



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 14, 2026 – 12:10 AM JST

PDB ID : 8IRA / pdb_00008ira
Title : XFEL structure of cyanobacterial photosystem II following one flash (1F) with a 200-microsecond delay
Authors : Li, H.; Suga, M.; Shen, J.R.
Deposited on : 2023-03-17
Resolution : 2.20 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

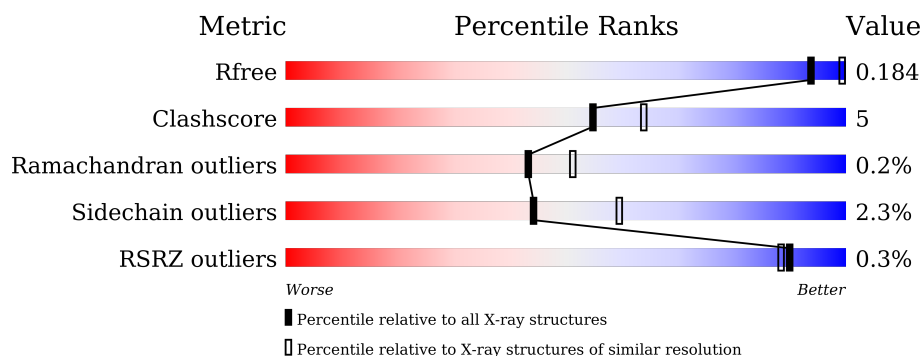
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	344	91% 6% .
1	a	344	89% 8% .
2	B	505	92% 7%
2	b	505	89% 10% .
3	C	455	91% 8% .
3	c	455	92% 8%

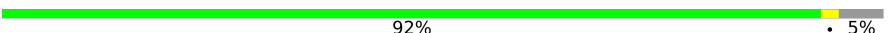
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Mol	Chain	Length	Quality of chain
4	D	342	
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V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

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Mol	Chain	Length	Quality of chain
16	v	137	 91% 9%
17	X	40	 85% 10% 5%
17	x	40	 92% 5%
18	Y	30	 3% 93% • •
18	y	30	 73% 23% •
19	Z	62	 87% 11% •
19	z	62	 77% 19% •
20	R	34	 6% 79% 21%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	GOL	D	412	-	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).

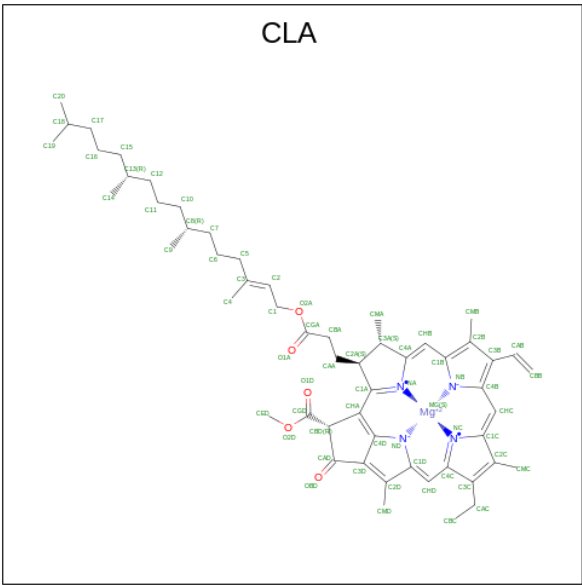
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	2
			4	4		

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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		

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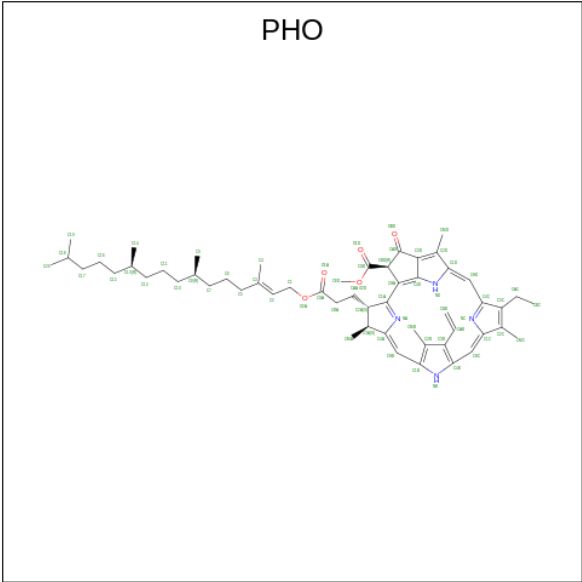
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	a	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	a	1	Total 65	C 55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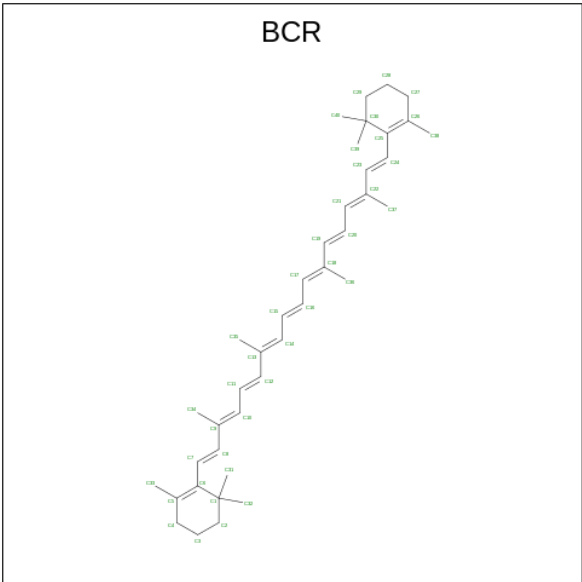
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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



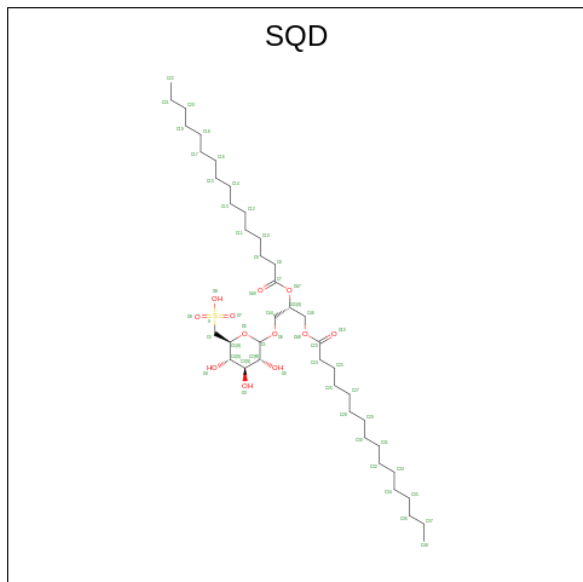
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	1
			128	110	8	10		
24	A	1	Total	C	N	O	0	1
			128	110	8	10		
24	a	1	Total	C	N	O	0	1
			128	110	8	10		
24	a	1	Total	C	N	O	0	1
			128	110	8	10		

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



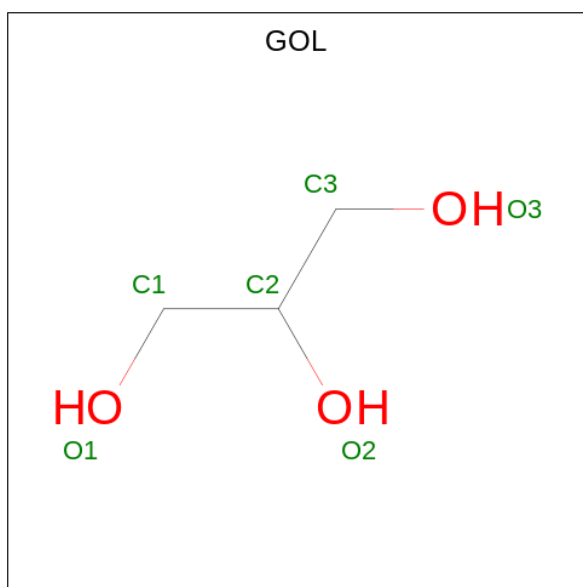
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total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



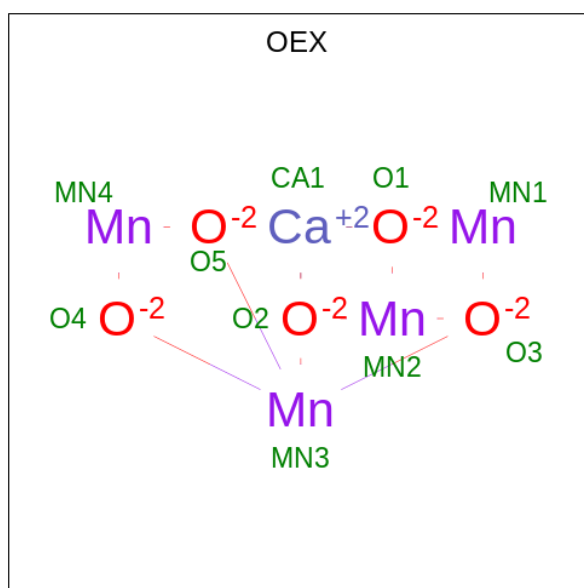
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			6	3	3		
27	A	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	1
			12	6	6		
27	D	1	Total	C	O	0	0
			6	3	3		
27	O	1	Total	C	O	0	0
			6	3	3		
27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

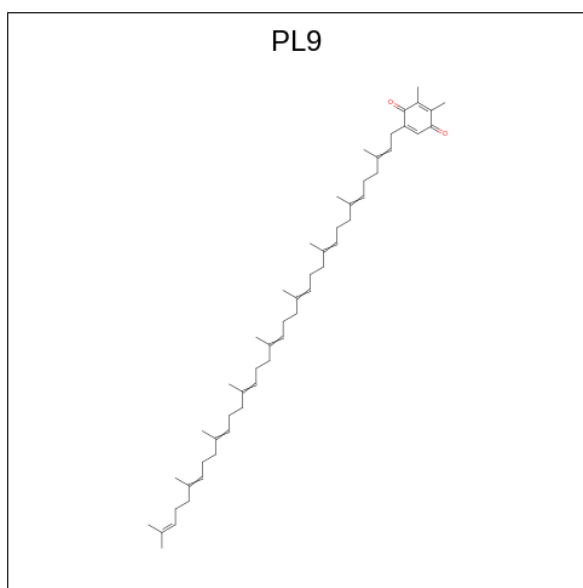
- Molecule 28 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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:).

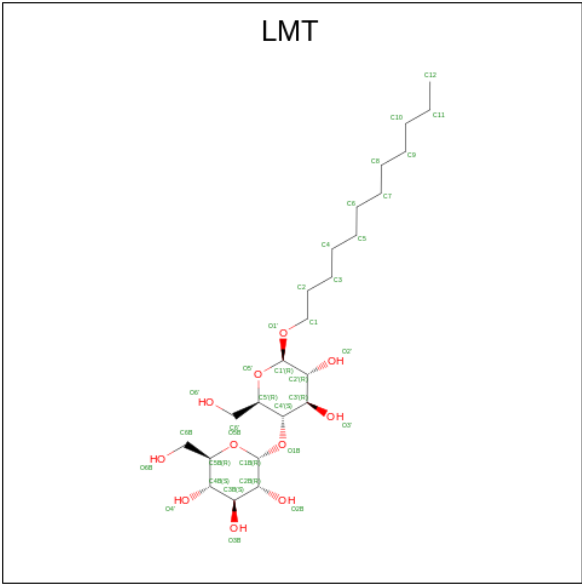
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			28	23	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	I	1	Total	C	O	0	0
			40	35	5		
30	J	1	Total	C		0	0
			10	10			
30	K	1	Total	C	O	0	1
			68	58	10		
30	M	1	Total	C		0	0
			10	10			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	X	1	Total	C	O	0	0
			18	16	2		
30	a	1	Total	C	O	0	0
			30	25	5		
30	b	1	Total	C	O	0	0
			33	28	5		
30	c	1	Total	C	O	0	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	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-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



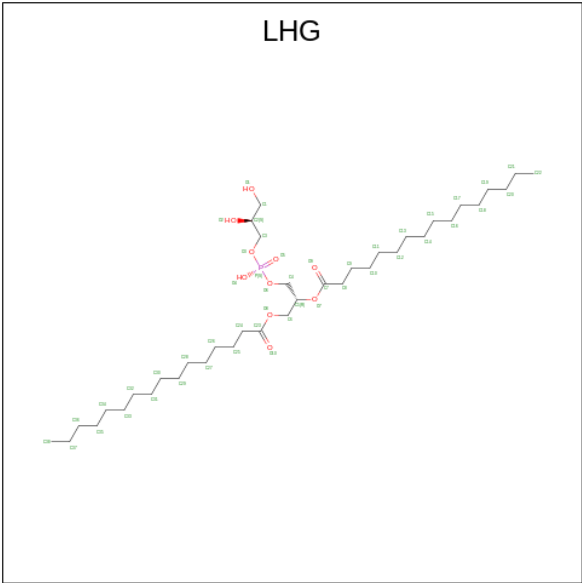
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			35	24	11		
31	A	1	Total	C	O	0	0
			35	24	11		

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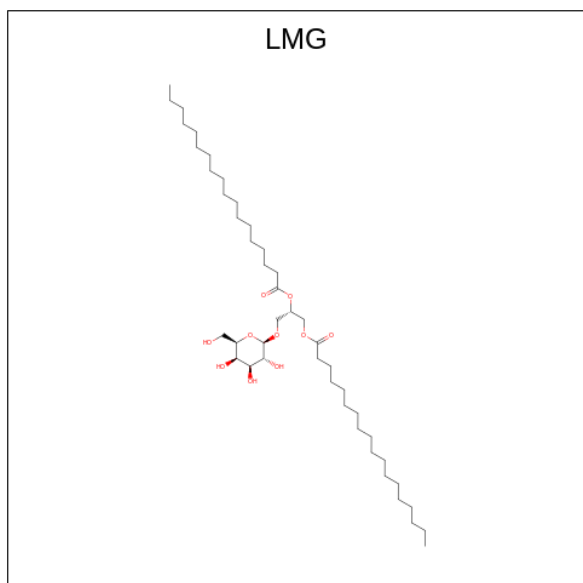
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			25	19	6		
31	F	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total	C	O	0	0
			35	24	11		
31	T	1	Total	C	O	0	0
			35	24	11		
31	a	1	Total	C	O	0	0
			35	24	11		
31	b	1	Total	C	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-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



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

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



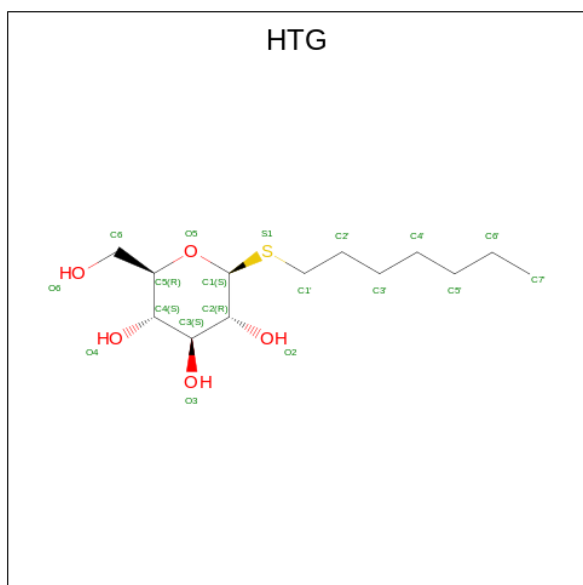
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	B	1	Total	C	O	0	0
			51	41	10		

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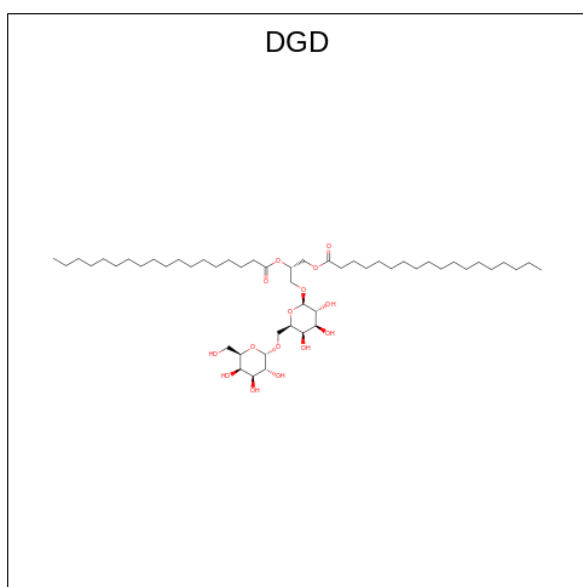
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	D	1	Total	C	O	0	0
			51	41	10		
33	a	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	d	1	Total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

- 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 19 13 5 1	0	0
34	B	1	Total C O S 19 13 5 1	0	0
34	B	1	Total C O S 19 13 5 1	0	0
34	C	1	Total C O S 19 13 5 1	0	0
34	D	1	Total C O S 16 10 5 1	0	0
34	V	1	Total C O 11 6 5	0	0
34	b	1	Total C O S 19 13 5 1	0	0
34	b	1	Total C O S 19 13 5 1	0	0
34	b	1	Total C O S 19 13 5 1	0	0
34	c	1	Total C O S 19 13 5 1	0	0
34	d	1	Total C O S 16 10 5 1	0	0

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

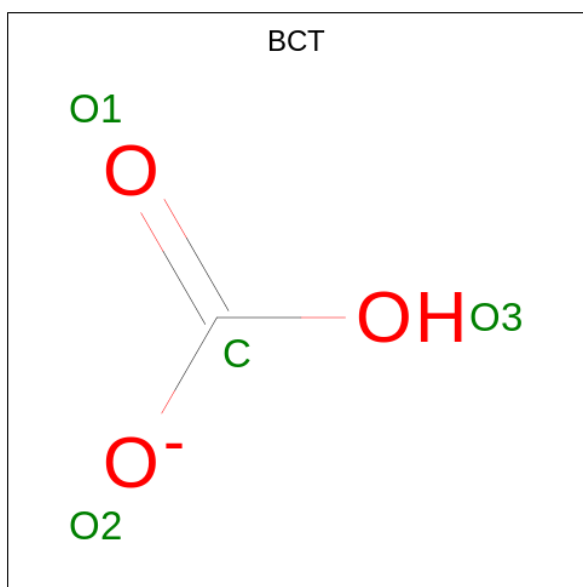


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	C	1	Total C O 124 94 30	0	1
35	C	1	Total C O 124 94 30	0	1
35	C	1	Total C O 62 47 15	0	0
35	H	1	Total C O 62 47 15	0	0
35	c	1	Total C O 124 94 30	0	1
35	c	1	Total C O 124 94 30	0	1
35	c	1	Total C O 62 47 15	0	0
35	h	1	Total C O 62 47 15	0	0

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

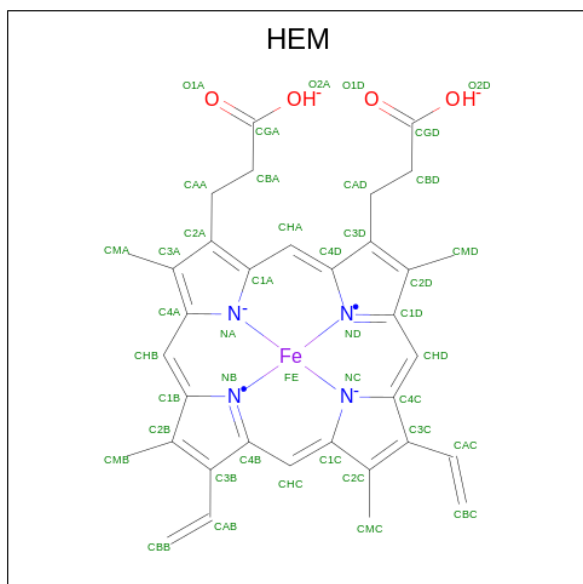
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	C	1	Total Ca 1 1	0	0
36	F	1	Total Ca 1 1	0	0
36	O	1	Total Ca 1 1	0	0
36	c	2	Total Ca 2 2	0	0
36	f	1	Total Ca 1 1	0	0
36	o	1	Total Ca 1 1	0	0

- 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 8 2 6	0	1
37	d	1	Total C O 8 2 6	0	1

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



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

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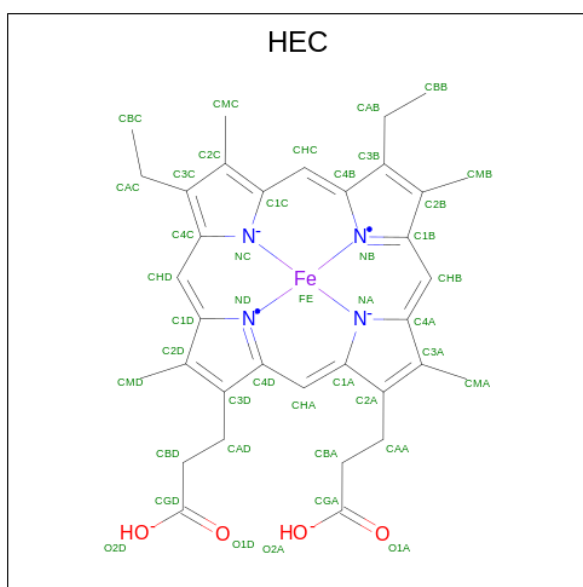
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	f	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

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

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

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



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	142	Total	O	0	86
			227	227		
41	B	187	Total	O	0	2
			189	189		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	C	169	Total 206	O 206	0	38
41	D	120	Total 155	O 155	0	35
41	E	17	Total 17	O 17	0	0
41	F	4	Total 4	O 4	0	0
41	H	22	Total 22	O 22	0	0
41	I	4	Total 4	O 4	0	0
41	J	6	Total 6	O 6	0	0
41	K	5	Total 5	O 5	0	0
41	L	9	Total 10	O 10	0	1
41	M	6	Total 6	O 6	0	0
41	O	104	Total 108	O 108	0	4
41	T	11	Total 14	O 14	0	3
41	U	47	Total 49	O 49	0	2
41	V	79	Total 80	O 80	0	1
41	X	7	Total 7	O 7	0	0
41	a	131	Total 211	O 211	0	81
41	b	201	Total 204	O 204	0	3
41	c	160	Total 193	O 193	0	34
41	d	117	Total 149	O 149	0	32
41	e	8	Total 8	O 8	0	0
41	f	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	h	17	Total 17	O 17	0	0
41	i	2	Total 2	O 2	0	0
41	j	1	Total 1	O 1	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	99	Total 103	O 103	0	4
41	t	8	Total 11	O 11	0	3
41	u	51	Total 52	O 52	0	1
41	v	56	Total 58	O 58	0	2
41	x	6	Total 6	O 6	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.

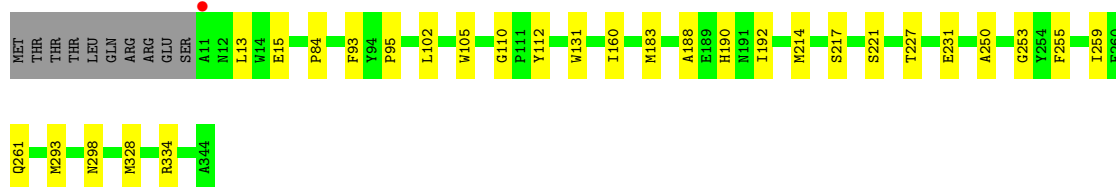
- Molecule 1: Photosystem II protein D1

Chain A: 



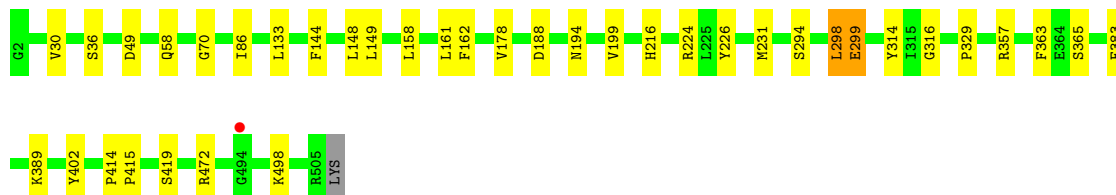
- Molecule 1: Photosystem II protein D1

Chain a: 



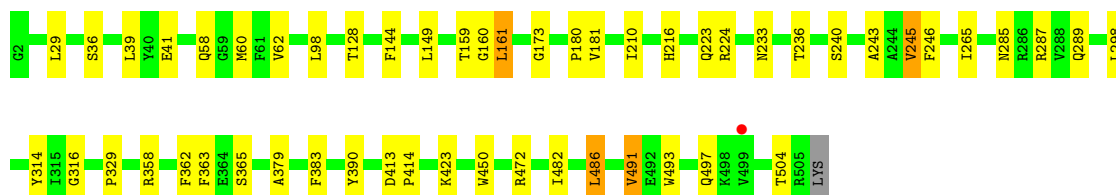
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B: 

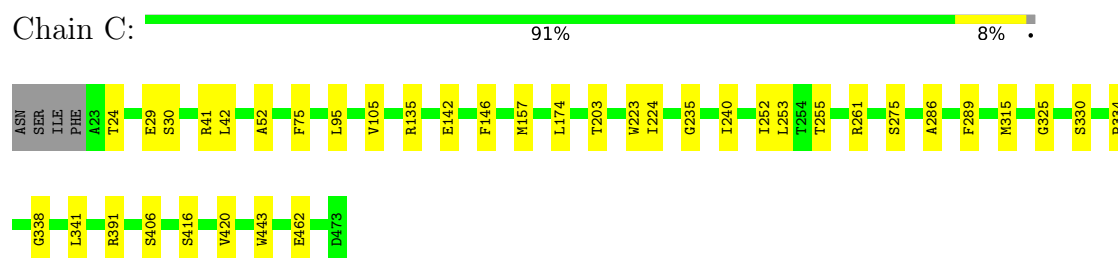


- Molecule 2: Photosystem II CP47 reaction center protein

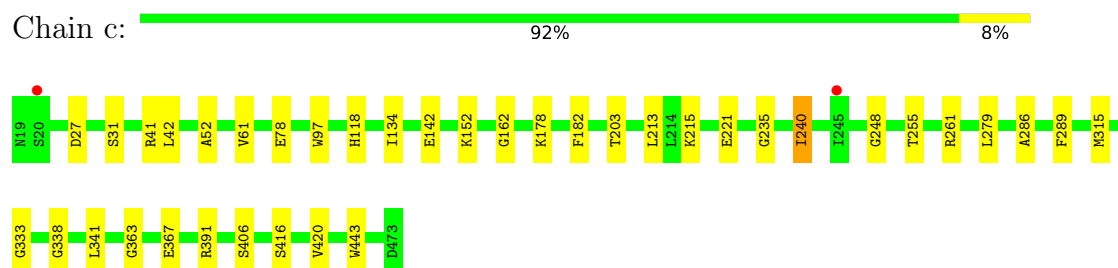
Chain b: 



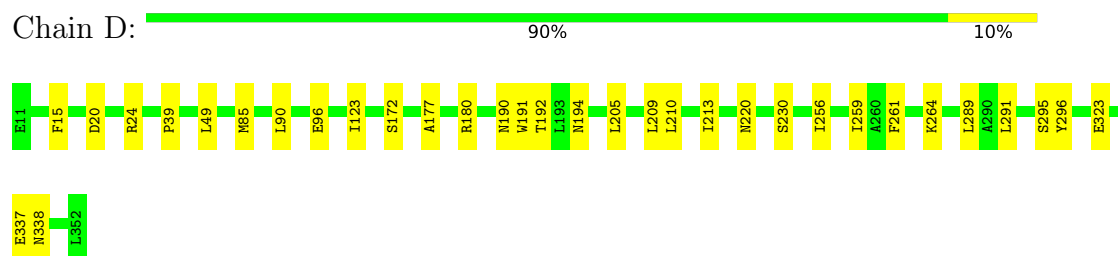
- Molecule 3: Photosystem II CP43 reaction center protein



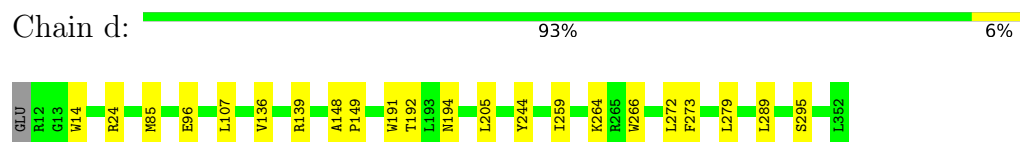
- Molecule 3: Photosystem II CP43 reaction center protein



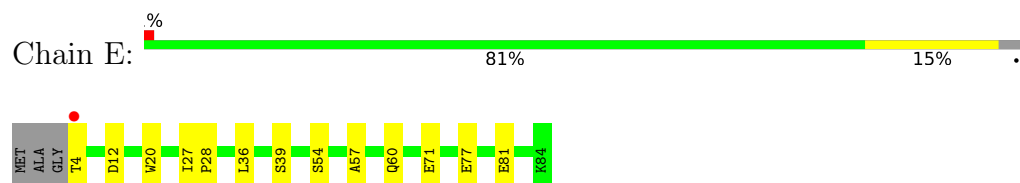
- Molecule 4: Photosystem II D2 protein



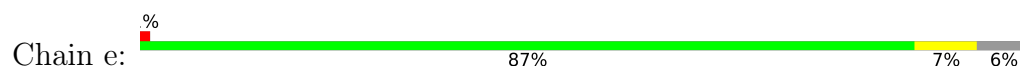
- Molecule 4: Photosystem II D2 protein



- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha

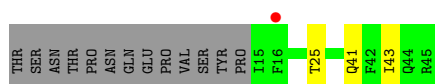




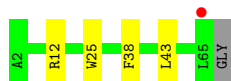
- Molecule 6: Cytochrome b559 subunit beta



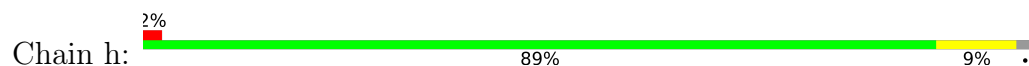
- Molecule 6: Cytochrome b559 subunit beta



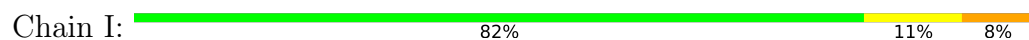
- Molecule 7: Photosystem II reaction center protein H



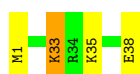
- Molecule 7: Photosystem II reaction center protein H



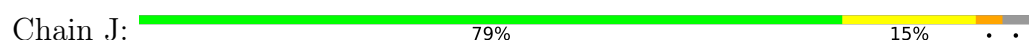
- Molecule 8: Photosystem II reaction center protein I

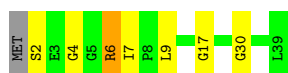


- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J





- Molecule 9: Photosystem II reaction center protein J

Chain j: 92% 8%



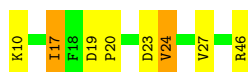
- Molecule 10: Photosystem II reaction center protein K

Chain K: 76% 19% 5%



- Molecule 10: Photosystem II reaction center protein K

Chain k: 78% 16% 5%



- Molecule 11: Photosystem II reaction center protein L

Chain L: 92% 5%



- Molecule 11: Photosystem II reaction center protein L

Chain l: 86% 11%



- Molecule 12: Photosystem II reaction center protein M

Chain M: 78% 8% 6% 8%



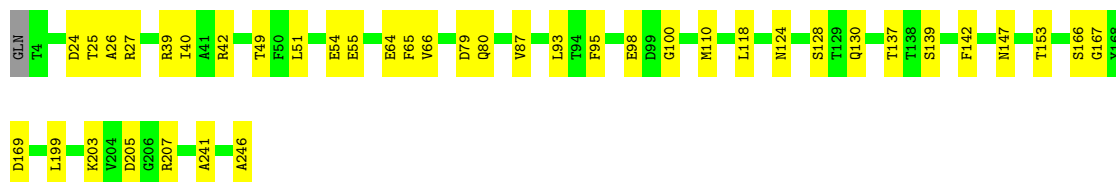
- Molecule 12: Photosystem II reaction center protein M

Chain m: 81% 11% 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 83% 16%



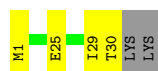
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 90% 9%



- Molecule 14: Photosystem II reaction center protein T

Chain T: 81% 12% 6%



- Molecule 14: Photosystem II reaction center protein T

Chain t: 3% 84% 9% 6%



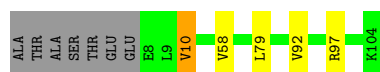
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 85% 8% 8%

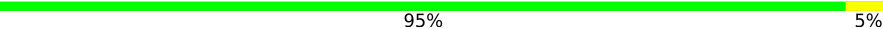


- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 88% 7% 7%



- Molecule 16: Cytochrome c-550

Chain V:  95% 5%



- Molecule 16: Cytochrome c-550

Chain v:  91% 9%



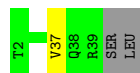
- Molecule 17: Photosystem II reaction center protein X

Chain X:  85% 10% 5%

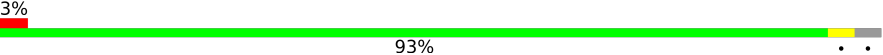


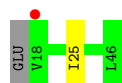
- Molecule 17: Photosystem II reaction center protein X

Chain x:  92% 5%



- Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:  3% 93%



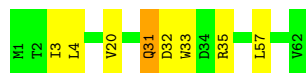
- Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:  73% 23%

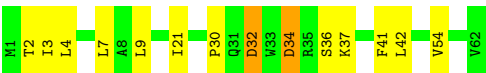
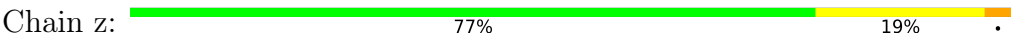


- Molecule 19: Photosystem II reaction center protein Z

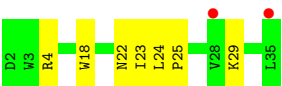
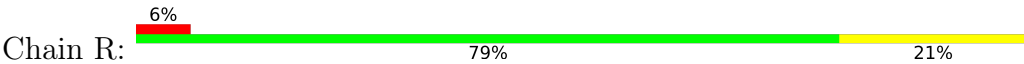
Chain Z:  87% 11%



- Molecule 19: Photosystem II reaction center protein Z



● Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	125.75Å 231.60Å 288.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.20 19.98 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.98-2.20) 99.7 (19.98-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.19Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.142 , 0.178 0.154 , 0.184	Depositor DCC
R_{free} test set	21187 reflections (2.60%)	wwPDB-VP
Wilson B-factor (Å ²)	50.0	Xtriage
Anisotropy	0.485	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 66.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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 1.73% 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: CLA, BCR, BCT, FME, CL, HTG, HEC, OEX, MG, SQD, LHG, PL9, LMG, CA, UNL, LMT, DGD, FE2, GOL, HEM, PHO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.27	0/4478	0.44	0/6098
1	a	0.25	0/4457	0.42	0/6069
2	B	0.34	0/4314	0.49	0/5879
2	b	0.31	0/4285	0.48	0/5841
3	C	0.28	0/4416	0.42	0/6013
3	c	0.28	0/4467	0.42	0/6082
4	D	0.32	0/3746	0.47	0/5102
4	d	0.30	0/3780	0.45	0/5147
5	E	0.31	0/681	0.48	0/928
5	e	0.29	0/690	0.46	0/939
6	F	0.30	0/284	0.44	0/387
6	f	0.26	0/269	0.41	0/365
7	H	0.31	0/519	0.48	0/708
7	h	0.27	0/530	0.46	0/722
8	I	0.29	0/311	0.40	0/419
8	i	0.35	0/311	0.50	0/419
9	J	0.30	0/278	0.37	0/376
9	j	0.28	0/283	0.41	0/383
10	K	0.31	0/303	0.51	0/416
10	k	0.31	0/303	0.50	0/416
11	L	0.37	0/318	0.44	0/433
11	l	0.37	0/318	0.49	0/433
12	M	0.43	0/261	0.52	0/357
12	m	0.33	0/279	0.47	0/380
13	O	0.33	0/1991	0.51	0/2698
13	o	0.31	0/1966	0.50	0/2665
14	T	0.32	0/310	0.40	0/419
14	t	0.33	0/301	0.42	0/406
15	U	0.35	0/811	0.53	0/1095
15	u	0.34	0/826	0.53	0/1116
16	V	0.34	0/1142	0.48	0/1545

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.30	0/1139	0.45	0/1542
17	X	0.23	0/292	0.37	0/395
17	x	0.23	0/284	0.36	0/384
18	Y	0.24	0/216	0.45	0/289
18	y	0.24	0/216	0.37	0/289
19	Z	0.21	0/490	0.35	0/669
19	z	0.21	0/490	0.33	0/669
20	R	0.24	0/279	0.35	0/383
All	All	0.30	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	18	0
1	a	4318	0	4124	31	0
2	B	4166	0	3999	28	0
2	b	4134	0	3976	41	0
3	C	4272	0	4138	24	0
3	c	4316	0	4184	27	0
4	D	3625	0	3489	33	0
4	d	3658	0	3522	21	0
5	E	662	0	648	7	0
5	e	670	0	655	4	0
6	F	275	0	282	6	0
6	f	261	0	269	4	0
7	H	506	0	529	3	0
7	h	517	0	541	4	0
8	I	314	0	328	5	0
8	i	314	0	328	2	0
9	J	272	0	279	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	277	0	284	2	0
10	K	293	0	305	6	0
10	k	293	0	305	7	0
11	L	311	0	320	2	0
11	l	311	0	320	4	0
12	M	268	0	285	3	0
12	m	286	0	305	8	0
13	O	1958	0	1920	24	0
13	o	1933	0	1900	11	0
14	T	311	0	318	1	0
14	t	302	0	311	4	0
15	U	800	0	796	4	0
15	u	815	0	817	3	0
16	V	1120	0	1122	4	0
16	v	1117	0	1131	9	0
17	X	289	0	322	3	0
17	x	281	0	312	1	0
18	Y	215	0	246	1	0
18	y	215	0	246	4	0
19	Z	479	0	516	3	0
19	z	479	0	516	4	0
20	R	273	0	305	3	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	36	0
23	D	195	0	216	7	0
23	a	325	0	360	14	0
23	b	1040	0	1152	28	0
23	c	845	0	936	37	0
23	d	325	0	360	11	0
24	A	256	0	296	5	0
24	a	256	0	296	4	0
25	A	40	0	56	2	0
25	B	120	0	168	7	0
25	C	80	0	112	3	0
25	D	40	0	56	1	0
25	H	40	0	56	3	0
25	K	40	0	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	T	40	0	56	7	0
25	Y	40	0	56	2	0
25	a	40	0	56	0	0
25	b	120	0	168	9	0
25	c	80	0	112	5	0
25	d	40	0	56	0	0
25	h	40	0	56	4	0
25	k	40	0	56	2	0
25	t	40	0	56	5	0
25	y	40	0	56	2	0
26	A	162	0	232	4	0
26	B	54	0	78	2	0
26	F	43	0	53	2	0
26	a	162	0	233	11	0
26	b	54	0	78	4	0
26	f	43	0	53	0	0
27	A	12	0	15	2	0
27	B	18	0	24	1	0
27	C	12	0	16	0	0
27	D	6	0	7	2	0
27	O	12	0	16	4	0
27	V	12	0	16	0	0
27	a	12	0	16	5	0
27	b	12	0	16	2	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	21	0
29	D	110	0	160	0	0
29	a	110	0	160	9	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	M	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	X	18	0	0	0	0
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	m	10	0	0	0	0
30	x	18	0	0	0	0
31	A	70	0	92	2	0
31	B	95	0	127	2	0
31	F	35	0	46	0	0
31	M	35	0	46	1	0
31	T	35	0	46	1	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	2	0
31	t	26	0	35	2	0
32	A	98	0	148	2	0
32	D	196	0	296	13	0
32	E	84	0	114	8	0
32	L	98	0	148	0	0
32	a	84	0	114	9	0
32	b	98	0	148	1	0
32	d	294	0	444	26	0
33	B	51	0	72	1	0
33	C	153	0	216	4	0
33	D	51	0	72	0	0
33	Z	37	0	44	1	0
33	a	51	0	72	0	0
33	c	102	0	144	2	0
33	d	51	0	72	3	0
33	m	51	0	72	0	0
33	z	39	0	48	2	0
34	B	57	0	78	4	0
34	C	19	0	26	0	0
34	D	16	0	17	1	0
34	V	11	0	10	0	0
34	b	57	0	78	3	0
34	c	19	0	26	1	0
34	d	16	0	17	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	C	310	0	410	6	0
35	H	62	0	82	2	0
35	c	310	0	410	9	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	E	43	0	30	1	0
38	f	43	0	30	0	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	227	0	0	2	0
41	B	189	0	0	0	0
41	C	206	0	0	1	0
41	D	155	0	0	3	0
41	E	17	0	0	0	0
41	F	4	0	0	0	0
41	H	22	0	0	0	0
41	I	4	0	0	0	0
41	J	6	0	0	2	0
41	K	5	0	0	0	0
41	L	10	0	0	0	0
41	M	6	0	0	0	0
41	O	108	0	0	1	0
41	T	14	0	0	0	0
41	U	49	0	0	0	0
41	V	80	0	0	0	0
41	X	7	0	0	0	0
41	a	211	0	0	2	0
41	b	204	0	0	0	0
41	c	193	0	0	4	0
41	d	149	0	0	1	0
41	e	8	0	0	0	0
41	f	3	0	0	0	0
41	h	17	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	i	2	0	0	0	0
41	j	1	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	103	0	0	0	0
41	t	11	0	0	1	0
41	u	52	0	0	1	0
41	v	58	0	0	0	0
41	x	6	0	0	0	0
41	y	2	0	0	0	0
All	All	62674	0	61528	589	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 589 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:A:418:GOL:H11	12:M:1:FME:HG2	1.41	1.01
23:B:604:CLA:H42	23:B:605:CLA:H2	1.49	0.93
1:a:250[B]:ALA:HA	2:b:491[B]:VAL:HG11	1.52	0.91
1:a:250[A]:ALA:HA	2:b:491[A]:VAL:HG11	1.53	0.88
23:b:605:CLA:HHC	23:b:605:CLA:HBB1	1.57	0.87

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	551/344 (160%)	540 (98%)	9 (2%)	2 (0%)	30	34
2	B	524/505 (104%)	517 (99%)	7 (1%)	0	100	100
2	b	521/505 (103%)	507 (97%)	14 (3%)	0	100	100
3	C	548/455 (120%)	540 (98%)	7 (1%)	1 (0%)	43	51
3	c	554/455 (122%)	545 (98%)	8 (1%)	1 (0%)	43	51
4	D	454/342 (133%)	439 (97%)	15 (3%)	0	100	100
4	d	457/342 (134%)	446 (98%)	11 (2%)	0	100	100
5	E	79/84 (94%)	78 (99%)	1 (1%)	0	100	100
5	e	79/84 (94%)	79 (100%)	0	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	62/65 (95%)	62 (100%)	0	0	100	100
7	h	63/65 (97%)	60 (95%)	2 (3%)	1 (2%)	7	6
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%)	33 (97%)	1 (3%)	0	100	100
13	O	251/244 (103%)	242 (96%)	8 (3%)	1 (0%)	30	34
13	o	249/244 (102%)	244 (98%)	5 (2%)	0	100	100
14	T	33/32 (103%)	33 (100%)	0	0	100	100
14	t	32/32 (100%)	32 (100%)	0	0	100	100
15	U	97/104 (93%)	93 (96%)	4 (4%)	0	100	100
15	u	99/104 (95%)	94 (95%)	5 (5%)	0	100	100
16	V	140/137 (102%)	136 (97%)	4 (3%)	0	100	100
16	v	140/137 (102%)	135 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
17	x	36/40 (90%)	36 (100%)	0	0	100	100
18	Y	27/30 (90%)	24 (89%)	3 (11%)	0	100	100
18	y	27/30 (90%)	27 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	5
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	7	5
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	6180/5384 (115%)	6042 (98%)	127 (2%)	11 (0%)	43	51

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	I	36	ASP
3	C	416	SER
13	O	26	ALA
3	c	416	SER
19	Z	31	GLN

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%)	442 (100%)	2 (0%)	81	90
1	a	442/279 (158%)	441 (100%)	1 (0%)	87	94
2	B	423/403 (105%)	416 (98%)	7 (2%)	53	69
2	b	420/403 (104%)	407 (97%)	13 (3%)	35	48
3	C	431/356 (121%)	422 (98%)	9 (2%)	47	63
3	c	437/356 (123%)	430 (98%)	7 (2%)	55	71
4	D	368/277 (133%)	365 (99%)	3 (1%)	73	85
4	d	372/277 (134%)	368 (99%)	4 (1%)	65	79
5	E	72/73 (99%)	69 (96%)	3 (4%)	26	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	e	72/73 (99%)	71 (99%)	1 (1%)	59	75
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	41
7	h	55/54 (102%)	55 (100%)	0	100	100
8	I	34/34 (100%)	32 (94%)	2 (6%)	18	22
8	i	34/34 (100%)	33 (97%)	1 (3%)	37	51
9	J	26/27 (96%)	24 (92%)	2 (8%)	12	13
9	j	26/27 (96%)	25 (96%)	1 (4%)	29	40
10	K	30/30 (100%)	26 (87%)	4 (13%)	4	3
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	7
11	L	36/35 (103%)	36 (100%)	0	100	100
11	l	36/35 (103%)	35 (97%)	1 (3%)	38	52
12	M	30/32 (94%)	27 (90%)	3 (10%)	7	7
12	m	32/32 (100%)	30 (94%)	2 (6%)	16	19
13	O	216/207 (104%)	210 (97%)	6 (3%)	38	52
13	o	213/207 (103%)	206 (97%)	7 (3%)	33	45
14	T	32/28 (114%)	28 (88%)	4 (12%)	4	4
14	t	31/28 (111%)	31 (100%)	0	100	100
15	U	86/89 (97%)	84 (98%)	2 (2%)	44	59
15	u	88/89 (99%)	86 (98%)	2 (2%)	44	59
16	V	123/117 (105%)	122 (99%)	1 (1%)	73	85
16	v	123/117 (105%)	120 (98%)	3 (2%)	43	58
17	X	32/33 (97%)	31 (97%)	1 (3%)	35	48
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	3
19	Z	52/52 (100%)	49 (94%)	3 (6%)	18	22
19	z	52/52 (100%)	44 (85%)	8 (15%)	2	2
20	R	29/29 (100%)	27 (93%)	2 (7%)	14	16
All	All	5110/4403 (116%)	4997 (98%)	113 (2%)	44	61

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

Mol	Chain	Res	Type
2	b	287	ARG
19	z	32	ASP
3	c	315[B]	MET
19	z	21	ILE
18	y	45	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
3	c	201	ASN
11	l	8	GLN
16	v	86	GLN
13	o	58	ASN
15	U	78	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	FME	M	1	12	8,9,10	0.64	0	7,9,11	1.18	1 (14%)
14	FME	T	1	14	8,9,10	0.63	0	7,9,11	1.31	1 (14%)
8	FME	i	1	8	8,9,10	0.66	0	7,9,11	1.16	1 (14%)
8	FME	I	1	8	8,9,10	0.58	0	7,9,11	1.16	1 (14%)
12	FME	m	1	12	8,9,10	0.58	0	7,9,11	1.51	2 (28%)
14	FME	t	1	14	8,9,10	0.71	0	7,9,11	1.53	2 (28%)

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

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

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	m	1	FME	O1-CN-N	-2.55	118.54	125.27
14	t	1	FME	O-C-CA	-2.40	118.48	124.78
14	T	1	FME	CG-CB-CA	2.39	119.60	112.95
12	m	1	FME	CA-N-CN	-2.26	119.34	122.82
14	t	1	FME	CA-N-CN	-2.22	119.40	122.82

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 4 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 274 ligands modelled in this entry, 21 are monoatomic and 20 are unknown - leaving 233 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	HTG	B	622	-	19,19,19	1.07	2 (10%)	23,24,24	1.59	5 (21%)
23	CLA	b	613	2	69,73,73	1.98	19 (27%)	83,113,113	2.79	30 (36%)
23	CLA	c	502	3	69,73,73	1.97	17 (24%)	83,113,113	2.80	27 (32%)
26	SQD	F	102	-	42,43,54	1.19	4 (9%)	51,54,65	2.18	14 (27%)
33	LMG	B	621	-	51,51,55	0.91	2 (3%)	59,59,63	1.32	5 (8%)
23	CLA	b	615	2	69,73,73	2.02	18 (26%)	83,113,113	2.82	30 (36%)
23	CLA	B	609	2	69,73,73	2.01	18 (26%)	83,113,113	2.85	28 (33%)
25	BCR	a	408	-	41,41,41	1.04	1 (2%)	56,56,56	1.29	7 (12%)
33	LMG	z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.08	3 (6%)
24	PHO	a	406[B]	-	58,69,69	2.78	13 (22%)	56,99,99	2.77	15 (26%)
26	SQD	a	409[A]	-	53,54,54	0.95	3 (5%)	62,65,65	1.77	13 (20%)
32	LHG	D	407[B]	-	48,48,48	0.92	2 (4%)	51,54,54	0.97	3 (5%)
23	CLA	C	512	3	69,73,73	2.01	20 (28%)	83,113,113	2.75	27 (32%)
23	CLA	b	602	2	69,73,73	2.09	20 (28%)	83,113,113	2.91	35 (42%)
23	CLA	c	505	3	69,73,73	2.03	18 (26%)	83,113,113	2.78	28 (33%)
23	CLA	d	404	4	69,73,73	2.04	19 (27%)	83,113,113	2.92	29 (34%)
25	BCR	B	618	-	41,41,41	1.00	1 (2%)	56,56,56	1.31	7 (12%)
23	CLA	b	610	41	69,73,73	2.02	20 (28%)	83,113,113	2.82	34 (40%)
25	BCR	d	405	-	41,41,41	1.13	2 (4%)	56,56,56	1.98	15 (26%)
27	GOL	B	629	-	5,5,5	0.99	0	5,5,5	1.00	0
27	GOL	O	302	-	5,5,5	0.91	0	5,5,5	0.87	0
27	GOL	B	627	-	5,5,5	1.00	0	5,5,5	1.06	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PL9	a	412[B]	-	55,55,55	0.64	2 (3%)	68,69,69	1.96	22 (32%)
35	DGD	c	516[A]	-	63,63,67	0.85	2 (3%)	77,77,81	1.12	6 (7%)
23	CLA	b	605	2	69,73,73	1.94	18 (26%)	83,113,113	2.98	30 (36%)
32	LHG	d	408[A]	-	48,48,48	0.92	2 (4%)	51,54,54	0.99	3 (5%)
33	LMG	d	412	39	51,51,55	0.88	2 (3%)	59,59,63	1.13	5 (8%)
23	CLA	b	608	2	69,73,73	1.97	19 (27%)	83,113,113	2.78	33 (39%)
33	LMG	c	519	-	51,51,55	0.93	2 (3%)	59,59,63	1.10	4 (6%)
34	HTG	b	623	-	19,19,19	1.01	1 (5%)	23,24,24	1.78	2 (8%)
23	CLA	C	513	3	69,73,73	2.04	19 (27%)	83,113,113	2.86	32 (38%)
23	CLA	c	503	3	69,73,73	2.04	19 (27%)	83,113,113	2.87	29 (34%)
23	CLA	A	408	1	69,73,73	2.00	20 (28%)	83,113,113	2.93	34 (40%)
23	CLA	a	405[B]	41	69,73,73	2.01	20 (28%)	83,113,113	2.84	30 (36%)
23	CLA	c	511	3	69,73,73	2.06	20 (28%)	83,113,113	2.82	33 (39%)
33	LMG	Z	101	-	37,37,55	1.01	2 (5%)	45,45,63	1.44	6 (13%)
24	PHO	A	416[A]	-	58,69,69	2.74	15 (25%)	56,99,99	2.87	17 (30%)
26	SQD	b	620	-	53,54,54	1.04	3 (5%)	62,65,65	1.68	11 (17%)
34	HTG	c	521	-	19,19,19	0.93	1 (5%)	23,24,24	1.51	1 (4%)
23	CLA	c	501	3	69,73,73	2.00	20 (28%)	83,113,113	2.93	29 (34%)
26	SQD	f	102	-	42,43,54	1.18	3 (7%)	51,54,65	1.55	11 (21%)
31	LMT	A	420	-	36,36,36	1.04	2 (5%)	47,47,47	1.15	4 (8%)
31	LMT	M	101	-	36,36,36	1.12	3 (8%)	47,47,47	1.17	4 (8%)
23	CLA	B	606	2	69,73,73	1.95	19 (27%)	83,113,113	2.96	32 (38%)
31	LMT	A	417	-	36,36,36	0.96	3 (8%)	47,47,47	0.99	1 (2%)
37	BCT	d	401[B]	21	2,3,3	0.61	0	2,3,3	1.23	0
23	CLA	C	510	3	69,73,73	2.05	19 (27%)	83,113,113	2.88	31 (37%)
25	BCR	c	514	-	41,41,41	1.00	1 (2%)	56,56,56	1.68	13 (23%)
31	LMT	b	627	-	25,25,36	0.89	1 (4%)	30,30,47	1.09	2 (6%)
25	BCR	h	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.44	11 (19%)
25	BCR	D	404	-	41,41,41	1.11	1 (2%)	56,56,56	1.80	17 (30%)
25	BCR	b	618	-	41,41,41	1.01	1 (2%)	56,56,56	1.16	6 (10%)
32	LHG	E	101[B]	-	41,41,48	1.06	2 (4%)	44,47,54	1.09	3 (6%)
26	SQD	B	620	-	53,54,54	1.07	4 (7%)	62,65,65	1.76	11 (17%)
23	CLA	a	407	1	69,73,73	1.97	19 (27%)	83,113,113	3.05	33 (39%)
24	PHO	a	414[B]	-	58,69,69	2.78	14 (24%)	56,99,99	2.85	16 (28%)
27	GOL	V	203[A]	-	5,5,5	1.22	0	5,5,5	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	508	3	69,73,73	2.12	20 (28%)	83,113,113	2.78	30 (36%)
27	GOL	a	418	-	5,5,5	1.23	1 (20%)	5,5,5	1.03	0
25	BCR	H	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.48	9 (16%)
34	HTG	C	522	-	19,19,19	0.86	1 (5%)	23,24,24	1.36	2 (8%)
35	DGD	C	518[B]	-	63,63,67	0.87	2 (3%)	77,77,81	1.07	5 (6%)
23	CLA	B	616	2	69,73,73	1.98	20 (28%)	83,113,113	2.90	28 (33%)
35	DGD	c	518	-	63,63,67	0.86	3 (4%)	77,77,81	1.04	4 (5%)
23	CLA	A	405[A]	41	69,73,73	1.93	18 (26%)	83,113,113	2.88	33 (39%)
23	CLA	B	612	2	69,73,73	2.03	21 (30%)	83,113,113	2.81	30 (36%)
31	LMT	B	631	-	25,25,36	0.88	2 (8%)	30,30,47	1.15	3 (10%)
34	HTG	V	202	-	11,11,19	0.29	0	15,15,24	1.17	1 (6%)
23	CLA	C	505	41	69,73,73	1.98	20 (28%)	83,113,113	2.78	28 (33%)
23	CLA	b	604	2	69,73,73	2.00	18 (26%)	83,113,113	2.78	28 (33%)
26	SQD	A	412	-	53,54,54	1.03	3 (5%)	62,65,65	1.22	7 (11%)
24	PHO	A	407[A]	-	58,69,69	2.69	14 (24%)	56,99,99	2.78	15 (26%)
25	BCR	C	516	-	41,41,41	1.03	1 (2%)	56,56,56	1.46	8 (14%)
27	GOL	b	628	-	5,5,5	0.54	0	5,5,5	1.35	1 (20%)
35	DGD	C	517[A]	-	63,63,67	0.81	2 (3%)	77,77,81	1.21	8 (10%)
23	CLA	A	404[A]	1	69,73,73	1.98	20 (28%)	83,113,113	2.82	32 (38%)
25	BCR	b	619	-	41,41,41	1.07	1 (2%)	56,56,56	1.36	6 (10%)
25	BCR	B	619	-	41,41,41	1.11	2 (4%)	56,56,56	1.31	8 (14%)
31	LMT	b	621	-	25,25,36	0.98	1 (4%)	30,30,47	1.20	2 (6%)
25	BCR	B	617	-	41,41,41	1.05	1 (2%)	56,56,56	1.32	6 (10%)
27	GOL	b	624	-	5,5,5	1.22	1 (20%)	5,5,5	0.81	0
28	OEX	a	411[A]	1,3,41	0,14,14	-	-	-	-	-
29	PL9	A	414[A]	-	55,55,55	0.68	2 (3%)	68,69,69	2.08	25 (36%)
32	LHG	D	406[B]	-	48,48,48	0.87	2 (4%)	51,54,54	0.93	3 (5%)
33	LMG	D	411	39	51,51,55	0.84	2 (3%)	59,59,63	0.99	4 (6%)
23	CLA	c	513	3	69,73,73	2.10	20 (28%)	83,113,113	2.86	30 (36%)
37	BCT	d	401[A]	21	2,3,3	0.57	0	2,3,3	1.58	1 (50%)
27	GOL	l	801[A]	-	5,5,5	0.96	0	5,5,5	0.97	0
32	LHG	E	101[A]	-	41,41,48	1.06	2 (4%)	44,47,54	1.11	3 (6%)
24	PHO	a	414[A]	-	58,69,69	2.75	14 (24%)	56,99,99	3.01	17 (30%)
33	LMG	c	520	-	51,51,55	1.00	2 (3%)	59,59,63	1.36	6 (10%)
26	SQD	A	410[A]	-	53,54,54	0.93	3 (5%)	62,65,65	1.81	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	K	102	-	41,41,41	1.02	1 (2%)	56,56,56	1.41	10 (17%)
33	LMG	a	415	-	51,51,55	0.92	2 (3%)	59,59,63	1.22	5 (8%)
23	CLA	B	607	41	69,73,73	1.95	20 (28%)	83,113,113	2.91	32 (38%)
23	CLA	C	507	3	69,73,73	2.03	21 (30%)	83,113,113	2.83	33 (39%)
23	CLA	d	403[B]	4	69,73,73	1.97	20 (28%)	83,113,113	2.86	27 (32%)
23	CLA	b	609	2	69,73,73	2.03	20 (28%)	83,113,113	2.82	33 (39%)
23	CLA	c	506	3	69,73,73	2.04	20 (28%)	83,113,113	2.80	30 (36%)
28	OEX	A	413[B]	1,3,41	0,14,14	-	-	-		
38	HEM	f	101	5,6	50,50,50	1.50	6 (12%)	66,82,82	1.75	13 (19%)
23	CLA	B	611	2	69,73,73	2.61	20 (28%)	83,113,113	4.03	31 (37%)
32	LHG	A	419[B]	-	48,48,48	0.87	2 (4%)	51,54,54	1.17	5 (9%)
23	CLA	a	404[B]	1	69,73,73	1.99	20 (28%)	83,113,113	2.86	33 (39%)
25	BCR	c	515	-	41,41,41	1.04	1 (2%)	56,56,56	1.45	13 (23%)
27	GOL	o	303	-	5,5,5	1.07	1 (20%)	5,5,5	1.08	0
32	LHG	b	629[B]	-	48,48,48	0.88	2 (4%)	51,54,54	1.02	3 (5%)
29	PL9	D	405[B]	-	55,55,55	0.63	2 (3%)	68,69,69	1.68	17 (25%)
27	GOL	A	418	-	5,5,5	1.62	2 (40%)	5,5,5	0.97	1 (20%)
24	PHO	a	406[A]	-	58,69,69	2.72	12 (20%)	56,99,99	2.76	15 (26%)
32	LHG	D	407[A]	-	48,48,48	0.92	2 (4%)	51,54,54	0.99	4 (7%)
23	CLA	c	510	3	69,73,73	2.03	20 (28%)	83,113,113	2.82	31 (37%)
25	BCR	b	617	-	41,41,41	1.04	1 (2%)	56,56,56	1.37	6 (10%)
27	GOL	v	202[B]	-	5,5,5	1.13	0	5,5,5	0.87	0
29	PL9	a	412[A]	-	55,55,55	0.65	2 (3%)	68,69,69	2.00	22 (32%)
38	HEM	E	102	5,6	50,50,50	1.54	6 (12%)	66,82,82	1.92	17 (25%)
34	HTG	B	625	-	19,19,19	0.97	2 (10%)	23,24,24	1.12	2 (8%)
32	LHG	L	101[B]	-	48,48,48	0.92	2 (4%)	51,54,54	1.09	4 (7%)
27	GOL	c	525[B]	-	5,5,5	1.04	0	5,5,5	0.87	0
32	LHG	a	419[B]	-	41,41,48	1.03	2 (4%)	44,47,54	0.92	2 (4%)
33	LMG	m	101	-	51,51,55	0.87	2 (3%)	59,59,63	1.24	6 (10%)
35	DGD	C	519	-	63,63,67	0.86	3 (4%)	77,77,81	0.98	3 (3%)
40	HEC	v	201	16	50,50,50	1.78	6 (12%)	68,82,82	1.43	9 (13%)
37	BCT	D	401[B]	21	2,3,3	0.63	0	2,3,3	1.06	0
23	CLA	a	405[A]	41	69,73,73	1.96	19 (27%)	83,113,113	2.86	30 (36%)
29	PL9	d	406[B]	-	55,55,55	0.68	1 (1%)	68,69,69	1.62	17 (25%)
23	CLA	c	512	3	69,73,73	2.08	20 (28%)	83,113,113	2.86	31 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	T	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.68	15 (26%)
23	CLA	d	403[A]	4	69,73,73	1.94	20 (28%)	83,113,113	2.78	29 (34%)
23	CLA	b	614	2	69,73,73	1.99	20 (28%)	83,113,113	2.92	33 (39%)
27	GOL	C	523[B]	-	5,5,5	1.07	0	5,5,5	0.91	0
33	LMG	C	501	-	51,51,55	0.92	2 (3%)	59,59,63	1.53	7 (11%)
23	CLA	B	608	2	69,73,73	1.92	21 (30%)	83,113,113	2.82	33 (39%)
27	GOL	A	411	-	5,5,5	1.13	0	5,5,5	0.74	0
35	DGD	H	102	-	63,63,67	0.85	3 (4%)	77,77,81	1.04	6 (7%)
23	CLA	b	601	41	69,73,73	2.10	20 (28%)	83,113,113	2.79	29 (34%)
31	LMT	T	101	-	36,36,36	1.05	3 (8%)	47,47,47	1.04	2 (4%)
31	LMT	B	630	-	36,36,36	1.02	3 (8%)	47,47,47	1.15	5 (10%)
34	HTG	D	410	-	16,16,19	1.04	1 (6%)	20,21,24	1.46	1 (5%)
23	CLA	B	601	41	69,73,73	2.09	20 (28%)	83,113,113	2.86	28 (33%)
23	CLA	C	503	3	69,73,73	2.01	20 (28%)	83,113,113	2.77	29 (34%)
23	CLA	b	611	2	69,73,73	1.98	20 (28%)	83,113,113	2.94	31 (37%)
32	LHG	b	629[A]	-	48,48,48	0.85	3 (6%)	51,54,54	1.03	4 (7%)
33	LMG	C	521	-	51,51,55	1.07	3 (5%)	59,59,63	1.33	6 (10%)
26	SQD	a	410	-	53,54,54	1.05	4 (7%)	62,65,65	1.21	8 (12%)
25	BCR	Y	101	-	41,41,41	0.99	1 (2%)	56,56,56	1.78	13 (23%)
23	CLA	B	603	2	69,73,73	2.00	20 (28%)	83,113,113	2.95	30 (36%)
27	GOL	v	202[A]	-	5,5,5	1.27	0	5,5,5	0.72	0
27	GOL	D	412	-	5,5,5	1.42	2 (40%)	5,5,5	0.81	0
26	SQD	a	409[B]	-	53,54,54	0.97	3 (5%)	62,65,65	1.64	12 (19%)
32	LHG	d	414[B]	-	48,48,48	0.91	2 (4%)	51,54,54	1.07	5 (9%)
23	CLA	b	603	2	69,73,73	2.01	18 (26%)	83,113,113	2.95	31 (37%)
27	GOL	C	523[A]	-	5,5,5	1.18	0	5,5,5	0.83	0
35	DGD	c	516[B]	-	63,63,67	0.86	2 (3%)	77,77,81	1.01	3 (3%)
27	GOL	c	525[A]	-	5,5,5	0.94	0	5,5,5	0.95	0
27	GOL	c	526	-	5,5,5	1.01	0	5,5,5	0.99	0
31	LMT	e	101	-	36,36,36	1.03	4 (11%)	47,47,47	0.98	1 (2%)
35	DGD	C	518[A]	-	63,63,67	0.89	3 (4%)	77,77,81	1.02	5 (6%)
25	BCR	C	515	-	41,41,41	1.05	1 (2%)	56,56,56	1.36	6 (10%)
25	BCR	A	409	-	41,41,41	1.01	1 (2%)	56,56,56	1.43	8 (14%)
34	HTG	B	623	-	19,19,19	0.81	1 (5%)	23,24,24	1.46	3 (13%)
29	PL9	d	406[A]	-	55,55,55	0.65	1 (1%)	68,69,69	1.63	17 (25%)
23	CLA	d	402[B]	41	69,73,73	2.07	19 (27%)	83,113,113	2.84	34 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	PHO	A	416[B]	-	58,69,69	2.74	12 (20%)	56,99,99	2.81	16 (28%)
35	DGD	h	102	-	63,63,67	0.87	3 (4%)	77,77,81	1.07	6 (7%)
23	CLA	B	615	2	69,73,73	2.07	19 (27%)	83,113,113	2.85	30 (36%)
34	HTG	b	625	-	19,19,19	1.03	2 (10%)	23,24,24	1.58	3 (13%)
32	LHG	D	406[A]	-	48,48,48	0.86	2 (4%)	51,54,54	0.99	3 (5%)
27	GOL	d	413	-	5,5,5	1.07	0	5,5,5	0.97	0
23	CLA	C	502	3	69,73,73	1.99	20 (28%)	83,113,113	2.81	31 (37%)
34	HTG	b	622	-	19,19,19	1.16	2 (10%)	23,24,24	1.96	7 (30%)
32	LHG	d	407[B]	-	48,48,48	0.88	2 (4%)	51,54,54	0.99	3 (5%)
23	CLA	B	610	41	69,73,73	2.07	19 (27%)	83,113,113	2.90	30 (36%)
32	LHG	d	414[A]	-	48,48,48	0.89	2 (4%)	51,54,54	1.12	4 (7%)
31	LMT	a	416	-	36,36,36	1.01	1 (2%)	47,47,47	1.03	1 (2%)
23	CLA	A	406[B]	41	69,73,73	2.05	19 (27%)	83,113,113	2.88	32 (38%)
23	CLA	C	514	3	69,73,73	2.04	20 (28%)	83,113,113	2.86	31 (37%)
25	BCR	y	101	-	41,41,41	1.09	1 (2%)	56,56,56	1.63	12 (21%)
23	CLA	c	504	41	69,73,73	2.06	21 (30%)	83,113,113	2.86	32 (38%)
23	CLA	D	402[B]	4	69,73,73	2.00	20 (28%)	83,113,113	2.88	32 (38%)
27	GOL	V	203[B]	-	5,5,5	1.10	0	5,5,5	0.89	0
35	DGD	c	517[B]	-	63,63,67	0.86	2 (3%)	77,77,81	0.97	5 (6%)
23	CLA	D	403	4	69,73,73	2.10	18 (26%)	83,113,113	2.79	31 (37%)
23	CLA	C	511	3	69,73,73	2.03	20 (28%)	83,113,113	2.94	33 (39%)
28	OEX	A	413[A]	1,3,41	0,14,14	-	-	-	-	-
23	CLA	b	607	41	69,73,73	1.96	20 (28%)	83,113,113	2.79	29 (34%)
23	CLA	B	605	2	69,73,73	2.01	19 (27%)	83,113,113	2.93	29 (34%)
23	CLA	A	405[B]	41	69,73,73	2.05	18 (26%)	83,113,113	2.82	32 (38%)
23	CLA	d	402[A]	41	69,73,73	2.01	17 (24%)	83,113,113	2.80	29 (34%)
27	GOL	o	302	-	5,5,5	1.00	0	5,5,5	1.00	0
27	GOL	a	417	-	5,5,5	0.99	0	5,5,5	1.03	0
31	LMT	m	103	-	36,36,36	1.10	3 (8%)	47,47,47	1.12	3 (6%)
25	BCR	t	102	-	41,41,41	1.00	1 (2%)	56,56,56	1.55	11 (19%)
32	LHG	A	419[A]	-	48,48,48	0.84	2 (4%)	51,54,54	1.31	6 (11%)
23	CLA	B	602	2	69,73,73	2.09	20 (28%)	83,113,113	2.86	33 (39%)
23	CLA	B	604	2	69,73,73	1.98	22 (31%)	83,113,113	2.67	31 (37%)
23	CLA	a	404[A]	1	69,73,73	1.96	19 (27%)	83,113,113	2.88	33 (39%)
27	GOL	O	303	-	5,5,5	0.98	0	5,5,5	1.11	1 (20%)
29	PL9	D	405[A]	-	55,55,55	0.62	2 (3%)	68,69,69	1.64	18 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LMT	t	101	-	26,26,36	0.93	2 (7%)	31,31,47	1.35	2 (6%)
24	PHO	A	407[B]	-	58,69,69	2.68	13 (22%)	56,99,99	2.88	15 (26%)
33	LMG	C	520	-	51,51,55	0.93	2 (3%)	59,59,63	1.18	6 (10%)
23	CLA	c	509	3	69,73,73	2.01	18 (26%)	83,113,113	2.87	32 (38%)
35	DGD	C	517[B]	-	63,63,67	0.84	2 (3%)	77,77,81	1.11	7 (9%)
23	CLA	A	404[B]	1	69,73,73	2.02	20 (28%)	83,113,113	2.87	32 (38%)
23	CLA	C	504	3	69,73,73	1.96	19 (27%)	83,113,113	2.93	28 (33%)
23	CLA	C	506	3	69,73,73	2.02	19 (27%)	83,113,113	2.78	32 (38%)
27	GOL	B	624	-	5,5,5	0.75	0	5,5,5	1.10	1 (20%)
31	LMT	F	101	-	36,36,36	1.07	1 (2%)	47,47,47	1.06	2 (4%)
23	CLA	B	614	2	69,73,73	2.05	21 (30%)	83,113,113	2.92	32 (38%)
28	OEX	a	411[B]	1,3,41	0,14,14	-	-	-	-	-
23	CLA	c	507	41	69,73,73	2.03	18 (26%)	83,113,113	2.91	30 (36%)
29	PL9	A	414[B]	-	55,55,55	0.65	2 (3%)	68,69,69	1.98	25 (36%)
32	LHG	L	101[A]	-	48,48,48	0.89	2 (4%)	51,54,54	1.15	3 (5%)
32	LHG	a	419[A]	-	41,41,48	1.04	2 (4%)	44,47,54	0.92	2 (4%)
32	LHG	d	407[A]	-	48,48,48	0.86	2 (4%)	51,54,54	1.08	4 (7%)
40	HEC	V	201	16	50,50,50	1.78	6 (12%)	68,82,82	1.60	13 (19%)
27	GOL	l	801[B]	-	5,5,5	0.88	0	5,5,5	0.97	0
31	LMT	B	628	-	36,36,36	1.19	4 (11%)	47,47,47	1.37	6 (12%)
37	BCT	D	401[A]	21	2,3,3	0.54	0	2,3,3	1.81	1 (50%)
32	LHG	d	408[B]	-	48,48,48	0.93	2 (4%)	51,54,54	1.01	3 (5%)
23	CLA	b	606	2	69,73,73	1.98	19 (27%)	83,113,113	2.92	32 (38%)
23	CLA	B	613	2	69,73,73	2.00	20 (28%)	83,113,113	2.80	30 (36%)
23	CLA	C	508	41	69,73,73	1.99	19 (27%)	83,113,113	2.82	30 (36%)
23	CLA	A	406[A]	41	69,73,73	1.99	18 (26%)	83,113,113	2.86	32 (38%)
23	CLA	b	616	2	69,73,73	1.98	20 (28%)	83,113,113	2.91	31 (37%)
34	HTG	d	411	-	16,16,19	0.96	1 (6%)	20,21,24	1.55	1 (5%)
35	DGD	c	517[A]	-	63,63,67	0.84	2 (3%)	77,77,81	0.97	5 (6%)
23	CLA	D	402[A]	4	69,73,73	1.98	19 (27%)	83,113,113	2.88	31 (37%)
23	CLA	b	612	2	69,73,73	2.00	20 (28%)	83,113,113	2.82	31 (37%)
26	SQD	A	410[B]	-	53,54,54	0.93	3 (5%)	62,65,65	1.79	11 (17%)
25	BCR	k	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.51	13 (23%)
23	CLA	C	509	3	69,73,73	2.03	20 (28%)	83,113,113	2.82	28 (33%)

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
34	HTG	B	622	-	-	4/10/30/30	0/1/1/1
23	CLA	b	613	2	-	5/39/115/115	-
23	CLA	c	502	3	-	6/39/115/115	-
26	SQD	F	102	-	-	14/38/58/69	0/1/1/1
33	LMG	B	621	-	-	19/46/66/70	0/1/1/1
23	CLA	b	615	2	-	7/39/115/115	-
23	CLA	B	609	2	-	2/39/115/115	-
25	BCR	a	408	-	-	1/29/63/63	0/2/2/2
33	LMG	z	101	-	-	9/34/54/70	0/1/1/1
24	PHO	a	406[B]	-	-	5/37/103/103	0/5/6/6
26	SQD	a	409[A]	-	-	10/49/69/69	0/1/1/1
32	LHG	D	407[B]	-	-	13/53/53/53	-
23	CLA	C	512	3	-	3/39/115/115	-
23	CLA	b	602	2	-	4/39/115/115	-
23	CLA	c	505	3	-	7/39/115/115	-
23	CLA	d	404	4	-	8/39/115/115	-
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
23	CLA	b	610	41	-	5/39/115/115	-
25	BCR	d	405	-	-	5/29/63/63	0/2/2/2
27	GOL	B	629	-	-	4/4/4/4	-
27	GOL	O	302	-	-	2/4/4/4	-
27	GOL	B	627	-	-	1/4/4/4	-
29	PL9	a	412[B]	-	-	15/53/73/73	0/1/1/1
35	DGD	c	516[A]	-	-	20/51/91/95	0/2/2/2
23	CLA	b	605	2	-	5/39/115/115	-
32	LHG	d	408[A]	-	-	11/53/53/53	-
33	LMG	d	412	39	-	11/46/66/70	0/1/1/1
23	CLA	b	608	2	-	5/39/115/115	-
33	LMG	c	519	-	-	12/46/66/70	0/1/1/1
34	HTG	b	623	-	-	5/10/30/30	0/1/1/1
23	CLA	C	513	3	-	9/39/115/115	-
23	CLA	c	503	3	-	2/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	A	408	1	-	9/39/115/115	-
23	CLA	a	405[B]	41	-	8/39/115/115	-
23	CLA	c	511	3	-	3/39/115/115	-
33	LMG	Z	101	-	-	10/31/51/70	0/1/1/1
24	PHO	A	416[A]	-	-	1/37/103/103	0/5/6/6
26	SQD	b	620	-	-	19/49/69/69	0/1/1/1
34	HTG	c	521	-	-	2/10/30/30	0/1/1/1
23	CLA	c	501	3	-	6/39/115/115	-
26	SQD	f	102	-	-	10/38/58/69	0/1/1/1
31	LMT	A	420	-	-	15/21/61/61	0/2/2/2
31	LMT	M	101	-	-	4/21/61/61	0/2/2/2
23	CLA	B	606	2	-	9/39/115/115	-
31	LMT	A	417	-	-	7/21/61/61	0/2/2/2
23	CLA	C	510	3	-	4/39/115/115	-
25	BCR	c	514	-	-	2/29/63/63	0/2/2/2
31	LMT	b	627	-	-	11/17/37/61	0/1/1/2
25	BCR	h	101	-	-	1/29/63/63	0/2/2/2
25	BCR	D	404	-	-	4/29/63/63	0/2/2/2
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
32	LHG	E	101[B]	-	-	23/46/46/53	-
26	SQD	B	620	-	-	13/49/69/69	0/1/1/1
23	CLA	a	407	1	-	10/39/115/115	-
24	PHO	a	414[B]	-	-	1/37/103/103	0/5/6/6
27	GOL	V	203[A]	-	-	2/4/4/4	-
23	CLA	c	508	3	-	5/39/115/115	-
27	GOL	a	418	-	-	0/4/4/4	-
25	BCR	H	101	-	-	2/29/63/63	0/2/2/2
34	HTG	C	522	-	-	0/10/30/30	0/1/1/1
35	DGD	C	518[B]	-	-	13/51/91/95	0/2/2/2
23	CLA	B	616	2	-	8/39/115/115	-
35	DGD	c	518	-	-	10/51/91/95	0/2/2/2
23	CLA	A	405[A]	41	-	4/39/115/115	-
23	CLA	B	612	2	-	6/39/115/115	-
31	LMT	B	631	-	-	11/17/37/61	0/1/1/2
34	HTG	V	202	-	-	0/2/19/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	505	41	-	8/39/115/115	-
23	CLA	b	604	2	-	12/39/115/115	-
26	SQD	A	412	-	-	14/49/69/69	0/1/1/1
24	PHO	A	407[A]	-	-	3/37/103/103	0/5/6/6
25	BCR	C	516	-	-	2/29/63/63	0/2/2/2
27	GOL	b	628	-	-	0/4/4/4	-
35	DGD	C	517[A]	-	-	11/51/91/95	0/2/2/2
23	CLA	A	404[A]	1	-	5/39/115/115	-
25	BCR	b	619	-	-	3/29/63/63	0/2/2/2
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
31	LMT	b	621	-	-	8/17/37/61	0/1/1/2
25	BCR	B	617	-	-	2/29/63/63	0/2/2/2
27	GOL	b	624	-	-	2/4/4/4	-
29	PL9	A	414[A]	-	-	15/53/73/73	0/1/1/1
32	LHG	D	406[B]	-	-	16/53/53/53	-
33	LMG	D	411	39	-	9/46/66/70	0/1/1/1
23	CLA	c	513	3	-	12/39/115/115	-
27	GOL	l	801[A]	-	-	2/4/4/4	-
32	LHG	E	101[A]	-	-	22/46/46/53	-
24	PHO	a	414[A]	-	-	1/37/103/103	0/5/6/6
33	LMG	c	520	-	-	10/46/66/70	0/1/1/1
26	SQD	A	410[A]	-	-	12/49/69/69	0/1/1/1
25	BCR	K	102	-	-	1/29/63/63	0/2/2/2
33	LMG	a	415	-	-	12/46/66/70	0/1/1/1
23	CLA	B	607	41	-	3/39/115/115	-
23	CLA	C	507	3	-	12/39/115/115	-
23	CLA	d	403[B]	4	-	4/39/115/115	-
23	CLA	b	609	2	-	3/39/115/115	-
23	CLA	c	506	3	-	8/39/115/115	-
38	HEM	f	101	5,6	-	8/14/54/54	-
23	CLA	B	611	2	-	2/39/115/115	-
32	LHG	A	419[B]	-	-	13/53/53/53	-
23	CLA	a	404[B]	1	-	2/39/115/115	-
25	BCR	c	515	-	-	0/29/63/63	0/2/2/2
27	GOL	o	303	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LHG	b	629[B]	-	-	18/53/53/53	-
29	PL9	D	405[B]	-	-	8/53/73/73	0/1/1/1
27	GOL	A	418	-	-	1/4/4/4	-
24	PHO	a	406[A]	-	-	5/37/103/103	0/5/6/6
32	LHG	D	407[A]	-	-	14/53/53/53	-
23	CLA	c	510	3	-	12/39/115/115	-
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
27	GOL	v	202[B]	-	-	2/4/4/4	-
29	PL9	a	412[A]	-	-	14/53/73/73	0/1/1/1
38	HEM	E	102	5,6	-	4/14/54/54	-
34	HTG	B	625	-	-	3/10/30/30	0/1/1/1
32	LHG	L	101[B]	-	-	18/53/53/53	-
27	GOL	c	525[B]	-	-	0/4/4/4	-
32	LHG	a	419[B]	-	-	16/46/46/53	-
33	LMG	m	101	-	-	10/46/66/70	0/1/1/1
35	DGD	C	519	-	-	16/51/91/95	0/2/2/2
40	HEC	v	201	16	1/1/3/7	6/14/54/54	-
23	CLA	a	405[A]	41	-	7/39/115/115	-
29	PL9	d	406[B]	-	-	6/53/73/73	0/1/1/1
23	CLA	c	512	3	-	13/39/115/115	-
25	BCR	T	102	-	-	1/29/63/63	0/2/2/2
23	CLA	d	403[A]	4	-	2/39/115/115	-
23	CLA	b	614	2	-	15/39/115/115	-
27	GOL	C	523[B]	-	-	0/4/4/4	-
33	LMG	C	501	-	-	13/46/66/70	0/1/1/1
23	CLA	B	608	2	-	4/39/115/115	-
27	GOL	A	411	-	-	2/4/4/4	-
35	DGD	H	102	-	-	9/51/91/95	0/2/2/2
23	CLA	b	601	41	-	19/39/115/115	-
31	LMT	T	101	-	-	10/21/61/61	0/2/2/2
31	LMT	B	630	-	-	12/21/61/61	0/2/2/2
34	HTG	D	410	-	-	3/7/27/30	0/1/1/1
23	CLA	B	601	41	-	13/39/115/115	-
23	CLA	C	503	3	-	10/39/115/115	-
23	CLA	b	611	2	-	2/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LHG	b	629[A]	-	-	20/53/53/53	-
33	LMG	C	521	-	-	13/46/66/70	0/1/1/1
26	SQD	a	410	-	-	14/49/69/69	0/1/1/1
25	BCR	Y	101	-	-	6/29/63/63	0/2/2/2
23	CLA	B	603	2	-	8/39/115/115	-
27	GOL	v	202[A]	-	-	1/4/4/4	-
27	GOL	D	412	-	-	4/4/4/4	-
26	SQD	a	409[B]	-	-	9/49/69/69	0/1/1/1
32	LHG	d	414[B]	-	-	12/53/53/53	-
23	CLA	b	603	2	-	4/39/115/115	-
27	GOL	C	523[A]	-	-	0/4/4/4	-
35	DGD	c	516[B]	-	-	21/51/91/95	0/2/2/2
27	GOL	c	525[A]	-	-	0/4/4/4	-
27	GOL	c	526	-	-	4/4/4/4	-
31	LMT	e	101	-	-	15/21/61/61	0/2/2/2
35	DGD	C	518[A]	-	-	15/51/91/95	0/2/2/2
25	BCR	C	515	-	-	2/29/63/63	0/2/2/2
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
34	HTG	B	623	-	-	4/10/30/30	0/1/1/1
29	PL9	d	406[A]	-	-	6/53/73/73	0/1/1/1
23	CLA	d	402[B]	41	-	6/39/115/115	-
24	PHO	A	416[B]	-	-	3/37/103/103	0/5/6/6
35	DGD	h	102	-	-	16/51/91/95	0/2/2/2
23	CLA	B	615	2	-	8/39/115/115	-
34	HTG	b	625	-	-	3/10/30/30	0/1/1/1
32	LHG	D	406[A]	-	-	16/53/53/53	-
27	GOL	d	413	-	-	3/4/4/4	-
23	CLA	C	502	3	-	5/39/115/115	-
34	HTG	b	622	-	-	5/10/30/30	0/1/1/1
32	LHG	d	407[B]	-	-	11/53/53/53	-
23	CLA	B	610	41	-	8/39/115/115	-
32	LHG	d	414[A]	-	-	13/53/53/53	-
31	LMT	a	416	-	-	10/21/61/61	0/2/2/2
23	CLA	A	406[B]	41	-	6/39/115/115	-
23	CLA	C	514	3	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	y	101	-	-	6/29/63/63	0/2/2/2
23	CLA	c	504	41	-	6/39/115/115	-
23	CLA	D	402[B]	4	-	2/39/115/115	-
27	GOL	V	203[B]	-	-	2/4/4/4	-
35	DGD	c	517[B]	-	-	17/51/91/95	0/2/2/2
23	CLA	D	403	4	-	14/39/115/115	-
23	CLA	C	511	3	-	12/39/115/115	-
23	CLA	b	607	41	-	3/39/115/115	-
23	CLA	B	605	2	-	6/39/115/115	-
23	CLA	A	405[B]	41	-	5/39/115/115	-
23	CLA	d	402[A]	41	-	8/39/115/115	-
27	GOL	o	302	-	-	2/4/4/4	-
27	GOL	a	417	-	-	2/4/4/4	-
31	LMT	m	103	-	-	4/21/61/61	0/2/2/2
25	BCR	t	102	-	-	1/29/63/63	0/2/2/2
32	LHG	A	419[A]	-	-	10/53/53/53	-
23	CLA	B	602	2	-	9/39/115/115	-
23	CLA	B	604	2	-	4/39/115/115	-
23	CLA	a	404[A]	1	-	3/39/115/115	-
27	GOL	O	303	-	-	2/4/4/4	-
29	PL9	D	405[A]	-	-	8/53/73/73	0/1/1/1
31	LMT	t	101	-	-	8/17/38/61	0/1/1/2
24	PHO	A	407[B]	-	-	2/37/103/103	0/5/6/6
33	LMG	C	520	-	-	9/46/66/70	0/1/1/1
23	CLA	c	509	3	-	14/39/115/115	-
35	DGD	C	517[B]	-	-	14/51/91/95	0/2/2/2
23	CLA	A	404[B]	1	-	4/39/115/115	-
23	CLA	C	504	3	-	2/39/115/115	-
23	CLA	C	506	3	-	7/39/115/115	-
27	GOL	B	624	-	-	2/4/4/4	-
31	LMT	F	101	-	-	8/21/61/61	0/2/2/2
23	CLA	B	614	2	-	14/39/115/115	-
32	LHG	L	101[A]	-	-	19/53/53/53	-
23	CLA	c	507	41	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PL9	A	414[B]	-	-	18/53/73/73	0/1/1/1
40	HEC	V	201	16	1/1/3/7	6/14/54/54	-
32	LHG	a	419[A]	-	-	16/46/46/53	-
32	LHG	d	407[A]	-	-	13/53/53/53	-
27	GOL	l	801[B]	-	-	3/4/4/4	-
31	LMT	B	628	-	-	12/21/61/61	0/2/2/2
32	LHG	d	408[B]	-	-	13/53/53/53	-
23	CLA	b	606	2	-	13/39/115/115	-
23	CLA	B	613	2	-	8/39/115/115	-
23	CLA	C	508	41	-	6/39/115/115	-
23	CLA	A	406[A]	41	-	7/39/115/115	-
23	CLA	b	616	2	-	9/39/115/115	-
34	HTG	d	411	-	-	1/7/27/30	0/1/1/1
35	DGD	c	517[A]	-	-	17/51/91/95	0/2/2/2
23	CLA	D	402[A]	4	-	0/39/115/115	-
23	CLA	b	612	2	-	3/39/115/115	-
26	SQD	A	410[B]	-	-	10/49/69/69	0/1/1/1
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2
23	CLA	C	509	3	-	3/39/115/115	-

The worst 5 of 1868 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	406[B]	PHO	C1B-C2B	9.19	1.49	1.39
24	A	407[A]	PHO	C1D-C2D	9.11	1.49	1.39
24	A	407[B]	PHO	C1D-C2D	9.08	1.49	1.39
24	a	414[B]	PHO	C1D-C2D	9.07	1.49	1.39
24	a	406[A]	PHO	C1B-C2B	8.96	1.49	1.39

The worst 5 of 3338 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	C2B-C1B-NB	17.33	121.85	110.23
23	B	611	CLA	C3B-C2B-C1B	-13.61	90.73	107.16
24	a	414[A]	PHO	C2D-C1D-ND	11.91	117.75	109.53
24	A	407[B]	PHO	C2D-C1D-ND	11.73	117.62	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 1666 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	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	C	507	CLA	C14-C13-C15-C16

There are no ring outliers.

175 monomers are involved in 370 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	B	622	HTG	2	0
23	b	613	CLA	2	0
23	c	502	CLA	2	0
26	F	102	SQD	2	0
33	B	621	LMG	1	0
23	b	615	CLA	2	0
23	B	609	CLA	3	0
33	z	101	LMG	2	0
24	a	406[B]	PHO	1	0
26	a	409[A]	SQD	4	0
32	D	407[B]	LHG	3	0
23	C	512	CLA	3	0
23	b	602	CLA	1	0
23	c	505	CLA	5	0
23	d	404	CLA	3	0
25	B	618	BCR	4	0
27	O	302	GOL	1	0
27	B	627	GOL	1	0
29	a	412[B]	PL9	5	0
35	c	516[A]	DGD	2	0
23	b	605	CLA	6	0
32	d	408[A]	LHG	10	0
33	d	412	LMG	3	0
33	c	519	LMG	1	0
23	C	513	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	c	503	CLA	3	0
23	A	408	CLA	4	0
23	a	405[B]	CLA	2	0
23	c	511	CLA	6	0
33	Z	101	LMG	1	0
24	A	416[A]	PHO	1	0
26	b	620	SQD	4	0
34	c	521	HTG	1	0
23	c	501	CLA	2	0
31	A	420	LMT	1	0
31	M	101	LMT	1	0
23	B	606	CLA	4	0
31	A	417	LMT	1	0
23	C	510	CLA	3	0
25	c	514	BCR	3	0
25	h	101	BCR	4	0
25	D	404	BCR	1	0
25	b	618	BCR	3	0
32	E	101[B]	LHG	4	0
26	B	620	SQD	2	0
23	a	407	CLA	4	0
24	a	414[B]	PHO	1	0
23	c	508	CLA	8	0
27	a	418	GOL	3	0
25	H	101	BCR	3	0
23	B	616	CLA	4	0
35	c	518	DGD	3	0
23	A	405[A]	CLA	4	0
23	B	612	CLA	2	0
31	B	631	LMT	1	0
23	C	505	CLA	1	0
23	b	604	CLA	2	0
24	A	407[A]	PHO	2	0
25	C	516	BCR	1	0
27	b	628	GOL	2	0
35	C	517[A]	DGD	2	0
23	A	404[A]	CLA	5	0
25	b	619	BCR	5	0
25	B	619	BCR	1	0
31	b	621	LMT	1	0
25	B	617	BCR	2	0
29	A	414[A]	PL9	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	D	406[B]	LHG	2	0
23	c	513	CLA	2	0
27	l	801[A]	GOL	1	0
32	E	101[A]	LHG	4	0
24	a	414[A]	PHO	2	0
33	c	520	LMG	1	0
26	A	410[A]	SQD	2	0
25	K	102	BCR	1	0
23	C	507	CLA	5	0
23	d	403[B]	CLA	2	0
23	b	609	CLA	5	0
23	c	506	CLA	3	0
32	A	419[B]	LHG	1	0
23	a	404[B]	CLA	3	0
25	c	515	BCR	2	0
32	b	629[B]	LHG	1	0
27	A	418	GOL	2	0
32	D	407[A]	LHG	6	0
25	b	617	BCR	1	0
27	v	202[B]	GOL	2	0
29	a	412[A]	PL9	4	0
38	E	102	HEM	1	0
34	B	625	HTG	1	0
32	a	419[B]	LHG	5	0
35	C	519	DGD	2	0
23	a	405[A]	CLA	2	0
23	c	512	CLA	7	0
25	T	102	BCR	7	0
23	d	403[A]	CLA	2	0
23	b	614	CLA	1	0
35	H	102	DGD	2	0
23	b	601	CLA	2	0
31	T	101	LMT	1	0
31	B	630	LMT	1	0
34	D	410	HTG	1	0
23	B	601	CLA	5	0
23	C	503	CLA	2	0
23	b	611	CLA	1	0
33	C	521	LMG	4	0
26	a	410	SQD	2	0
25	Y	101	BCR	2	0
27	v	202[A]	GOL	1	0

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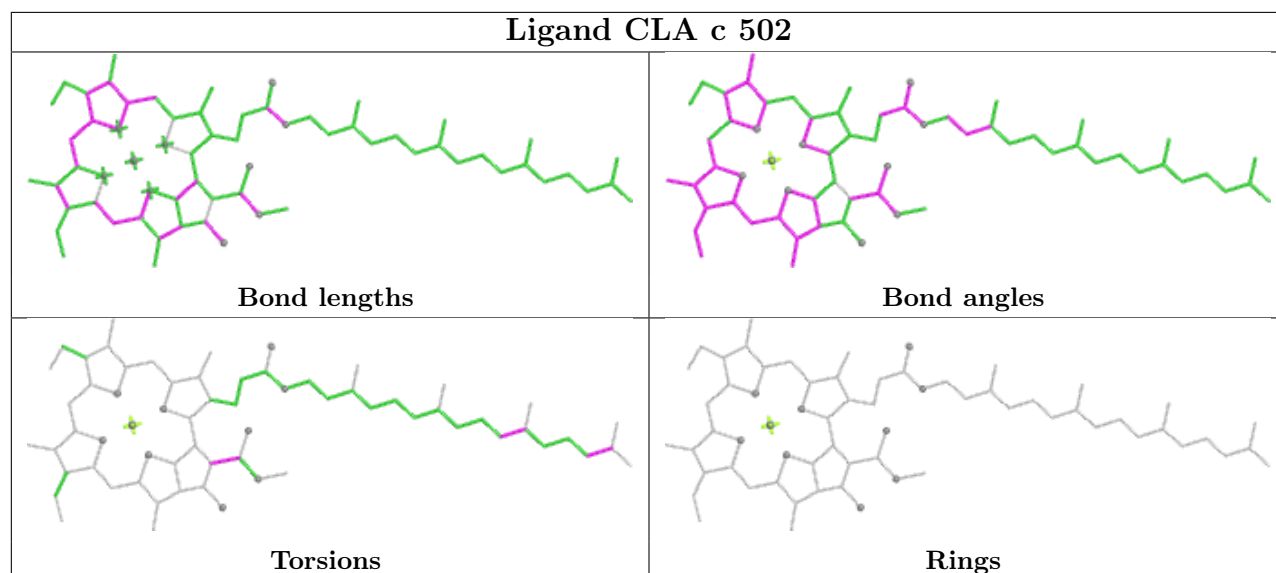
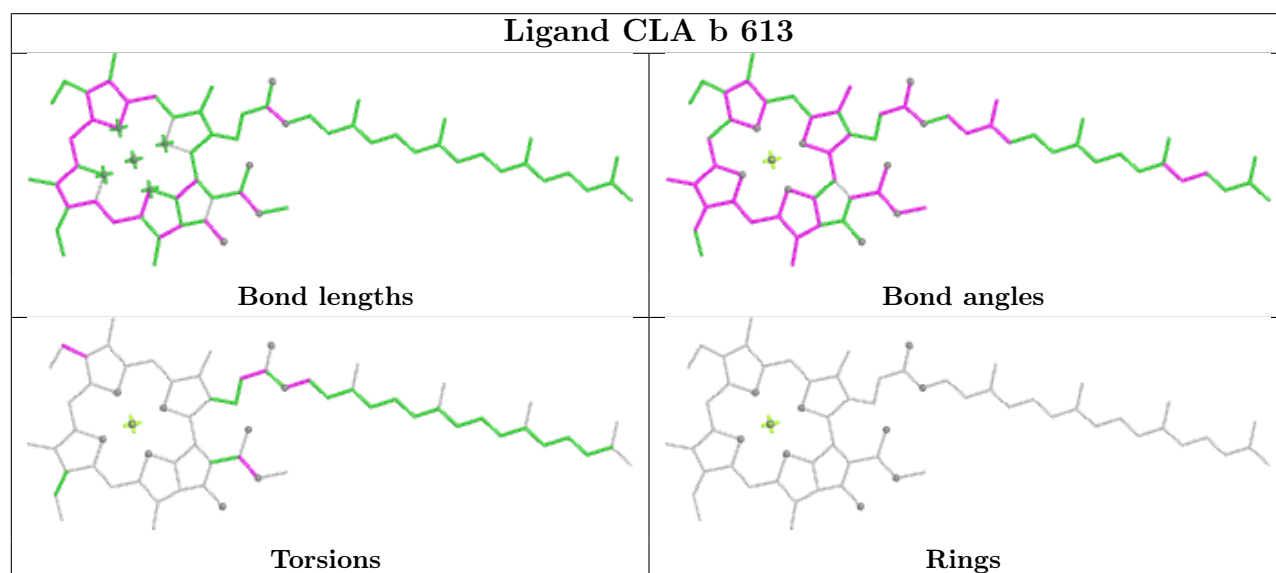
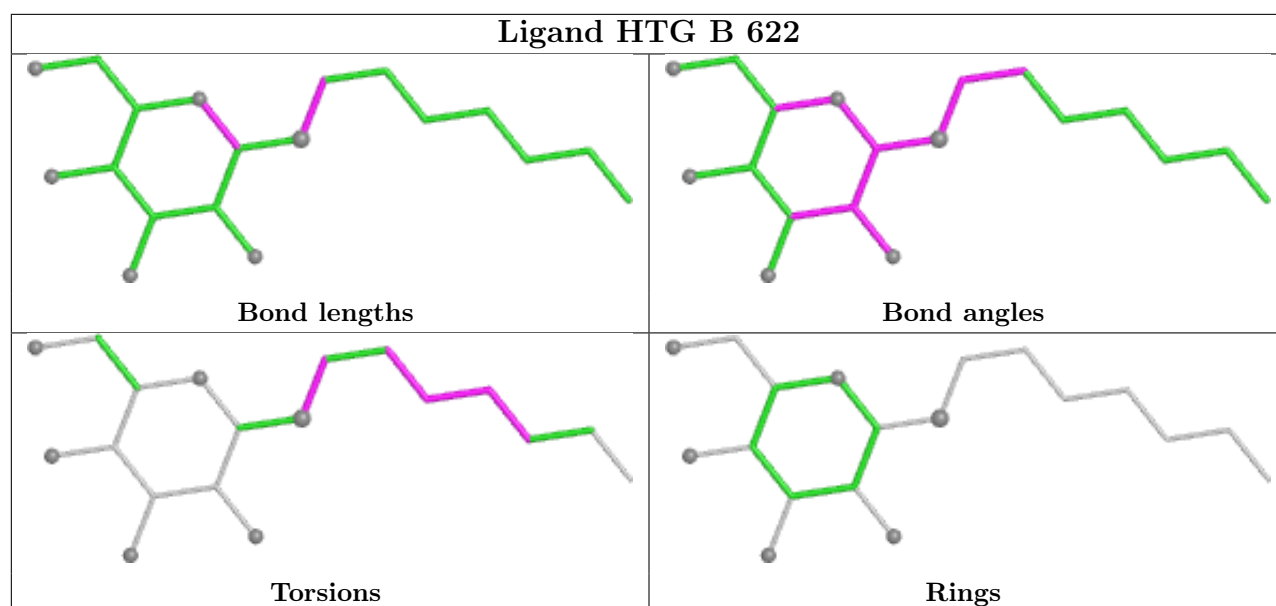
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	D	412	GOL	2	0
26	a	409[B]	SQD	5	0
32	d	414[B]	LHG	1	0
23	b	603	CLA	1	0
35	c	516[B]	DGD	2	0
31	e	101	LMT	1	0
35	C	518[A]	DGD	2	0
25	C	515	BCR	2	0
25	A	409	BCR	2	0
34	B	623	HTG	1	0
23	d	402[B]	CLA	2	0
24	A	416[B]	PHO	1	0
23	B	615	CLA	4	0
34	b	625	HTG	1	0
32	D	406[A]	LHG	2	0
23	C	502	CLA	5	0
34	b	622	HTG	2	0
32	d	407[B]	LHG	2	0
23	B	610	CLA	1	0
32	d	414[A]	LHG	1	0
31	a	416	LMT	1	0
23	A	406[B]	CLA	2	0
23	C	514	CLA	3	0
25	y	101	BCR	2	0
23	c	504	CLA	2	0
23	D	402[B]	CLA	4	0
35	c	517[B]	DGD	1	0
23	C	511	CLA	4	0
23	b	607	CLA	2	0
23	B	605	CLA	3	0
23	A	405[B]	CLA	4	0
23	d	402[A]	CLA	2	0
27	a	417	GOL	2	0
31	m	103	LMT	2	0
25	t	102	BCR	5	0
32	A	419[A]	LHG	1	0
23	B	604	CLA	1	0
23	a	404[A]	CLA	3	0
27	O	303	GOL	3	0
31	t	101	LMT	2	0
24	A	407[B]	PHO	1	0
23	c	509	CLA	3	0

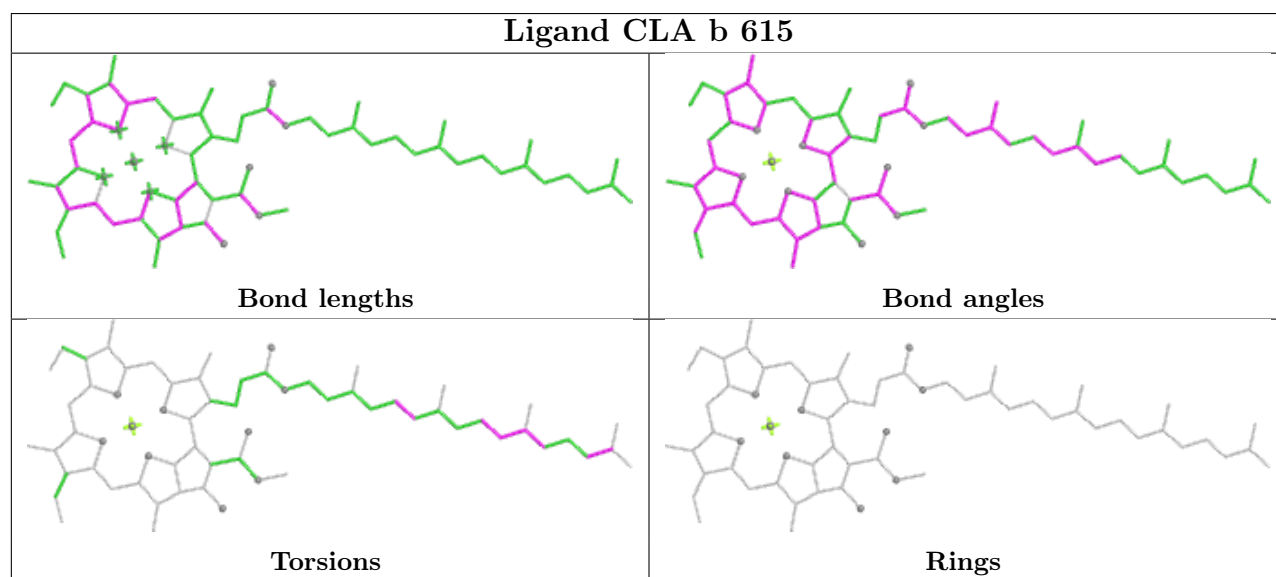
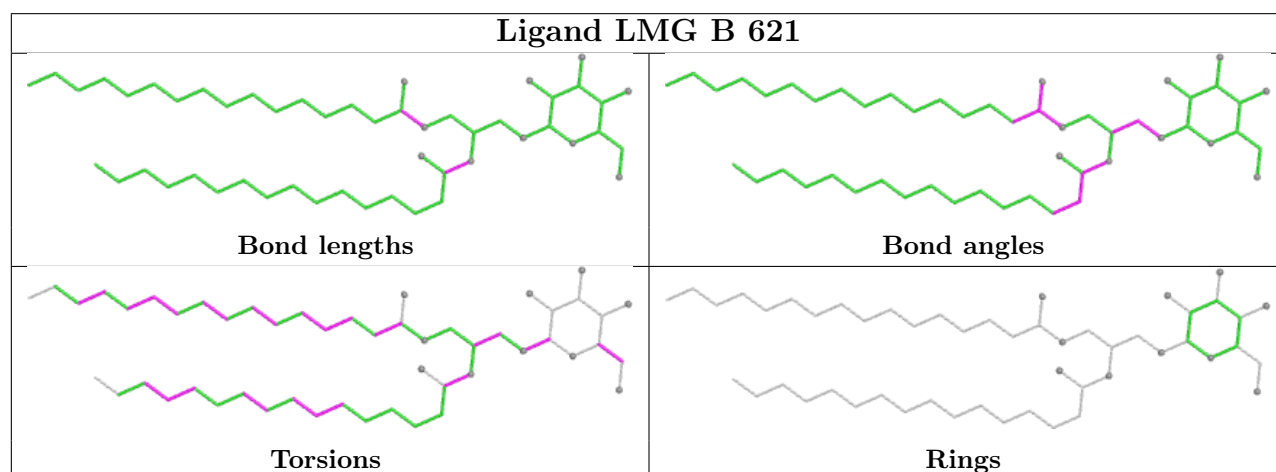
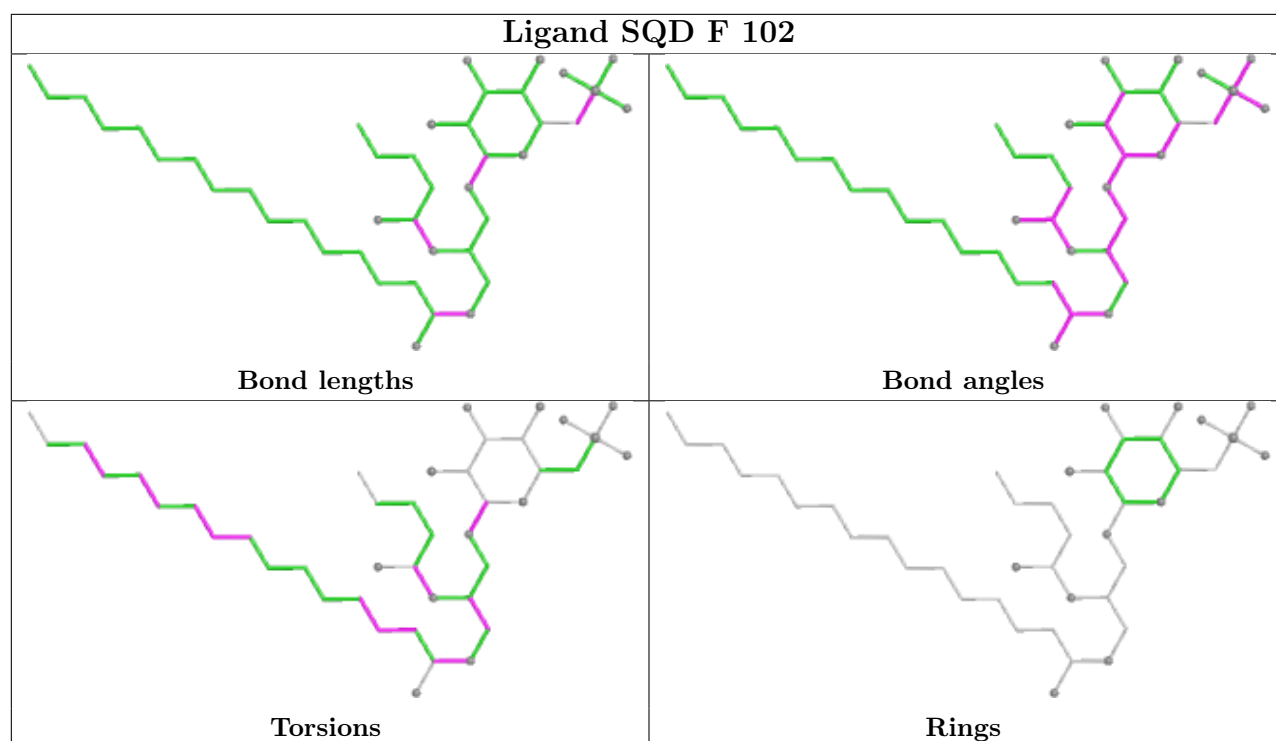
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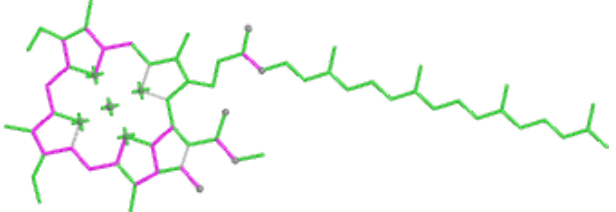
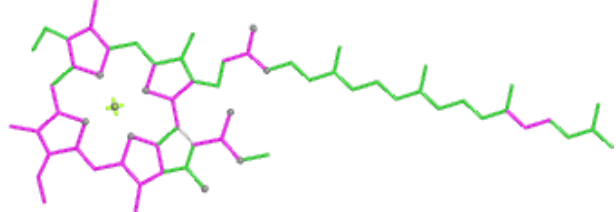
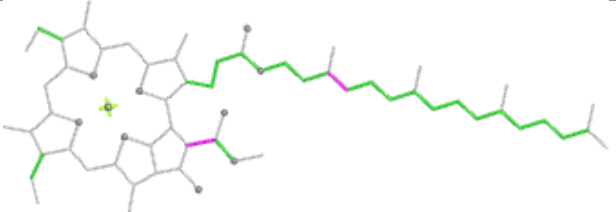
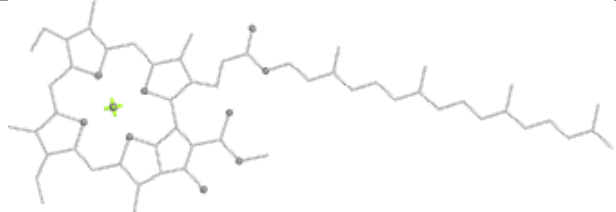
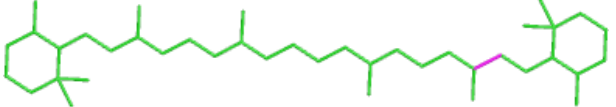
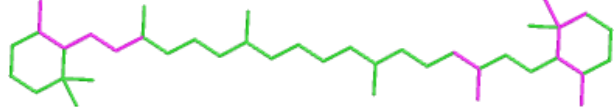
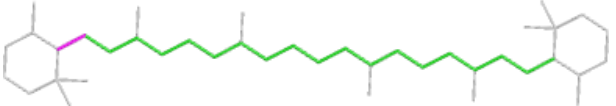
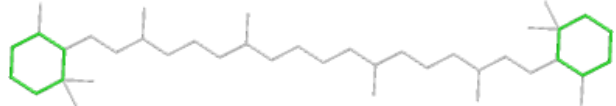
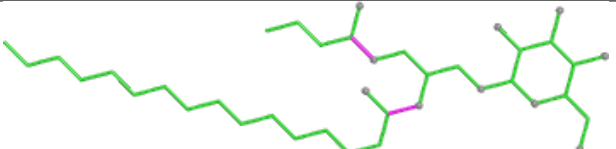
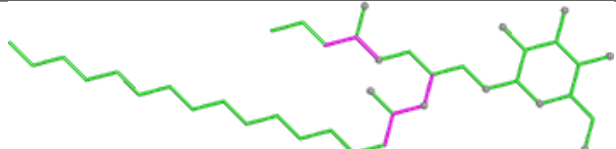
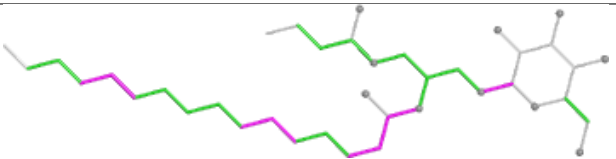
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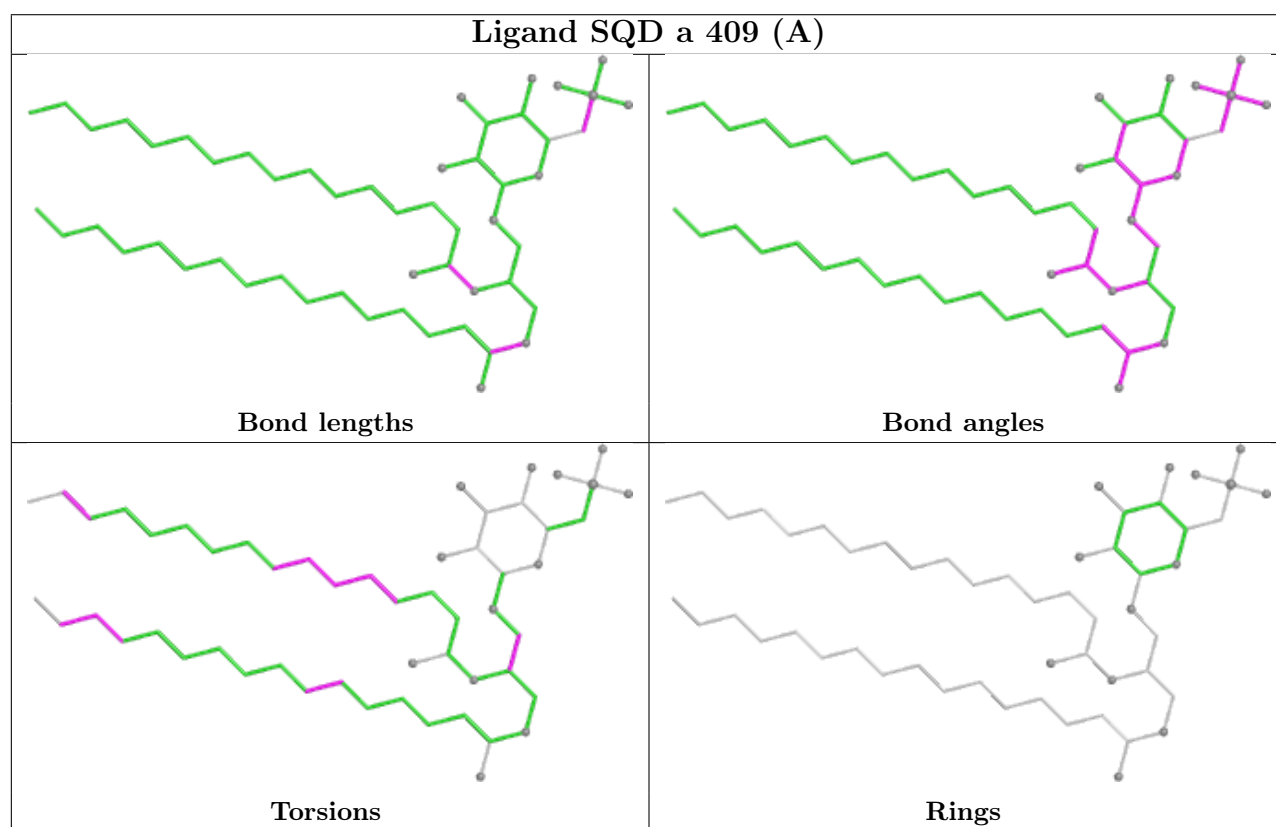
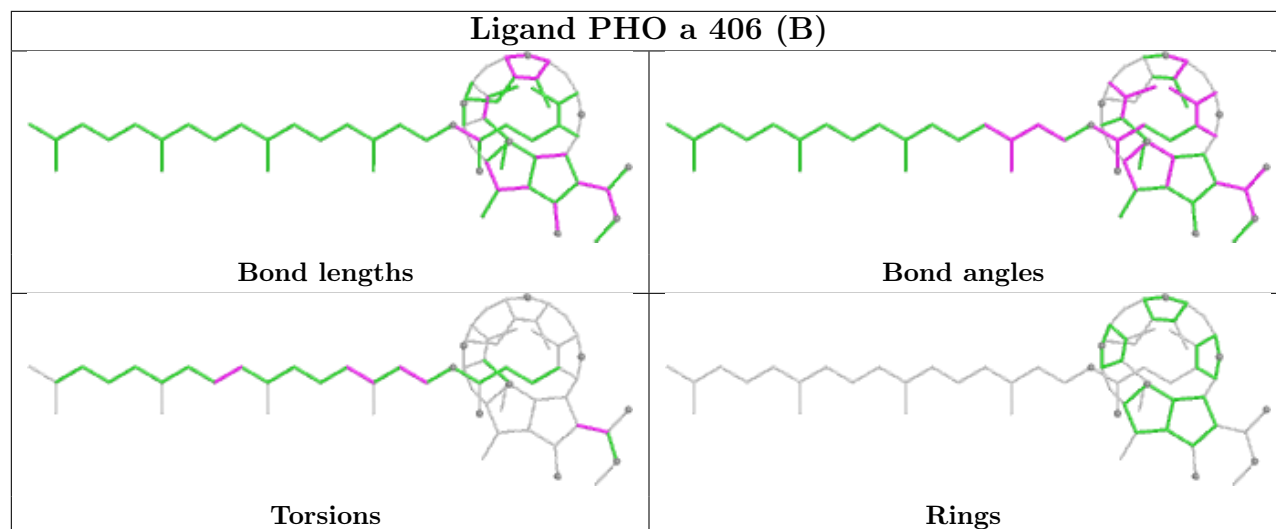
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	C	517[B]	DGD	1	0
23	A	404[B]	CLA	2	0
23	C	504	CLA	4	0
23	C	506	CLA	5	0
23	B	614	CLA	2	0
23	c	507	CLA	2	0
29	A	414[B]	PL9	11	0
32	a	419[A]	LHG	4	0
32	d	407[A]	LHG	3	0
40	V	201	HEC	1	0
27	l	801[B]	GOL	1	0
32	d	408[B]	LHG	9	0
23	b	606	CLA	1	0
23	B	613	CLA	4	0
23	C	508	CLA	2	0
23	A	406[A]	CLA	1	0
23	b	616	CLA	1	0
34	d	411	HTG	1	0
35	c	517[A]	DGD	1	0
23	D	402[A]	CLA	3	0
23	b	612	CLA	2	0
26	A	410[B]	SQD	2	0
25	k	101	BCR	2	0
23	C	509	CLA	3	0

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

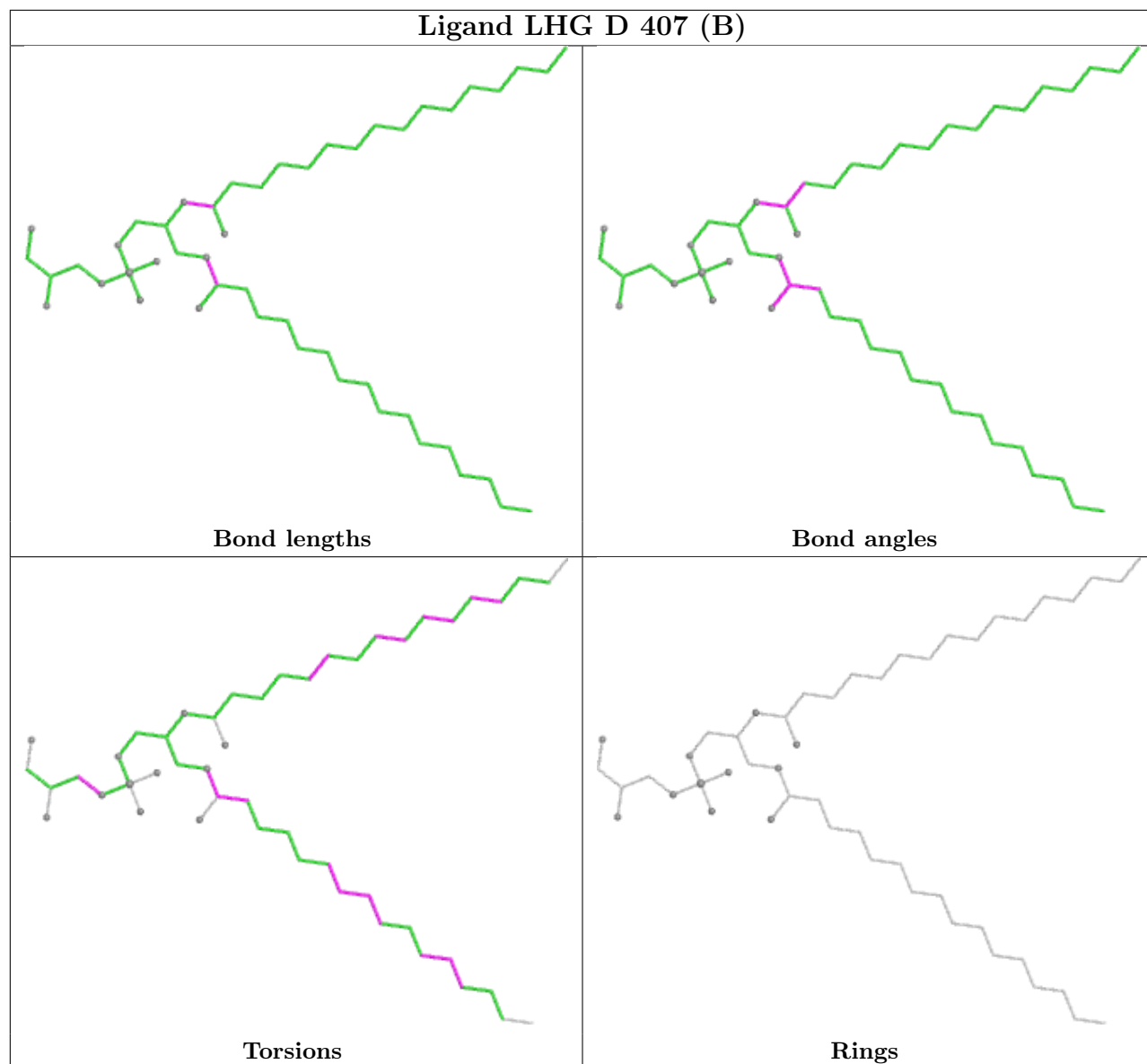




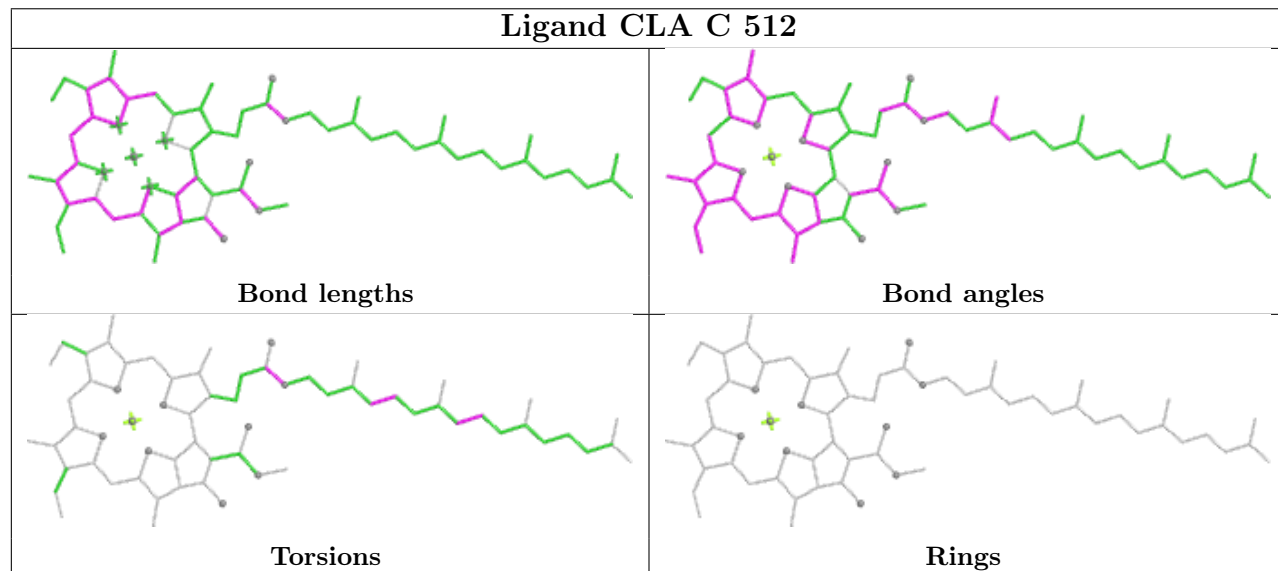
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 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR a 408	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG z 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

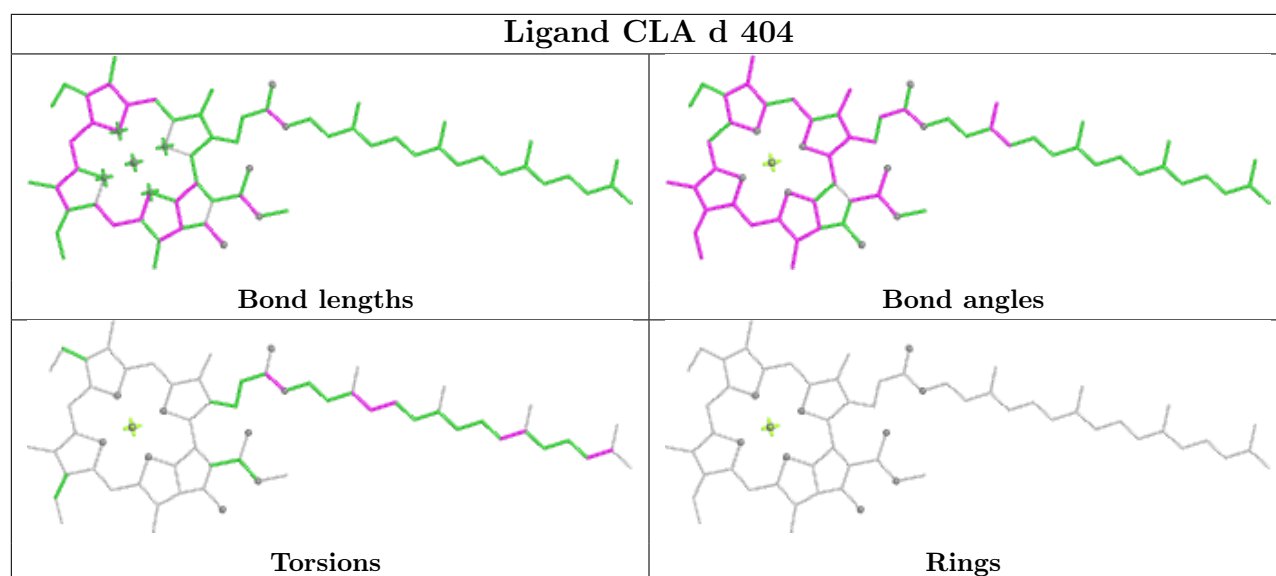
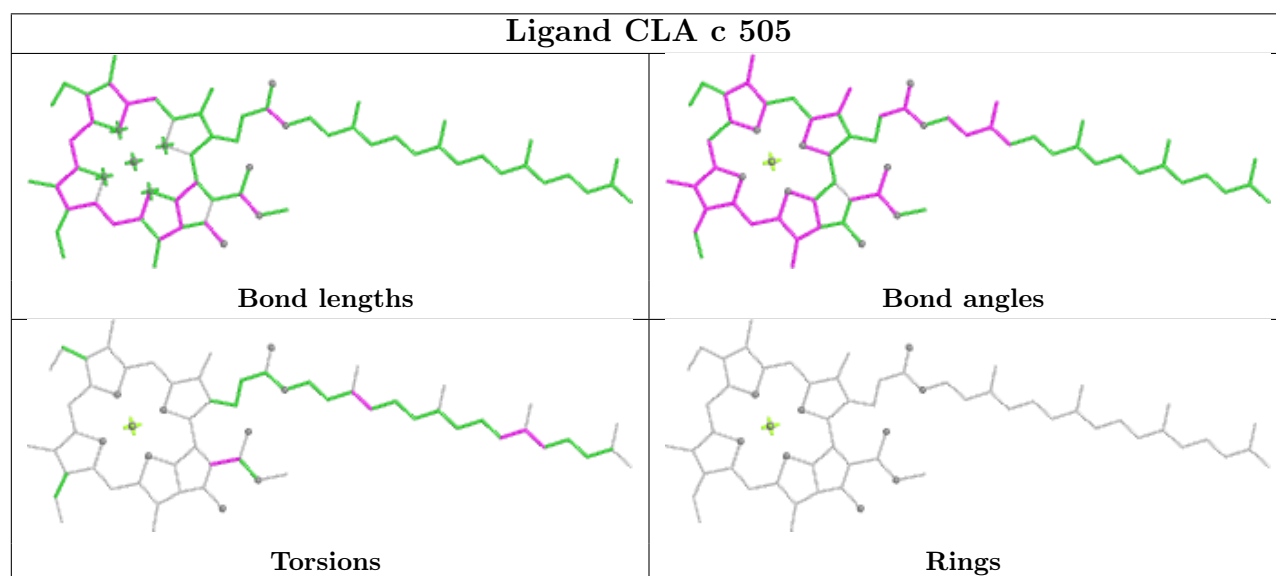
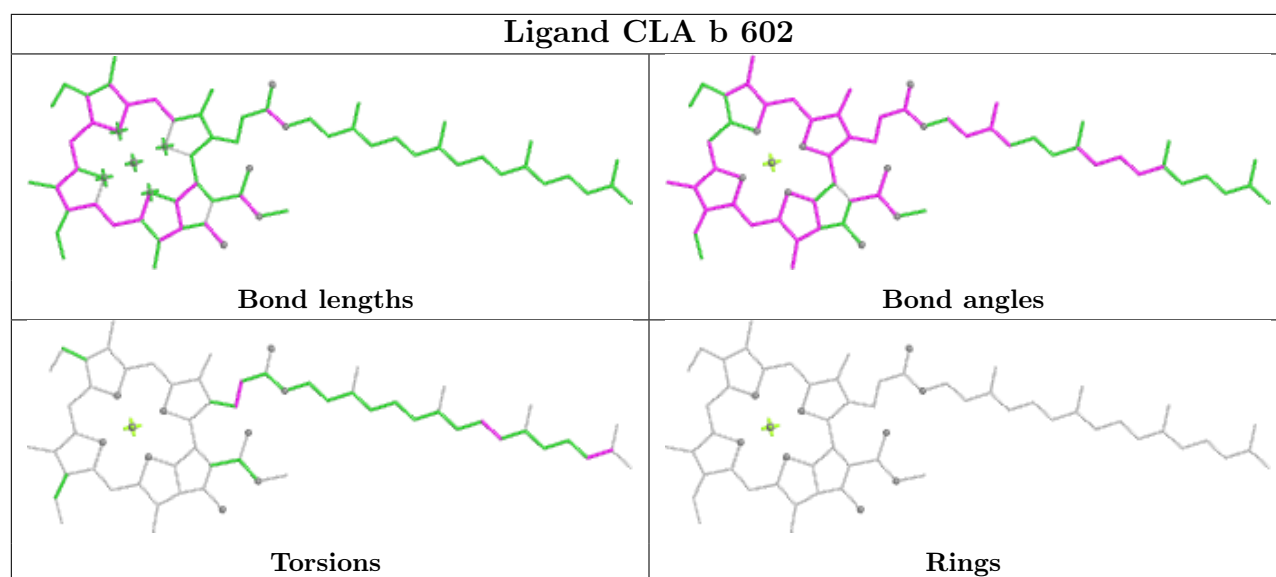


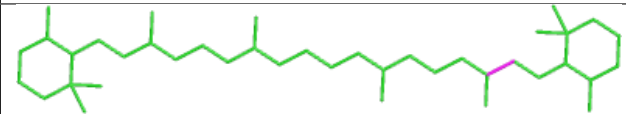
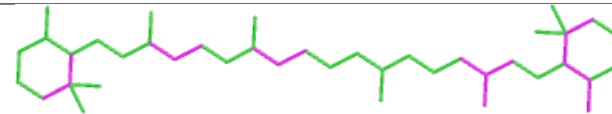
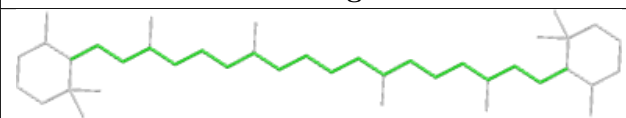
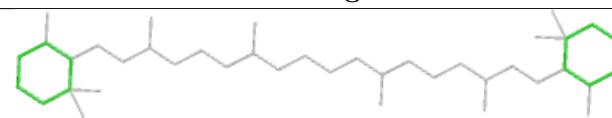
Ligand LHG D 407 (B)

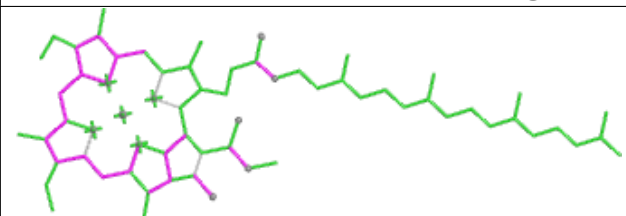
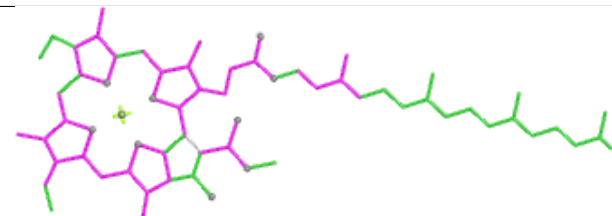
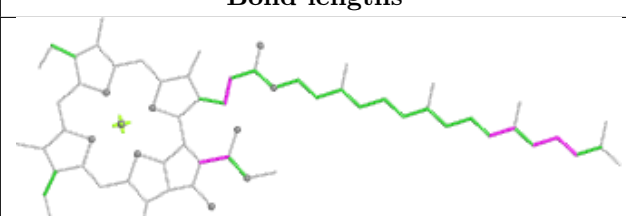
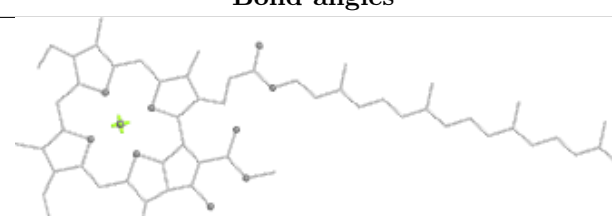


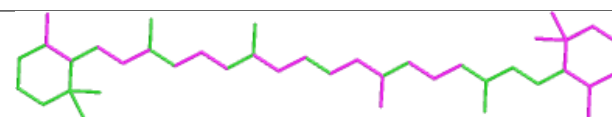
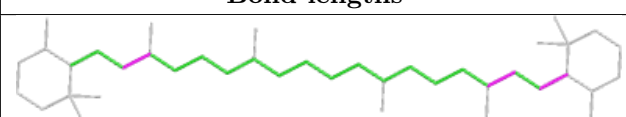
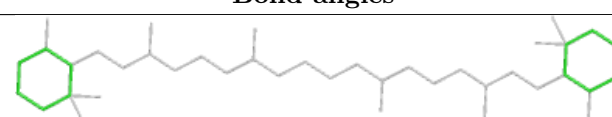
Ligand CLA C 512

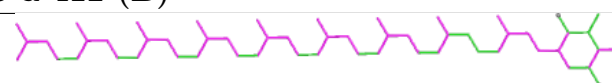
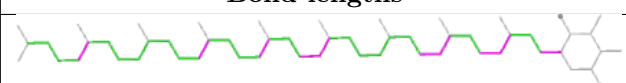
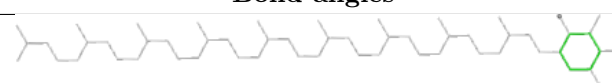


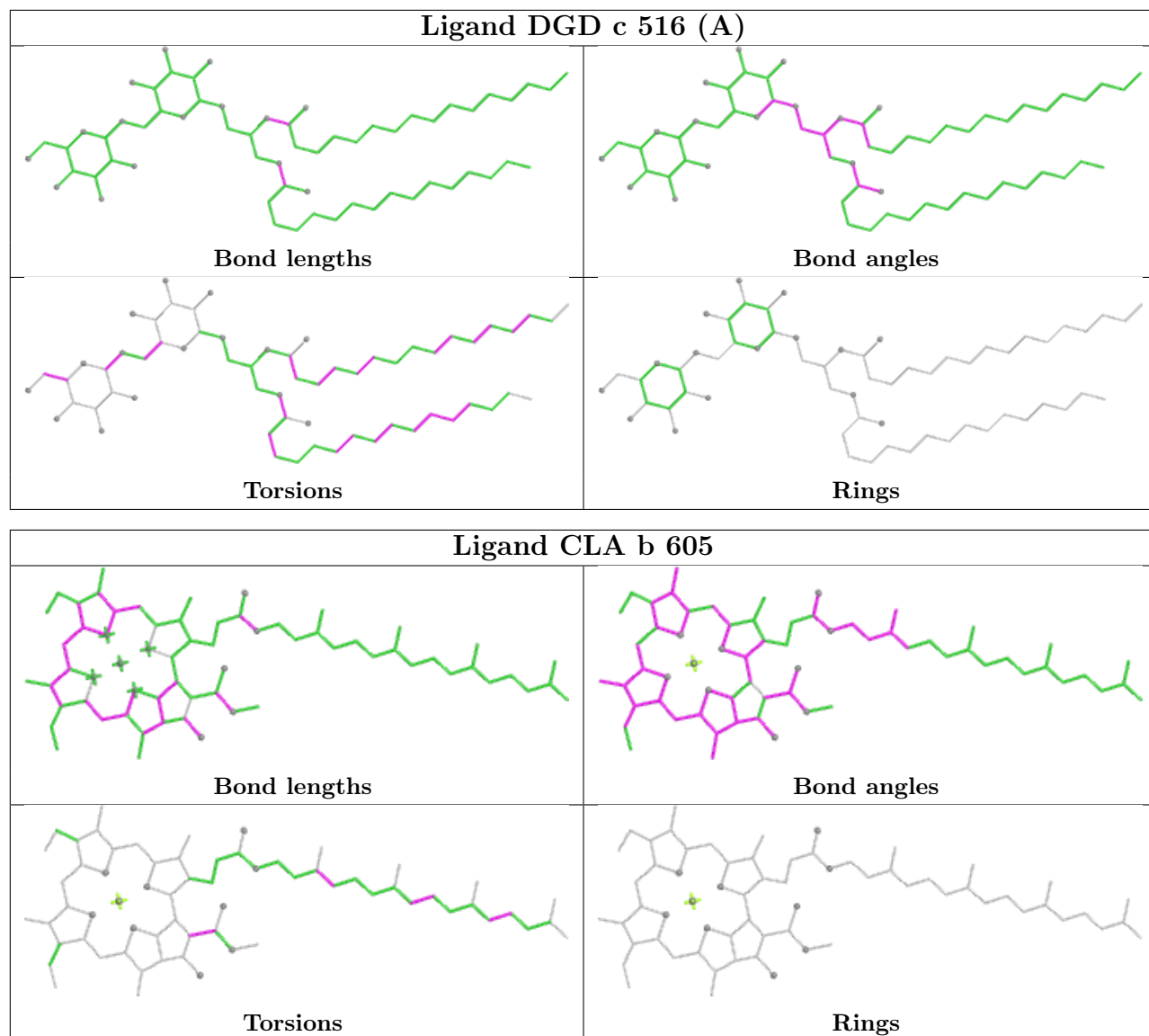


Ligand BCR B 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

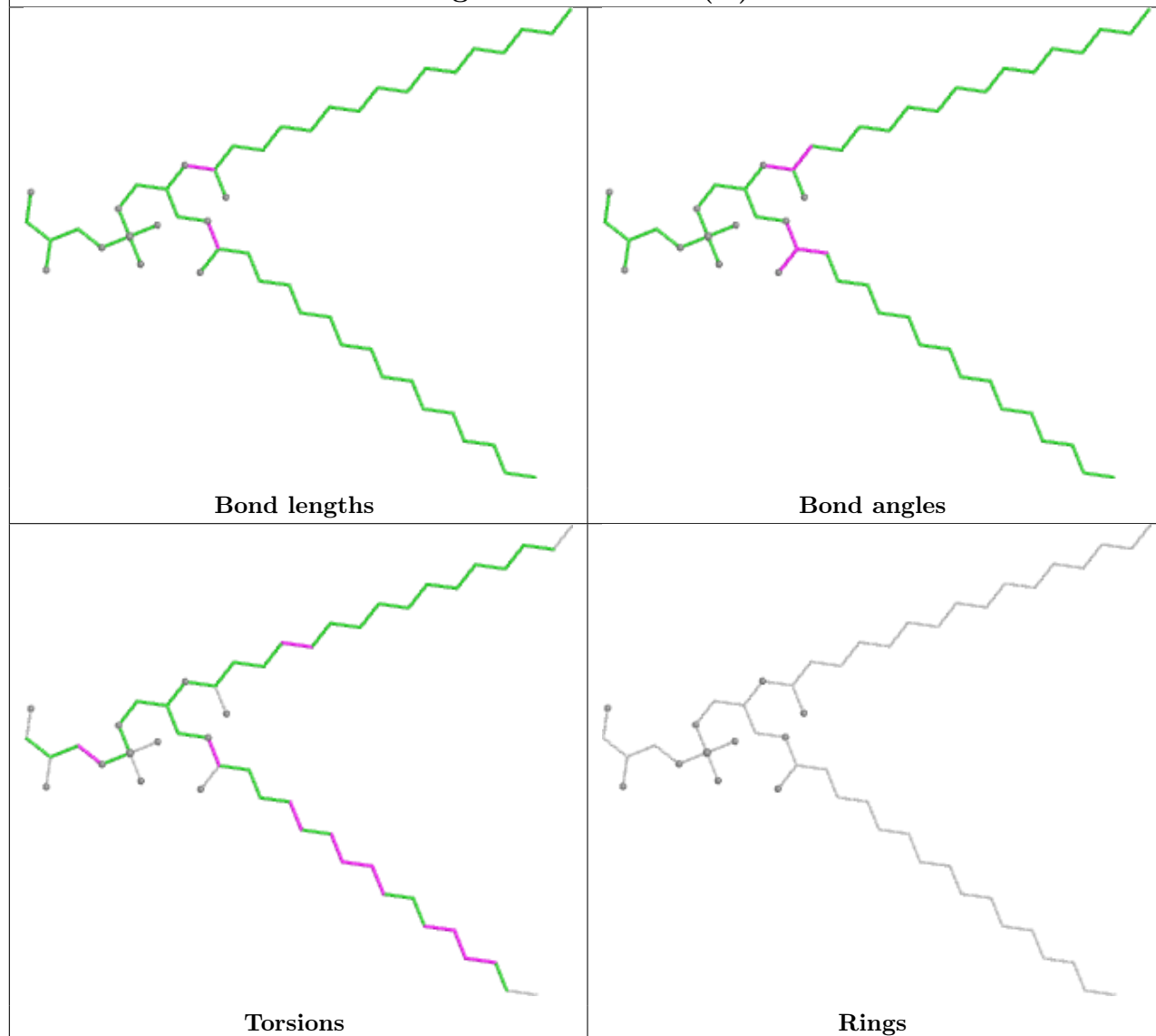
Ligand CLA b 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR d 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

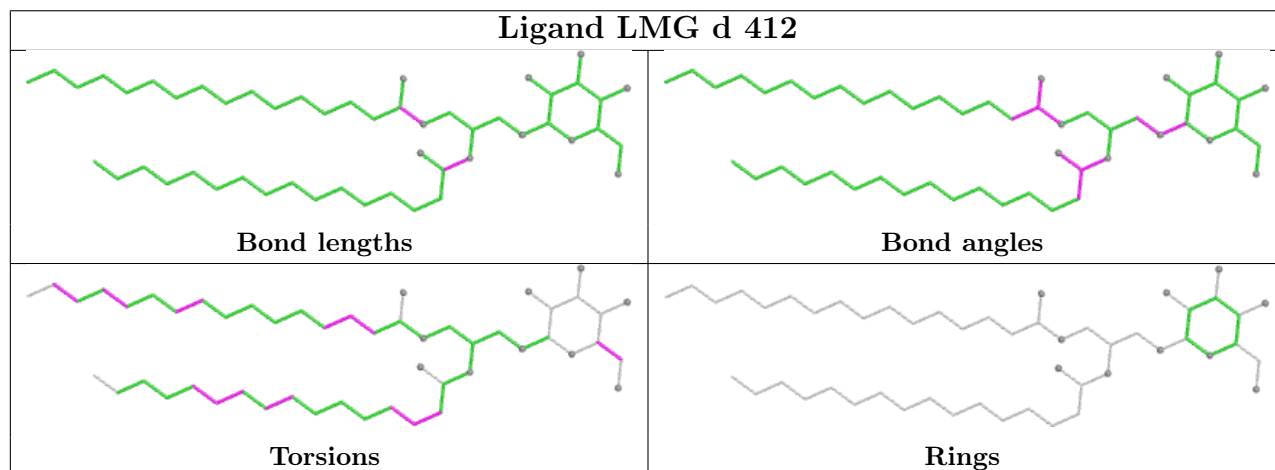
Ligand PL9 a 412 (B)	
	
Bond lengths	Bond angles
	
Torsions	Rings

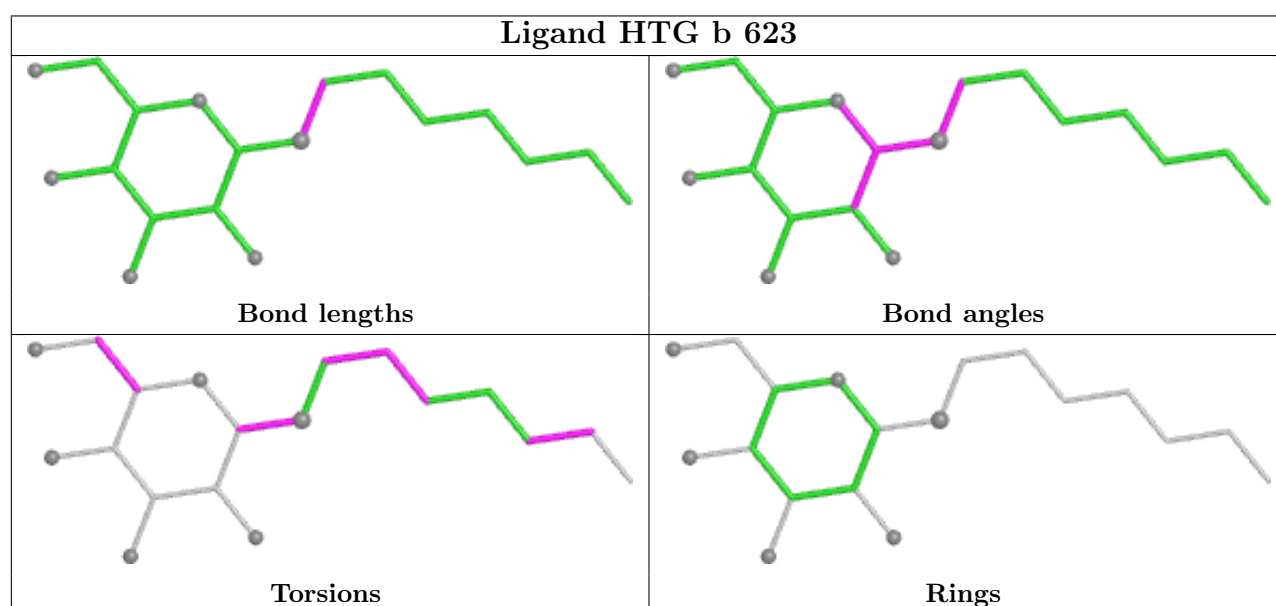
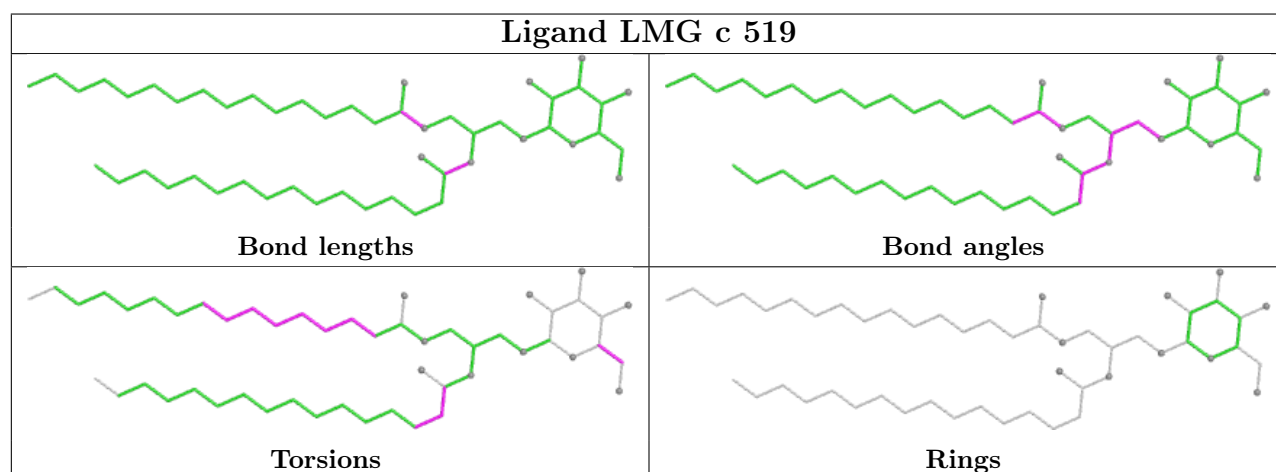
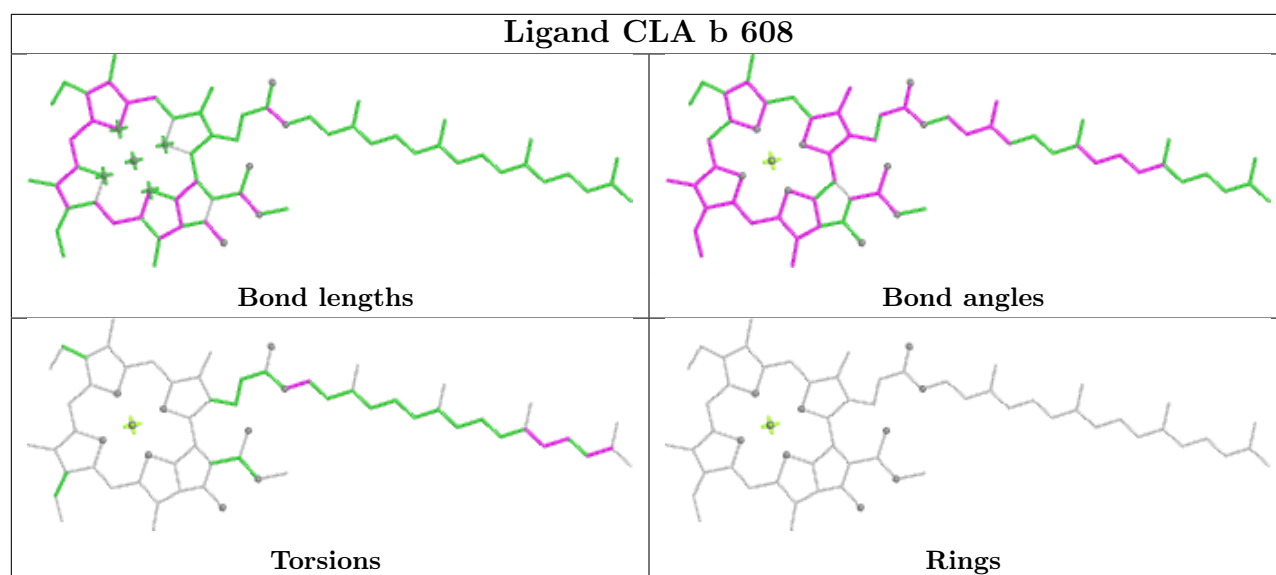


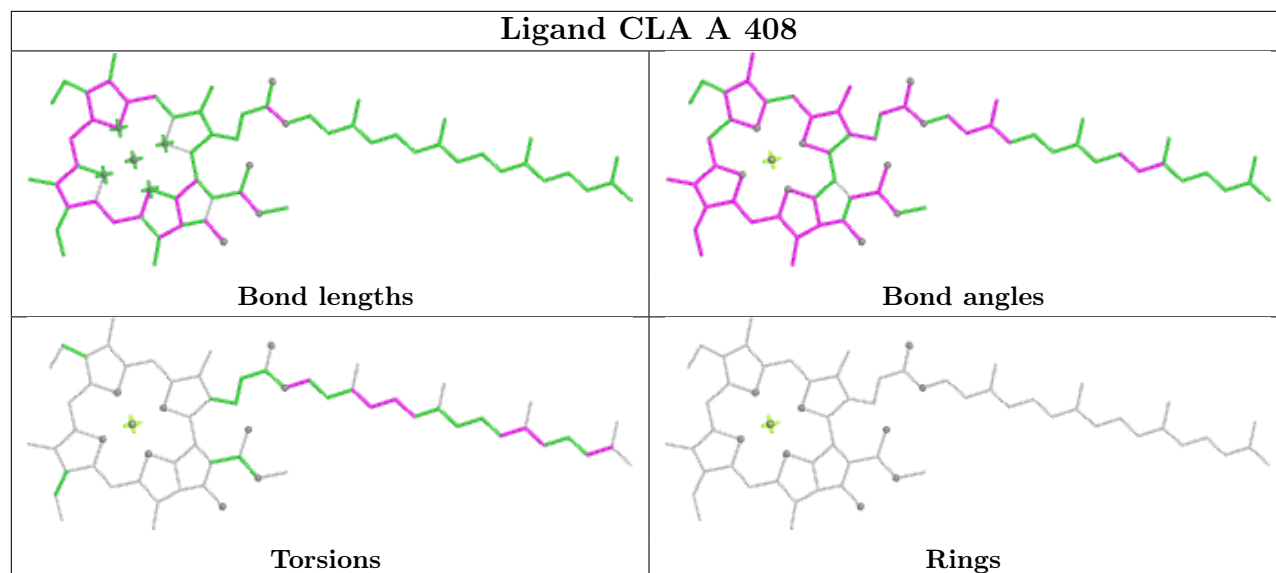
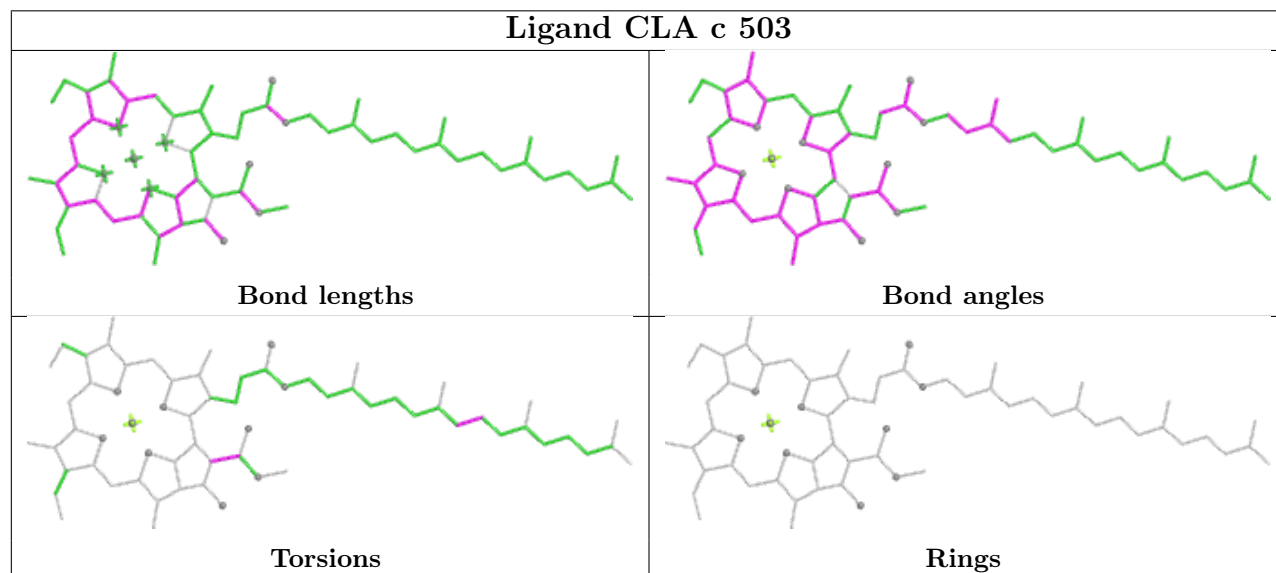
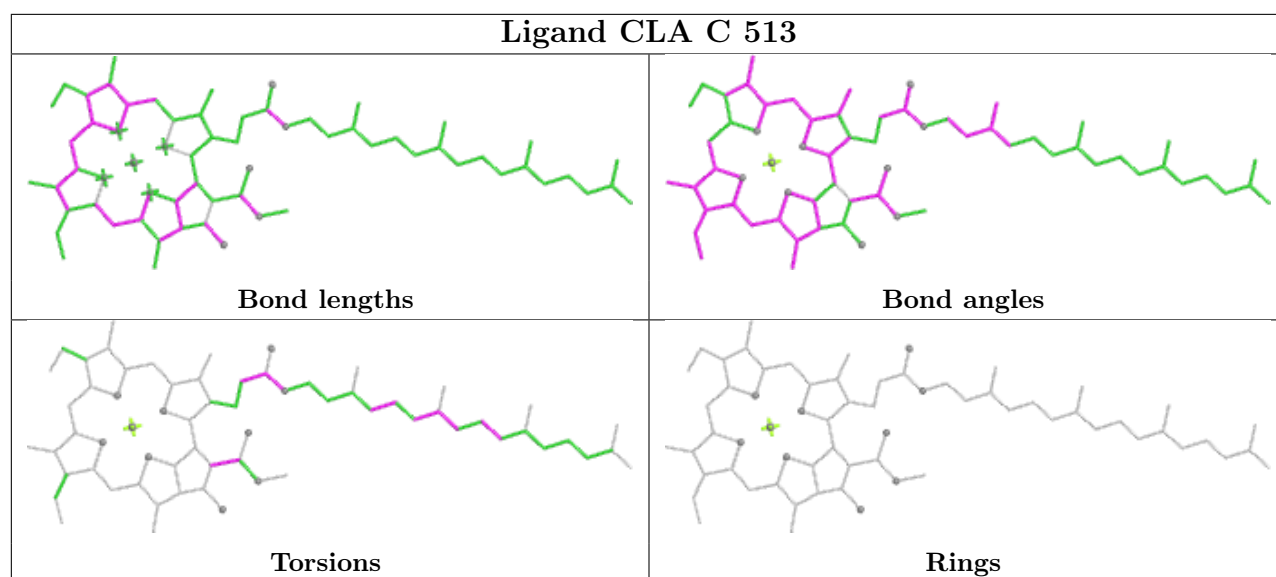
Ligand LHG d 408 (A)

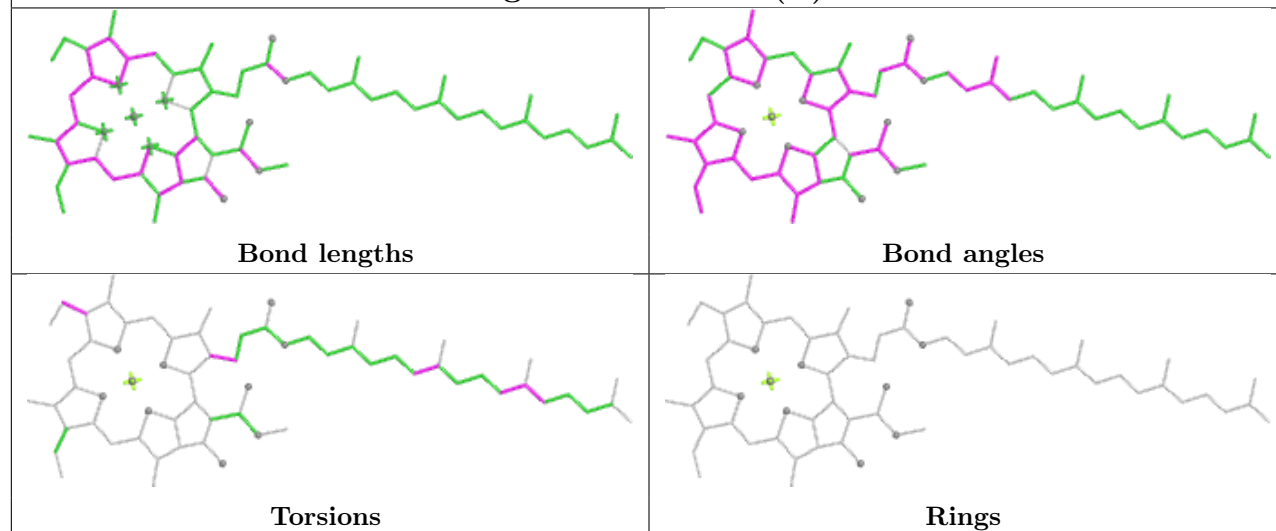
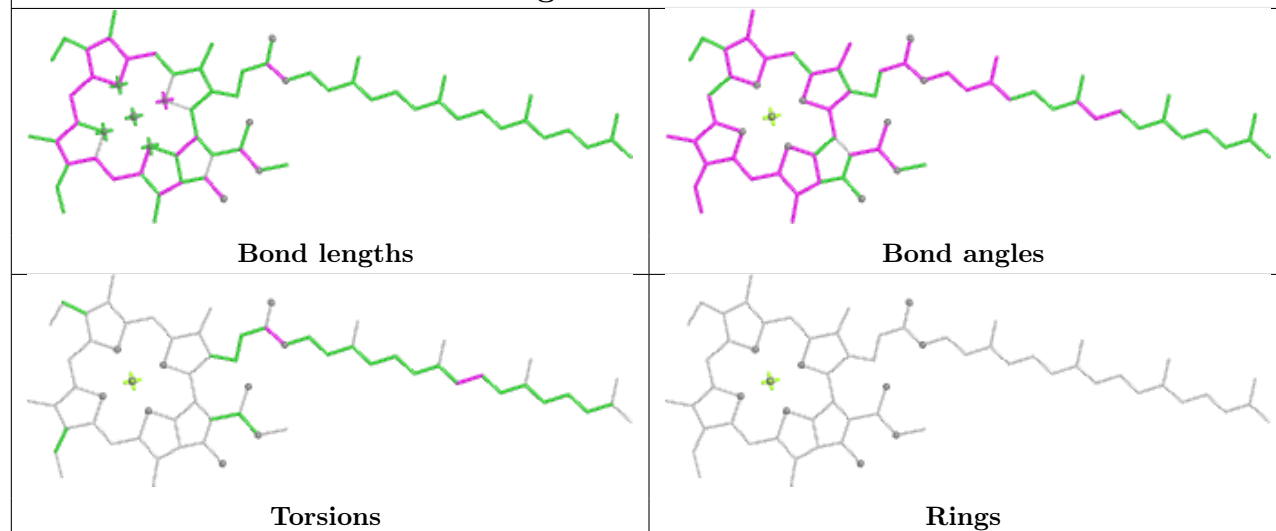
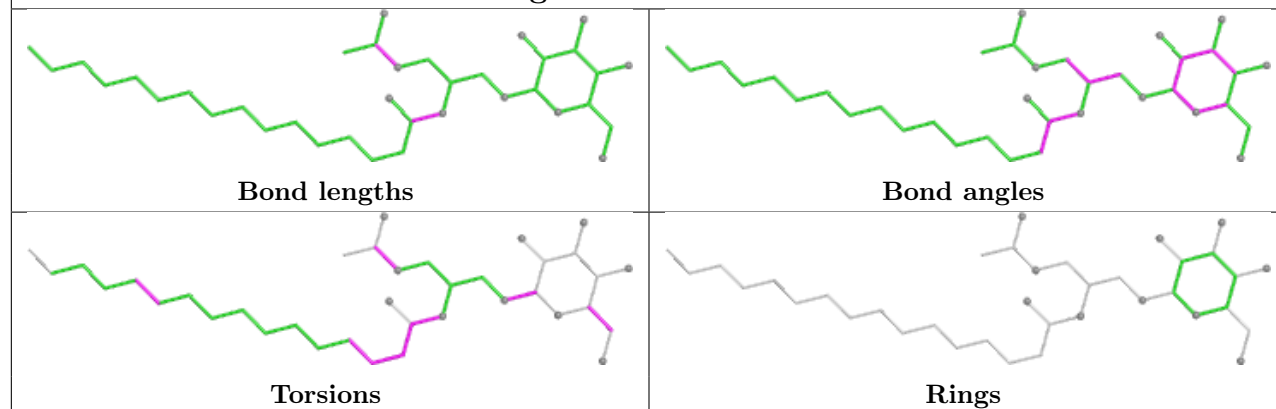


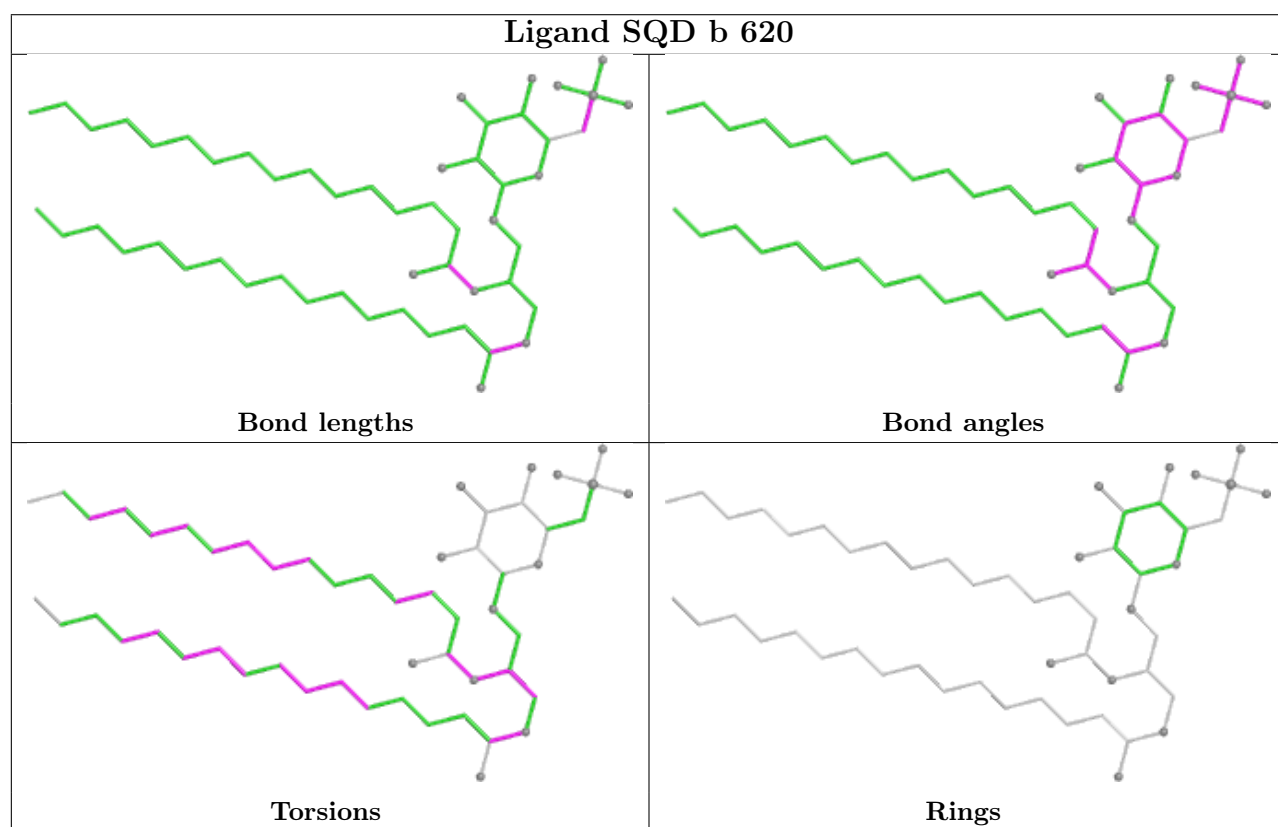
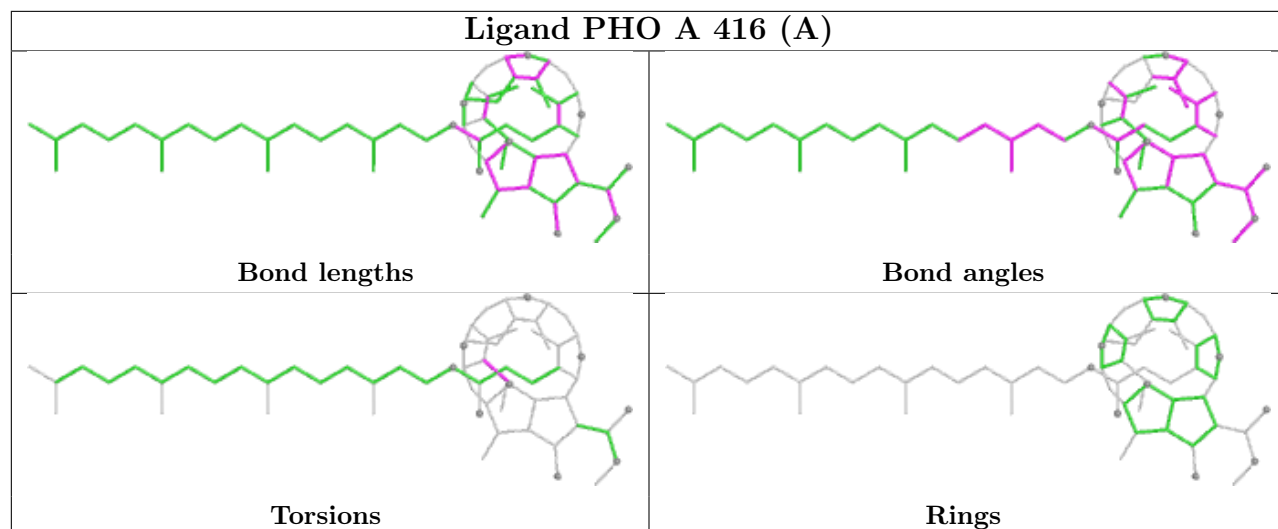
Ligand LMG d 412

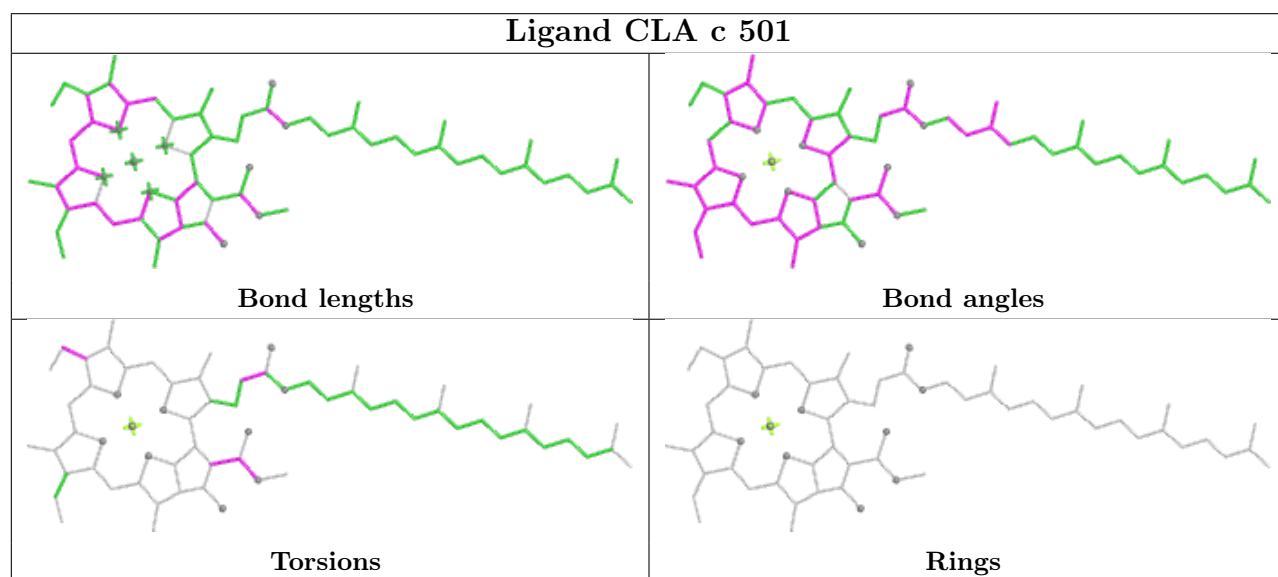
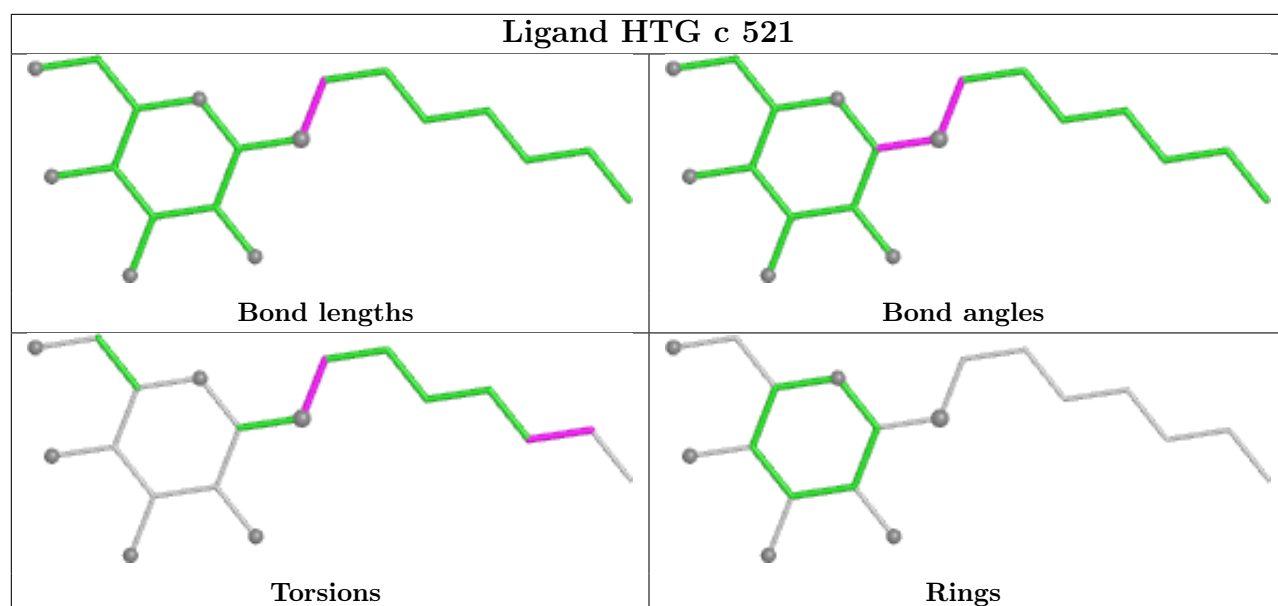


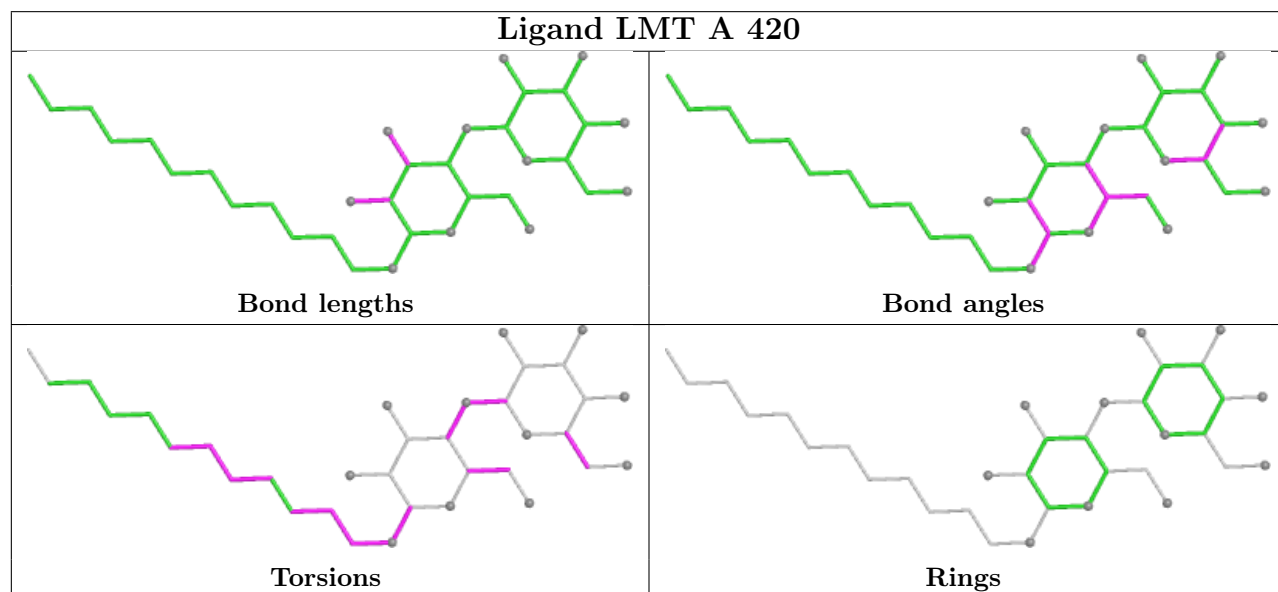
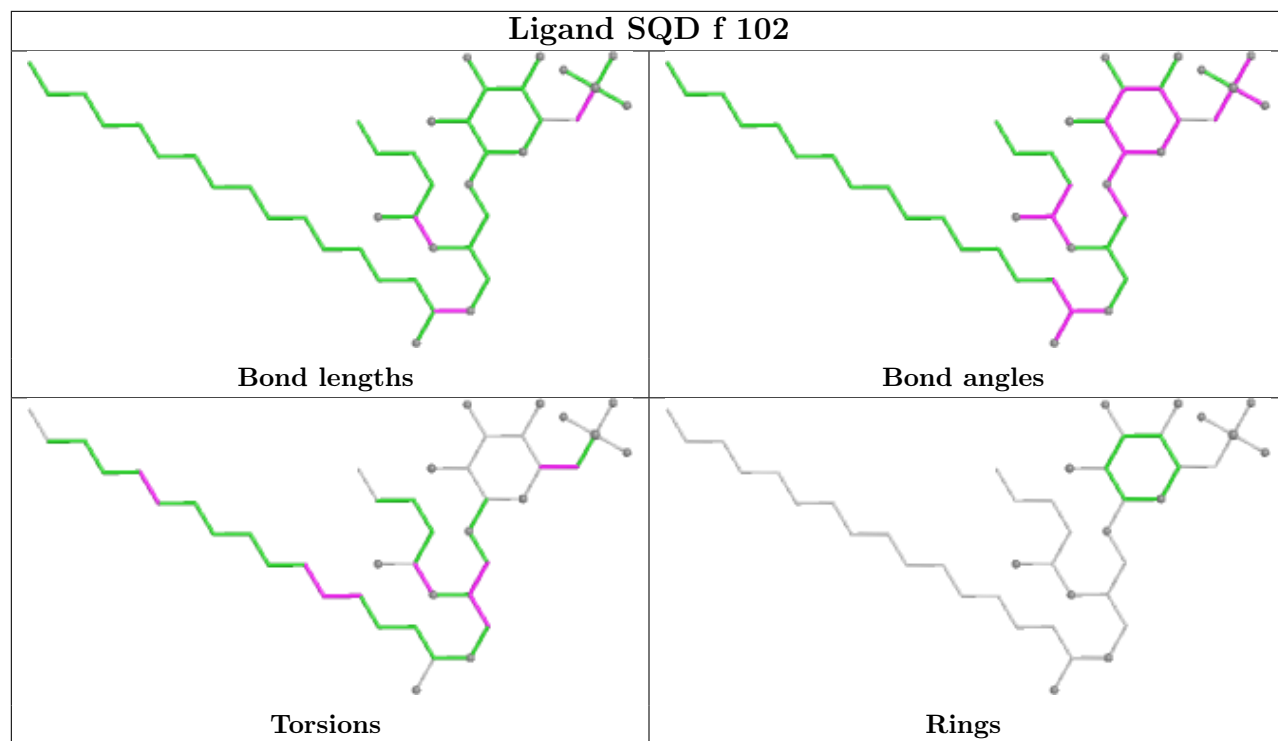


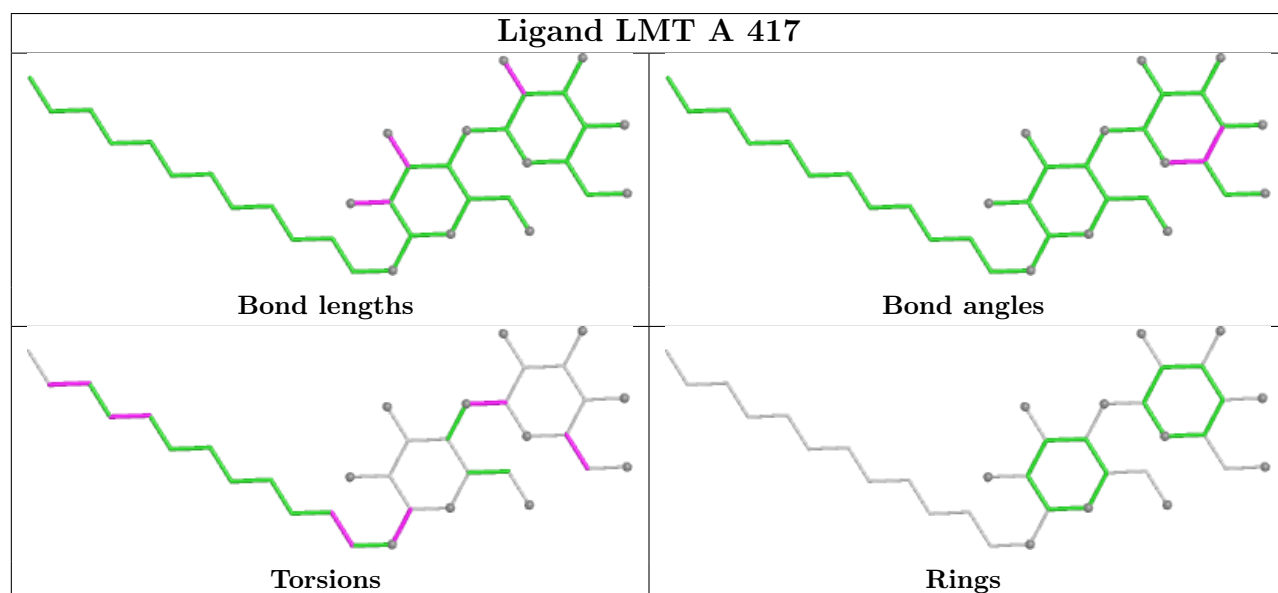
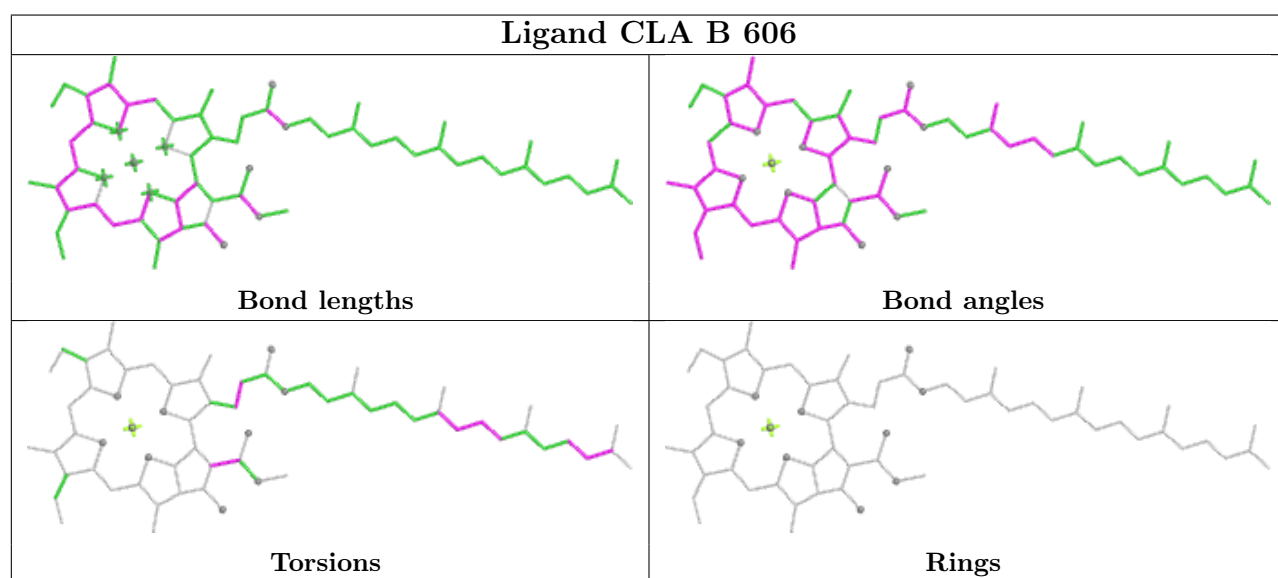
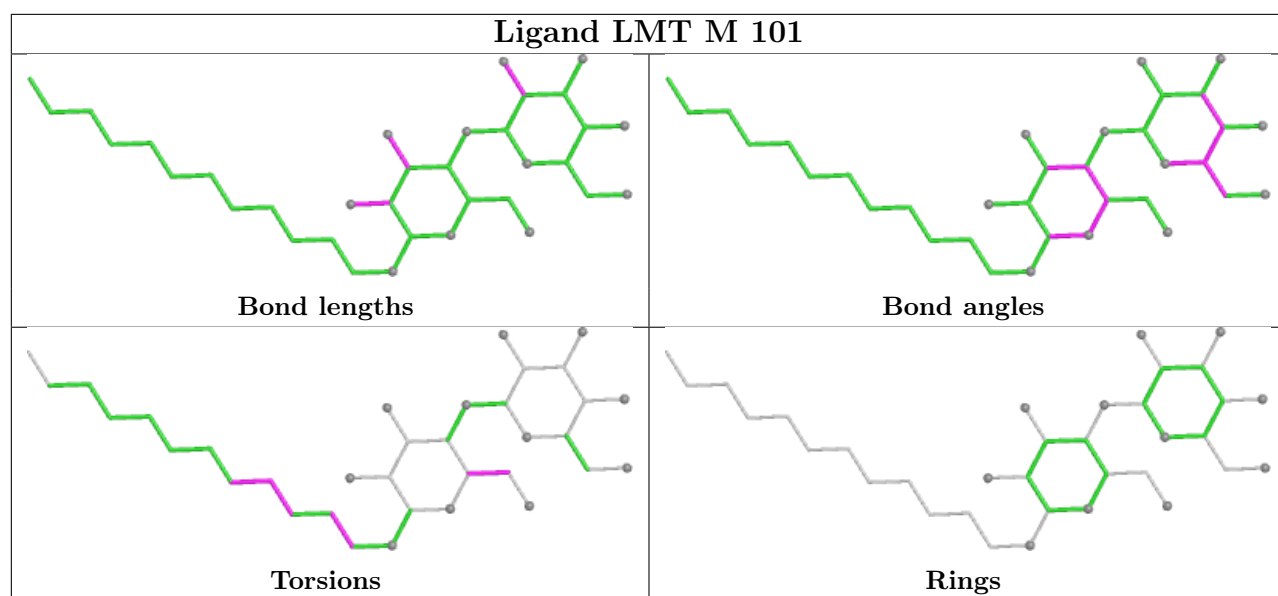


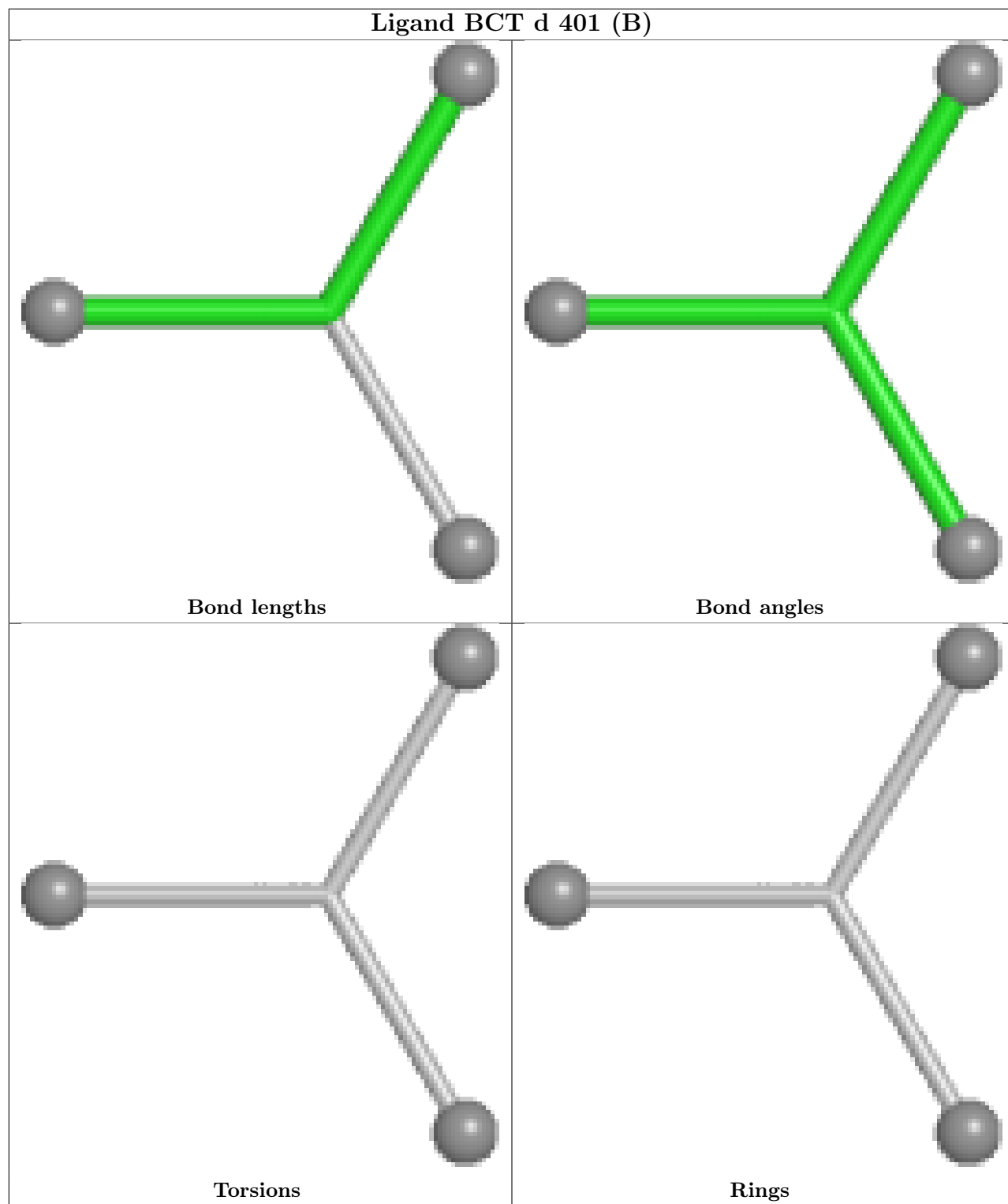
Ligand CLA a 405 (B)**Ligand CLA c 511****Ligand LMG Z 101**

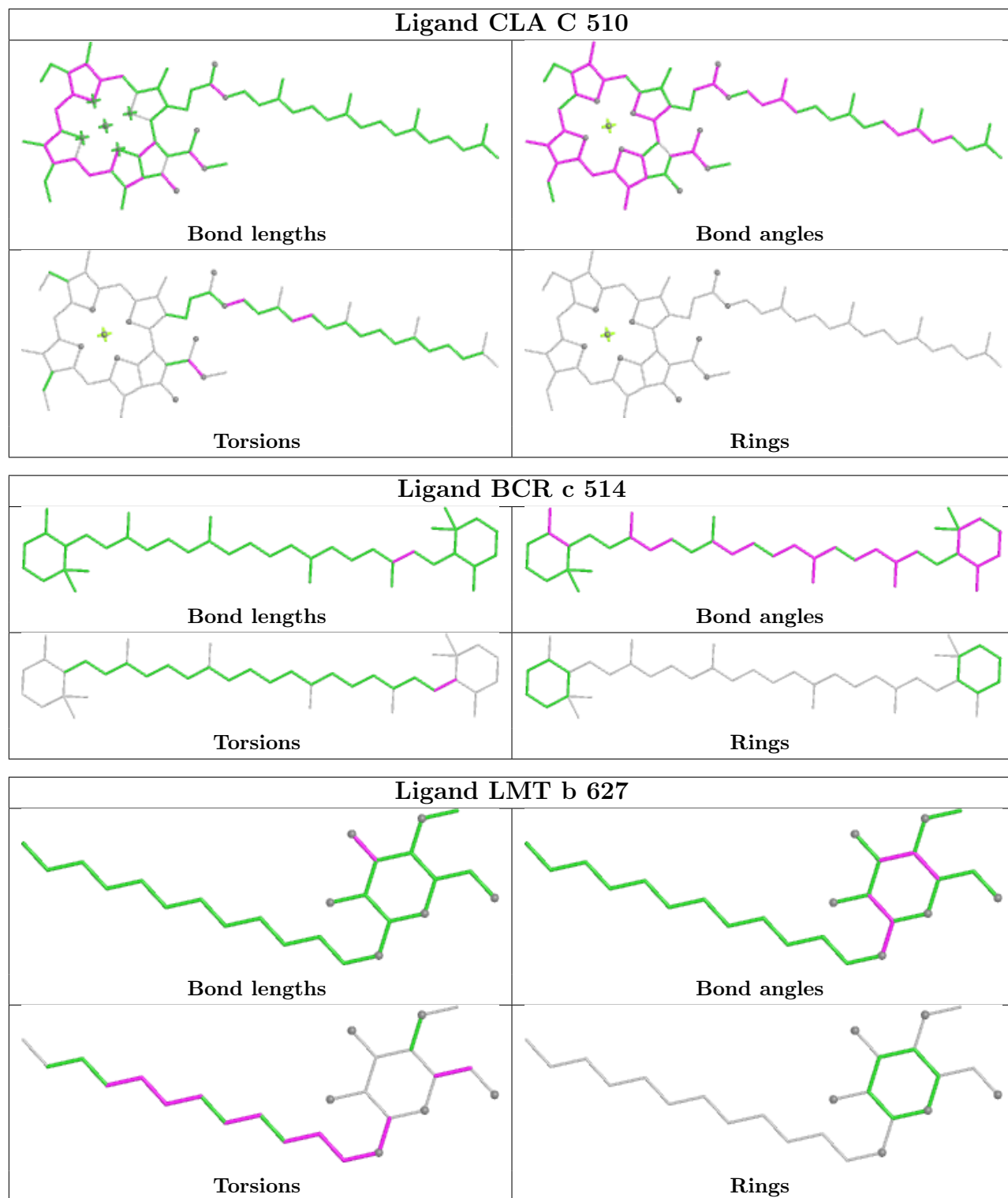


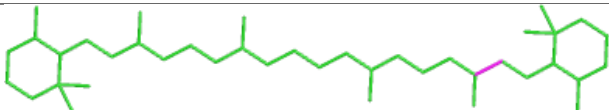
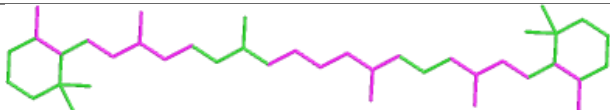
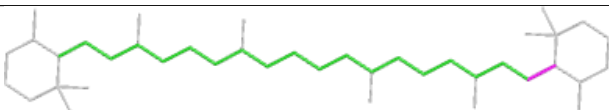
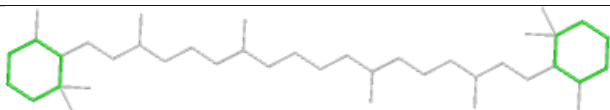


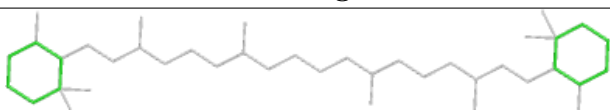


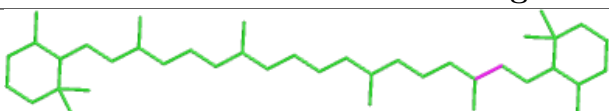
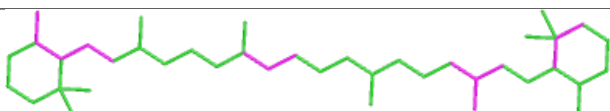
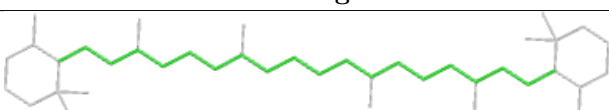
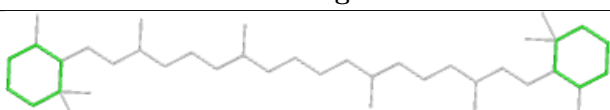




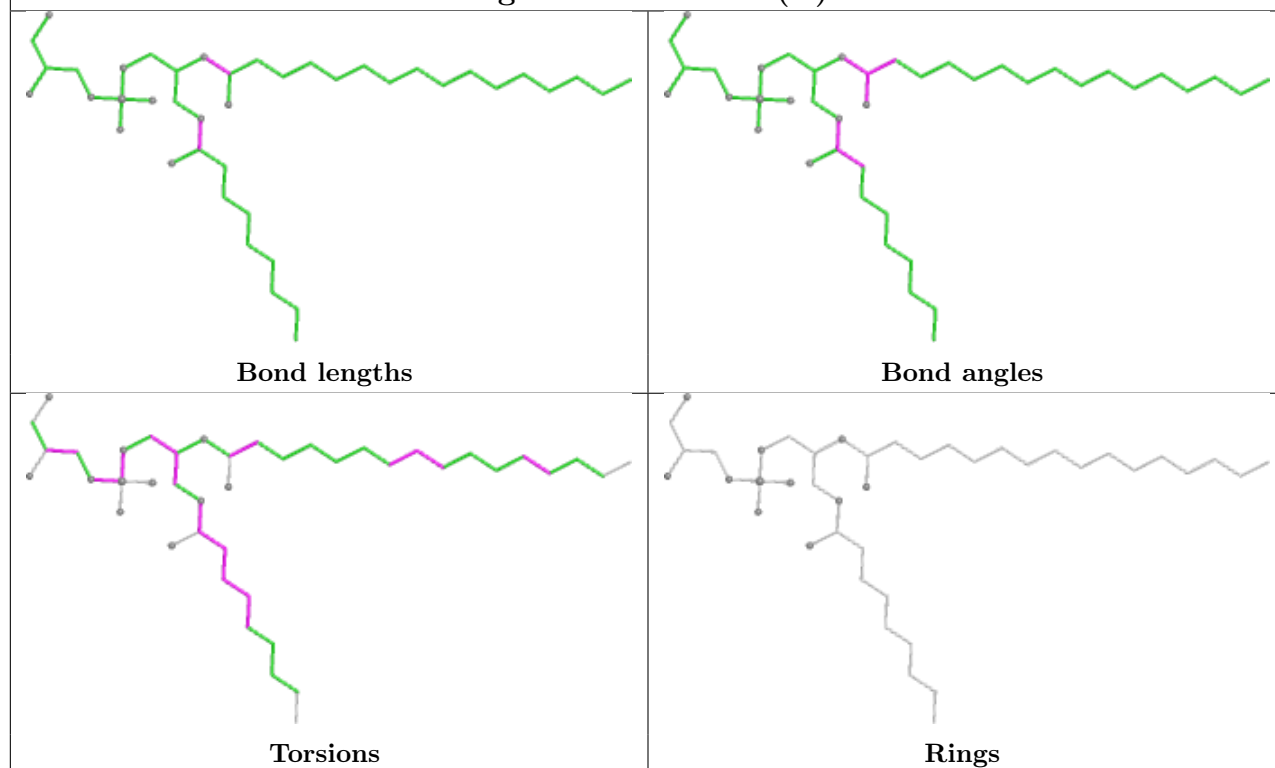


Ligand BCR h 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

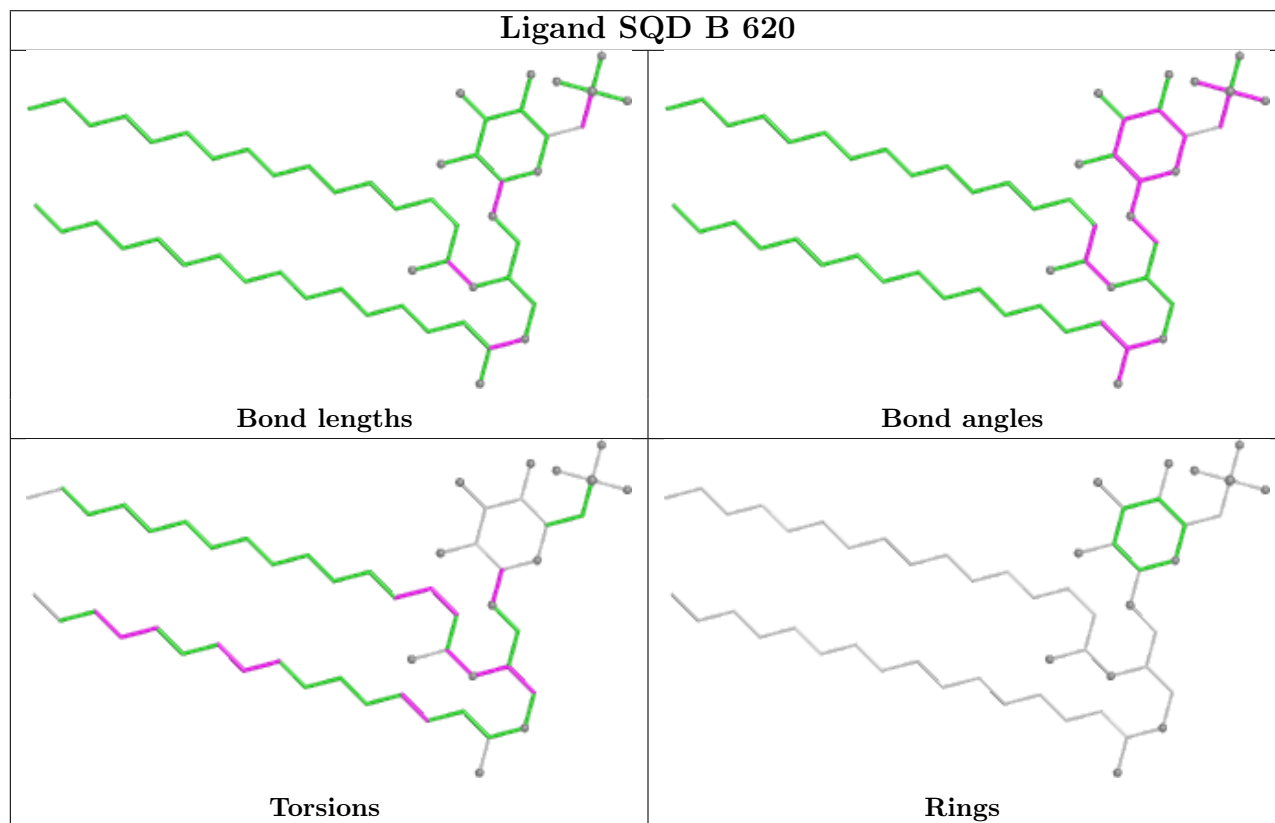
Ligand BCR D 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

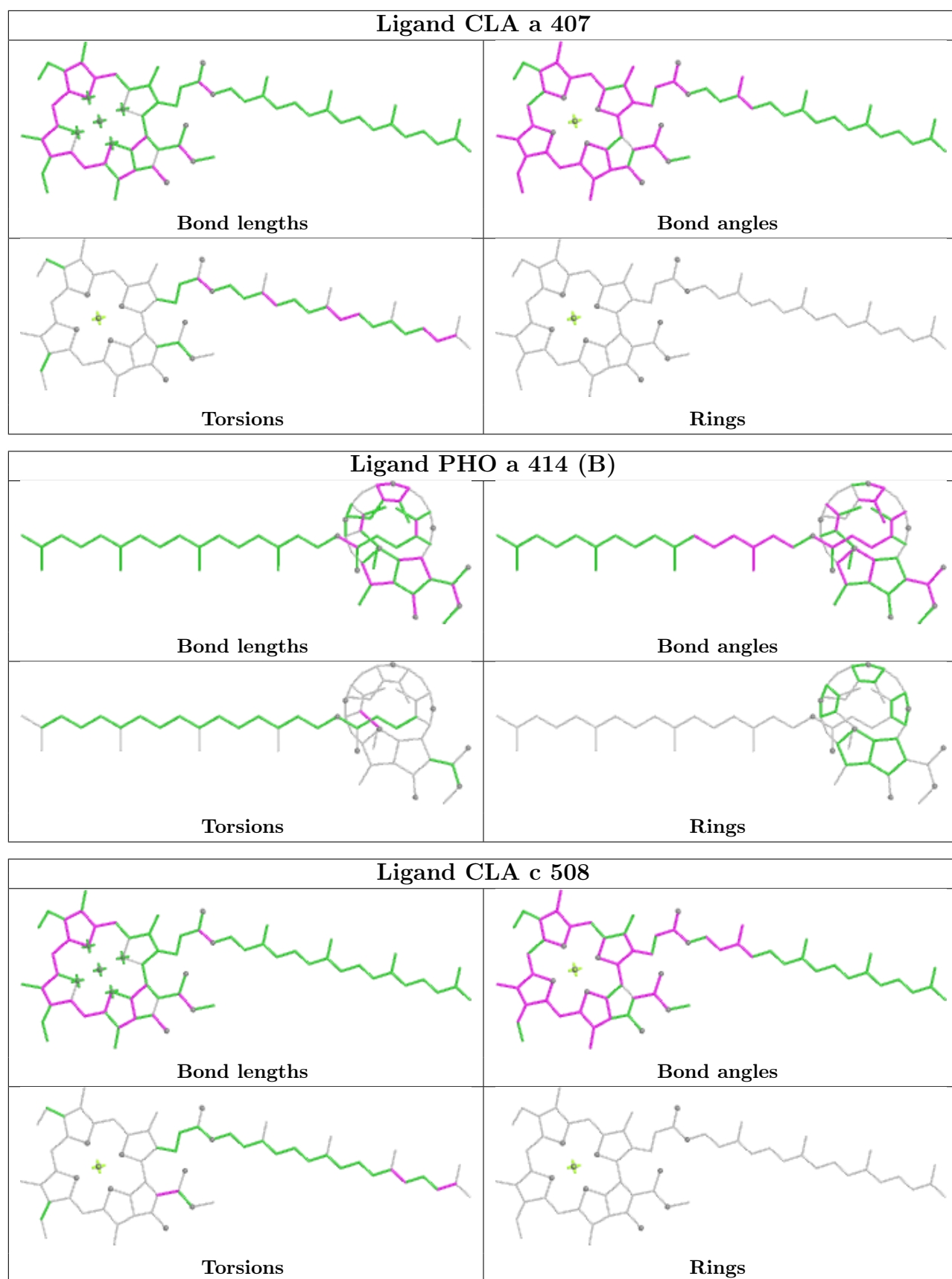
Ligand BCR b 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

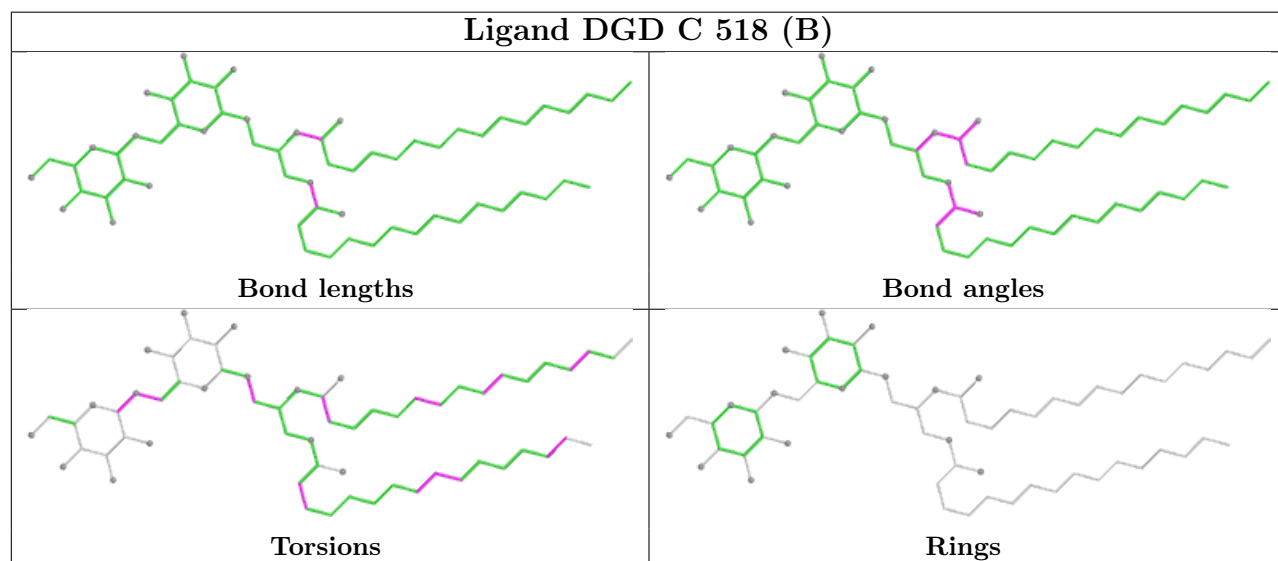
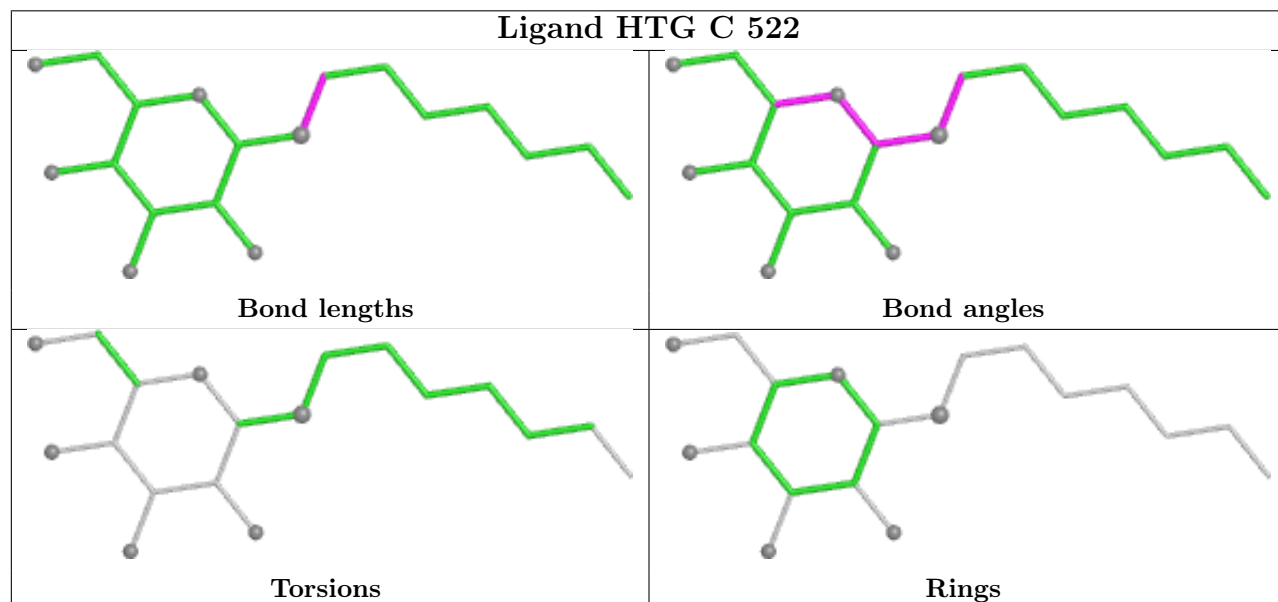
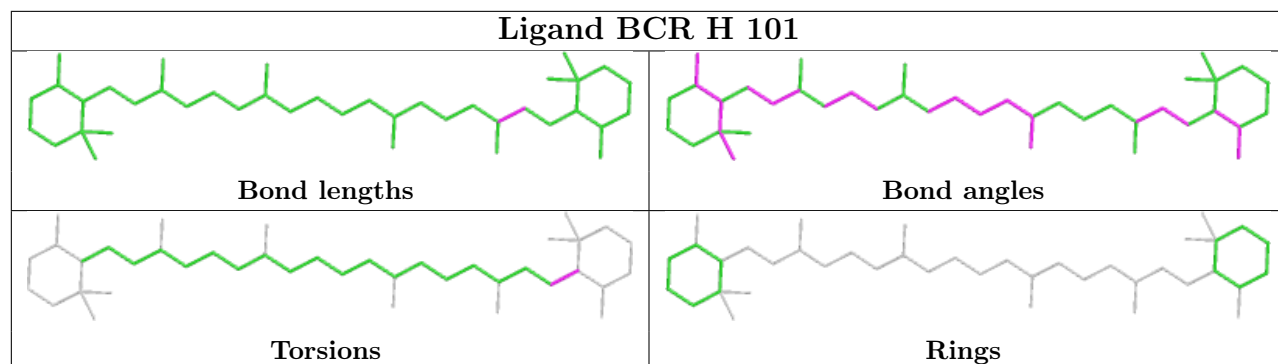
Ligand LHG E 101 (B)

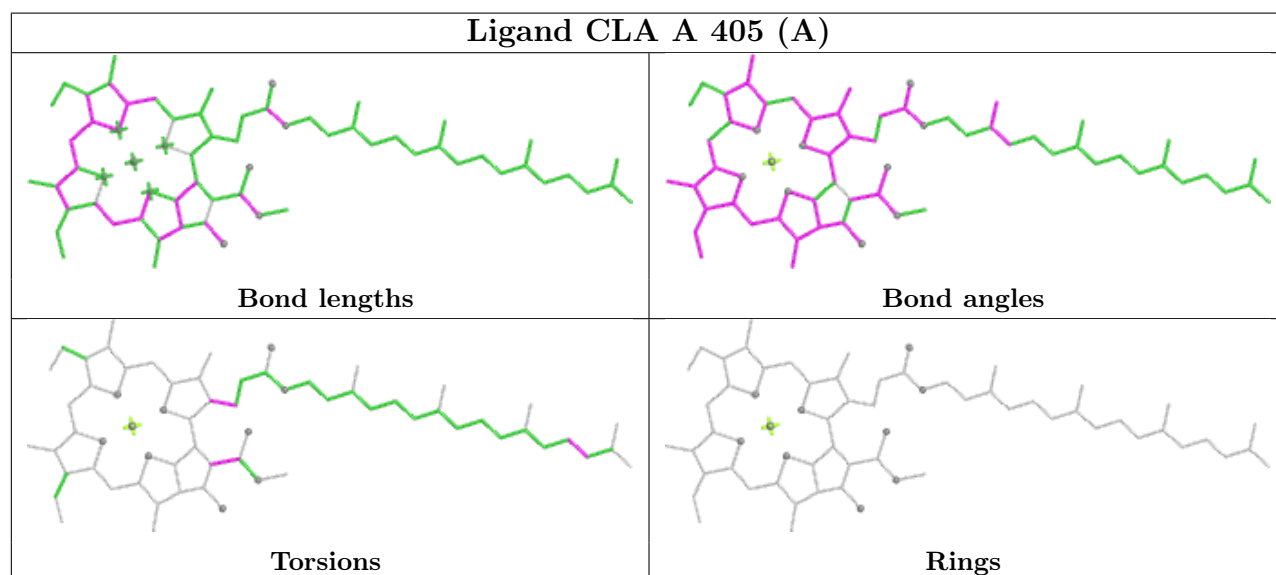
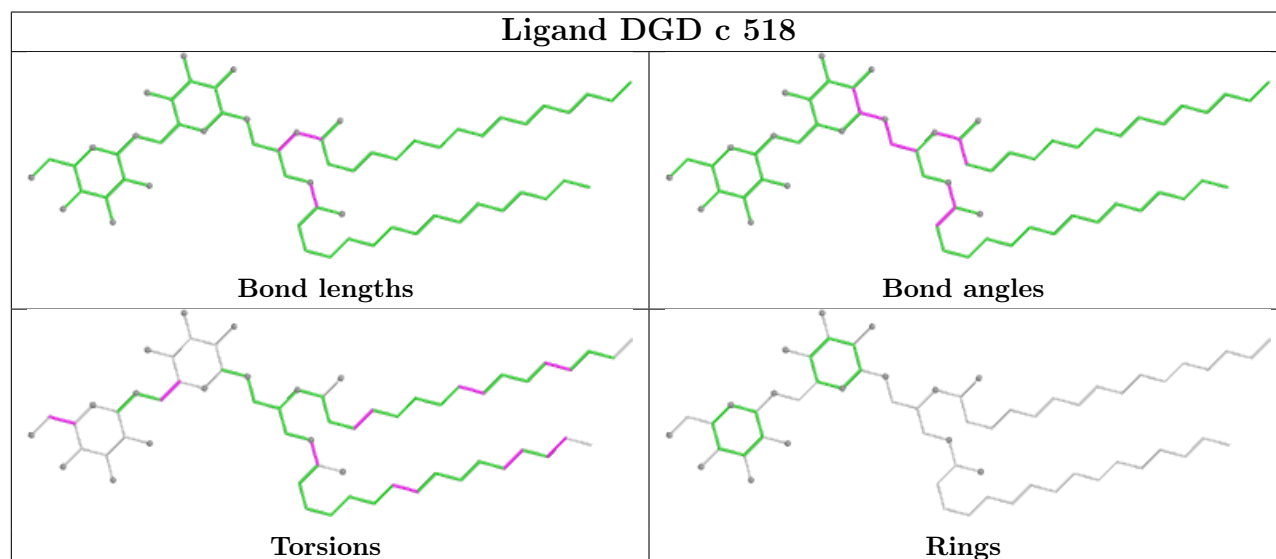
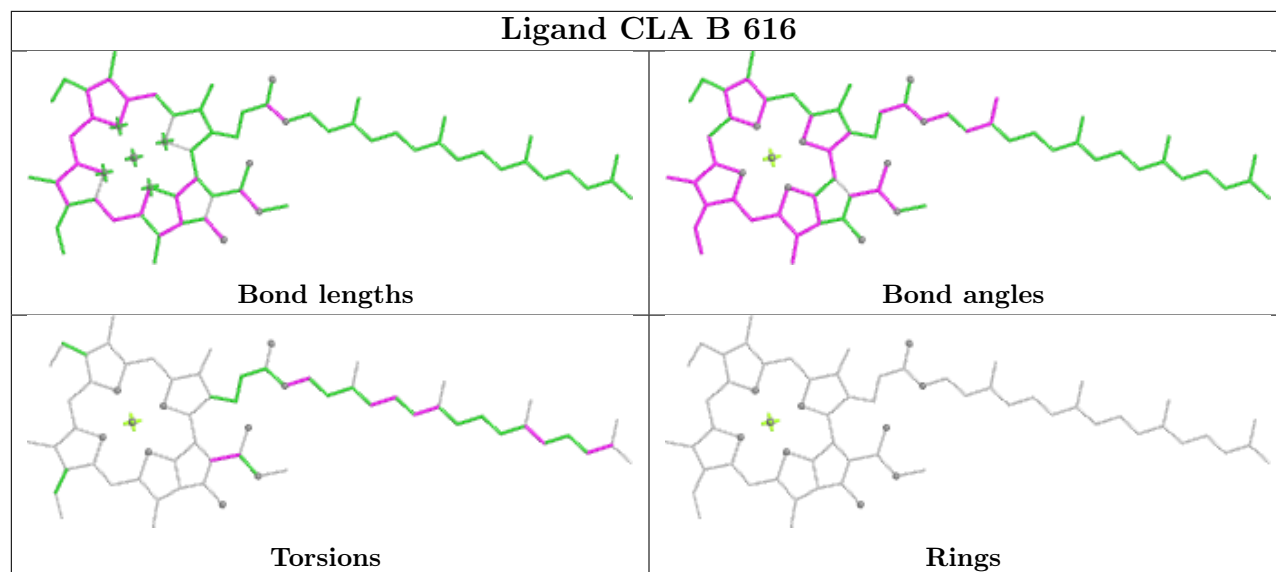


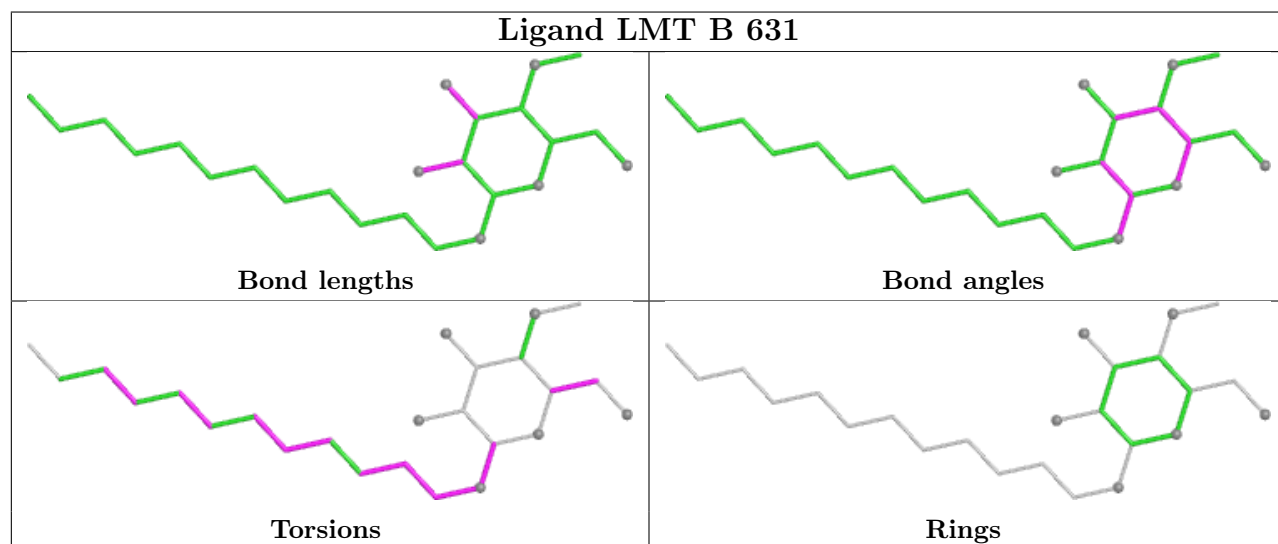
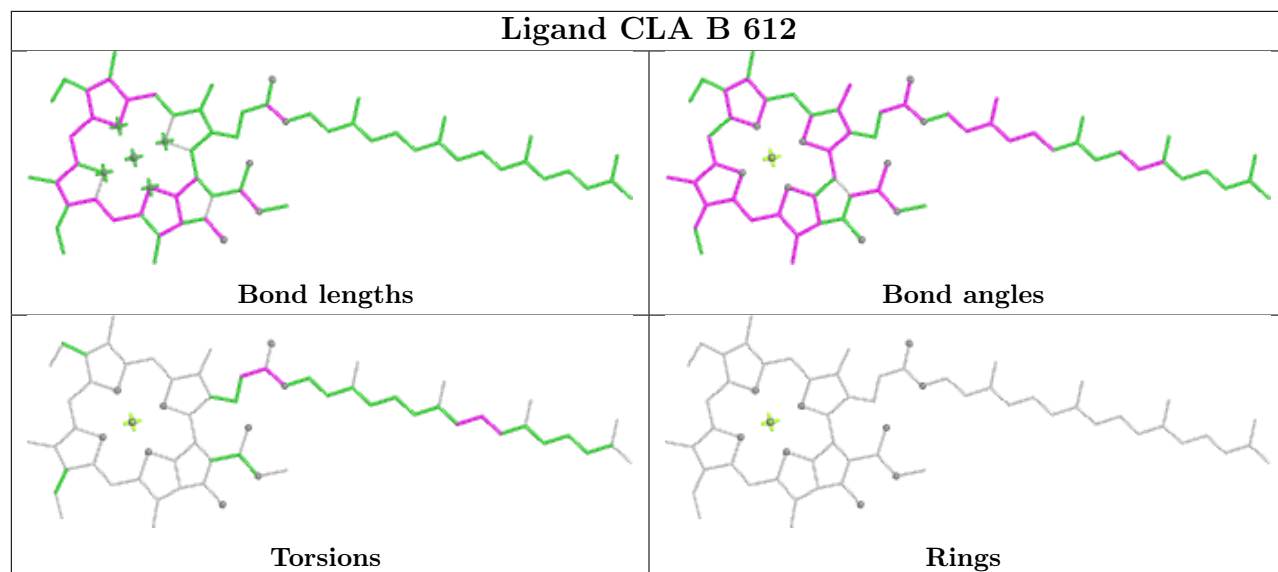
Ligand SQD B 620

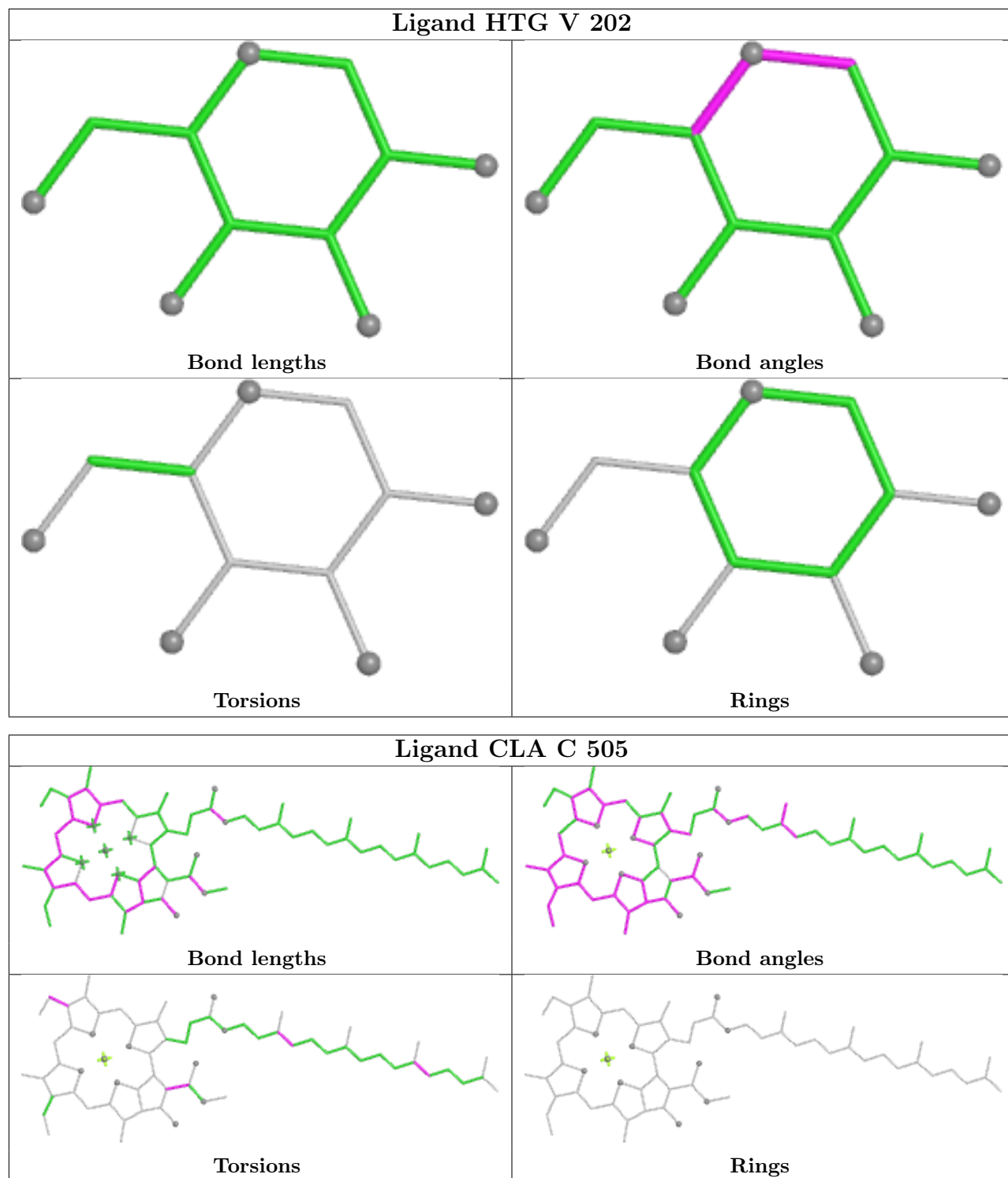


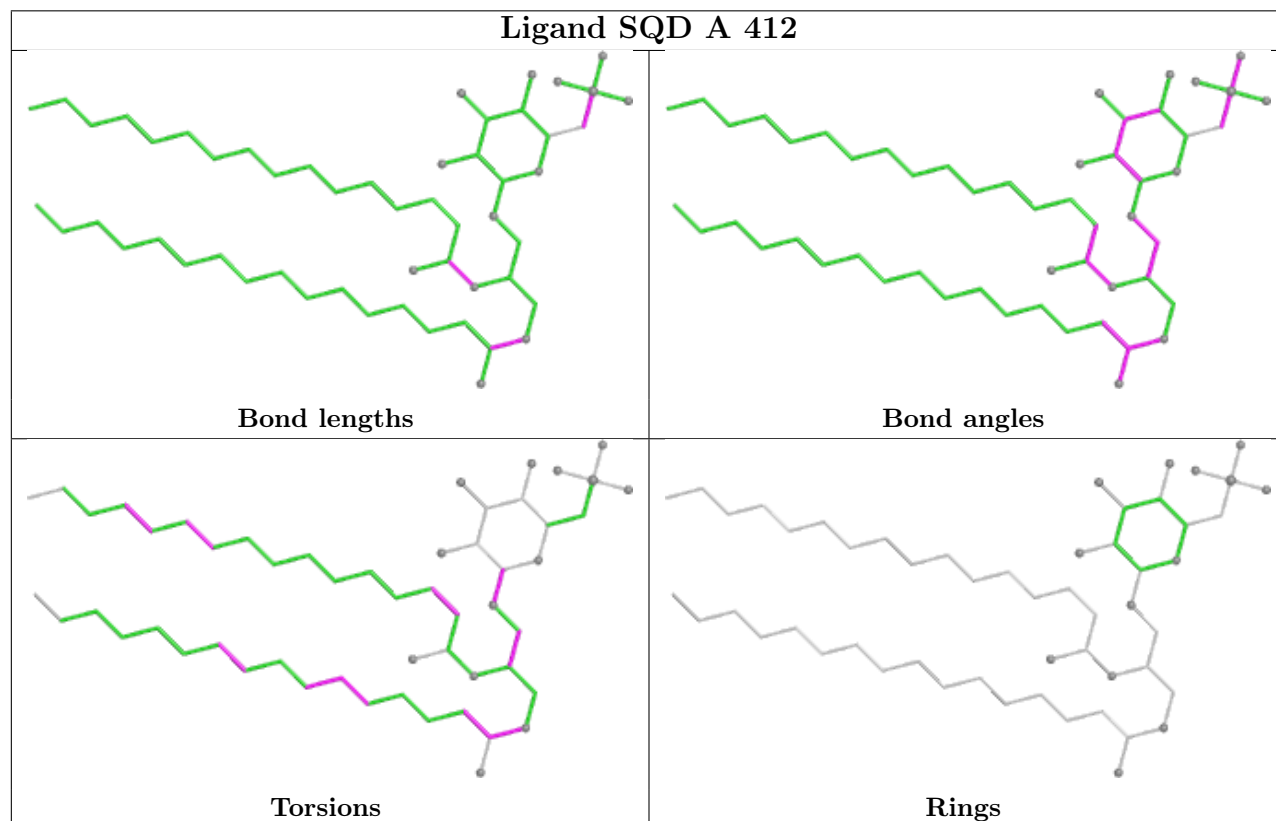
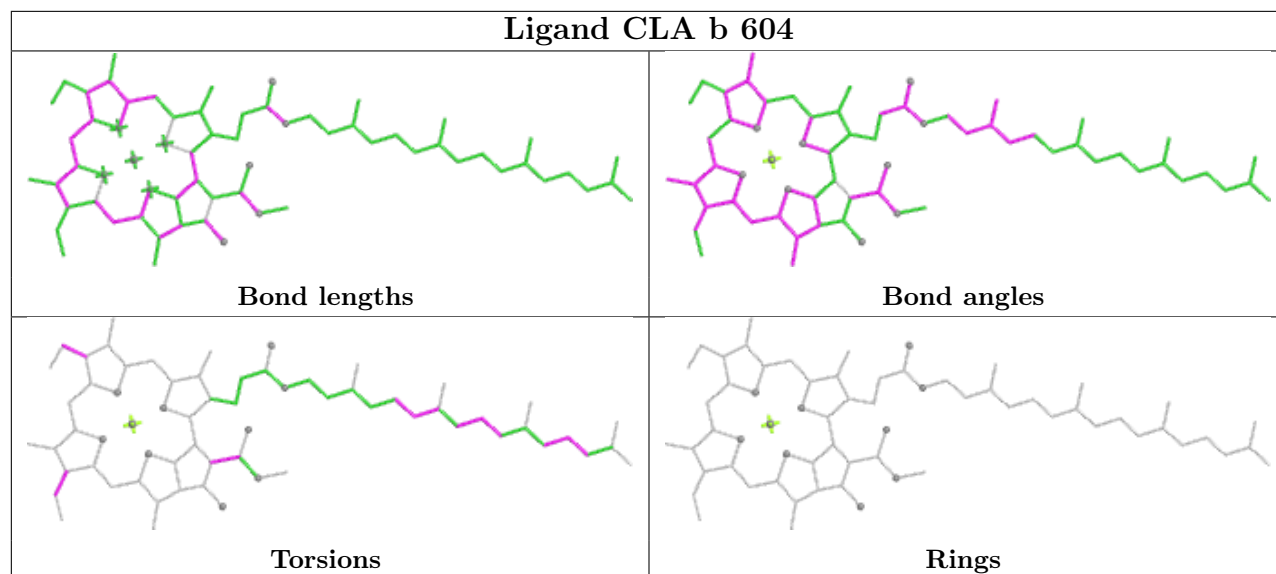


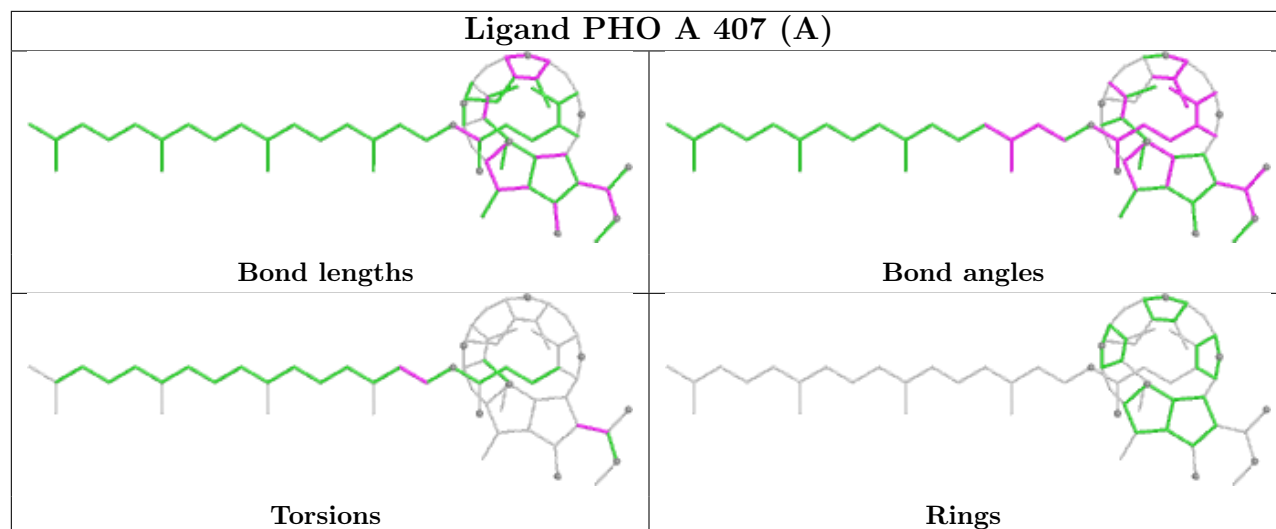
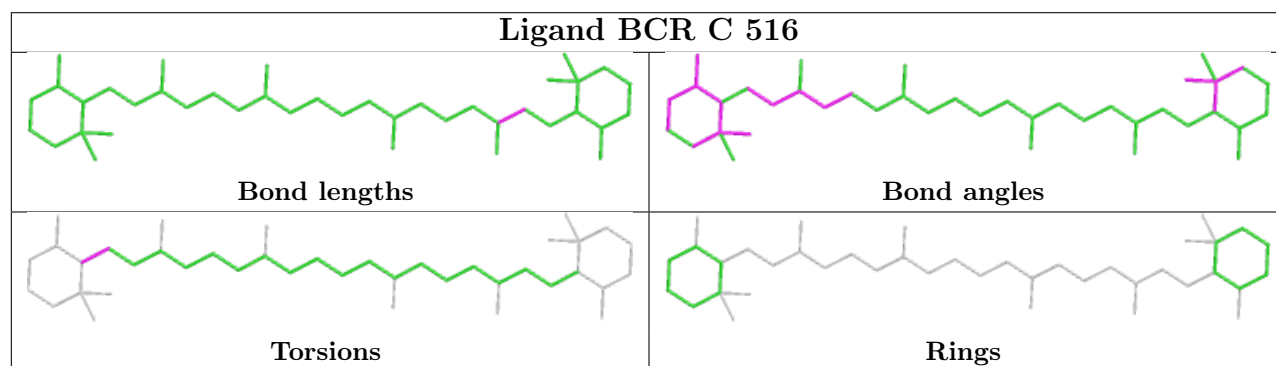
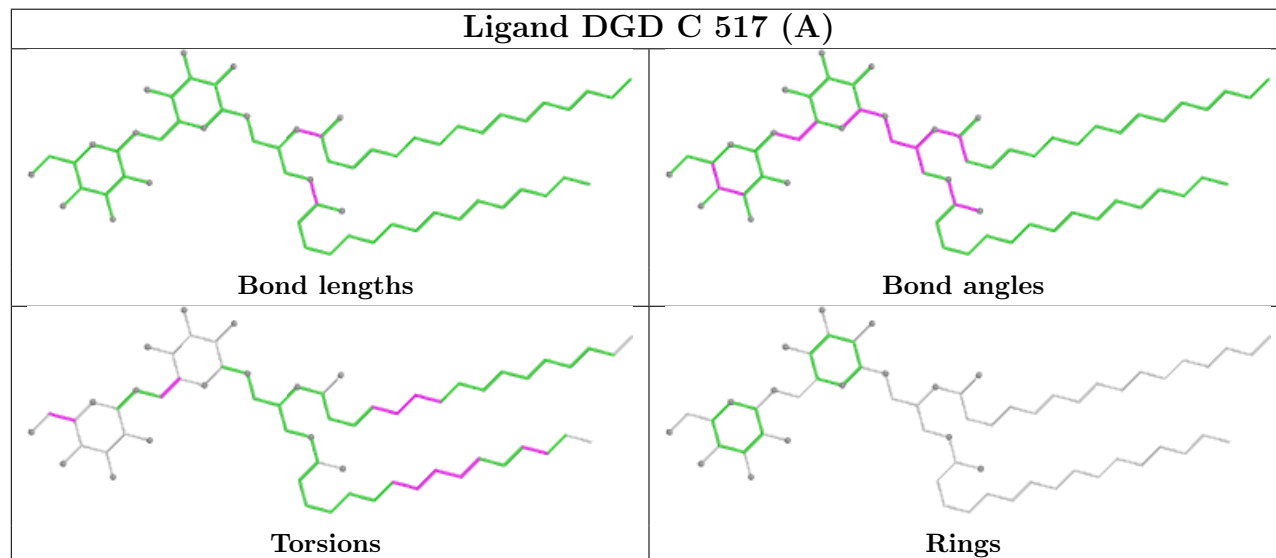


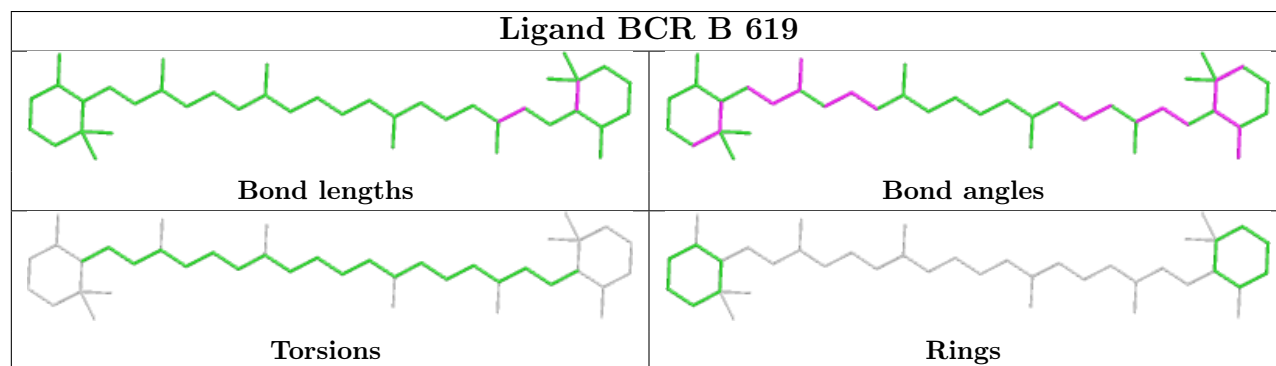
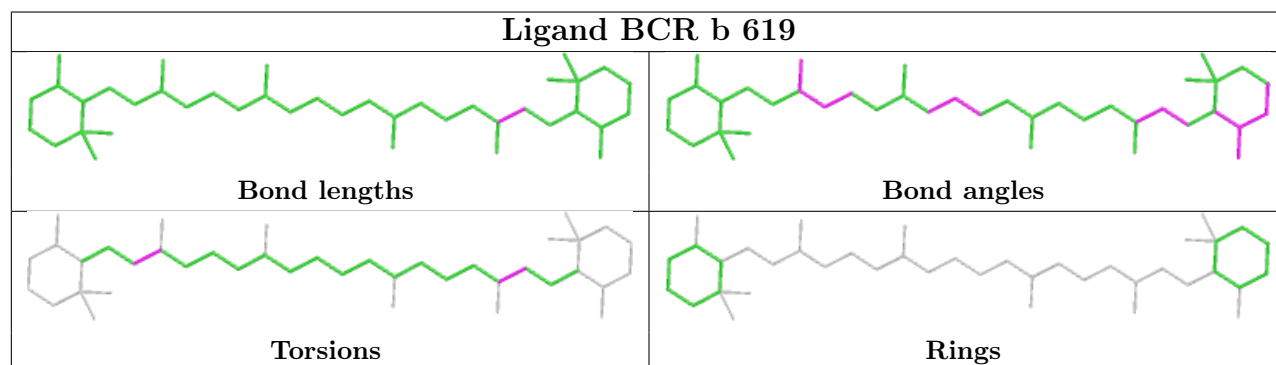
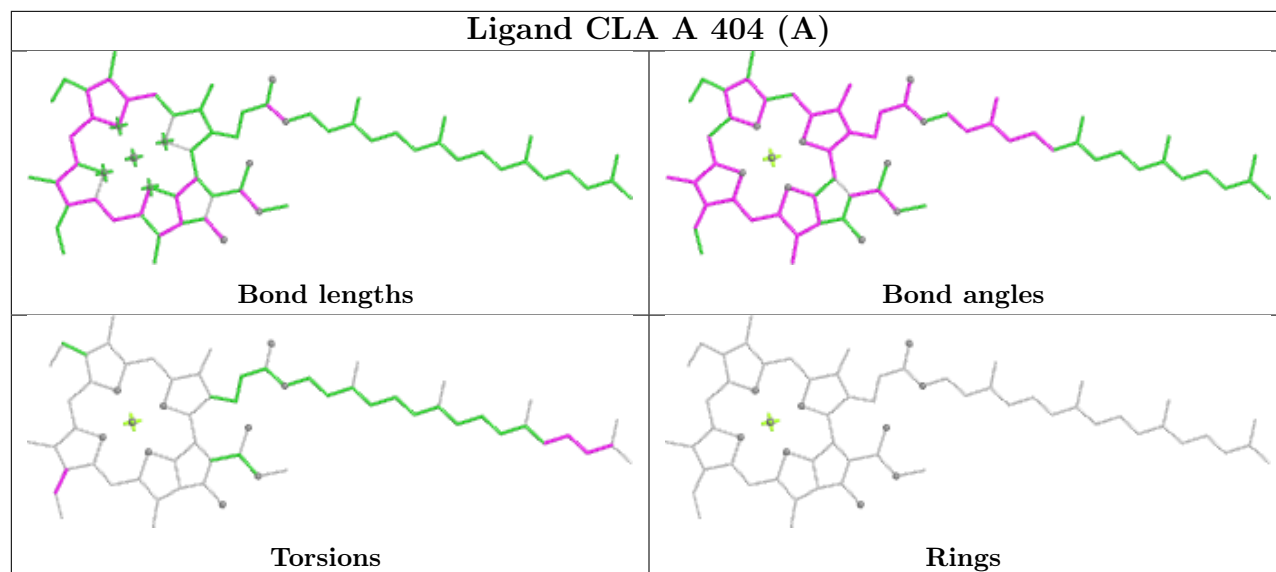


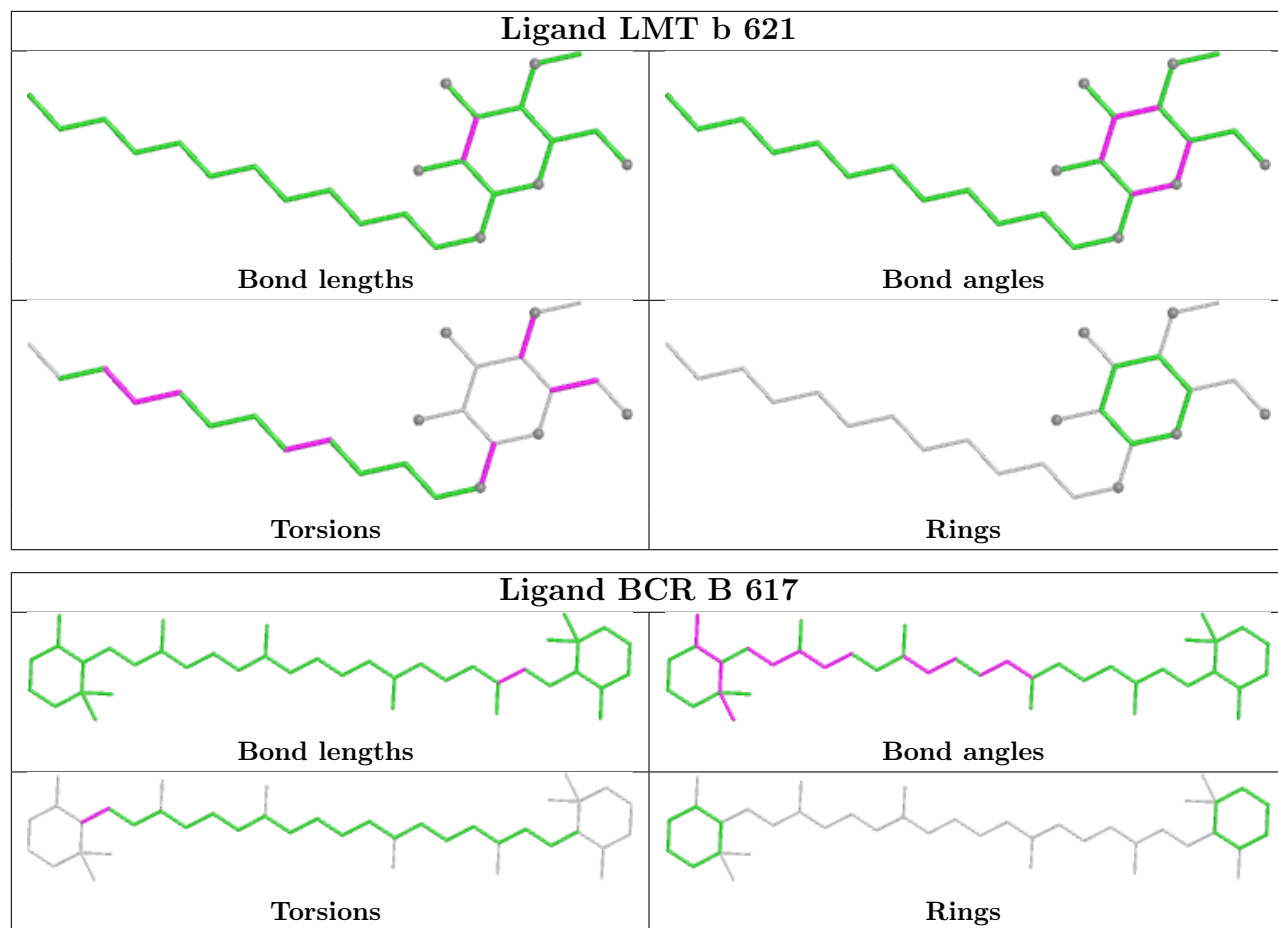


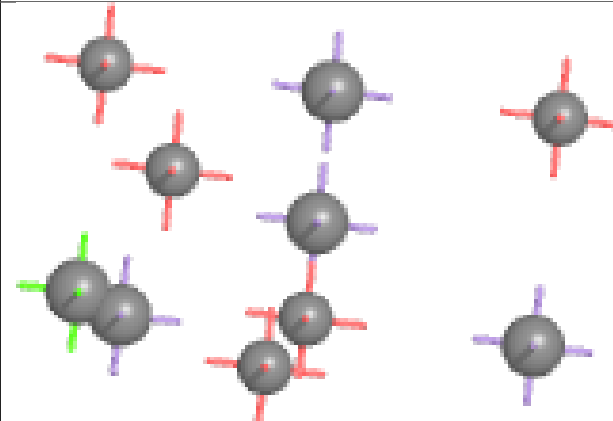
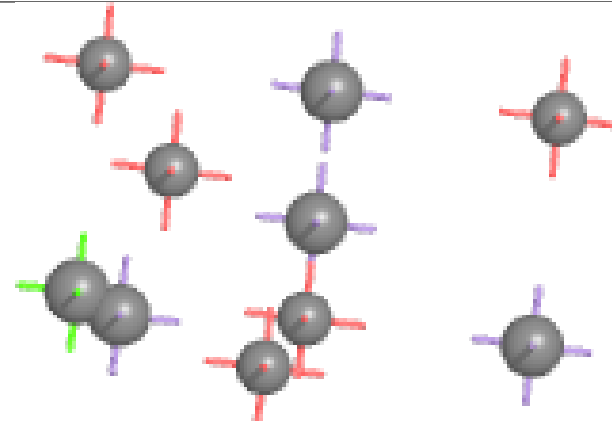
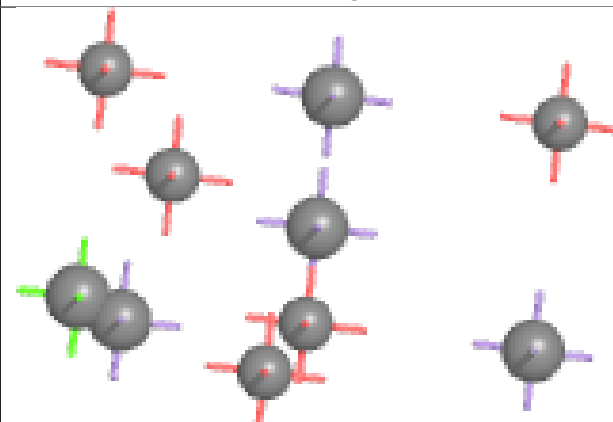
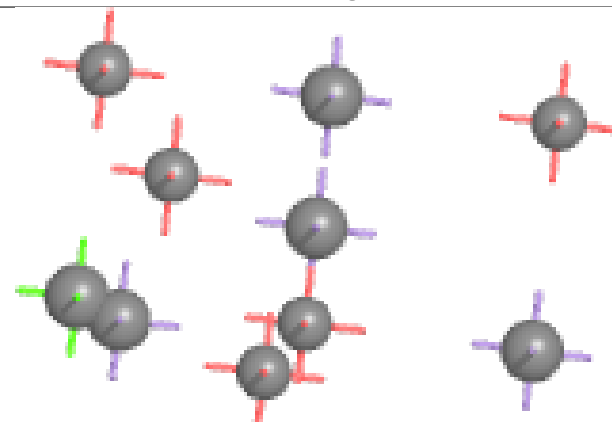


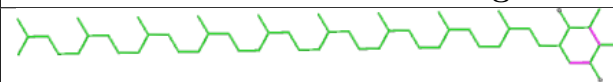
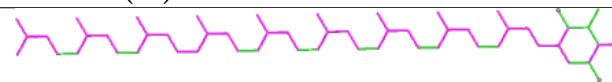
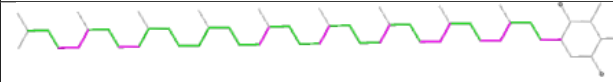
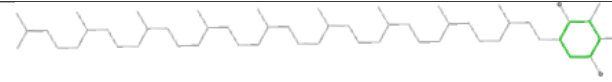


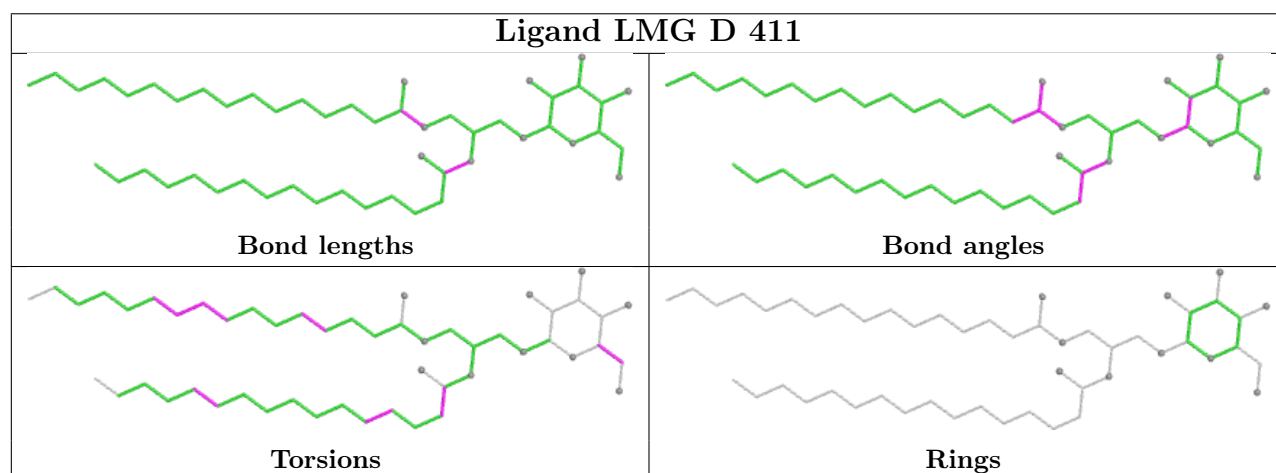
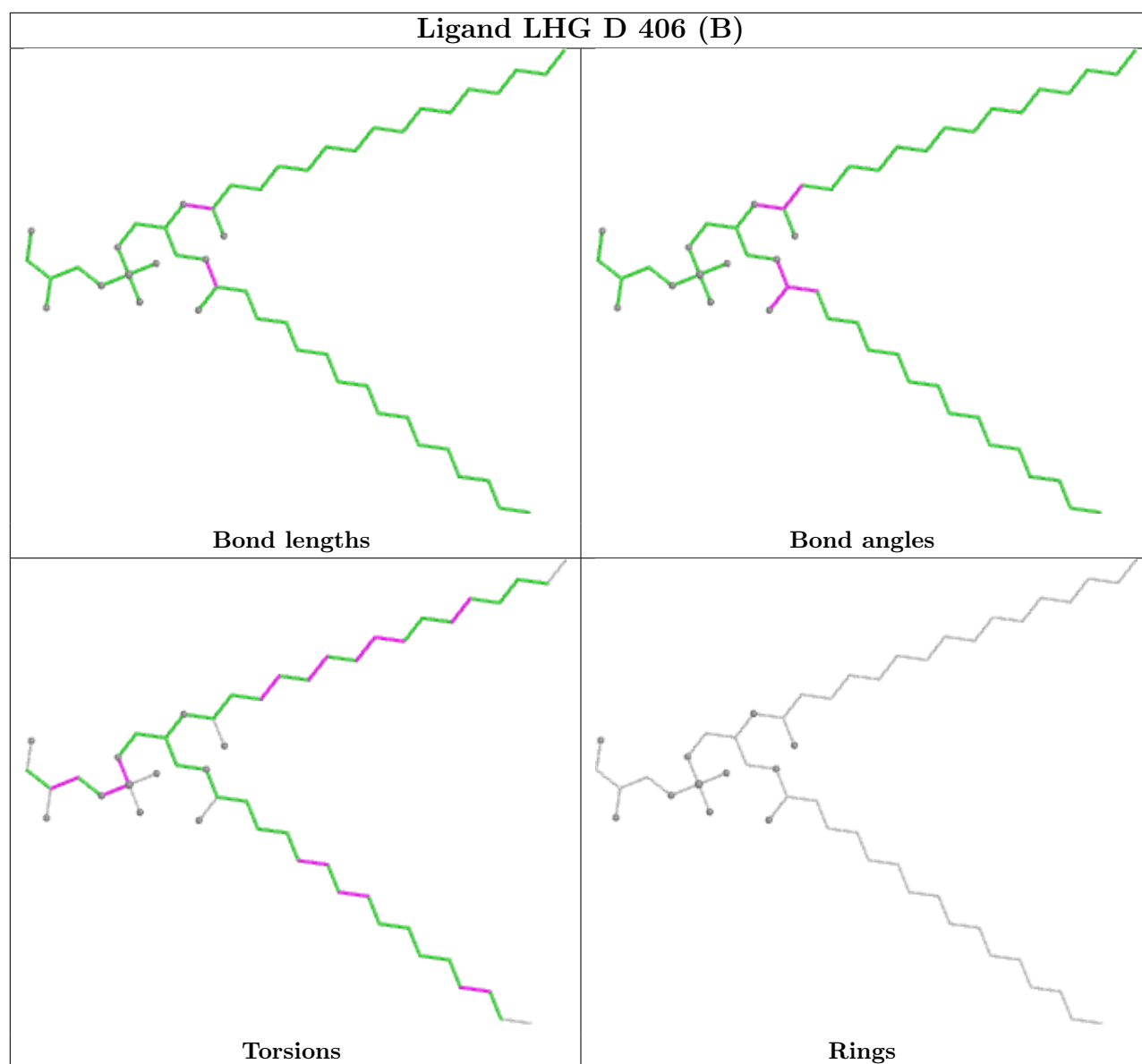
Ligand PHO A 407 (A)**Ligand BCR C 516****Ligand DGD C 517 (A)**

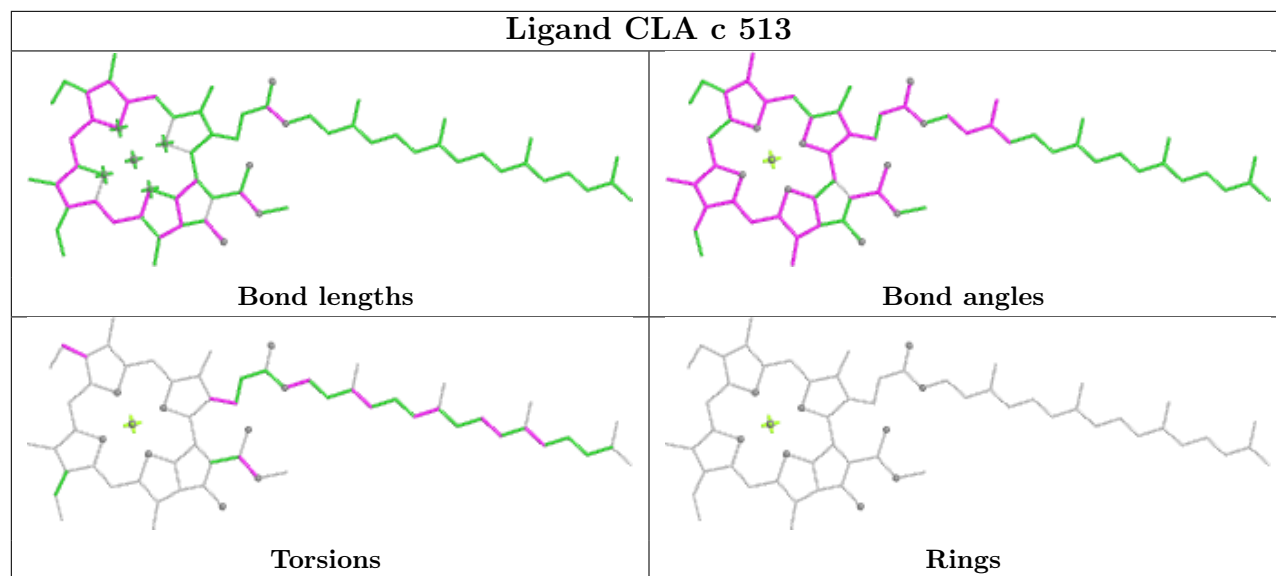


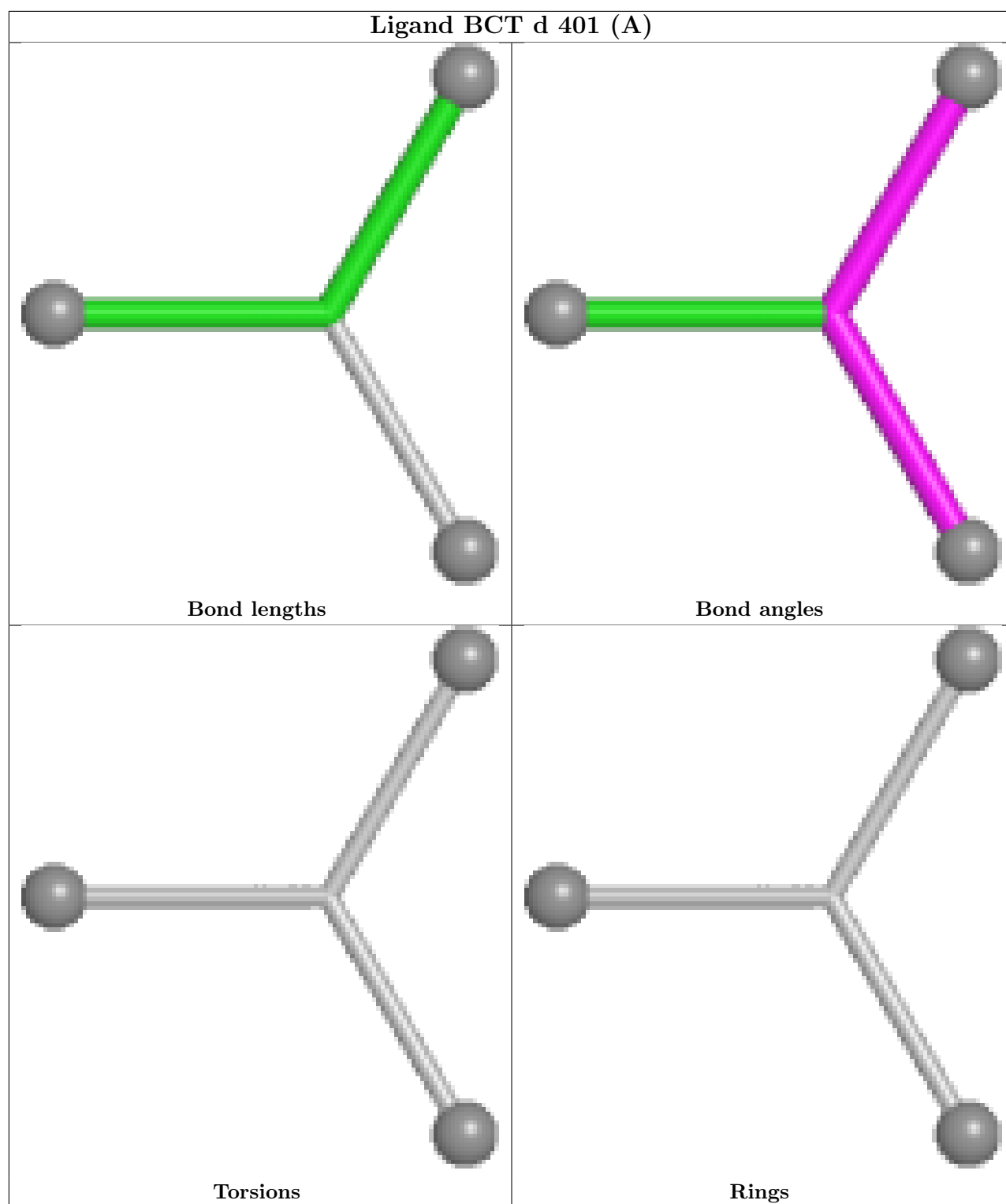


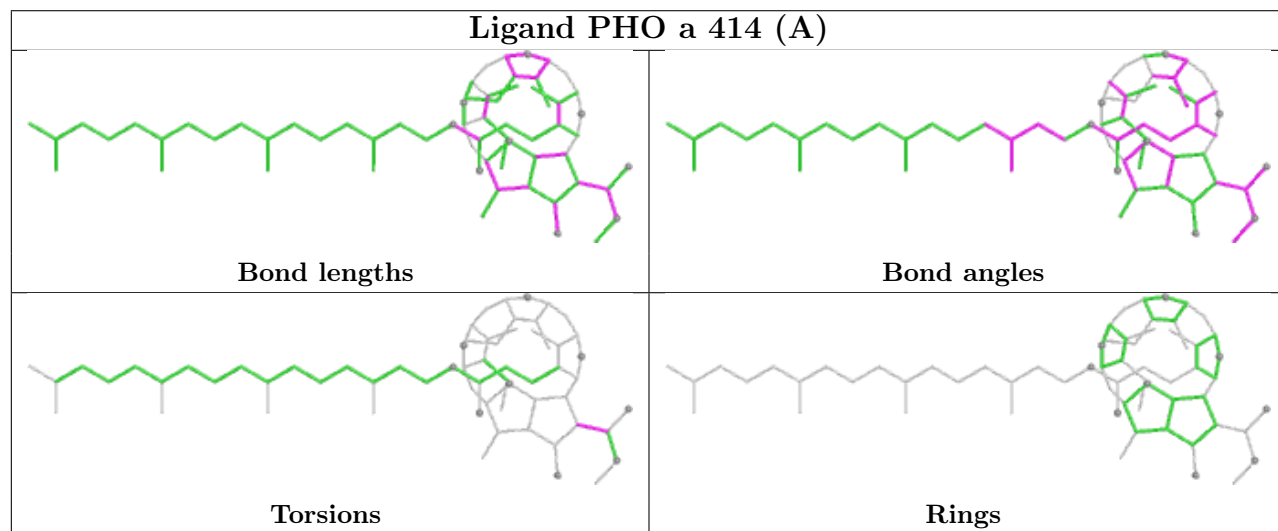
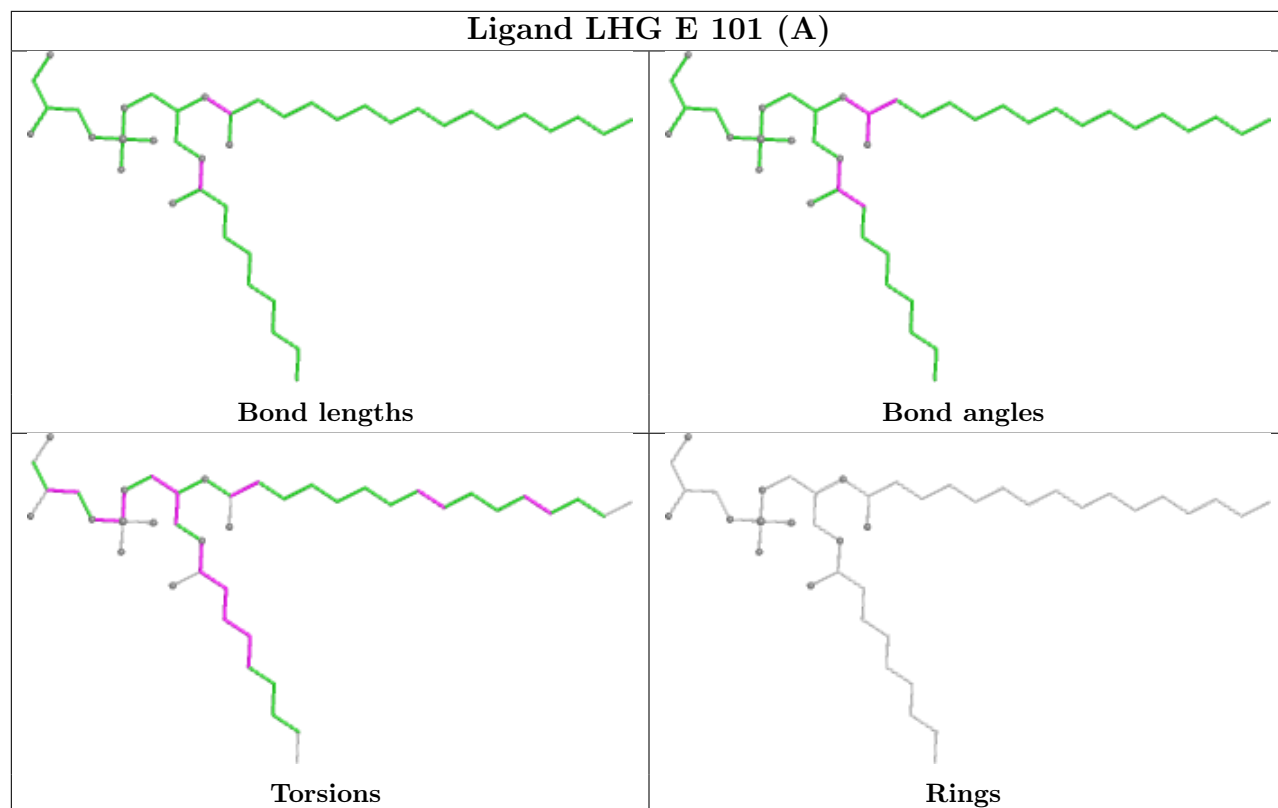
Ligand OEX a 411 (A)	
	
Bond lengths	Bond angles
	
Torsions	Rings

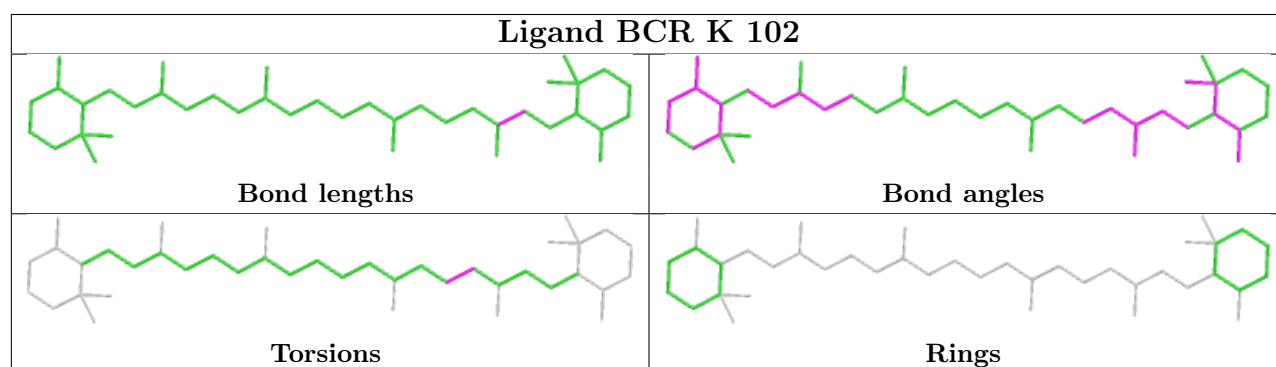
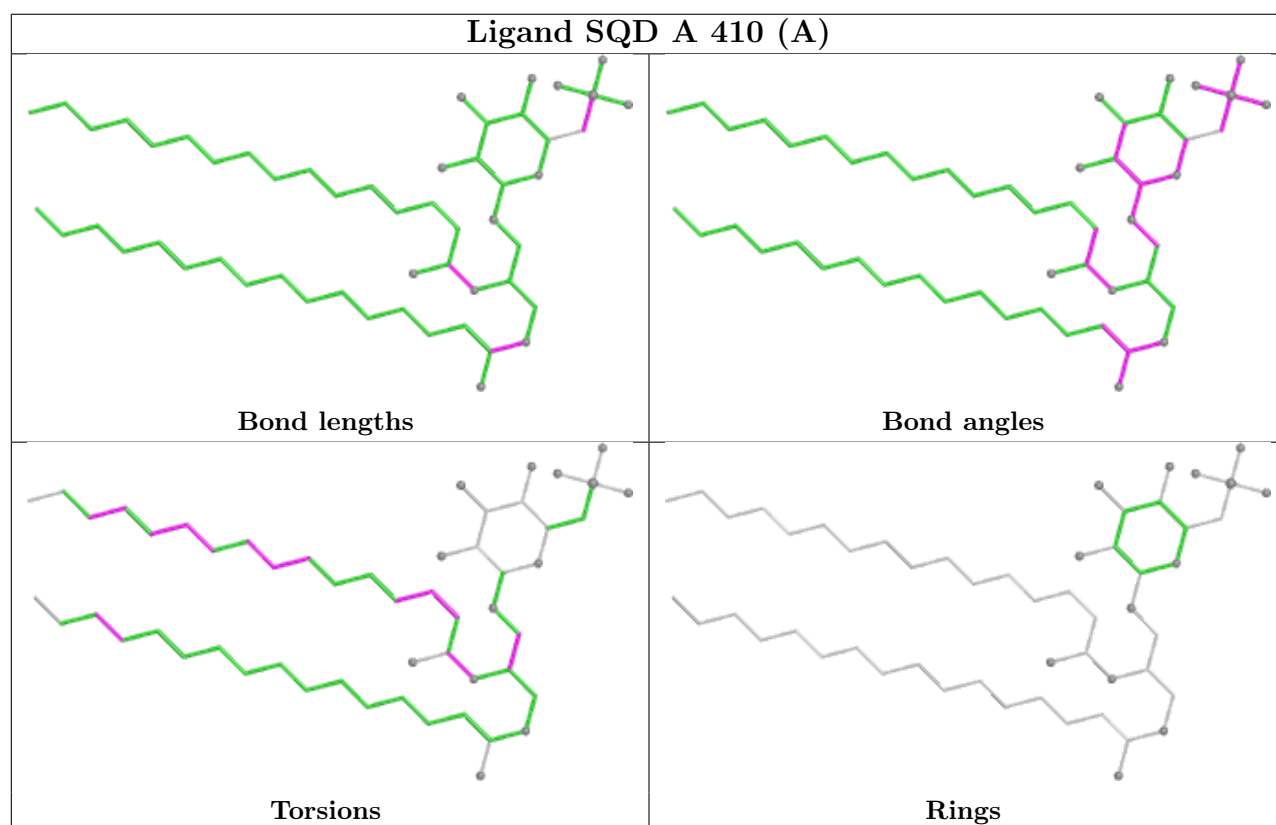
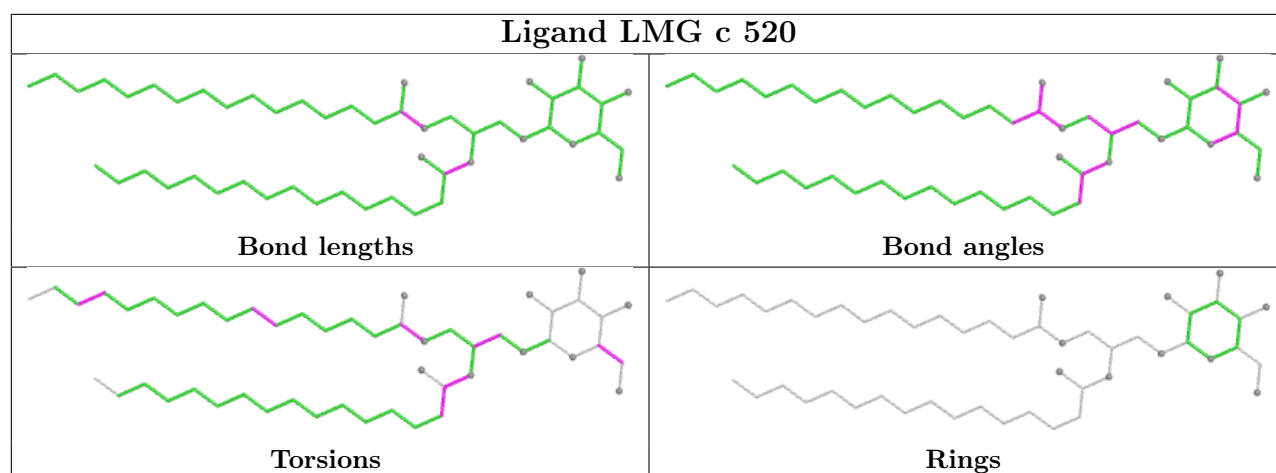
Ligand PL9 A 414 (A)	
	
Bond lengths	Bond angles
	
Torsions	Rings

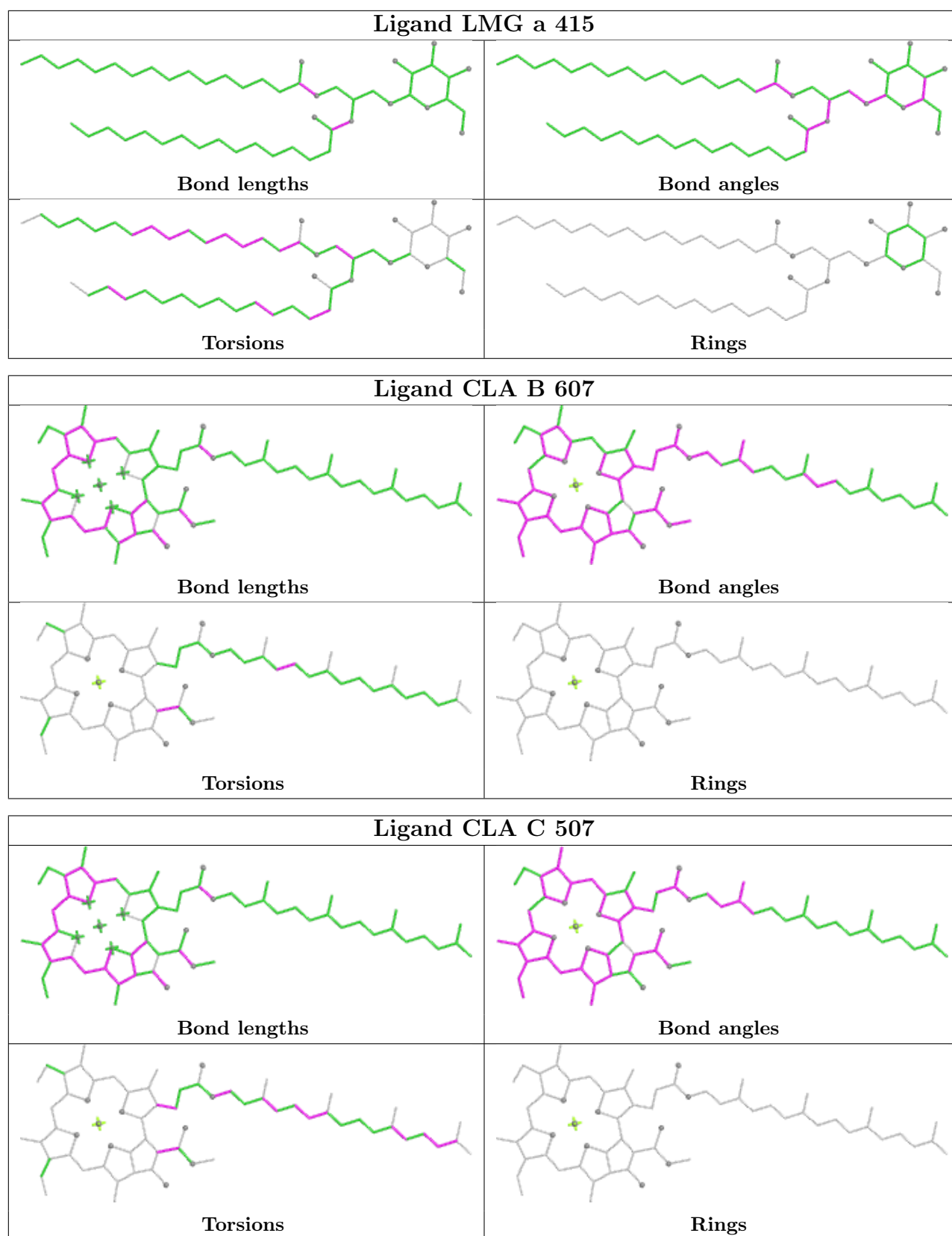


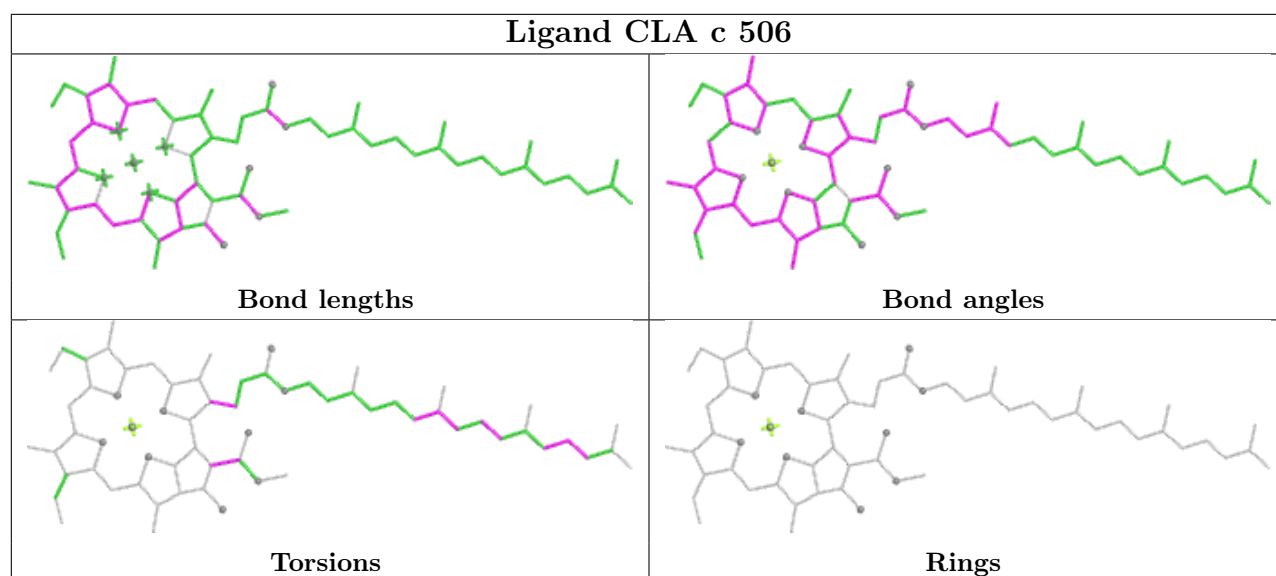
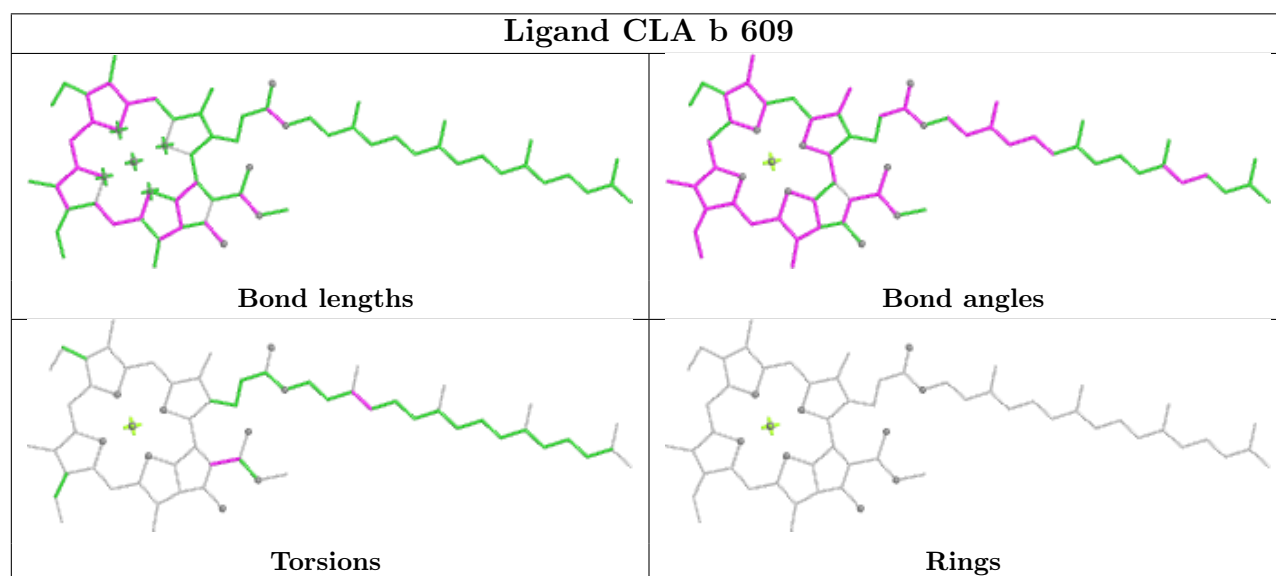
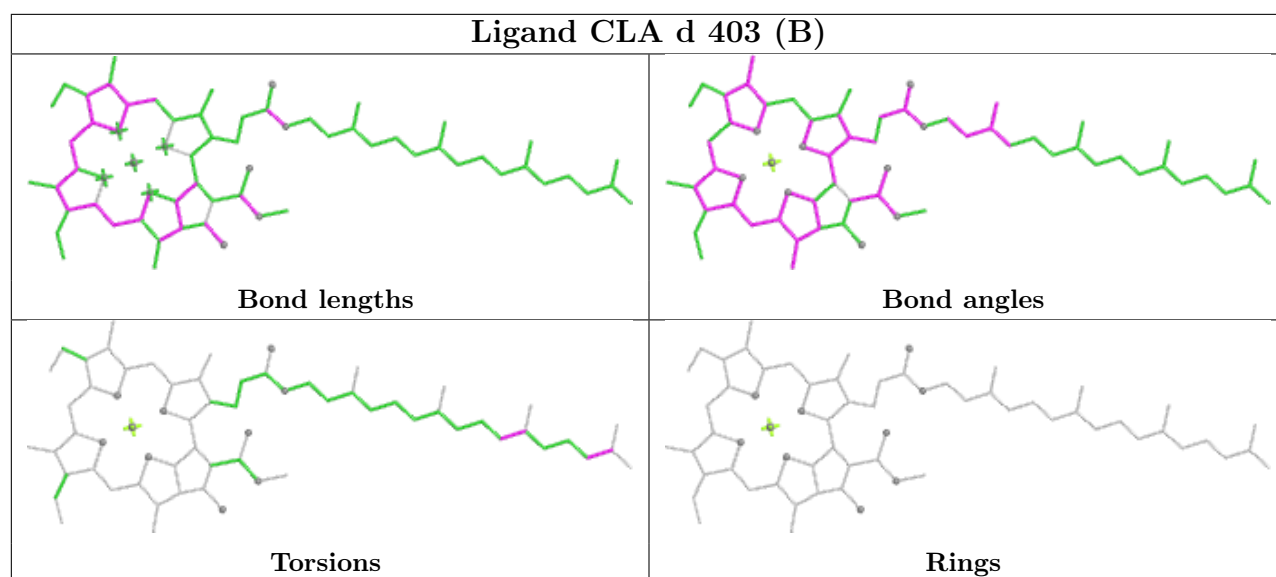


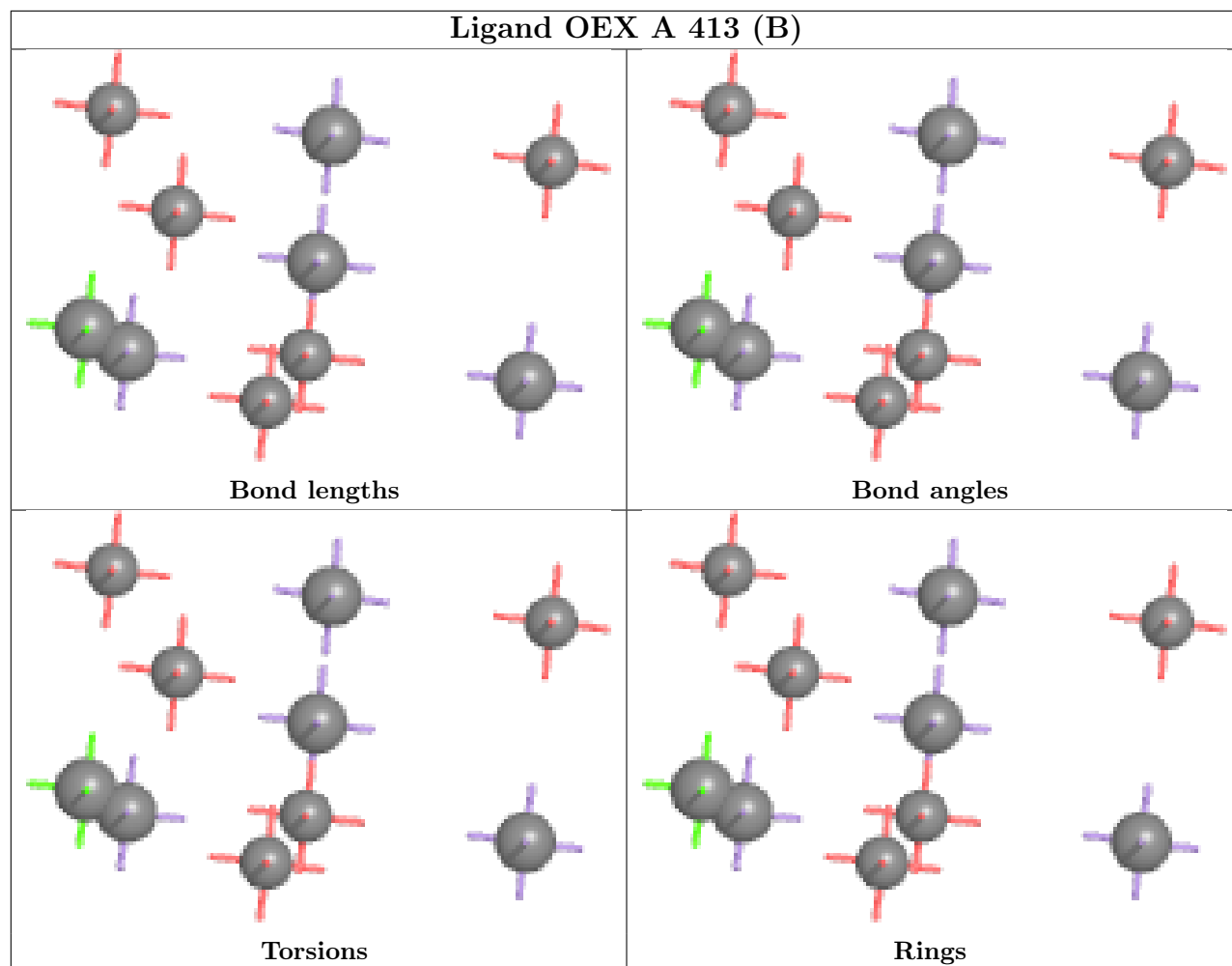




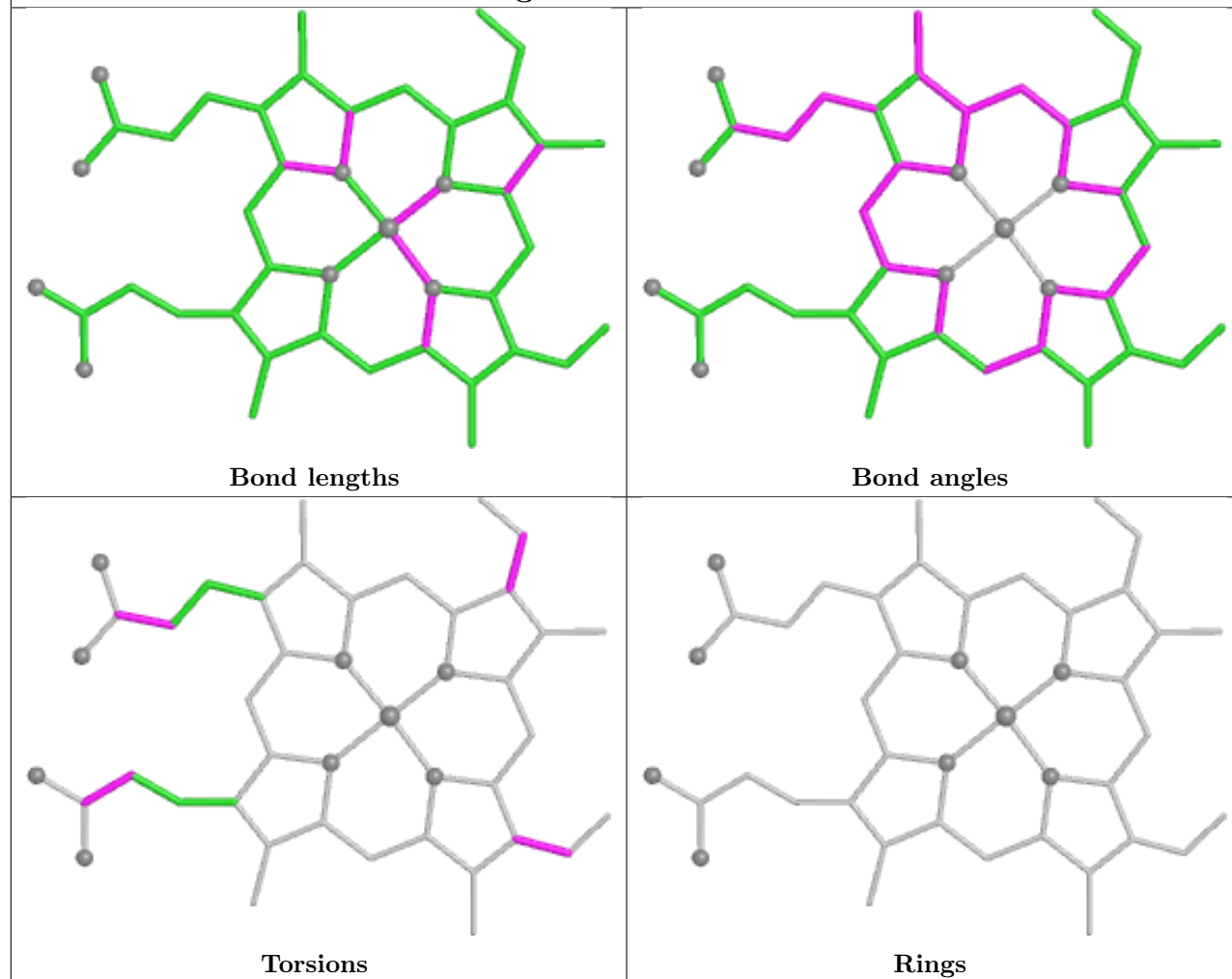




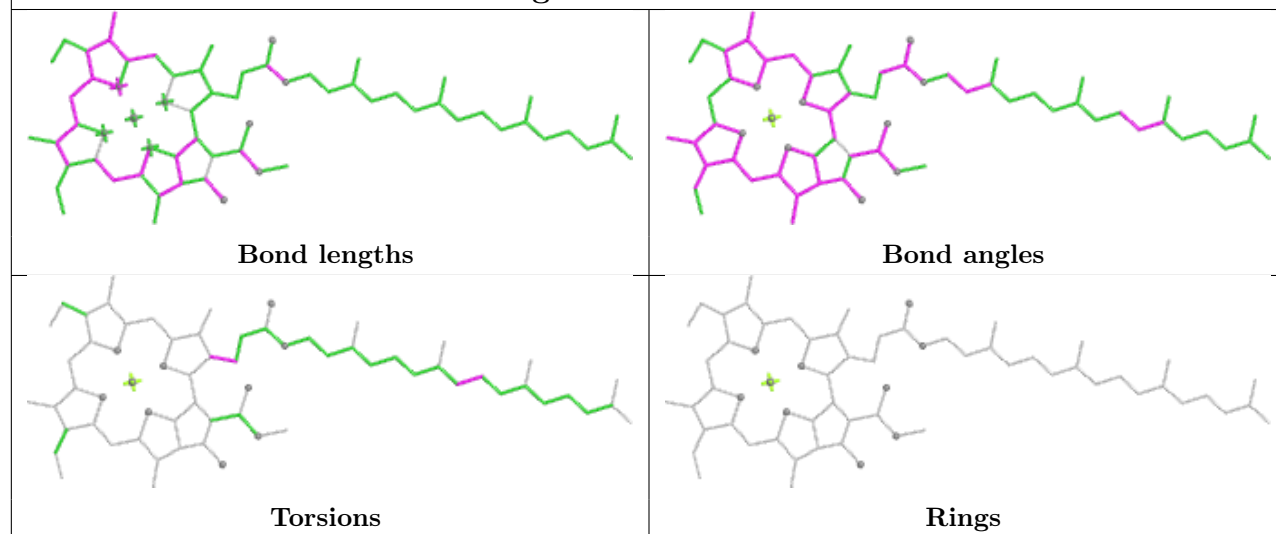


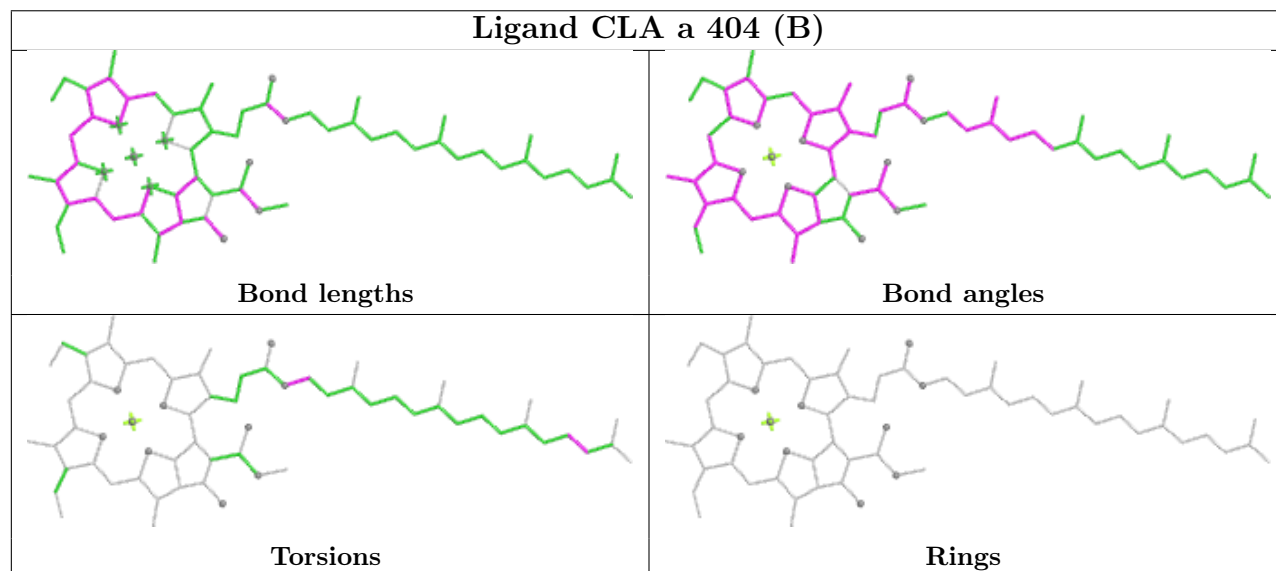
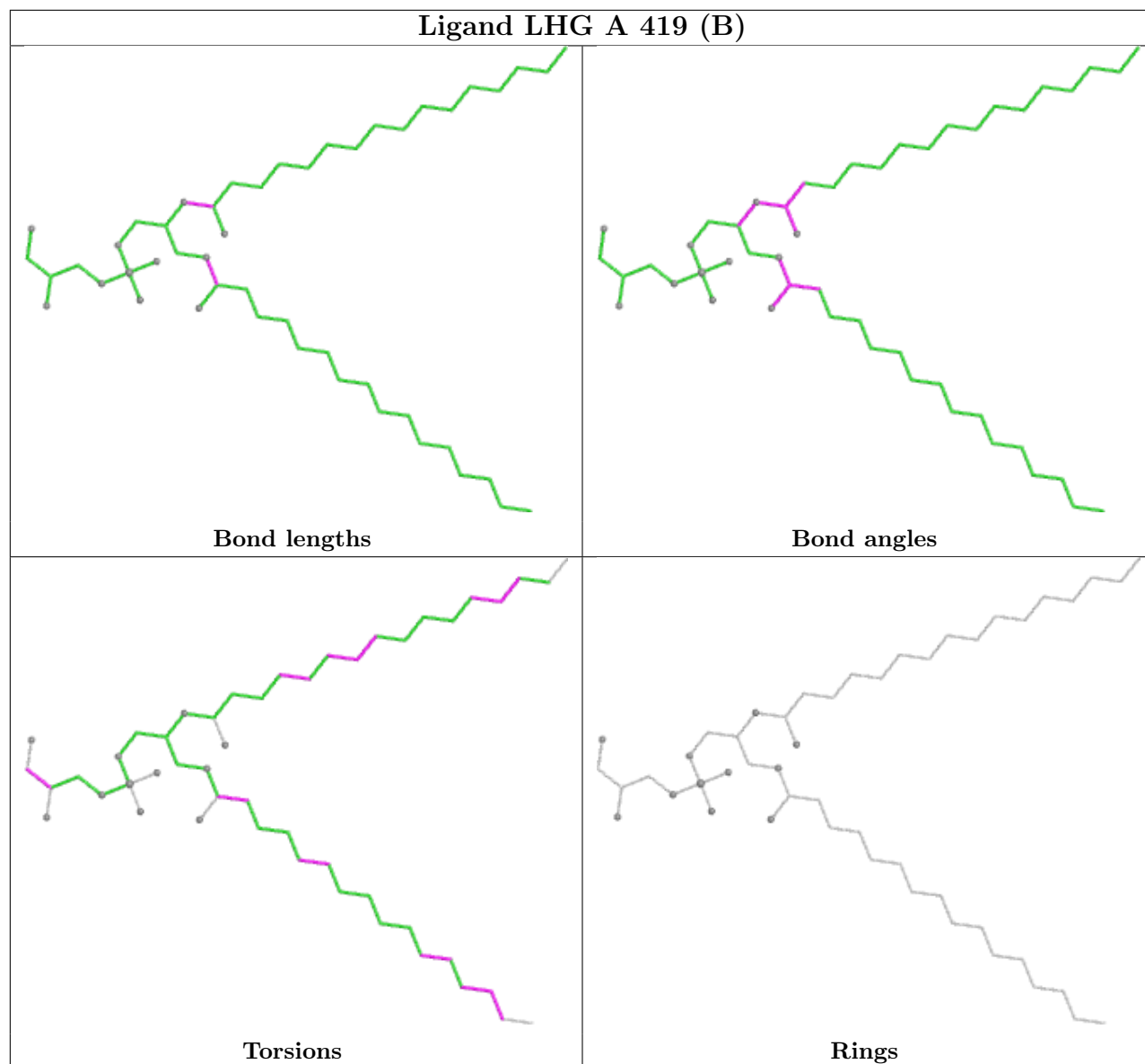


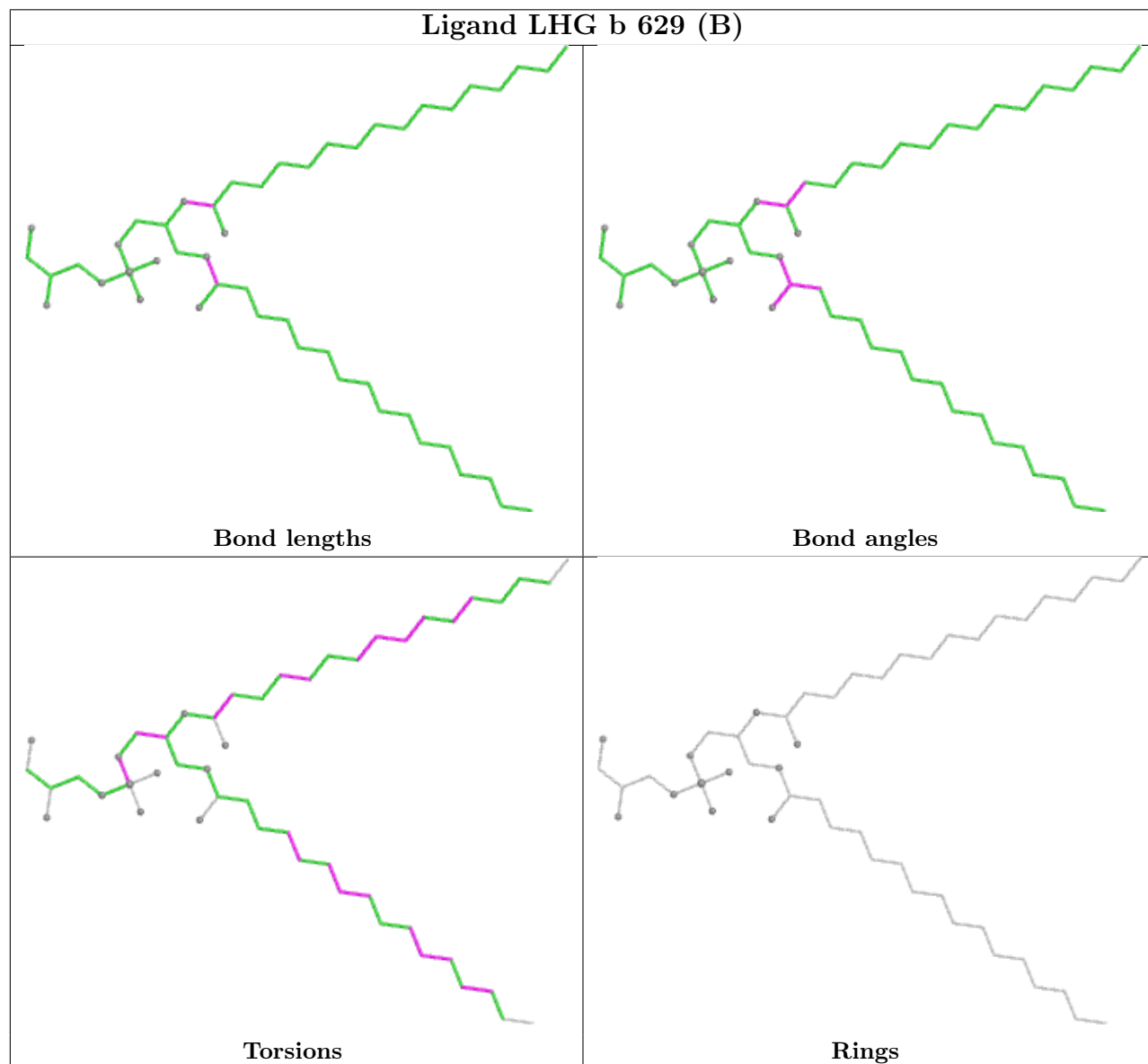
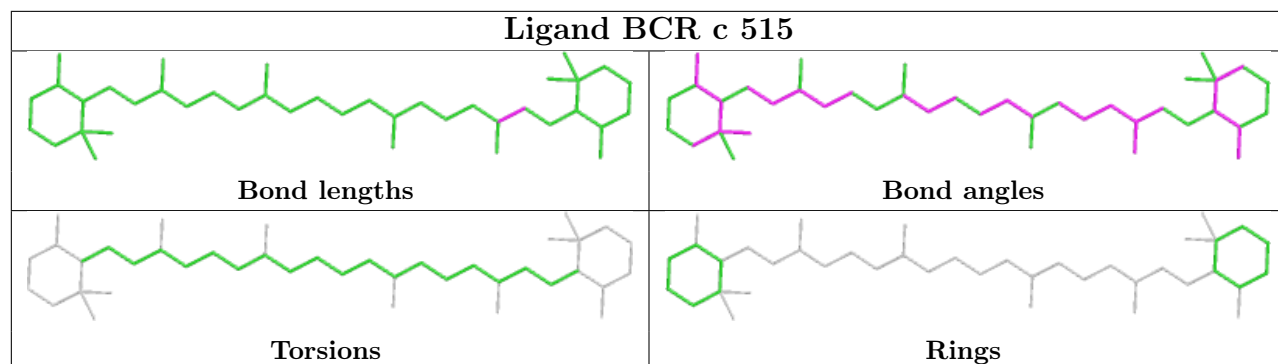
Ligand HEM f 101

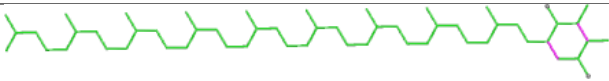
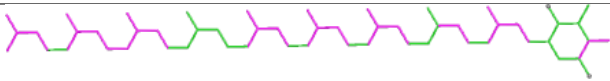
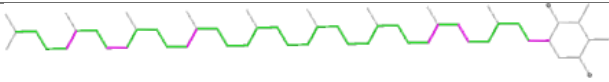
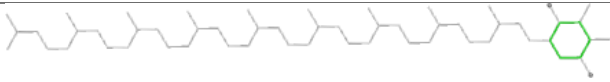


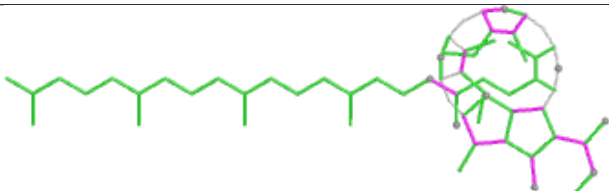
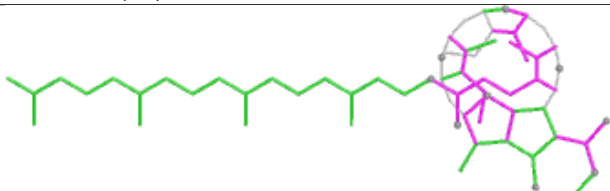
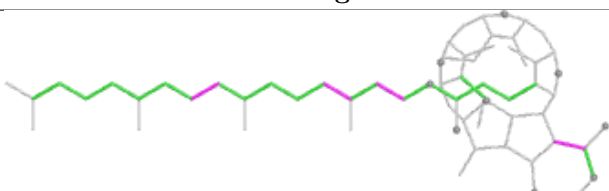
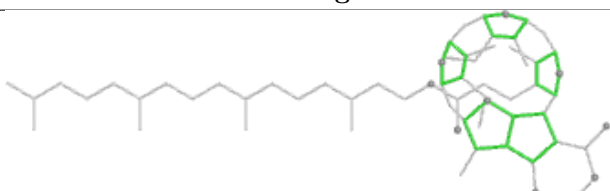
Ligand CLA B 611

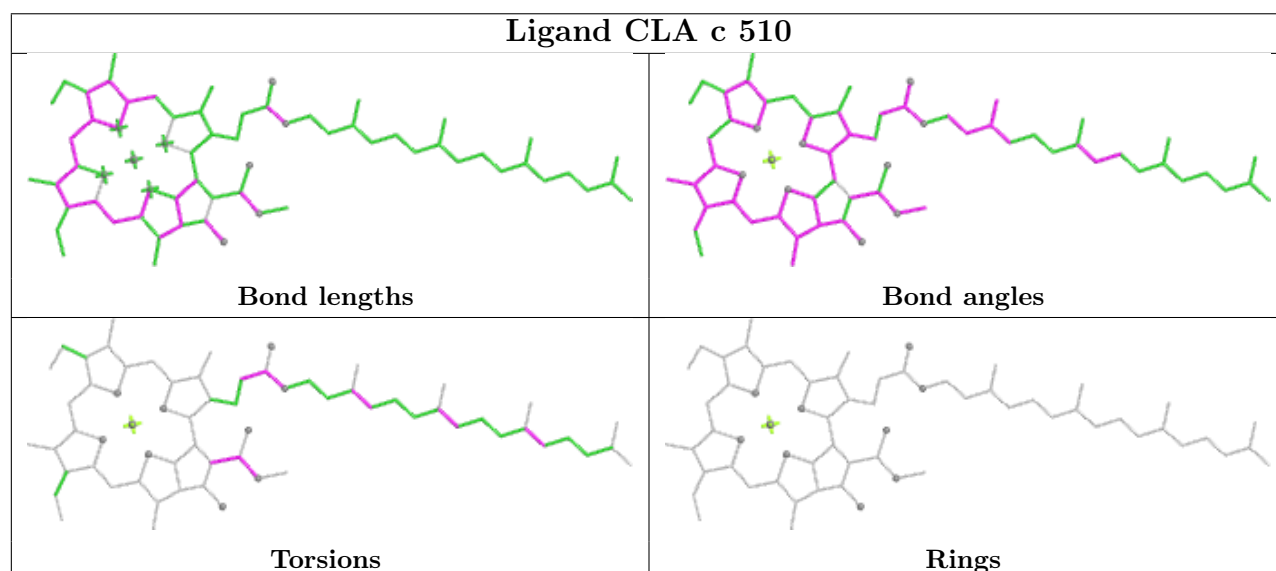
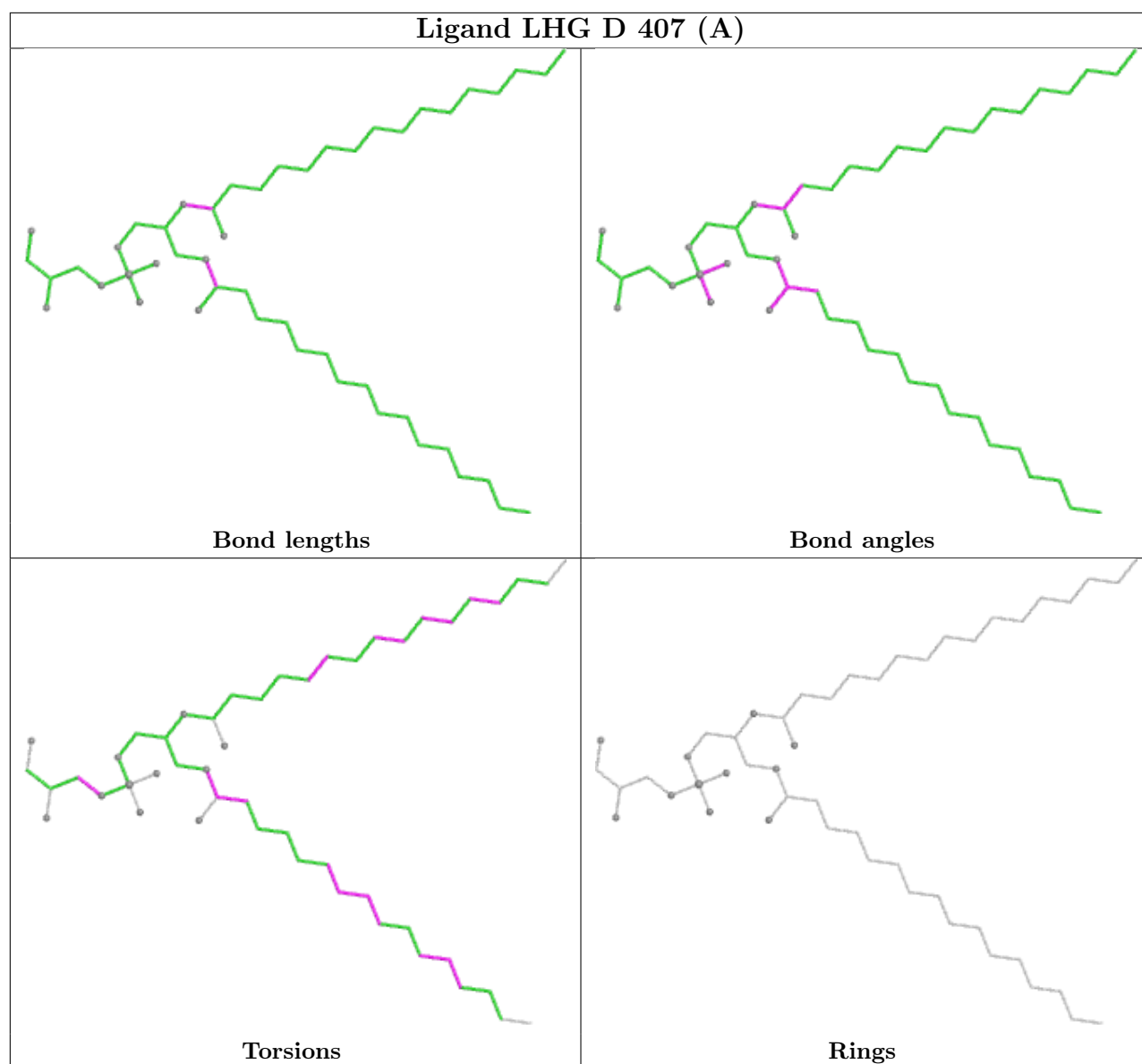


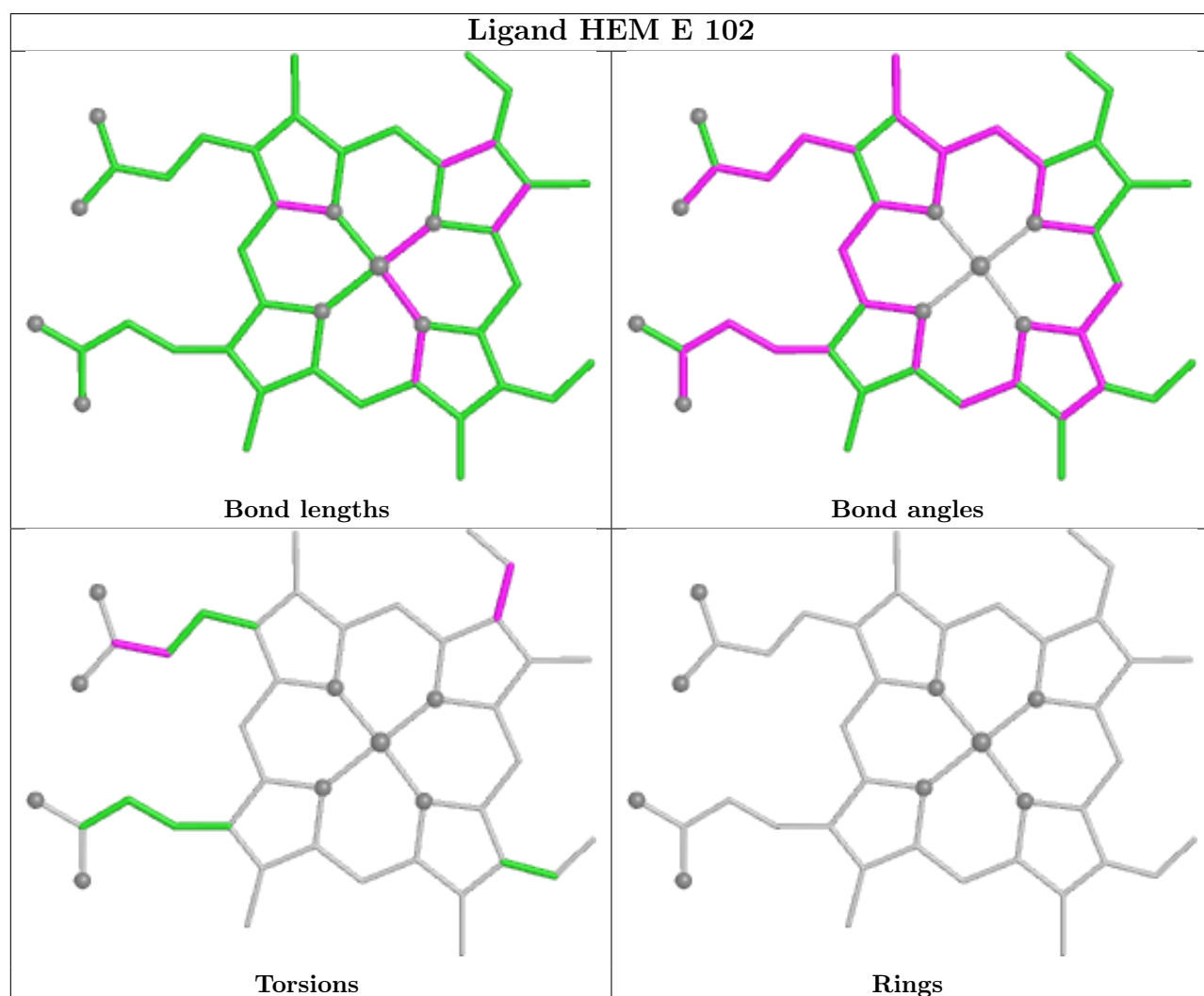
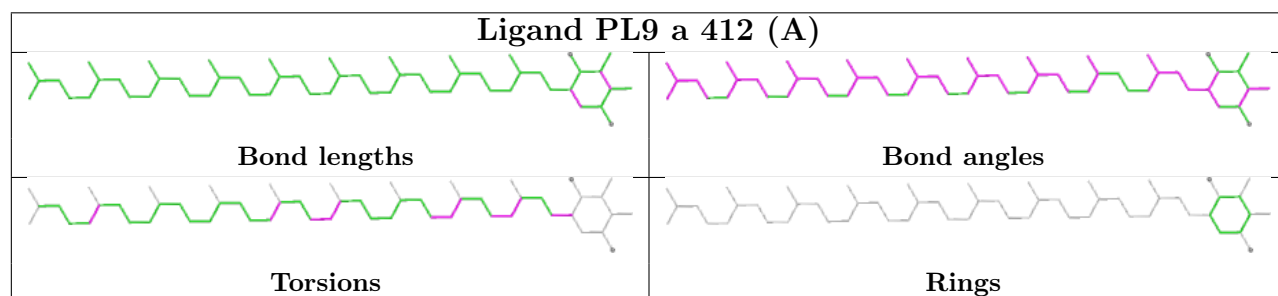
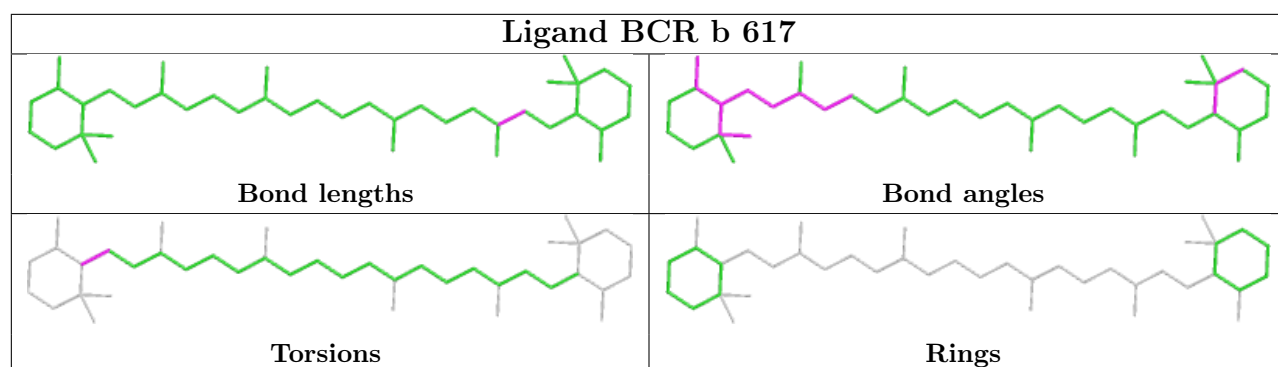


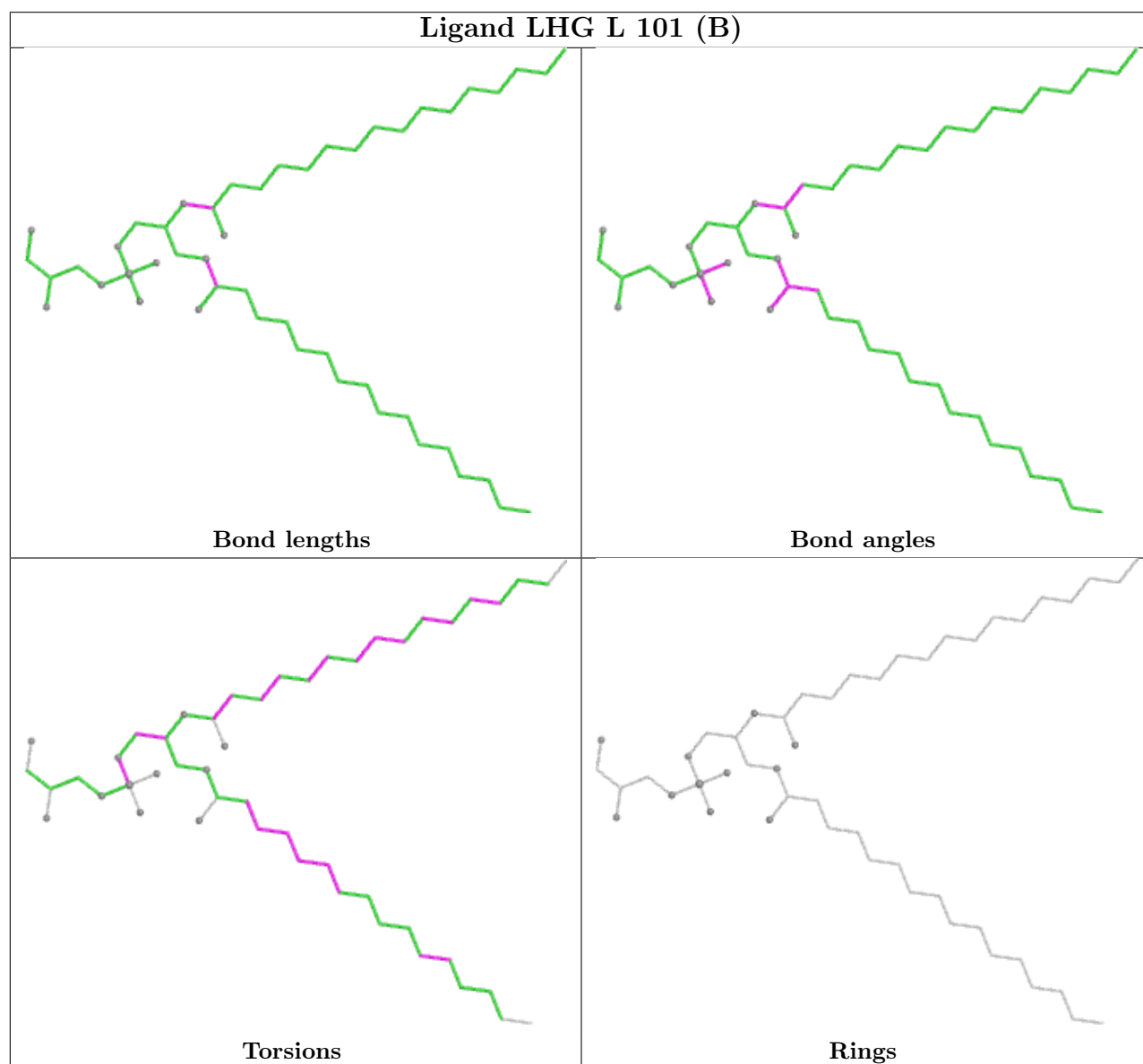
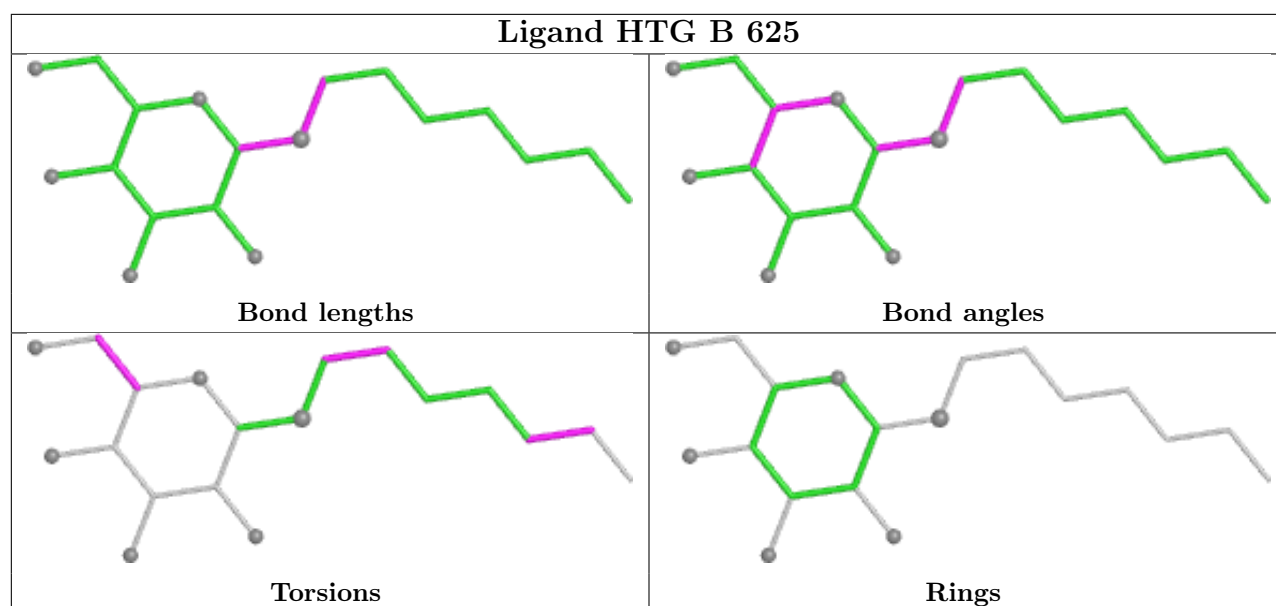


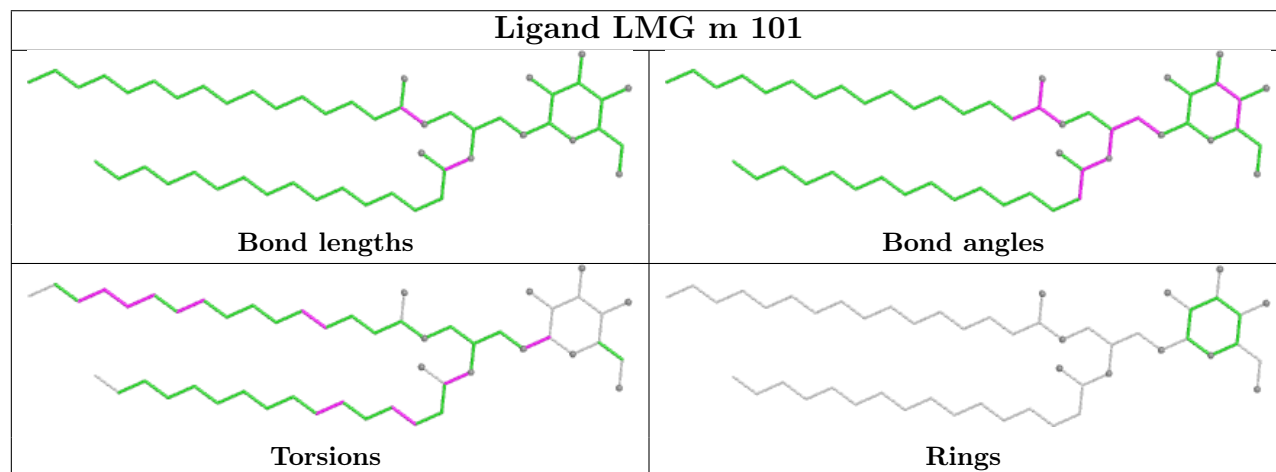
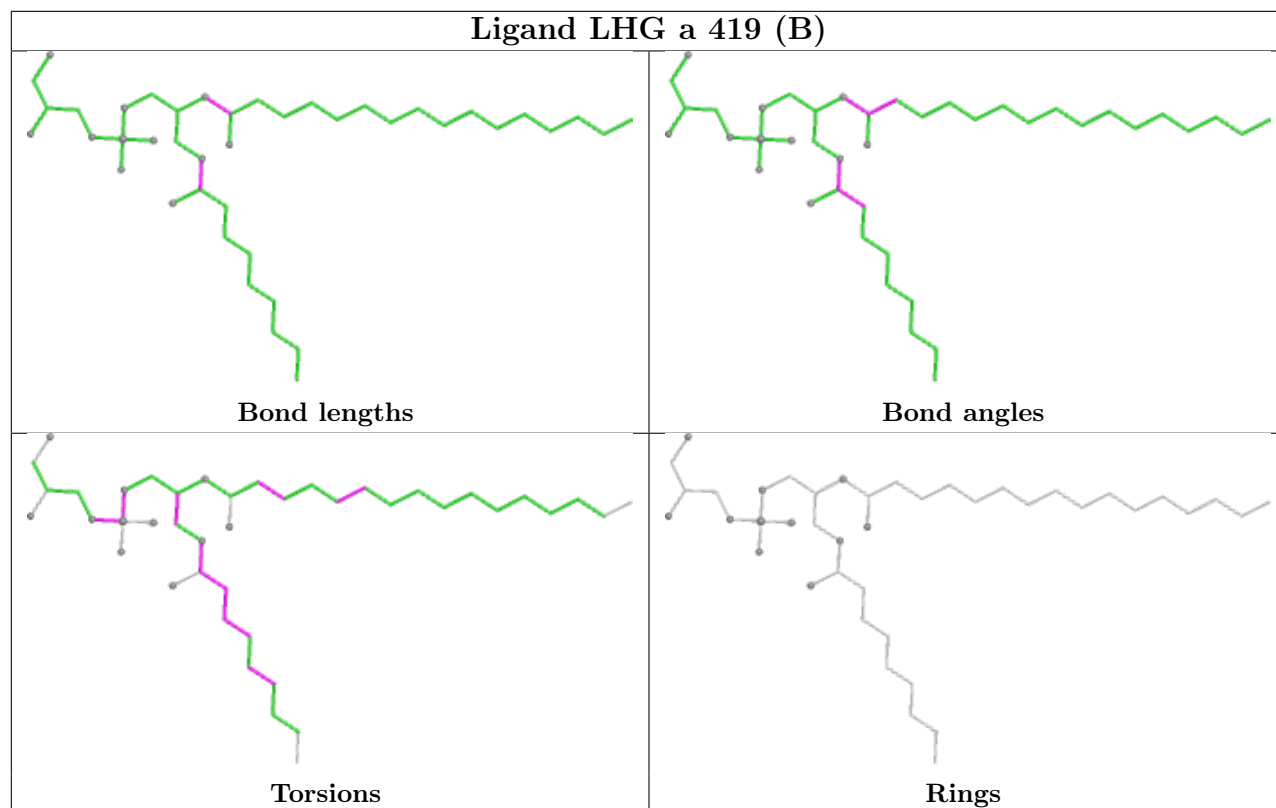
Ligand PL9 D 405 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings

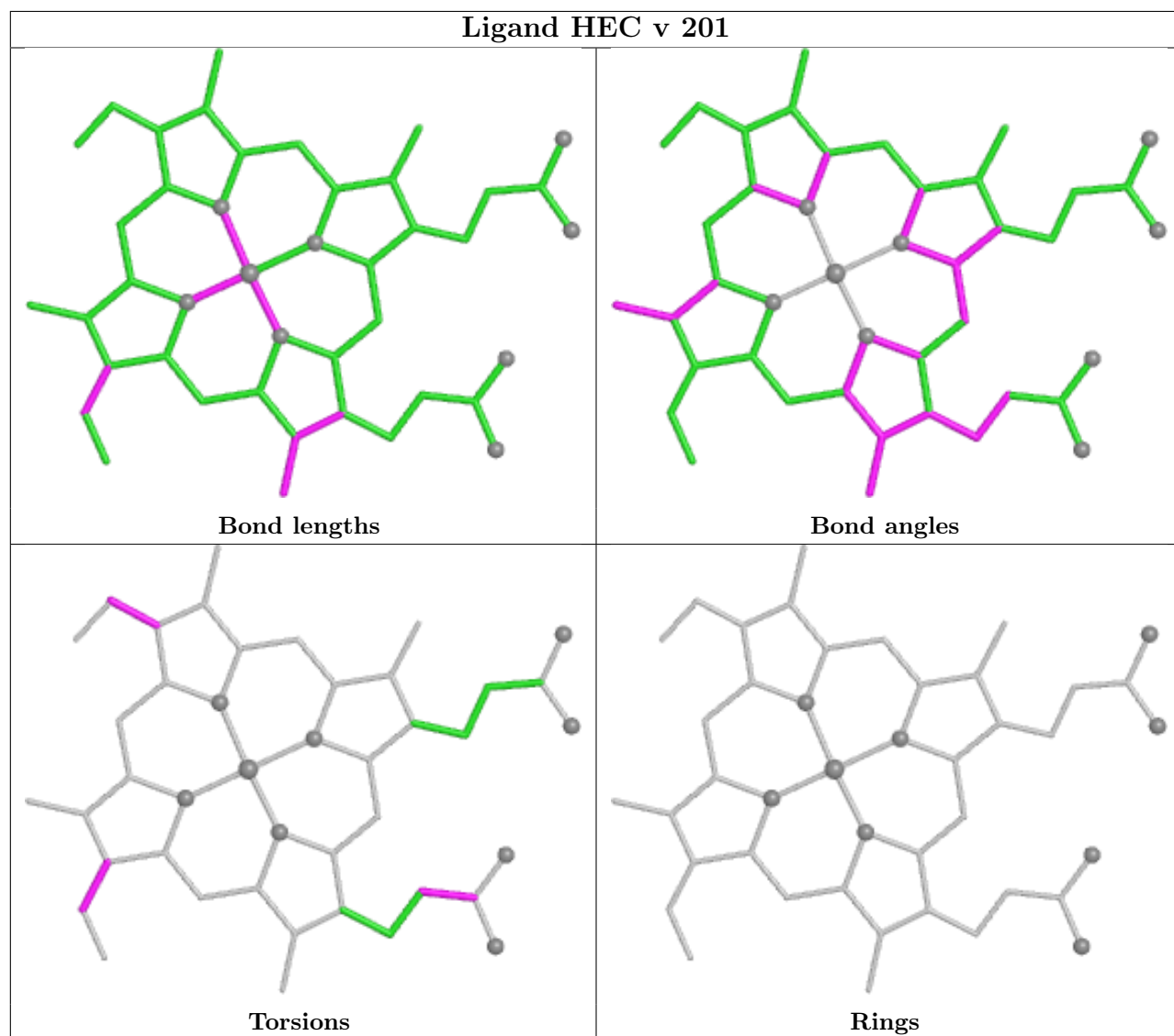
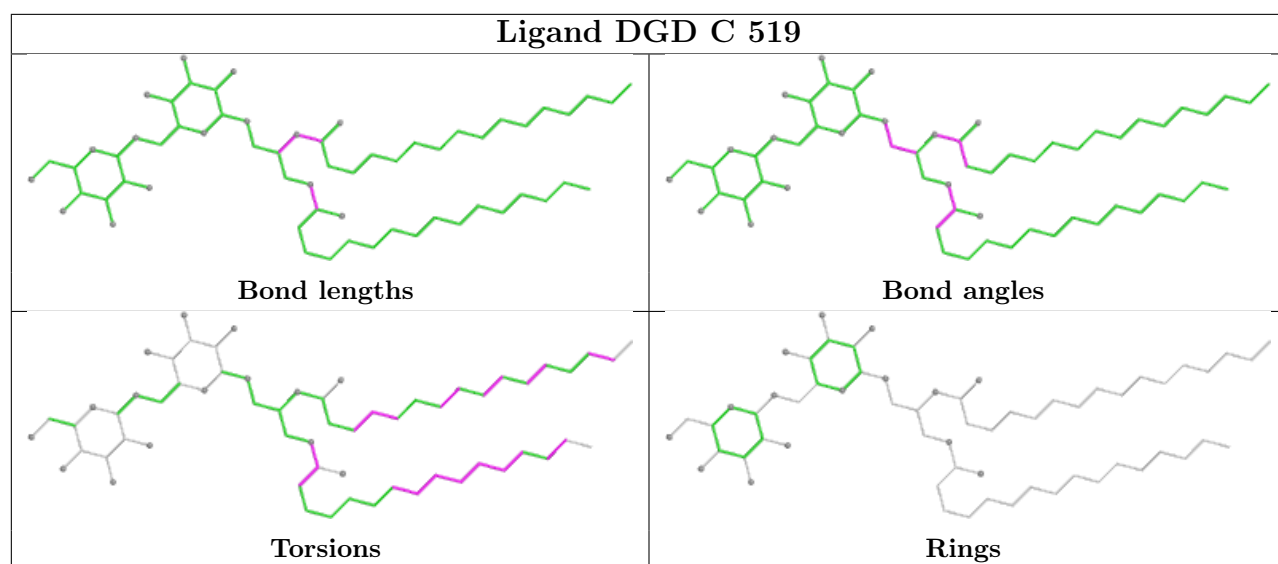
Ligand PHO a 406 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings

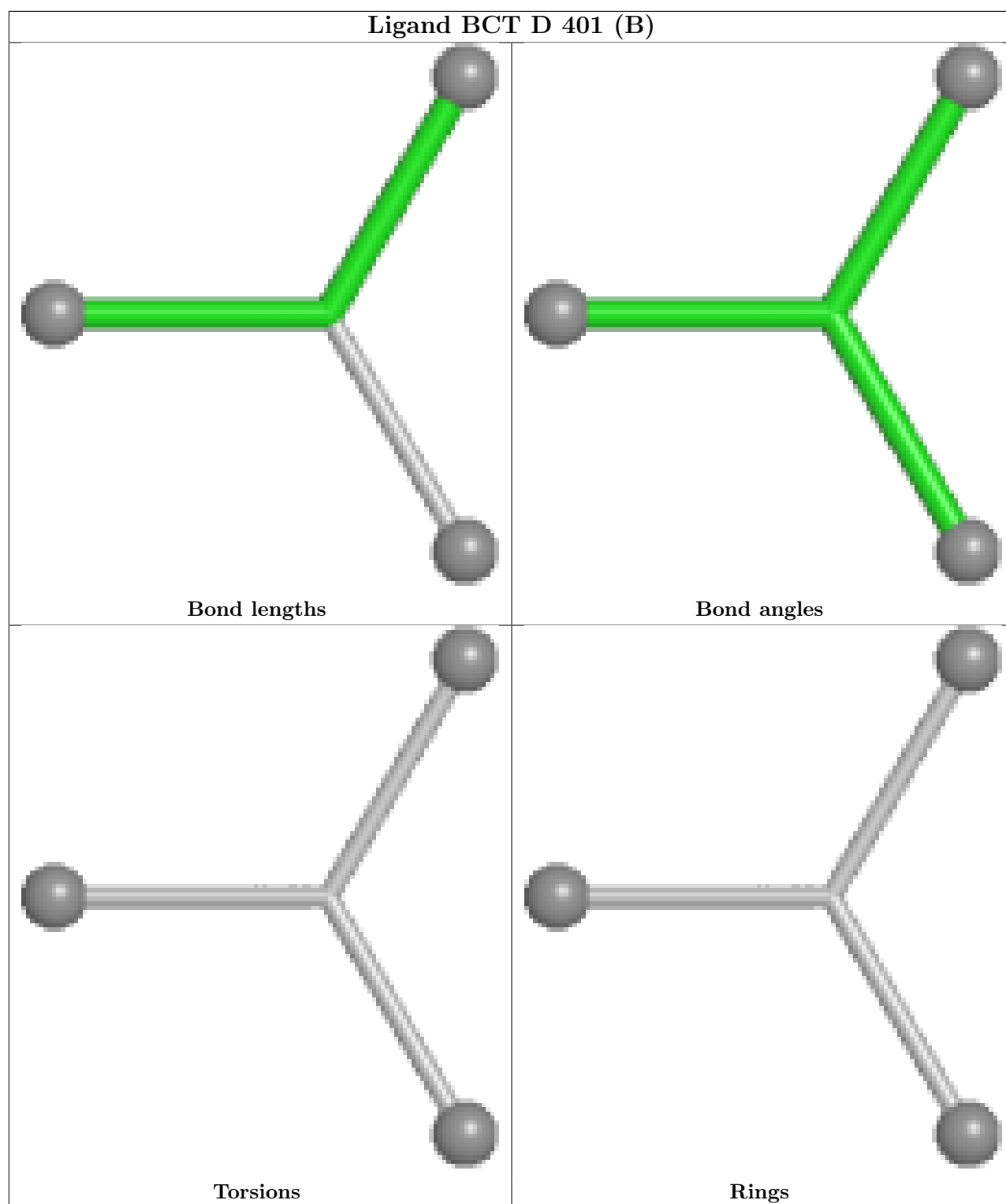


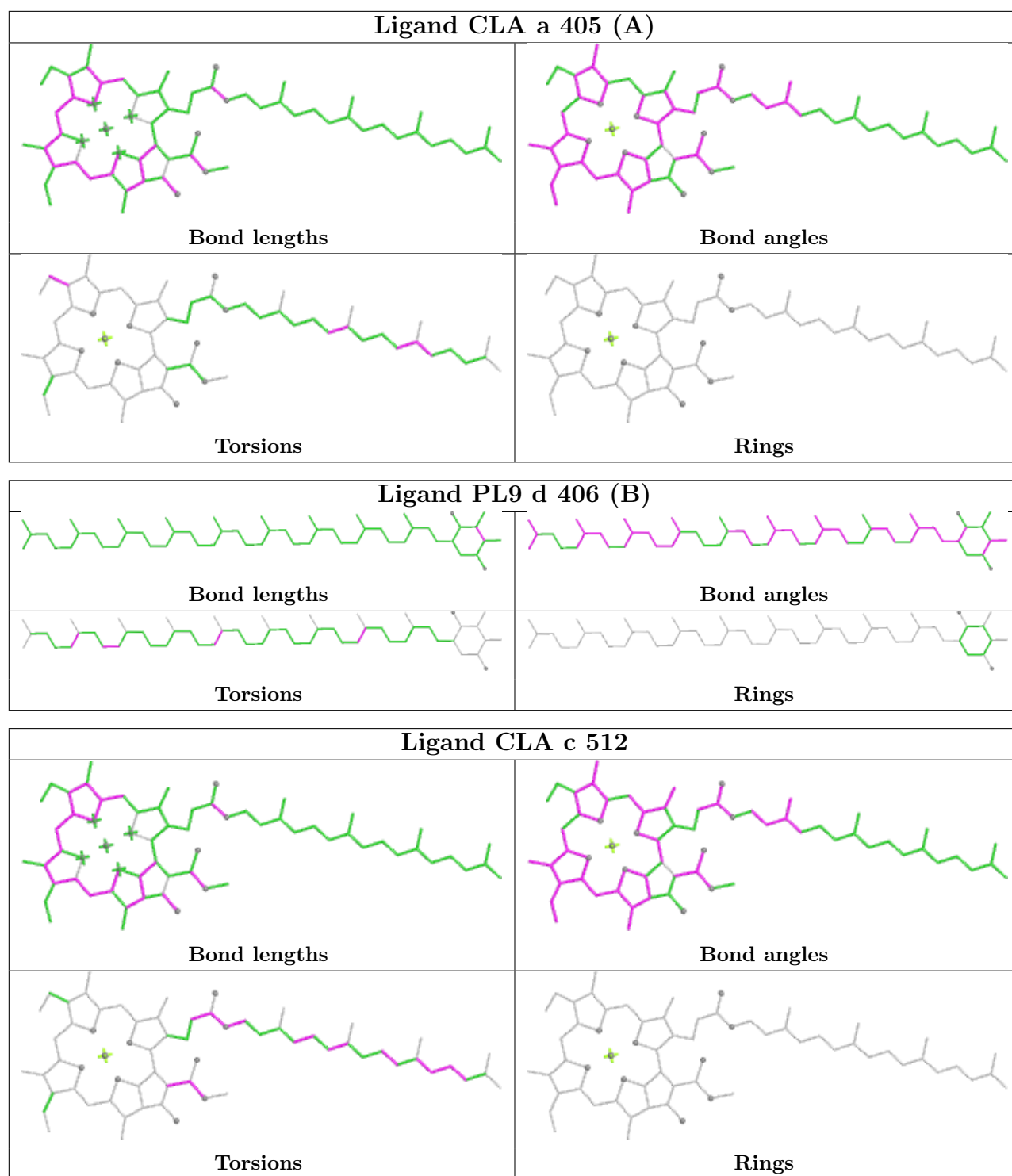


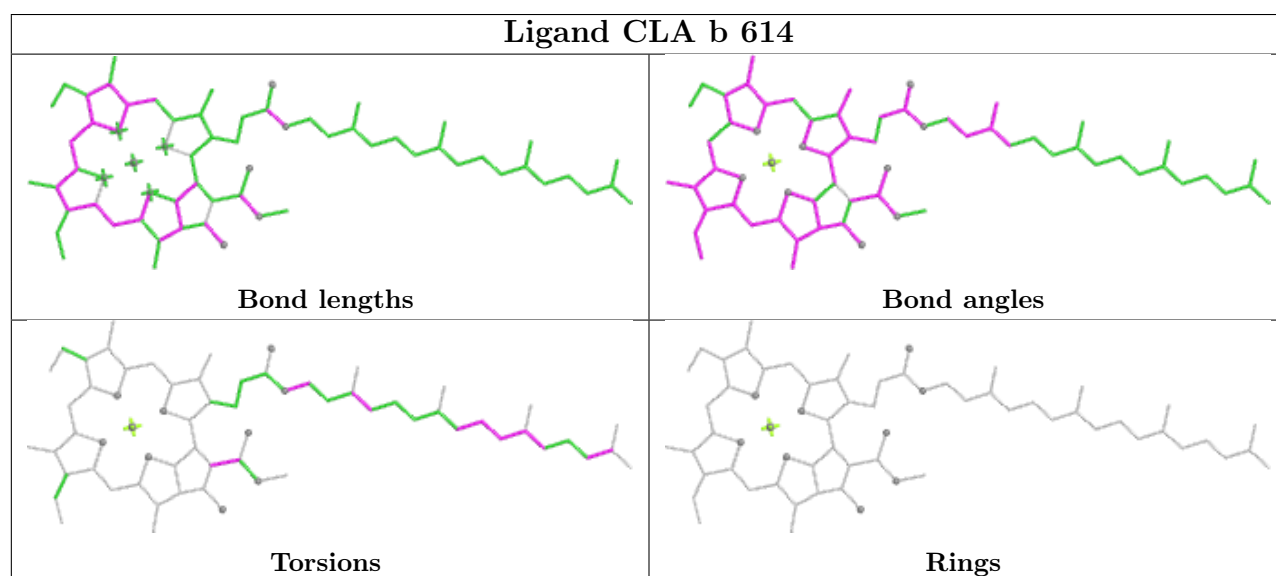
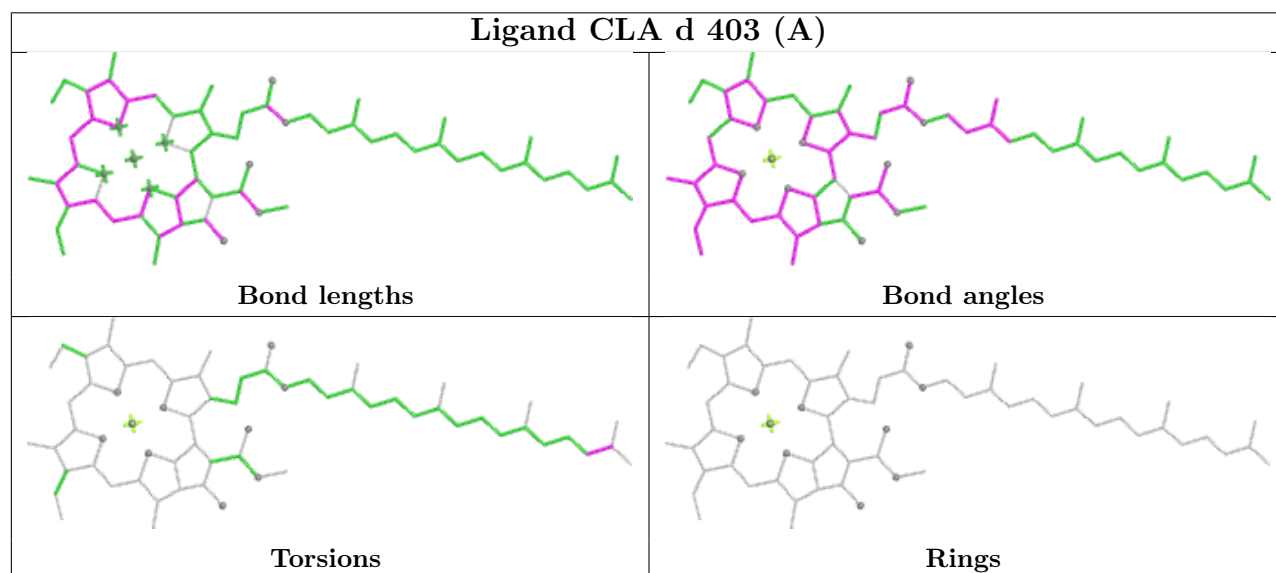
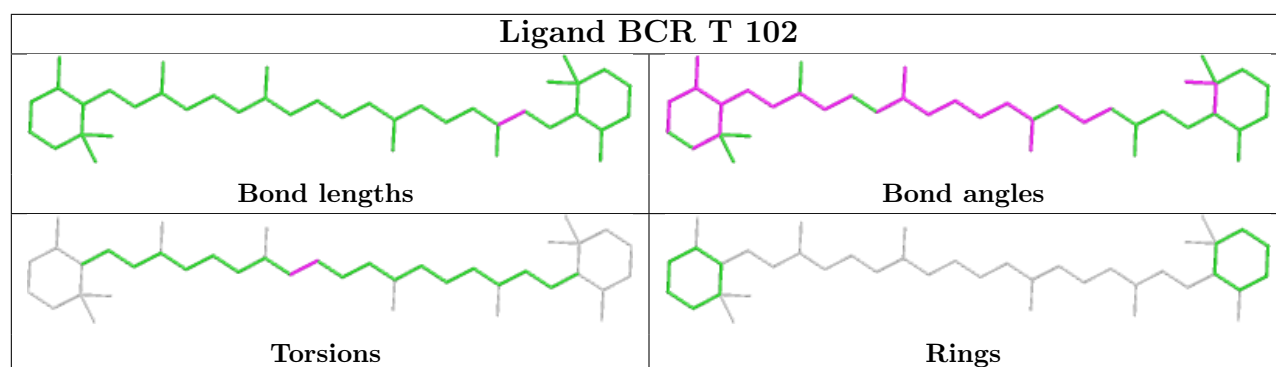


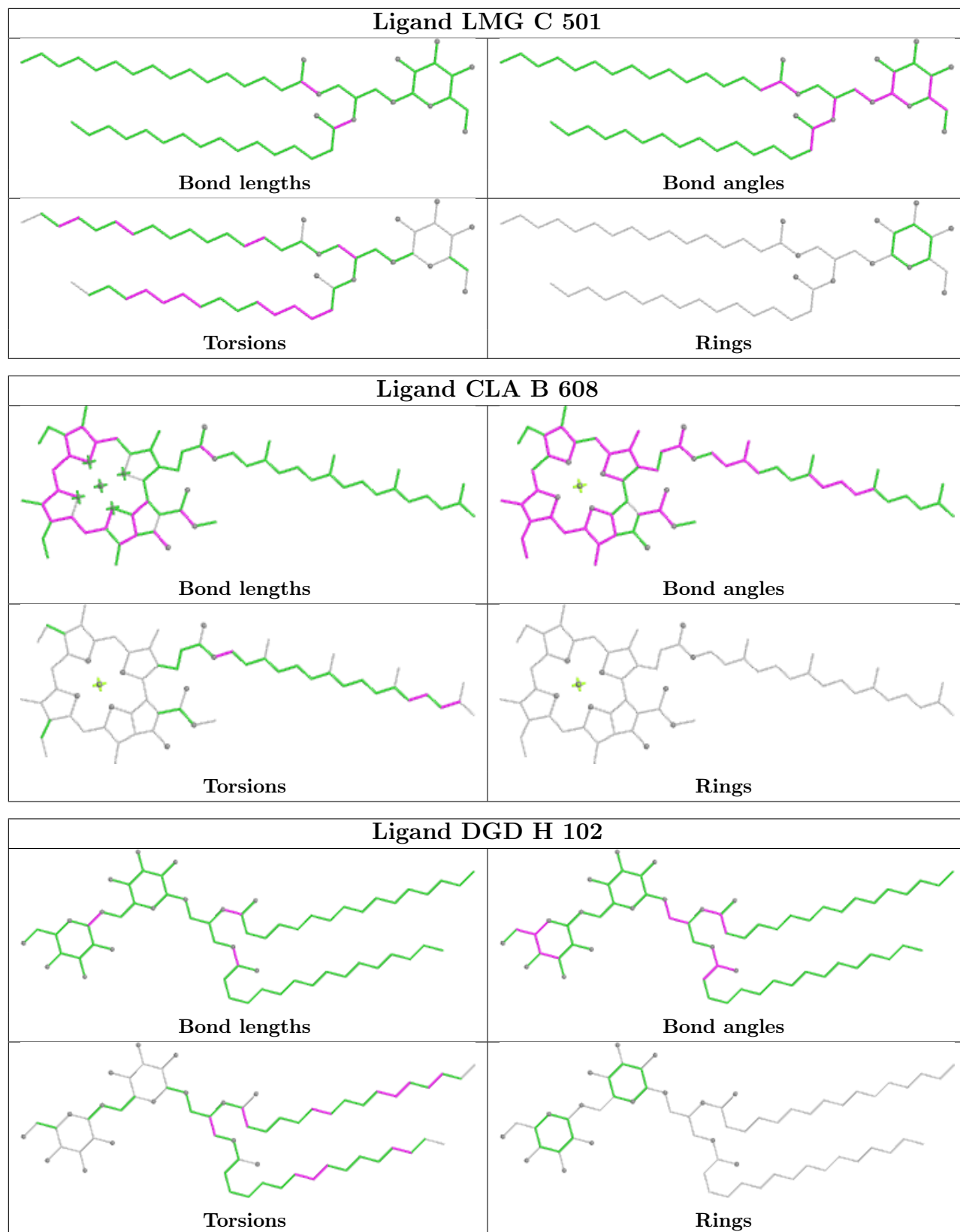


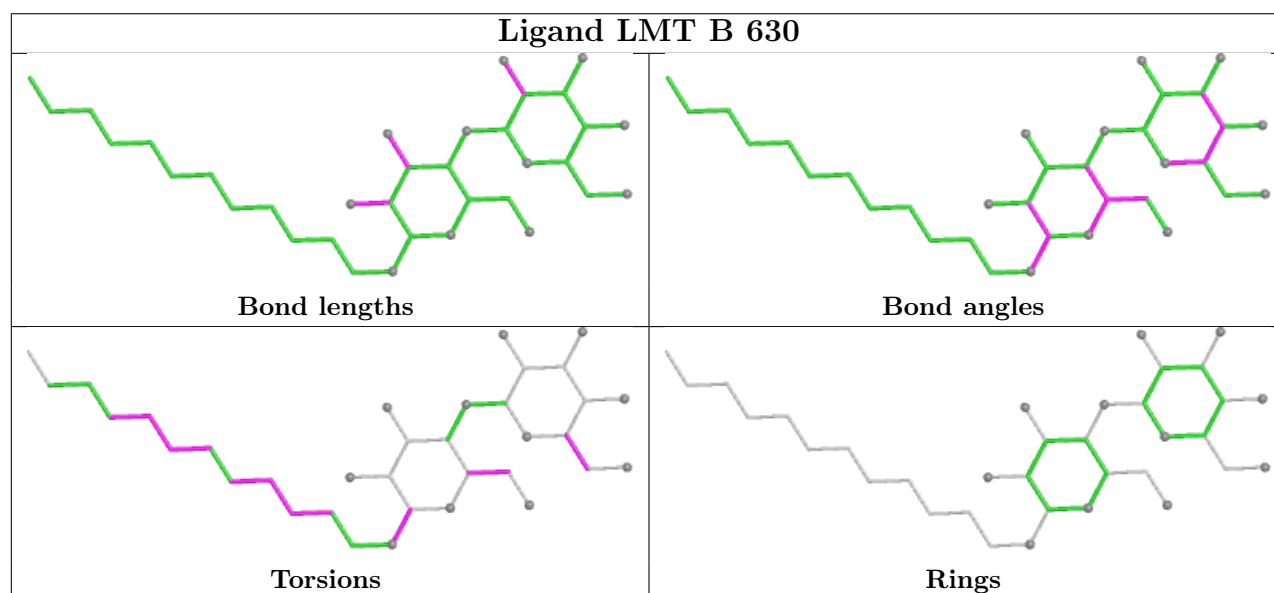
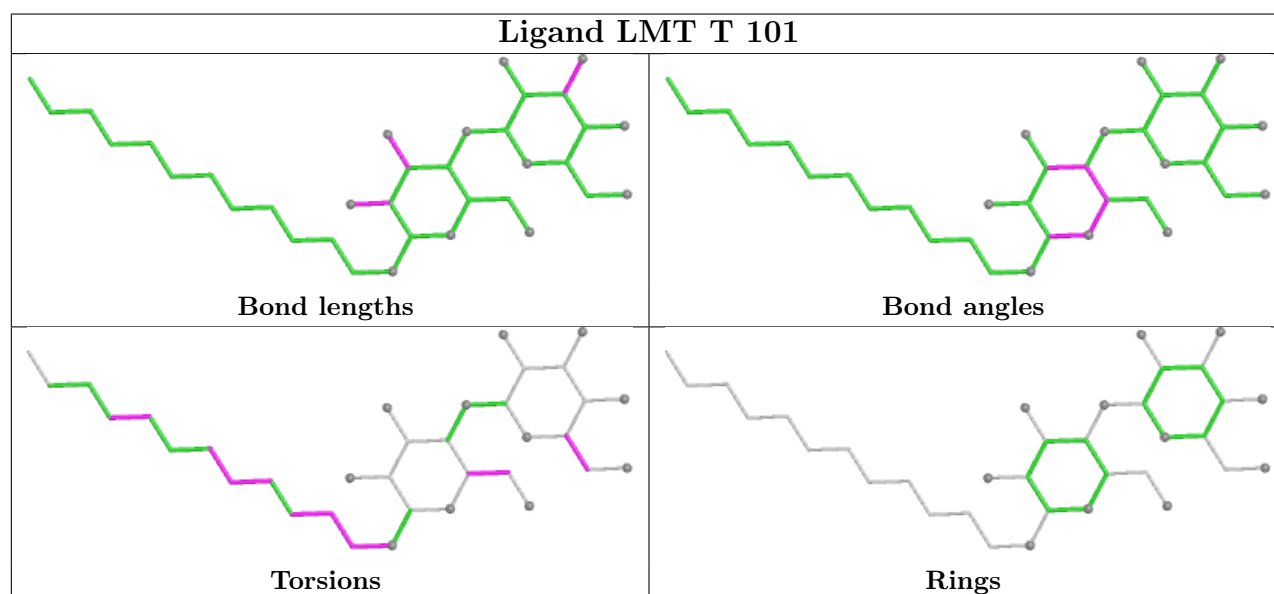
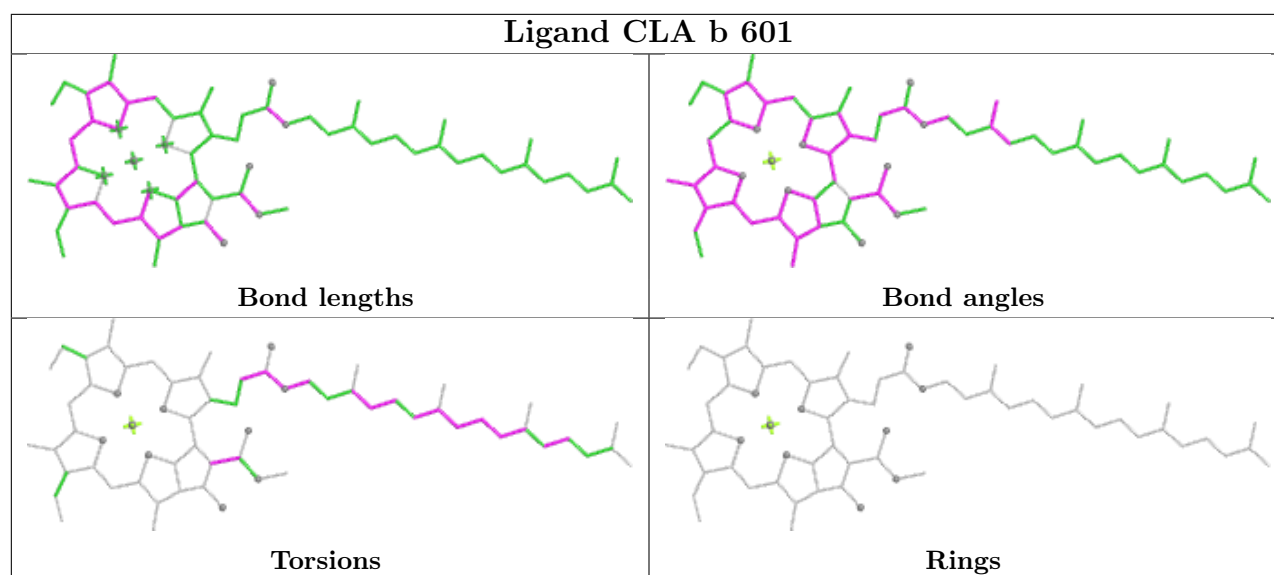


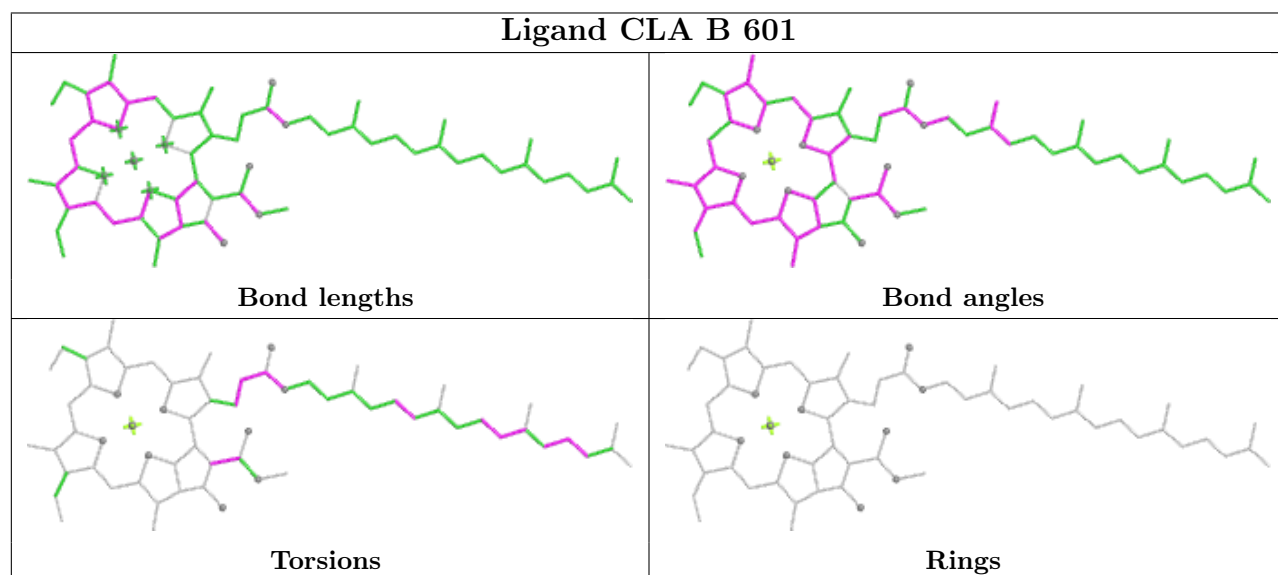
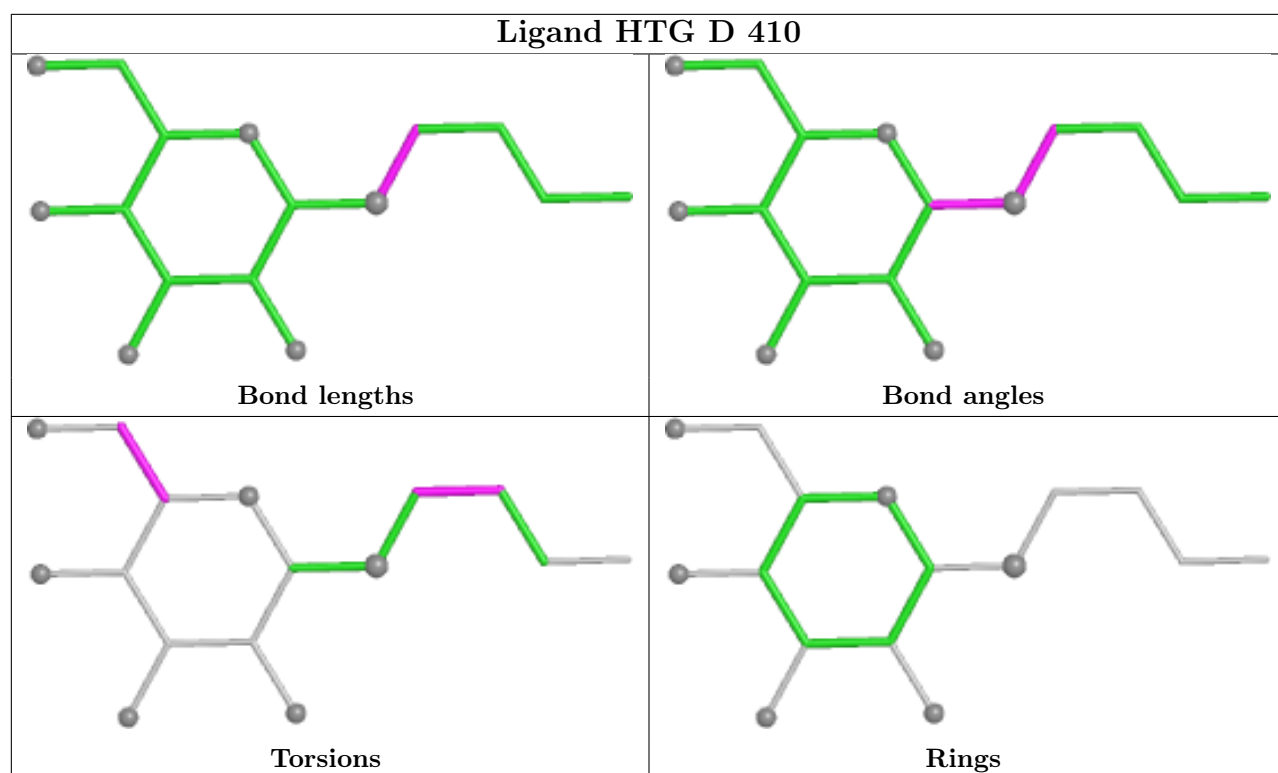


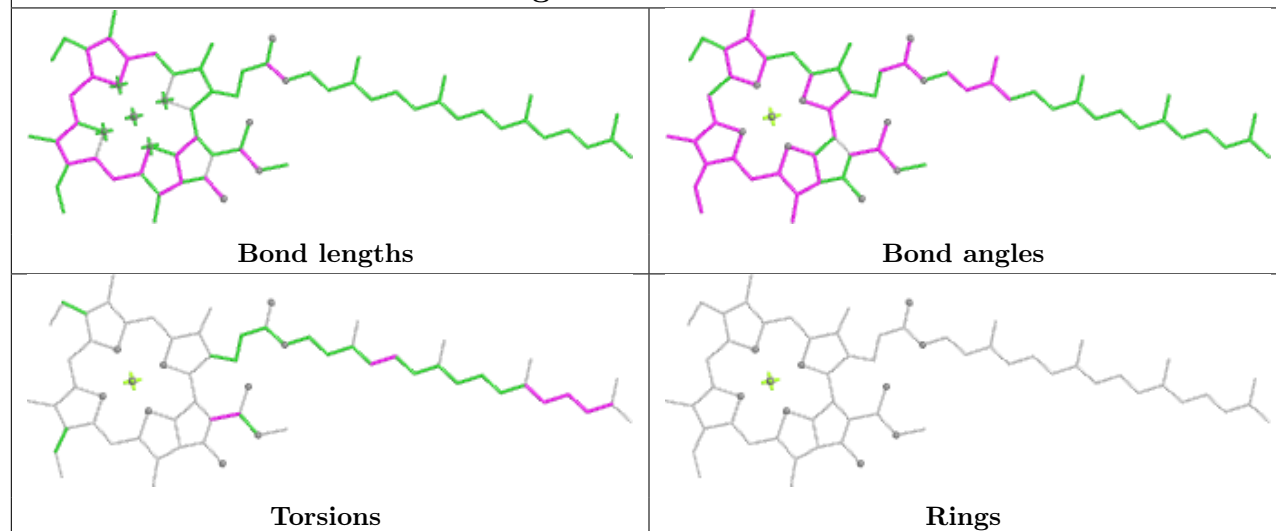
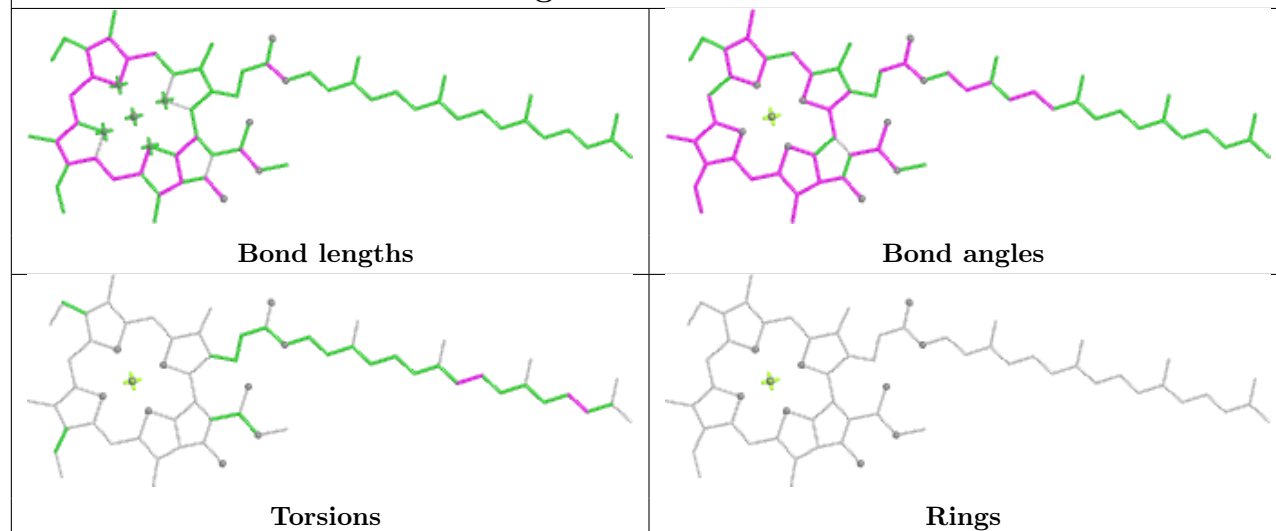


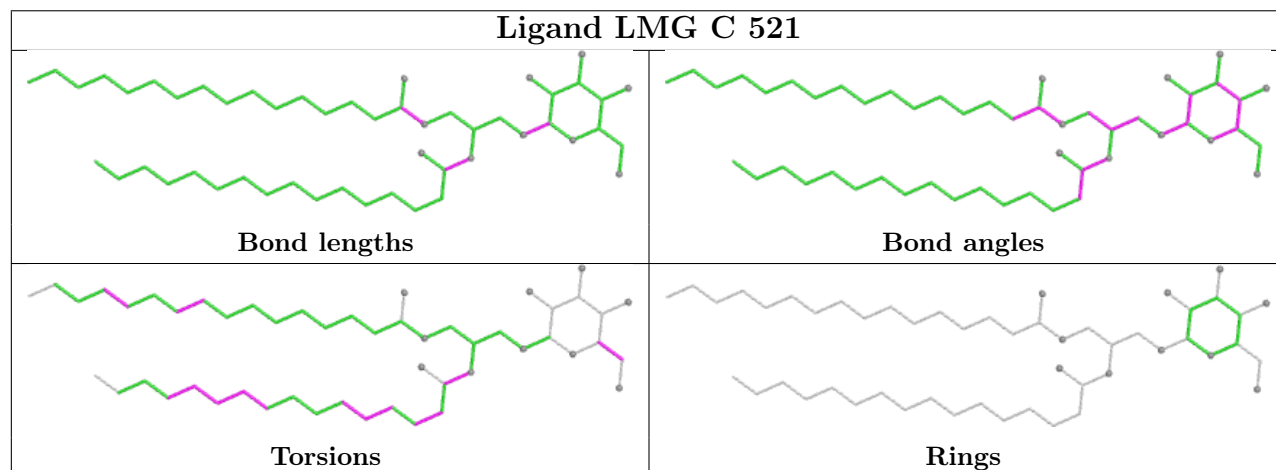
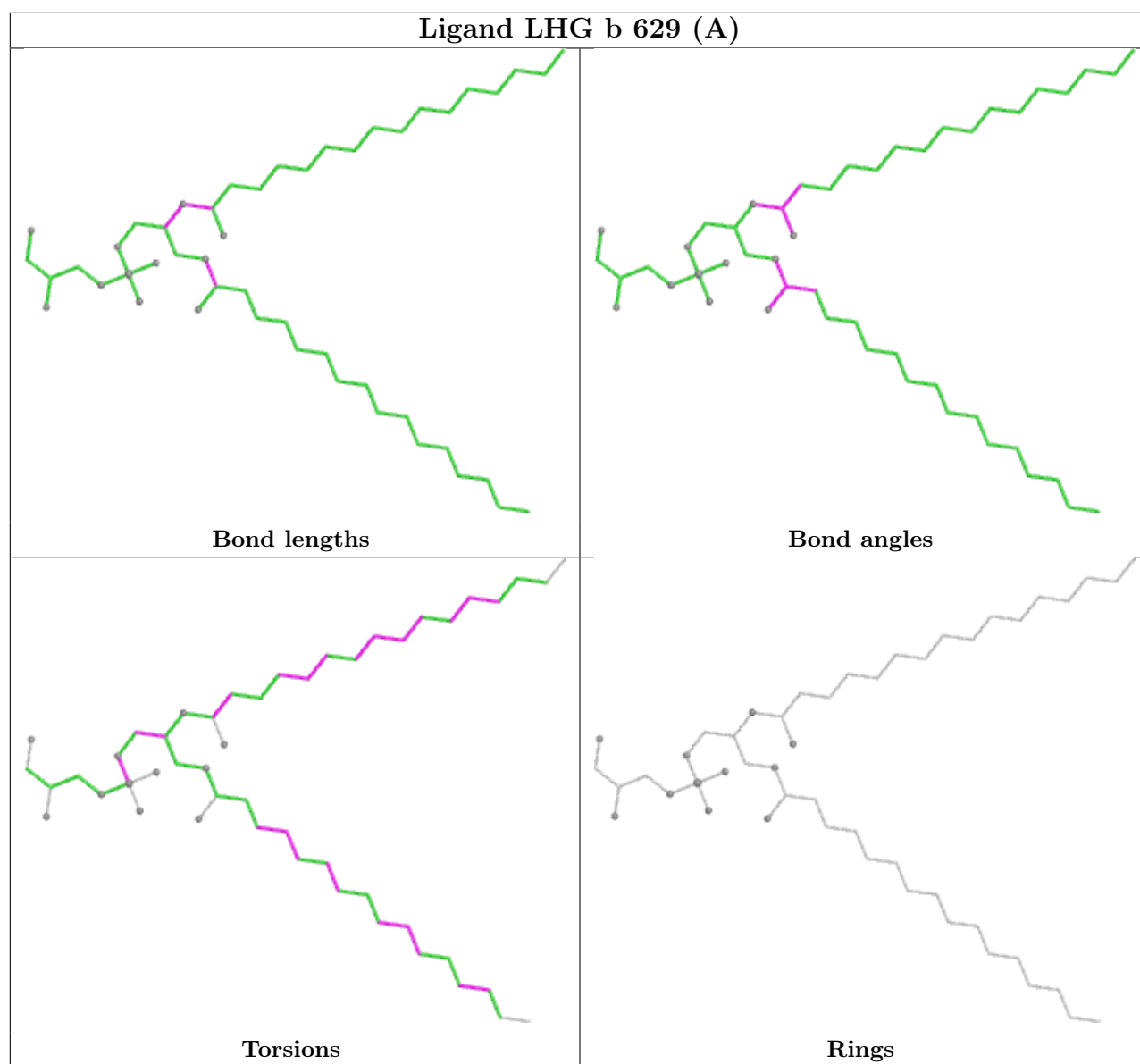


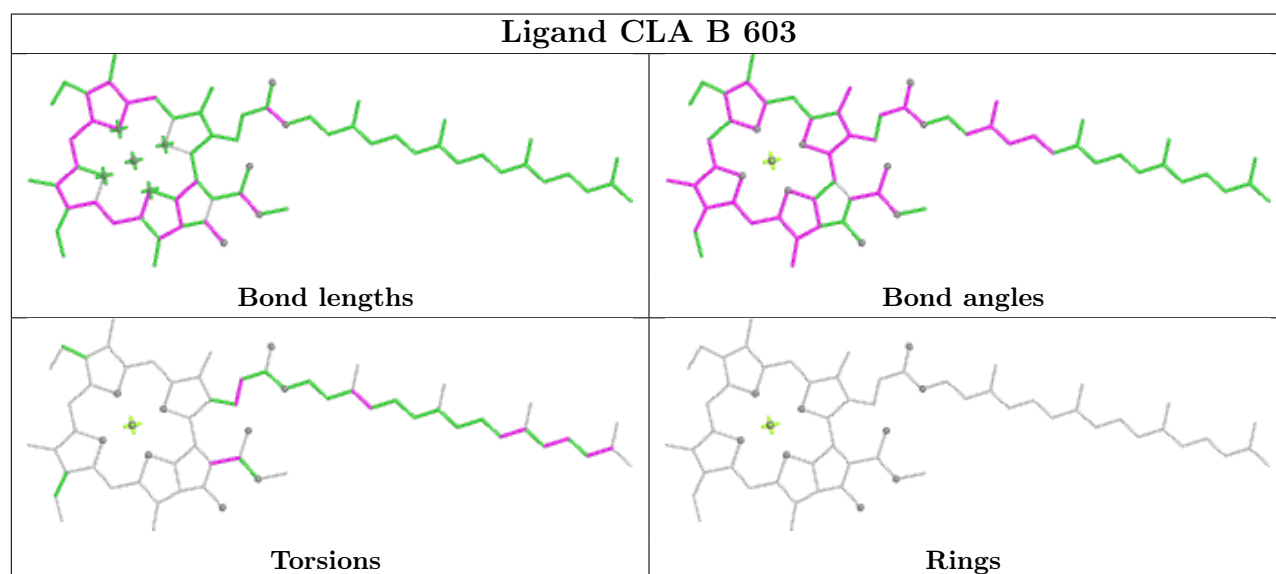
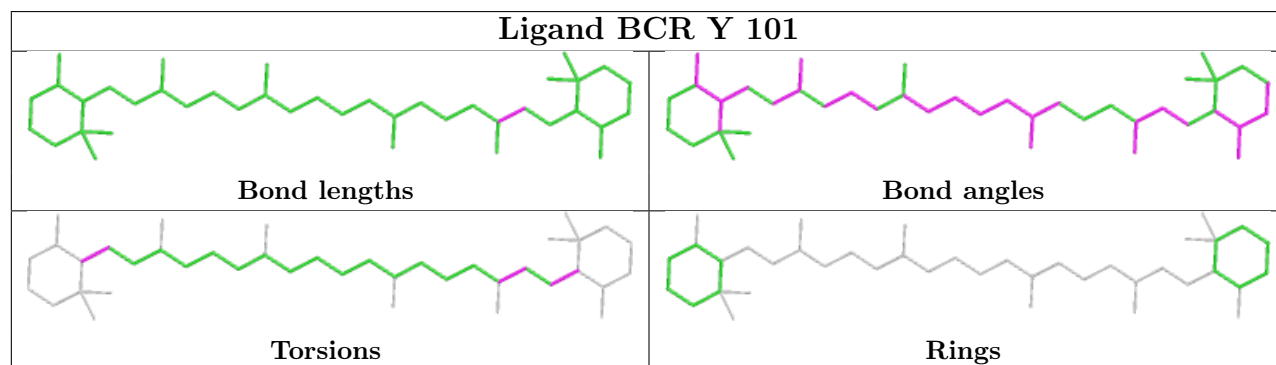
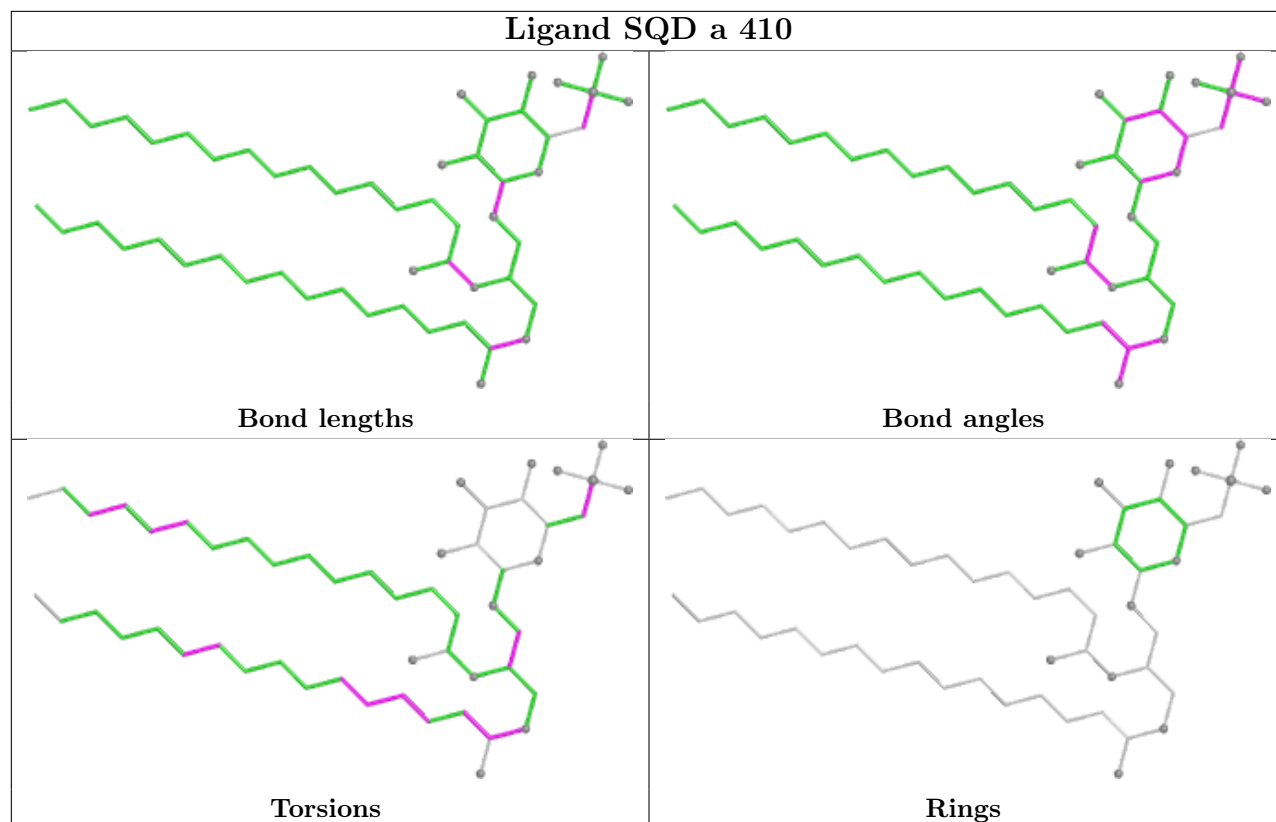


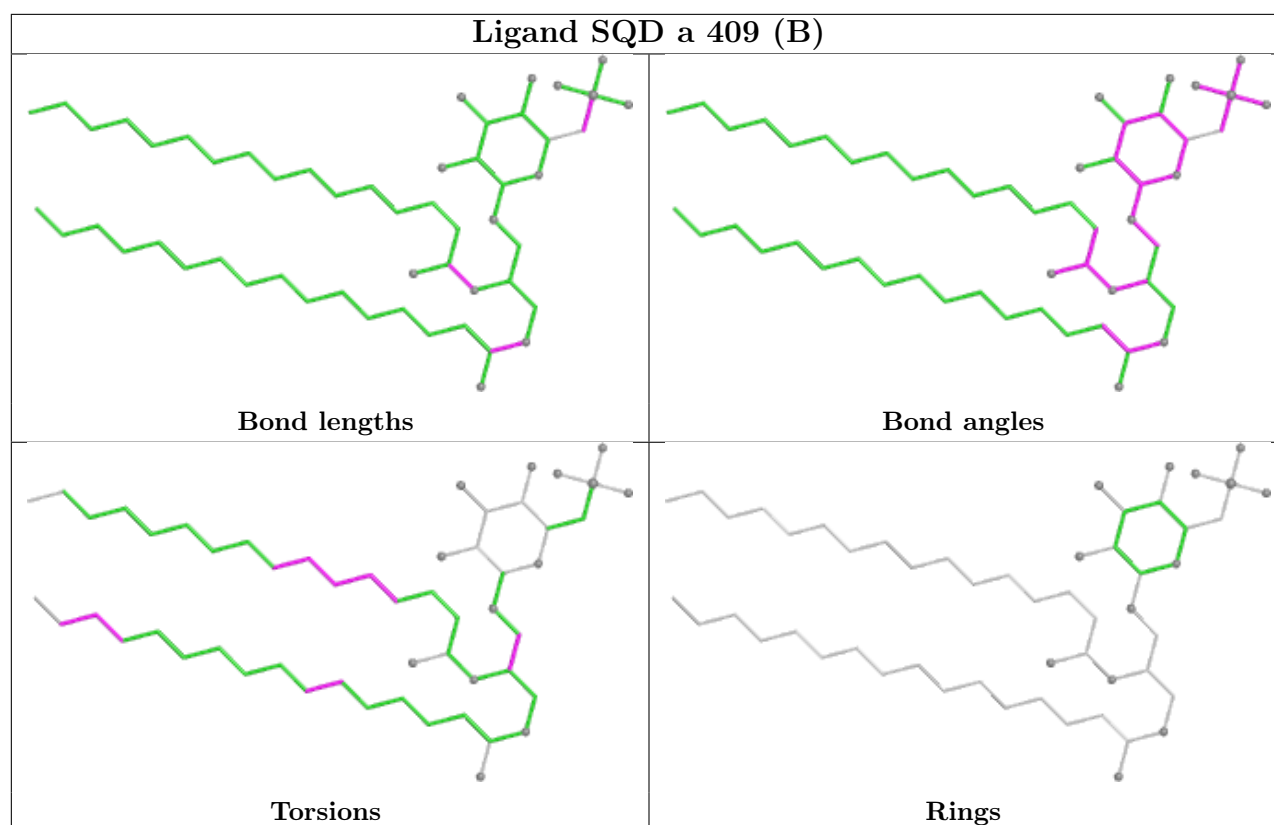




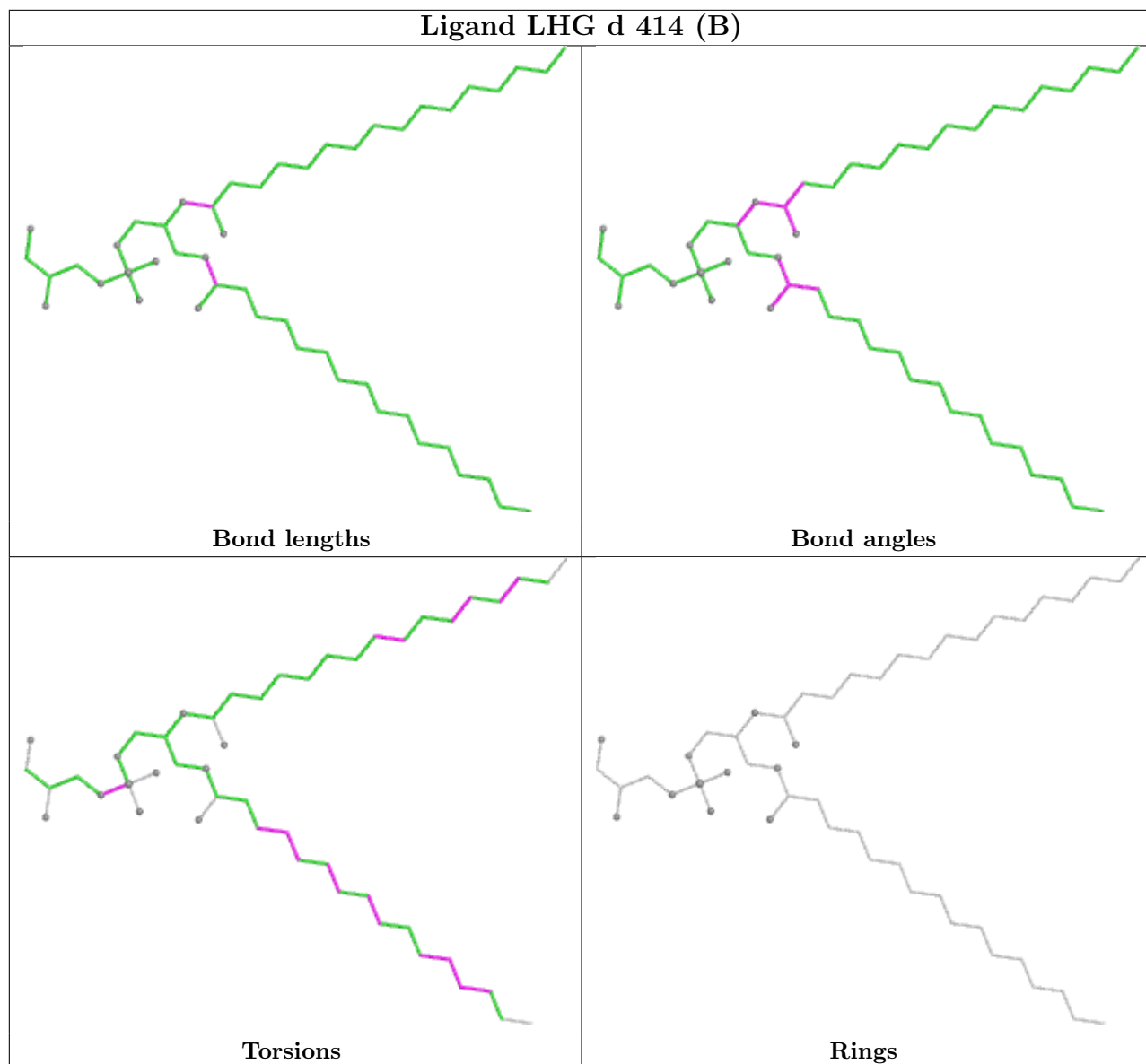
Ligand CLA C 503**Ligand CLA b 611**



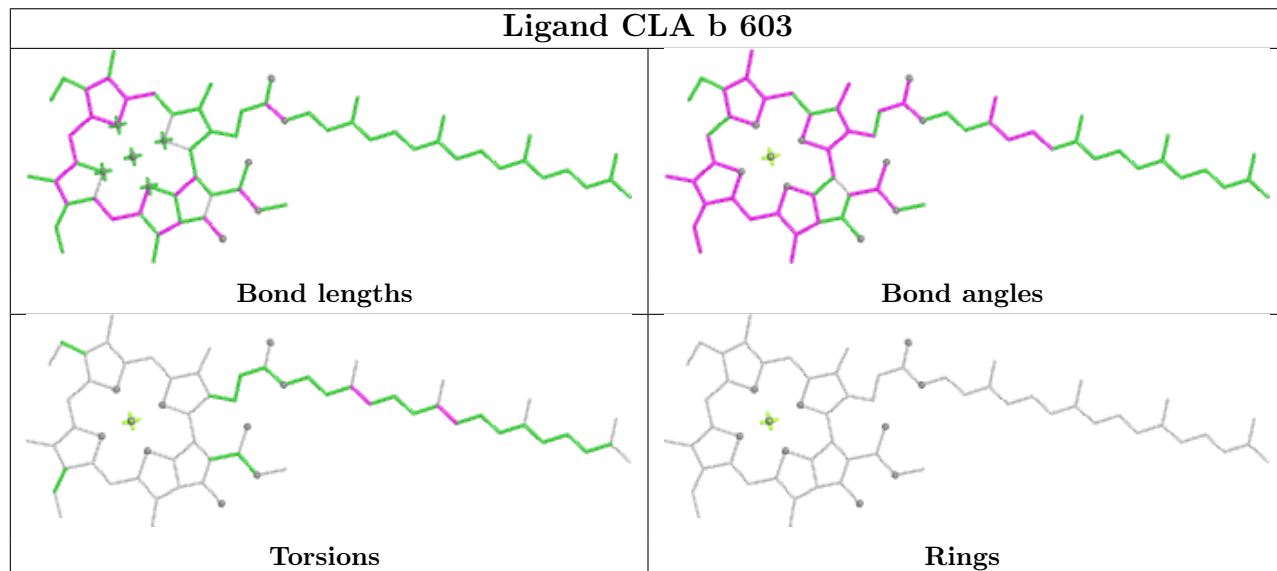


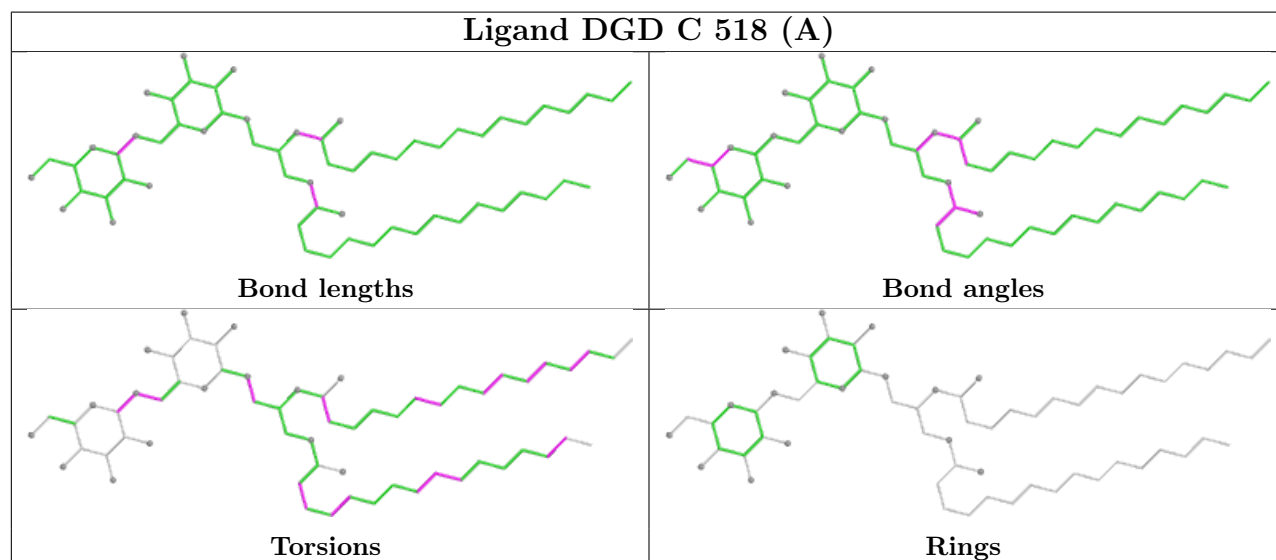
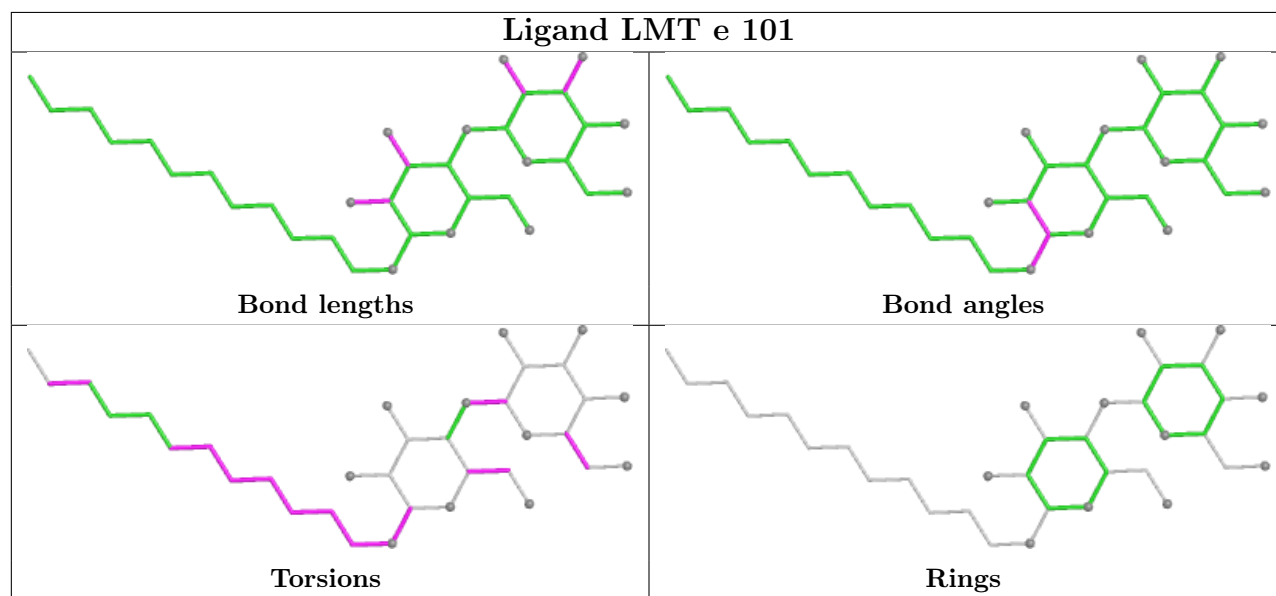
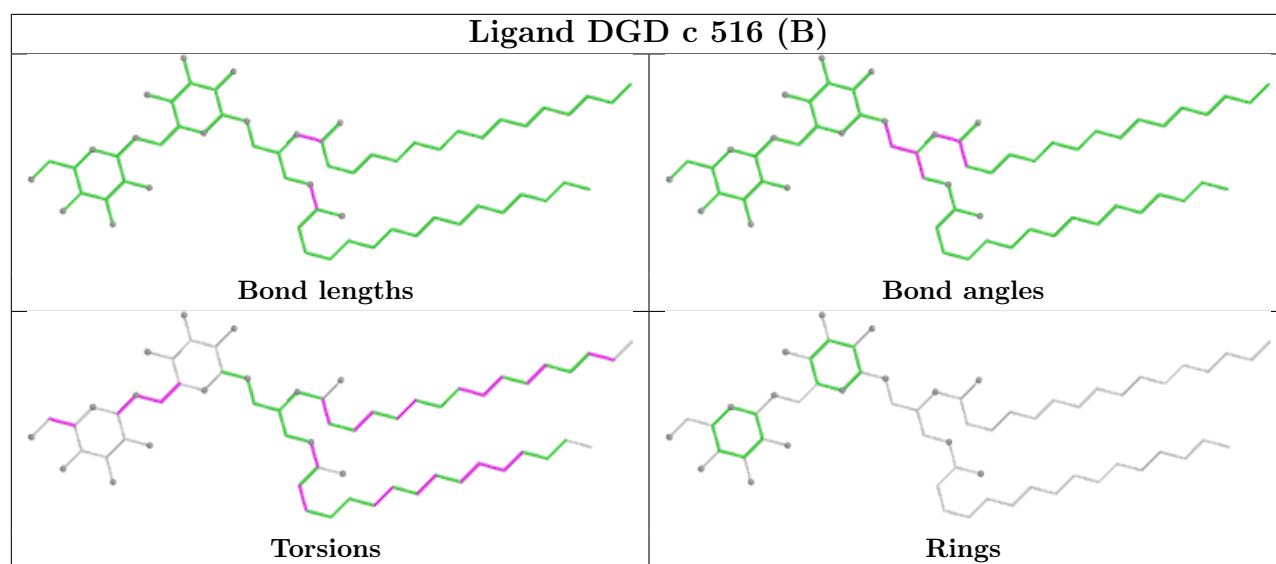


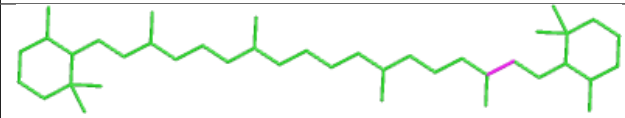
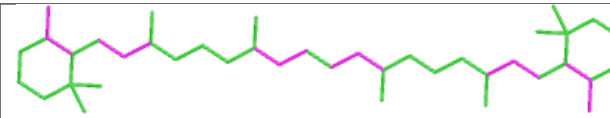
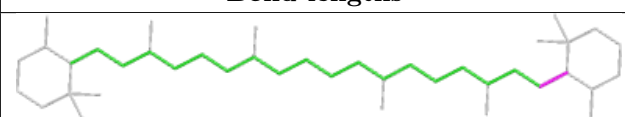
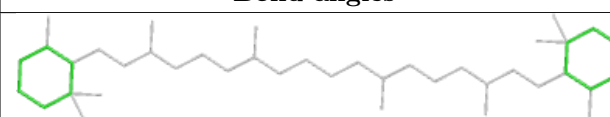
Ligand LHG d 414 (B)

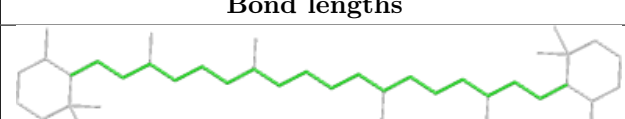
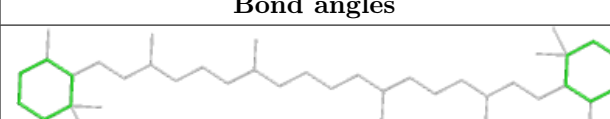


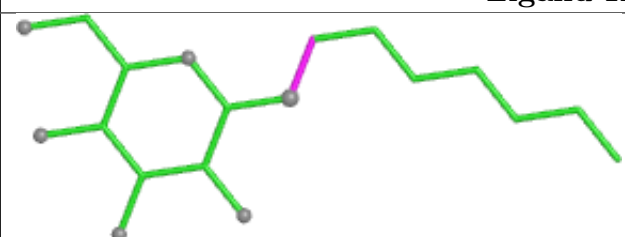
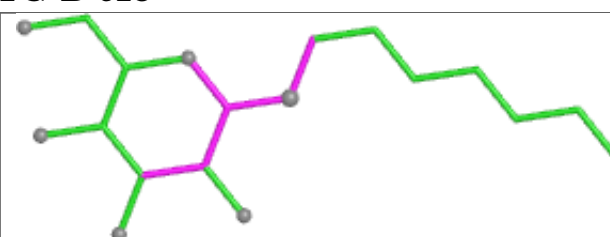
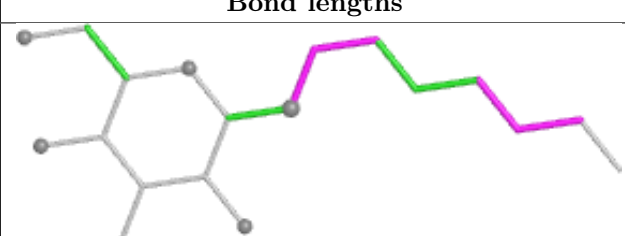
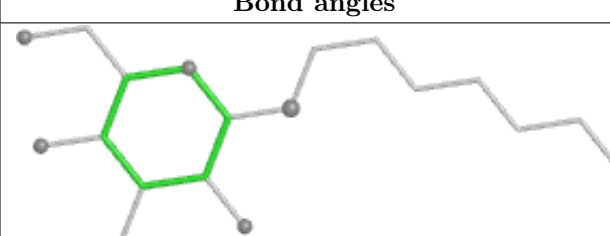
Ligand CLA b 603

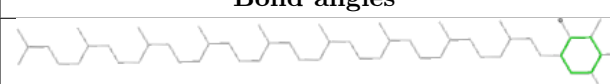


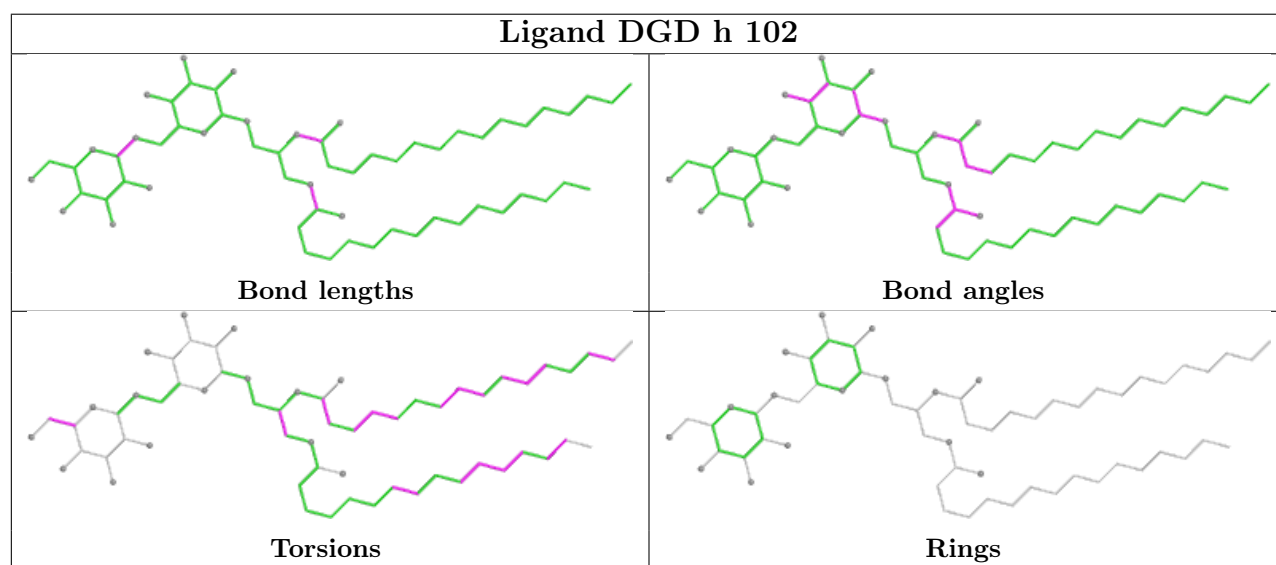
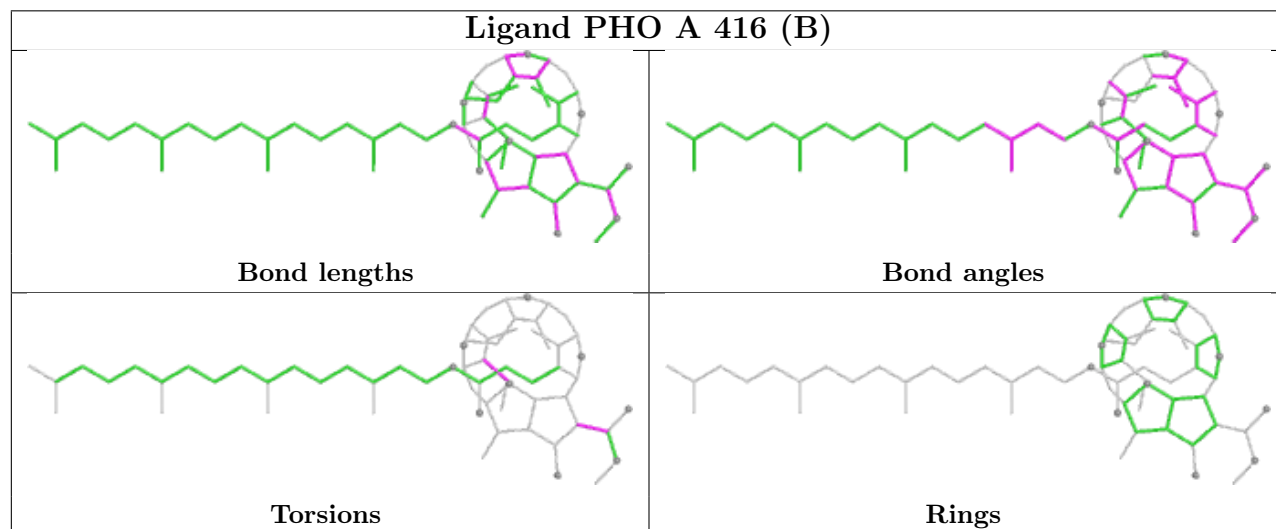
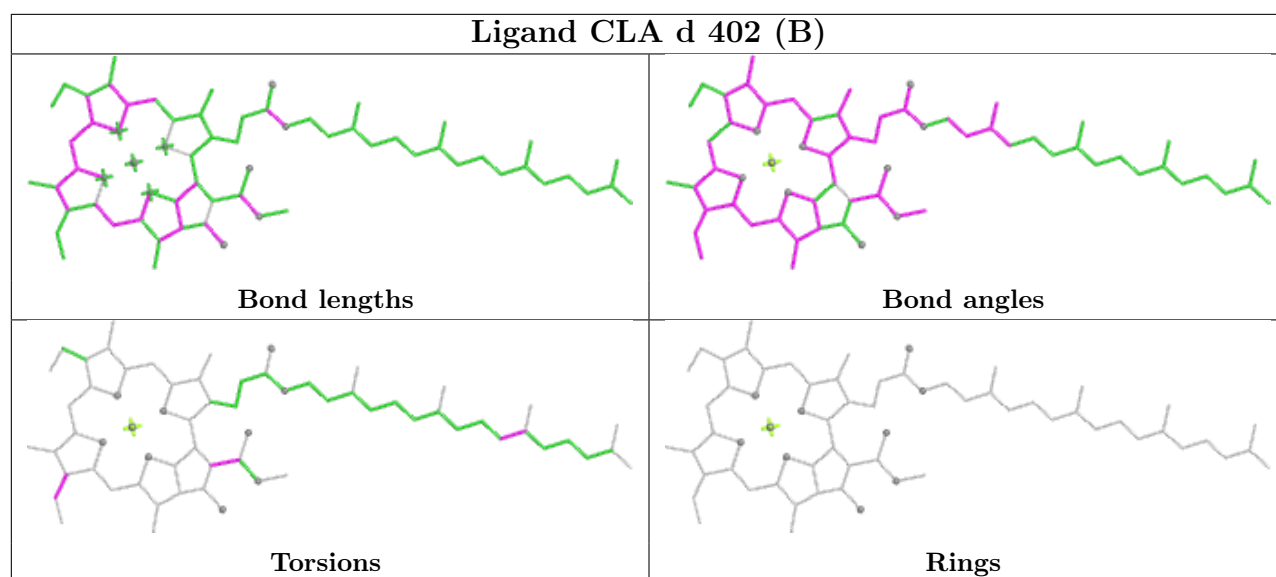


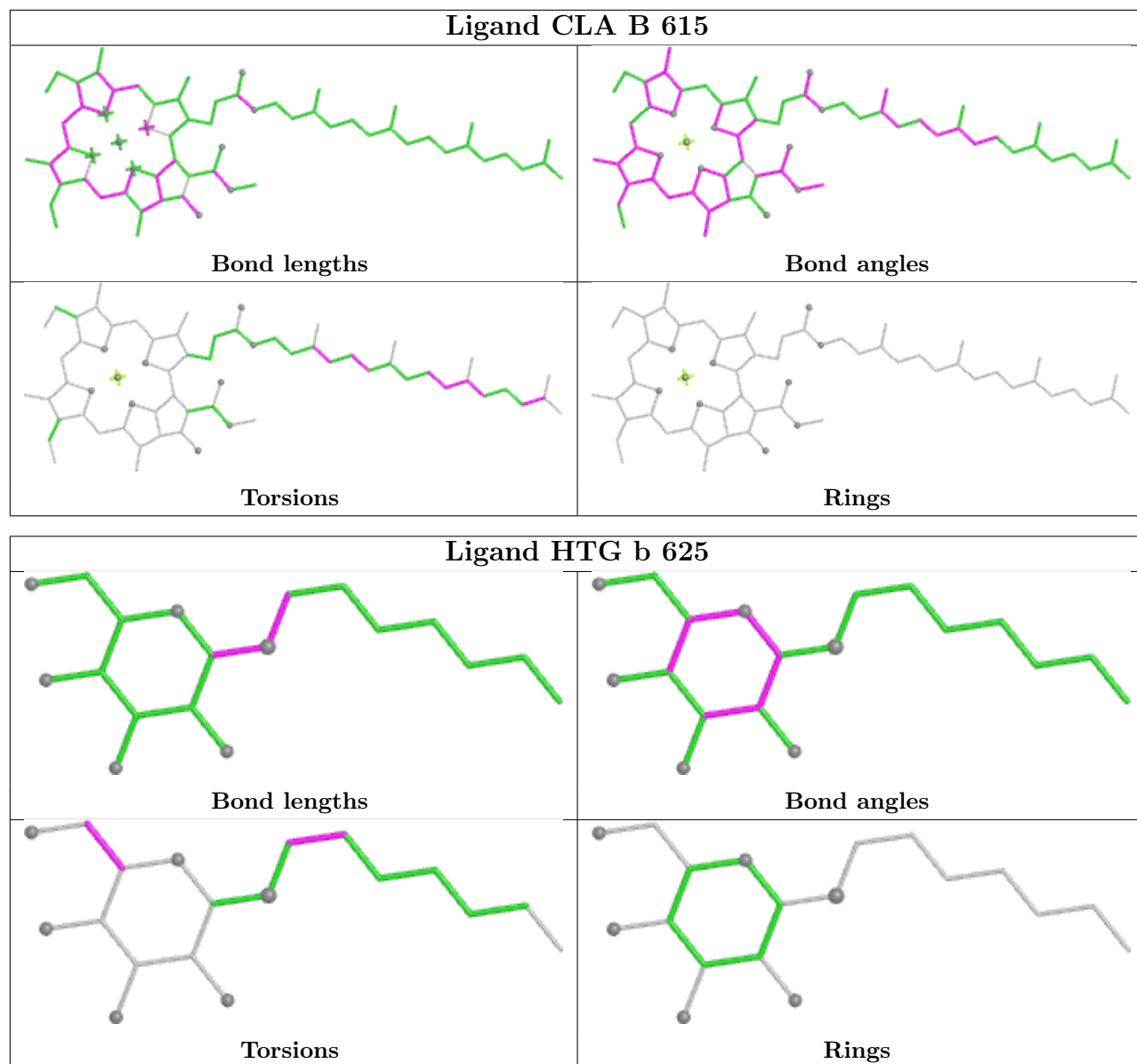
Ligand BCR C 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

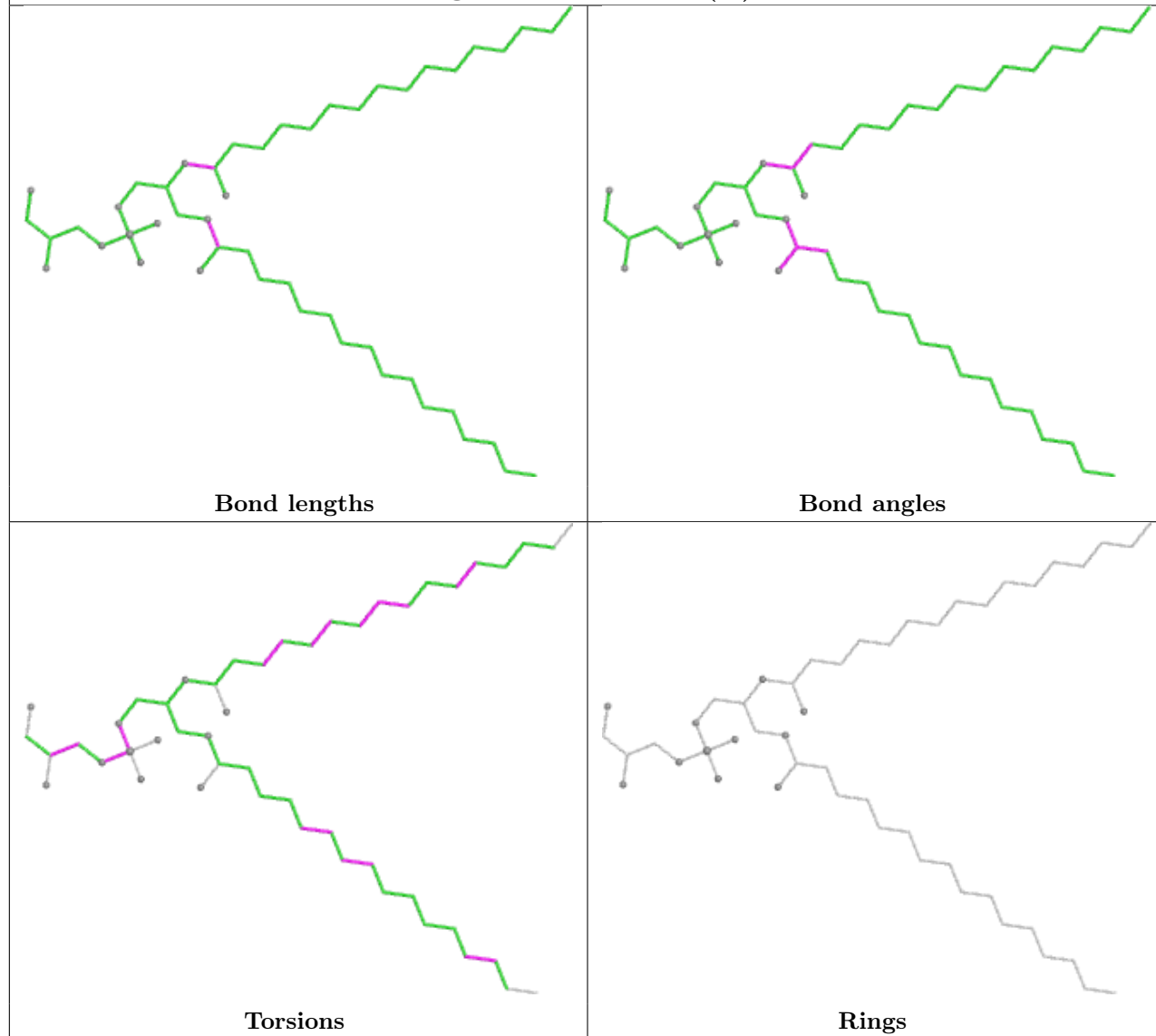
Ligand HTG B 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

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

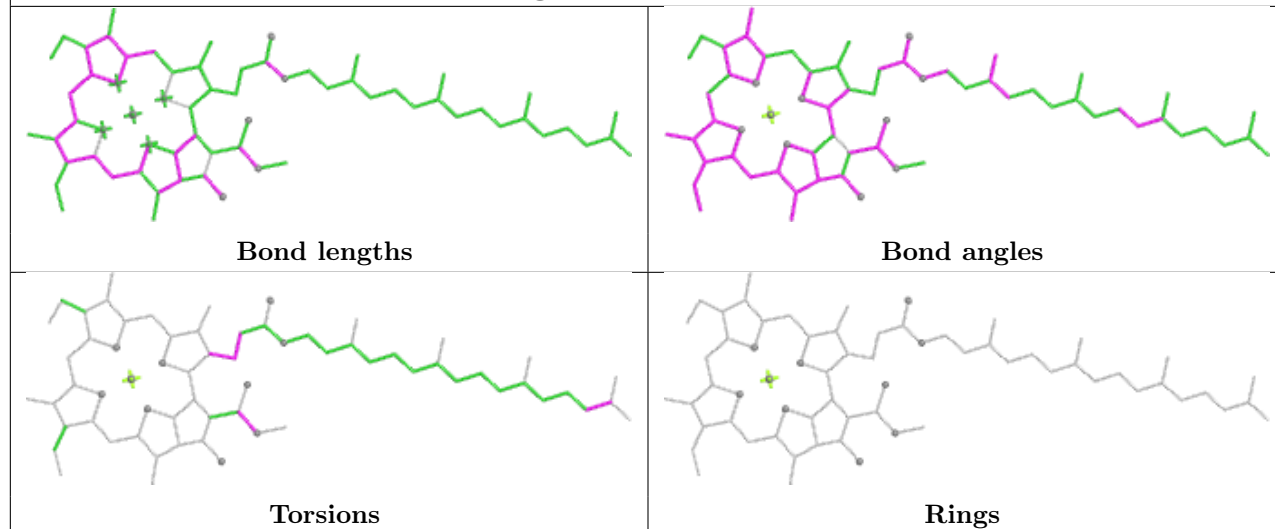


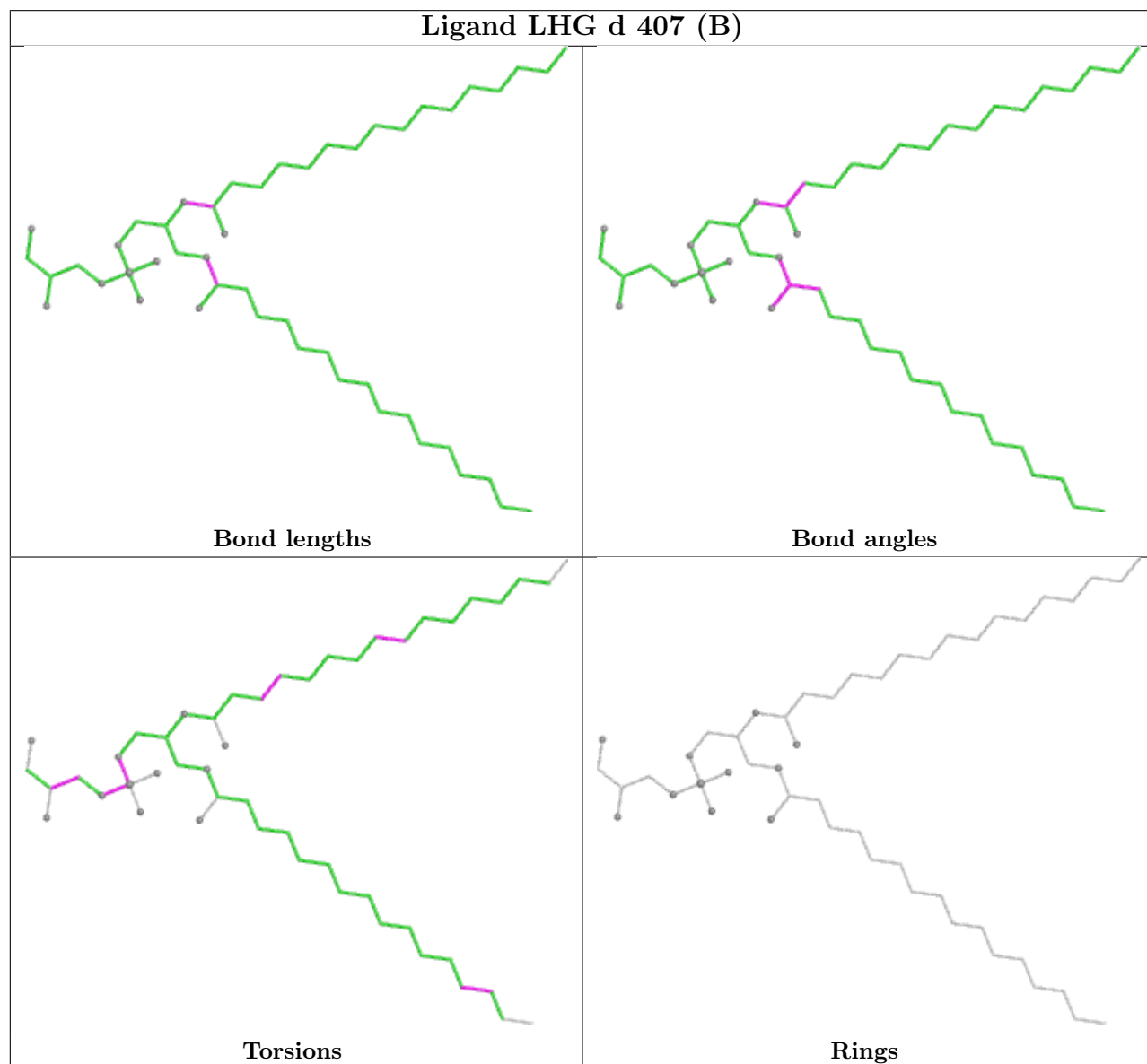
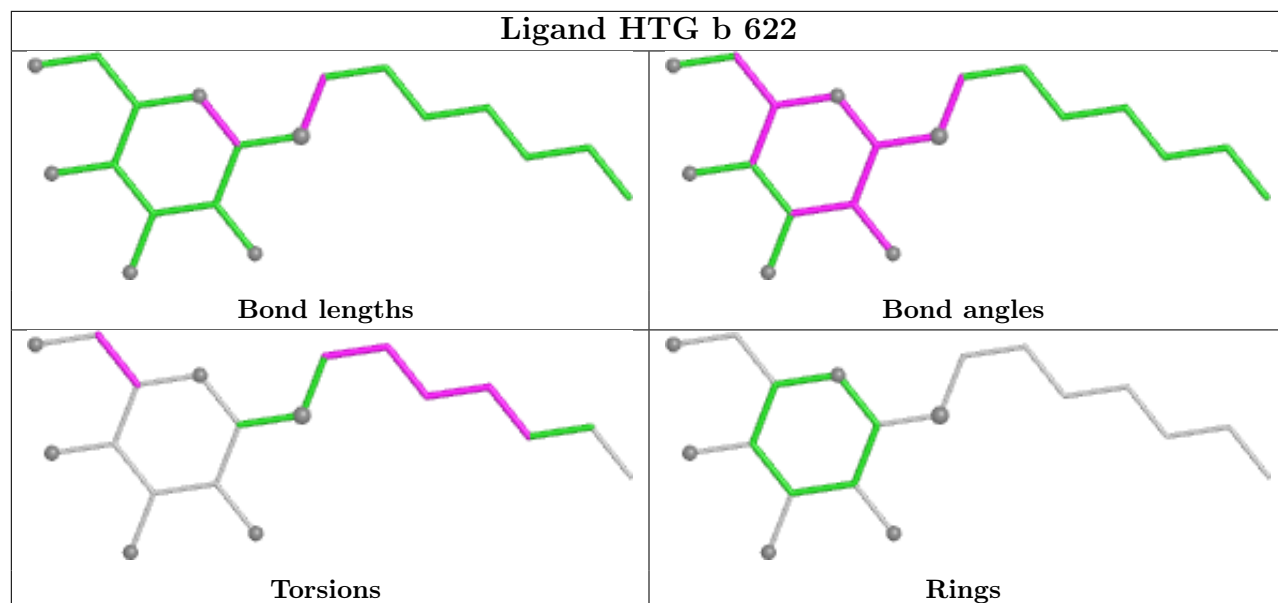


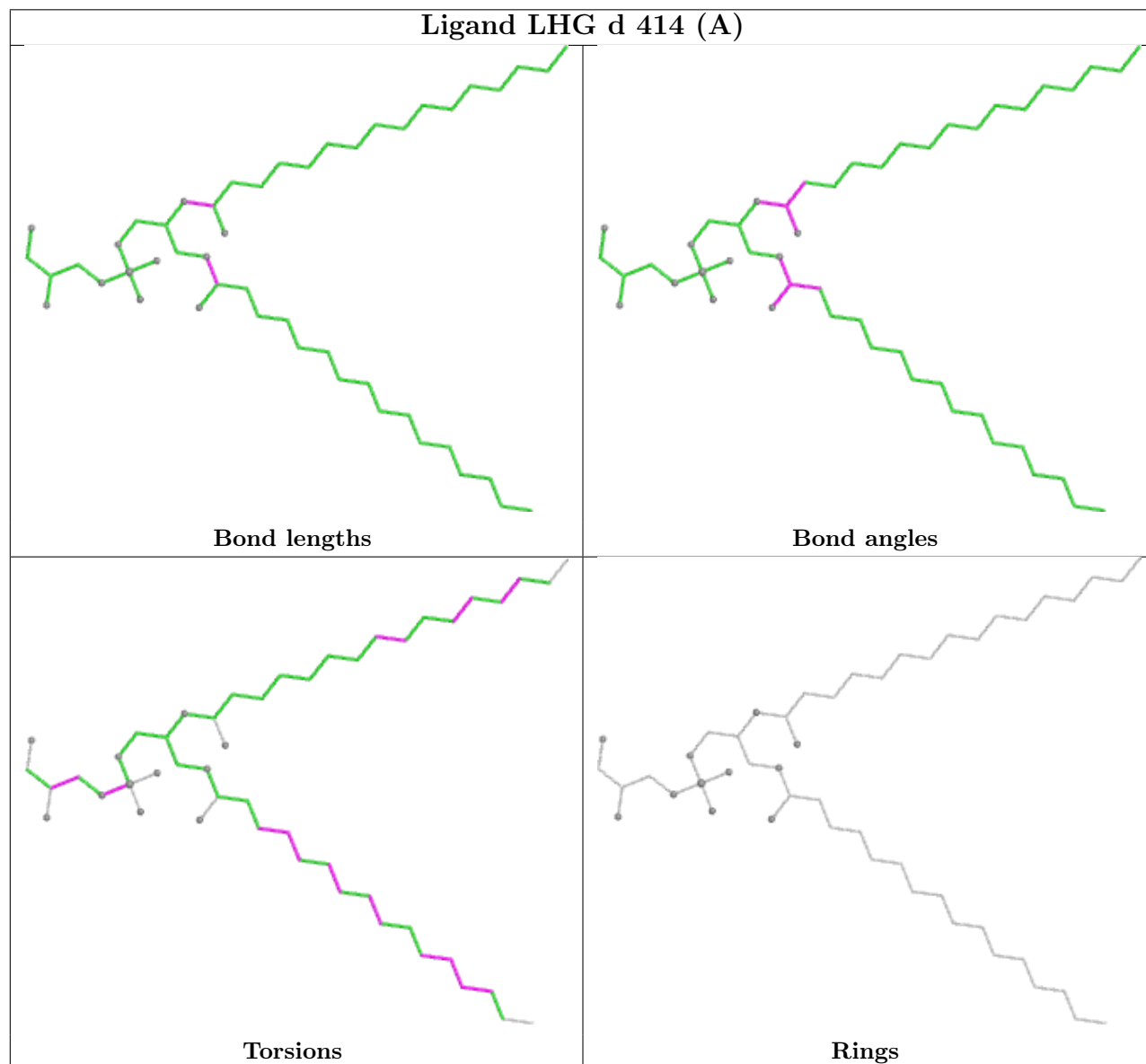
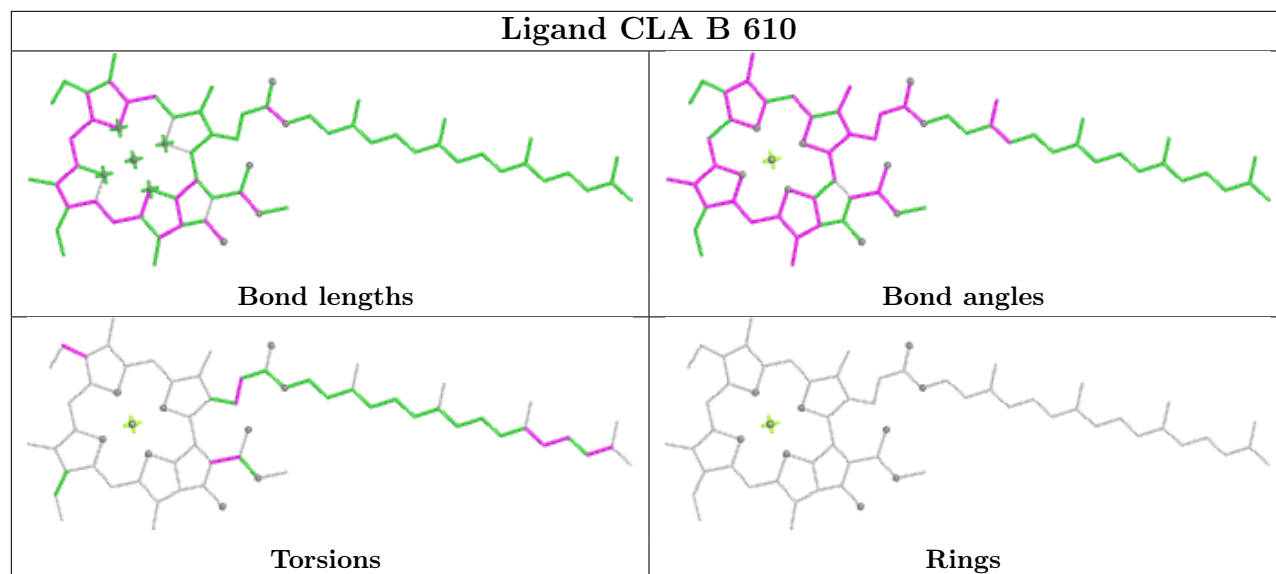
Ligand LHG D 406 (A)

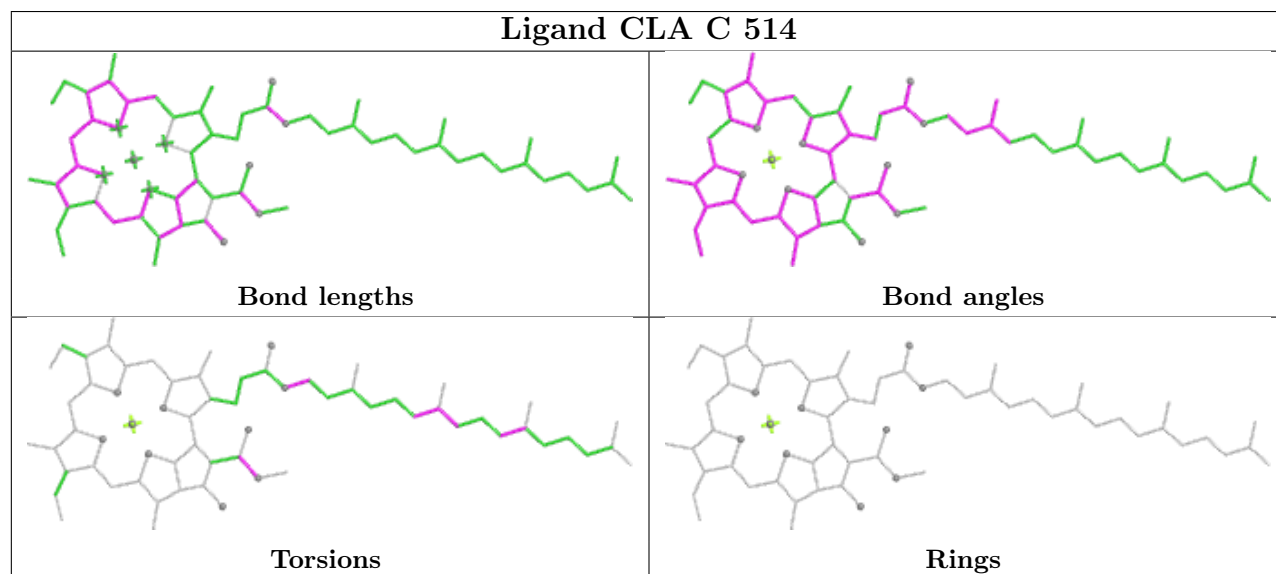
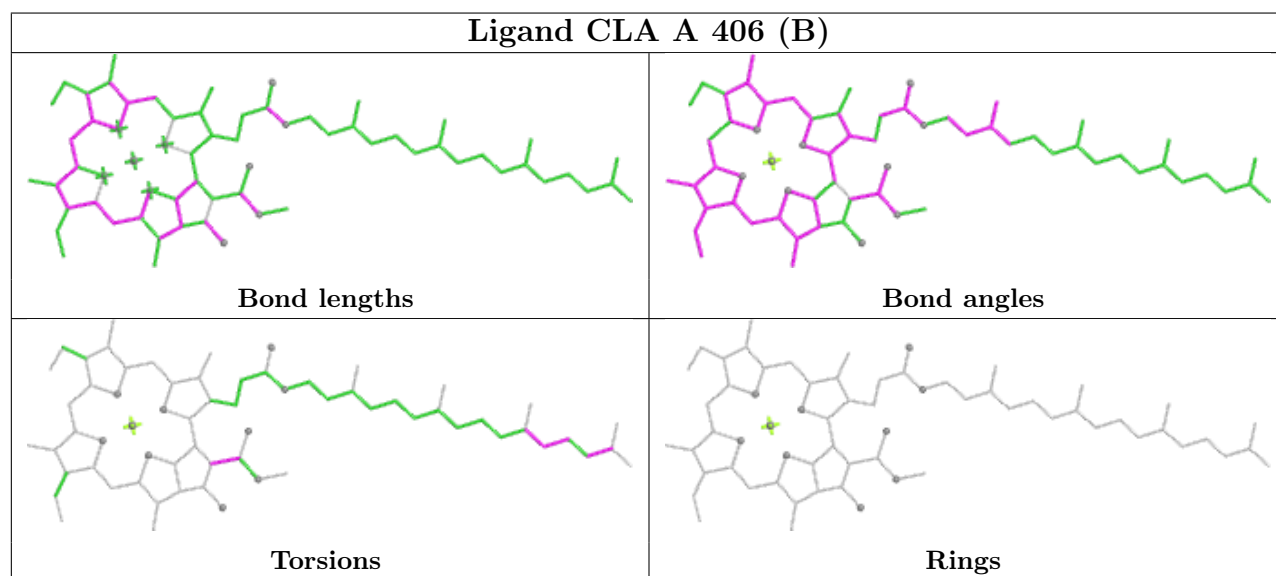
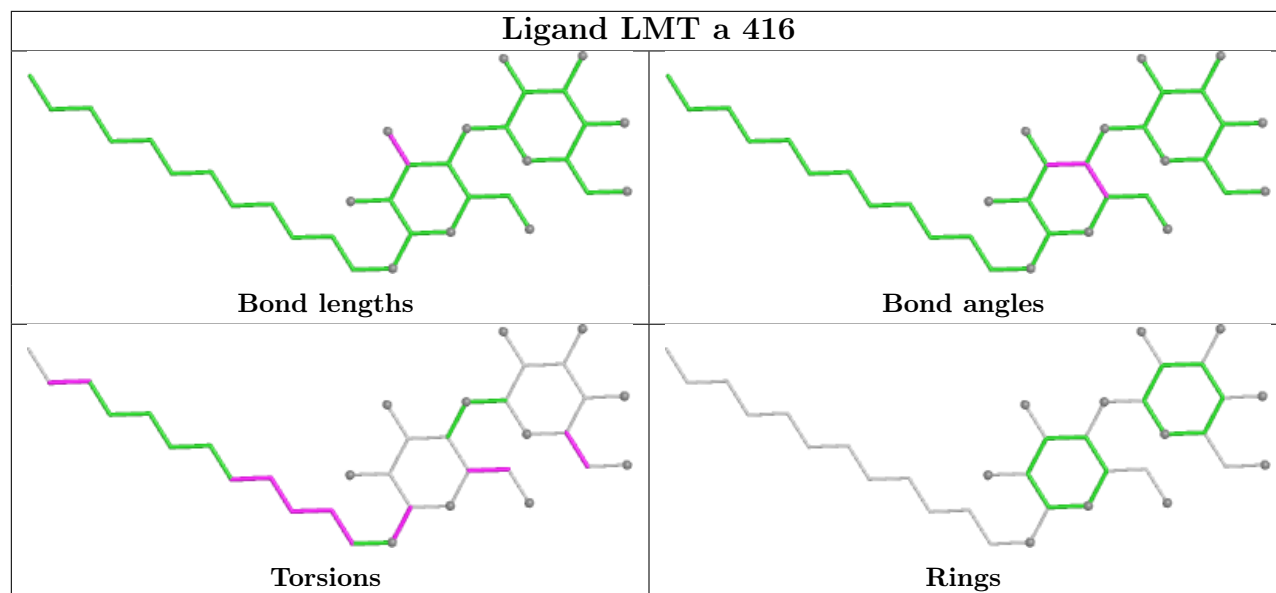


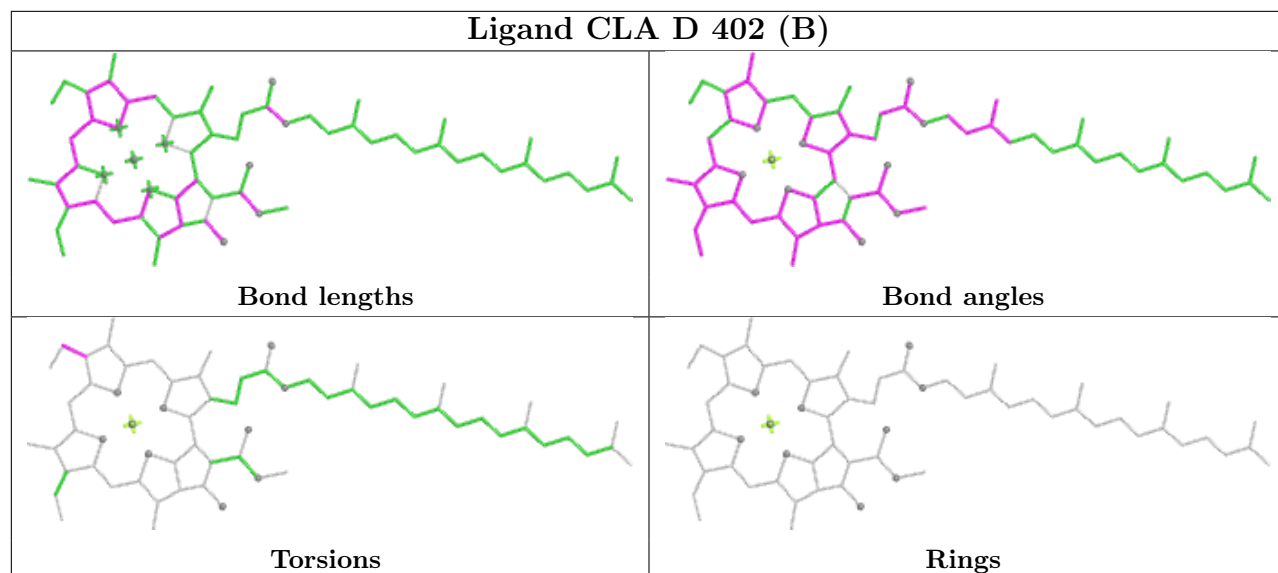
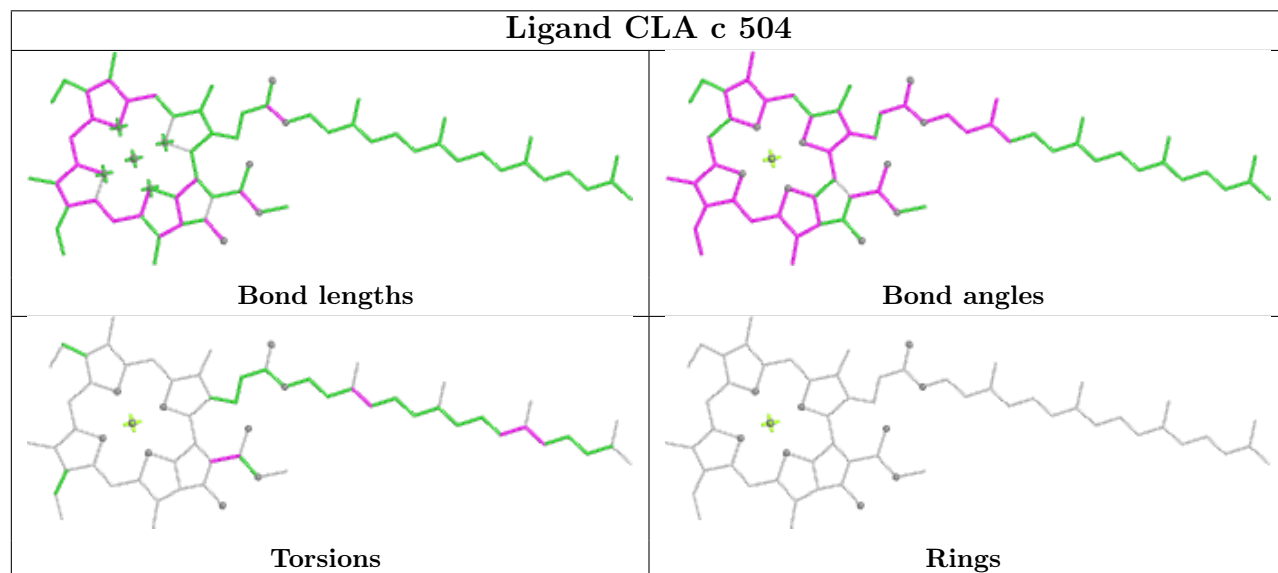
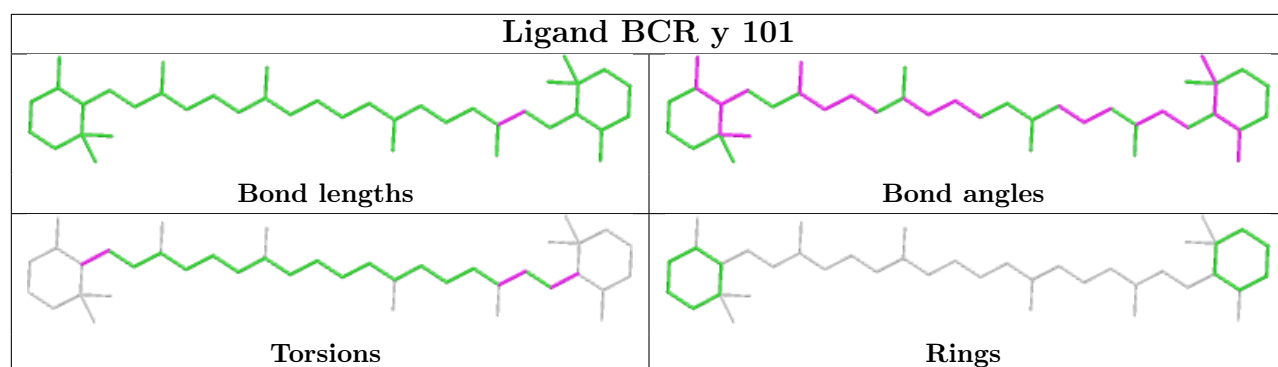
Ligand CLA C 502

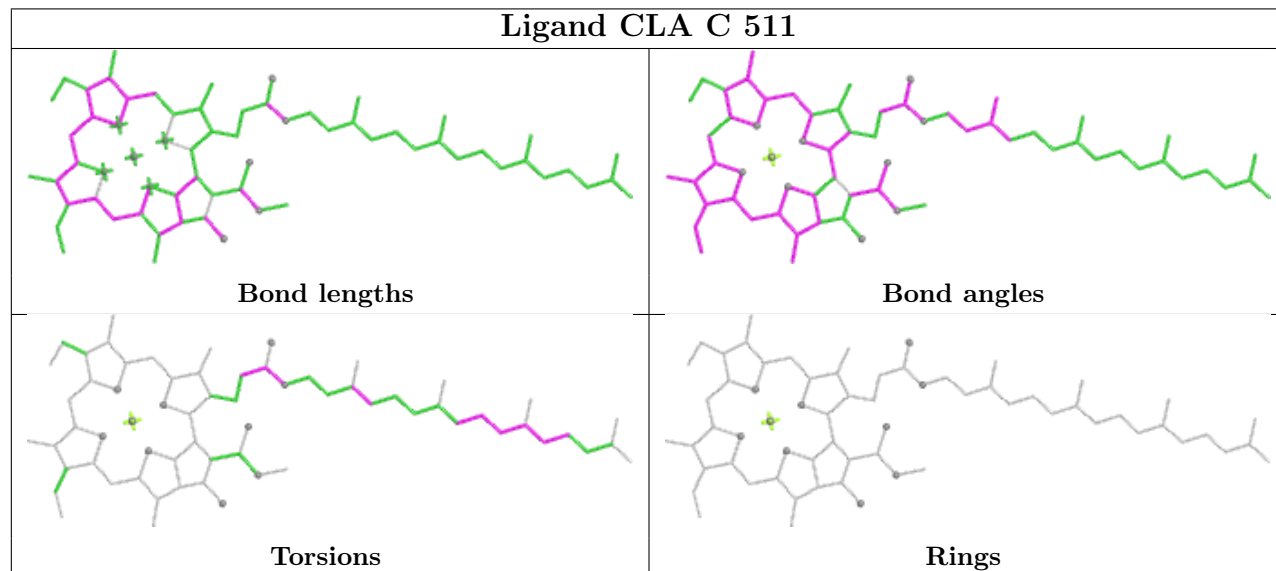
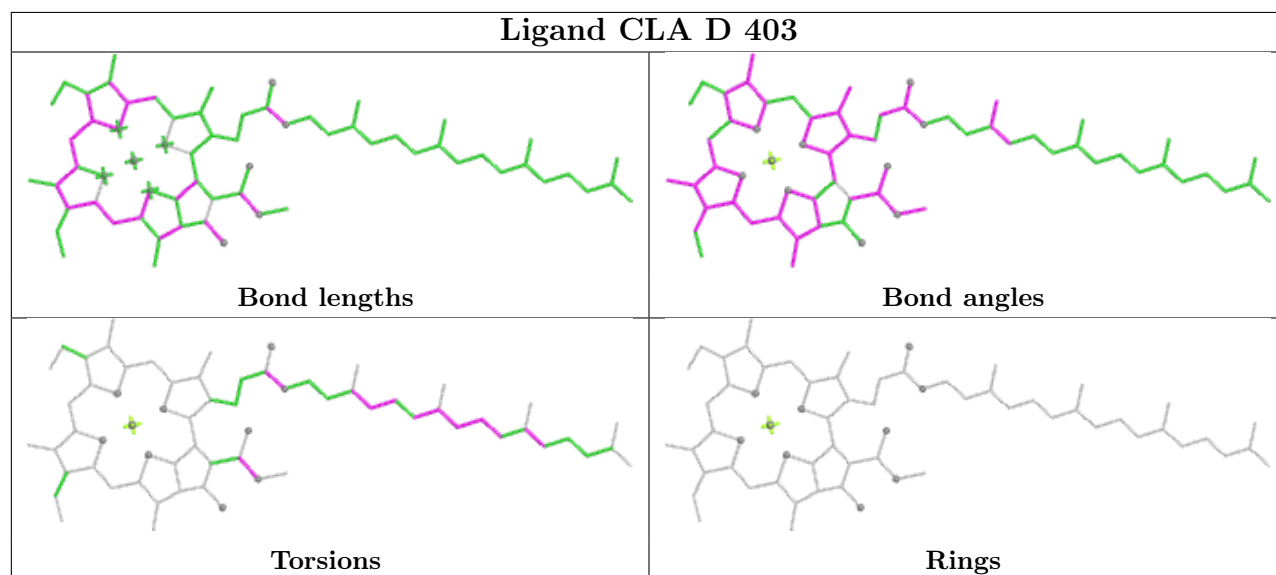
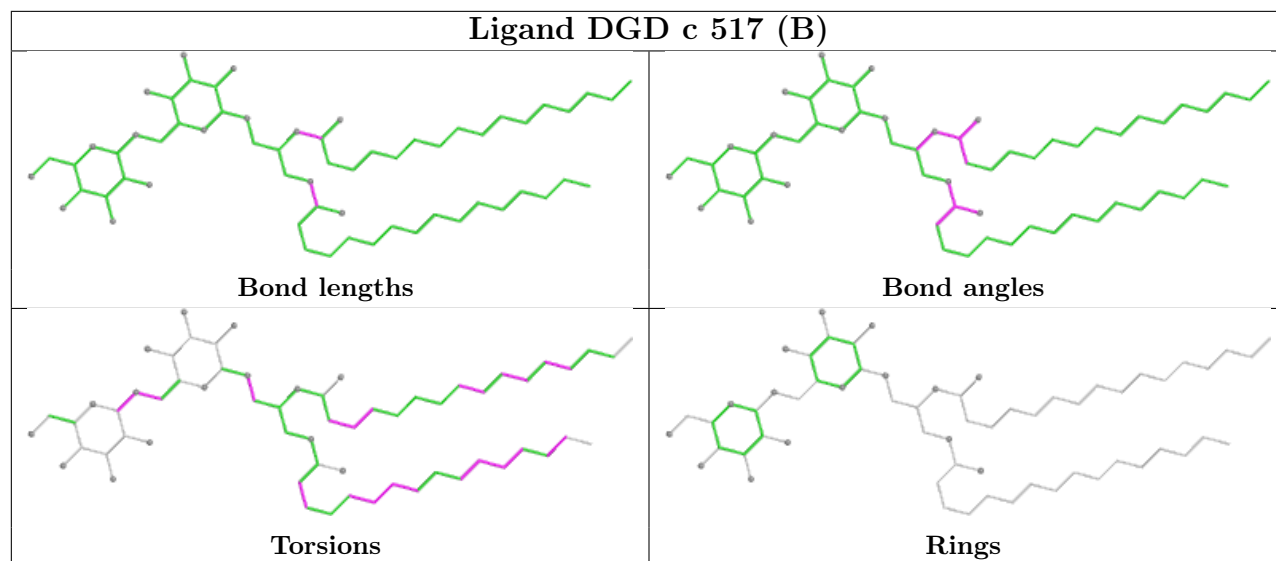




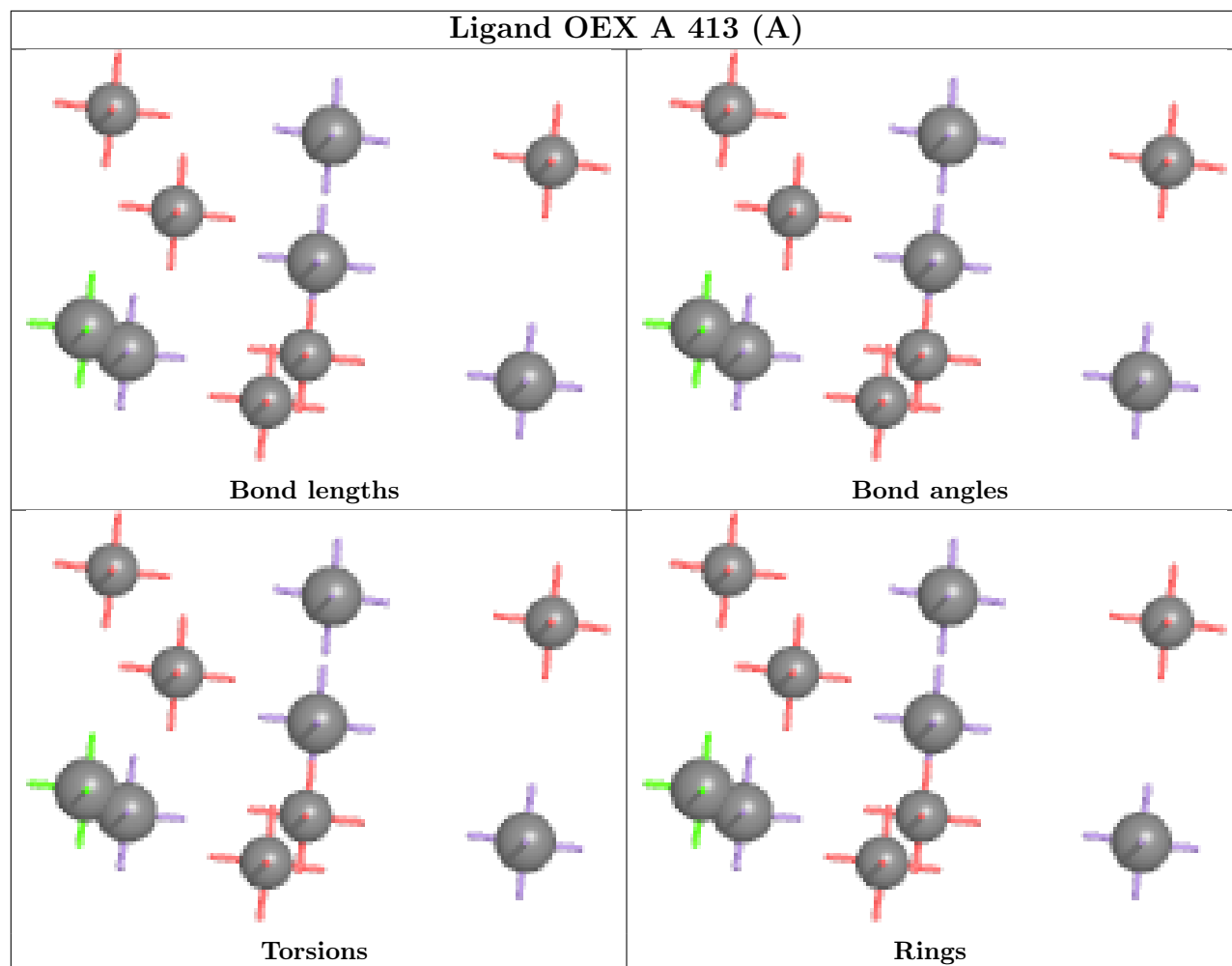




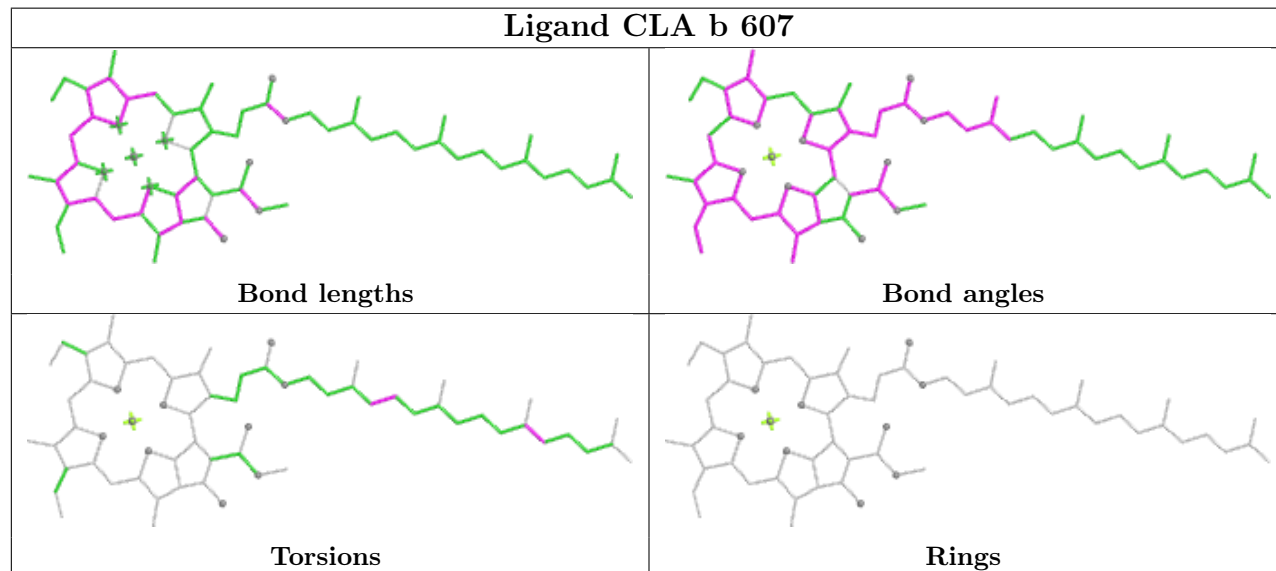


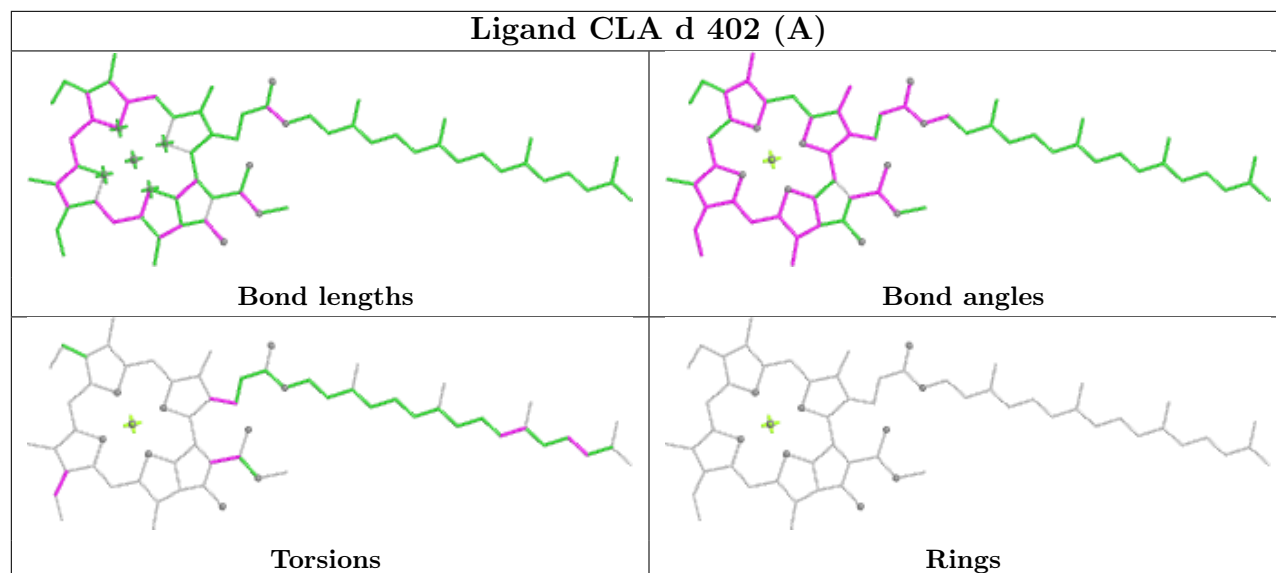
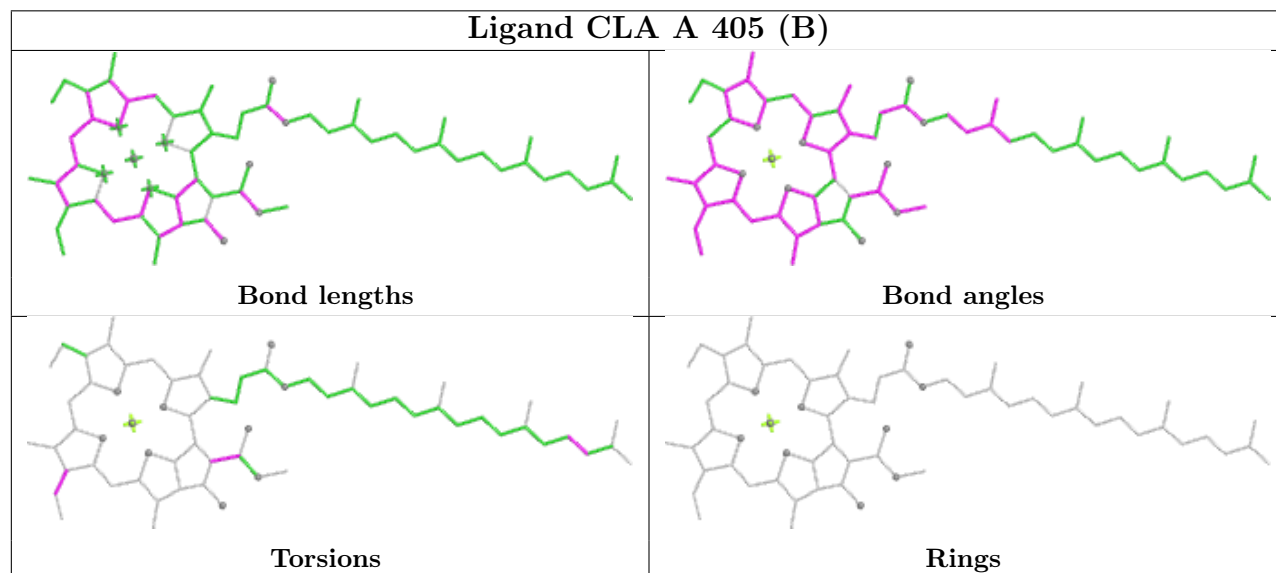
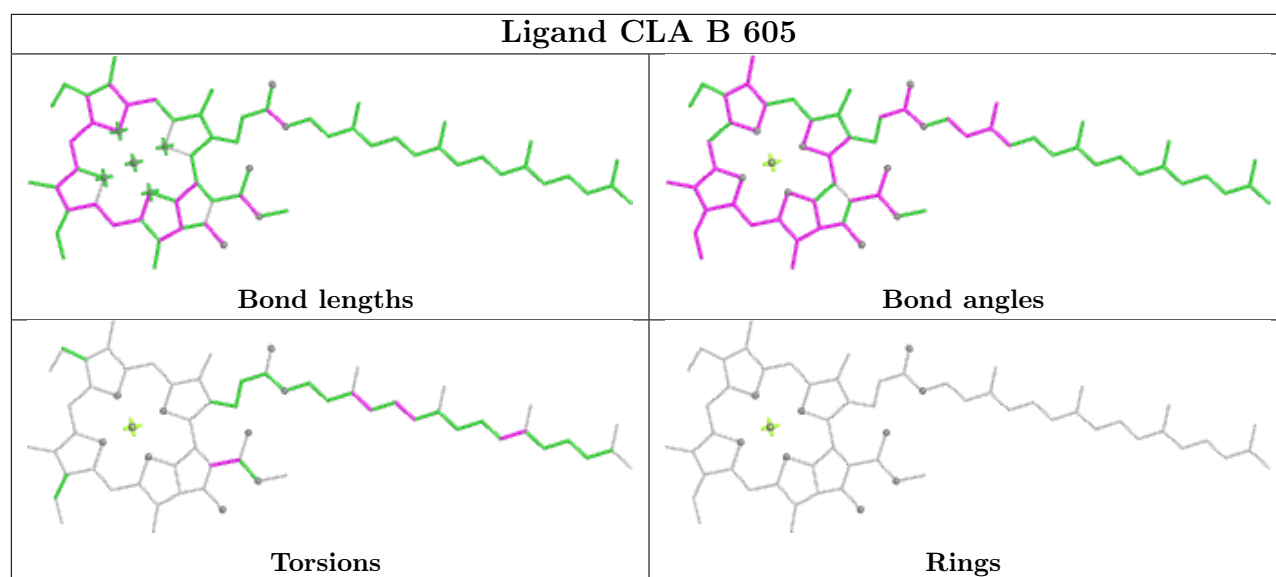


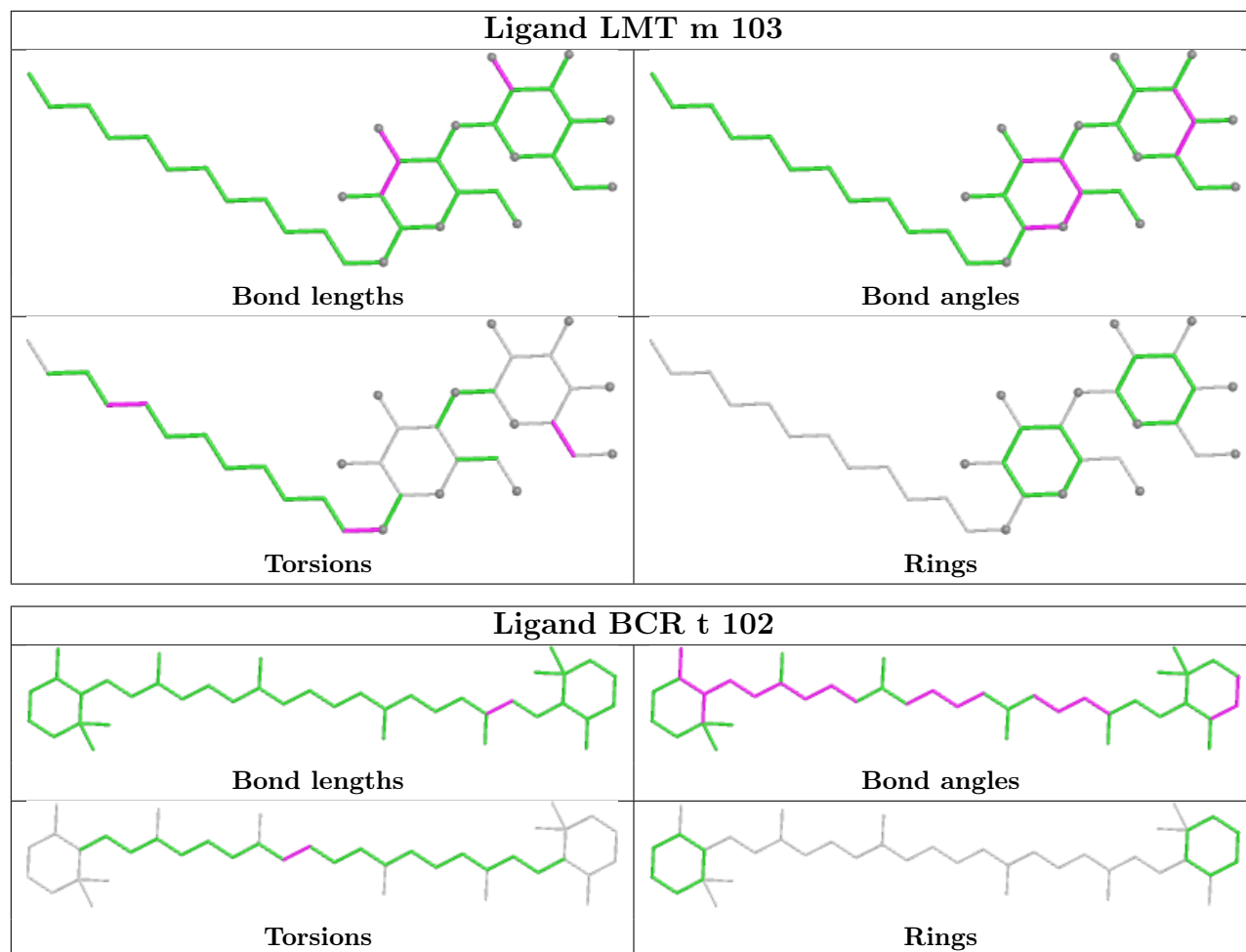
Ligand OEX A 413 (A)



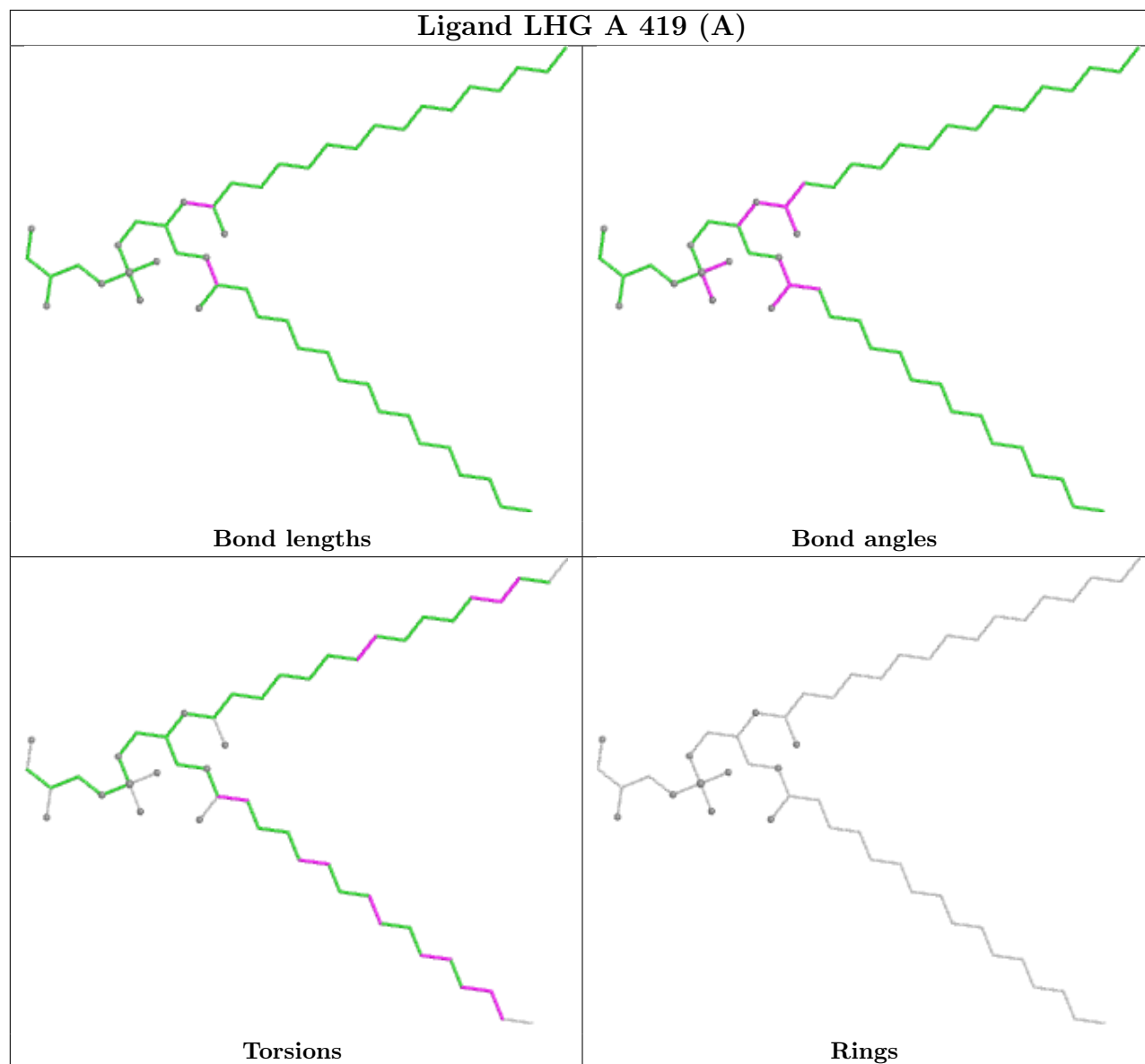
Ligand CLA b 607



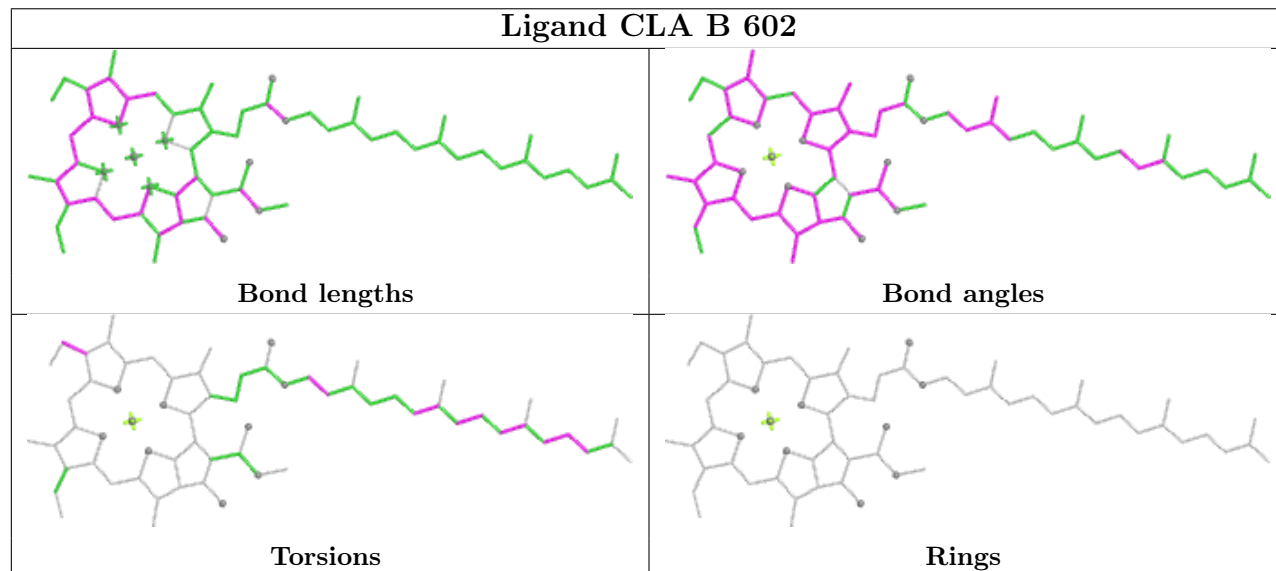


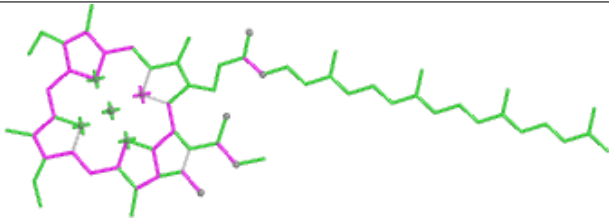
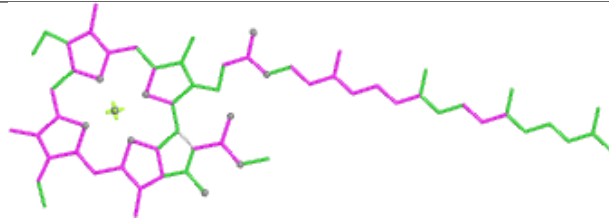
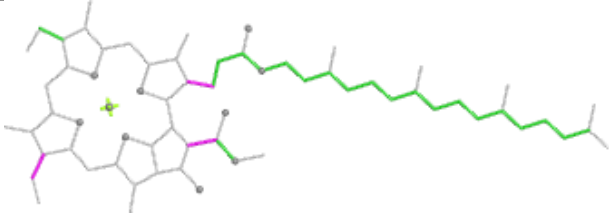
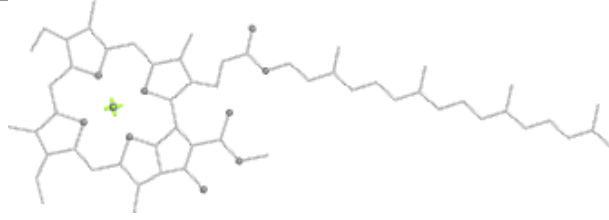


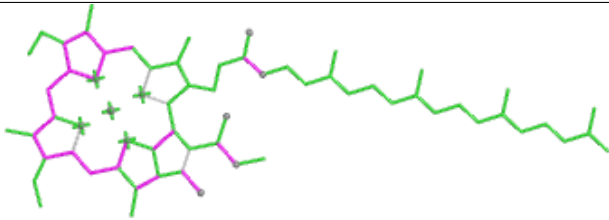
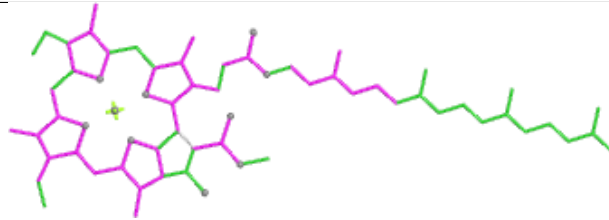
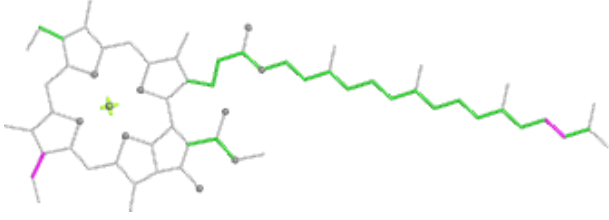
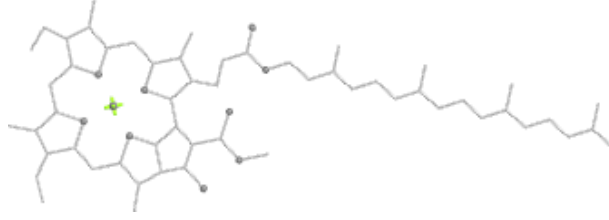
Ligand LHG A 419 (A)

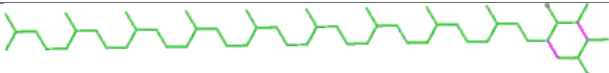
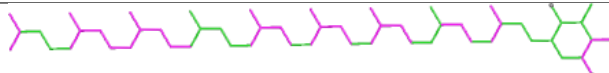


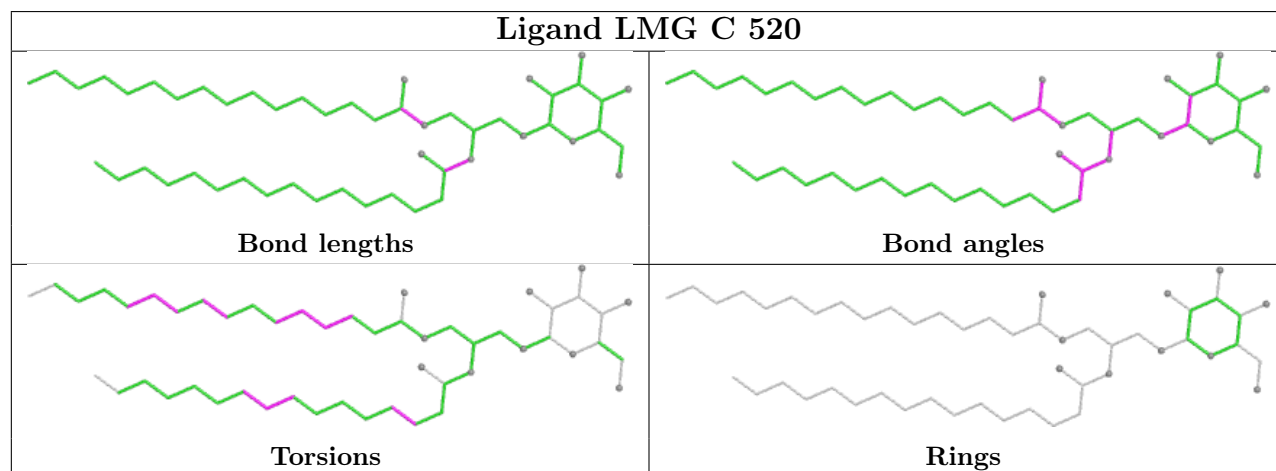
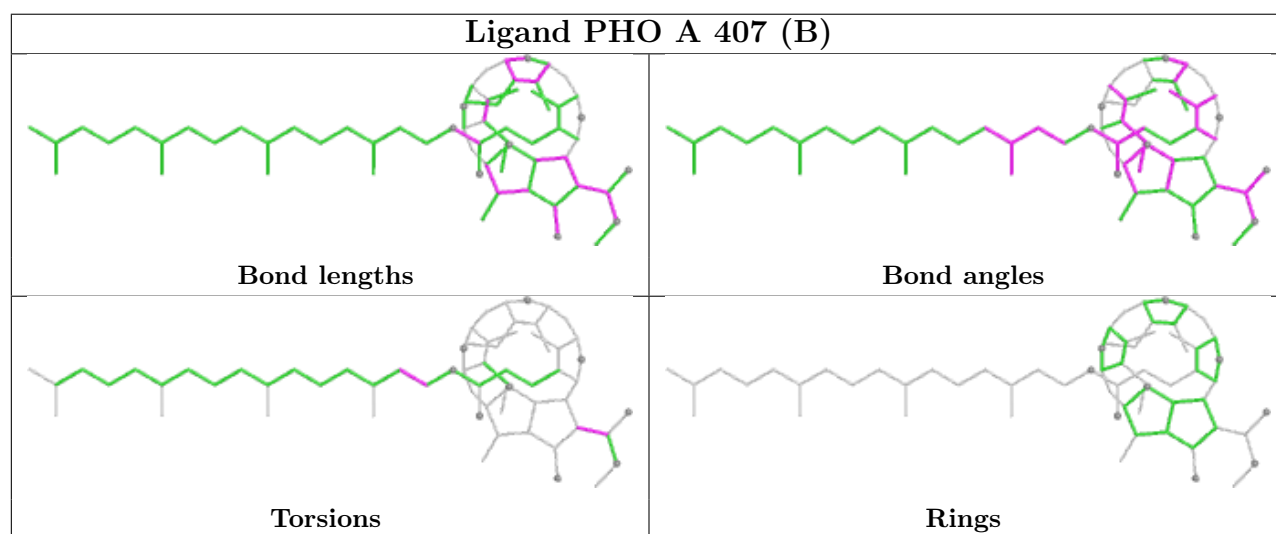
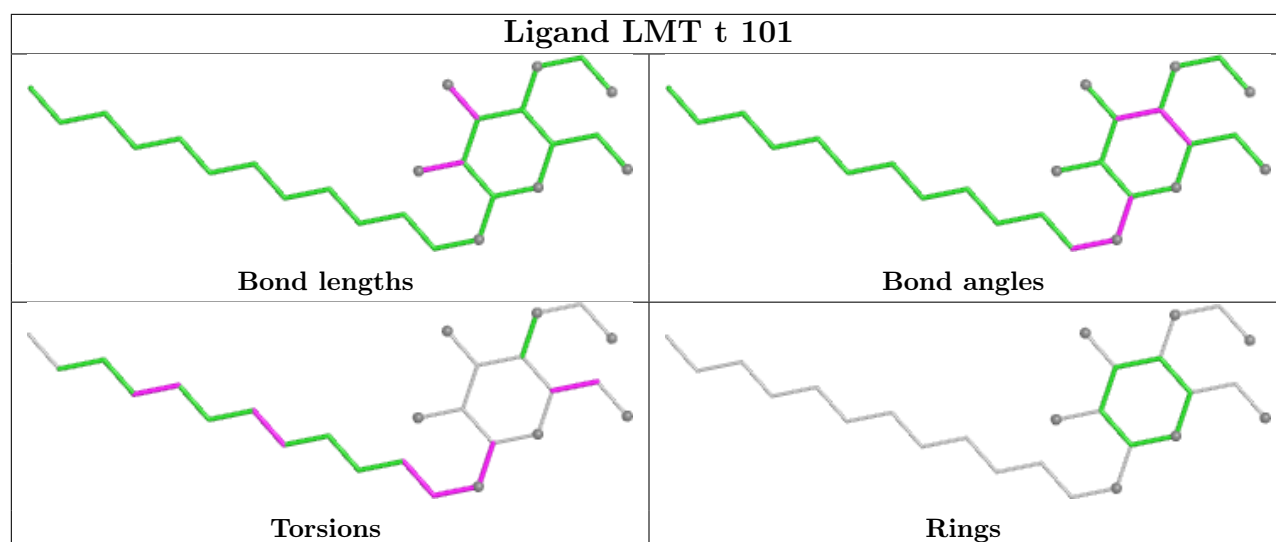
Ligand CLA B 602

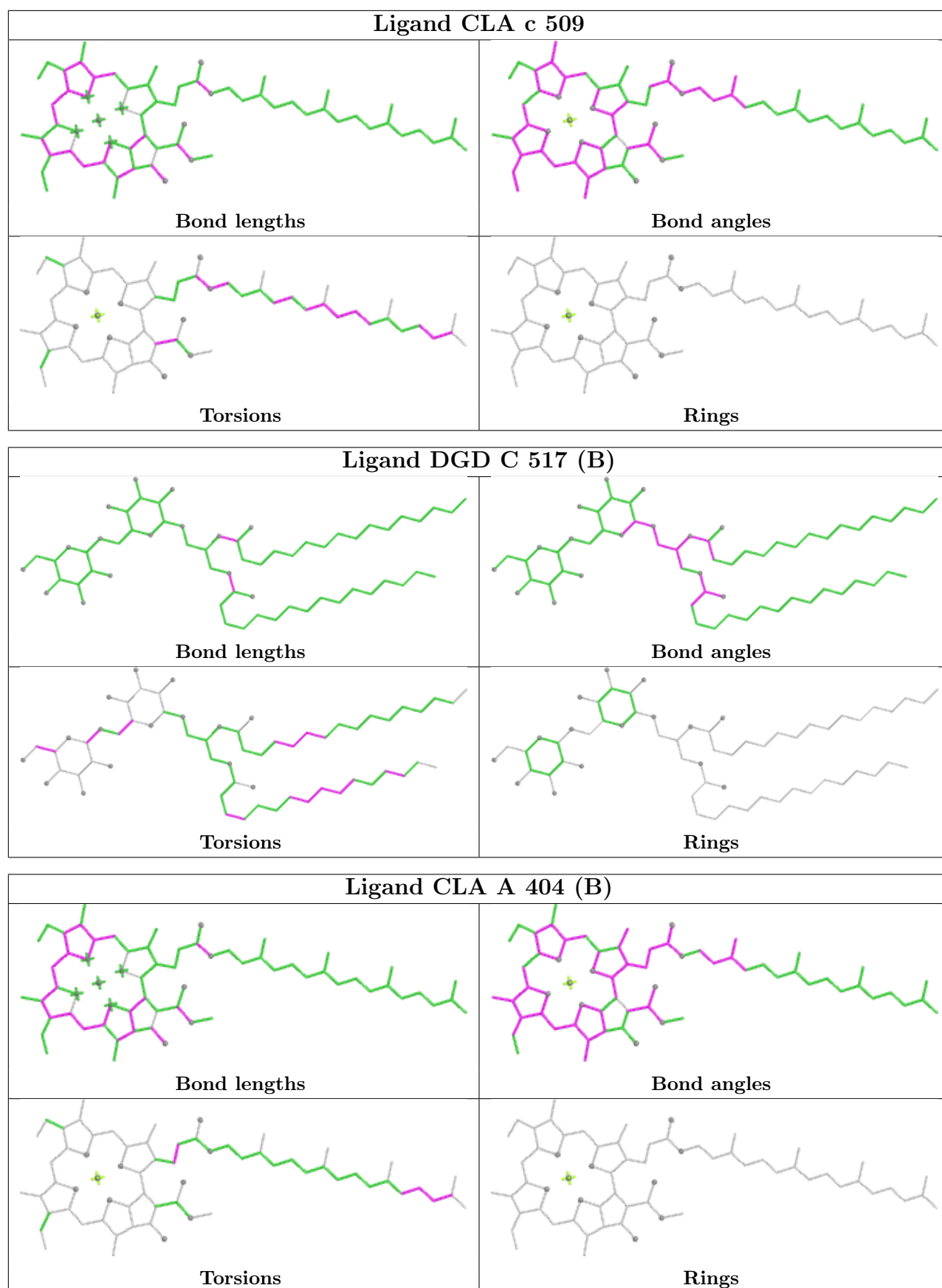


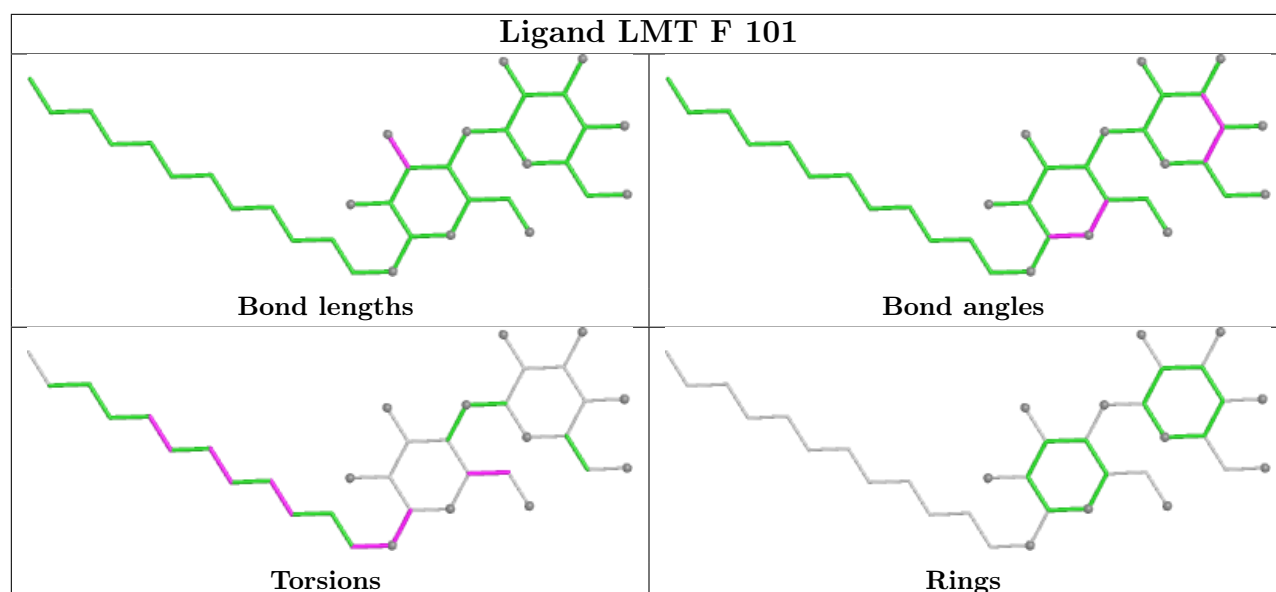
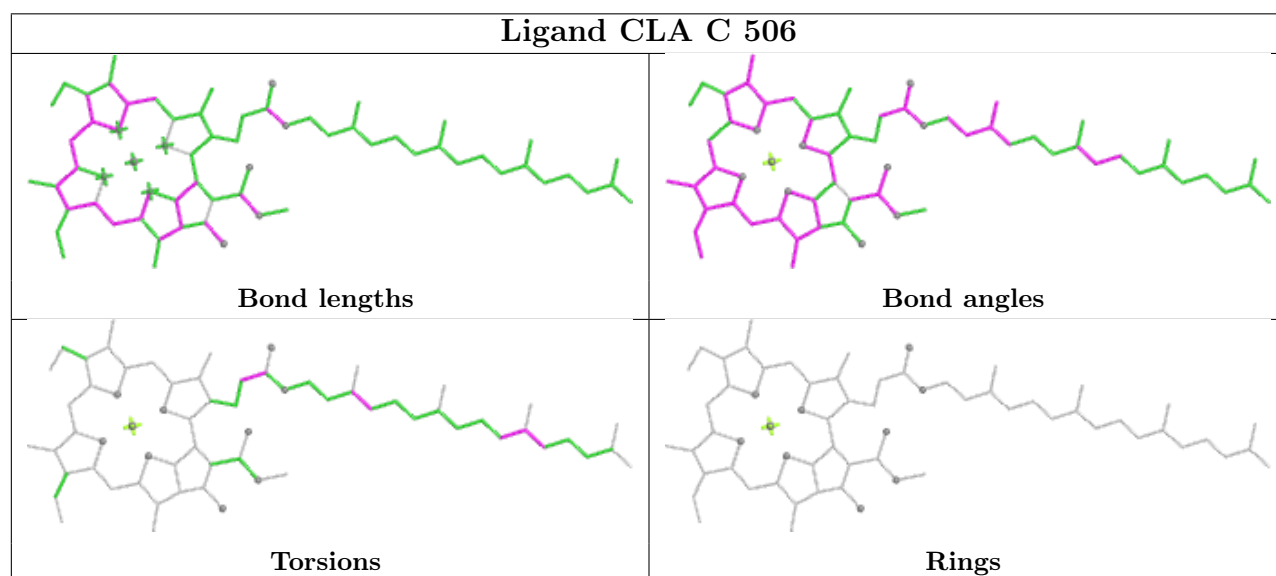
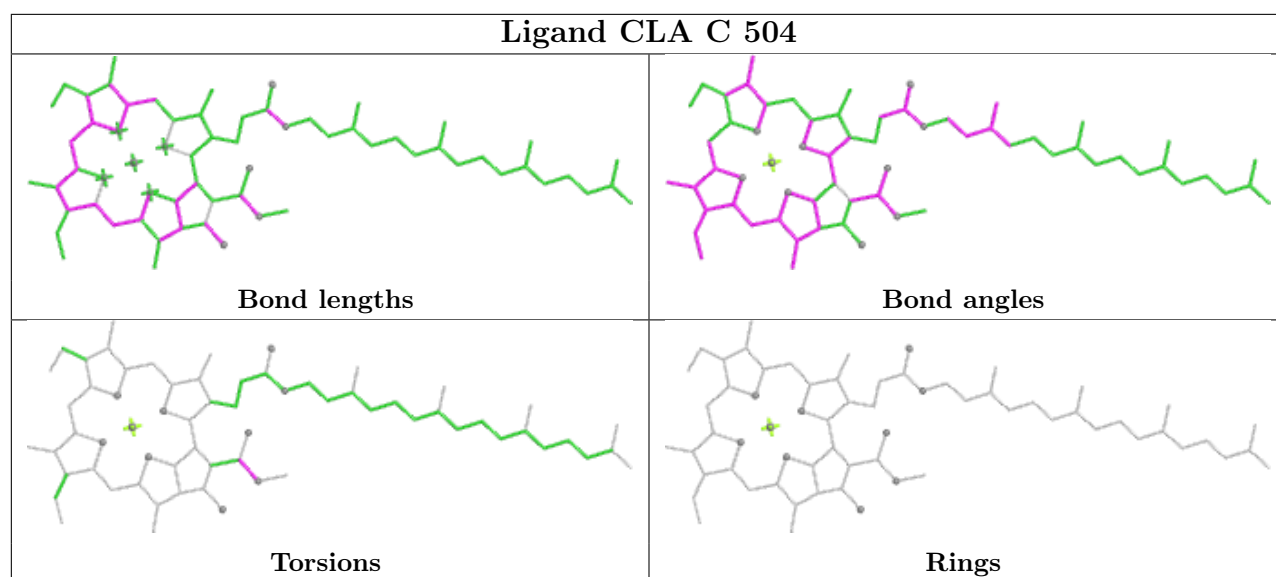
Ligand CLA B 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

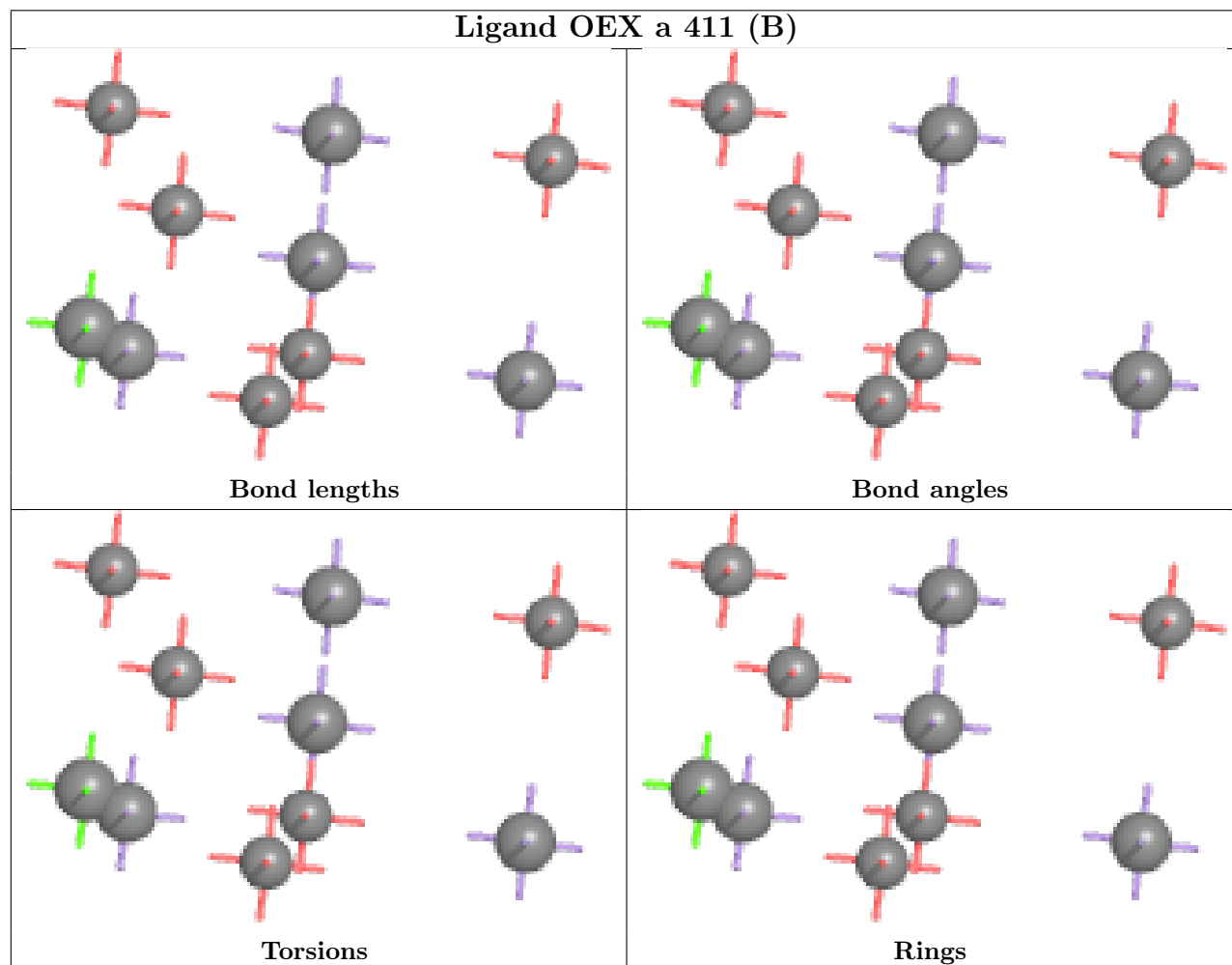
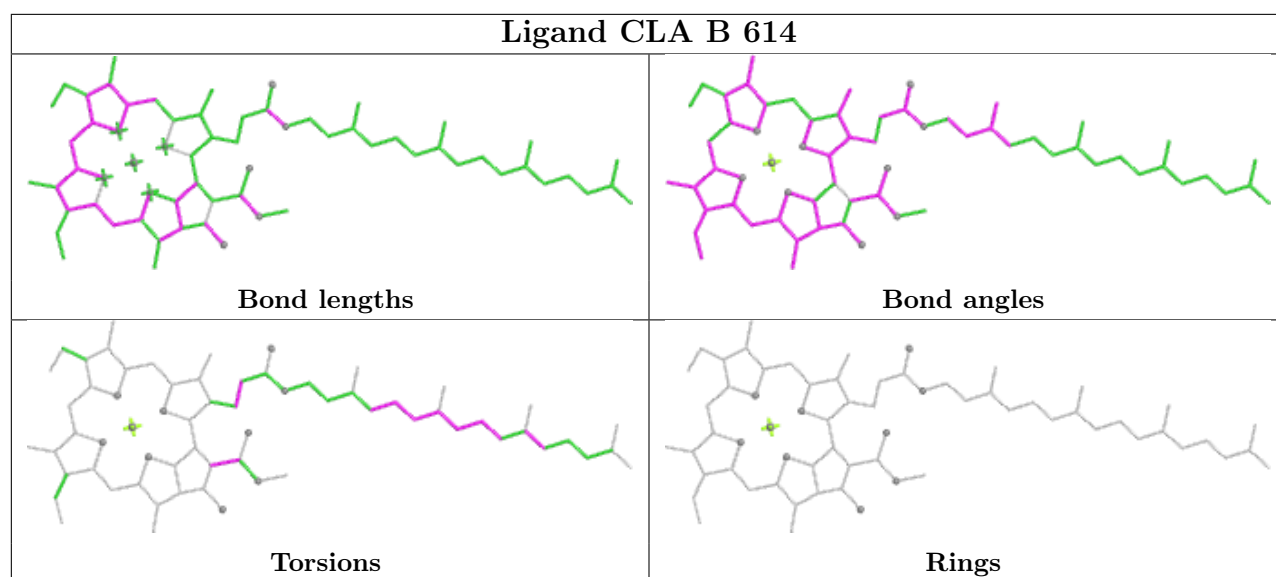
Ligand CLA a 404 (A)	
	
Bond lengths	Bond angles
	
Torsions	Rings

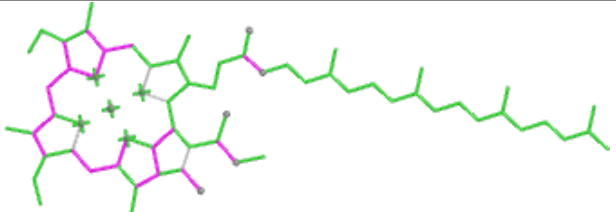
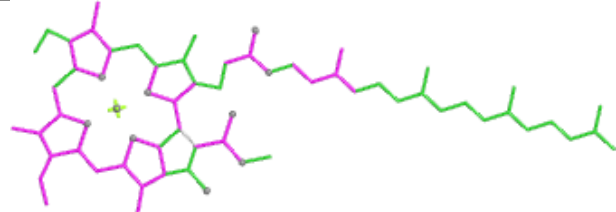
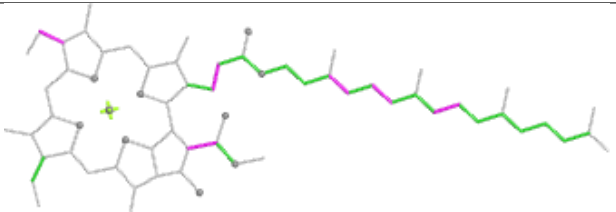
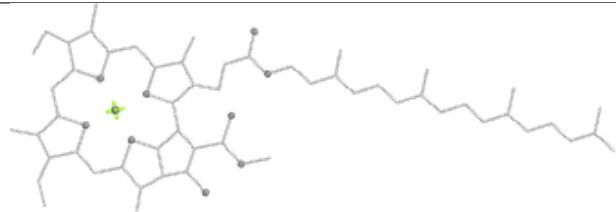
Ligand PL9 D 405 (A)	
	
Bond lengths	Bond angles
	
Torsions	Rings

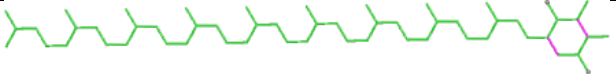
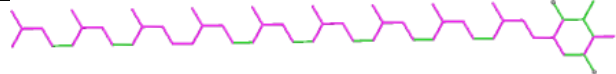
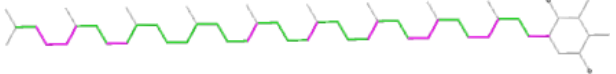
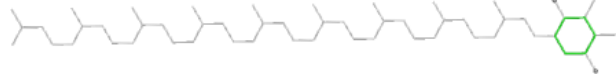


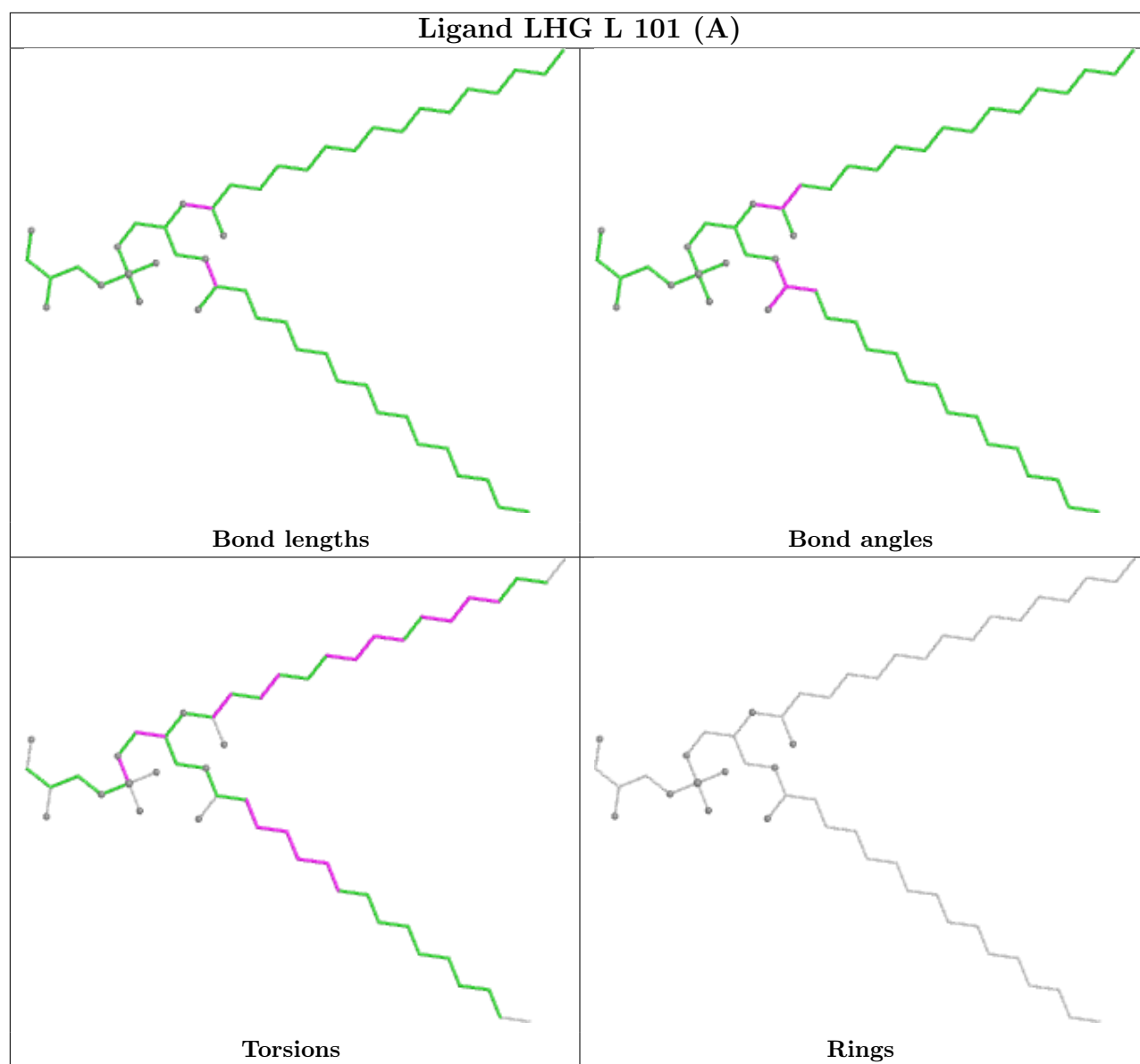


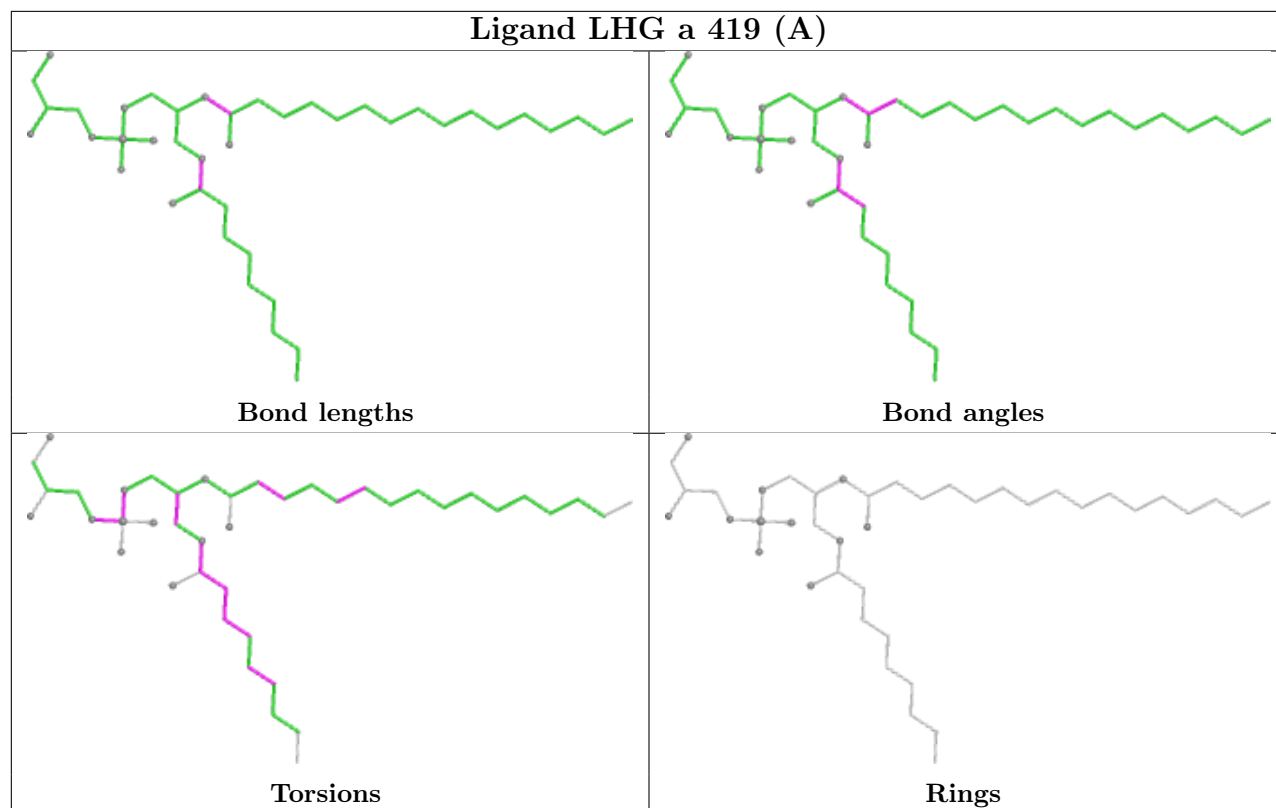


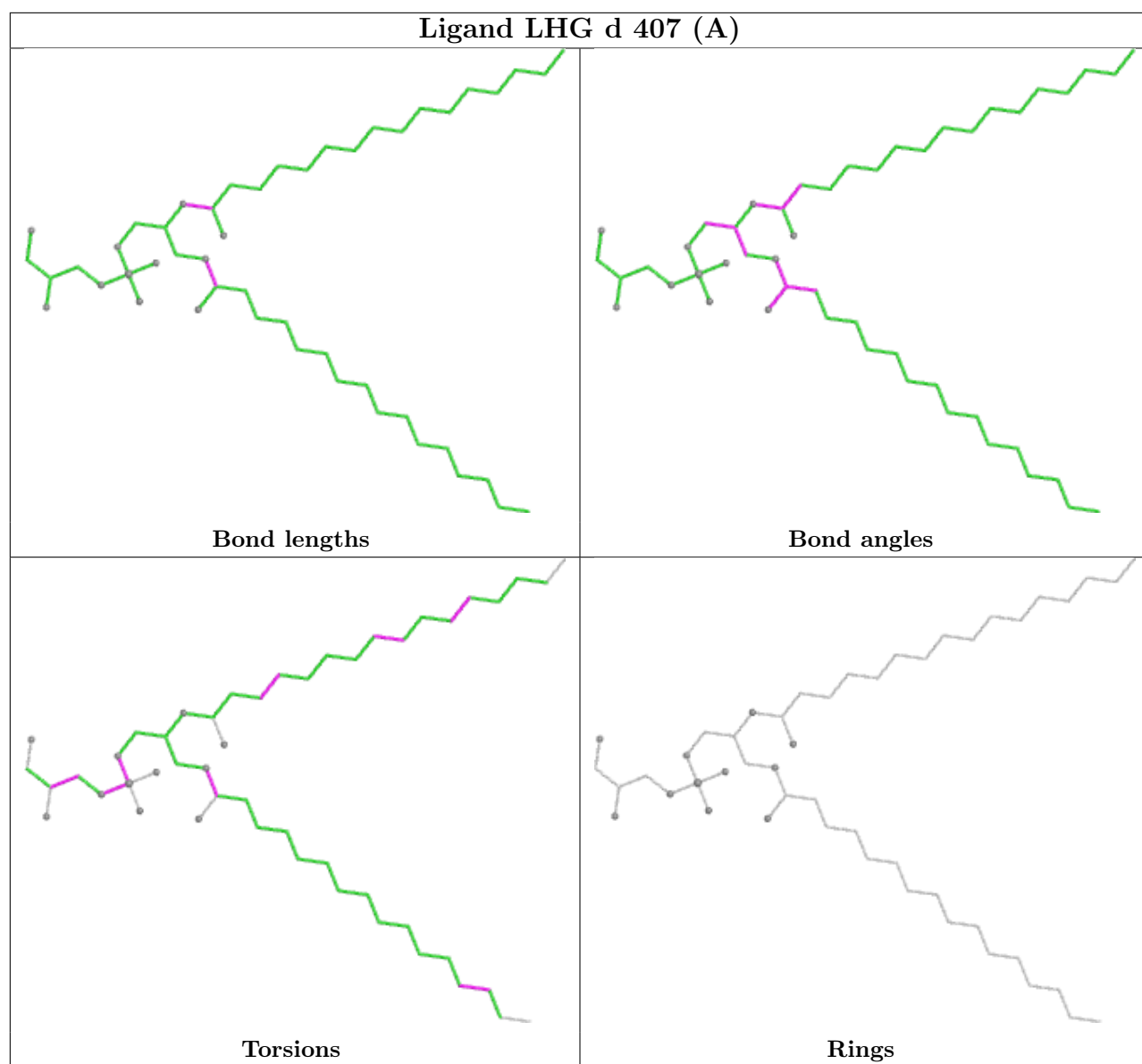


Ligand CLA c 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

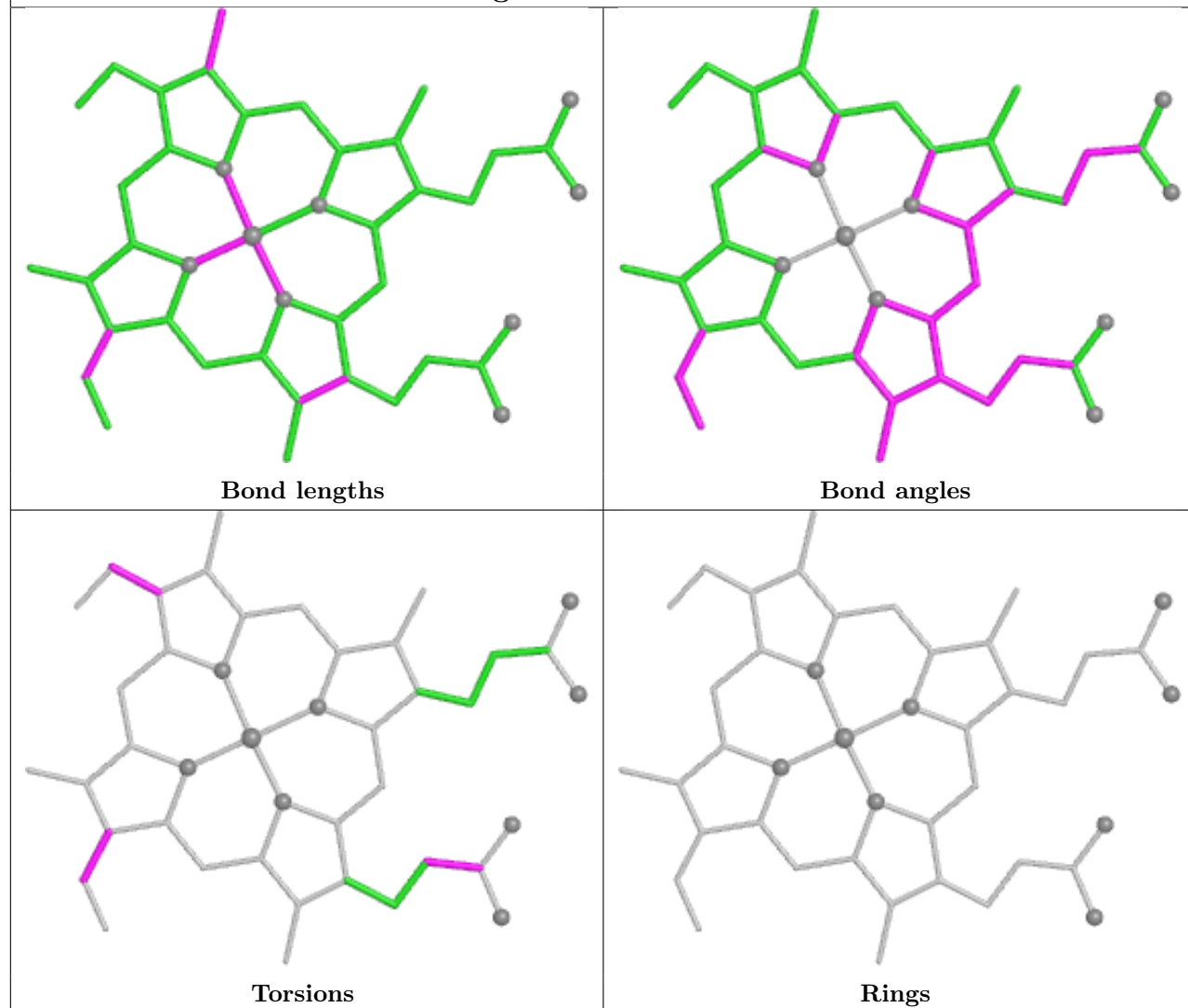
Ligand PL9 A 414 (B)	
	
Bond lengths	Bond angles
	
Torsions	Rings



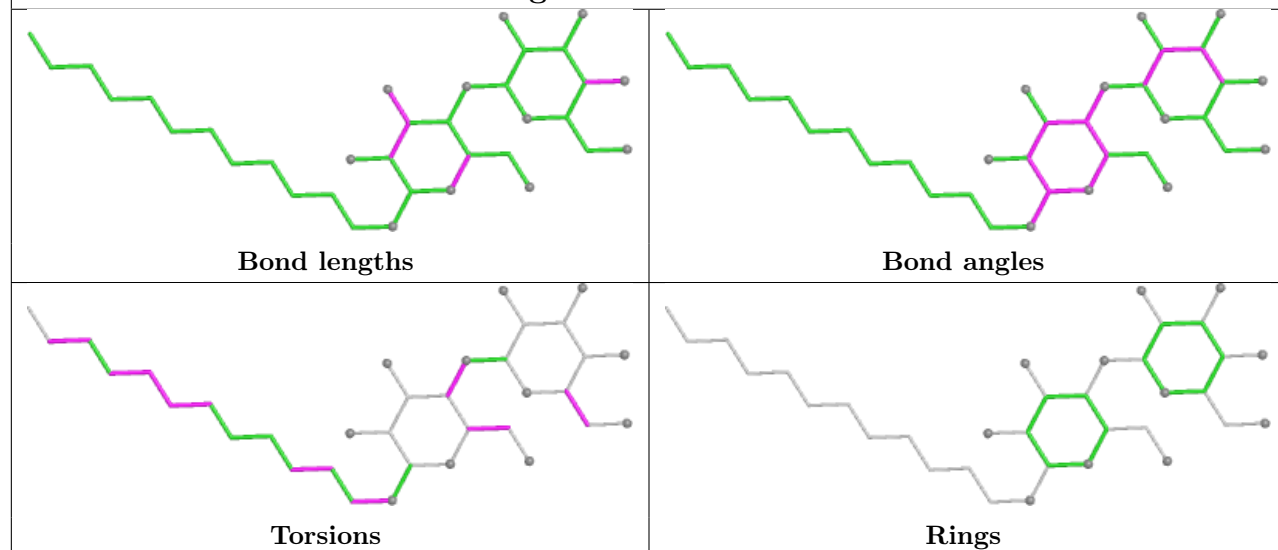




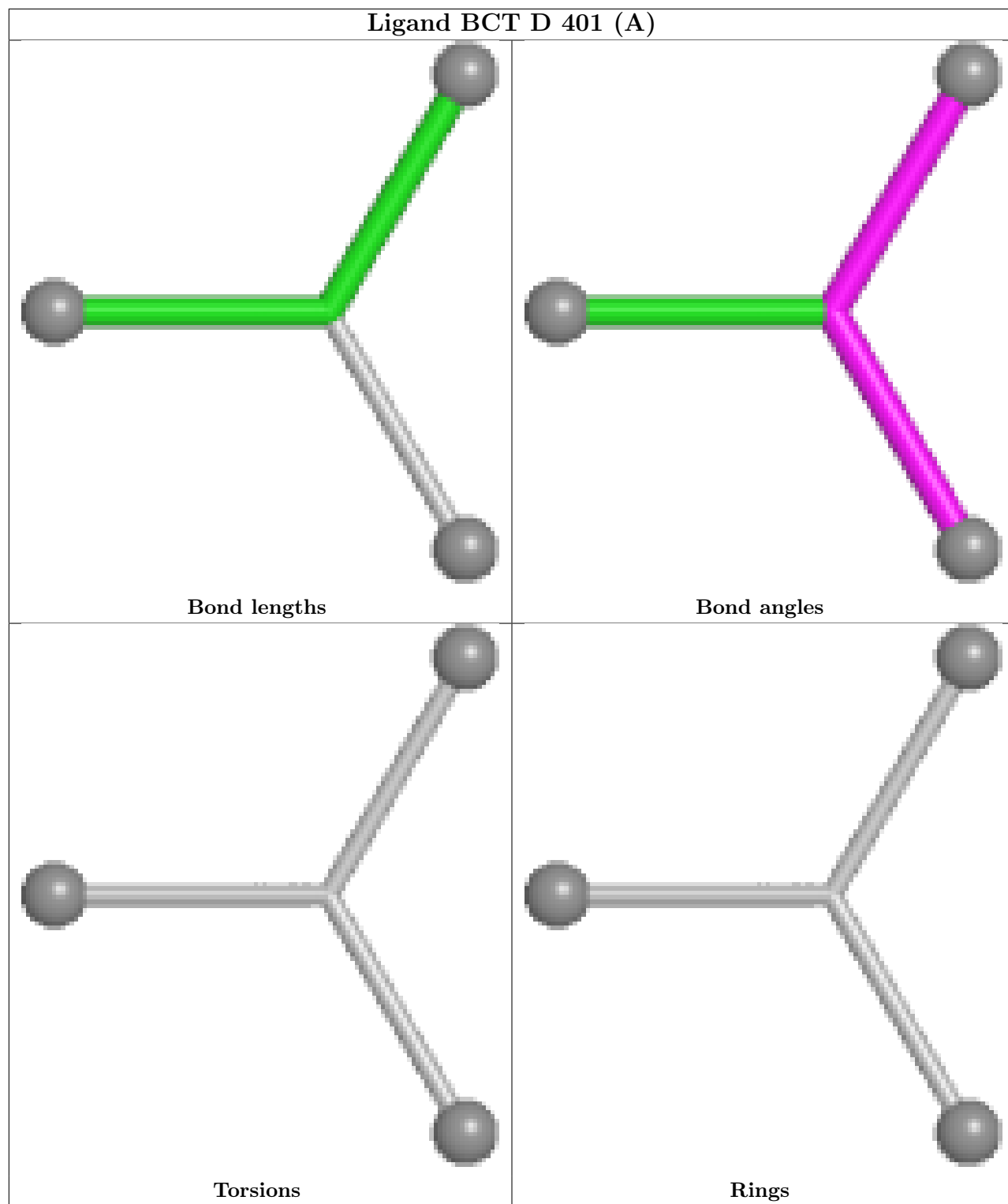
Ligand HEC V 201



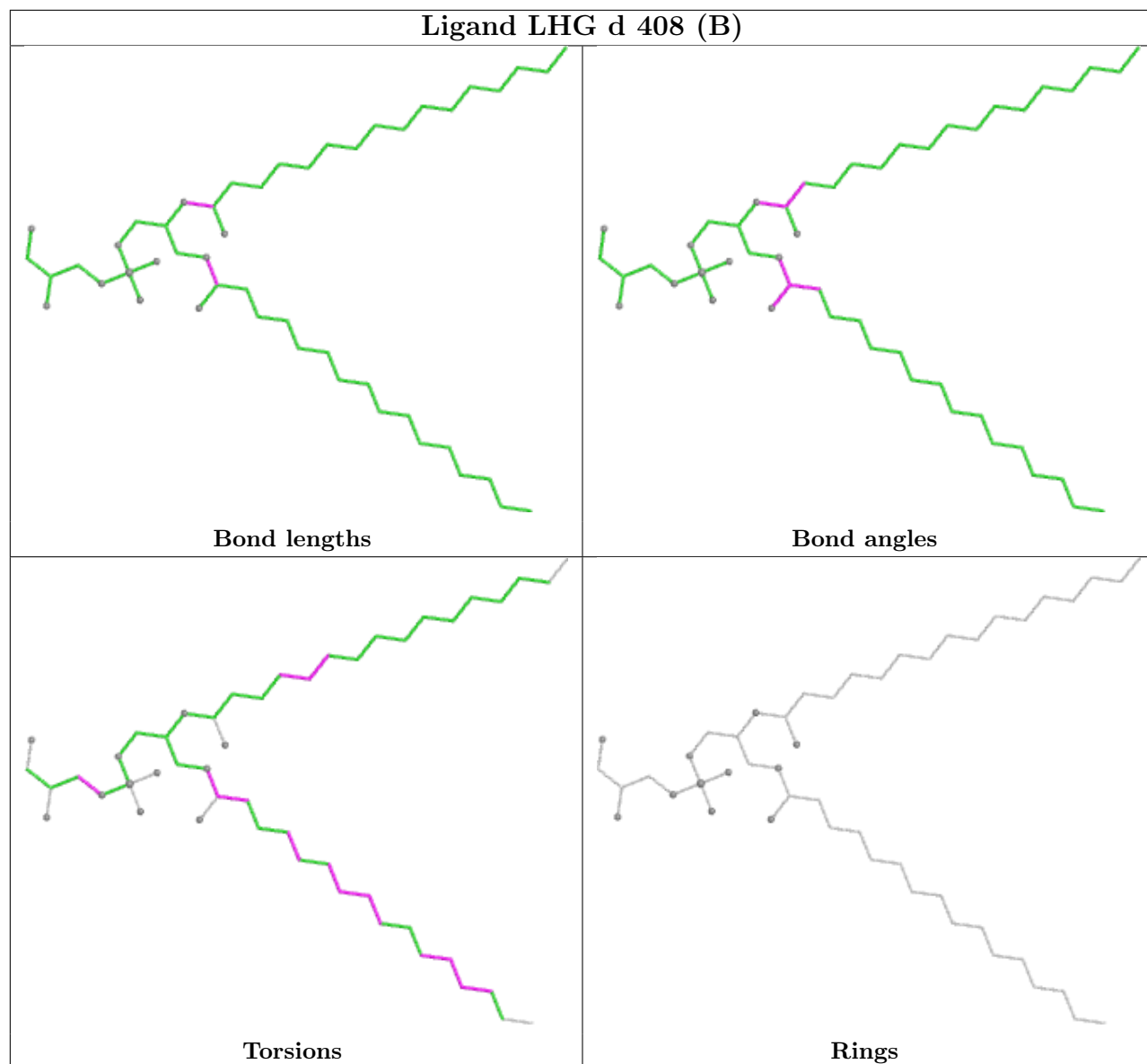
Ligand LMT B 628



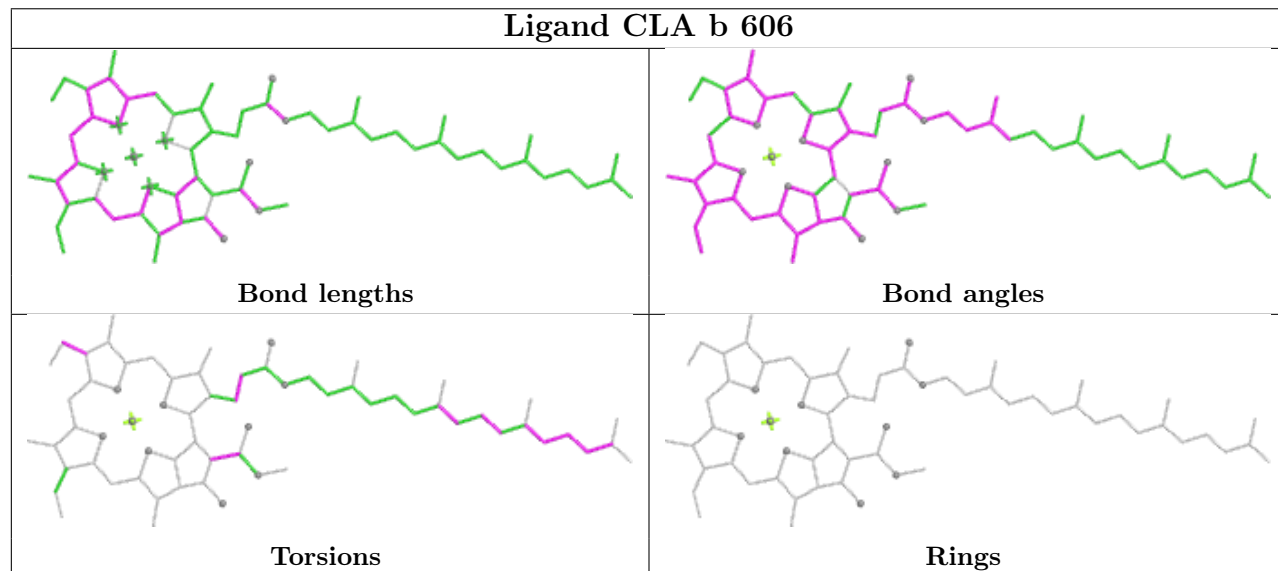
Ligand BCT D 401 (A)

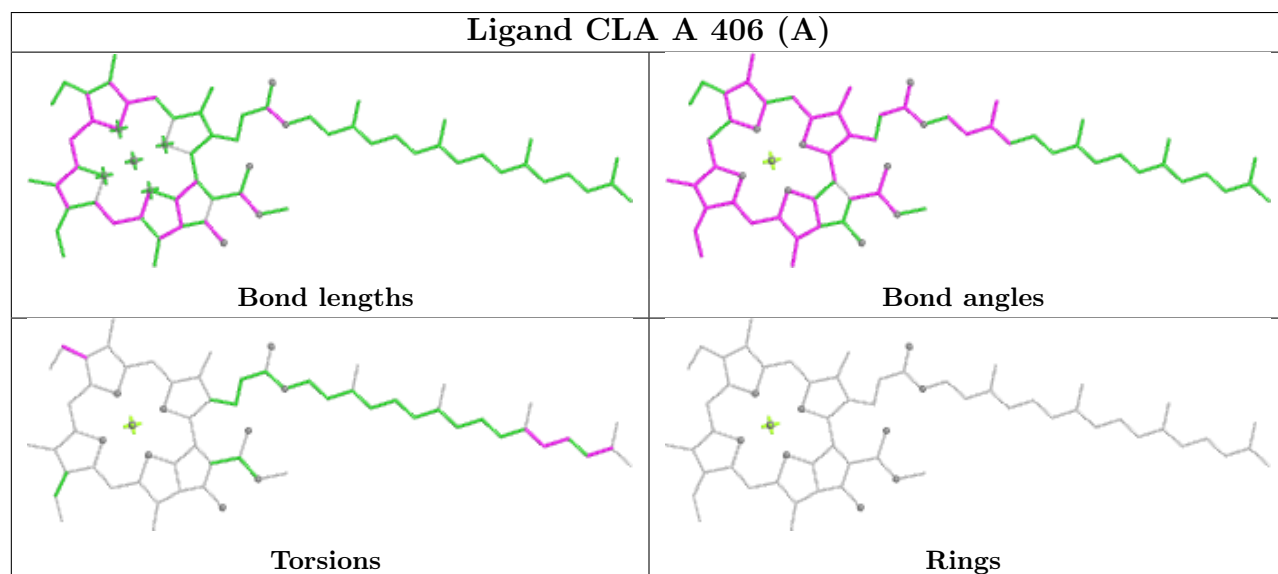
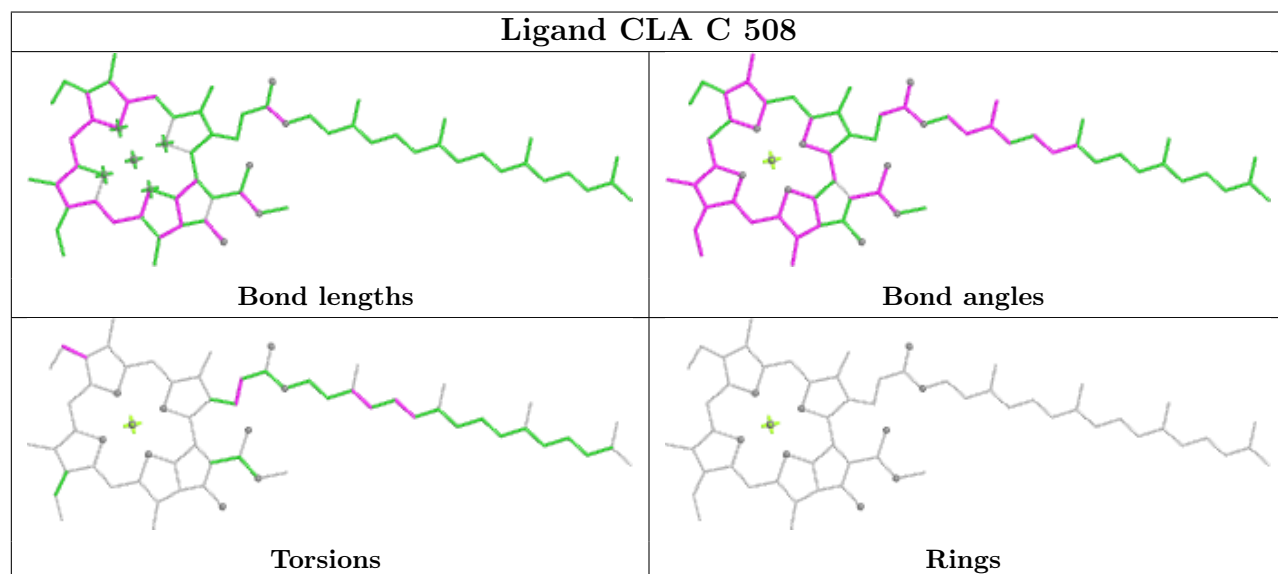
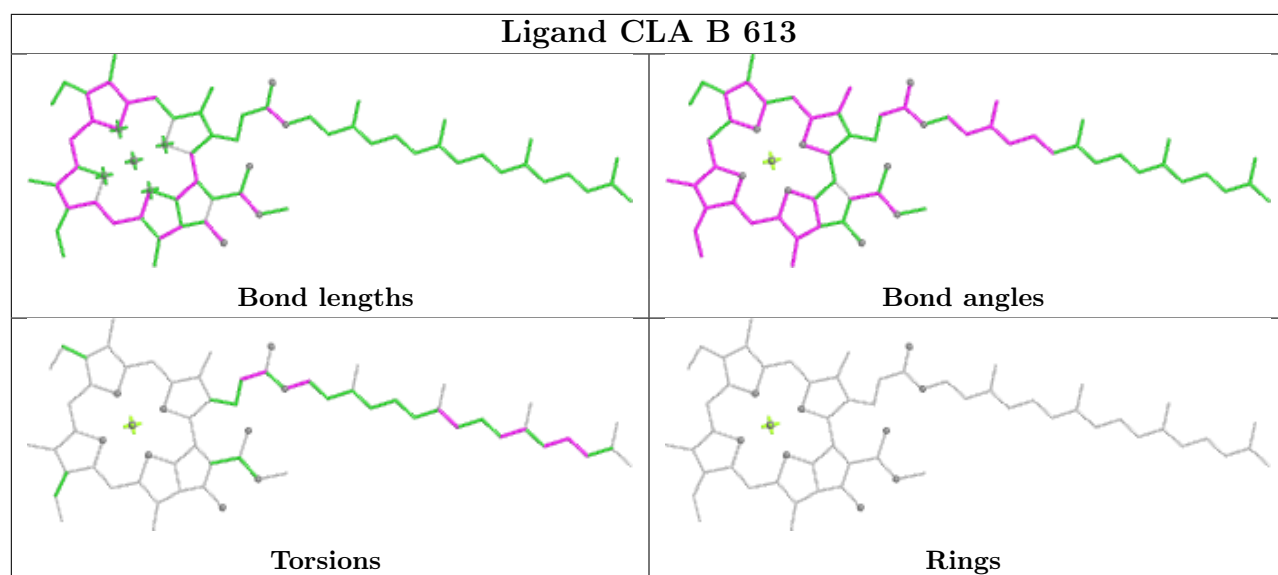


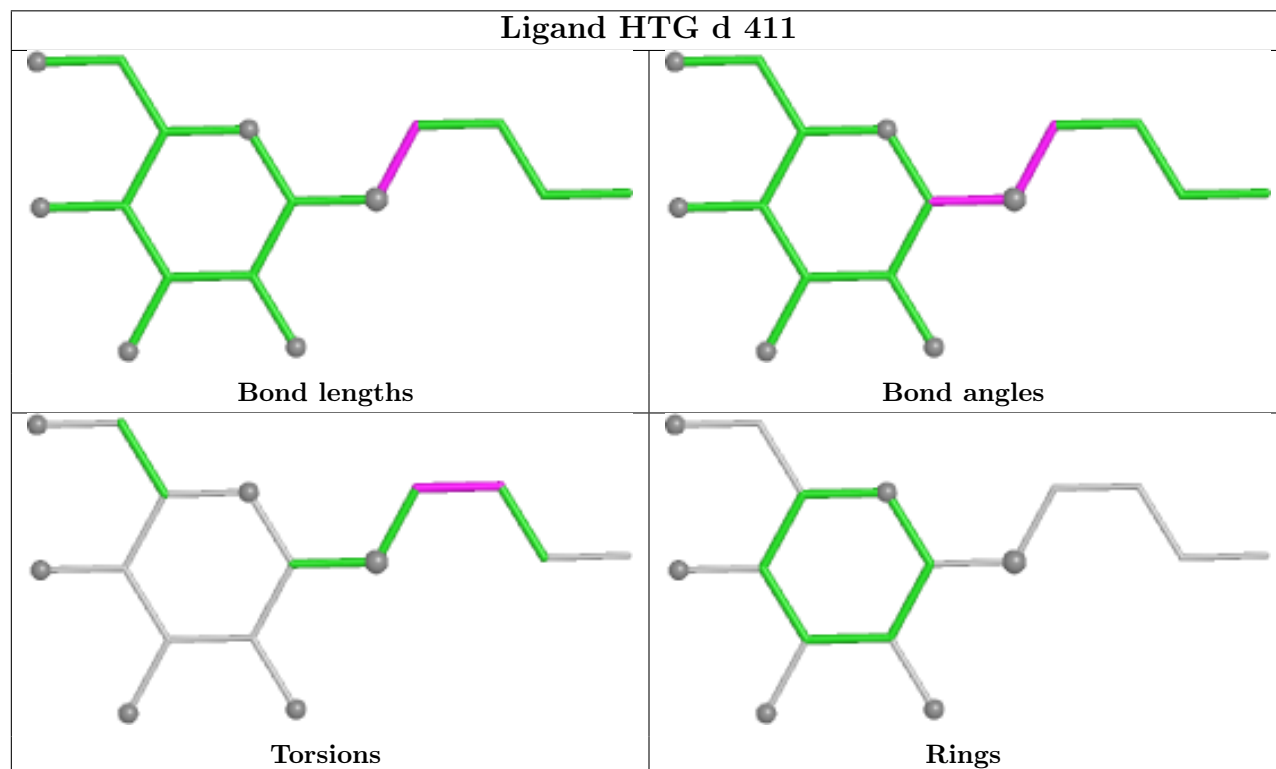
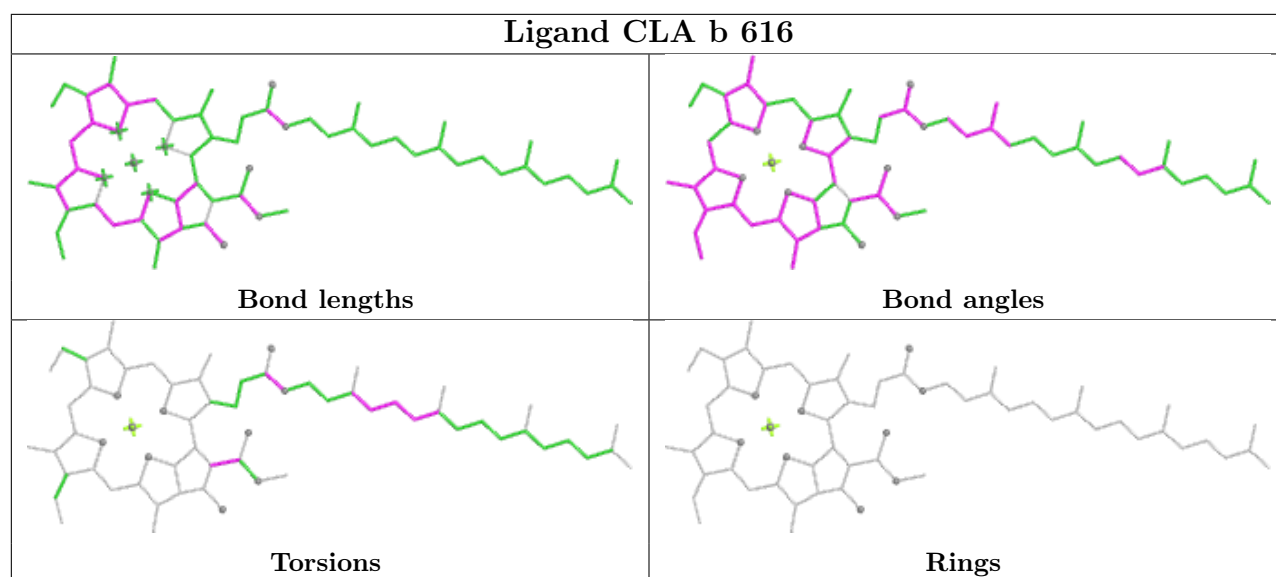
Ligand LHG d 408 (B)

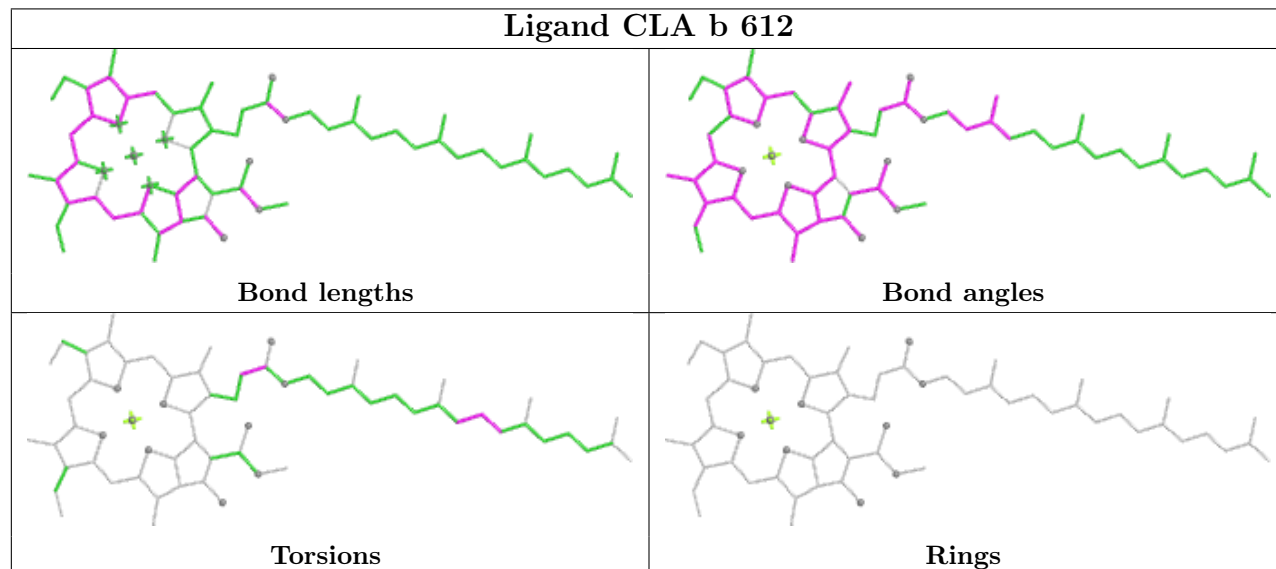
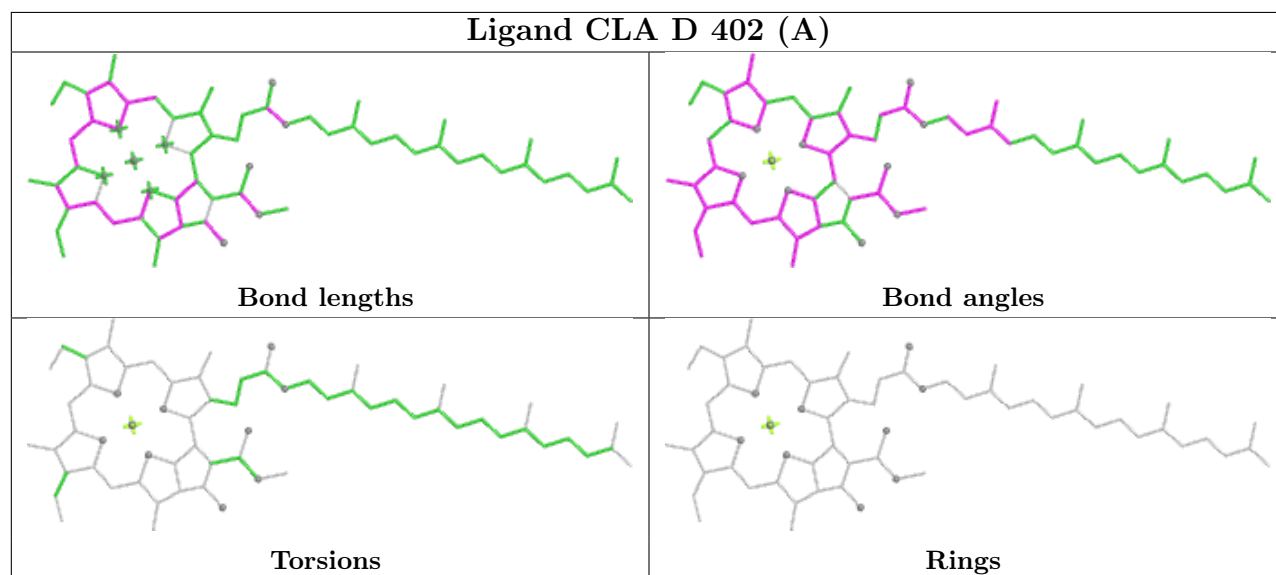
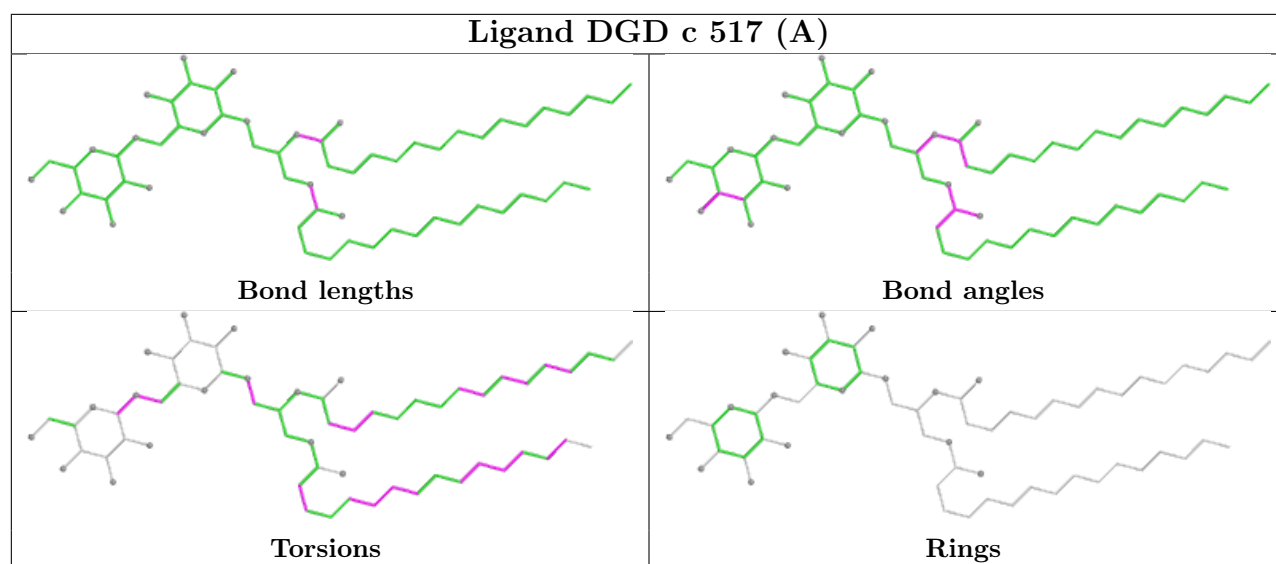


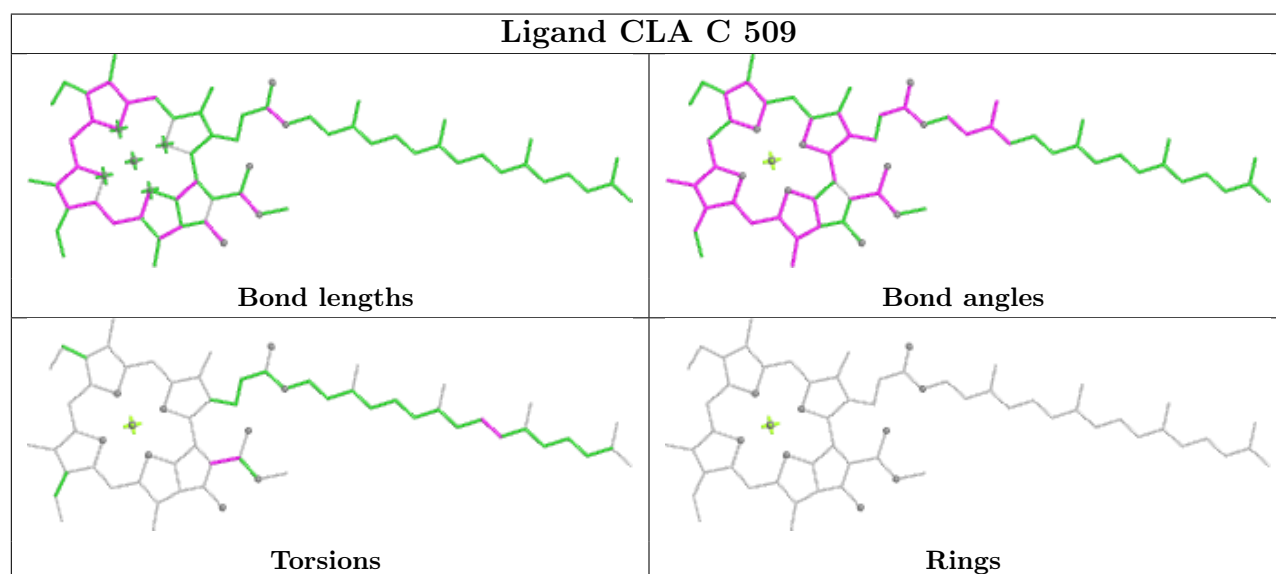
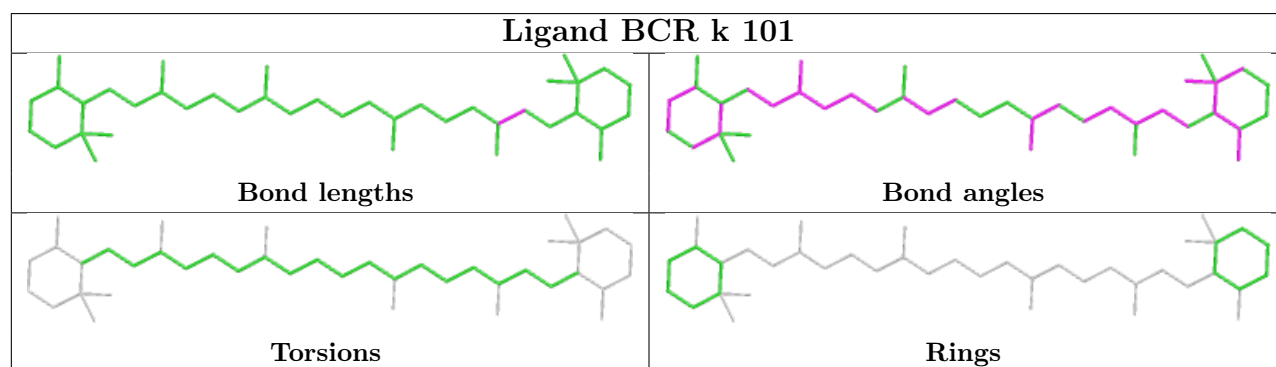
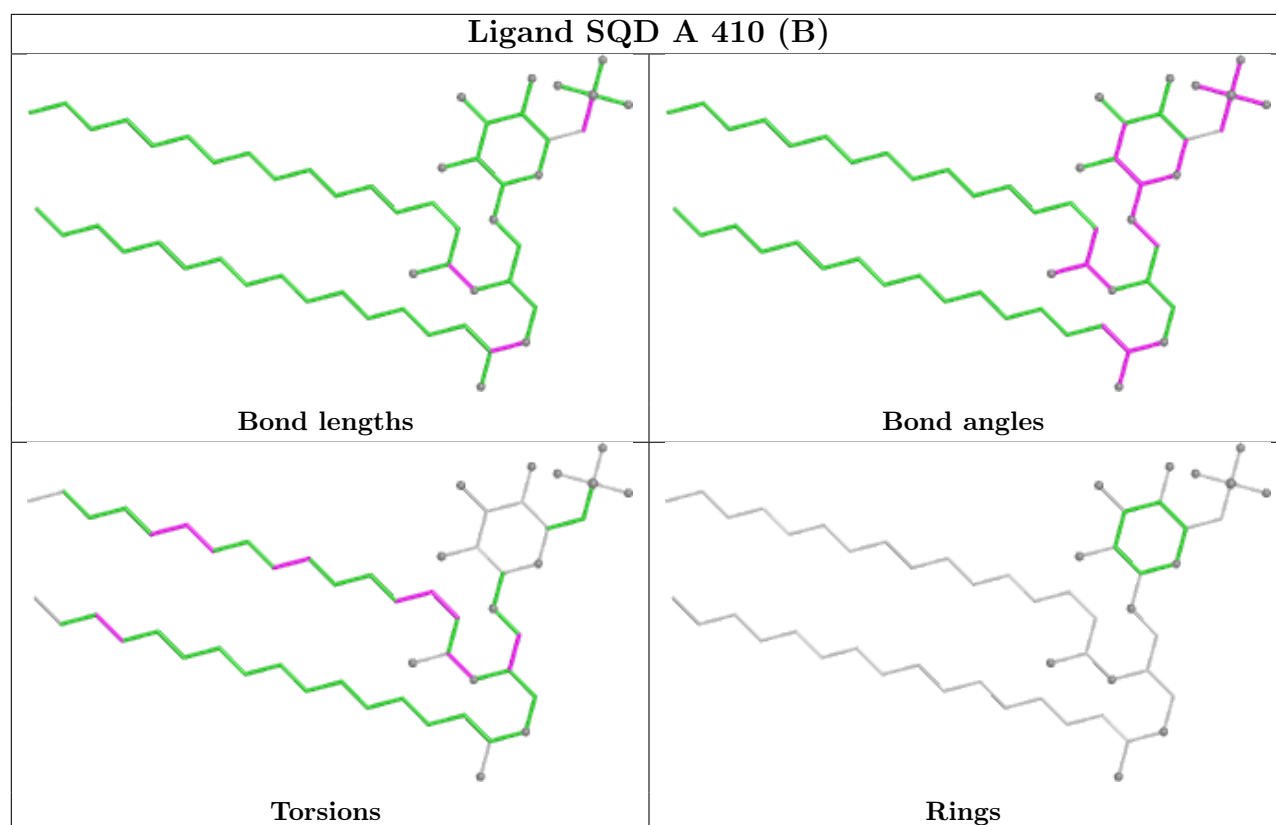
Ligand CLA b 606











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.57	1 (0%) 90 88	20, 26, 58, 126	222 (66%)
1	a	334/344 (97%)	-0.51	1 (0%) 90 88	22, 29, 65, 132	220 (65%)
2	B	504/505 (99%)	-0.43	1 (0%) 91 90	23, 54, 81, 116	22 (4%)
2	b	504/505 (99%)	-0.36	1 (0%) 91 90	24, 57, 94, 167	19 (3%)
3	C	451/455 (99%)	-0.50	0 100 100	23, 59, 79, 163	99 (21%)
3	c	455/455 (100%)	-0.39	2 (0%) 88 87	24, 65, 85, 134	101 (22%)
4	D	342/342 (100%)	-0.57	0 100 100	20, 46, 65, 141	115 (33%)
4	d	341/342 (99%)	-0.56	0 100 100	22, 51, 72, 133	119 (34%)
5	E	81/84 (96%)	-0.30	1 (1%) 76 74	53, 70, 102, 166	0
5	e	79/84 (94%)	-0.24	1 (1%) 75 73	32, 76, 116, 153	2 (2%)
6	F	34/44 (77%)	-0.54	0 100 100	54, 62, 84, 115	0
6	f	31/44 (70%)	-0.45	1 (3%) 50 47	54, 66, 95, 156	1 (3%)
7	H	64/65 (98%)	-0.15	1 (1%) 70 67	51, 63, 86, 111	0
7	h	64/65 (98%)	-0.29	1 (1%) 70 67	38, 69, 94, 113	1 (1%)
8	I	37/38 (97%)	-0.20	0 100 100	57, 63, 124, 169	0
8	i	37/38 (97%)	-0.22	0 100 100	54, 64, 122, 146	0
9	J	38/39 (97%)	-0.29	0 100 100	52, 69, 117, 183	0
9	j	39/39 (100%)	-0.29	0 100 100	59, 77, 129, 165	0
10	K	37/37 (100%)	-0.61	0 100 100	60, 68, 88, 105	0
10	k	37/37 (100%)	-0.49	0 100 100	68, 74, 95, 113	0
11	L	36/37 (97%)	-0.55	0 100 100	23, 47, 103, 147	2 (5%)
11	l	36/37 (97%)	-0.52	0 100 100	24, 48, 100, 124	2 (5%)
12	M	32/36 (88%)	-0.58	0 100 100	27, 49, 77, 136	1 (3%)
12	m	33/36 (91%)	-0.46	0 100 100	25, 49, 70, 153	2 (6%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.43	0 100 100	22, 64, 120, 188	10 (4%)
13	o	243/244 (99%)	-0.38	0 100 100	23, 66, 124, 171	8 (3%)
14	T	29/32 (90%)	-0.57	0 100 100	26, 47, 57, 65	6 (20%)
14	t	29/32 (90%)	-0.56	1 (3%) 48 45	27, 49, 63, 74	5 (17%)
15	U	96/104 (92%)	-0.56	0 100 100	26, 59, 92, 102	4 (4%)
15	u	97/104 (93%)	-0.55	0 100 100	29, 62, 83, 137	5 (5%)
16	V	137/137 (100%)	-0.62	0 100 100	24, 57, 83, 109	6 (4%)
16	v	137/137 (100%)	-0.54	0 100 100	27, 71, 102, 138	6 (4%)
17	X	38/40 (95%)	-0.28	0 100 100	35, 71, 90, 114	1 (2%)
17	x	38/40 (95%)	0.04	0 100 100	64, 77, 119, 164	0
18	Y	29/30 (96%)	0.01	1 (3%) 48 45	67, 84, 127, 131	0
18	y	29/30 (96%)	-0.16	0 100 100	75, 92, 112, 119	0
19	Z	62/62 (100%)	-0.28	0 100 100	67, 80, 132, 162	0
19	z	62/62 (100%)	0.14	0 100 100	80, 94, 140, 206	0
20	R	34/34 (100%)	0.47	2 (5%) 28 25	79, 101, 130, 137	0
All	All	5283/5384 (98%)	-0.44	15 (0%) 90 88	20, 58, 99, 206	979 (18%)

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	3.9
5	e	79[A]	PHE	3.8
6	f	16[A]	PHE	2.6
1	a	11	ALA	2.5
5	E	4	THR	2.5

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	T	1	10/11	0.94	0.08	45,55,64,72	0
8	FME	I	1	10/11	0.95	0.07	58,69,79,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	FME	m	1	10/11	0.96	0.07	53,63,88,122	0
14	FME	t	1	10/11	0.96	0.07	44,51,65,75	0
8	FME	i	1	10/11	0.97	0.07	53,68,77,90	0
12	FME	M	1	10/11	0.98	0.06	52,60,89,108	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	417	6/6	0.63	0.15	78,98,110,112	0
31	LMT	A	417	35/35	0.67	0.15	65,116,144,148	0
31	LMT	B	630	35/35	0.67	0.15	66,117,148,156	0
31	LMT	F	101	35/35	0.69	0.15	102,138,184,189	0
30	UNL	j	101	10/-	0.70	0.18	80,93,103,106	0
30	UNL	I	101	40/-	0.71	0.16	73,111,158,166	0
30	UNL	a	413	30/-	0.71	0.12	93,119,146,161	0
30	UNL	A	415	28/-	0.71	0.15	93,117,135,155	0
34	HTG	B	623	19/19	0.71	0.17	67,93,117,125	0
30	UNL	J	101	10/-	0.72	0.24	72,81,90,95	0
30	UNL	m	102	10/-	0.72	0.21	73,77,96,102	0
30	UNL	K	101[A]	34/-	0.74	0.14	88,115,128,132	34
30	UNL	K	101[B]	34/-	0.74	0.14	88,115,128,133	34
31	LMT	A	420	35/35	0.74	0.13	100,135,156,170	0
34	HTG	C	522	19/19	0.74	0.13	112,130,148,148	0
31	LMT	a	416	35/35	0.75	0.13	109,138,152,164	0
31	LMT	e	101	35/35	0.76	0.13	110,151,197,199	0
30	UNL	M	102	10/-	0.77	0.16	69,78,93,96	0
26	SQD	f	102	43/54	0.77	0.13	90,133,179,195	0
30	UNL	i	101	40/-	0.78	0.14	73,110,160,171	0
30	UNL	b	626	33/-	0.79	0.13	68,97,161,173	0
30	UNL	c	524[A]	32/-	0.79	0.15	98,113,127,139	32
31	LMT	b	621	25/35	0.79	0.13	84,112,164,173	0
30	UNL	c	524[B]	32/-	0.79	0.15	98,113,127,139	32

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	LMG	C	521	51/55	0.79	0.11	63,117,164,179	0
30	UNL	d	410	36/-	0.79	0.12	65,93,136,146	0
27	GOL	o	302	6/6	0.79	0.17	84,102,112,116	0
34	HTG	D	410	16/19	0.79	0.12	84,104,134,149	0
27	GOL	d	413	6/6	0.80	0.14	55,75,76,91	0
30	UNL	D	409	40/-	0.80	0.13	67,94,139,151	0
36	CA	F	103	1/1	0.81	0.24	127,127,127,127	0
30	UNL	B	626	33/-	0.82	0.15	54,117,145,149	0
34	HTG	V	202	11/19	0.82	0.10	83,111,123,130	0
34	HTG	b	623	19/19	0.82	0.11	84,135,161,168	0
34	HTG	c	521	19/19	0.82	0.10	105,125,141,151	0
31	LMT	B	628	35/35	0.82	0.12	67,102,138,150	0
32	LHG	a	419[B]	42/49	0.83	0.11	94,140,157,165	42
26	SQD	a	410	54/54	0.83	0.11	67,97,136,154	0
27	GOL	o	303	6/6	0.83	0.14	82,91,102,110	0
27	GOL	v	202[A]	6/6	0.83	0.13	65,79,85,86	6
27	GOL	v	202[B]	6/6	0.83	0.13	65,79,85,87	6
27	GOL	a	418	6/6	0.83	0.15	58,78,84,88	0
27	GOL	b	624	6/6	0.83	0.15	88,95,107,111	0
27	GOL	O	303	6/6	0.83	0.13	82,95,107,108	0
32	LHG	a	419[A]	42/49	0.83	0.11	94,140,157,165	42
27	GOL	l	801[B]	6/6	0.84	0.19	73,105,107,111	6
31	LMT	B	631	25/35	0.84	0.12	63,87,150,170	0
27	GOL	B	627	6/6	0.84	0.13	71,88,97,112	0
34	HTG	d	411	16/19	0.84	0.11	89,122,140,154	0
27	GOL	l	801[A]	6/6	0.84	0.19	73,104,107,111	6
33	LMG	c	520	51/55	0.85	0.10	73,135,172,190	0
33	LMG	z	101	39/55	0.85	0.13	78,132,153,170	0
29	PL9	A	414[A]	55/55	0.85	0.15	74,100,115,120	55
29	PL9	A	414[B]	55/55	0.85	0.15	74,100,115,120	55
31	LMT	T	101	35/35	0.85	0.11	77,131,185,192	0
36	CA	f	103	1/1	0.85	0.10	120,120,120,120	0
27	GOL	A	411	6/6	0.86	0.12	64,81,85,91	0
34	HTG	b	622	19/19	0.86	0.12	58,80,121,125	0
33	LMG	Z	101	37/55	0.86	0.14	72,123,151,171	0
31	LMT	t	101	26/35	0.86	0.12	78,105,148,163	0
29	PL9	a	412[A]	55/55	0.86	0.15	82,109,121,129	55
29	PL9	a	412[B]	55/55	0.86	0.15	82,109,121,129	55
26	SQD	A	412	54/54	0.86	0.11	65,90,140,150	0
31	LMT	M	101	35/35	0.87	0.10	63,96,120,125	0
31	LMT	m	103	35/35	0.87	0.10	66,90,109,125	0
27	GOL	B	629	6/6	0.87	0.13	74,79,93,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	HTG	B	622	19/19	0.87	0.13	61,87,121,126	0
27	GOL	O	302	6/6	0.87	0.08	77,86,99,113	0
27	GOL	c	526	6/6	0.87	0.16	102,111,120,127	0
31	LMT	b	627	25/35	0.87	0.12	59,100,155,167	0
27	GOL	A	418	6/6	0.88	0.15	51,82,88,93	0
26	SQD	F	102	43/54	0.88	0.12	69,107,131,145	0
23	CLA	b	601	65/65	0.88	0.11	59,84,128,166	0
27	GOL	D	412	6/6	0.88	0.12	51,68,73,94	0
26	SQD	b	620	54/54	0.89	0.10	65,96,118,130	0
32	LHG	E	101[A]	42/49	0.89	0.12	76,106,118,123	42
32	LHG	E	101[B]	42/49	0.89	0.12	76,106,118,124	42
26	SQD	B	620	54/54	0.89	0.10	66,93,135,146	0
30	UNL	D	408	17/-	0.89	0.11	62,78,99,122	0
36	CA	o	301	1/1	0.89	0.07	103,103,103,103	0
27	GOL	V	203[B]	6/6	0.90	0.13	60,70,77,77	6
23	CLA	c	513	65/65	0.90	0.10	66,93,129,148	0
23	CLA	B	601	65/65	0.90	0.10	57,78,114,156	0
33	LMG	C	501	51/55	0.90	0.10	68,90,118,136	0
27	GOL	V	203[A]	6/6	0.90	0.13	60,70,77,77	6
33	LMG	a	415	51/55	0.91	0.09	71,96,115,119	0
33	LMG	c	519	51/55	0.91	0.10	62,91,136,161	0
27	GOL	B	624	6/6	0.91	0.09	70,73,86,91	0
33	LMG	m	101	51/55	0.91	0.09	63,76,98,115	0
34	HTG	B	625	19/19	0.91	0.08	68,82,98,105	0
30	UNL	d	409	17/-	0.92	0.10	69,79,114,116	0
33	LMG	D	411	51/55	0.92	0.10	50,72,124,138	0
23	CLA	b	616	65/65	0.92	0.09	48,62,133,146	0
33	LMG	C	520	51/55	0.92	0.09	55,85,123,134	0
34	HTG	b	625	19/19	0.92	0.08	68,79,97,110	0
37	BCT	d	401[A]	4/4	0.92	0.09	59,61,69,78	4
37	BCT	d	401[B]	4/4	0.92	0.09	60,61,69,80	4
25	BCR	t	102	40/40	0.93	0.07	44,59,80,89	0
26	SQD	A	410[A]	54/54	0.93	0.09	57,81,115,119	54
26	SQD	A	410[B]	54/54	0.93	0.09	57,81,115,119	54
23	CLA	B	603	65/65	0.93	0.09	43,54,73,83	0
23	CLA	C	507	65/65	0.93	0.08	53,71,125,144	0
33	LMG	d	412	51/55	0.93	0.09	54,72,124,155	0
23	CLA	c	506	65/65	0.93	0.09	54,72,126,142	0
26	SQD	a	409[A]	54/54	0.93	0.10	61,83,121,123	54
26	SQD	a	409[B]	54/54	0.93	0.10	61,83,121,123	54
23	CLA	c	512	65/65	0.93	0.09	60,81,126,140	0
23	CLA	C	514	65/65	0.93	0.08	59,83,115,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	CLA	d	404	65/65	0.93	0.09	52,67,130,157	0
25	BCR	B	619	40/40	0.93	0.09	47,60,90,101	0
25	BCR	D	404	40/40	0.93	0.09	44,62,108,115	0
32	LHG	A	419[A]	49/49	0.93	0.10	50,66,89,93	49
32	LHG	A	419[B]	49/49	0.93	0.10	50,66,89,93	49
32	LHG	D	407[A]	49/49	0.93	0.09	49,61,110,113	49
32	LHG	D	407[B]	49/49	0.93	0.09	49,61,110,114	49
25	BCR	H	101	40/40	0.93	0.09	53,68,90,93	0
25	BCR	T	102	40/40	0.93	0.07	45,57,73,86	0
35	DGD	C	518[A]	62/66	0.93	0.08	49,63,114,118	62
35	DGD	C	518[B]	62/66	0.93	0.08	49,63,114,118	62
25	BCR	a	408	40/40	0.93	0.07	45,53,67,69	0
27	GOL	C	523[A]	6/6	0.93	0.11	59,62,67,72	6
33	LMG	B	621	51/55	0.93	0.08	55,72,95,116	0
27	GOL	C	523[B]	6/6	0.93	0.11	59,63,67,72	6
25	BCR	d	405	40/40	0.93	0.08	51,69,109,113	0
32	LHG	d	414[B]	49/49	0.94	0.09	51,69,82,94	49
23	CLA	D	403	65/65	0.94	0.09	47,60,132,138	0
23	CLA	a	407	65/65	0.94	0.10	42,57,141,161	0
25	BCR	K	102	40/40	0.94	0.09	56,65,76,82	0
23	CLA	B	614	65/65	0.94	0.08	39,50,104,118	0
25	BCR	Y	101	40/40	0.94	0.08	54,65,84,92	0
29	PL9	D	405[A]	55/55	0.94	0.07	38,50,57,72	55
29	PL9	D	405[B]	55/55	0.94	0.07	38,50,58,72	55
23	CLA	b	606	65/65	0.94	0.08	43,58,117,132	0
25	BCR	b	619	40/40	0.94	0.08	48,64,90,95	0
25	BCR	c	514	40/40	0.94	0.09	71,83,93,98	0
23	CLA	b	614	65/65	0.94	0.07	42,53,102,117	0
25	BCR	h	101	40/40	0.94	0.09	55,70,91,97	0
23	CLA	B	616	65/65	0.94	0.09	48,59,132,147	0
25	BCR	y	101	40/40	0.94	0.08	59,71,89,100	0
23	CLA	c	504	65/65	0.94	0.07	53,64,107,142	0
23	CLA	C	505	65/65	0.94	0.08	42,58,106,131	0
23	CLA	c	507	65/65	0.94	0.10	50,67,85,92	0
23	CLA	A	408	65/65	0.94	0.09	43,54,128,149	0
30	UNL	X	101	18/-	0.94	0.11	64,73,112,112	0
27	GOL	b	628	6/6	0.94	0.07	78,88,92,92	0
23	CLA	C	508	65/65	0.94	0.09	47,61,83,93	0
23	CLA	C	513	65/65	0.94	0.09	54,72,117,136	0
25	BCR	A	409	40/40	0.94	0.07	40,52,67,71	0
25	BCR	B	618	40/40	0.94	0.06	43,55,73,80	0
23	CLA	B	606	65/65	0.94	0.09	44,56,114,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	DGD	C	519	62/66	0.94	0.08	45,61,103,122	0
35	DGD	H	102	62/66	0.94	0.09	47,63,75,90	0
35	DGD	c	516[A]	62/66	0.94	0.08	48,64,103,113	62
35	DGD	c	516[B]	62/66	0.94	0.08	47,64,103,114	62
35	DGD	c	517[A]	62/66	0.94	0.08	56,69,123,138	62
35	DGD	c	517[B]	62/66	0.94	0.08	56,69,123,139	62
35	DGD	c	518	62/66	0.94	0.08	50,67,106,131	0
35	DGD	h	102	62/66	0.94	0.08	52,65,79,82	0
32	LHG	b	629[A]	49/49	0.94	0.08	51,60,72,95	49
32	LHG	b	629[B]	49/49	0.94	0.08	51,60,72,95	49
32	LHG	d	408[A]	49/49	0.94	0.09	52,64,117,134	49
32	LHG	d	408[B]	49/49	0.94	0.09	52,64,117,134	49
32	LHG	d	414[A]	49/49	0.94	0.09	51,69,81,93	49
23	CLA	c	508	65/65	0.95	0.07	46,63,133,152	0
23	CLA	C	509	65/65	0.95	0.07	47,56,122,147	0
23	CLA	C	502	65/65	0.95	0.07	49,60,74,81	0
25	BCR	b	617	40/40	0.95	0.06	43,53,64,69	0
25	BCR	b	618	40/40	0.95	0.07	47,57,76,94	0
23	CLA	b	612	65/65	0.95	0.08	41,54,65,76	0
24	PHO	A	416[A]	64/64	0.95	0.07	39,51,56,63	64
25	BCR	c	515	40/40	0.95	0.07	57,65,78,86	0
24	PHO	A	416[B]	64/64	0.95	0.07	38,51,56,64	64
24	PHO	a	414[A]	64/64	0.95	0.07	44,56,64,72	64
32	LHG	d	407[A]	49/49	0.95	0.08	49,57,72,79	49
32	LHG	d	407[B]	49/49	0.95	0.08	49,58,72,79	49
35	DGD	C	517[A]	62/66	0.95	0.07	47,57,103,109	62
35	DGD	C	517[B]	62/66	0.95	0.07	47,57,103,109	62
30	UNL	x	101	18/-	0.95	0.11	68,84,140,141	0
25	BCR	k	101	40/40	0.95	0.09	59,75,85,87	0
24	PHO	a	414[B]	64/64	0.95	0.07	44,56,64,72	64
23	CLA	B	611	65/65	0.95	0.07	38,46,65,74	0
29	PL9	d	406[A]	55/55	0.95	0.07	41,52,63,72	55
29	PL9	d	406[B]	55/55	0.95	0.07	40,52,63,72	55
23	CLA	B	609	65/65	0.95	0.07	47,59,72,83	0
23	CLA	c	501	65/65	0.95	0.08	55,67,80,93	0
25	BCR	C	515	40/40	0.95	0.07	55,75,91,93	0
25	BCR	C	516	40/40	0.95	0.07	51,61,76,90	0
23	CLA	a	405[A]	65/65	0.95	0.07	43,55,126,133	65
23	CLA	a	405[B]	65/65	0.95	0.07	42,55,126,133	65
27	GOL	c	525[A]	6/6	0.95	0.08	65,72,77,77	6
37	BCT	D	401[A]	4/4	0.95	0.08	54,55,61,68	4
37	BCT	D	401[B]	4/4	0.95	0.08	54,55,62,69	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
27	GOL	c	525[B]	6/6	0.95	0.08	65,73,77,78	6
23	CLA	B	610	65/65	0.95	0.09	42,55,68,84	0
23	CLA	b	607	65/65	0.96	0.07	38,48,81,94	0
23	CLA	b	609	65/65	0.96	0.07	49,65,77,90	0
23	CLA	b	611	65/65	0.96	0.07	41,51,72,81	0
23	CLA	C	506	65/65	0.96	0.07	46,60,96,109	0
23	CLA	b	613	65/65	0.96	0.06	43,50,88,108	0
23	CLA	B	607	65/65	0.96	0.07	38,48,72,85	0
23	CLA	b	615	65/65	0.96	0.06	48,59,83,95	0
23	CLA	A	406[A]	65/65	0.96	0.06	41,48,114,125	65
32	LHG	D	406[A]	49/49	0.96	0.08	46,57,70,80	49
32	LHG	D	406[B]	49/49	0.96	0.08	46,57,71,80	49
23	CLA	A	406[B]	65/65	0.96	0.06	41,48,114,125	65
23	CLA	c	503	65/65	0.96	0.07	49,70,86,93	0
23	CLA	C	510	65/65	0.96	0.08	50,59,83,94	0
23	CLA	c	505	65/65	0.96	0.07	51,64,92,97	0
32	LHG	L	101[A]	49/49	0.96	0.07	49,58,71,94	49
32	LHG	L	101[B]	49/49	0.96	0.07	48,58,71,94	49
23	CLA	C	512	65/65	0.96	0.07	49,64,80,84	0
22	CL	a	402[A]	1/1	0.96	0.06	50,50,50,50	1
23	CLA	B	613	65/65	0.96	0.06	39,48,100,109	0
23	CLA	c	509	65/65	0.96	0.08	46,62,90,101	0
23	CLA	c	511	65/65	0.96	0.08	56,68,87,107	0
22	CL	a	402[B]	1/1	0.96	0.06	50,50,50,50	1
23	CLA	B	615	65/65	0.96	0.06	45,55,78,96	0
23	CLA	B	602	65/65	0.96	0.07	46,56,74,88	0
23	CLA	A	404[A]	65/65	0.96	0.07	37,45,63,71	65
23	CLA	C	504	65/65	0.96	0.06	46,62,72,88	0
24	PHO	a	406[A]	64/64	0.96	0.06	43,50,55,60	64
36	CA	C	524	1/1	0.96	0.05	72,72,72,72	0
24	PHO	a	406[B]	64/64	0.96	0.06	43,50,56,60	64
36	CA	O	301	1/1	0.96	0.04	104,104,104,104	0
36	CA	c	522	1/1	0.96	0.10	73,73,73,73	0
23	CLA	b	602	65/65	0.96	0.07	47,61,80,92	0
23	CLA	b	603	65/65	0.96	0.07	43,56,80,101	0
23	CLA	b	604	65/65	0.96	0.07	42,52,106,121	0
25	BCR	B	617	40/40	0.96	0.06	42,55,65,69	0
23	CLA	b	605	65/65	0.96	0.08	38,52,73,83	0
23	CLA	A	404[B]	65/65	0.96	0.07	37,45,63,71	65
23	CLA	A	405[A]	65/65	0.97	0.06	37,45,58,74	65
23	CLA	A	405[B]	65/65	0.97	0.06	37,45,58,75	65
23	CLA	c	502	65/65	0.97	0.07	46,60,92,112	0

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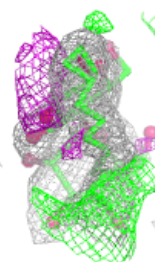
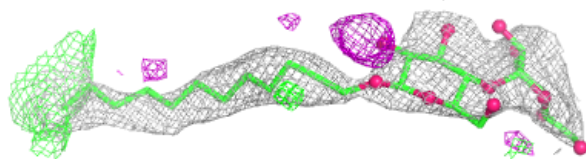
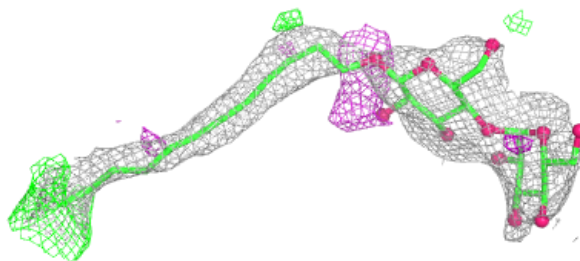
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	B	608	65/65	0.97	0.05	40,50,69,83	0
23	CLA	C	511	65/65	0.97	0.06	48,59,81,89	0
22	CL	a	403[A]	1/1	0.97	0.07	54,54,54,54	1
23	CLA	C	503	65/65	0.97	0.06	43,55,84,91	0
22	CL	a	403[B]	1/1	0.97	0.07	54,54,54,54	1
23	CLA	D	402[A]	65/65	0.97	0.07	36,45,69,80	65
23	CLA	b	608	65/65	0.97	0.06	41,57,79,95	0
23	CLA	c	510	65/65	0.97	0.06	51,62,80,95	0
23	CLA	D	402[B]	65/65	0.97	0.07	36,45,69,80	65
23	CLA	b	610	65/65	0.97	0.07	46,57,68,71	0
23	CLA	B	604	65/65	0.97	0.06	37,49,118,134	0
23	CLA	d	402[A]	65/65	0.97	0.05	40,46,64,73	65
23	CLA	d	402[B]	65/65	0.97	0.05	40,46,64,73	65
23	CLA	d	403[A]	65/65	0.97	0.06	38,48,76,95	65
23	CLA	d	403[B]	65/65	0.97	0.06	37,48,76,95	65
23	CLA	a	404[A]	65/65	0.97	0.07	41,46,64,77	65
24	PHO	A	407[A]	64/64	0.97	0.05	38,47,53,59	64
24	PHO	A	407[B]	64/64	0.97	0.05	38,47,53,60	64
23	CLA	a	404[B]	65/65	0.97	0.07	41,46,65,78	65
23	CLA	B	612	65/65	0.97	0.06	38,50,63,72	0
23	CLA	B	605	65/65	0.97	0.06	39,49,69,86	0
22	CL	A	402[B]	1/1	0.98	0.05	44,44,44,44	1
22	CL	A	403[A]	1/1	0.98	0.04	49,49,49,49	1
22	CL	A	403[B]	1/1	0.98	0.04	49,49,49,49	1
21	FE2	a	401[A]	1/1	0.98	0.04	55,55,55,55	1
21	FE2	a	401[B]	1/1	0.98	0.04	55,55,55,55	1
22	CL	A	402[A]	1/1	0.98	0.05	44,44,44,44	1
38	HEM	E	102	43/43	0.98	0.07	53,69,82,94	0
38	HEM	f	101	43/43	0.98	0.08	61,80,114,135	0
40	HEC	V	201	43/43	0.98	0.06	40,51,58,62	0
40	HEC	v	201	43/43	0.98	0.07	50,62,67,75	0
28	OEX	A	413[A]	10/10	0.99	0.03	42,44,48,50	10
28	OEX	A	413[B]	10/10	0.99	0.03	42,45,49,50	10
28	OEX	a	411[A]	10/10	0.99	0.03	48,51,52,56	10
36	CA	c	523	1/1	0.99	0.03	77,77,77,77	0
28	OEX	a	411[B]	10/10	0.99	0.03	48,50,52,54	10
39	MG	J	102	1/1	0.99	0.03	57,57,57,57	0
39	MG	j	102	1/1	0.99	0.06	62,62,62,62	0
21	FE2	A	401[A]	1/1	0.99	0.02	51,51,51,51	1
21	FE2	A	401[B]	1/1	0.99	0.02	51,51,51,51	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.

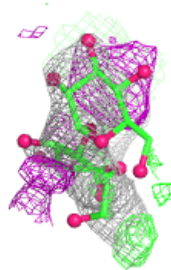
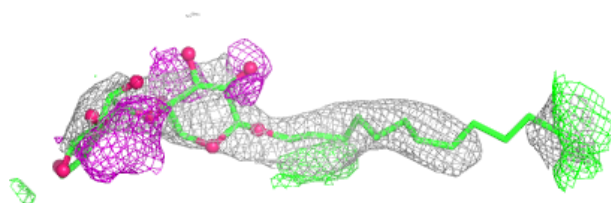
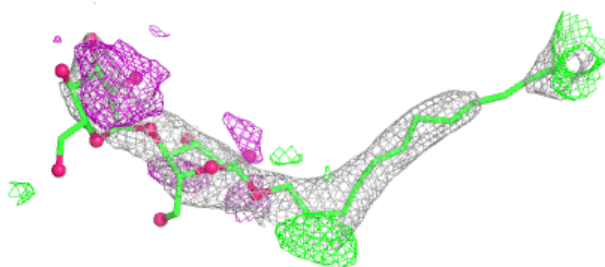
Electron density around LMT A 417:

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

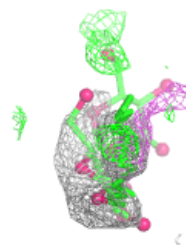
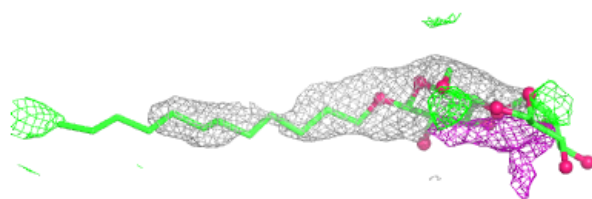
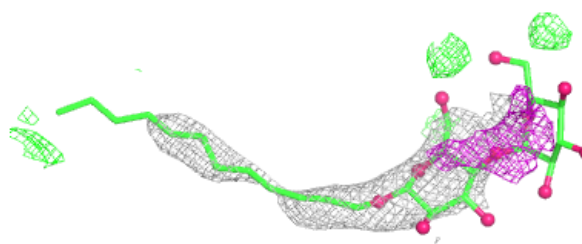


Electron density around LMT B 630:

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

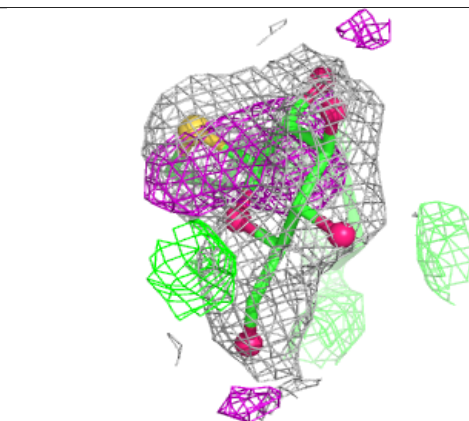
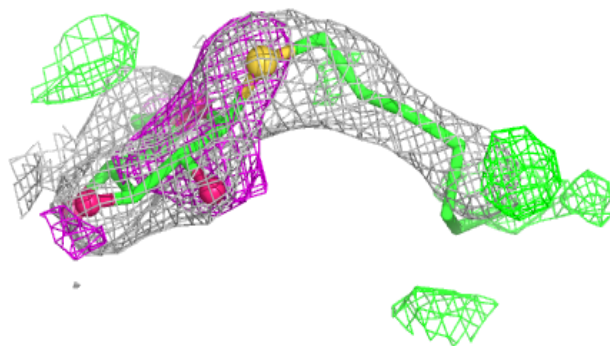
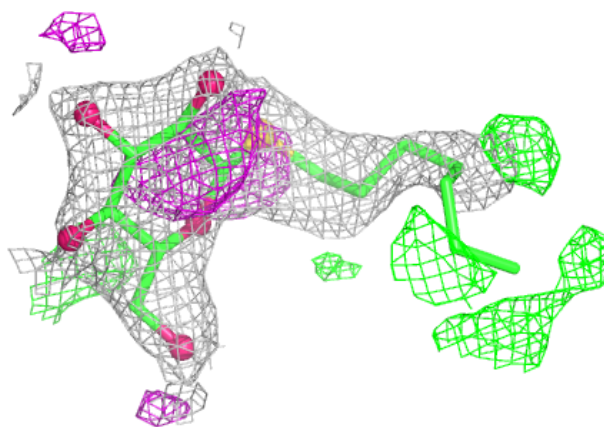
**Electron density around LMT F 101:**

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

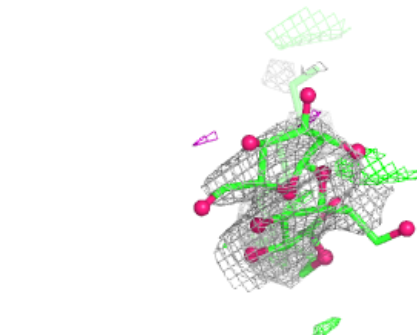
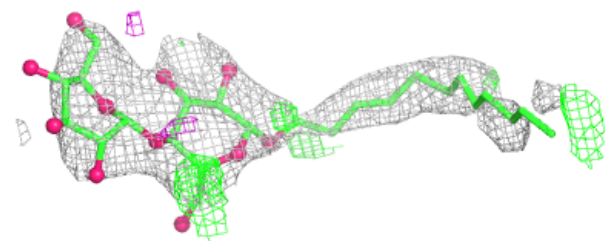
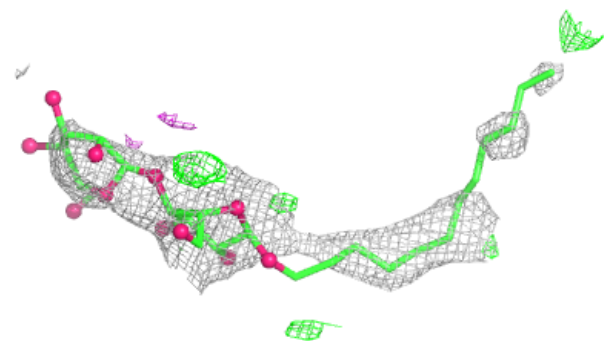


Electron density around HTG B 623:

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

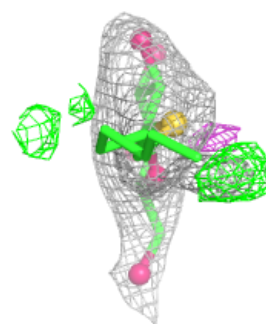
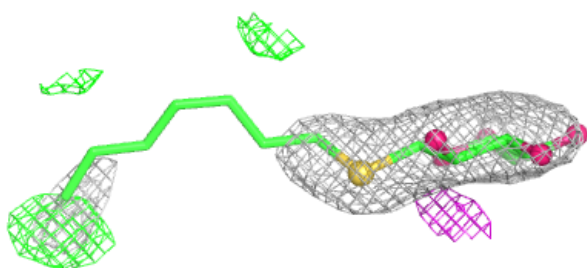
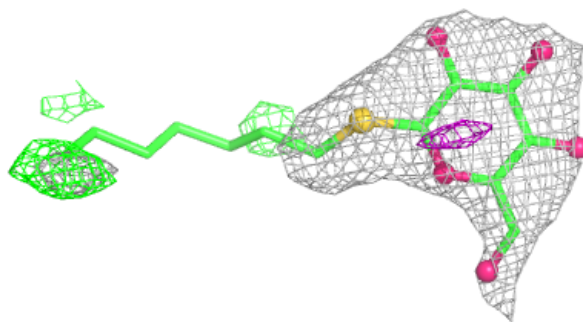
**Electron density around LMT A 420:**

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

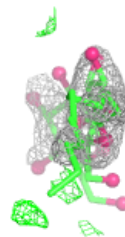
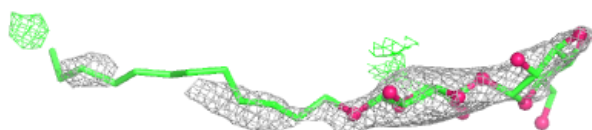
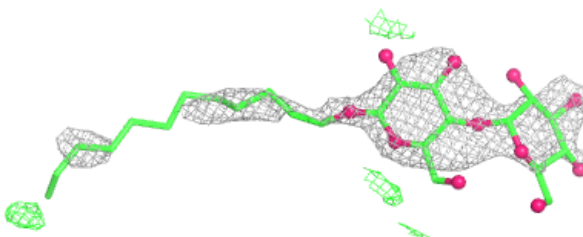


Electron density around HTG C 522:

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

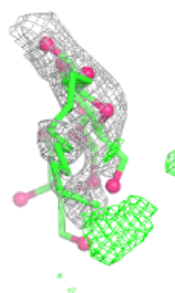
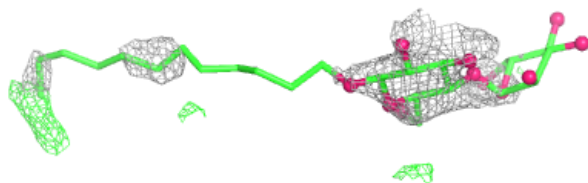
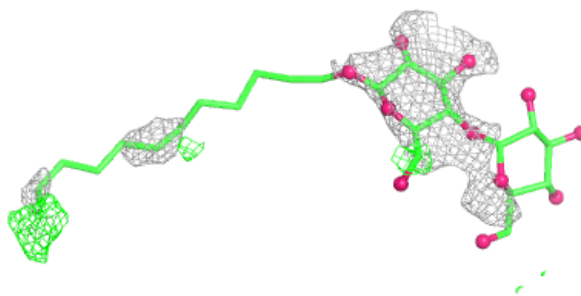
**Electron density around LMT a 416:**

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

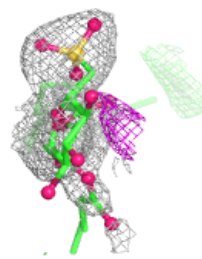
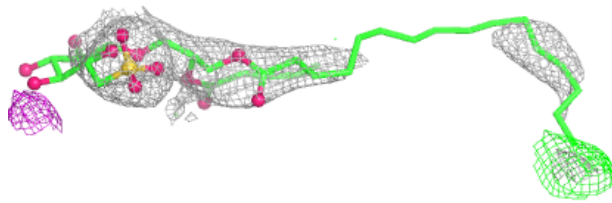
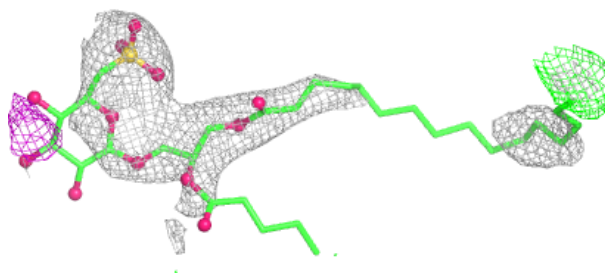


Electron density around LMT e 101:

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

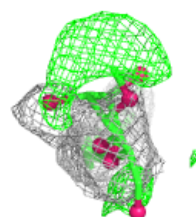
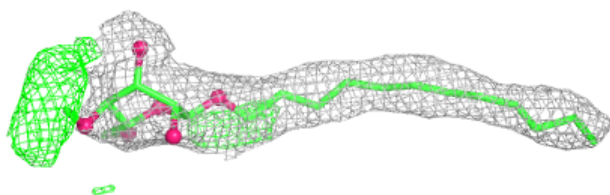
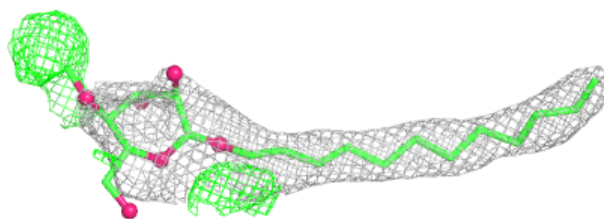
**Electron density around SQD f 102:**

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

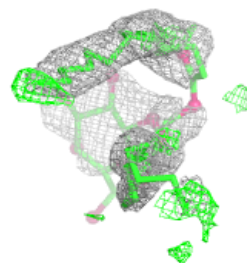
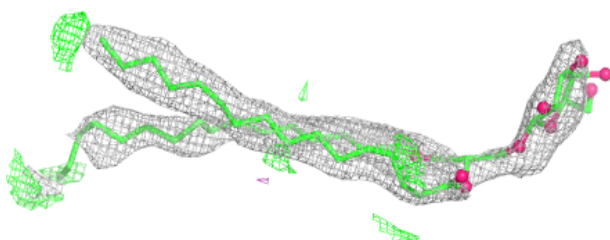
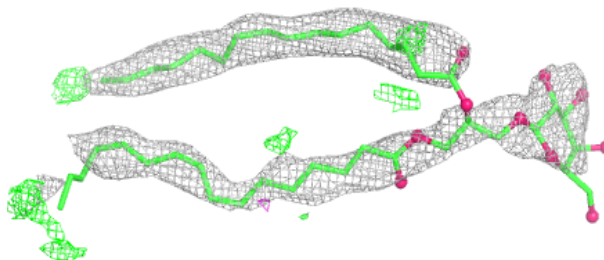


Electron density around LMT b 621:

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

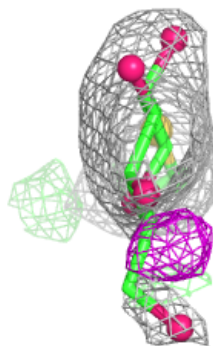
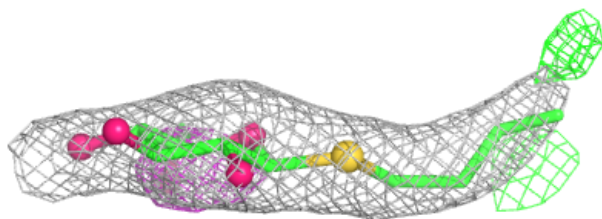
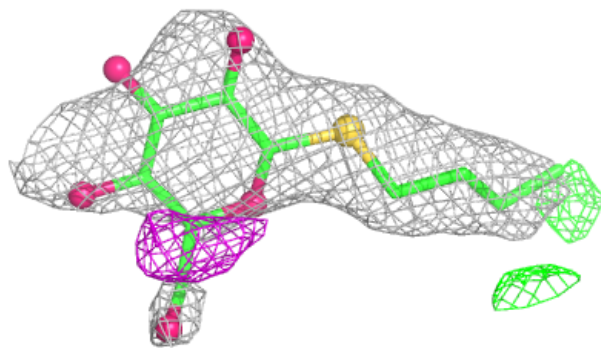
**Electron density around LMG C 521:**

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



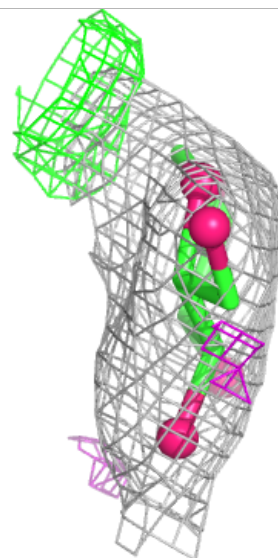
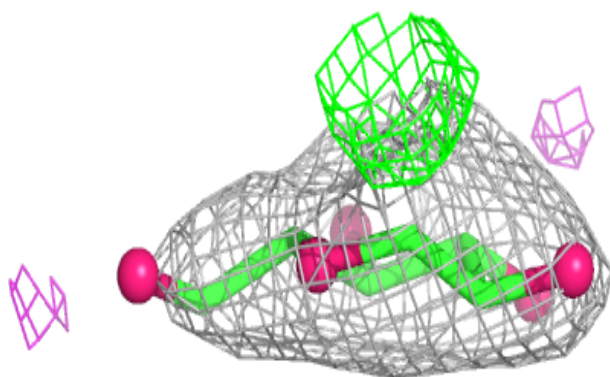
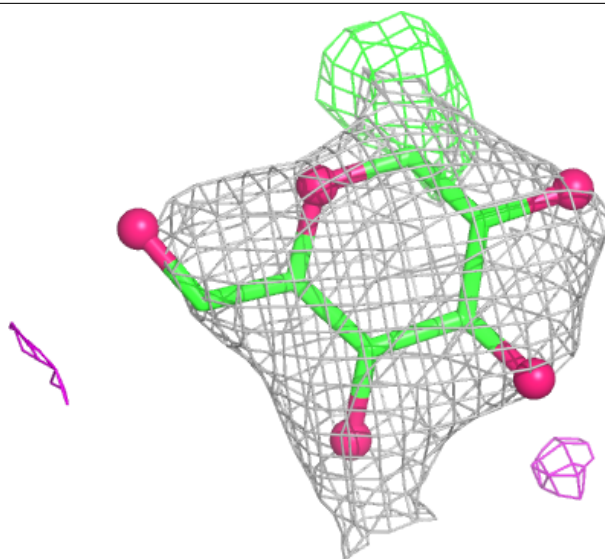
Electron density around HTG D 410:

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



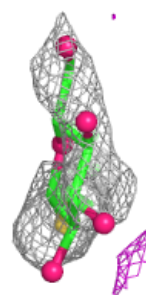
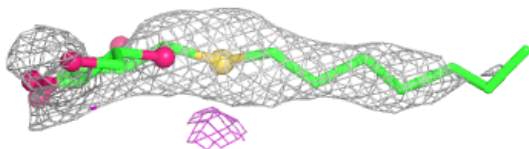
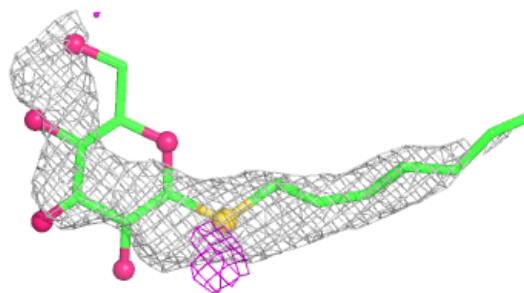
Electron density around HTG V 202:

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

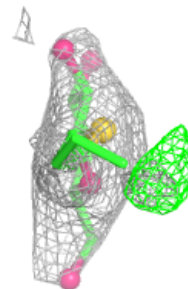
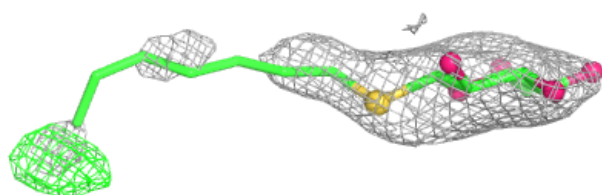
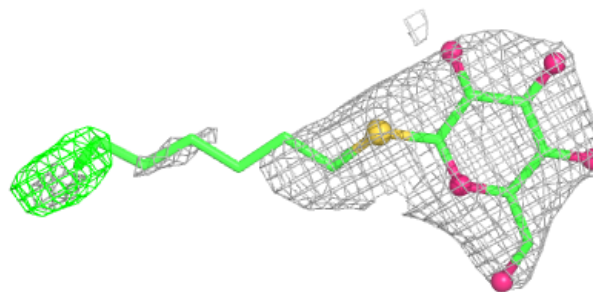


Electron density around HTG b 623:

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

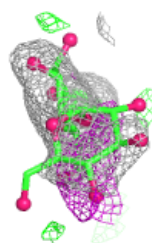
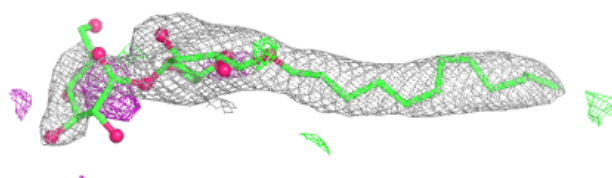
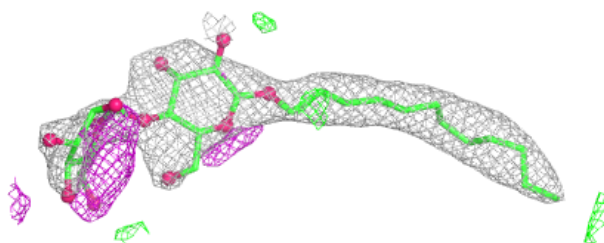
**Electron density around HTG c 521:**

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

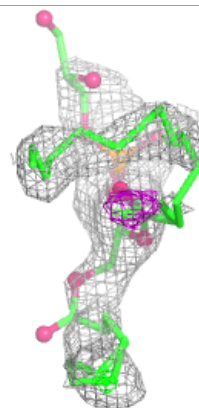
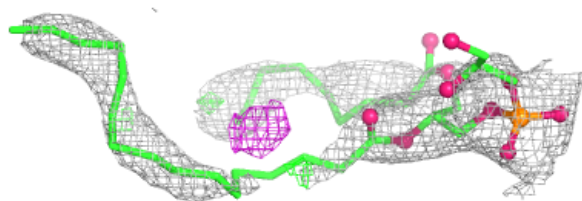
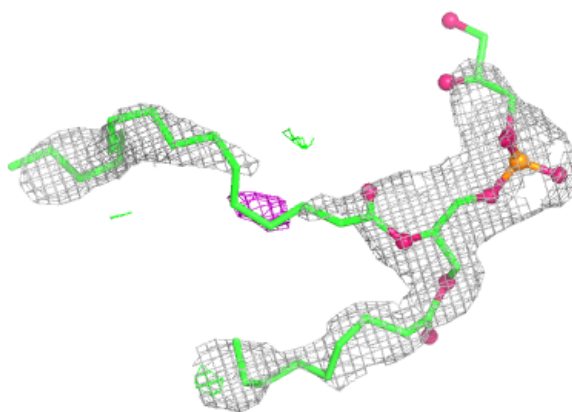


Electron density around LMT B 628:

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

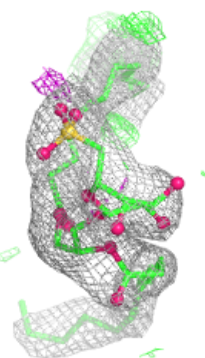
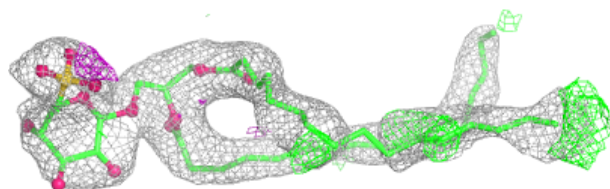
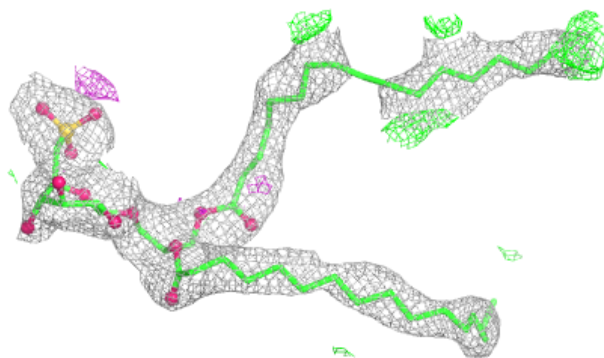
**Electron density around LHG a 419 (B):**

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

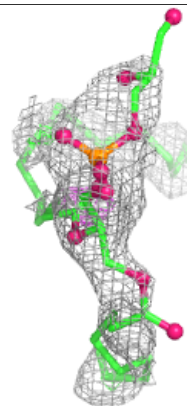
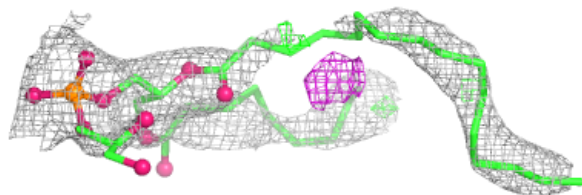
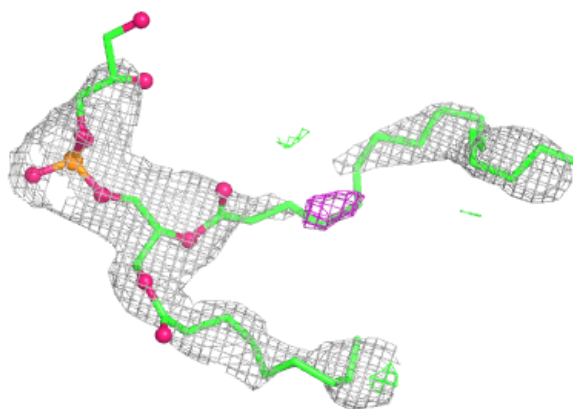


Electron density around SQD a 410:

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

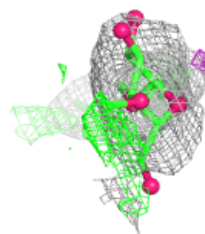
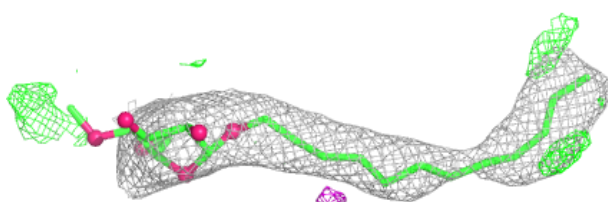
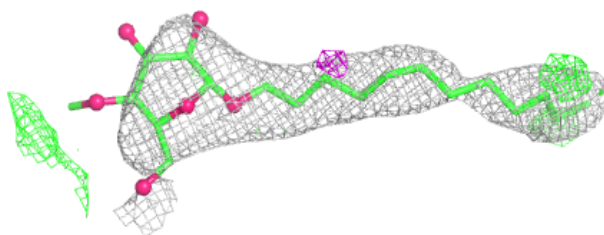
**Electron density around LHG a 419 (A):**

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

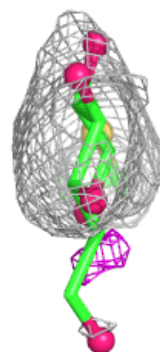
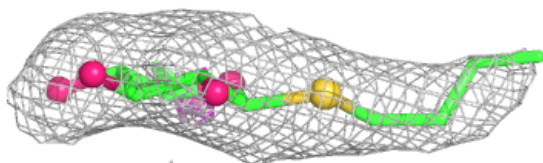
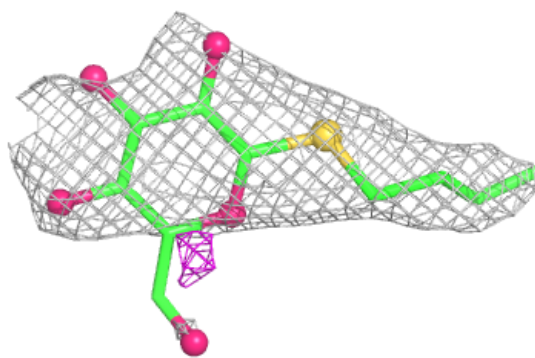


Electron density around LMT B 631:

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

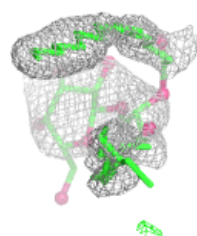
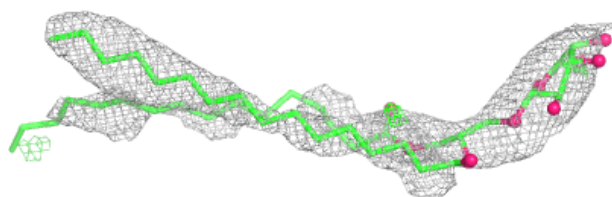
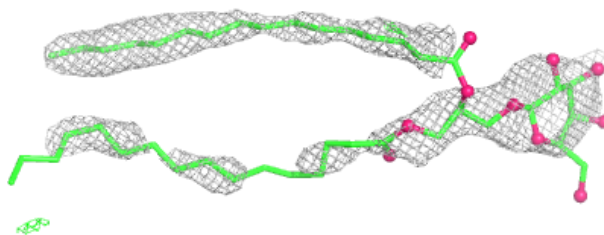
**Electron density around HTG d 411:**

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

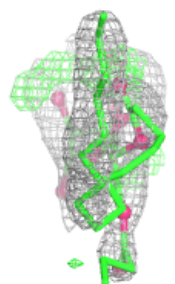
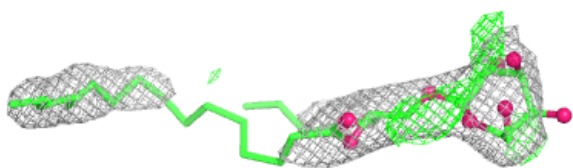
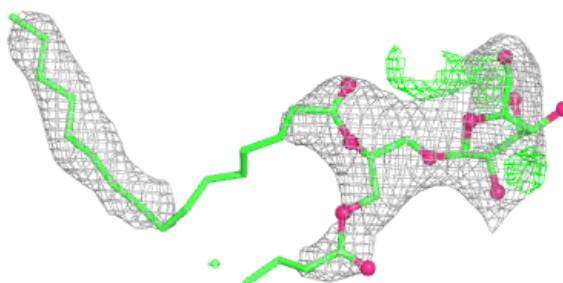


Electron density around LMG c 520:

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

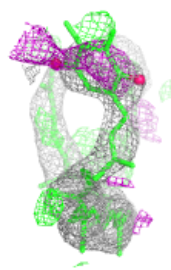
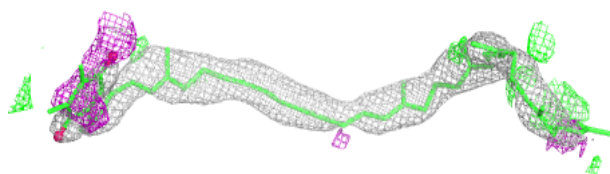
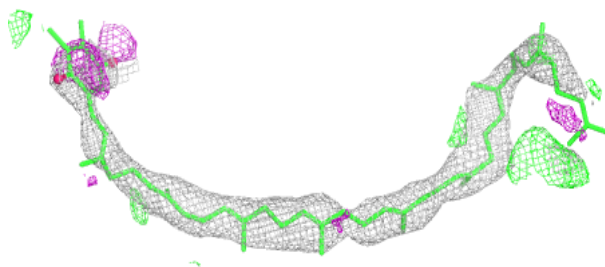
**Electron density around LMG z 101:**

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

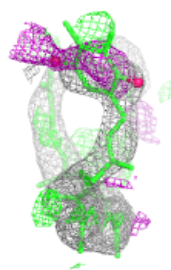
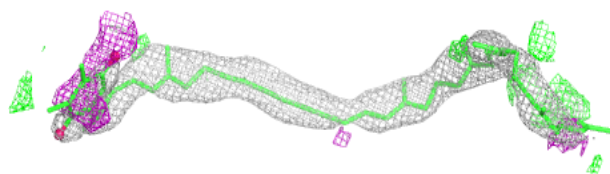
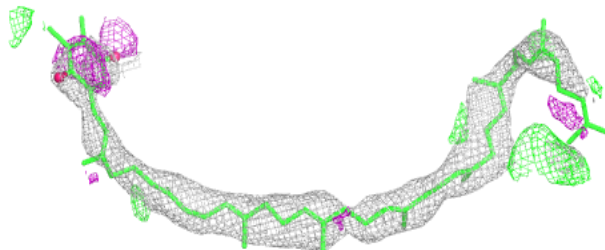


Electron density around PL9 A 414 (A):

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

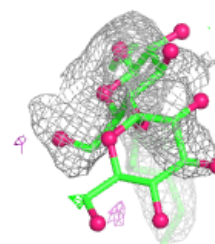
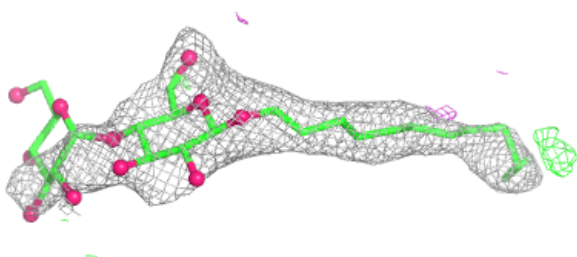
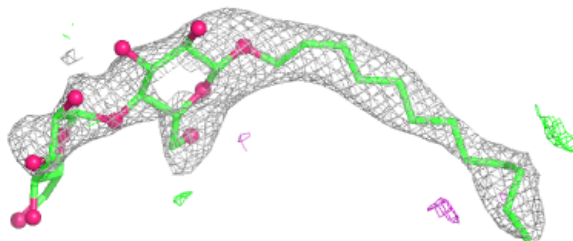
**Electron density around PL9 A 414 (B):**

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

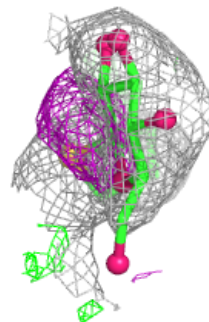
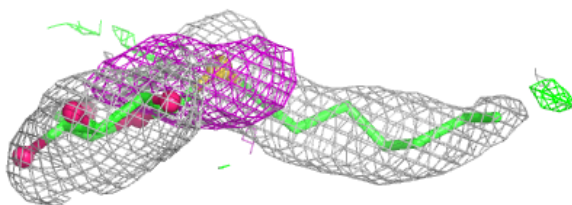
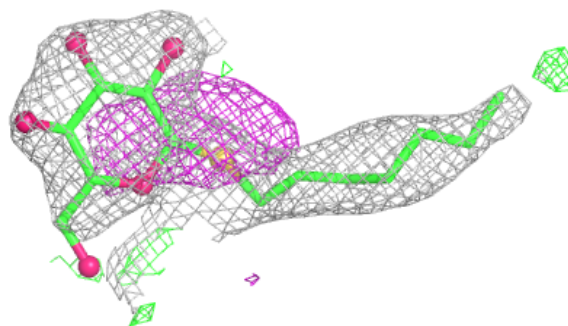


Electron density around LMT T 101:

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

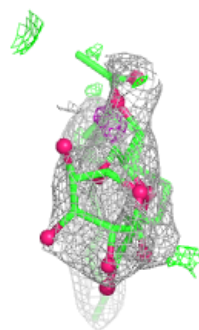
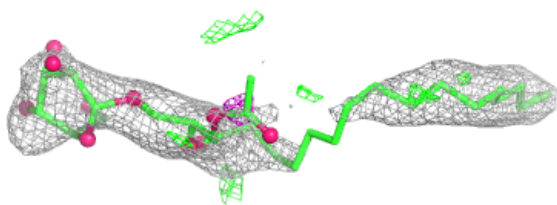
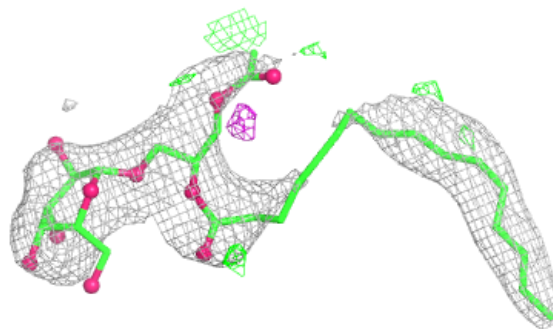
**Electron density around HTG b 622:**

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

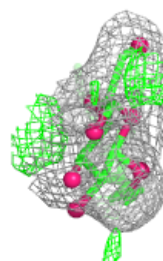
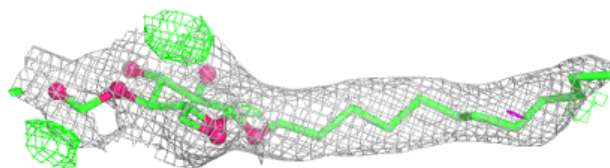
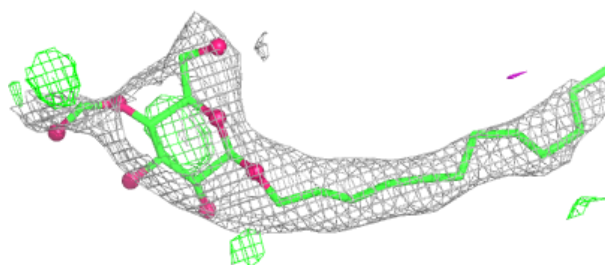


Electron density around LMG Z 101:

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

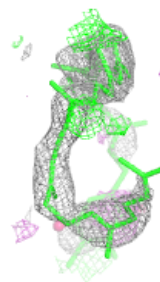
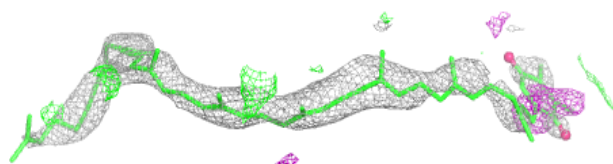
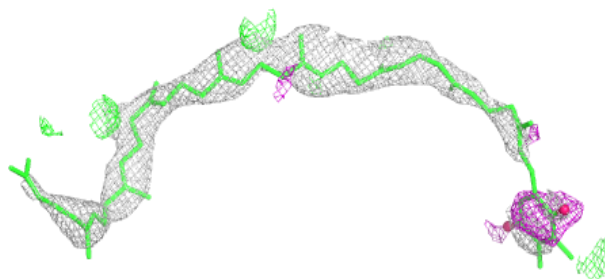
**Electron density around LMT t 101:**

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

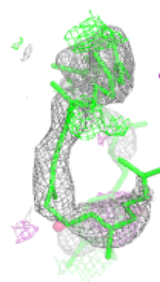
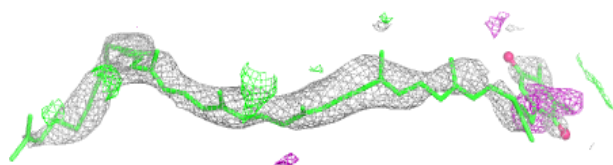
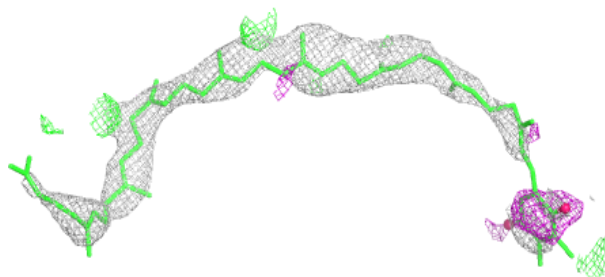


Electron density around PL9 a 412 (A):

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

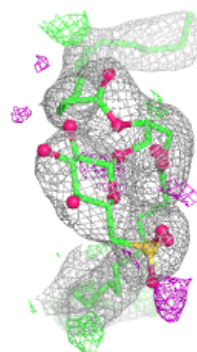
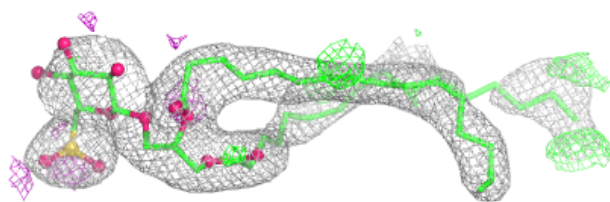
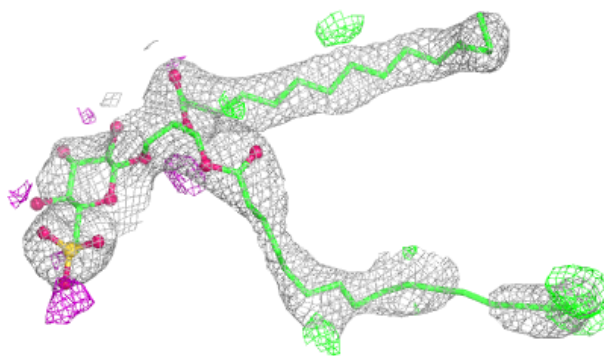
**Electron density around PL9 a 412 (B):**

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

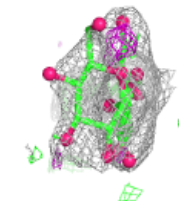
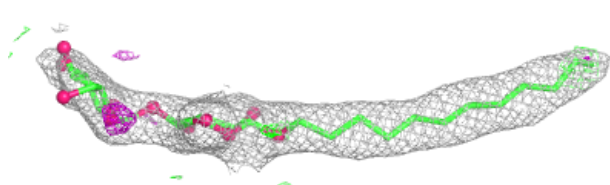
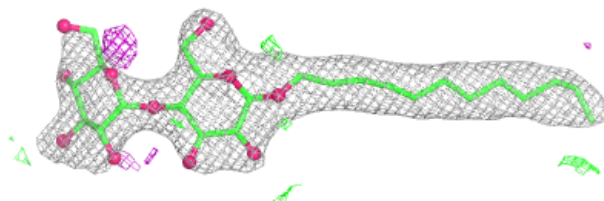


Electron density around SQD A 412:

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

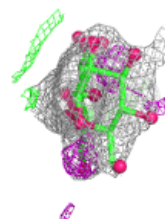
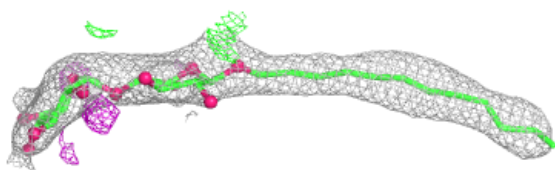
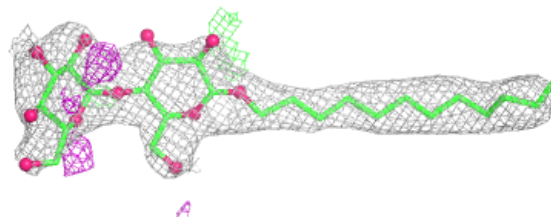
**Electron density around LMT M 101:**

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

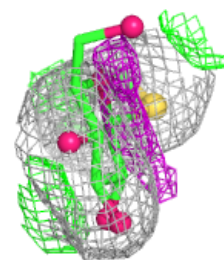
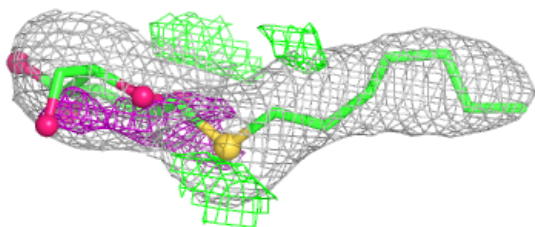
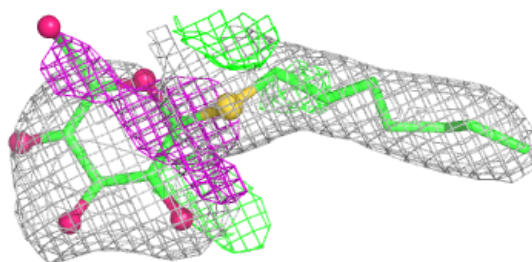


Electron density around LMT m 103:

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

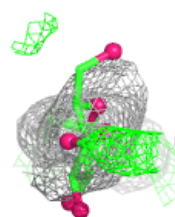
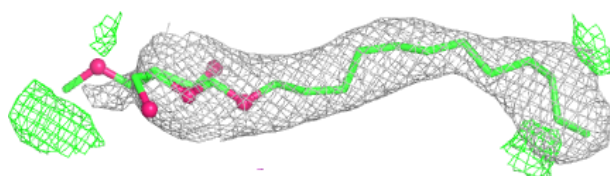
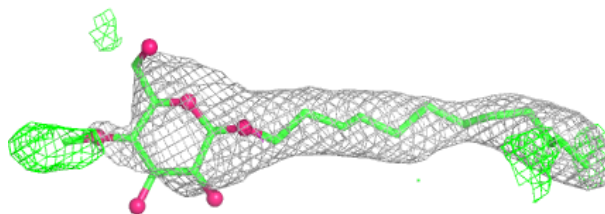
**Electron density around HTG B 622:**

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

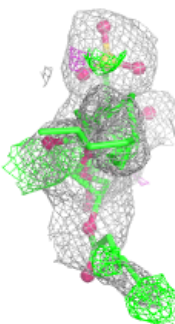
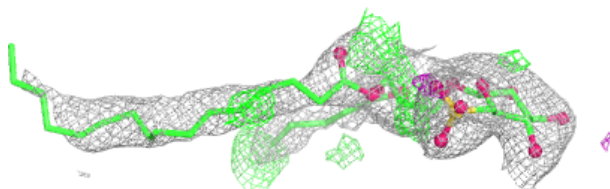
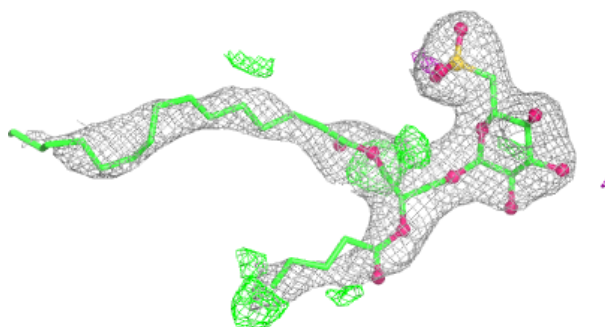


Electron density around LMT b 627:

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

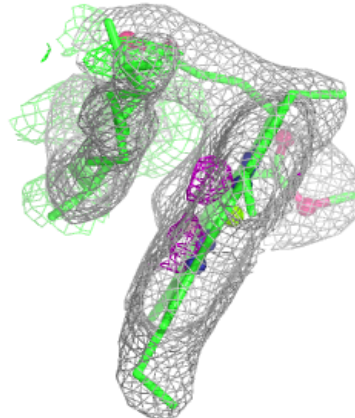
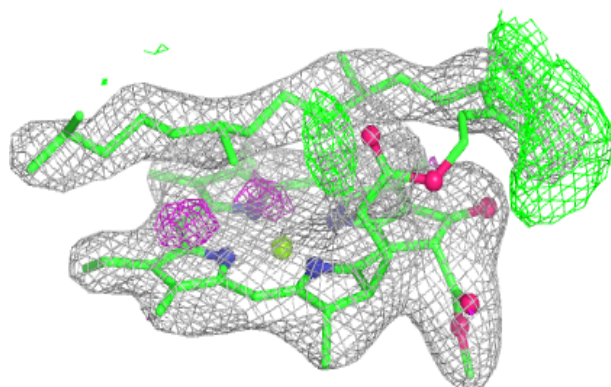
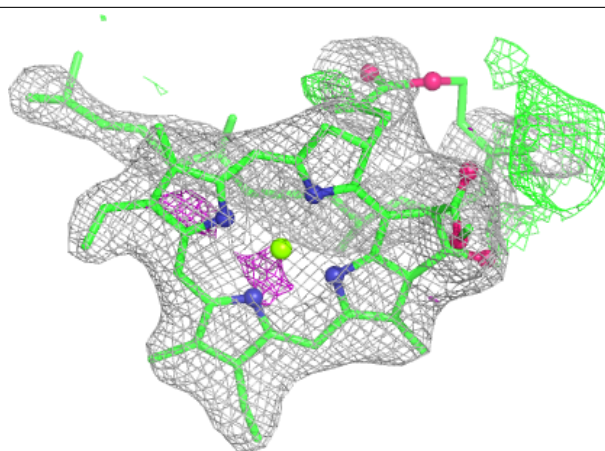
**Electron density around SQD F 102:**

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

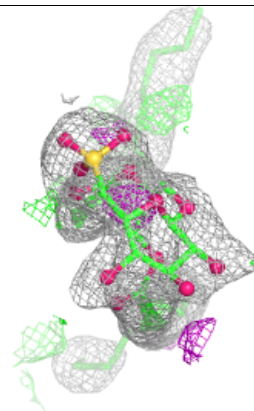
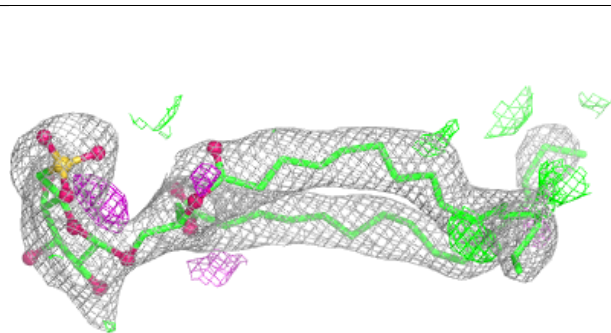
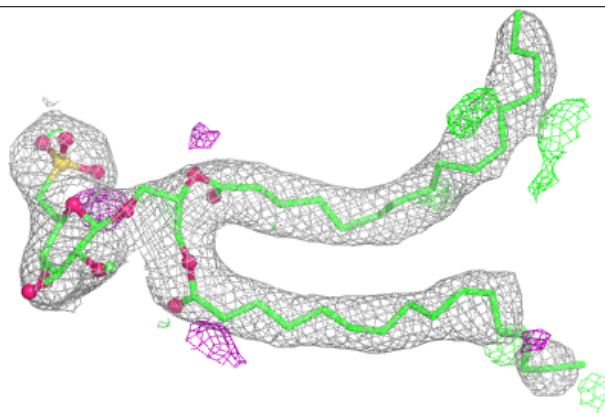


Electron density around CLA b 601:

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

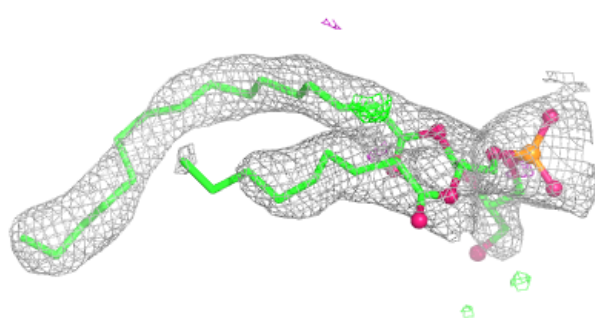
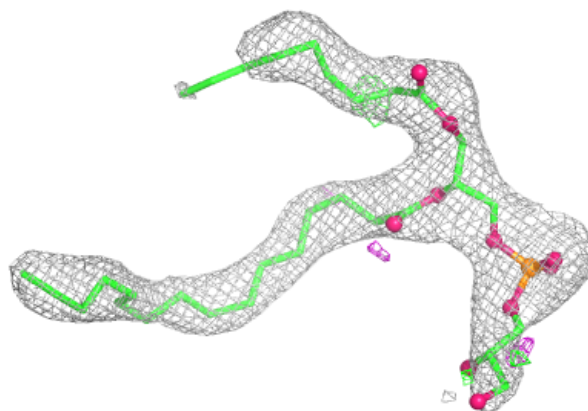
**Electron density around SQD b 620:**

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

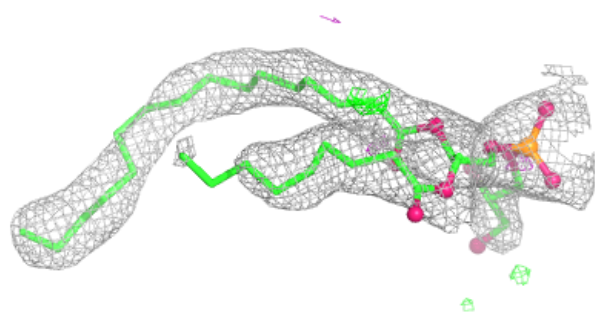
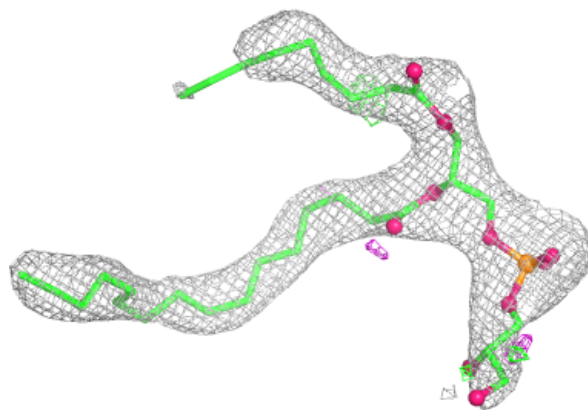


Electron density around LHG E 101 (A):

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

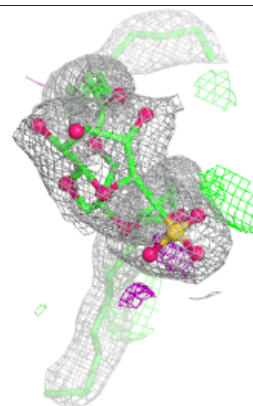
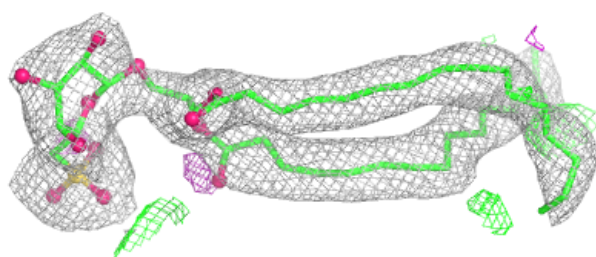
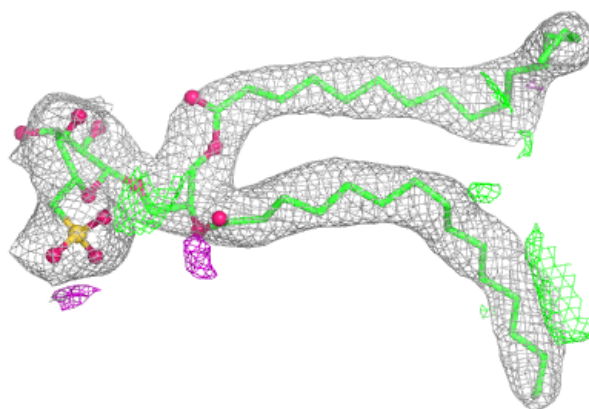
**Electron density around LHG E 101 (B):**

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

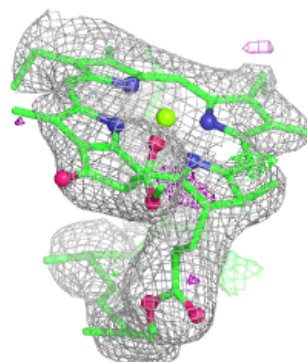
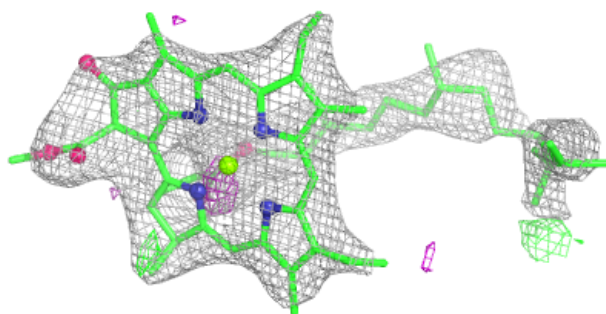
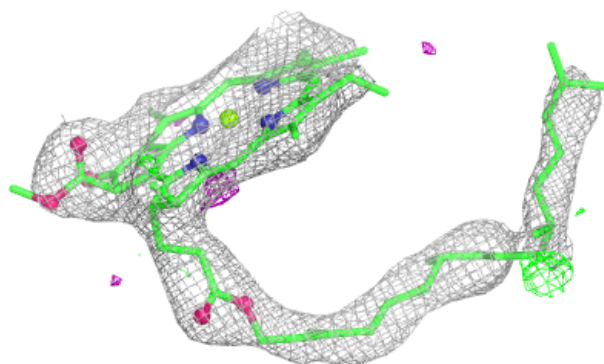


Electron density around SQD B 620:

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

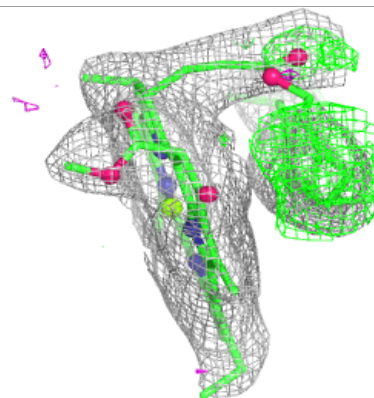
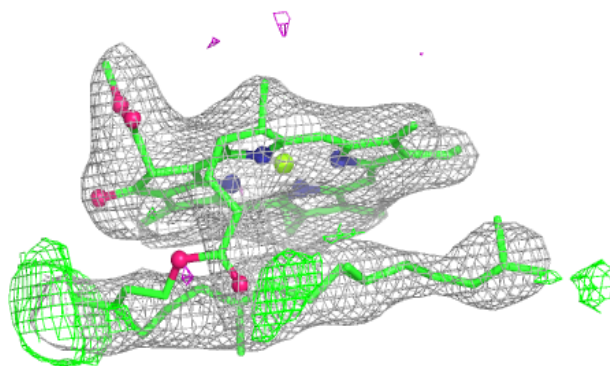
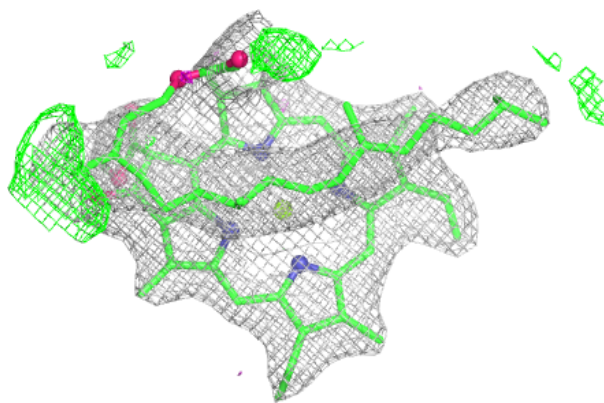
**Electron density around CLA c 513:**

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

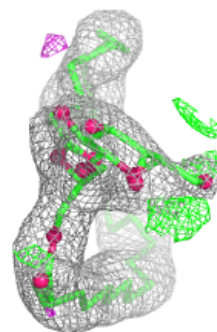
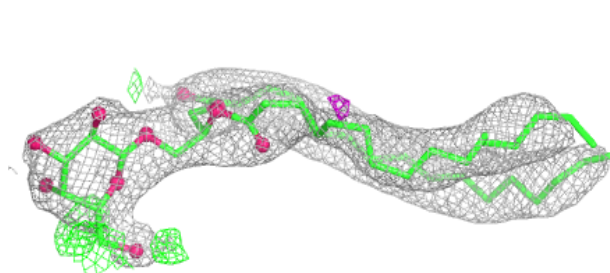
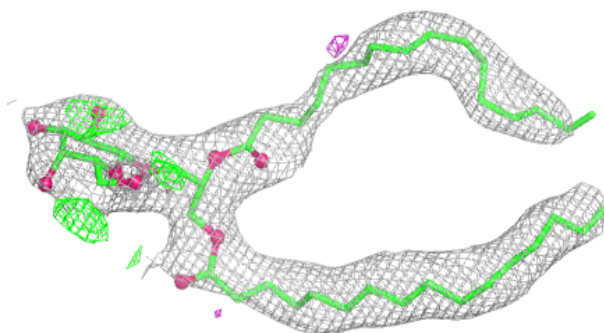


Electron density around CLA B 601:

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

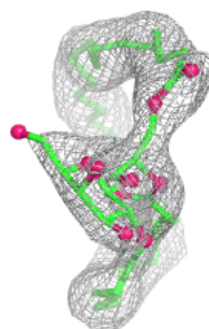
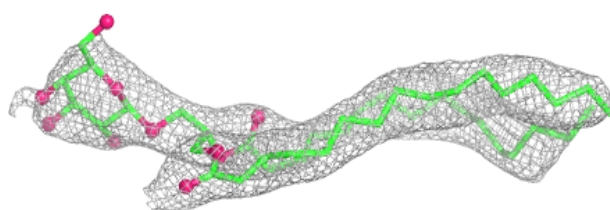
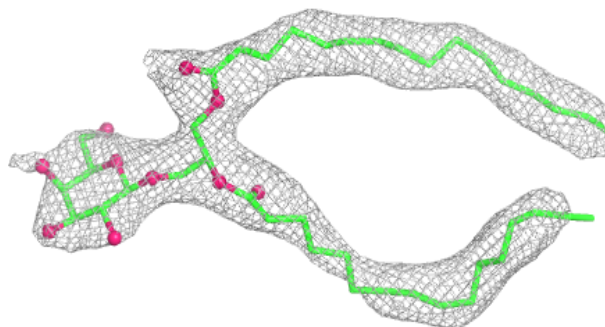
**Electron density around LMG C 501:**

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

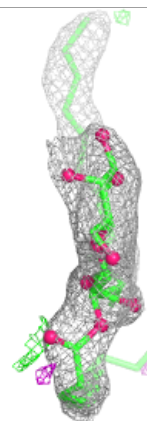
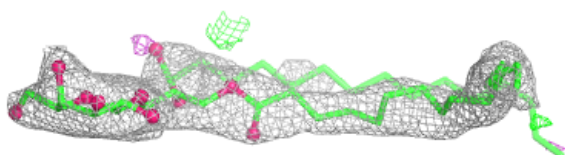
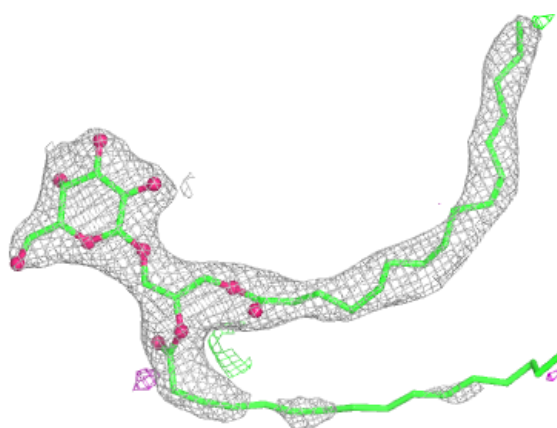


Electron density around LMG a 415:

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

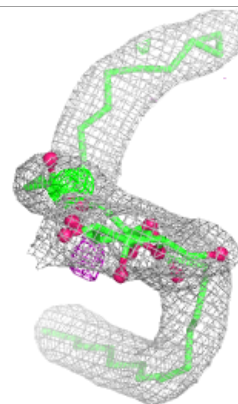
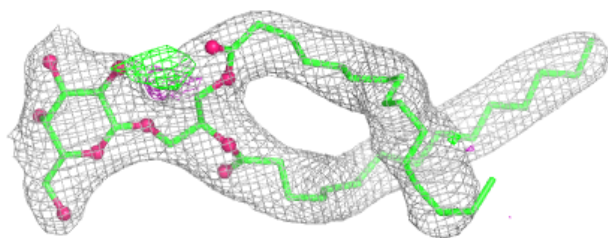
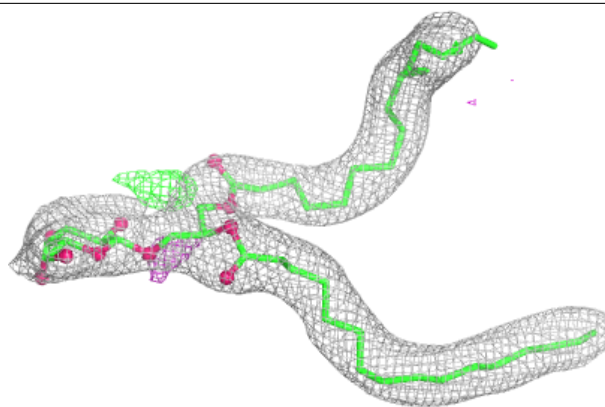
**Electron density around LMG c 519:**

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

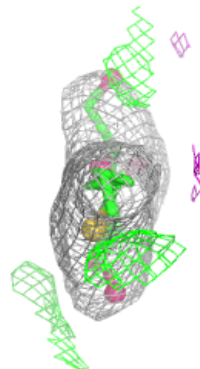
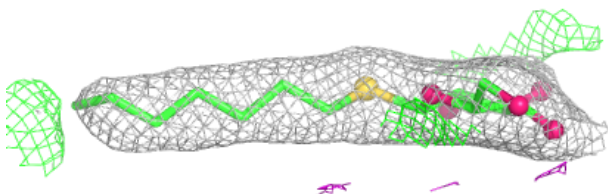
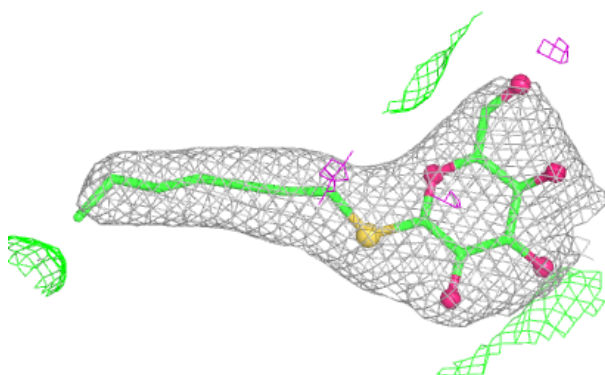


Electron density around LMG m 101:

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

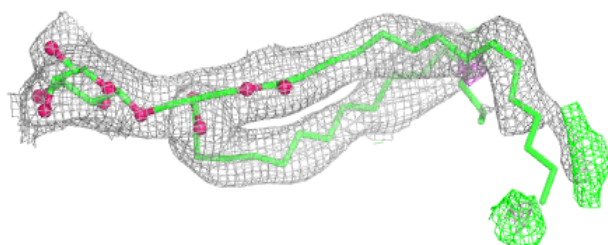
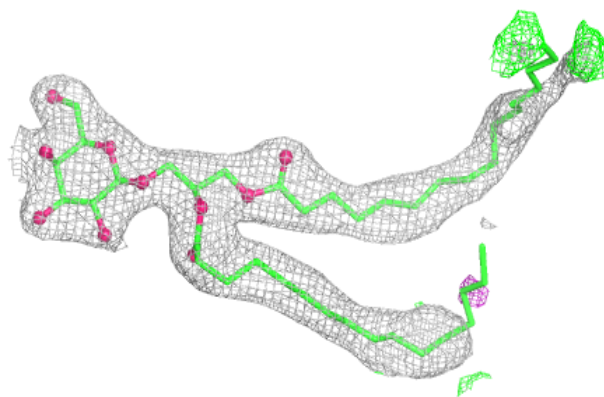
**Electron density around HTG B 625:**

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



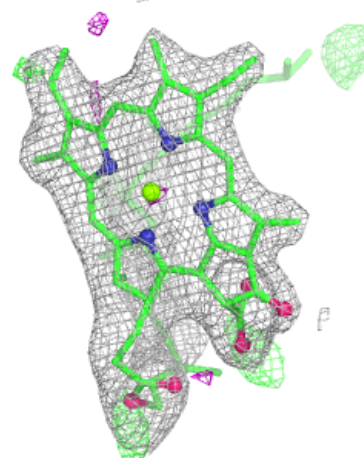
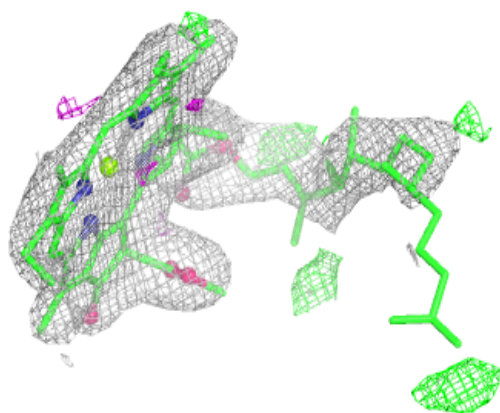
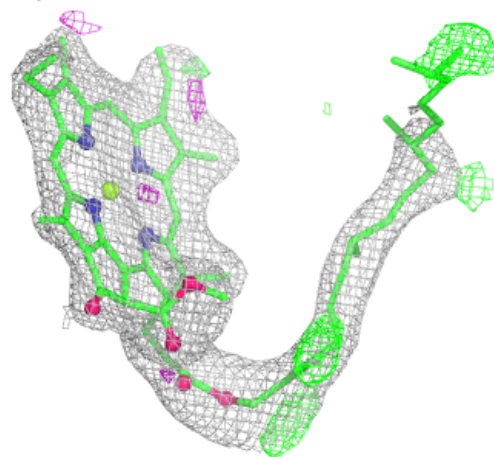
Electron density around LMG D 411:

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



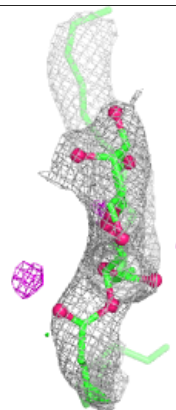
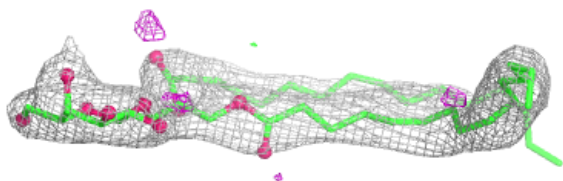
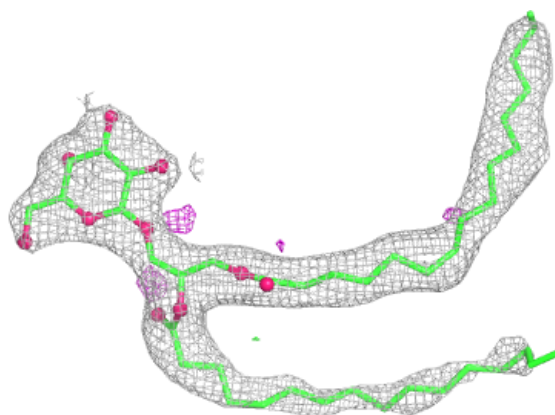
Electron density around CLA b 616:

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

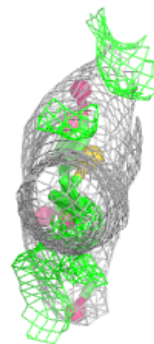
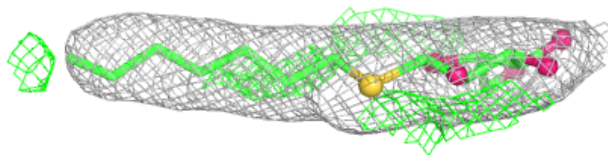
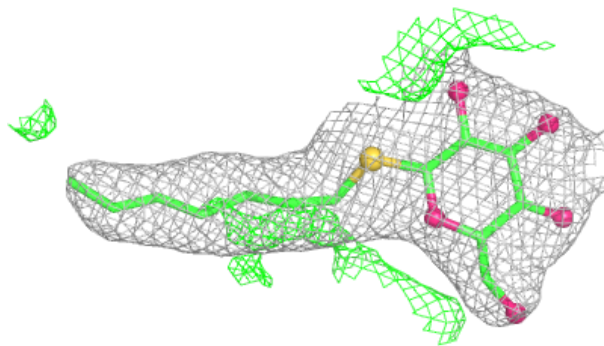


Electron density around LMG C 520:

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

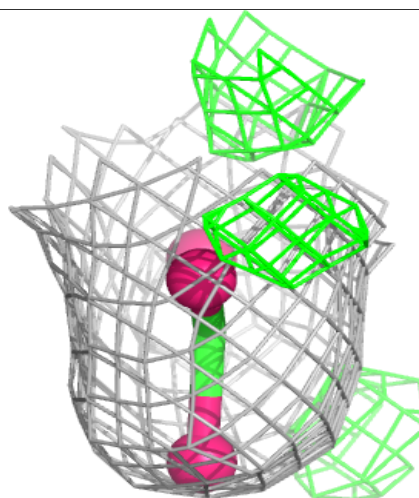
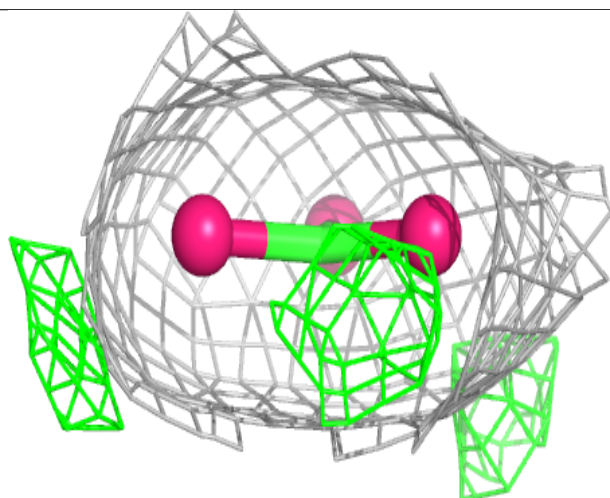
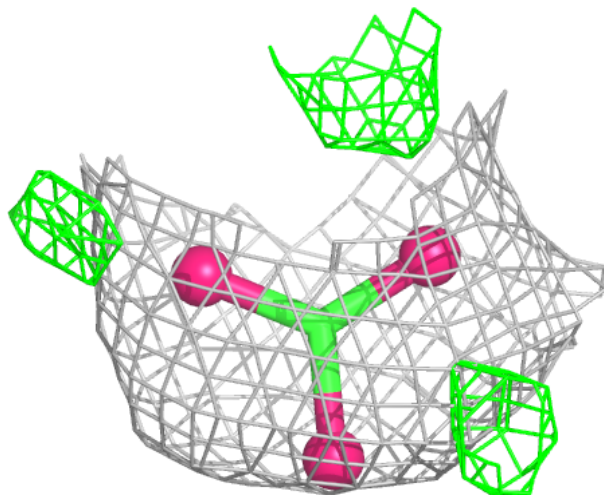
**Electron density around HTG b 625:**

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



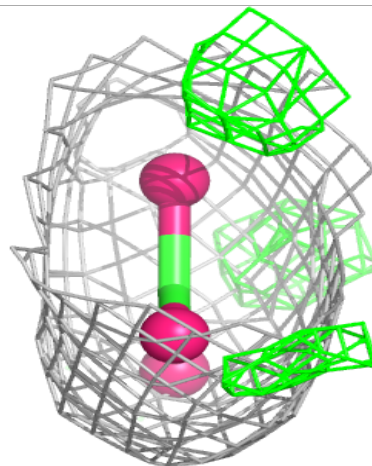
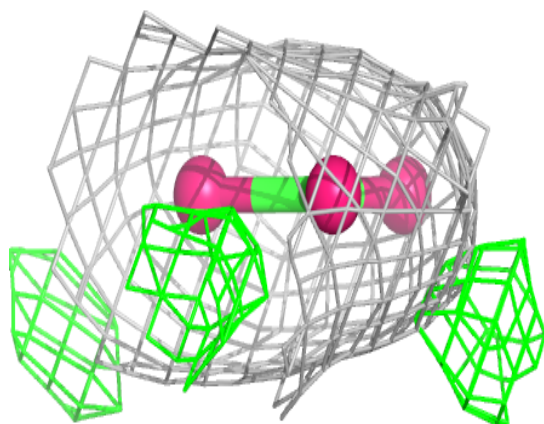
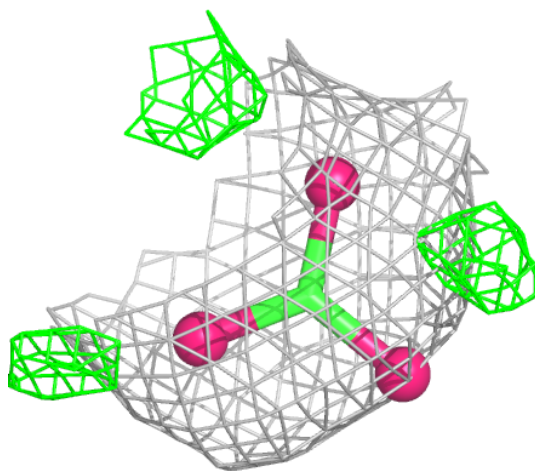
Electron density around BCT d 401 (A):

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



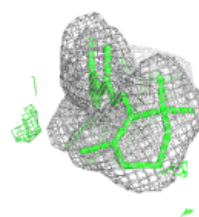
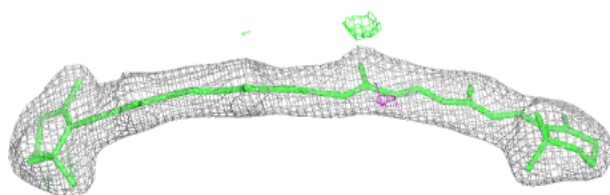
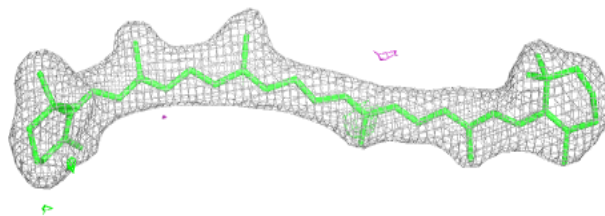
Electron density around BCT d 401 (B):

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

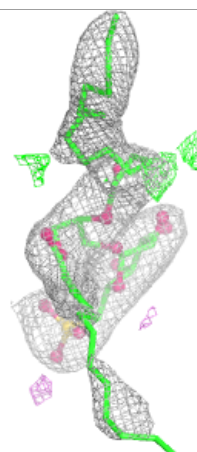
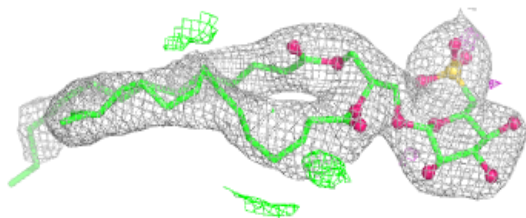
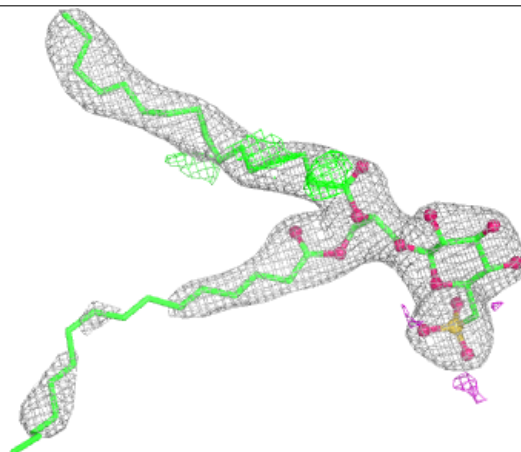


Electron density around BCR t 102:

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

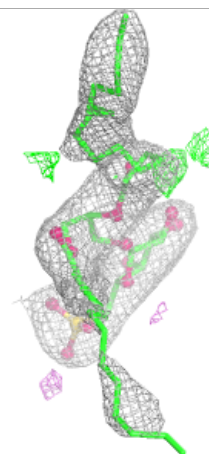
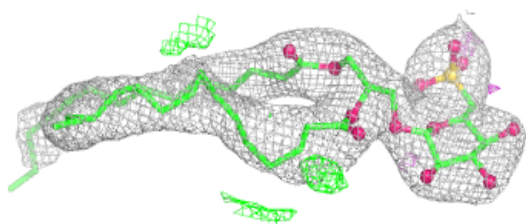
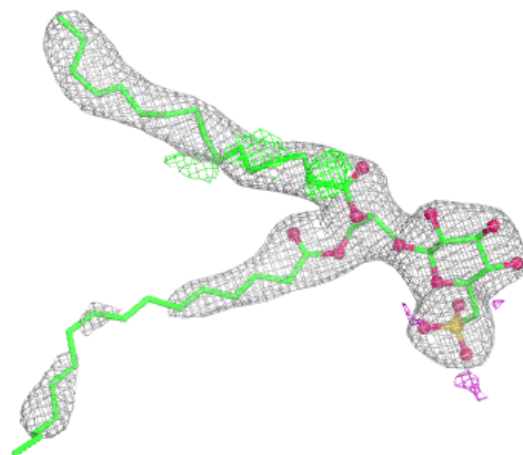
**Electron density around SQD A 410 (A):**

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



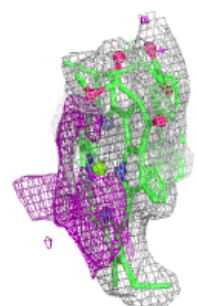
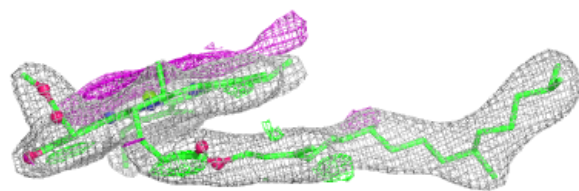
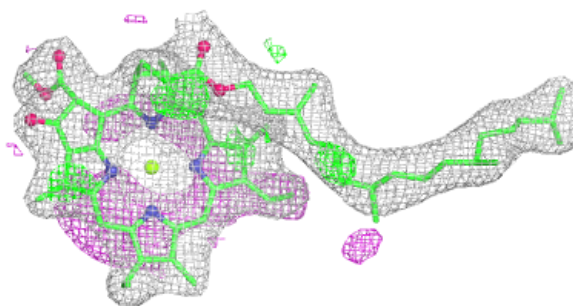
Electron density around SQD A 410 (B):

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

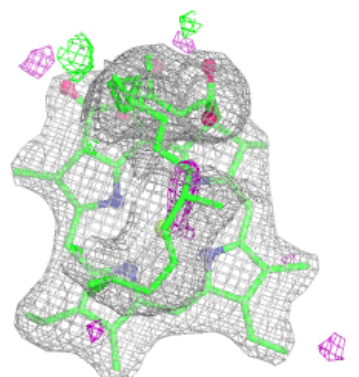
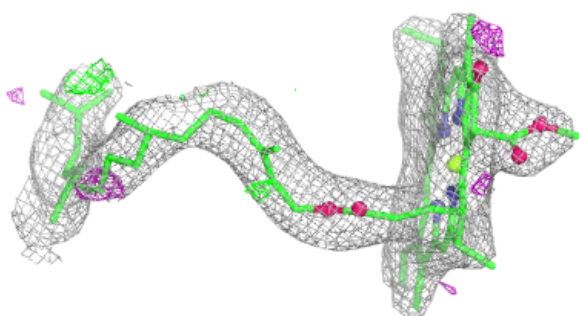
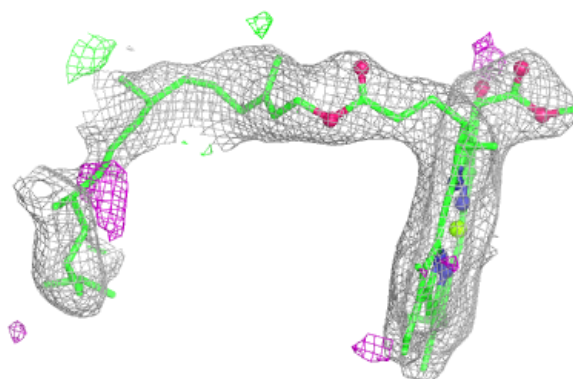


Electron density around CLA B 603:

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

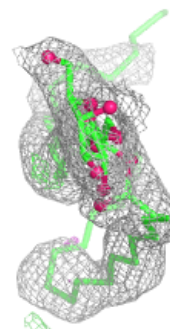
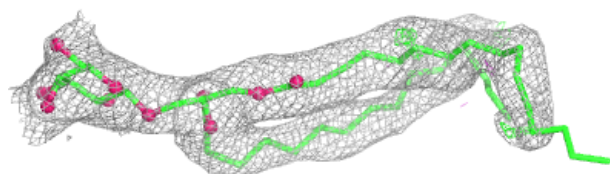
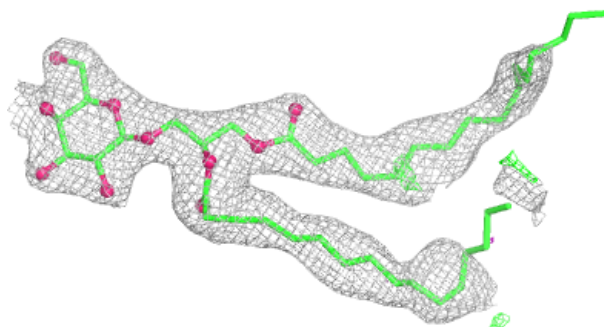
**Electron density around CLA C 507:**

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

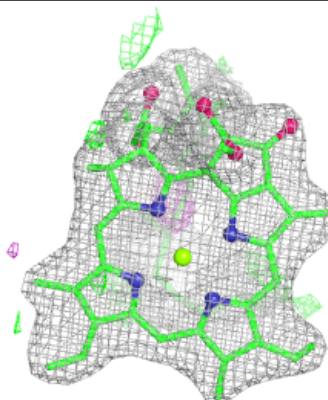
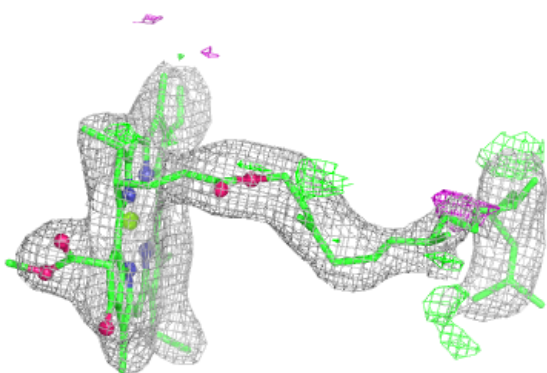
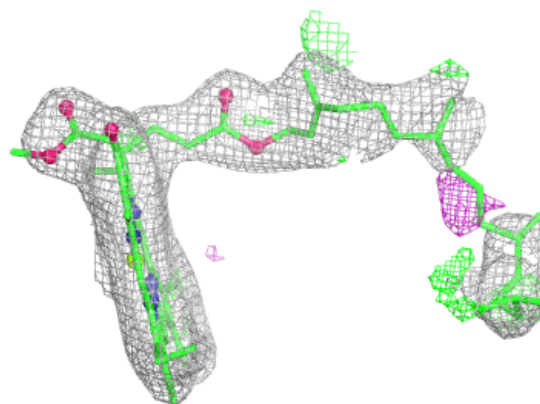


Electron density around LMG d 412:

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

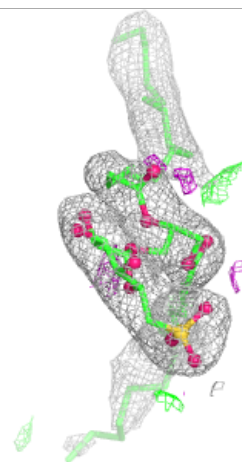
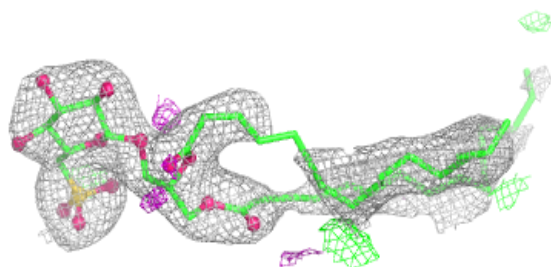
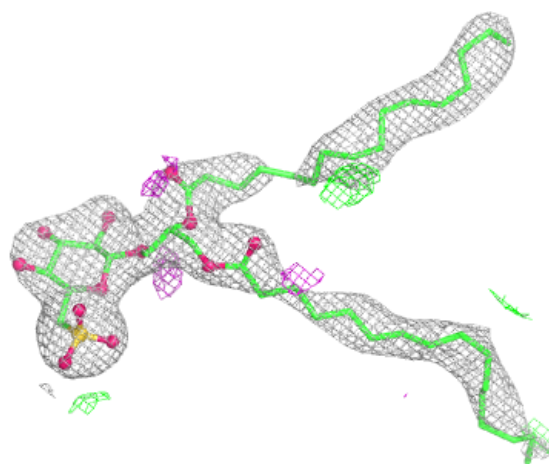
**Electron density around CLA c 506:**

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



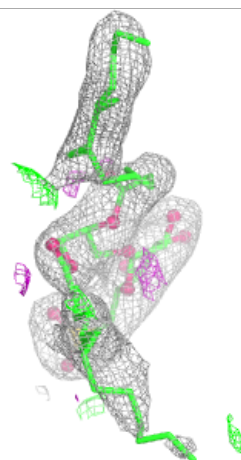
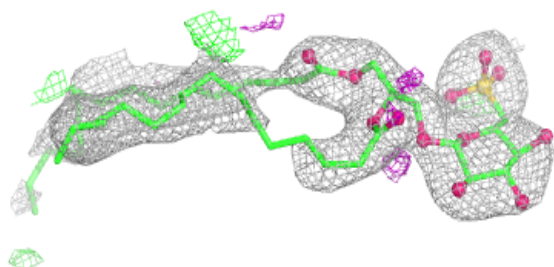
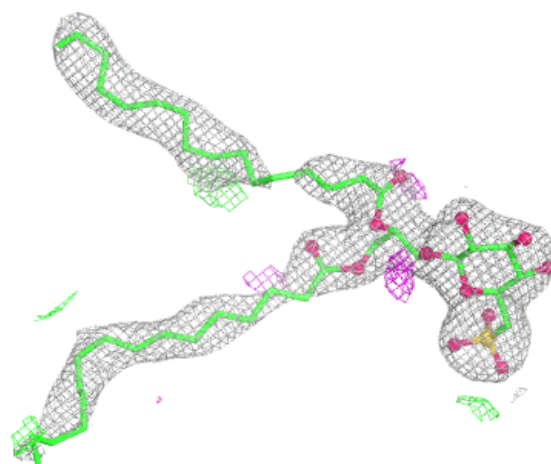
Electron density around SQD a 409 (A):

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



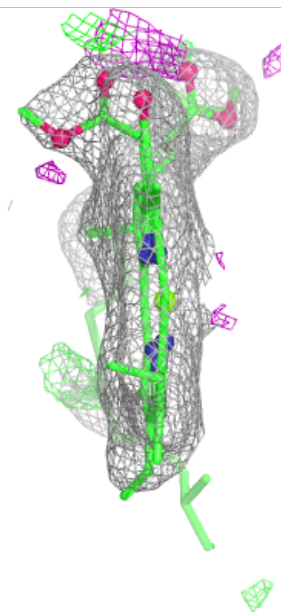
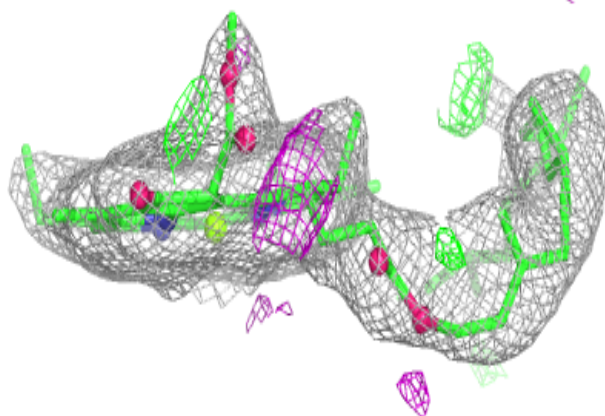
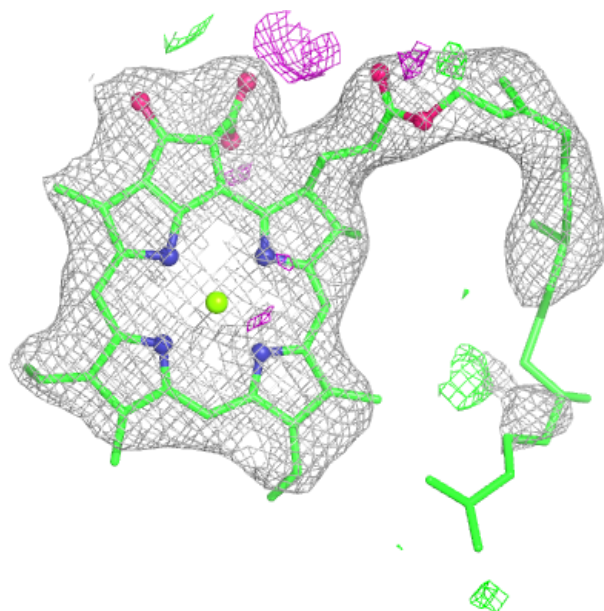
Electron density around SQD a 409 (B):

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



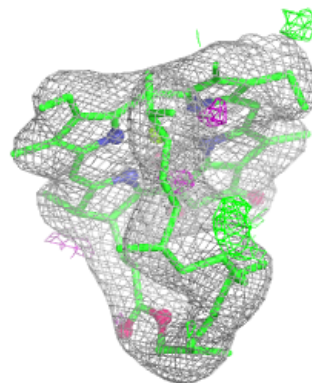
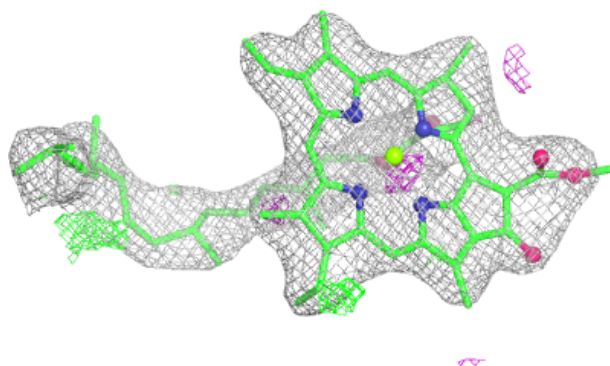
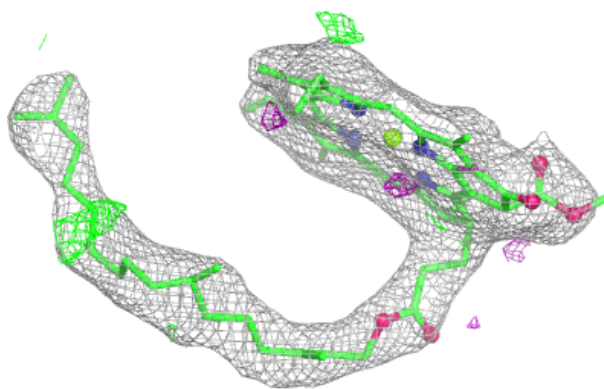
Electron density around CLA c 512:

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

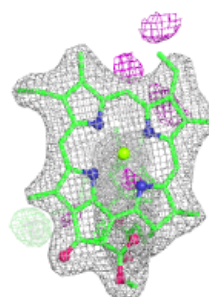
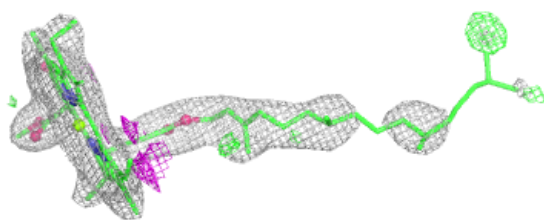
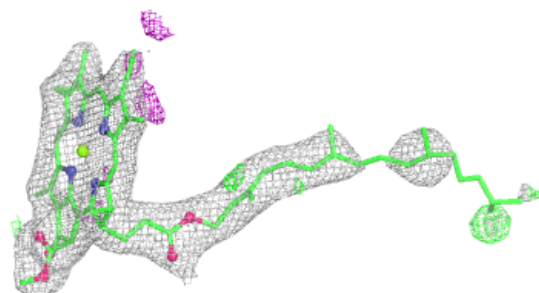


Electron density around CLA C 514:

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

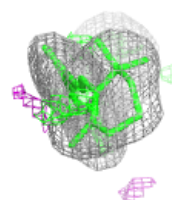
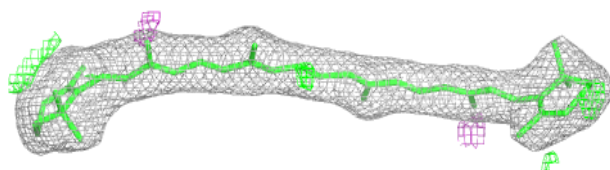
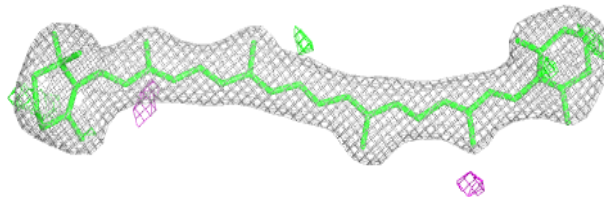
**Electron density around CLA d 404:**

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

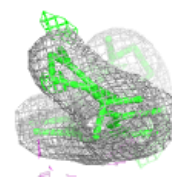
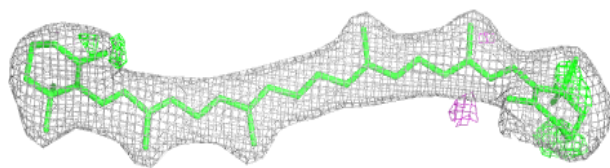
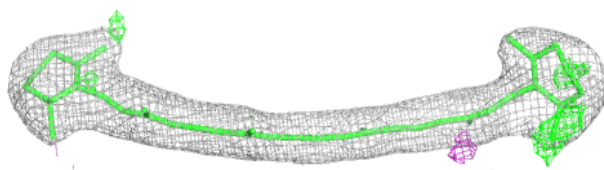


Electron density around BCR B 619:

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

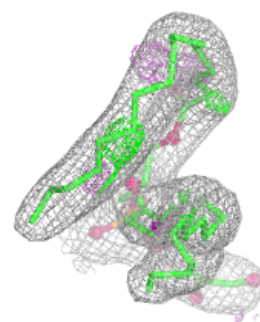
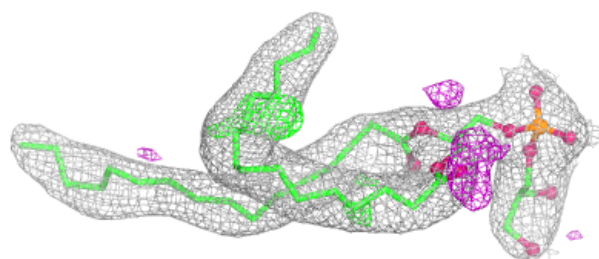
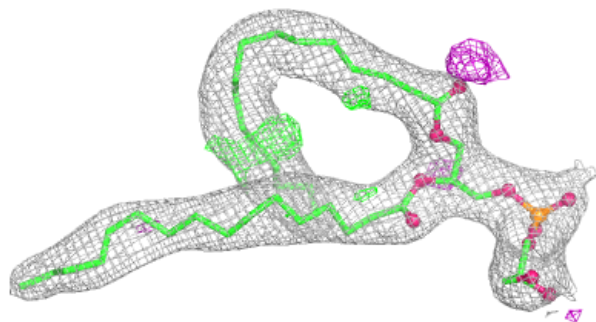
**Electron density around BCR D 404:**

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

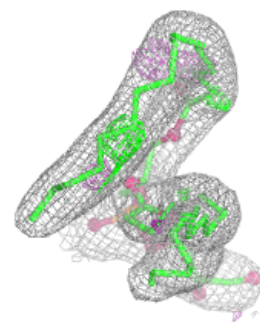
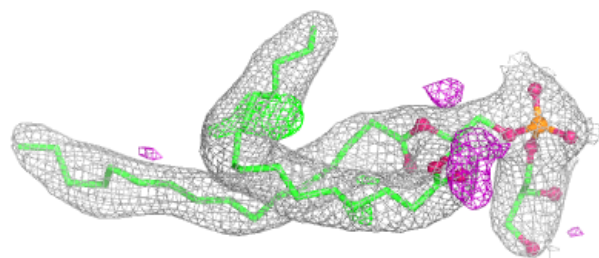
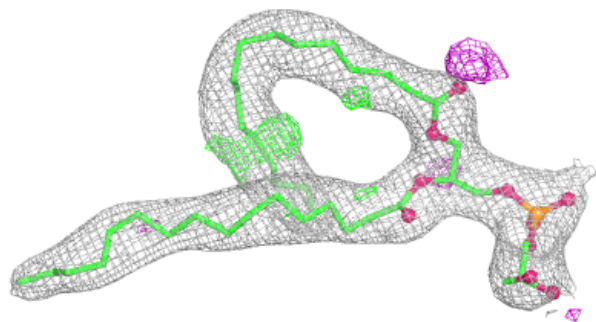


Electron density around LHG A 419 (A):

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

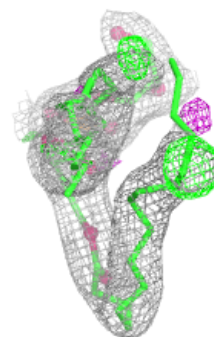
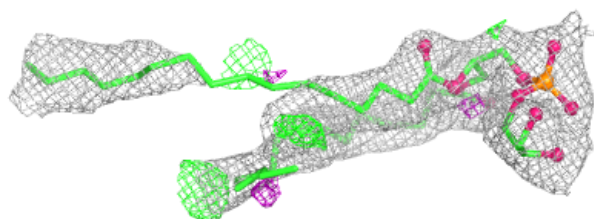
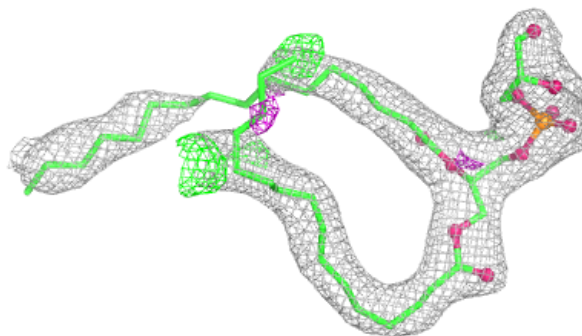
**Electron density around LHG A 419 (B):**

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

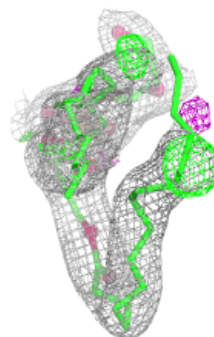
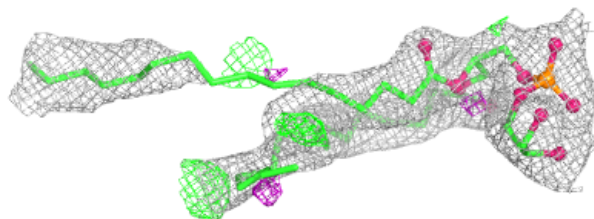
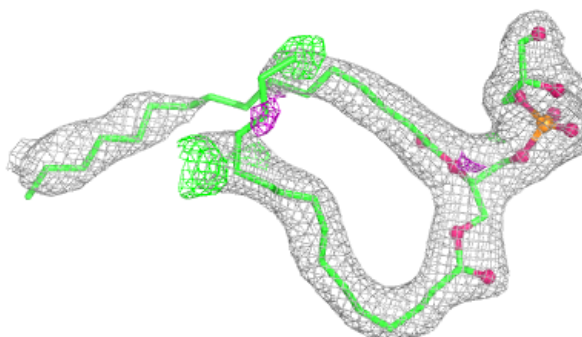


Electron density around LHG D 407 (A):

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

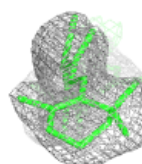
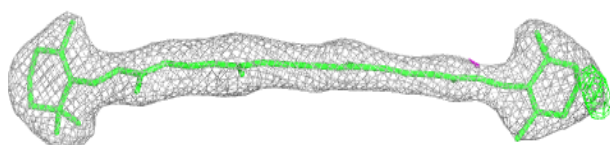
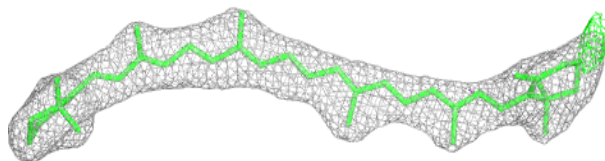
**Electron density around LHG D 407 (B):**

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

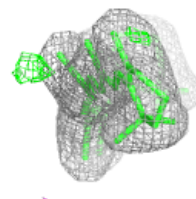
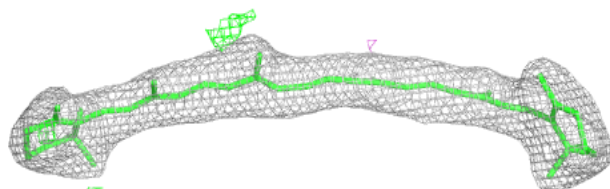
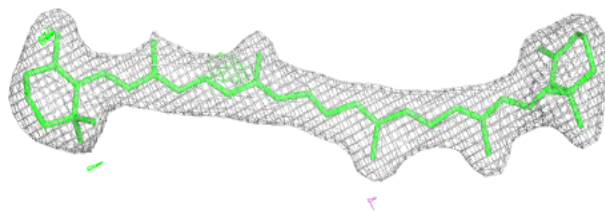


Electron density around BCR H 101:

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

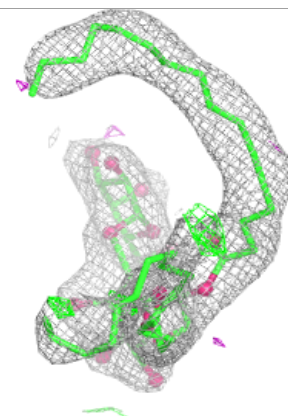
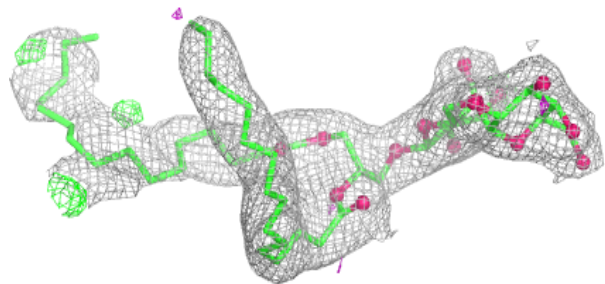
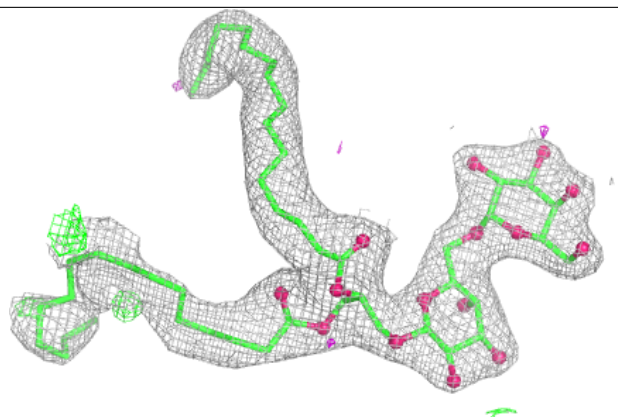
**Electron density around BCR T 102:**

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

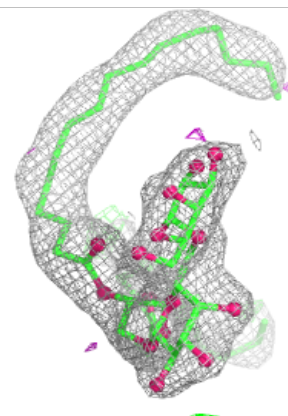
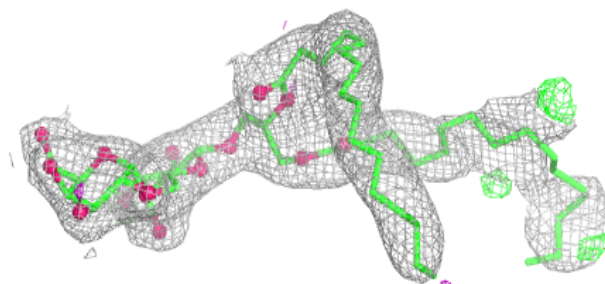
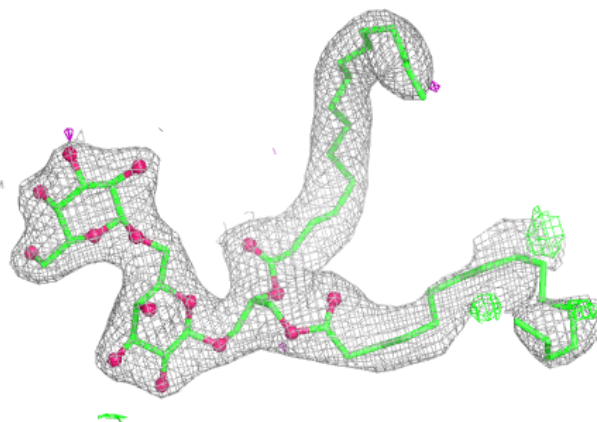


Electron density around DGD C 518 (A):

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

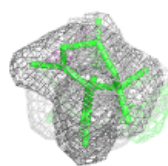
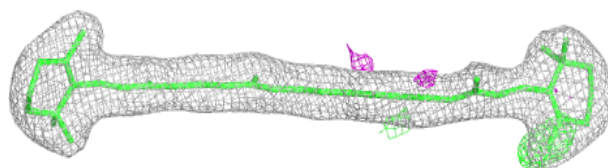
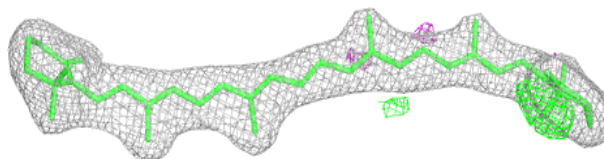
**Electron density around DGD C 518 (B):**

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

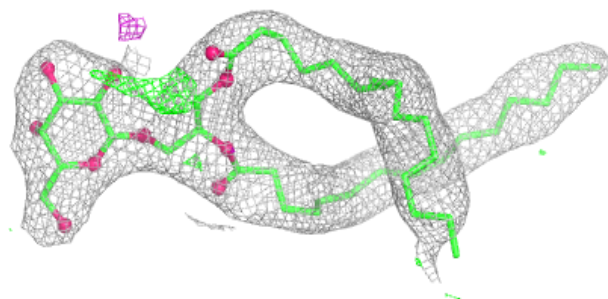
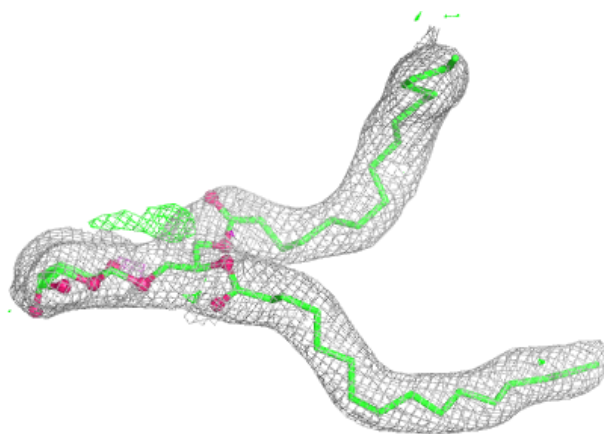


Electron density around BCR a 408:

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

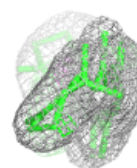
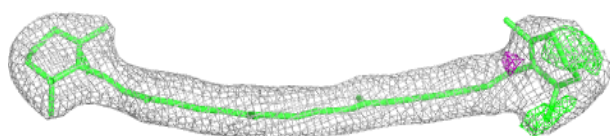
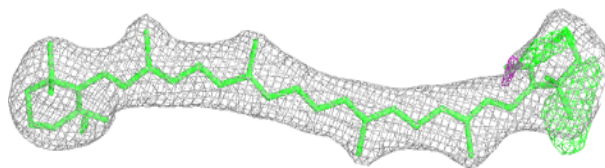
**Electron density around LMG B 621:**

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

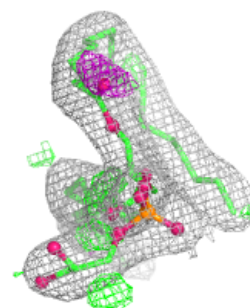
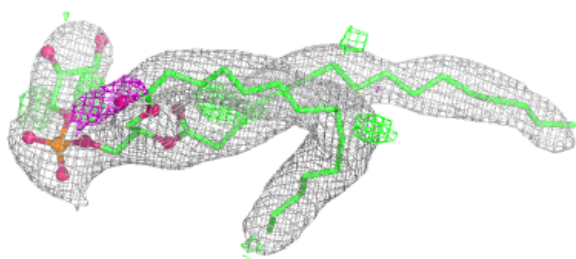
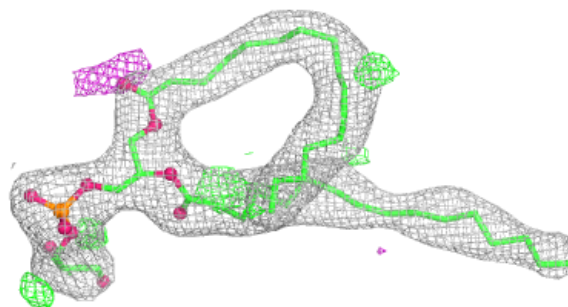


Electron density around BCR d 405:

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

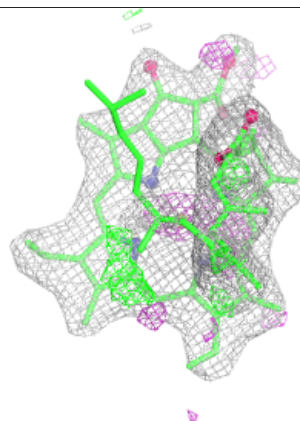
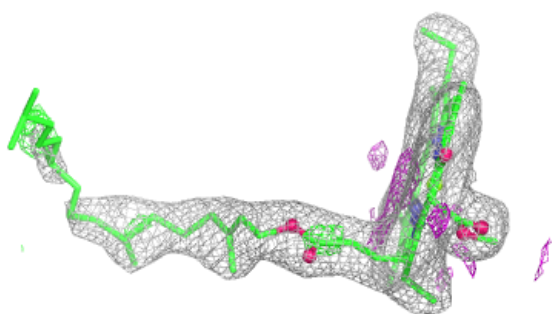
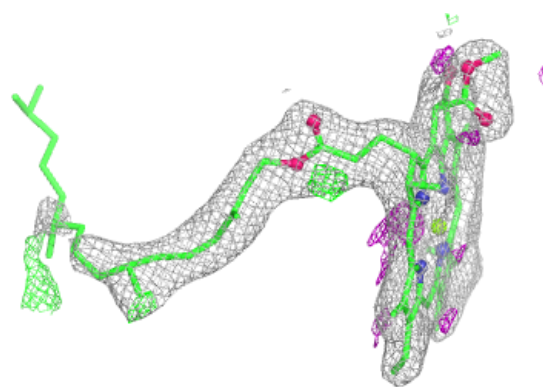
**Electron density around LHG d 414 (B):**

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

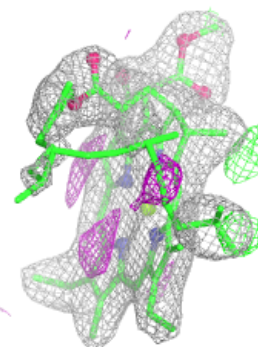
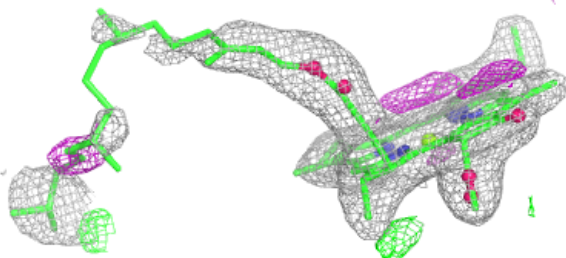
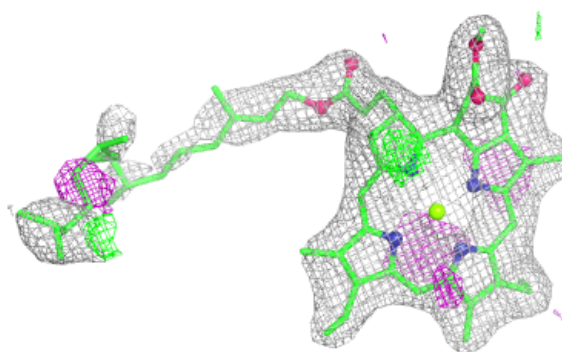


Electron density around CLA D 403:

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

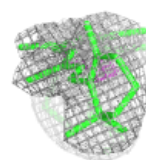
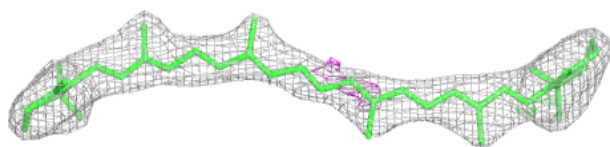
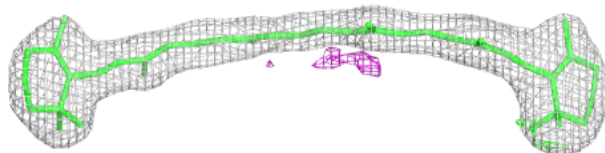
**Electron density around CLA a 407:**

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

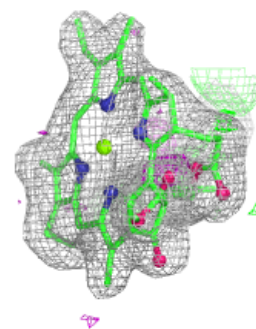
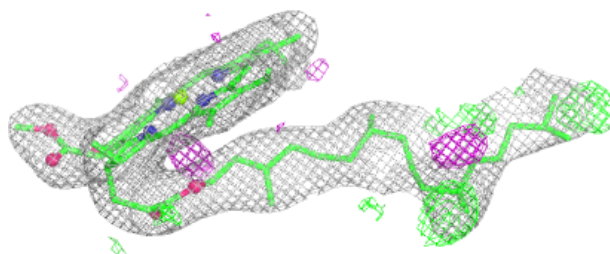
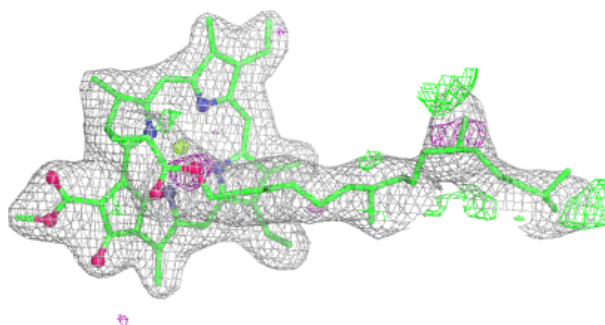


Electron density around BCR K 102:

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

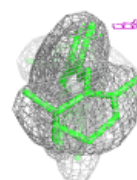
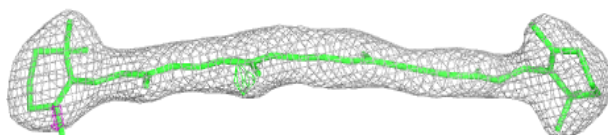
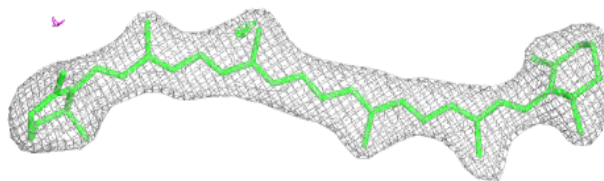
**Electron density around CLA B 614:**

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

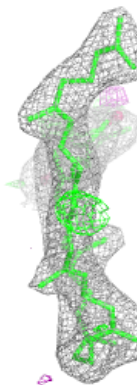
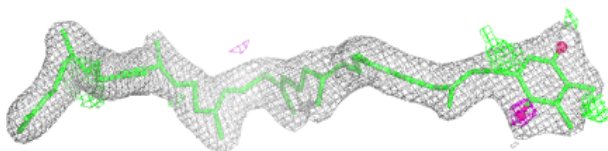
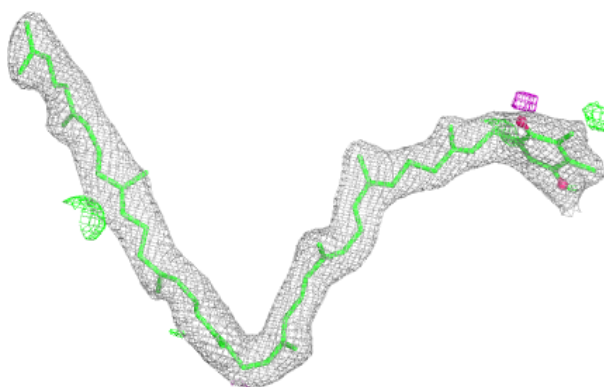


Electron density around BCR Y 101:

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

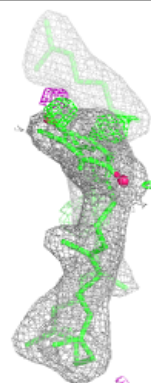
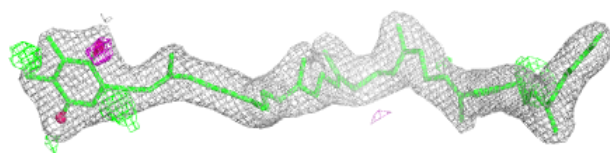
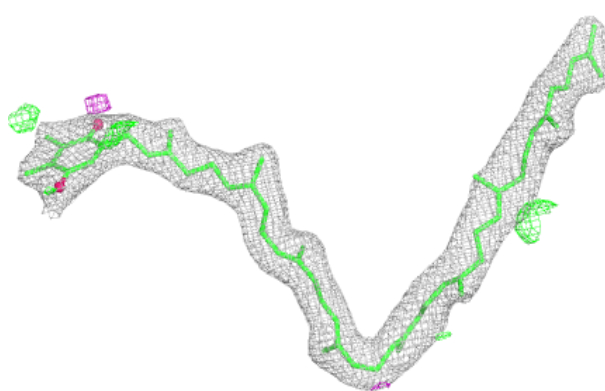
**Electron density around PL9 D 405 (A):**

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

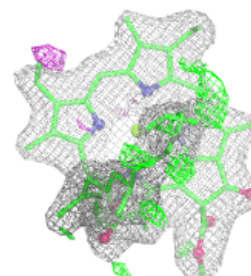
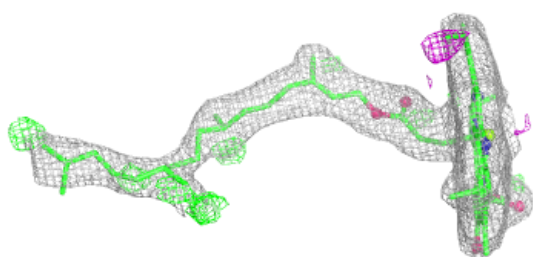
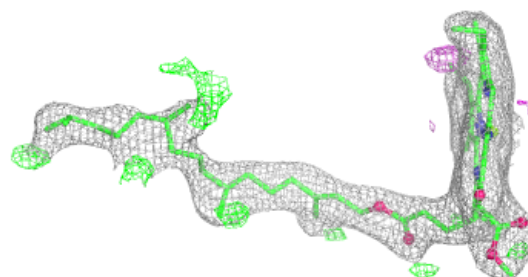


Electron density around PL9 D 405 (B):

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

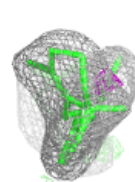
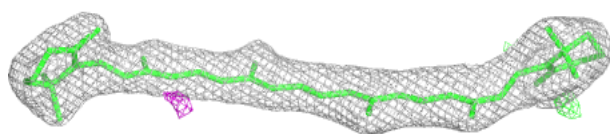
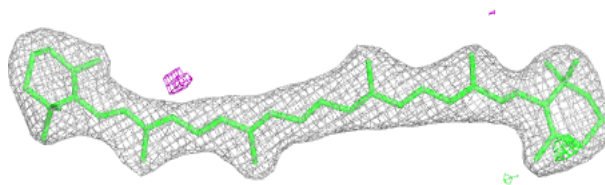
**Electron density around CLA b 606:**

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

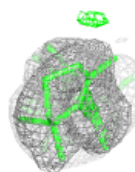
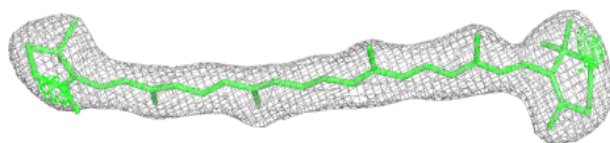
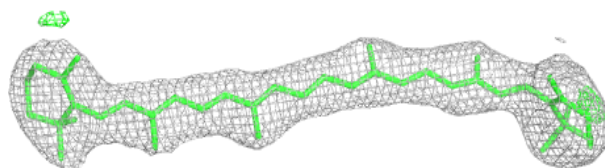


Electron density around BCR b 619:

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

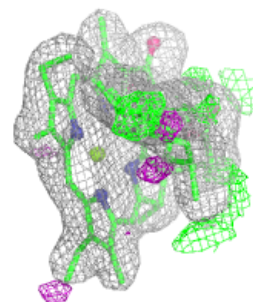
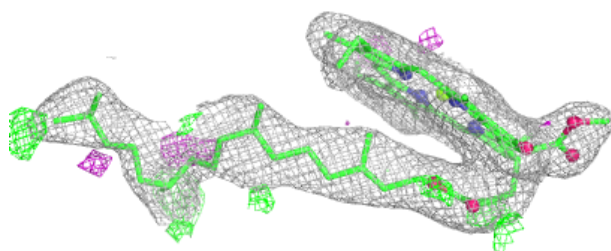
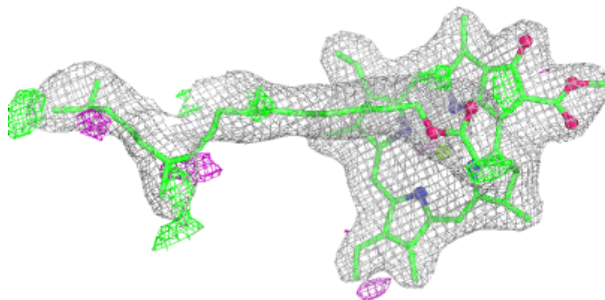
**Electron density around BCR c 514:**

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

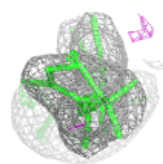
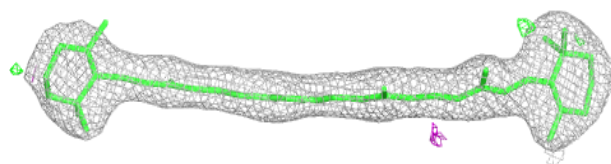
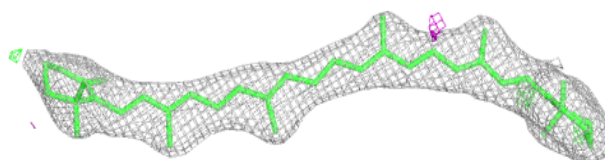


Electron density around CLA b 614:

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

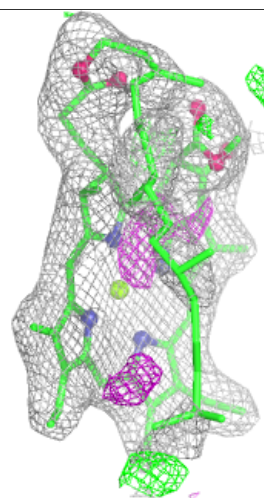
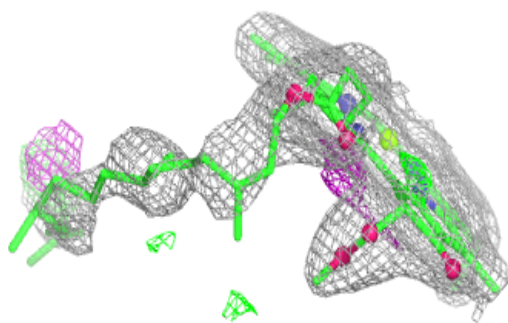
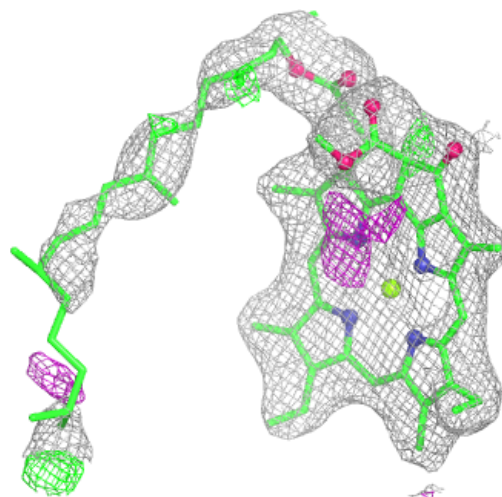
**Electron density around BCR h 101:**

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



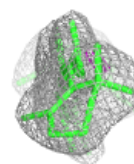
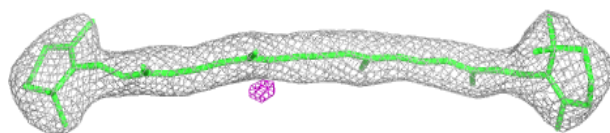
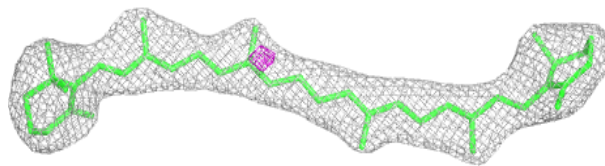
Electron density around CLA B 616:

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

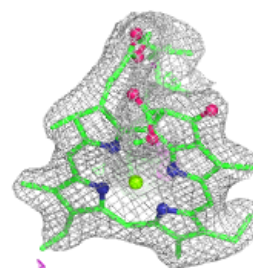
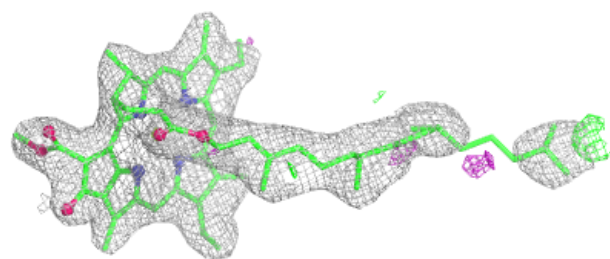
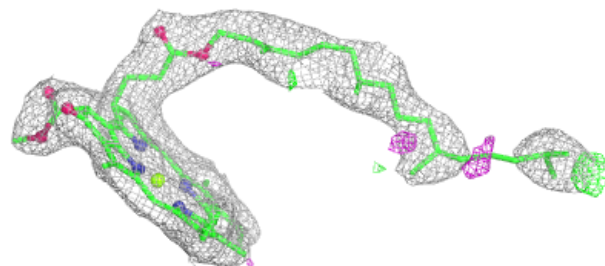


Electron density around BCR y 101:

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

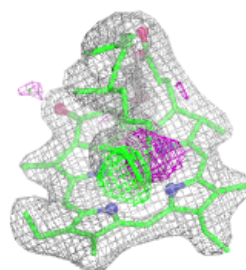
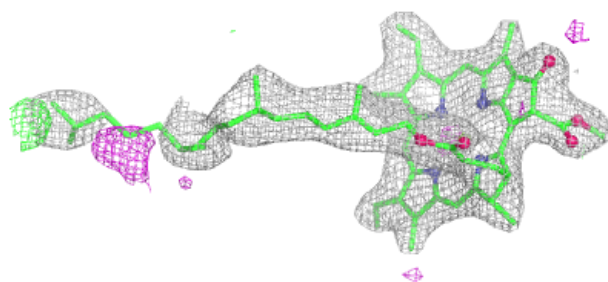
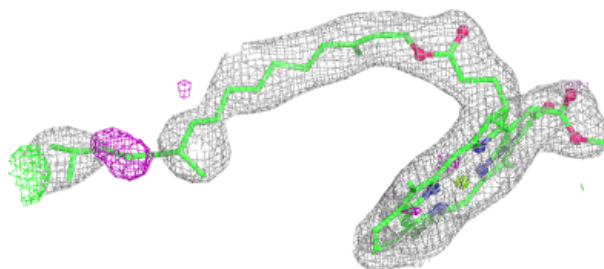
**Electron density around CLA c 504:**

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



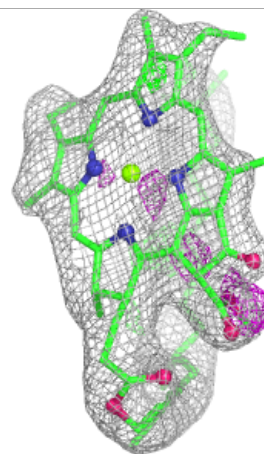
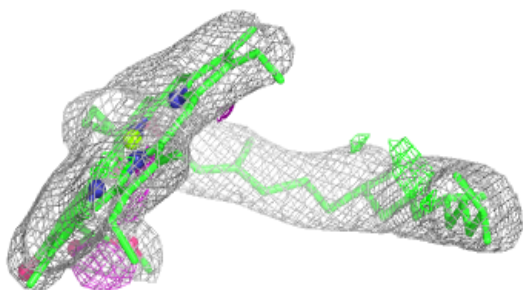
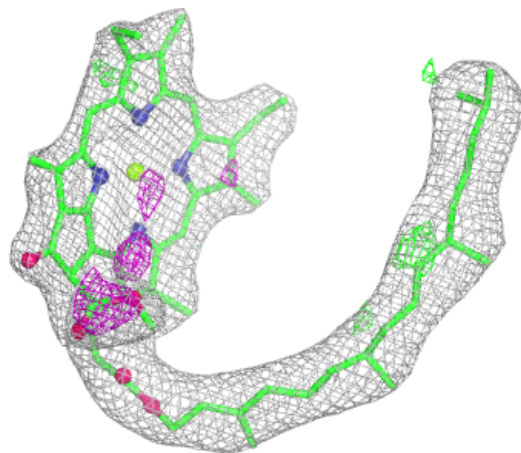
Electron density around CLA C 505:

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



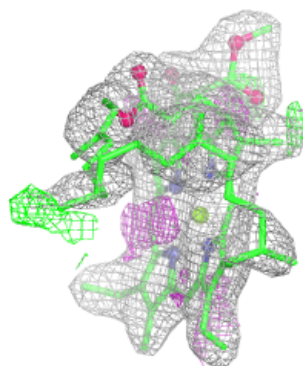
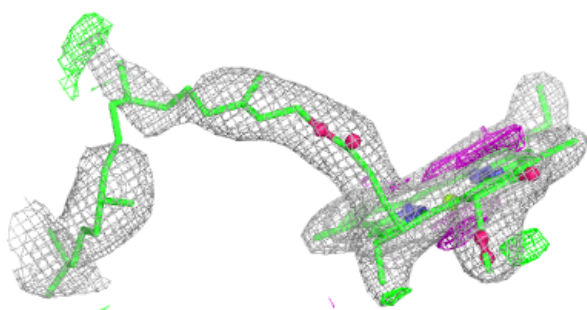
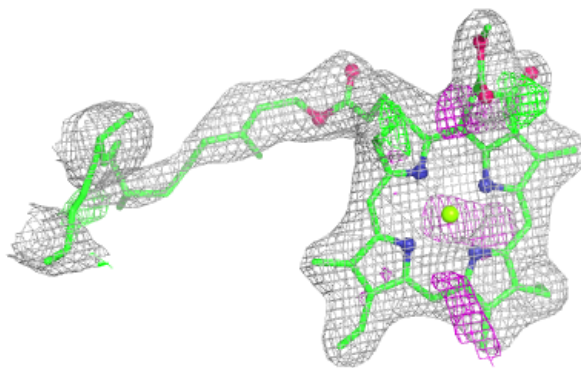
Electron density around CLA c 507:

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

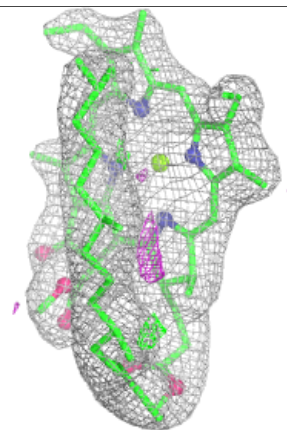
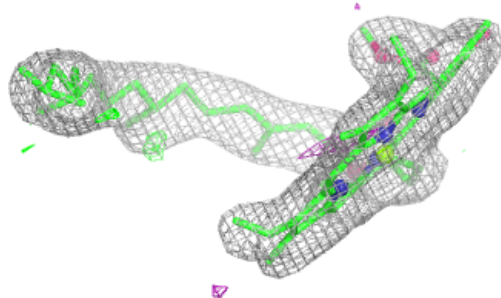
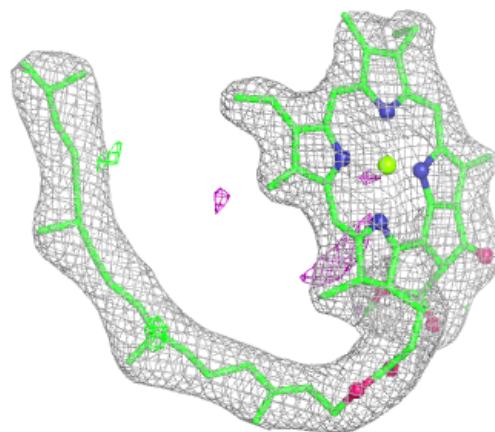


Electron density around CLA A 408:

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

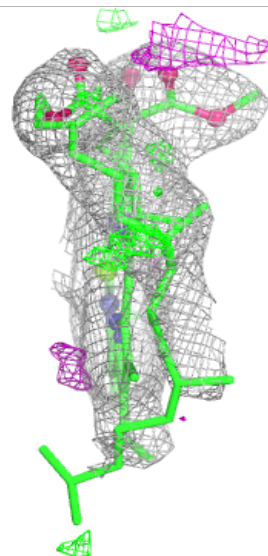
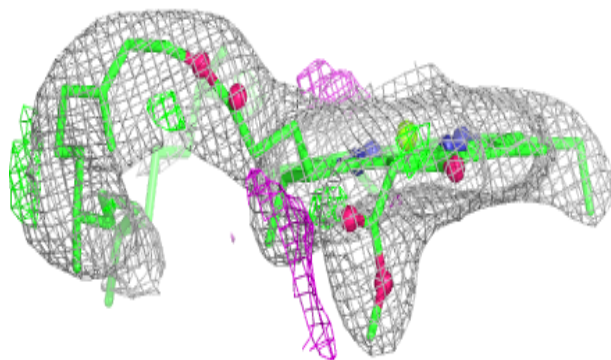
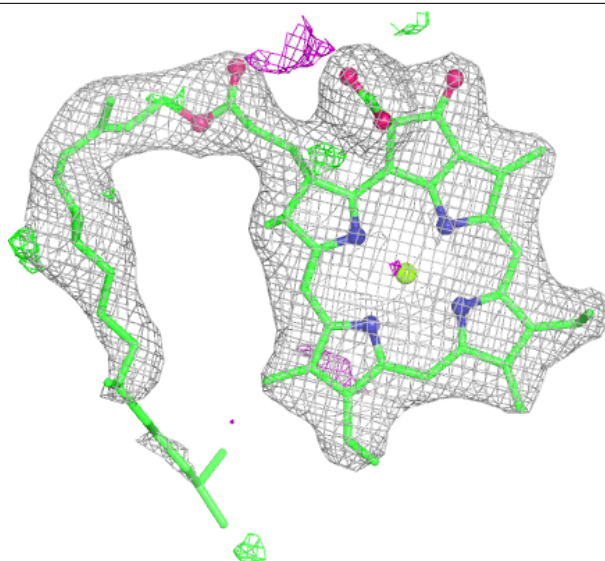
**Electron density around CLA C 508:**

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



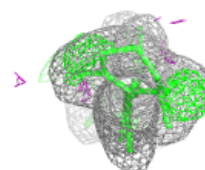
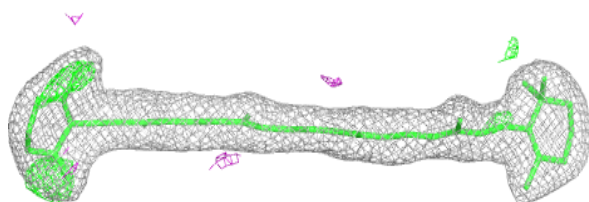
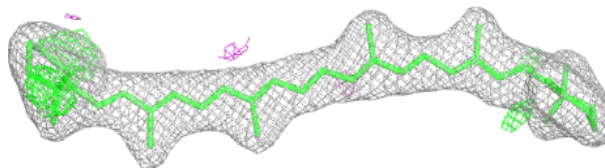
Electron density around CLA C 513:

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

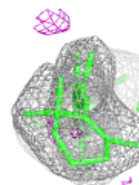
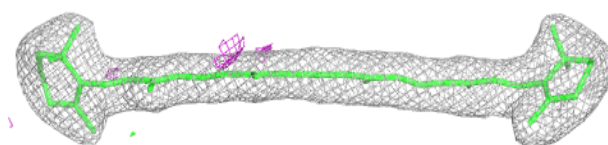
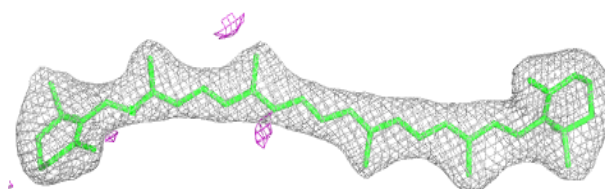


Electron density around BCR A 409:

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

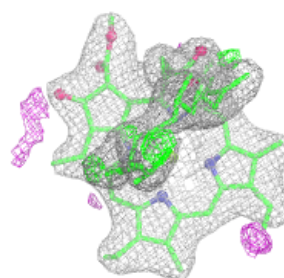
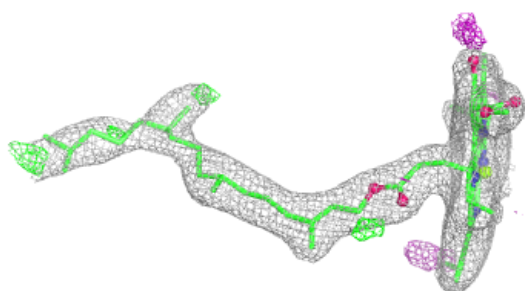
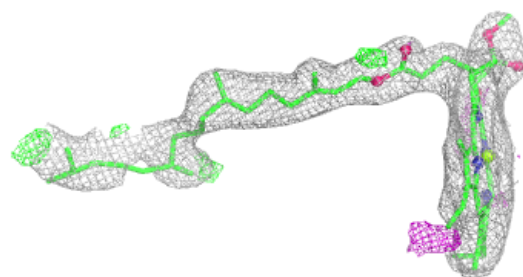
**Electron density around BCR B 618:**

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

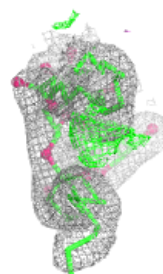
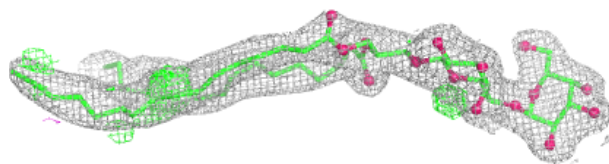
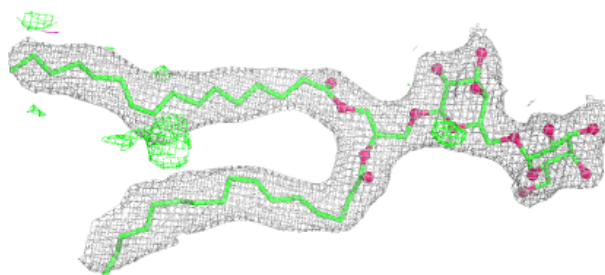


Electron density around CLA B 606:

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

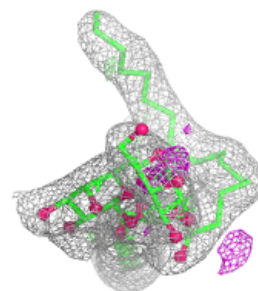
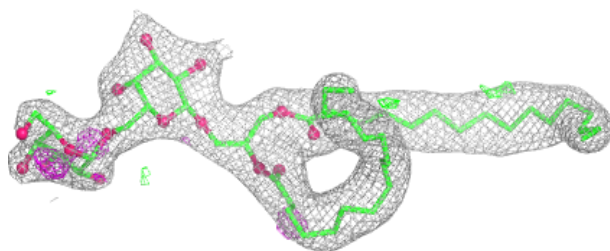
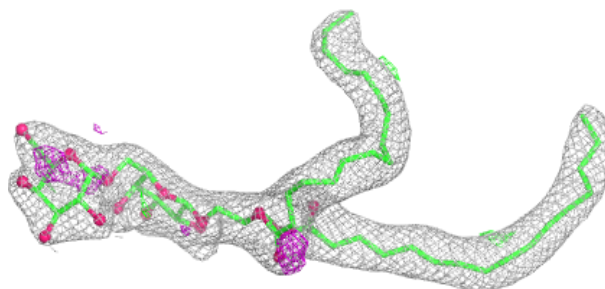
**Electron density around DGD C 519:**

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

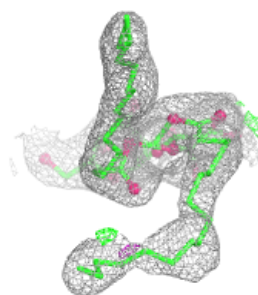
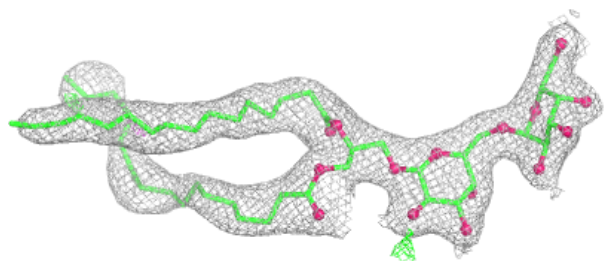
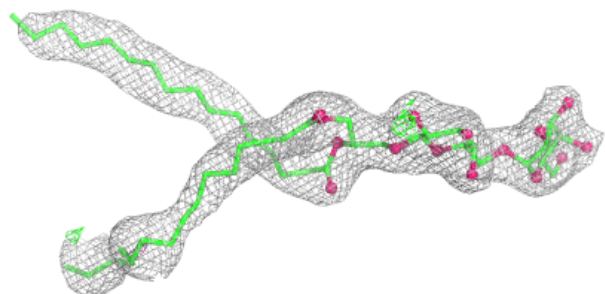


Electron density around DGD H 102:

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

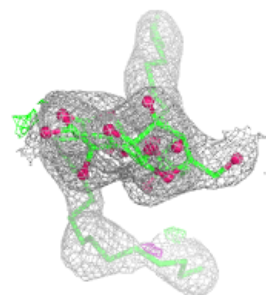
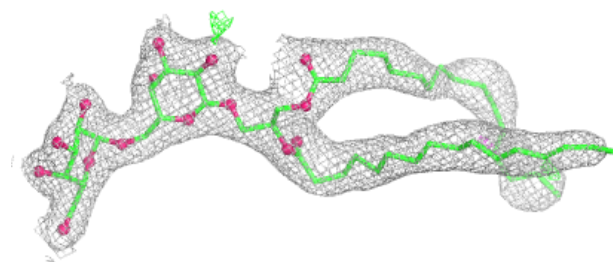
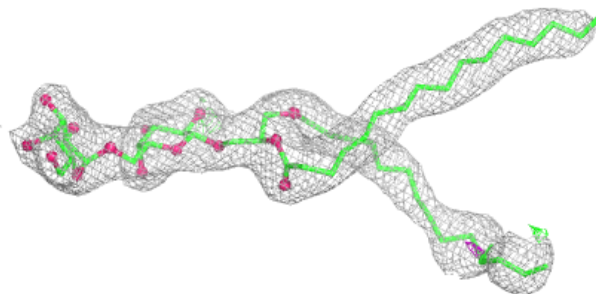
**Electron density around DGD c 516 (A):**

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

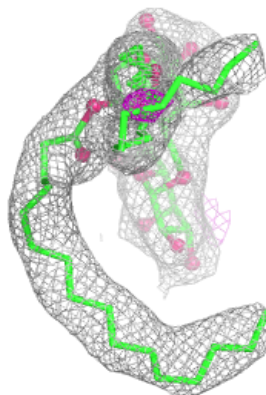
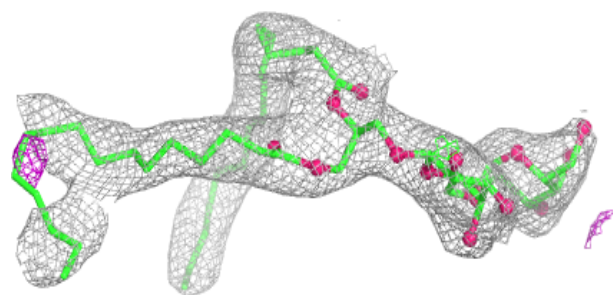
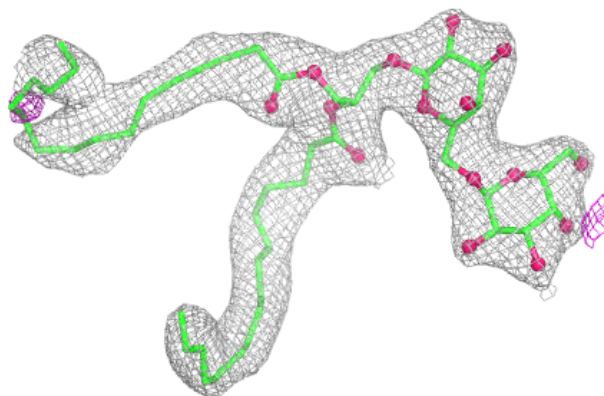


Electron density around DGD c 516 (B):

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

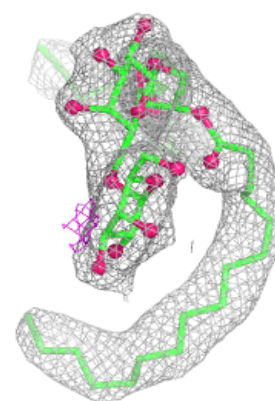
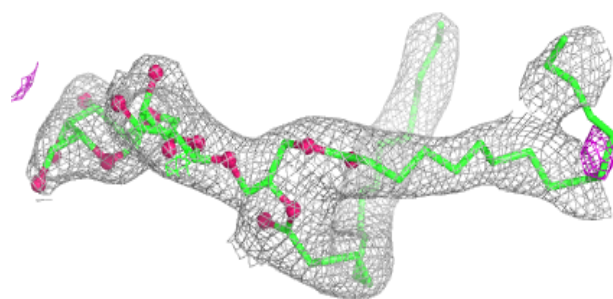
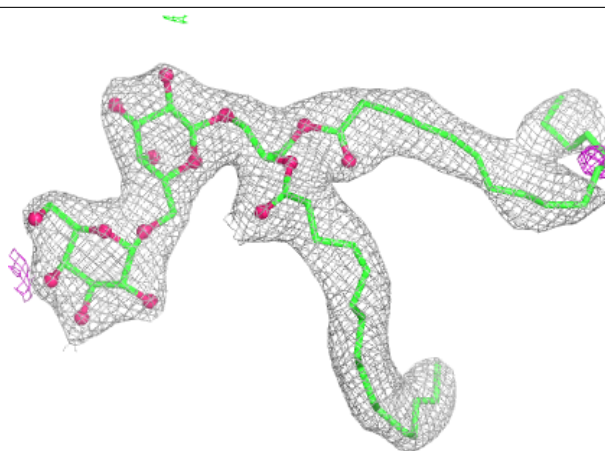
**Electron density around DGD c 517 (A):**

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

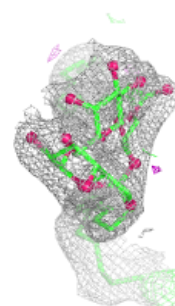
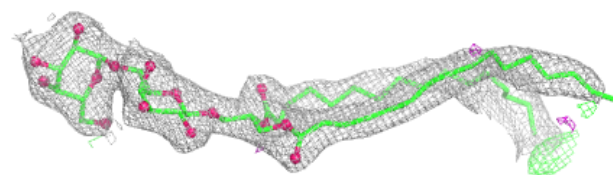
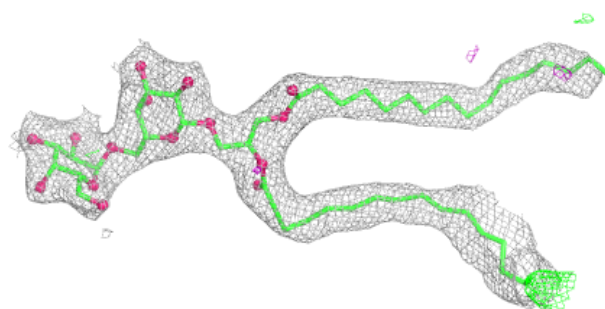


Electron density around DGD c 517 (B):

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

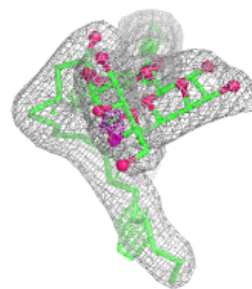
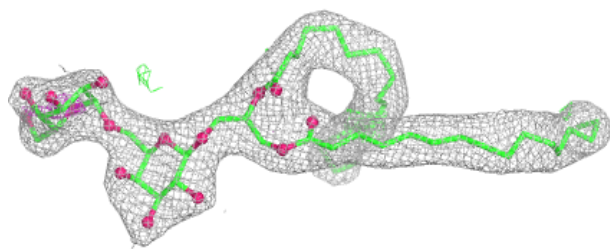
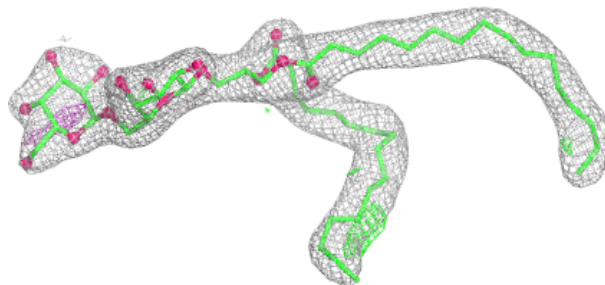
**Electron density around DGD c 518:**

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



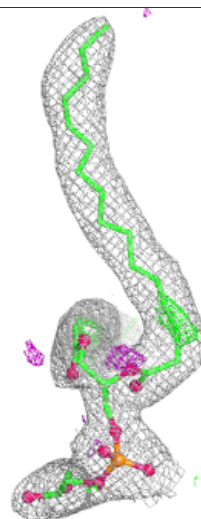
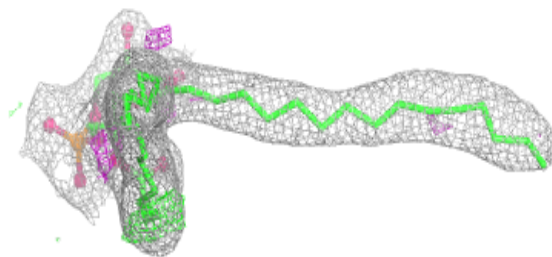
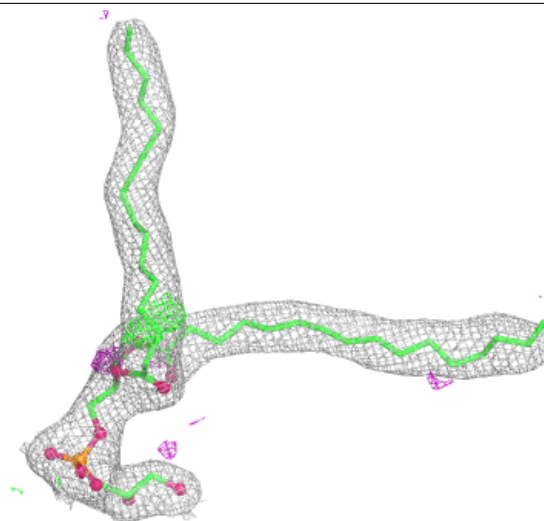
Electron density around DGD h 102:

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



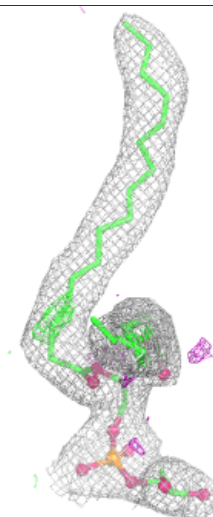
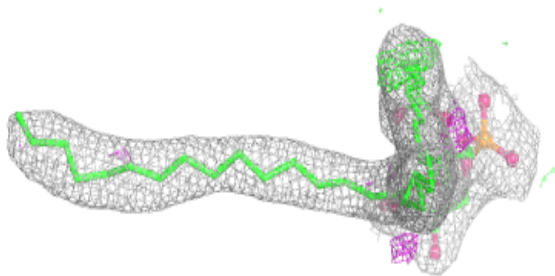
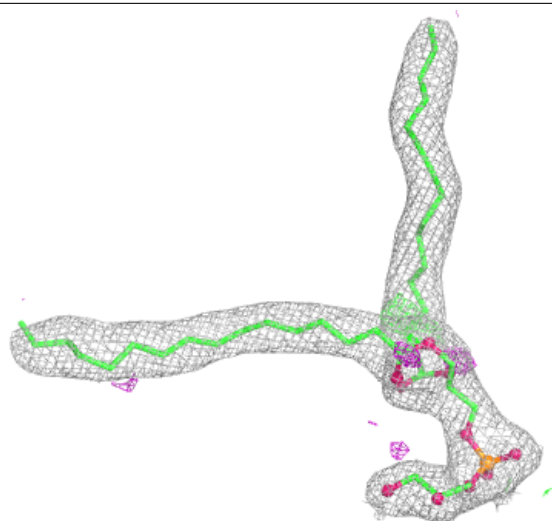
Electron density around LHG b 629 (A):

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



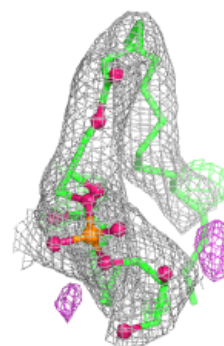
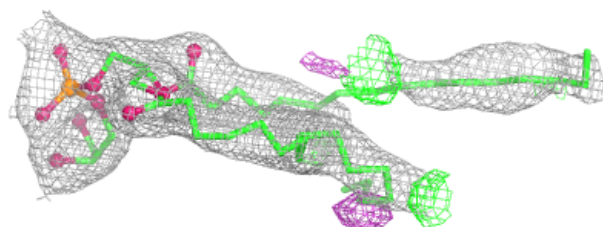
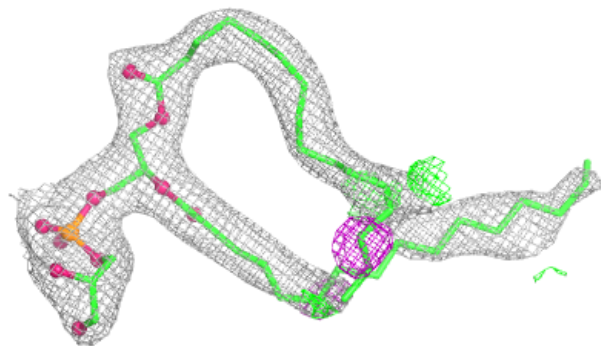
Electron density around LHG b 629 (B):

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

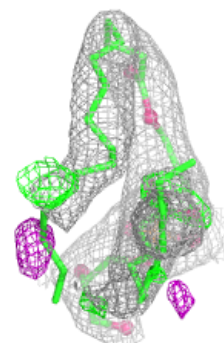
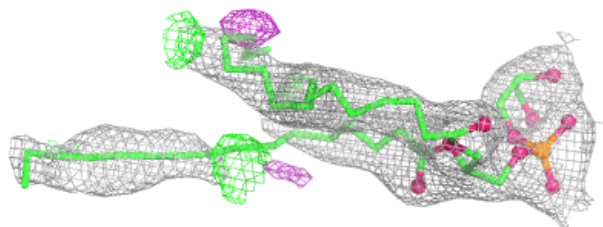
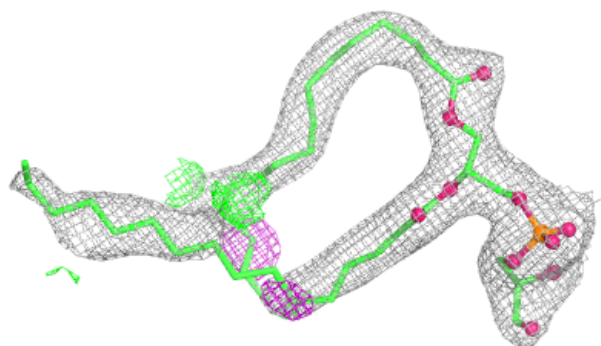


Electron density around LHG d 408 (A):

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

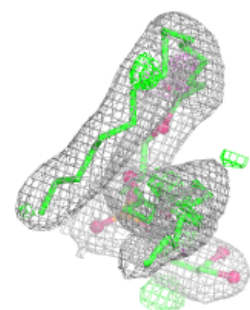
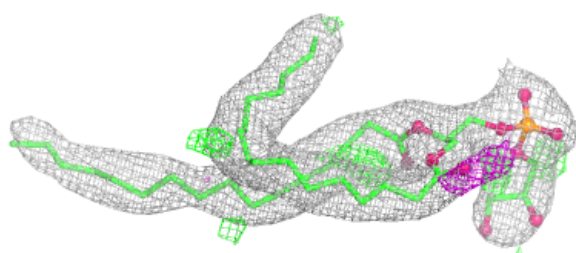
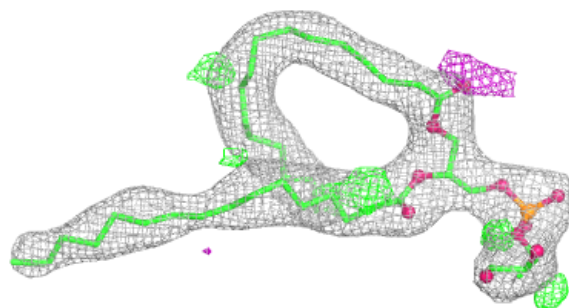
**Electron density around LHG d 408 (B):**

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

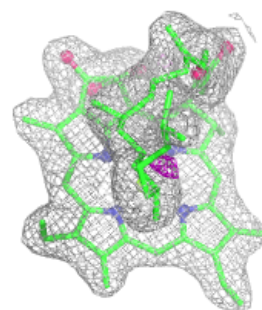
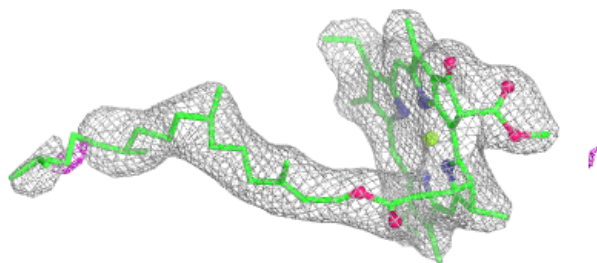
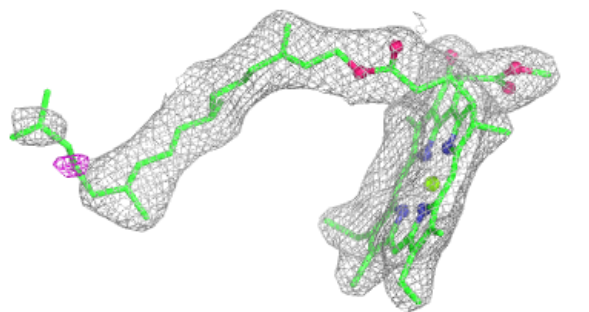


Electron density around LHG d 414 (A):

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

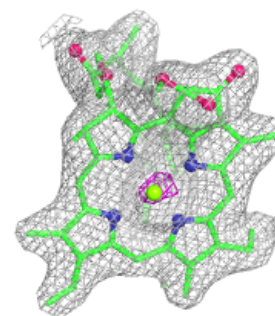
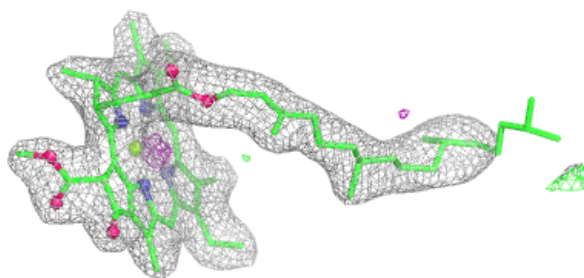
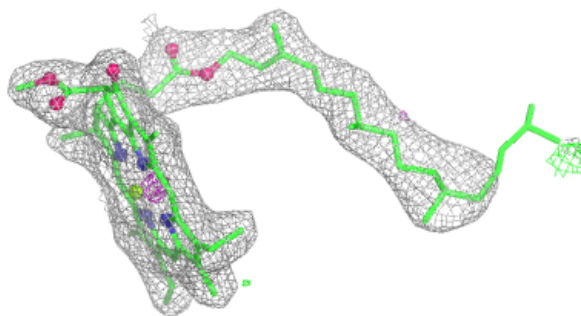
**Electron density around CLA c 508:**

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

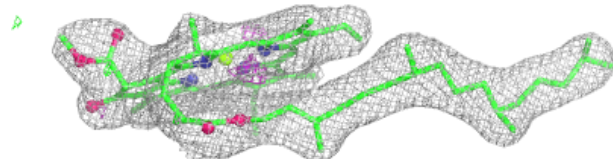
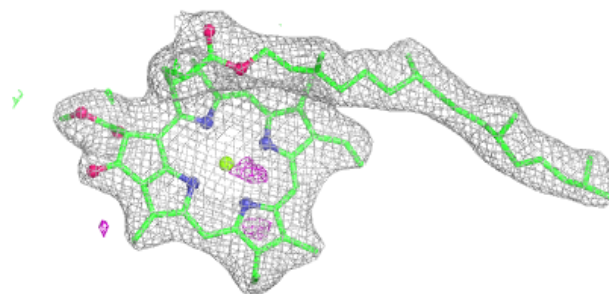


Electron density around CLA C 509:

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

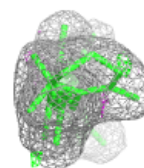
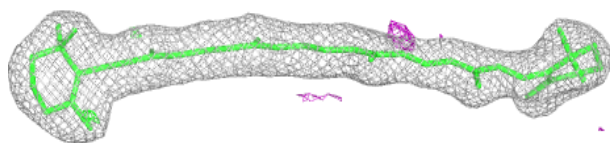
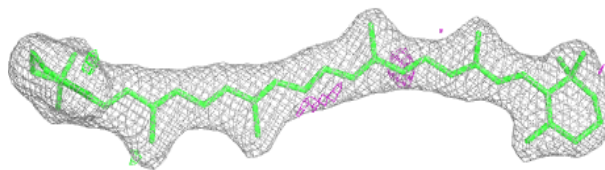
**Electron density around CLA C 502:**

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

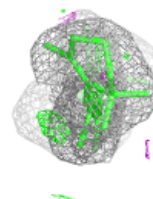
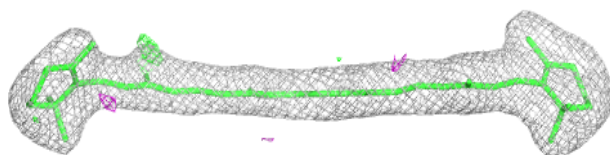
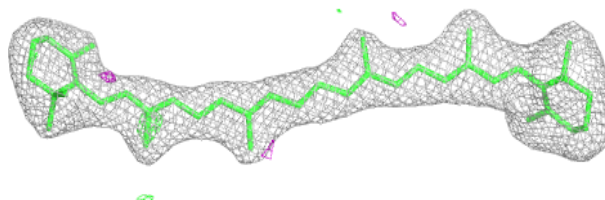


Electron density around BCR b 617:

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

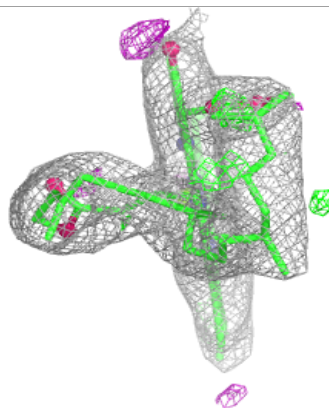
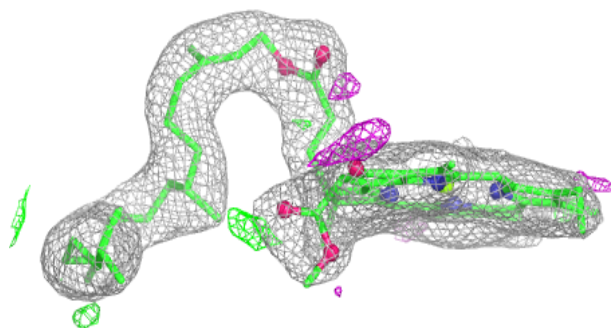
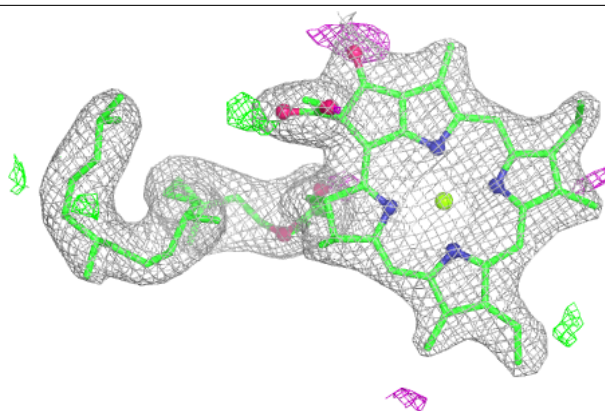
**Electron density around BCR b 618:**

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



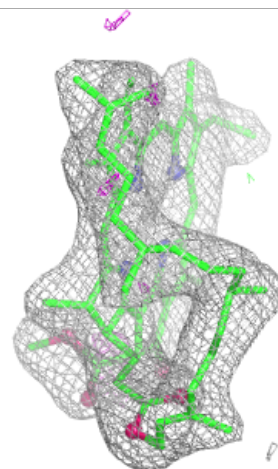
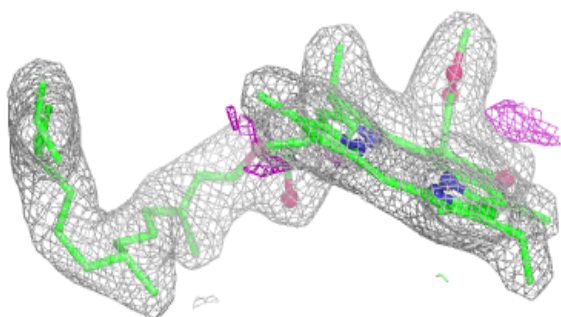
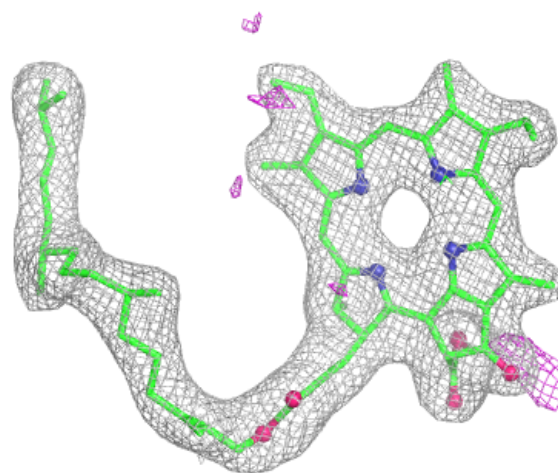
Electron density around CLA b 612:

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



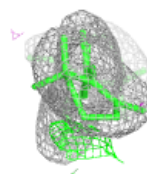
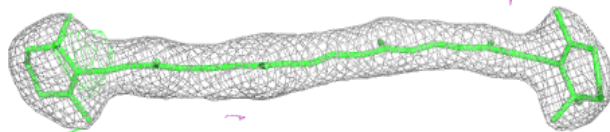
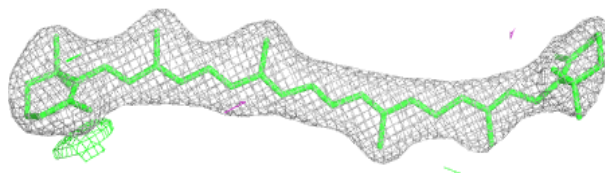
Electron density around PHO A 416 (A):

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



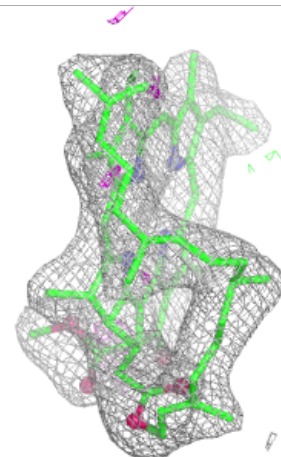
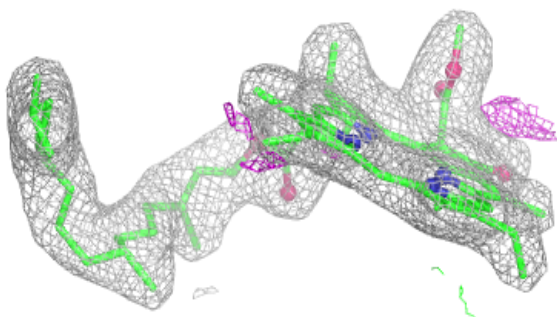
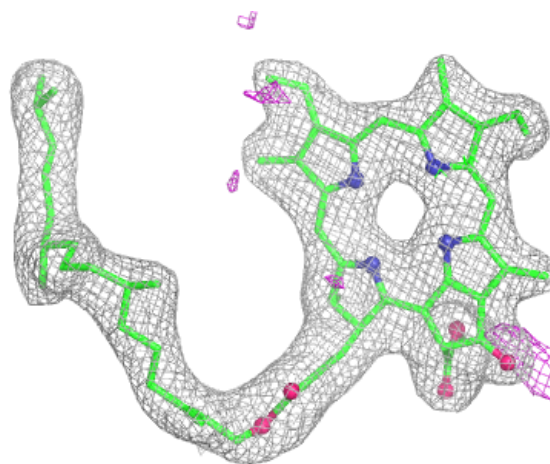
Electron density around BCR c 515:

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



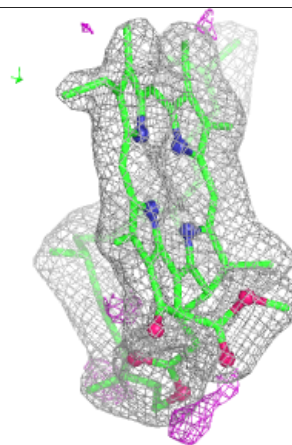
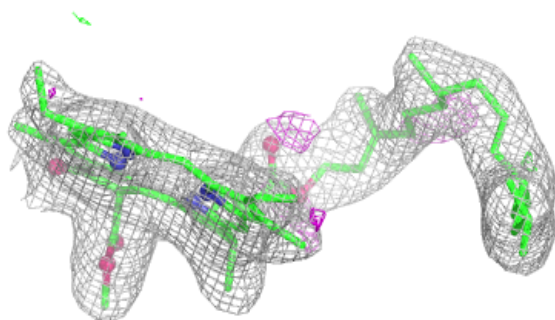
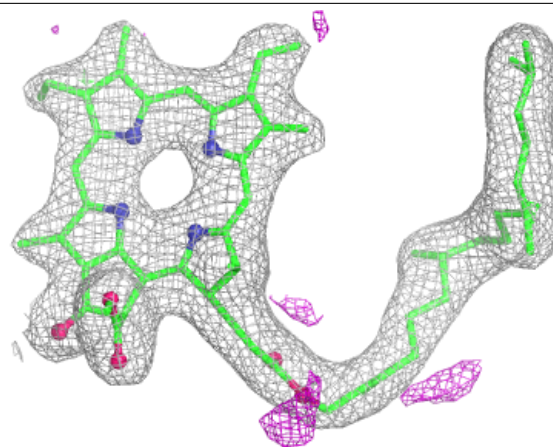
Electron density around PHO A 416 (B):

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



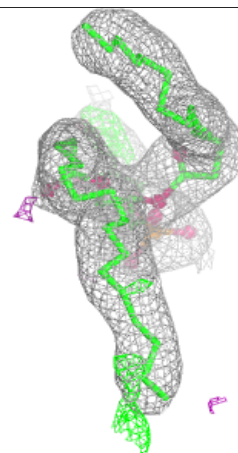
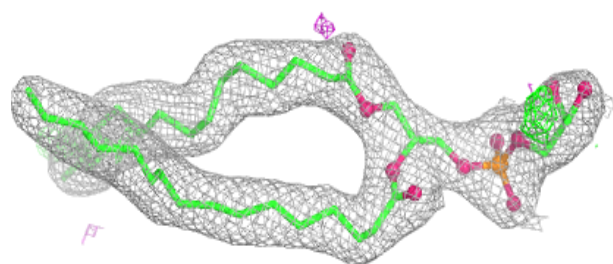
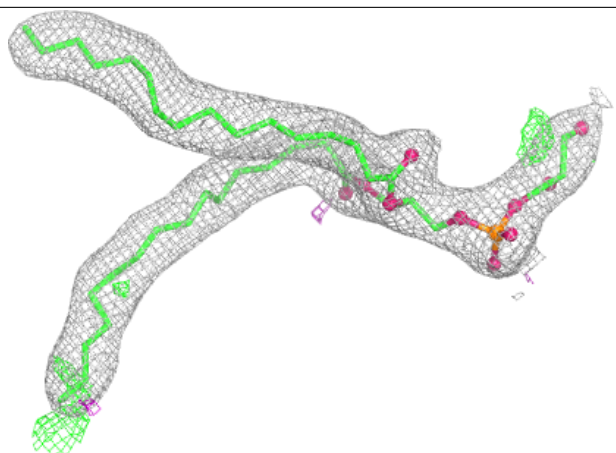
Electron density around PHO a 414 (A):

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



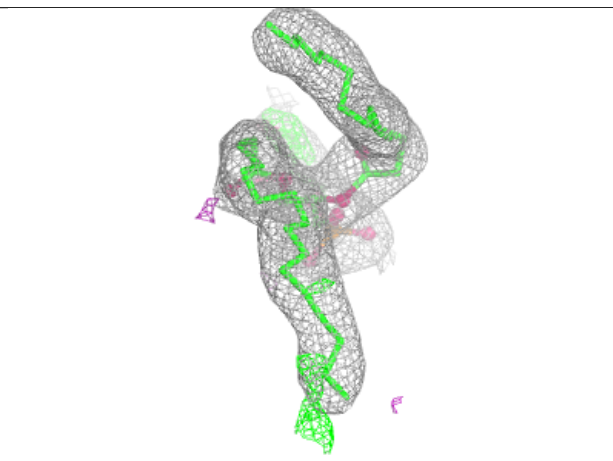
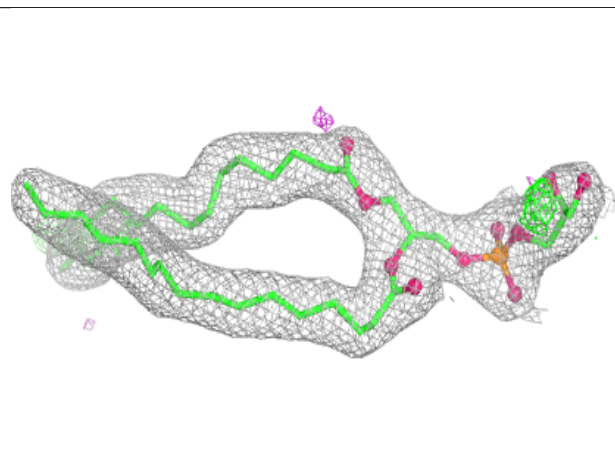
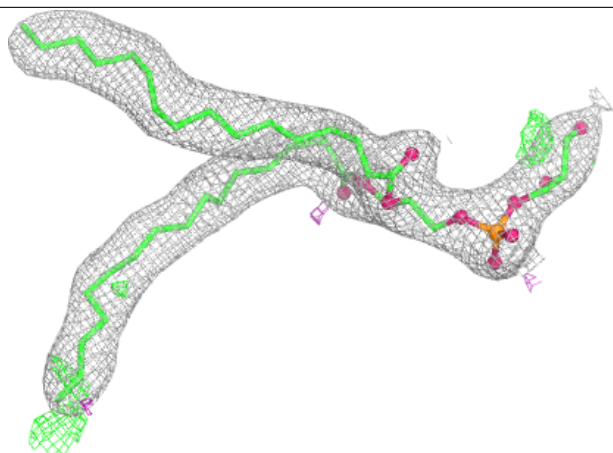
Electron density around LHG d 407 (A):

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

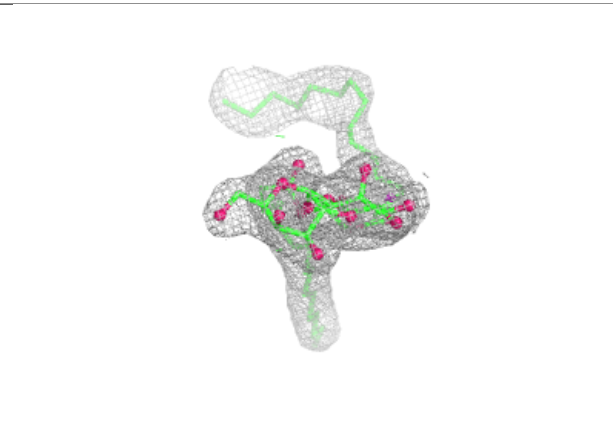
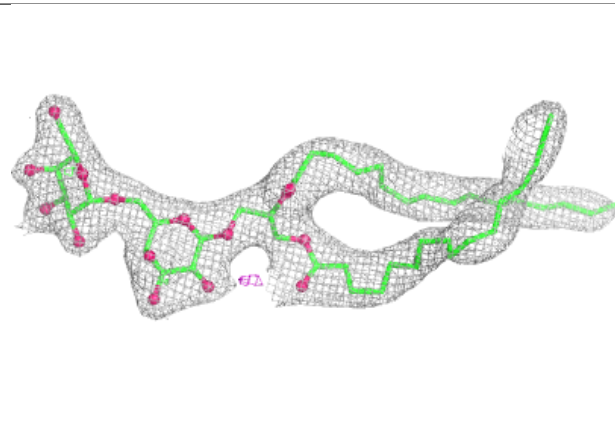
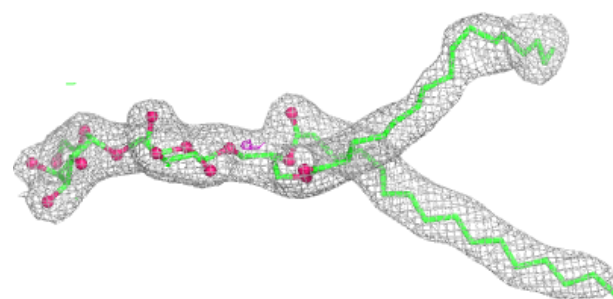


Electron density around LHG d 407 (B):

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

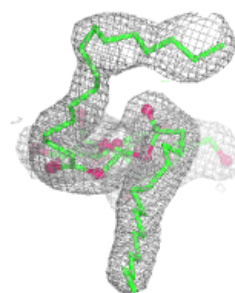
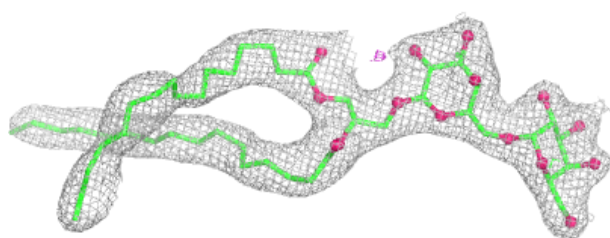
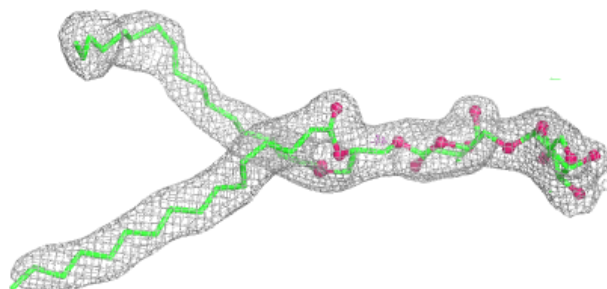
**Electron density around DGD C 517 (A):**

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

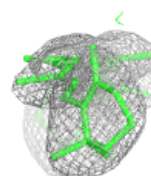
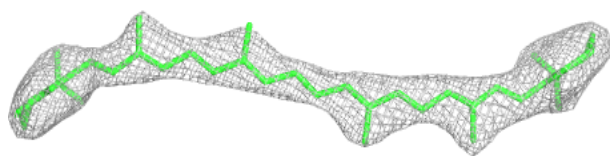
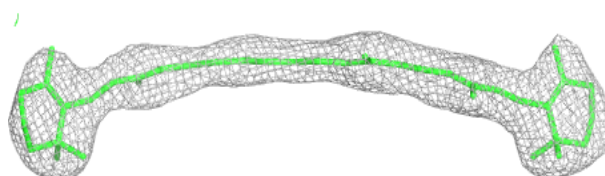


Electron density around DGD C 517 (B):

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

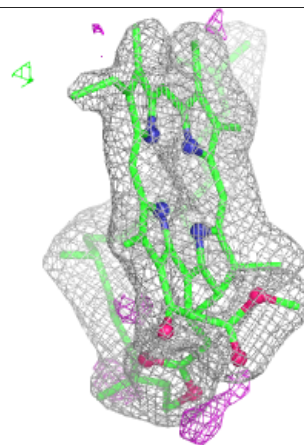
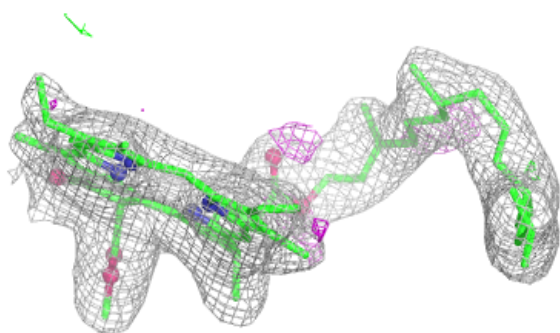
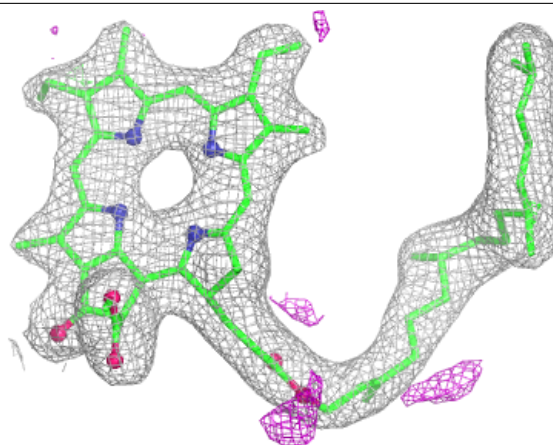
**Electron density around BCR k 101:**

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



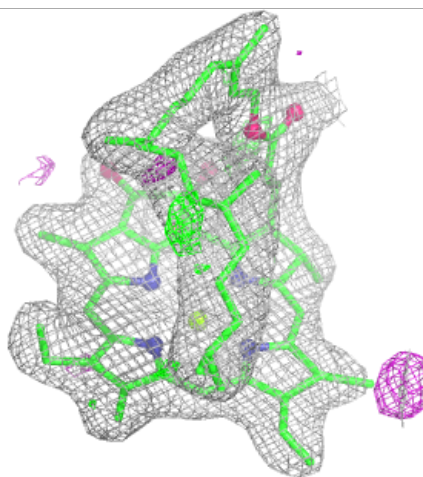
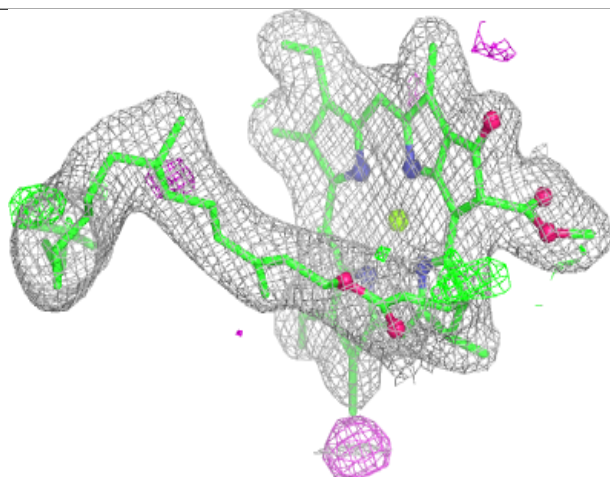
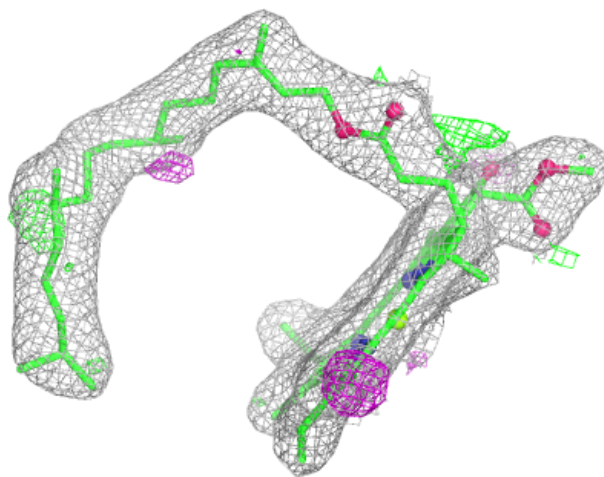
Electron density around PHO a 414 (B):

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



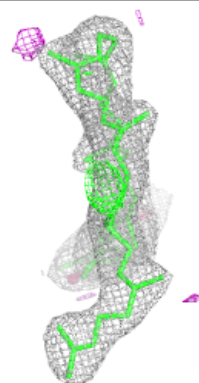
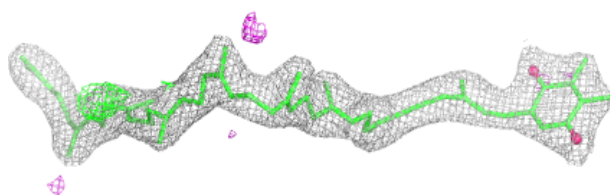
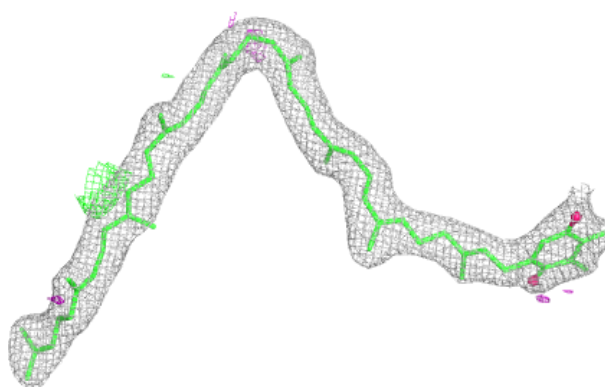
Electron density around CLA B 611:

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

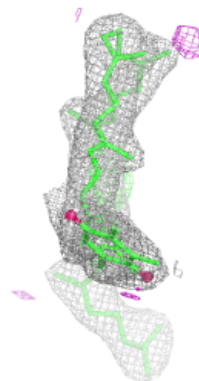
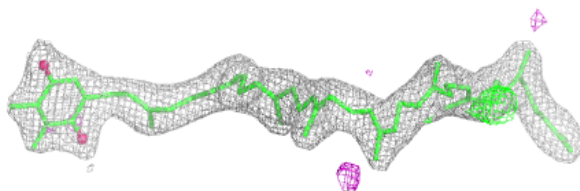
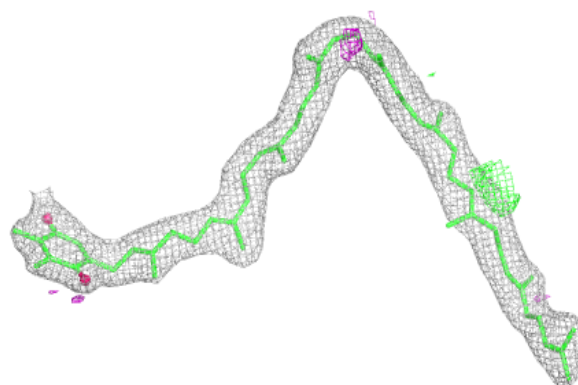


Electron density around PL9 d 406 (A):

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

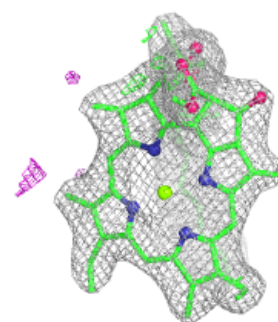
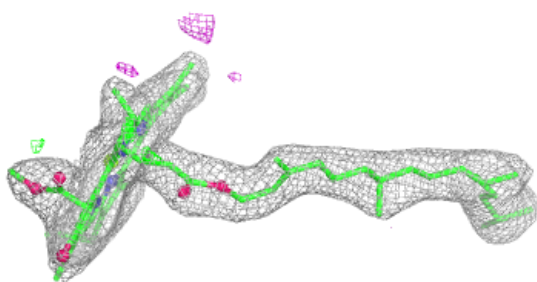
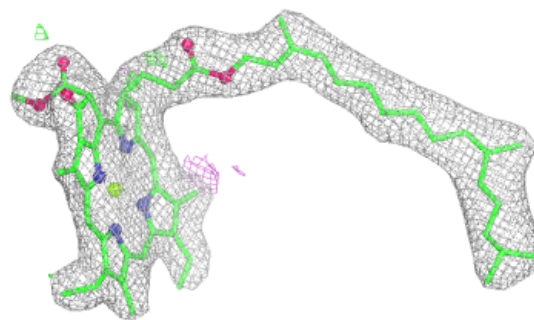
**Electron density around PL9 d 406 (B):**

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

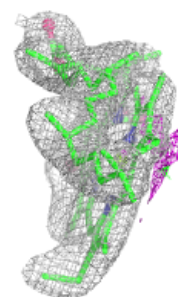
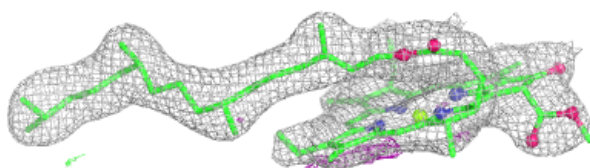
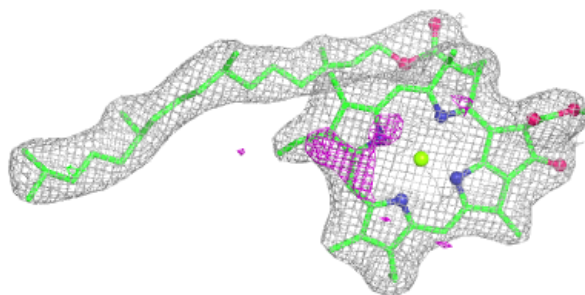


Electron density around CLA B 609:

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

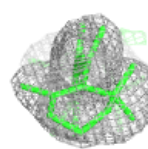
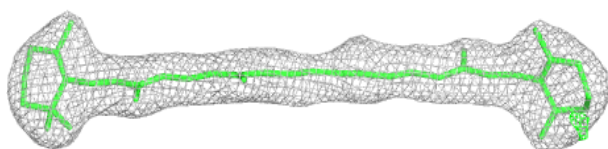
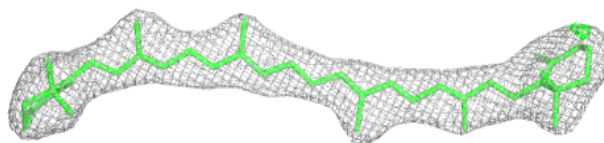
**Electron density around CLA c 501:**

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

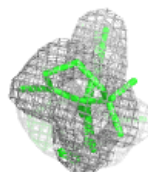
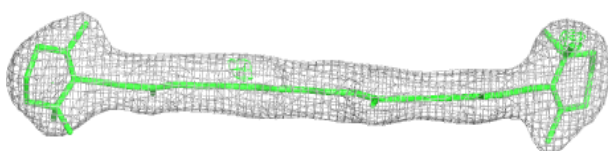
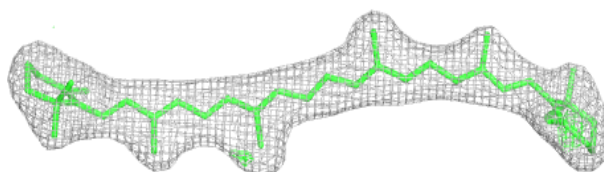


Electron density around BCR C 515:

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

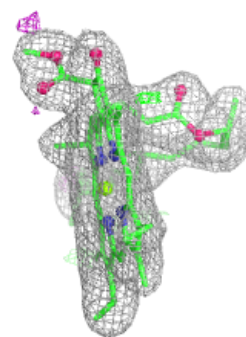
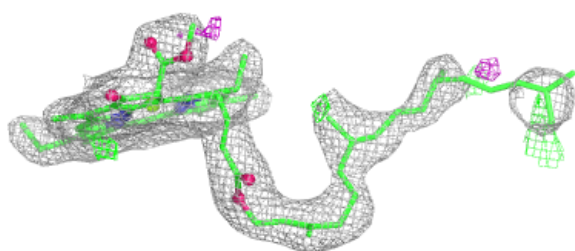
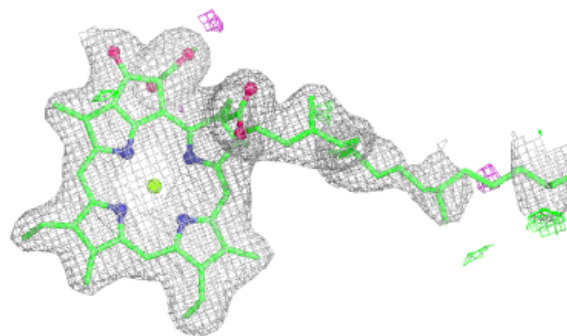
**Electron density around BCR C 516:**

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

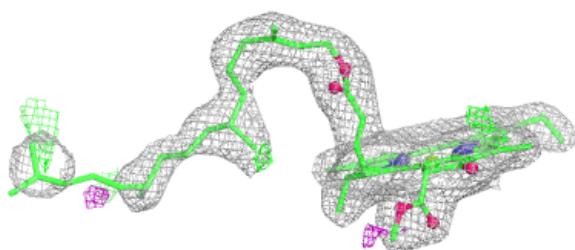
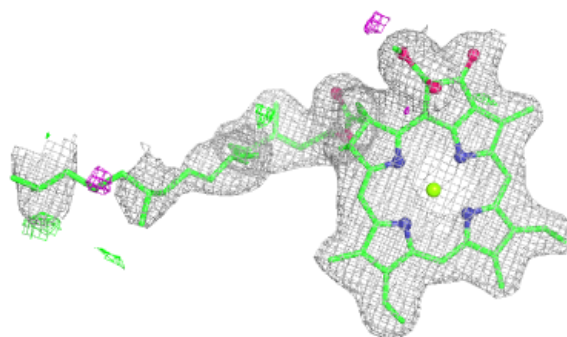


Electron density around CLA a 405 (A):

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

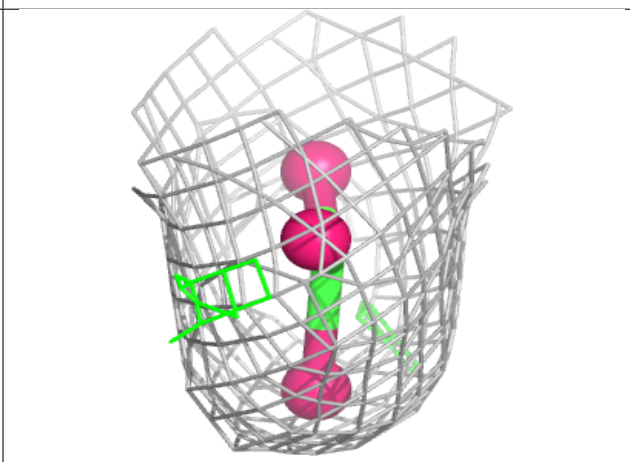
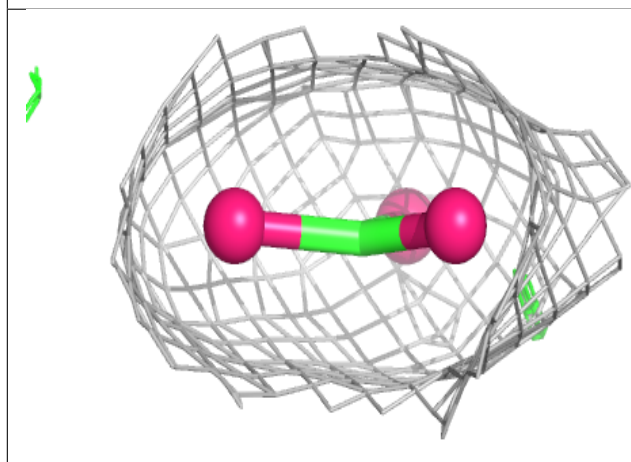
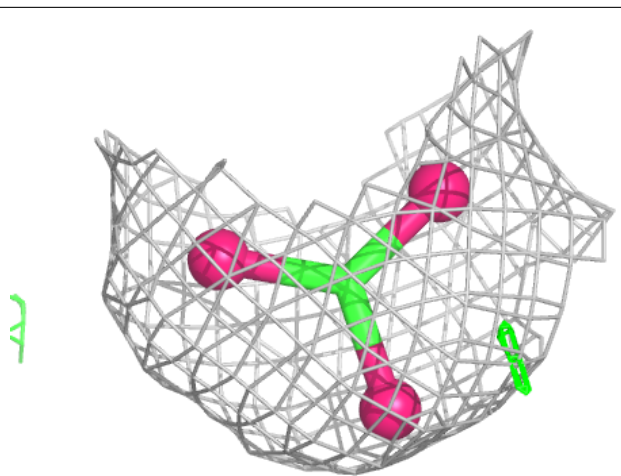
**Electron density around CLA a 405 (B):**

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



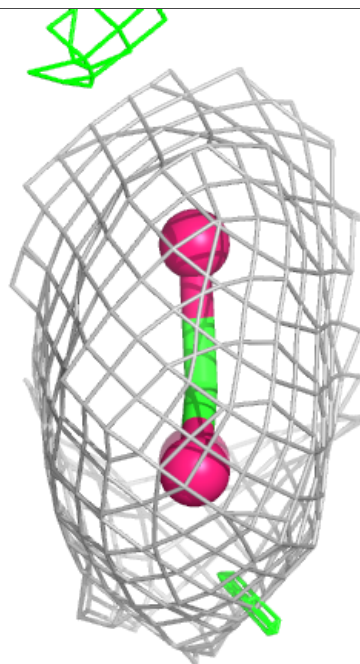
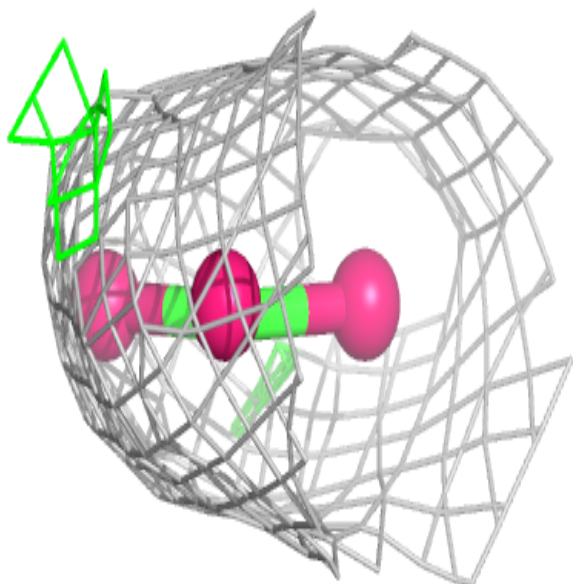
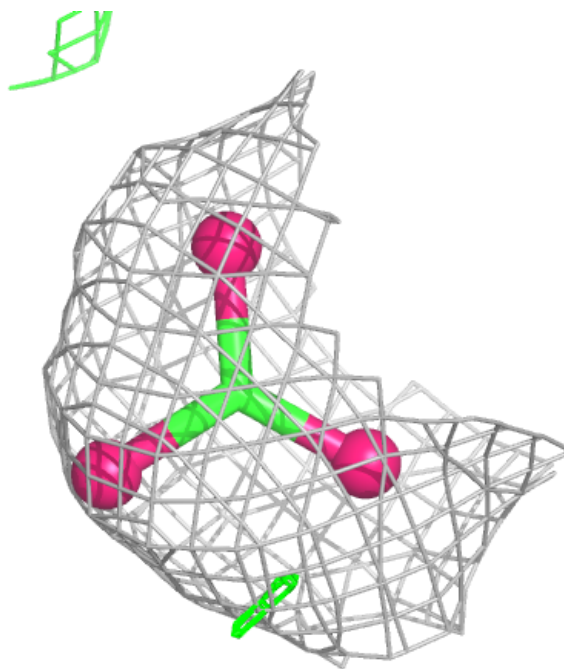
Electron density around BCT D 401 (A):

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



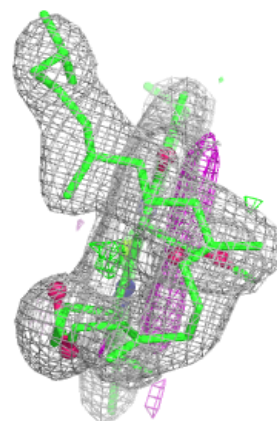
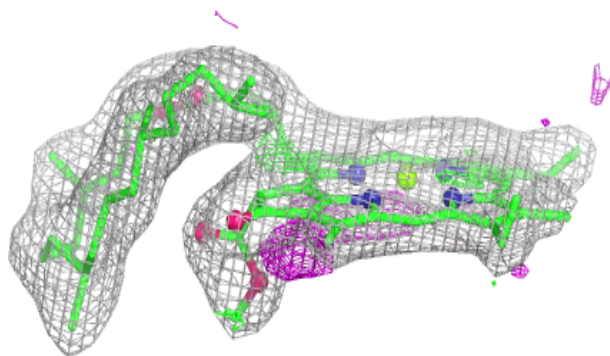
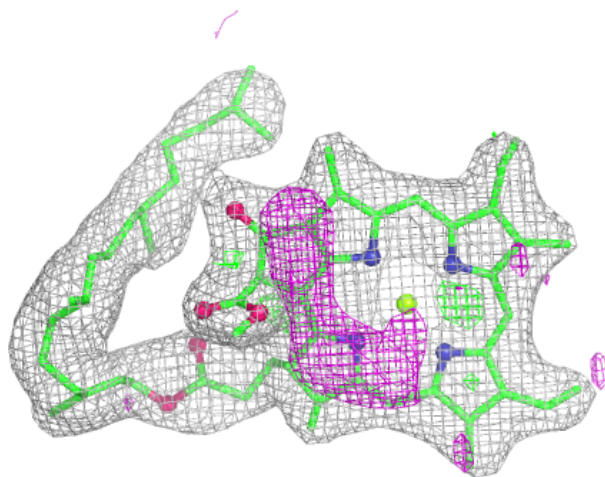
Electron density around BCT D 401 (B):

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



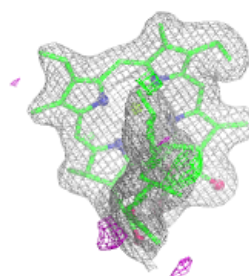
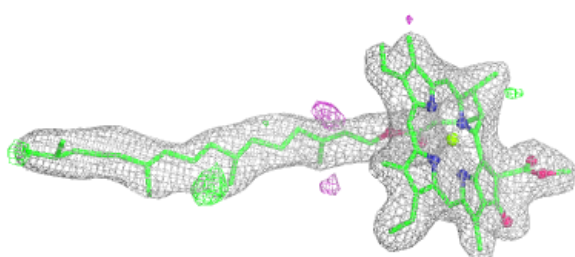
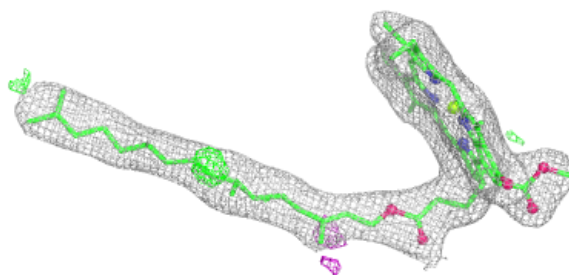
Electron density around CLA B 610:

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

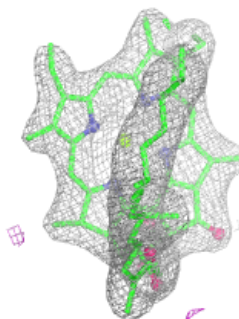
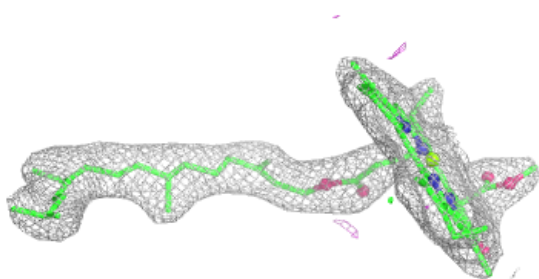
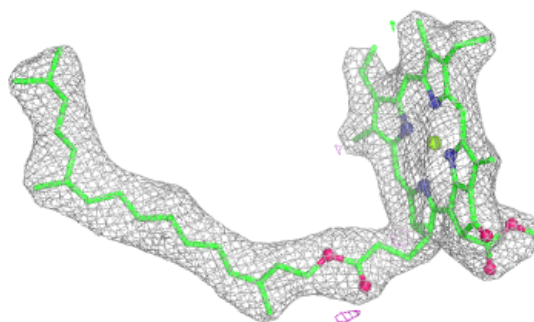


Electron density around CLA b 607:

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

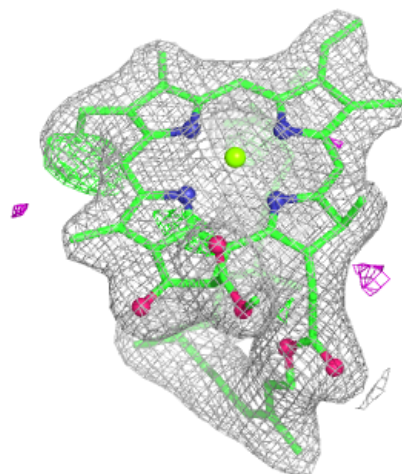
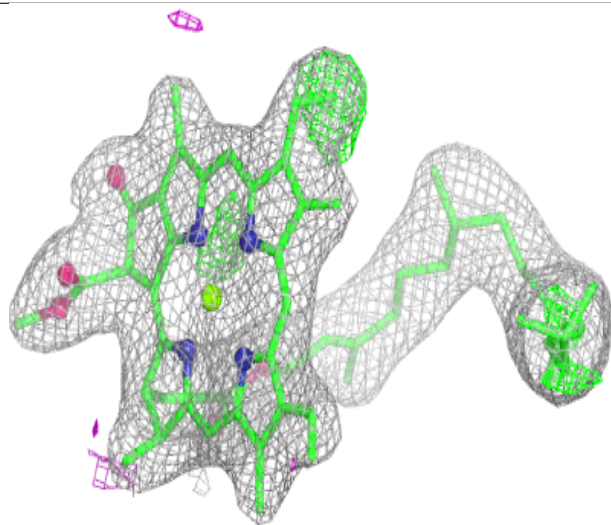
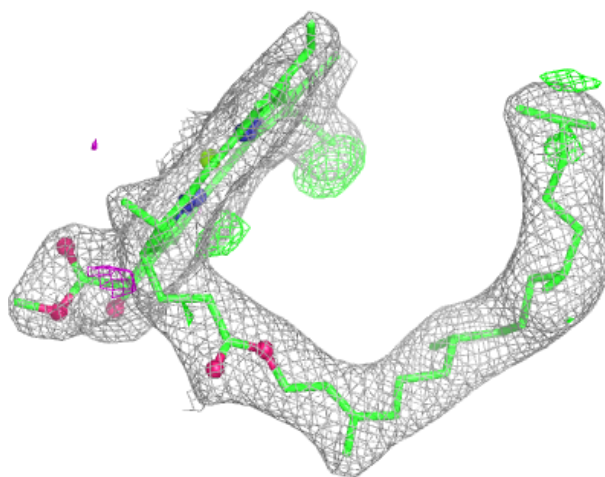
**Electron density around CLA b 609:**

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



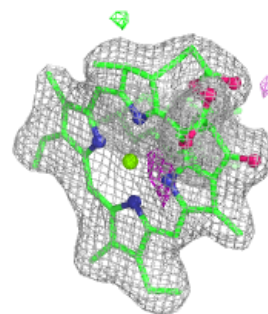
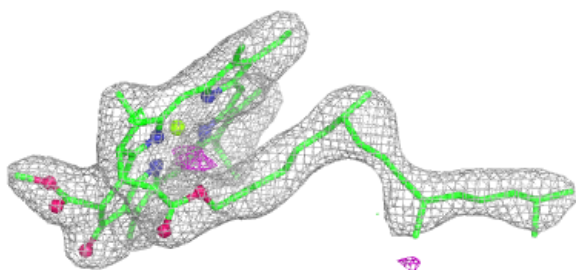
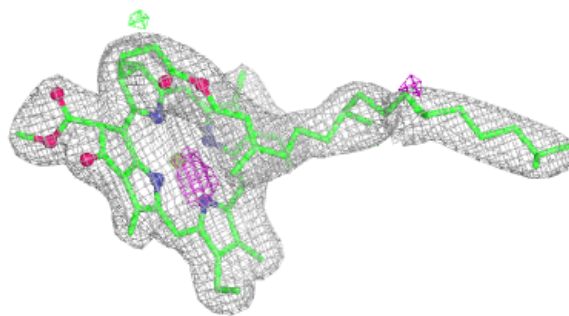
Electron density around CLA b 611:

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



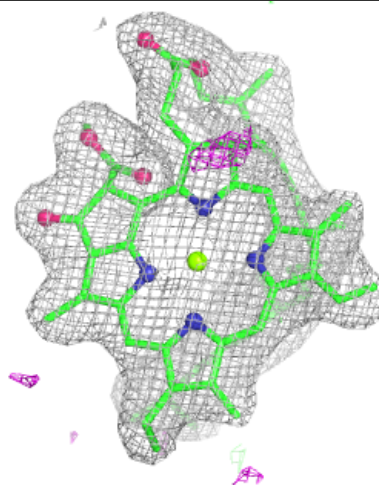
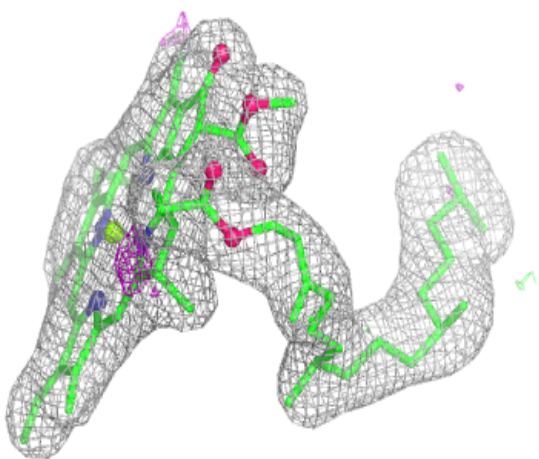
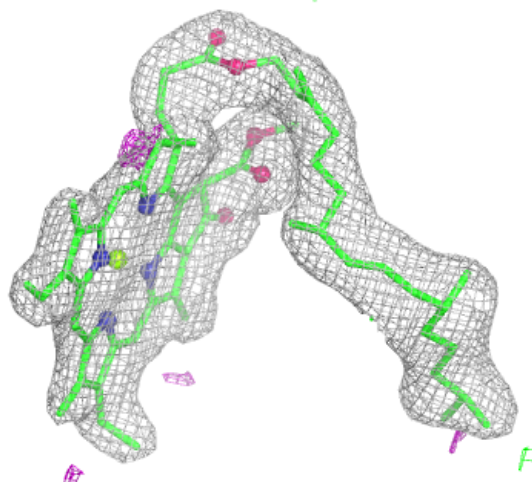
Electron density around CLA C 506:

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



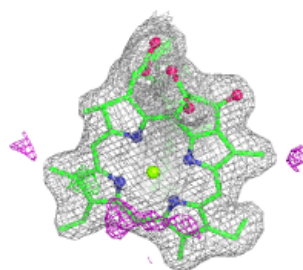
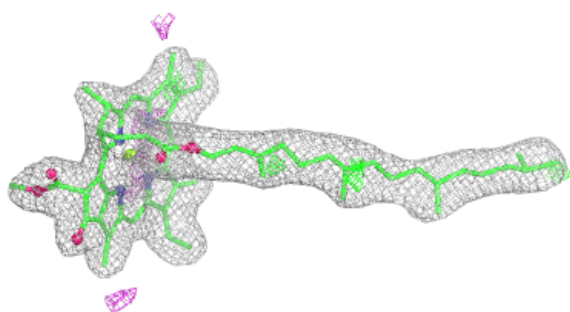
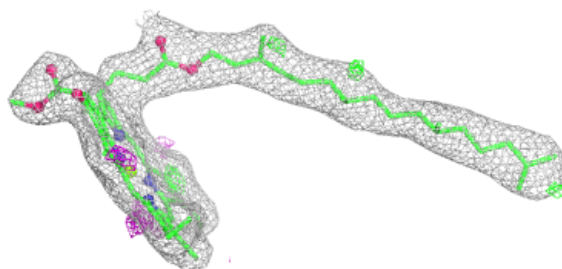
Electron density around CLA b 613:

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



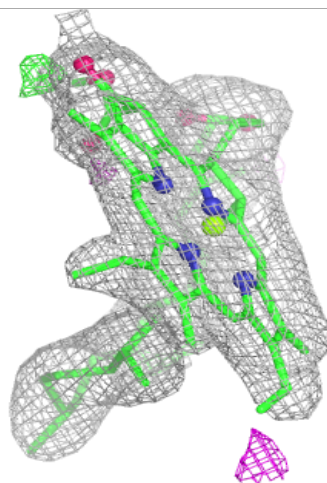
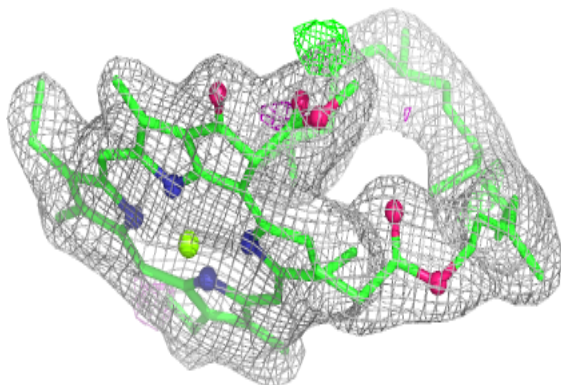
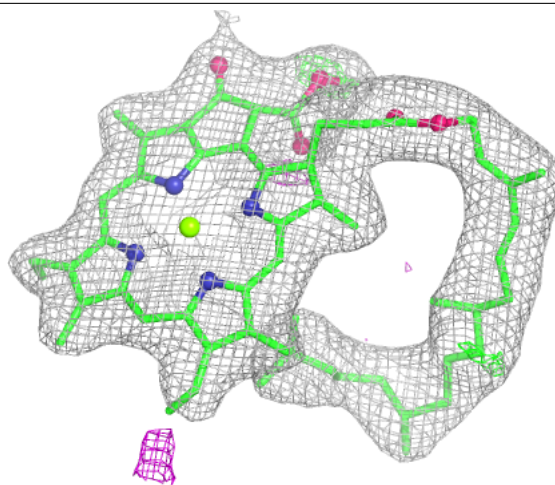
Electron density around CLA B 607:

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



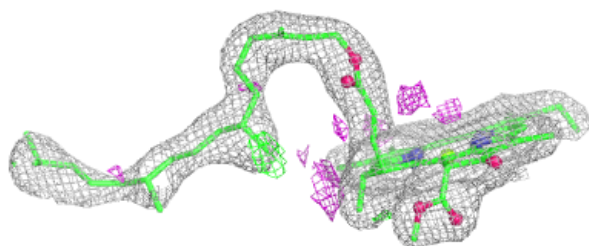
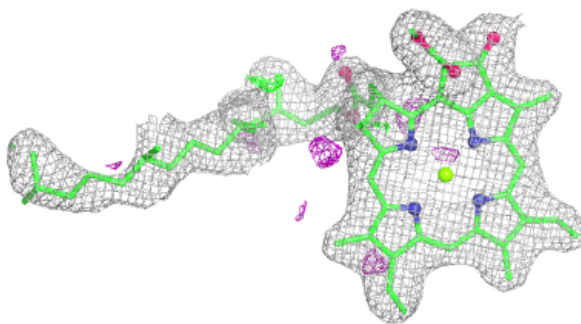
Electron density around CLA b 615:

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



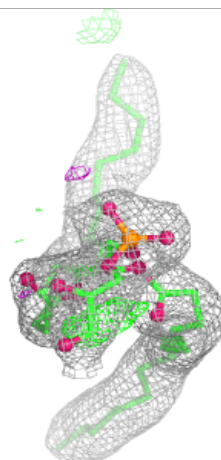
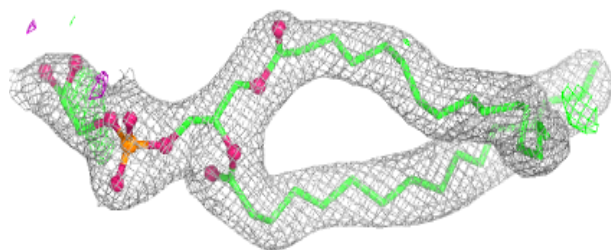
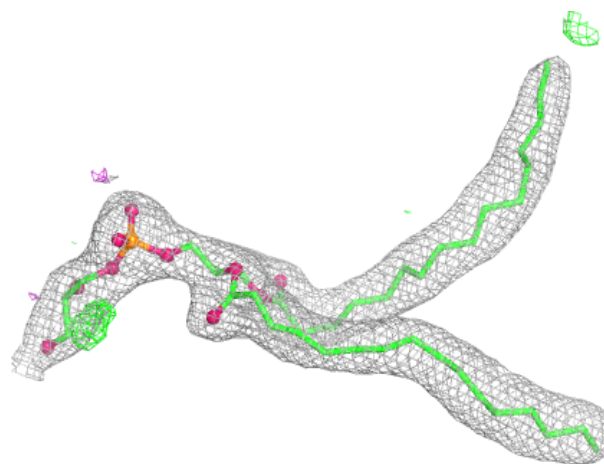
Electron density around CLA A 406 (A):

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



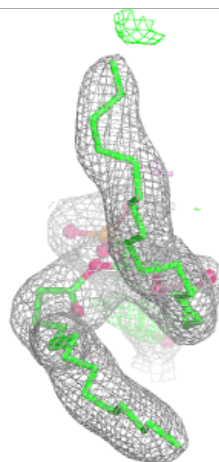
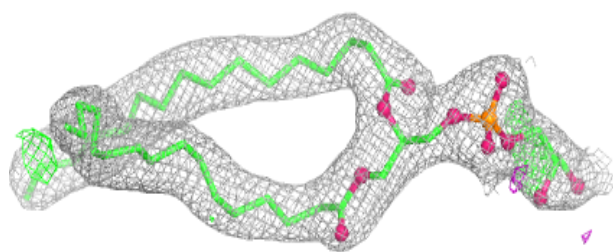
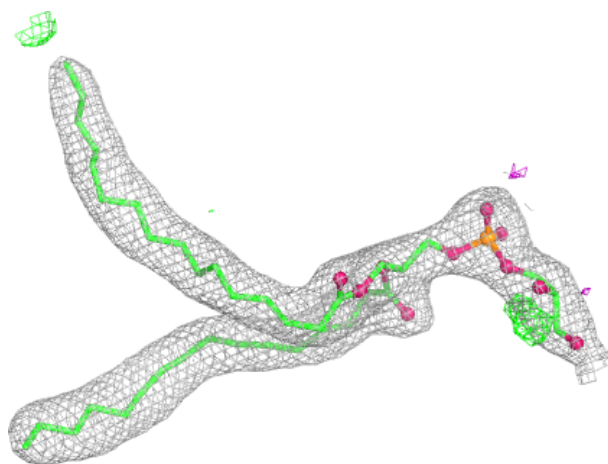
Electron density around LHG D 406 (A):

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



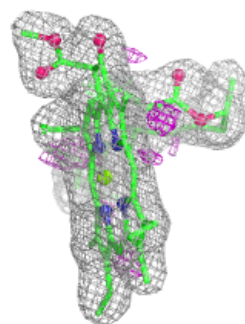
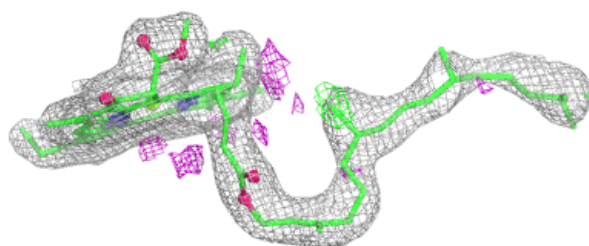
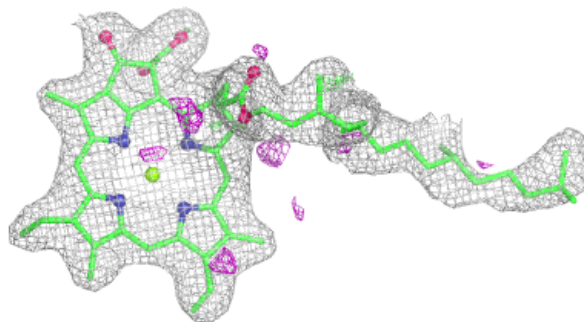
Electron density around LHG D 406 (B):

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



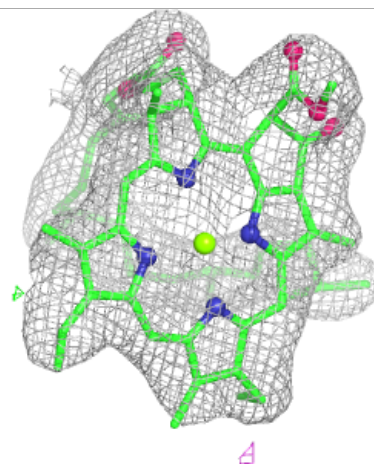
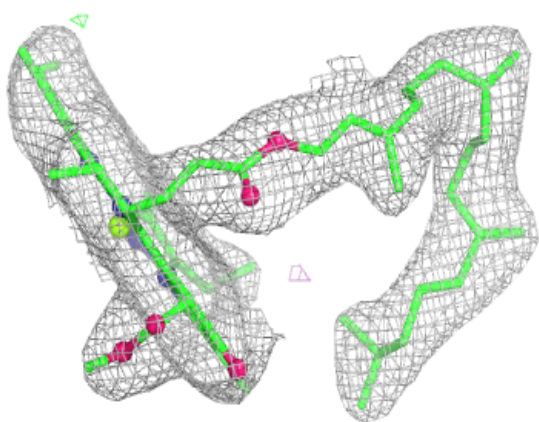
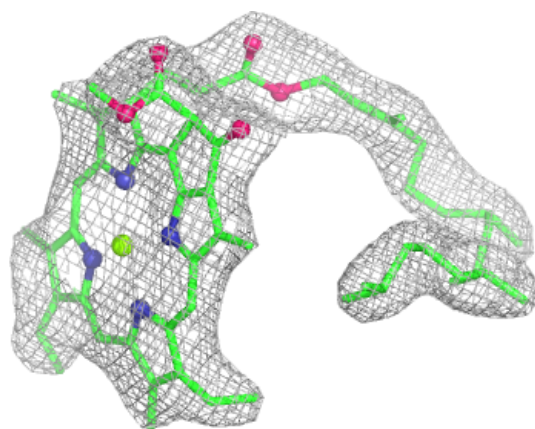
Electron density around CLA A 406 (B):

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



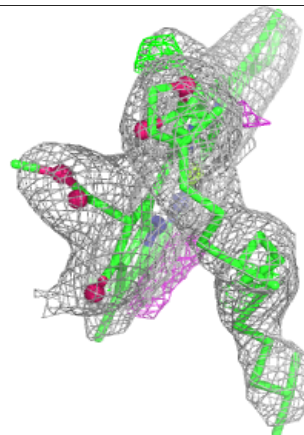
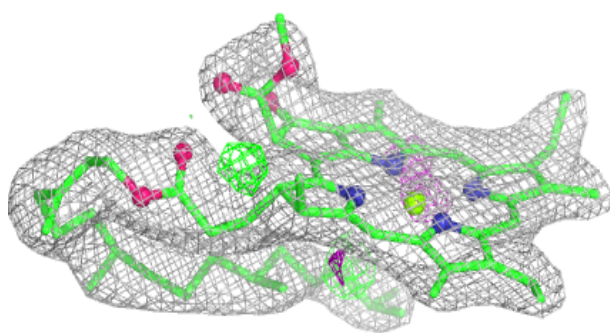
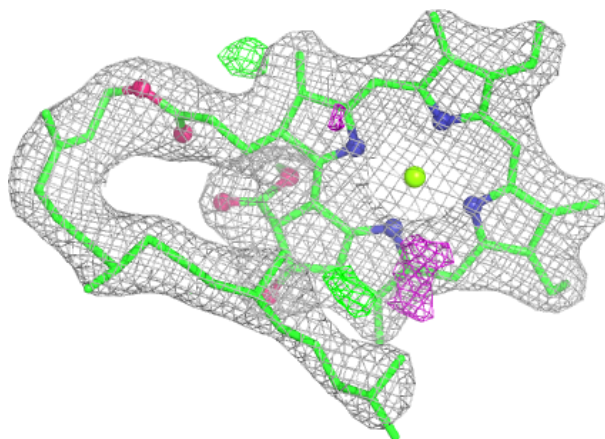
Electron density around CLA c 503:

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



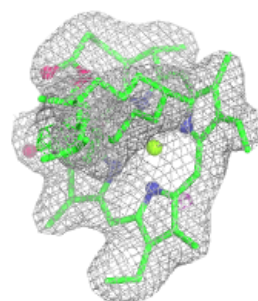
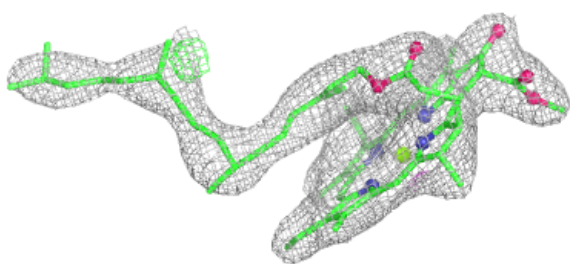
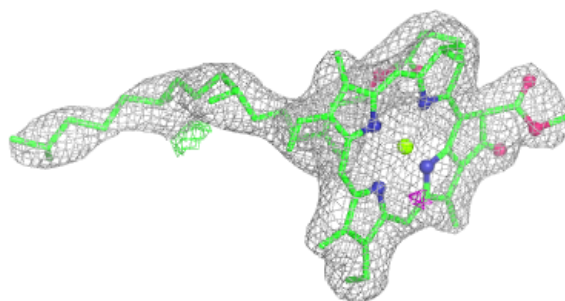
Electron density around CLA C 510:

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



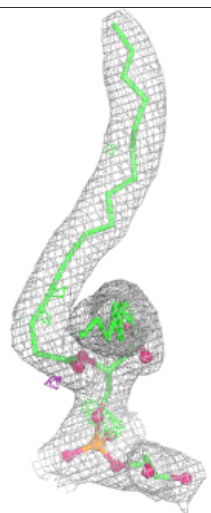
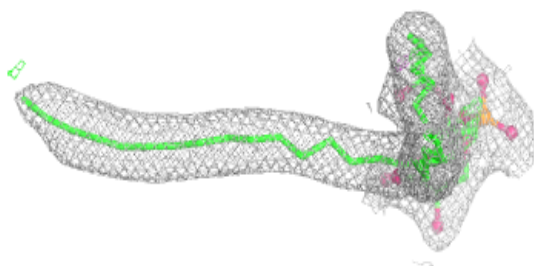
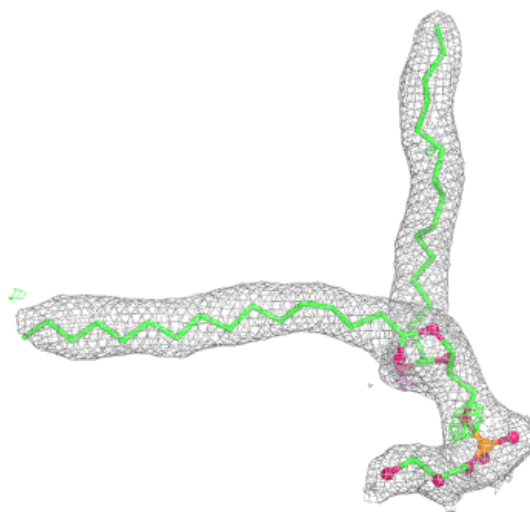
Electron density around CLA c 505:

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



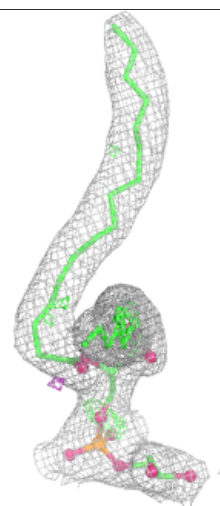
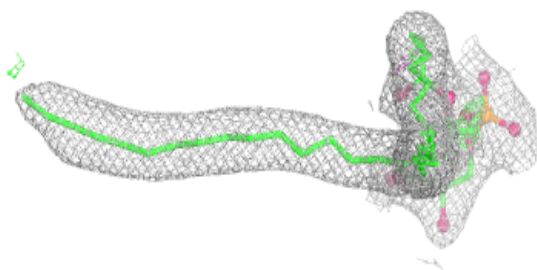
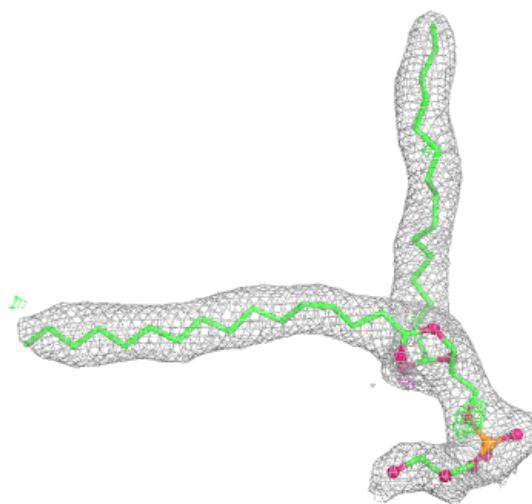
Electron density around LHG L 101 (A):

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



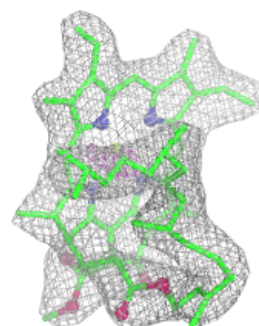
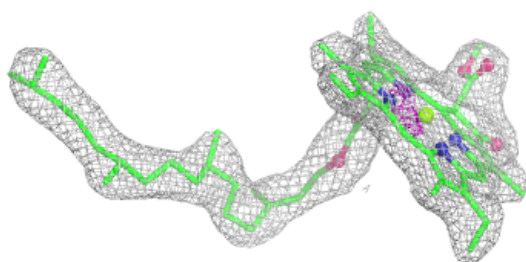
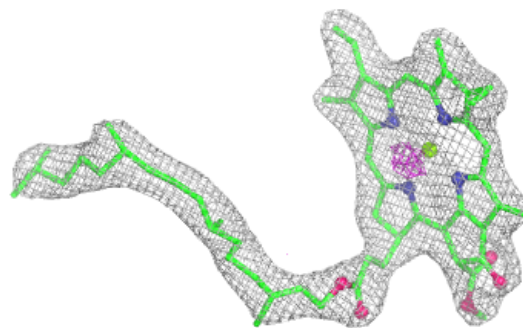
Electron density around LHG L 101 (B):

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



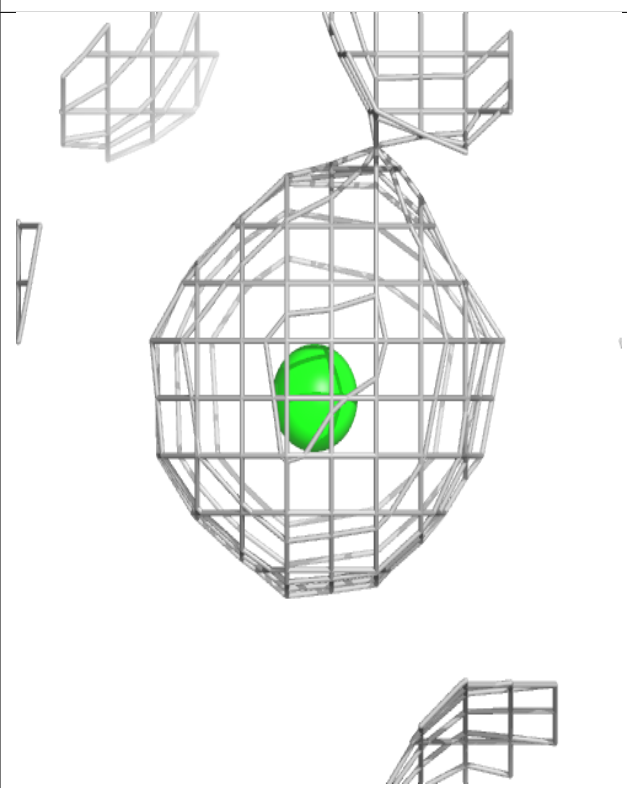
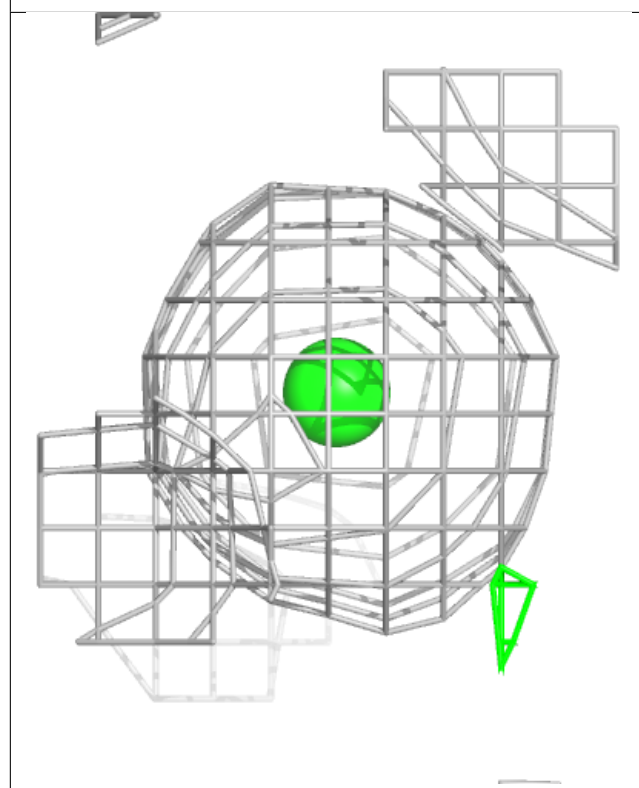
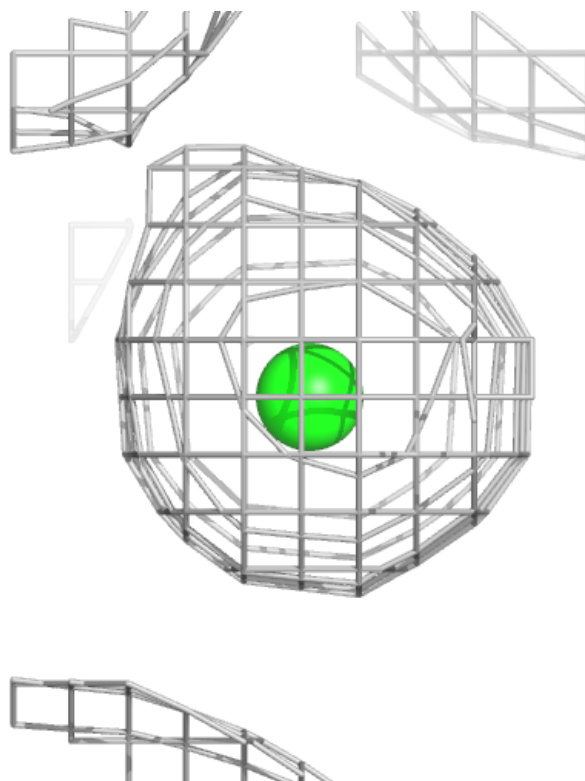
Electron density around CLA C 512:

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



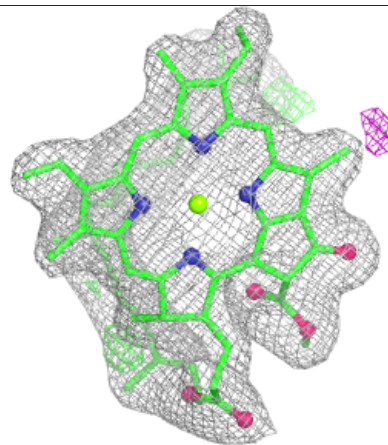
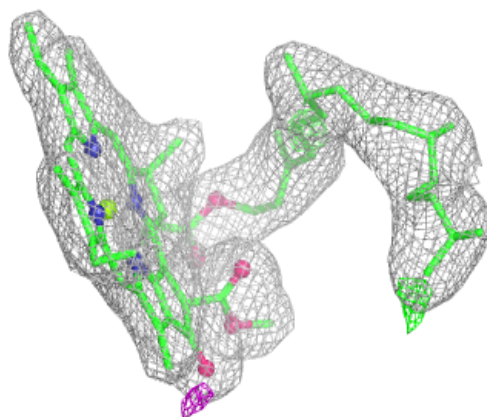
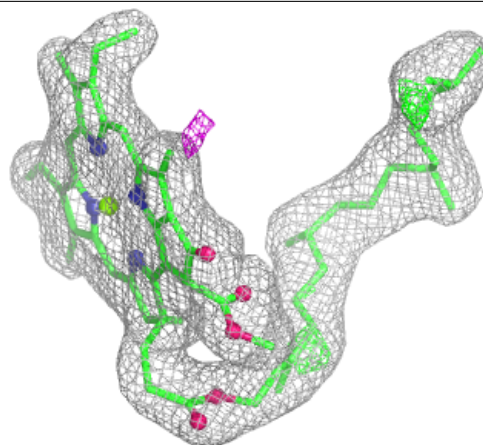
Electron density around CL a 402 (A):

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



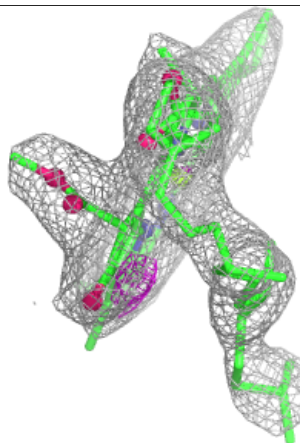
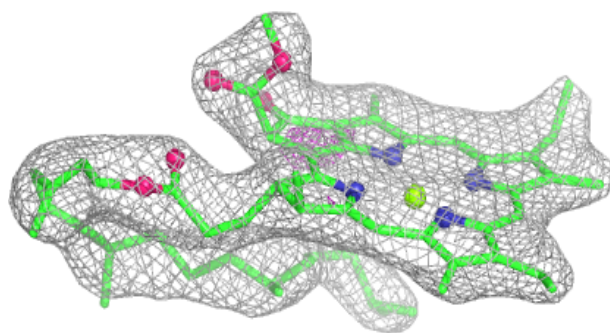
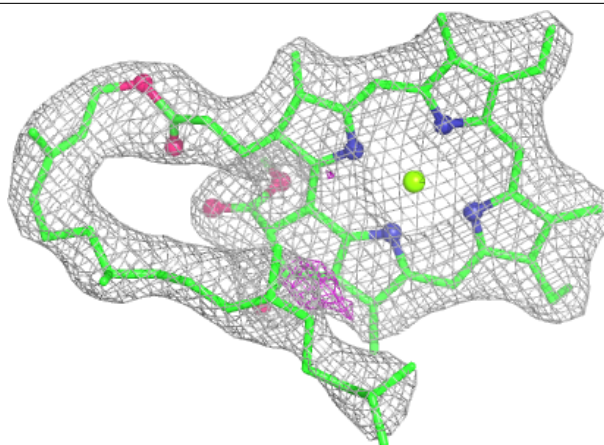
Electron density around CLA B 613:

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



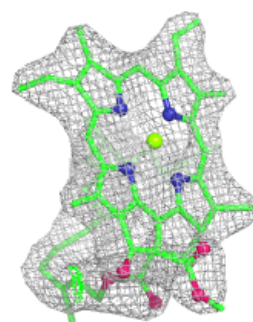
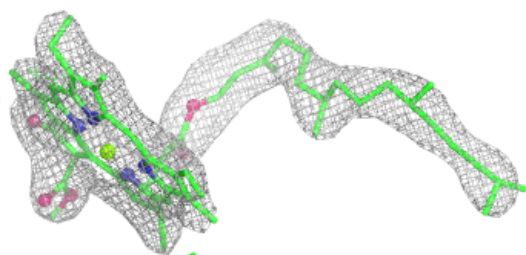
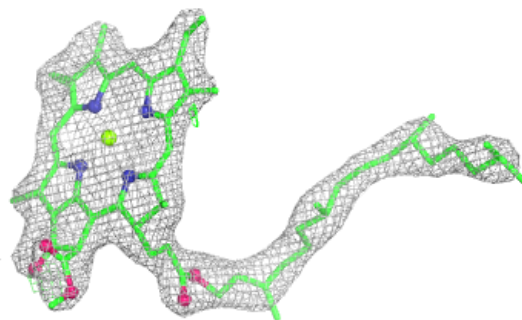
Electron density around CLA c 509:

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



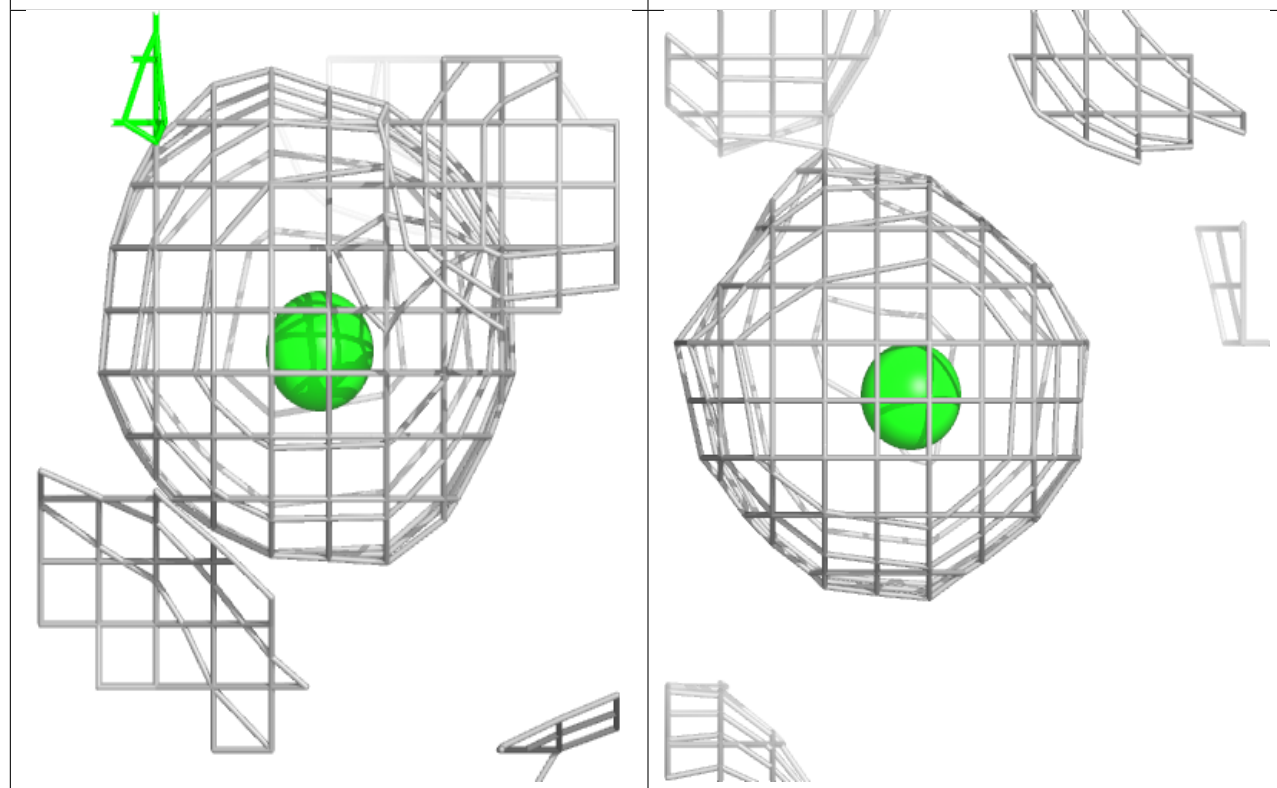
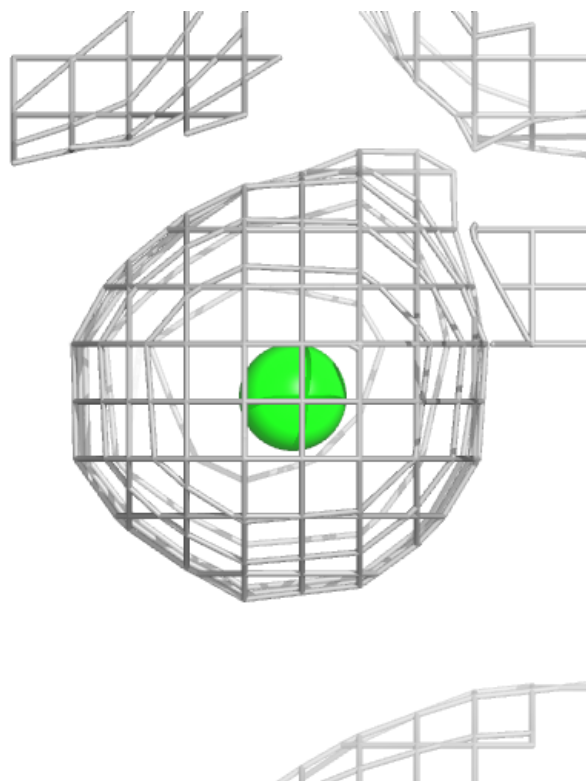
Electron density around CLA c 511:

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



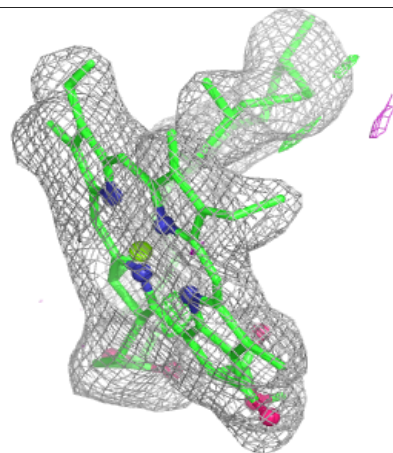
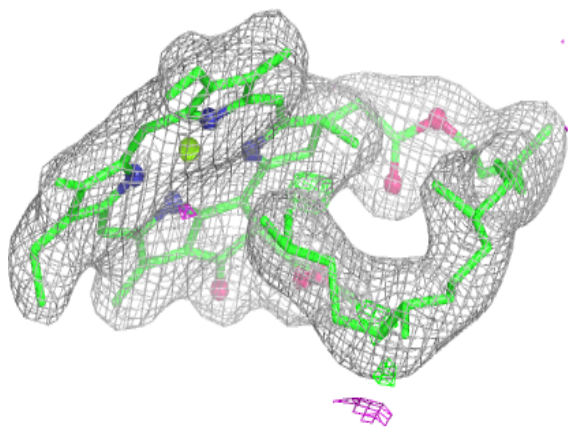
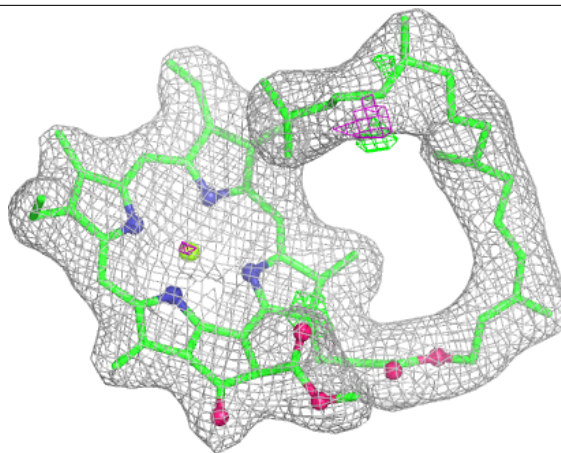
Electron density around CL a 402 (B):

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

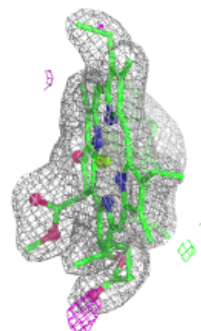
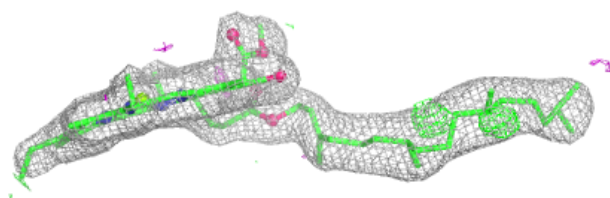
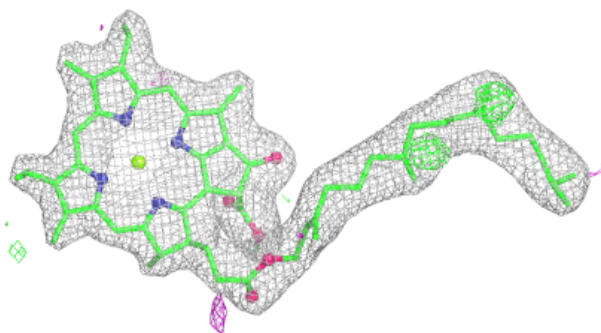


Electron density around CLA B 615:

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

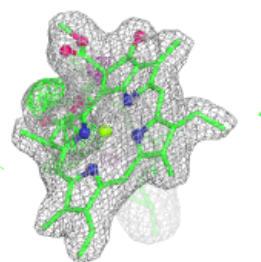
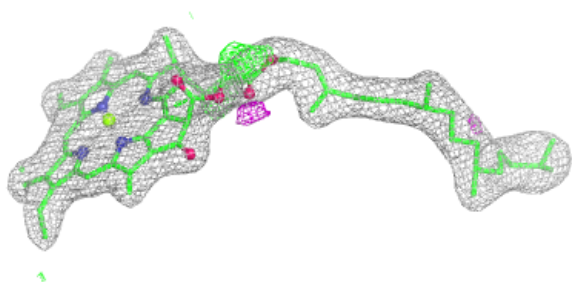
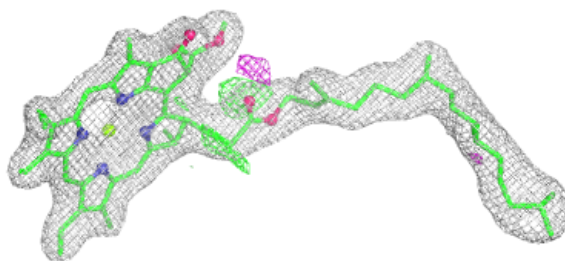
**Electron density around CLA B 602:**

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



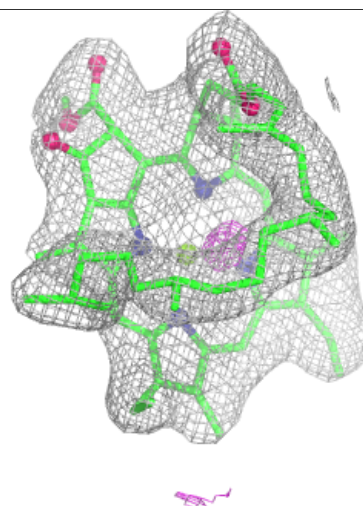
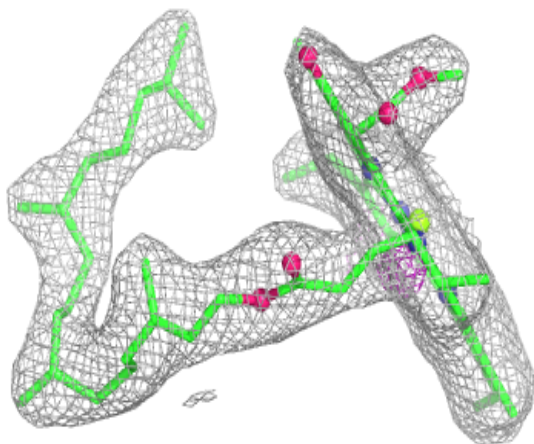
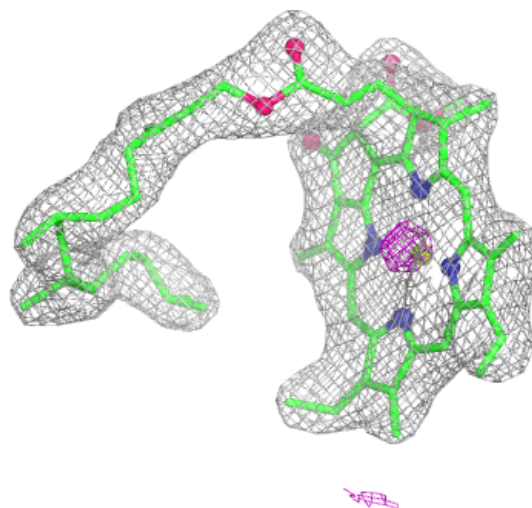
Electron density around CLA A 404 (A):

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



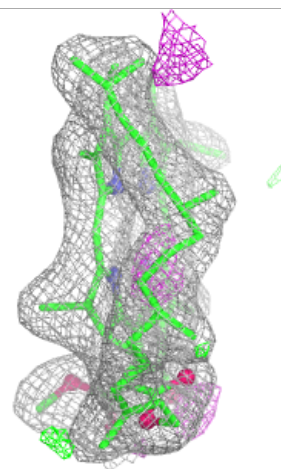
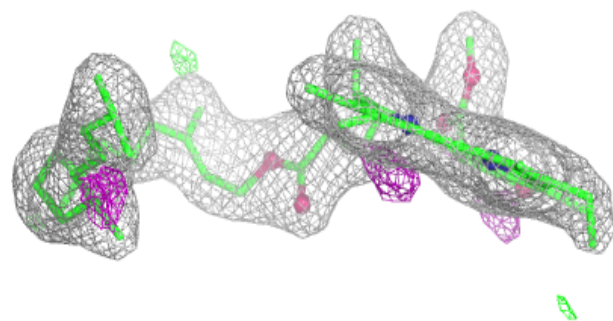
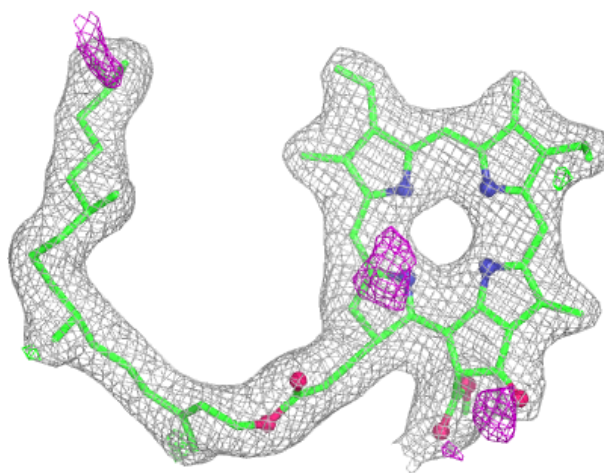
Electron density around CLA C 504:

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



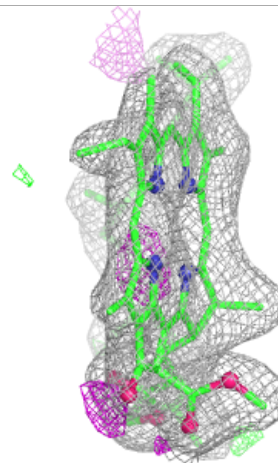
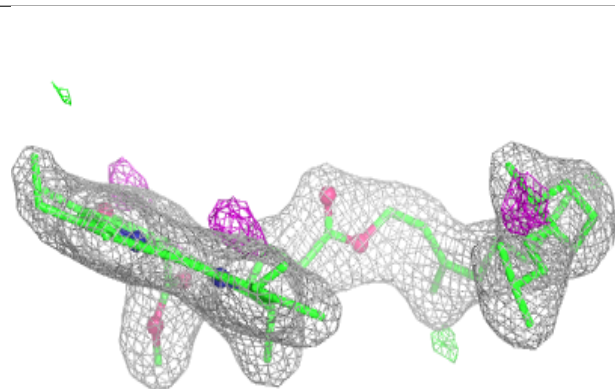
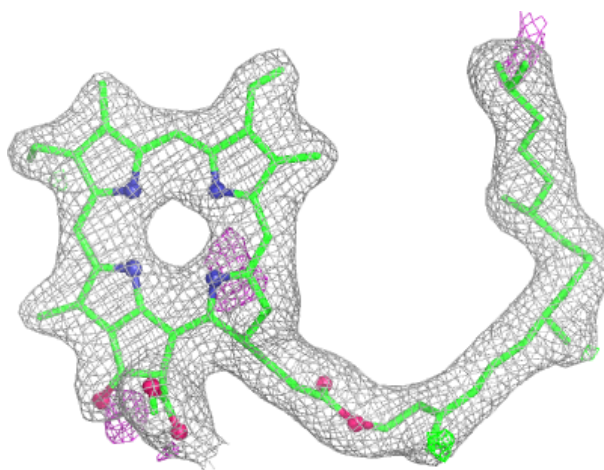
Electron density around PHO a 406 (A):

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



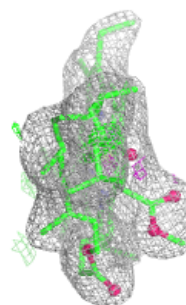
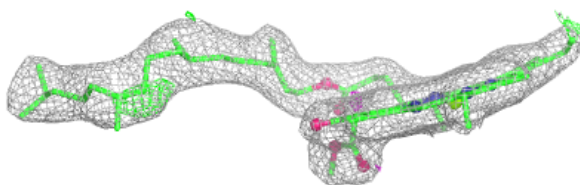
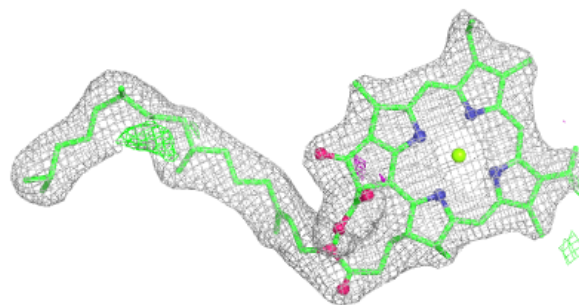
Electron density around PHO a 406 (B):

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

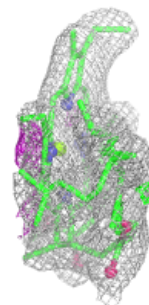
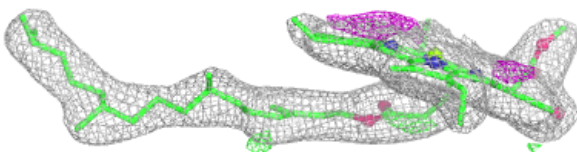
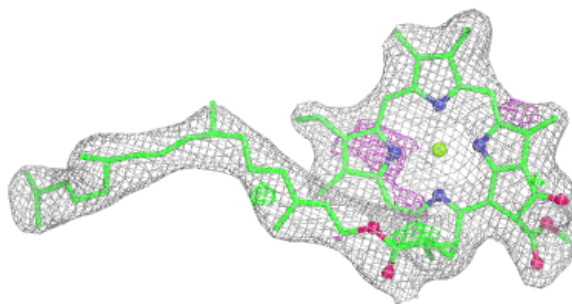


Electron density around CLA b 602:

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

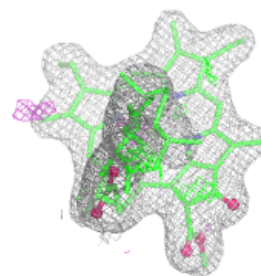
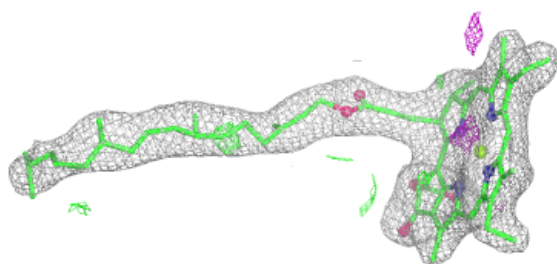
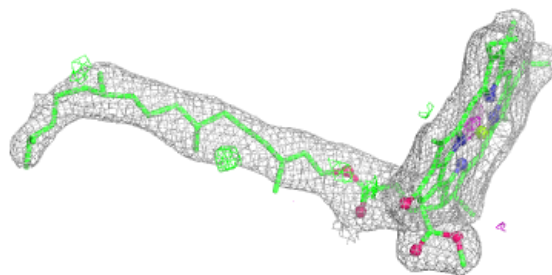
**Electron density around CLA b 603:**

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

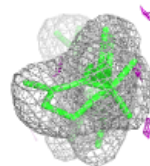
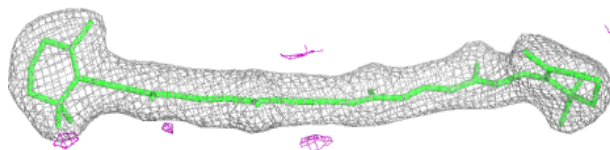
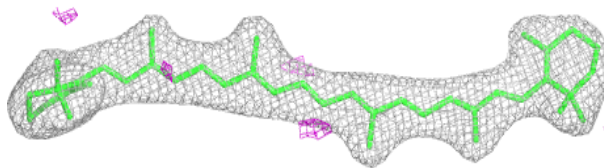


Electron density around CLA b 604:

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

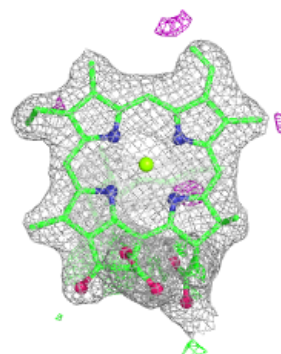
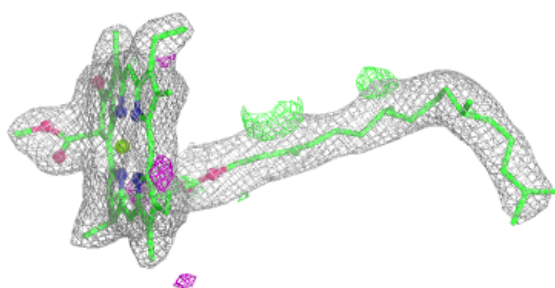
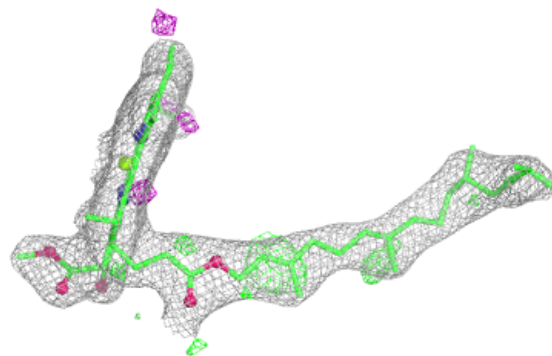
**Electron density around BCR B 617:**

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

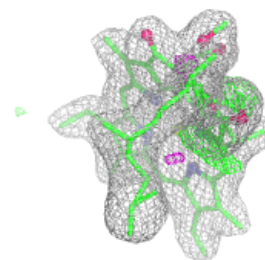
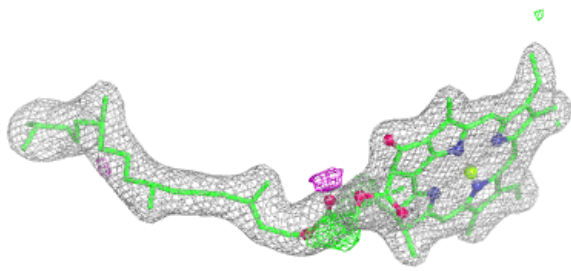
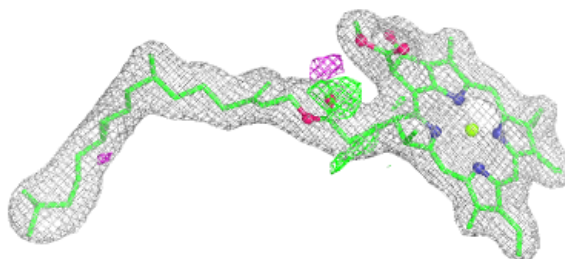


Electron density around CLA b 605:

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

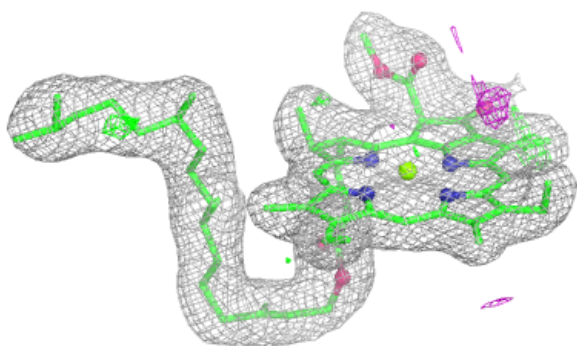
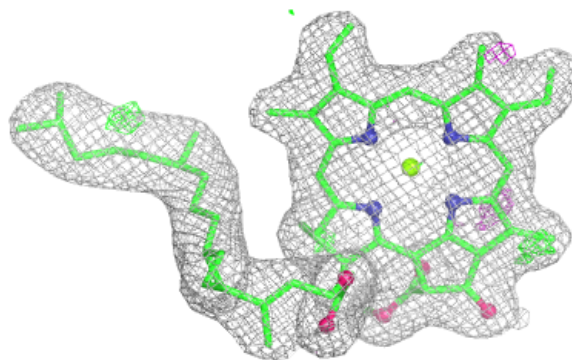
**Electron density around CLA A 404 (B):**

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

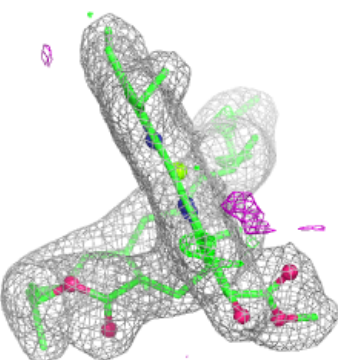
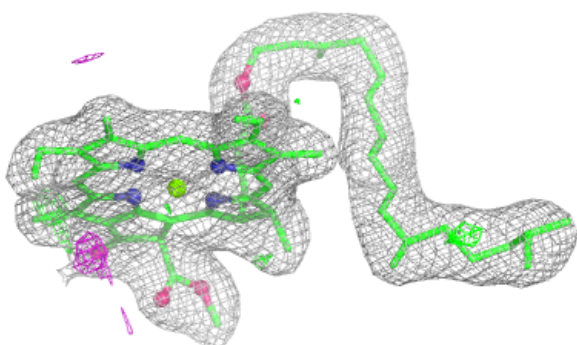
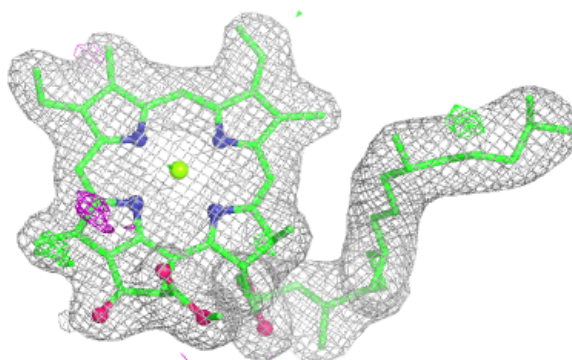


Electron density around CLA A 405 (A):

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

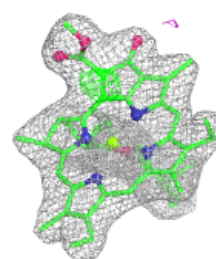
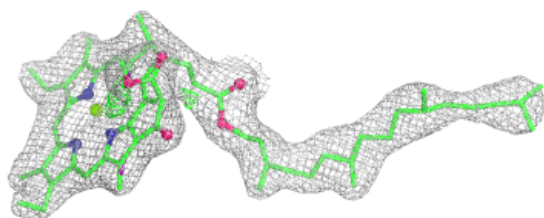
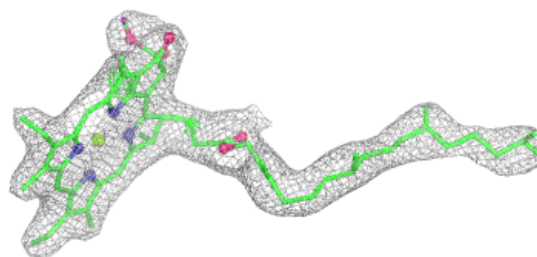
**Electron density around CLA A 405 (B):**

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

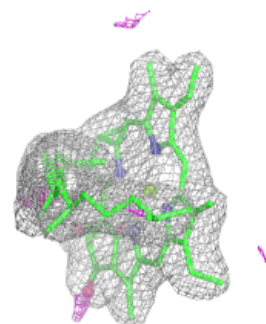
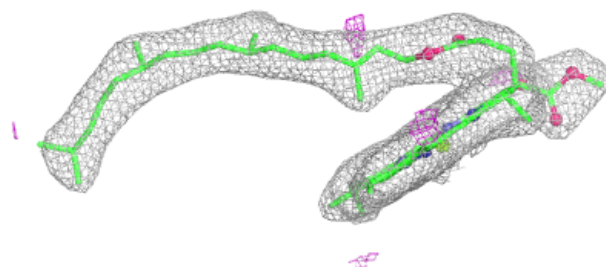
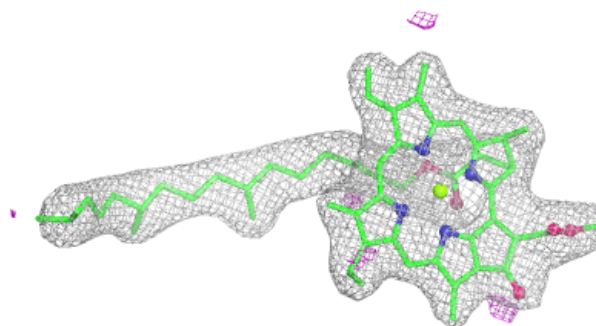


Electron density around CLA c 502:

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

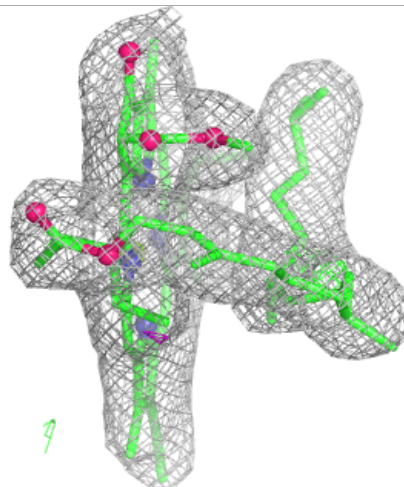
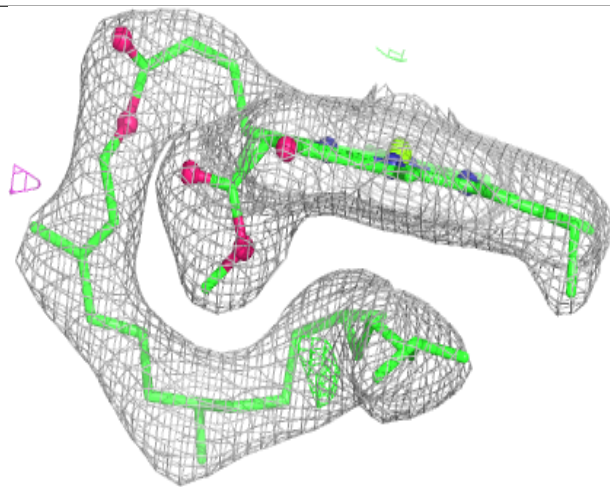
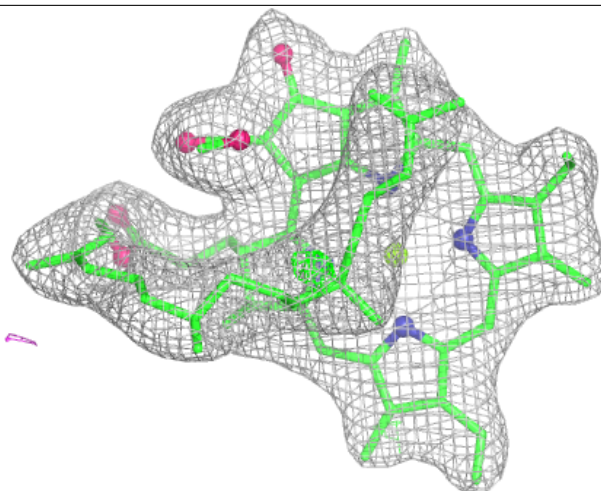
**Electron density around CLA B 608:**

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



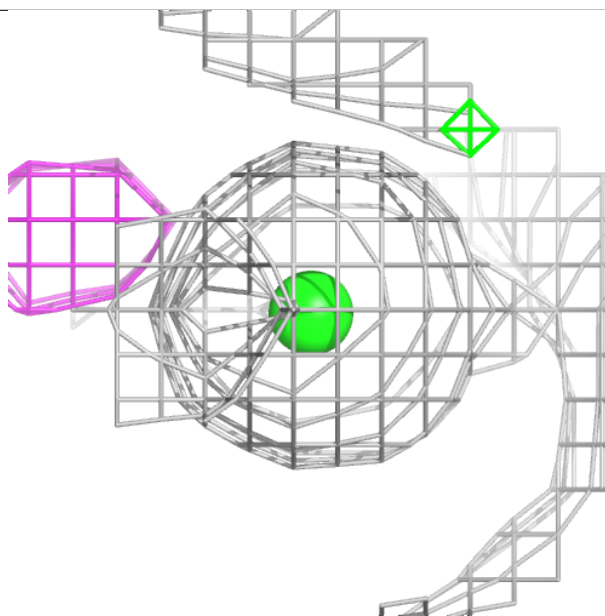
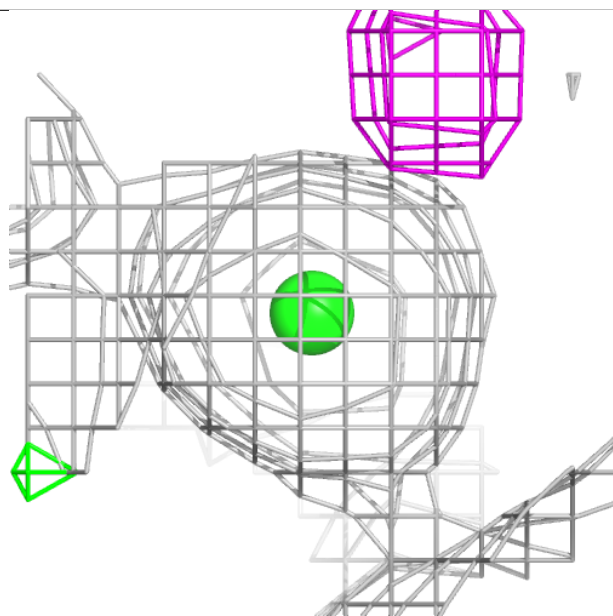
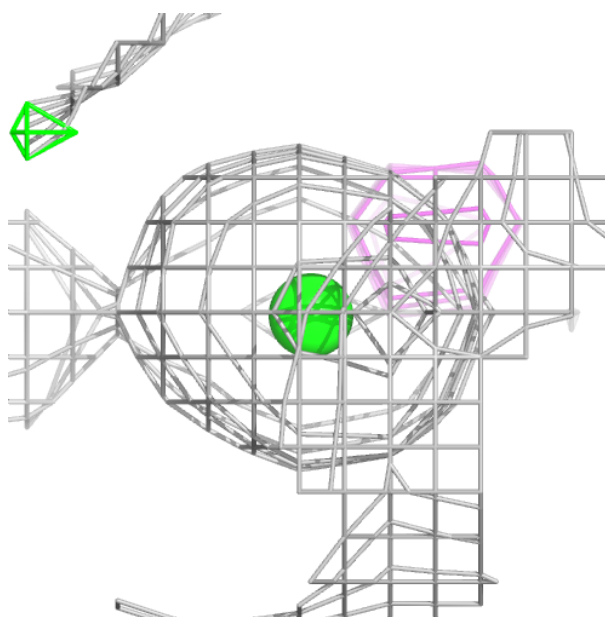
Electron density around CLA C 511:

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



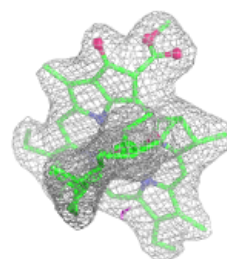
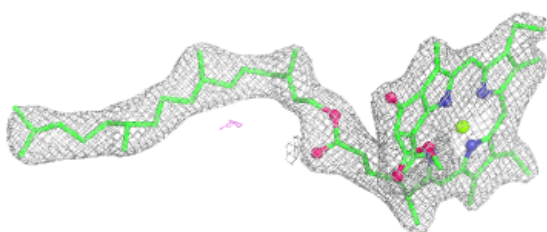
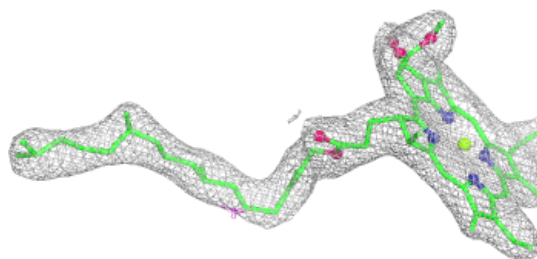
Electron density around CL a 403 (A):

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



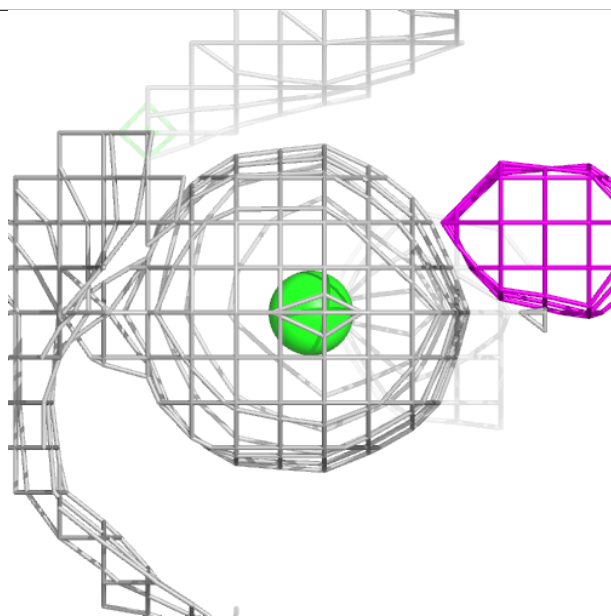
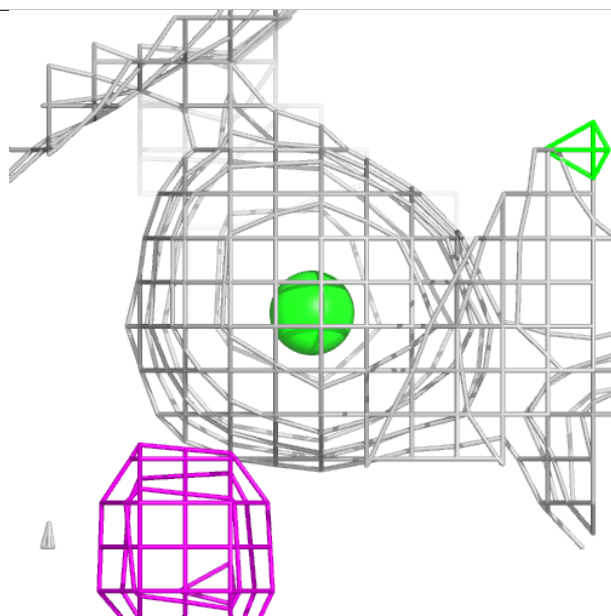
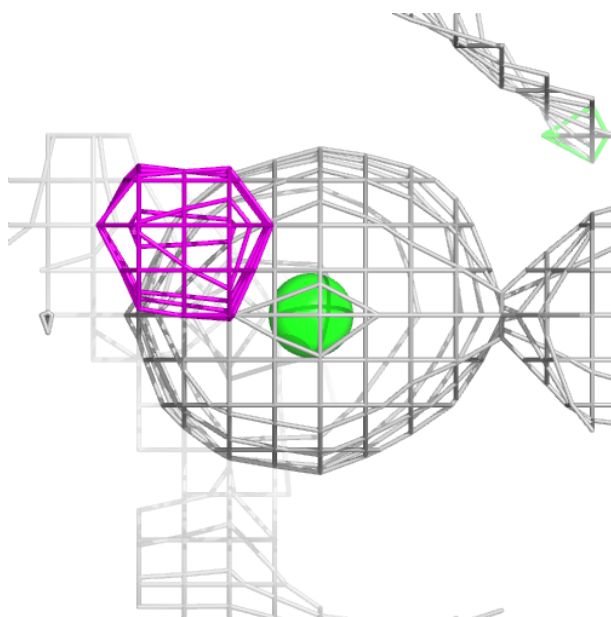
Electron density around CLA C 503:

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



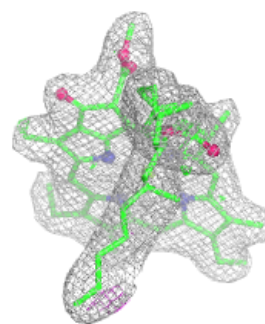
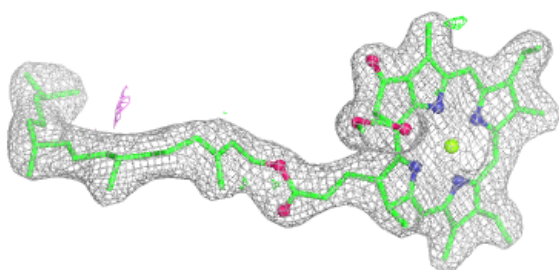
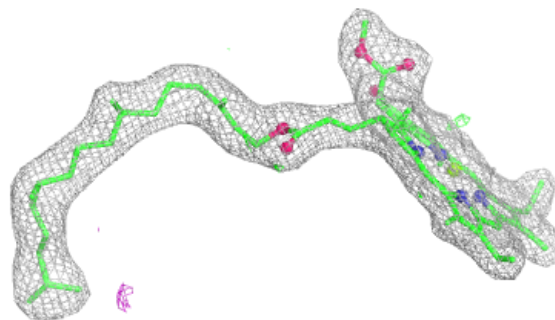
Electron density around CL a 403 (B):

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

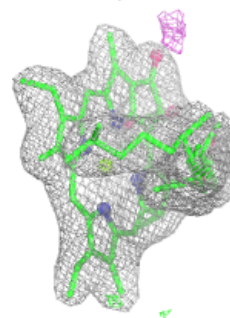
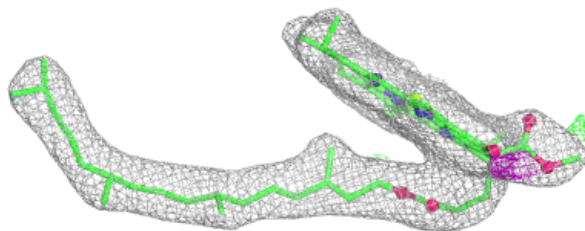
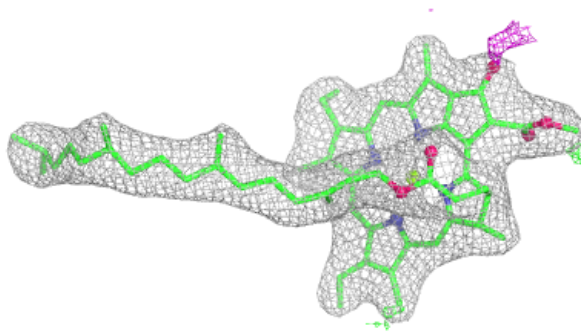


Electron density around CLA D 402 (A):

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

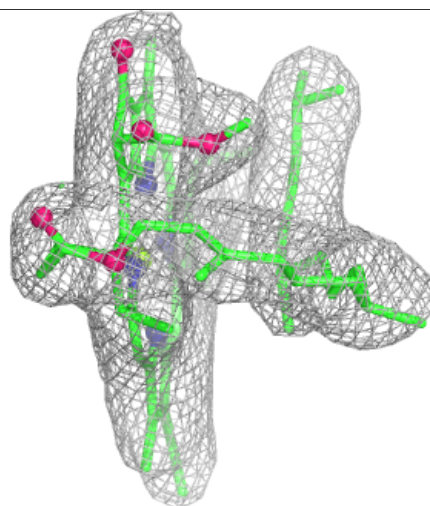
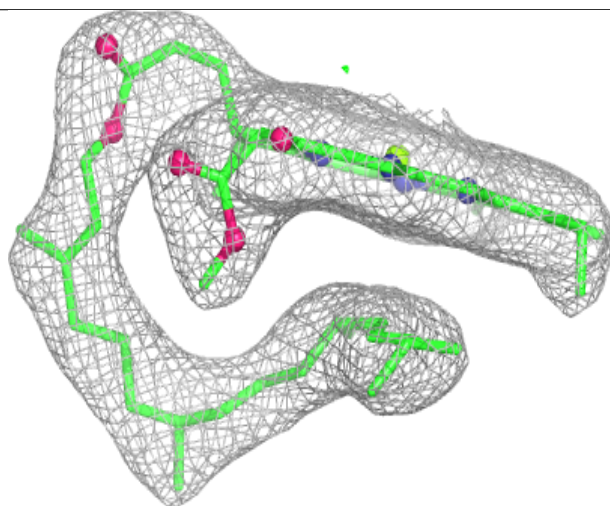
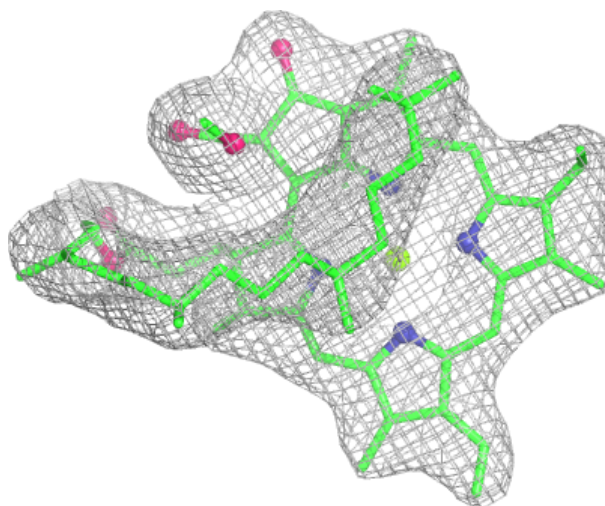
**Electron density around CLA b 608:**

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



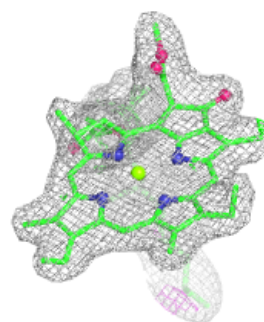
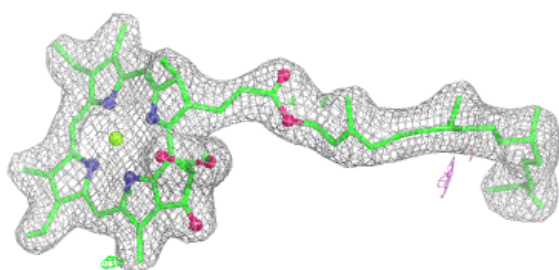
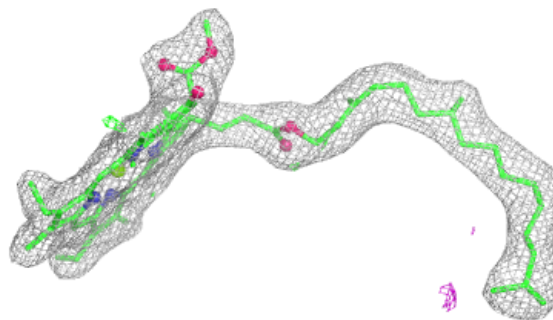
Electron density around CLA c 510:

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

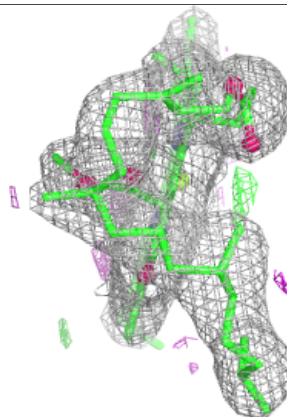
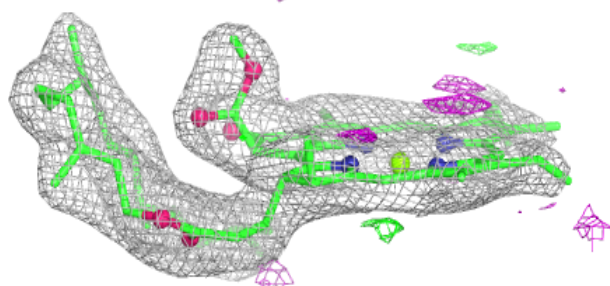
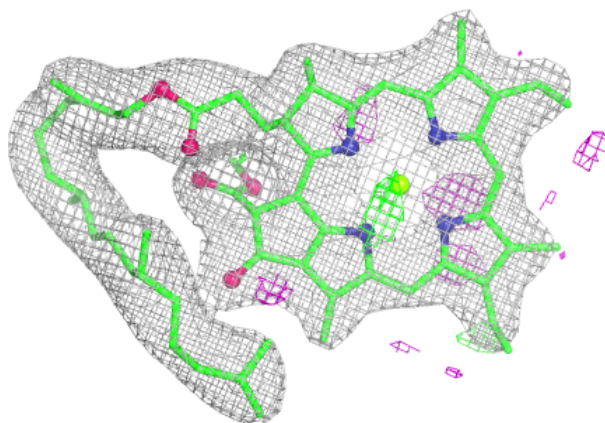


Electron density around CLA D 402 (B):

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

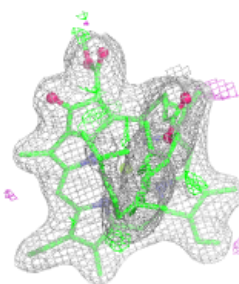
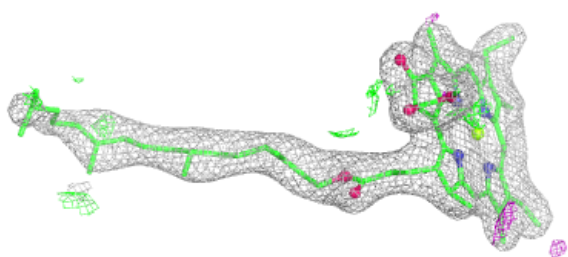
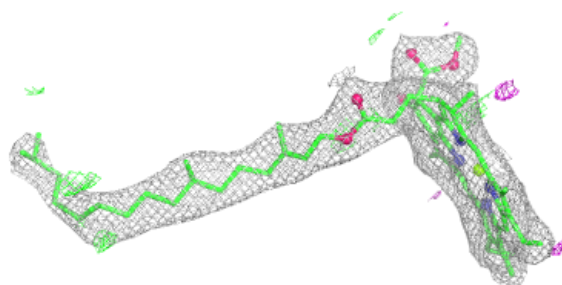
**Electron density around CLA b 610:**

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

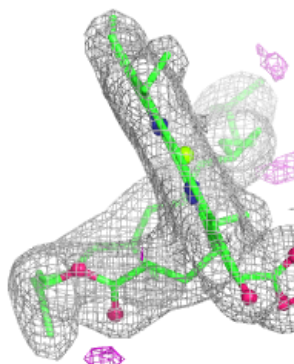
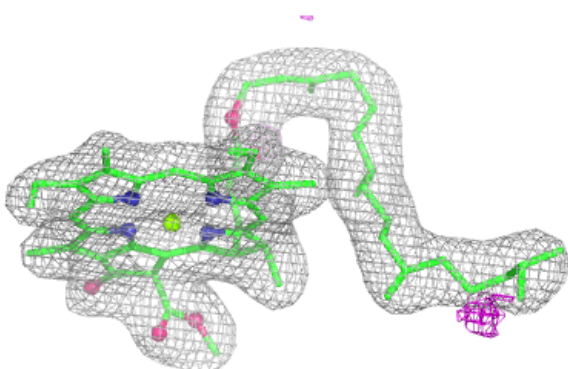
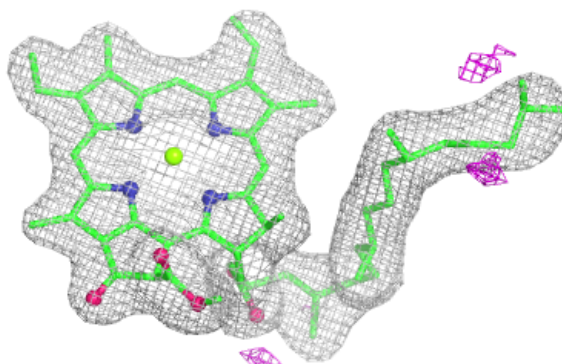


Electron density around CLA B 604:

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

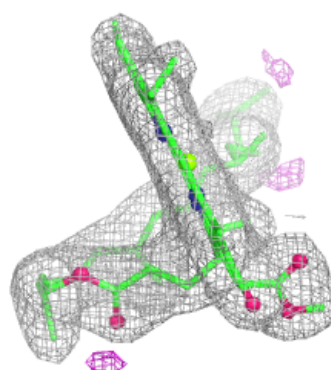
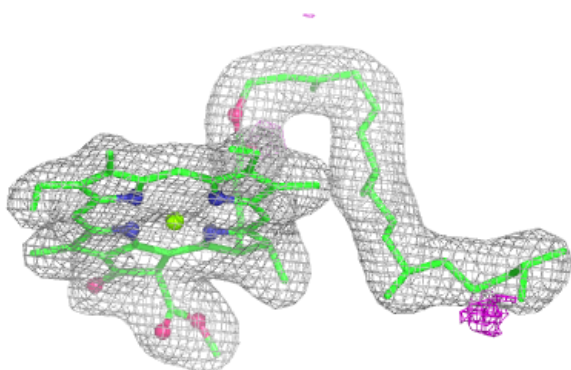
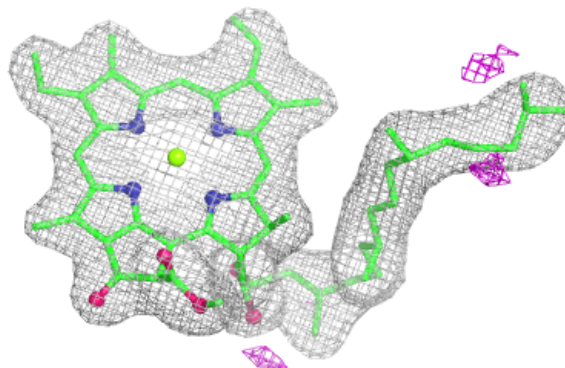
**Electron density around CLA d 402 (A):**

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

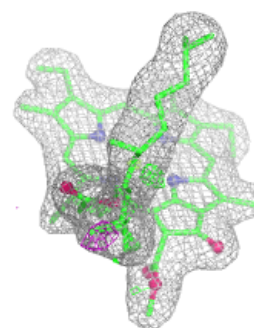
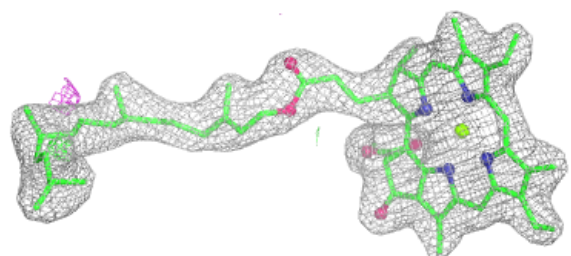
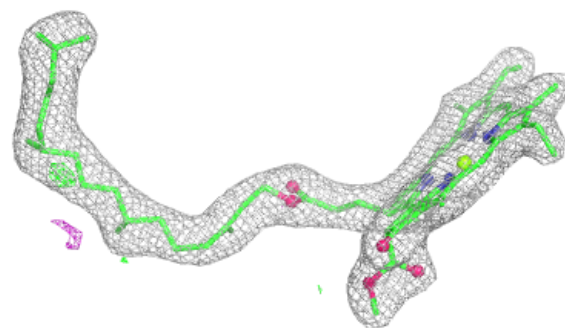


Electron density around CLA d 402 (B):

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

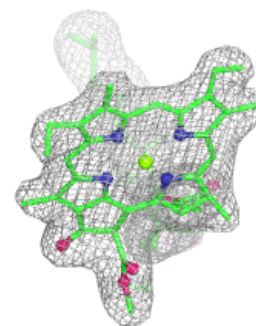
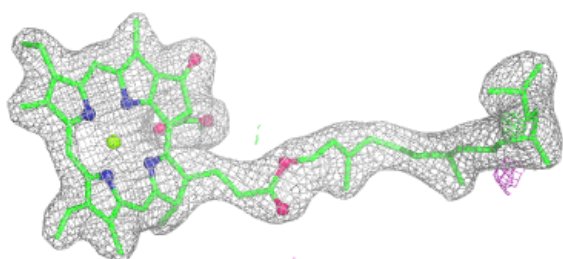
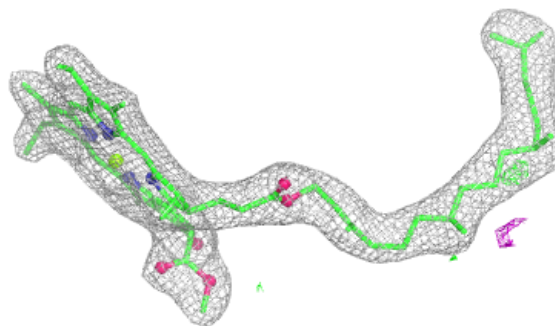
**Electron density around CLA d 403 (A):**

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

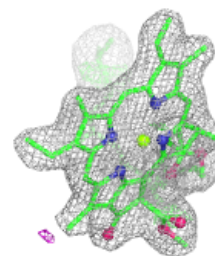
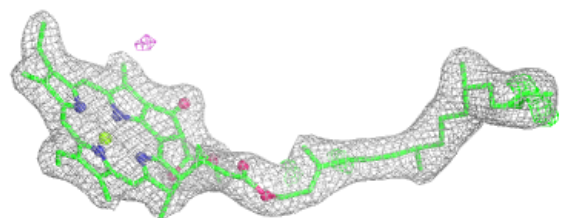
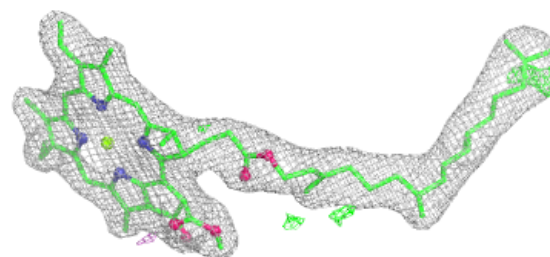


Electron density around CLA d 403 (B):

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

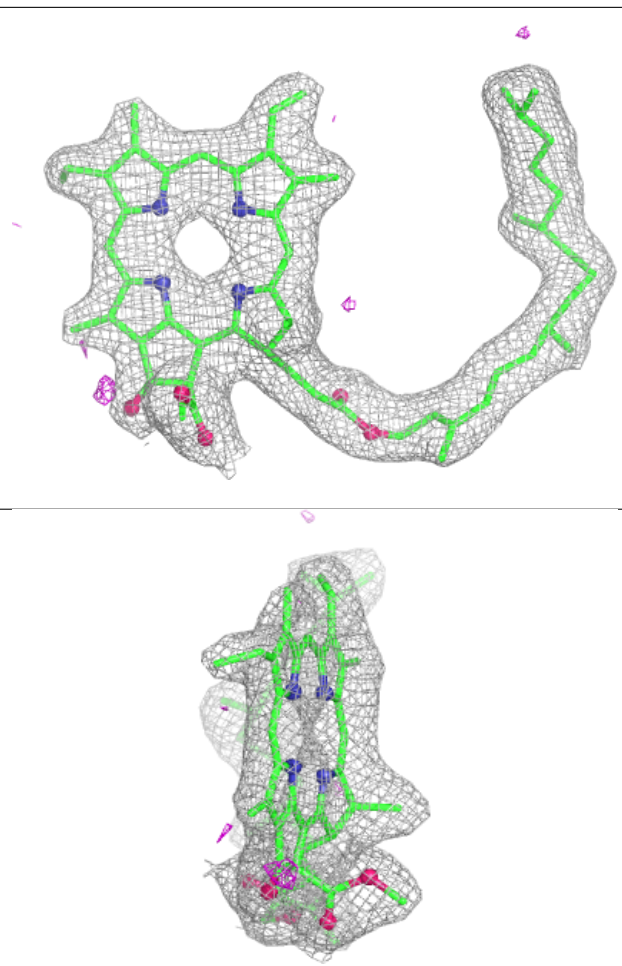
**Electron density around CLA a 404 (A):**

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



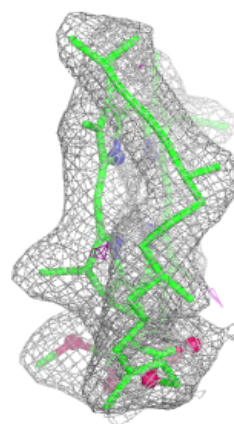
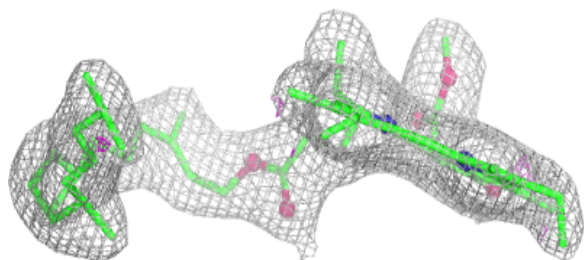
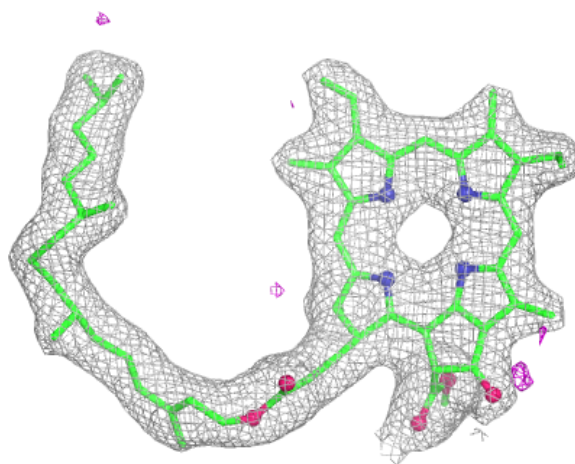
Electron density around PHO A 407 (A):

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



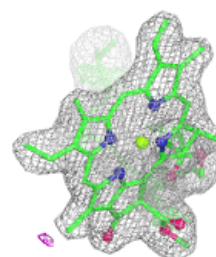
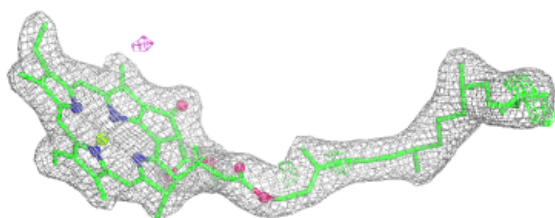
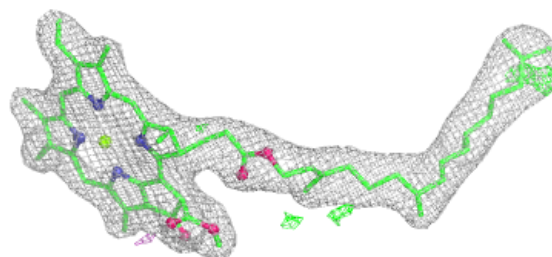
Electron density around PHO A 407 (B):

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

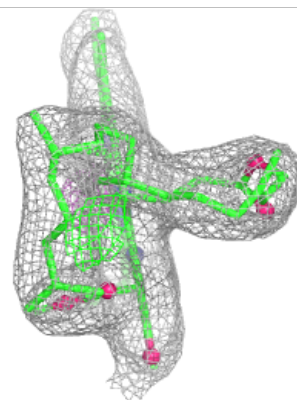
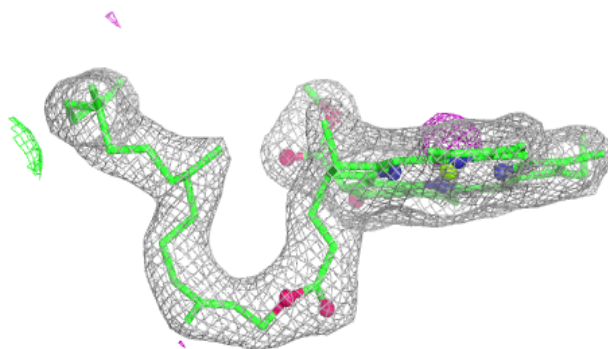
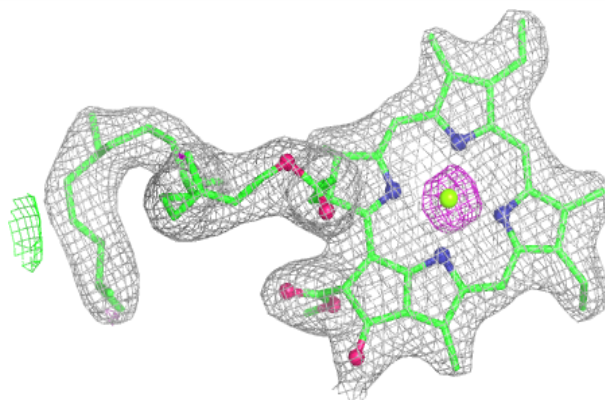


Electron density around CLA a 404 (B):

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

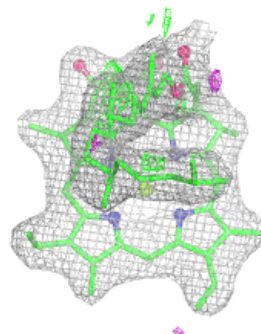
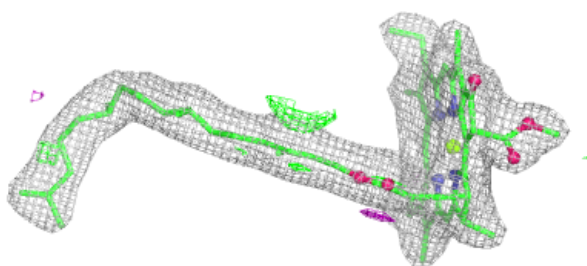
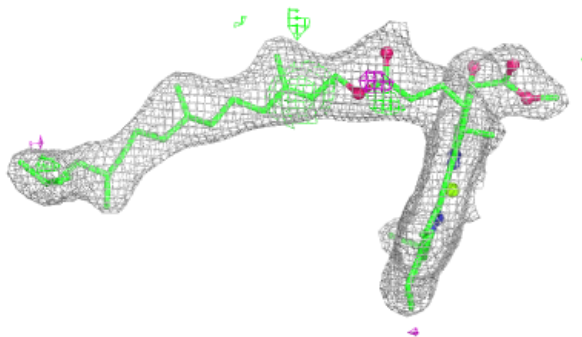
**Electron density around CLA B 612:**

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



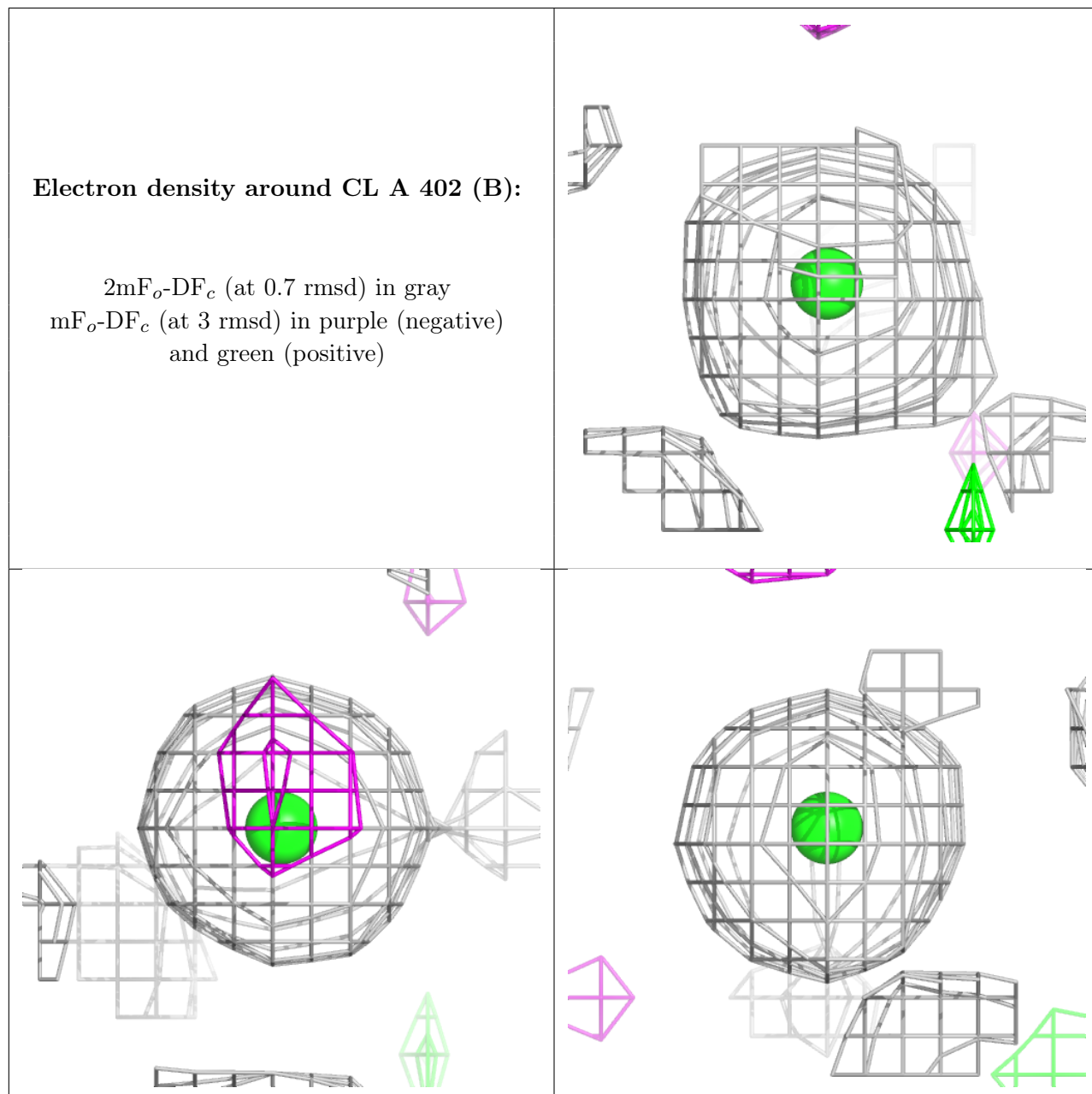
Electron density around CLA B 605:

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



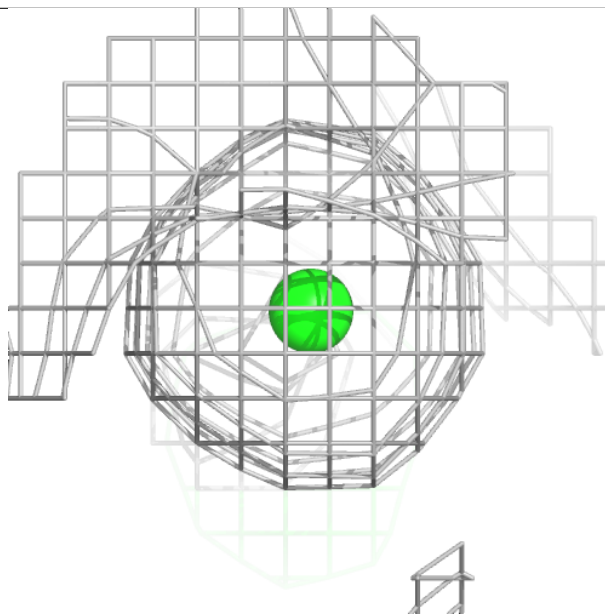
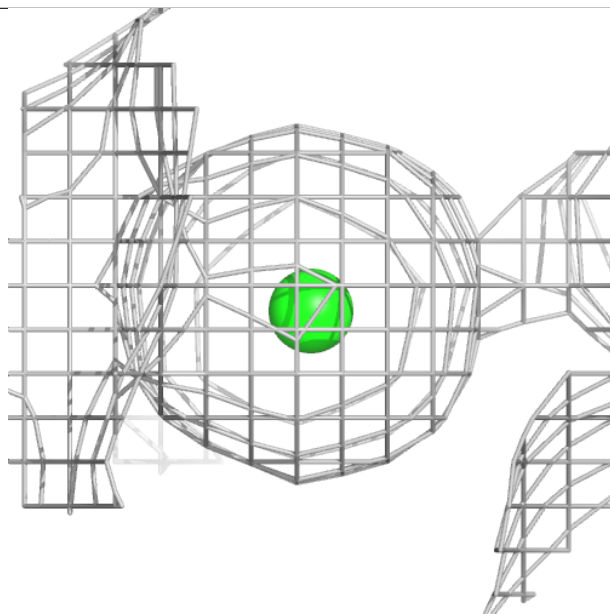
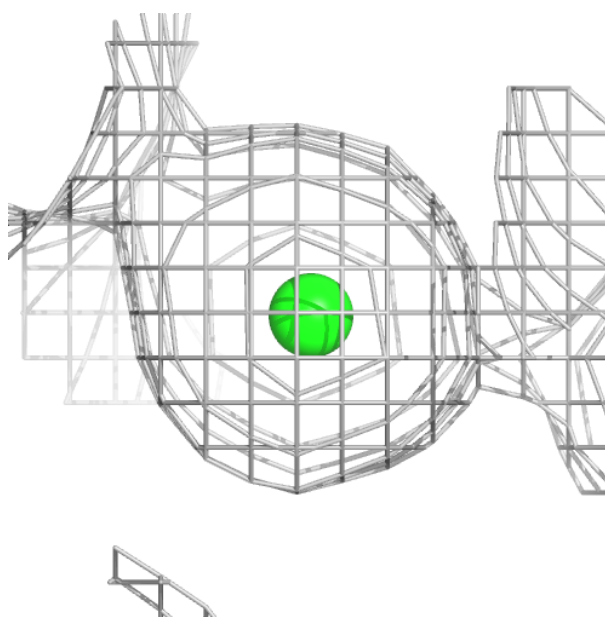
Electron density around CL A 402 (B):

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



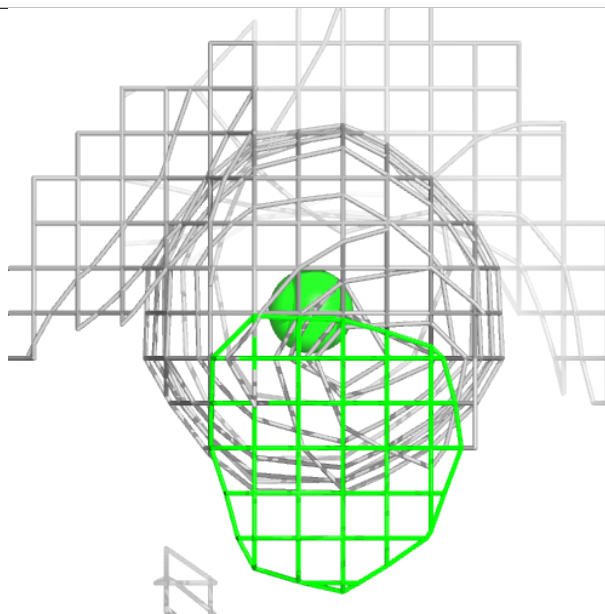
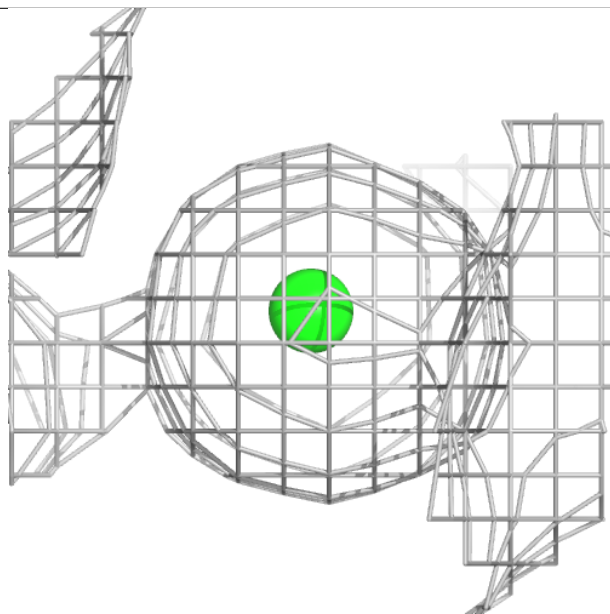
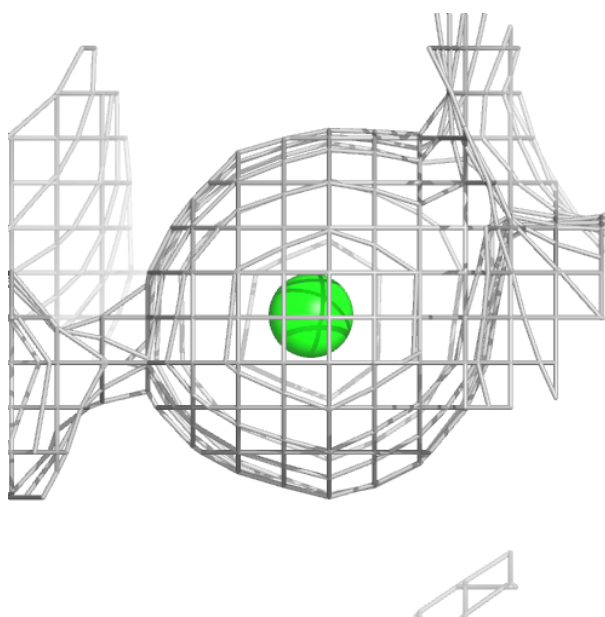
Electron density around CL A 403 (A):

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



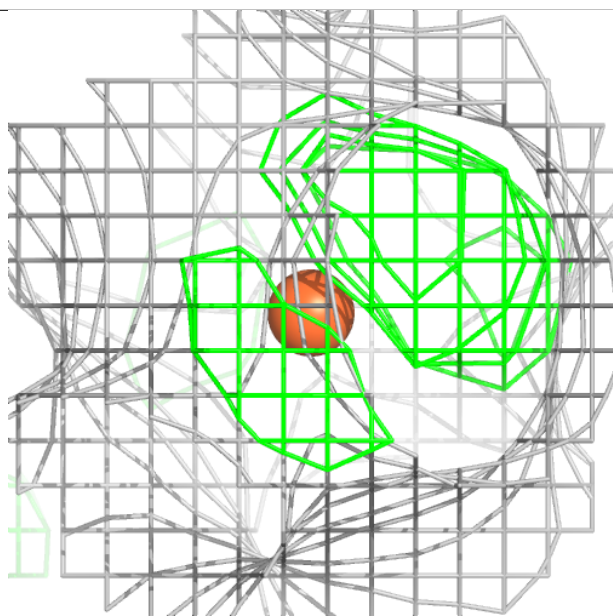
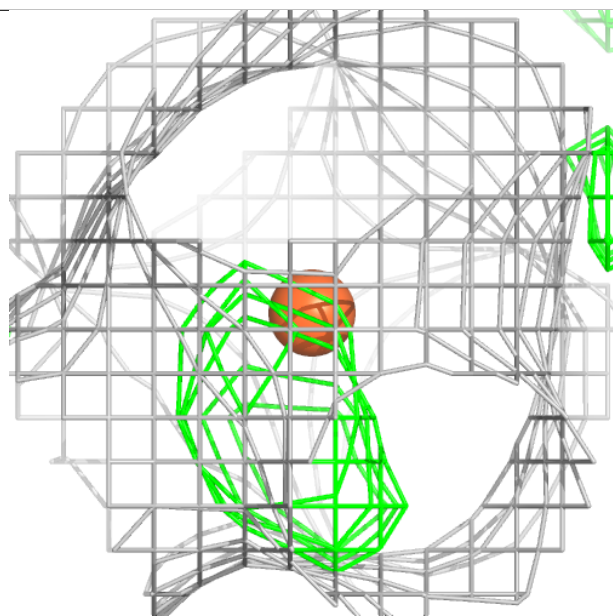
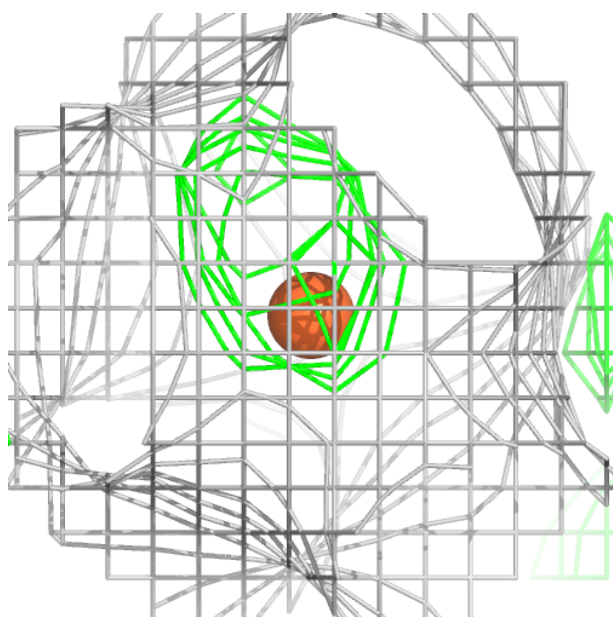
Electron density around CL A 403 (B):

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



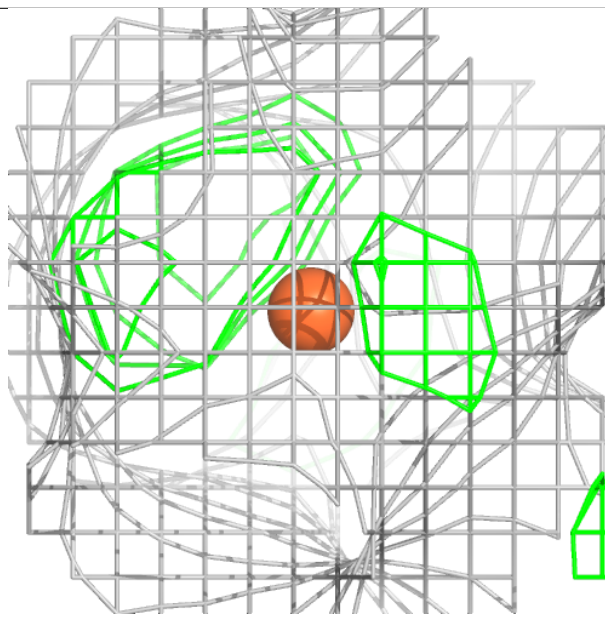
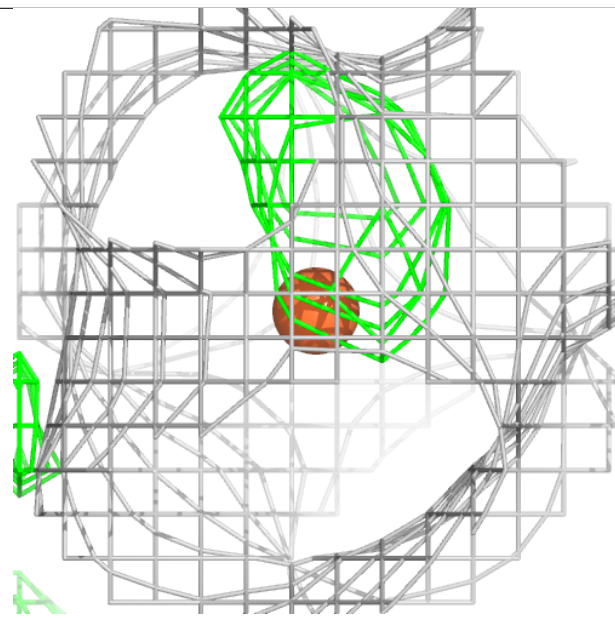
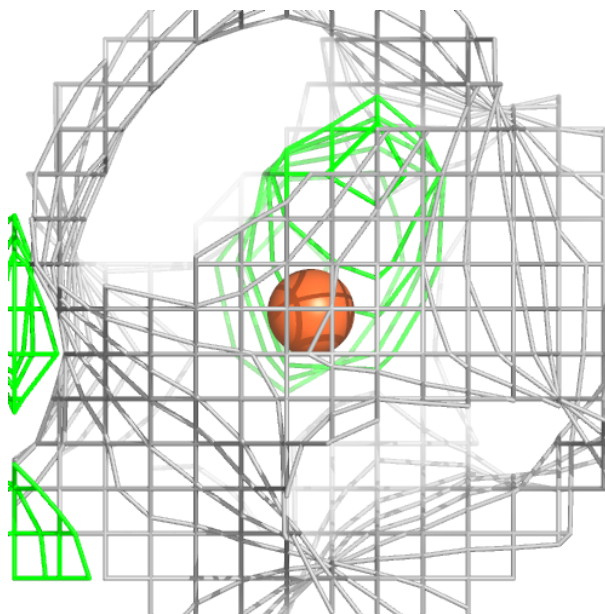
Electron density around FE2 a 401 (A):

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



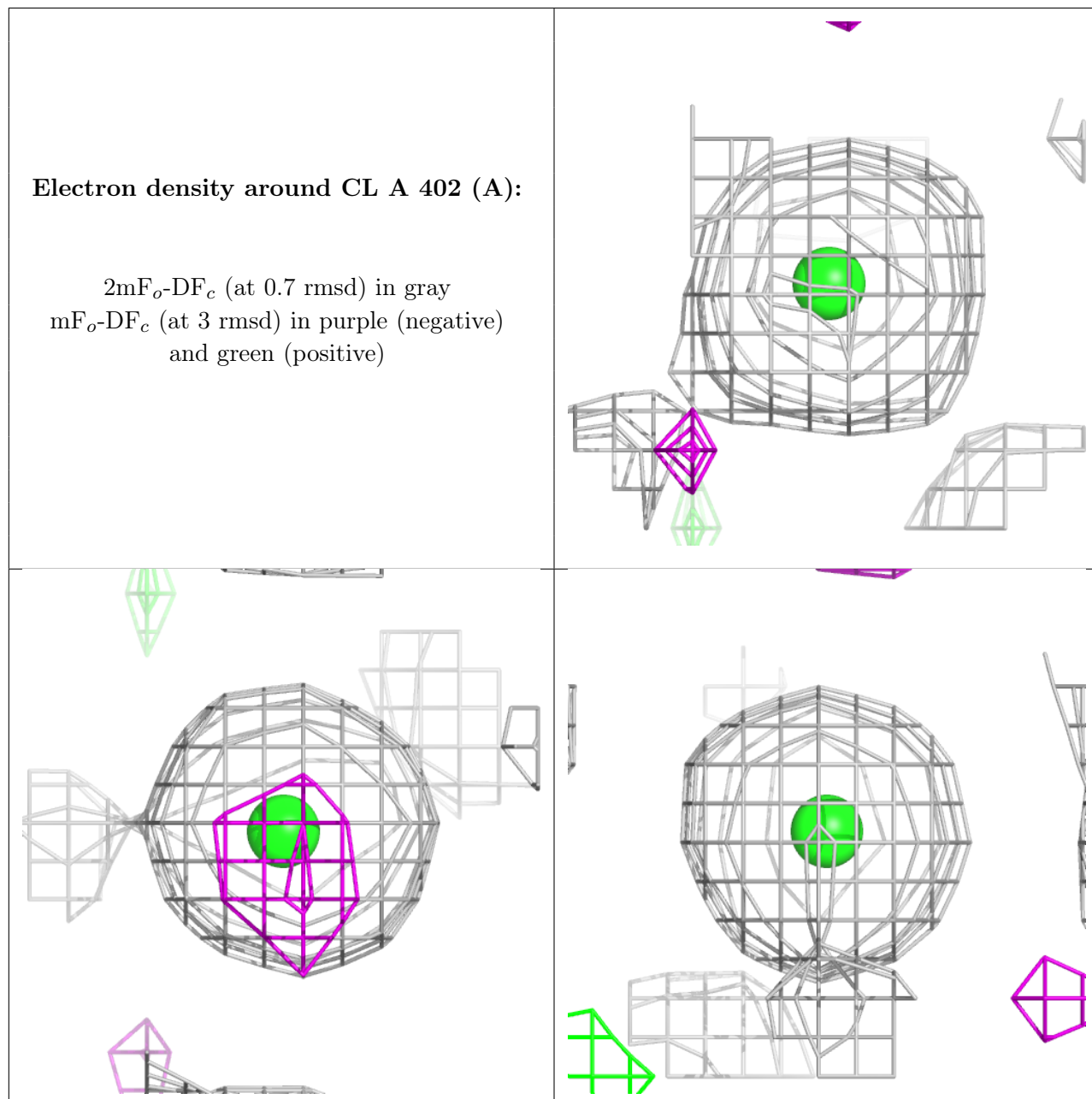
Electron density around FE2 a 401 (B):

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



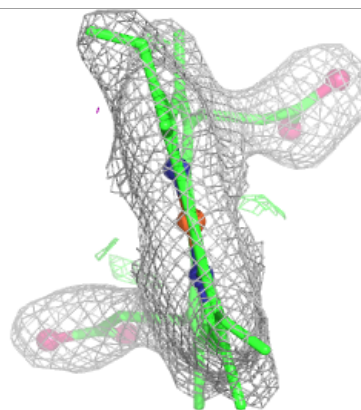
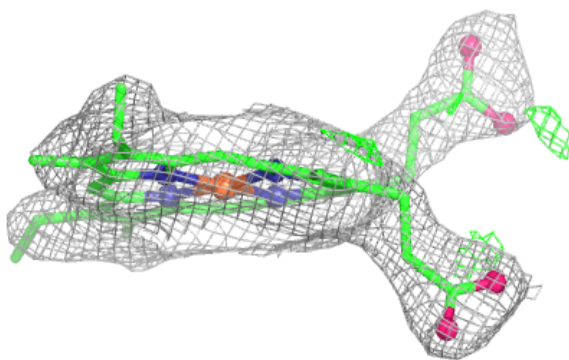
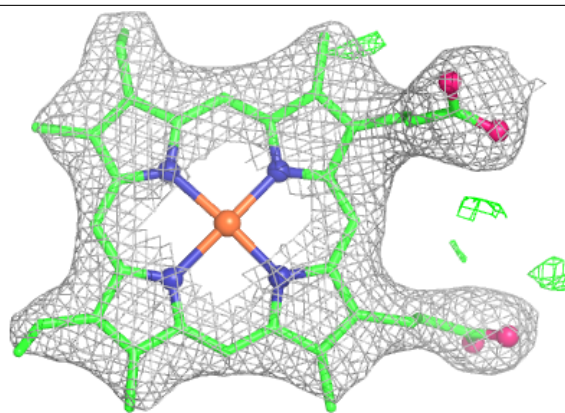
Electron density around CL A 402 (A):

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



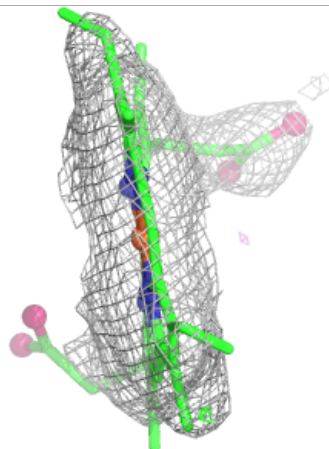
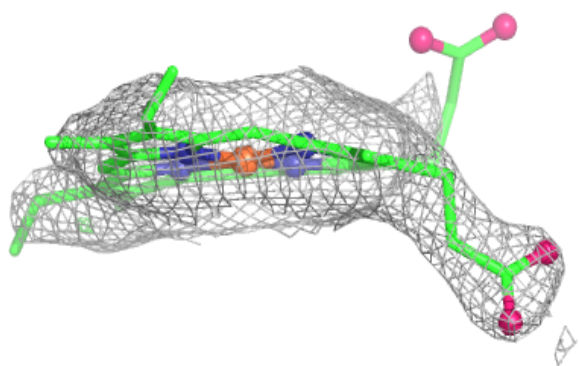
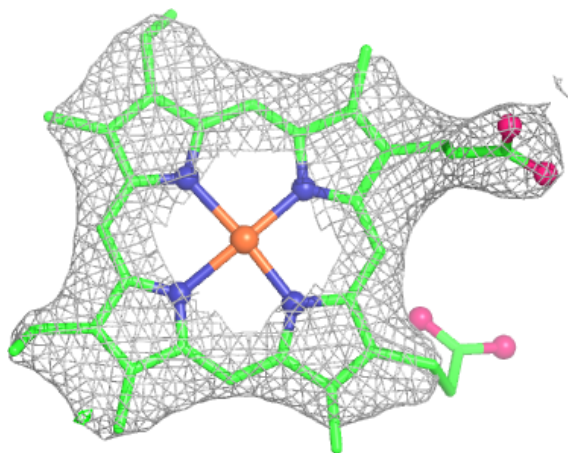
Electron density around HEM E 102:

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



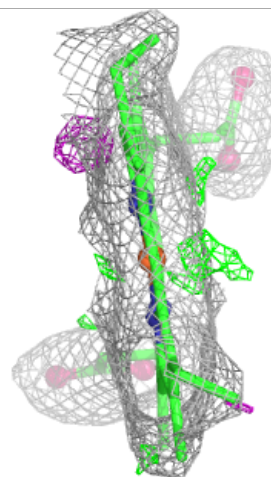
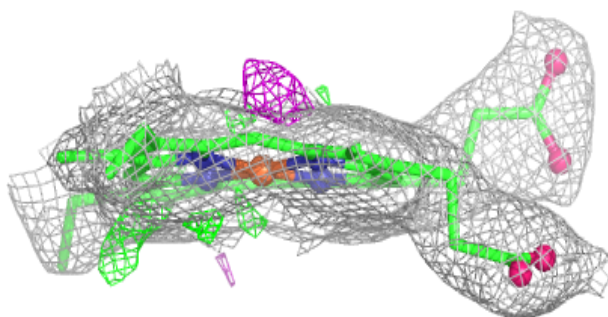
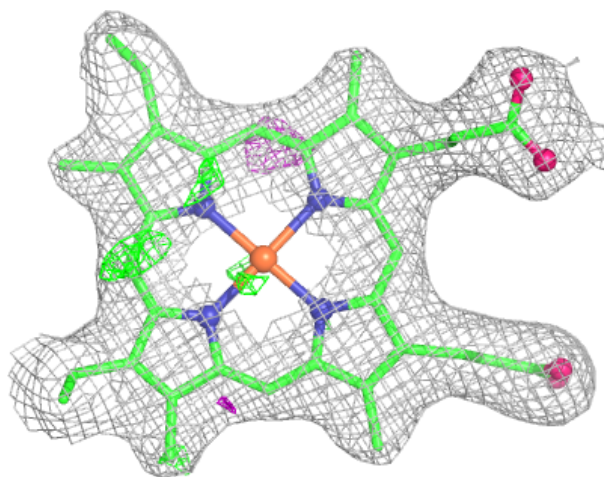
Electron density around HEM f 101:

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



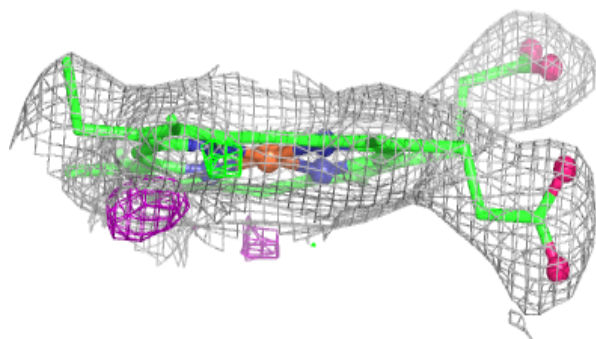
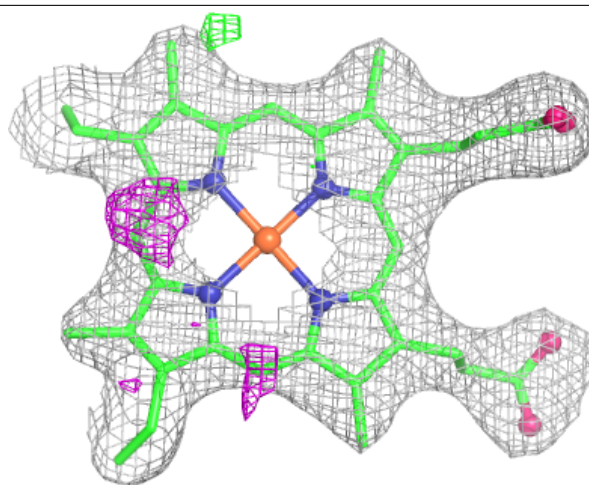
Electron density around HEC V 201:

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



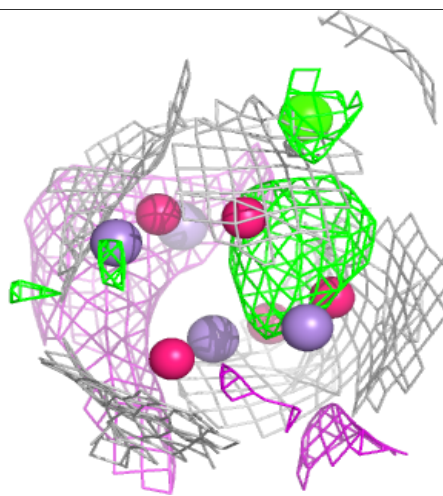
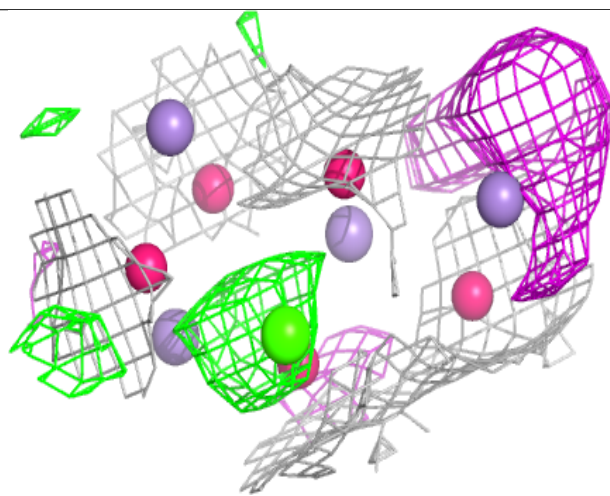
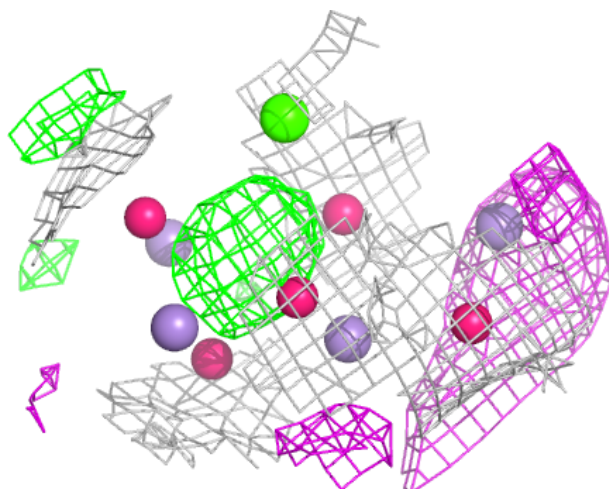
Electron density around HEC v 201:

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



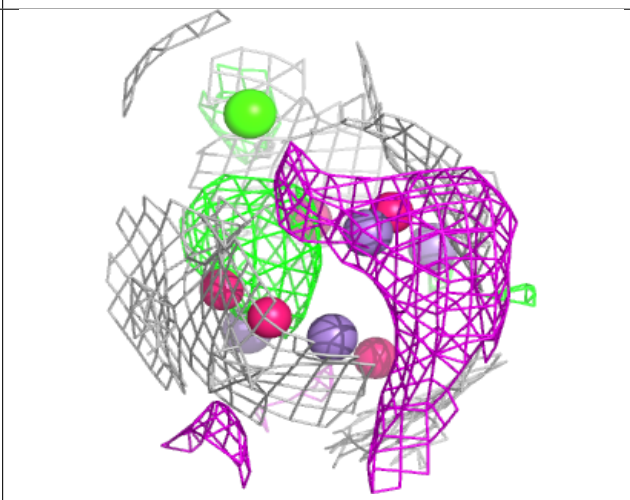
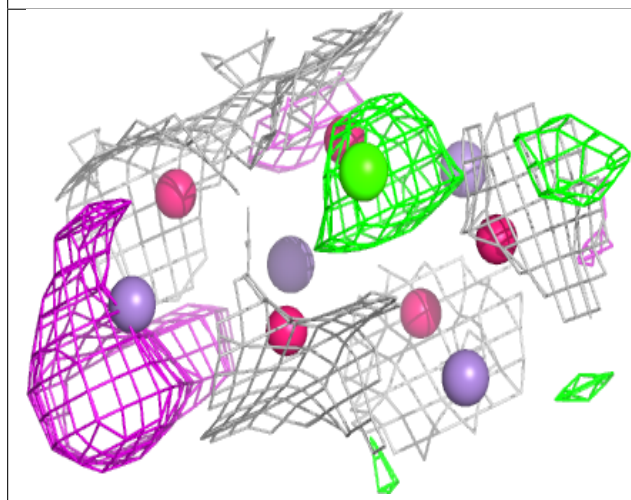
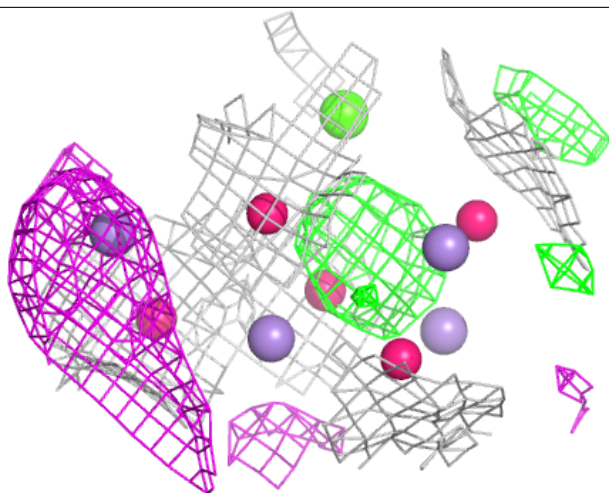
Electron density around OEX A 413 (A):

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



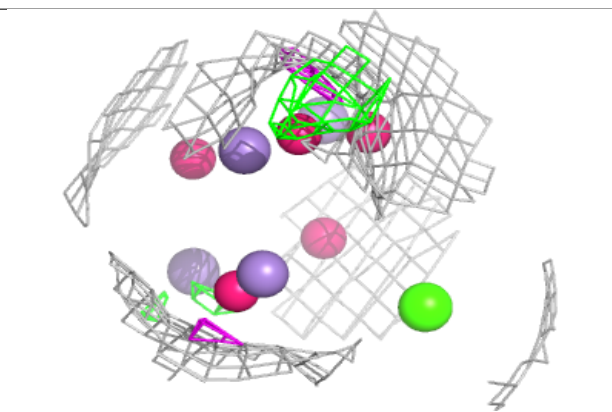
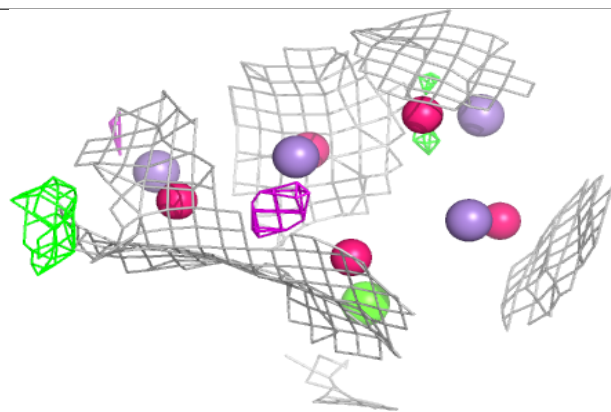
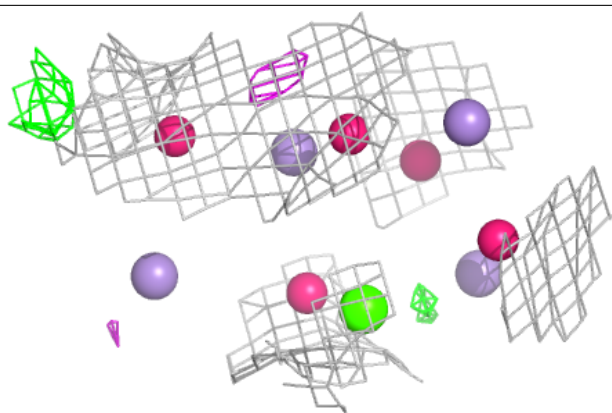
Electron density around OEX A 413 (B):

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

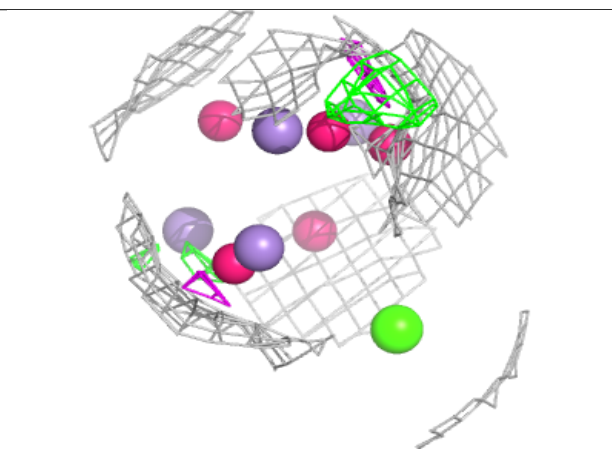
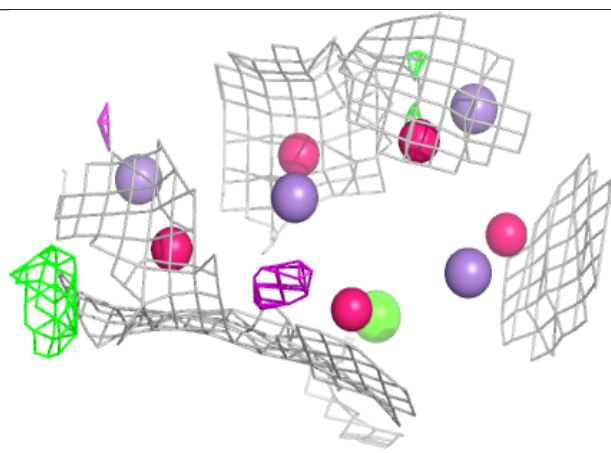
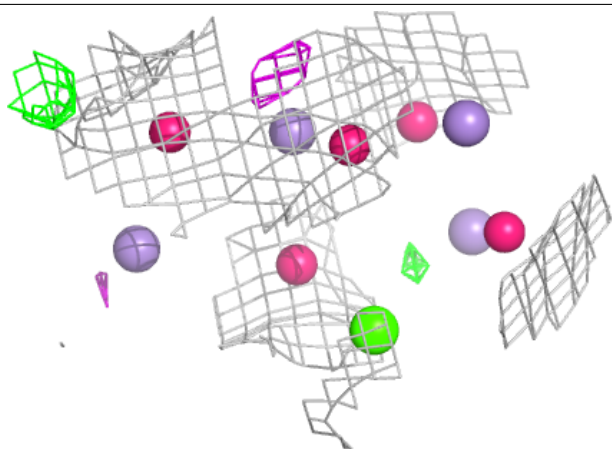


Electron density around OEX a 411 (A):

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

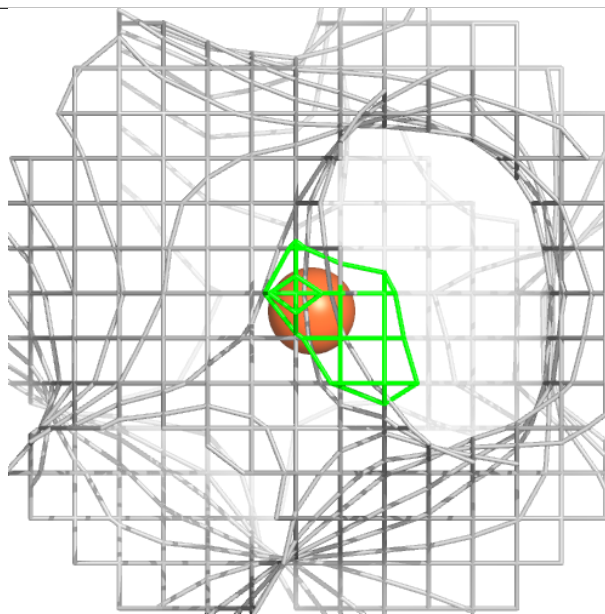
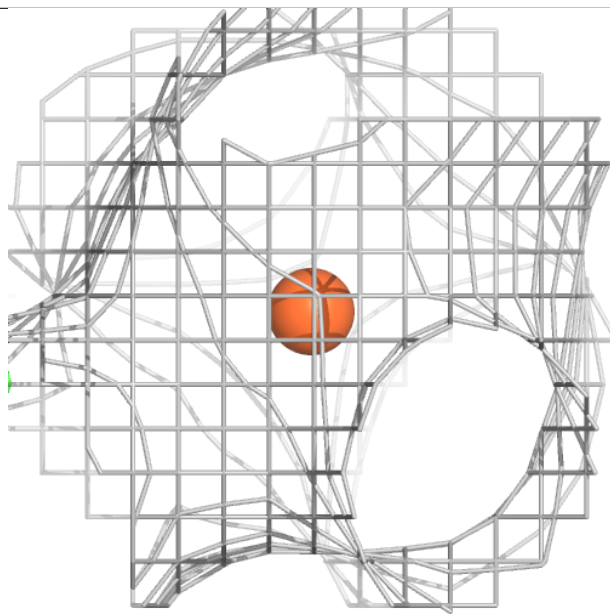
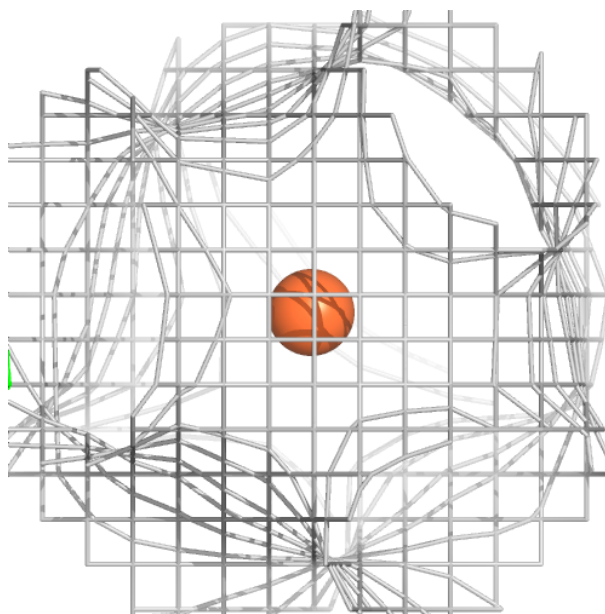
**Electron density around OEX a 411 (B):**

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



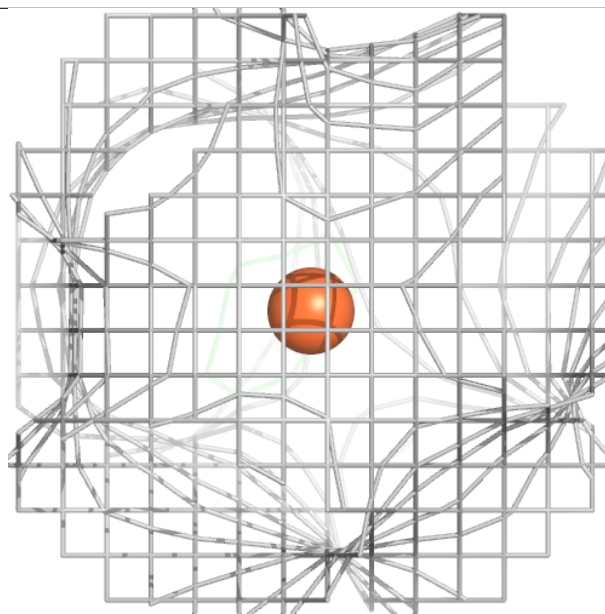
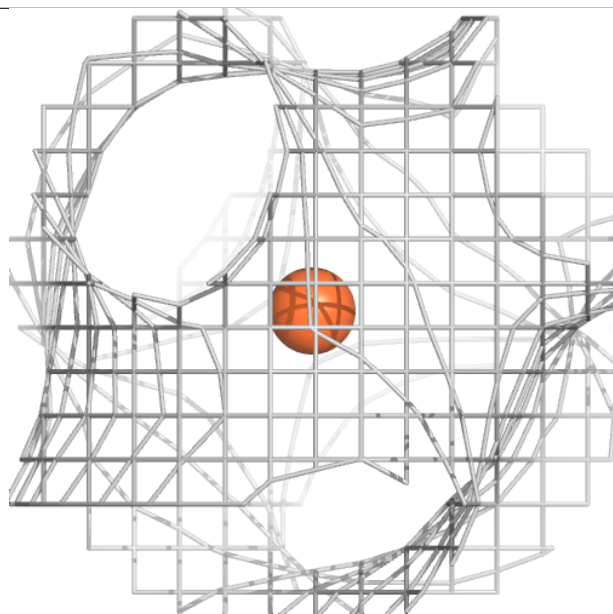
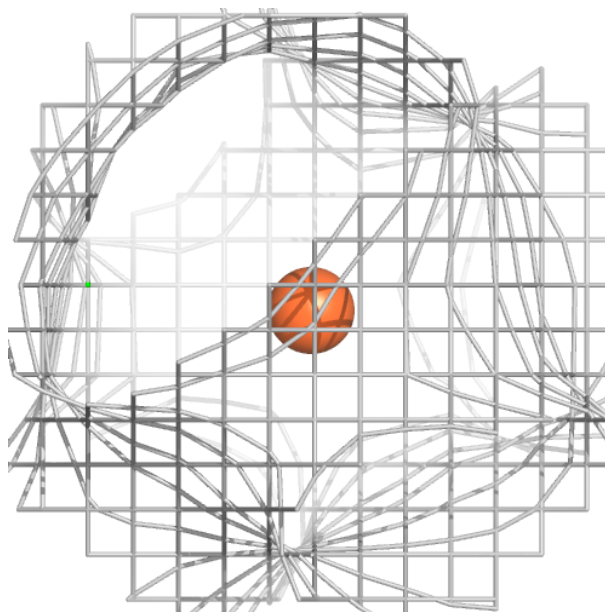
Electron density around FE2 A 401 (A):

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.