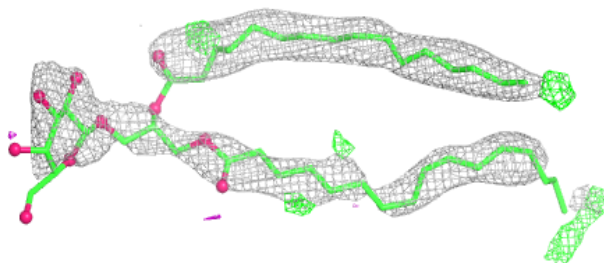


Electron density around HTG D 411:

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

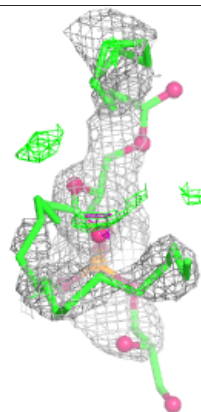
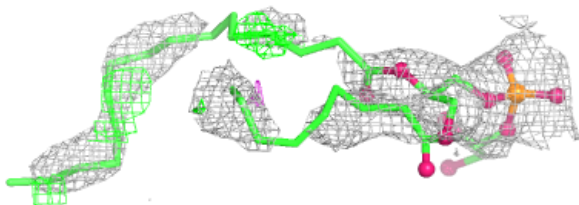
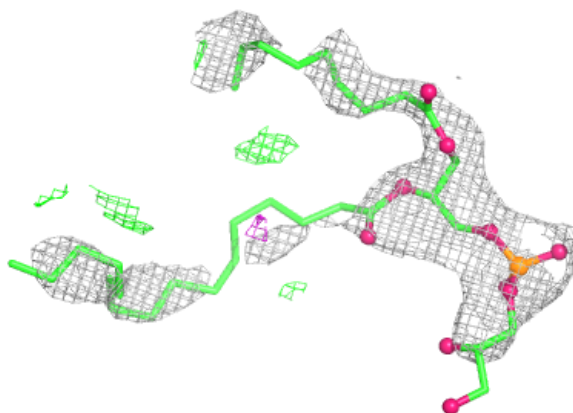
**Electron density around LMG C 520:**

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

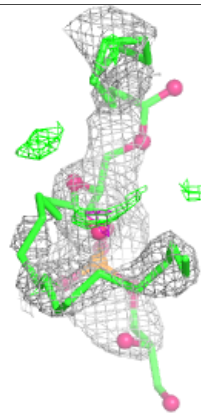
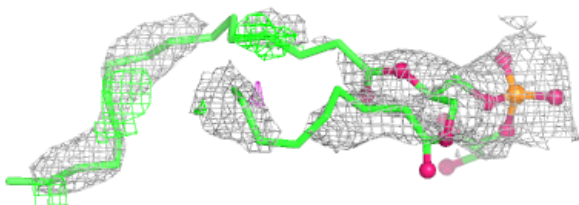
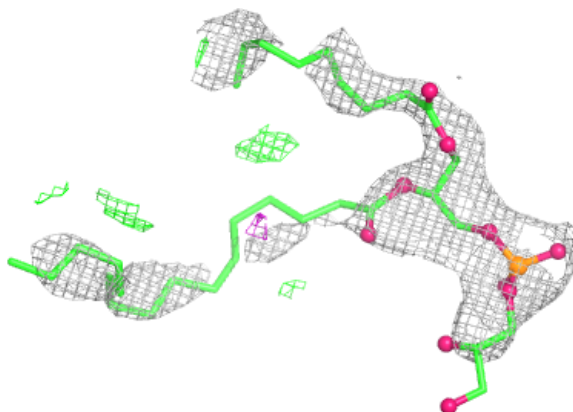


Electron density around LHG a 418 (A):

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

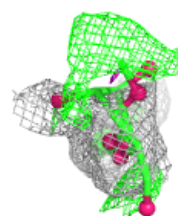
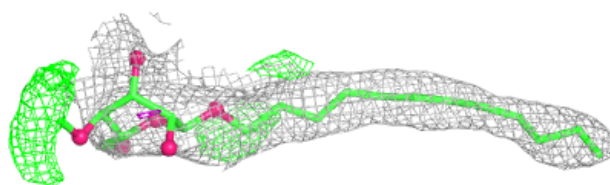
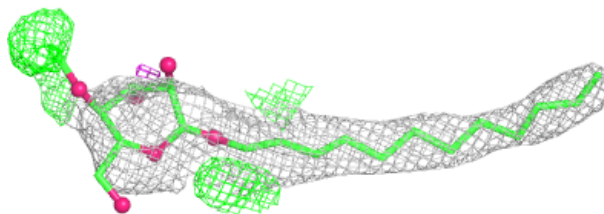
**Electron density around LHG a 418 (B):**

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



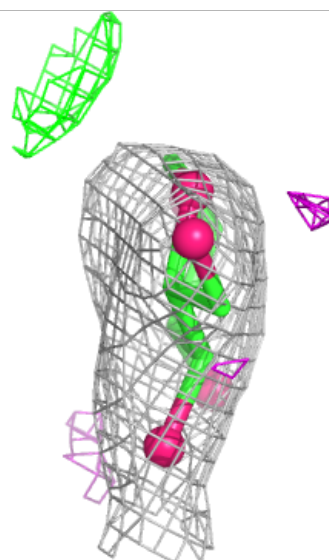
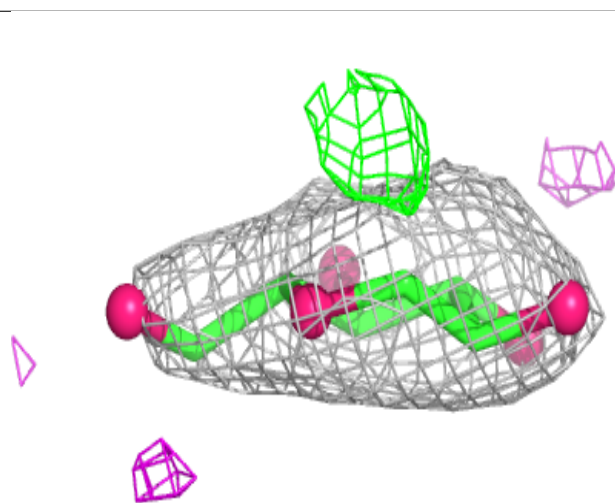
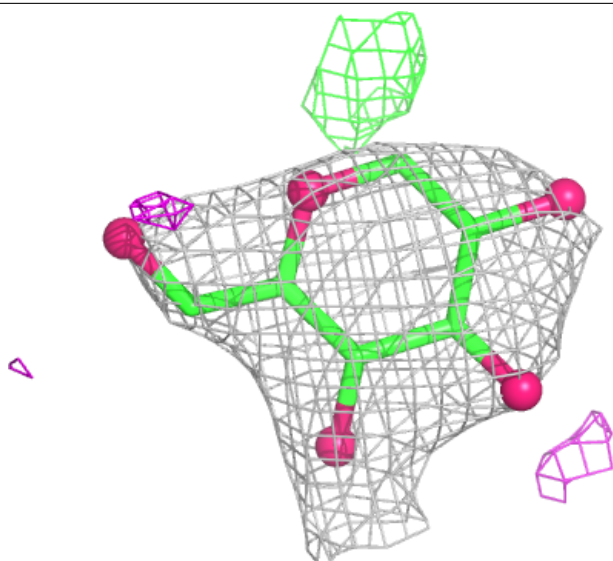
Electron density around LMT b 621:

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



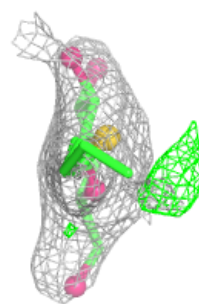
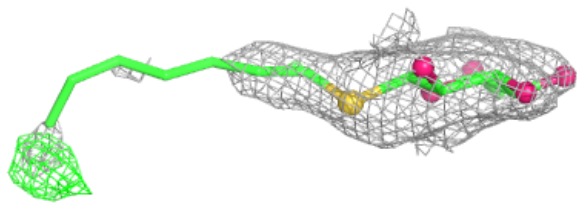
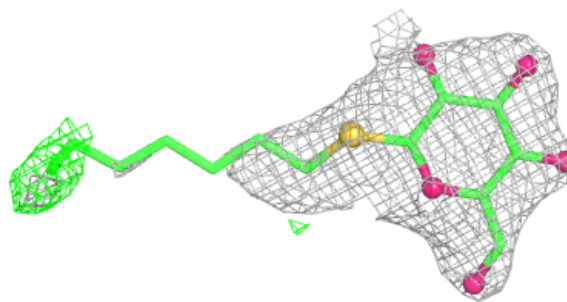
Electron density around HTG V 202:

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

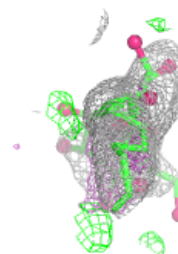
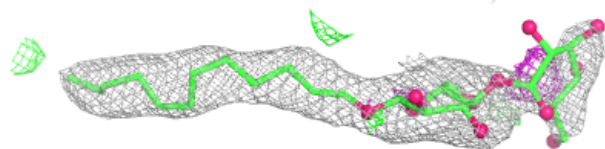
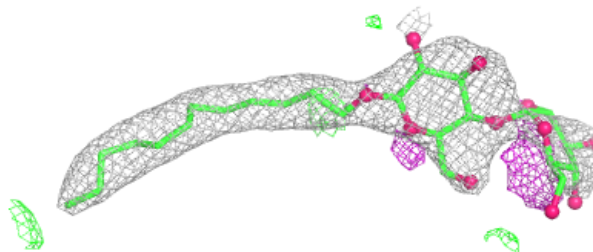


Electron density around HTG c 522:

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

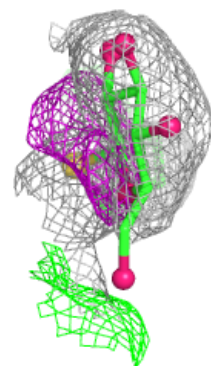
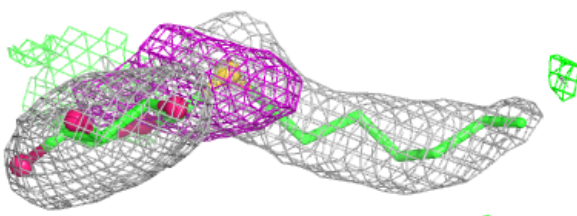
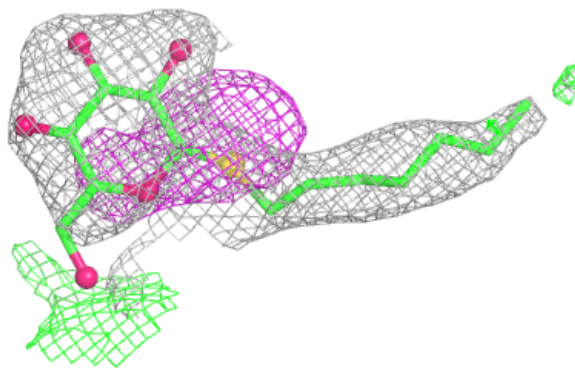
**Electron density around LMT B 628:**

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

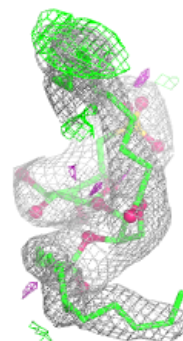
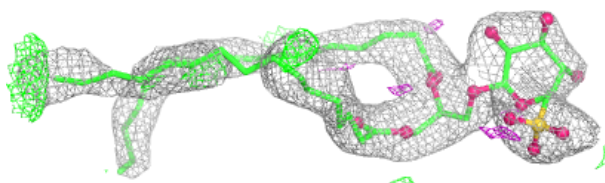
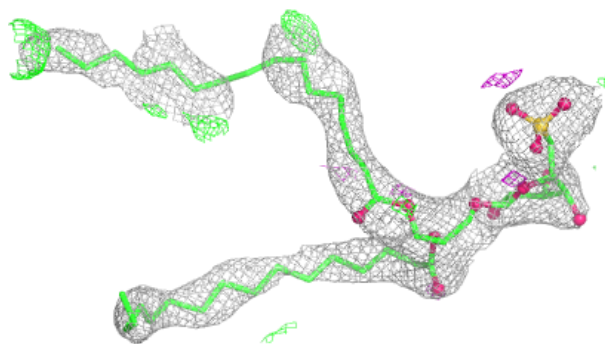


Electron density around HTG b 622:

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

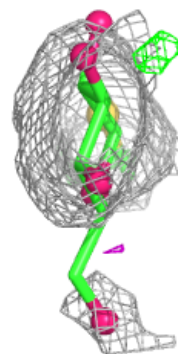
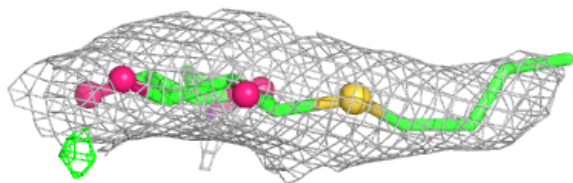
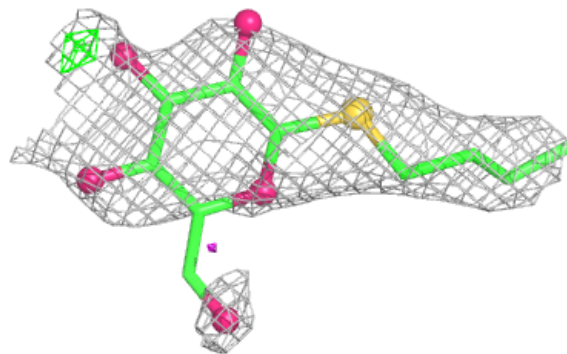
**Electron density around SQD a 410:**

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

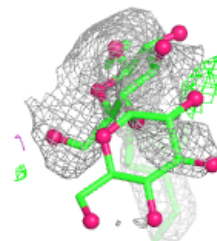
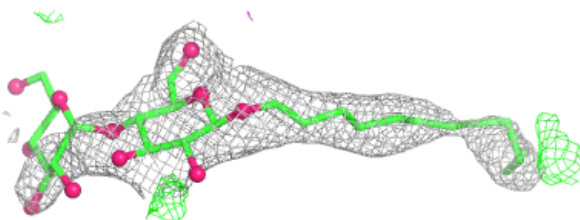
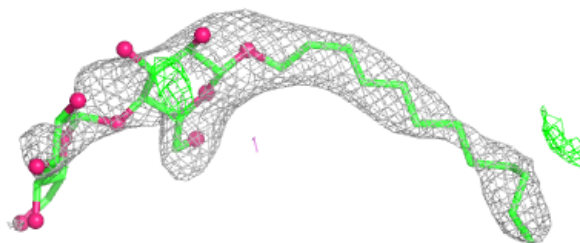


Electron density around HTG d 411:

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

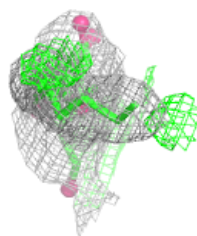
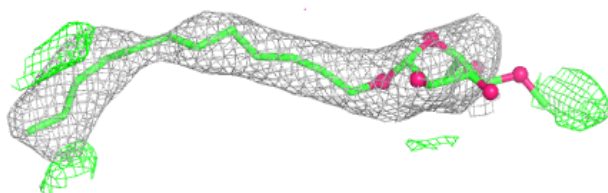
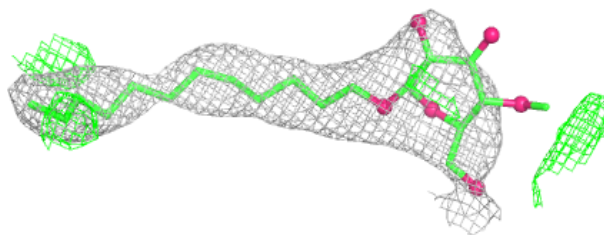
**Electron density around LMT M 102:**

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

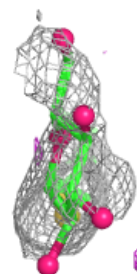
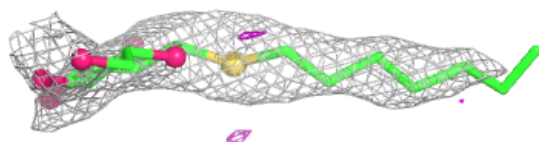
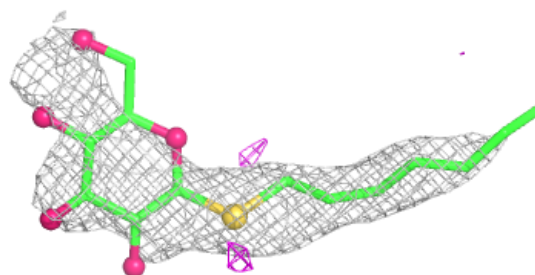


Electron density around LMT B 631:

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

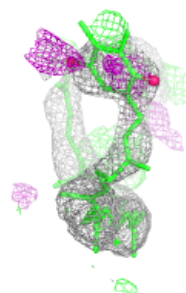
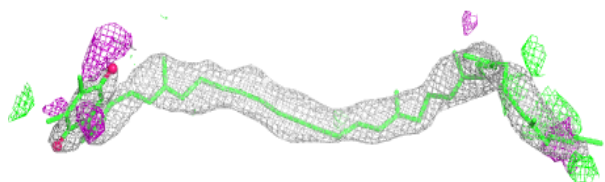
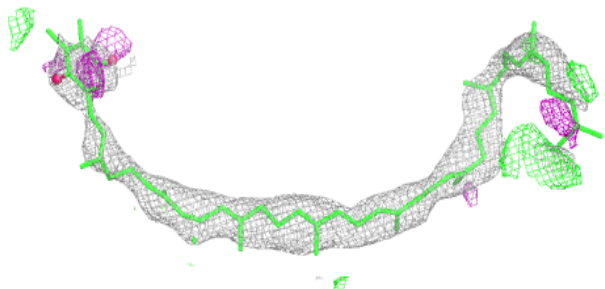
**Electron density around HTG b 623:**

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

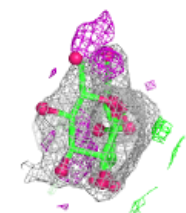
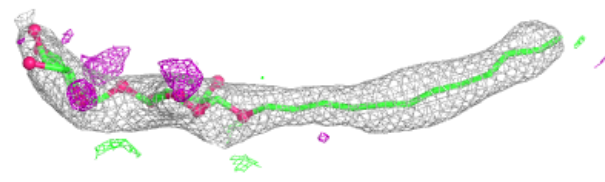
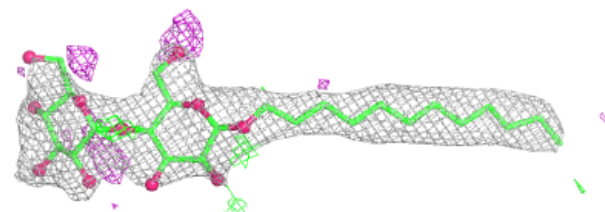


Electron density around PL9 A 414 (B):

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

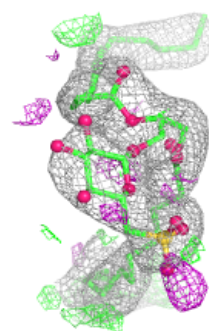
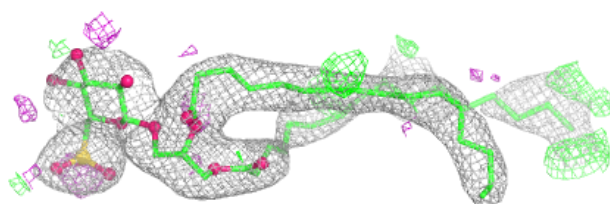
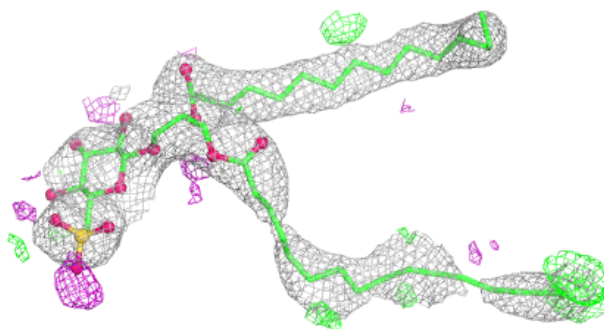
**Electron density around LMT m 103:**

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

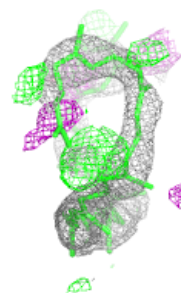
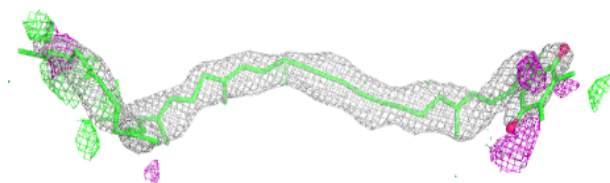
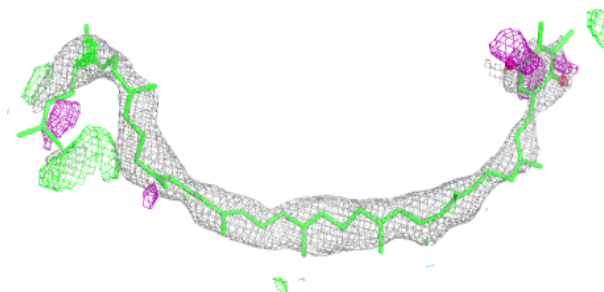


Electron density around SQD A 412:

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

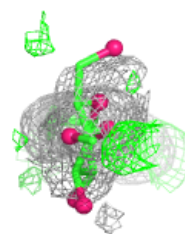
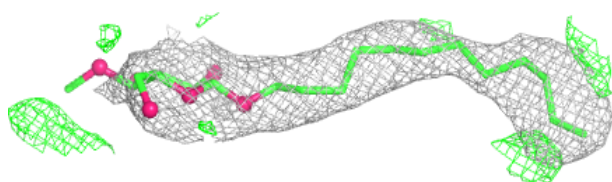
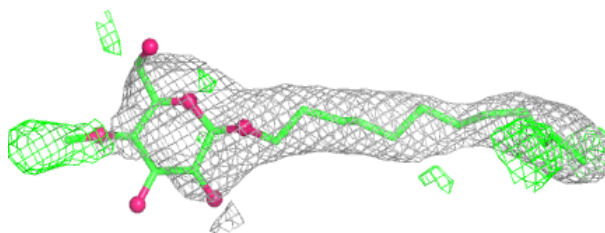
**Electron density around PL9 A 414 (A):**

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

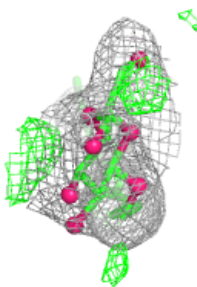
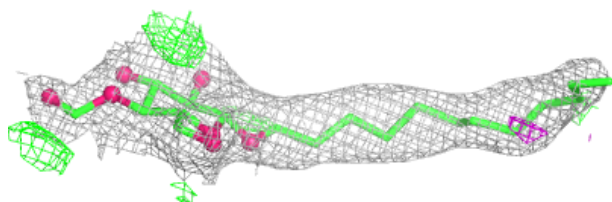
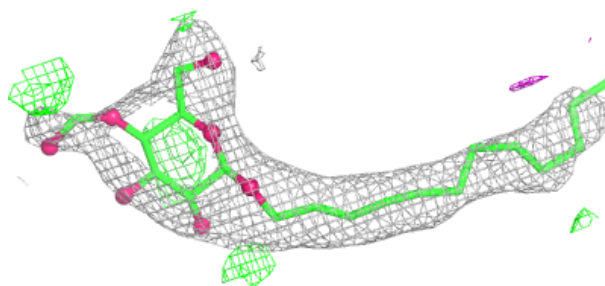


Electron density around LMT b 627:

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

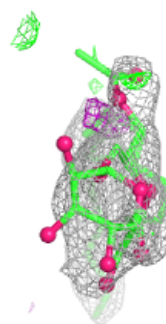
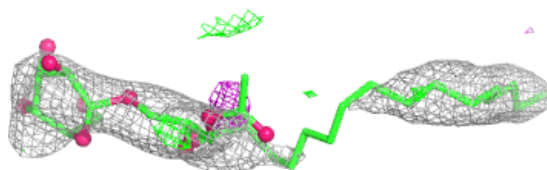
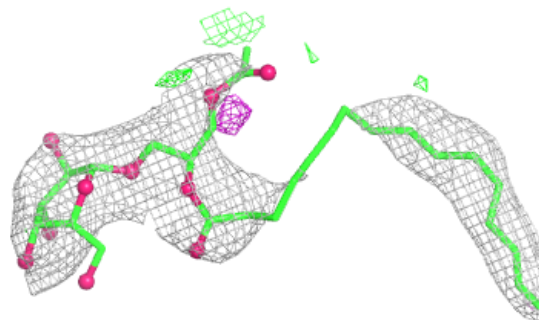
**Electron density around LMT t 101:**

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

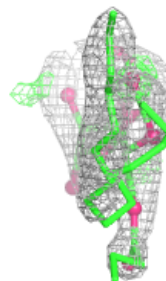
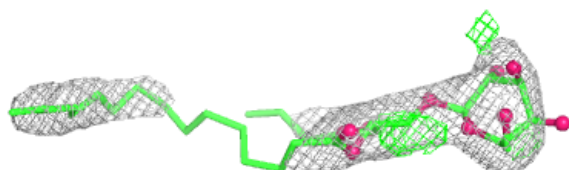
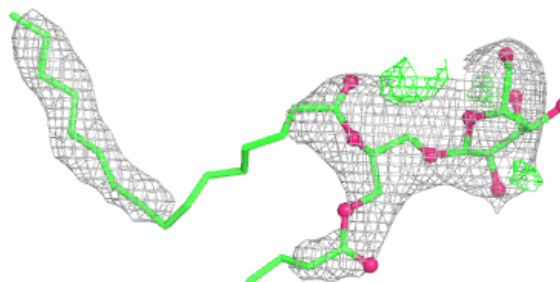


Electron density around LMG Z 101:

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

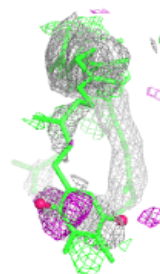
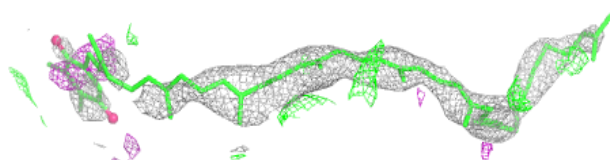
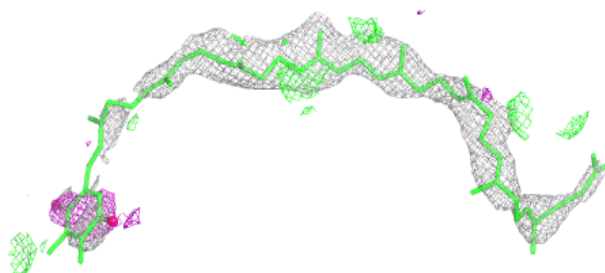
**Electron density around LMG z 101:**

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

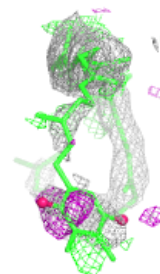
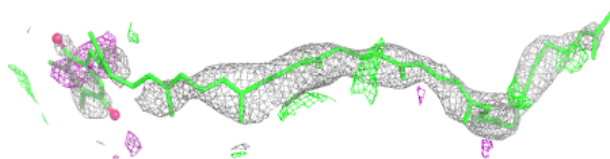
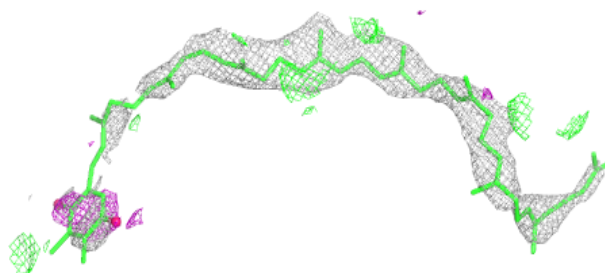


Electron density around PL9 a 412 (A):

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

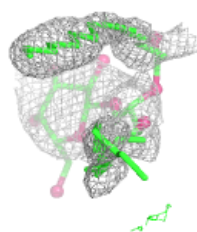
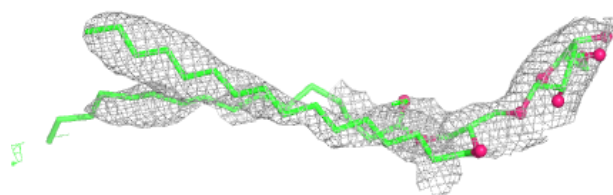
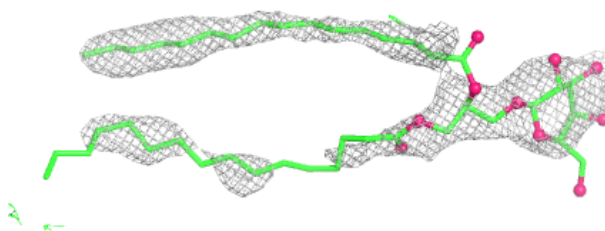
**Electron density around PL9 a 412 (B):**

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

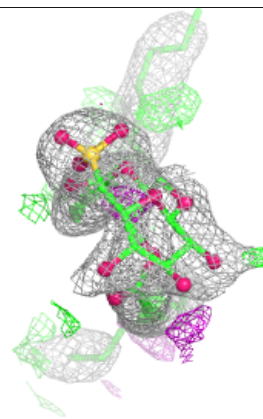
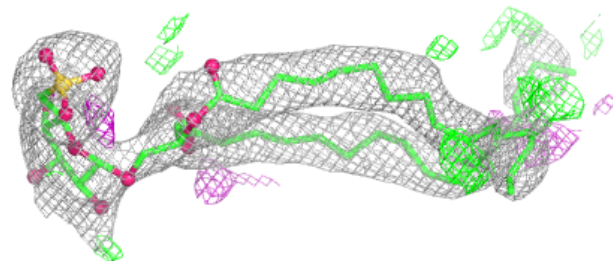
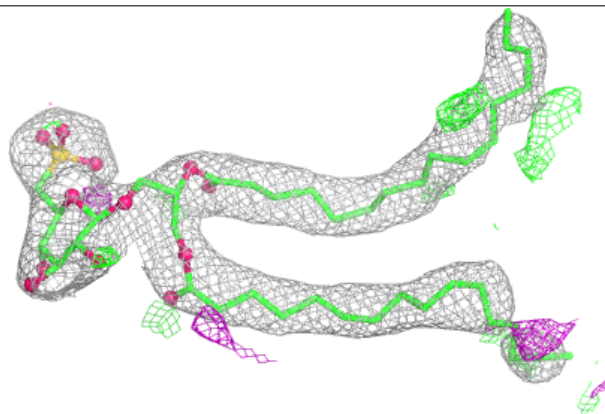


Electron density around LMG c 521:

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

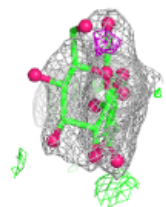
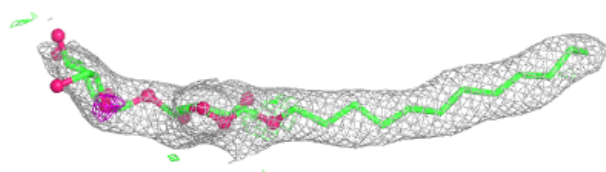
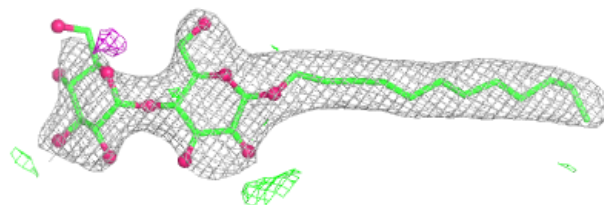
**Electron density around SQD b 620:**

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

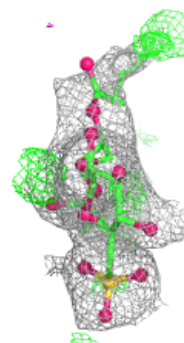
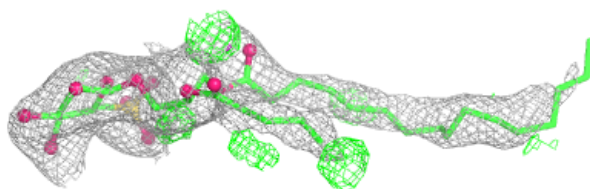
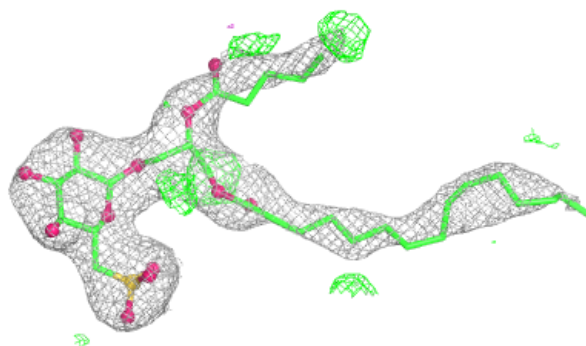


Electron density around LMT M 101:

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

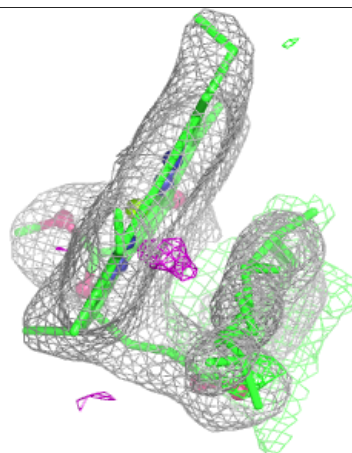
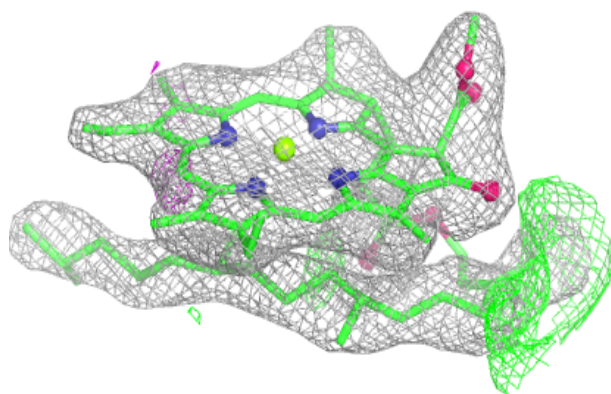
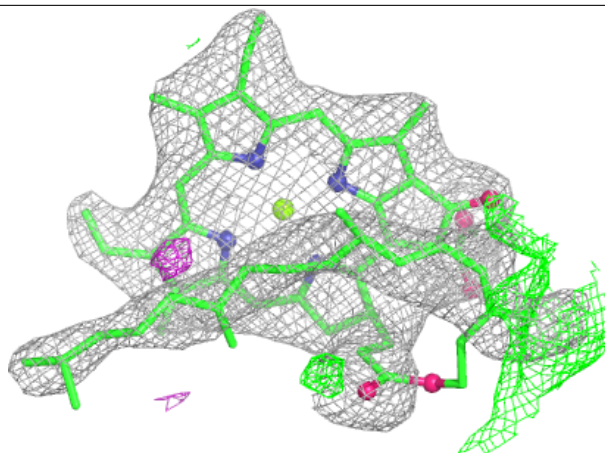
**Electron density around SQD F 103:**

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



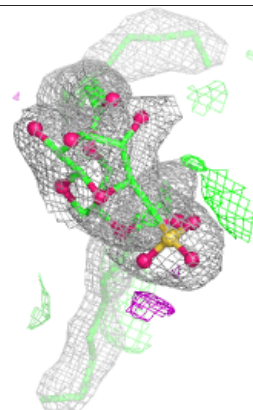
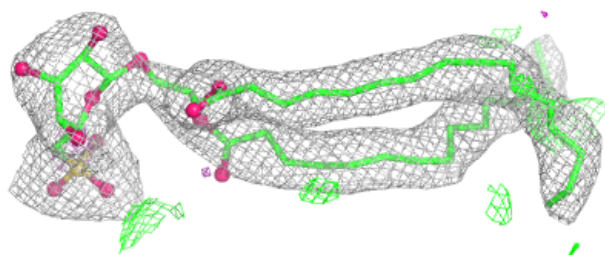
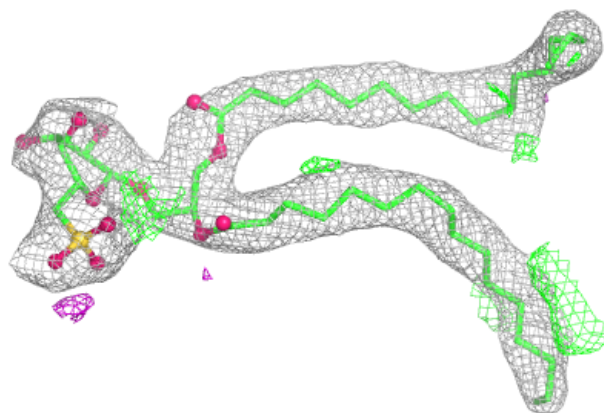
Electron density around CLA b 601:

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



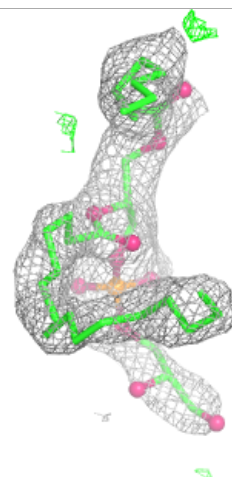
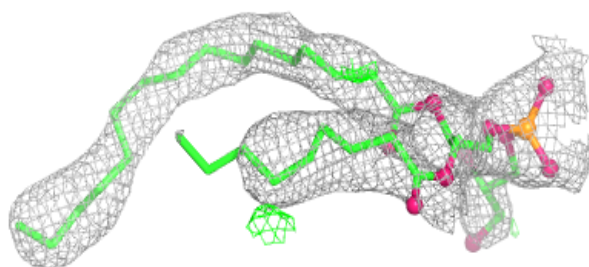
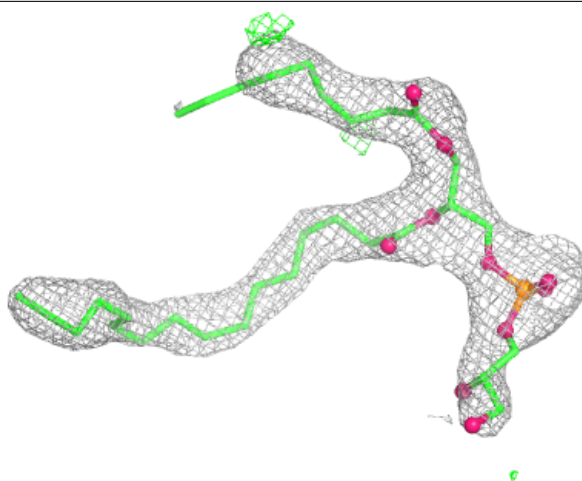
Electron density around SQD B 620:

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



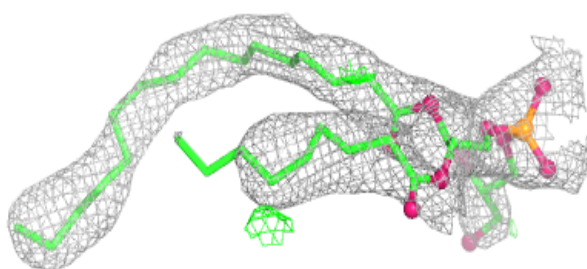
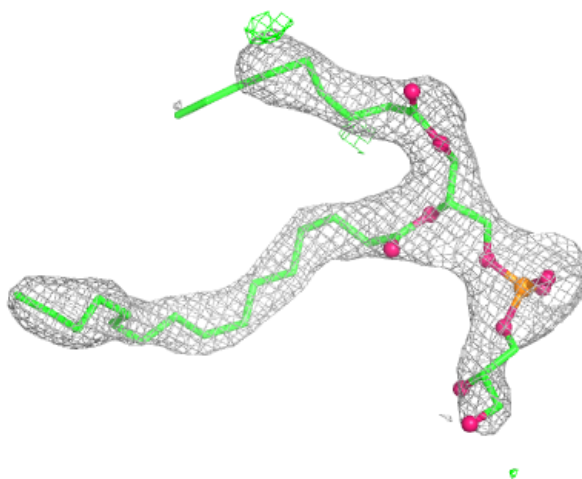
Electron density around LHG E 101 (A):

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



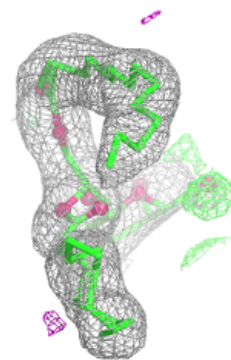
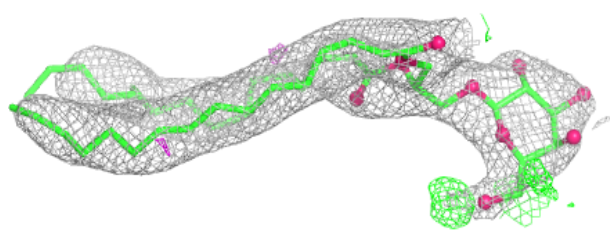
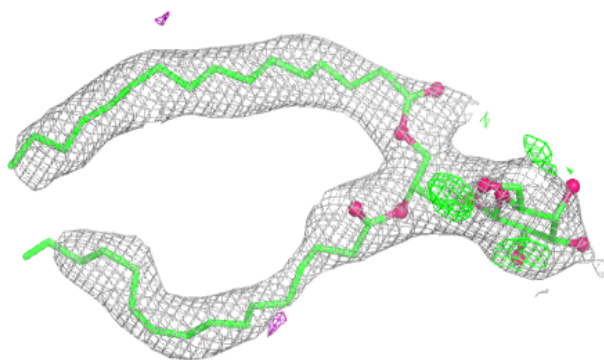
Electron density around LHG E 101 (B):

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

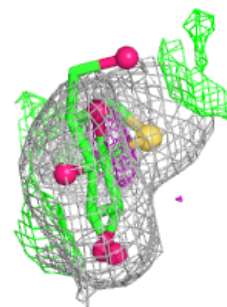
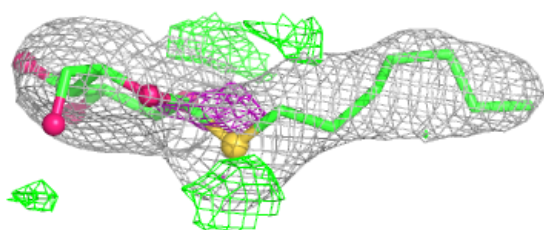
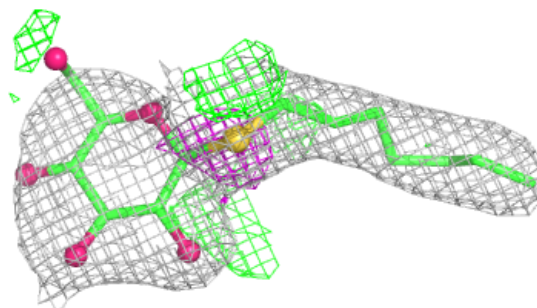


Electron density around LMG A 418:

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

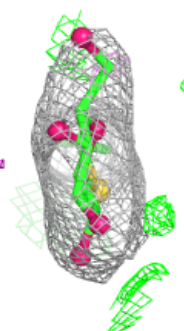
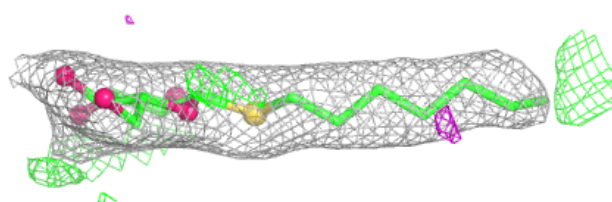
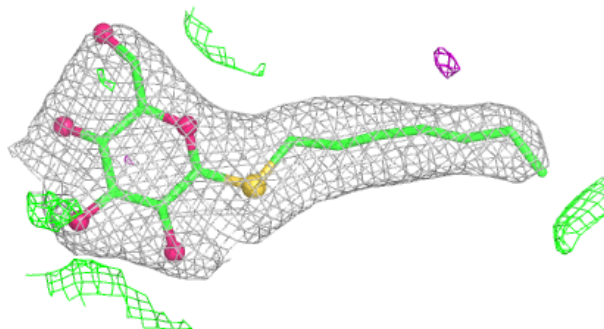
**Electron density around HTG B 622:**

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

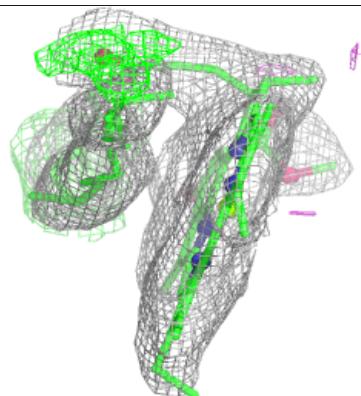
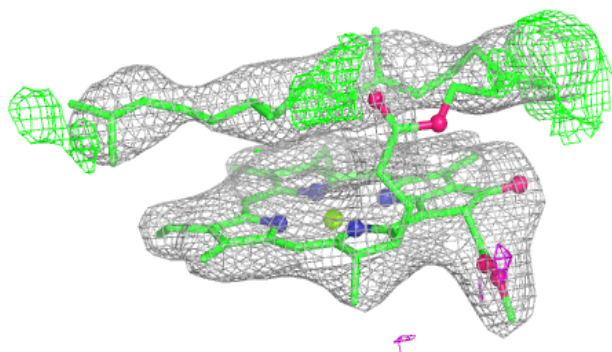
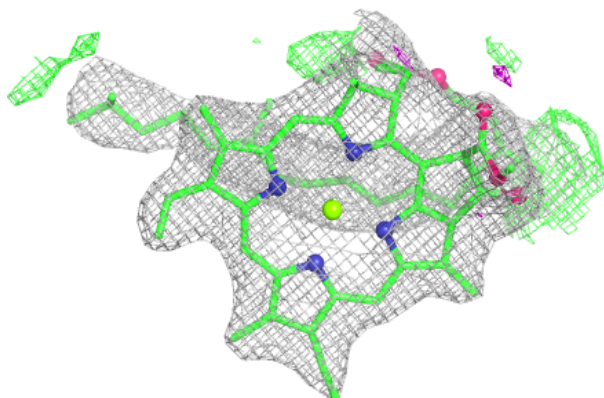


Electron density around HTG B 625:

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

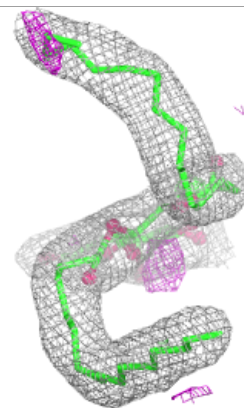
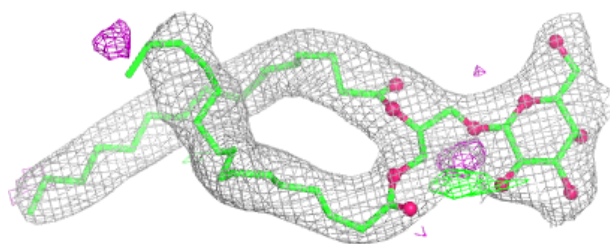
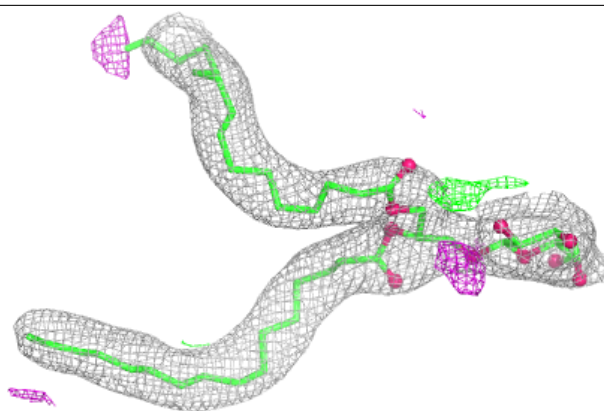
**Electron density around CLA B 601:**

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

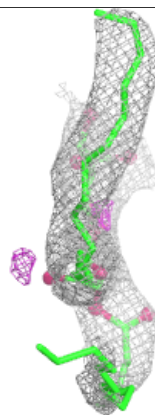
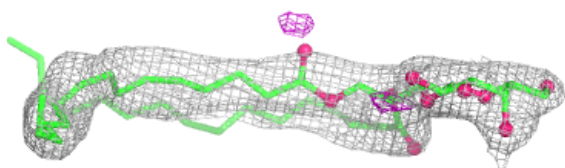
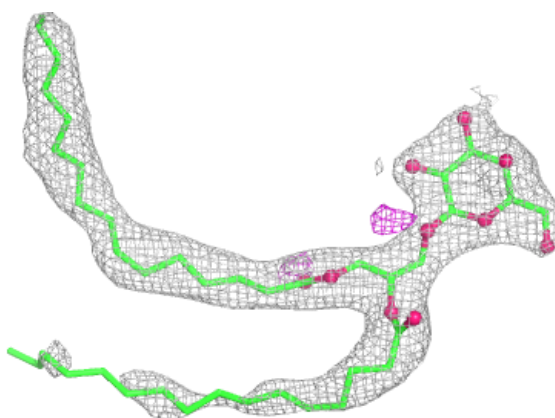


Electron density around LMG m 101:

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

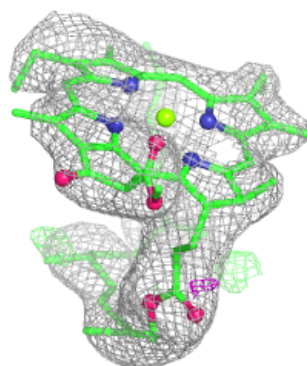
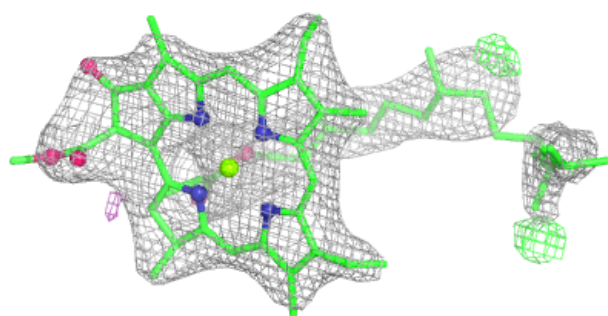
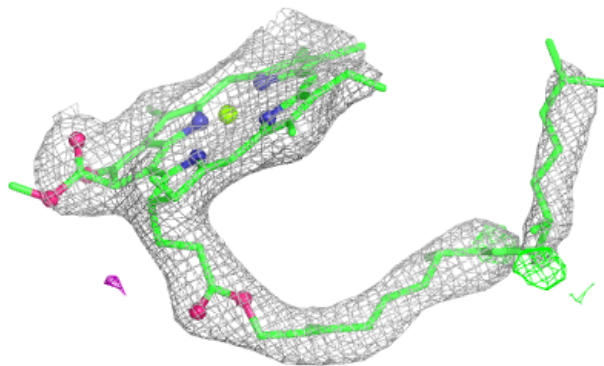
**Electron density around LMG C 519:**

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

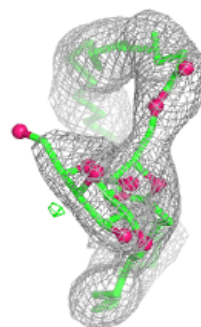
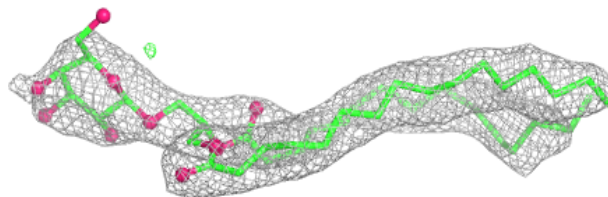
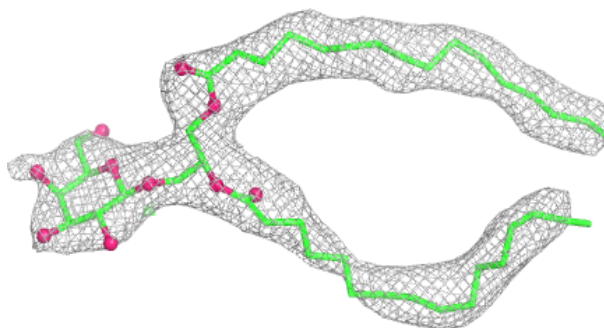


Electron density around CLA c 514:

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

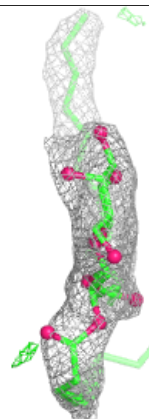
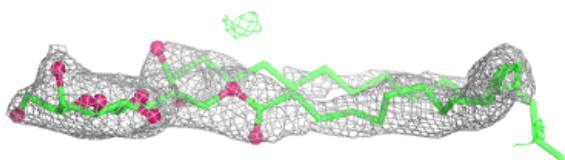
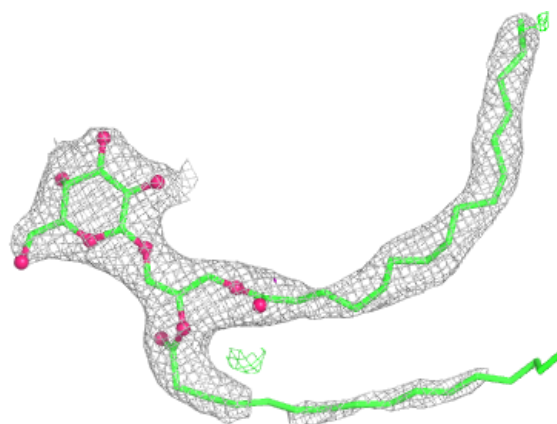
**Electron density around LMG c 501:**

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

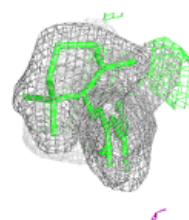
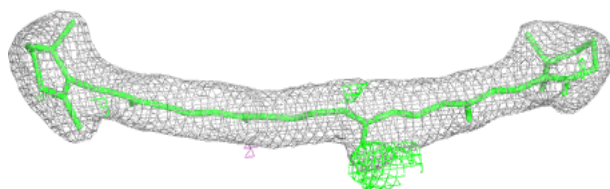
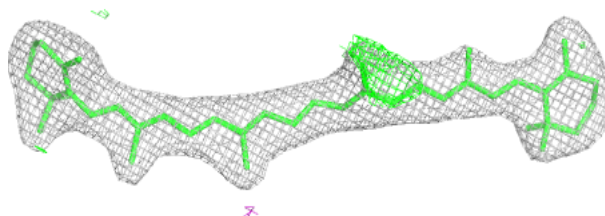


Electron density around LMG c 520:

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

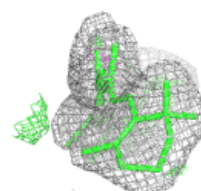
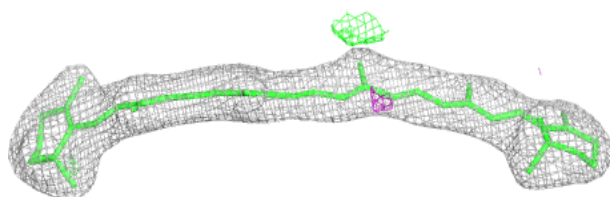
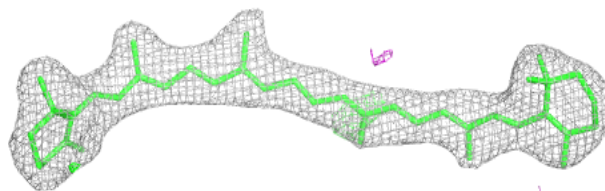
**Electron density around BCR T 101:**

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

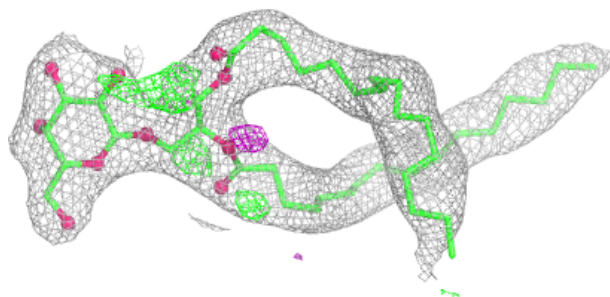
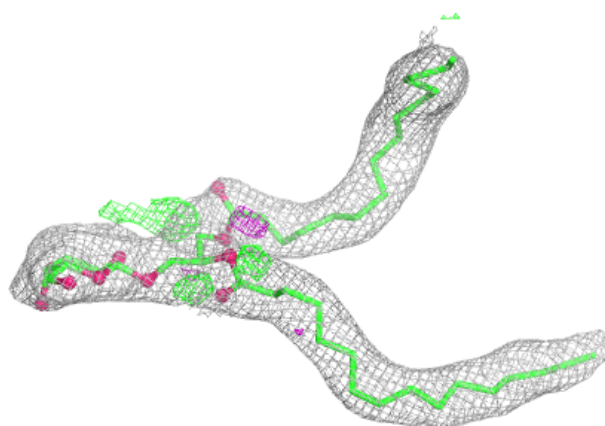


Electron density around BCR t 102:

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

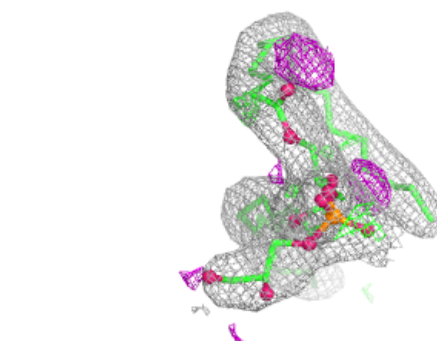
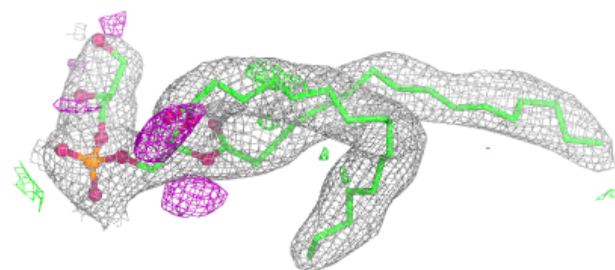
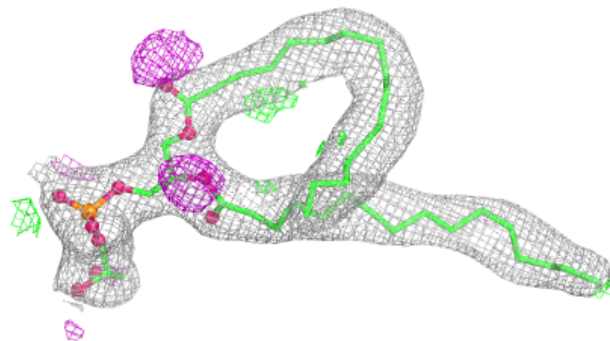
**Electron density around LMG B 621:**

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

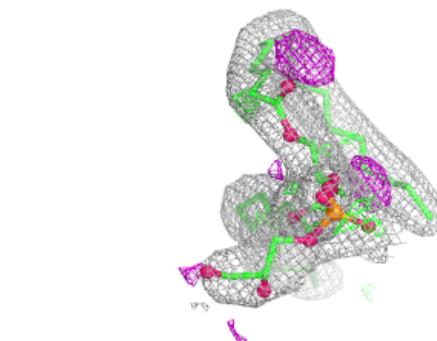
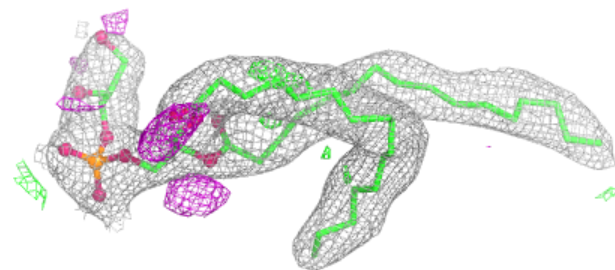
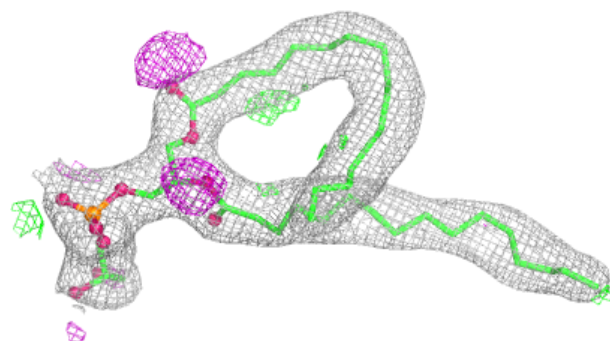


Electron density around LHG A 419 (A):

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

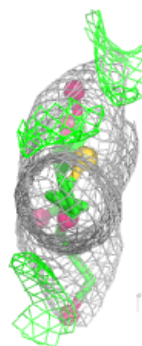
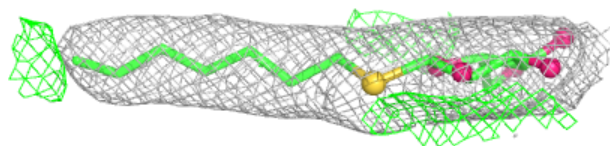
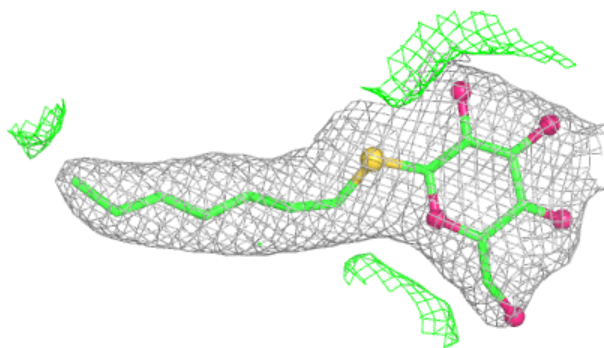
**Electron density around LHG A 419 (B):**

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

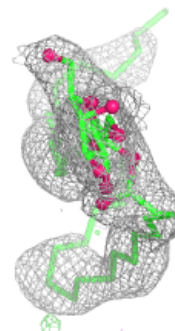
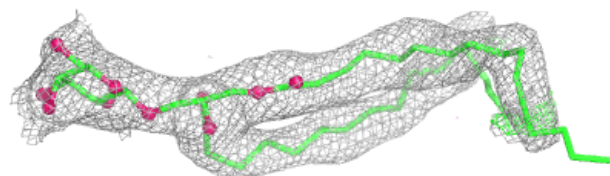
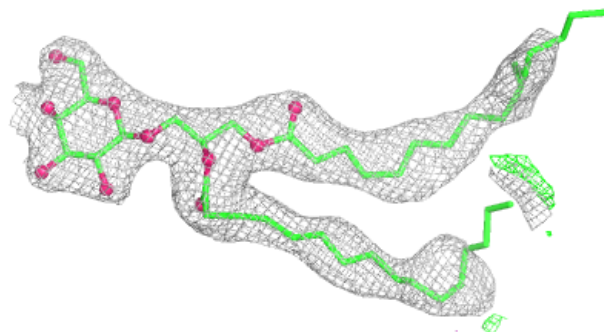


Electron density around HTG b 625:

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

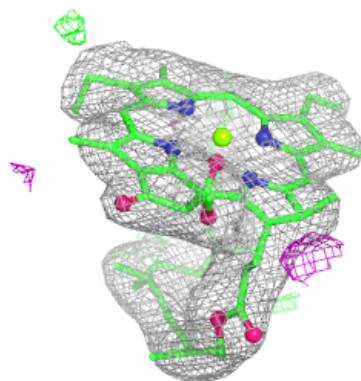
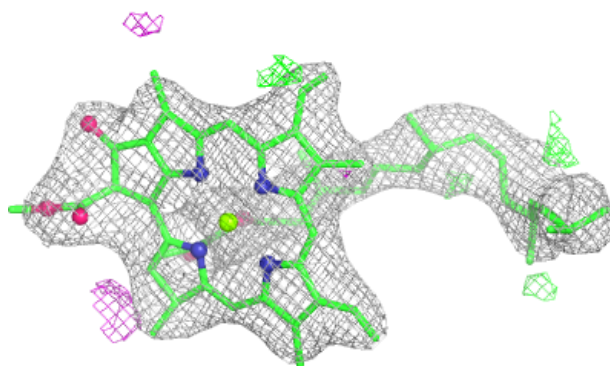
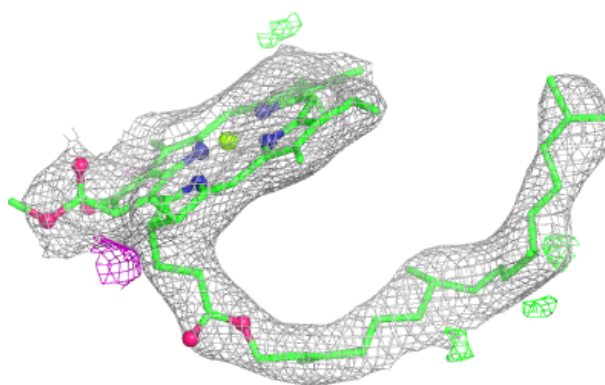
**Electron density around LMG d 412:**

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

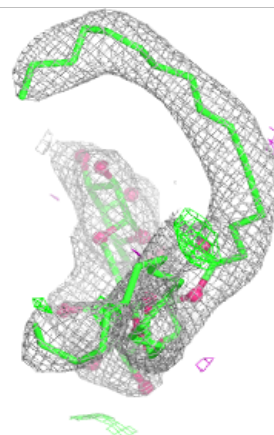
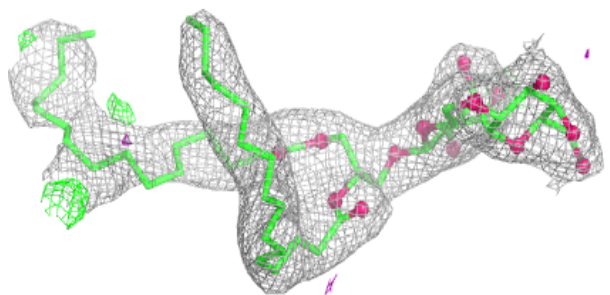
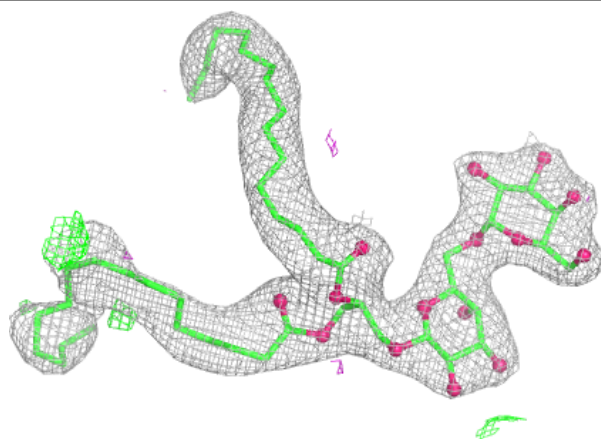


Electron density around CLA C 513:

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

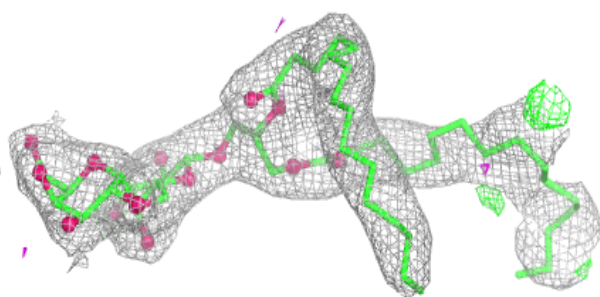
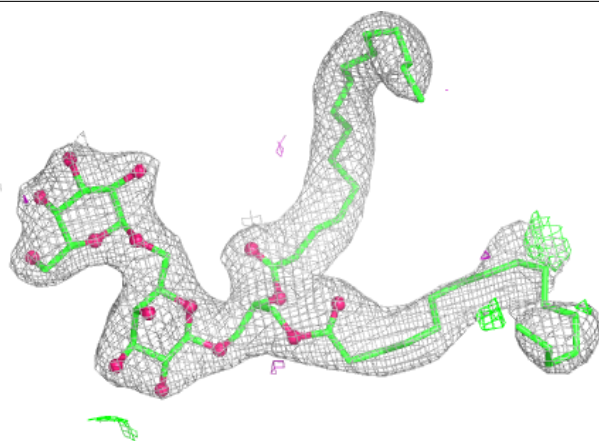
**Electron density around DGD C 517 (A):**

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

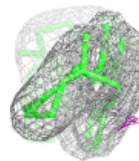
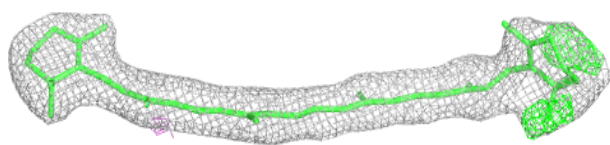
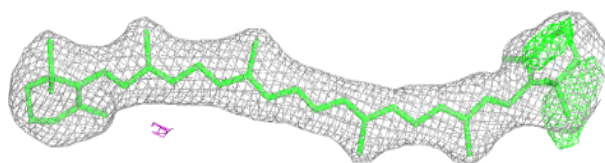


Electron density around DGD C 517 (B):

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

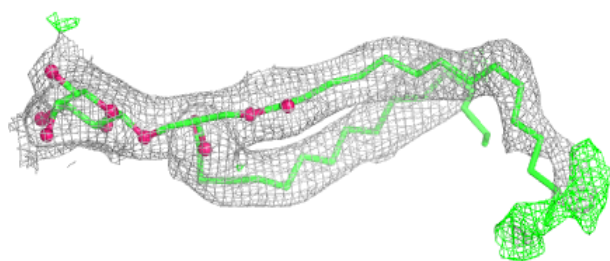
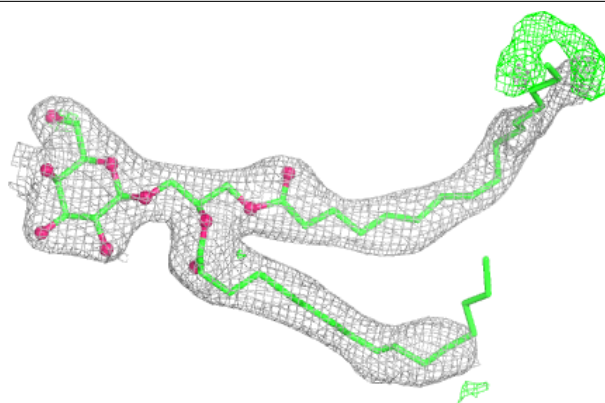
**Electron density around BCR d 405:**

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



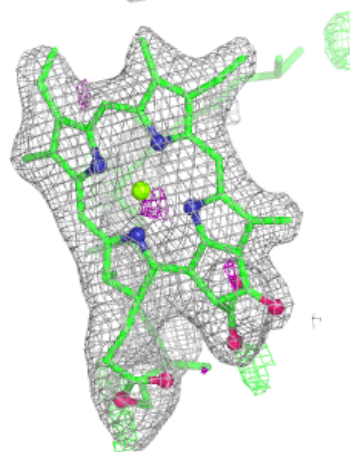
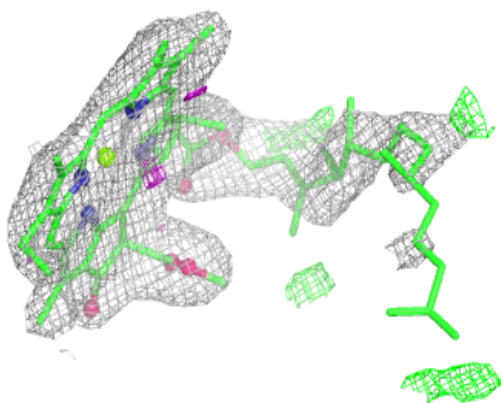
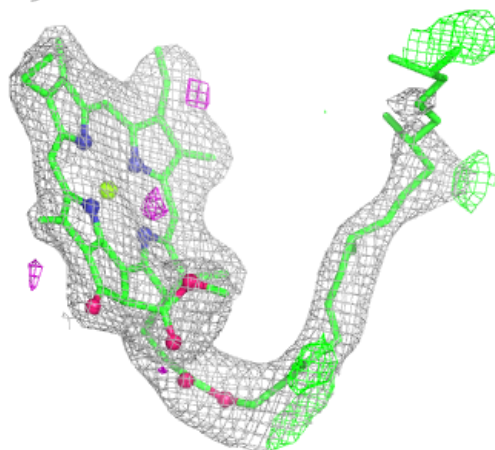
Electron density around LMG D 412:

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



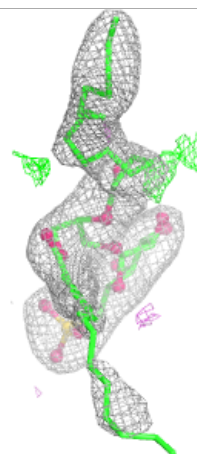
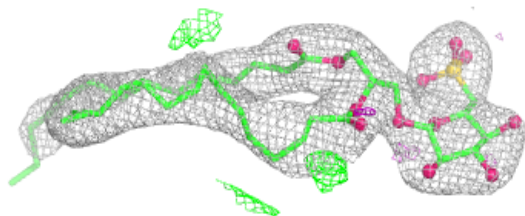
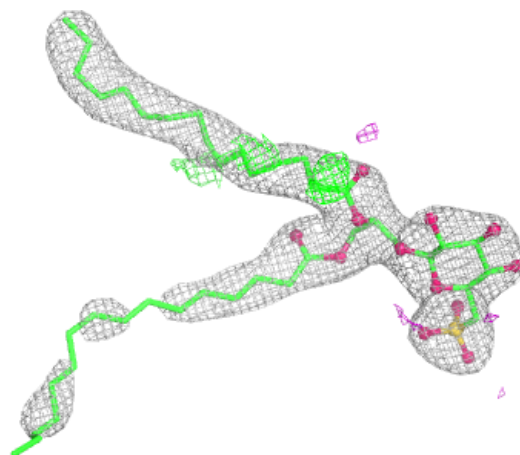
Electron density around CLA b 616:

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



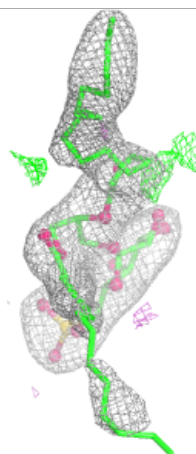
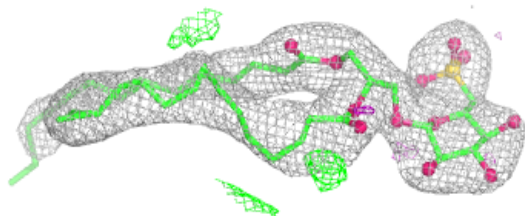
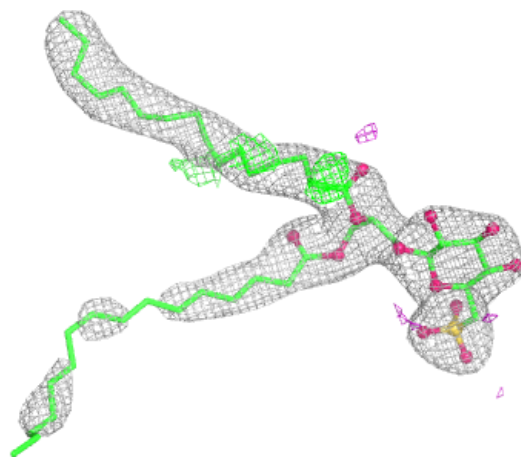
Electron density around SQD A 410 (A):

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



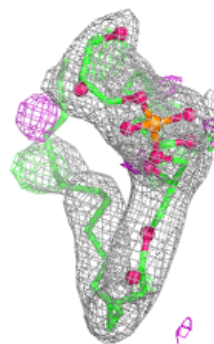
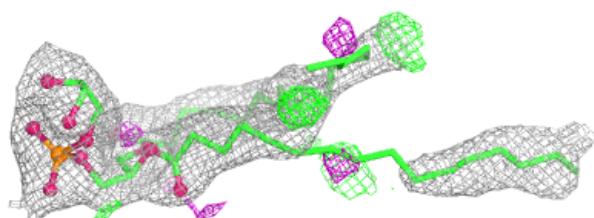
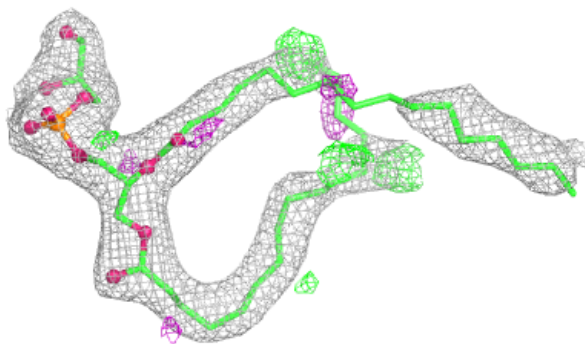
Electron density around SQD A 410 (B):

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

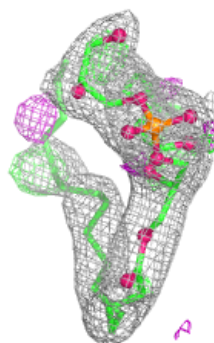
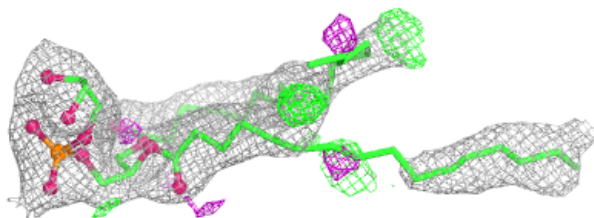
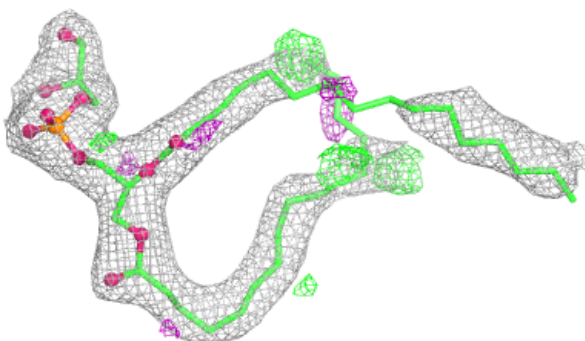


Electron density around LHG D 408 (A):

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

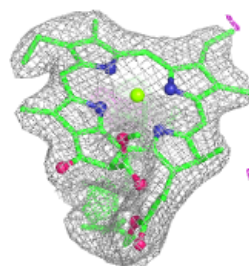
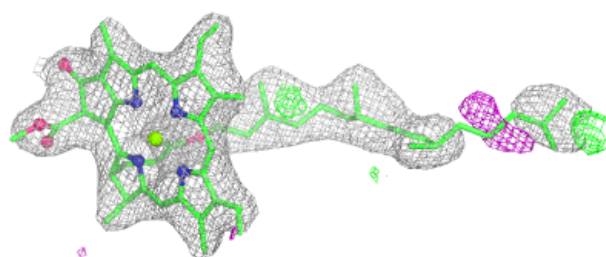
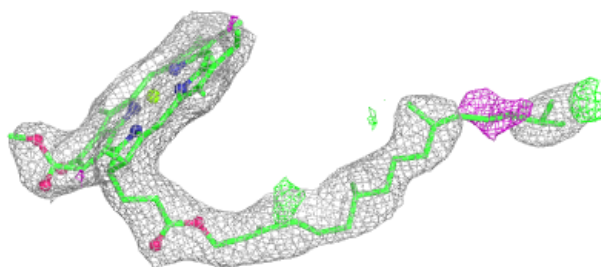
**Electron density around LHG D 408 (B):**

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

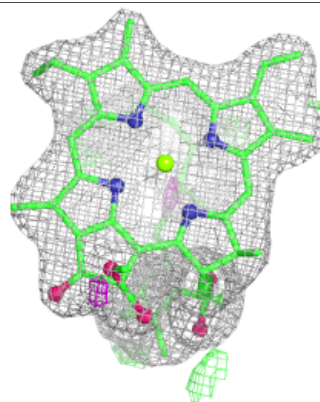
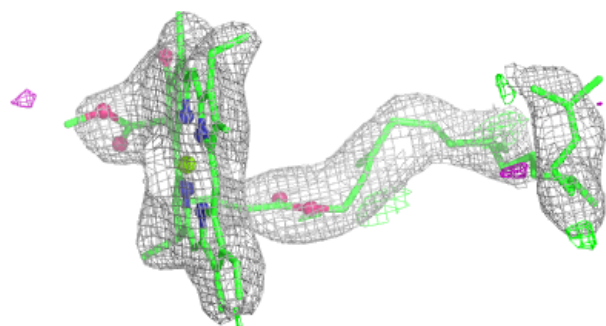
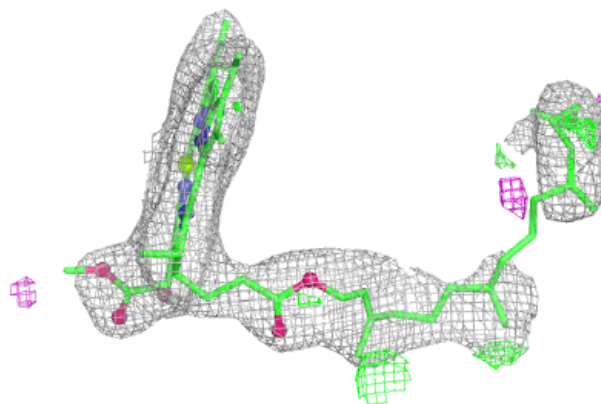


Electron density around CLA c 505:

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

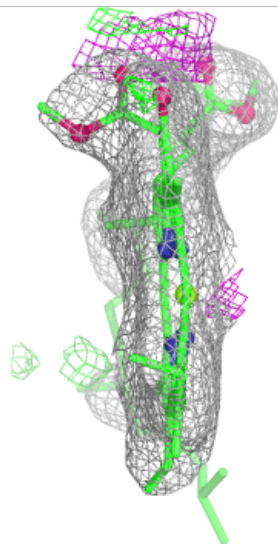
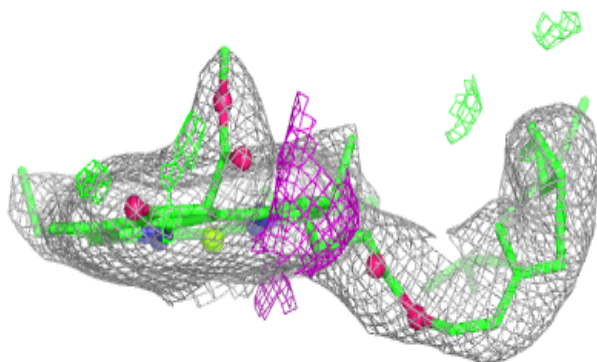
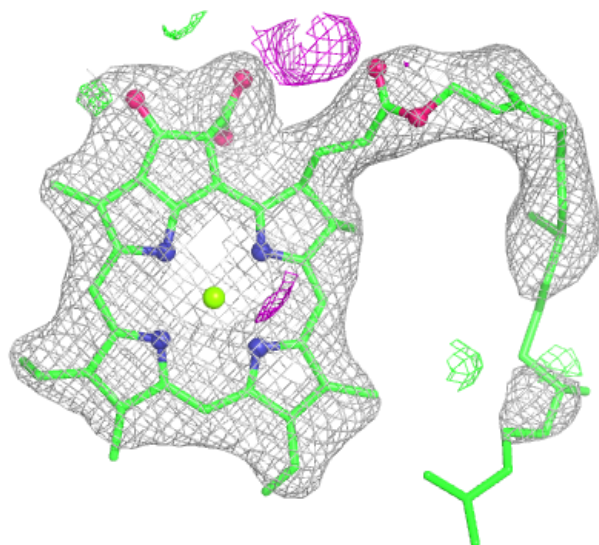
**Electron density around CLA c 507:**

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



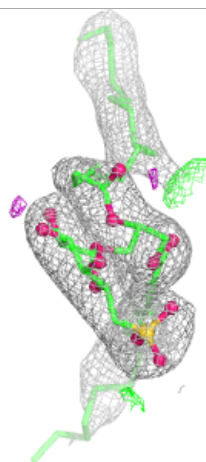
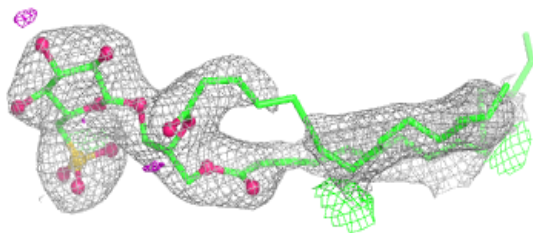
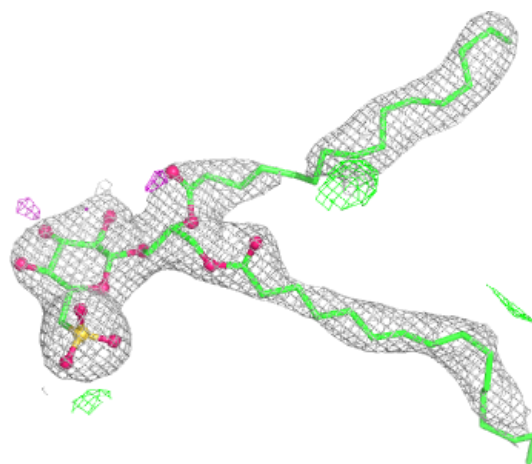
Electron density around CLA c 513:

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



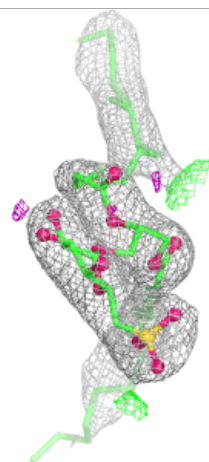
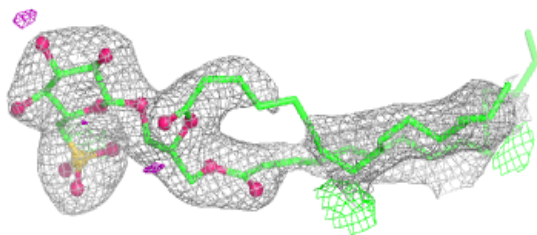
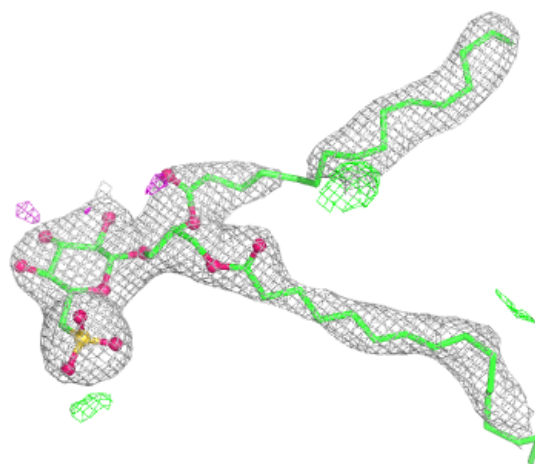
Electron density around SQD a 409 (A):

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



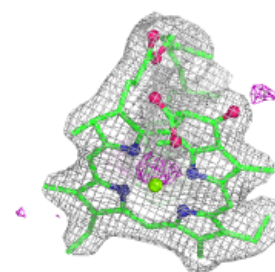
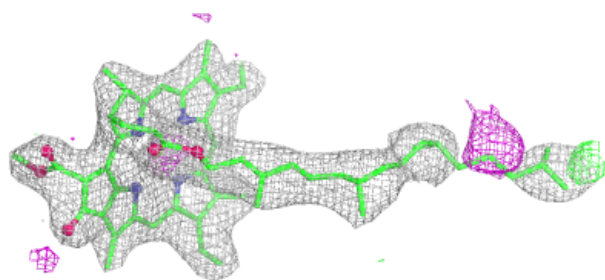
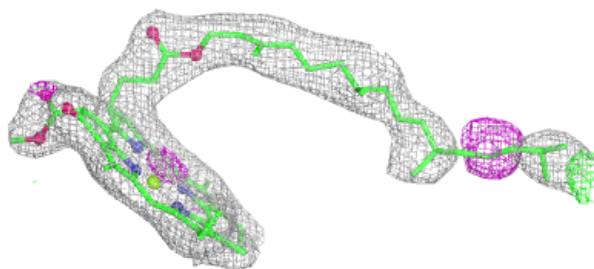
Electron density around SQD a 409 (B):

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

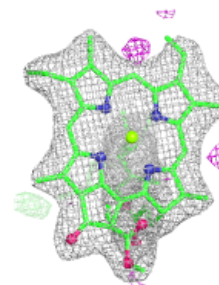
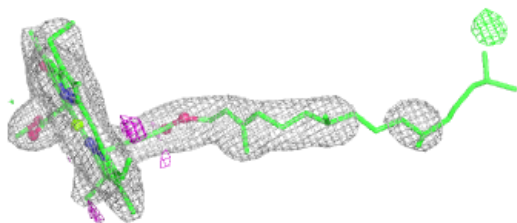
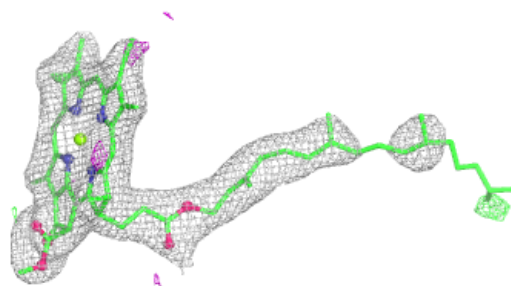


Electron density around CLA C 504:

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

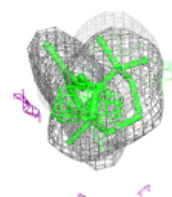
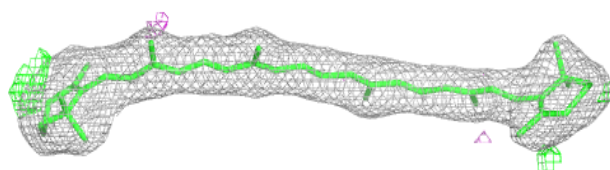
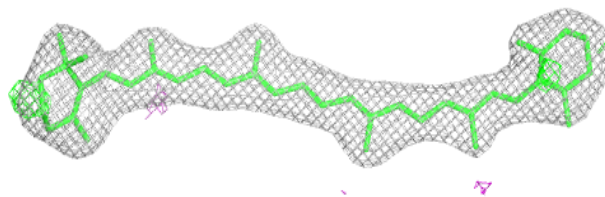
**Electron density around CLA d 404:**

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

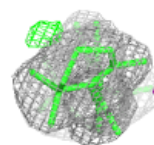
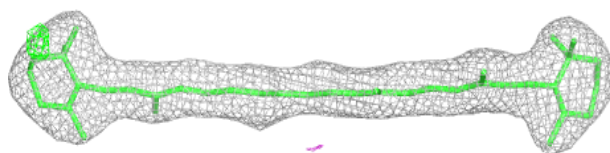
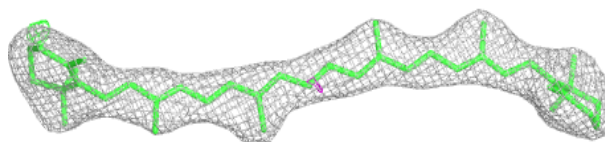


Electron density around BCR B 619:

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

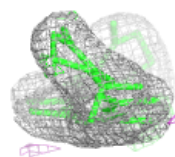
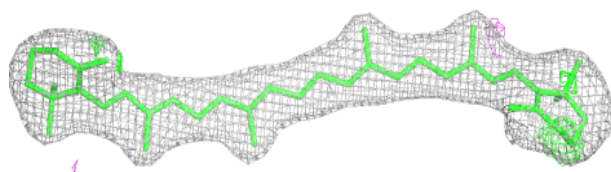
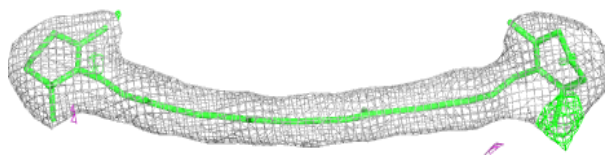
**Electron density around BCR C 514:**

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

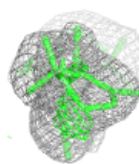
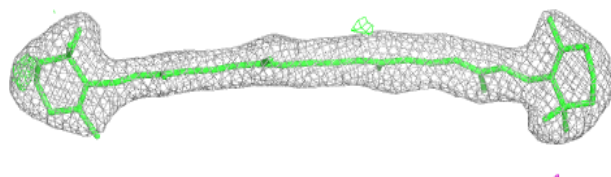
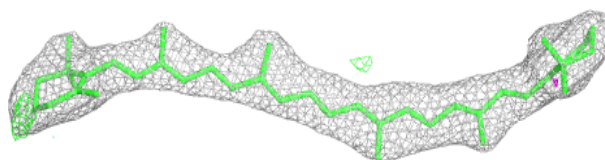


Electron density around BCR D 405:

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

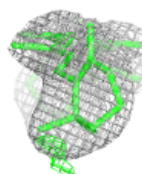
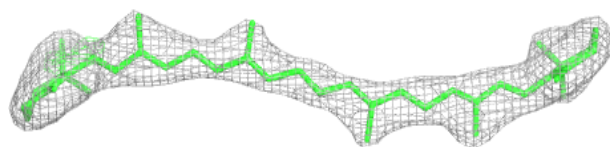
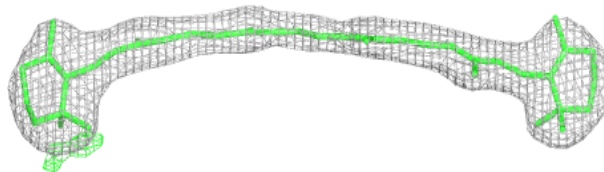
**Electron density around BCR H 101:**

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

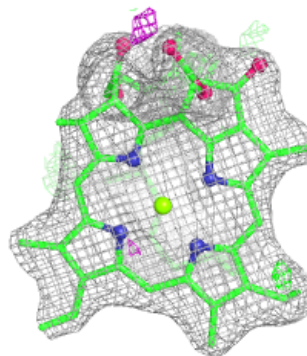
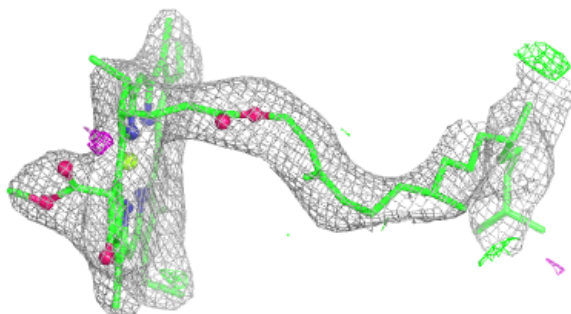
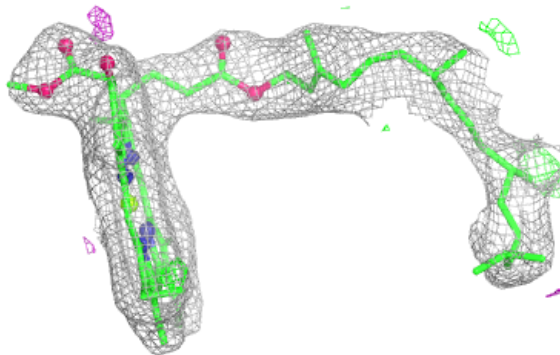


Electron density around BCR K 102:

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

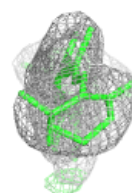
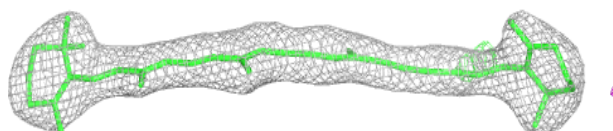
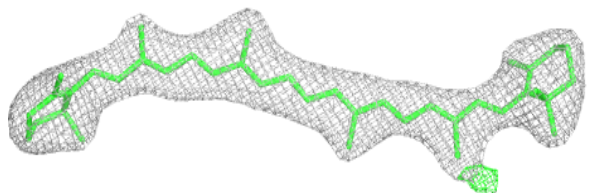
**Electron density around CLA C 506:**

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

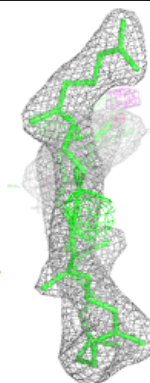
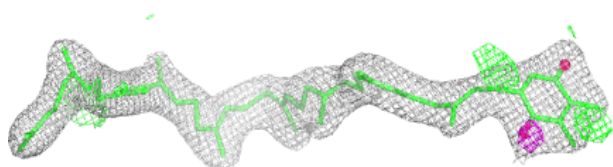
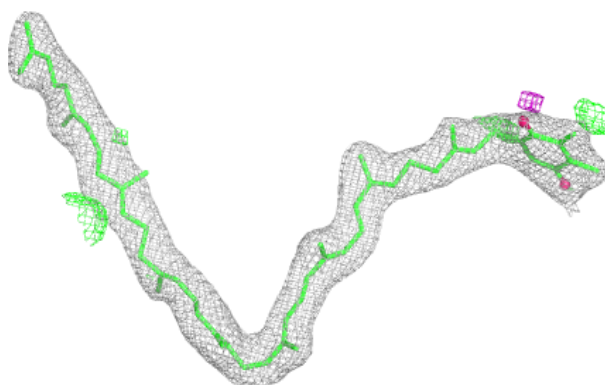


Electron density around BCR Y 101:

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

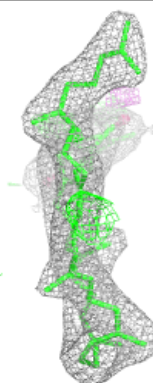
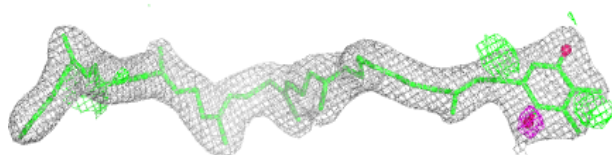
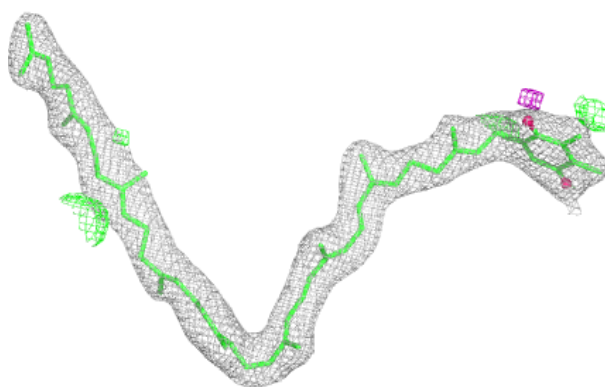
**Electron density around PL9 D 406 (A):**

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

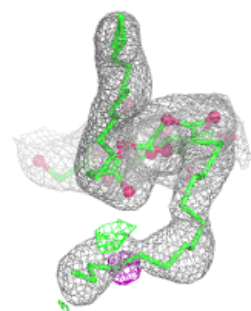
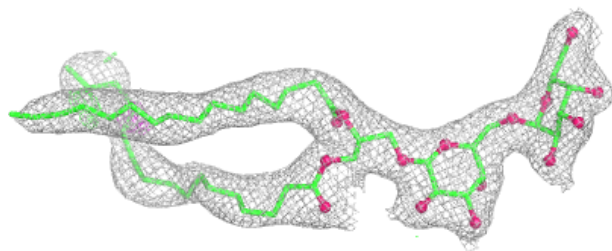
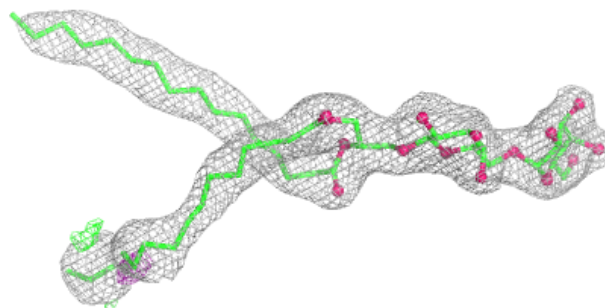


Electron density around PL9 D 406 (B):

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

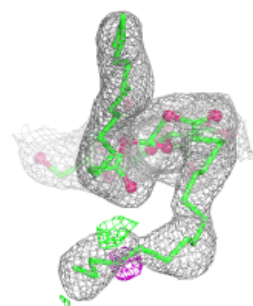
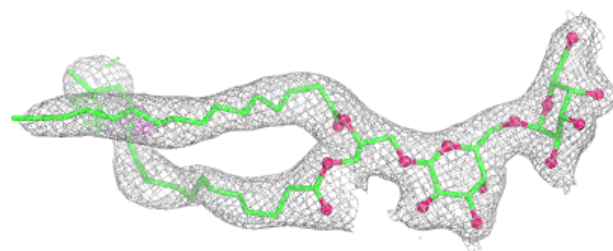
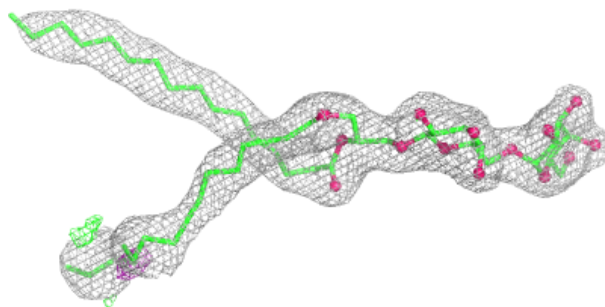
**Electron density around DGD c 517 (A):**

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

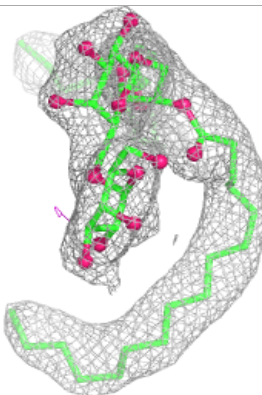
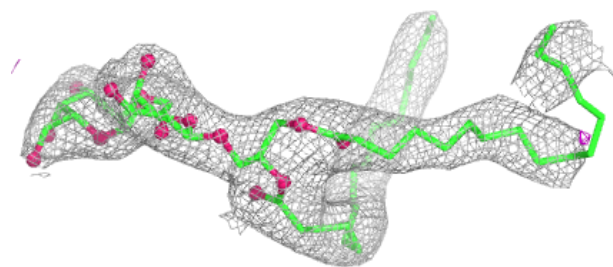
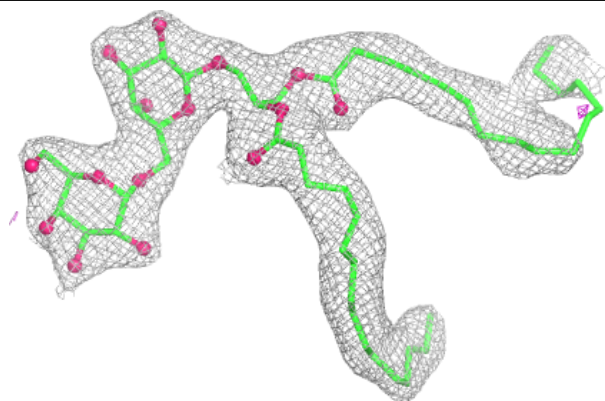


Electron density around DGD c 517 (B):

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

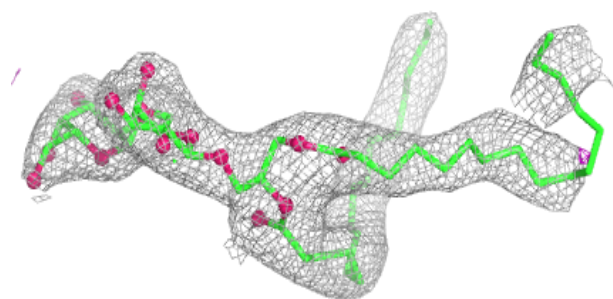
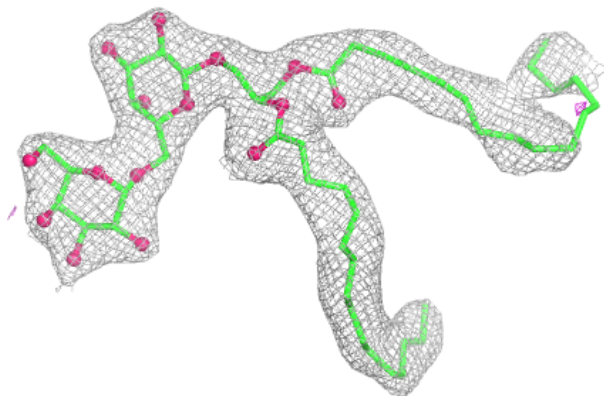
**Electron density around DGD c 518 (A):**

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

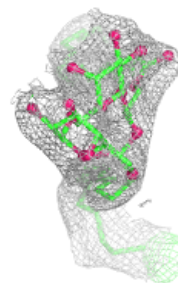
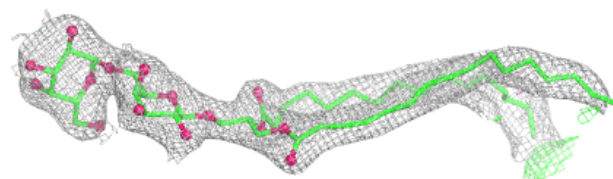
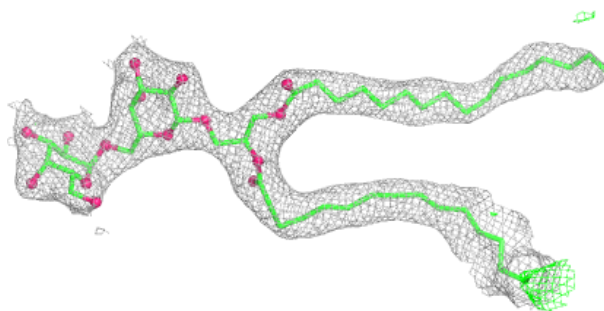


Electron density around DGD c 518 (B):

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

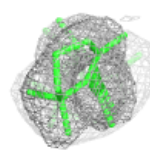
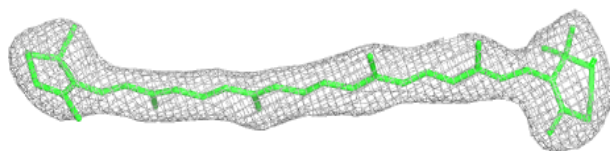
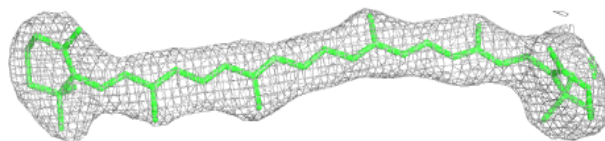
**Electron density around DGD c 519:**

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

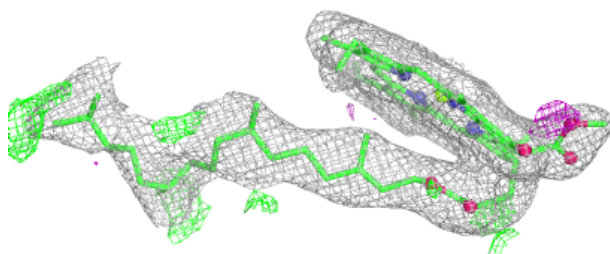
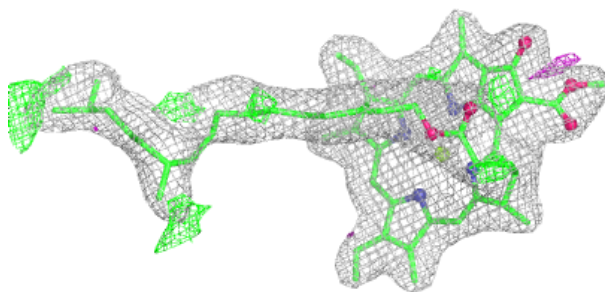


Electron density around BCR c 515:

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

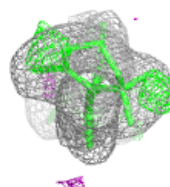
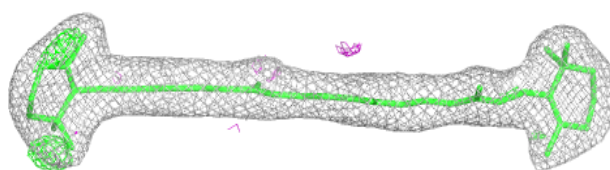
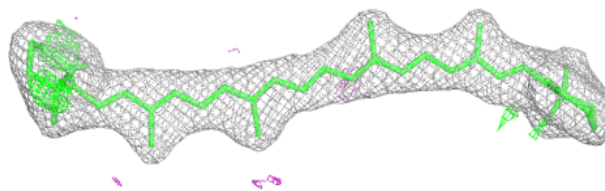
**Electron density around CLA b 614:**

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

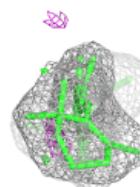
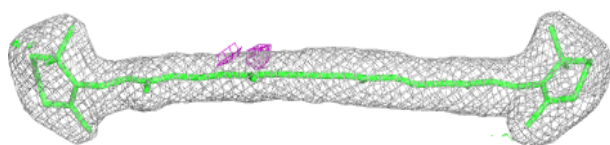
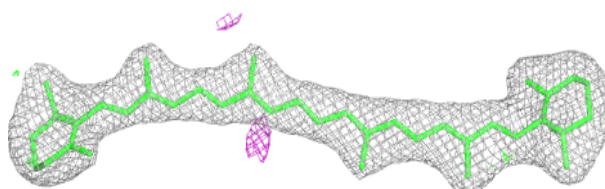


Electron density around BCR A 409:

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

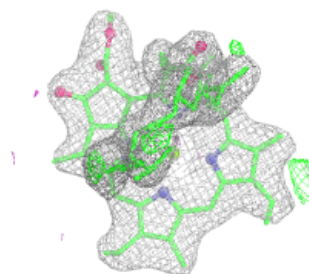
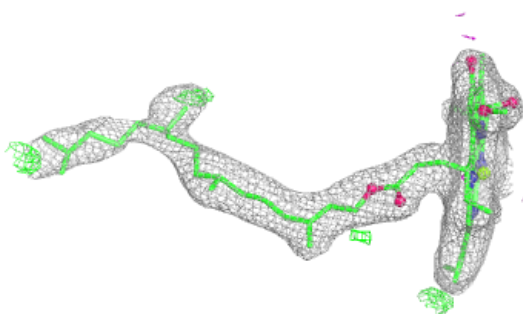
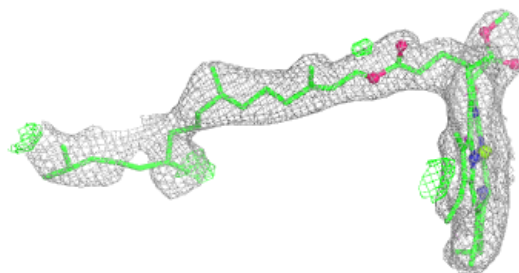
**Electron density around BCR B 618:**

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

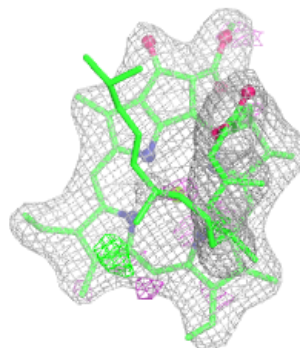
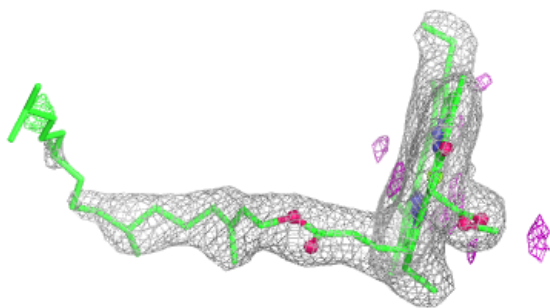
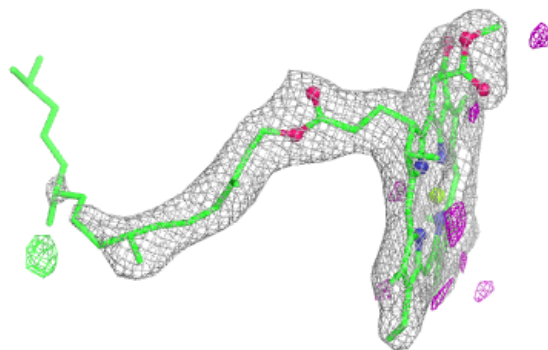


Electron density around CLA B 606:

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

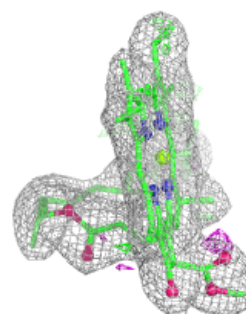
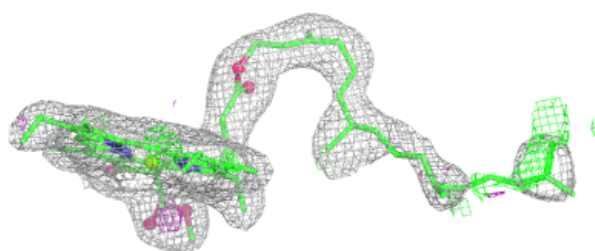
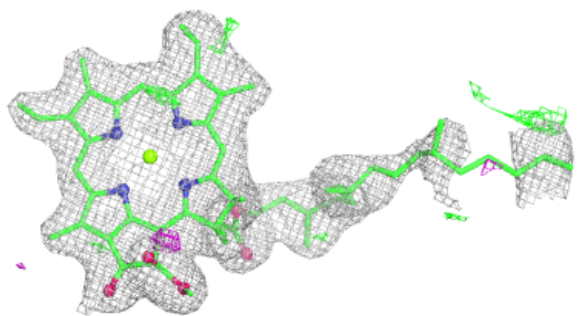
**Electron density around CLA D 404:**

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

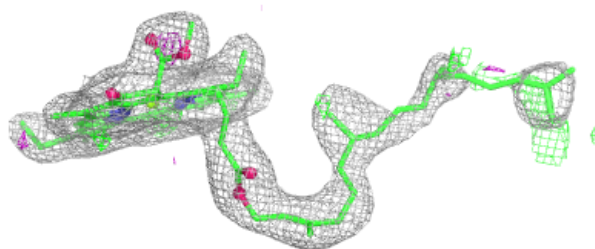
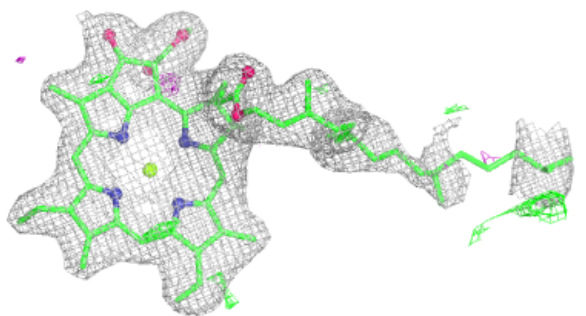


Electron density around CLA a 405 (A):

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

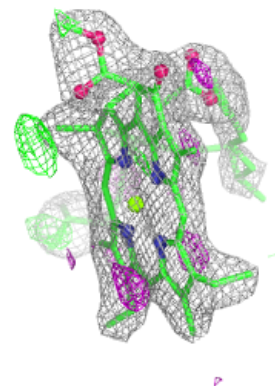
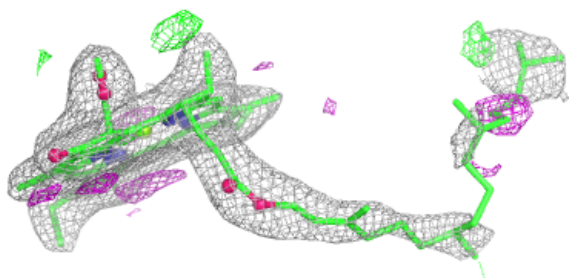
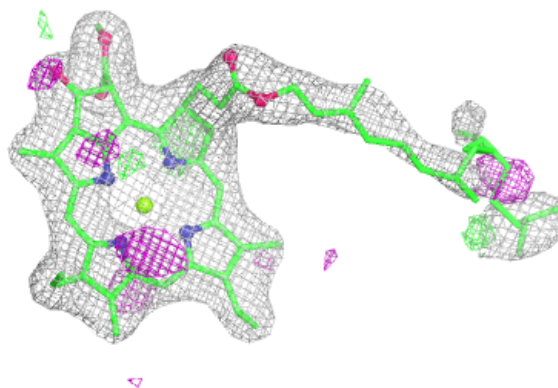
**Electron density around CLA a 405 (B):**

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



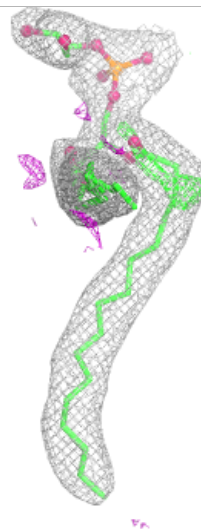
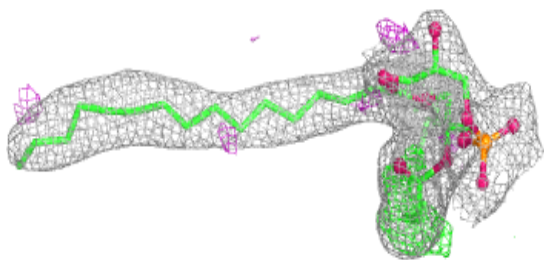
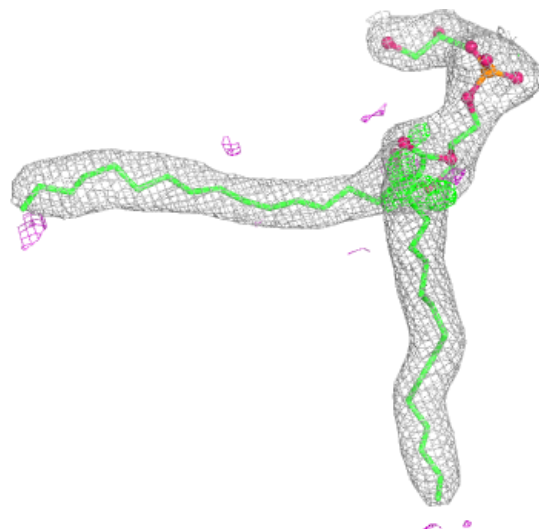
Electron density around CLA a 407:

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



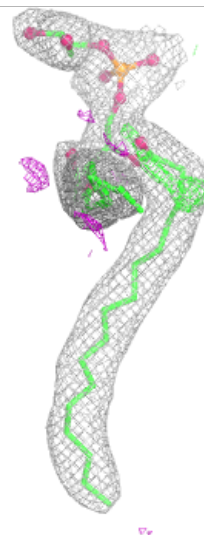
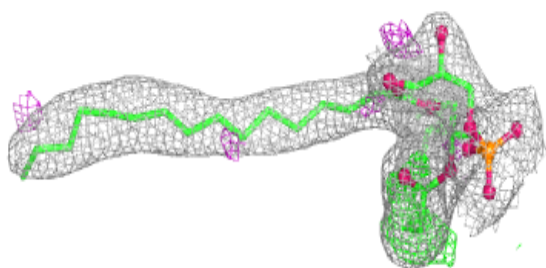
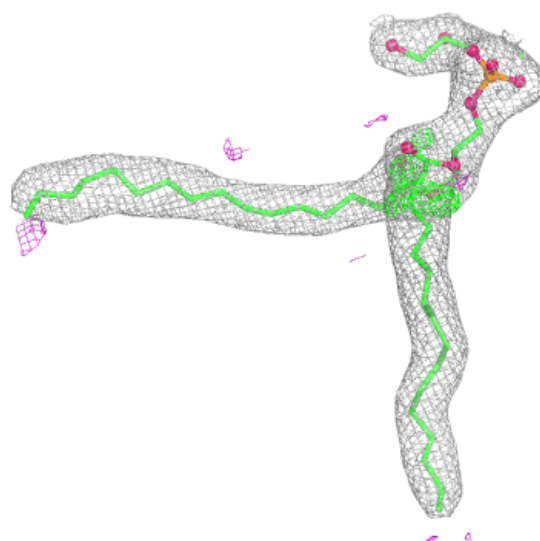
Electron density around LHG b 629 (A):

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



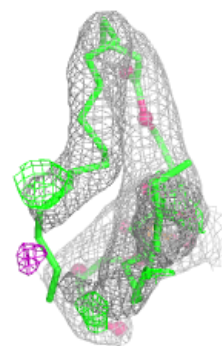
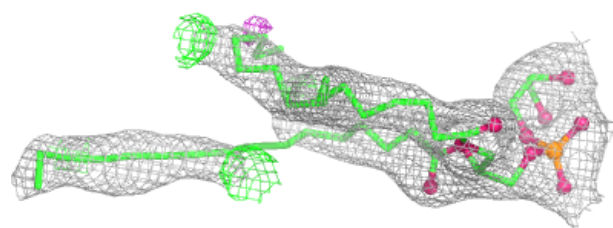
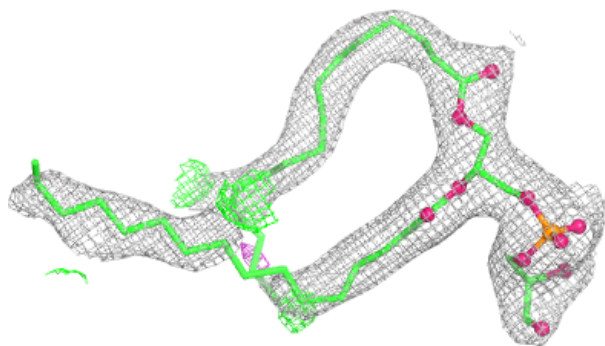
Electron density around LHG b 629 (B):

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

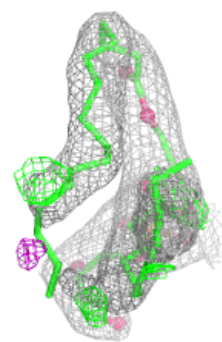
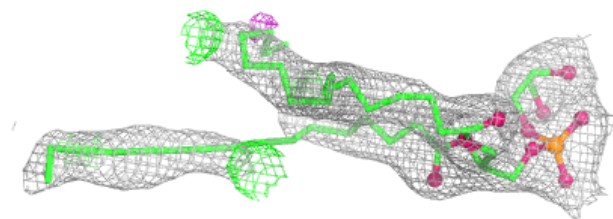
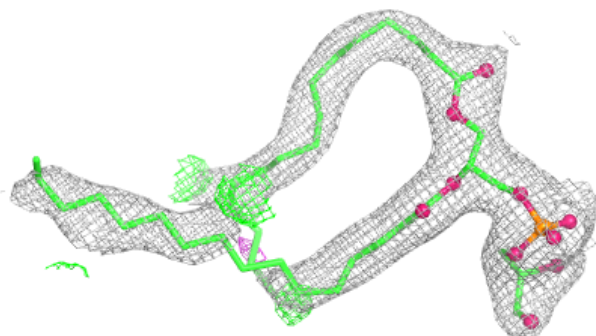


Electron density around LHG d 408 (A):

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

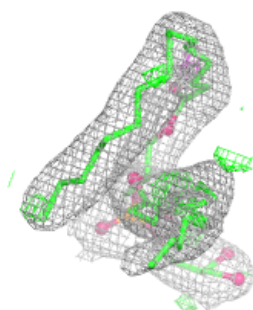
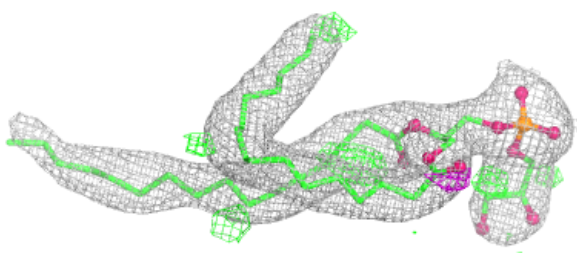
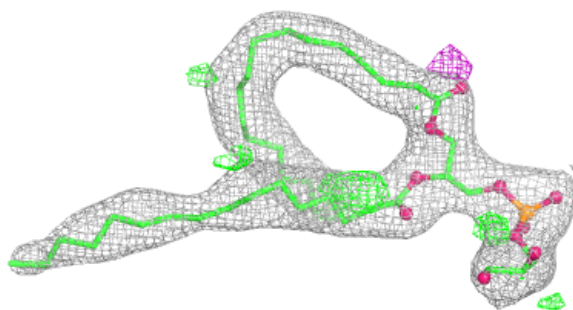
**Electron density around LHG d 408 (B):**

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

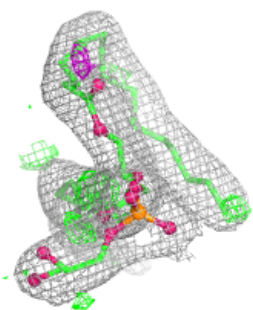
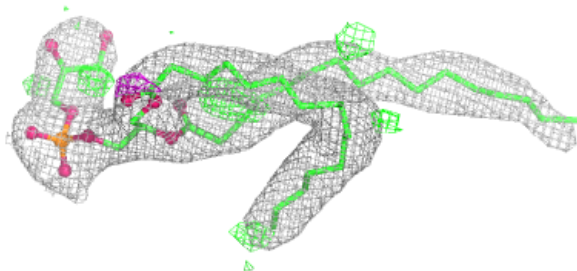
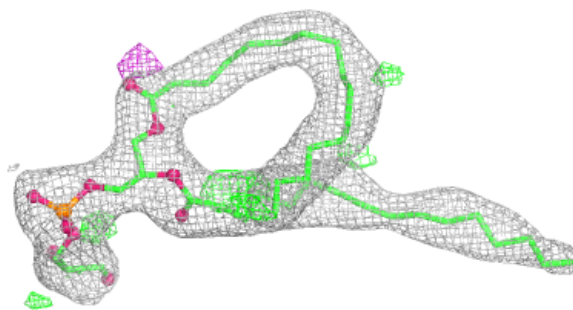


Electron density around LHG d 414 (A):

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

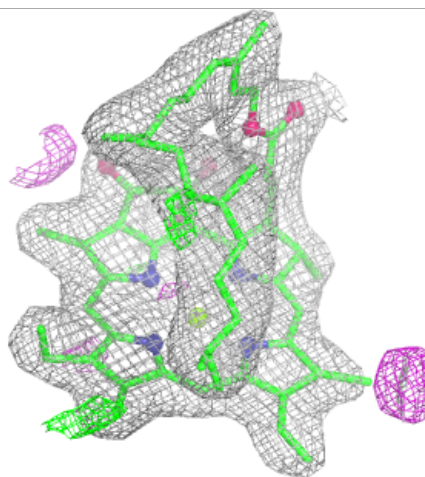
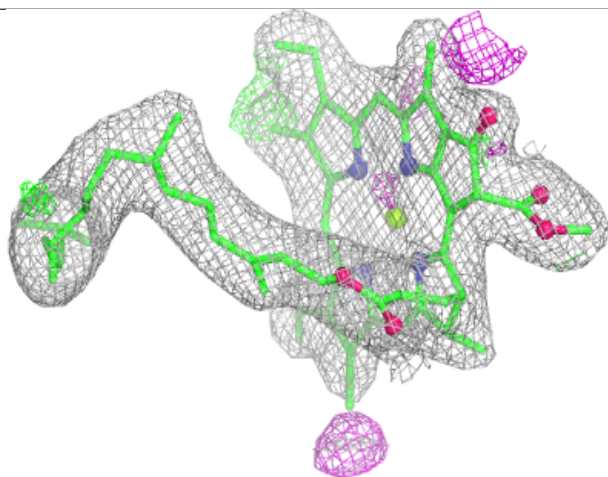
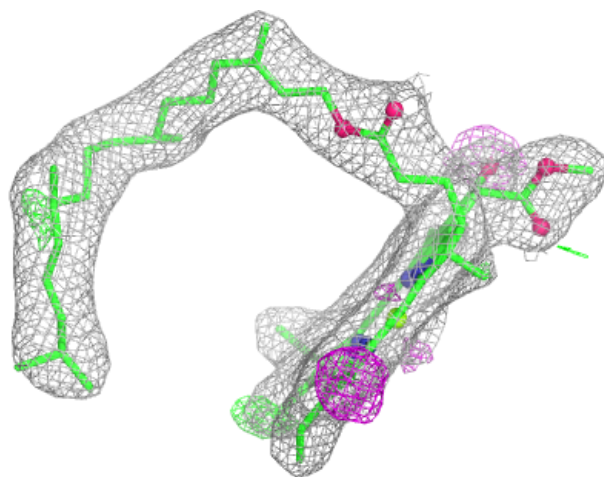
**Electron density around LHG d 414 (B):**

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



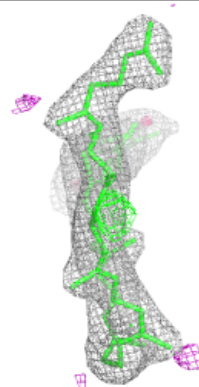
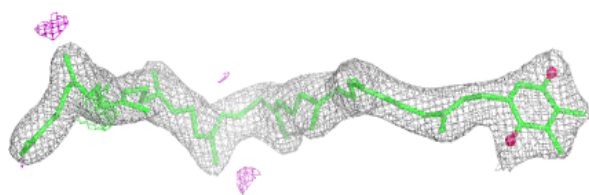
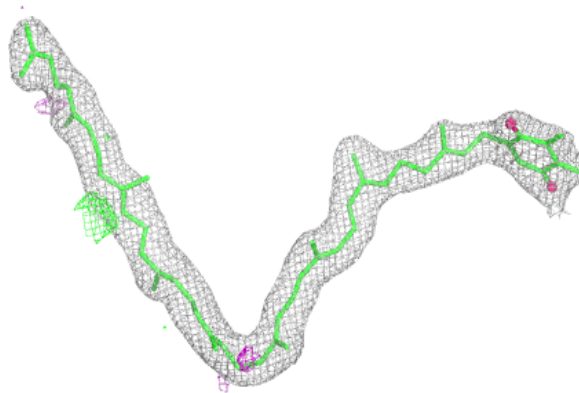
Electron density around CLA B 611:

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

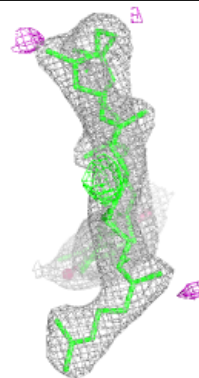
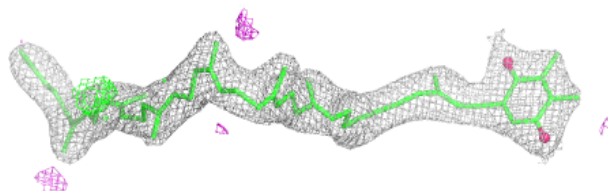
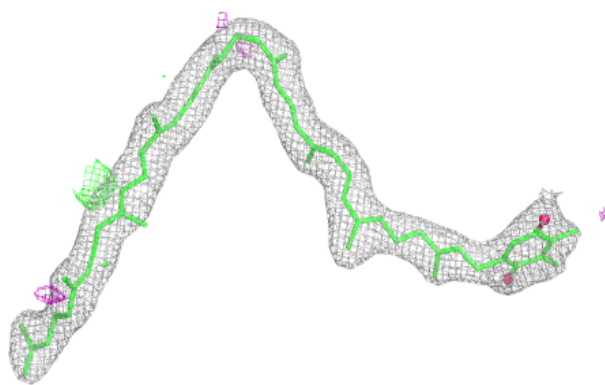


Electron density around PL9 d 406 (A):

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

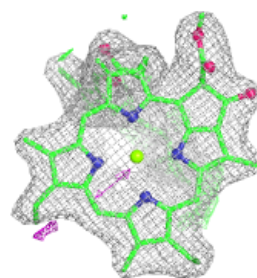
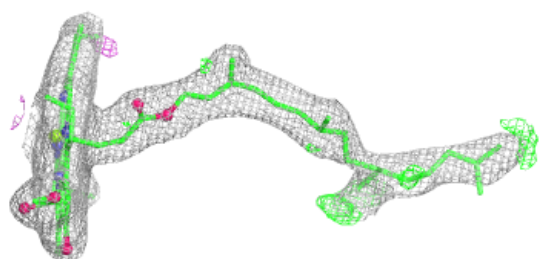
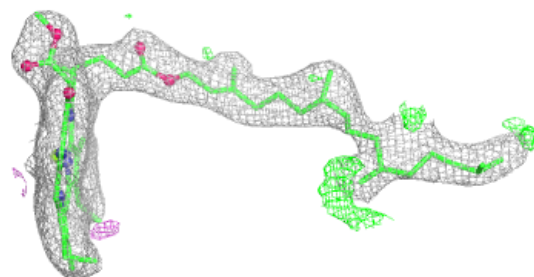
**Electron density around PL9 d 406 (B):**

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

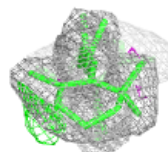
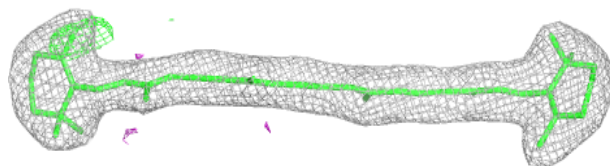
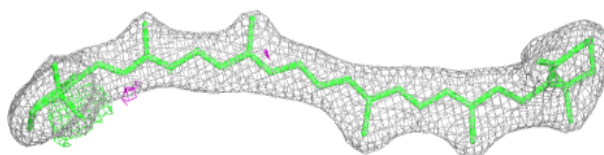


Electron density around CLA b 606:

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

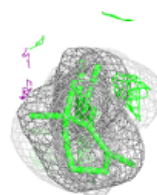
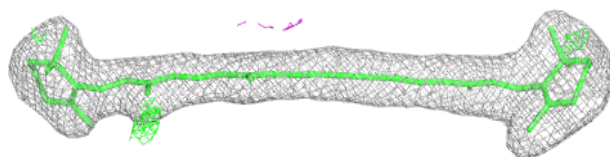
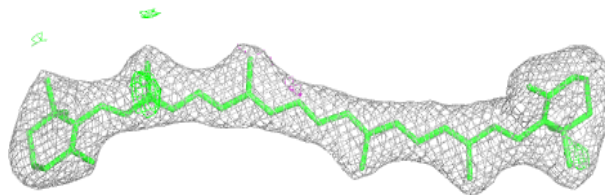
**Electron density around BCR a 408:**

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

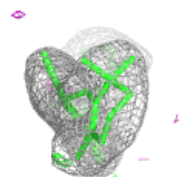
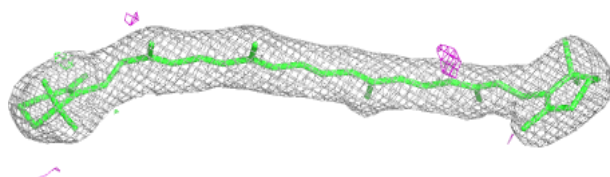
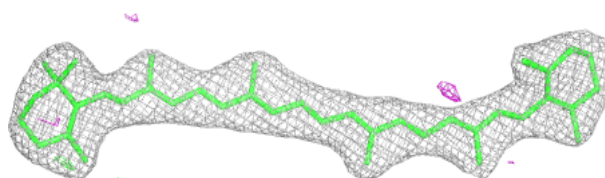


Electron density around BCR b 618:

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

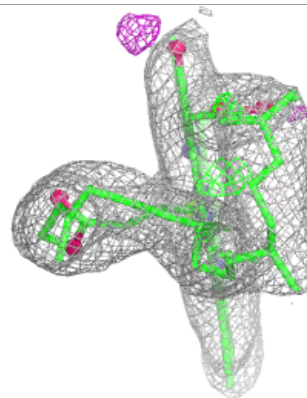
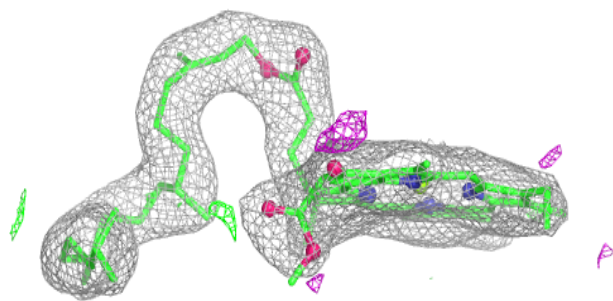
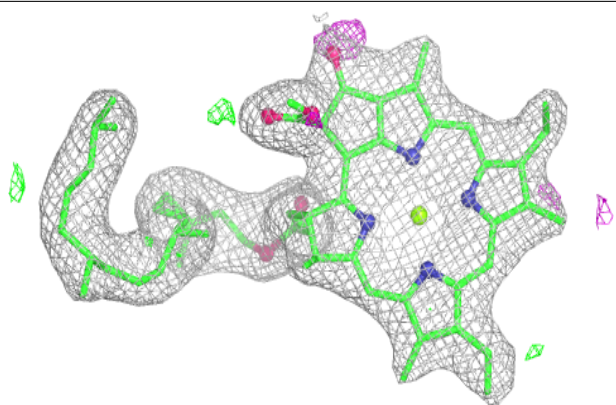
**Electron density around BCR b 619:**

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

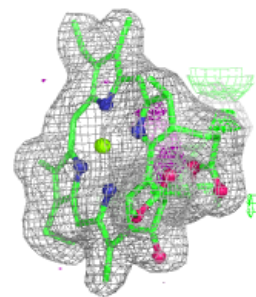
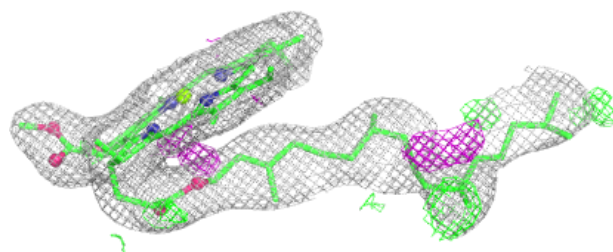
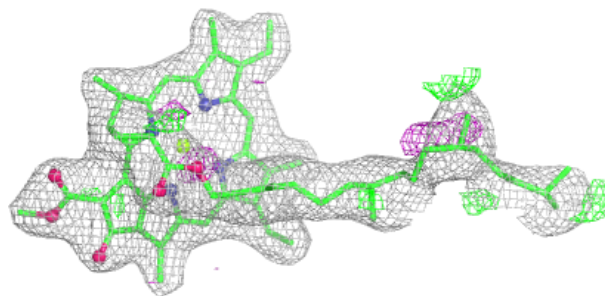


Electron density around CLA b 612:

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

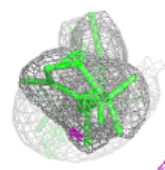
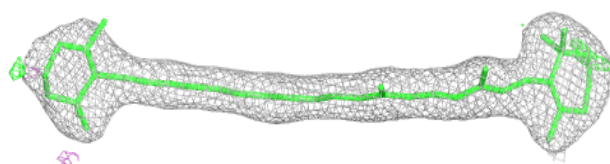
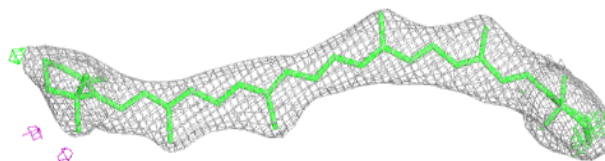
**Electron density around CLA B 614:**

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



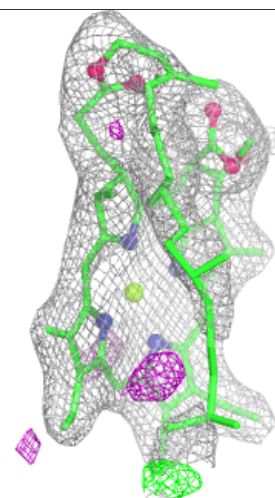
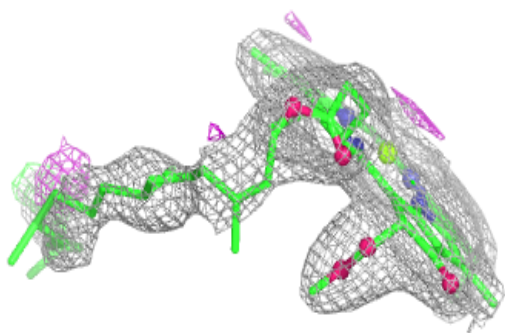
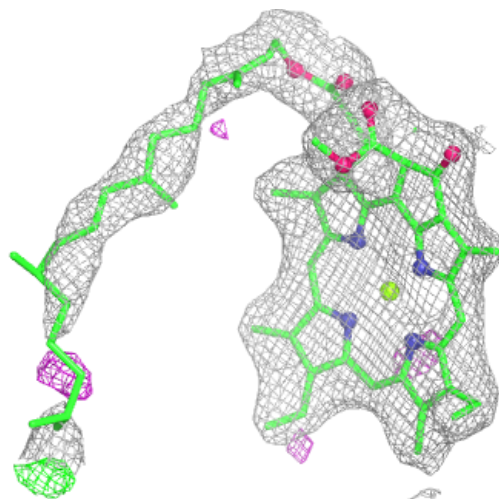
Electron density around BCR h 101:

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



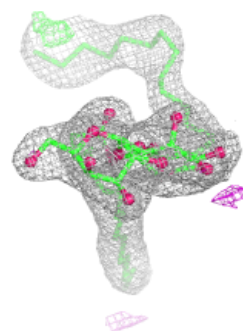
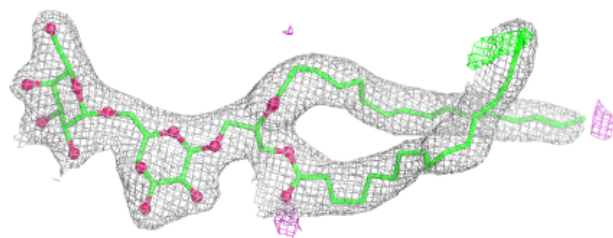
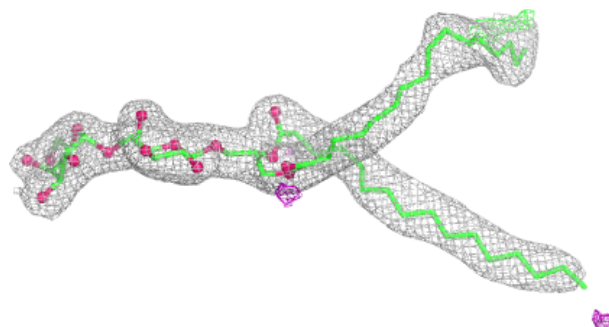
Electron density around CLA B 616:

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

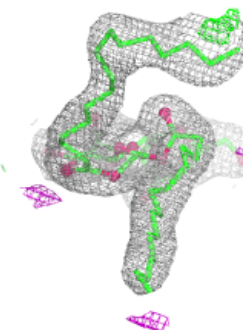
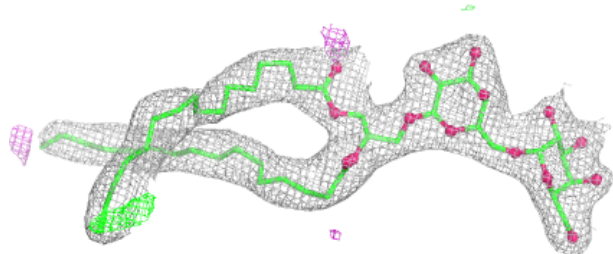
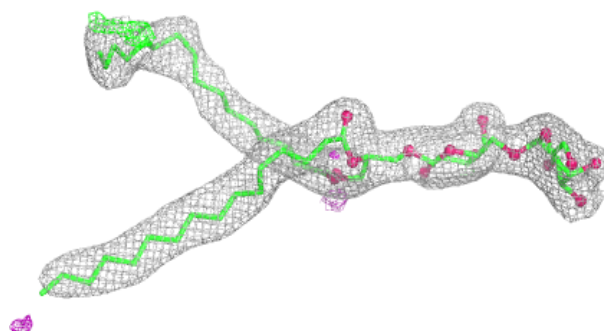


Electron density around DGD C 516 (A):

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

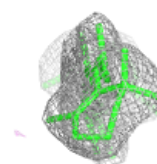
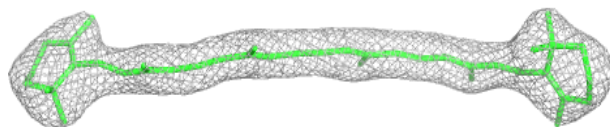
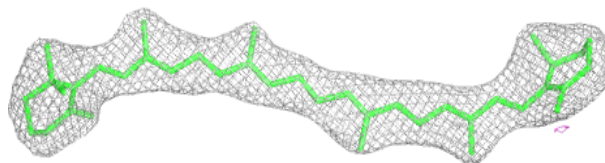
**Electron density around DGD C 516 (B):**

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

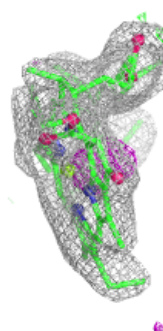
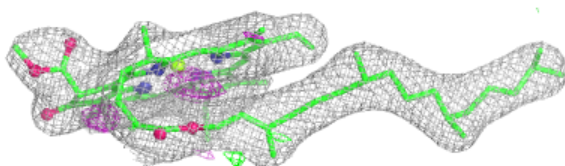
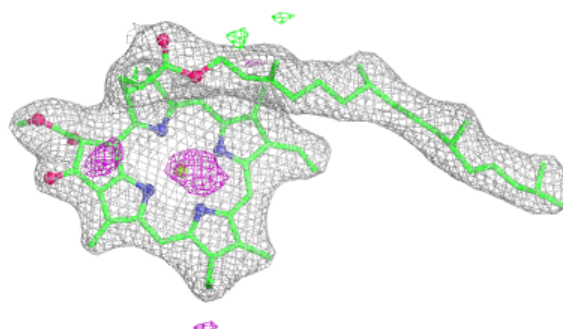


Electron density around BCR y 101:

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

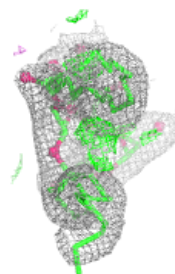
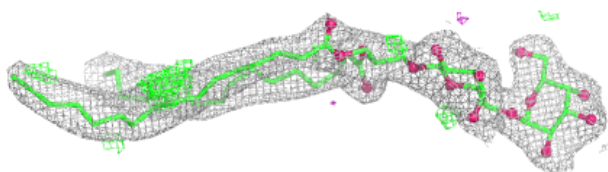
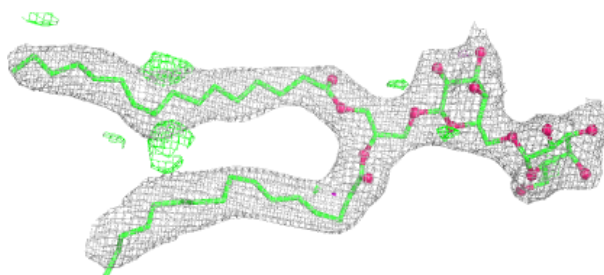
**Electron density around CLA C 501:**

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

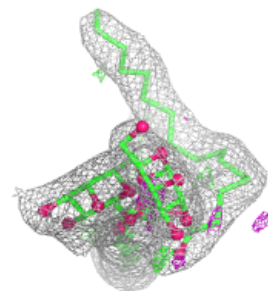
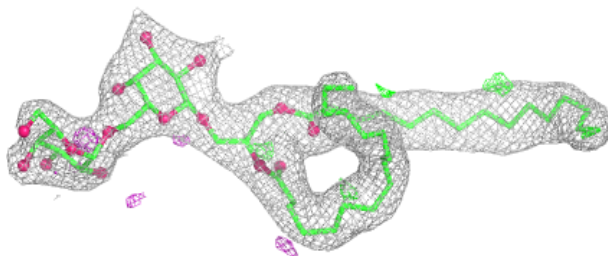
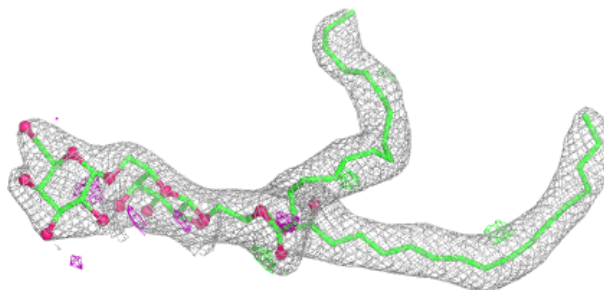


Electron density around DGD C 518:

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

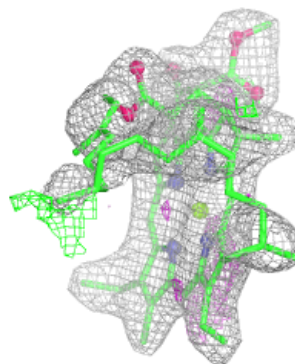
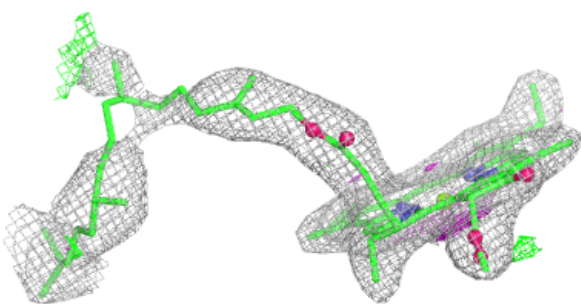
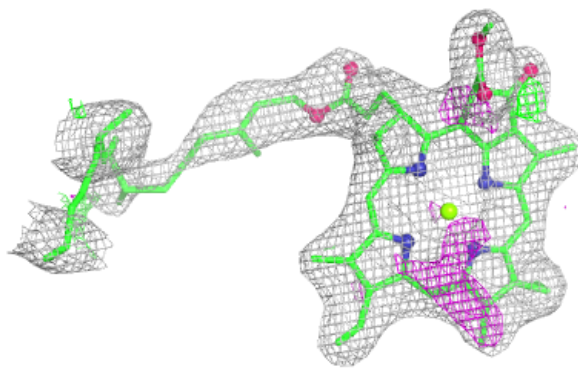
**Electron density around DGD H 102:**

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



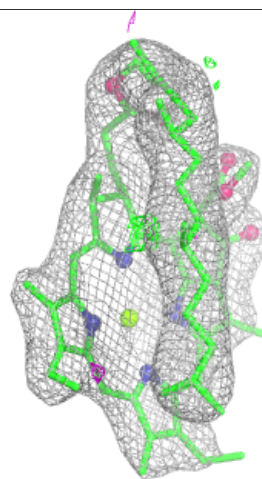
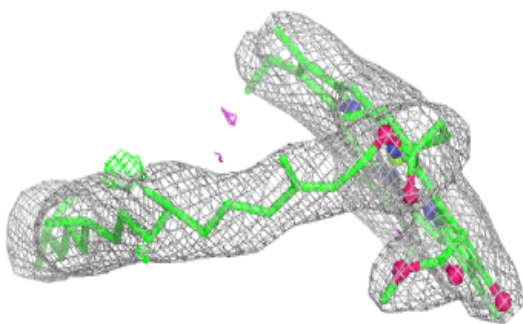
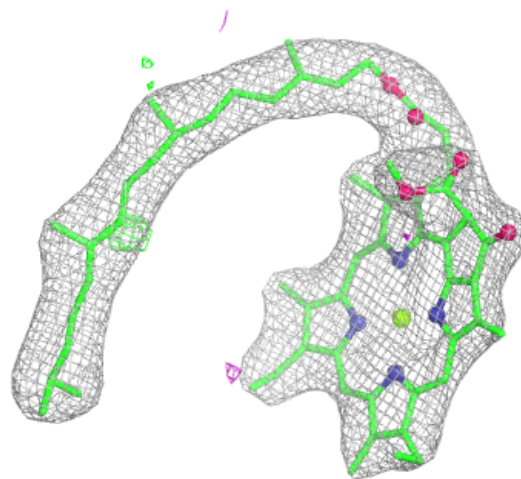
Electron density around CLA A 408:

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



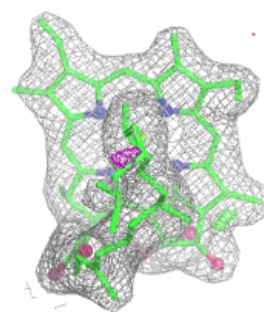
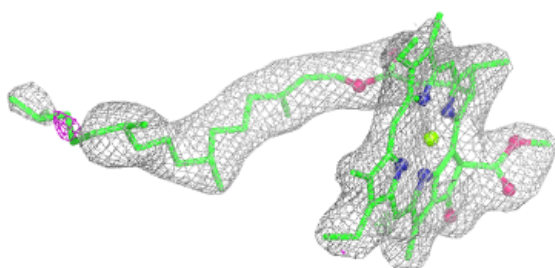
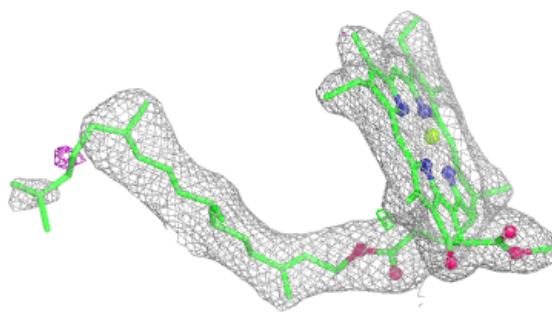
Electron density around CLA c 508:

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

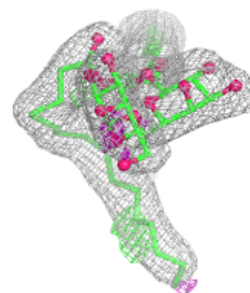
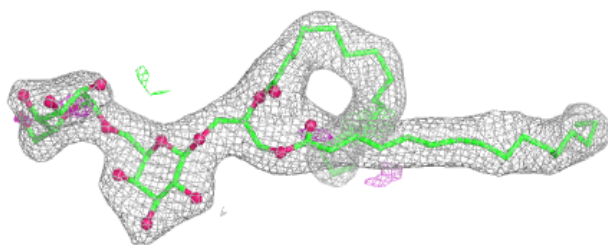
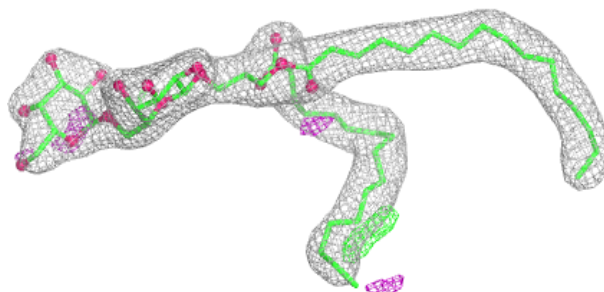


Electron density around CLA c 509:

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

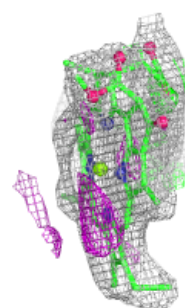
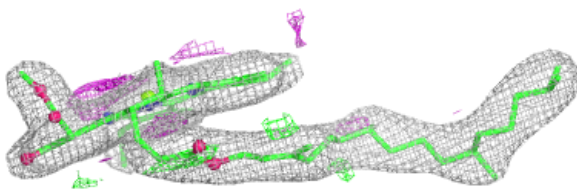
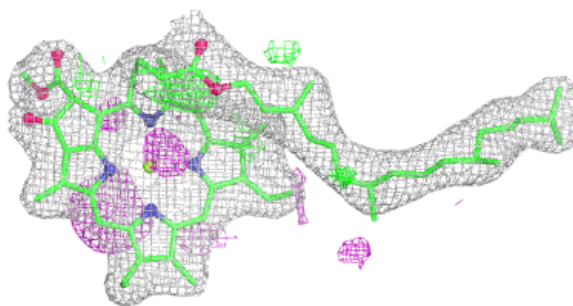
**Electron density around DGD h 102:**

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

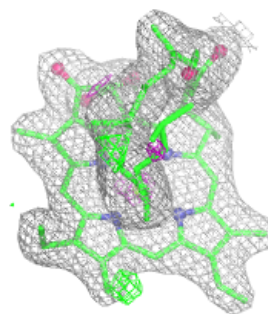
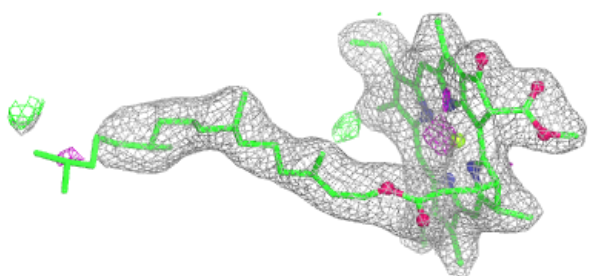
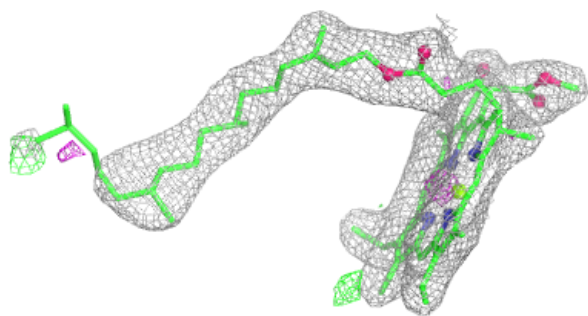


Electron density around CLA B 603:

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

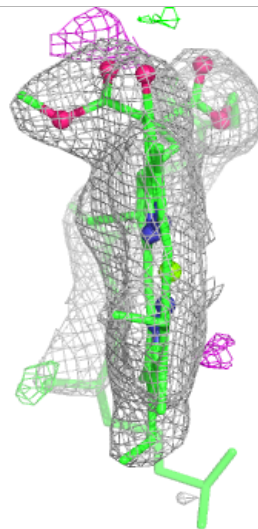
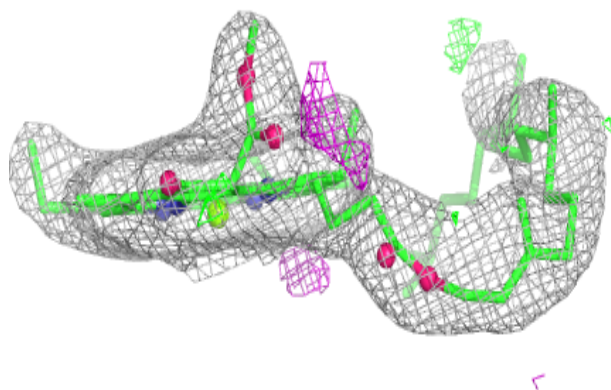
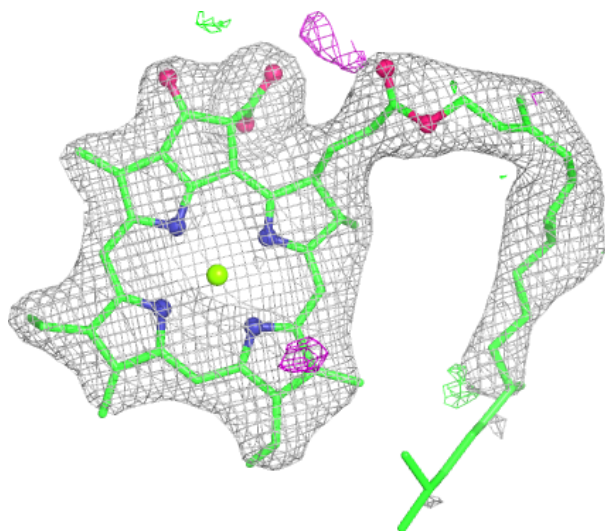
**Electron density around CLA C 508:**

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



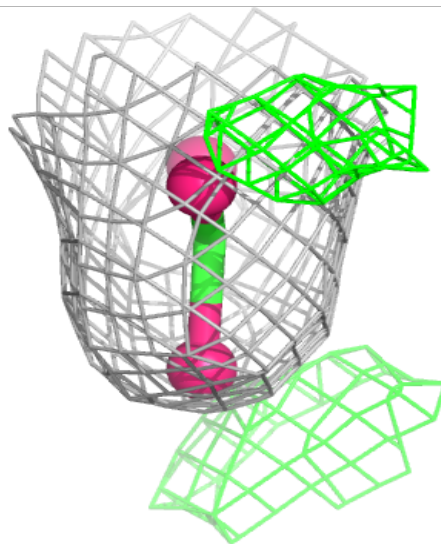
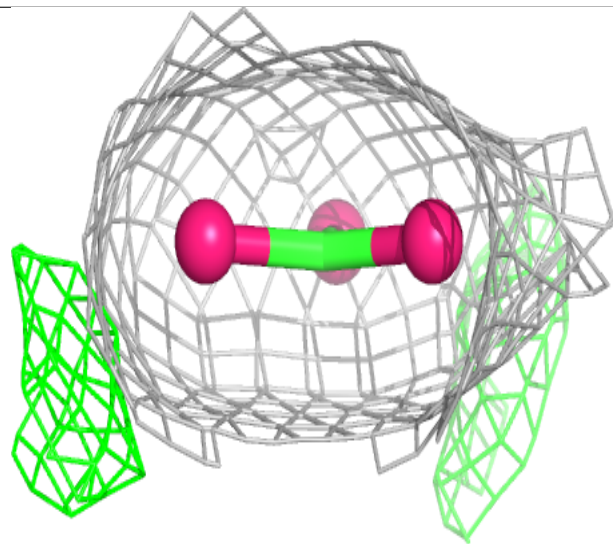
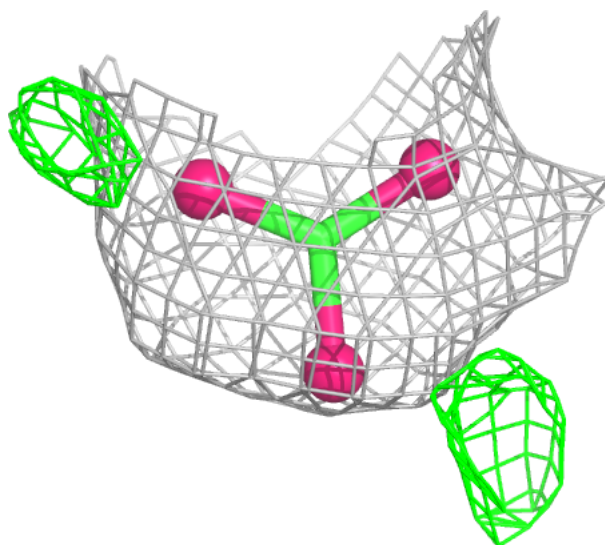
Electron density around CLA C 512:

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



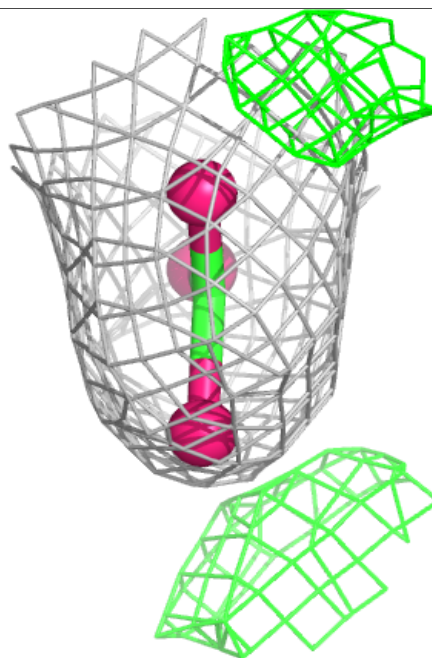
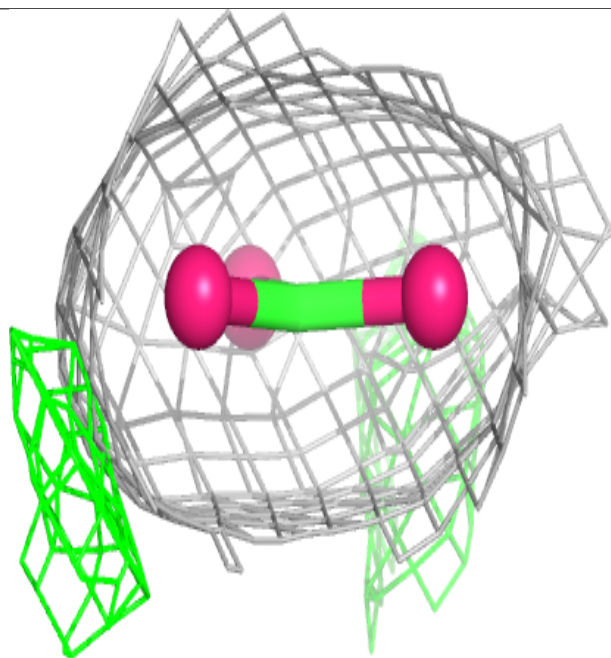
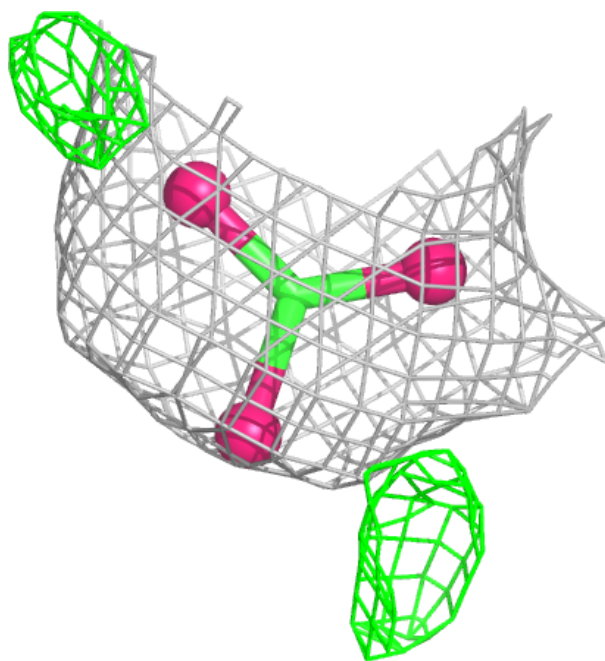
Electron density around BCT d 401 (A):

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



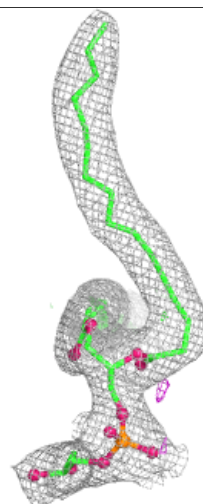
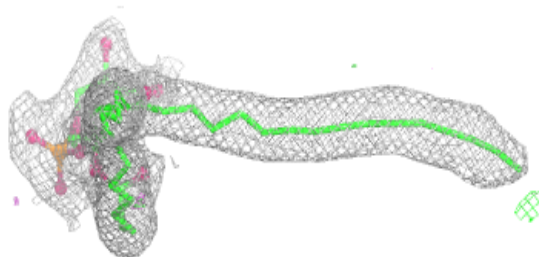
Electron density around BCT d 401 (B):

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



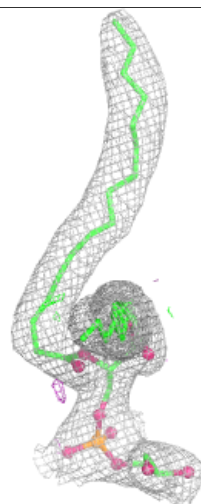
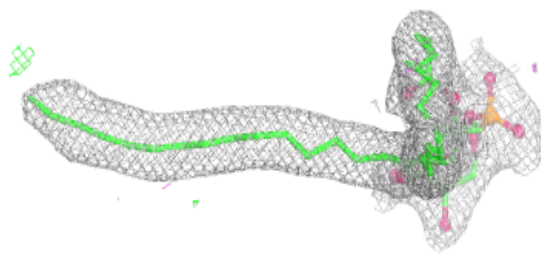
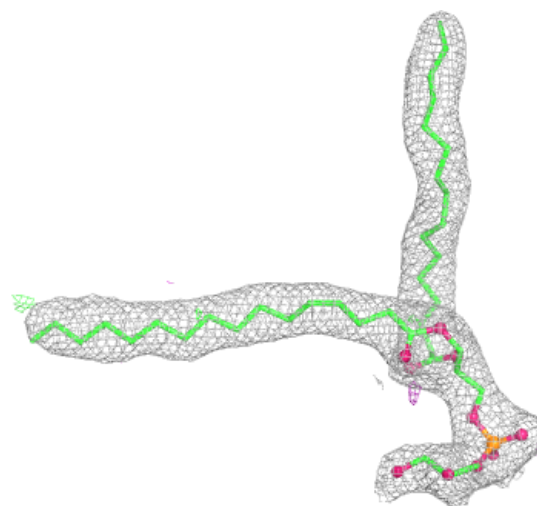
Electron density around LHG L 101 (A):

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



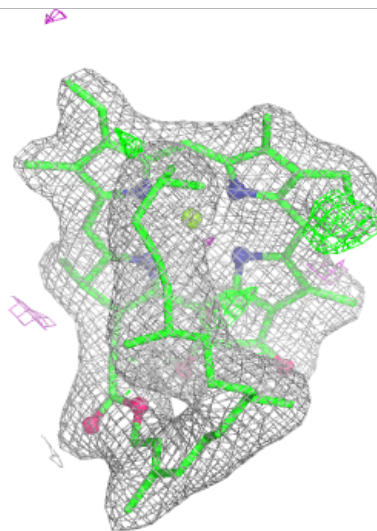
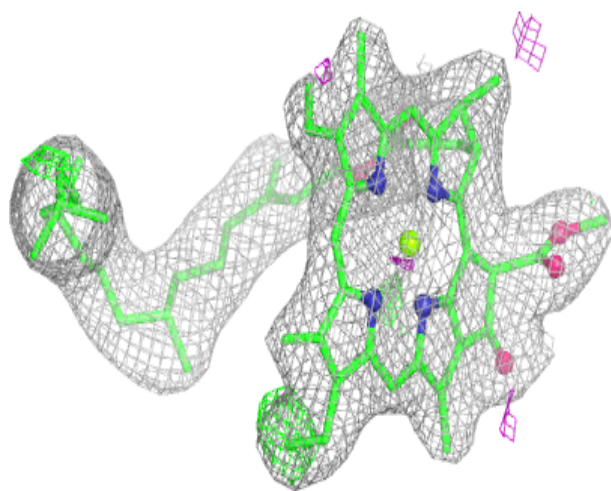
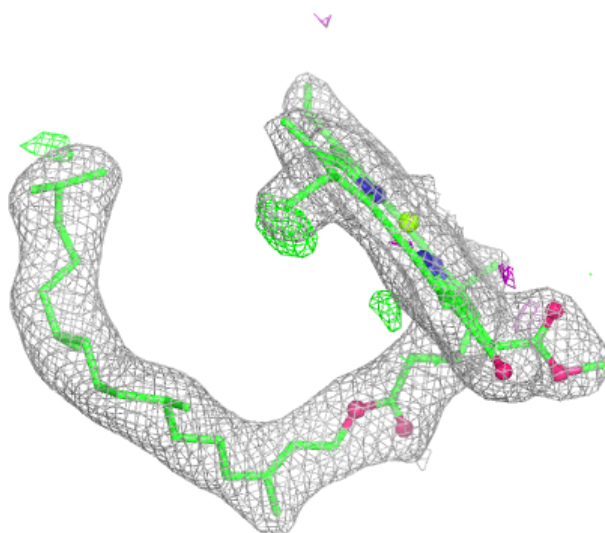
Electron density around LHG L 101 (B):

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



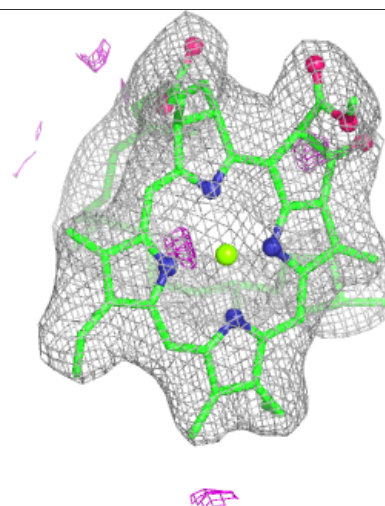
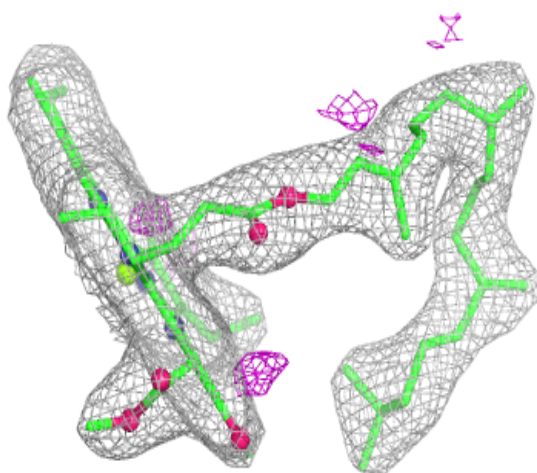
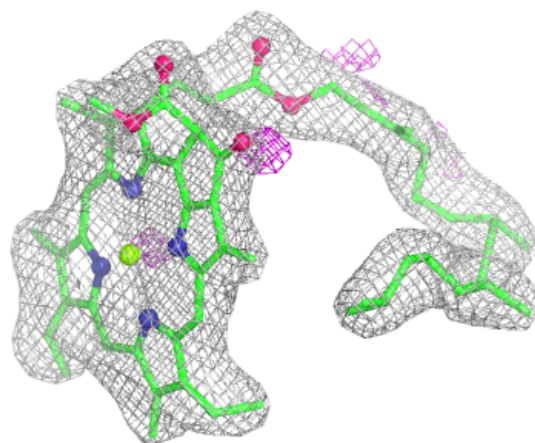
Electron density around CLA b 611:

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



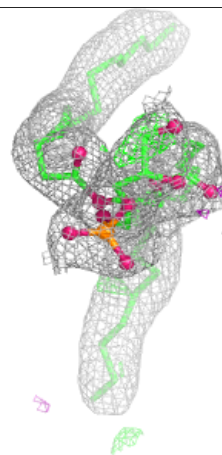
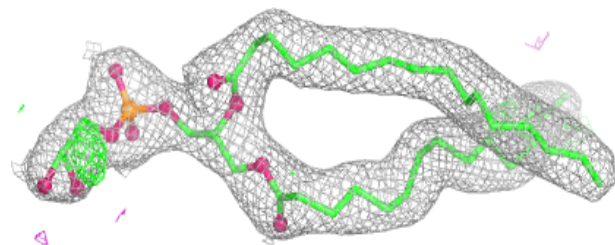
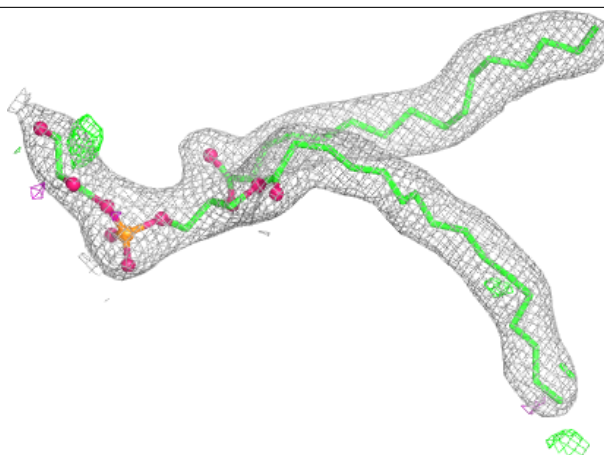
Electron density around CLA C 503:

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



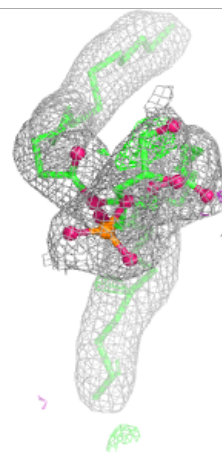
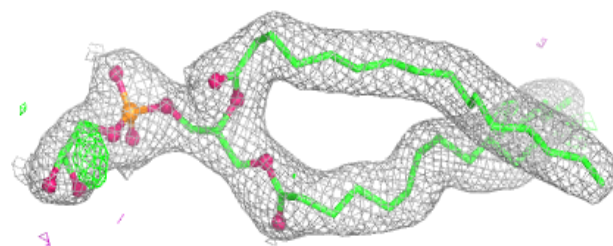
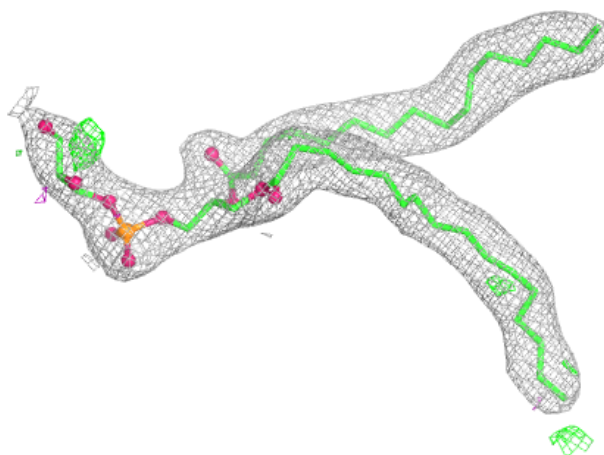
Electron density around LHG d 407 (A):

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



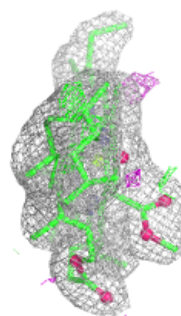
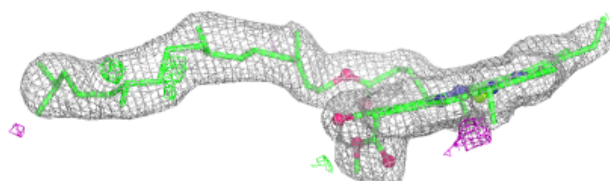
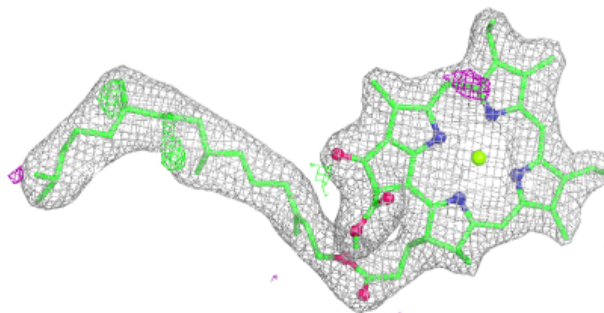
Electron density around LHG d 407 (B):

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

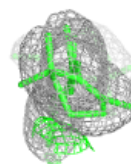
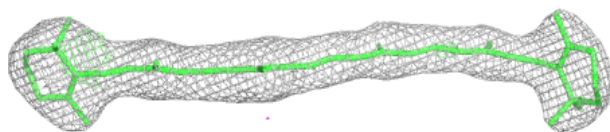
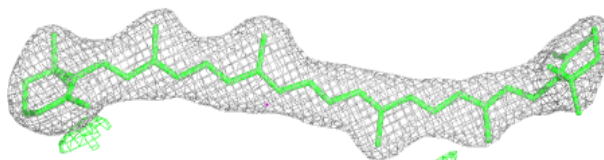


Electron density around CLA B 602:

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

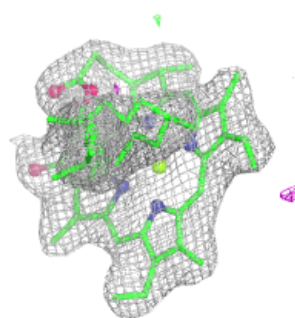
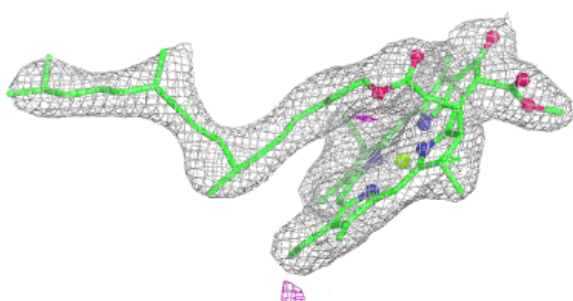
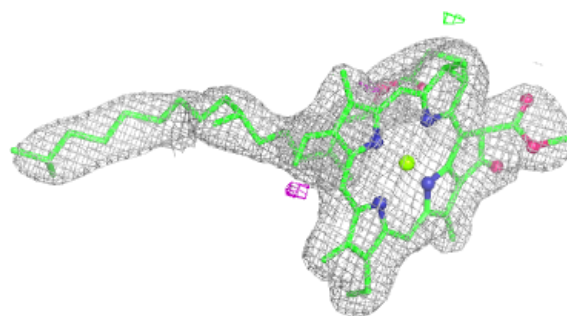
**Electron density around BCR c 516:**

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

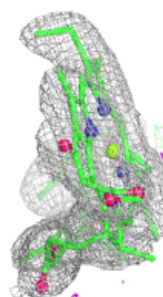
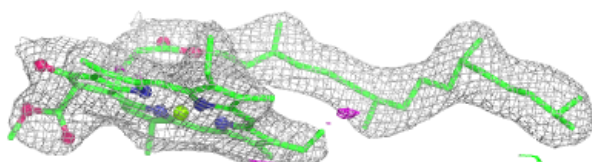
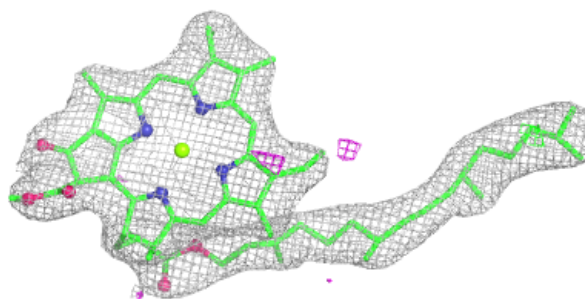


Electron density around CLA C 505:

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

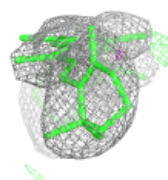
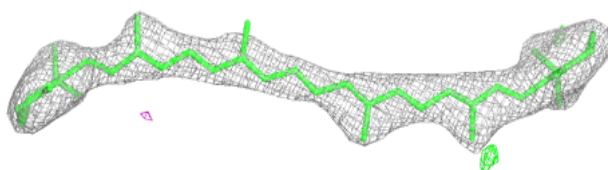
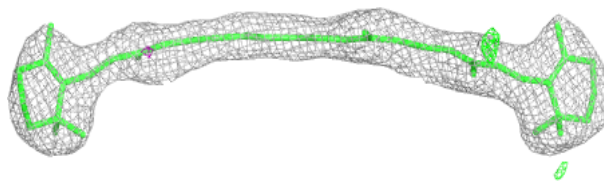
**Electron density around CLA c 502:**

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



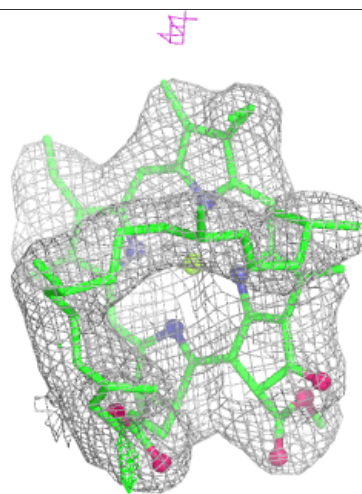
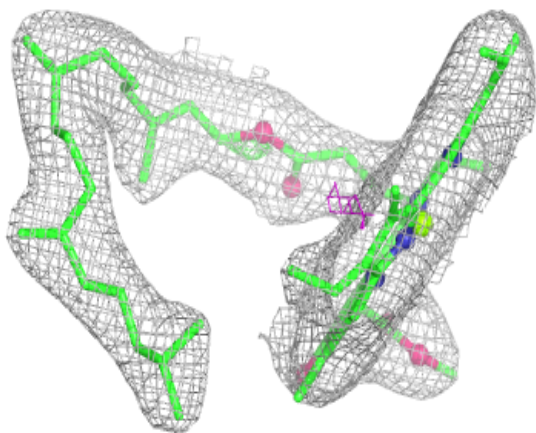
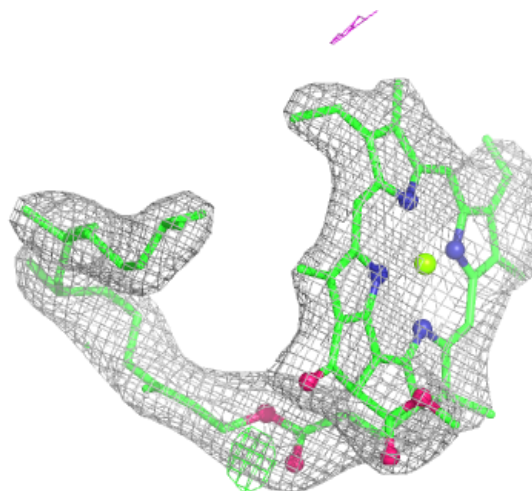
Electron density around BCR k 101:

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



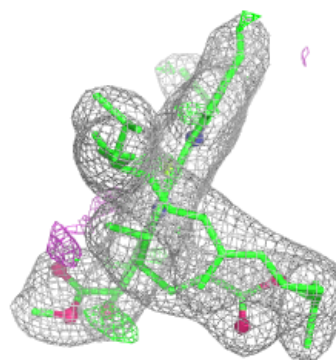
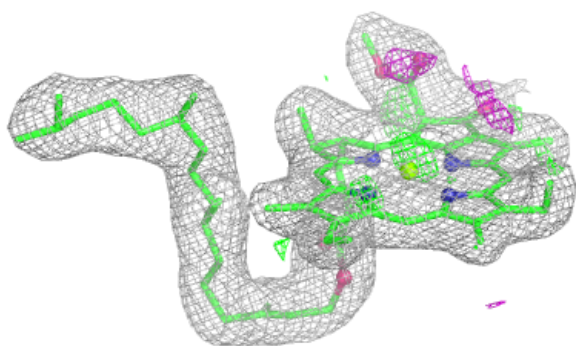
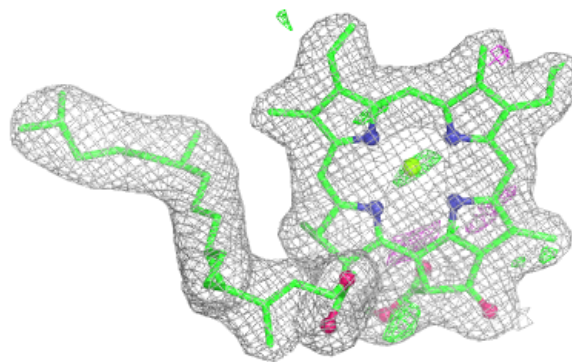
Electron density around CLA c 504:

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

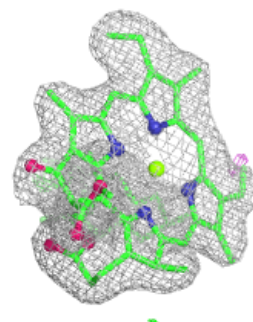
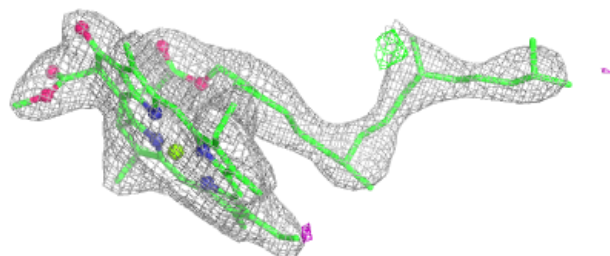
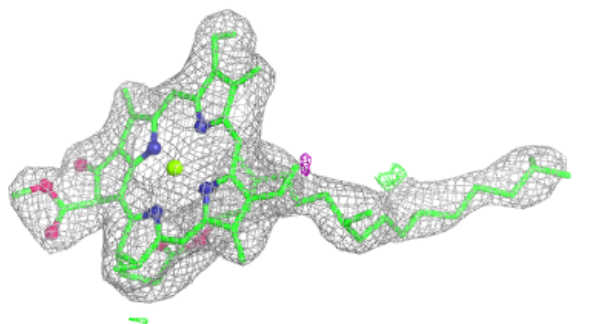


Electron density around CLA A 405 (A):

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

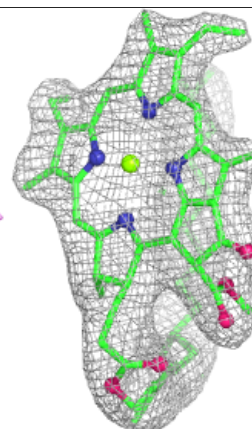
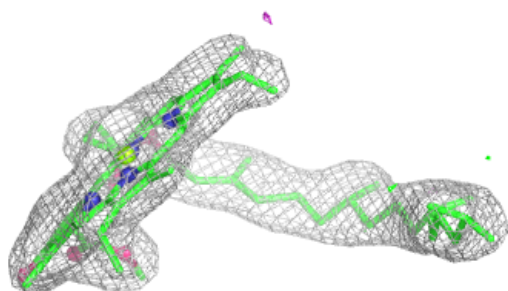
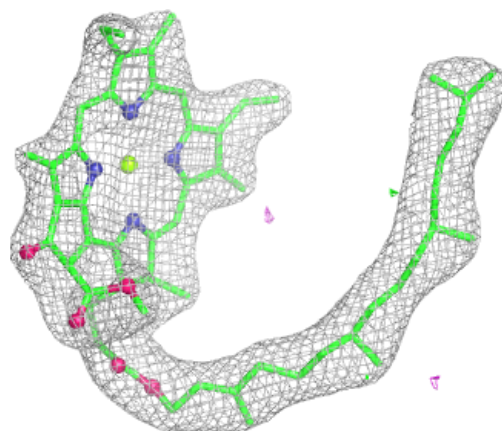
**Electron density around CLA c 506:**

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

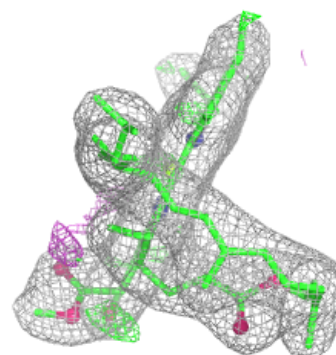
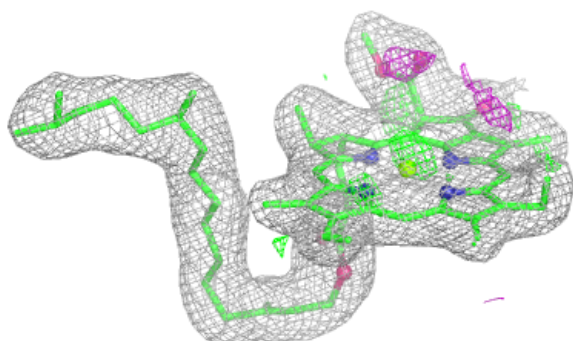
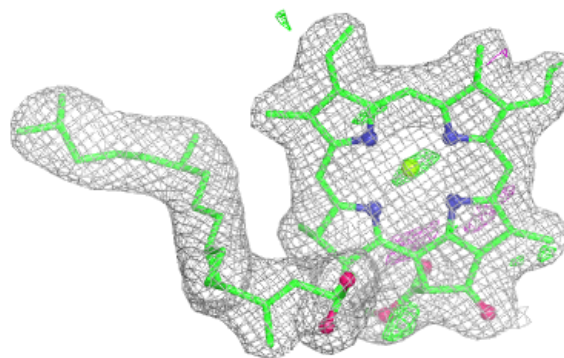


Electron density around CLA C 507:

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

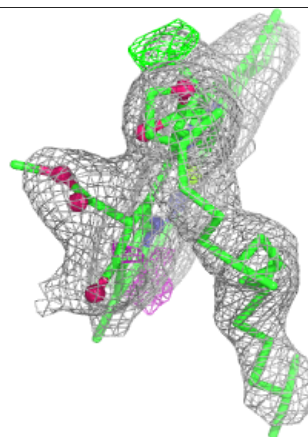
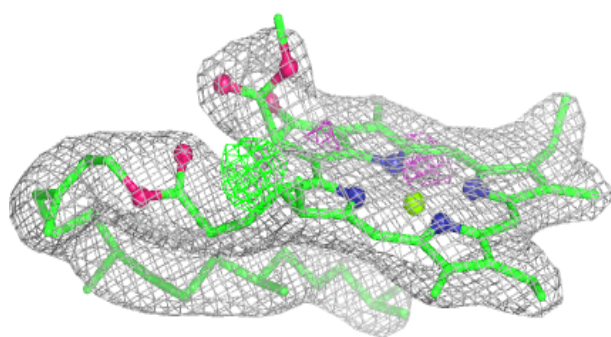
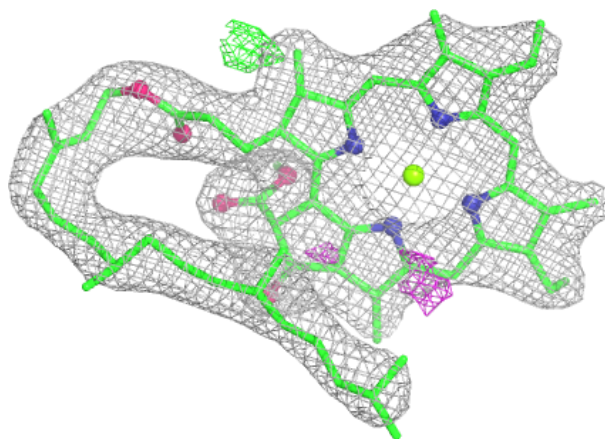
**Electron density around CLA A 405 (B):**

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



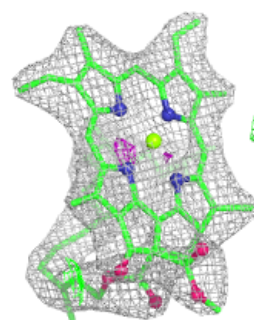
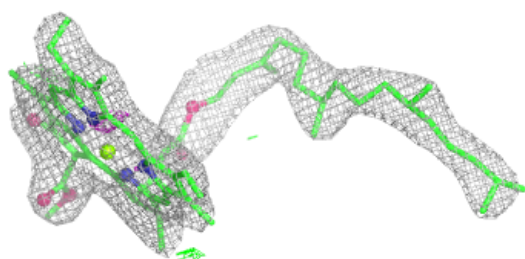
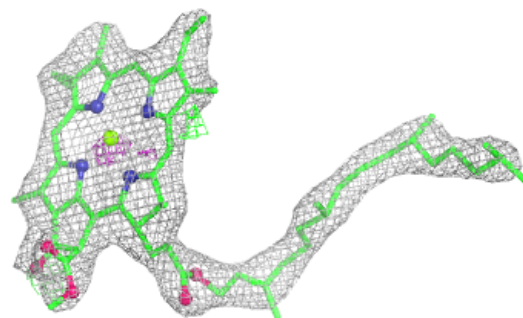
Electron density around CLA C 509:

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

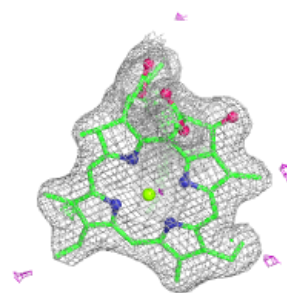
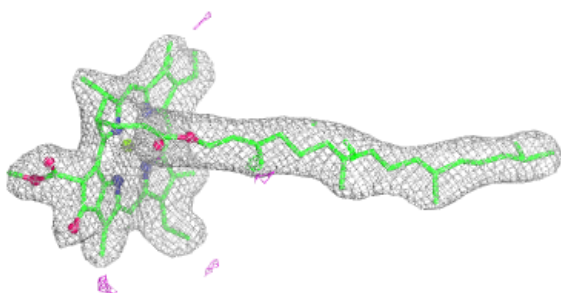
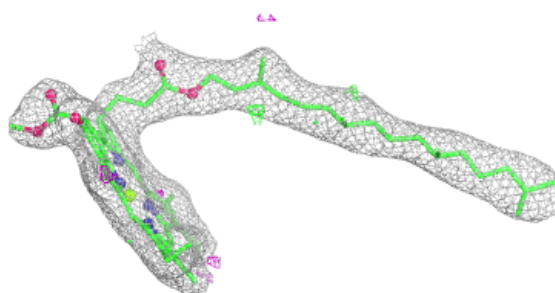


Electron density around CLA c 512:

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

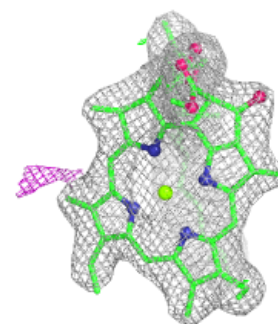
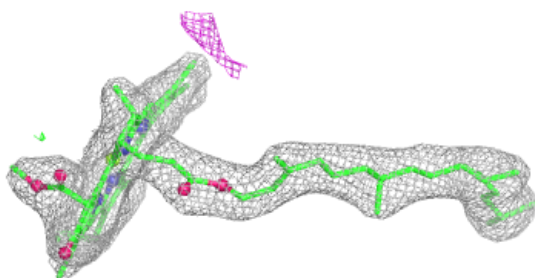
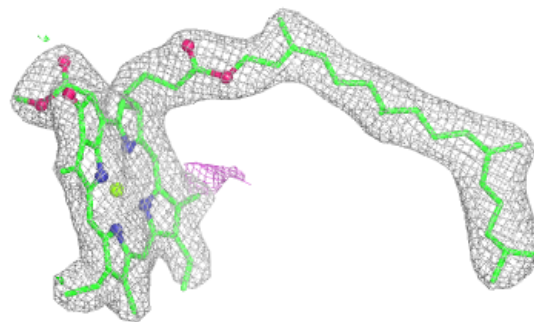
**Electron density around CLA B 607:**

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

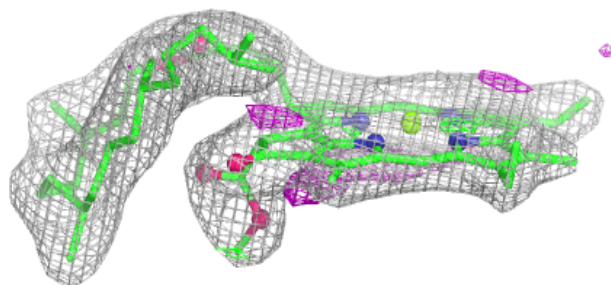
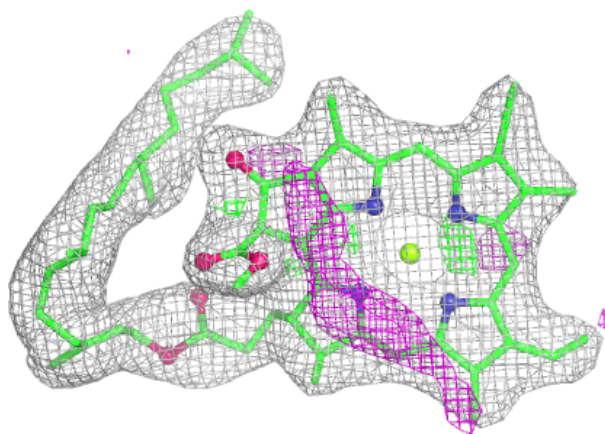


Electron density around CLA B 609:

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

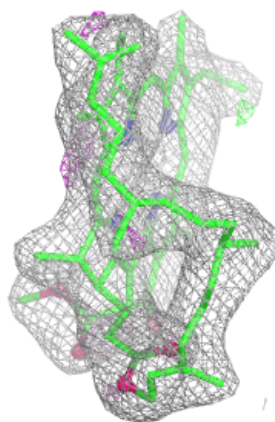
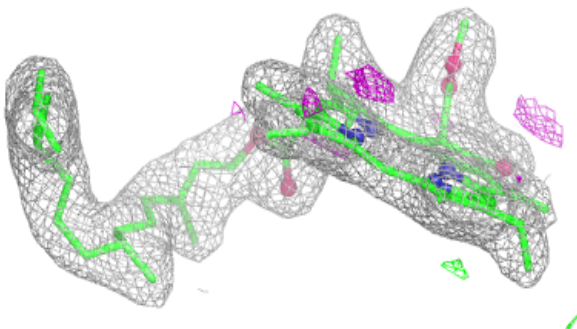
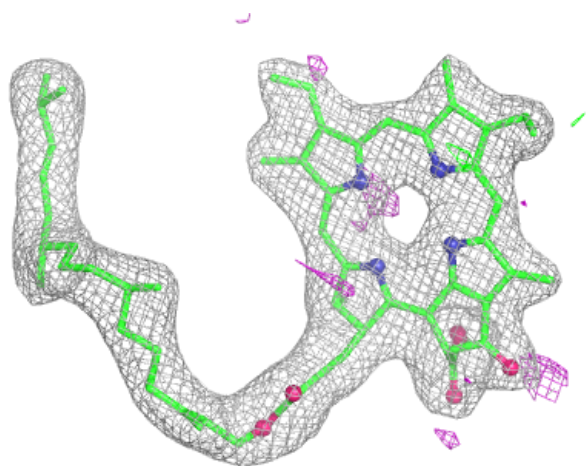
**Electron density around CLA B 610:**

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



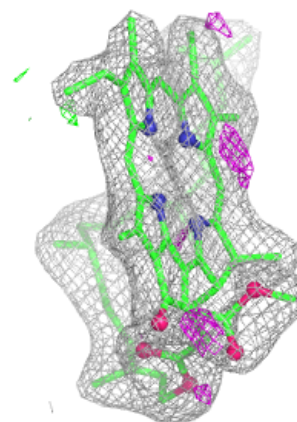
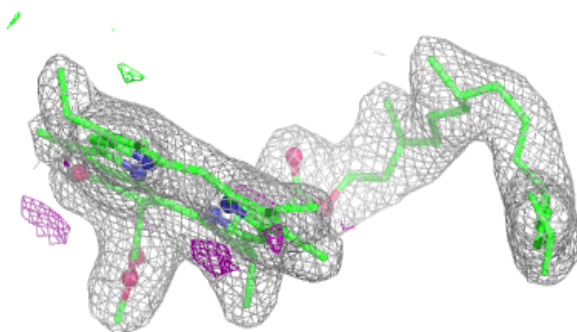
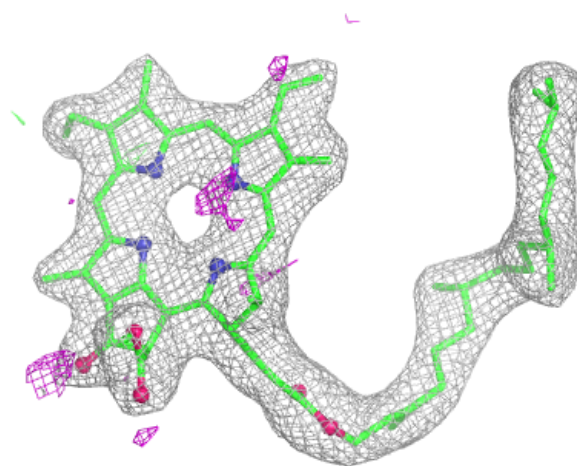
Electron density around PHO A 416 (A):

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



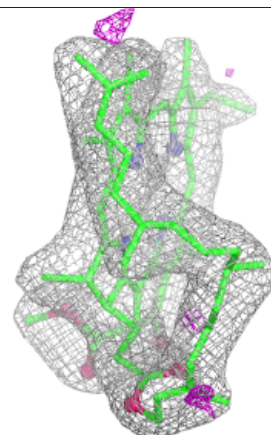
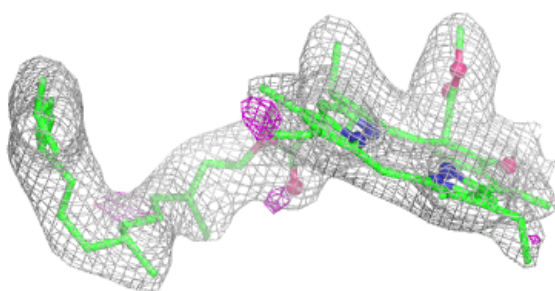
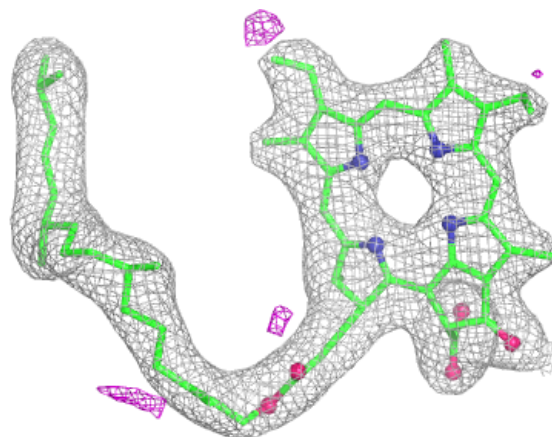
Electron density around PHO A 416 (B):

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



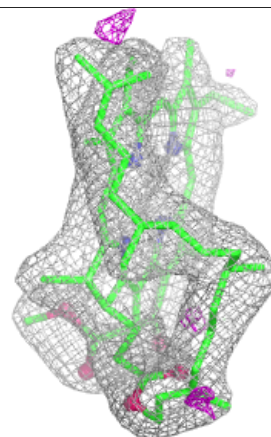
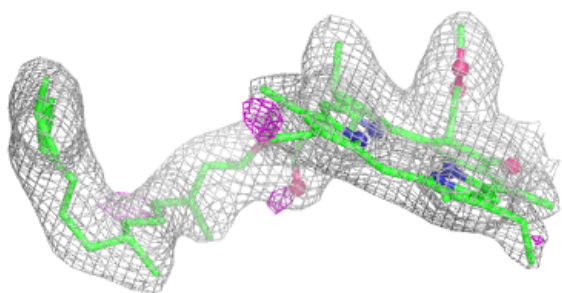
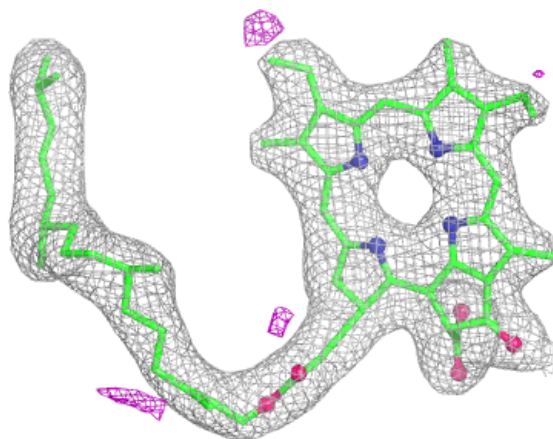
Electron density around PHO a 414 (A):

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



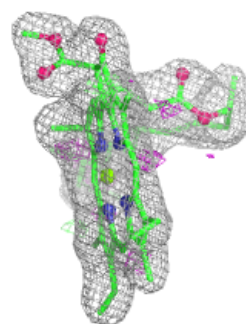
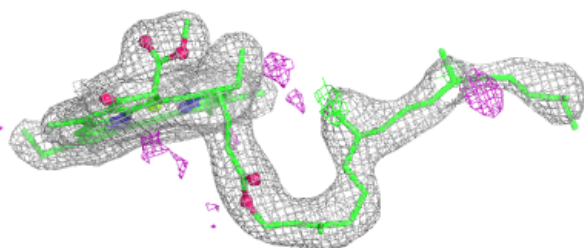
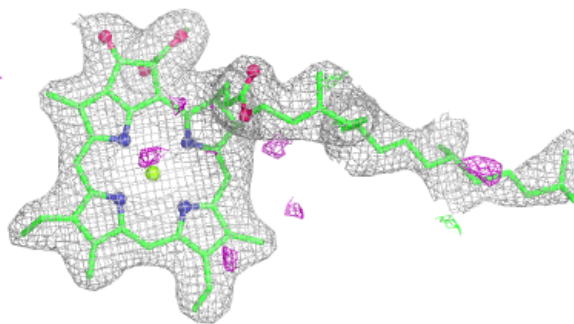
Electron density around PHO a 414 (B):

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

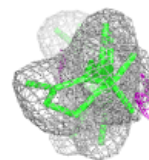
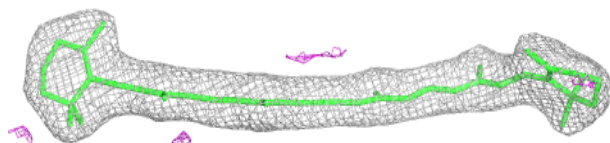
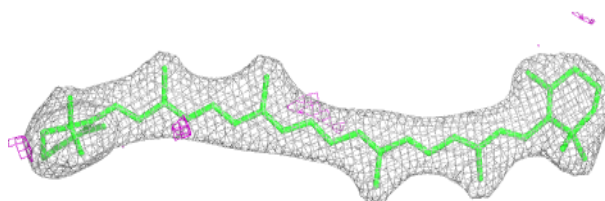


Electron density around CLA A 406 (A):

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

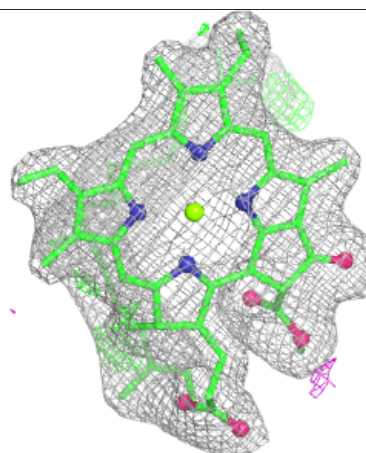
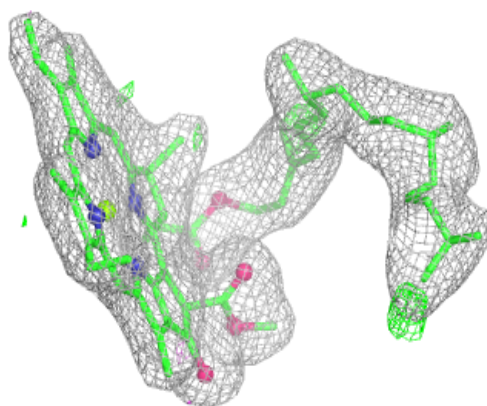
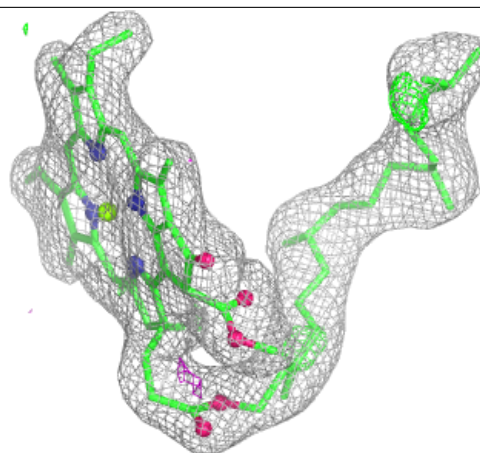
**Electron density around BCR B 617:**

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



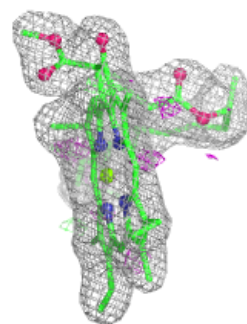
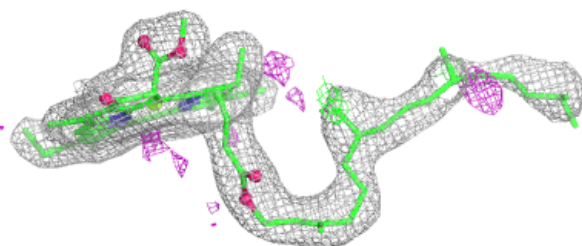
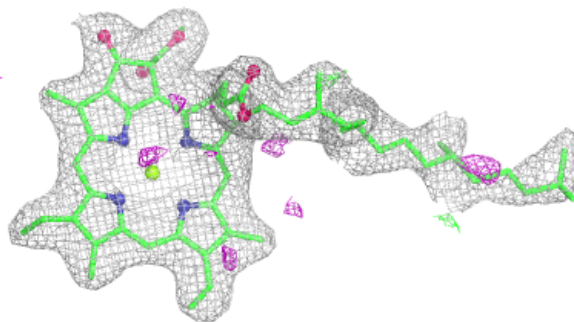
Electron density around CLA B 613:

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

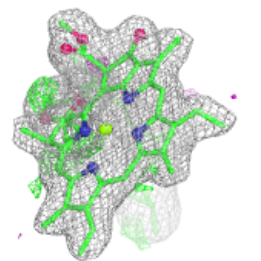
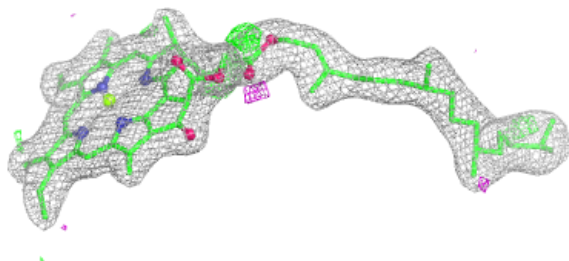
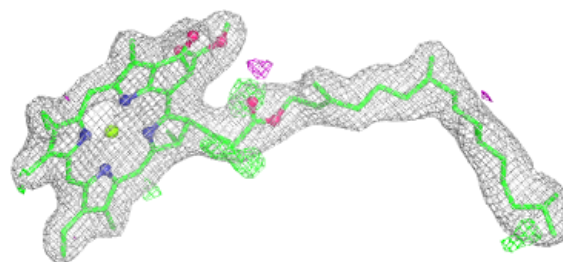


Electron density around CLA A 406 (B):

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

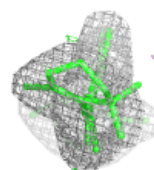
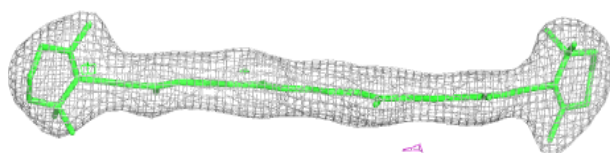
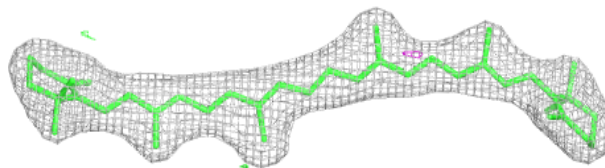
**Electron density around CLA A 404 (A):**

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

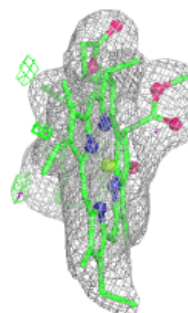
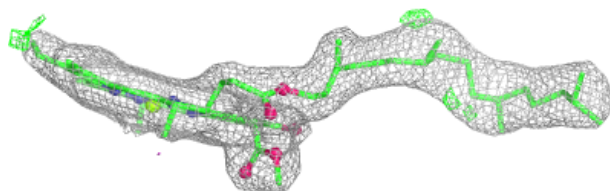
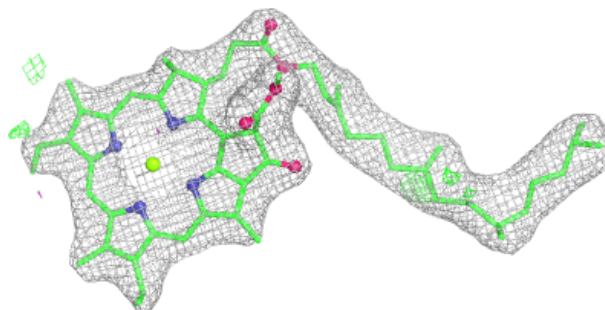


Electron density around BCR C 515:

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

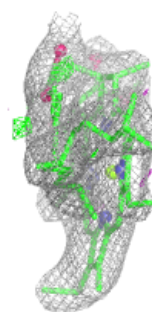
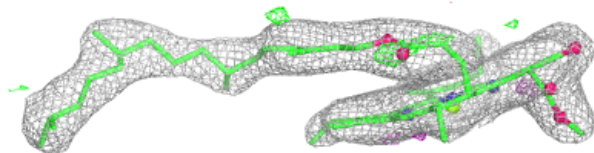
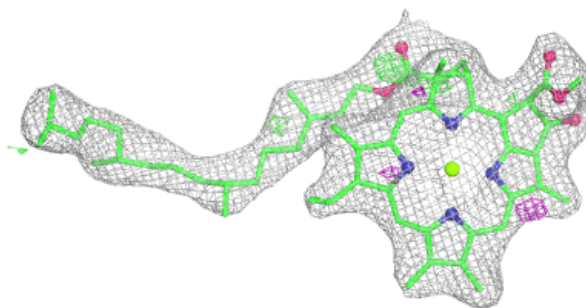
**Electron density around CLA b 602:**

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

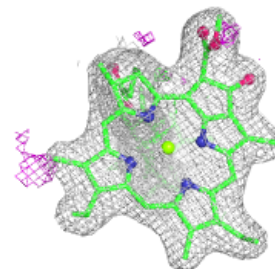
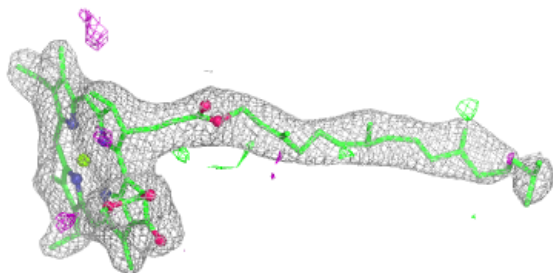
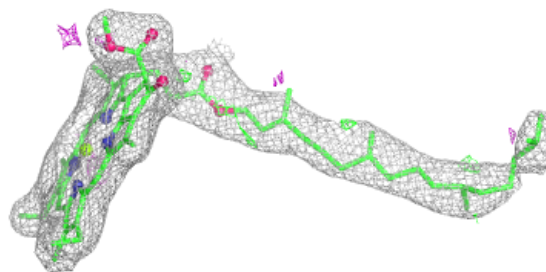


Electron density around CLA b 603:

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

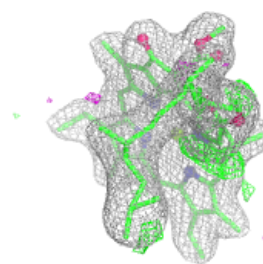
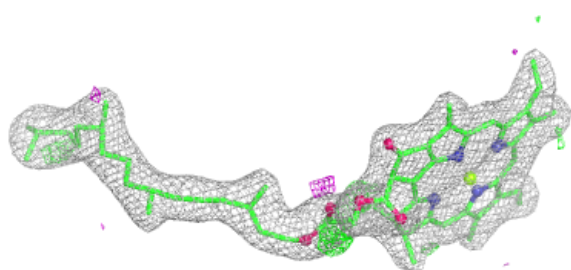
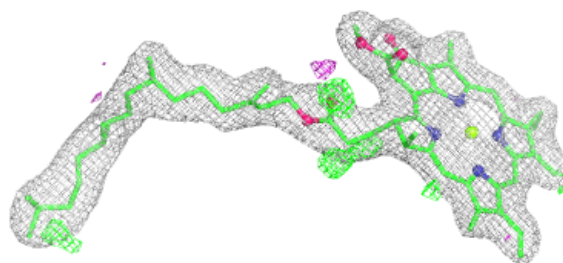
**Electron density around CLA b 604:**

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

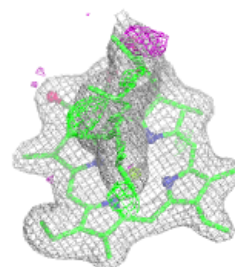
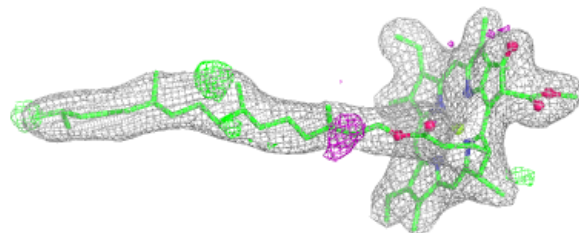


Electron density around CLA A 404 (B):

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

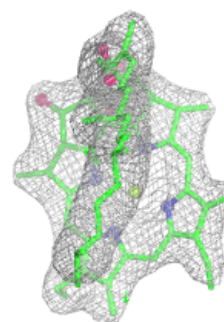
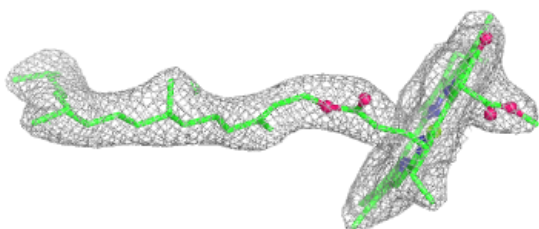
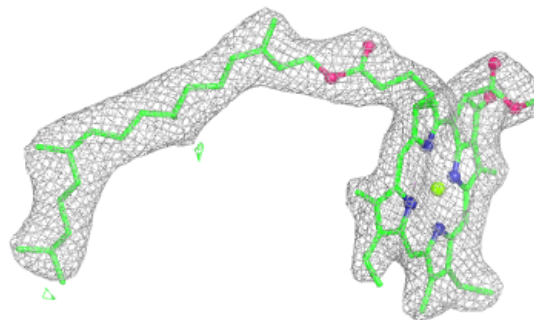
**Electron density around CLA b 607:**

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

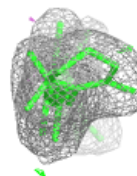
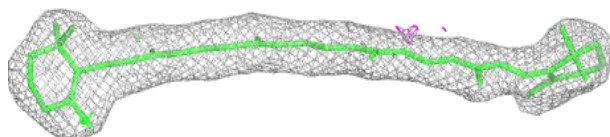
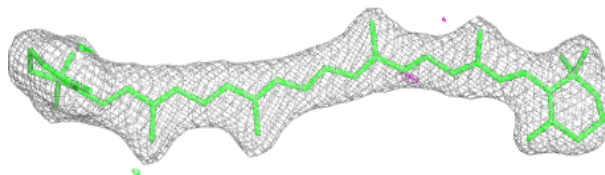


Electron density around CLA b 609:

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

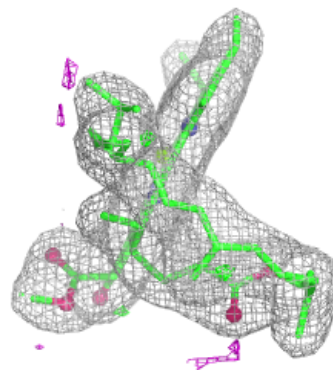
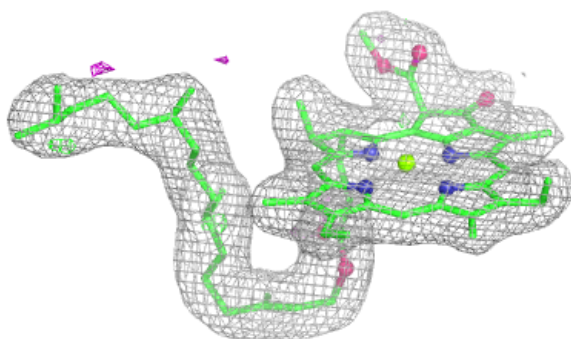
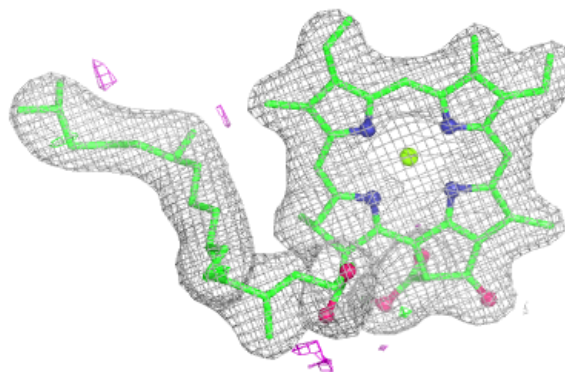
**Electron density around BCR b 617:**

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

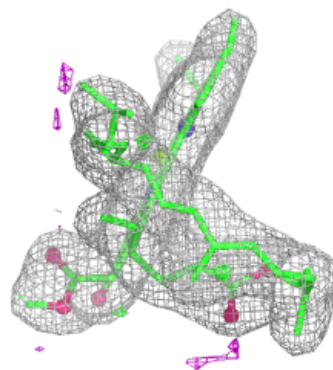
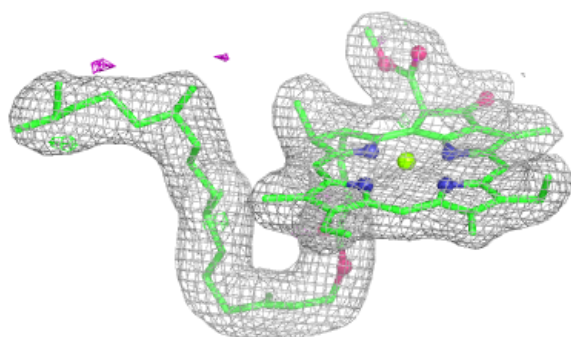
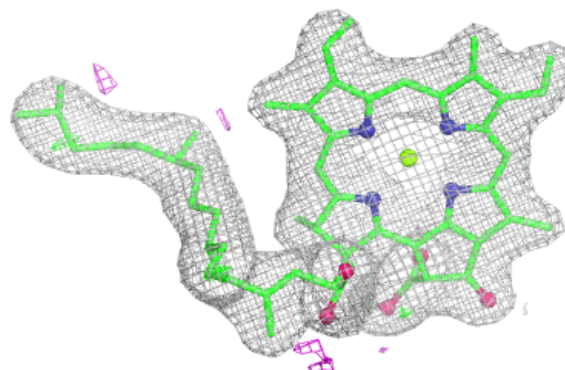


Electron density around CLA d 402 (A):

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

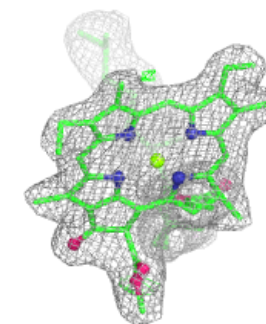
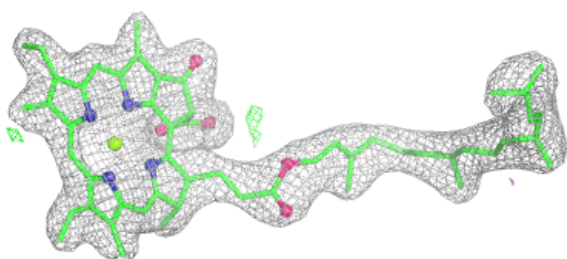
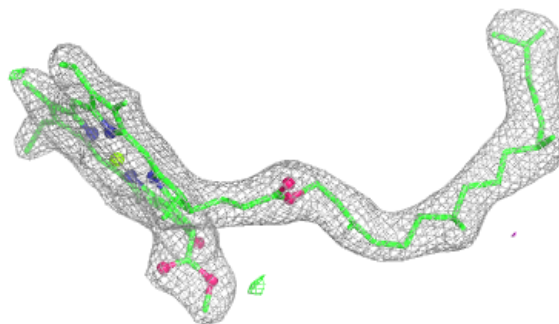
**Electron density around CLA d 402 (B):**

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

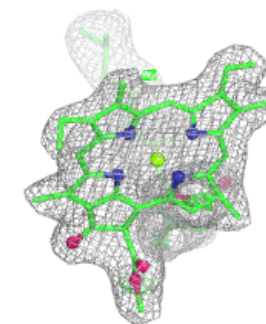
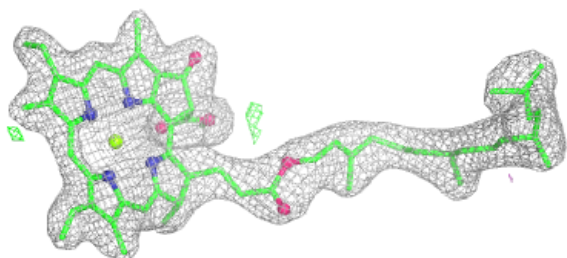
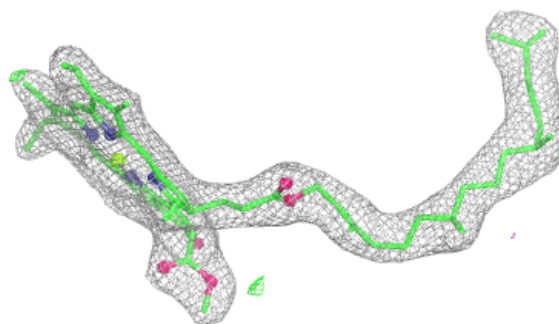


Electron density around CLA d 403 (A):

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

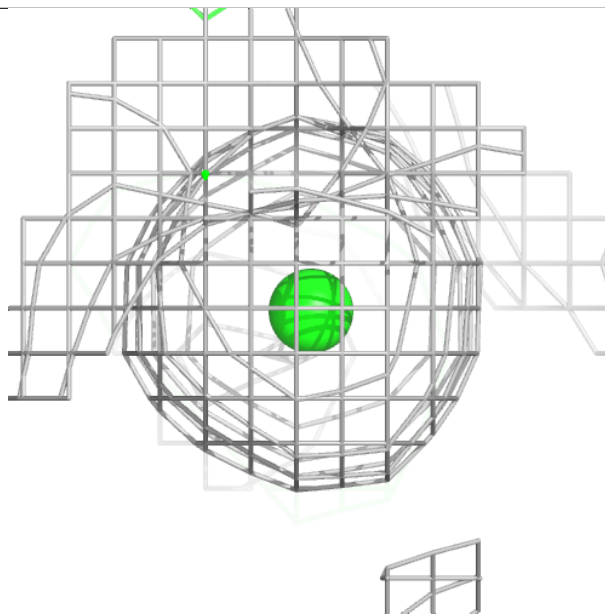
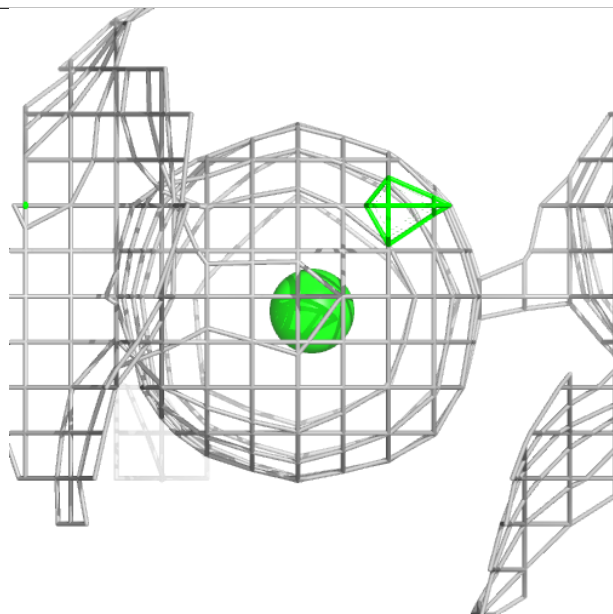
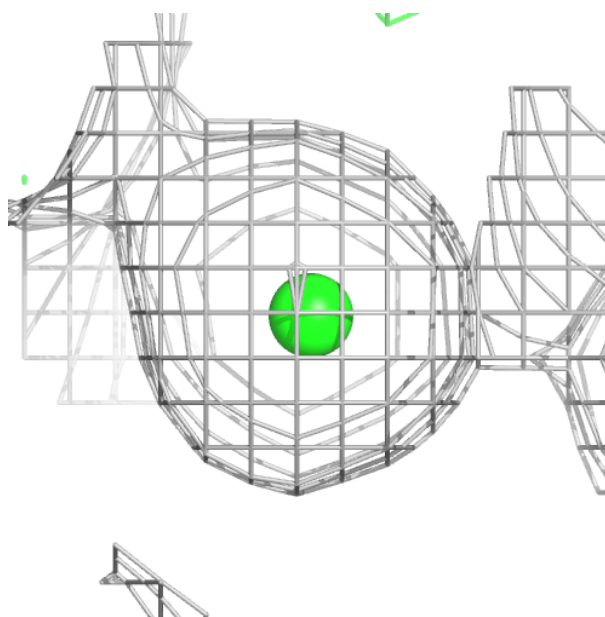
**Electron density around CLA d 403 (B):**

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



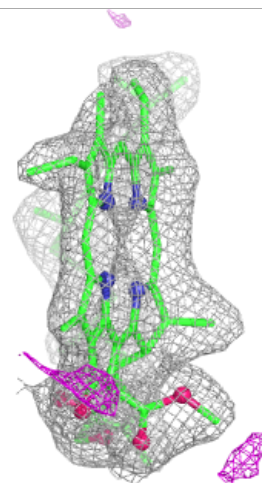
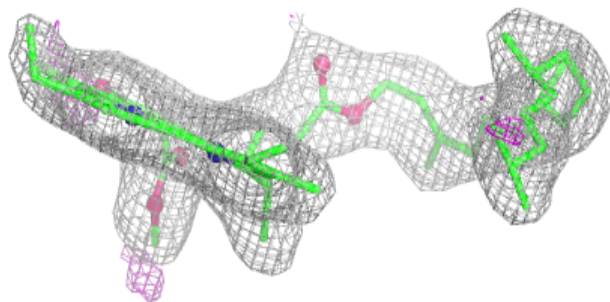
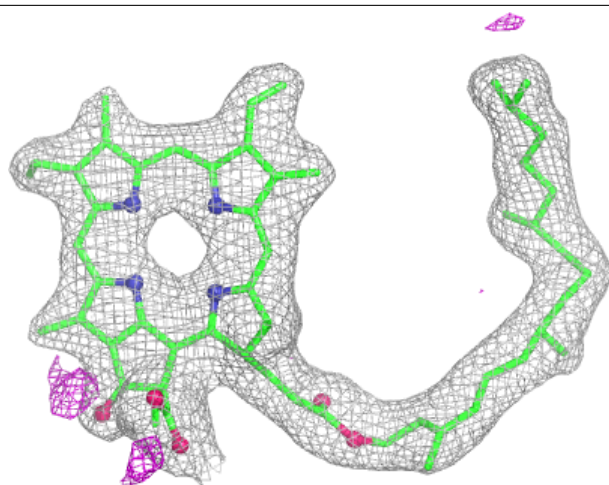
Electron density around CL A 403 (A):

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



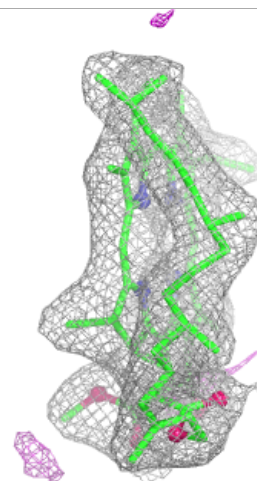
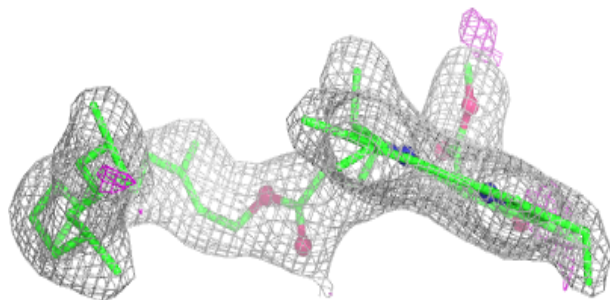
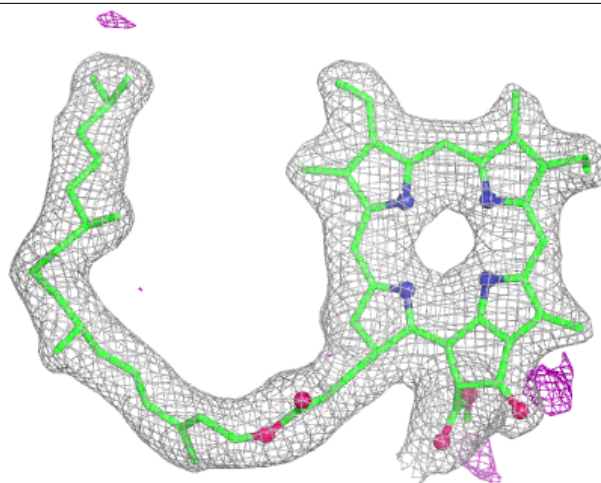
Electron density around PHO A 407 (A):

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



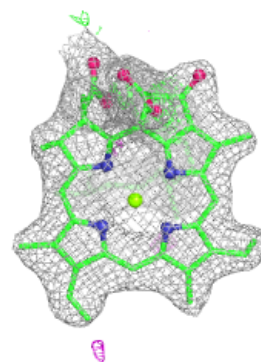
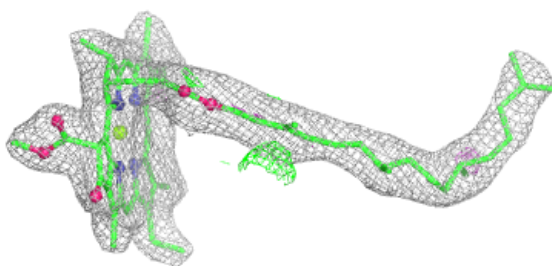
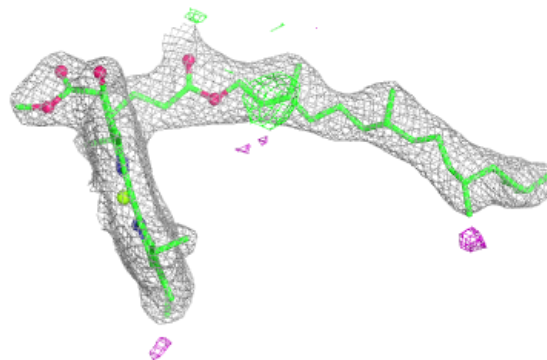
Electron density around PHO A 407 (B):

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

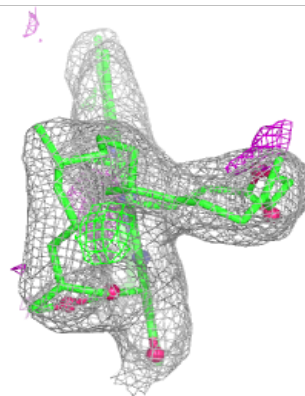
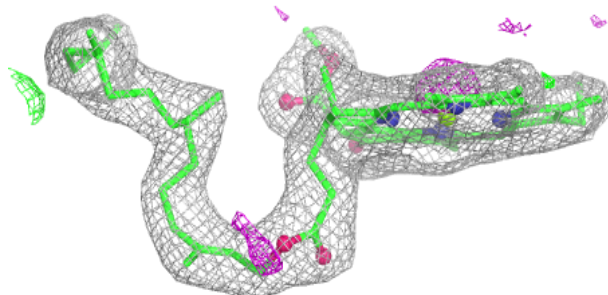
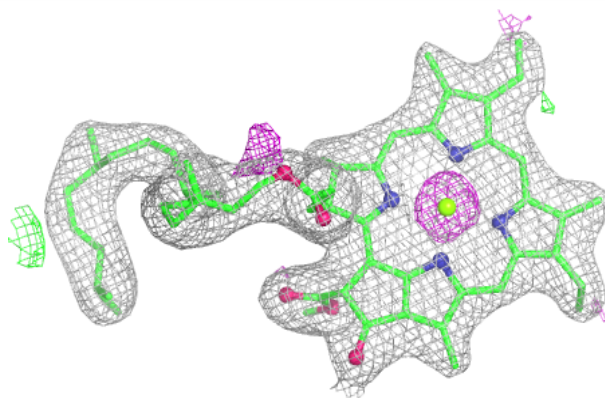


Electron density around CLA b 605:

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

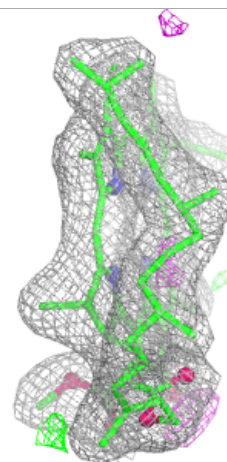
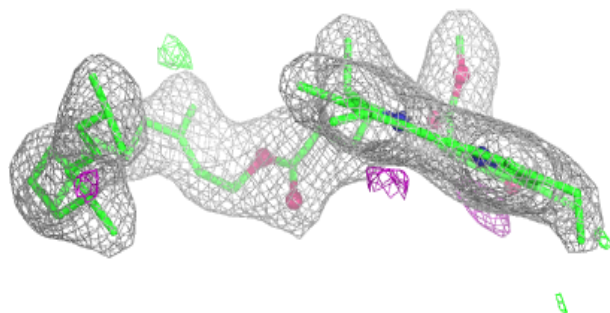
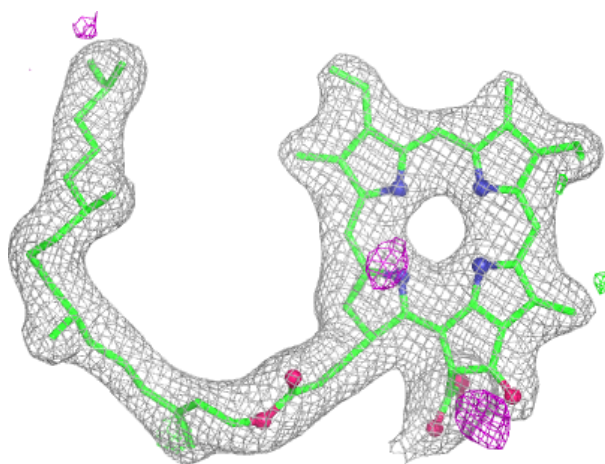
**Electron density around CLA B 612:**

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



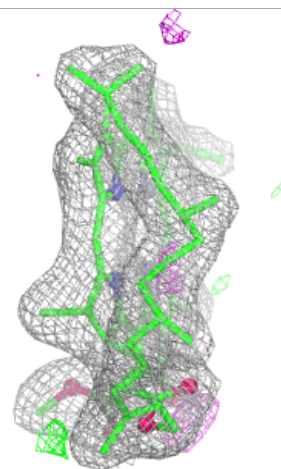
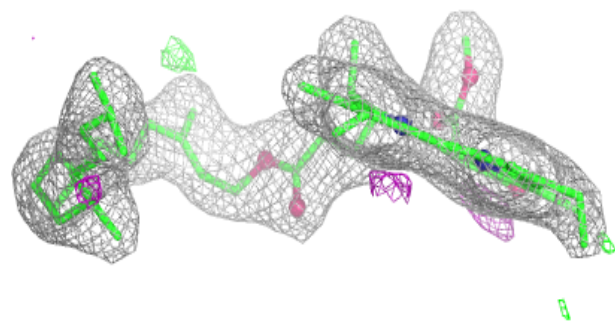
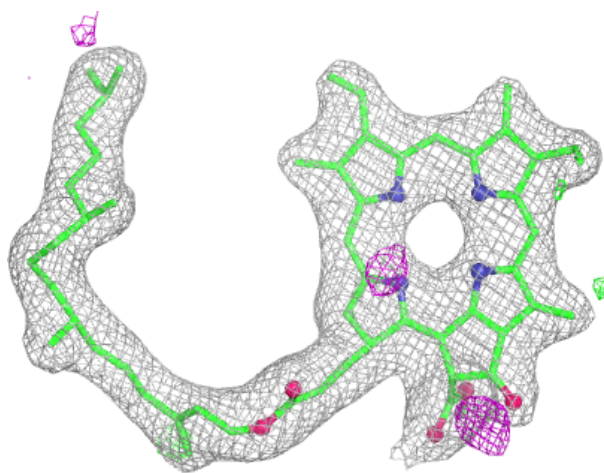
Electron density around PHO a 406 (A):

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



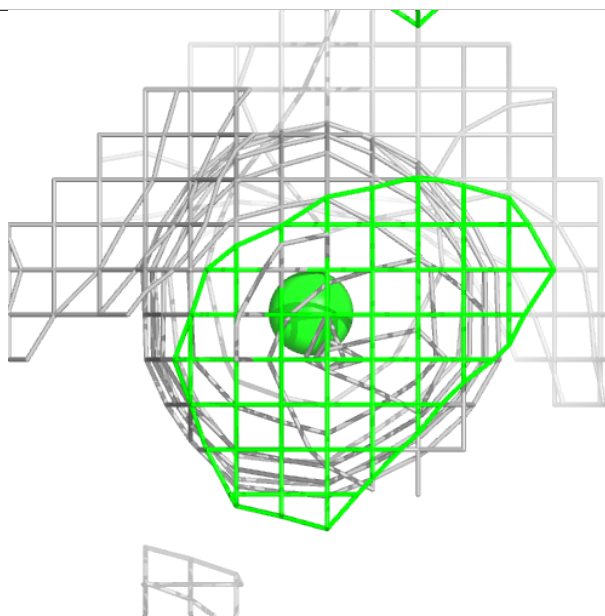
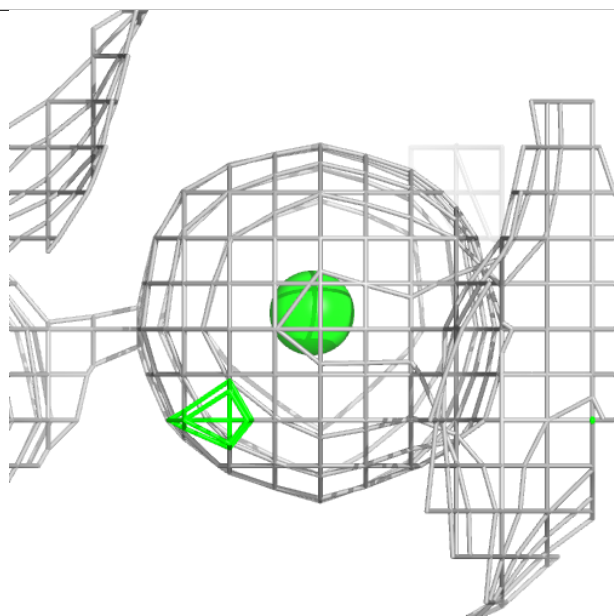
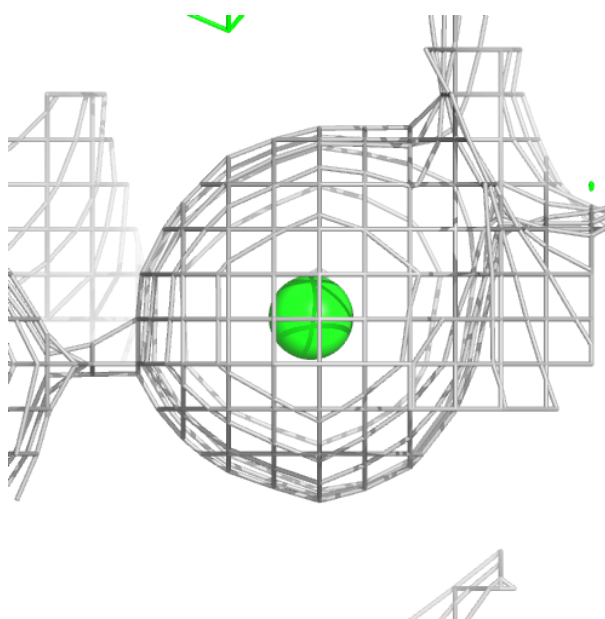
Electron density around PHO a 406 (B):

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



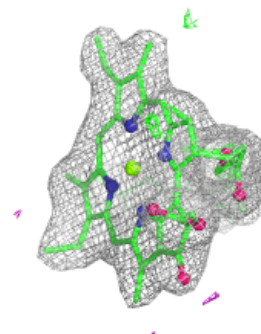
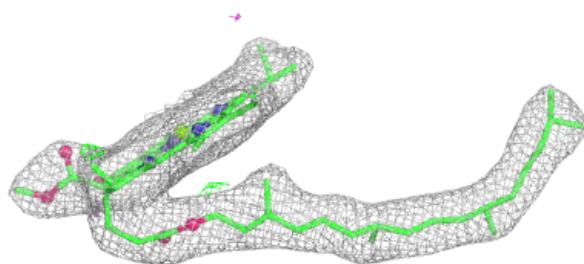
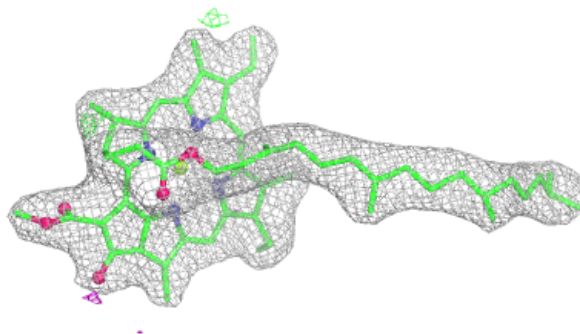
Electron density around CL A 403 (B):

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



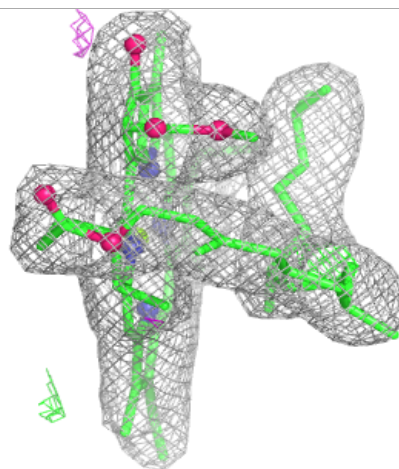
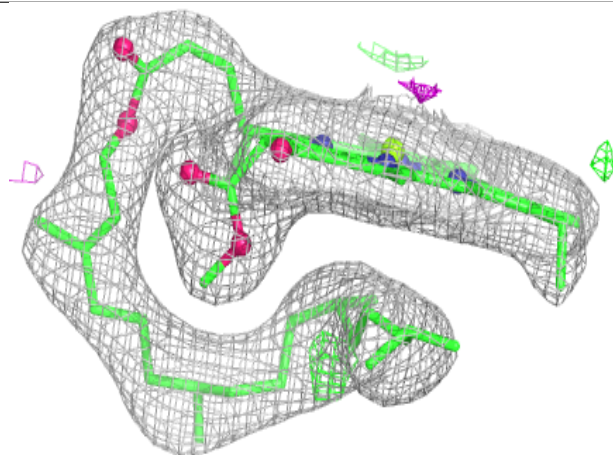
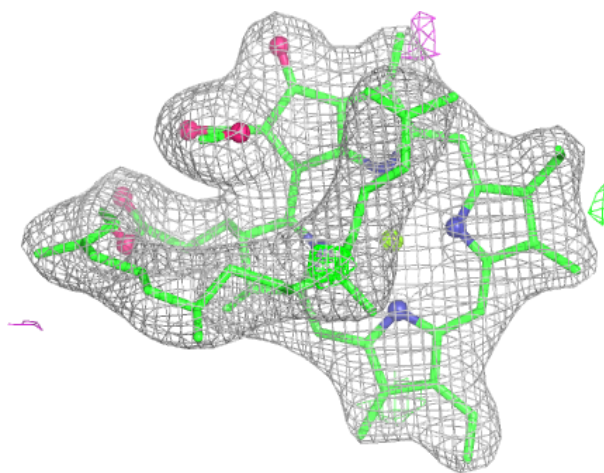
Electron density around CLA b 608:

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



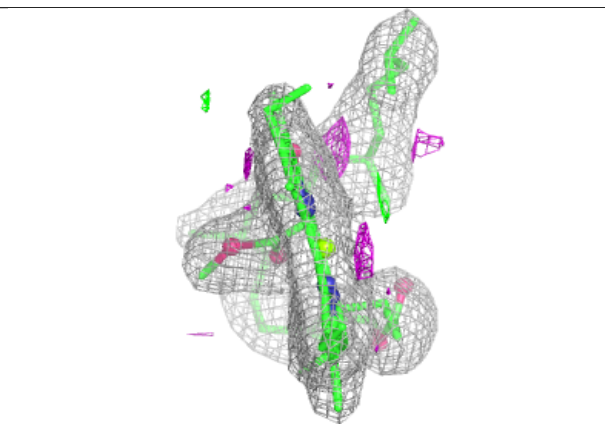
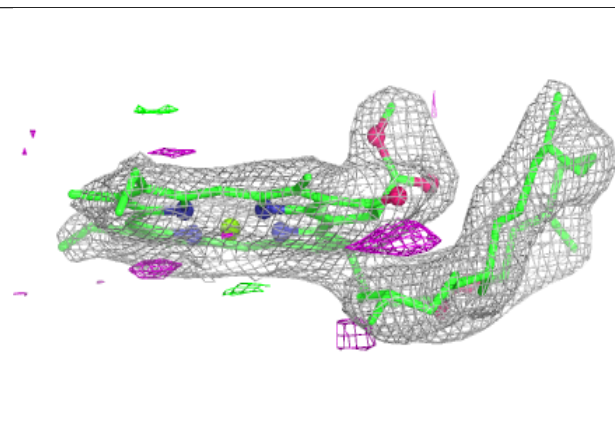
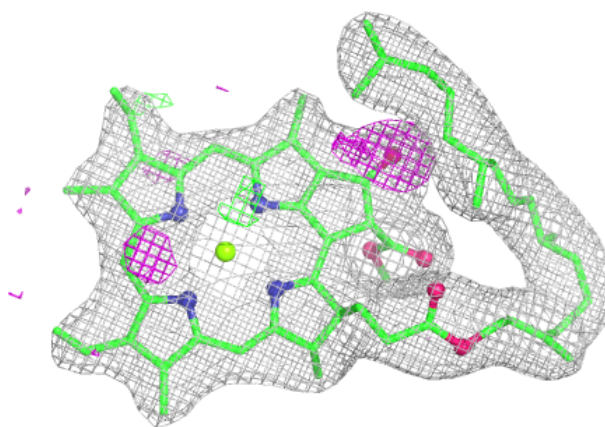
Electron density around CLA C 510:

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

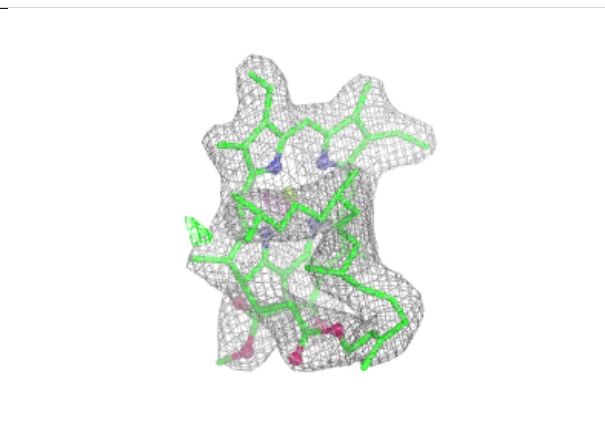
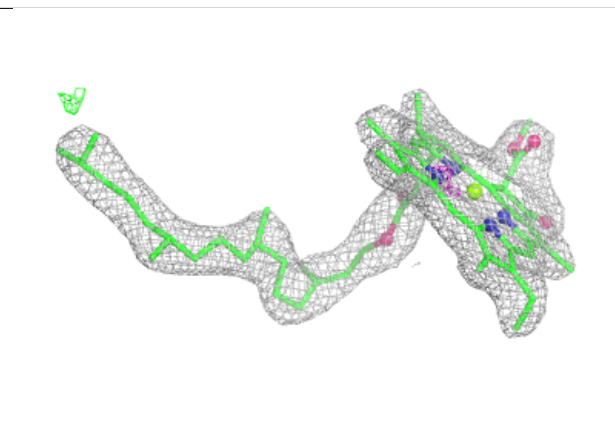
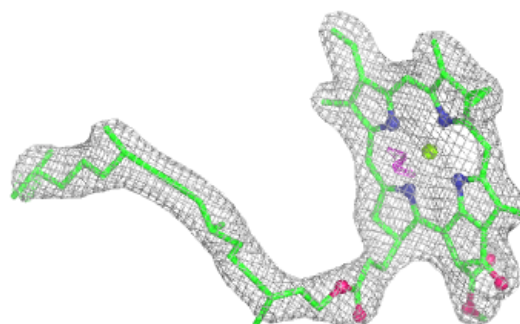


Electron density around CLA b 610:

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

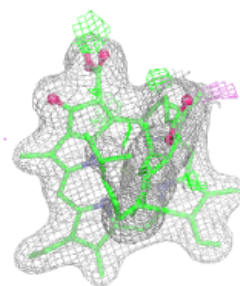
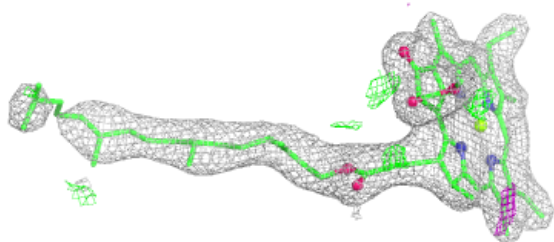
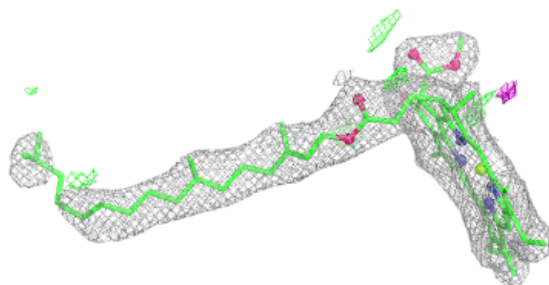
**Electron density around CLA C 511:**

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



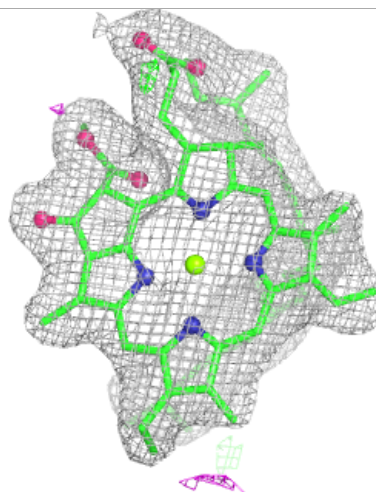
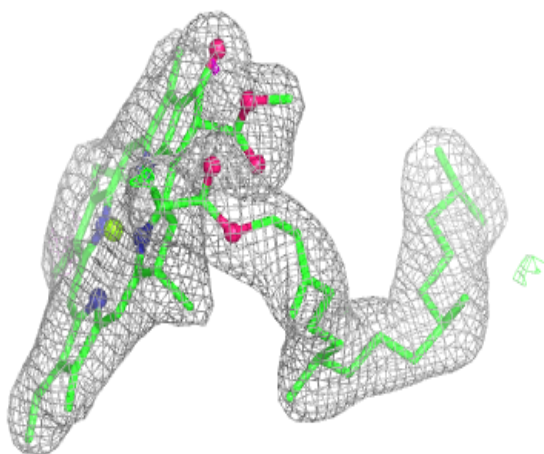
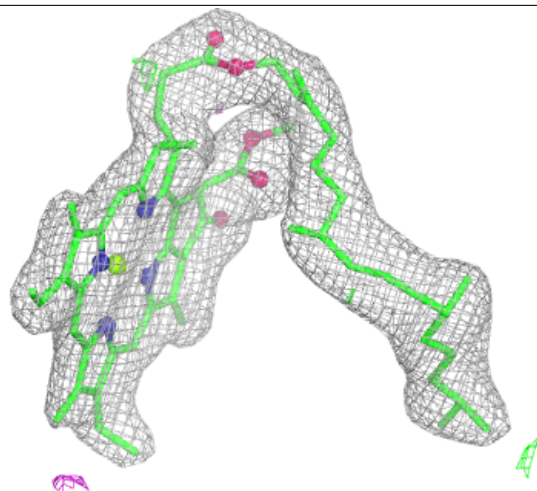
Electron density around CLA B 604:

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



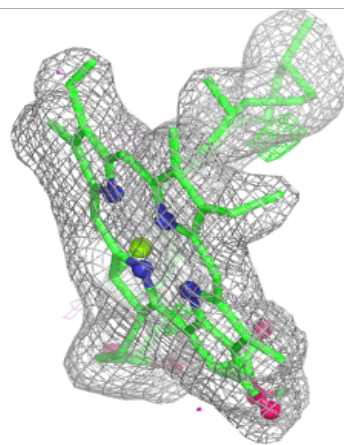
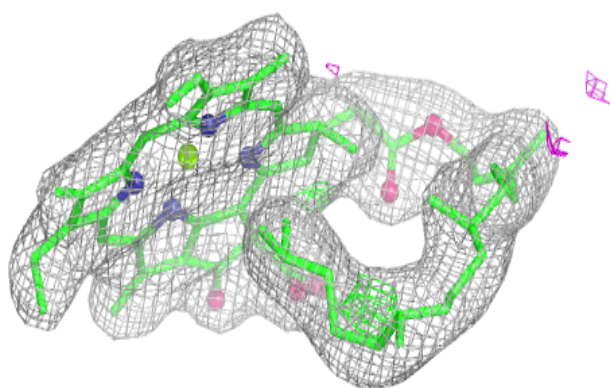
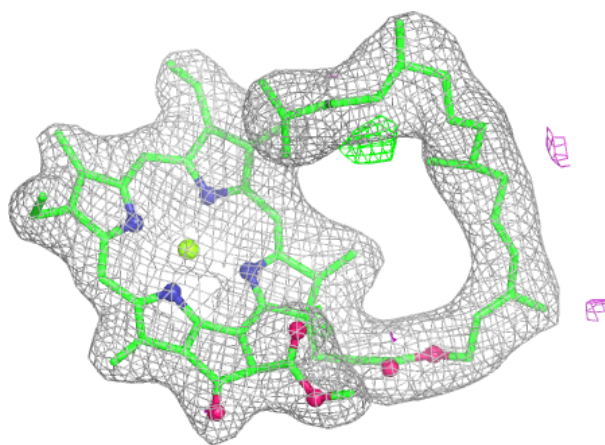
Electron density around CLA b 613:

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



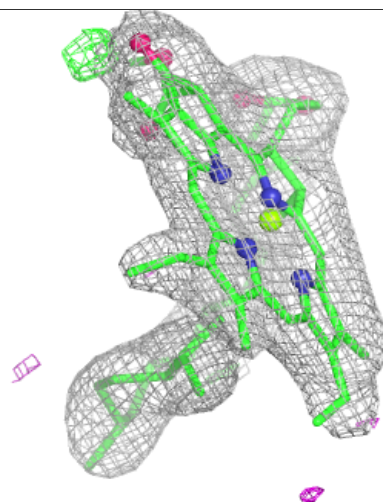
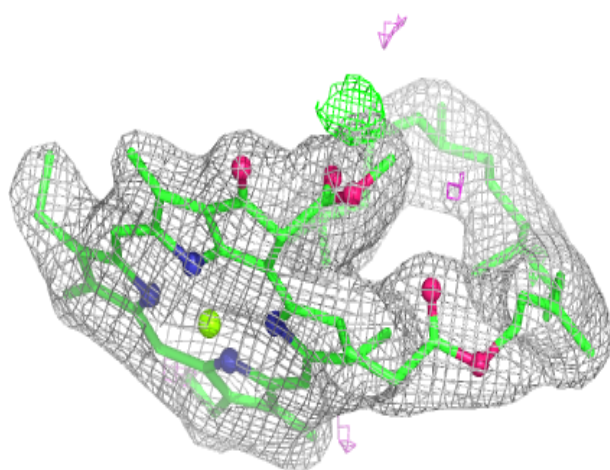
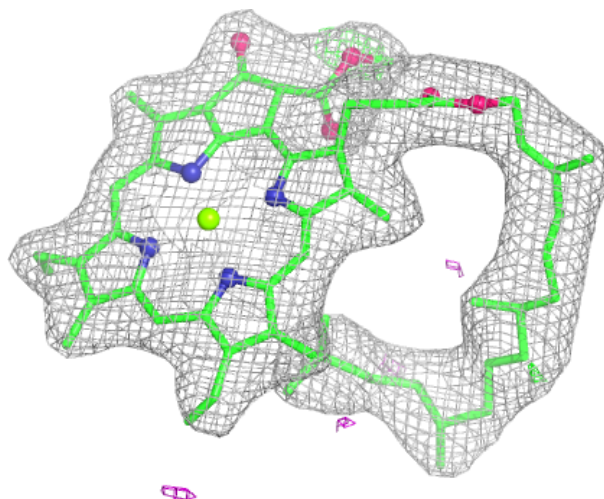
Electron density around CLA B 615:

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



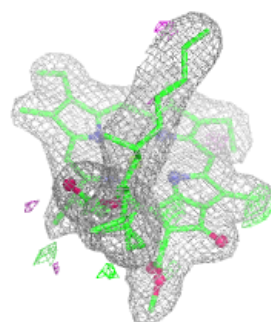
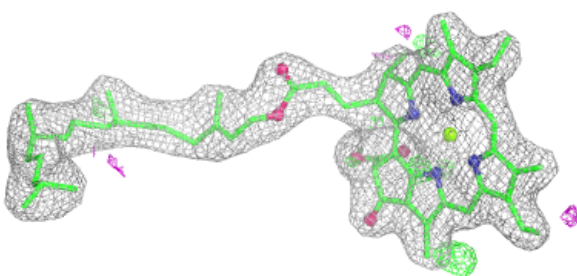
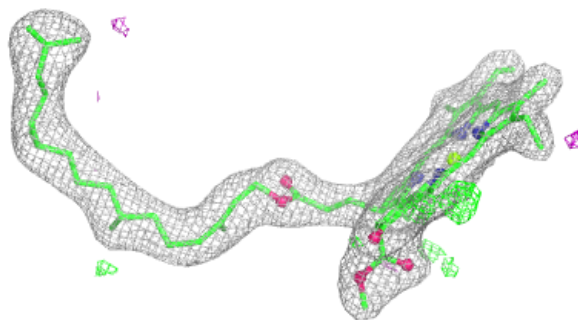
Electron density around CLA b 615:

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

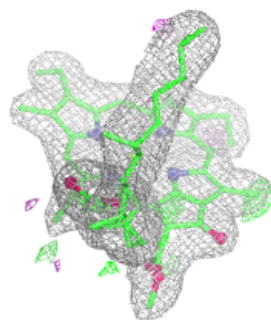
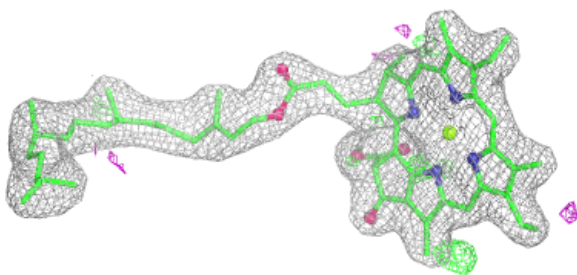
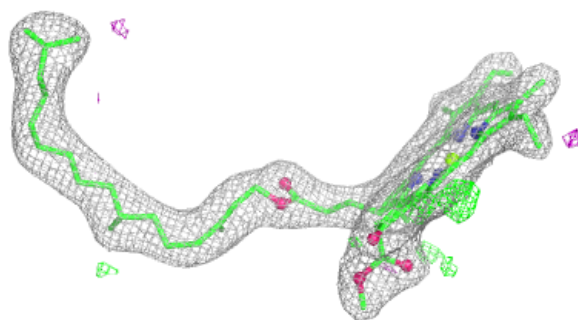


Electron density around CLA D 403 (A):

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

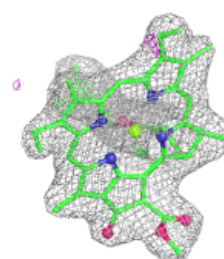
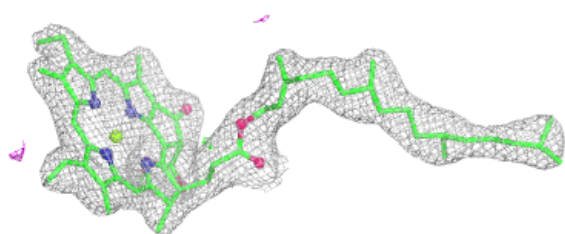
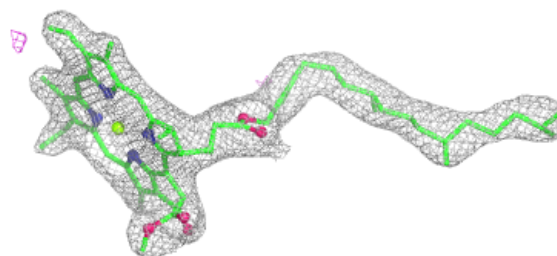
**Electron density around CLA D 403 (B):**

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

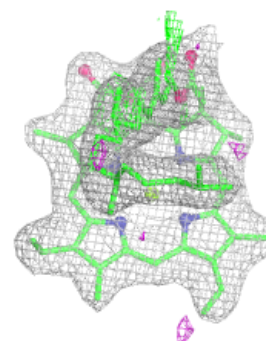
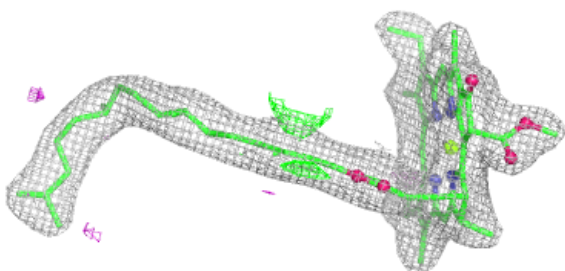
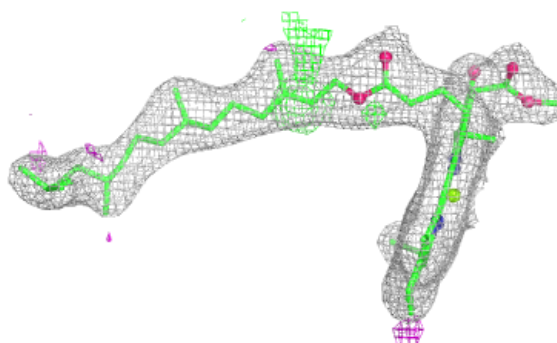


Electron density around CLA c 503:

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

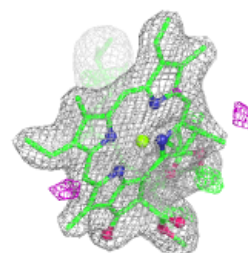
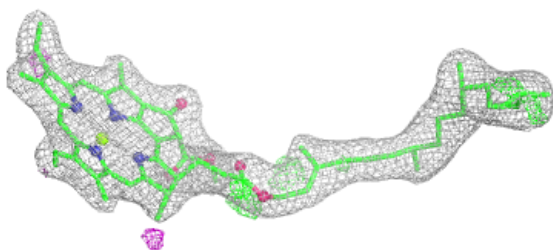
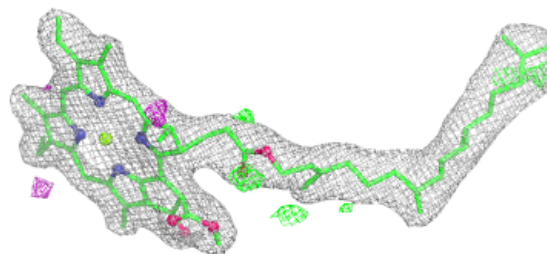
**Electron density around CLA B 605:**

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



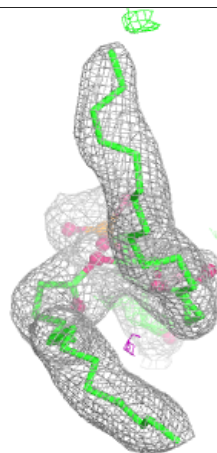
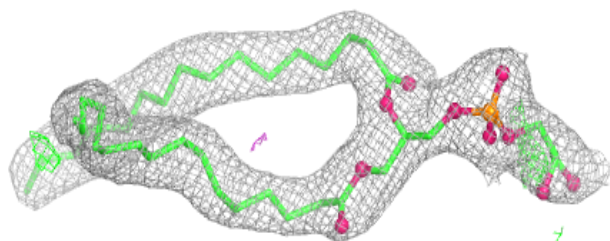
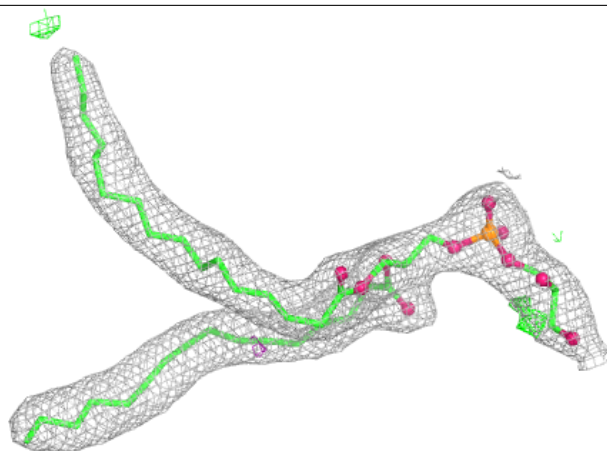
Electron density around CLA a 404 (A):

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



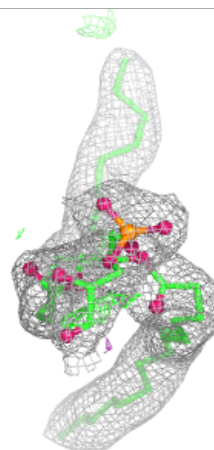
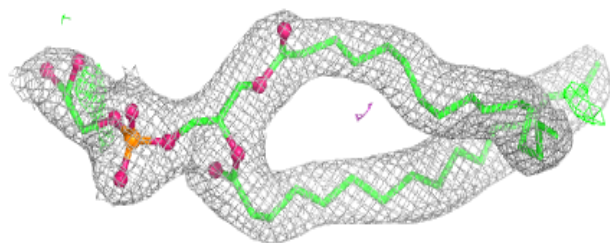
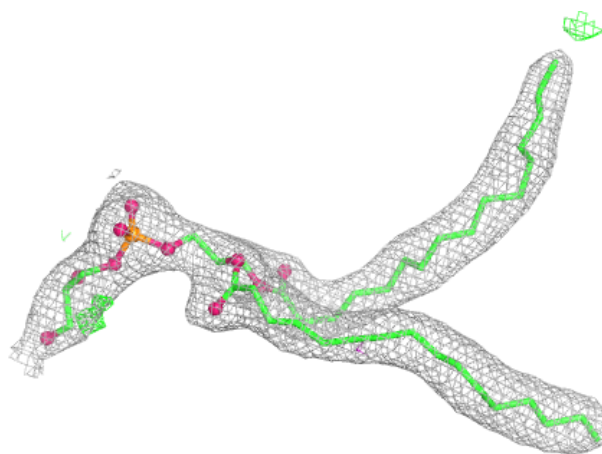
Electron density around LHG D 407 (A):

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



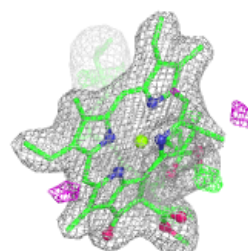
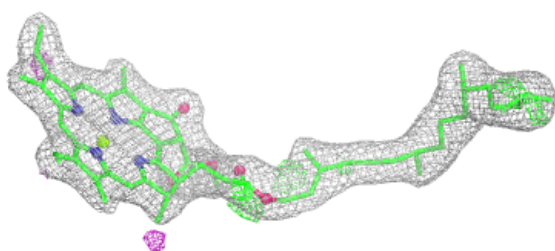
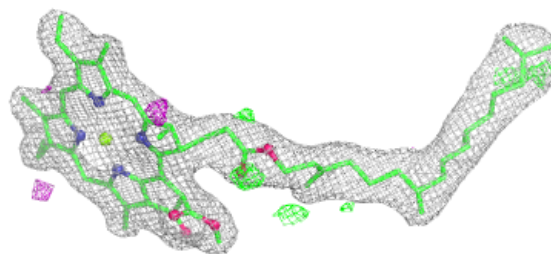
Electron density around LHG D 407 (B):

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



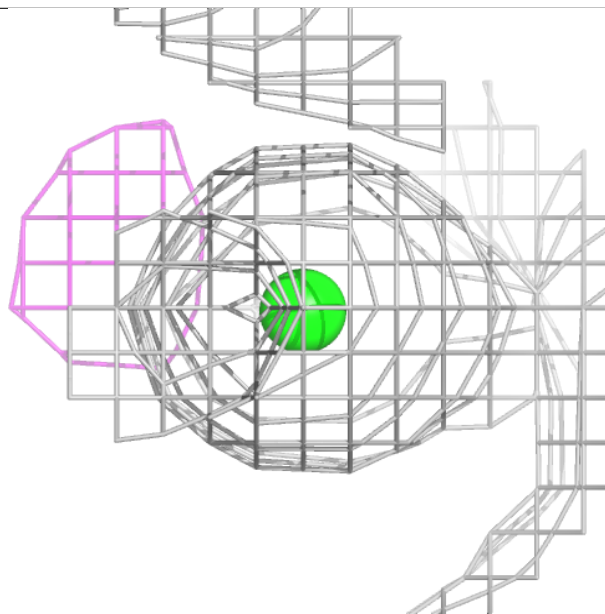
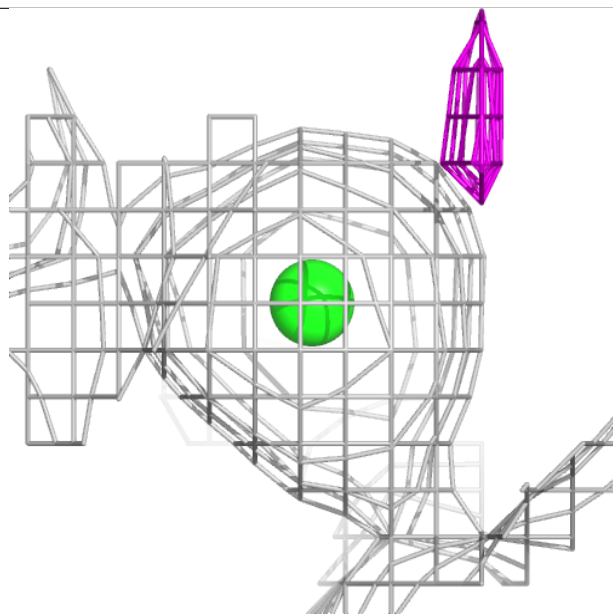
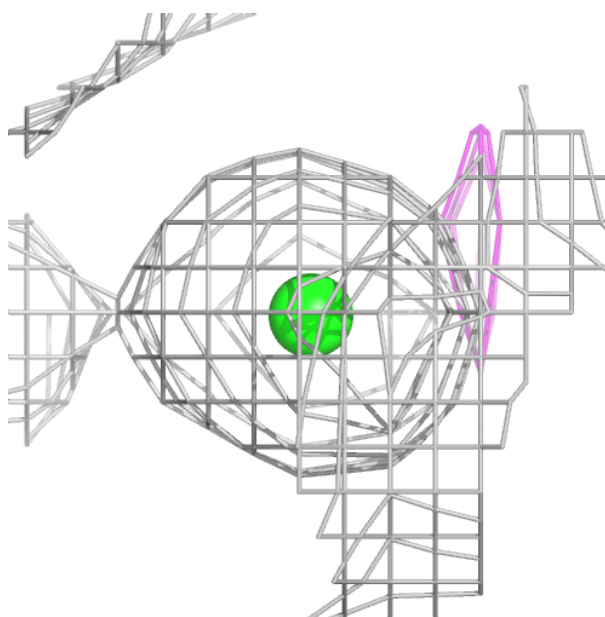
Electron density around CLA a 404 (B):

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



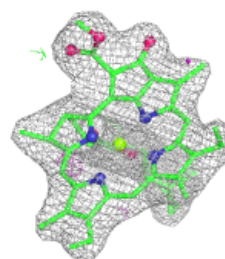
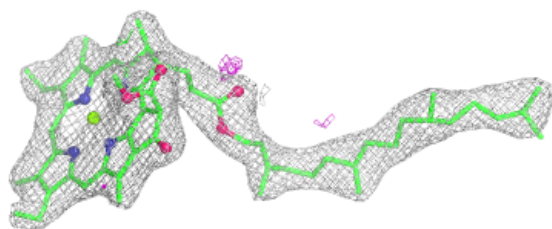
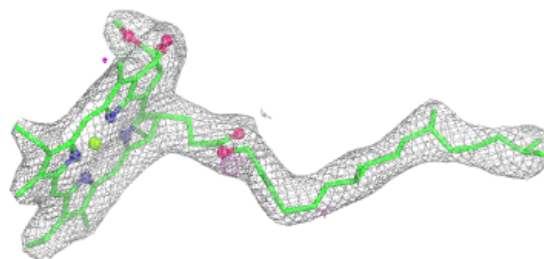
Electron density around CL a 403 (A):

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



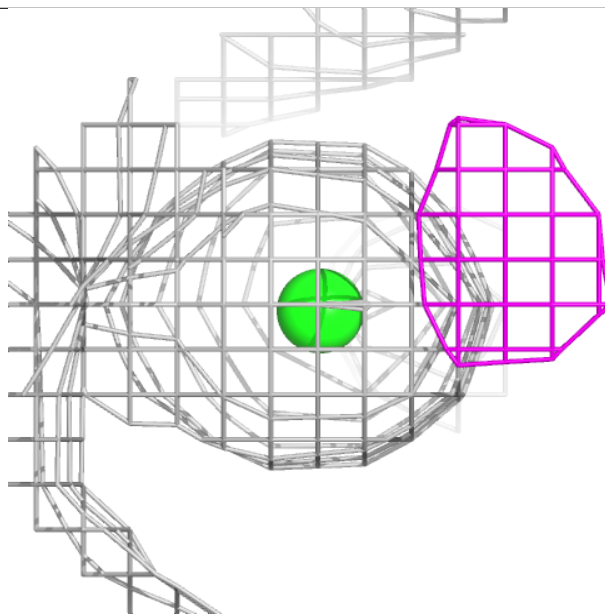
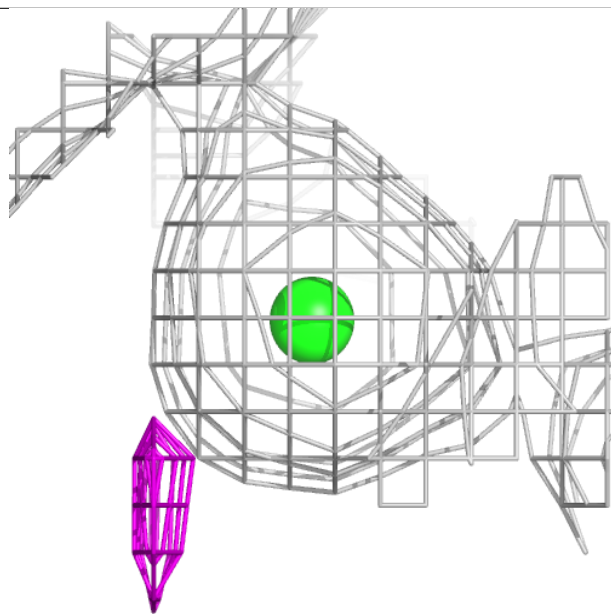
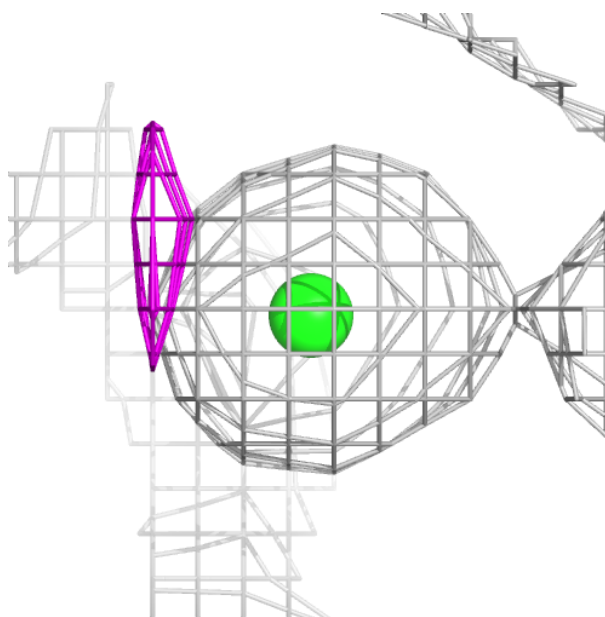
Electron density around CLA C 502:

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



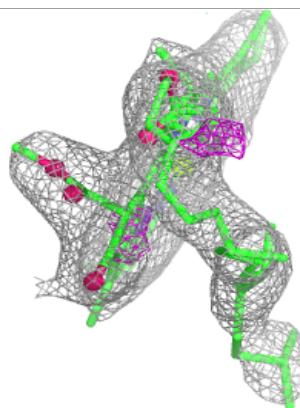
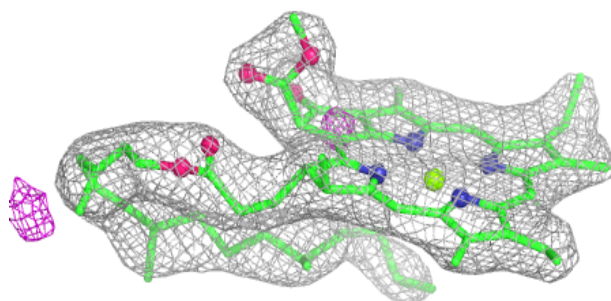
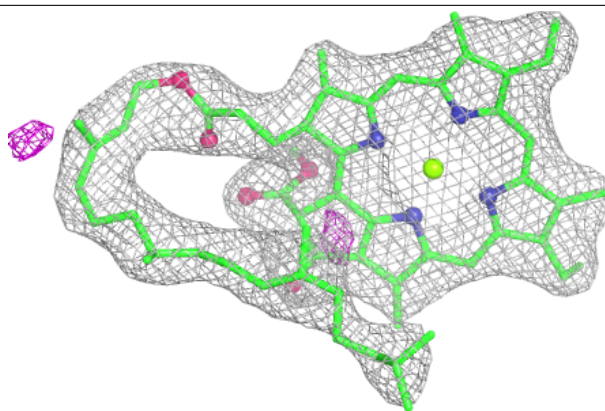
Electron density around CL a 403 (B):

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



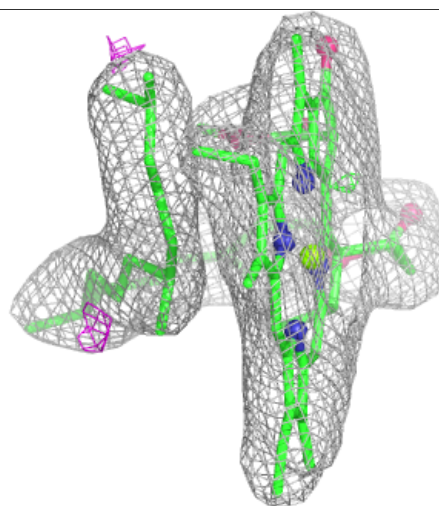
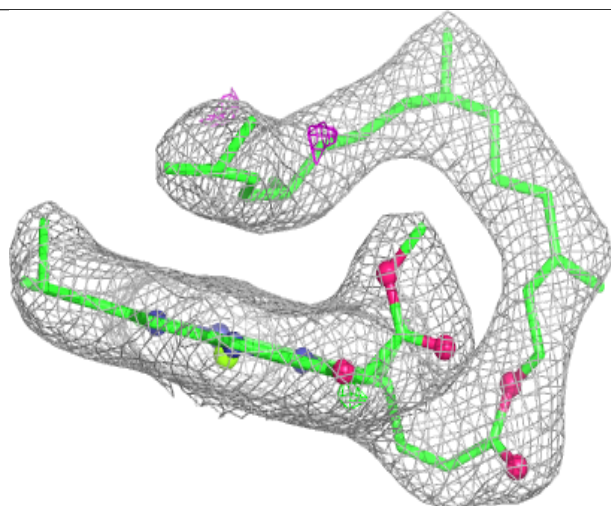
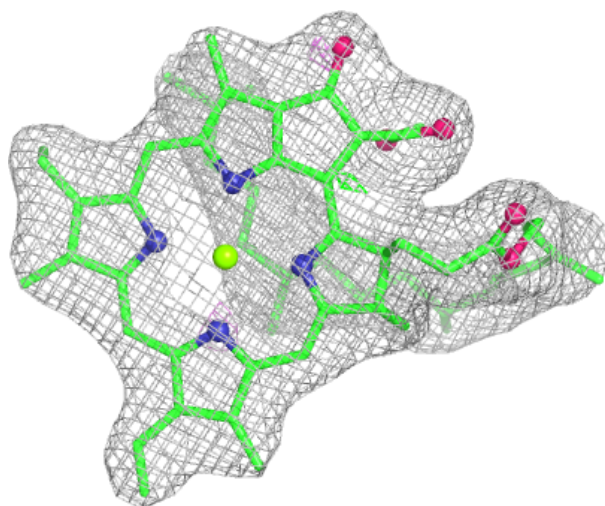
Electron density around CLA c 510:

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



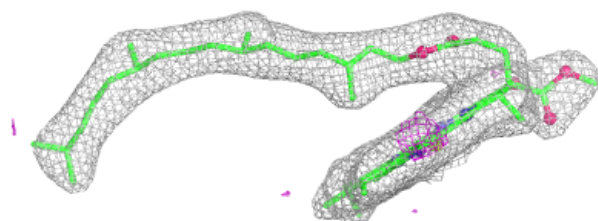
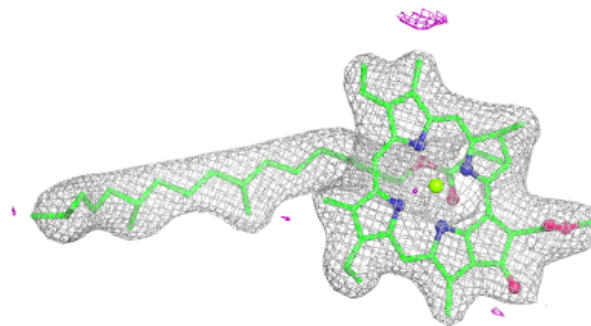
Electron density around CLA c 511:

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



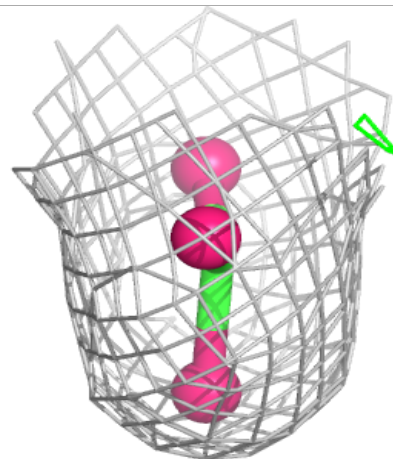
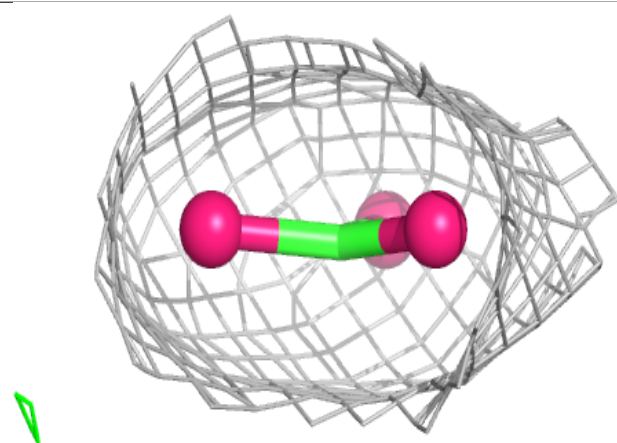
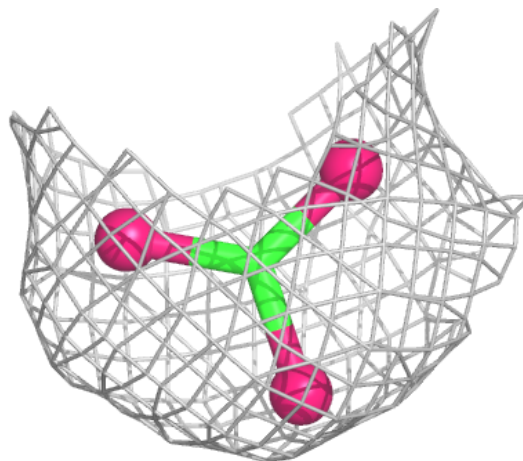
Electron density around CLA B 608:

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



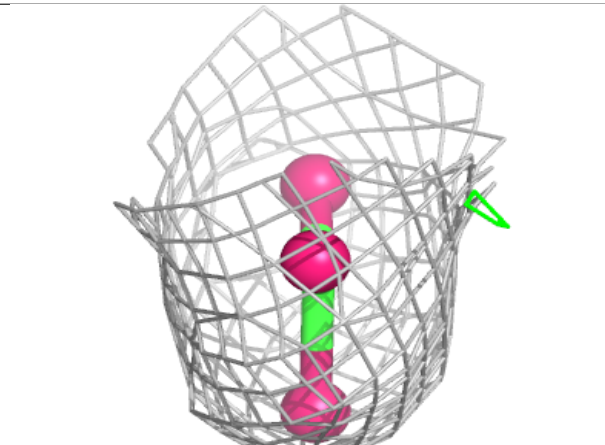
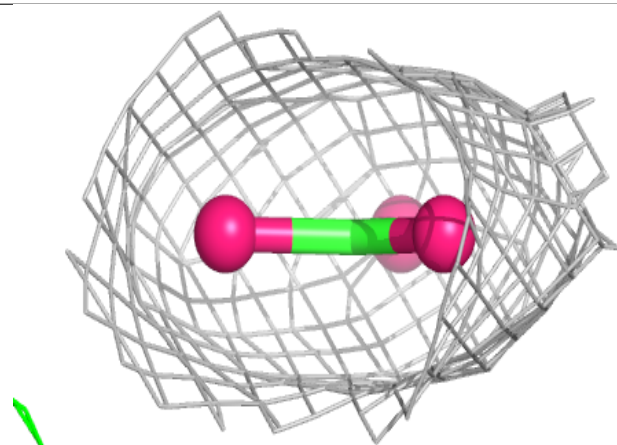
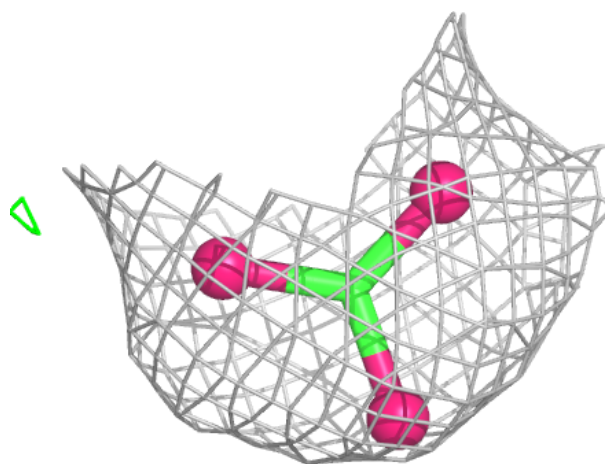
Electron density around BCT D 401 (A):

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



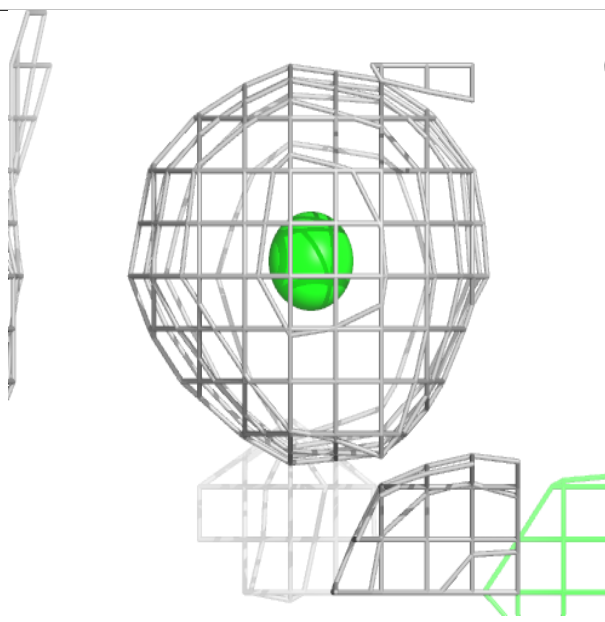
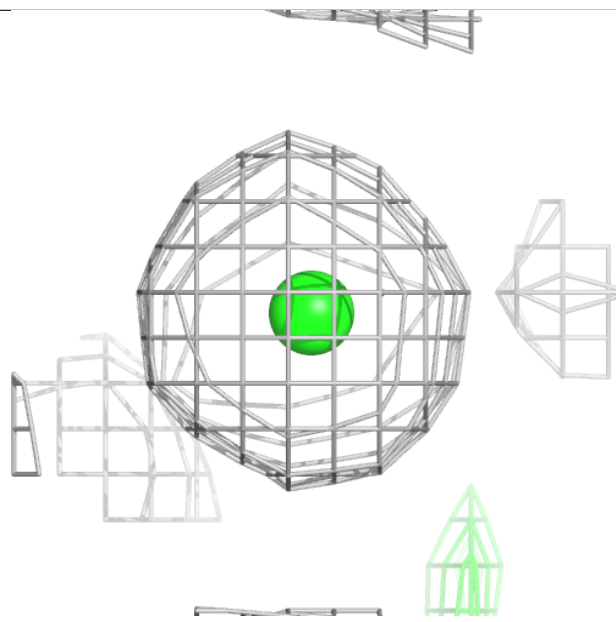
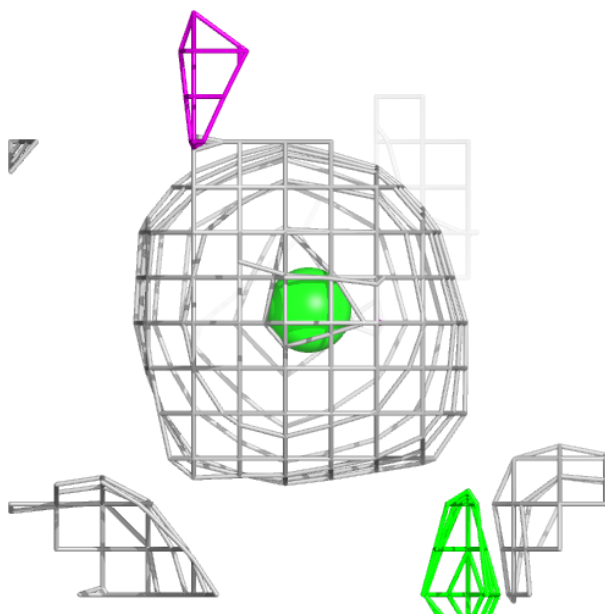
Electron density around BCT D 401 (B):

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



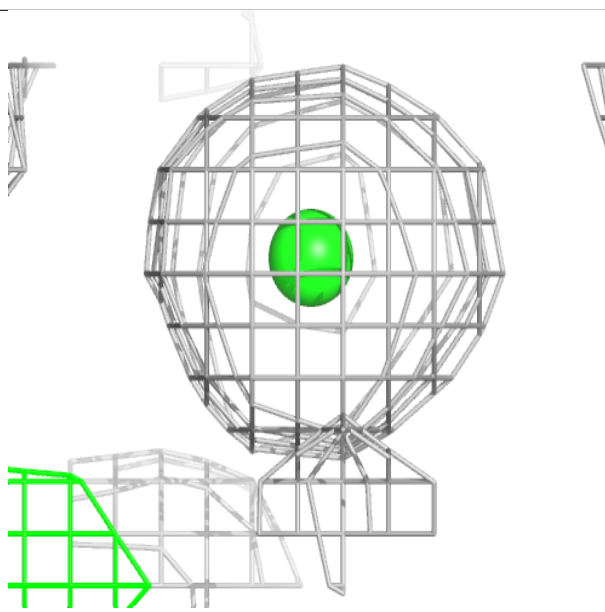
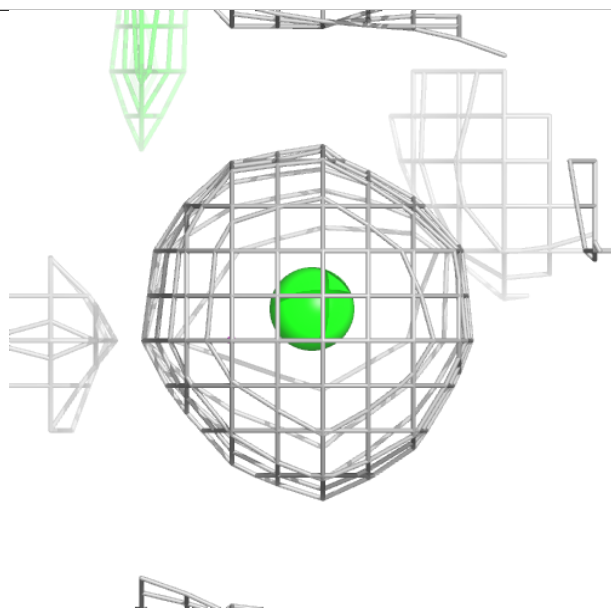
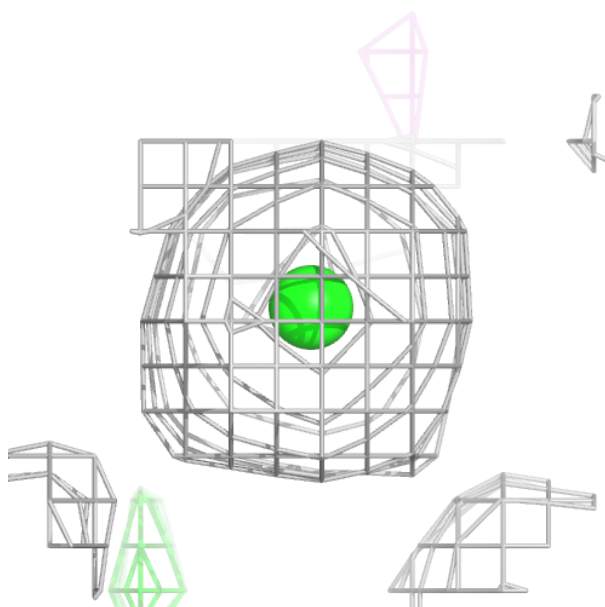
Electron density around CL A 402 (A):

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



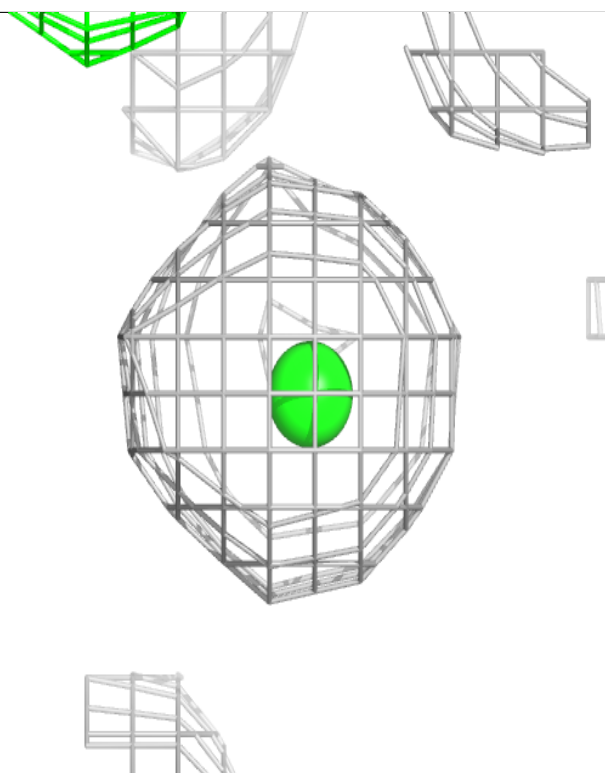
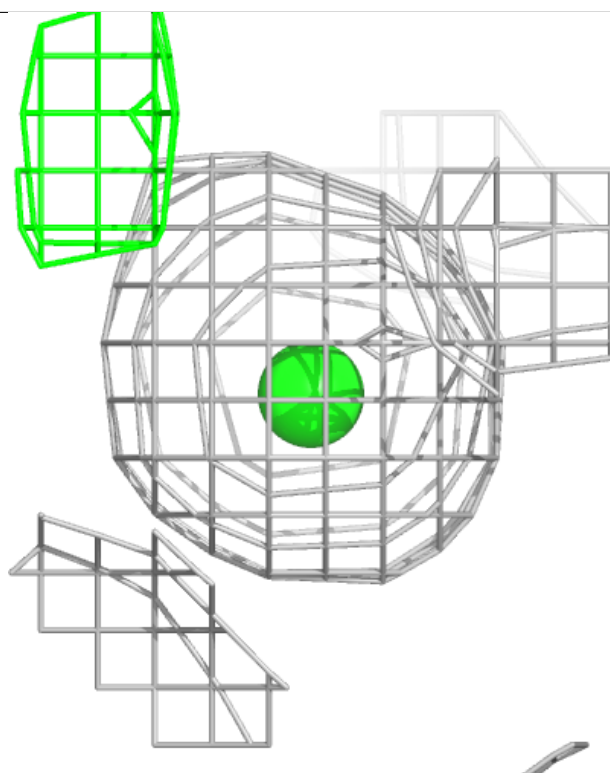
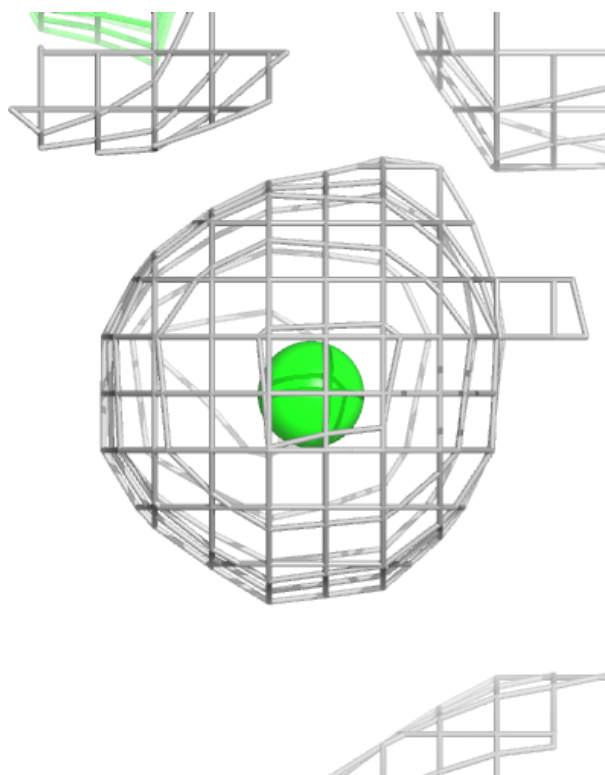
Electron density around CL A 402 (B):

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



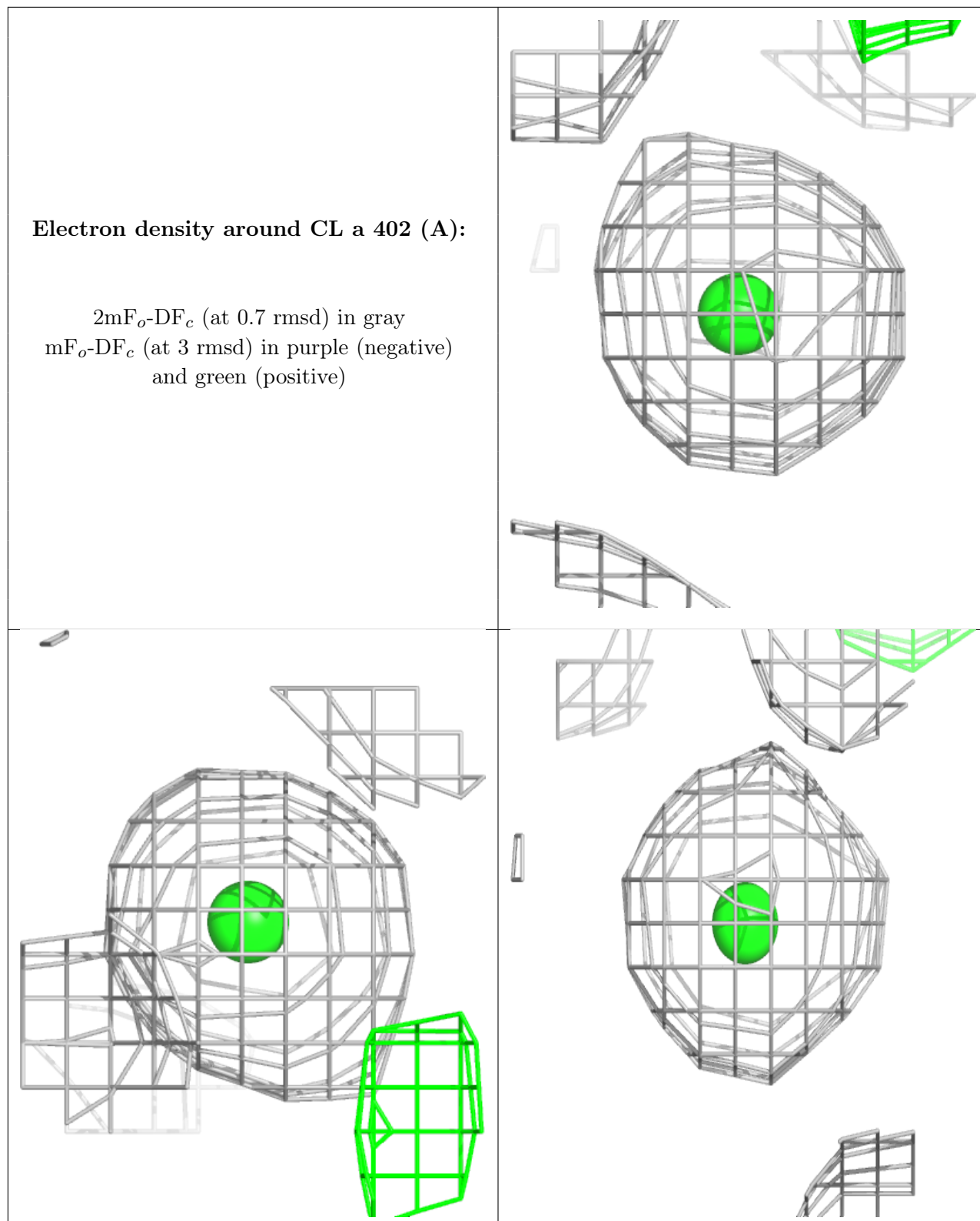
Electron density around CL a 402 (B):

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



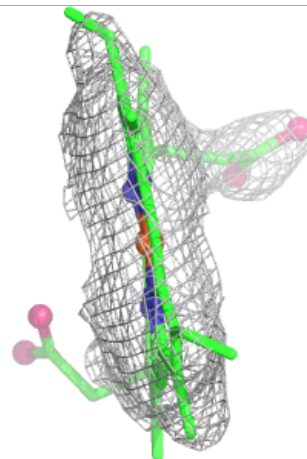
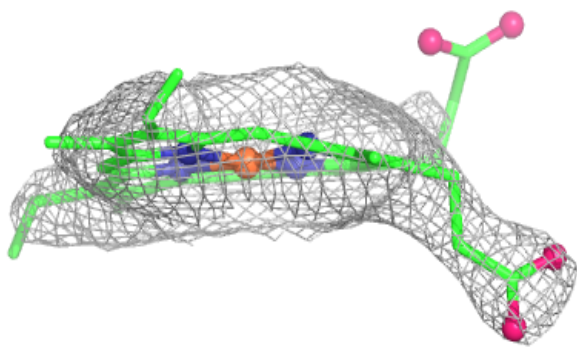
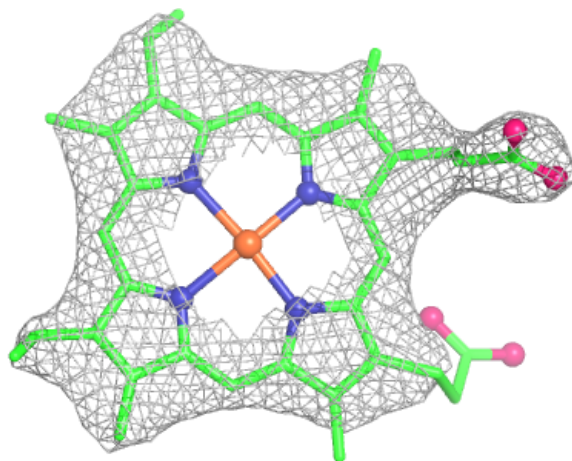
Electron density around CL a 402 (A):

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



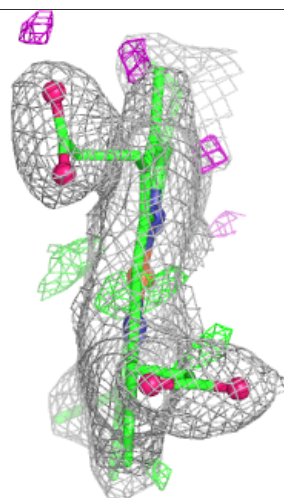
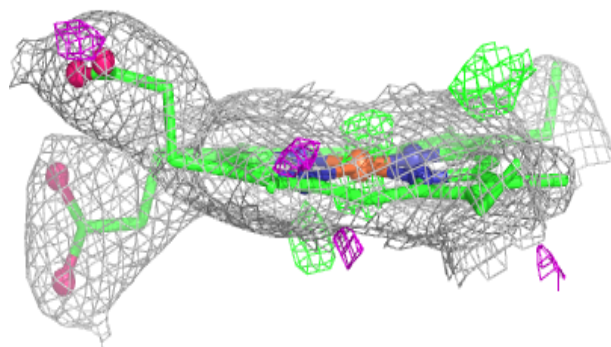
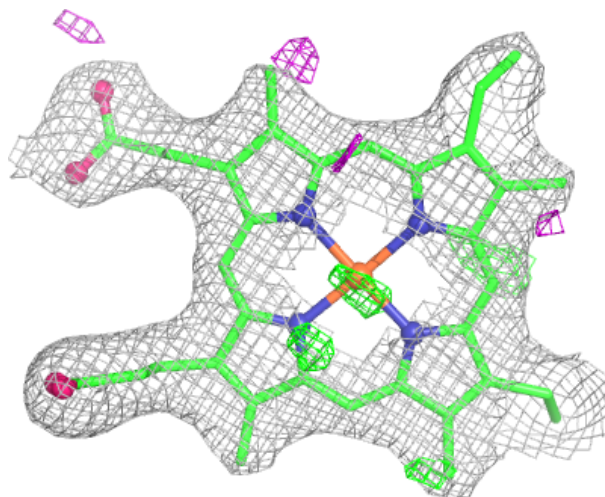
Electron density around HEM f 101:

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



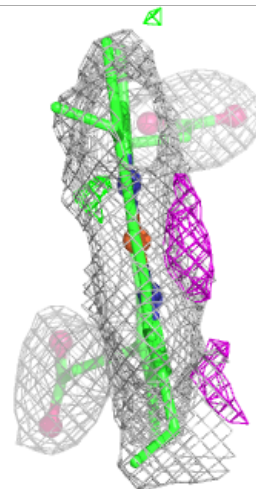
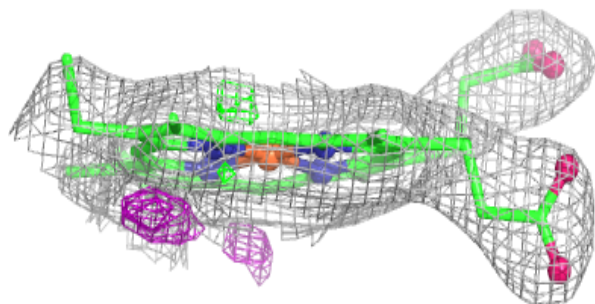
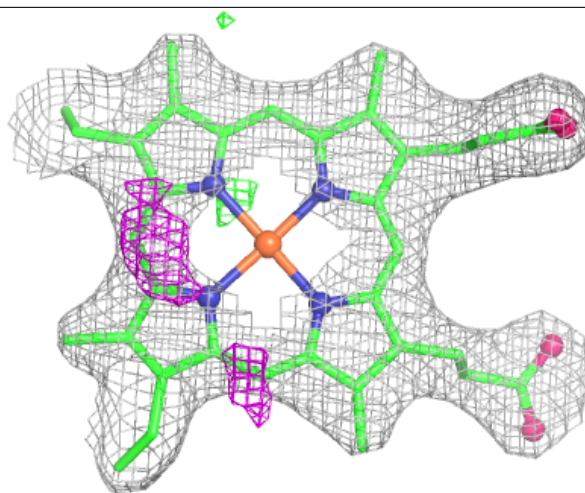
Electron density around HEC V 201:

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



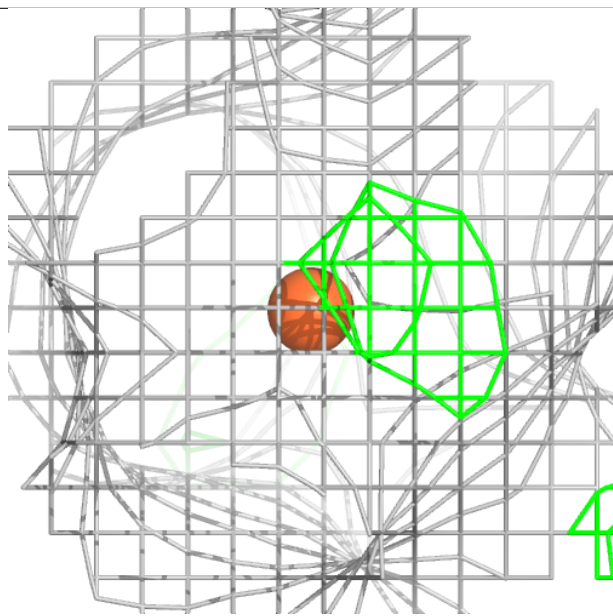
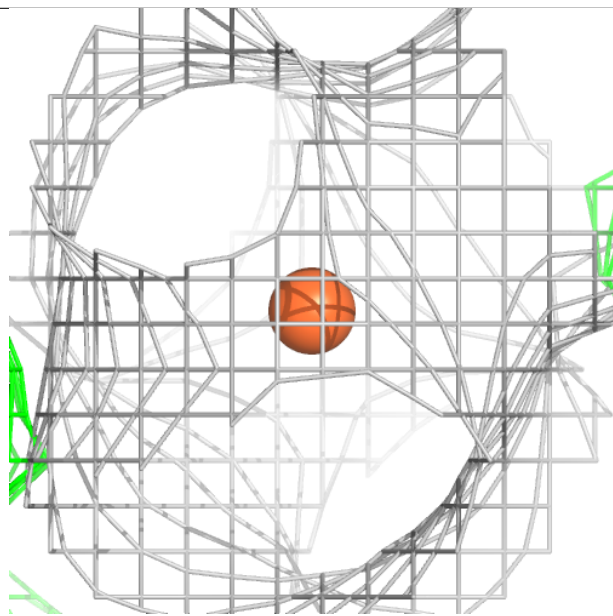
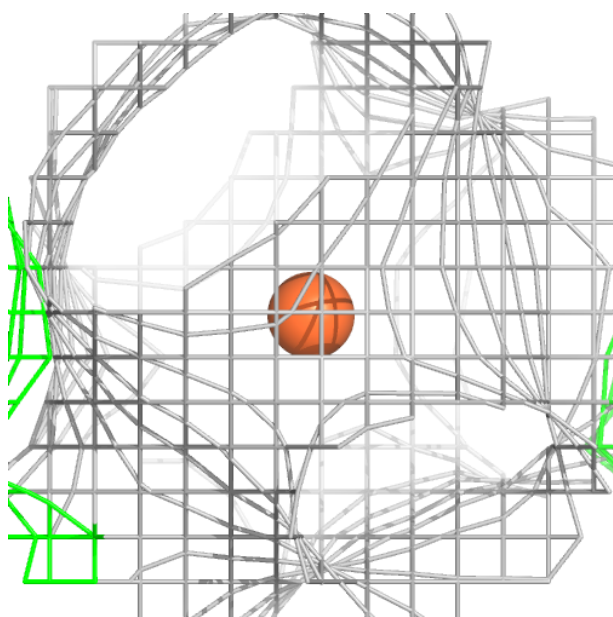
Electron density around HEC v 201:

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



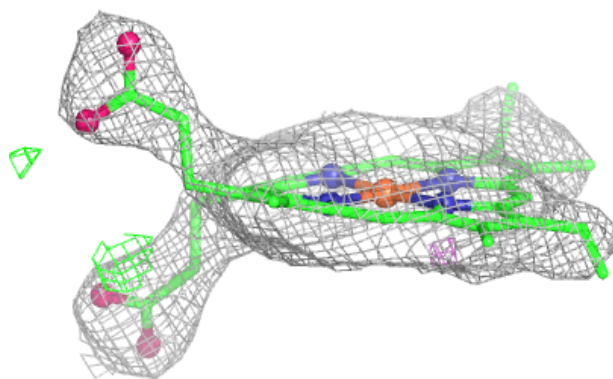
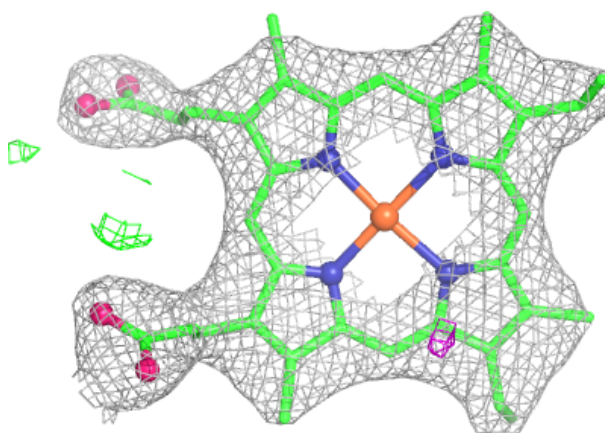
Electron density around FE2 a 401 (B):

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



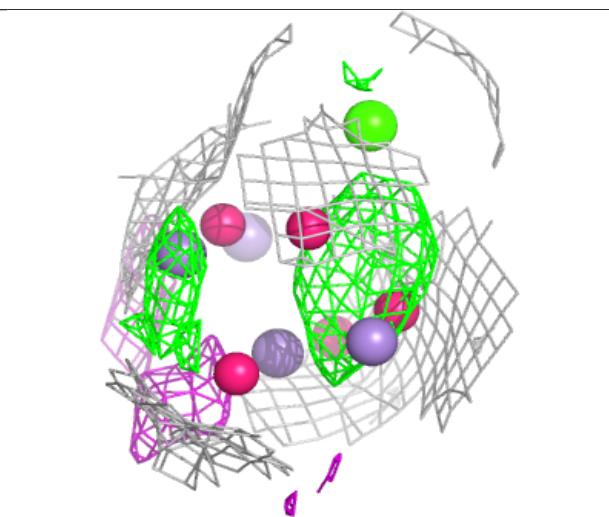
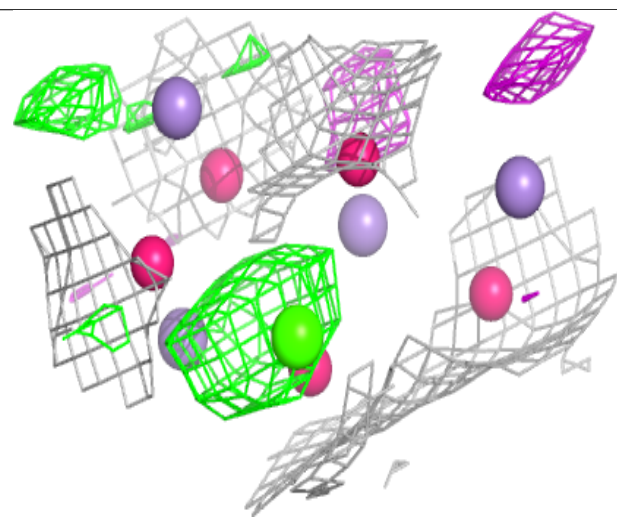
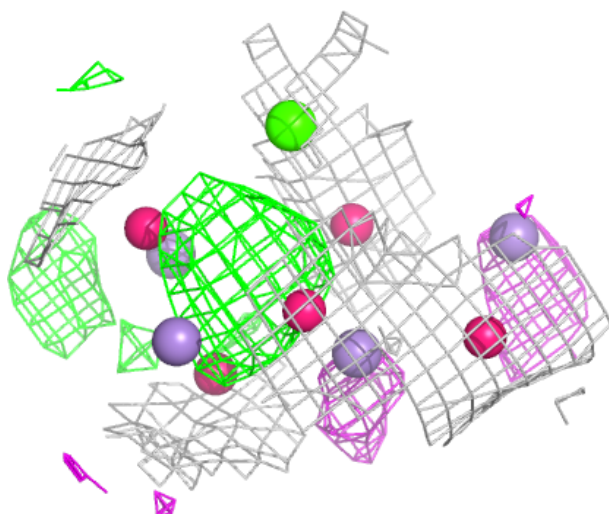
Electron density around HEM F 102:

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



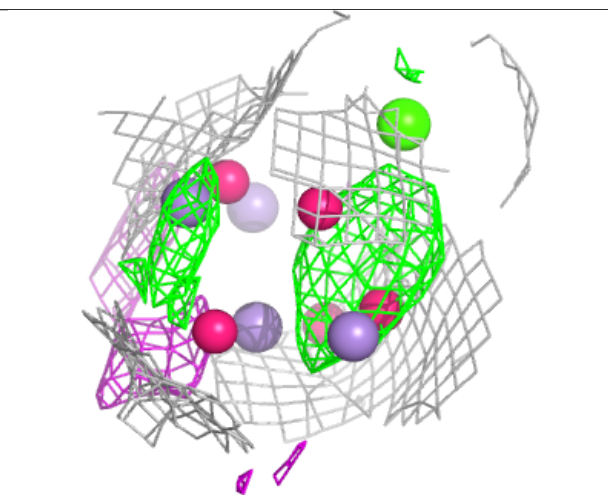
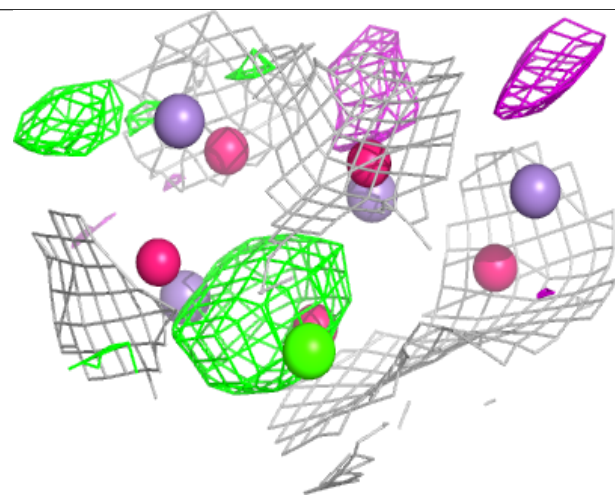
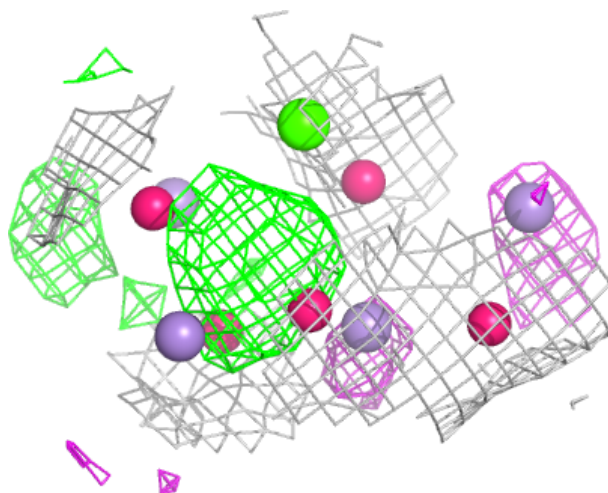
Electron density around OEX A 413 (A):

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



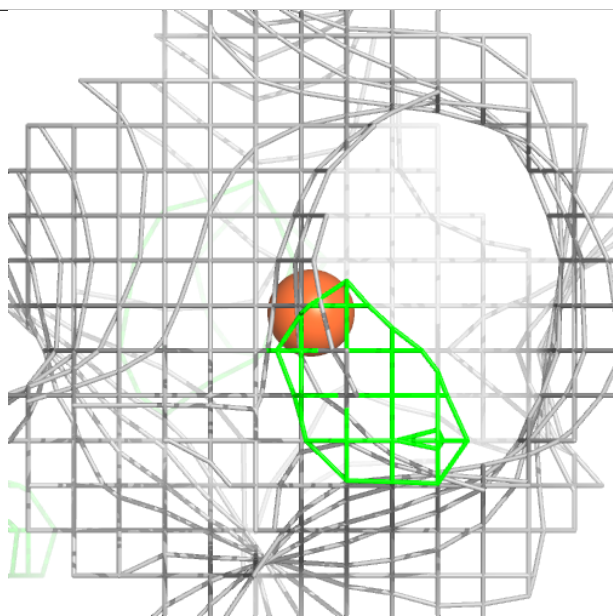
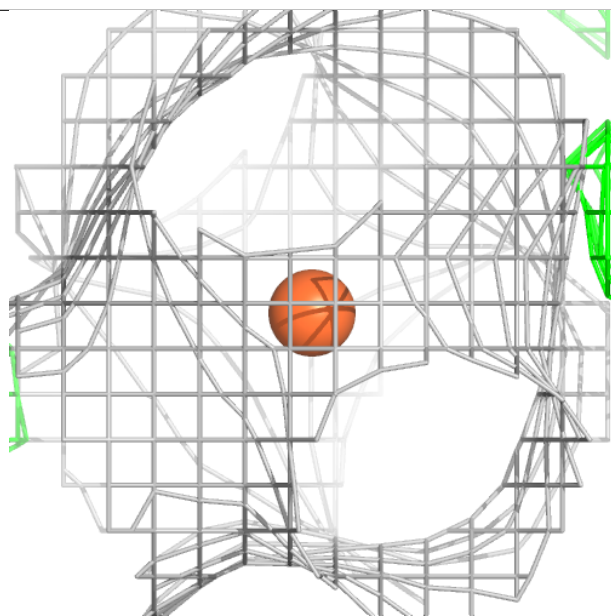
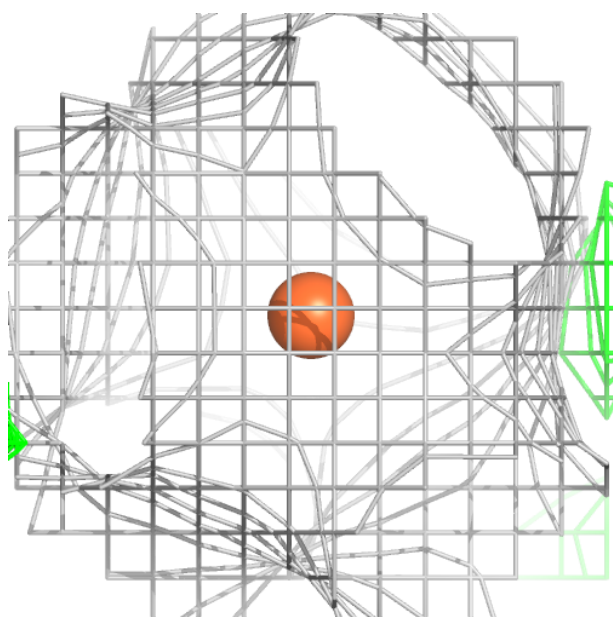
Electron density around OEX A 413 (B):

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



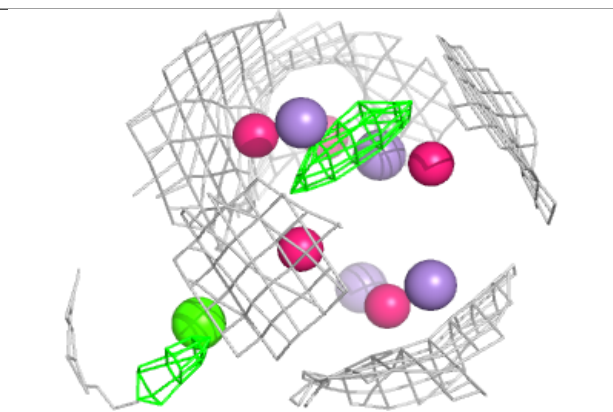
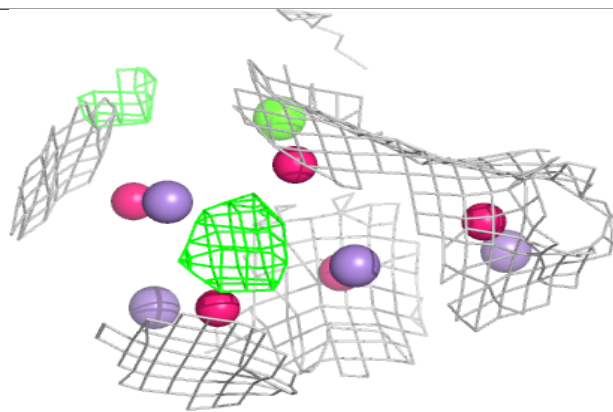
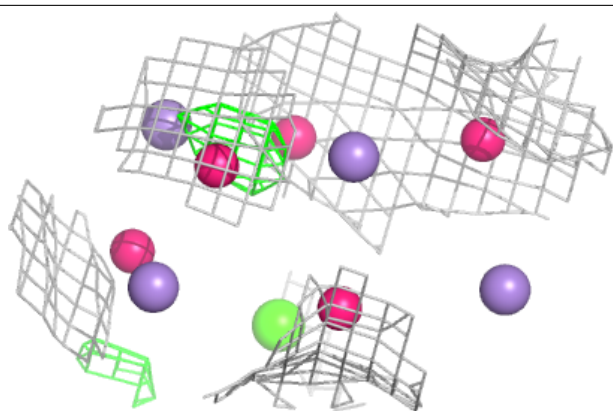
Electron density around FE2 a 401 (A):

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

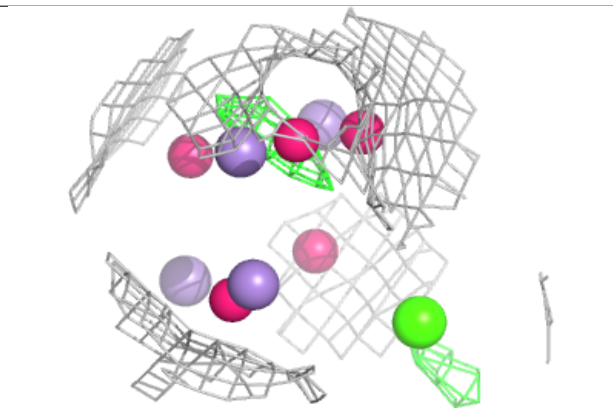
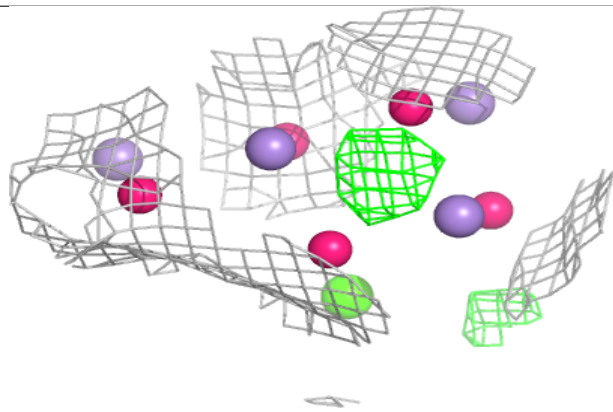
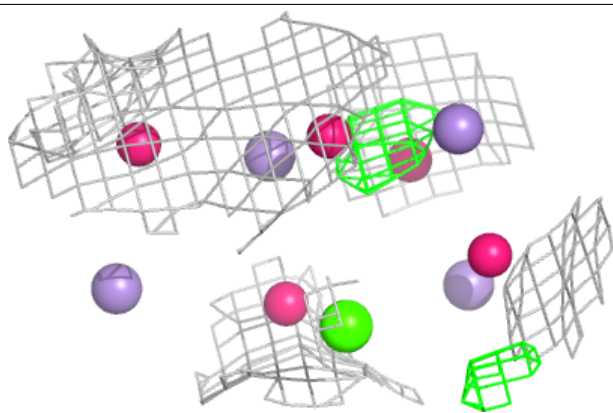


Electron density around OEX a 411 (A):

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

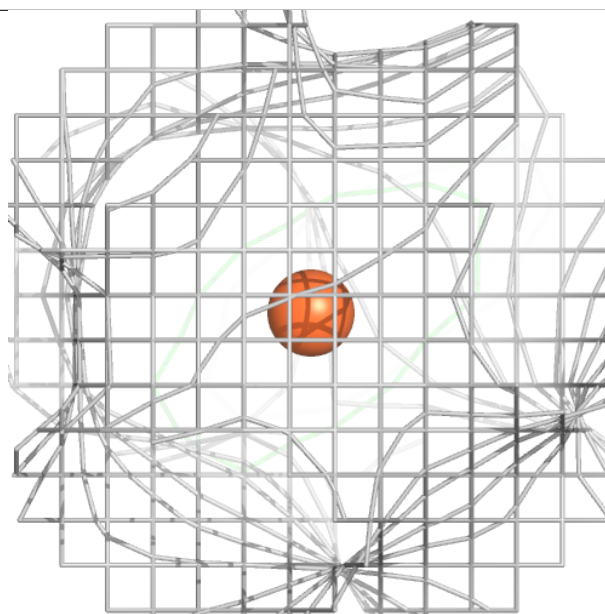
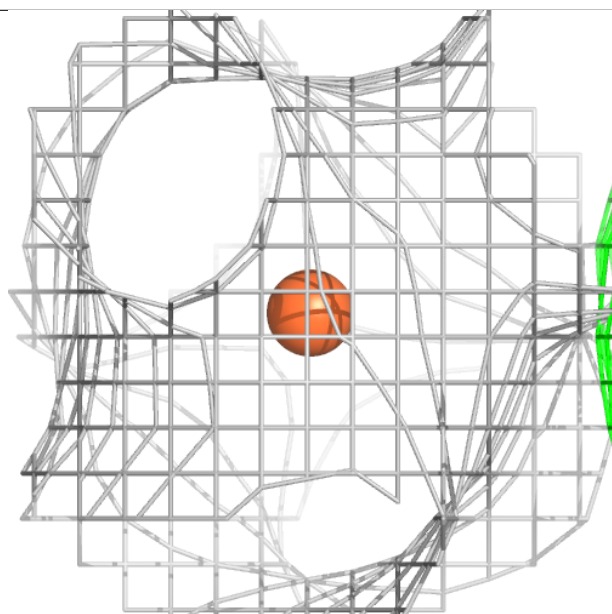
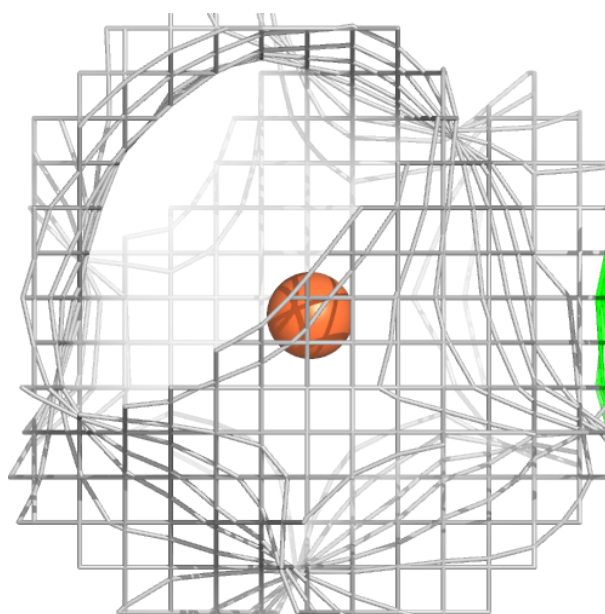
**Electron density around OEX a 411 (B):**

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



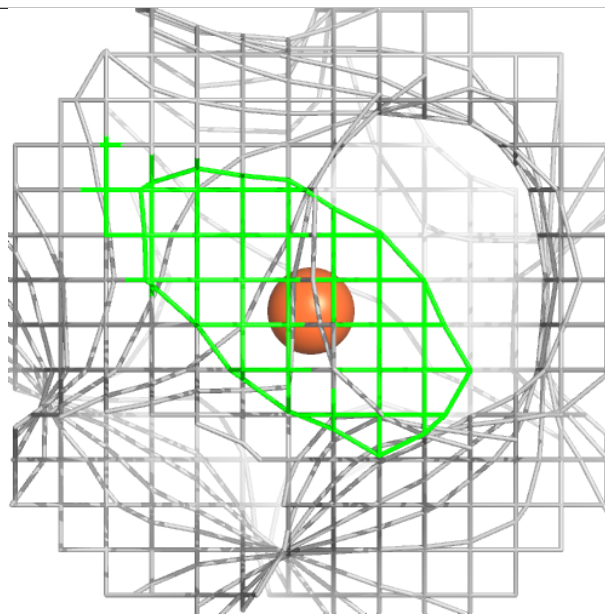
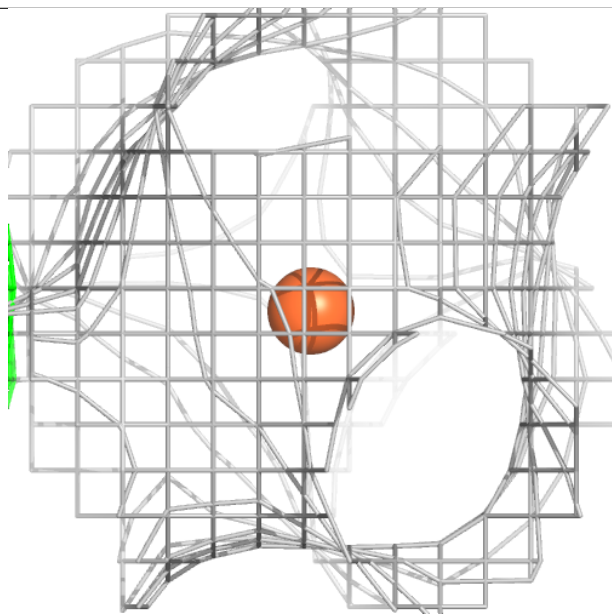
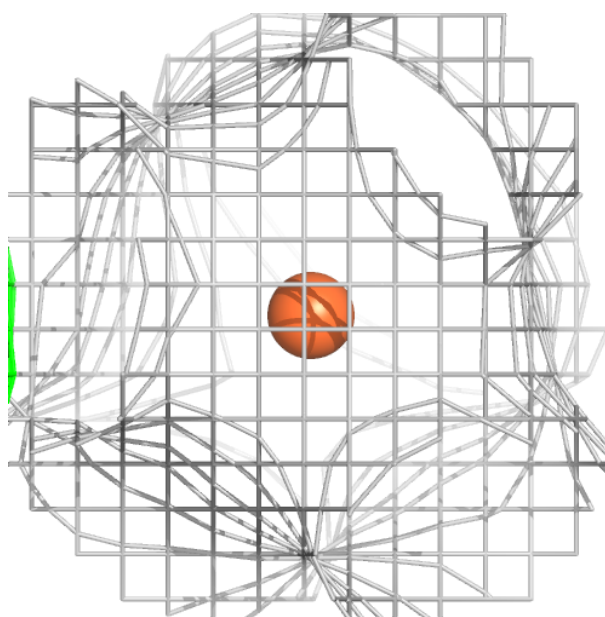
Electron density around FE2 A 401 (A):

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



Electron density around FE2 A 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.