



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 13, 2026 – 02:29 PM JST

PDB ID : 8IR9 / pdb_00008ir9
Title : XFEL structure of cyanobacterial photosystem II following one flash (1F) with a 30-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

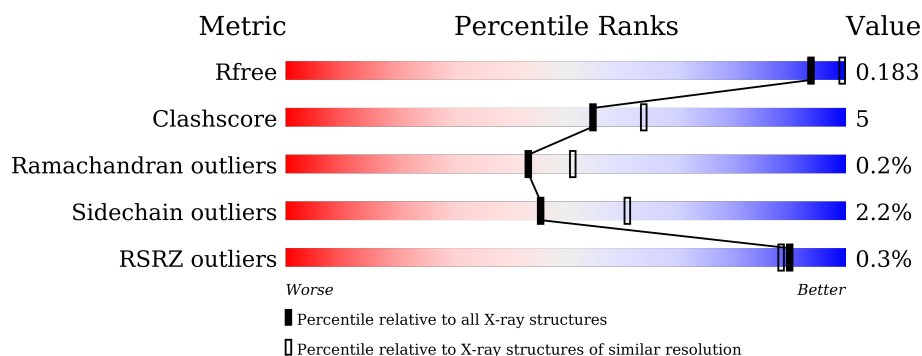
1 Overall quality at a glance

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.



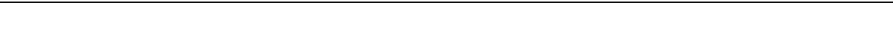
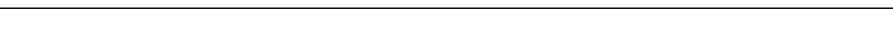
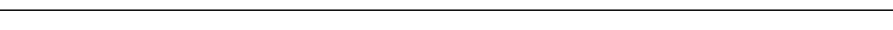
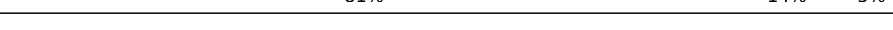
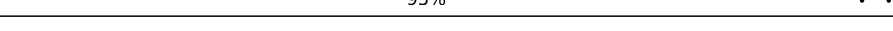
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	90% 7% .
1	a	344	88% 9% .
2	B	505	92% 7%
2	b	505	90% 9% .
3	C	455	92% 7% .
3	c	455	91% 8%

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Mol	Chain	Length	Quality of chain
4	D	342	 92% 8%
4	d	342	 92% 8%
5	E	84	 % 81% 15% .
5	e	84	 % 87% 7% 6%
6	F	44	 73% 5% 23%
6	f	44	 2% 61% 9% 30%
7	H	65	 2% 94% 5% .
7	h	65	 2% 86% 12% .
8	I	38	 82% 16% .
8	i	38	 84% 13% .
9	J	39	 87% 8% . .
9	j	39	 90% 10%
10	K	37	 78% 16% 5%
10	k	37	 81% 14% 5%
11	L	37	 95% . .
11	l	37	 86% 11% .
12	M	36	 81% 6% 6% 8%
12	m	36	 78% 14% . 6%
13	O	244	 83% 16%
13	o	244	 92% 7%
14	T	32	 81% 12% 6%
14	t	32	 3% 81% 12% 6%
15	U	104	 84% 9% 8%
15	u	104	 87% 6% . 7%
16	V	137	 95% 5%

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Mol	Chain	Length	Quality of chain
16	v	137	 91% 9%
17	X	40	 90% 5% 5%
17	x	40	 90% 5% 5%
18	Y	30	 3% 87% 10% •
18	y	30	 60% 37% •
19	Z	62	 90% 8% •
19	z	62	 77% 21% •
20	R	34	 6% 74% 26%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	GOL	D	412	-	X	-	-
27	GOL	a	418	-	-	X	-
40	HEC	V	201	X	-	-	-
40	HEC	v	201	X	-	-	-

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 62674 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	222	0
			4338	2836	717	760	25			
1	a	334	Total	C	N	O	S	0	220	0
			4318	2821	715	757	25			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	22	0
			4166	2735	694	724	13			
2	b	504	Total	C	N	O	S	0	19	0
			4134	2718	687	716	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	99	0
			4272	2796	715	743	18			
3	c	455	Total	C	N	O	S	0	101	0
			4316	2827	720	751	18			

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	115	0
			3625	2390	597	623	15			
4	d	341	Total	C	N	O	S	0	119	0
			3658	2412	605	626	15			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	0	0
			662	432	107	123			
5	e	79	Total	C	N	O	0	2	0
			670	439	110	121			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	31	Total	C	N	O	S	0	1	0
			261	179	43	38	1			

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

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

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	10	0
			1958	1221	335	398	4			
13	o	243	Total	C	N	O	S	0	8	0
			1933	1207	330	392	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	6	0
			311	213	48	48	2			
14	t	30	Total	C	N	O	S	0	5	0
			302	208	47	45	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	96	Total	C	N	O		0	4	0
			800	508	133	159				
15	u	97	Total	C	N	O		0	5	0
			815	519	135	161				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	6	0
			1120	711	185	220	4			
16	v	137	Total	C	N	O	S	0	6	0
			1117	712	185	216	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	38	Total	C	N	O	0	1	0
			289	194	46	49			
17	x	38	Total	C	N	O	0	0	0
			281	188	45	48			

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

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

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

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

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

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

- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

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

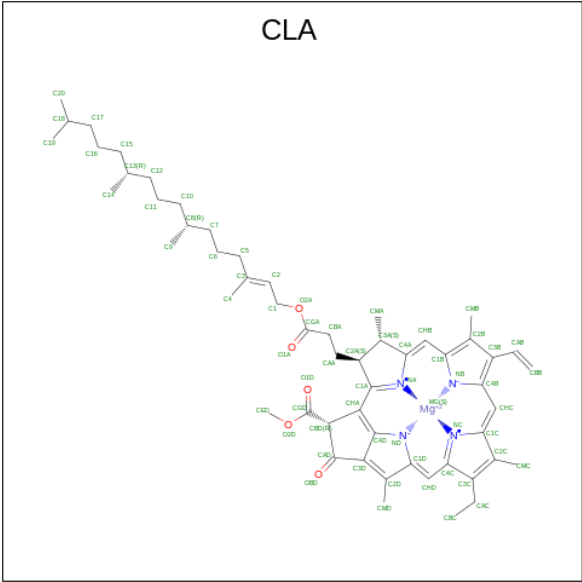
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	2
			4	4		

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

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



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

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

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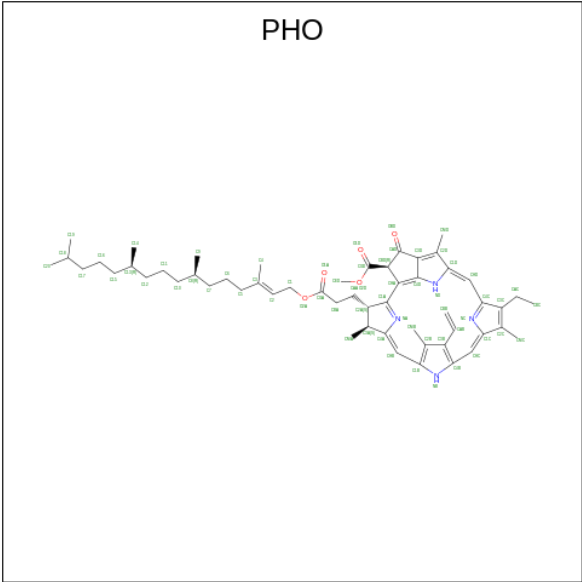
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	a	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	a	1	Total 130	C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

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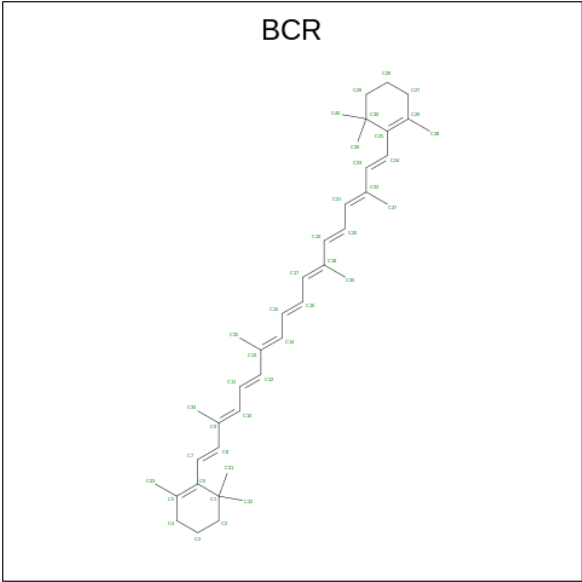
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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



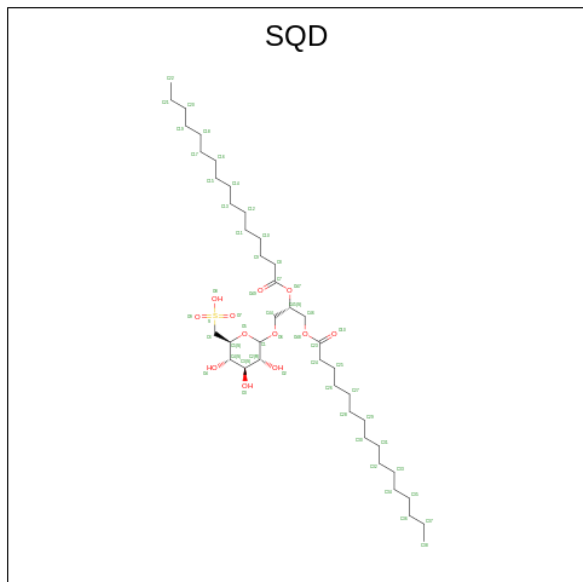
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	1
			128	110	8	10		
24	A	1	Total	C	N	O	0	1
			128	110	8	10		
24	a	1	Total	C	N	O	0	1
			128	110	8	10		
24	a	1	Total	C	N	O	0	1
			128	110	8	10		

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



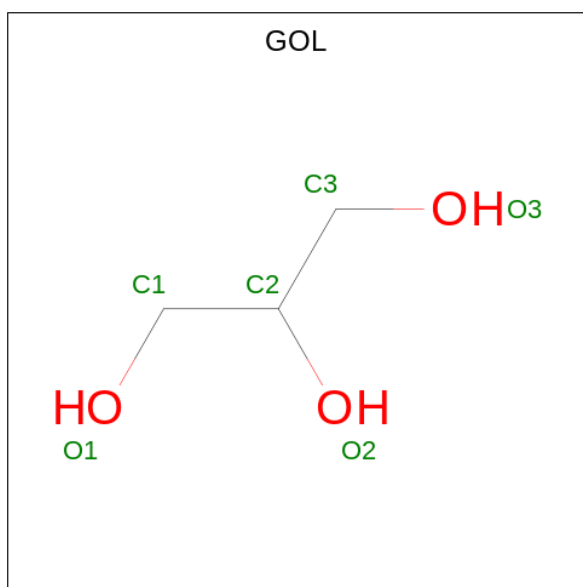
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total 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	F	1	Total	C	O	S	0	0
			43	30	12	1		
26	L	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	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: $C_3H_8O_3$).



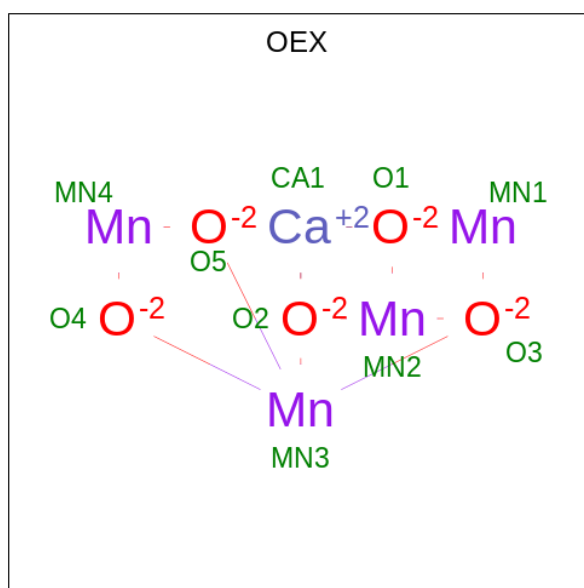
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			6	3	3		
27	A	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	1
			12	6	6		
27	D	1	Total	C	O	0	0
			6	3	3		
27	O	1	Total	C	O	0	0
			6	3	3		
27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

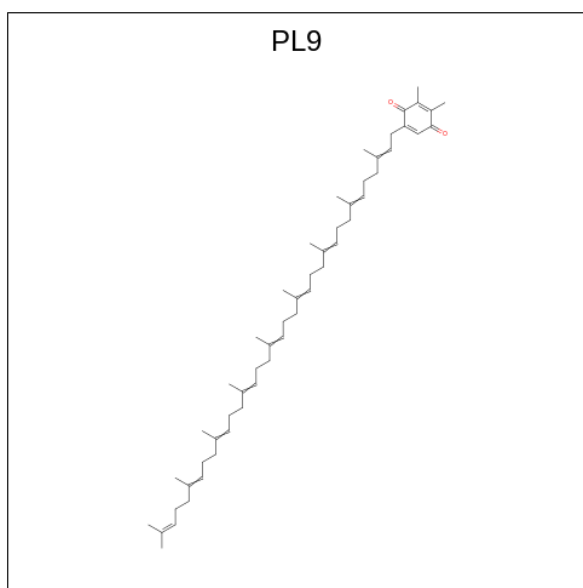
- Molecule 28 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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:).

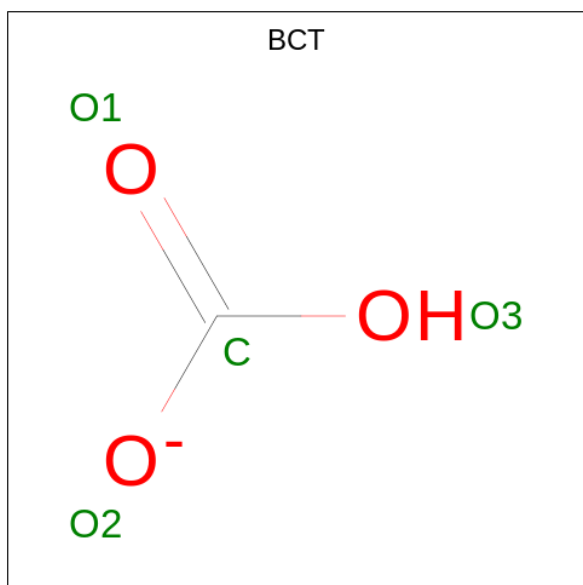
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			28	23	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	I	1	Total	C	O	0	0
			40	35	5		
30	J	1	Total	C		0	0
			10	10			
30	K	1	Total	C	O	0	1
			68	58	10		
30	X	1	Total	C	O	0	0
			18	16	2		

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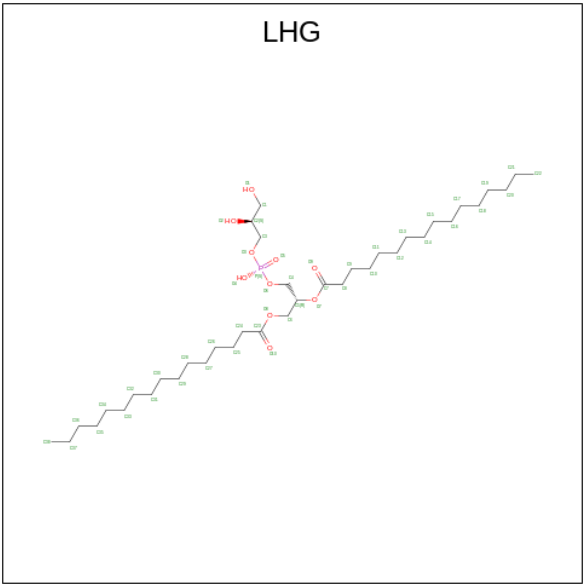
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	a	1	Total	C	O	0	0
			30	25	5		
30	b	2	Total	C	O	0	0
			69	59	10		
30	c	1	Total	C	O	0	1
			64	54	10		
30	d	1	Total	C	O	0	0
			17	16	1		
30	i	1	Total	C	O	0	0
			40	35	5		
30	j	1	Total	C		0	0
			10	10			
30	l	1	Total	C		0	0
			10	10			
30	m	1	Total	C		0	0
			10	10			
30	x	1	Total	C	O	0	0
			18	16	2		

- Molecule 31 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



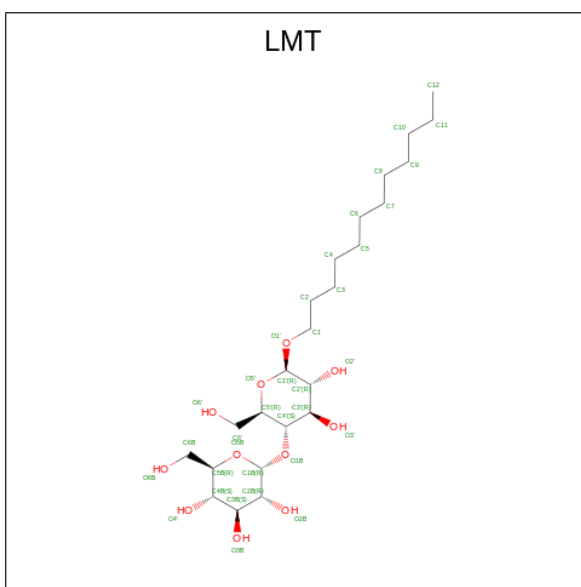
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	1
			8	2	6		
31	d	1	Total	C	O	0	1
			8	2	6		

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



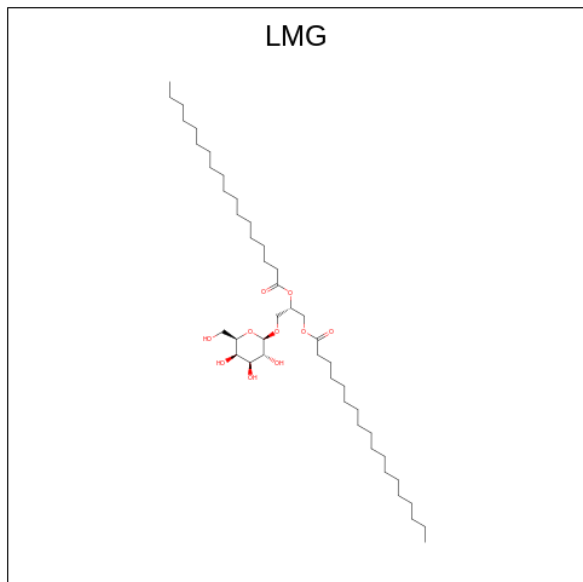
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	A	1	Total	C	O	P	0	1
			98	76	20	2		
32	D	1	Total	C	O	P	0	1
			98	76	20	2		
32	D	1	Total	C	O	P	0	1
			98	76	20	2		
32	E	1	Total	C	O	P	0	1
			84	62	20	2		
32	L	1	Total	C	O	P	0	1
			98	76	20	2		
32	a	1	Total	C	O	P	0	1
			84	62	20	2		
32	b	1	Total	C	O	P	0	1
			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 DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



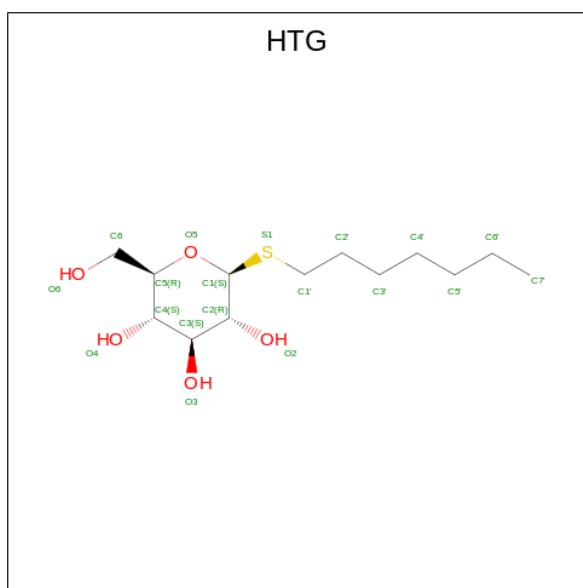
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	A	1	Total 35	C 24	O 11	0	0
33	B	1	Total 35	C 24	O 11	0	0
33	B	1	Total 35	C 24	O 11	0	0
33	B	1	Total 25	C 19	O 6	0	0
33	D	1	Total 35	C 24	O 11	0	0
33	F	1	Total 35	C 24	O 11	0	0
33	M	1	Total 35	C 24	O 11	0	0
33	T	1	Total 35	C 24	O 11	0	0
33	a	1	Total 35	C 24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

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



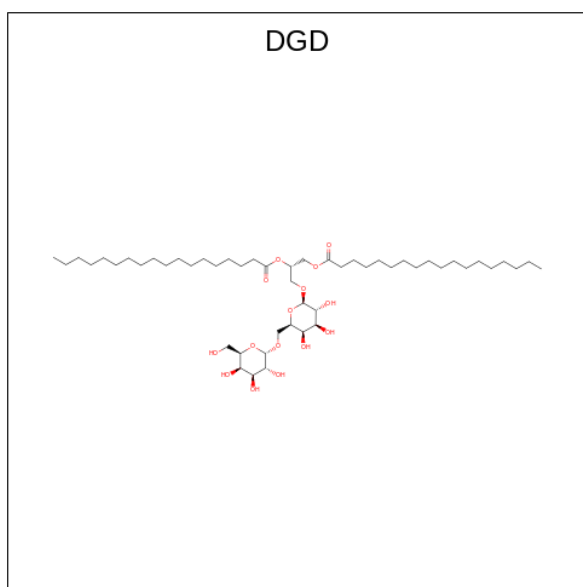
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	B	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	D	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total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

- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: $C_{13}H_{26}O_5S$).



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

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



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

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

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

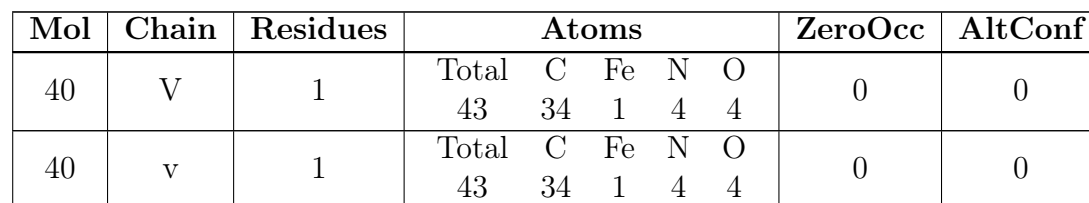
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	f	1	Total Ca 1 1	0	0
37	o	1	Total Ca 1 1	0	0

- # HEM

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

- 
- WORLD WIDE
PDB
PROTEIN DATA BANK



- | Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 41 | A | 136 | Total
220 | O
220 | 0 | 85 |
| 41 | B | 187 | Total
189 | O
189 | 0 | 2 |
| 41 | C | 169 | Total
206 | O
206 | 0 | 38 |
| 41 | D | 122 | Total
156 | O
156 | 0 | 34 |
| 41 | E | 17 | Total
17 | O
17 | 0 | 0 |
| 41 | F | 5 | Total
5 | O
5 | 0 | 0 |
| 41 | H | 22 | Total
22 | O
22 | 0 | 0 |
| 41 | I | 5 | Total
5 | O
5 | 0 | 0 |
| 41 | J | 7 | Total
7 | O
7 | 0 | 0 |
| 41 | K | 5 | Total
5 | O
5 | 0 | 0 |



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	L	9	Total O 10 10	0	1
41	M	6	Total O 6 6	0	0
41	O	104	Total O 109 109	0	5
41	T	10	Total O 13 13	0	3
41	U	46	Total O 49 49	0	3
41	V	82	Total O 83 83	0	1
41	X	8	Total O 8 8	0	0
41	a	130	Total O 211 211	0	82
41	b	200	Total O 203 203	0	3
41	c	160	Total O 193 193	0	34
41	d	115	Total O 146 146	0	31
41	e	9	Total O 9 9	0	0
41	f	3	Total O 3 3	0	0
41	h	17	Total O 17 17	0	0
41	i	2	Total O 2 2	0	0
41	j	1	Total O 1 1	0	0
41	k	3	Total O 3 3	0	0
41	l	8	Total O 10 10	0	2
41	m	12	Total O 12 12	0	0
41	o	100	Total O 104 104	0	4
41	t	7	Total O 10 10	0	3

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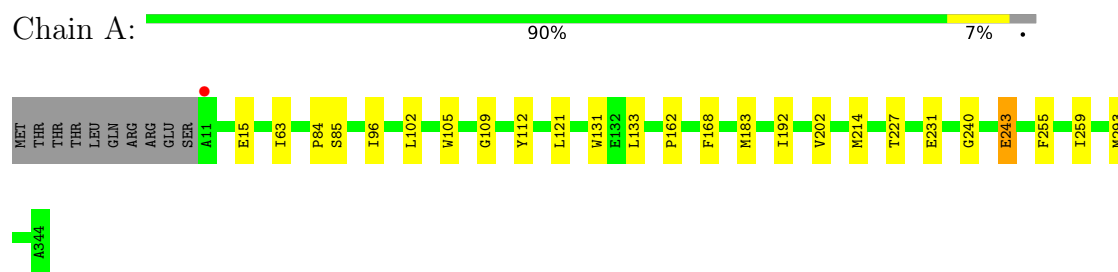
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	u	50	Total 51	O 51	0	1
41	v	58	Total 60	O 60	0	2
41	x	8	Total 8	O 8	0	0
41	y	2	Total 2	O 2	0	0

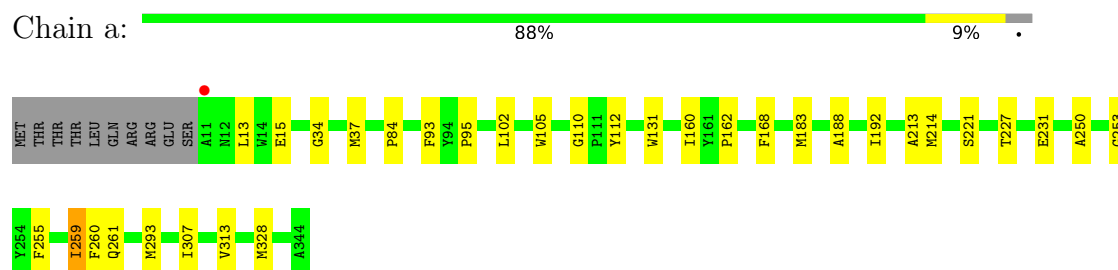
3 Residue-property plots [i](#)

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

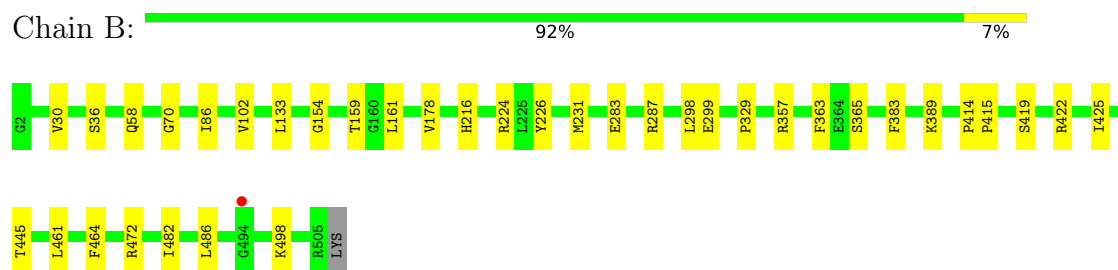
- Molecule 1: Photosystem II protein D1



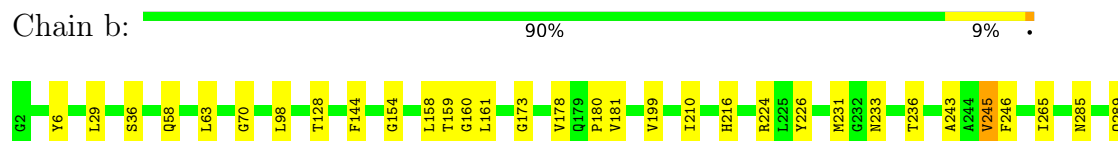
- Molecule 1: Photosystem II protein D1



- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein





- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 92% 7%



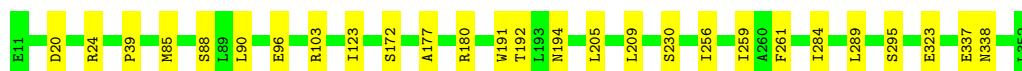
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 91% 8%



- Molecule 4: Photosystem II D2 protein

Chain D: 92% 8%



- Molecule 4: Photosystem II D2 protein

Chain d: 92% 8%



- Molecule 5: Cytochrome b559 subunit alpha

Chain E: 81% 15%



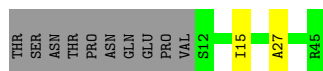
- Molecule 5: Cytochrome b559 subunit alpha

Chain e: 87% 7% 6%



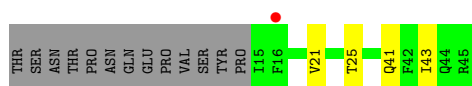
- Molecule 6: Cytochrome b559 subunit beta

Chain F: 73% 5% 23%



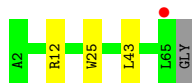
- Molecule 6: Cytochrome b559 subunit beta

Chain f: 2% 61% 9% 30%



- Molecule 7: Photosystem II reaction center protein H

Chain H: 2% 94% 5%



- Molecule 7: Photosystem II reaction center protein H

Chain h: 2% 86% 12%



- Molecule 8: Photosystem II reaction center protein I

Chain I: 82% 16%



- Molecule 8: Photosystem II reaction center protein I

Chain i: 84% 13%



- Molecule 9: Photosystem II reaction center protein J

Chain J: 87% 8%



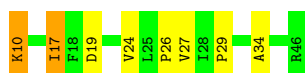
- Molecule 9: Photosystem II reaction center protein J

Chain j: 90% 10%



- Molecule 10: Photosystem II reaction center protein K

Chain K: 78% 16% 5%



- Molecule 10: Photosystem II reaction center protein K

Chain k: 81% 14% 5%



- Molecule 11: Photosystem II reaction center protein L

Chain L: 95% . .



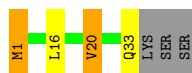
- Molecule 11: Photosystem II reaction center protein L

Chain l: 86% 11% .



- Molecule 12: Photosystem II reaction center protein M

Chain M: 81% 6% 6% 8%



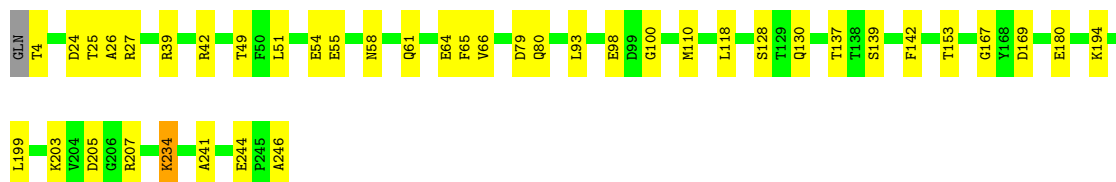
- Molecule 12: Photosystem II reaction center protein M

Chain m: 78% 14% . 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 83% 16%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 92% 7%



- Molecule 14: Photosystem II reaction center protein T

Chain T: 81% 12% 6%



- Molecule 14: Photosystem II reaction center protein T

Chain t: 3% 81% 12% 6%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 84% 9% 8%

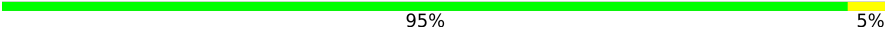


- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 87% 6% 7%



- Molecule 16: Cytochrome c-550

Chain V:  95% 5%



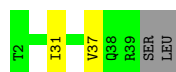
- Molecule 16: Cytochrome c-550

Chain v:  91% 9%



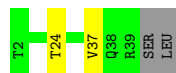
- Molecule 17: Photosystem II reaction center protein X

Chain X:  90% 5% 5%



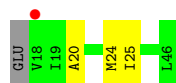
- Molecule 17: Photosystem II reaction center protein X

Chain x:  90% 5% 5%



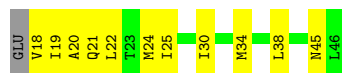
- Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:  3% 87% 10% .



- Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:  60% 37% .



- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  90% 8% .

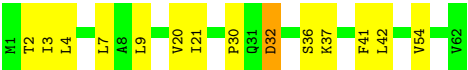


- Molecule 19: Photosystem II reaction center protein Z

Chain z:

77%

21%



● Molecule 20: Photosystem II protein Y

Chain R:

6%

74%

26%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	125.75Å 231.60Å 288.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.20 19.98 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (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}	0.140 , 0.176 0.153 , 0.183	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 , 67.2	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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.26	0/4478	0.45	0/6098
1	a	0.25	0/4457	0.41	0/6069
2	B	0.34	0/4314	0.49	0/5879
2	b	0.31	0/4285	0.48	0/5841
3	C	0.27	0/4416	0.42	0/6013
3	c	0.27	0/4467	0.42	0/6082
4	D	0.32	0/3746	0.46	0/5102
4	d	0.29	0/3780	0.45	0/5147
5	E	0.31	0/681	0.48	0/928
5	e	0.28	0/690	0.46	0/939
6	F	0.31	0/284	0.43	0/387
6	f	0.26	0/269	0.41	0/365
7	H	0.30	0/519	0.47	0/708
7	h	0.28	0/530	0.46	0/722
8	I	0.27	0/311	0.41	0/419
8	i	0.31	0/311	0.45	0/419
9	J	0.29	0/278	0.36	0/376
9	j	0.27	0/283	0.38	0/383
10	K	0.33	0/303	0.50	0/416
10	k	0.30	0/303	0.45	0/416
11	L	0.35	0/318	0.46	0/433
11	l	0.36	0/318	0.50	0/433
12	M	0.37	0/261	0.52	0/357
12	m	0.31	0/279	0.46	0/380
13	O	0.33	0/1991	0.50	0/2698
13	o	0.31	0/1966	0.49	0/2665
14	T	0.33	0/310	0.41	0/419
14	t	0.33	0/301	0.41	0/406
15	U	0.35	0/811	0.54	0/1095
15	u	0.34	0/826	0.52	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	0.29	0/1139	0.46	0/1542
17	X	0.23	0/292	0.34	0/395
17	x	0.23	0/284	0.36	0/384
18	Y	0.24	0/216	0.42	0/289
18	y	0.22	0/216	0.36	0/289
19	Z	0.21	0/490	0.34	0/669
19	z	0.21	0/490	0.39	0/669
20	R	0.24	0/279	0.34	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	21	0
1	a	4318	0	4124	36	0
2	B	4166	0	3999	26	0
2	b	4134	0	3976	38	0
3	C	4272	0	4138	22	0
3	c	4316	0	4184	32	0
4	D	3625	0	3489	28	0
4	d	3658	0	3522	26	0
5	E	662	0	648	10	0
5	e	670	0	655	6	0
6	F	275	0	282	2	0
6	f	261	0	269	5	0
7	H	506	0	529	2	0
7	h	517	0	541	6	0
8	I	314	0	328	4	0
8	i	314	0	328	3	0
9	J	272	0	279	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	277	0	284	3	0
10	K	293	0	305	6	0
10	k	293	0	305	5	0
11	L	311	0	320	2	0
11	l	311	0	320	4	0
12	M	268	0	285	4	0
12	m	286	0	305	8	0
13	O	1958	0	1920	24	0
13	o	1933	0	1900	8	0
14	T	311	0	318	2	0
14	t	302	0	311	4	0
15	U	800	0	796	5	0
15	u	815	0	817	4	0
16	V	1120	0	1122	4	0
16	v	1117	0	1131	7	0
17	X	289	0	322	2	0
17	x	281	0	312	2	0
18	Y	215	0	246	2	0
18	y	215	0	246	5	0
19	Z	479	0	516	2	0
19	z	479	0	516	3	0
20	R	273	0	305	4	0
21	A	2	0	0	0	0
21	a	2	0	0	0	0
22	A	4	0	0	0	0
22	a	4	0	0	0	0
23	A	455	0	504	19	0
23	B	1040	0	1152	27	0
23	C	845	0	936	33	0
23	D	195	0	216	7	0
23	a	455	0	504	20	0
23	b	1040	0	1152	21	0
23	c	845	0	936	38	0
23	d	195	0	216	5	0
24	A	256	0	296	5	0
24	a	256	0	296	5	0
25	A	40	0	56	1	0
25	B	120	0	168	5	0
25	C	80	0	112	1	0
25	D	40	0	56	0	0
25	H	40	0	56	2	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	5	0
25	Y	40	0	56	1	0
25	a	40	0	56	1	0
25	b	120	0	168	8	0
25	c	80	0	112	1	0
25	d	40	0	56	3	0
25	h	40	0	56	6	0
25	k	40	0	56	2	0
25	t	40	0	56	4	0
25	y	40	0	56	1	0
26	A	162	0	232	4	0
26	F	43	0	53	3	0
26	L	54	0	78	1	0
26	a	162	0	232	11	0
26	b	54	0	78	4	0
26	f	43	0	53	1	0
27	A	12	0	15	4	0
27	B	18	0	24	2	0
27	C	12	0	16	0	0
27	D	6	0	8	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	3	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	17	0
29	D	110	0	160	0	0
29	a	110	0	160	10	0
29	d	110	0	160	0	0
30	A	28	0	0	0	0
30	B	33	0	0	0	0
30	D	57	0	0	0	0
30	I	40	0	0	0	0
30	J	10	0	0	0	0
30	K	68	0	0	0	0
30	X	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	a	30	0	0	0	0
30	b	69	0	0	0	0
30	c	64	0	0	0	0
30	d	17	0	0	0	0
30	i	40	0	0	0	0
30	j	10	0	0	0	0
30	l	10	0	0	0	0
30	m	10	0	0	0	0
30	x	18	0	0	0	0
31	A	8	0	0	0	0
31	d	8	0	0	0	0
32	A	98	0	148	3	0
32	D	196	0	296	13	0
32	E	84	0	114	6	0
32	L	98	0	148	0	0
32	a	84	0	114	8	0
32	b	98	0	148	1	0
32	d	294	0	444	25	0
33	A	35	0	46	2	0
33	B	95	0	127	3	0
33	D	35	0	46	1	0
33	F	35	0	46	0	0
33	M	35	0	46	2	0
33	T	35	0	46	0	0
33	a	35	0	46	2	0
33	b	50	0	70	1	0
33	e	35	0	46	1	0
33	m	35	0	46	0	0
33	t	26	0	35	2	0
34	B	51	0	72	0	0
34	C	153	0	216	2	0
34	D	51	0	72	0	0
34	Z	37	0	44	2	0
34	c	153	0	216	3	0
34	d	51	0	72	4	0
34	m	51	0	72	0	0
34	z	39	0	48	2	0
35	B	38	0	52	2	0
35	C	19	0	26	0	0
35	D	16	0	17	0	0
35	V	11	0	10	0	0
35	b	57	0	78	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	c	19	0	26	1	0
35	d	16	0	17	1	0
35	o	19	0	26	1	0
36	C	310	0	410	7	0
36	H	62	0	82	1	0
36	c	310	0	410	8	0
36	h	62	0	82	2	0
37	C	1	0	0	0	0
37	F	1	0	0	0	0
37	O	1	0	0	0	0
37	c	2	0	0	0	0
37	f	1	0	0	0	0
37	o	1	0	0	0	0
38	F	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	220	0	0	1	0
41	B	189	0	0	2	0
41	C	206	0	0	2	0
41	D	156	0	0	2	0
41	E	17	0	0	2	0
41	F	5	0	0	0	0
41	H	22	0	0	0	0
41	I	5	0	0	0	0
41	J	7	0	0	0	0
41	K	5	0	0	1	0
41	L	10	0	0	0	0
41	M	6	0	0	0	0
41	O	109	0	0	1	0
41	T	13	0	0	0	0
41	U	49	0	0	0	0
41	V	83	0	0	0	0
41	X	8	0	0	0	0
41	a	211	0	0	2	0
41	b	203	0	0	0	0
41	c	193	0	0	3	0
41	d	146	0	0	0	0
41	e	9	0	0	0	0
41	f	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	h	17	0	0	0	0
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	12	0	0	0	0
41	o	104	0	0	0	0
41	t	10	0	0	0	0
41	u	51	0	0	1	0
41	v	60	0	0	0	0
41	x	8	0	0	0	0
41	y	2	0	0	0	0
All	All	62674	0	61528	582	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 582 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:604:CLA:H42	23:B:605:CLA:H2	1.47	0.94
1:a:250[B]:ALA:HA	2:b:491[B]:VAL:HG11	1.51	0.92
27:A:418:GOL:H11	12:M:1:FME:HG2	1.52	0.91
1:a:250[A]:ALA:HA	2:b:491[A]:VAL:HG11	1.53	0.88
23:c:504:CLA:HBB1	23:c:513:CLA:H41	1.55	0.87

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	553/344 (161%)	544 (98%)	7 (1%)	2 (0%)	30	34
1	a	551/344 (160%)	541 (98%)	8 (2%)	2 (0%)	30	34
2	B	524/505 (104%)	518 (99%)	6 (1%)	0	100	100
2	b	521/505 (103%)	509 (98%)	12 (2%)	0	100	100
3	C	548/455 (120%)	540 (98%)	7 (1%)	1 (0%)	43	51
3	c	554/455 (122%)	544 (98%)	9 (2%)	1 (0%)	43	51
4	D	454/342 (133%)	438 (96%)	16 (4%)	0	100	100
4	d	457/342 (134%)	445 (97%)	12 (3%)	0	100	100
5	E	79/84 (94%)	78 (99%)	1 (1%)	0	100	100
5	e	79/84 (94%)	79 (100%)	0	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	62/65 (95%)	62 (100%)	0	0	100	100
7	h	63/65 (97%)	60 (95%)	2 (3%)	1 (2%)	7	6
8	I	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	4	2
8	i	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
9	J	36/39 (92%)	36 (100%)	0	0	100	100
9	j	37/39 (95%)	37 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	34/36 (94%)	34 (100%)	0	0	100	100
13	O	251/244 (103%)	242 (96%)	8 (3%)	1 (0%)	30	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%)	92 (95%)	5 (5%)	0	100	100
15	u	99/104 (95%)	95 (96%)	4 (4%)	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%)	25 (93%)	2 (7%)	0	100	100
18	y	27/30 (90%)	27 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	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%)	6047 (98%)	122 (2%)	11 (0%)	43	51

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
8	I	36	ASP
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%)	441 (99%)	3 (1%)	76	87
1	a	442/279 (158%)	441 (100%)	1 (0%)	87	94
2	B	423/403 (105%)	417 (99%)	6 (1%)	59	75
2	b	420/403 (104%)	410 (98%)	10 (2%)	43	58
3	C	431/356 (121%)	422 (98%)	9 (2%)	47	63
3	c	437/356 (123%)	431 (99%)	6 (1%)	59	75
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%)	70 (97%)	2 (3%)	38	52

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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%)	25 (96%)	1 (4%)	29	40
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%)	36 (100%)	0	100	100
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%)	207 (96%)	9 (4%)	26	36
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%)	119 (97%)	4 (3%)	33	45
17	X	32/33 (97%)	32 (100%)	0	100	100
17	x	31/33 (94%)	31 (100%)	0	100	100
18	Y	22/23 (96%)	22 (100%)	0	100	100
18	y	22/23 (96%)	18 (82%)	4 (18%)	2	1
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%)	5000 (98%)	110 (2%)	45	61

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	362	PHE
4	d	272[B]	LEU
19	z	42	LEU
19	Z	31	GLN
2	b	486[B]	LEU

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

Mol	Chain	Res	Type
2	b	14	ASN
2	b	331	ASN
19	Z	31	GLN
15	u	78	ASN
16	v	86	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	i	1	8	8,9,10	0.70	0	7,9,11	1.20	1 (14%)
12	FME	m	1	12	8,9,10	0.52	0	7,9,11	1.52	2 (28%)
14	FME	T	1	14	8,9,10	0.63	0	7,9,11	1.62	2 (28%)
12	FME	M	1	12	8,9,10	0.57	0	7,9,11	1.33	1 (14%)
8	FME	I	1	8	8,9,10	0.58	0	7,9,11	1.20	1 (14%)
14	FME	t	1	14	8,9,10	0.65	0	7,9,11	1.47	2 (28%)

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

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

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	m	1	FME	CA-N-CN	-2.62	118.80	122.82
14	T	1	FME	CA-N-CN	2.49	126.66	122.82
14	t	1	FME	O-C-CA	-2.39	118.50	124.78
14	T	1	FME	CG-CB-CA	2.39	119.59	112.95
14	t	1	FME	CA-N-CN	-2.38	119.17	122.82

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	m	1	FME	3	0
12	M	1	FME	2	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
35	HTG	C	522	-	19,19,19	0.89	1 (5%)	23,24,24	1.43	1 (4%)
24	PHO	A	417[B]	-	58,69,69	2.70	14 (24%)	56,99,99	2.97	18 (32%)
26	SQD	A	412	-	53,54,54	1.02	3 (5%)	62,65,65	1.24	6 (9%)
36	DGD	h	102	-	63,63,67	0.86	3 (4%)	77,77,81	1.11	7 (9%)
35	HTG	o	301	-	19,19,19	1.06	2 (10%)	23,24,24	1.49	4 (17%)
25	BCR	B	619	-	41,41,41	1.06	1 (2%)	56,56,56	1.32	7 (12%)
27	GOL	c	526[B]	-	5,5,5	1.02	0	5,5,5	0.91	0
27	GOL	C	523[A]	-	5,5,5	1.18	0	5,5,5	0.83	0
34	LMG	d	410	39	51,51,55	0.87	2 (3%)	59,59,63	1.14	5 (8%)
23	CLA	B	610	41	69,73,73	2.07	19 (27%)	83,113,113	2.87	32 (38%)
27	GOL	o	304	-	5,5,5	0.97	0	5,5,5	1.10	0
32	LHG	d	407[A]	-	48,48,48	0.92	2 (4%)	51,54,54	0.99	3 (5%)
38	HEM	F	102	6,5	50,50,50	1.54	7 (14%)	66,82,82	1.94	15 (22%)
23	CLA	C	511	3	69,73,73	2.04	21 (30%)	83,113,113	2.96	32 (38%)
23	CLA	C	505	41	69,73,73	1.99	20 (28%)	83,113,113	2.85	29 (34%)
26	SQD	A	410[A]	-	53,54,54	0.93	3 (5%)	62,65,65	1.81	10 (16%)
23	CLA	b	602	2	69,73,73	2.09	18 (26%)	83,113,113	2.95	35 (42%)
25	BCR	b	618	-	41,41,41	0.98	1 (2%)	56,56,56	1.31	9 (16%)
25	BCR	A	409	-	41,41,41	0.98	1 (2%)	56,56,56	1.43	9 (16%)
35	HTG	b	625	-	19,19,19	1.10	2 (10%)	23,24,24	1.46	4 (17%)
23	CLA	b	614	2	69,73,73	1.97	20 (28%)	83,113,113	2.97	31 (37%)
23	CLA	a	404[B]	1	69,73,73	1.99	20 (28%)	83,113,113	2.89	32 (38%)
23	CLA	a	408	1	69,73,73	1.98	19 (27%)	83,113,113	2.94	31 (37%)
32	LHG	d	406[B]	-	48,48,48	0.90	2 (4%)	51,54,54	1.07	4 (7%)
35	HTG	b	623	-	19,19,19	1.06	1 (5%)	23,24,24	1.88	2 (8%)
25	BCR	d	404	-	41,41,41	1.11	2 (4%)	56,56,56	1.96	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	D	404	-	41,41,41	1.13	2 (4%)	56,56,56	1.83	17 (30%)
23	CLA	d	402[B]	4	69,73,73	1.99	20 (28%)	83,113,113	2.84	30 (36%)
36	DGD	c	519	-	63,63,67	0.88	4 (6%)	77,77,81	1.02	5 (6%)
34	LMG	c	501	-	51,51,55	0.91	2 (3%)	59,59,63	1.23	6 (10%)
23	CLA	b	611	2	69,73,73	1.95	21 (30%)	83,113,113	2.90	28 (33%)
32	LHG	a	419[A]	-	41,41,48	1.04	2 (4%)	44,47,54	0.92	2 (4%)
27	GOL	c	527	-	5,5,5	1.13	0	5,5,5	0.92	0
36	DGD	C	518[B]	-	63,63,67	0.88	2 (3%)	77,77,81	0.97	4 (5%)
29	PL9	d	405[B]	-	55,55,55	0.66	1 (1%)	68,69,69	1.63	17 (25%)
24	PHO	A	407[B]	-	58,69,69	2.65	12 (20%)	56,99,99	2.87	17 (30%)
36	DGD	c	518[B]	-	63,63,67	0.86	3 (4%)	77,77,81	0.96	5 (6%)
40	HEC	v	201	16	50,50,50	1.71	7 (14%)	68,82,82	1.39	8 (11%)
27	GOL	O	302	-	5,5,5	0.87	0	5,5,5	0.90	0
25	BCR	c	516	-	41,41,41	1.02	1 (2%)	56,56,56	1.40	11 (19%)
38	HEM	f	101	6,5	50,50,50	1.49	6 (12%)	66,82,82	1.74	11 (16%)
36	DGD	c	517[A]	-	63,63,67	0.85	2 (3%)	77,77,81	1.12	6 (7%)
23	CLA	c	513	3	69,73,73	2.08	19 (27%)	83,113,113	2.89	32 (38%)
33	LMT	b	621	-	25,25,36	0.95	1 (4%)	30,30,47	1.17	2 (6%)
24	PHO	A	417[A]	-	58,69,69	2.74	15 (25%)	56,99,99	2.87	17 (30%)
25	BCR	b	619	-	41,41,41	1.09	1 (2%)	56,56,56	1.35	9 (16%)
23	CLA	C	507	3	69,73,73	2.03	20 (28%)	83,113,113	2.80	32 (38%)
29	PL9	a	413[A]	-	55,55,55	0.65	2 (3%)	68,69,69	2.00	22 (32%)
23	CLA	c	509	3	69,73,73	2.11	20 (28%)	83,113,113	2.77	30 (36%)
27	GOL	c	526[A]	-	5,5,5	0.94	0	5,5,5	0.95	0
36	DGD	C	519	-	63,63,67	0.89	3 (4%)	77,77,81	1.00	4 (5%)
26	SQD	f	102	-	42,43,54	1.18	3 (7%)	51,54,65	1.57	11 (21%)
23	CLA	b	616	2	69,73,73	2.01	18 (26%)	83,113,113	2.92	30 (36%)
40	HEC	V	201	16	50,50,50	1.71	6 (12%)	68,82,82	1.53	13 (19%)
25	BCR	B	617	-	41,41,41	1.08	1 (2%)	56,56,56	1.29	4 (7%)
27	GOL	D	412	-	5,5,5	1.42	2 (40%)	5,5,5	0.89	0
35	HTG	B	623	-	19,19,19	0.99	2 (10%)	23,24,24	1.13	3 (13%)
25	BCR	k	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.50	11 (19%)
32	LHG	D	406[A]	-	48,48,48	0.86	2 (4%)	51,54,54	0.99	3 (5%)
23	CLA	B	603	2	69,73,73	2.01	19 (27%)	83,113,113	2.90	31 (37%)
23	CLA	a	404[A]	1	69,73,73	1.96	19 (27%)	83,113,113	2.88	33 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LHG	d	406[A]	-	48,48,48	0.86	2 (4%)	51,54,54	1.08	4 (7%)
29	PL9	A	414[B]	-	55,55,55	0.65	1 (1%)	68,69,69	2.01	25 (36%)
33	LMT	t	101	-	26,26,36	0.90	2 (7%)	31,31,47	1.32	3 (9%)
23	CLA	B	606	2	69,73,73	1.98	20 (28%)	83,113,113	2.88	32 (38%)
32	LHG	L	102[B]	-	48,48,48	0.92	2 (4%)	51,54,54	1.08	2 (3%)
23	CLA	d	402[A]	4	69,73,73	1.94	20 (28%)	83,113,113	2.78	29 (34%)
23	CLA	C	503	3	69,73,73	2.03	20 (28%)	83,113,113	2.72	28 (33%)
23	CLA	C	502	3	69,73,73	1.97	19 (27%)	83,113,113	2.84	33 (39%)
23	CLA	c	511	3	69,73,73	2.00	20 (28%)	83,113,113	2.84	32 (38%)
27	GOL	a	418	-	5,5,5	1.31	1 (20%)	5,5,5	0.85	0
23	CLA	C	513	3	69,73,73	2.06	19 (27%)	83,113,113	2.84	35 (42%)
32	LHG	A	419[B]	-	48,48,48	0.86	2 (4%)	51,54,54	1.19	5 (9%)
26	SQD	a	410[B]	-	53,54,54	0.97	3 (5%)	62,65,65	1.64	11 (17%)
23	CLA	b	609	2	69,73,73	2.02	18 (26%)	83,113,113	2.79	31 (37%)
31	BCT	A	416[B]	21	2,3,3	0.63	0	2,3,3	1.15	0
34	LMG	c	520	-	51,51,55	0.90	2 (3%)	59,59,63	1.15	5 (8%)
36	DGD	C	517[B]	-	63,63,67	0.85	2 (3%)	77,77,81	1.09	7 (9%)
36	DGD	C	518[A]	-	63,63,67	0.89	3 (4%)	77,77,81	1.02	5 (6%)
23	CLA	D	402[B]	4	69,73,73	2.04	20 (28%)	83,113,113	2.88	30 (36%)
29	PL9	d	405[A]	-	55,55,55	0.65	1 (1%)	68,69,69	1.63	17 (25%)
34	LMG	Z	101	-	37,37,55	1.01	2 (5%)	45,45,63	1.48	6 (13%)
23	CLA	b	601	41	69,73,73	2.09	19 (27%)	83,113,113	2.79	28 (33%)
23	CLA	a	405[A]	41	69,73,73	2.01	17 (24%)	83,113,113	2.80	29 (34%)
36	DGD	c	518[A]	-	63,63,67	0.84	2 (3%)	77,77,81	0.97	5 (6%)
27	GOL	B	622	-	5,5,5	0.97	0	5,5,5	1.14	1 (20%)
23	CLA	c	508	41	69,73,73	2.03	19 (27%)	83,113,113	2.88	29 (34%)
23	CLA	B	613	2	69,73,73	2.02	20 (28%)	83,113,113	2.73	31 (37%)
33	LMT	e	101	-	36,36,36	1.02	2 (5%)	47,47,47	0.99	1 (2%)
33	LMT	B	628	-	36,36,36	1.02	3 (8%)	47,47,47	1.15	5 (10%)
27	GOL	o	303	-	5,5,5	0.97	0	5,5,5	0.97	0
32	LHG	b	630[B]	-	48,48,48	0.87	2 (4%)	51,54,54	1.02	3 (5%)
27	GOL	v	202[A]	-	5,5,5	1.27	0	5,5,5	0.72	0
29	PL9	D	405[B]	-	55,55,55	0.63	2 (3%)	68,69,69	1.67	17 (25%)
25	BCR	H	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.44	7 (12%)
32	LHG	D	407[B]	-	48,48,48	0.91	2 (4%)	51,54,54	1.00	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LHG	d	412[B]	-	48,48,48	0.92	2 (4%)	51,54,54	1.08	5 (9%)
25	BCR	Y	101	-	41,41,41	0.99	1 (2%)	56,56,56	1.73	12 (21%)
34	LMG	C	520	-	51,51,55	0.92	2 (3%)	59,59,63	1.12	4 (6%)
23	CLA	c	504	3	69,73,73	2.08	19 (27%)	83,113,113	2.85	28 (33%)
35	HTG	b	622	-	19,19,19	1.15	2 (10%)	23,24,24	1.94	7 (30%)
23	CLA	c	507	3	69,73,73	2.03	20 (28%)	83,113,113	2.78	30 (36%)
35	HTG	V	202	-	11,11,19	0.31	0	15,15,24	1.01	1 (6%)
27	GOL	a	417	-	5,5,5	1.14	0	5,5,5	1.06	1 (20%)
23	CLA	B	607	41	69,73,73	1.97	21 (30%)	83,113,113	2.84	31 (37%)
23	CLA	A	405[A]	41	69,73,73	1.93	18 (26%)	83,113,113	2.88	33 (39%)
23	CLA	C	506	3	69,73,73	2.00	19 (27%)	83,113,113	2.81	30 (36%)
27	GOL	A	418	-	5,5,5	1.42	1 (20%)	5,5,5	0.96	1 (20%)
23	CLA	b	603	2	69,73,73	2.01	20 (28%)	83,113,113	2.90	34 (40%)
27	GOL	d	411	-	5,5,5	0.98	0	5,5,5	1.10	0
27	GOL	l	102[B]	-	5,5,5	0.91	0	5,5,5	0.96	0
23	CLA	a	406[B]	41	69,73,73	2.01	19 (27%)	83,113,113	2.89	30 (36%)
28	OEX	a	412[B]	1,3,41	0,14,14	-	-	-	-	-
33	LMT	T	101	-	36,36,36	1.06	3 (8%)	47,47,47	1.06	3 (6%)
23	CLA	b	610	41	69,73,73	2.02	20 (28%)	83,113,113	2.82	33 (39%)
35	HTG	c	522	-	19,19,19	0.94	1 (5%)	23,24,24	1.64	3 (13%)
23	CLA	b	606	2	69,73,73	1.97	19 (27%)	83,113,113	2.92	31 (37%)
23	CLA	c	514	3	69,73,73	2.10	21 (30%)	83,113,113	2.86	32 (38%)
29	PL9	A	414[A]	-	55,55,55	0.68	2 (3%)	68,69,69	2.08	25 (36%)
25	BCR	B	618	-	41,41,41	0.97	1 (2%)	56,56,56	1.37	9 (16%)
32	LHG	L	102[A]	-	48,48,48	0.89	2 (4%)	51,54,54	1.15	3 (5%)
23	CLA	C	510	3	69,73,73	2.06	19 (27%)	83,113,113	2.83	31 (37%)
23	CLA	b	608	2	69,73,73	1.98	19 (27%)	83,113,113	2.76	32 (38%)
24	PHO	a	415[B]	-	58,69,69	2.79	14 (24%)	56,99,99	2.90	16 (28%)
28	OEX	A	413[B]	1,3,41	0,14,14	-	-	-	-	-
32	LHG	A	419[A]	-	48,48,48	0.84	2 (4%)	51,54,54	1.31	6 (11%)
26	SQD	F	103	-	42,43,54	1.19	4 (9%)	51,54,65	2.14	14 (27%)
25	BCR	T	102	-	41,41,41	1.00	1 (2%)	56,56,56	1.57	12 (21%)
26	SQD	a	410[A]	-	53,54,54	0.95	3 (5%)	62,65,65	1.77	13 (20%)
25	BCR	C	516	-	41,41,41	1.03	1 (2%)	56,56,56	1.29	6 (10%)
36	DGD	C	517[A]	-	63,63,67	0.81	2 (3%)	77,77,81	1.21	8 (10%)
27	GOL	A	411	-	5,5,5	1.11	0	5,5,5	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	HTG	D	410	-	16,16,19	1.04	1 (6%)	20,21,24	1.59	1 (5%)
23	CLA	B	611	2	69,73,73	2.55	19 (27%)	83,113,113	4.09	31 (37%)
23	CLA	D	402[A]	4	69,73,73	1.98	19 (27%)	83,113,113	2.88	31 (37%)
23	CLA	A	406[B]	41	69,73,73	2.05	19 (27%)	83,113,113	2.84	32 (38%)
34	LMG	C	501	-	51,51,55	0.92	2 (3%)	59,59,63	1.44	7 (11%)
23	CLA	B	614	2	69,73,73	2.02	20 (28%)	83,113,113	3.01	30 (36%)
23	CLA	c	502	3	69,73,73	1.97	19 (27%)	83,113,113	2.83	30 (36%)
33	LMT	B	629	-	25,25,36	0.89	2 (8%)	30,30,47	1.14	3 (10%)
27	GOL	B	625	-	5,5,5	1.01	0	5,5,5	0.95	0
34	LMG	c	521	-	51,51,55	1.00	2 (3%)	59,59,63	1.37	7 (11%)
25	BCR	y	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.68	13 (23%)
23	CLA	D	403	4	69,73,73	2.10	19 (27%)	83,113,113	2.86	34 (40%)
23	CLA	B	604	2	69,73,73	2.00	21 (30%)	83,113,113	2.68	30 (36%)
32	LHG	b	630[A]	-	48,48,48	0.85	3 (6%)	51,54,54	1.03	4 (7%)
25	BCR	a	409	-	41,41,41	1.02	1 (2%)	56,56,56	1.35	7 (12%)
24	PHO	A	407[A]	-	58,69,69	2.69	14 (24%)	56,99,99	2.78	15 (26%)
23	CLA	d	403	4	69,73,73	2.03	20 (28%)	83,113,113	2.89	31 (37%)
23	CLA	B	615	2	69,73,73	1.99	18 (26%)	83,113,113	2.90	28 (33%)
29	PL9	D	405[A]	-	55,55,55	0.62	2 (3%)	68,69,69	1.64	18 (26%)
32	LHG	D	407[A]	-	48,48,48	0.92	2 (4%)	51,54,54	0.99	4 (7%)
32	LHG	E	101[B]	-	41,41,48	1.05	2 (4%)	44,47,54	1.10	4 (9%)
34	LMG	z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.05	2 (4%)
33	LMT	a	416	-	36,36,36	1.00	1 (2%)	47,47,47	1.01	1 (2%)
23	CLA	A	408	1	69,73,73	1.97	19 (27%)	83,113,113	2.99	35 (42%)
26	SQD	L	101	-	53,54,54	1.06	4 (7%)	62,65,65	1.75	10 (16%)
23	CLA	b	607	41	69,73,73	1.99	20 (28%)	83,113,113	2.77	29 (34%)
23	CLA	c	503	3	69,73,73	1.97	18 (26%)	83,113,113	2.71	29 (34%)
31	BCT	d	401[B]	21	2,3,3	0.60	0	2,3,3	1.27	0
33	LMT	b	627	-	25,25,36	0.87	0	30,30,47	1.12	3 (10%)
28	OEX	a	412[A]	1,3,41	0,14,14	-	-	-	-	-
27	GOL	l	102[A]	-	5,5,5	0.96	0	5,5,5	0.97	0
23	CLA	a	406[A]	41	69,73,73	1.96	19 (27%)	83,113,113	2.86	30 (36%)
33	LMT	F	101	-	36,36,36	1.08	1 (2%)	47,47,47	1.06	3 (6%)
35	HTG	d	409	-	16,16,19	1.01	1 (6%)	20,21,24	1.60	2 (10%)
33	LMT	m	103	-	36,36,36	1.03	2 (5%)	47,47,47	1.08	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	GOL	O	303	-	5,5,5	1.00	0	5,5,5	1.07	1 (20%)
23	CLA	C	508	41	69,73,73	1.95	19 (27%)	83,113,113	2.84	29 (34%)
26	SQD	b	620	-	53,54,54	1.05	3 (5%)	62,65,65	1.69	12 (19%)
23	CLA	B	608	2	69,73,73	1.92	19 (27%)	83,113,113	2.86	34 (40%)
24	PHO	a	415[A]	-	58,69,69	2.75	14 (24%)	56,99,99	3.01	17 (30%)
28	OEX	A	413[A]	1,3,41	0,14,14	-	-	-	-	-
25	BCR	c	515	-	41,41,41	0.98	1 (2%)	56,56,56	1.64	11 (19%)
34	LMG	C	521	-	51,51,55	1.06	3 (5%)	59,59,63	1.34	6 (10%)
26	SQD	a	411	-	53,54,54	1.07	3 (5%)	62,65,65	1.19	8 (12%)
27	GOL	V	203[B]	-	5,5,5	1.01	0	5,5,5	0.94	0
23	CLA	B	605	2	69,73,73	2.01	19 (27%)	83,113,113	2.95	30 (36%)
23	CLA	B	609	2	69,73,73	2.01	18 (26%)	83,113,113	2.80	29 (34%)
24	PHO	a	407[B]	-	58,69,69	2.77	12 (20%)	56,99,99	2.71	15 (26%)
25	BCR	t	102	-	41,41,41	1.00	1 (2%)	56,56,56	1.67	13 (23%)
29	PL9	a	413[B]	-	55,55,55	0.64	2 (3%)	68,69,69	1.90	22 (32%)
23	CLA	A	404[B]	1	69,73,73	2.05	20 (28%)	83,113,113	2.85	31 (37%)
23	CLA	B	602	2	69,73,73	2.02	20 (28%)	83,113,113	2.83	31 (37%)
25	BCR	b	617	-	41,41,41	1.04	1 (2%)	56,56,56	1.37	5 (8%)
34	LMG	D	411	39	51,51,55	0.82	3 (5%)	59,59,63	1.04	3 (5%)
35	HTG	B	621	-	19,19,19	0.77	1 (5%)	23,24,24	1.49	1 (4%)
33	LMT	A	420	-	36,36,36	1.03	2 (5%)	47,47,47	1.14	4 (8%)
23	CLA	A	406[A]	41	69,73,73	1.99	18 (26%)	83,113,113	2.86	32 (38%)
32	LHG	D	406[B]	-	48,48,48	0.85	2 (4%)	51,54,54	0.99	3 (5%)
27	GOL	C	523[B]	-	5,5,5	1.31	0	5,5,5	0.75	0
23	CLA	C	512	3	69,73,73	2.01	20 (28%)	83,113,113	2.77	28 (33%)
31	BCT	A	416[A]	21	2,3,3	0.54	0	2,3,3	1.81	1 (50%)
32	LHG	d	407[B]	-	48,48,48	0.91	2 (4%)	51,54,54	1.03	3 (5%)
23	CLA	C	514	3	69,73,73	2.03	20 (28%)	83,113,113	2.80	31 (37%)
23	CLA	c	506	3	69,73,73	2.03	18 (26%)	83,113,113	2.75	28 (33%)
25	BCR	K	102	-	41,41,41	1.06	1 (2%)	56,56,56	1.43	10 (17%)
26	SQD	A	410[B]	-	53,54,54	0.93	3 (5%)	62,65,65	1.77	11 (17%)
34	LMG	m	101	-	51,51,55	0.87	2 (3%)	59,59,63	1.29	7 (11%)
23	CLA	b	613	2	69,73,73	1.95	18 (26%)	83,113,113	2.80	31 (37%)
23	CLA	C	509	3	69,73,73	2.05	21 (30%)	83,113,113	2.79	27 (32%)
25	BCR	h	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.43	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	GOL	b	628	-	5,5,5	0.31	0	5,5,5	1.43	1 (20%)
32	LHG	E	101[A]	-	41,41,48	1.06	2 (4%)	44,47,54	1.11	3 (6%)
34	LMG	B	620	-	51,51,55	0.92	2 (3%)	59,59,63	1.34	5 (8%)
33	LMT	M	101	-	36,36,36	1.10	3 (8%)	47,47,47	1.17	4 (8%)
27	GOL	b	624	-	5,5,5	1.12	1 (20%)	5,5,5	0.79	0
25	BCR	C	515	-	41,41,41	1.04	1 (2%)	56,56,56	1.42	8 (14%)
33	LMT	D	401	-	36,36,36	0.93	2 (5%)	47,47,47	1.07	2 (4%)
23	CLA	c	510	3	69,73,73	2.04	18 (26%)	83,113,113	2.84	31 (37%)
23	CLA	a	405[B]	41	69,73,73	2.07	18 (26%)	83,113,113	2.81	32 (38%)
31	BCT	d	401[A]	21	2,3,3	0.57	0	2,3,3	1.58	1 (50%)
32	LHG	d	412[A]	-	48,48,48	0.89	2 (4%)	51,54,54	1.12	4 (7%)
23	CLA	B	601	41	69,73,73	2.08	20 (28%)	83,113,113	2.90	30 (36%)
32	LHG	a	419[B]	-	41,41,48	1.03	2 (4%)	44,47,54	0.94	2 (4%)
23	CLA	b	615	2	69,73,73	1.97	18 (26%)	83,113,113	2.86	31 (37%)
33	LMT	B	626	-	36,36,36	1.18	4 (11%)	47,47,47	1.38	5 (10%)
36	DGD	H	102	-	63,63,67	0.86	4 (6%)	77,77,81	1.03	6 (7%)
23	CLA	c	512	3	69,73,73	2.06	21 (30%)	83,113,113	2.86	33 (39%)
23	CLA	c	505	41	69,73,73	2.06	21 (30%)	83,113,113	2.84	30 (36%)
27	GOL	v	202[B]	-	5,5,5	1.07	0	5,5,5	0.84	0
23	CLA	B	616	2	69,73,73	1.99	20 (28%)	83,113,113	2.91	28 (33%)
23	CLA	b	604	2	69,73,73	2.03	21 (30%)	83,113,113	2.74	28 (33%)
23	CLA	B	612	2	69,73,73	2.03	21 (30%)	83,113,113	2.82	30 (36%)
23	CLA	C	504	3	69,73,73	2.00	19 (27%)	83,113,113	2.89	29 (34%)
23	CLA	b	605	2	69,73,73	1.95	18 (26%)	83,113,113	2.98	30 (36%)
27	GOL	V	203[A]	-	5,5,5	1.22	0	5,5,5	0.91	0
24	PHO	a	407[A]	-	58,69,69	2.72	12 (20%)	56,99,99	2.76	15 (26%)
23	CLA	A	404[A]	1	69,73,73	1.98	20 (28%)	83,113,113	2.82	32 (38%)
23	CLA	b	612	2	69,73,73	2.01	20 (28%)	83,113,113	2.75	30 (36%)
23	CLA	A	405[B]	41	69,73,73	2.01	19 (27%)	83,113,113	2.78	31 (37%)
36	DGD	c	517[B]	-	63,63,67	0.86	2 (3%)	77,77,81	1.07	5 (6%)
27	GOL	B	627	-	5,5,5	0.97	0	5,5,5	1.01	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HTG	C	522	-	-	0/10/30/30	0/1/1/1
24	PHO	A	417[B]	-	-	1/37/103/103	0/5/6/6
26	SQD	A	412	-	-	12/49/69/69	0/1/1/1
36	DGD	h	102	-	-	13/51/91/95	0/2/2/2
35	HTG	o	301	-	-	3/10/30/30	0/1/1/1
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
27	GOL	c	526[B]	-	-	0/4/4/4	-
27	GOL	C	523[A]	-	-	0/4/4/4	-
34	LMG	d	410	39	-	9/46/66/70	0/1/1/1
23	CLA	B	610	41	-	10/39/115/115	-
27	GOL	o	304	-	-	2/4/4/4	-
32	LHG	d	407[A]	-	-	11/53/53/53	-
38	HEM	F	102	6,5	-	6/14/54/54	-
23	CLA	C	511	3	-	14/39/115/115	-
23	CLA	C	505	41	-	7/39/115/115	-
26	SQD	A	410[A]	-	-	12/49/69/69	0/1/1/1
23	CLA	b	602	2	-	4/39/115/115	-
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
35	HTG	b	625	-	-	4/10/30/30	0/1/1/1
23	CLA	b	614	2	-	14/39/115/115	-
23	CLA	a	404[B]	1	-	4/39/115/115	-
23	CLA	a	408	1	-	9/39/115/115	-
32	LHG	d	406[B]	-	-	15/53/53/53	-
35	HTG	b	623	-	-	3/10/30/30	0/1/1/1
25	BCR	d	404	-	-	4/29/63/63	0/2/2/2
25	BCR	D	404	-	-	4/29/63/63	0/2/2/2
23	CLA	d	402[B]	4	-	4/39/115/115	-
36	DGD	c	519	-	-	9/51/91/95	0/2/2/2
34	LMG	c	501	-	-	14/46/66/70	0/1/1/1
23	CLA	b	611	2	-	3/39/115/115	-
32	LHG	a	419[A]	-	-	16/46/46/53	-
27	GOL	c	527	-	-	3/4/4/4	-
36	DGD	C	518[B]	-	-	13/51/91/95	0/2/2/2
29	PL9	d	405[B]	-	-	9/53/73/73	0/1/1/1
24	PHO	A	407[B]	-	-	2/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	DGD	c	518[B]	-	-	17/51/91/95	0/2/2/2
40	HEC	v	201	16	1/1/3/7	6/14/54/54	-
27	GOL	O	302	-	-	2/4/4/4	-
25	BCR	c	516	-	-	0/29/63/63	0/2/2/2
38	HEM	f	101	6,5	-	6/14/54/54	-
36	DGD	c	517[A]	-	-	20/51/91/95	0/2/2/2
23	CLA	c	513	3	-	15/39/115/115	-
33	LMT	b	621	-	-	8/17/37/61	0/1/1/2
24	PHO	A	417[A]	-	-	1/37/103/103	0/5/6/6
25	BCR	b	619	-	-	5/29/63/63	0/2/2/2
23	CLA	C	507	3	-	10/39/115/115	-
29	PL9	a	413[A]	-	-	14/53/73/73	0/1/1/1
23	CLA	c	509	3	-	4/39/115/115	-
27	GOL	c	526[A]	-	-	0/4/4/4	-
36	DGD	C	519	-	-	15/51/91/95	0/2/2/2
26	SQD	f	102	-	-	11/38/58/69	0/1/1/1
23	CLA	b	616	2	-	8/39/115/115	-
40	HEC	V	201	16	1/1/3/7	6/14/54/54	-
25	BCR	B	617	-	-	2/29/63/63	0/2/2/2
27	GOL	D	412	-	-	4/4/4/4	-
35	HTG	B	623	-	-	5/10/30/30	0/1/1/1
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2
32	LHG	D	406[A]	-	-	16/53/53/53	-
23	CLA	B	603	2	-	7/39/115/115	-
23	CLA	a	404[A]	1	-	3/39/115/115	-
32	LHG	d	406[A]	-	-	13/53/53/53	-
29	PL9	A	414[B]	-	-	16/53/73/73	0/1/1/1
33	LMT	t	101	-	-	9/17/38/61	0/1/1/2
23	CLA	B	606	2	-	10/39/115/115	-
32	LHG	L	102[B]	-	-	16/53/53/53	-
23	CLA	d	402[A]	4	-	2/39/115/115	-
23	CLA	C	503	3	-	11/39/115/115	-
23	CLA	C	502	3	-	6/39/115/115	-
23	CLA	c	511	3	-	10/39/115/115	-
27	GOL	a	418	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	513	3	-	12/39/115/115	-
32	LHG	A	419[B]	-	-	12/53/53/53	-
26	SQD	a	410[B]	-	-	10/49/69/69	0/1/1/1
23	CLA	b	609	2	-	3/39/115/115	-
34	LMG	c	520	-	-	12/46/66/70	0/1/1/1
36	DGD	C	517[B]	-	-	14/51/91/95	0/2/2/2
36	DGD	C	518[A]	-	-	15/51/91/95	0/2/2/2
23	CLA	D	402[B]	4	-	2/39/115/115	-
29	PL9	d	405[A]	-	-	6/53/73/73	0/1/1/1
34	LMG	Z	101	-	-	11/31/51/70	0/1/1/1
23	CLA	b	601	41	-	17/39/115/115	-
23	CLA	a	405[A]	41	-	8/39/115/115	-
36	DGD	c	518[A]	-	-	17/51/91/95	0/2/2/2
27	GOL	B	622	-	-	2/4/4/4	-
23	CLA	c	508	41	-	9/39/115/115	-
23	CLA	B	613	2	-	8/39/115/115	-
33	LMT	e	101	-	-	15/21/61/61	0/2/2/2
33	LMT	B	628	-	-	12/21/61/61	0/2/2/2
27	GOL	o	303	-	-	1/4/4/4	-
32	LHG	b	630[B]	-	-	20/53/53/53	-
27	GOL	v	202[A]	-	-	1/4/4/4	-
29	PL9	D	405[B]	-	-	8/53/73/73	0/1/1/1
25	BCR	H	101	-	-	2/29/63/63	0/2/2/2
32	LHG	D	407[B]	-	-	16/53/53/53	-
32	LHG	d	412[B]	-	-	11/53/53/53	-
25	BCR	Y	101	-	-	2/29/63/63	0/2/2/2
34	LMG	C	520	-	-	9/46/66/70	0/1/1/1
23	CLA	c	504	3	-	3/39/115/115	-
35	HTG	b	622	-	-	5/10/30/30	0/1/1/1
23	CLA	c	507	3	-	8/39/115/115	-
35	HTG	V	202	-	-	0/2/19/30	0/1/1/1
27	GOL	a	417	-	-	2/4/4/4	-
23	CLA	B	607	41	-	4/39/115/115	-
23	CLA	A	405[A]	41	-	4/39/115/115	-
23	CLA	C	506	3	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	GOL	A	418	-	-	2/4/4/4	-
23	CLA	b	603	2	-	5/39/115/115	-
27	GOL	d	411	-	-	3/4/4/4	-
27	GOL	l	102[B]	-	-	3/4/4/4	-
23	CLA	a	406[B]	41	-	7/39/115/115	-
33	LMT	T	101	-	-	7/21/61/61	0/2/2/2
35	HTG	c	522	-	-	2/10/30/30	0/1/1/1
23	CLA	b	610	41	-	5/39/115/115	-
23	CLA	b	606	2	-	14/39/115/115	-
23	CLA	c	514	3	-	12/39/115/115	-
29	PL9	A	414[A]	-	-	15/53/73/73	0/1/1/1
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
32	LHG	L	102[A]	-	-	19/53/53/53	-
23	CLA	C	510	3	-	5/39/115/115	-
23	CLA	b	608	2	-	4/39/115/115	-
24	PHO	a	415[B]	-	-	1/37/103/103	0/5/6/6
32	LHG	A	419[A]	-	-	10/53/53/53	-
26	SQD	F	103	-	-	15/38/58/69	0/1/1/1
25	BCR	T	102	-	-	3/29/63/63	0/2/2/2
26	SQD	a	410[A]	-	-	10/49/69/69	0/1/1/1
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
36	DGD	C	517[A]	-	-	11/51/91/95	0/2/2/2
27	GOL	A	411	-	-	2/4/4/4	-
35	HTG	D	410	-	-	3/7/27/30	0/1/1/1
23	CLA	B	611	2	-	2/39/115/115	-
23	CLA	D	402[A]	4	-	0/39/115/115	-
23	CLA	A	406[B]	41	-	6/39/115/115	-
34	LMG	C	501	-	-	11/46/66/70	0/1/1/1
23	CLA	B	614	2	-	13/39/115/115	-
23	CLA	c	502	3	-	4/39/115/115	-
33	LMT	B	629	-	-	11/17/37/61	0/1/1/2
27	GOL	B	625	-	-	1/4/4/4	-
34	LMG	c	521	-	-	13/46/66/70	0/1/1/1
25	BCR	y	101	-	-	5/29/63/63	0/2/2/2
23	CLA	D	403	4	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	604	2	-	2/39/115/115	-
32	LHG	b	630[A]	-	-	20/53/53/53	-
25	BCR	a	409	-	-	0/29/63/63	0/2/2/2
24	PHO	A	407[A]	-	-	3/37/103/103	0/5/6/6
23	CLA	d	403	4	-	8/39/115/115	-
23	CLA	B	615	2	-	7/39/115/115	-
29	PL9	D	405[A]	-	-	8/53/73/73	0/1/1/1
32	LHG	D	407[A]	-	-	14/53/53/53	-
32	LHG	E	101[B]	-	-	21/46/46/53	-
34	LMG	z	101	-	-	9/34/54/70	0/1/1/1
33	LMT	a	416	-	-	11/21/61/61	0/2/2/2
23	CLA	A	408	1	-	9/39/115/115	-
26	SQD	L	101	-	-	12/49/69/69	0/1/1/1
23	CLA	b	607	41	-	2/39/115/115	-
23	CLA	c	503	3	-	9/39/115/115	-
33	LMT	b	627	-	-	11/17/37/61	0/1/1/2
33	LMT	F	101	-	-	8/21/61/61	0/2/2/2
27	GOL	l	102[A]	-	-	2/4/4/4	-
23	CLA	a	406[A]	41	-	7/39/115/115	-
35	HTG	d	409	-	-	1/7/27/30	0/1/1/1
33	LMT	m	103	-	-	6/21/61/61	0/2/2/2
27	GOL	O	303	-	-	2/4/4/4	-
23	CLA	C	508	41	-	9/39/115/115	-
26	SQD	b	620	-	-	17/49/69/69	0/1/1/1
23	CLA	B	608	2	-	4/39/115/115	-
24	PHO	a	415[A]	-	-	1/37/103/103	0/5/6/6
25	BCR	c	515	-	-	1/29/63/63	0/2/2/2
34	LMG	C	521	-	-	13/46/66/70	0/1/1/1
26	SQD	a	411	-	-	14/49/69/69	0/1/1/1
27	GOL	V	203[B]	-	-	2/4/4/4	-
23	CLA	B	605	2	-	7/39/115/115	-
23	CLA	B	609	2	-	1/39/115/115	-
24	PHO	a	407[B]	-	-	5/37/103/103	0/5/6/6
25	BCR	t	102	-	-	3/29/63/63	0/2/2/2
29	PL9	a	413[B]	-	-	15/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	A	404[B]	1	-	6/39/115/115	-
23	CLA	B	602	2	-	9/39/115/115	-
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
34	LMG	D	411	39	-	10/46/66/70	0/1/1/1
35	HTG	B	621	-	-	4/10/30/30	0/1/1/1
33	LMT	A	420	-	-	15/21/61/61	0/2/2/2
23	CLA	A	406[A]	41	-	7/39/115/115	-
32	LHG	D	406[B]	-	-	19/53/53/53	-
27	GOL	C	523[B]	-	-	0/4/4/4	-
23	CLA	C	512	3	-	2/39/115/115	-
32	LHG	d	407[B]	-	-	13/53/53/53	-
23	CLA	C	514	3	-	7/39/115/115	-
23	CLA	c	506	3	-	7/39/115/115	-
25	BCR	K	102	-	-	0/29/63/63	0/2/2/2
26	SQD	A	410[B]	-	-	10/49/69/69	0/1/1/1
34	LMG	m	101	-	-	10/46/66/70	0/1/1/1
23	CLA	b	613	2	-	6/39/115/115	-
23	CLA	C	509	3	-	7/39/115/115	-
25	BCR	h	101	-	-	2/29/63/63	0/2/2/2
27	GOL	b	628	-	-	0/4/4/4	-
32	LHG	E	101[A]	-	-	22/46/46/53	-
34	LMG	B	620	-	-	14/46/66/70	0/1/1/1
33	LMT	M	101	-	-	5/21/61/61	0/2/2/2
27	GOL	b	624	-	-	2/4/4/4	-
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
33	LMT	D	401	-	-	6/21/61/61	0/2/2/2
23	CLA	c	510	3	-	14/39/115/115	-
23	CLA	a	405[B]	41	-	6/39/115/115	-
32	LHG	d	412[A]	-	-	13/53/53/53	-
23	CLA	B	601	41	-	11/39/115/115	-
32	LHG	a	419[B]	-	-	16/46/46/53	-
23	CLA	b	615	2	-	7/39/115/115	-
33	LMT	B	626	-	-	11/21/61/61	0/2/2/2
36	DGD	H	102	-	-	10/51/91/95	0/2/2/2
23	CLA	c	512	3	-	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	505	41	-	8/39/115/115	-
27	GOL	v	202[B]	-	-	2/4/4/4	-
23	CLA	B	616	2	-	5/39/115/115	-
23	CLA	b	604	2	-	11/39/115/115	-
23	CLA	B	612	2	-	7/39/115/115	-
23	CLA	C	504	3	-	4/39/115/115	-
23	CLA	b	605	2	-	7/39/115/115	-
27	GOL	V	203[A]	-	-	2/4/4/4	-
24	PHO	a	407[A]	-	-	5/37/103/103	0/5/6/6
23	CLA	A	404[A]	1	-	5/39/115/115	-
23	CLA	b	612	2	-	4/39/115/115	-
23	CLA	A	405[B]	41	-	4/39/115/115	-
36	DGD	c	517[B]	-	-	19/51/91/95	0/2/2/2
27	GOL	B	627	-	-	4/4/4/4	-

The worst 5 of 1860 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	407[B]	PHO	C1B-C2B	9.39	1.50	1.39
24	A	407[A]	PHO	C1D-C2D	9.11	1.49	1.39
24	a	415[B]	PHO	C1D-C2D	9.08	1.49	1.39
24	a	407[A]	PHO	C1B-C2B	8.96	1.49	1.39
24	a	415[B]	PHO	C1B-C2B	8.82	1.49	1.39

The worst 5 of 3339 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	C2B-C1B-NB	17.25	121.80	110.23
23	B	611	CLA	C3B-C2B-C1B	-13.68	90.65	107.16
23	B	611	CLA	C1D-ND-C4D	-12.02	97.79	106.33
24	a	415[A]	PHO	C2D-C1D-ND	11.91	117.75	109.53
24	A	417[B]	PHO	C2D-C1D-ND	11.65	117.57	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 1668 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	408	CLA	C4-C3-C5-C6
23	B	606	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CAD-CBD-CGD-O1D

There are no ring outliers.

173 monomers are involved in 354 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	417[B]	PHO	2	0
36	h	102	DGD	2	0
35	o	301	HTG	1	0
34	d	410	LMG	4	0
23	B	610	CLA	1	0
32	d	407[A]	LHG	10	0
38	F	102	HEM	1	0
23	C	511	CLA	3	0
23	C	505	CLA	1	0
26	A	410[A]	SQD	2	0
25	b	618	BCR	4	0
25	A	409	BCR	1	0
35	b	625	HTG	1	0
23	b	614	CLA	2	0
23	a	404[B]	CLA	4	0
23	a	408	CLA	5	0
32	d	406[B]	LHG	2	0
25	d	404	BCR	3	0
23	d	402[B]	CLA	2	0
36	c	519	DGD	2	0
34	c	501	LMG	1	0
32	a	419[A]	LHG	4	0
36	C	518[B]	DGD	1	0
36	c	518[B]	DGD	1	0
27	O	302	GOL	1	0
36	c	517[A]	DGD	2	0
23	c	513	CLA	6	0
33	b	621	LMT	1	0
24	A	417[A]	PHO	1	0
25	b	619	BCR	3	0
23	C	507	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	a	413[A]	PL9	4	0
23	c	509	CLA	7	0
36	C	519	DGD	2	0
26	f	102	SQD	1	0
23	b	616	CLA	1	0
40	V	201	HEC	1	0
25	B	617	BCR	1	0
27	D	412	GOL	2	0
35	B	623	HTG	1	0
25	k	101	BCR	2	0
32	D	406[A]	LHG	2	0
23	B	603	CLA	1	0
23	a	404[A]	CLA	3	0
32	d	406[A]	LHG	3	0
29	A	414[B]	PL9	7	0
33	t	101	LMT	2	0
23	B	606	CLA	1	0
23	d	402[A]	CLA	2	0
23	C	503	CLA	4	0
23	C	502	CLA	6	0
23	c	511	CLA	1	0
27	a	418	GOL	4	0
23	C	513	CLA	4	0
32	A	419[B]	LHG	1	0
26	a	410[B]	SQD	5	0
23	b	609	CLA	5	0
34	c	520	LMG	1	0
36	C	517[B]	DGD	2	0
36	C	518[A]	DGD	2	0
23	D	402[B]	CLA	4	0
34	Z	101	LMG	2	0
23	b	601	CLA	3	0
23	a	405[A]	CLA	2	0
36	c	518[A]	DGD	1	0
27	B	622	GOL	1	0
23	c	508	CLA	2	0
23	B	613	CLA	4	0
33	e	101	LMT	1	0
33	B	628	LMT	1	0
32	b	630[B]	LHG	1	0
27	v	202[A]	GOL	1	0
25	H	101	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	D	407[B]	LHG	3	0
25	Y	101	BCR	1	0
23	c	504	CLA	3	0
35	b	622	HTG	3	0
23	c	507	CLA	3	0
27	a	417	GOL	1	0
23	A	405[A]	CLA	4	0
23	C	506	CLA	5	0
27	A	418	GOL	3	0
23	b	603	CLA	1	0
27	l	102[B]	GOL	1	0
23	a	406[B]	CLA	2	0
35	c	522	HTG	1	0
23	b	606	CLA	1	0
23	c	514	CLA	3	0
29	A	414[A]	PL9	10	0
25	B	618	BCR	4	0
23	C	510	CLA	1	0
24	a	415[B]	PHO	1	0
32	A	419[A]	LHG	2	0
26	F	103	SQD	3	0
25	T	102	BCR	5	0
26	a	410[A]	SQD	4	0
36	C	517[A]	DGD	2	0
27	A	411	GOL	1	0
23	D	402[A]	CLA	3	0
23	A	406[B]	CLA	2	0
23	B	614	CLA	4	0
23	c	502	CLA	3	0
33	B	629	LMT	1	0
27	B	625	GOL	1	0
34	c	521	LMG	1	0
25	y	101	BCR	1	0
23	B	604	CLA	1	0
25	a	409	BCR	1	0
24	A	407[A]	PHO	2	0
23	d	403	CLA	1	0
23	B	615	CLA	7	0
32	D	407[A]	LHG	5	0
32	E	101[B]	LHG	3	0
34	z	101	LMG	2	0
33	a	416	LMT	2	0

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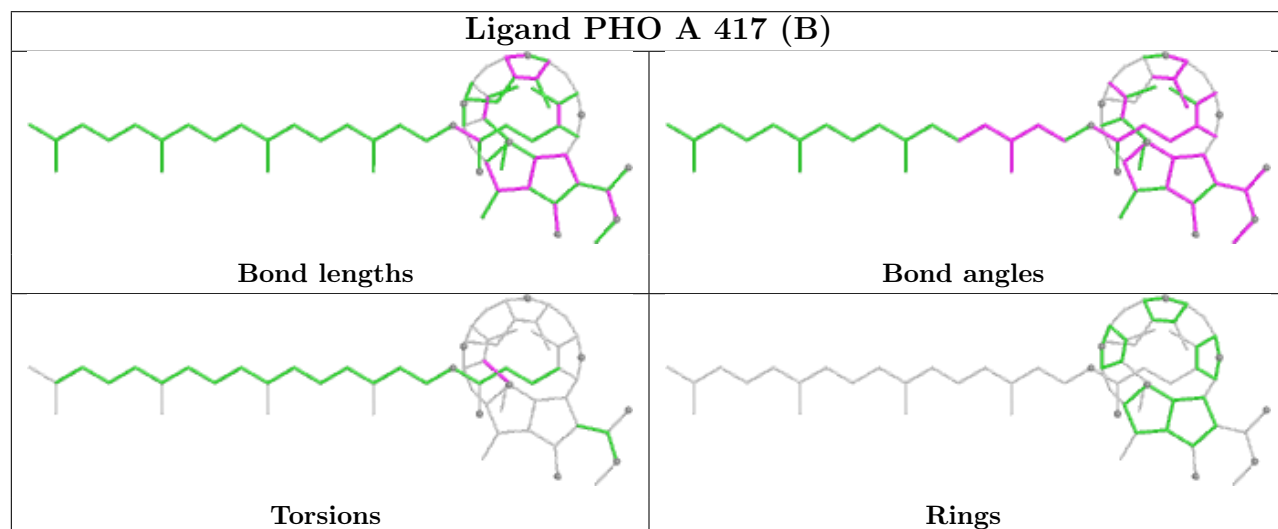
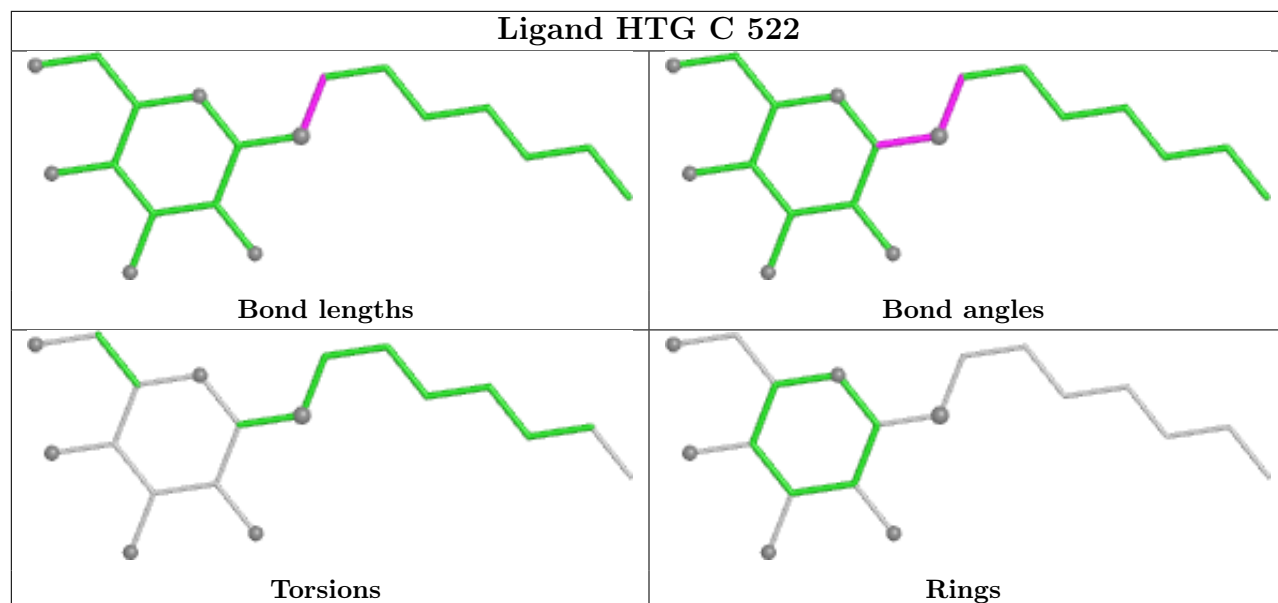
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	408	CLA	4	0
26	L	101	SQD	1	0
23	b	607	CLA	1	0
23	c	503	CLA	2	0
27	l	102[A]	GOL	1	0
23	a	406[A]	CLA	2	0
35	d	409	HTG	1	0
27	O	303	GOL	3	0
23	C	508	CLA	2	0
26	b	620	SQD	4	0
24	a	415[A]	PHO	2	0
25	c	515	BCR	1	0
34	C	521	LMG	2	0
26	a	411	SQD	2	0
23	B	605	CLA	4	0
23	B	609	CLA	2	0
24	a	407[B]	PHO	2	0
25	t	102	BCR	4	0
29	a	413[B]	PL9	6	0
23	A	404[B]	CLA	3	0
23	B	602	CLA	1	0
25	b	617	BCR	1	0
35	B	621	HTG	1	0
33	A	420	LMT	2	0
23	A	406[A]	CLA	1	0
32	D	406[B]	LHG	3	0
23	C	512	CLA	2	0
32	d	407[B]	LHG	10	0
23	C	514	CLA	2	0
23	c	506	CLA	6	0
25	K	102	BCR	1	0
26	A	410[B]	SQD	2	0
23	b	613	CLA	1	0
23	C	509	CLA	3	0
25	h	101	BCR	6	0
27	b	628	GOL	3	0
32	E	101[A]	LHG	3	0
33	M	101	LMT	2	0
25	C	515	BCR	1	0
33	D	401	LMT	1	0
23	c	510	CLA	3	0
23	a	405[B]	CLA	2	0

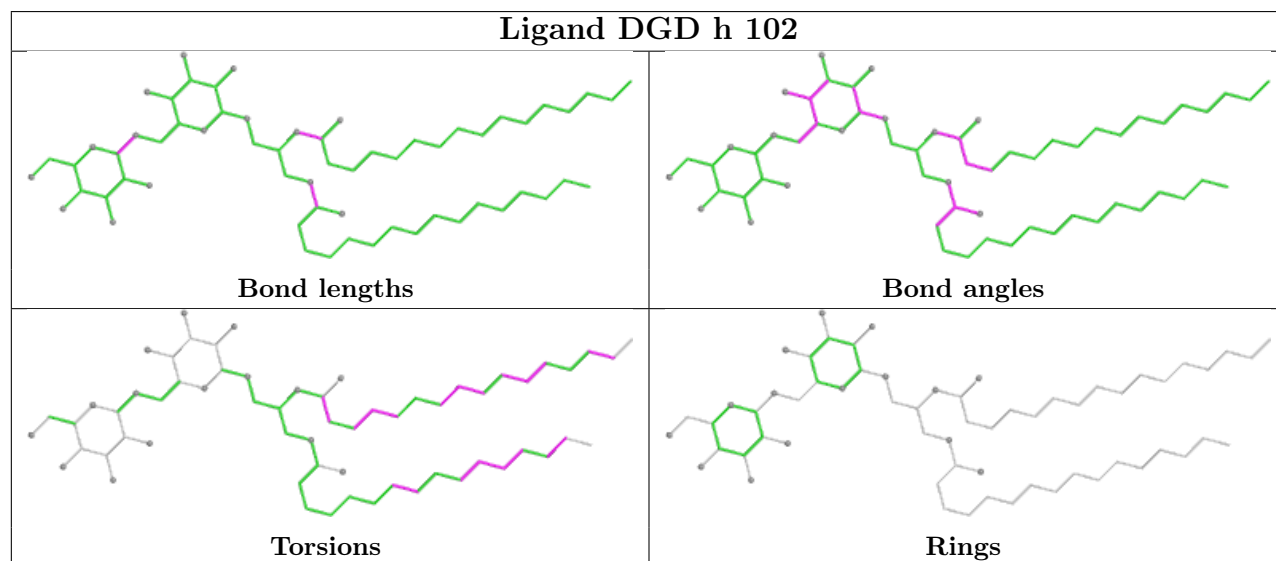
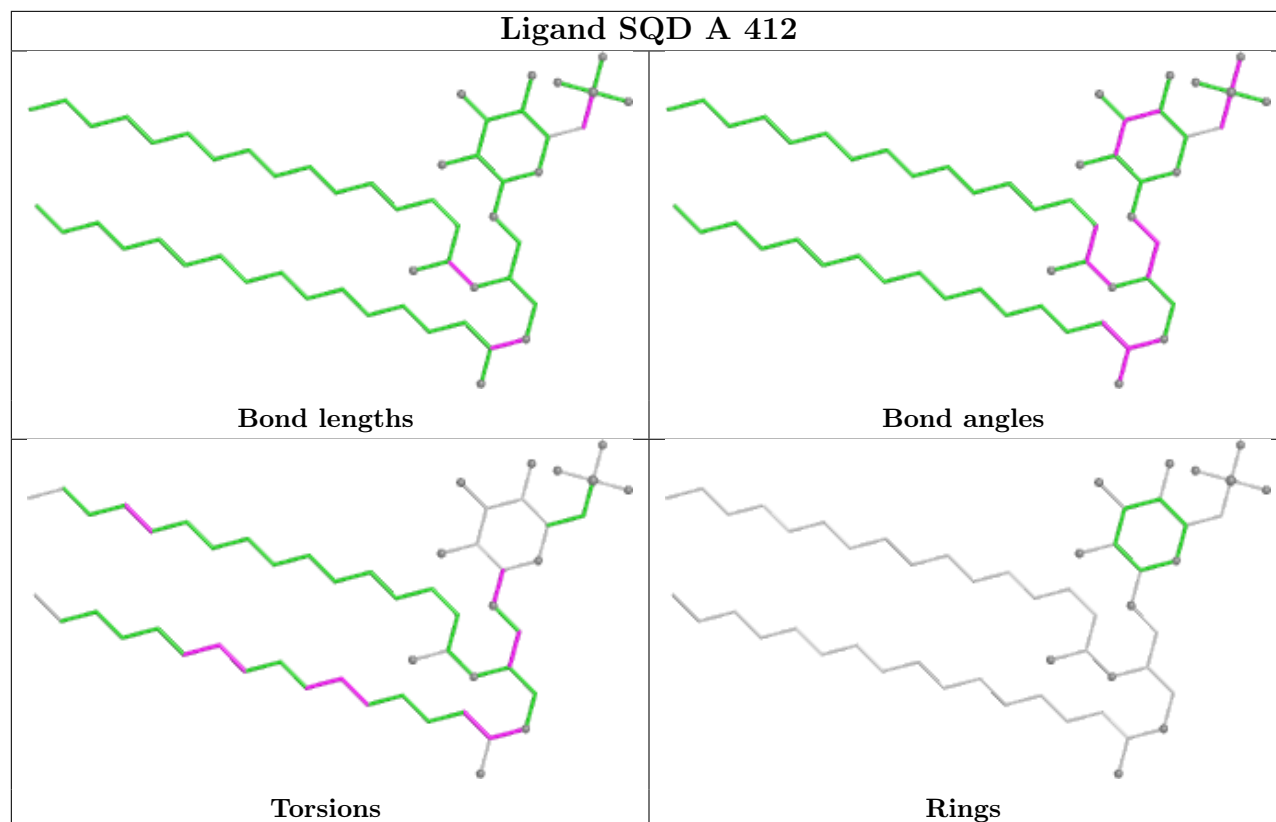
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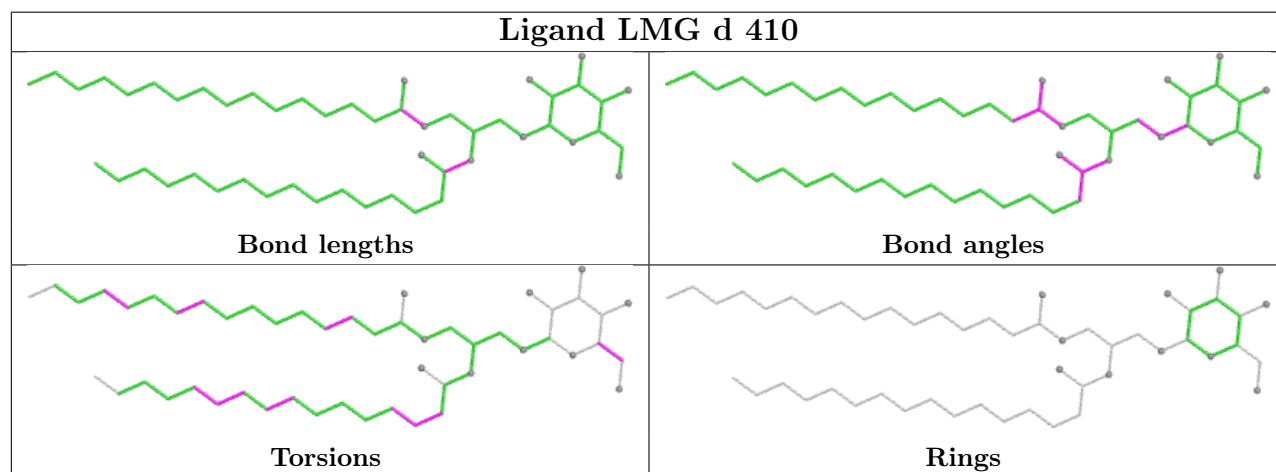
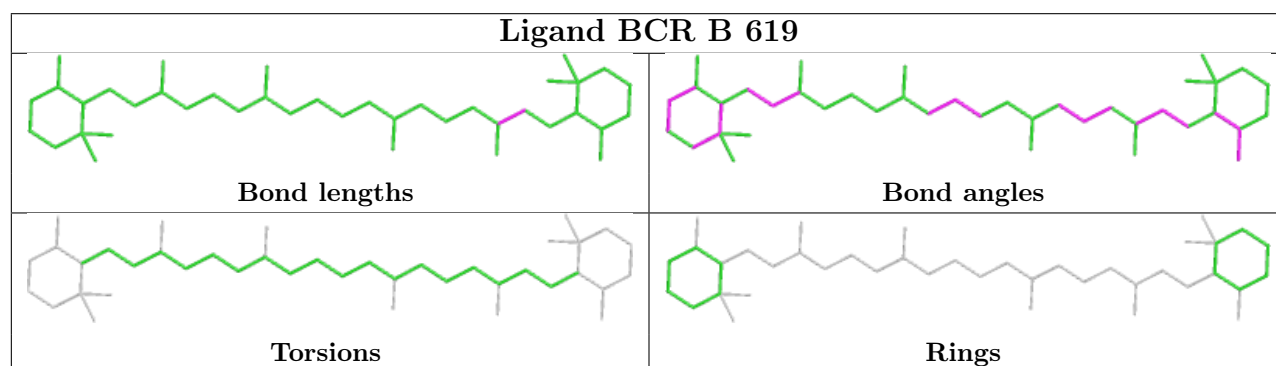
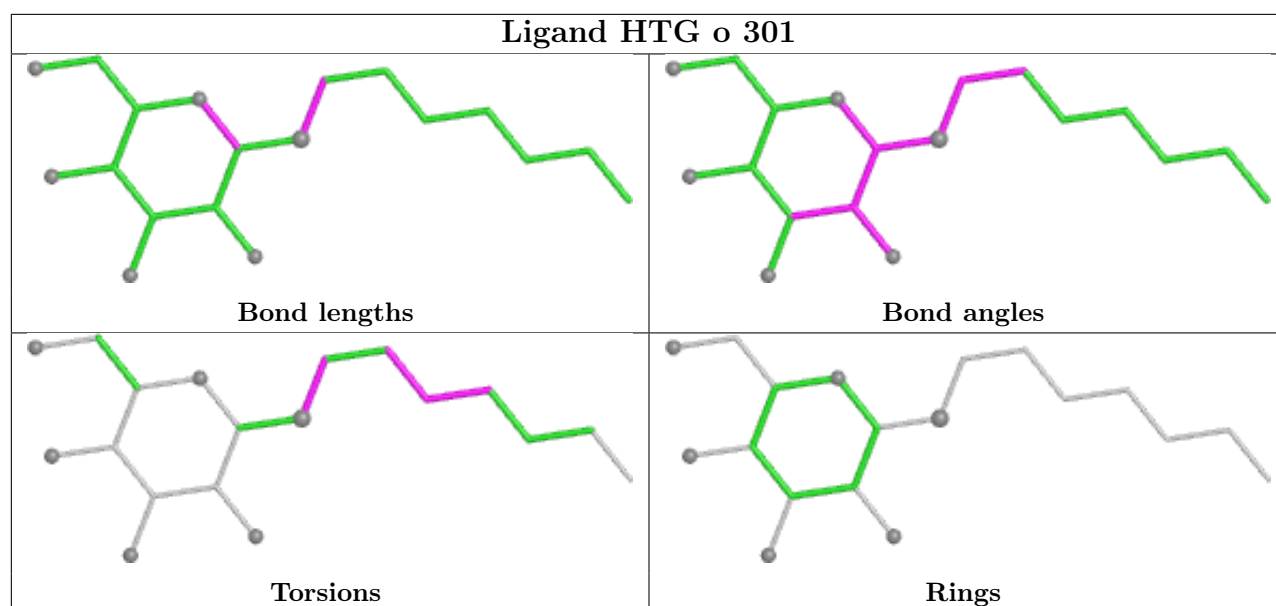
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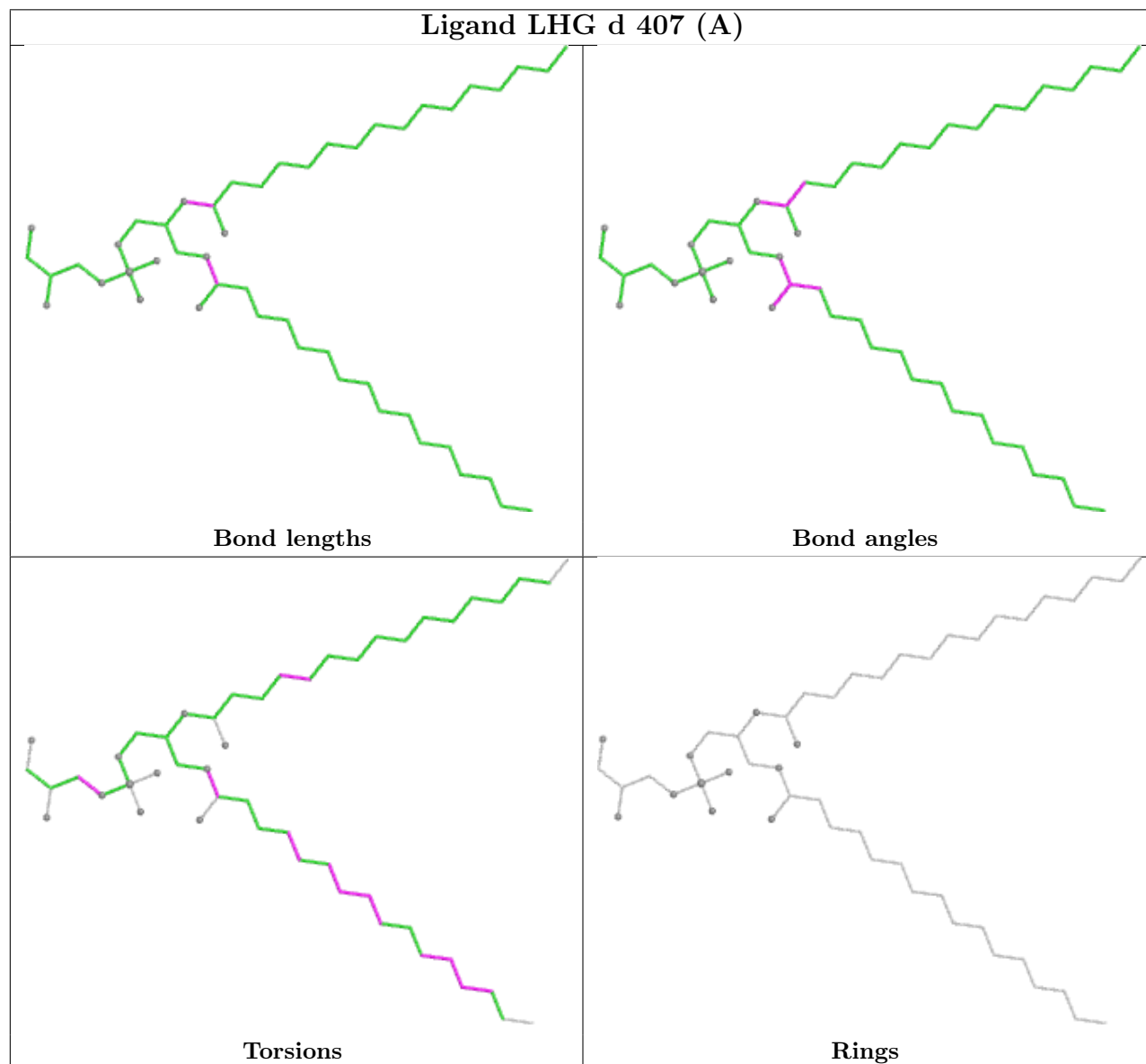
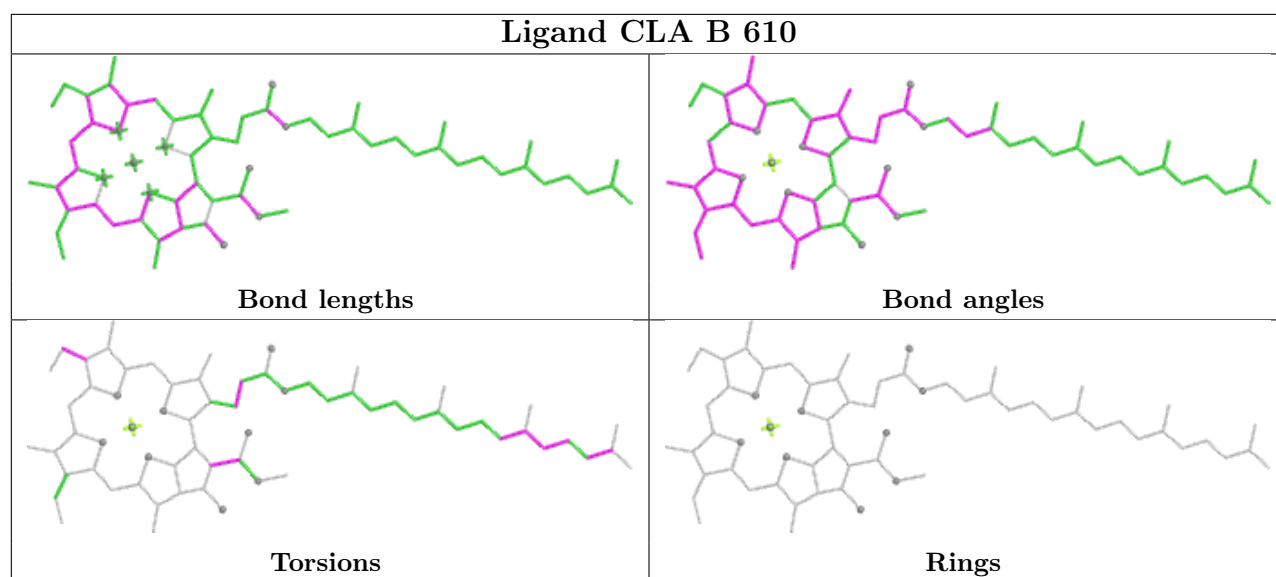
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	601	CLA	2	0
32	a	419[B]	LHG	4	0
23	b	615	CLA	2	0
33	B	626	LMT	1	0
36	H	102	DGD	1	0
23	c	512	CLA	6	0
23	c	505	CLA	2	0
27	v	202[B]	GOL	2	0
23	B	616	CLA	4	0
23	b	604	CLA	1	0
23	C	504	CLA	5	0
23	b	605	CLA	3	0
23	A	404[A]	CLA	5	0
23	b	612	CLA	1	0
23	A	405[B]	CLA	3	0
36	c	517[B]	DGD	2	0

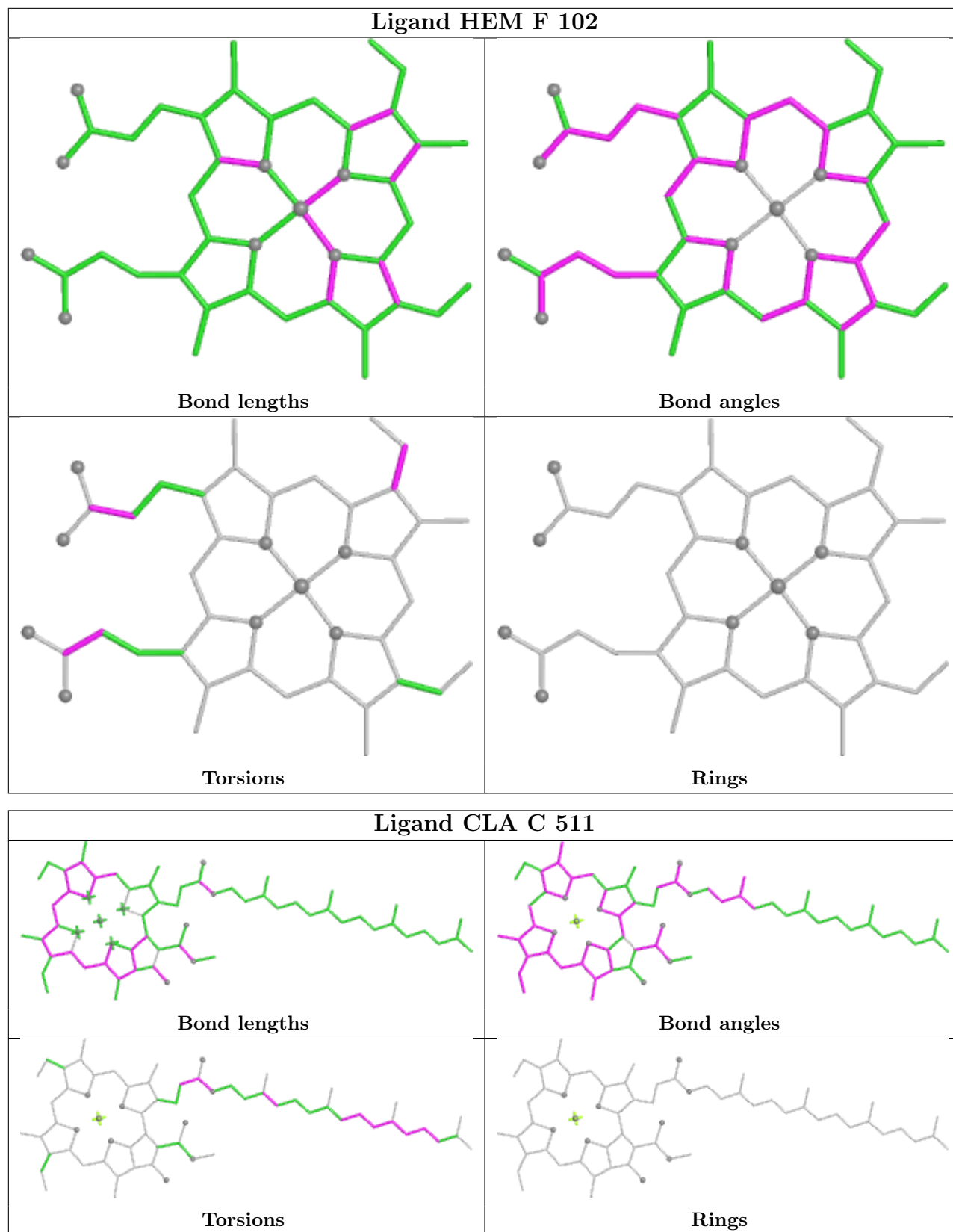
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

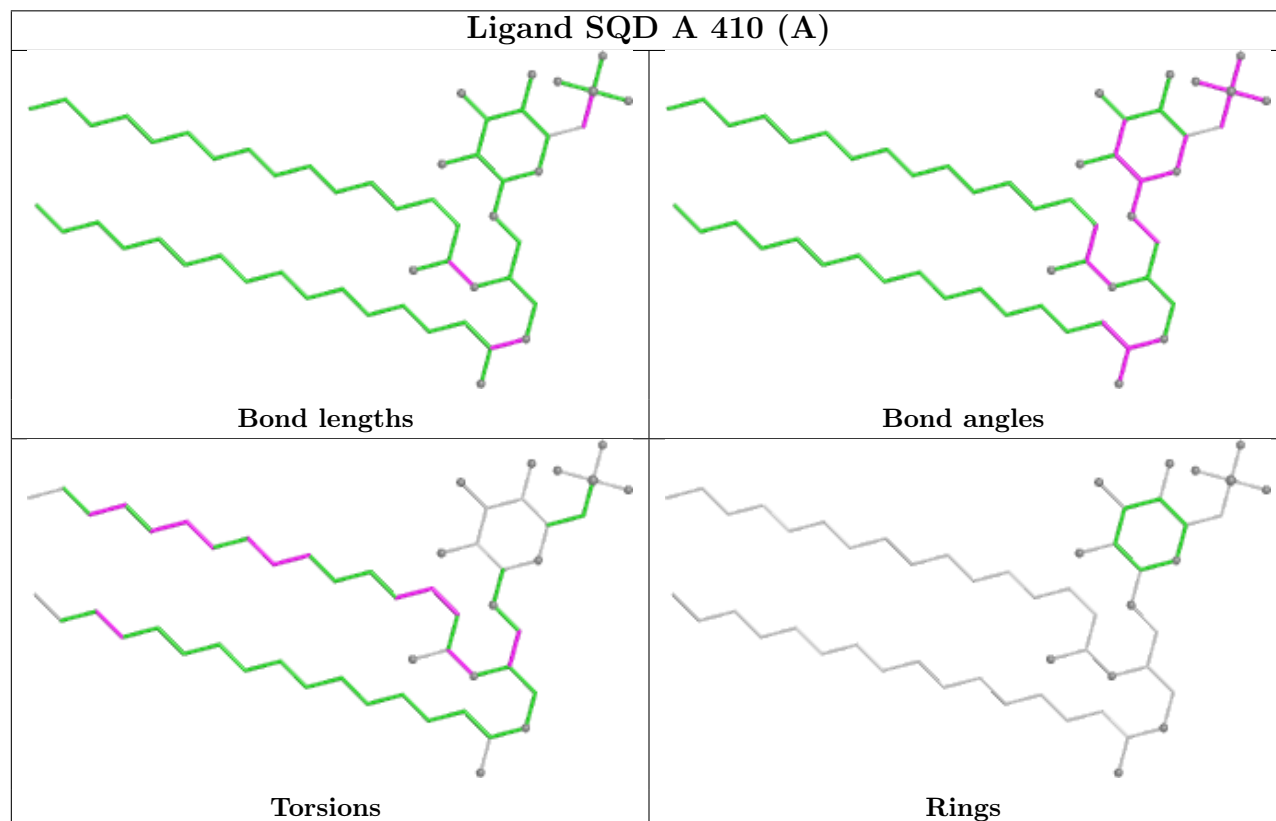
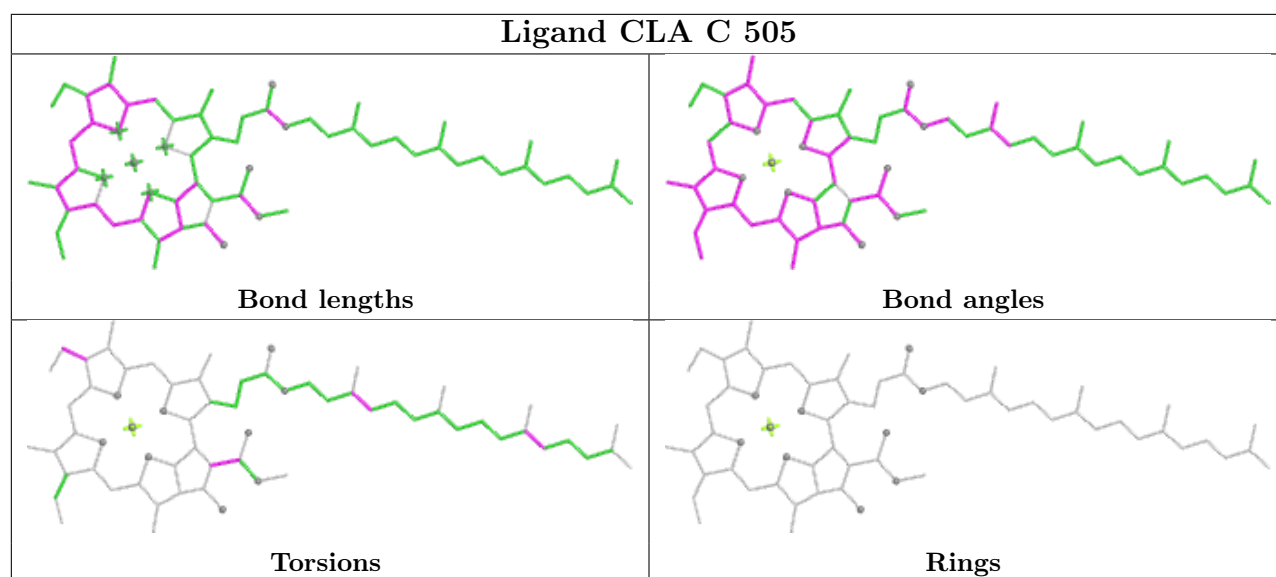


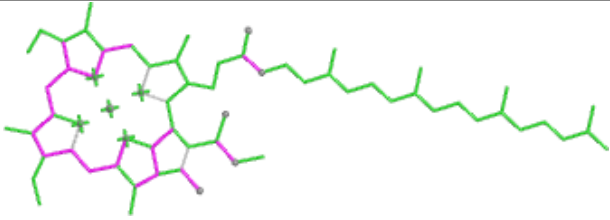
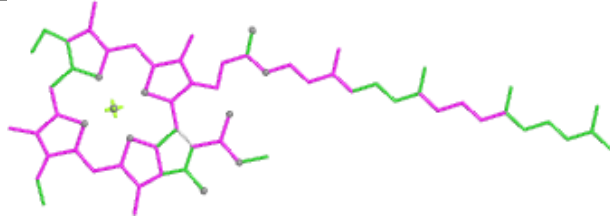
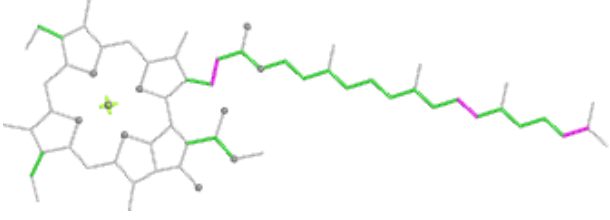
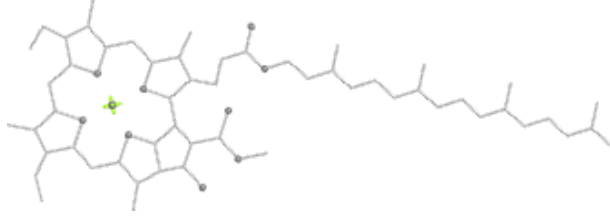
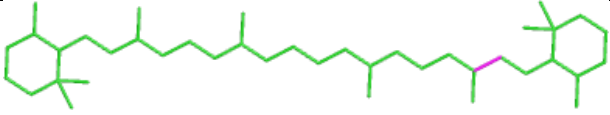
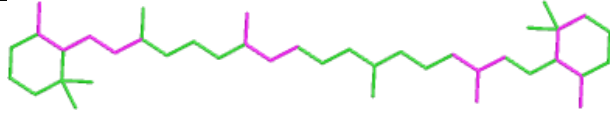
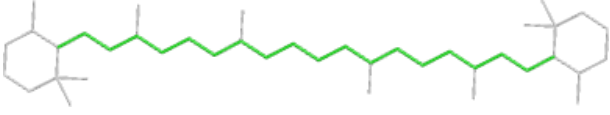
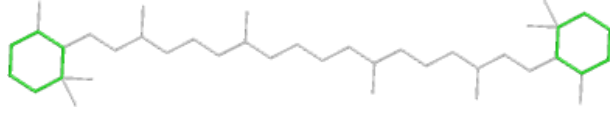
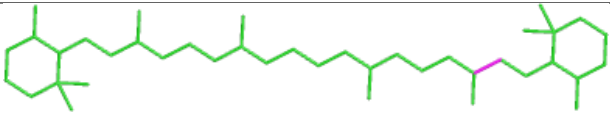
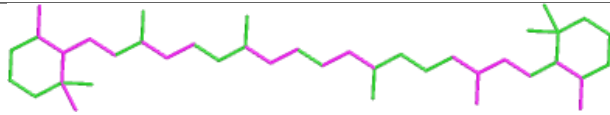
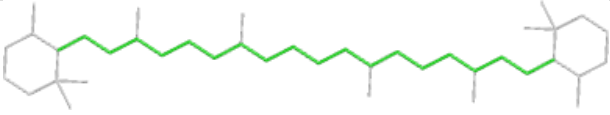
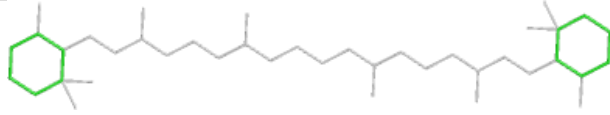


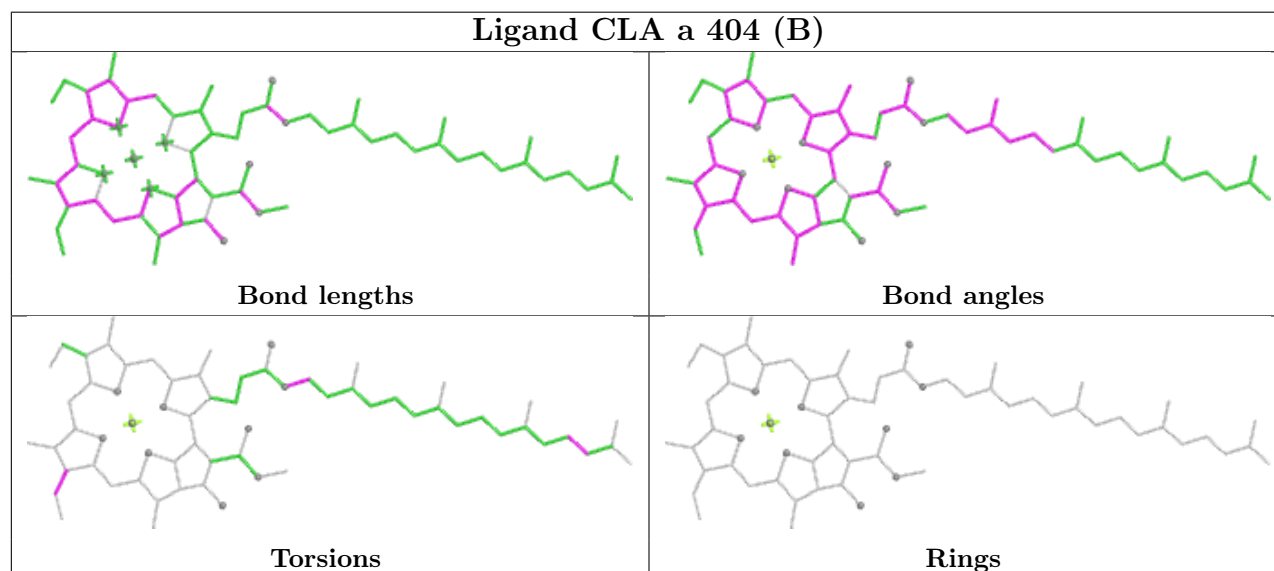
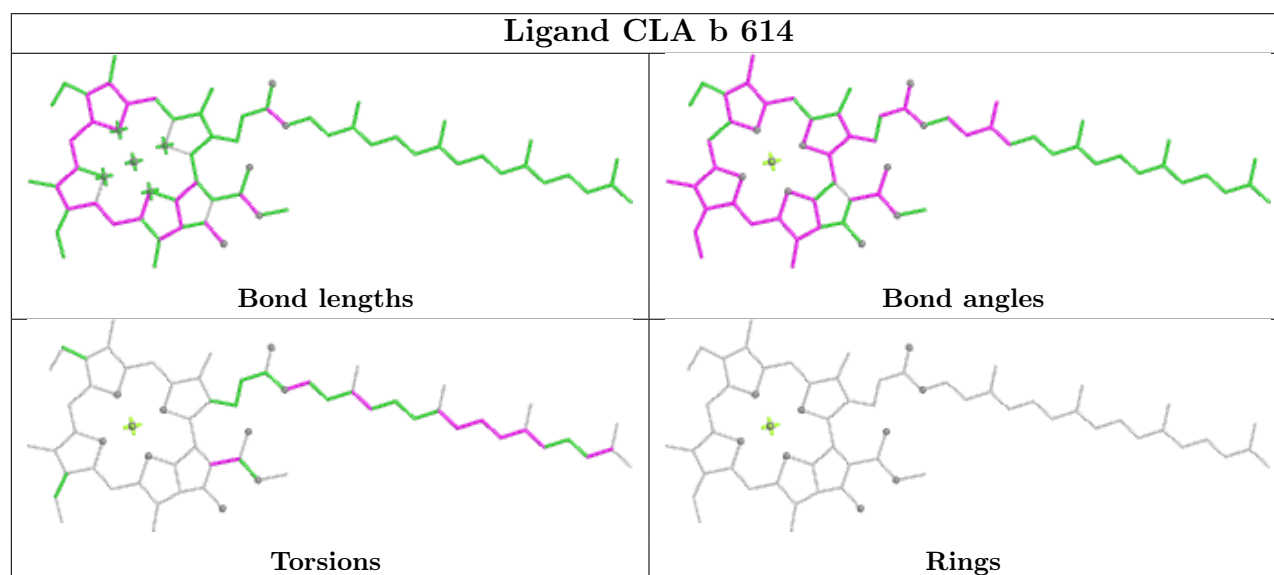
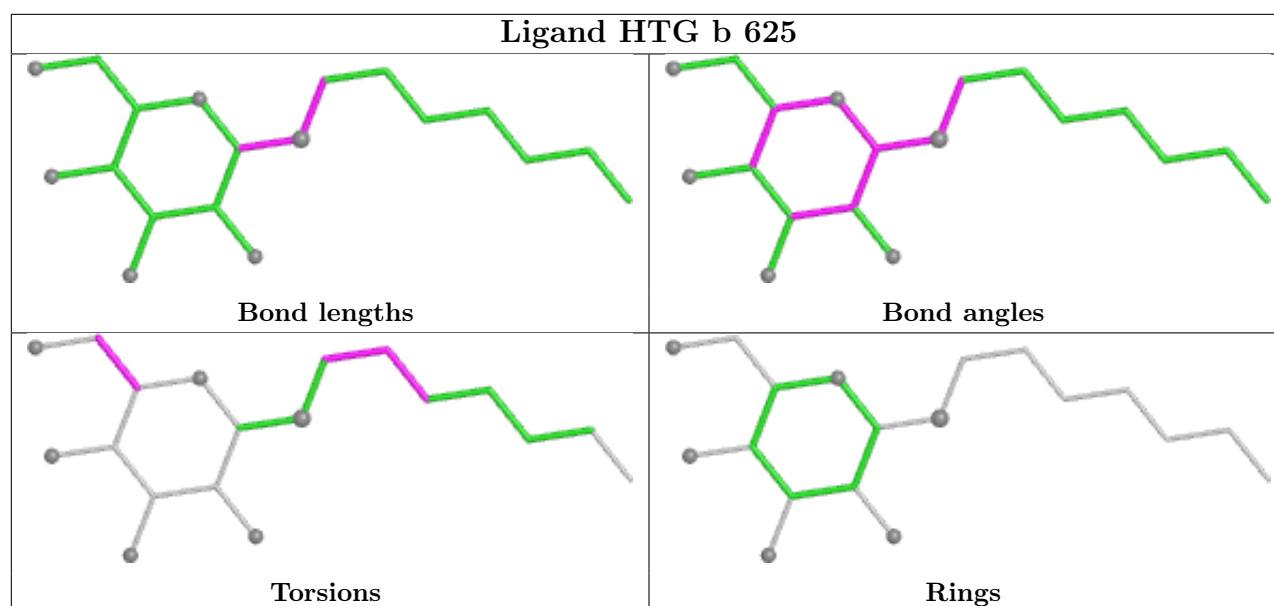


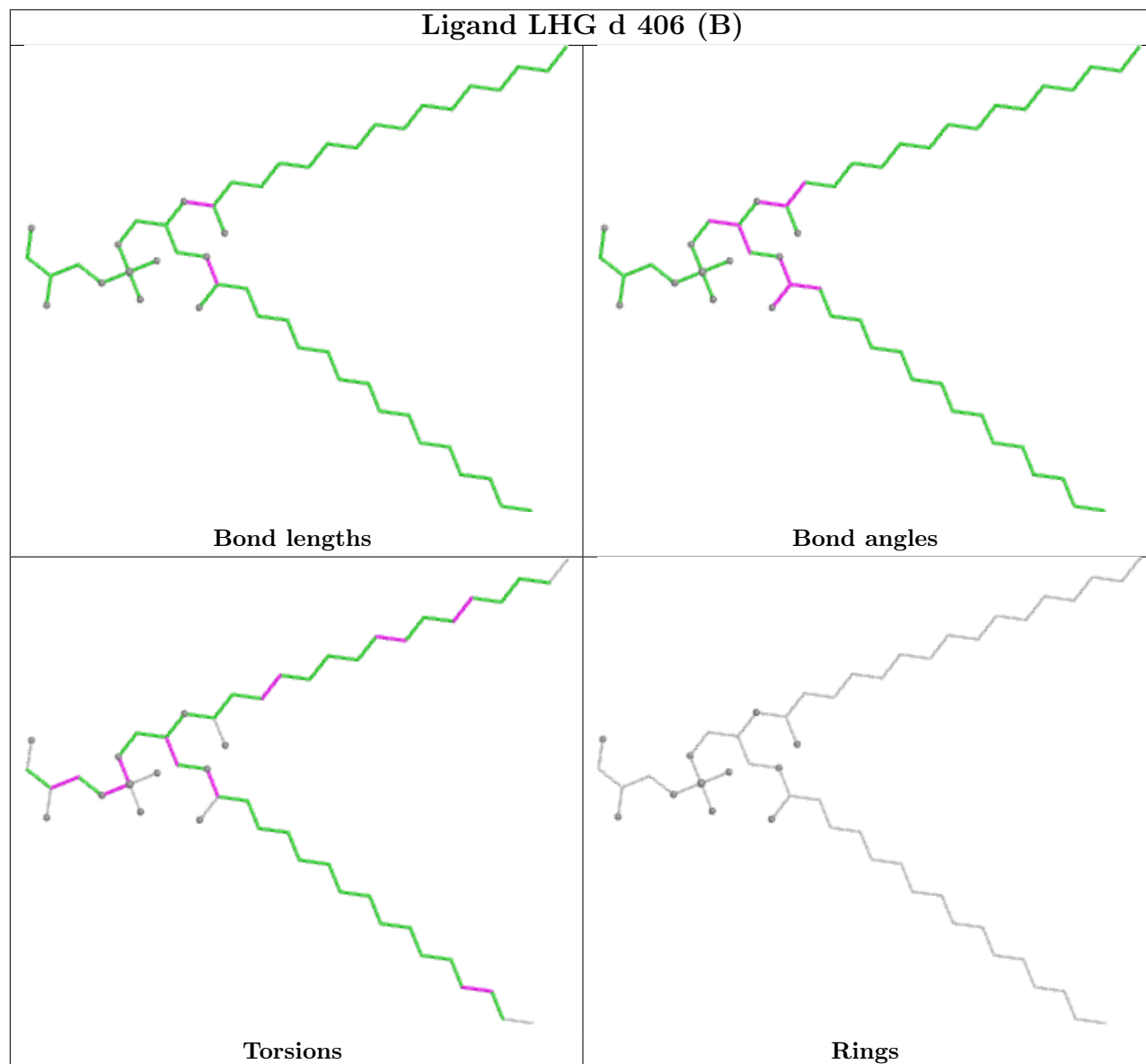
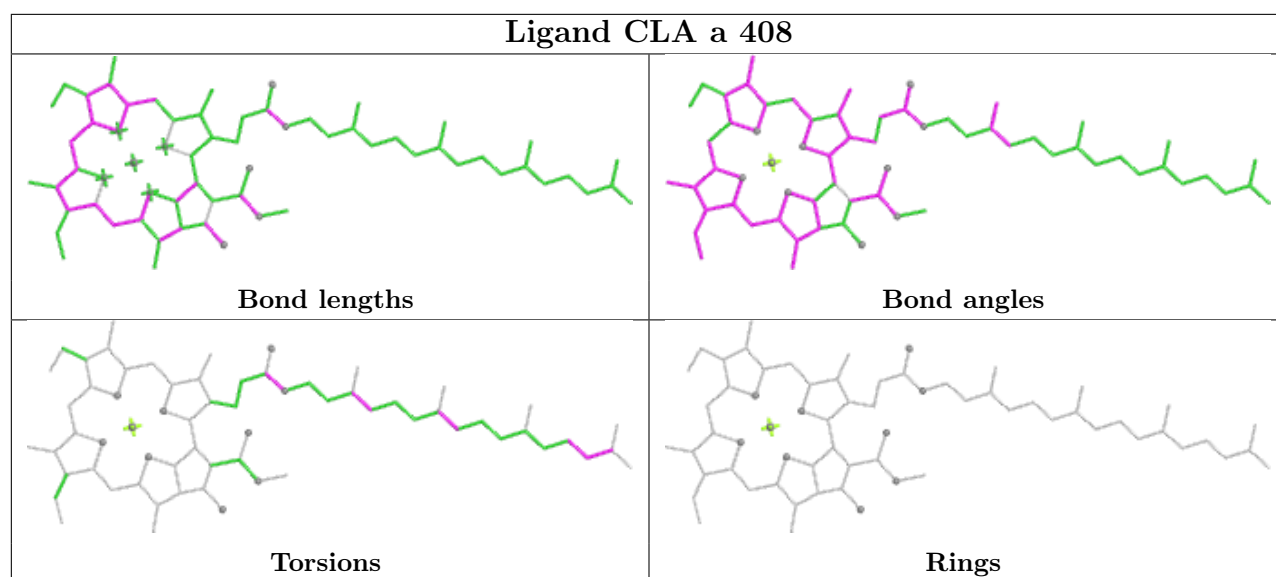


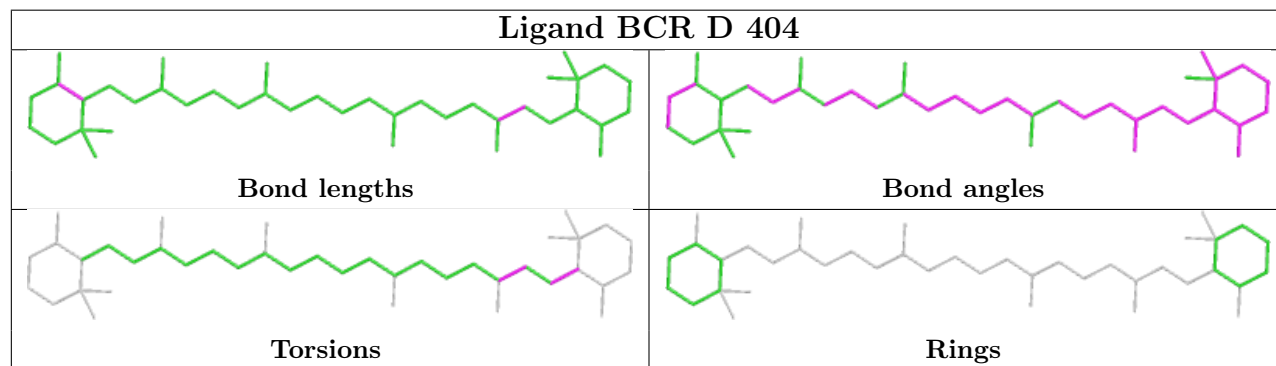
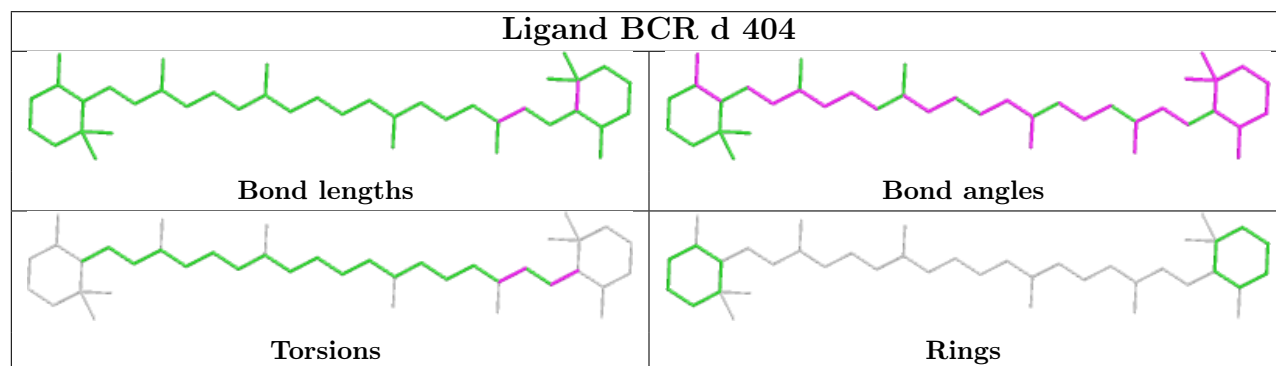
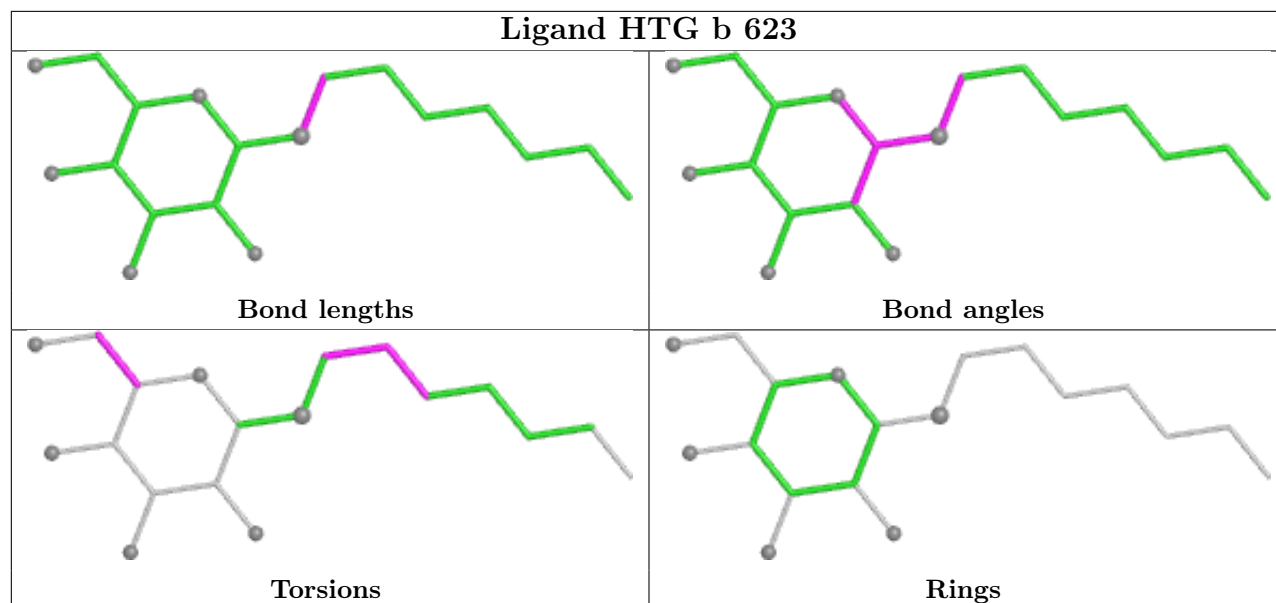


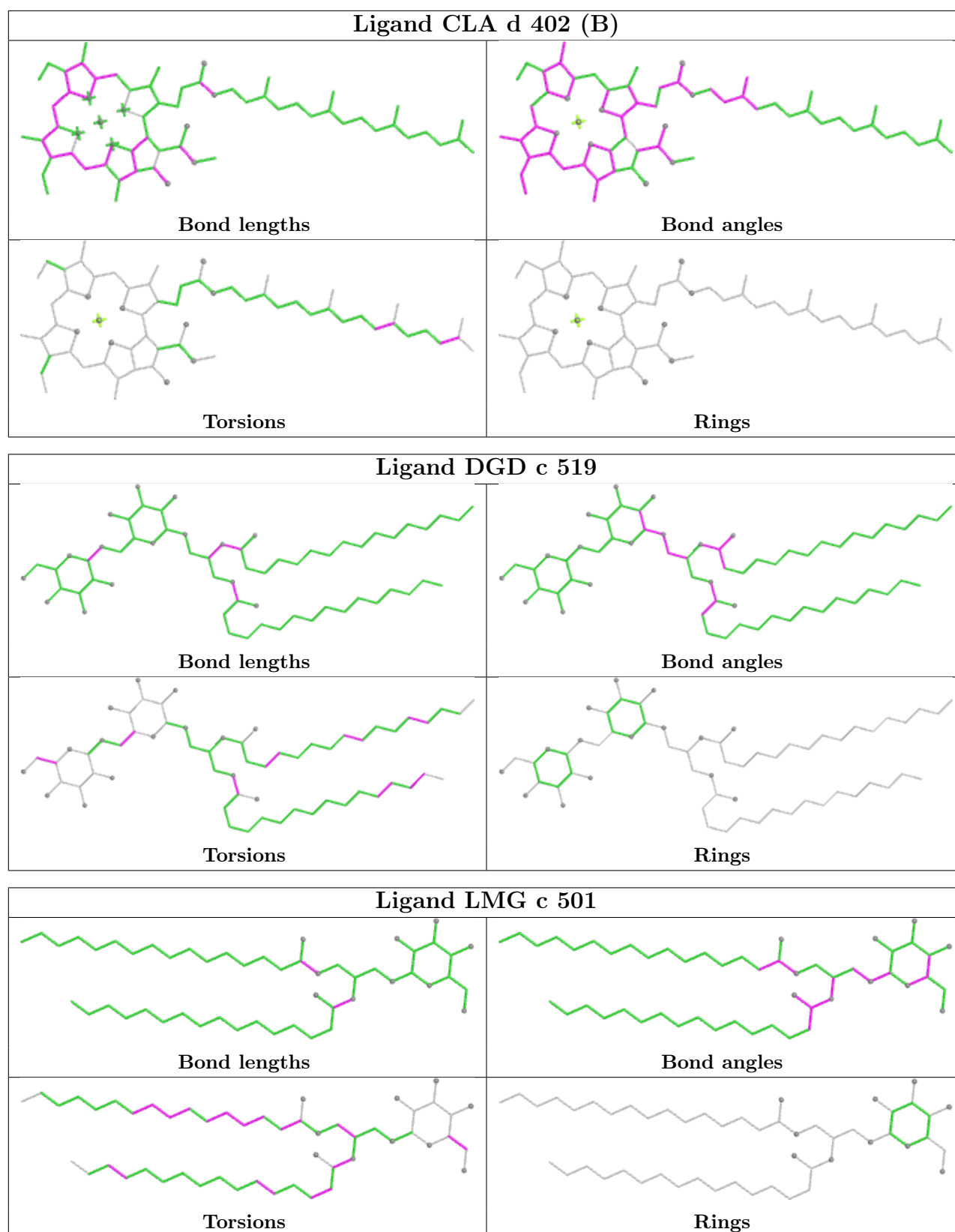


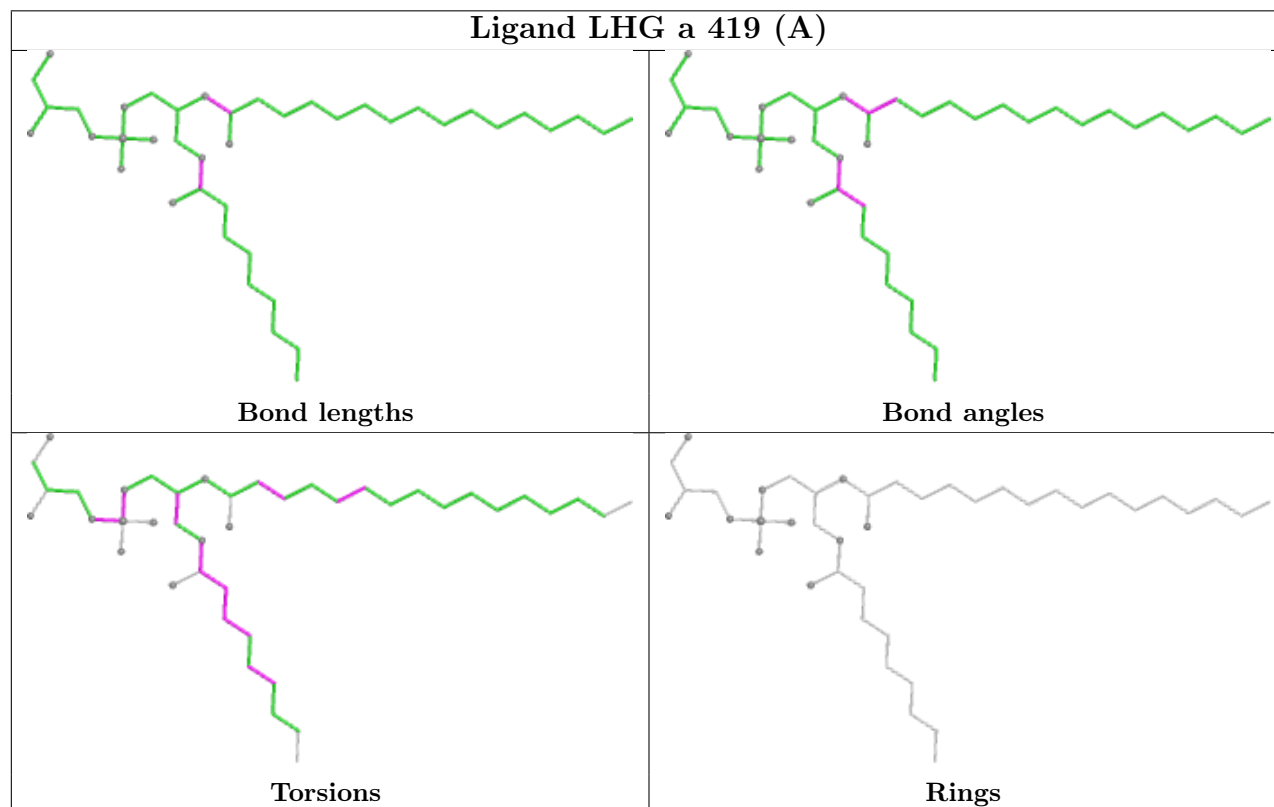
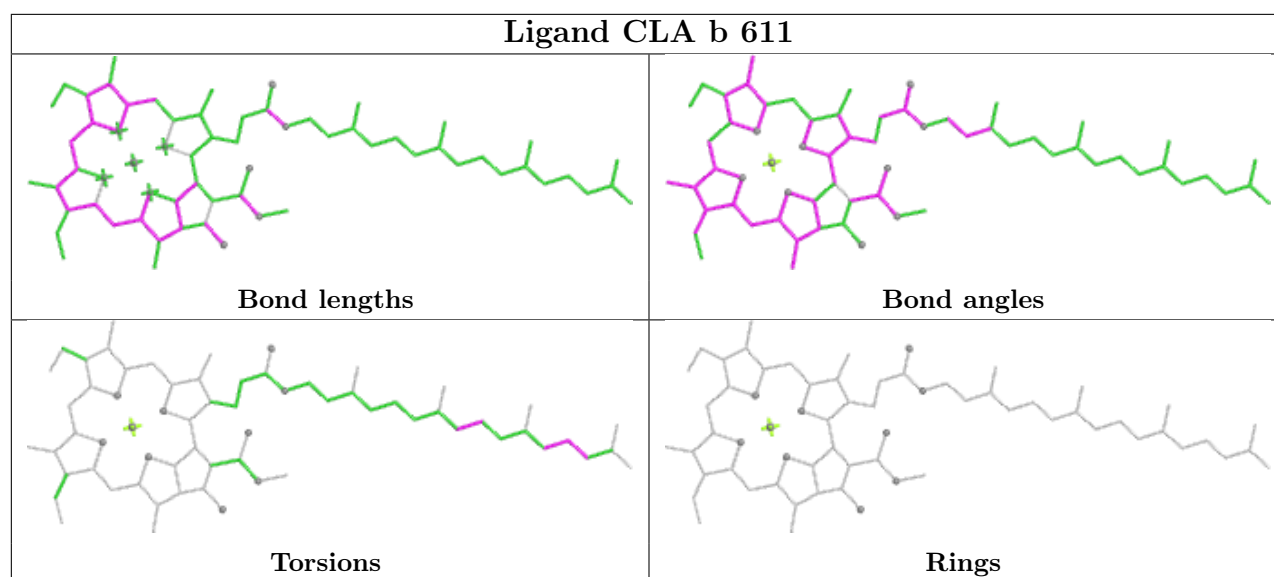
Ligand CLA b 602	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b 618	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR A 409	
 Bond lengths	 Bond angles
 Torsions	 Rings

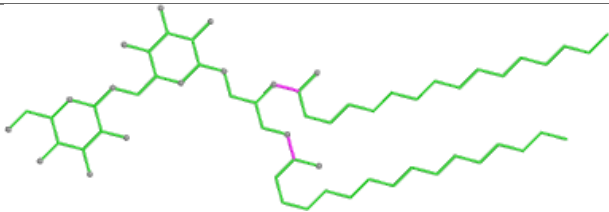
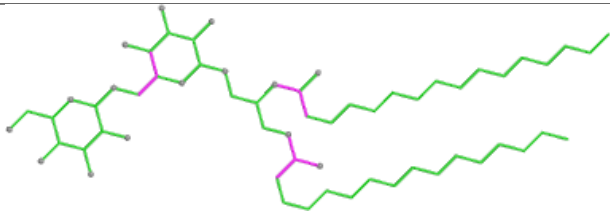
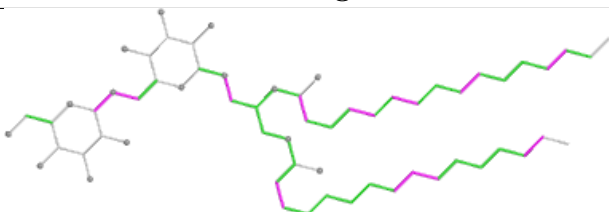
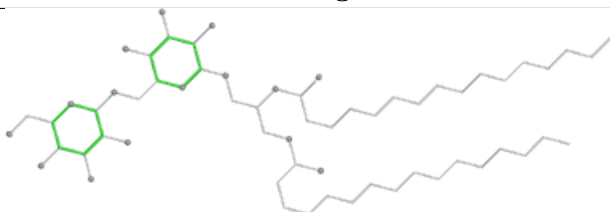


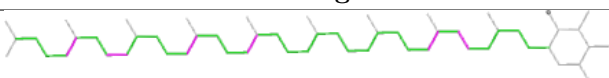
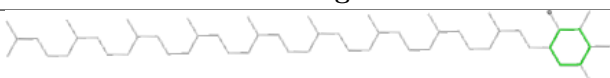


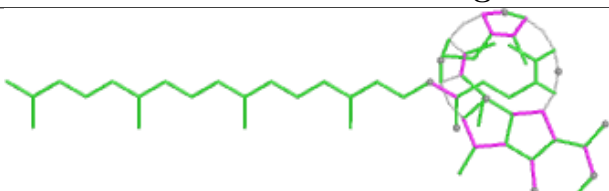
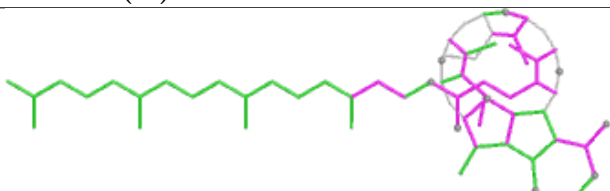
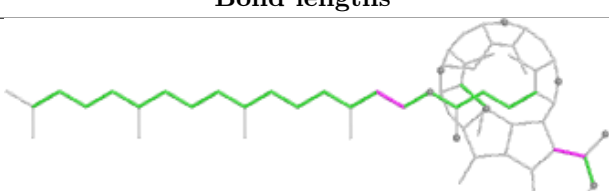
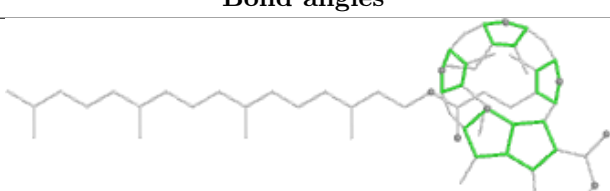


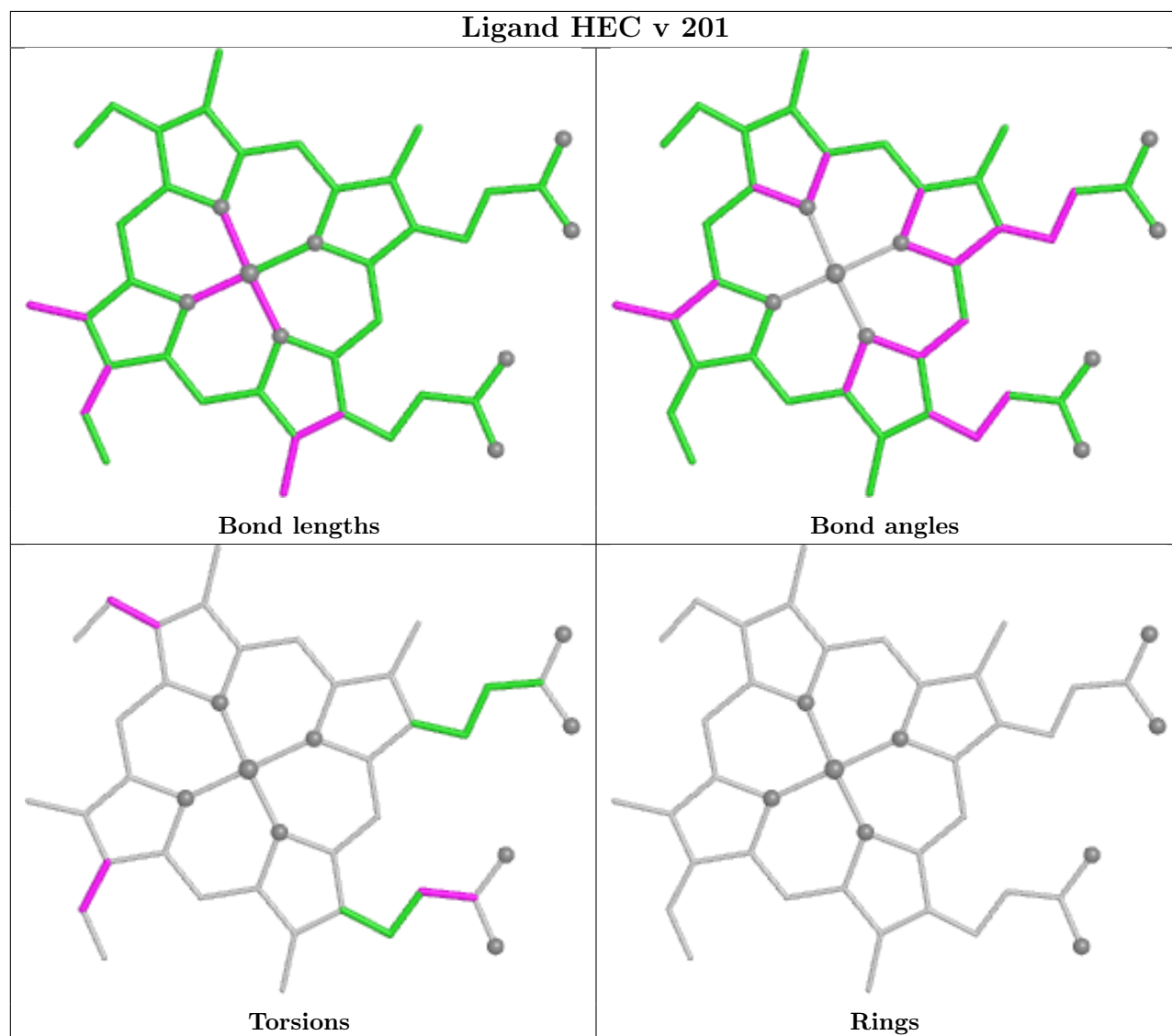
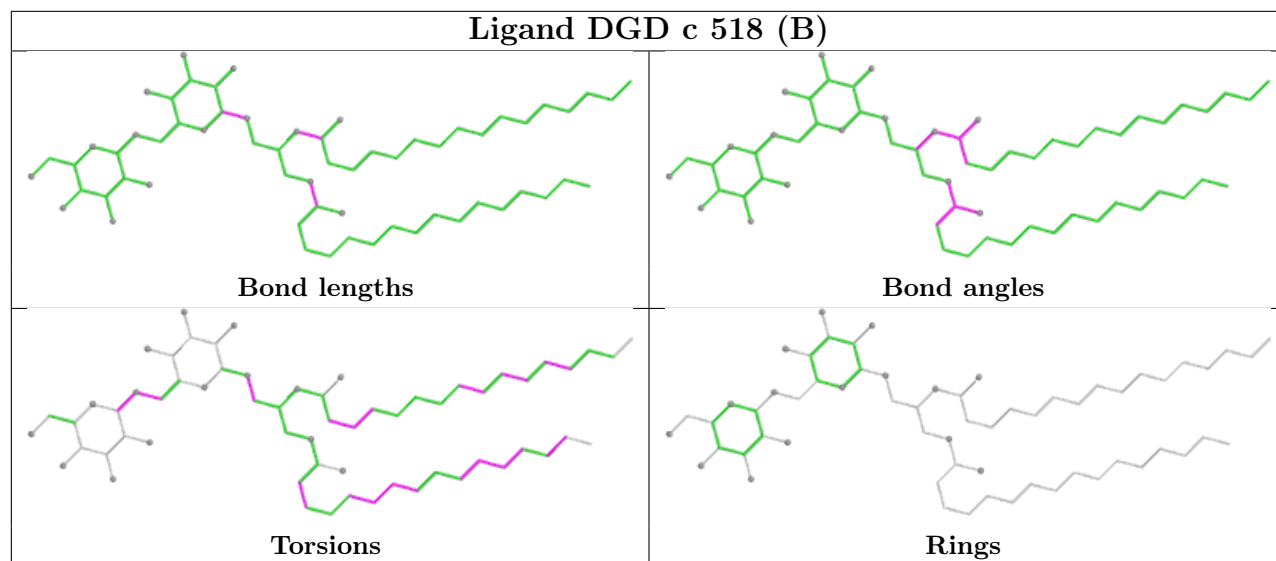


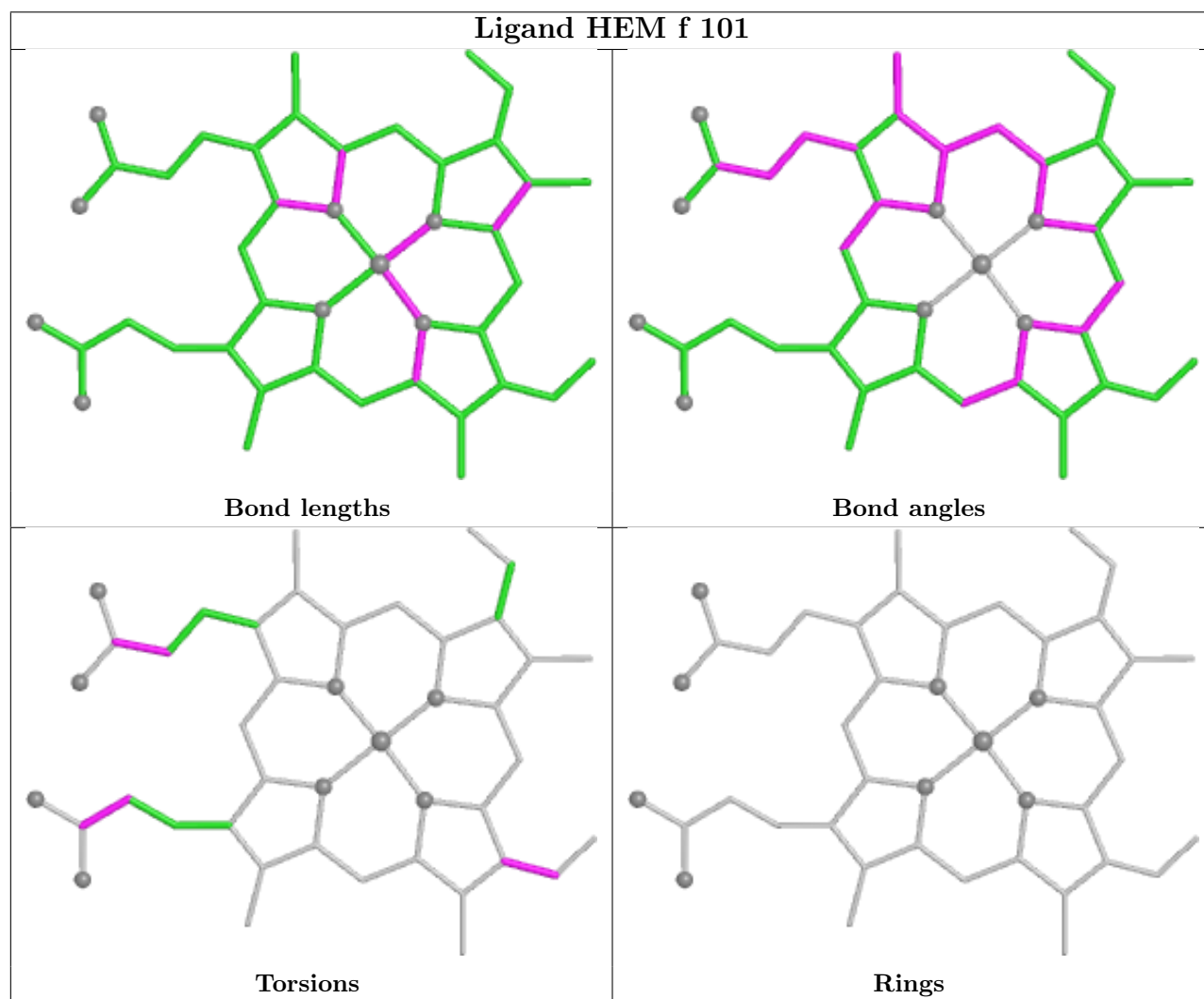
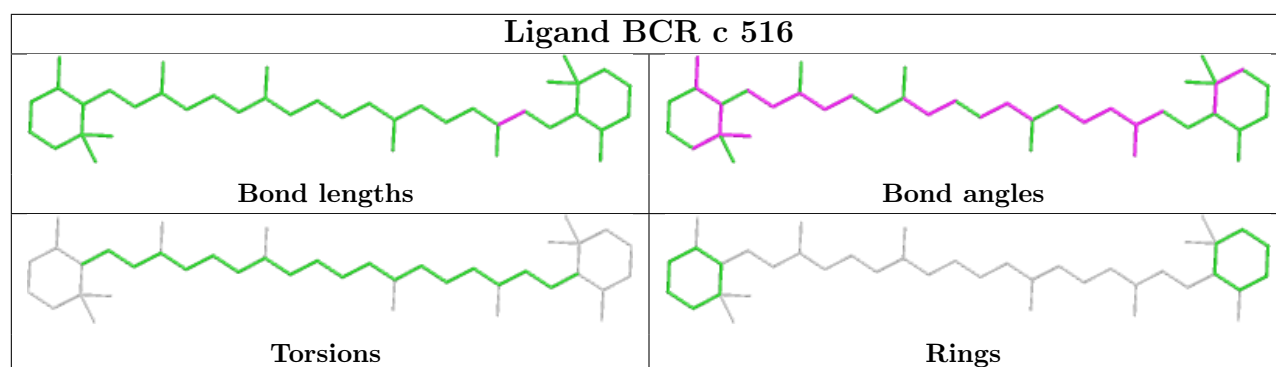


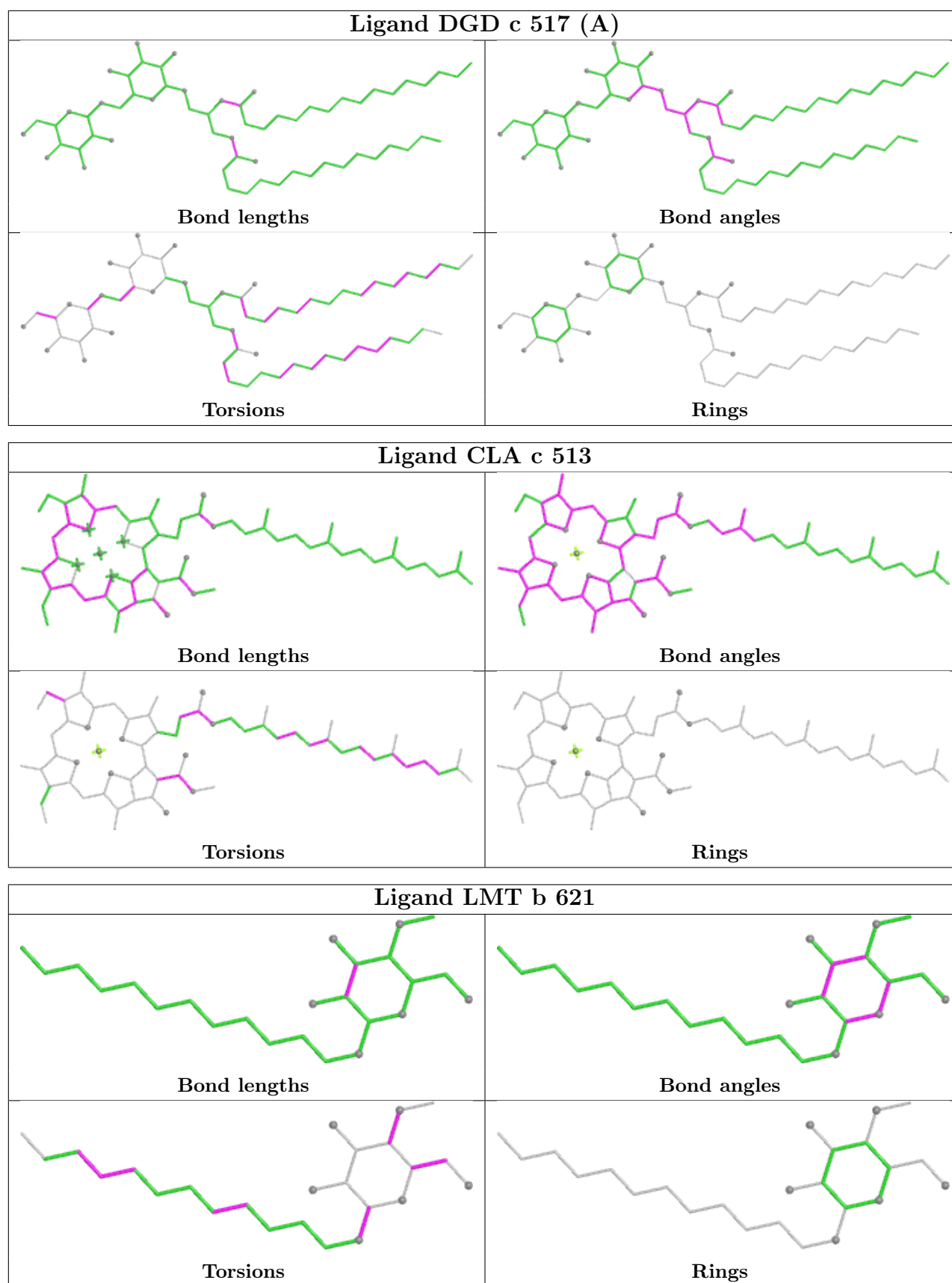
Ligand DGD C 518 (B)	
	
Bond lengths	Bond angles
	
Torsions	Rings

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

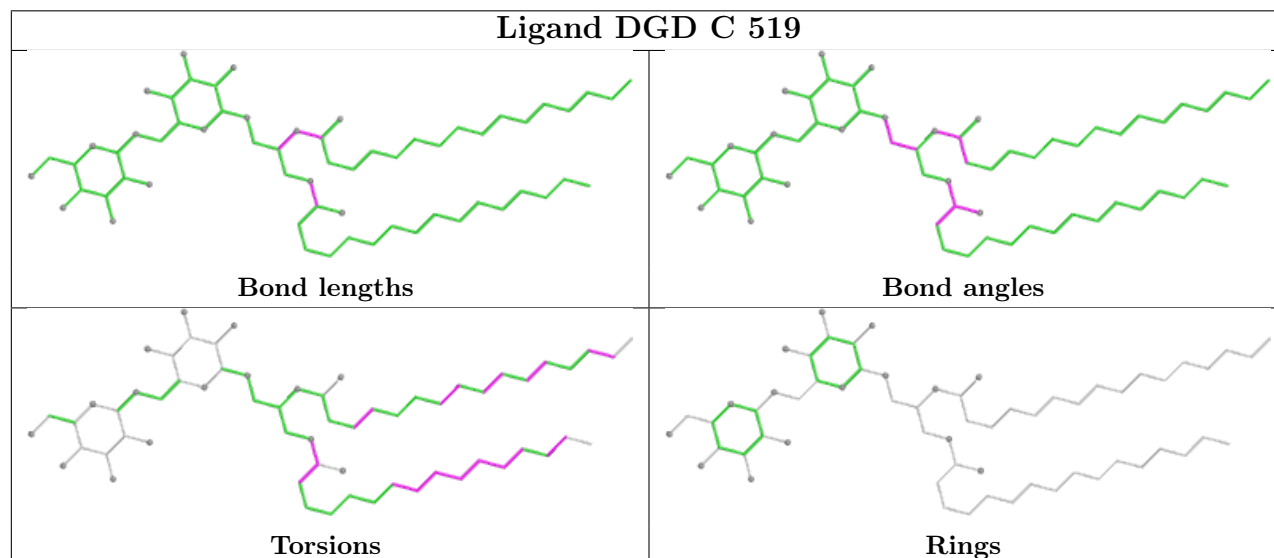
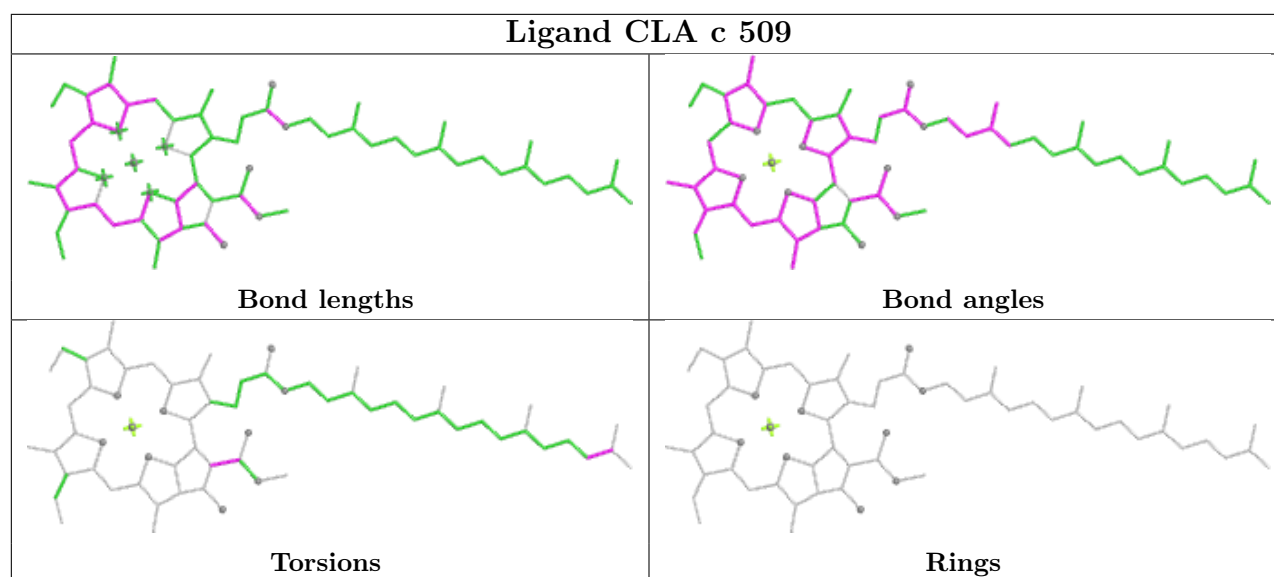
Ligand PHO A 407 (B)	
	
Bond lengths	Bond angles
	
Torsions	Rings

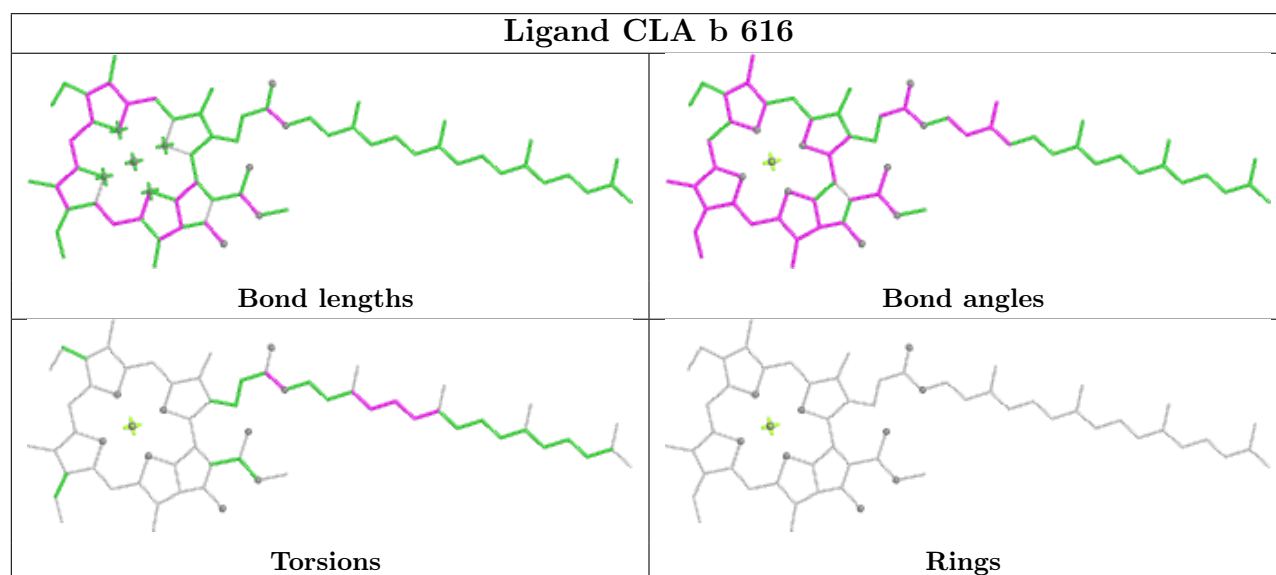
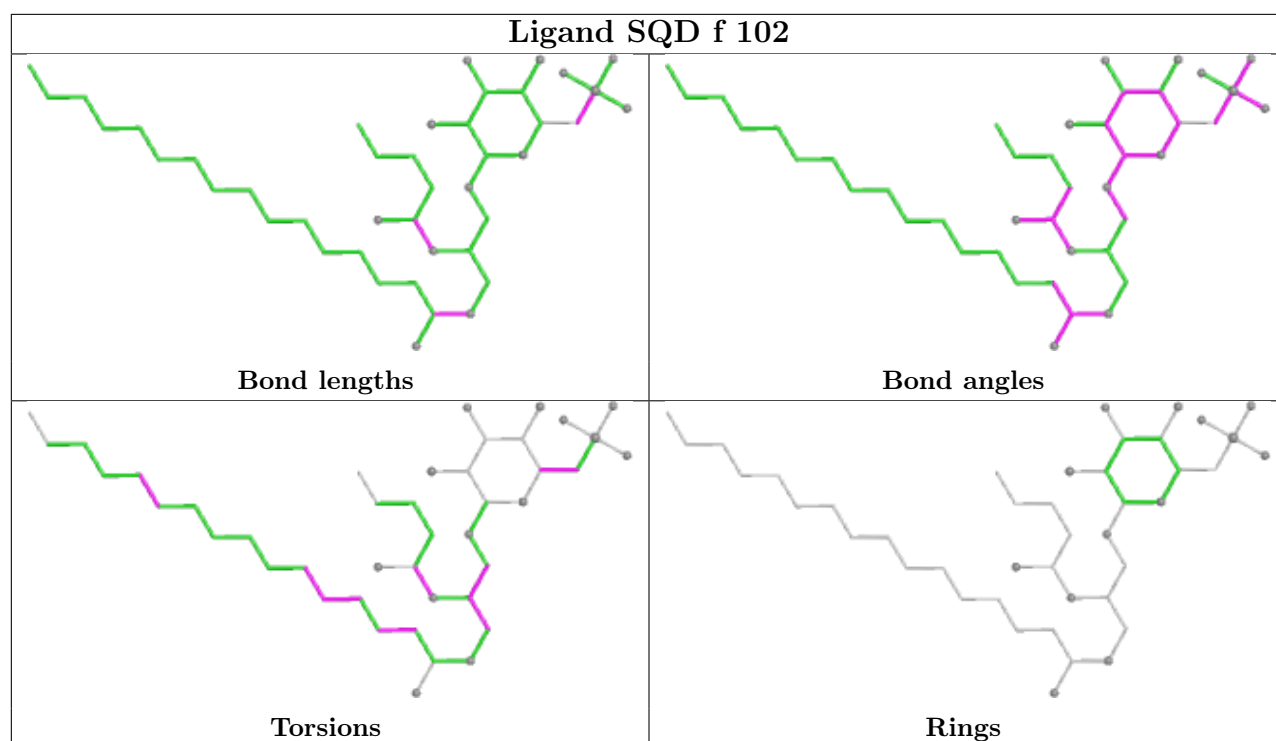




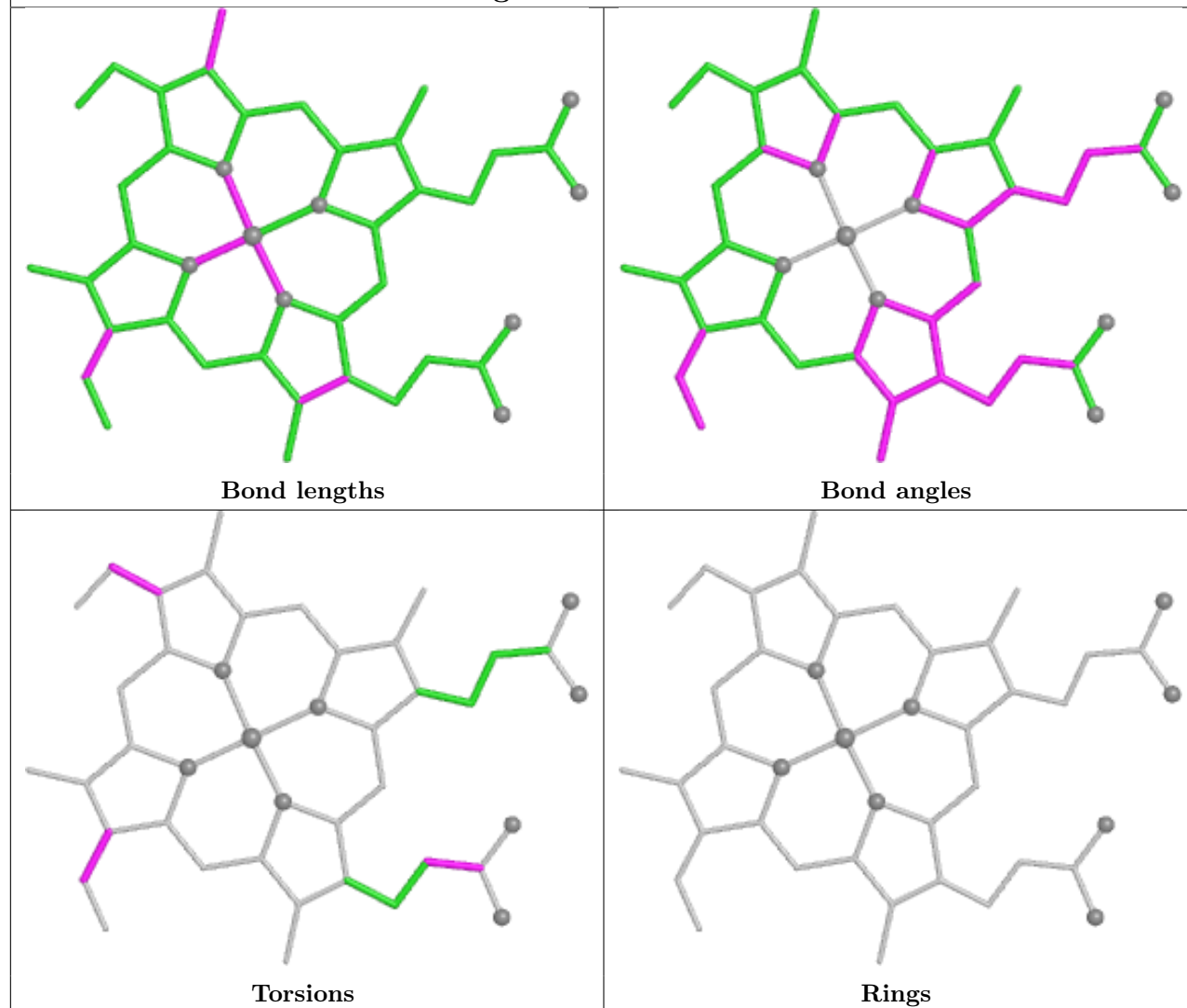


Ligand PHO A 417 (A)	
Bond lengths	Bond angles
Torsions	Rings
Ligand BCR b 619	
Bond lengths	Bond angles
Torsions	Rings
Ligand CLA C 507	
Bond lengths	Bond angles
Torsions	Rings
Ligand PL9 a 413 (A)	
Bond lengths	Bond angles
Torsions	Rings

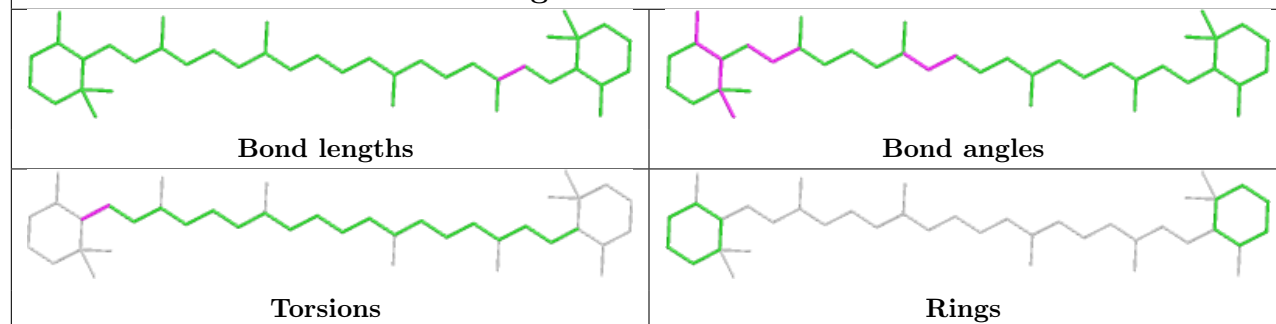


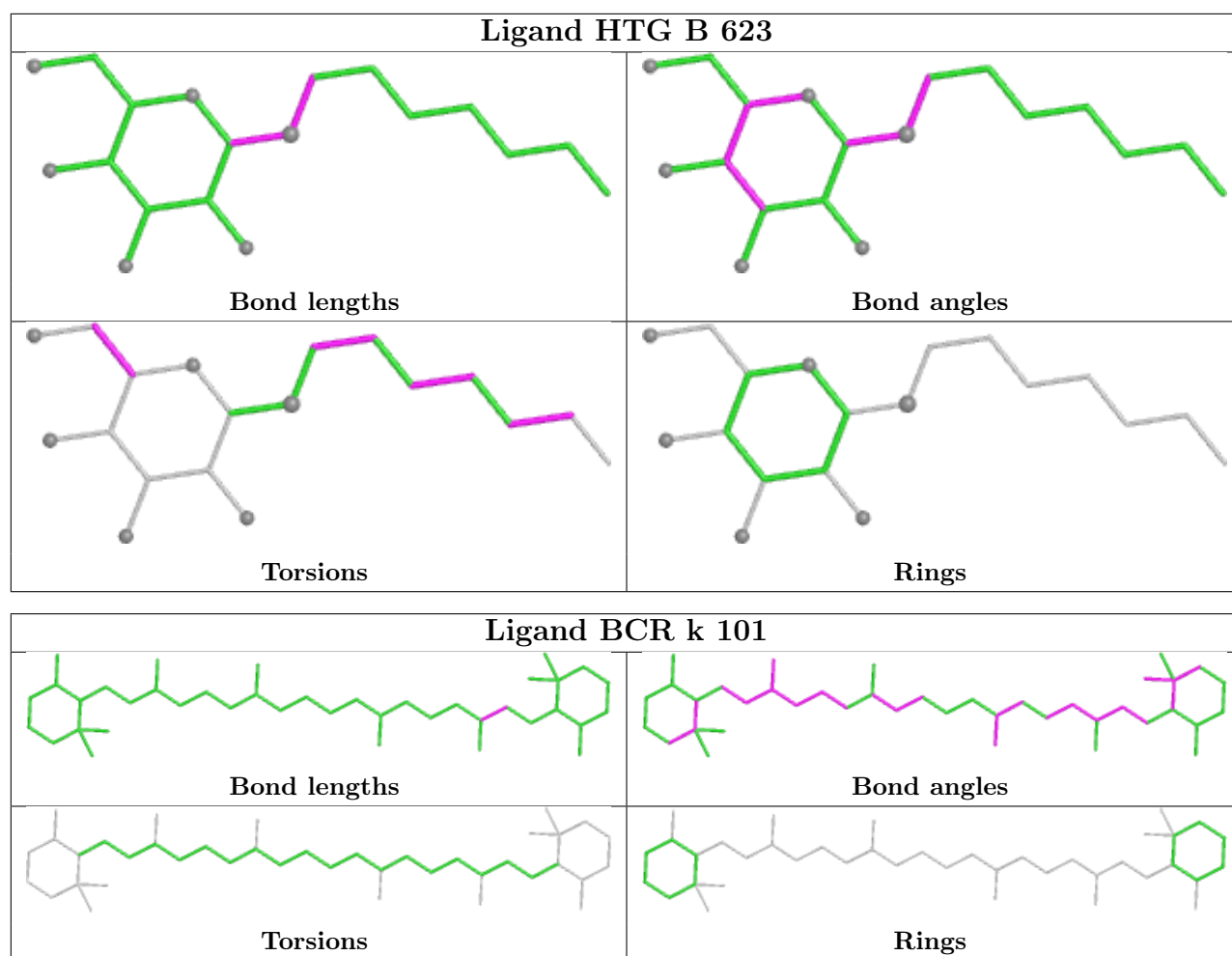


Ligand HEC V 201

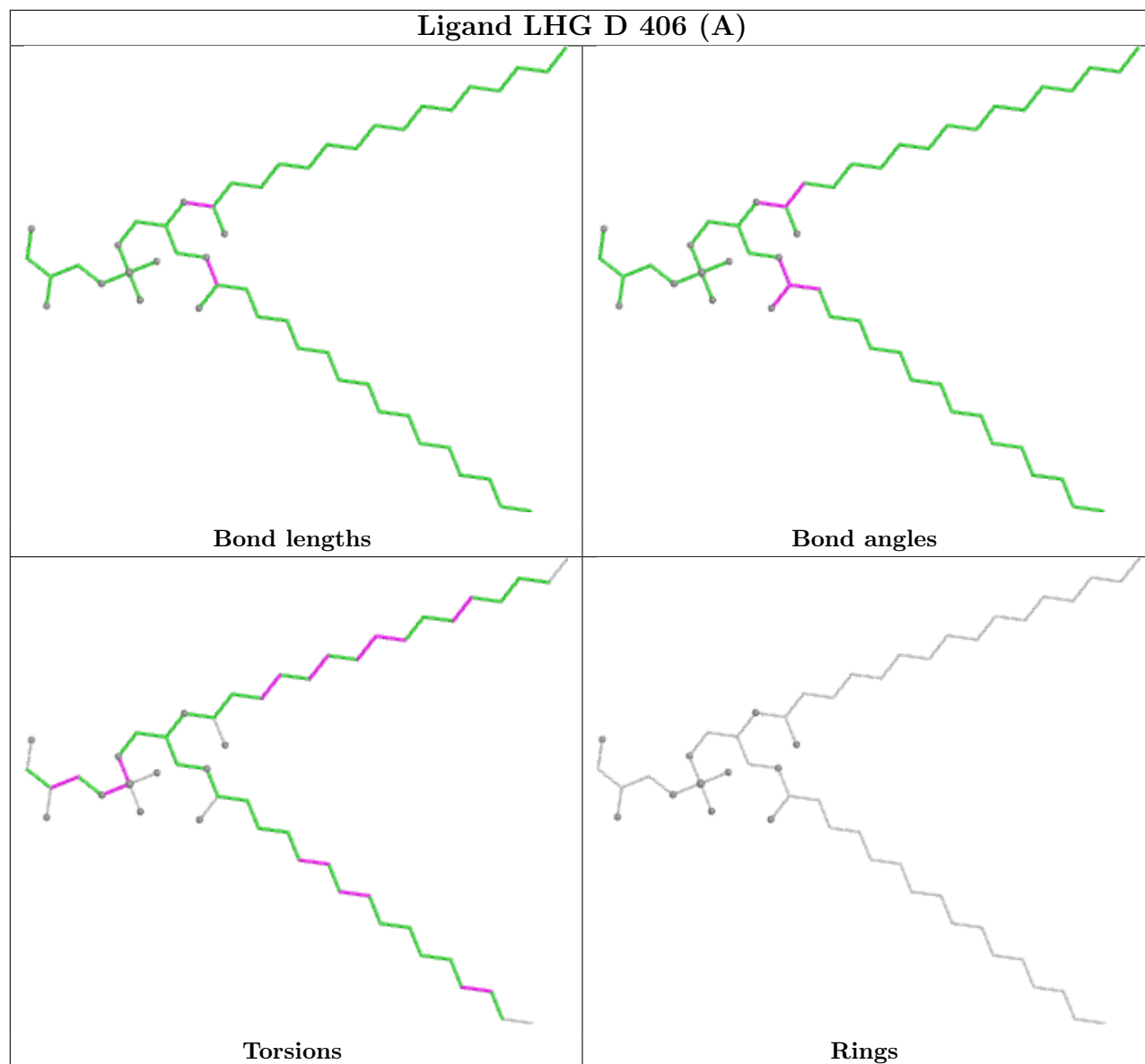


Ligand BCR B 617

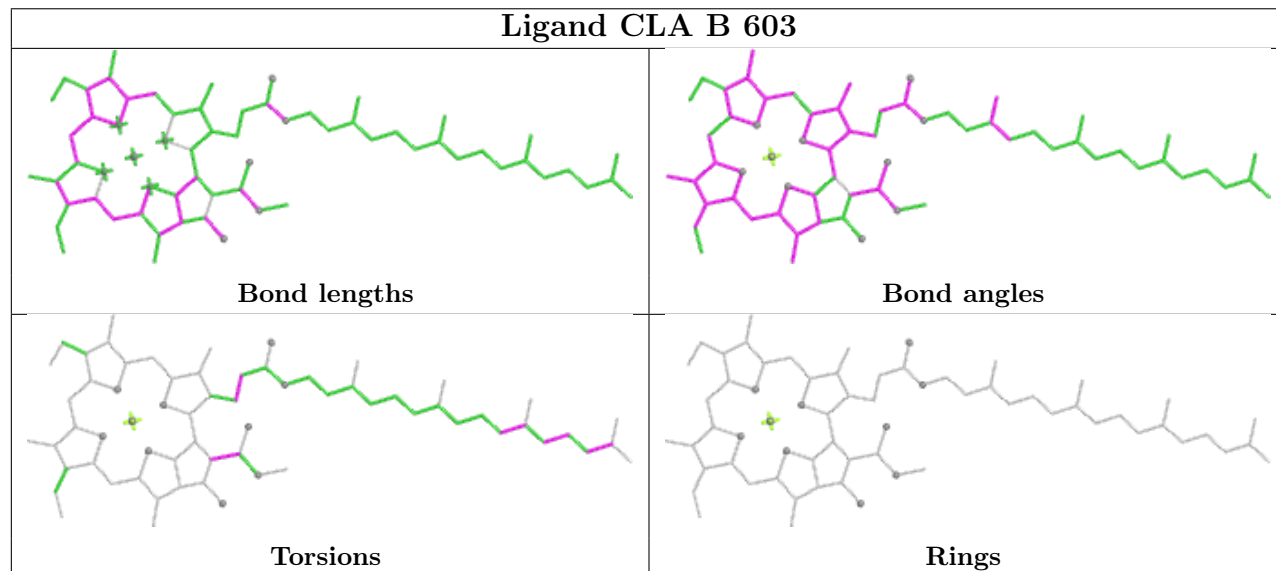


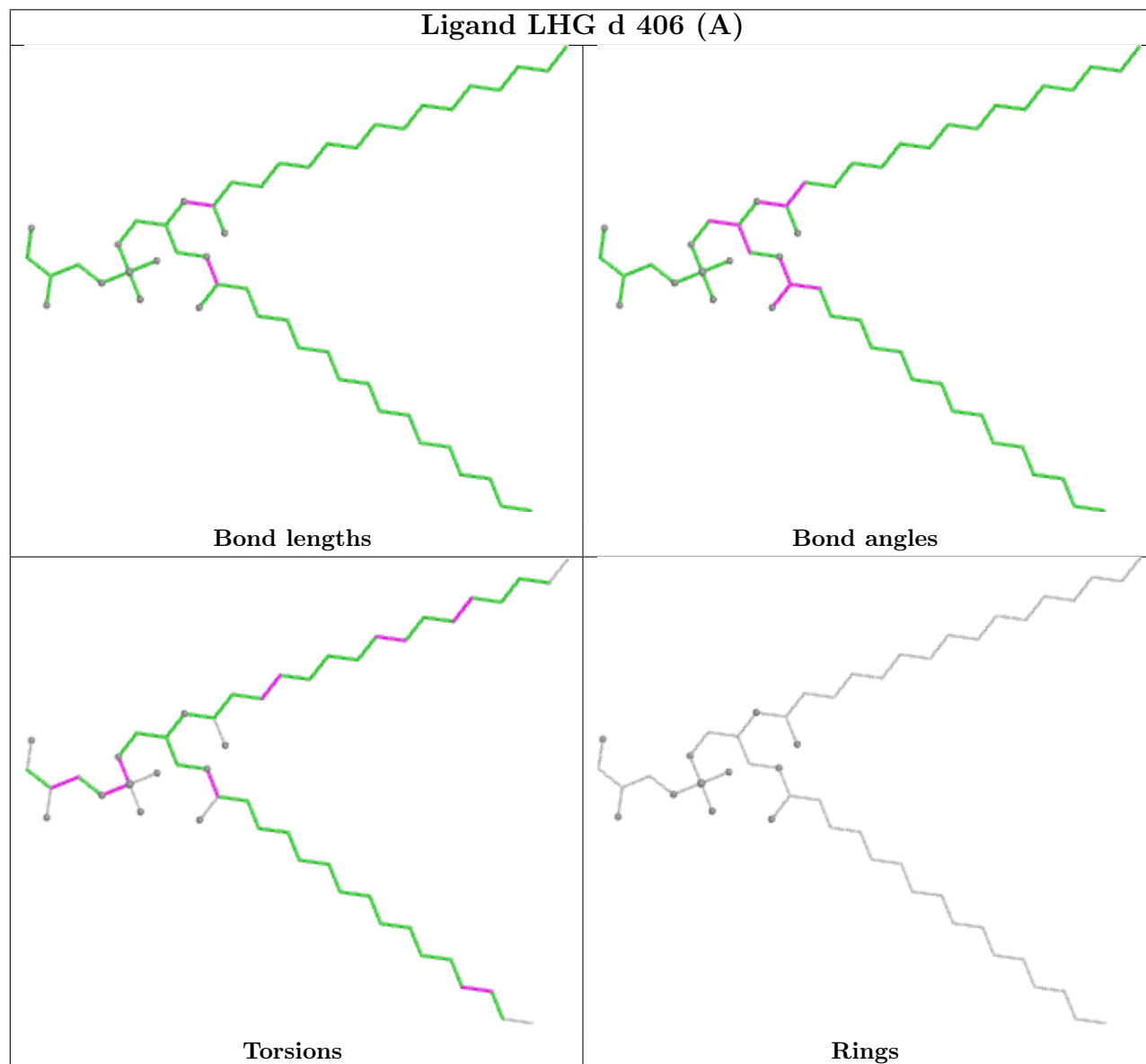
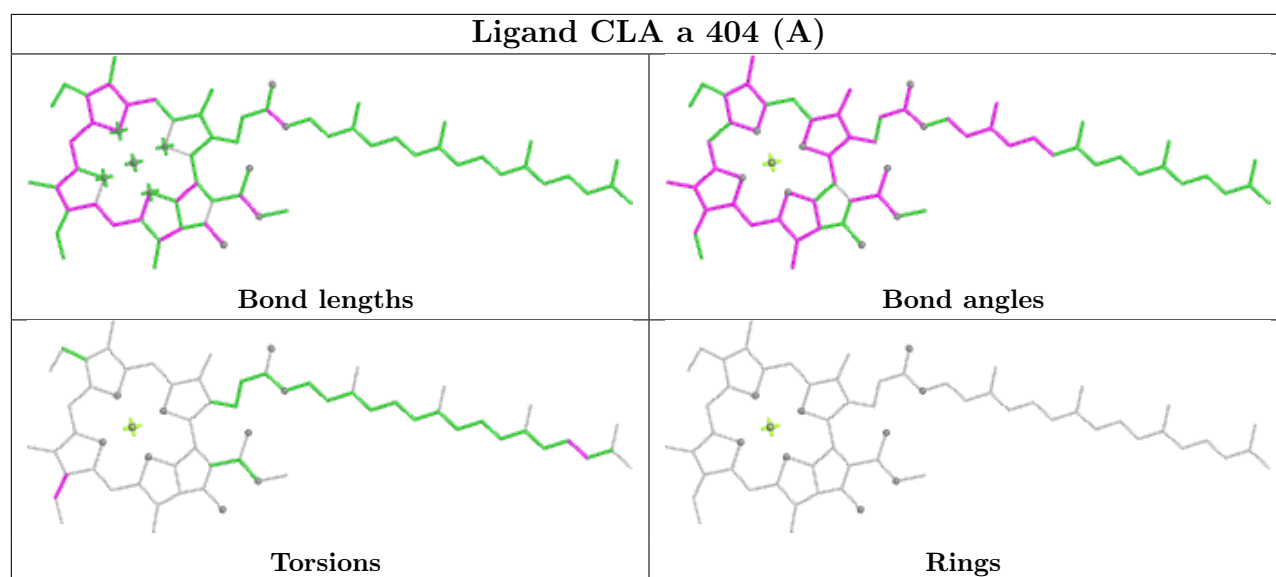


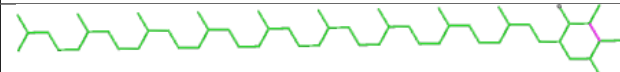
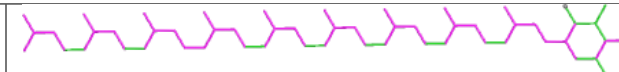
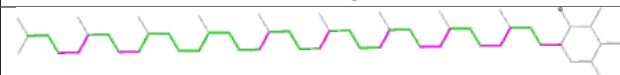
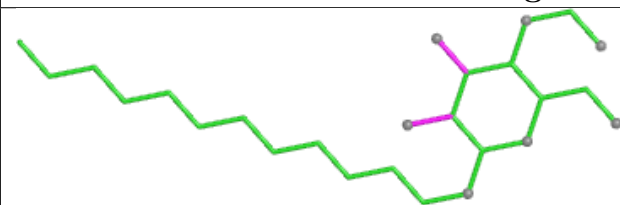
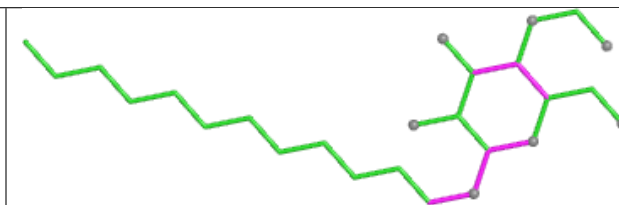
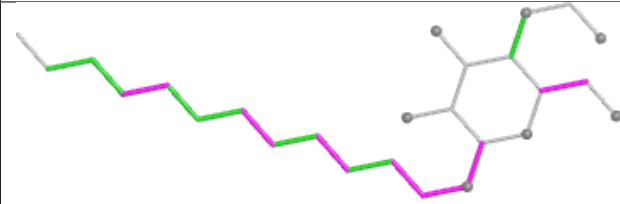
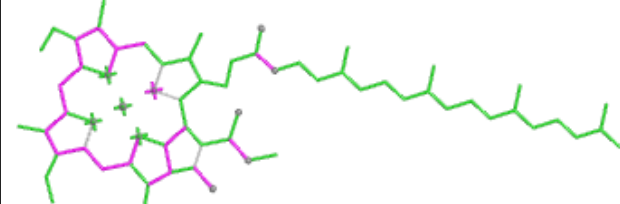
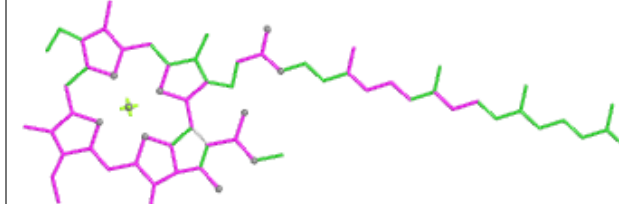
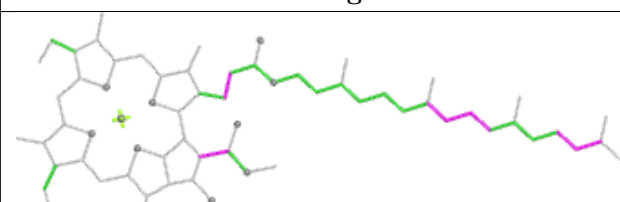
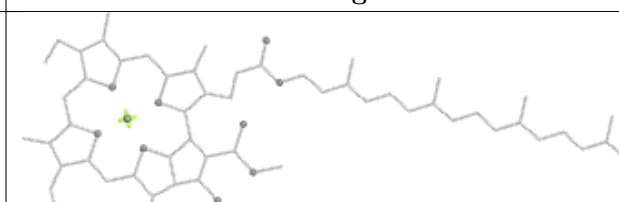
Ligand LHG D 406 (A)



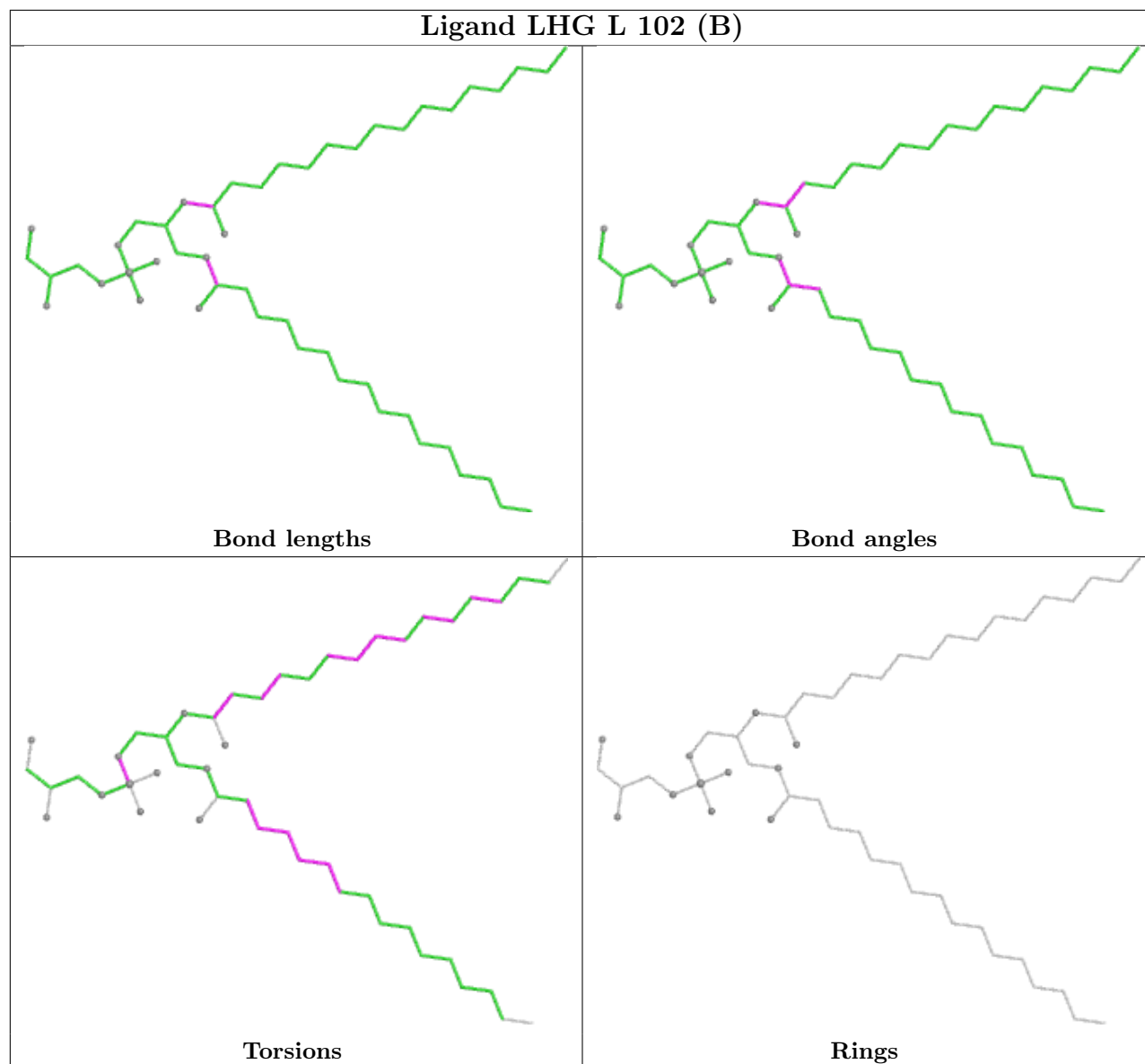
Ligand CLA B 603



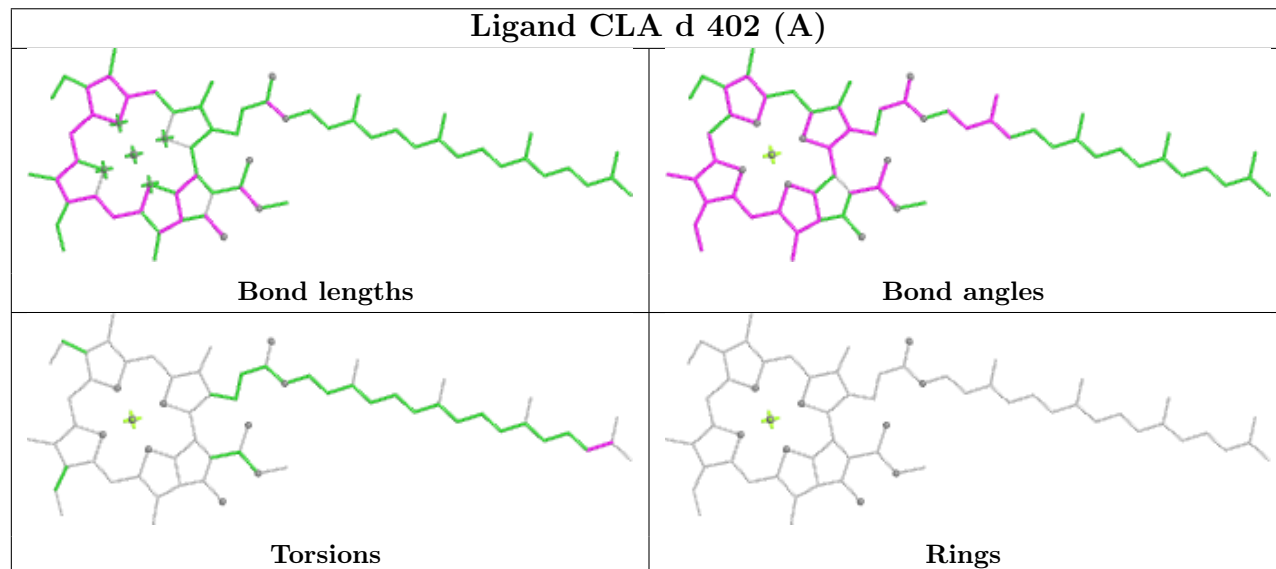


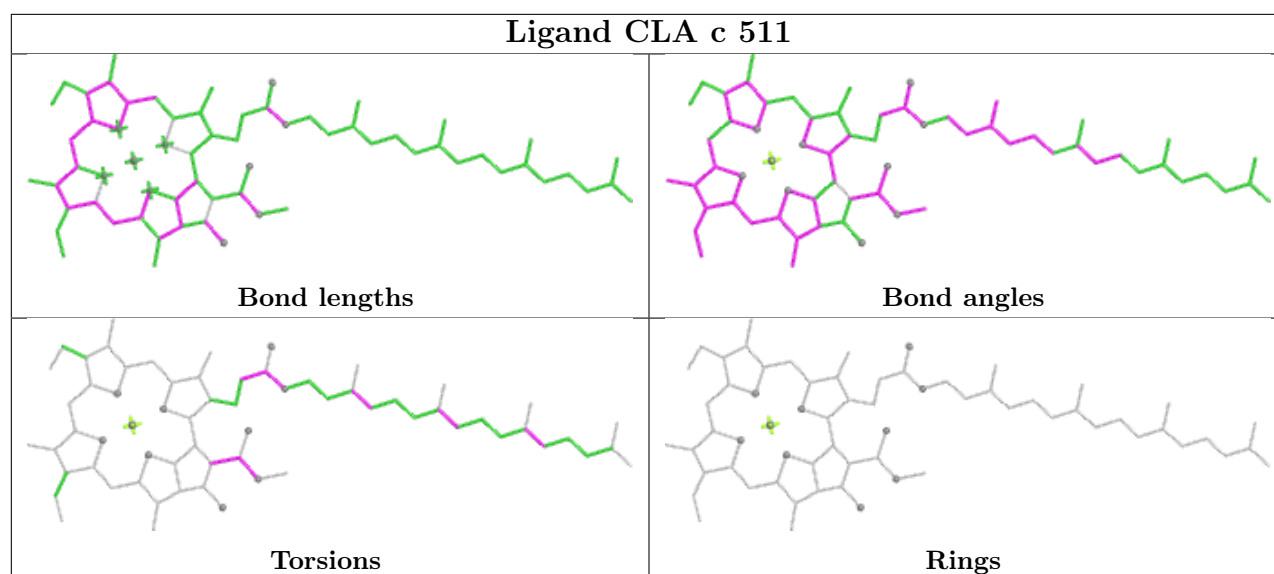
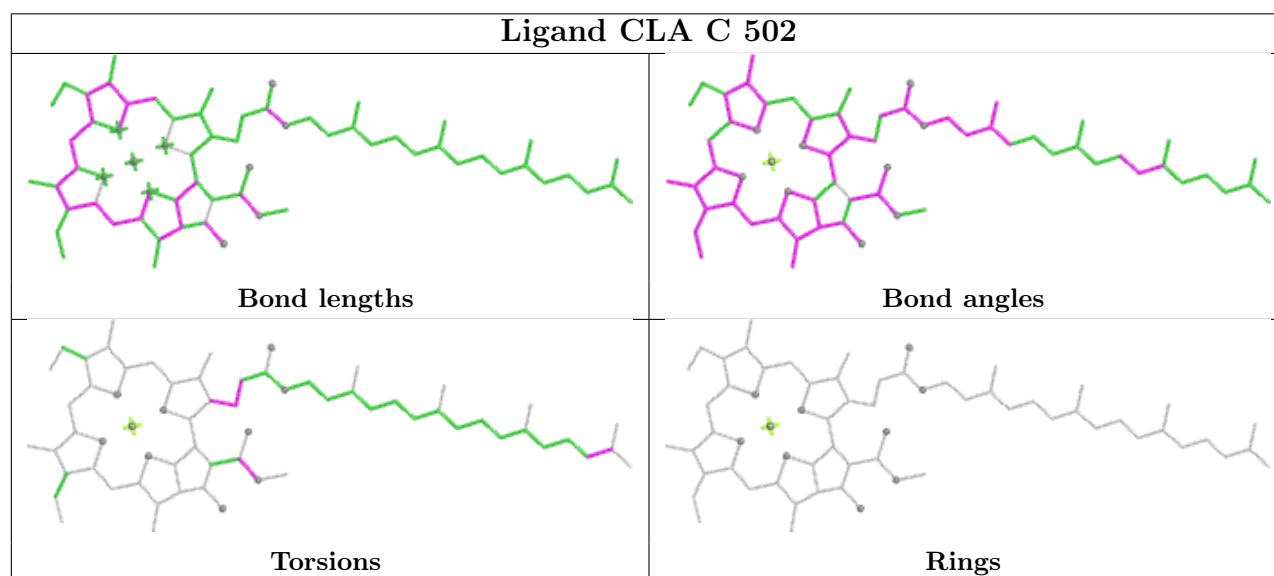
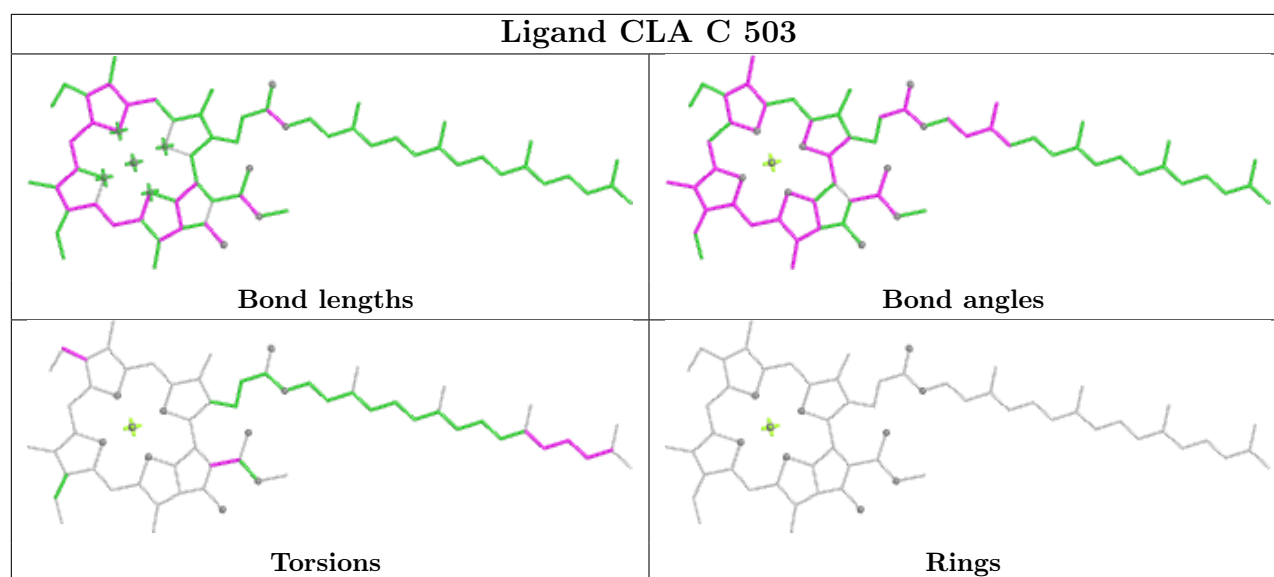
Ligand PL9 A 414 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMT t 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

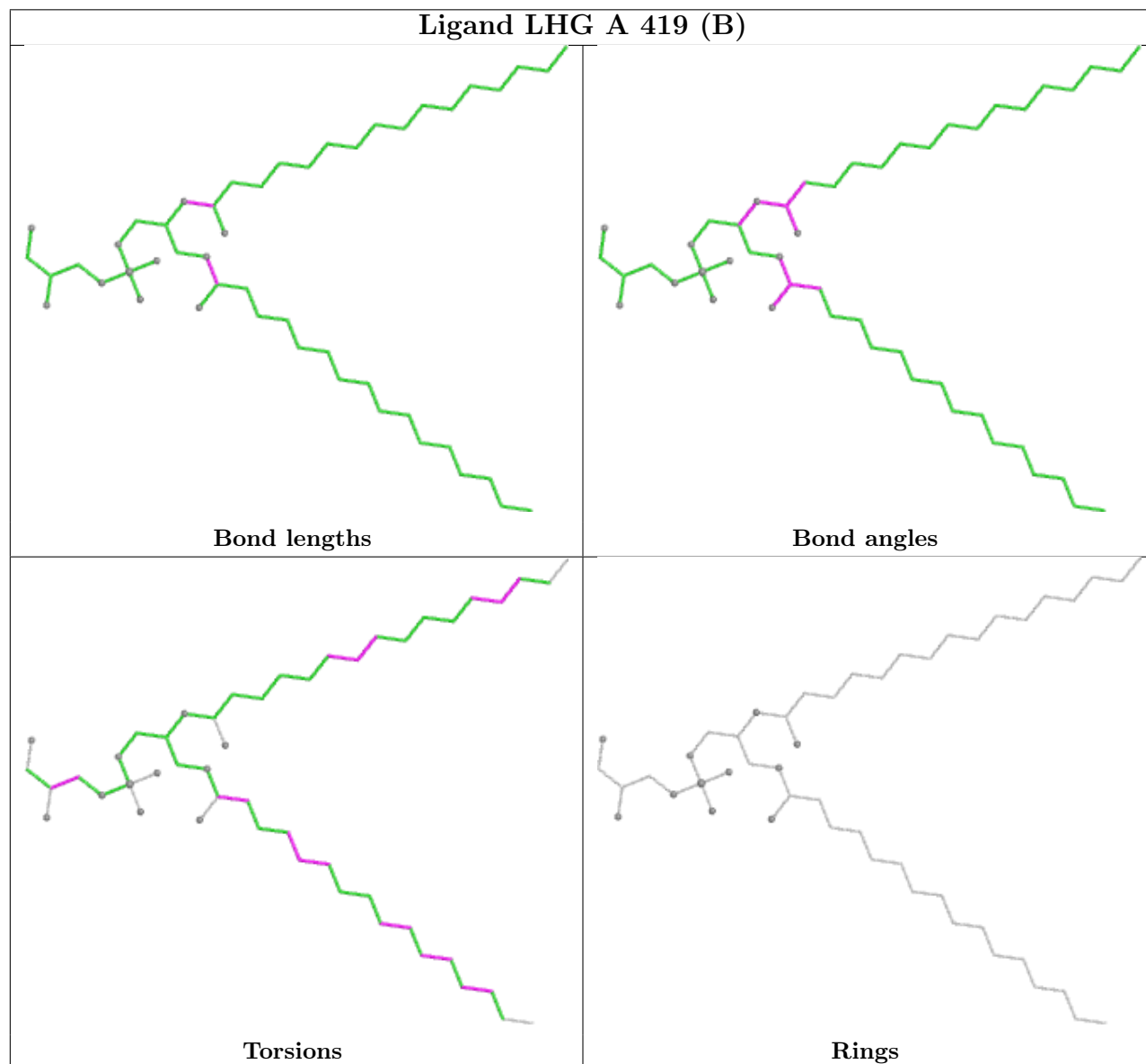
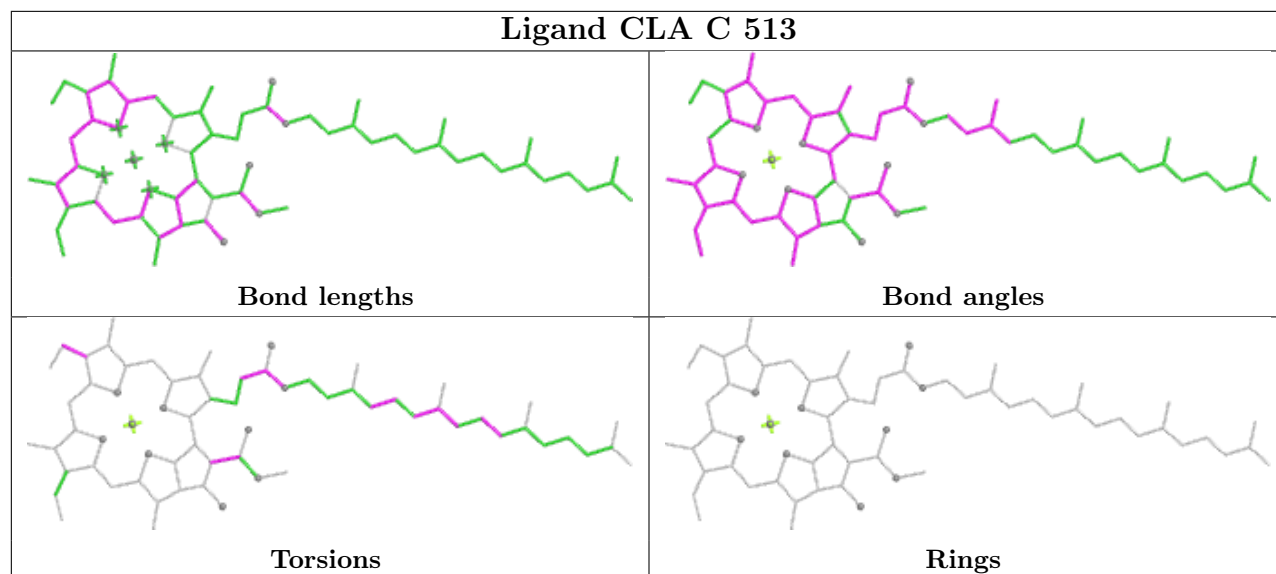
Ligand LHG L 102 (B)

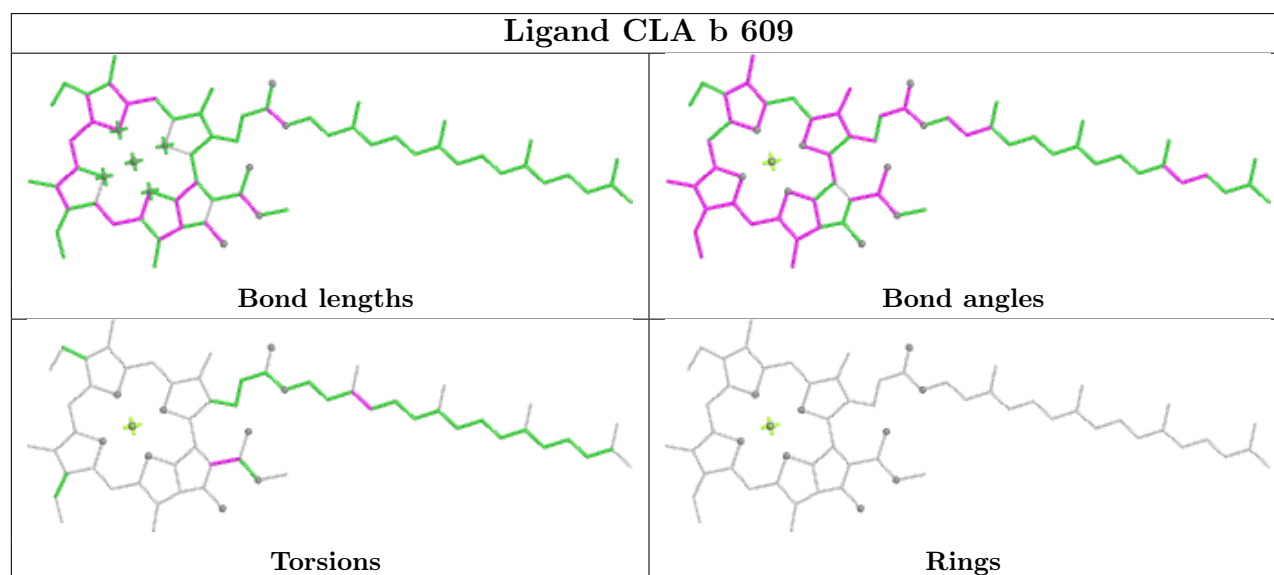
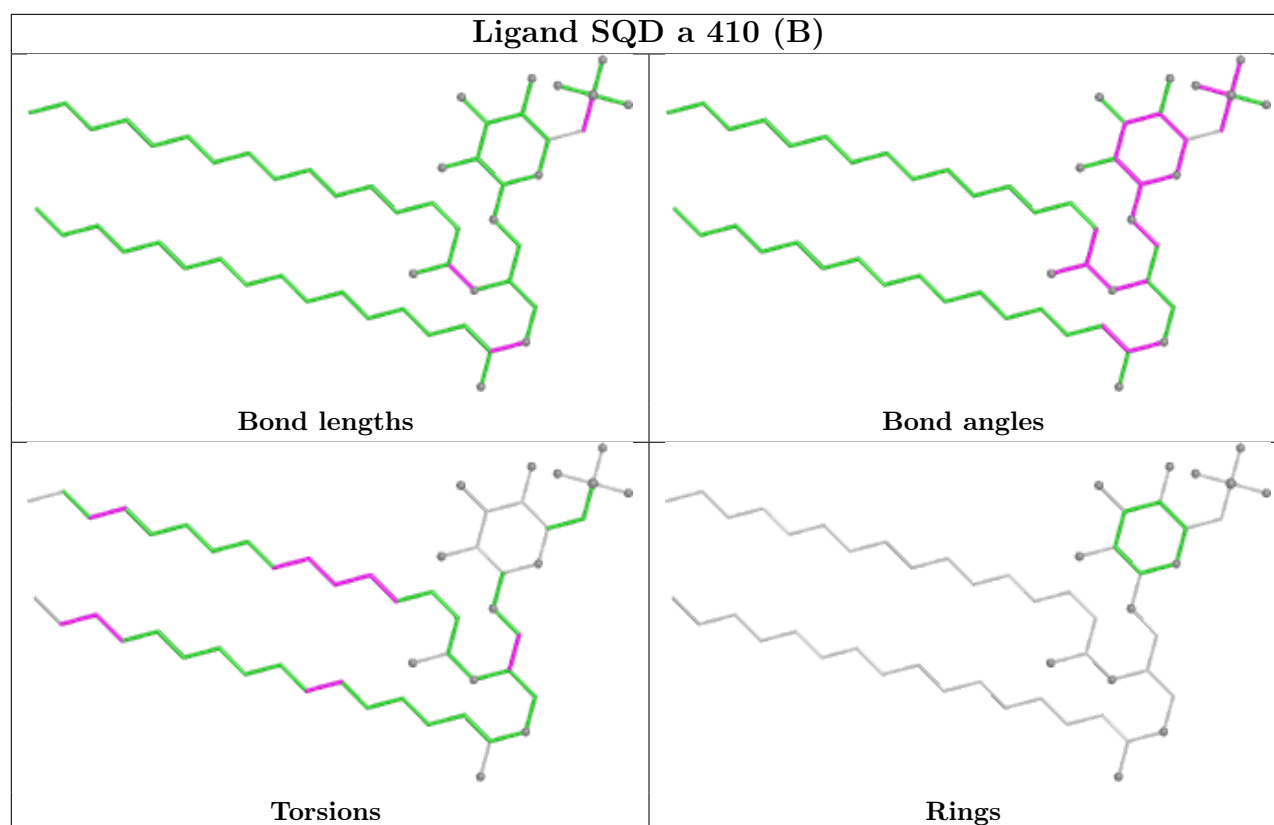


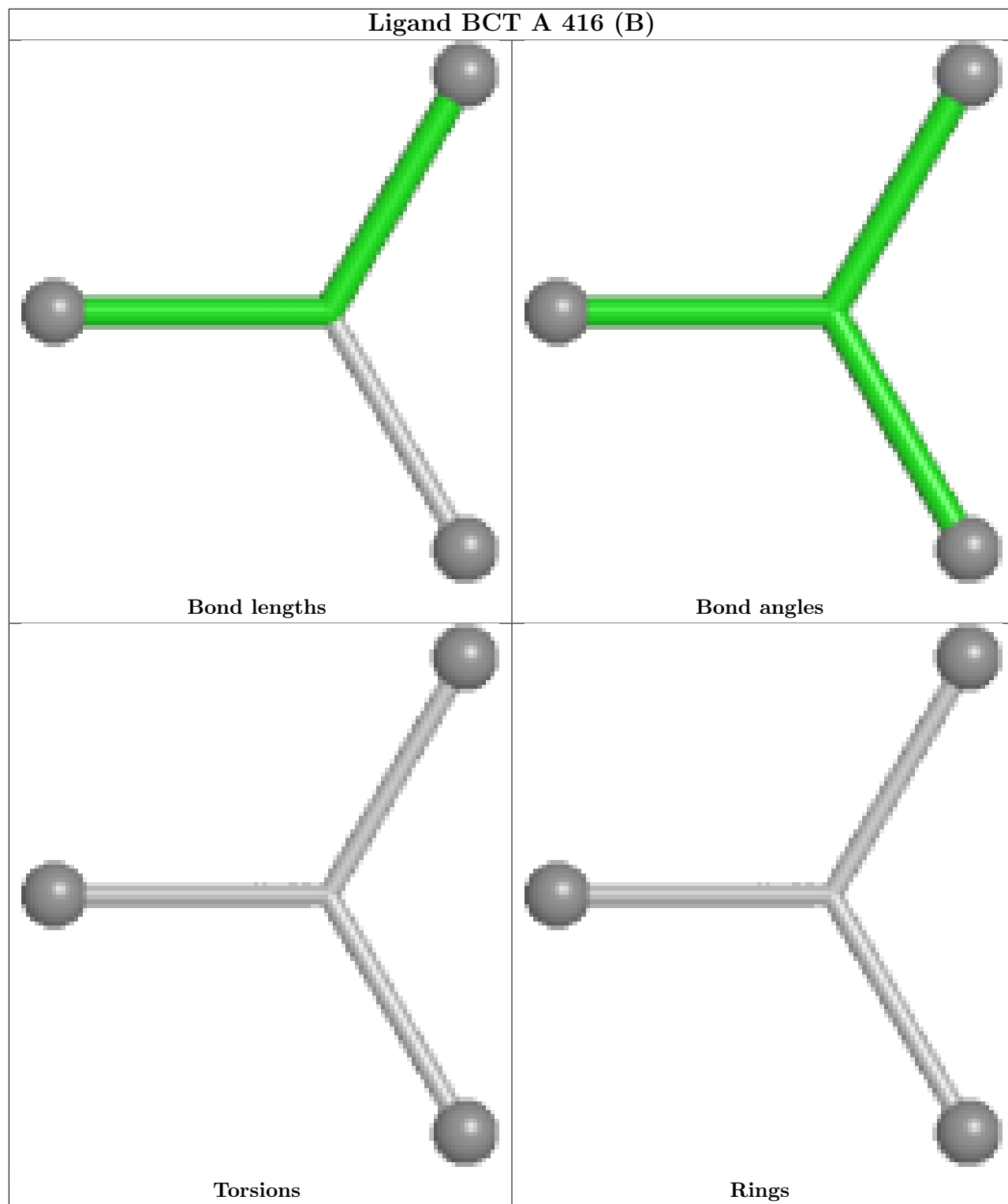
Ligand CLA d 402 (A)

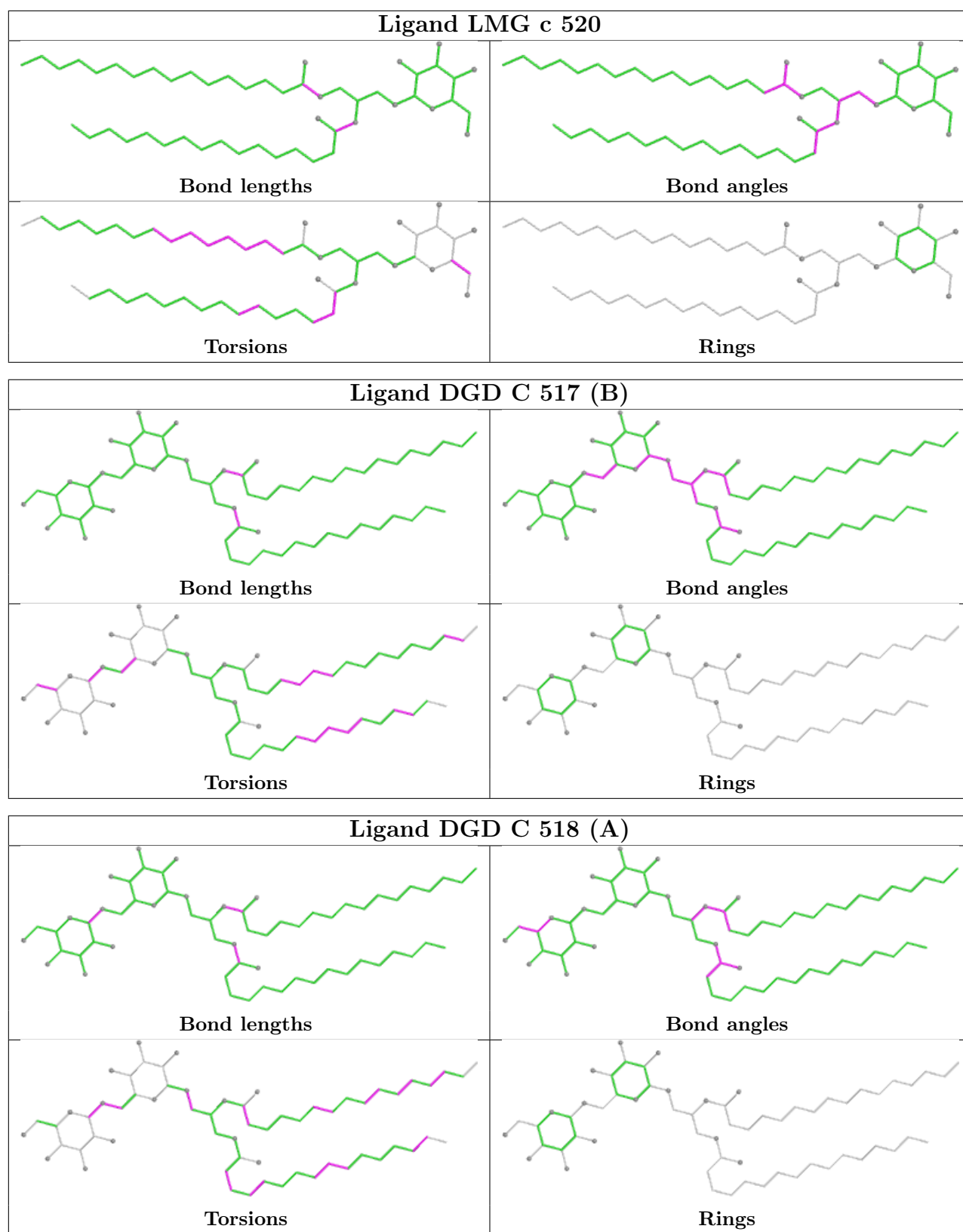


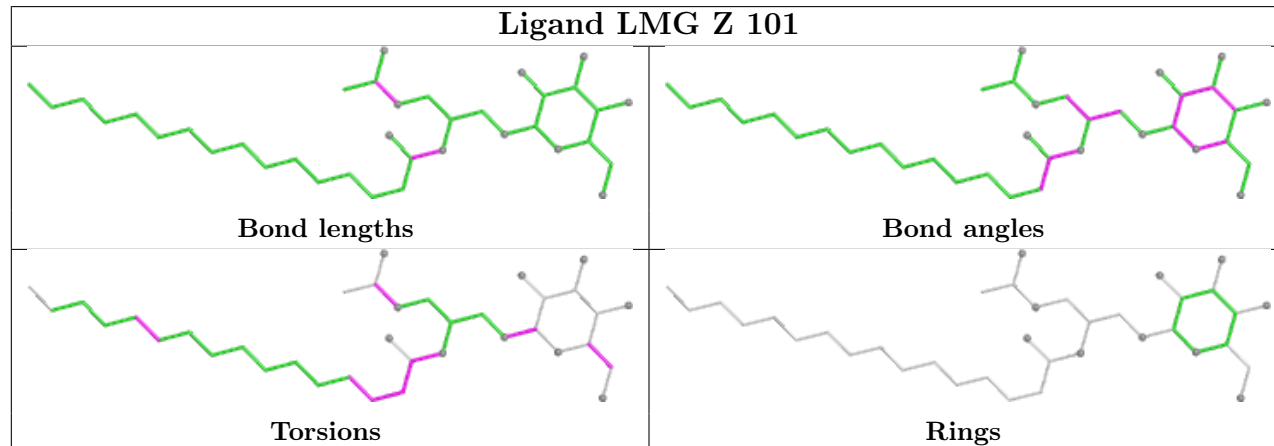
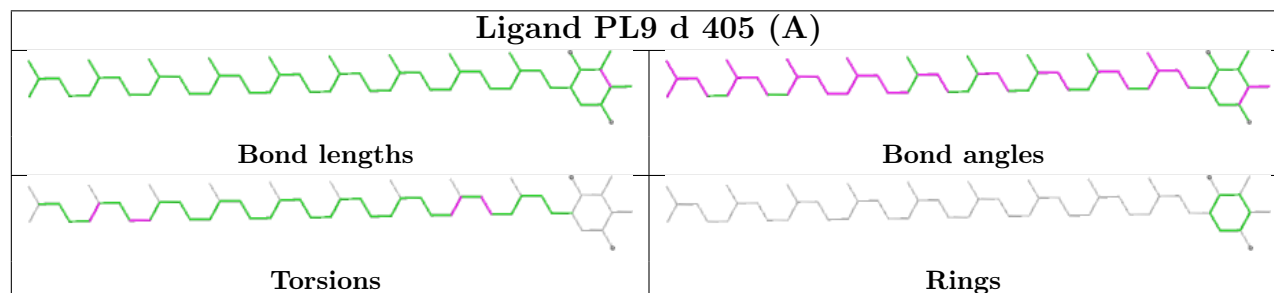
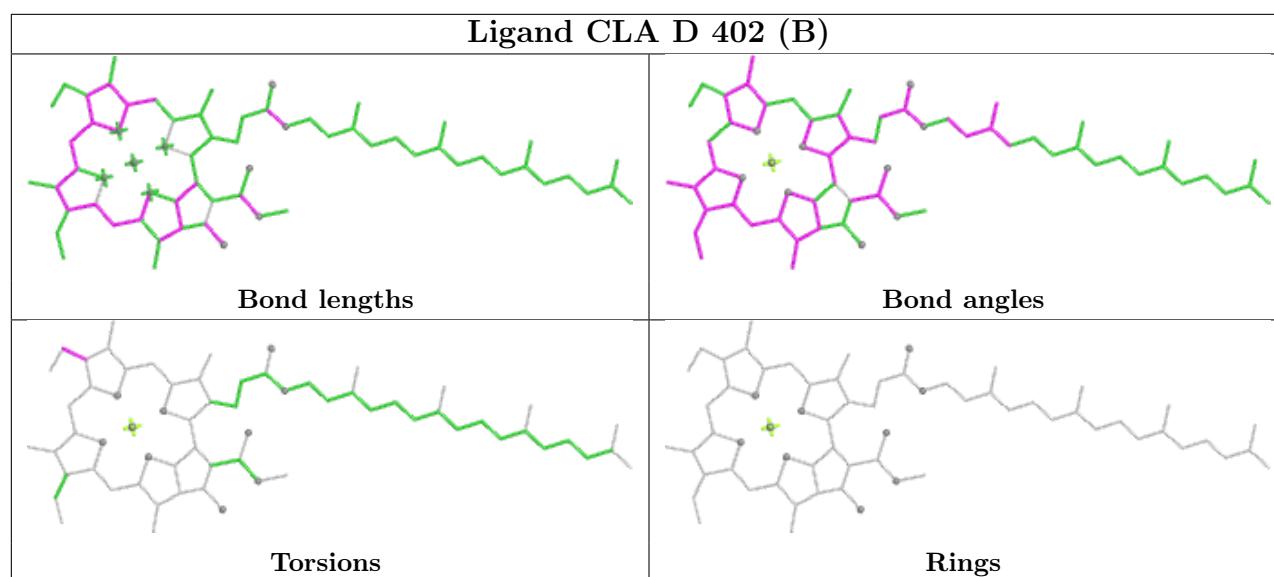


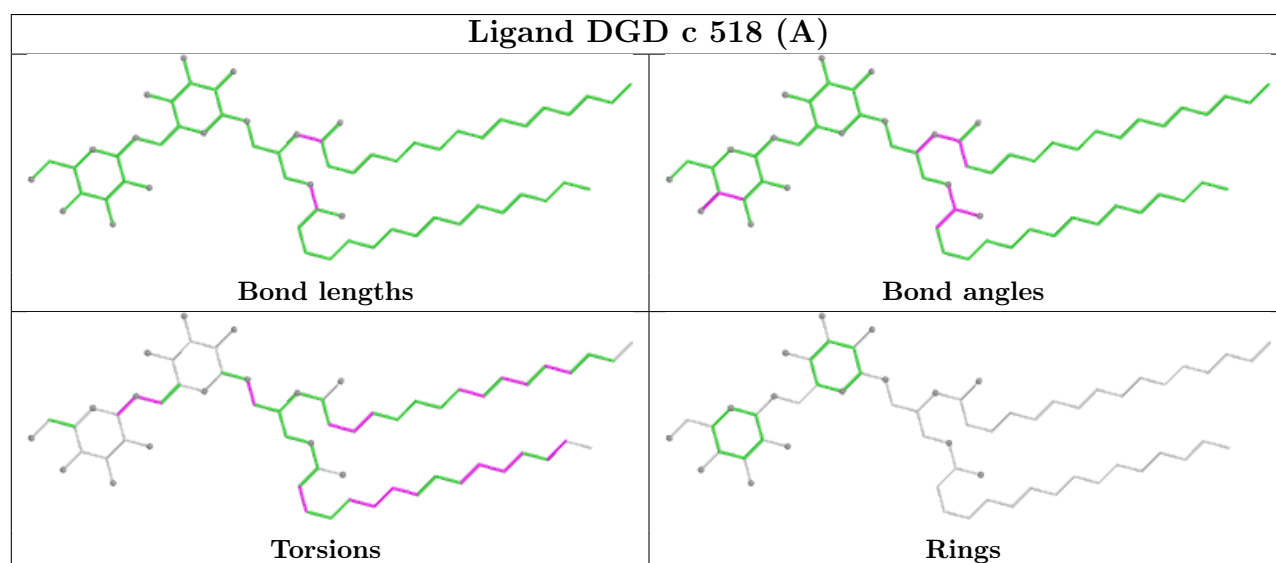
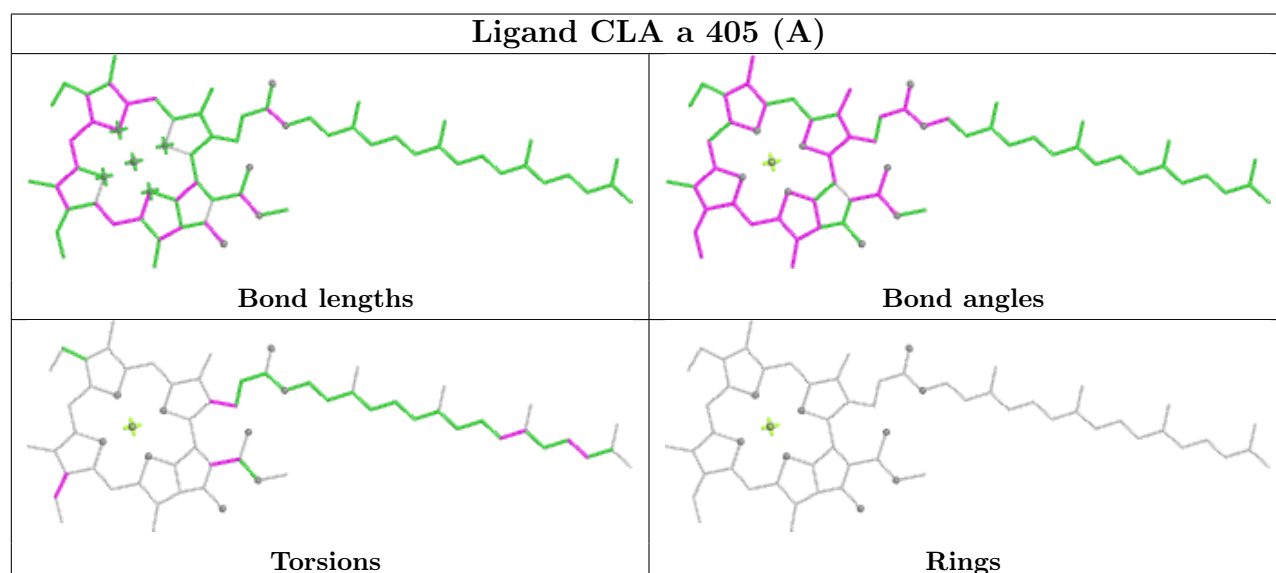
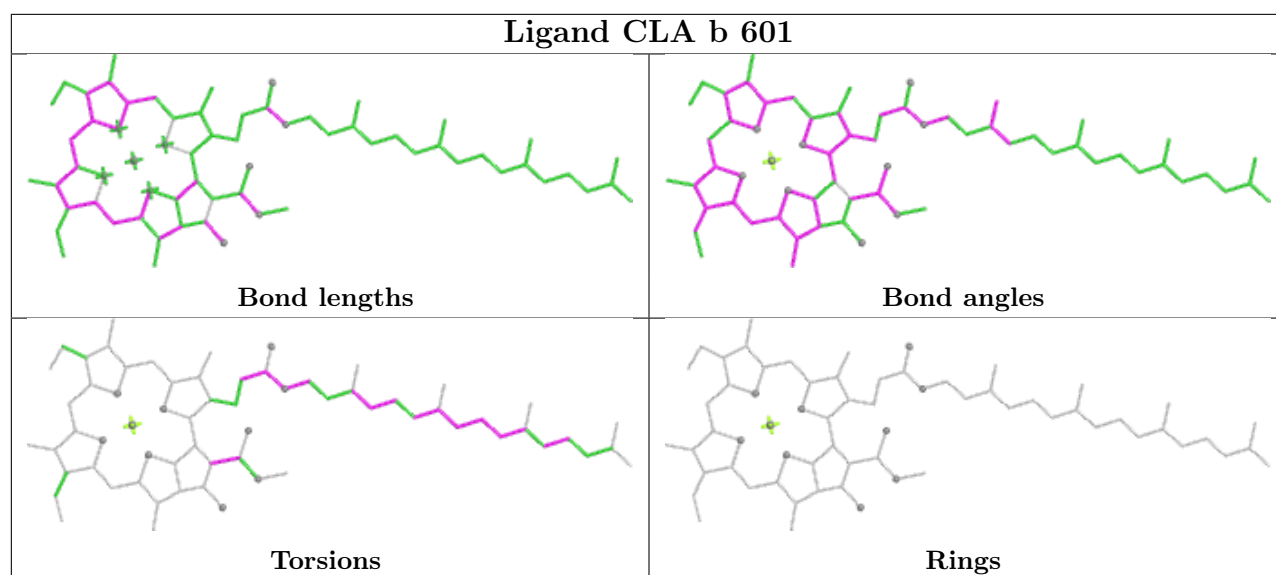


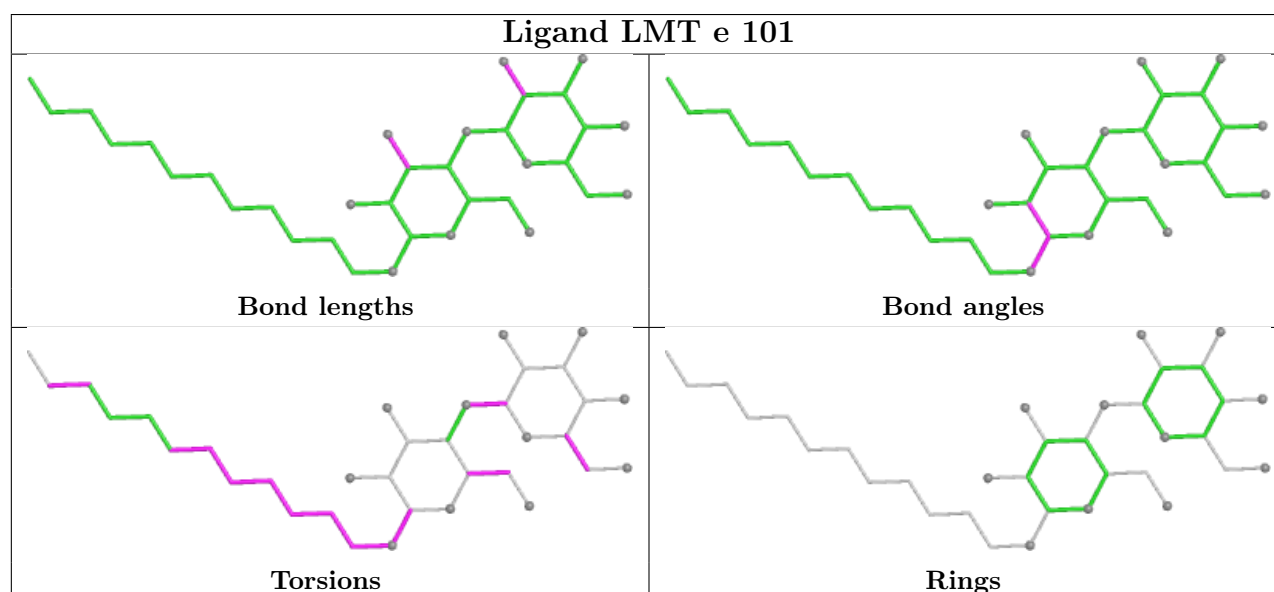
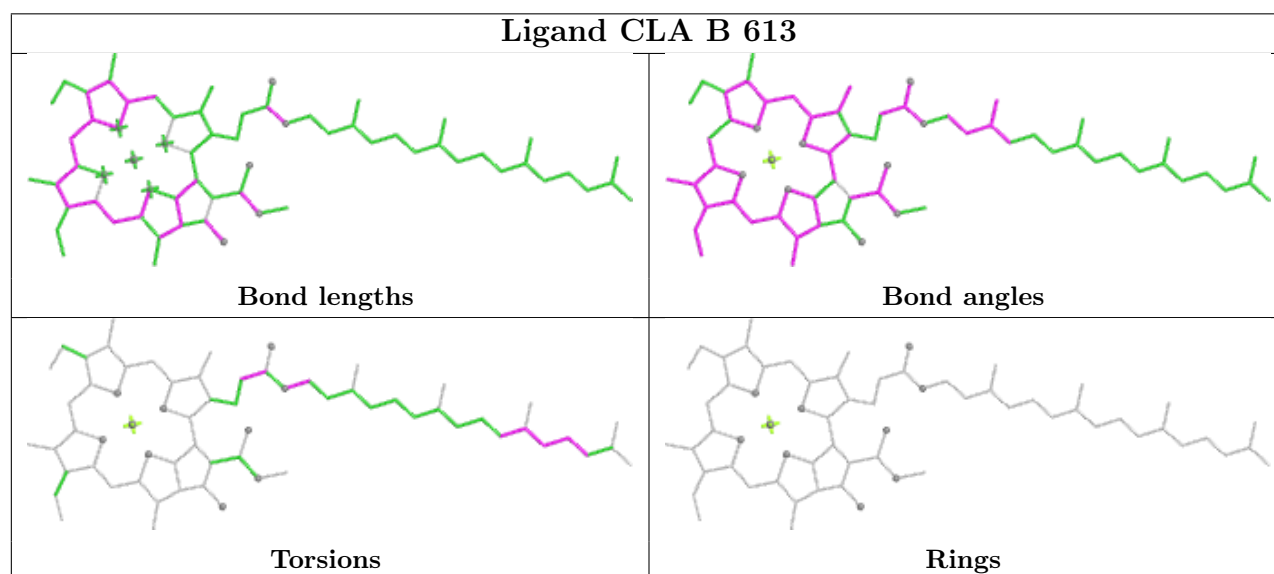
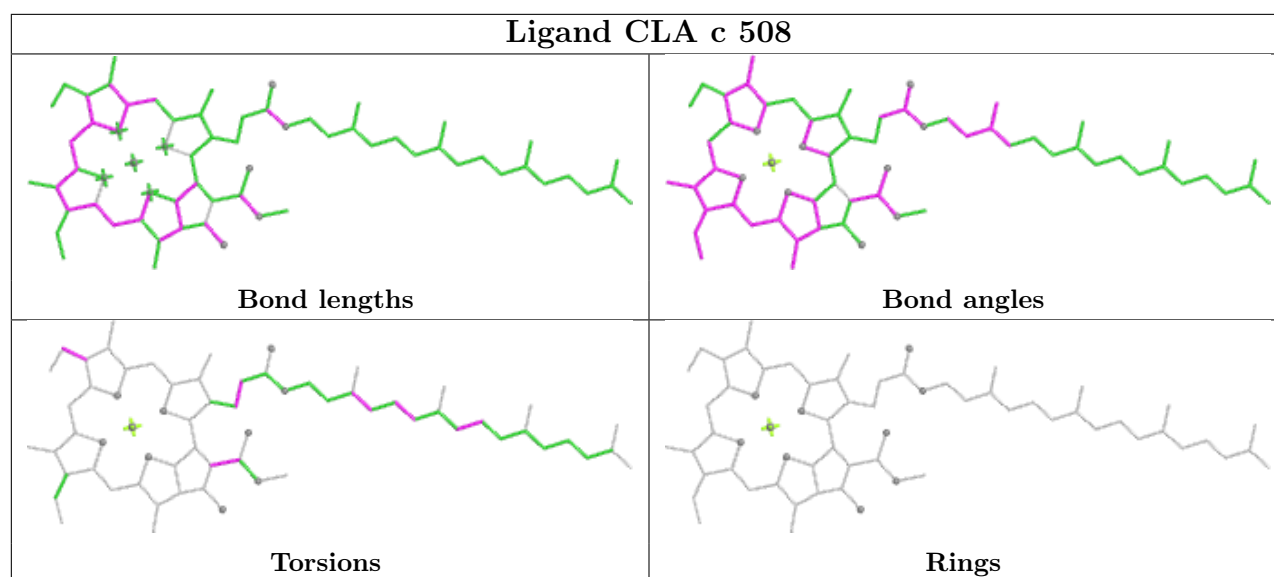


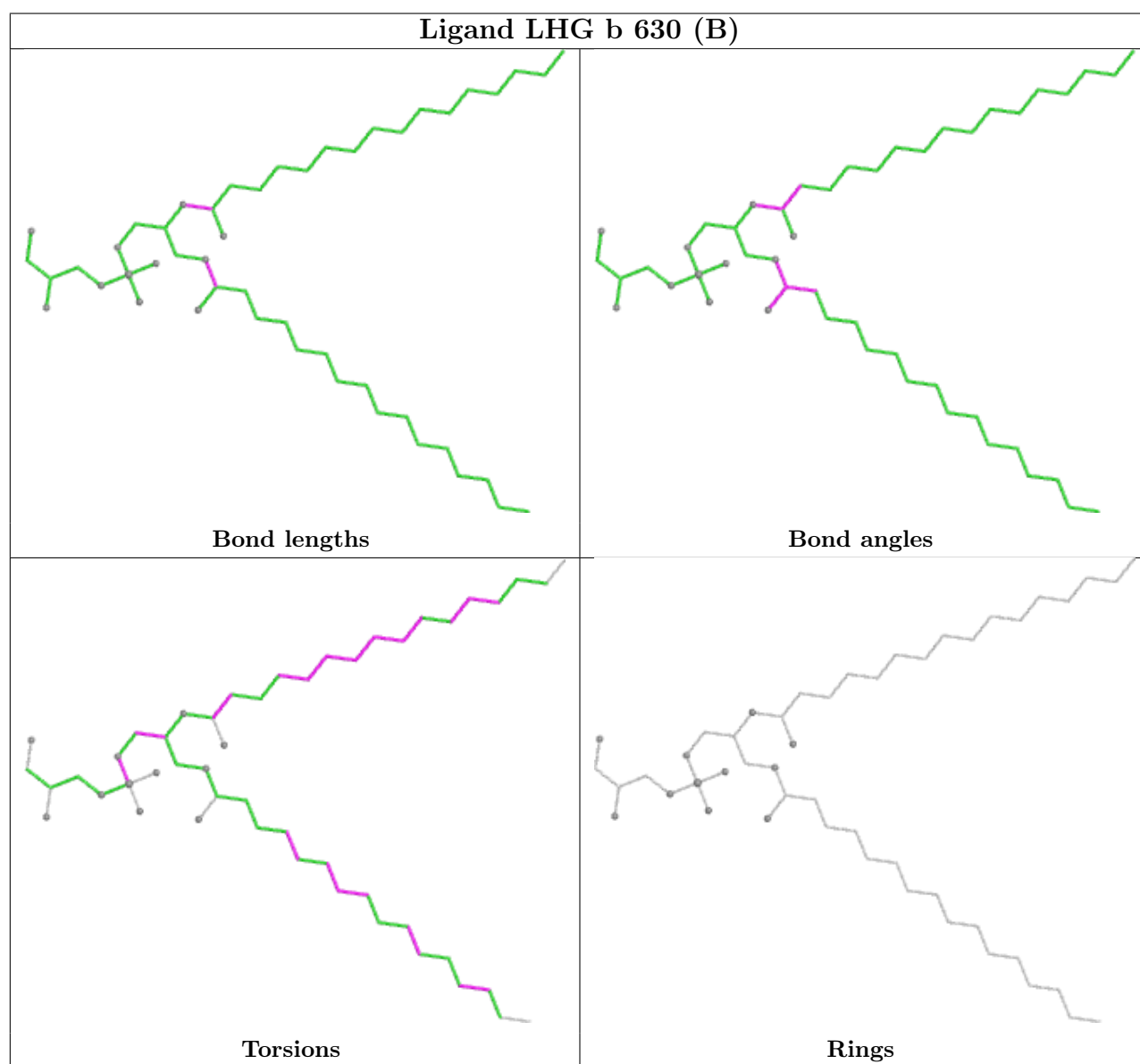
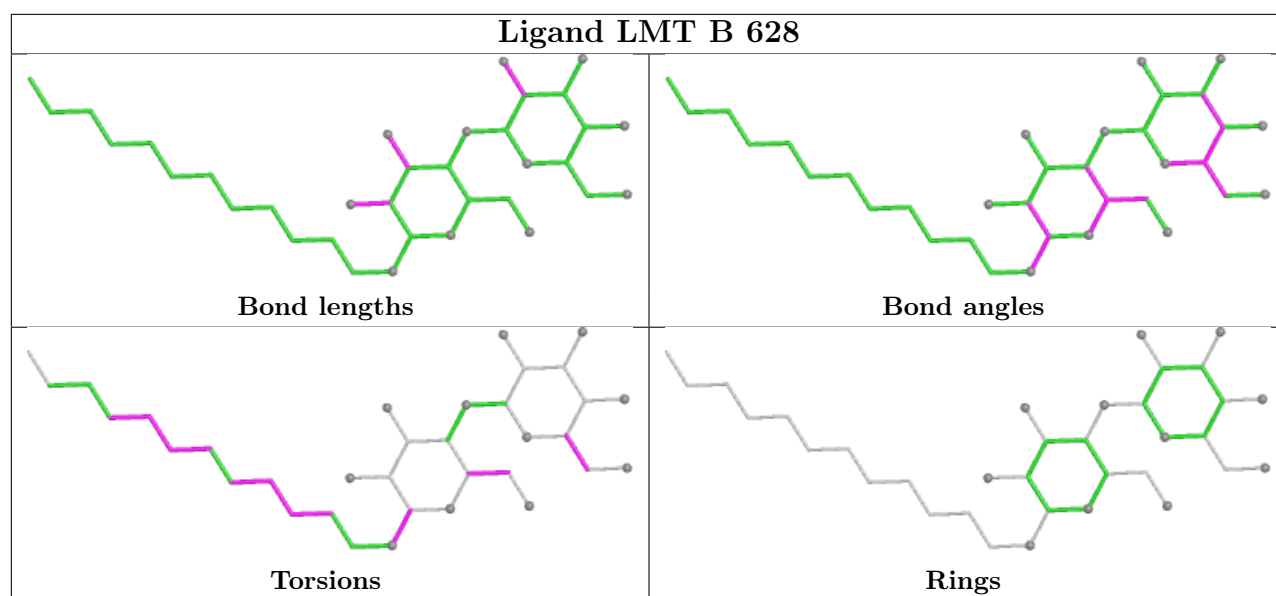


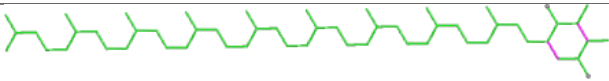
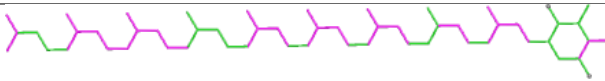
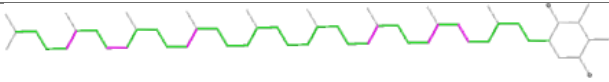
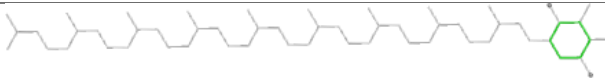


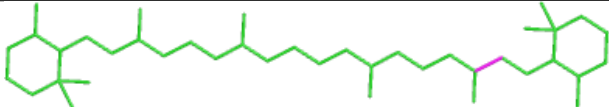
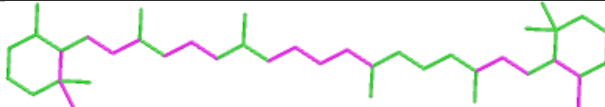
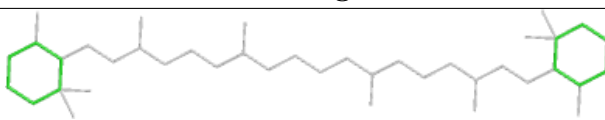


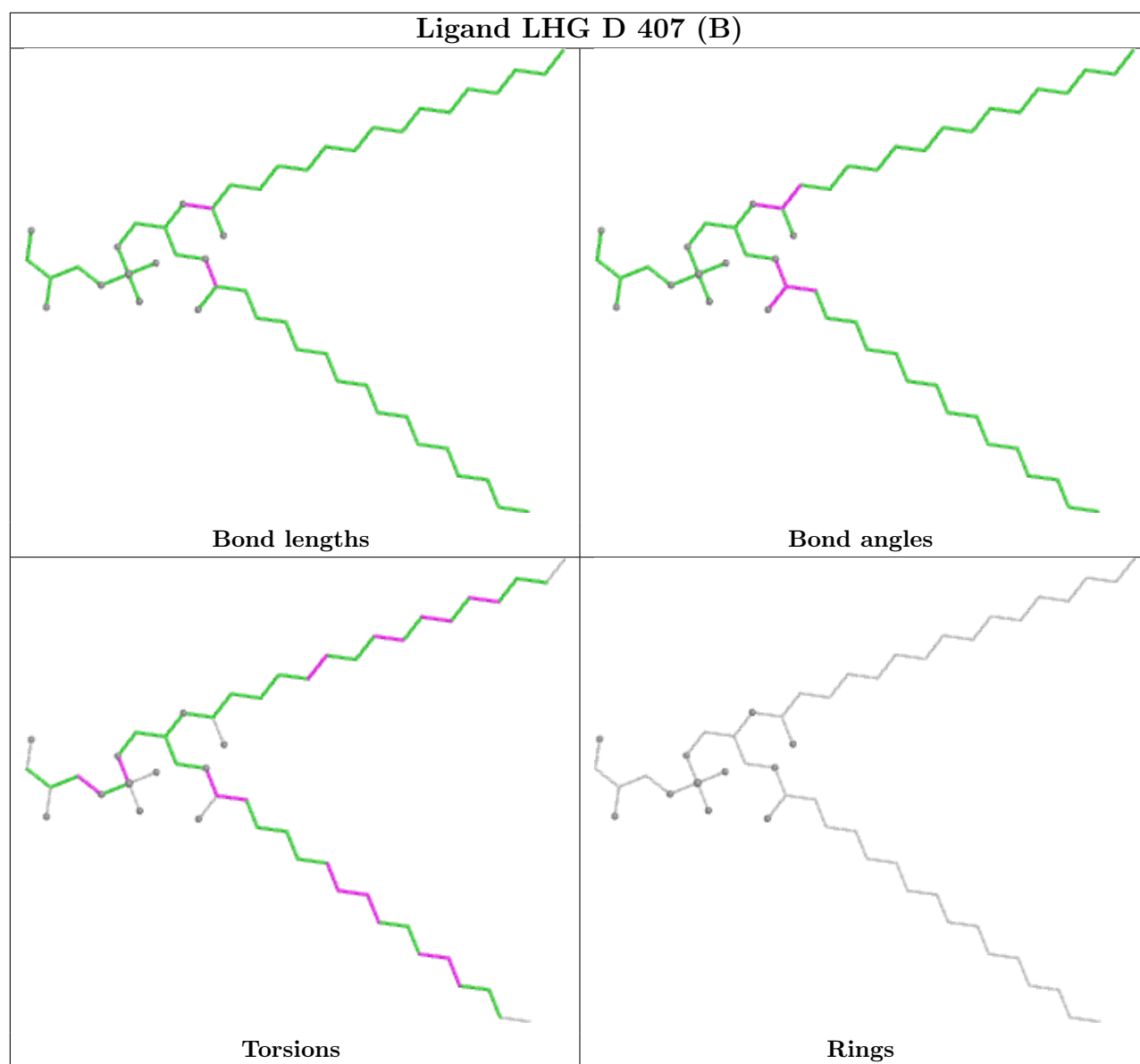




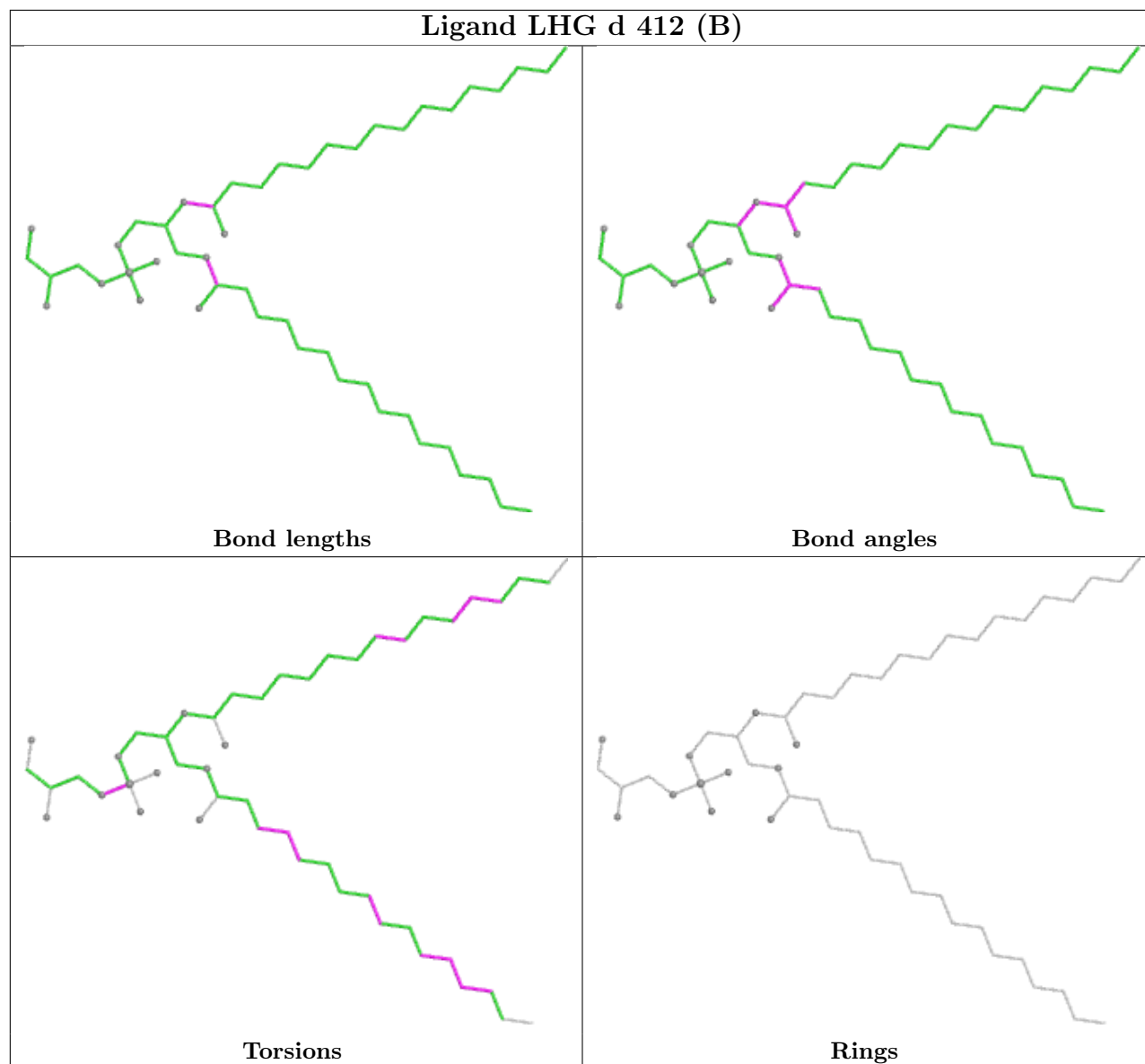


Ligand PL9 D 405 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings

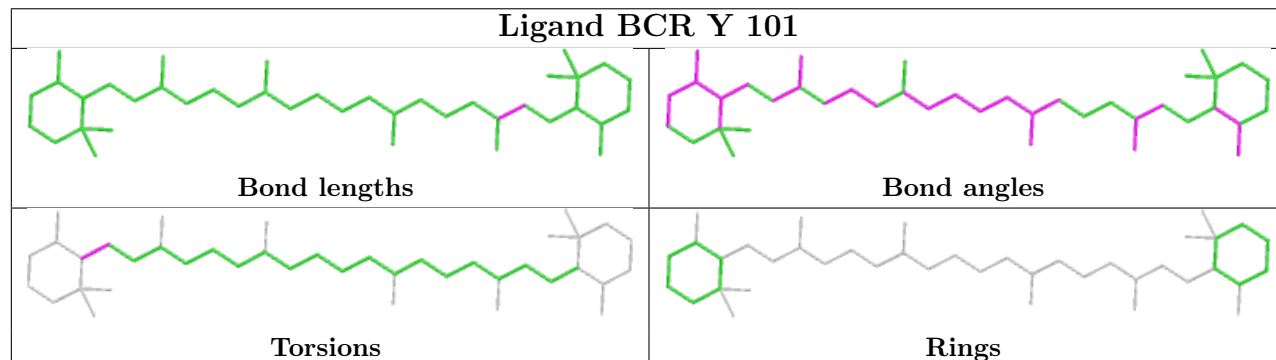
Ligand BCR H 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

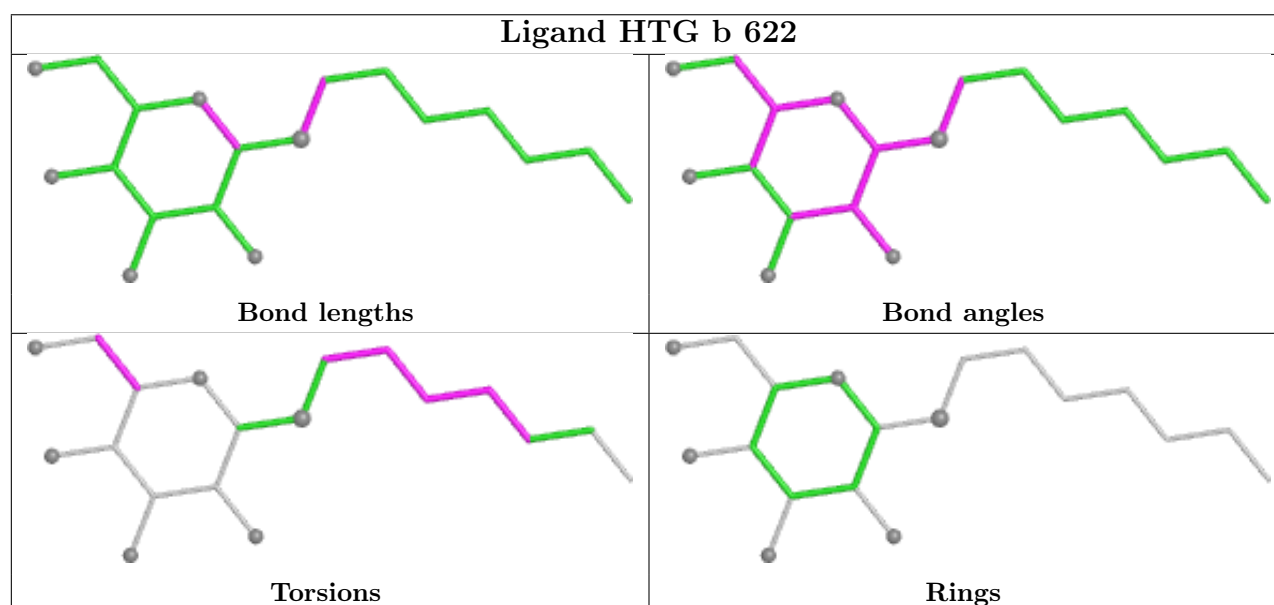
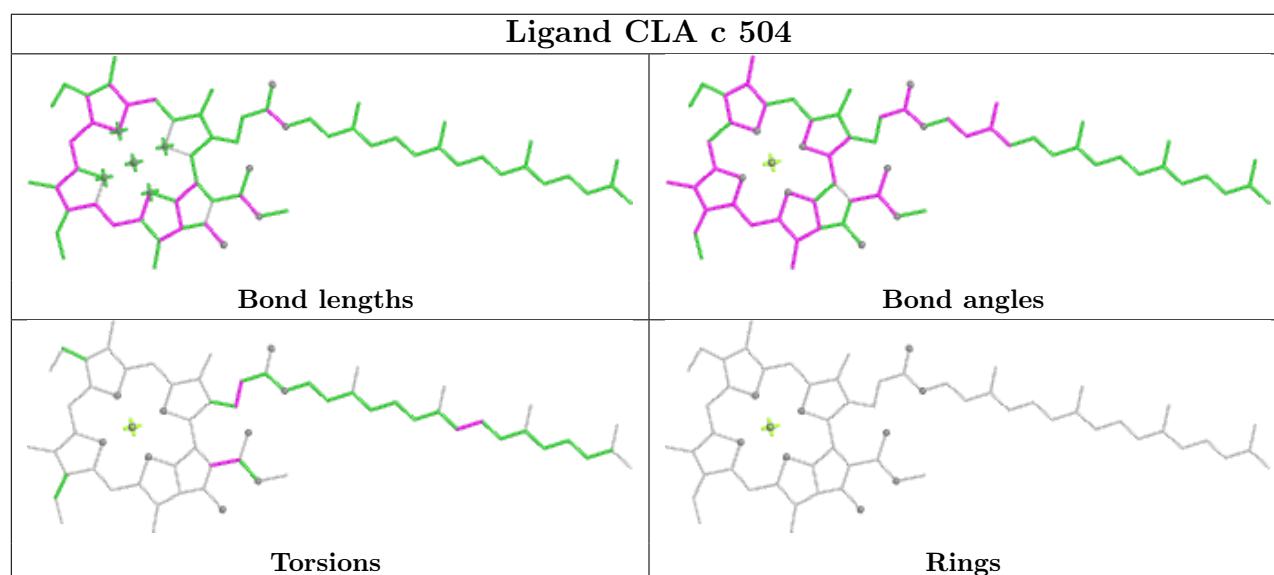
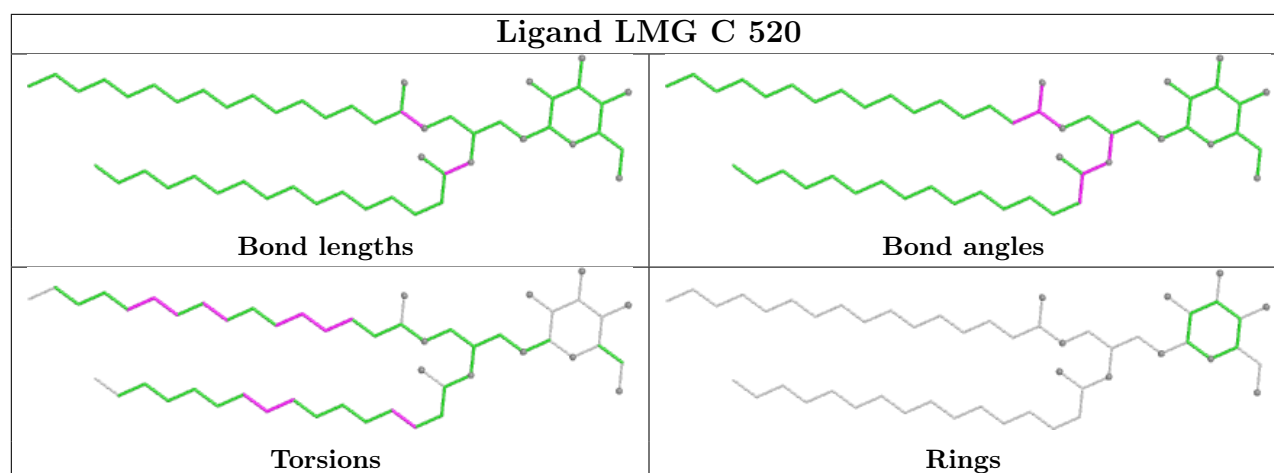


Ligand LHG d 412 (B)

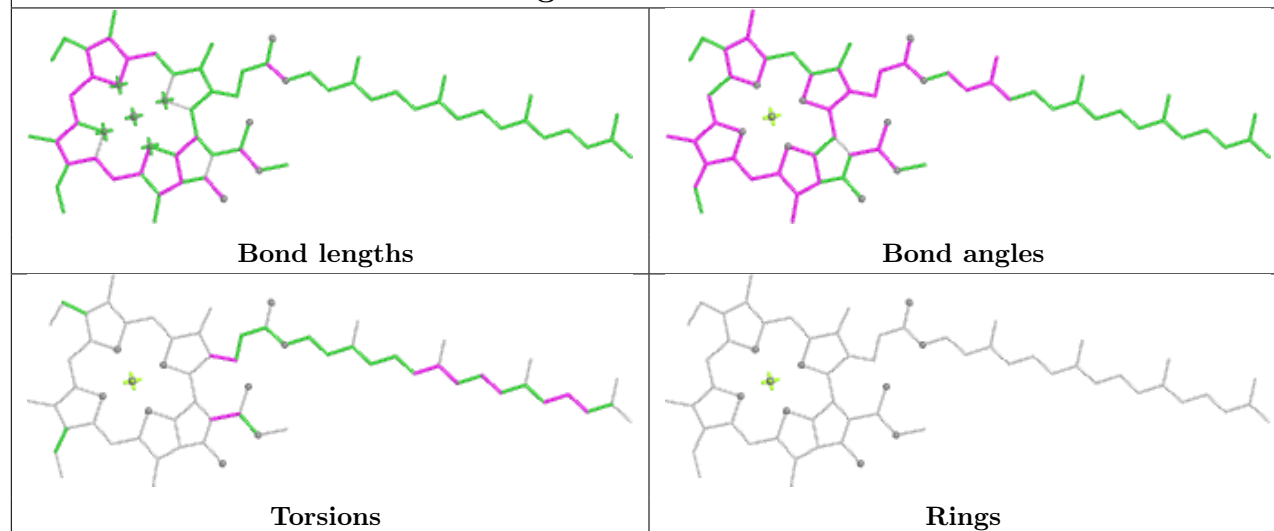


Ligand BCR Y 101

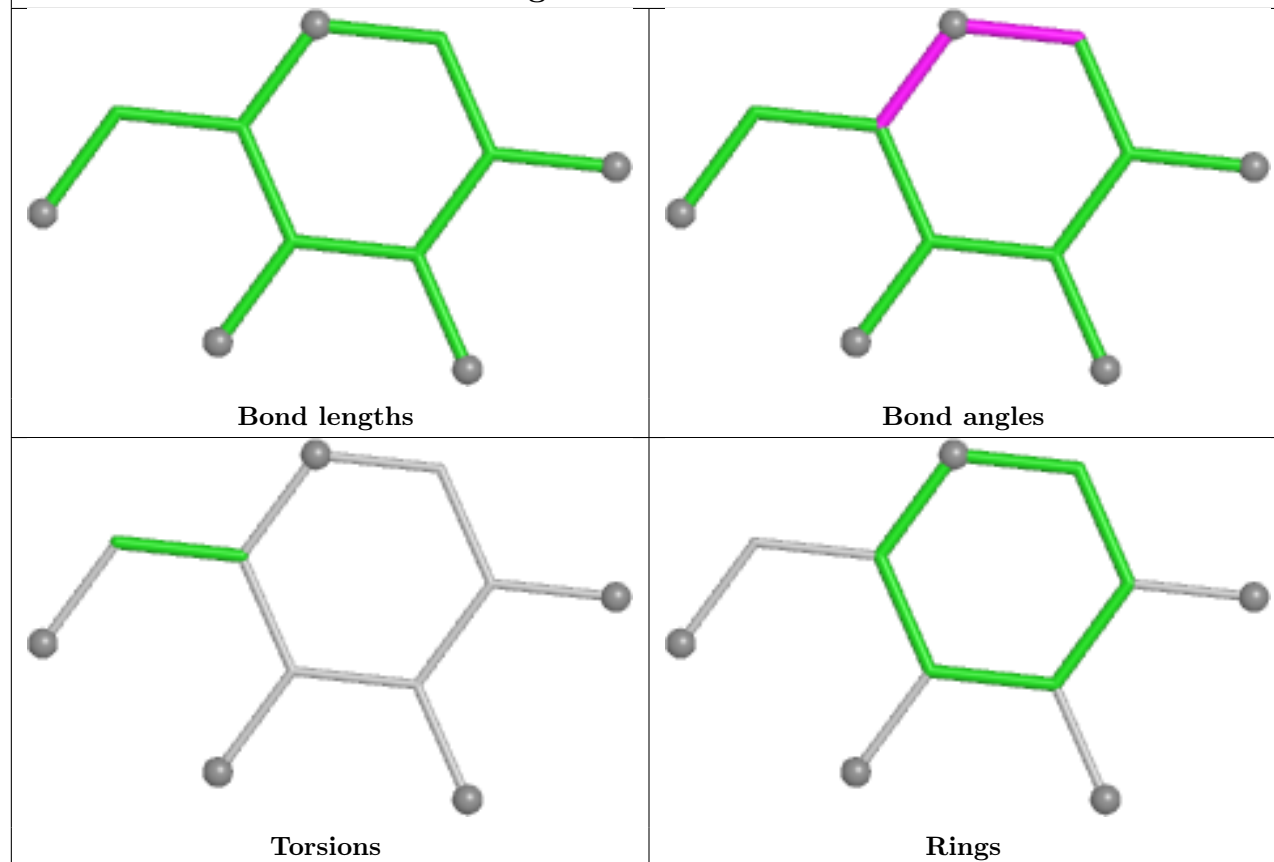


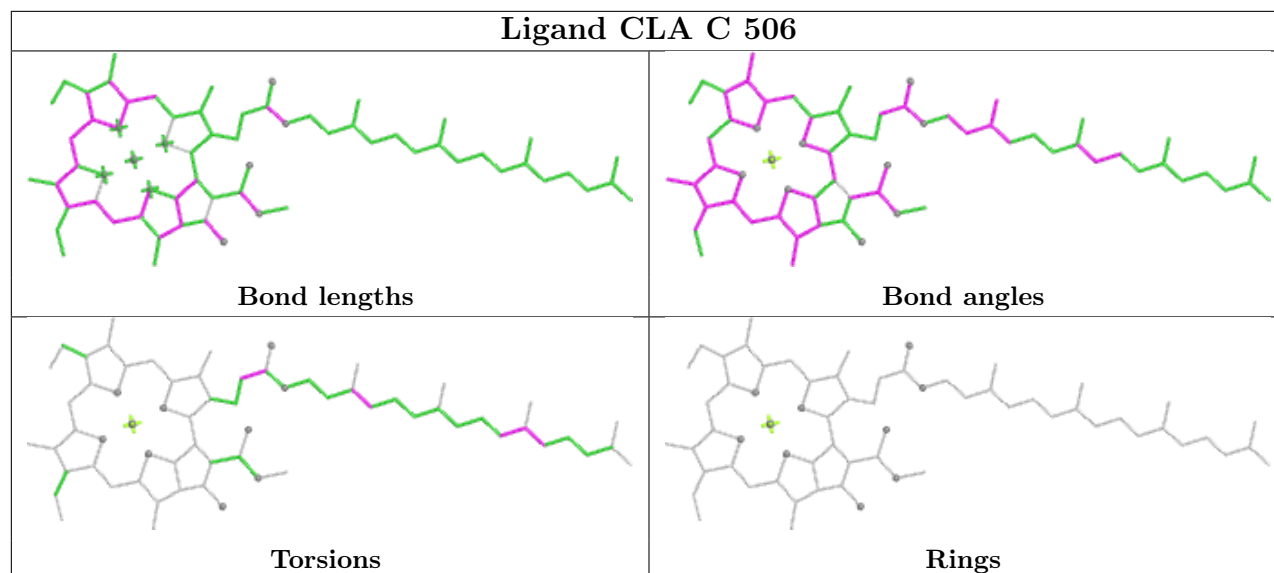
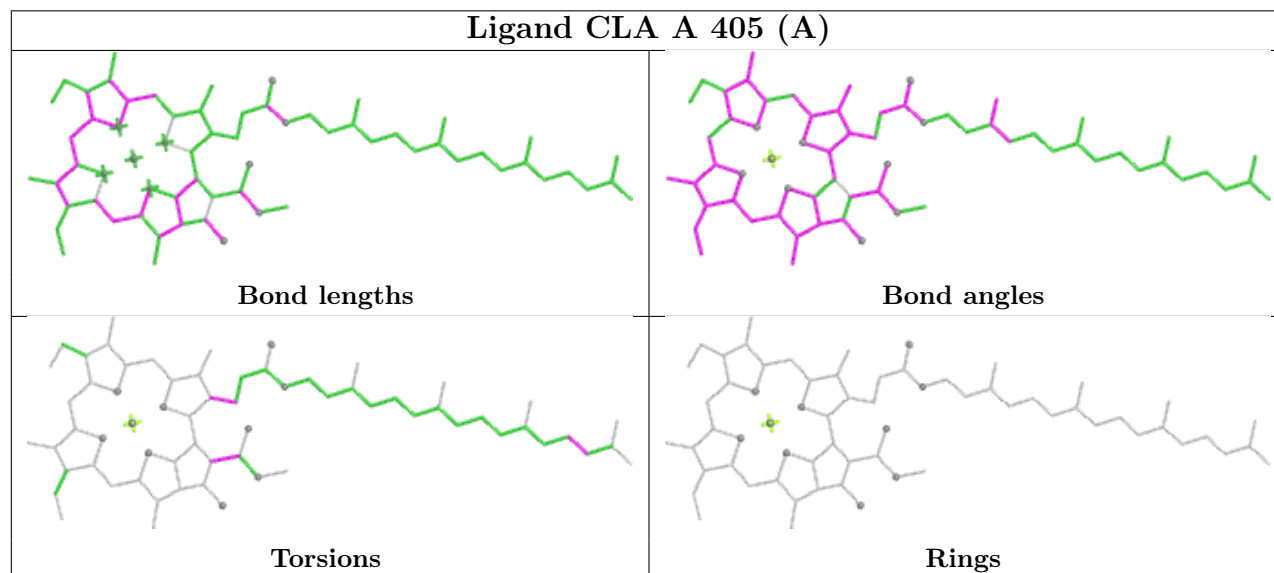
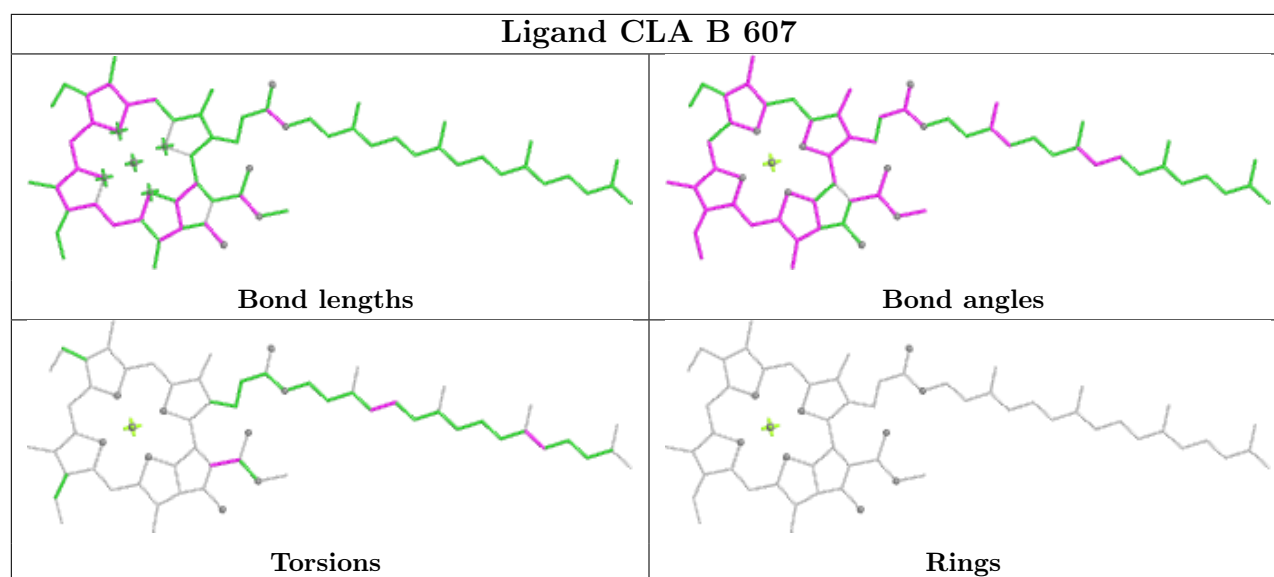


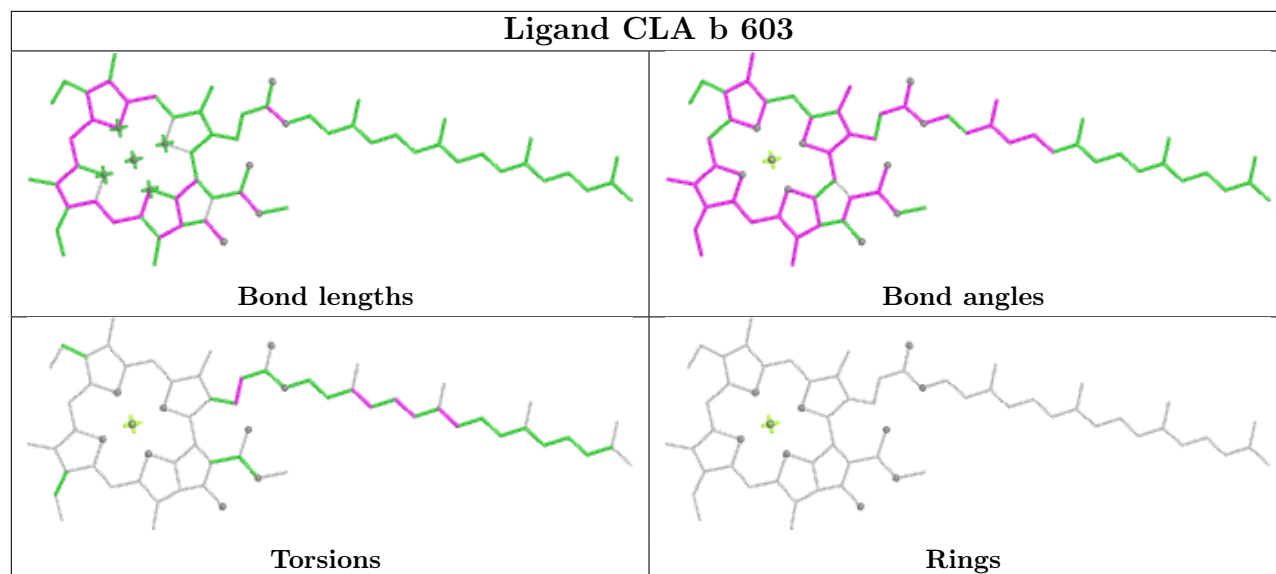
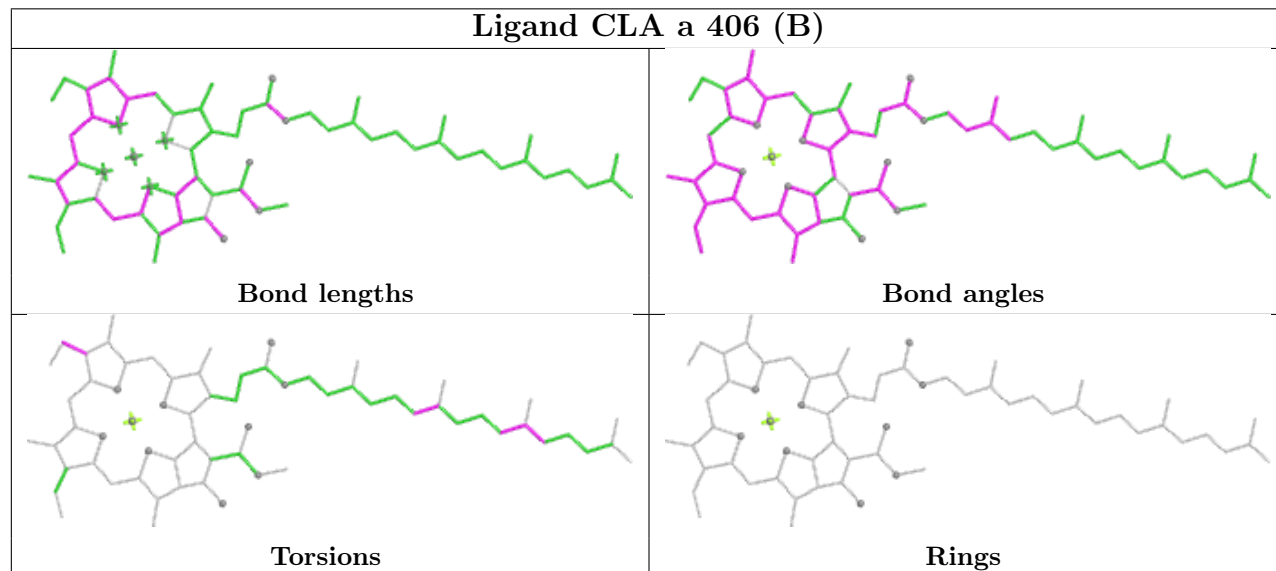
Ligand CLA c 507



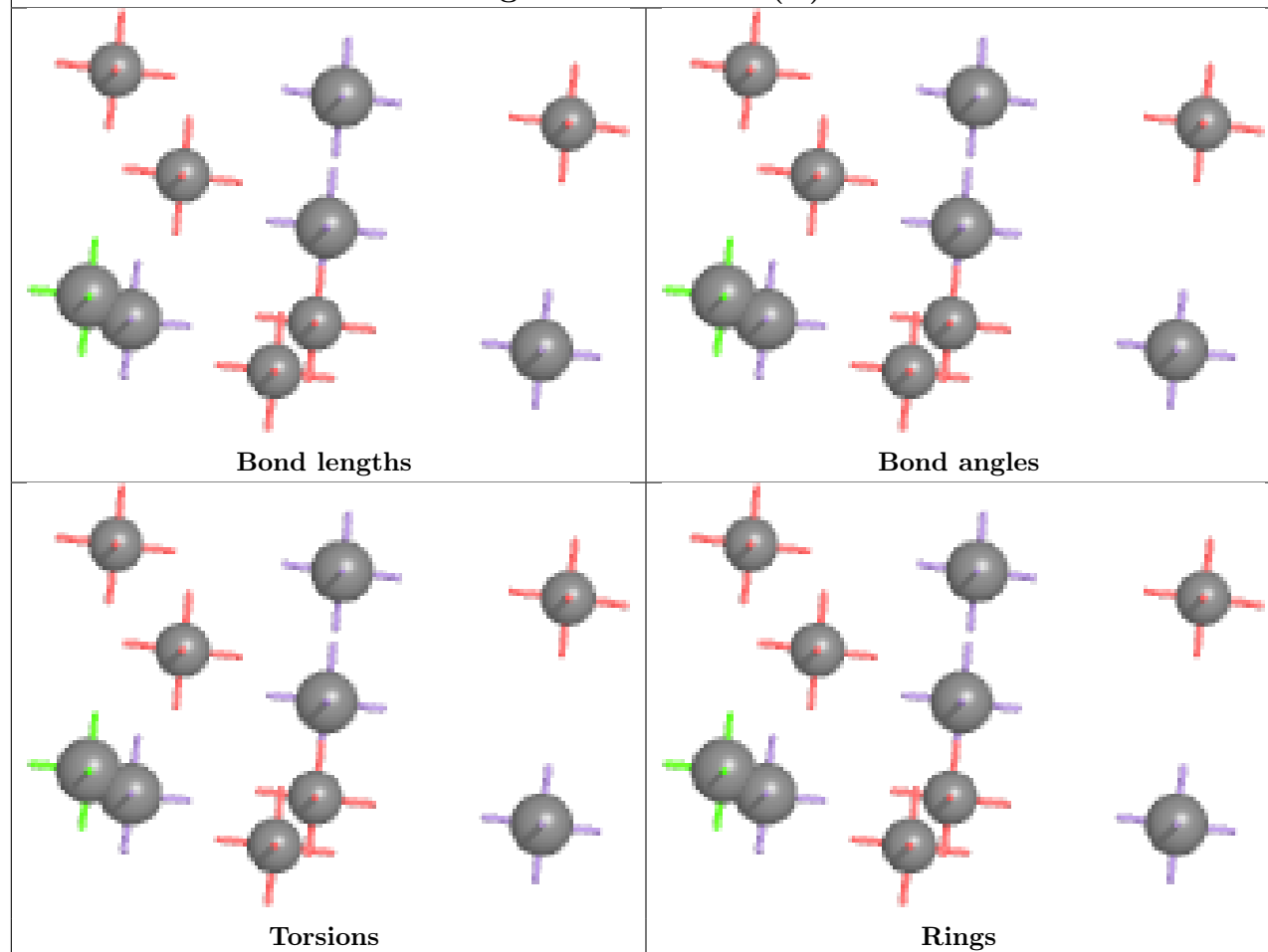
Ligand HTG V 202



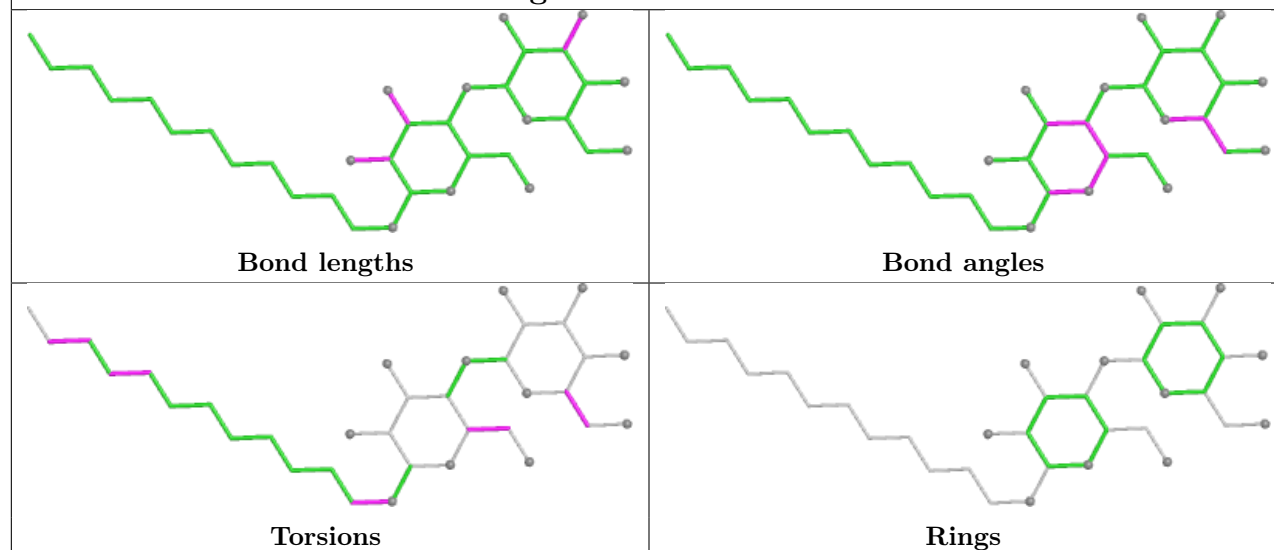


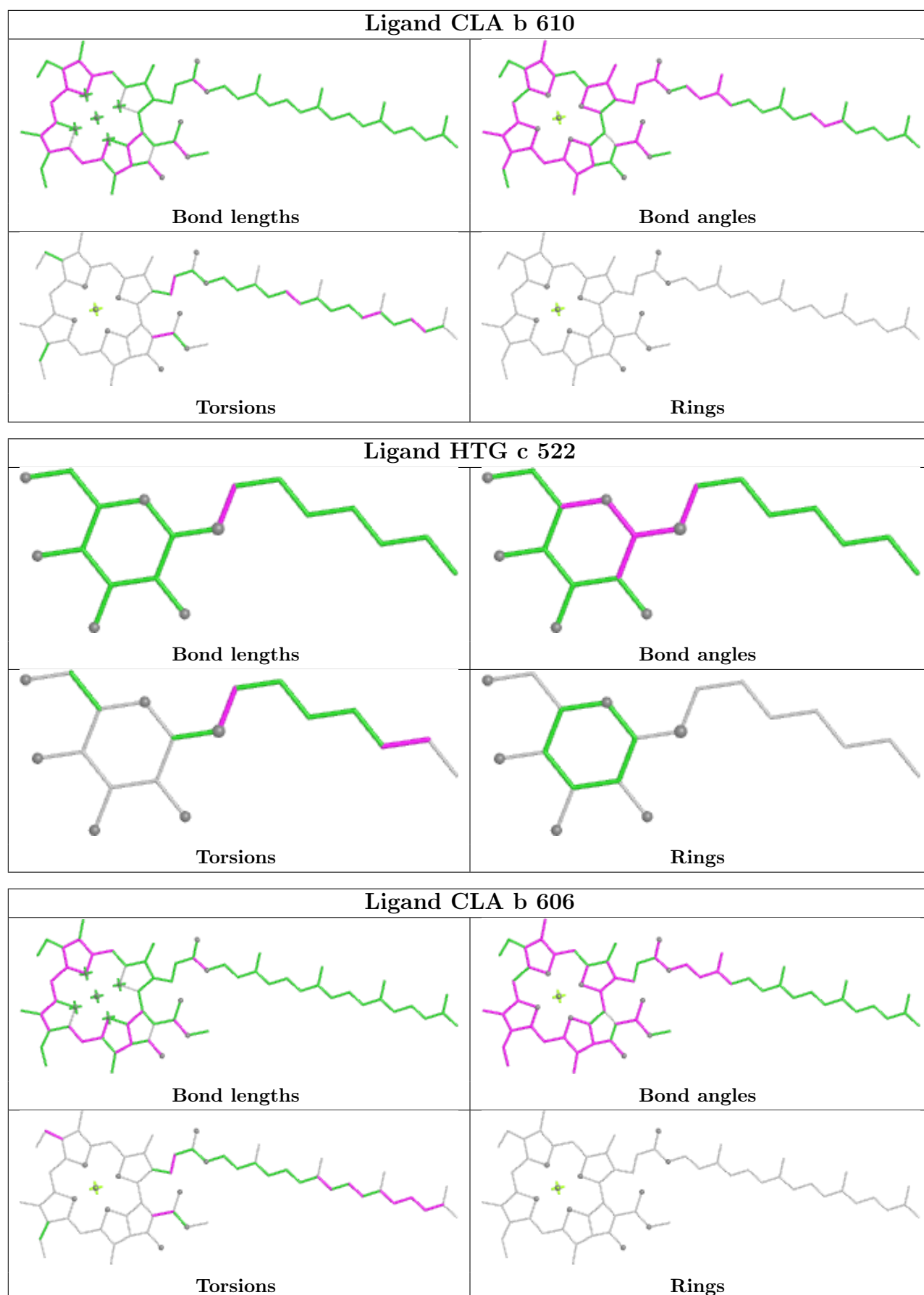
Ligand CLA b 603**Ligand CLA a 406 (B)**

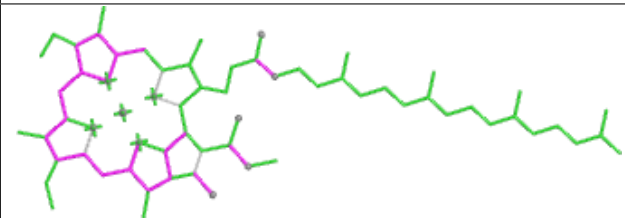
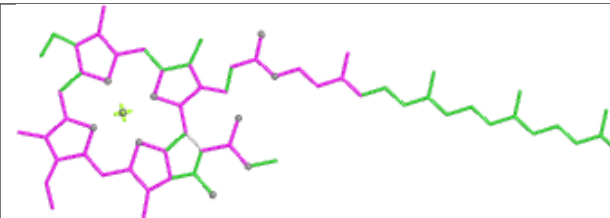
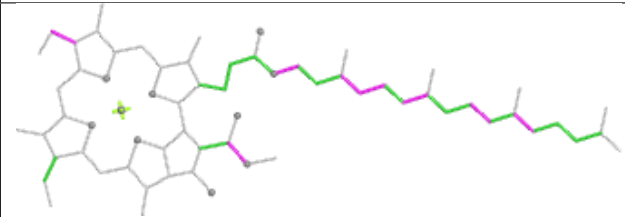
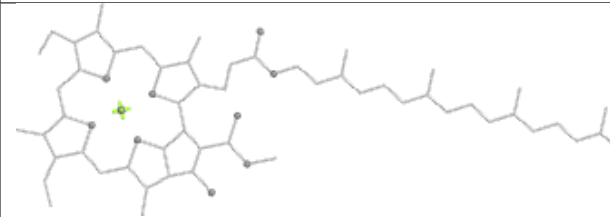
Ligand OEX a 412 (B)

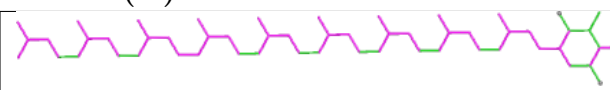
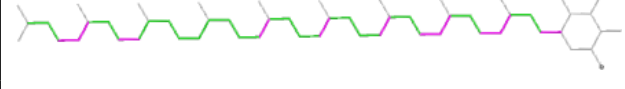


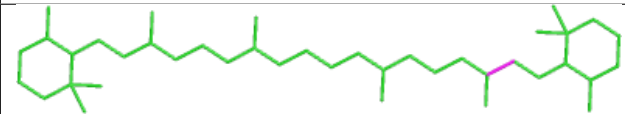
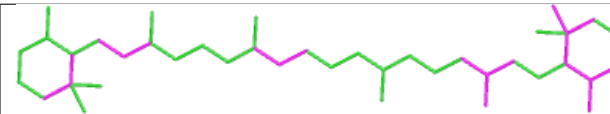
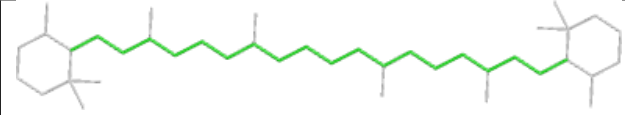
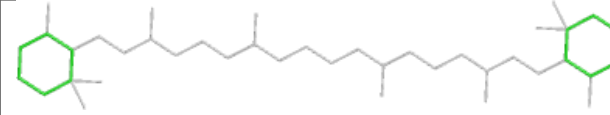
Ligand LMT T 101



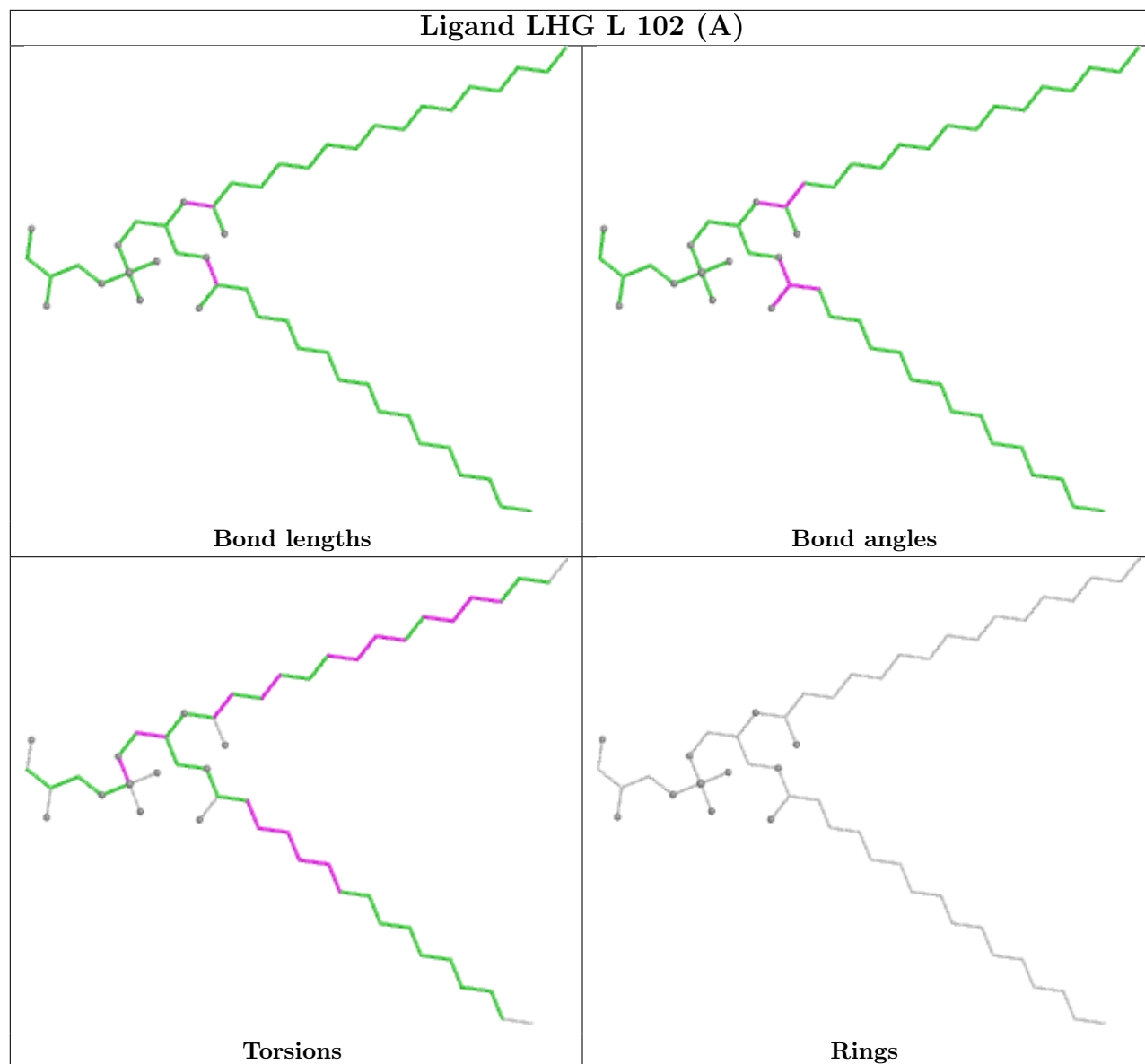


Ligand CLA c 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

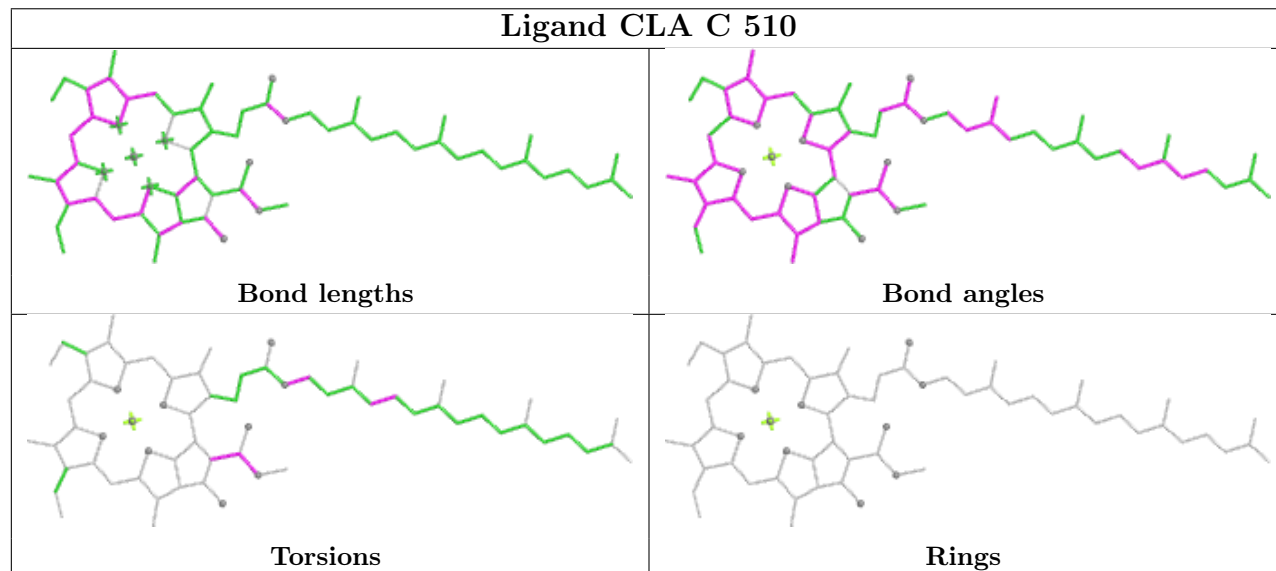
Ligand PL9 A 414 (A)	
	
Bond lengths	Bond angles
	
Torsions	Rings

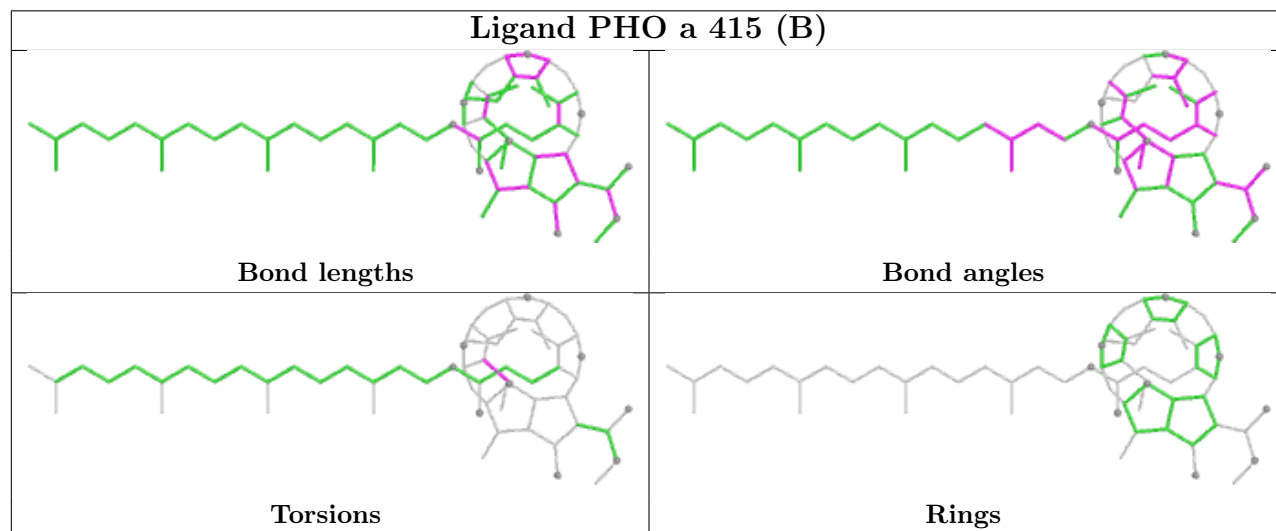
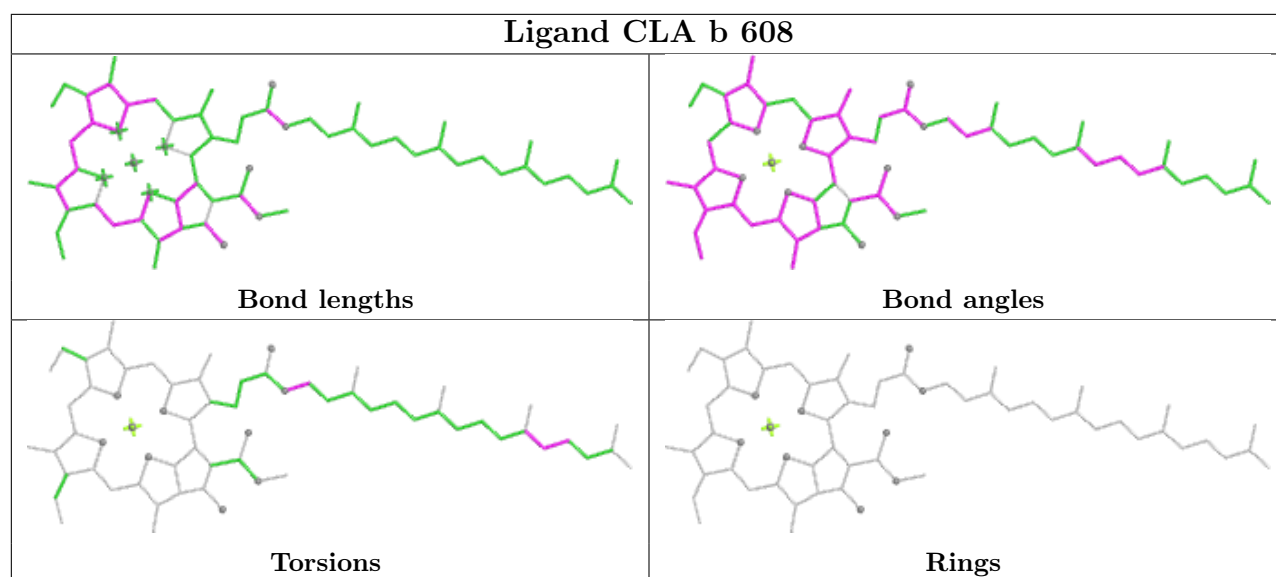
Ligand BCR B 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

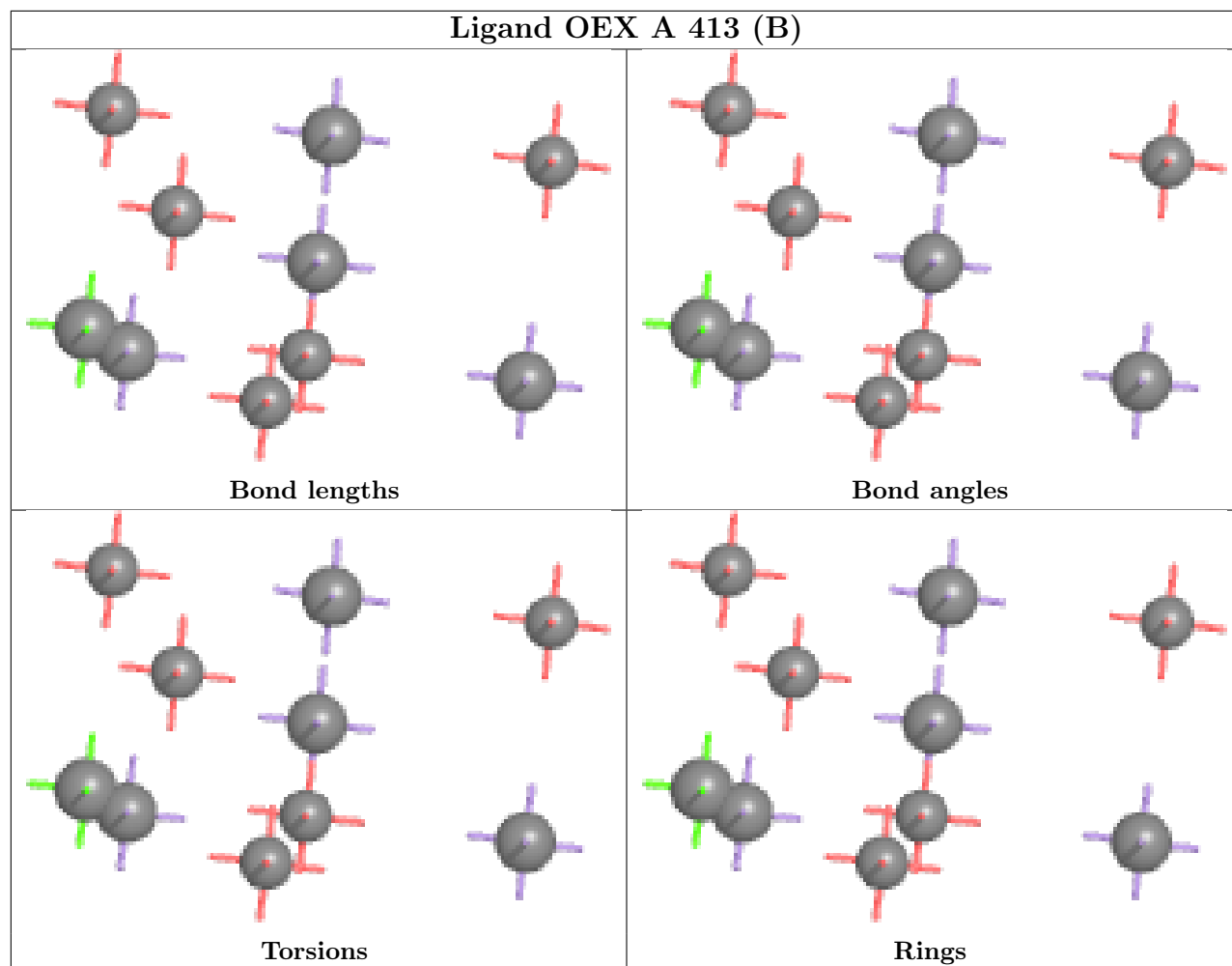
Ligand LHG L 102 (A)

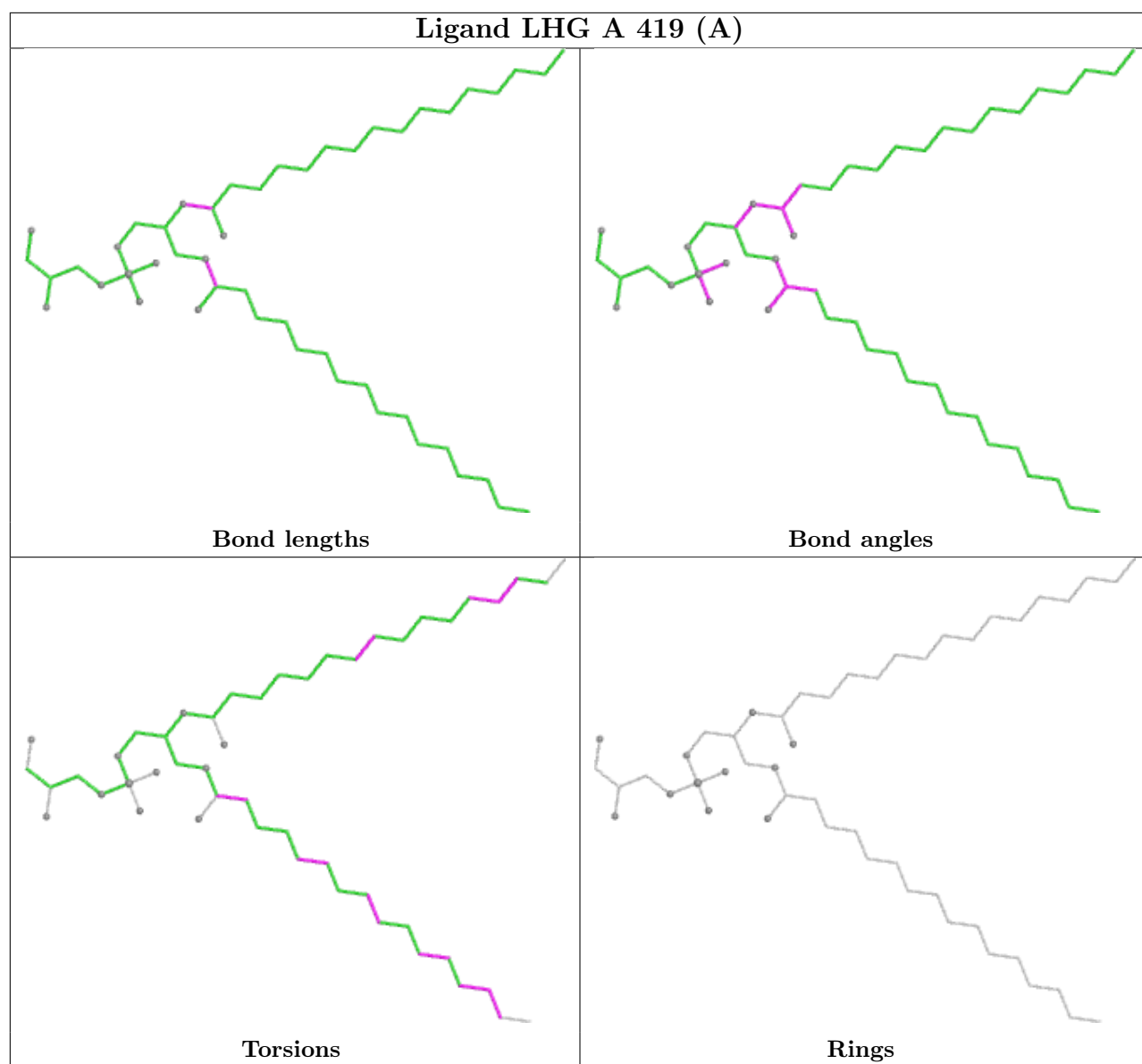


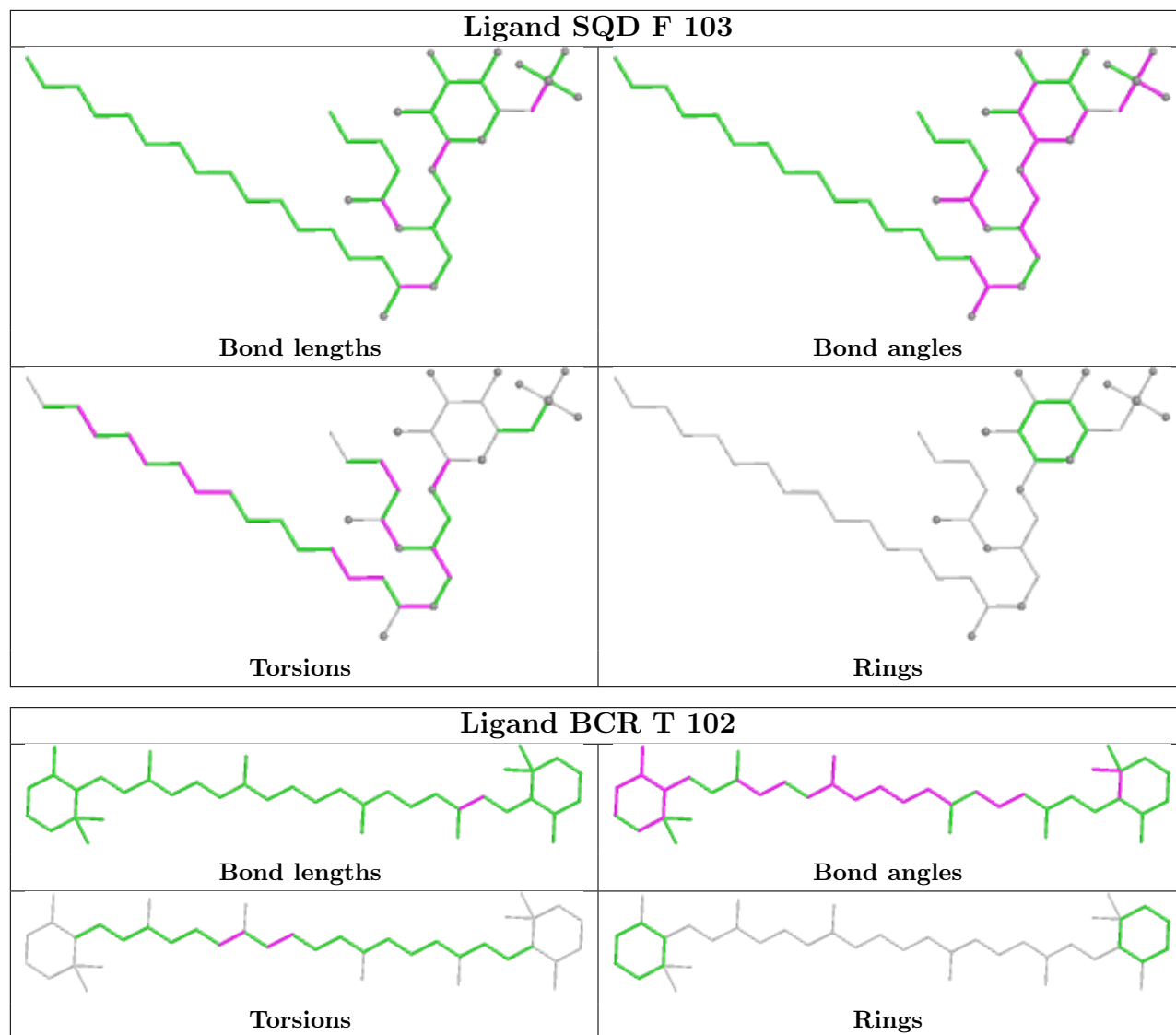
Ligand CLA C 510

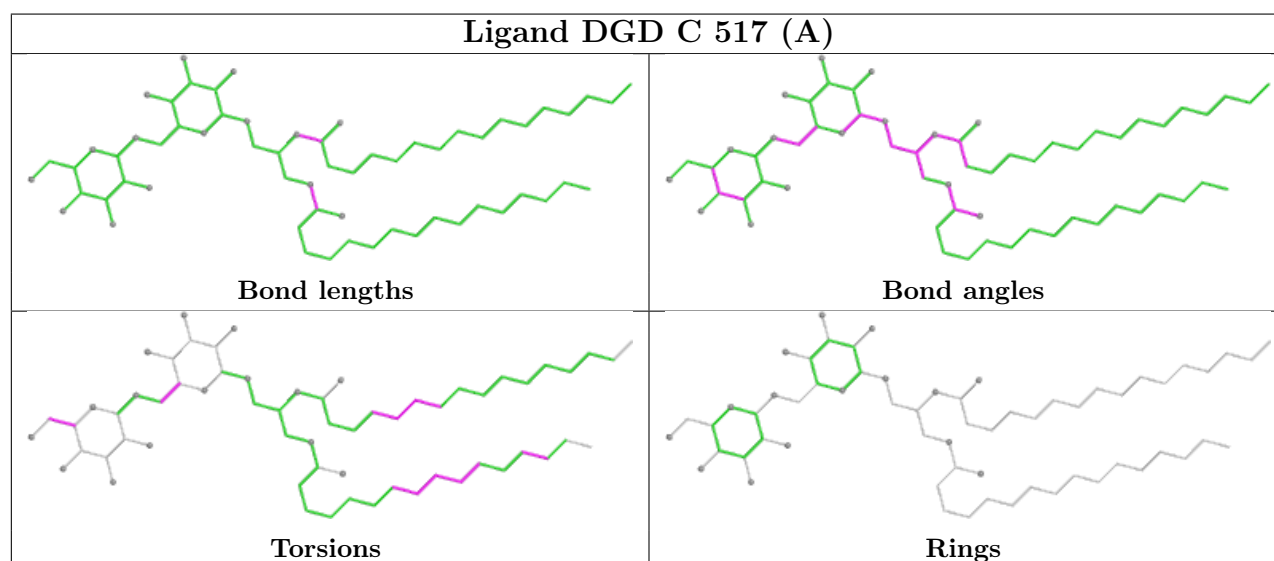
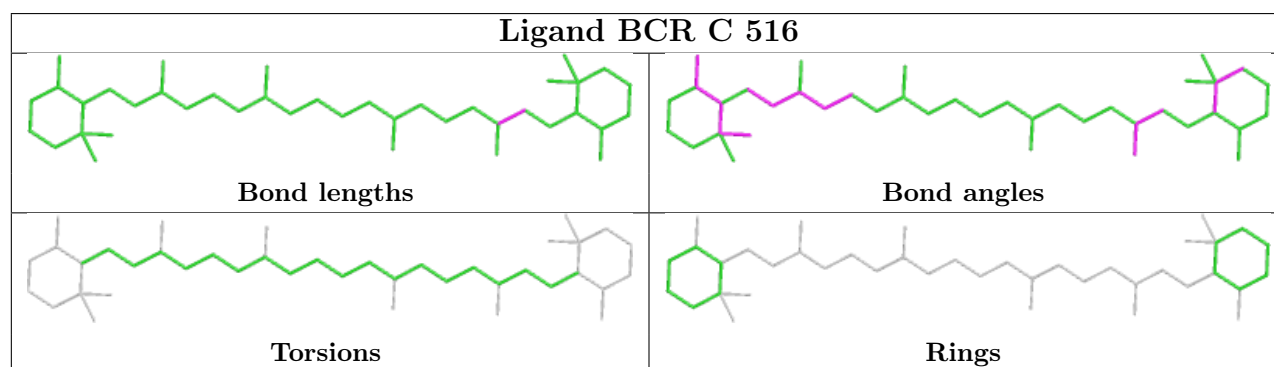
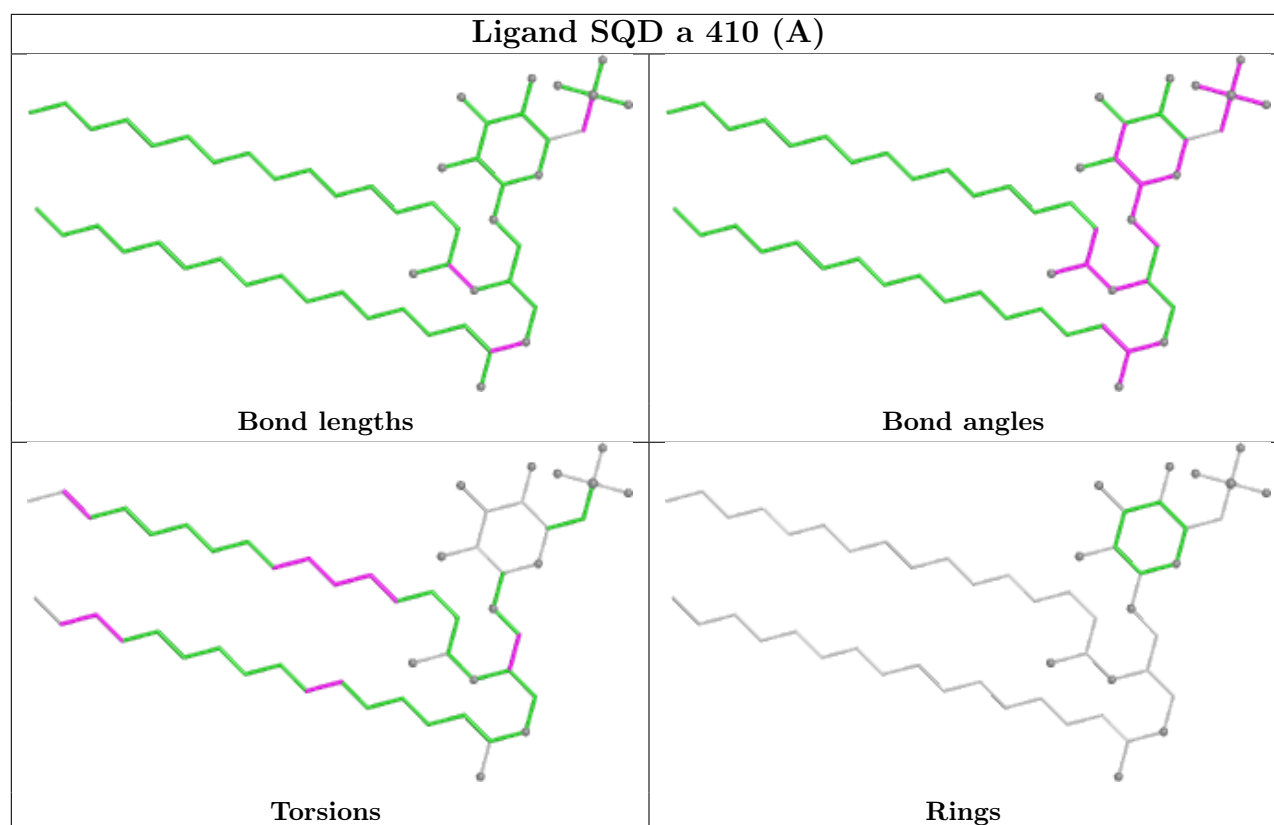


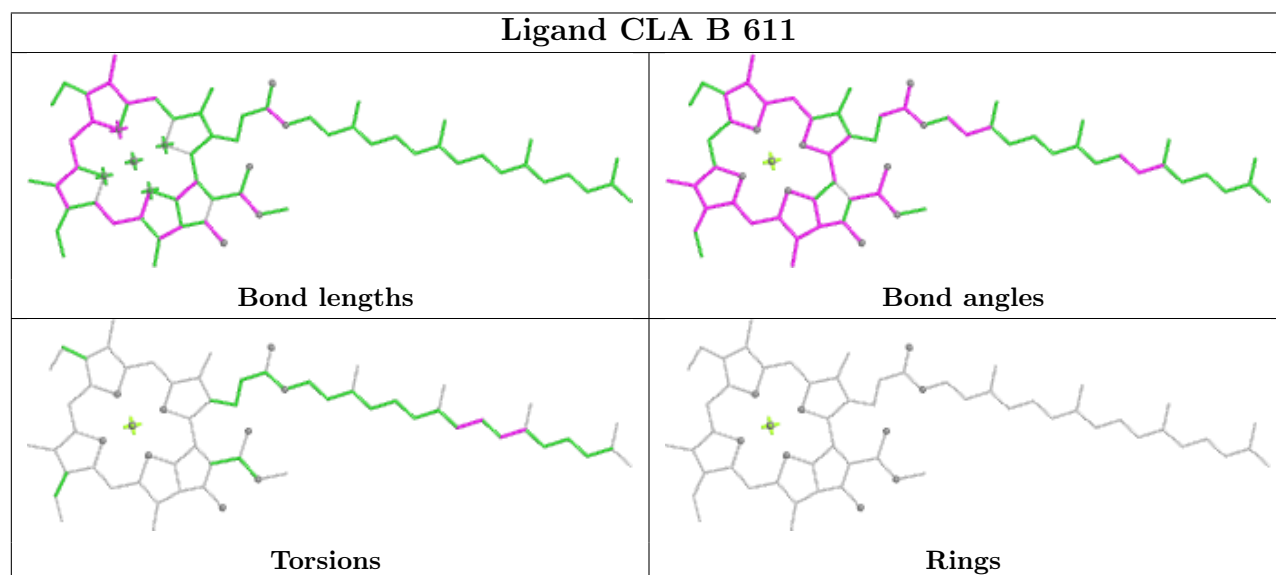
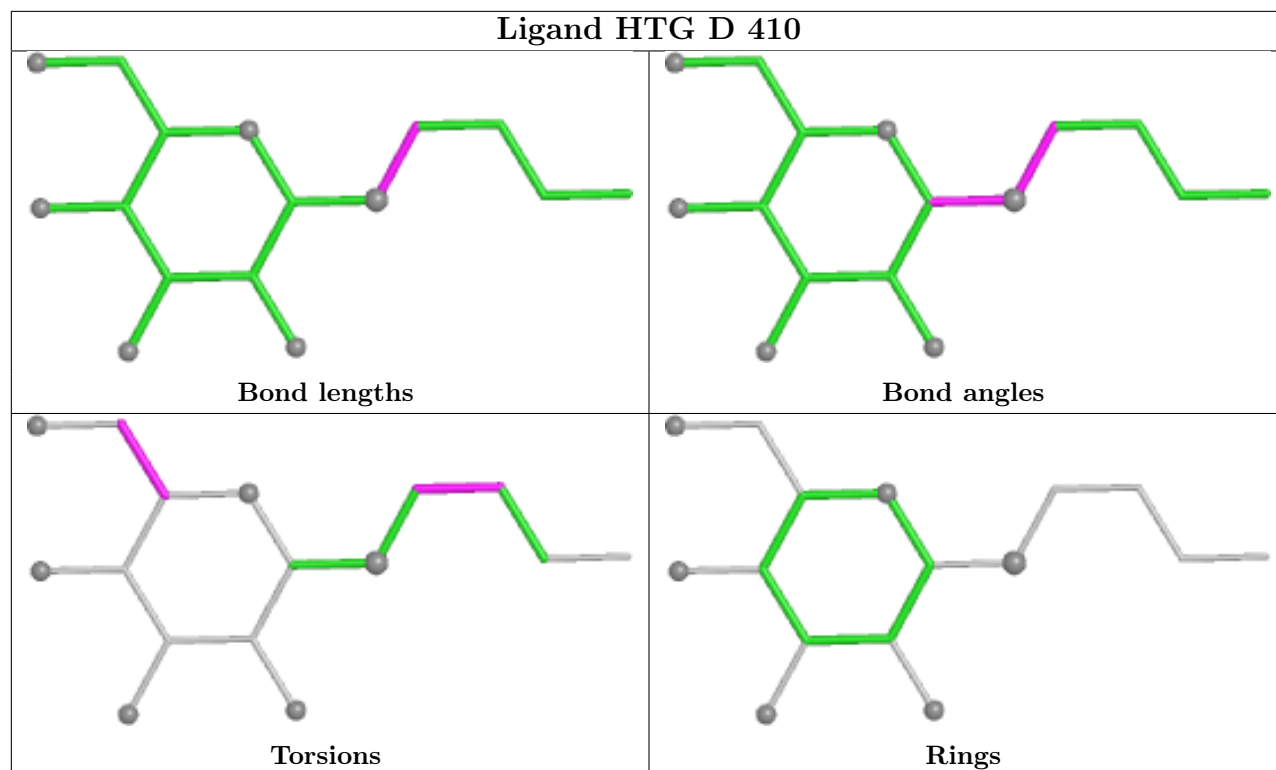


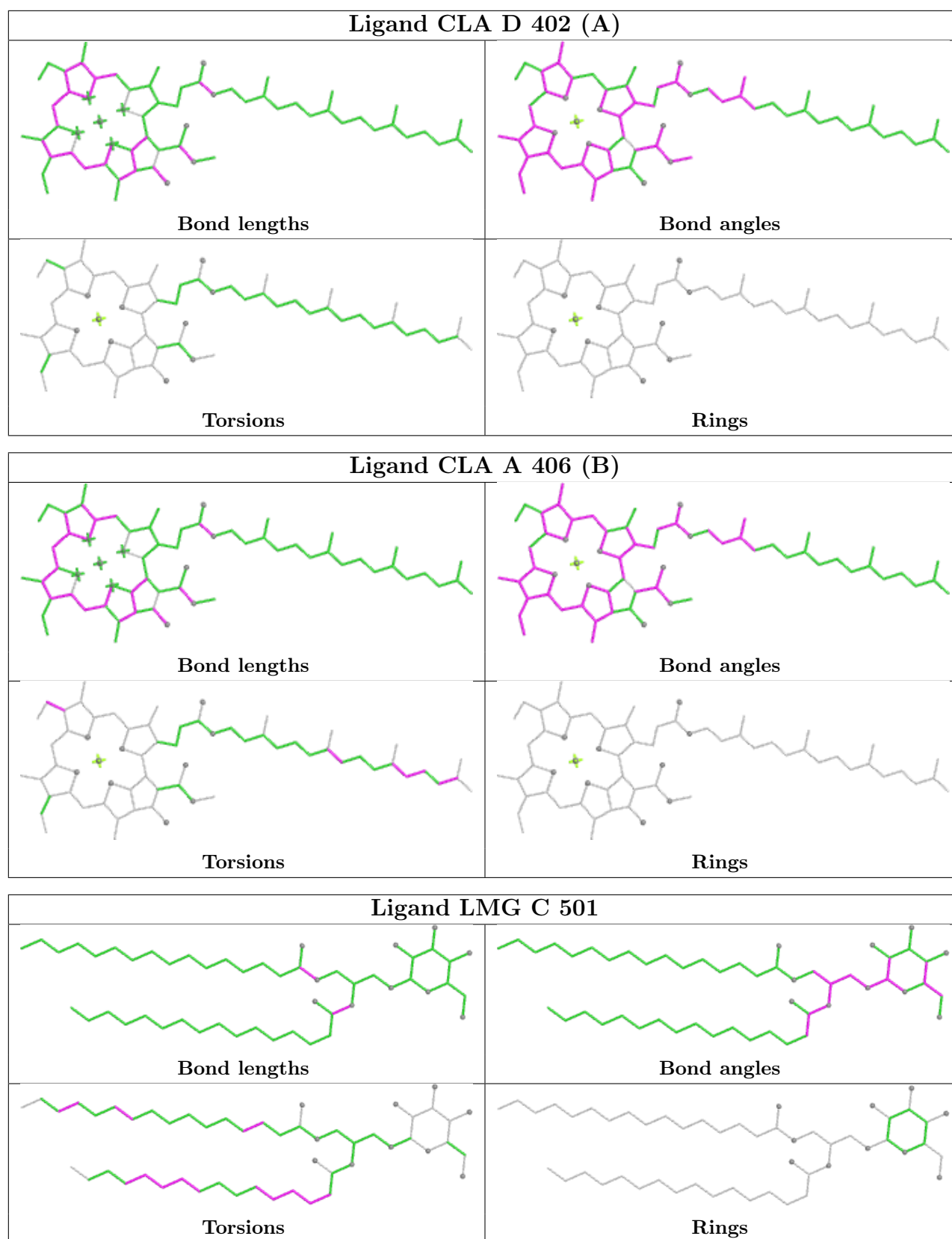


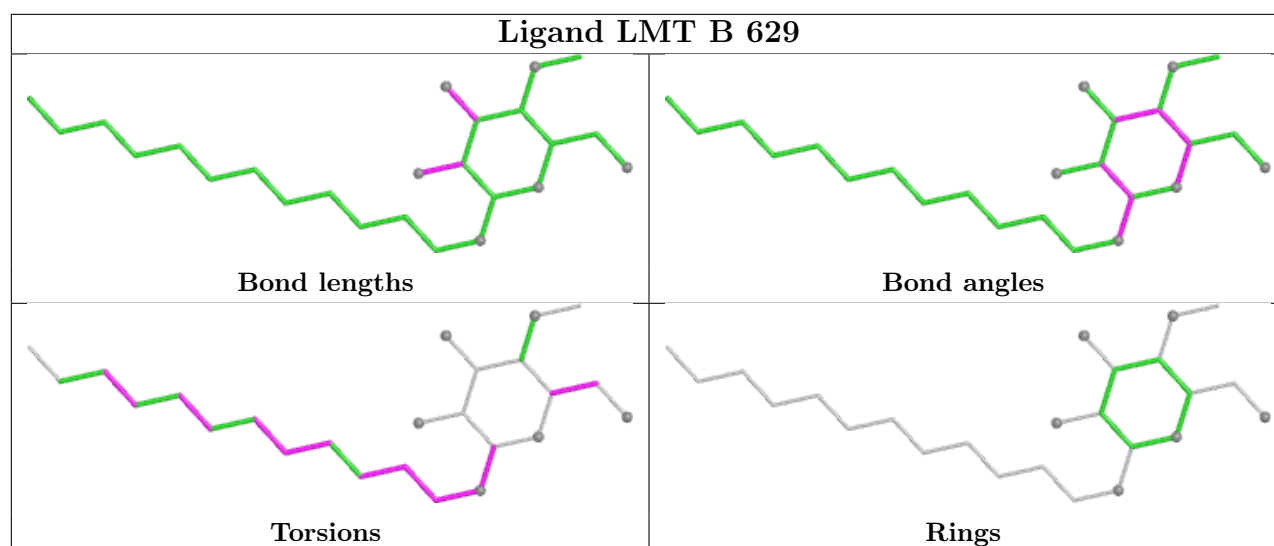
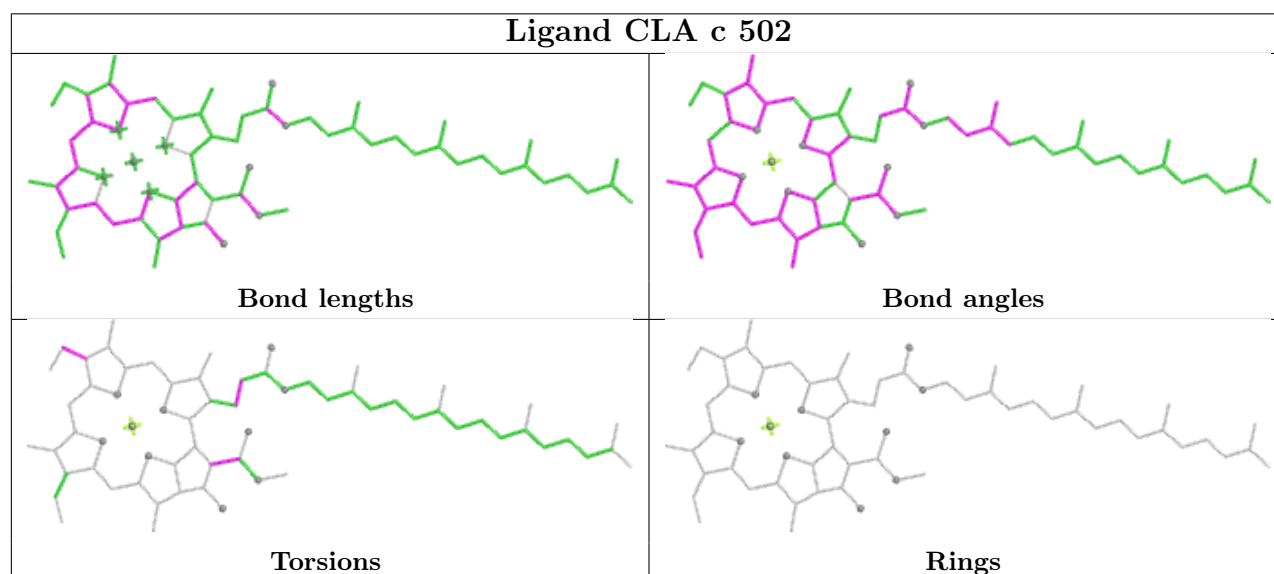
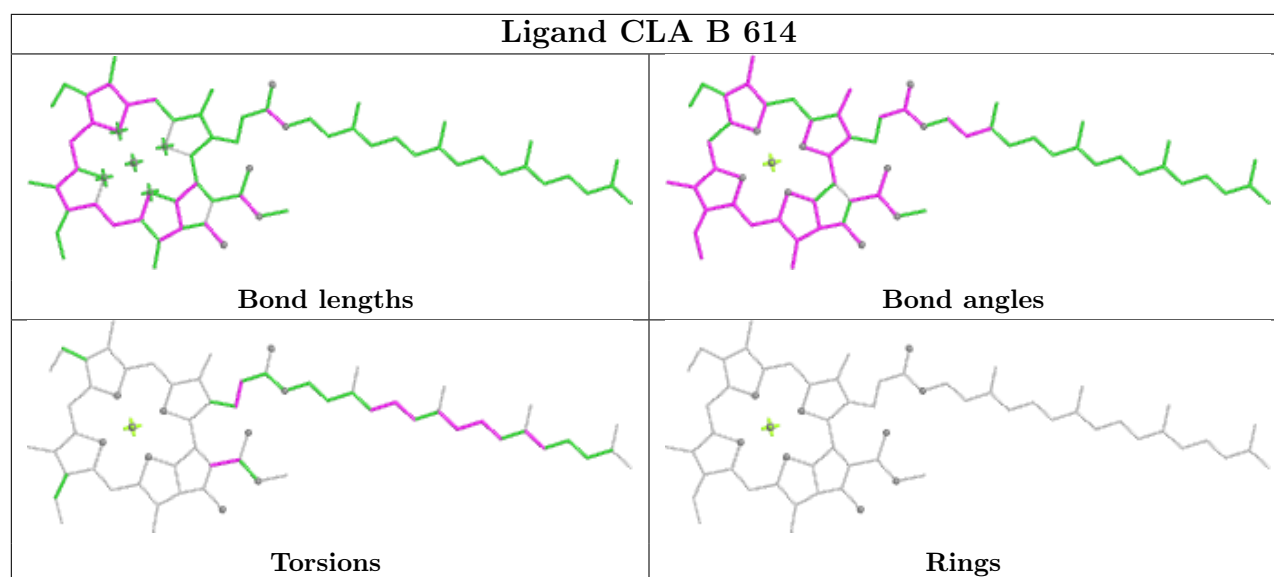


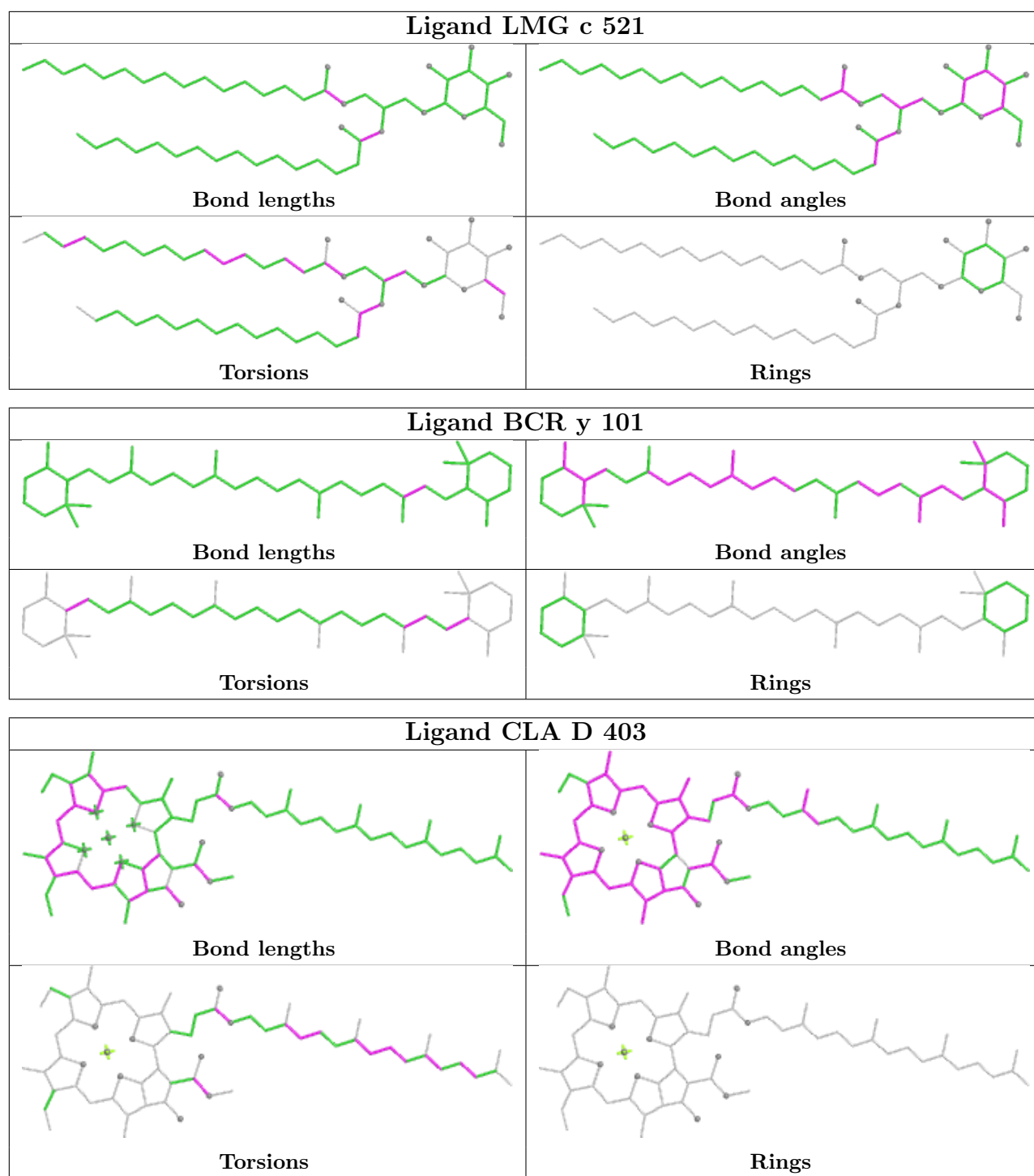


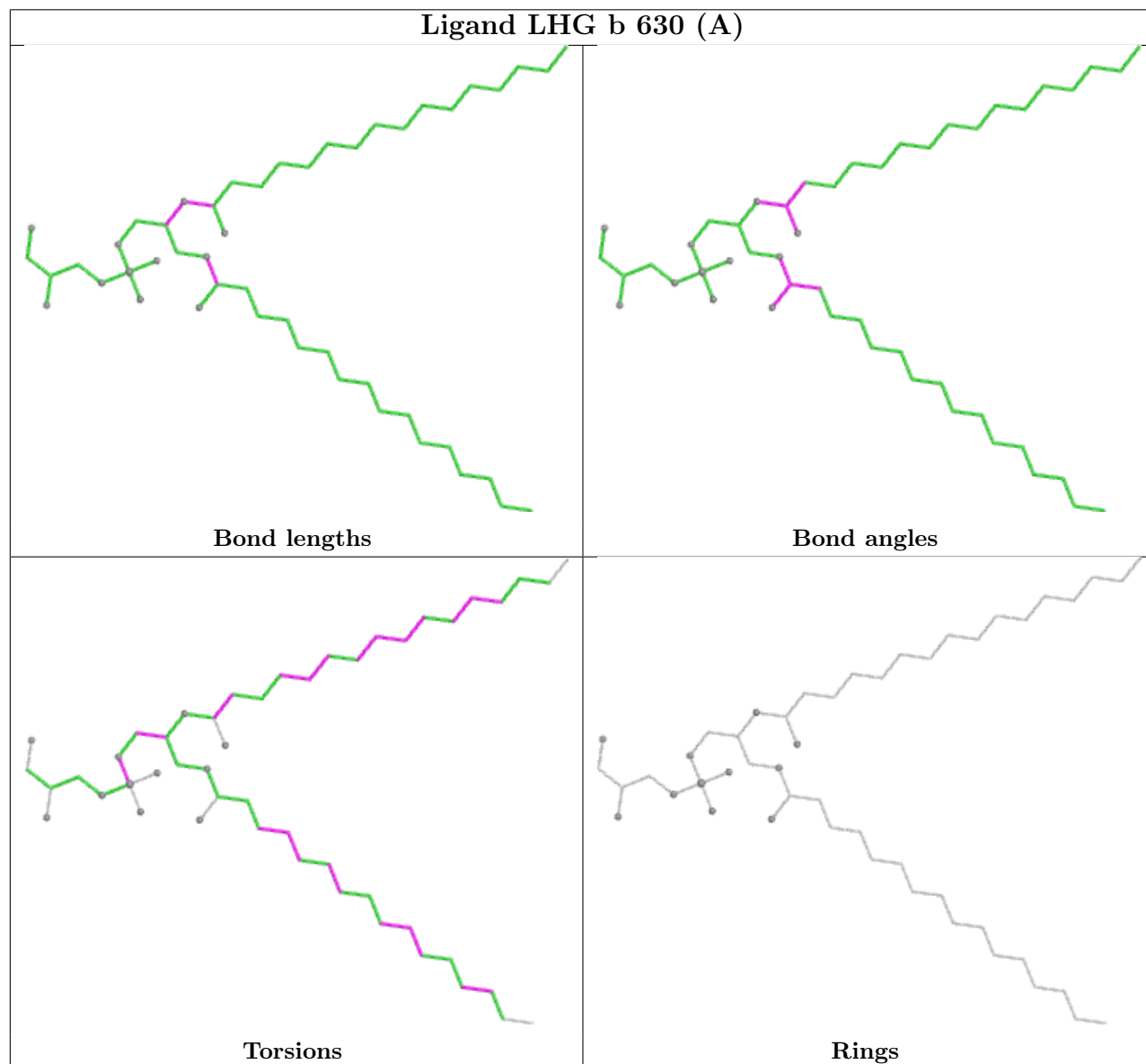
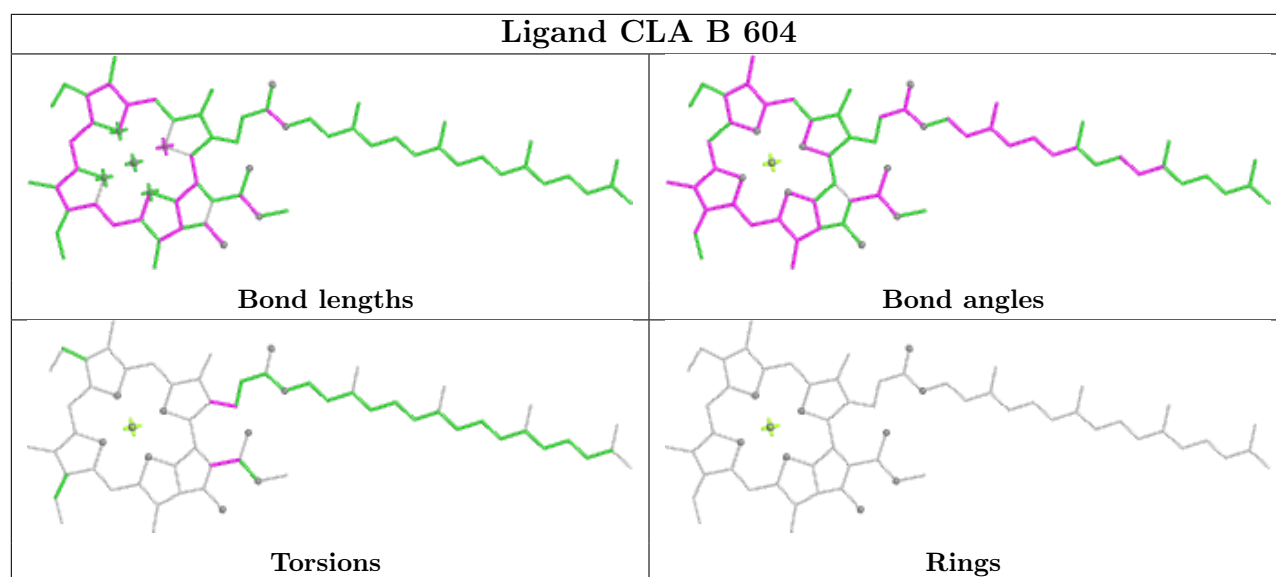


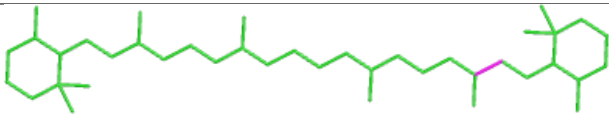
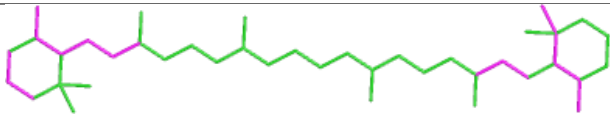
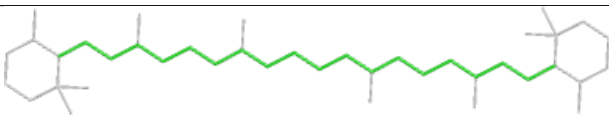
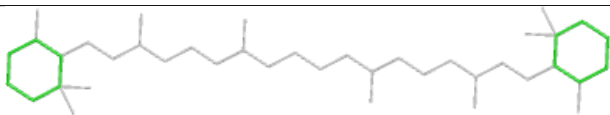


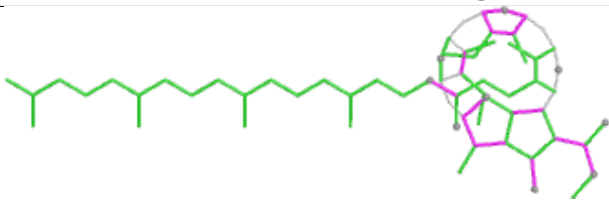
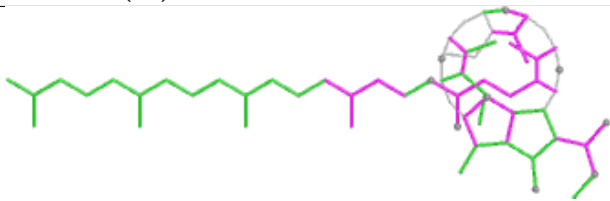
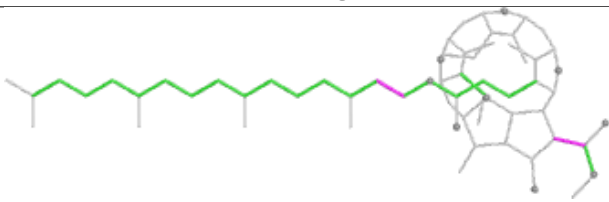
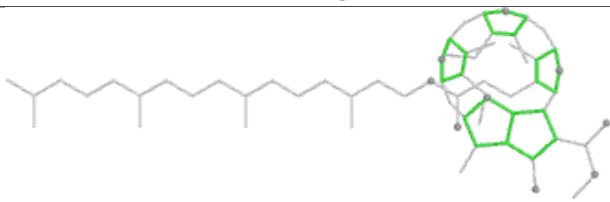


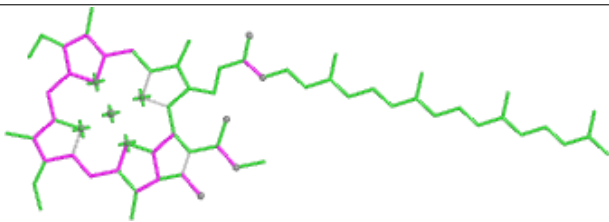
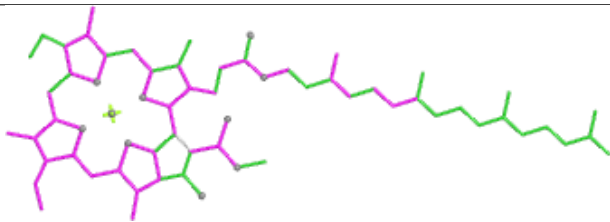
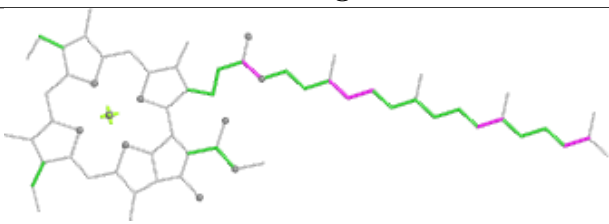
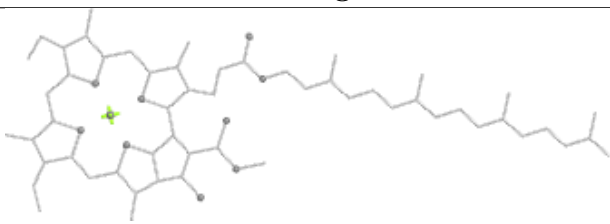


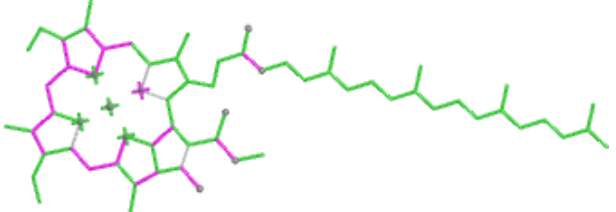
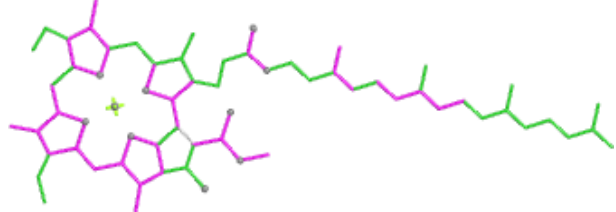
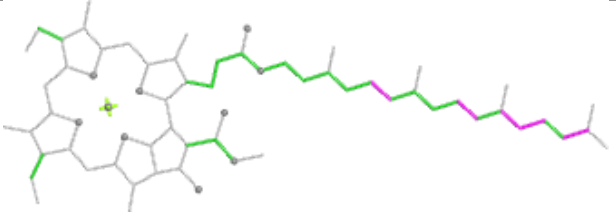
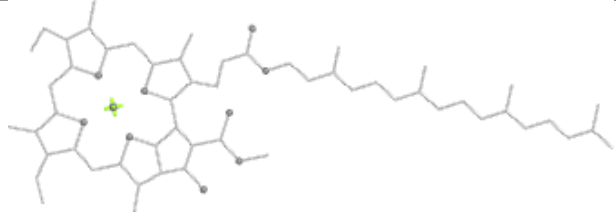
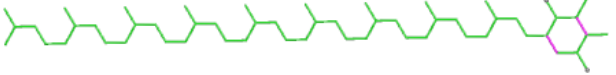
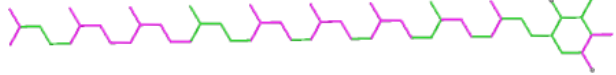
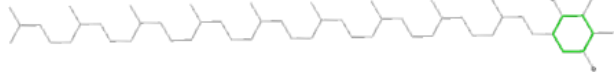


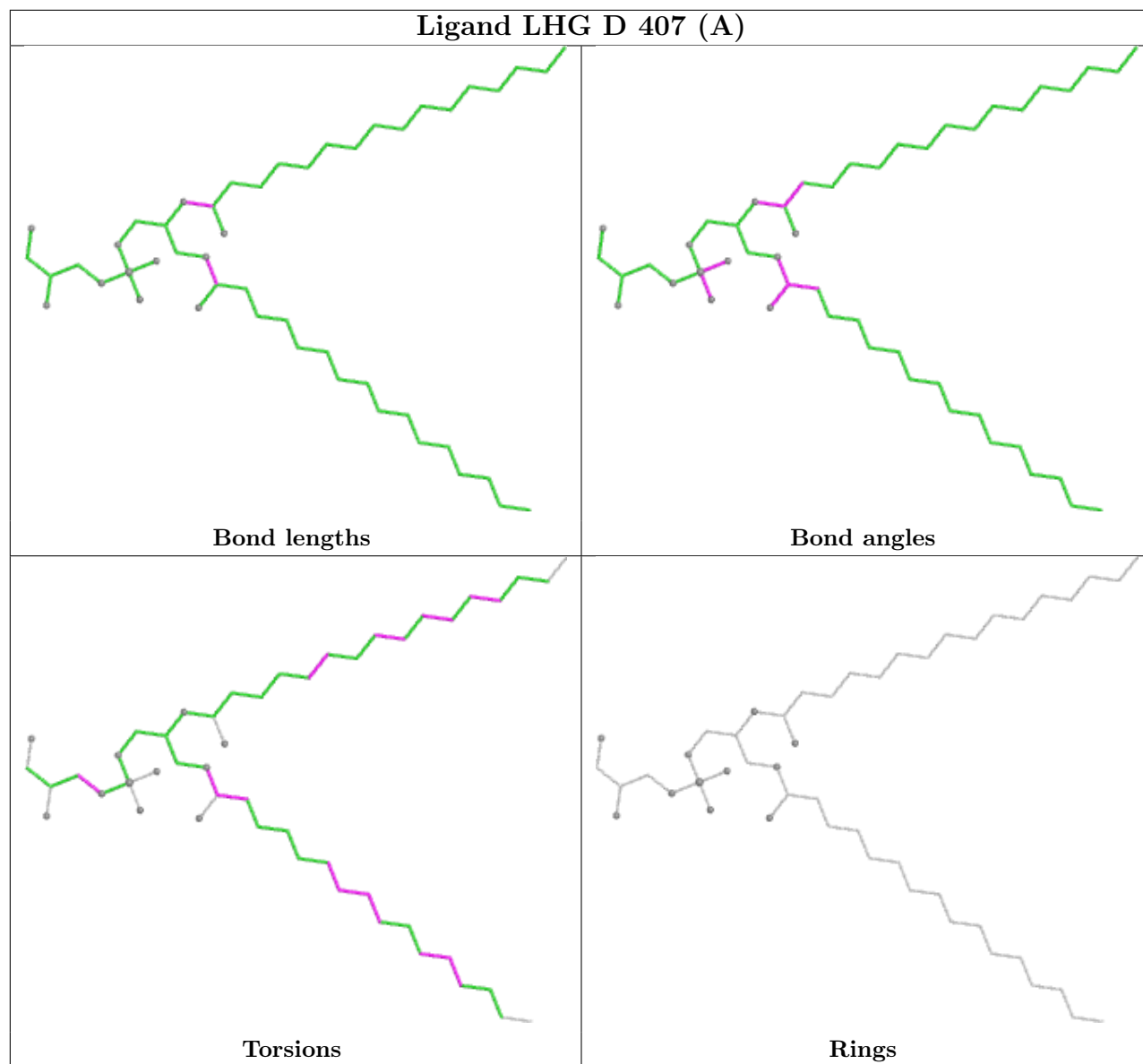


Ligand BCR a 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

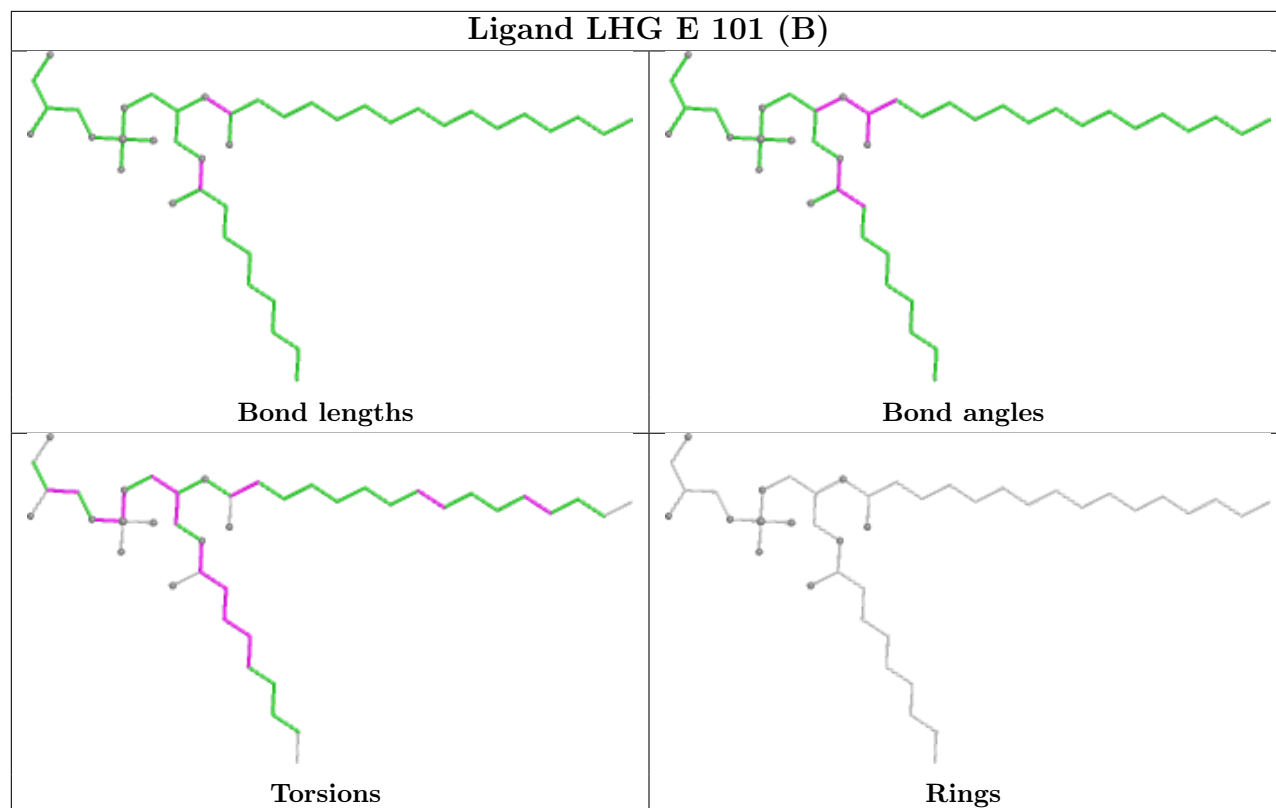
Ligand PHO A 407 (A)	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA d 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

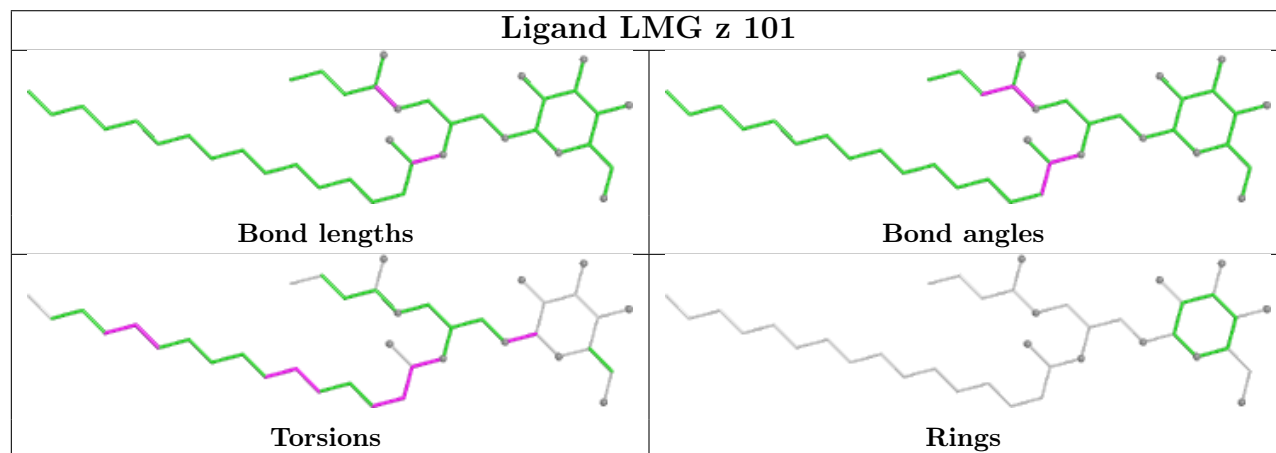
Ligand CLA B 615	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 D 405 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings

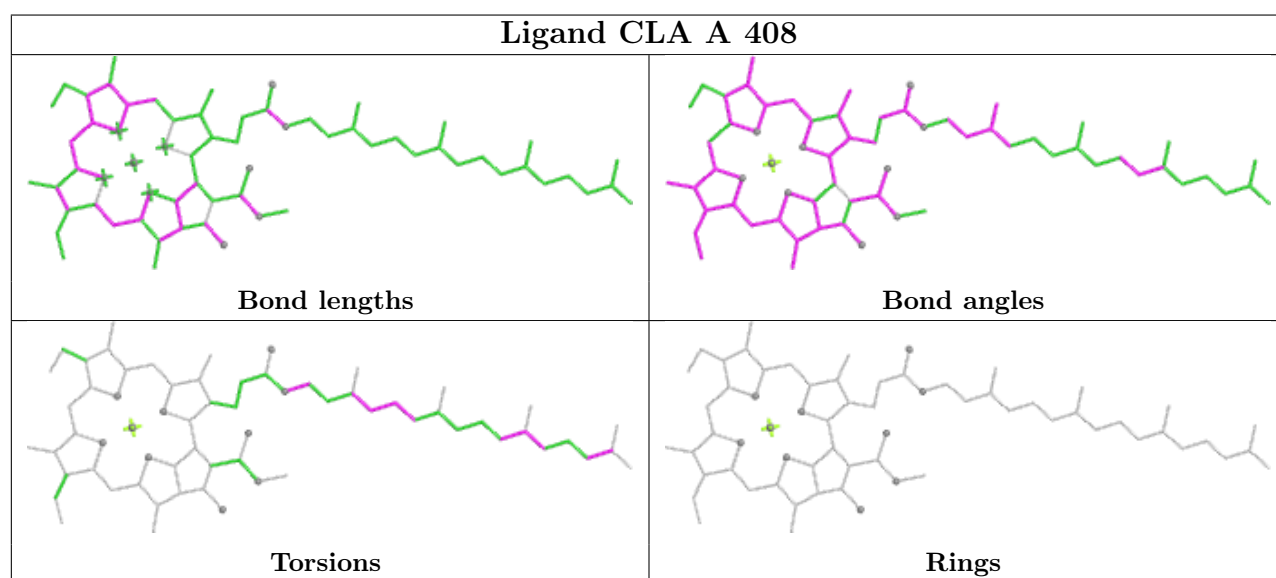
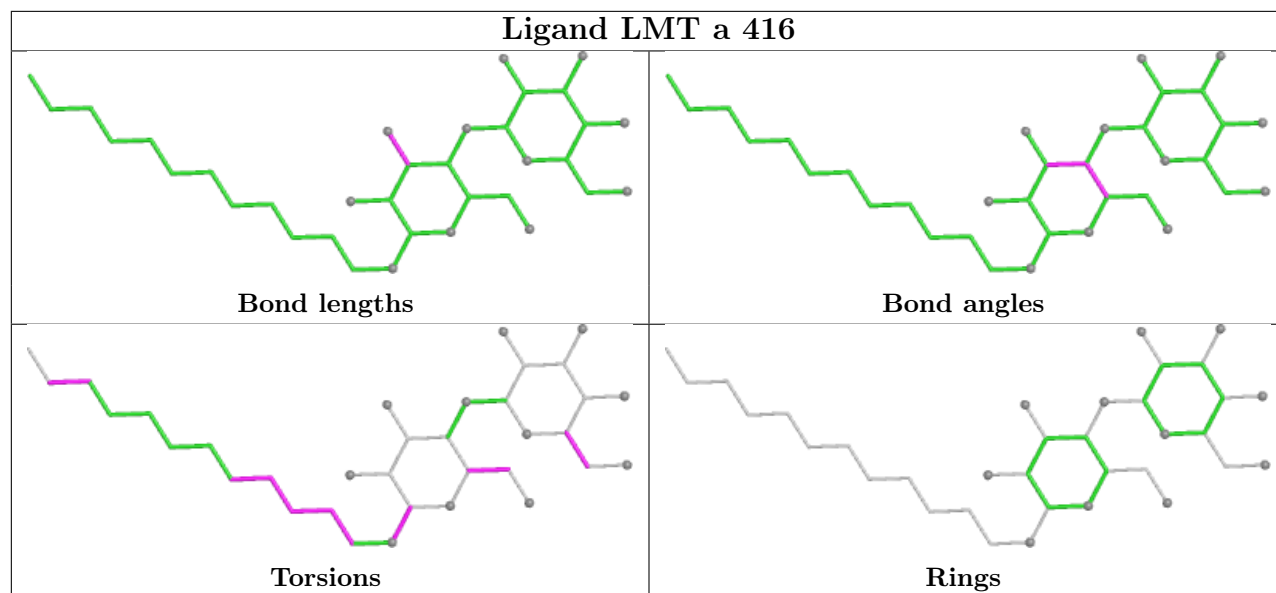


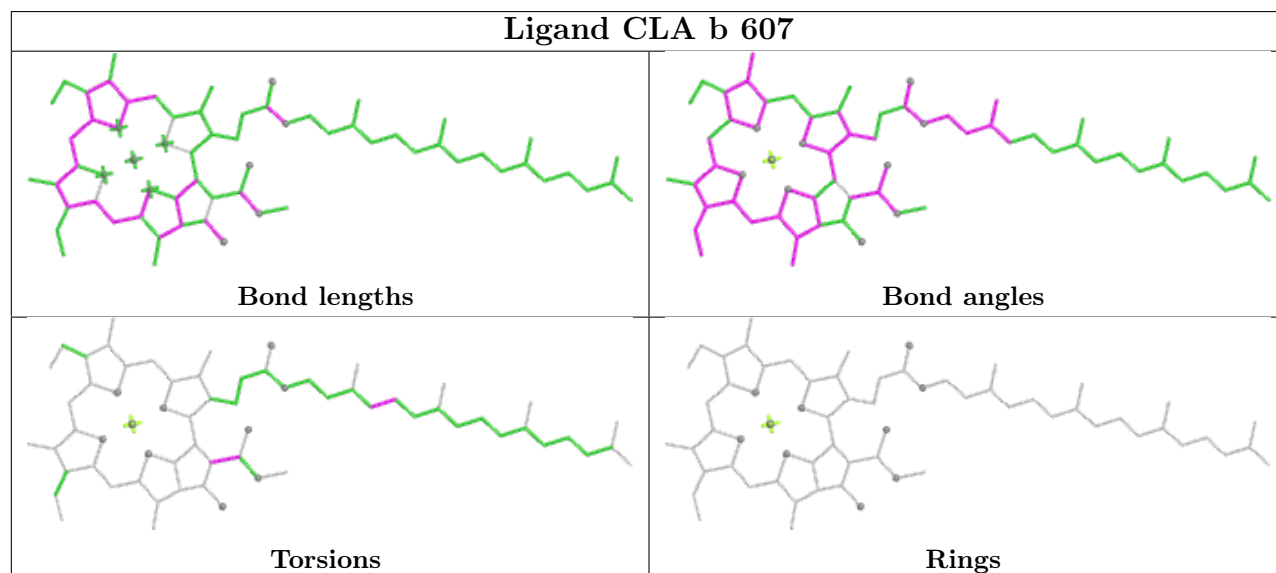
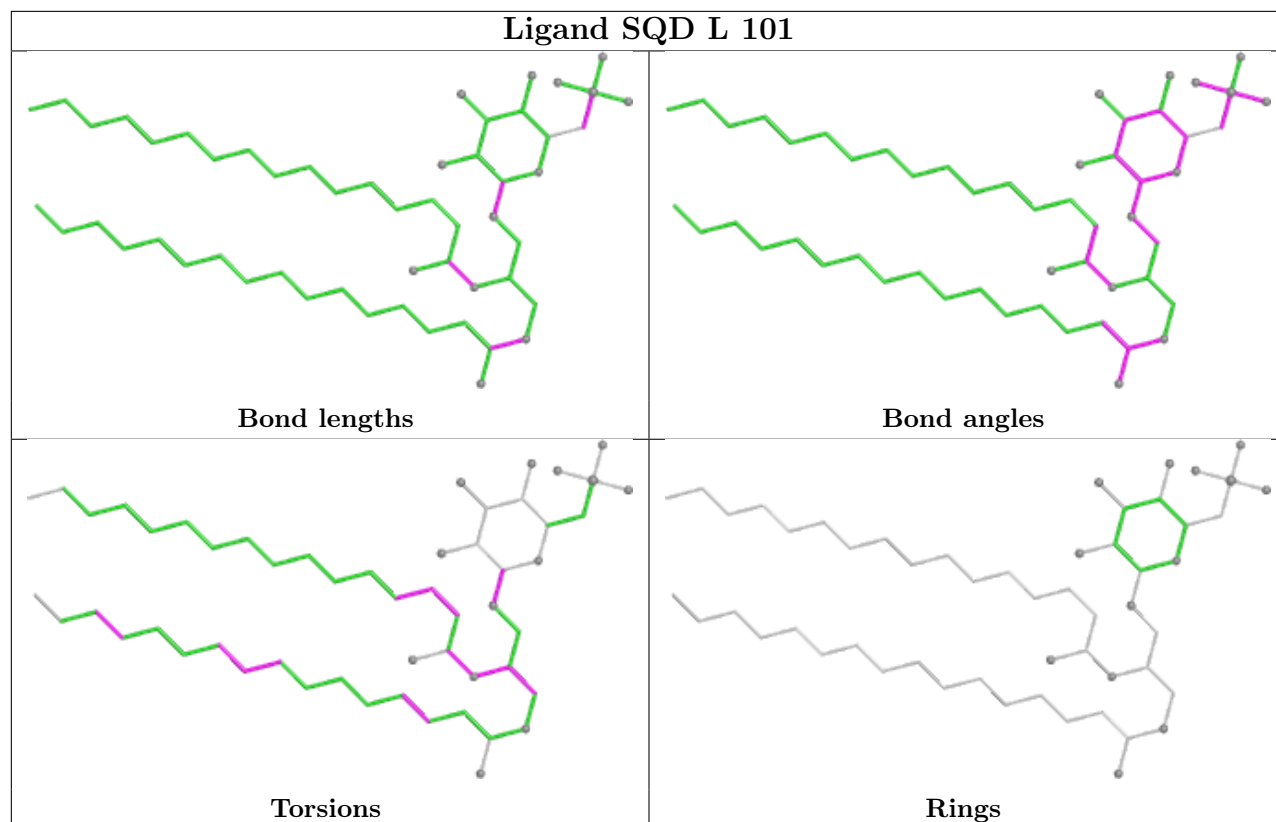
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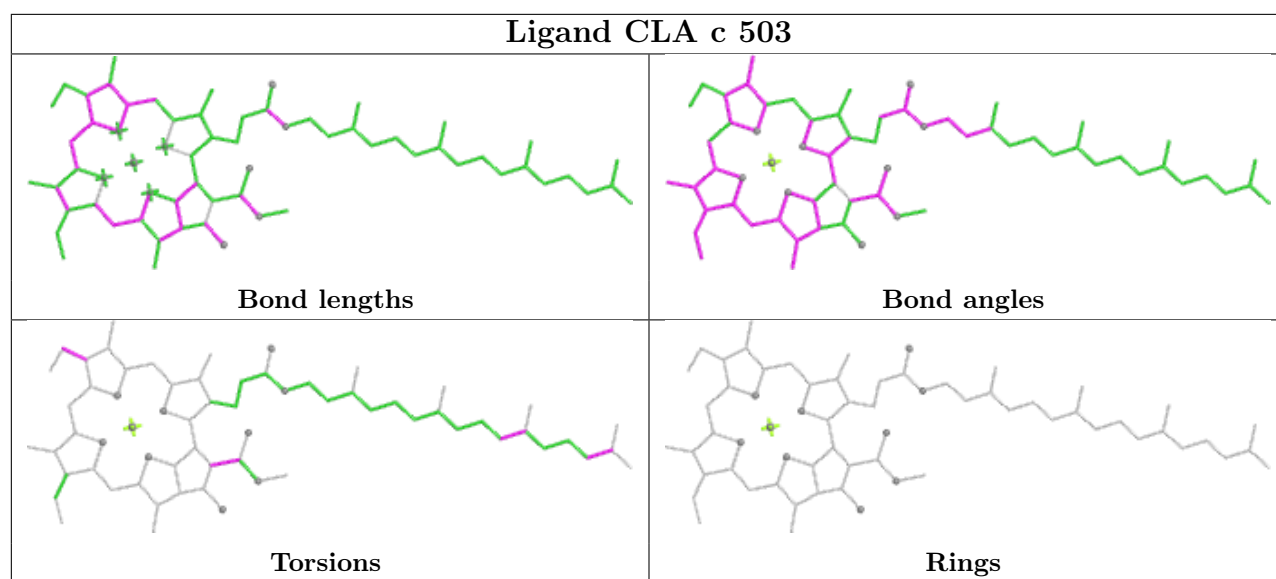


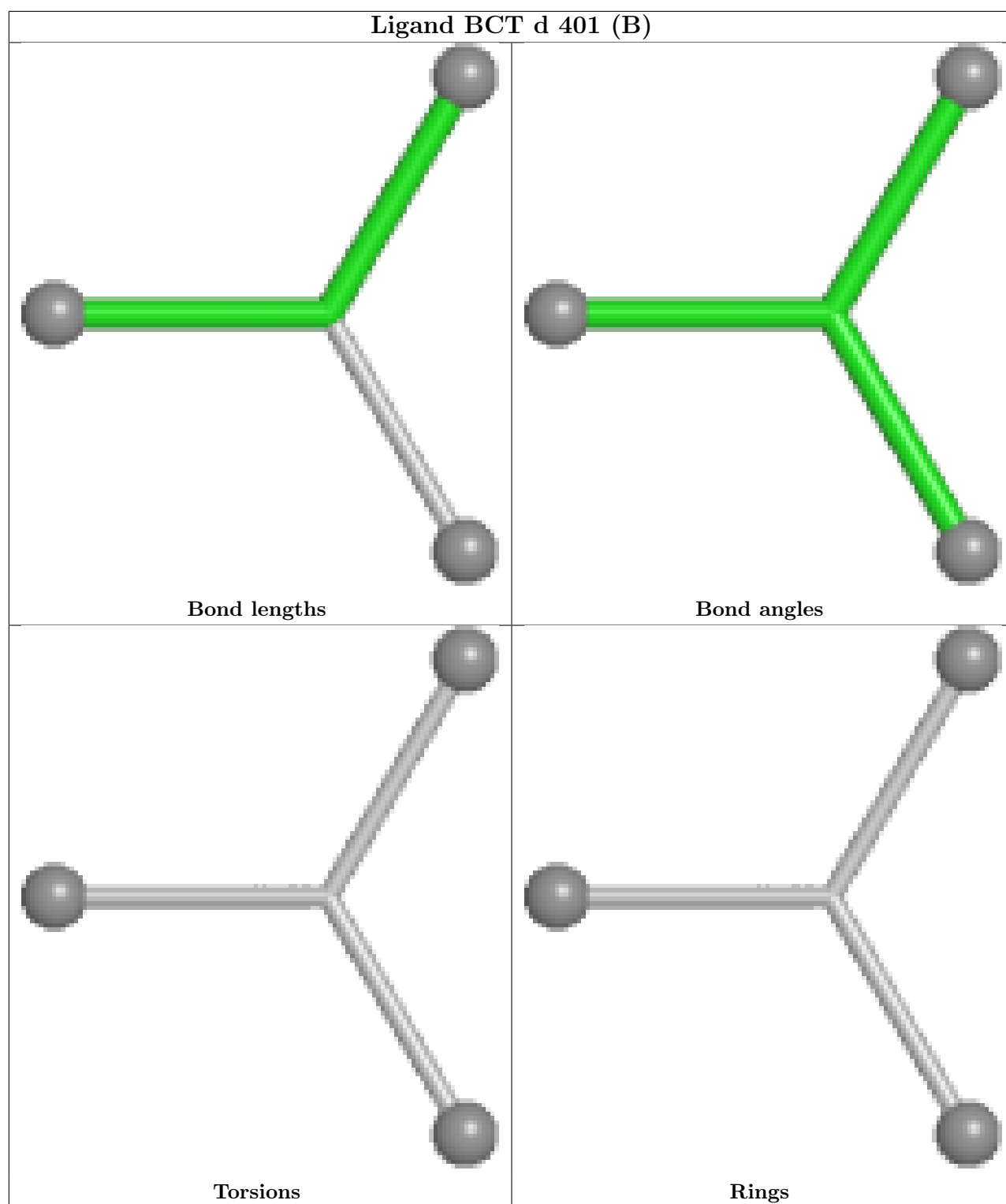
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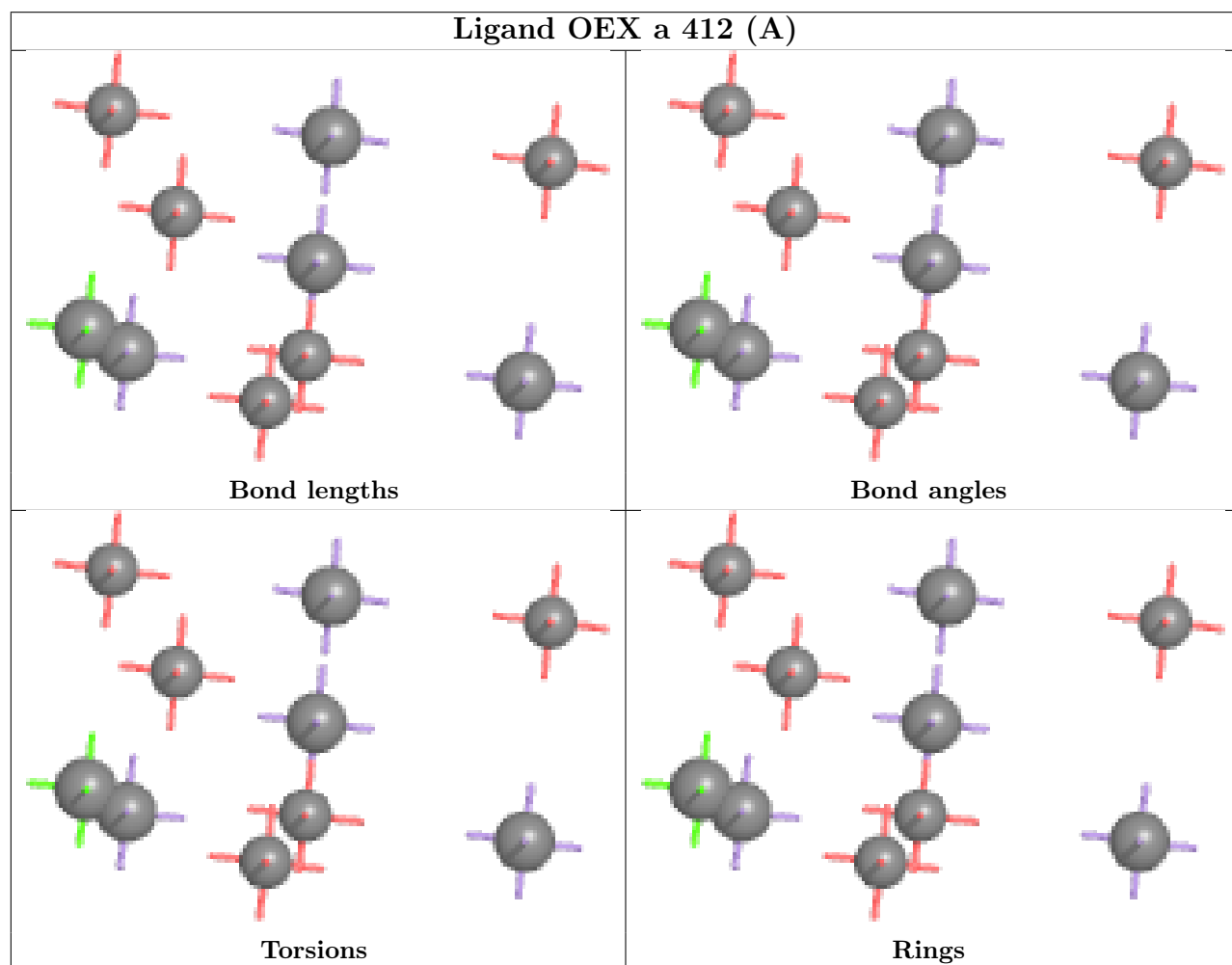
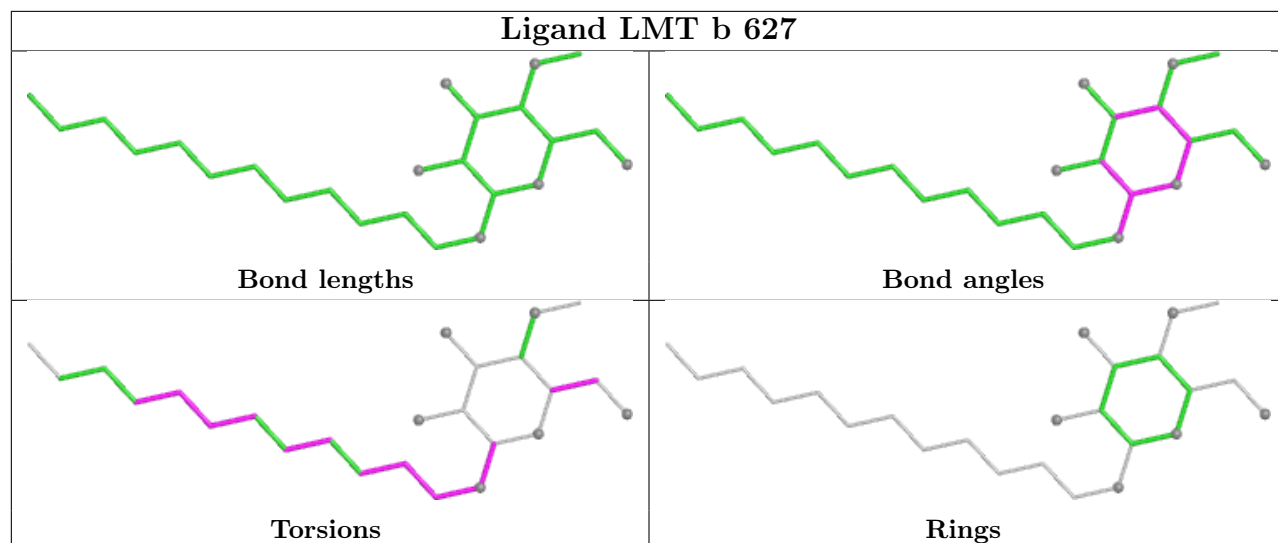


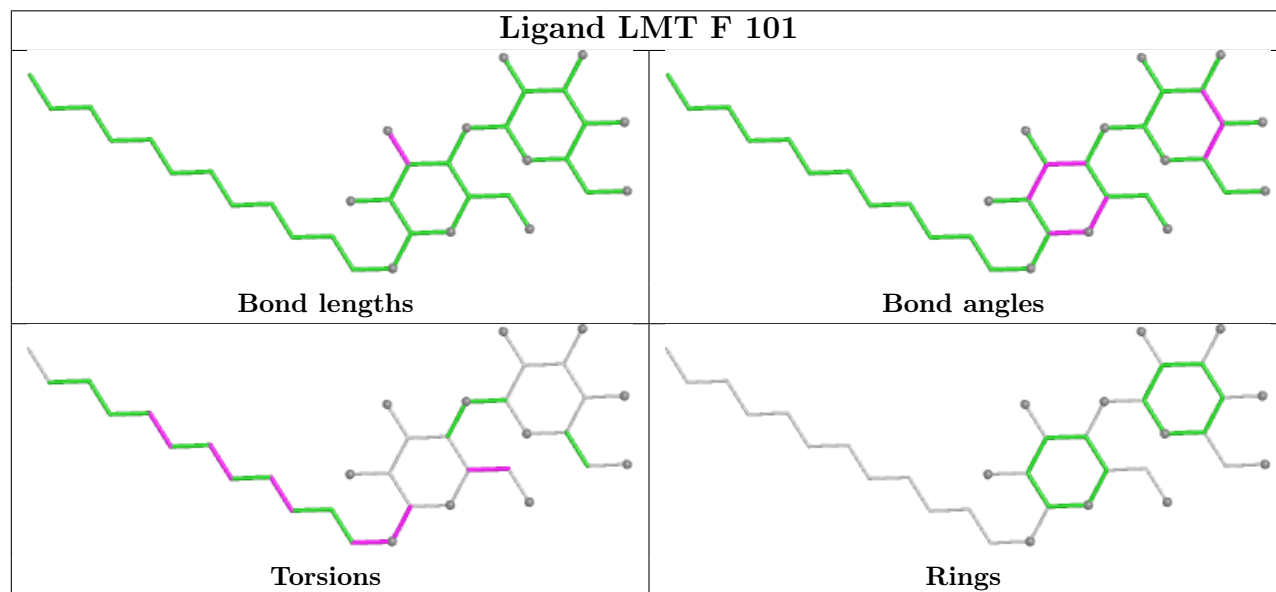
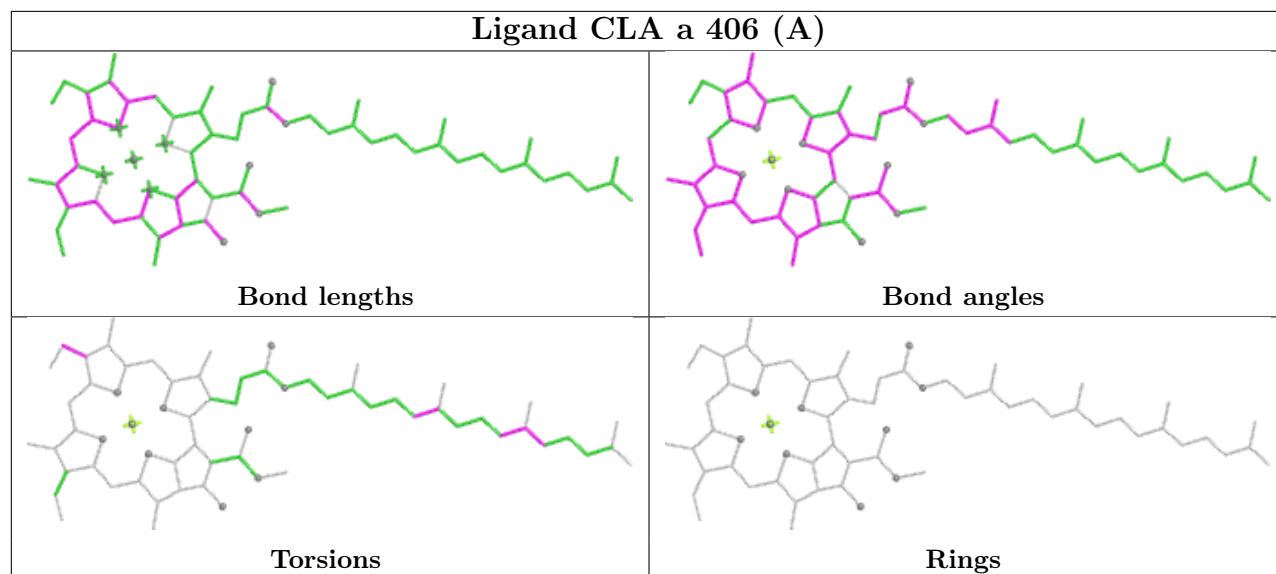


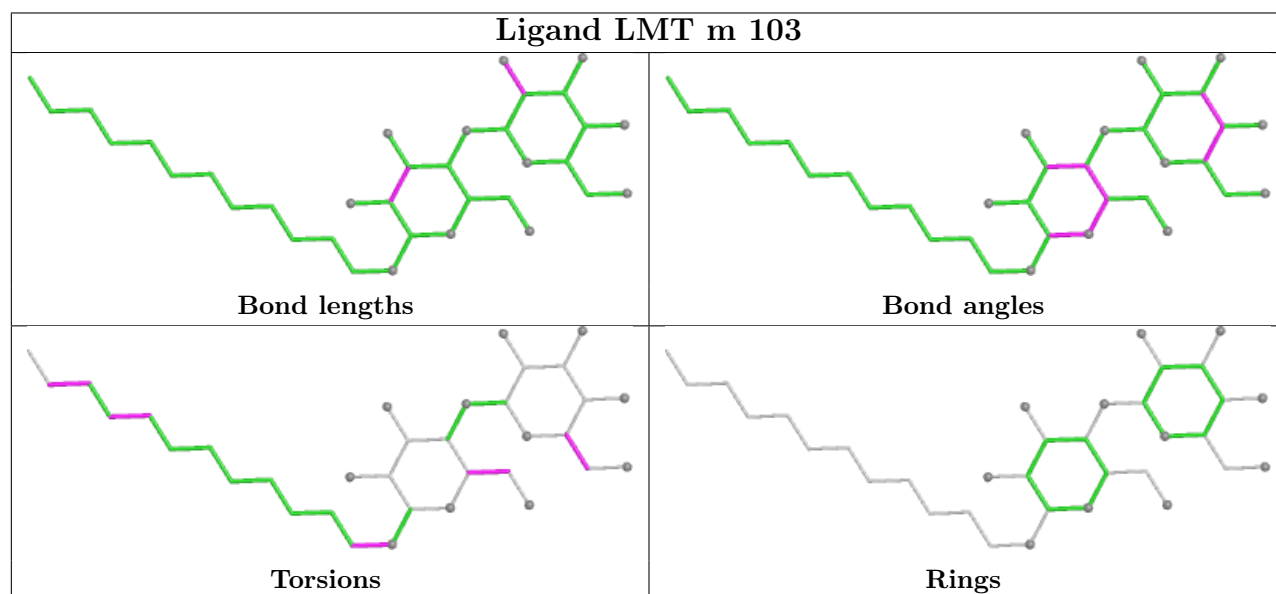
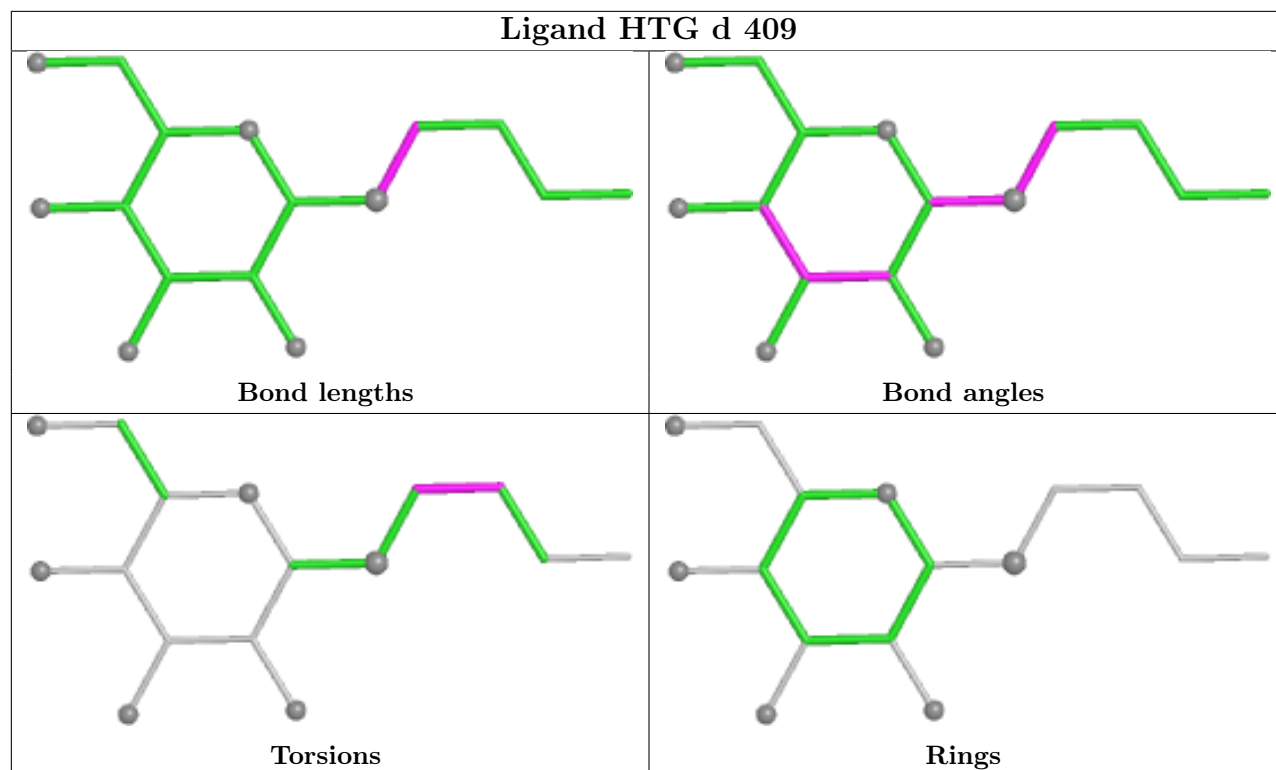


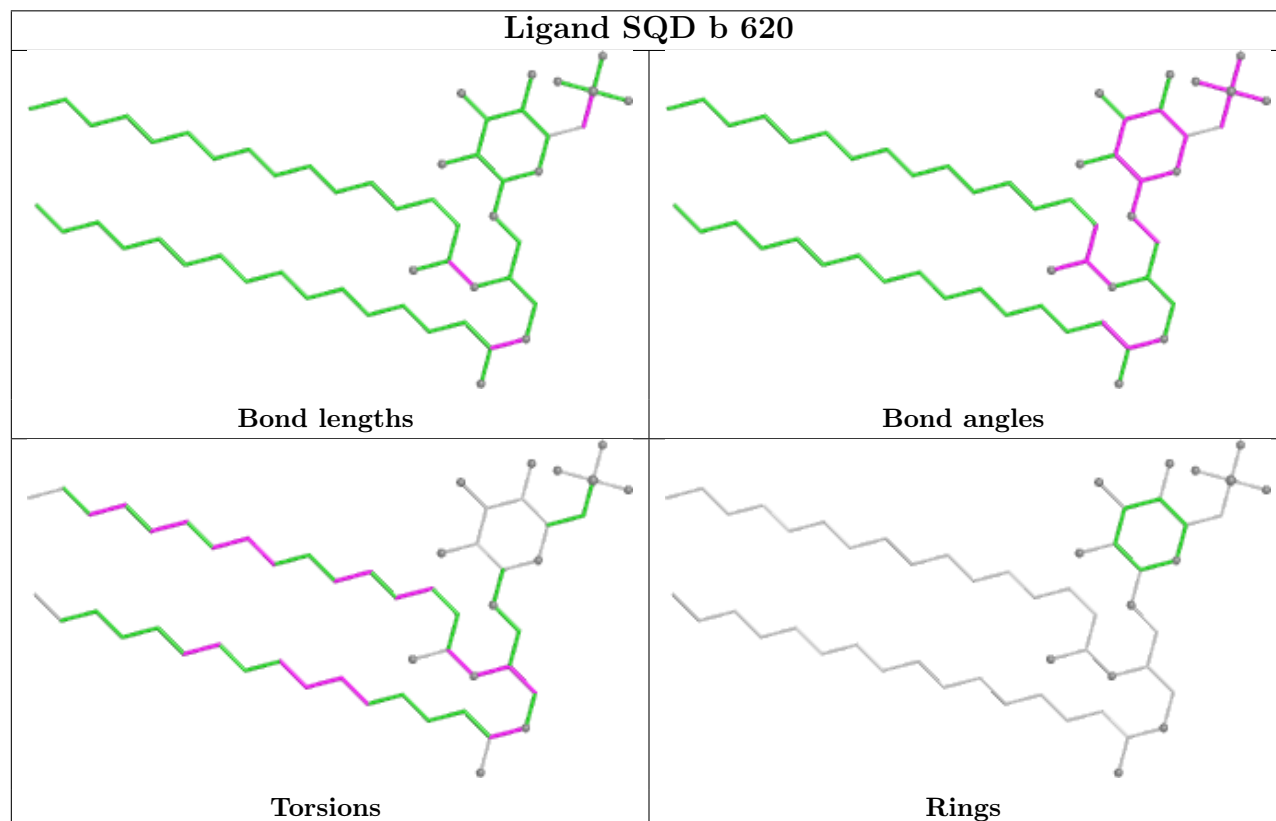
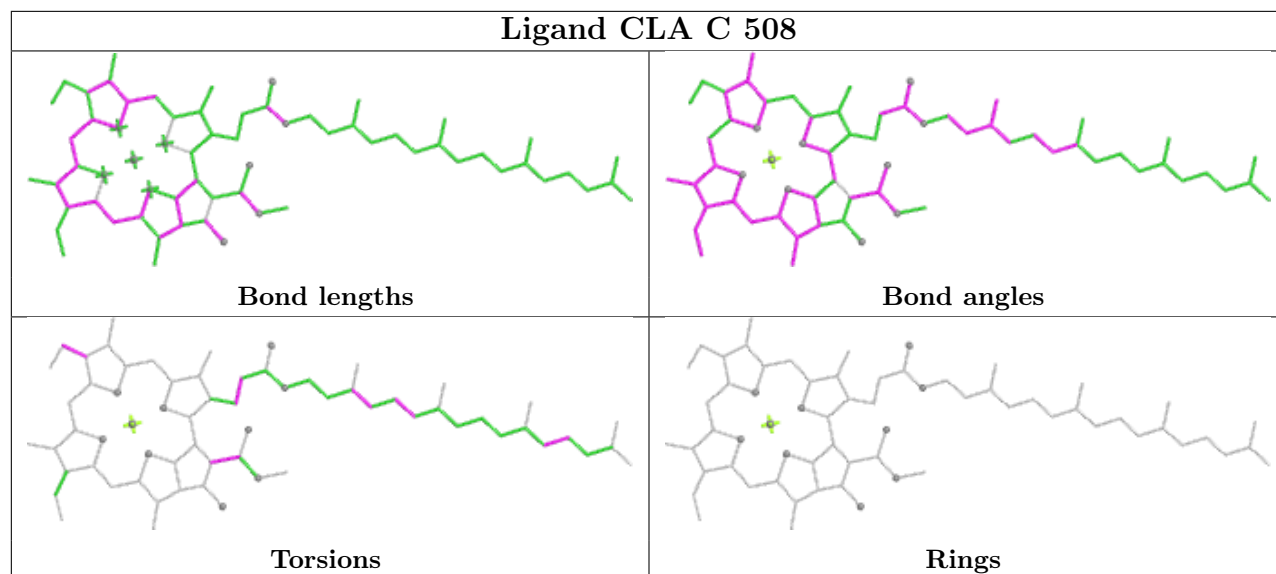


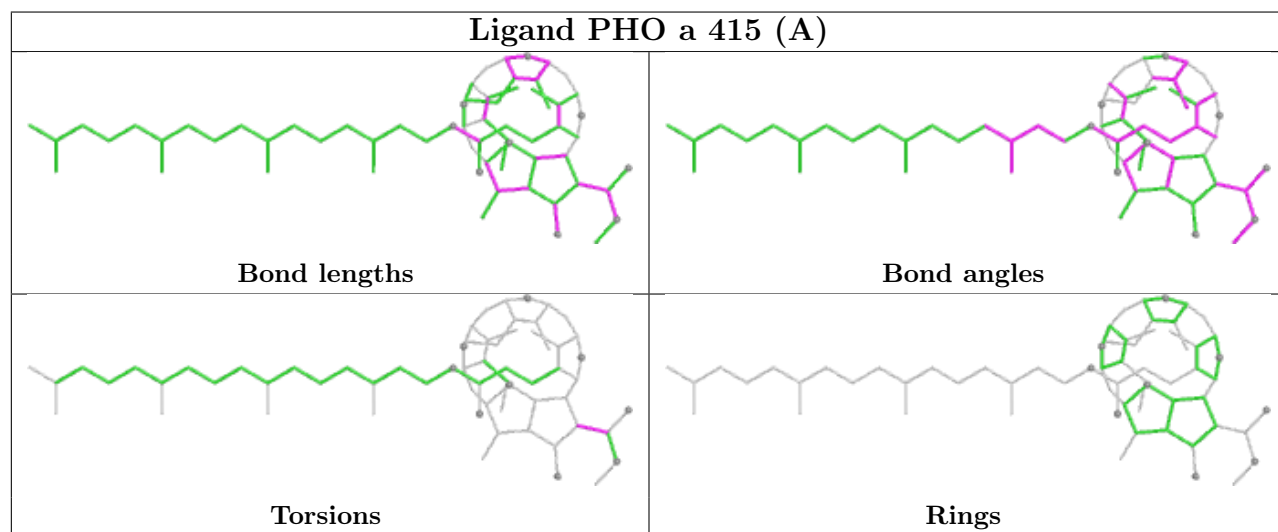
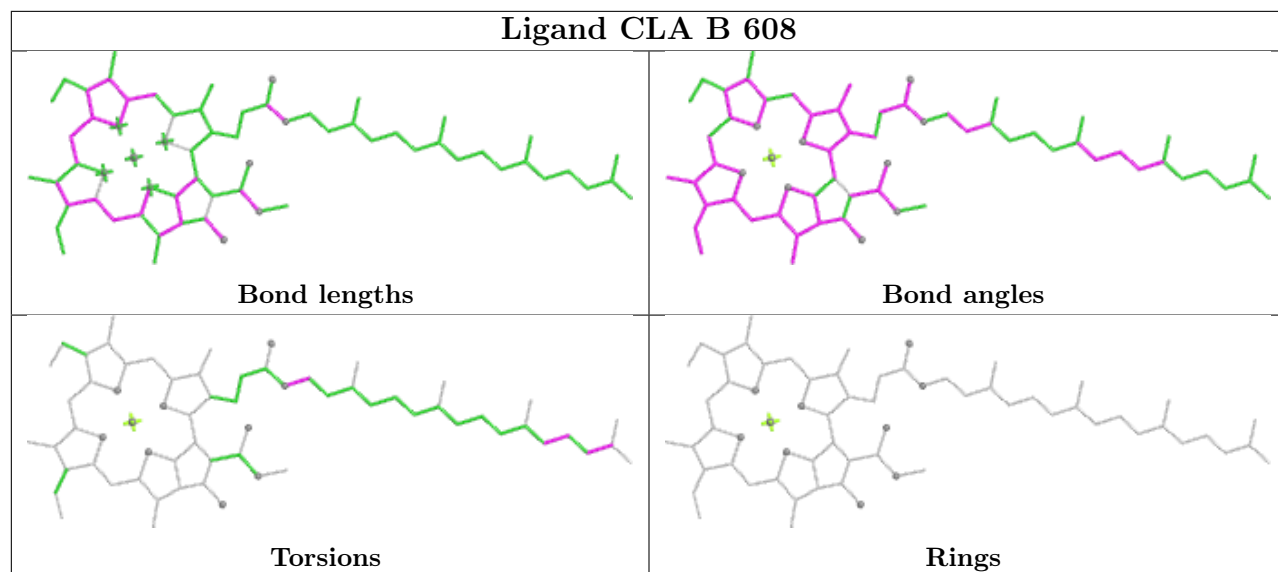




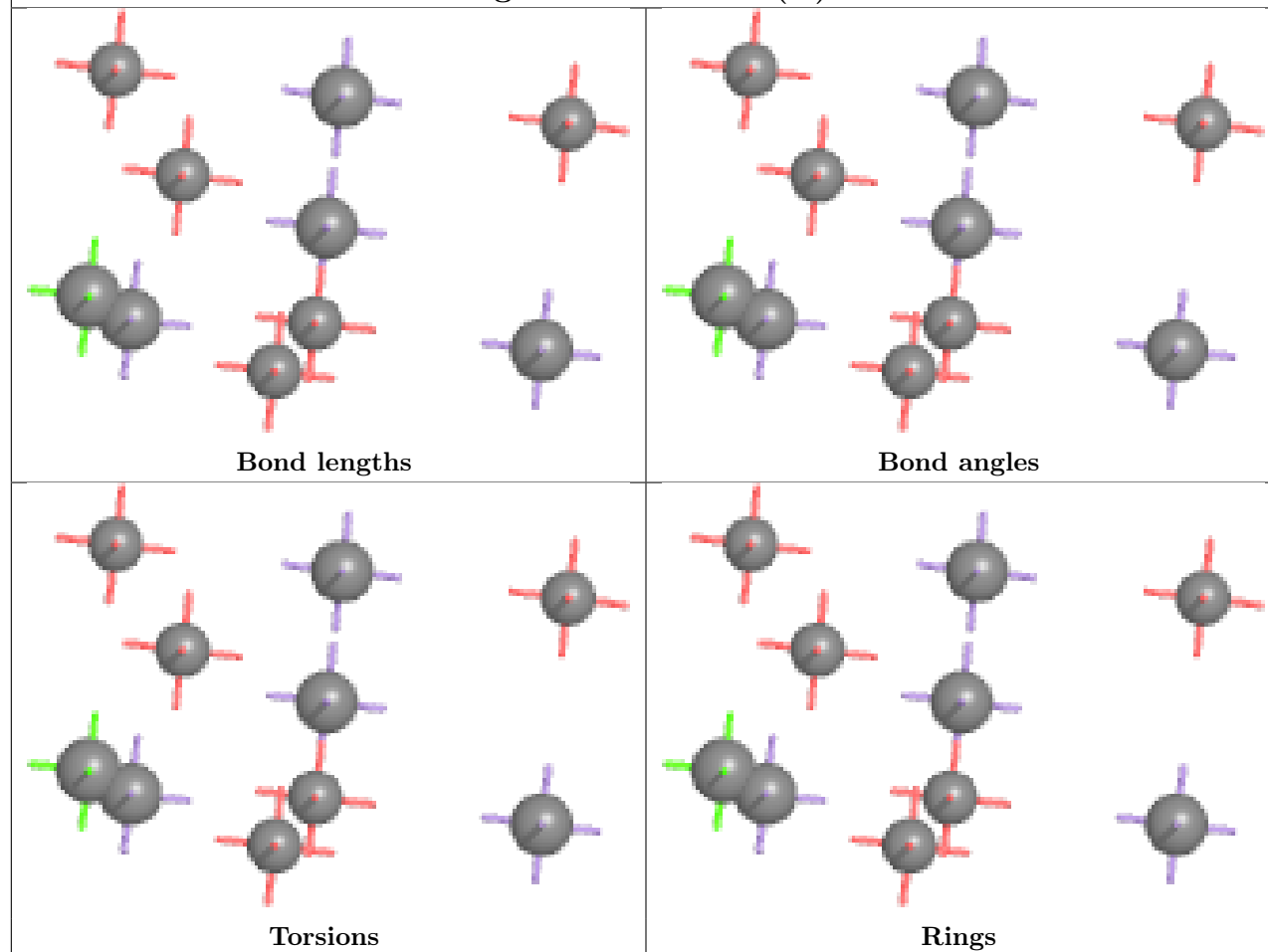




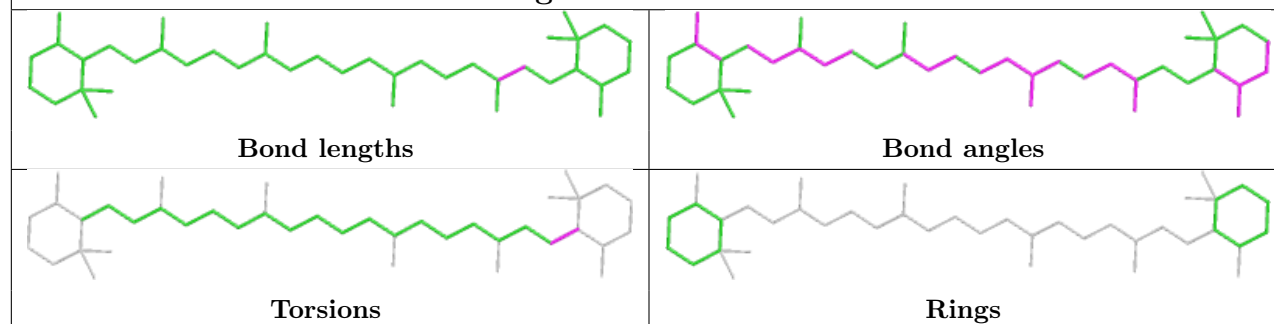


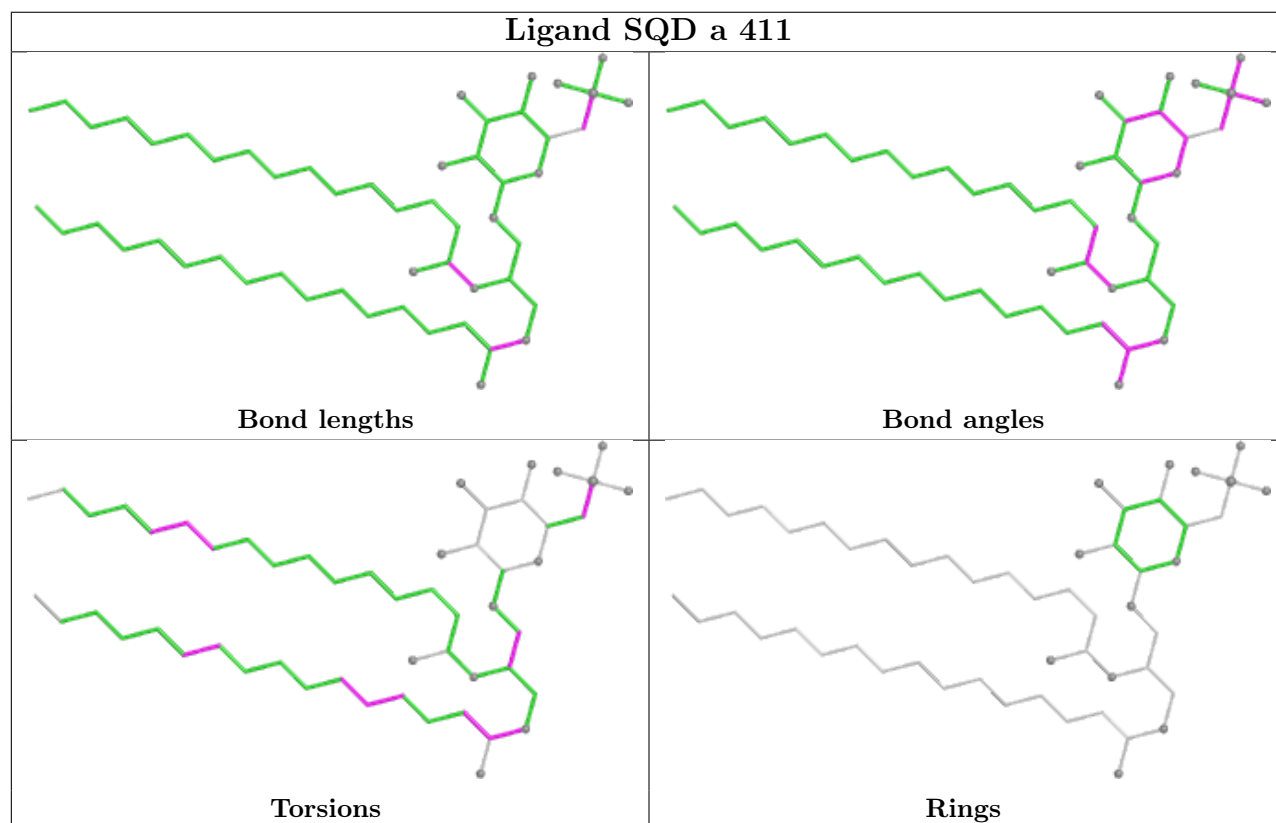
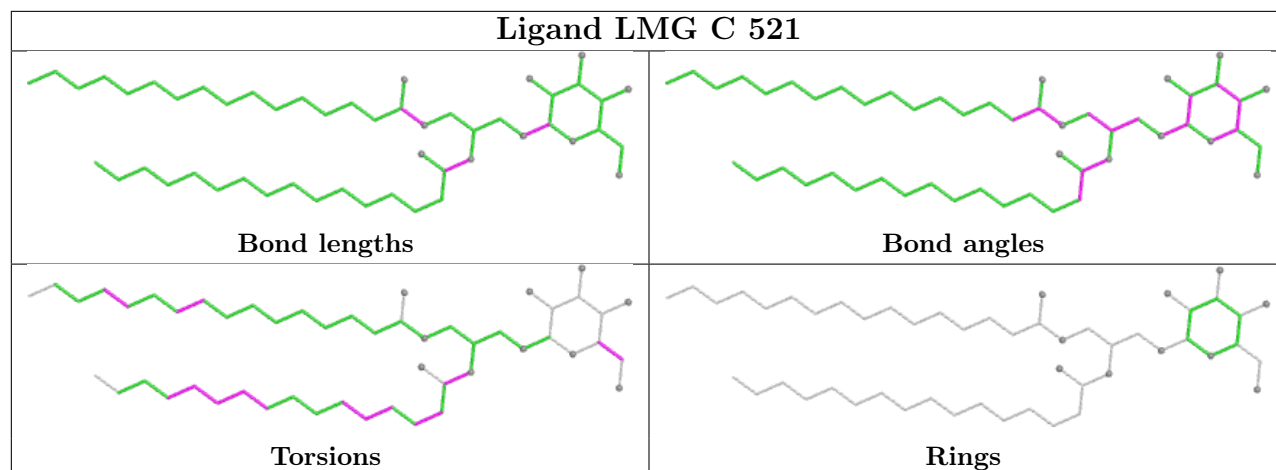


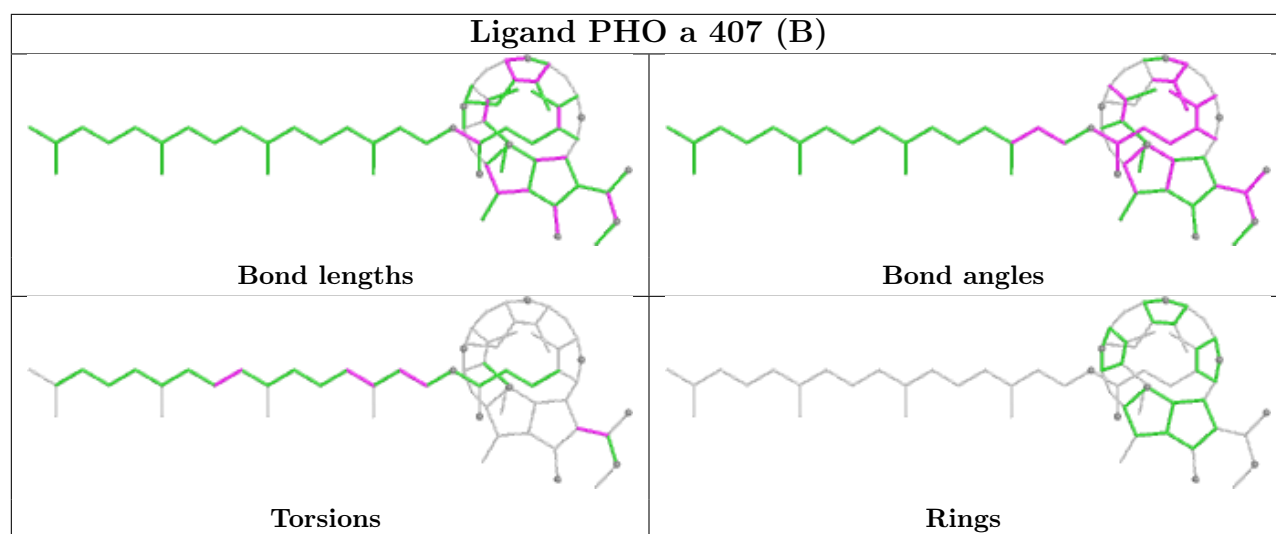
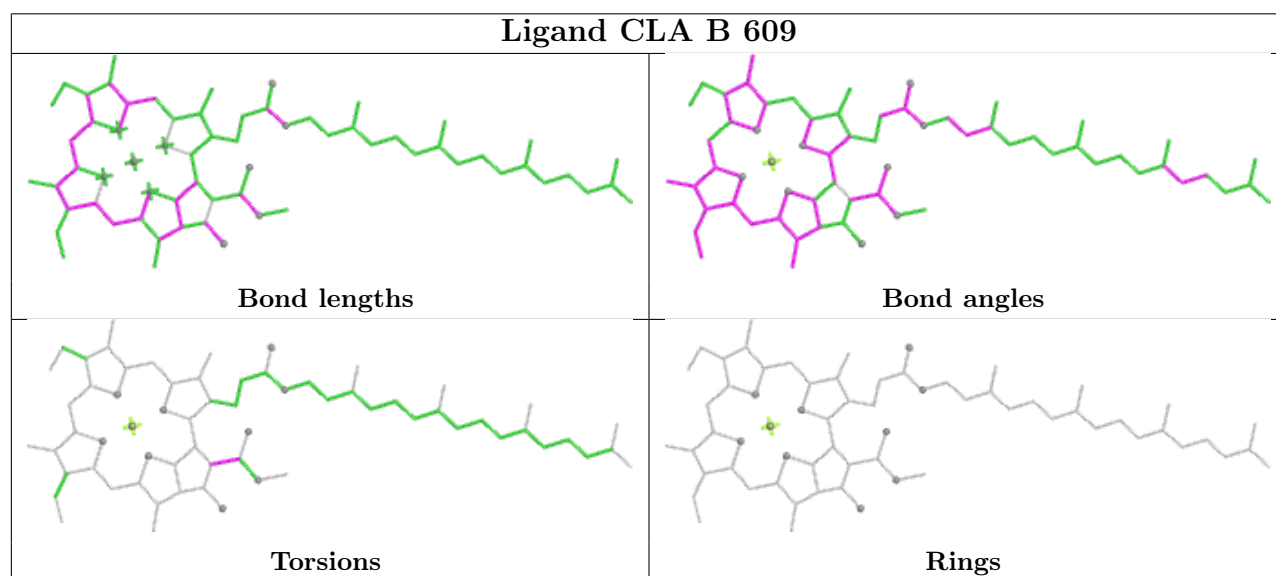
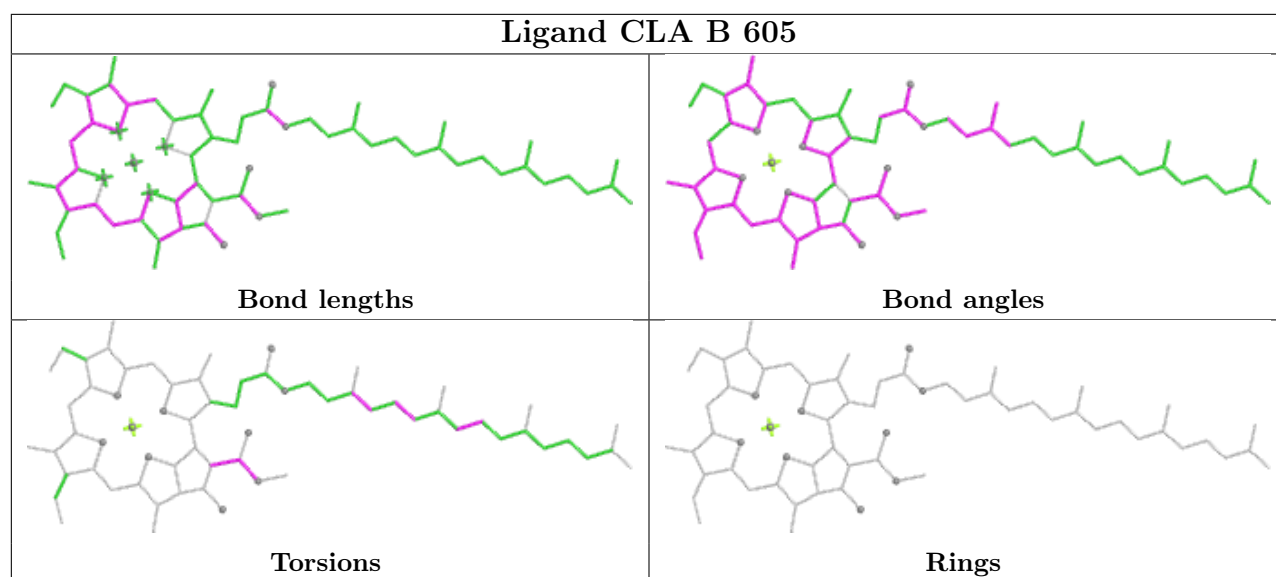
Ligand OEX A 413 (A)

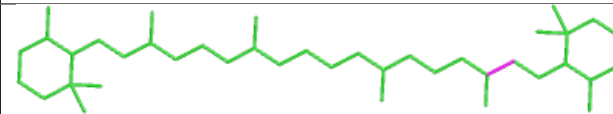
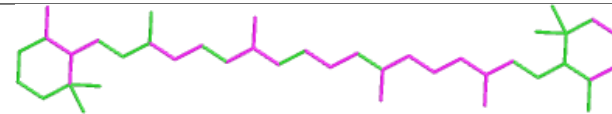
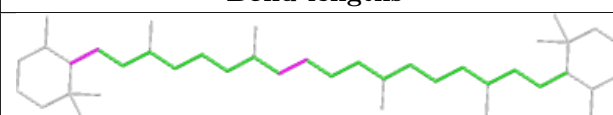
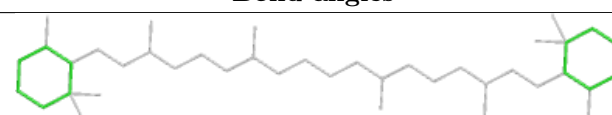


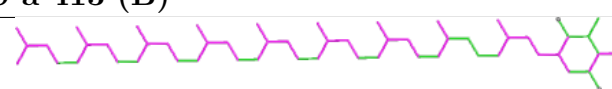
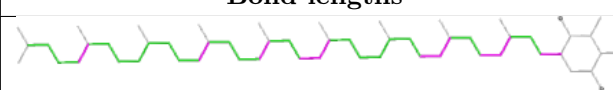
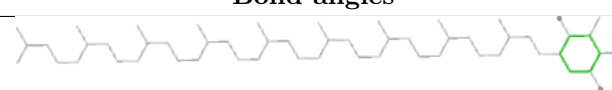
Ligand BCR c 515

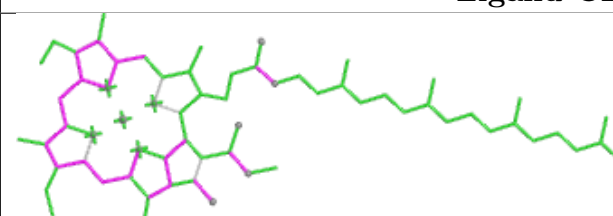
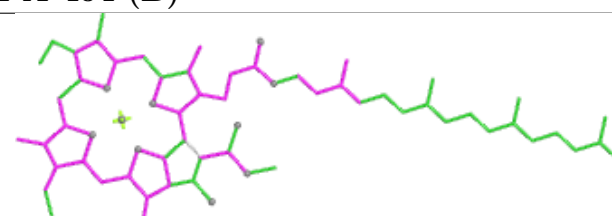
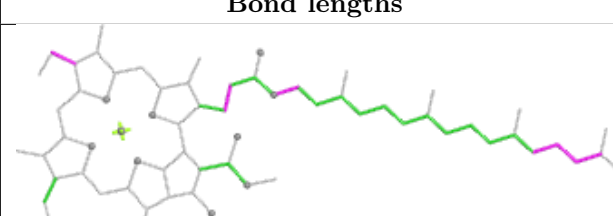
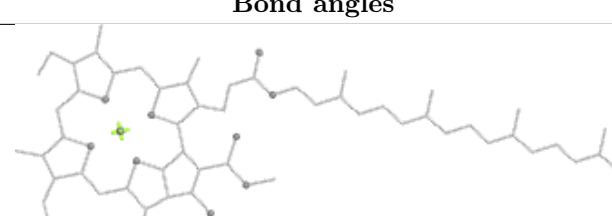


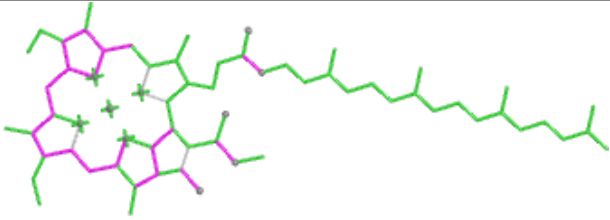
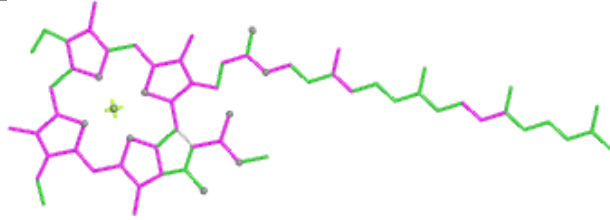
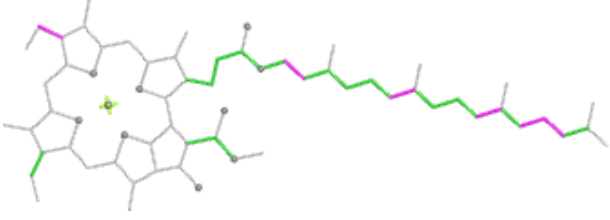
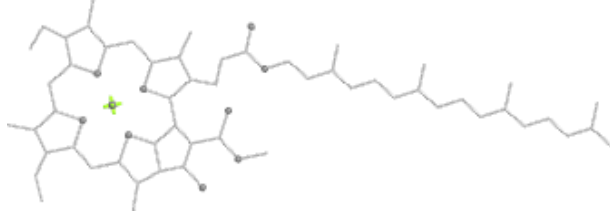
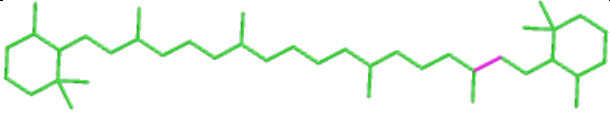
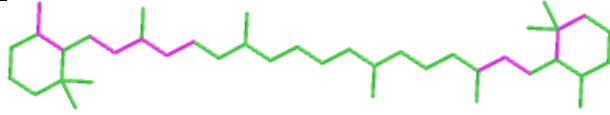
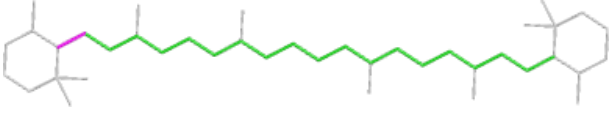
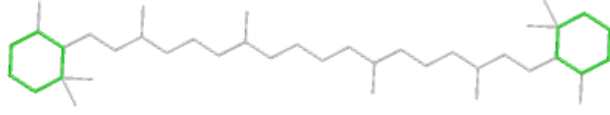
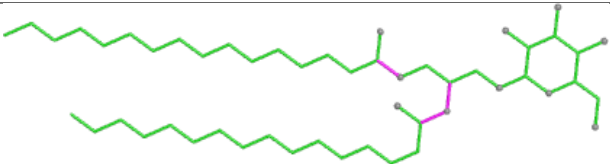
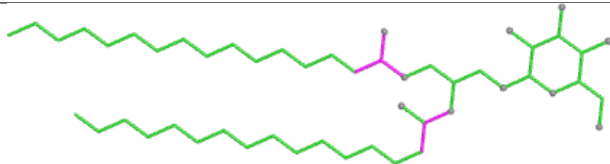
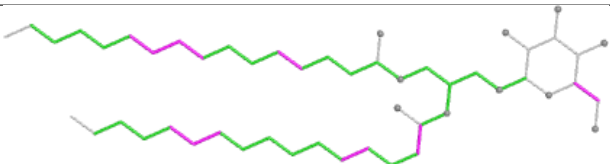
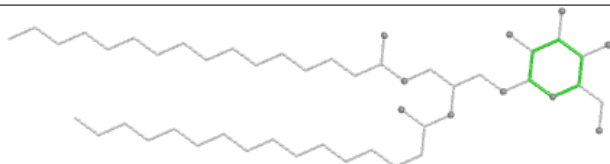


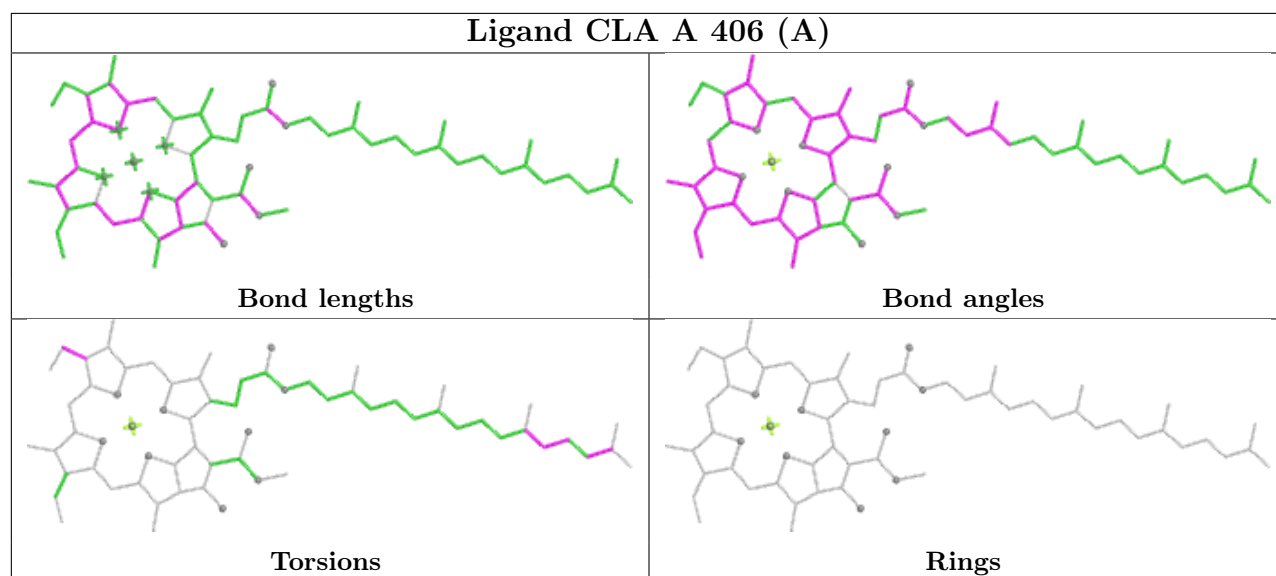
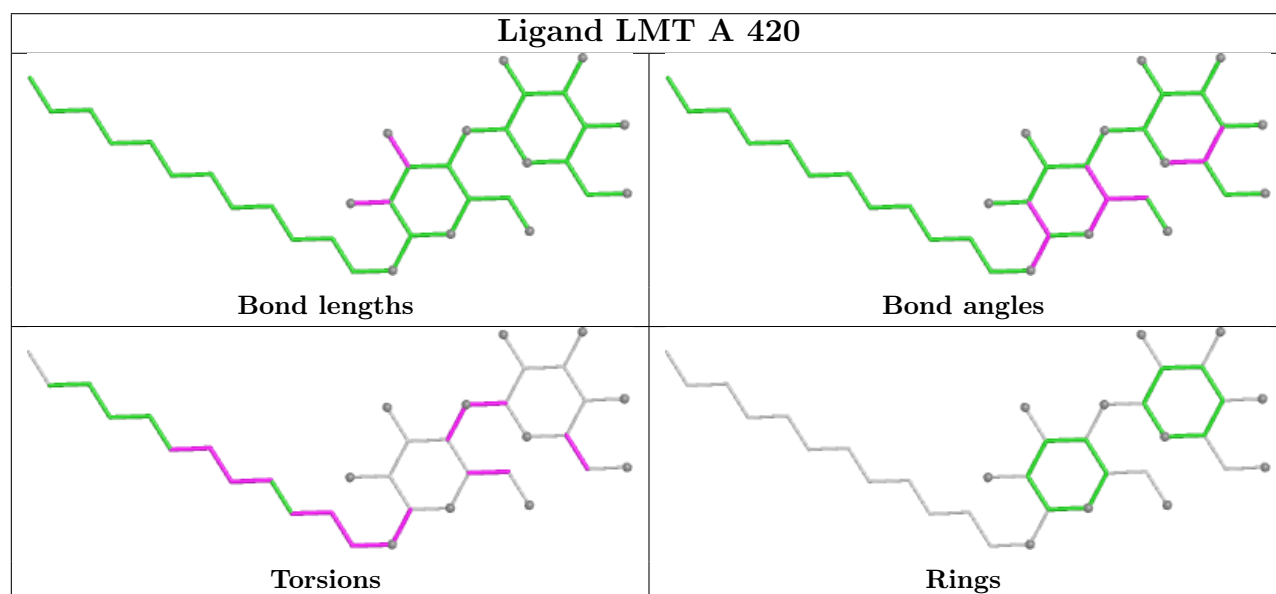
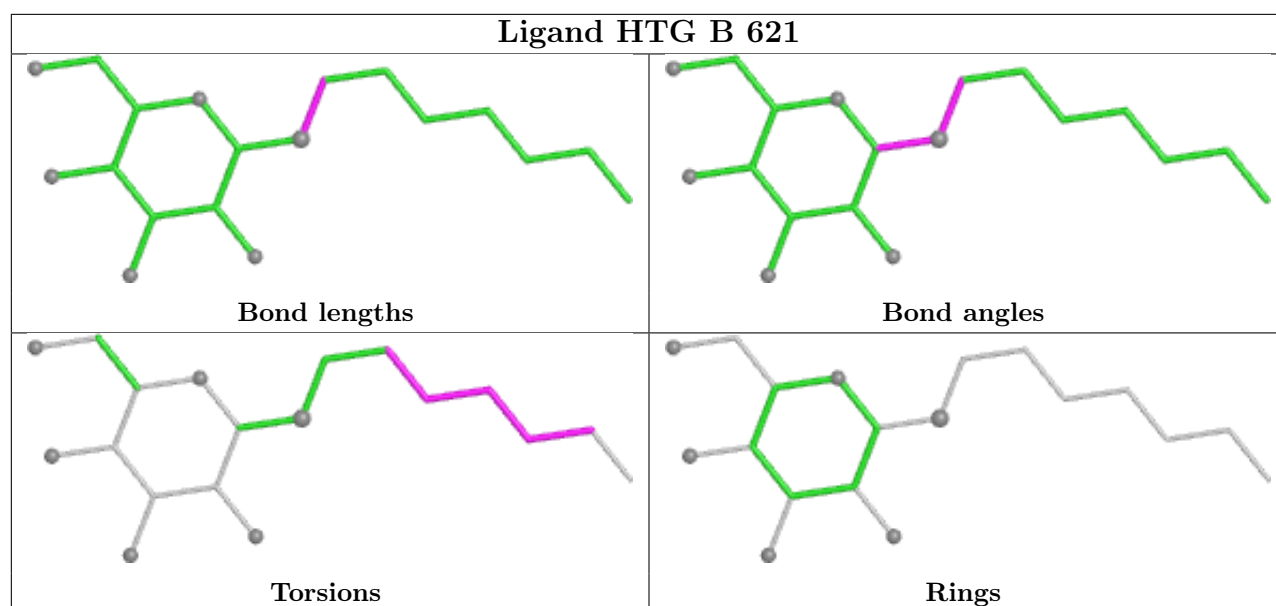


Ligand BCR t 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

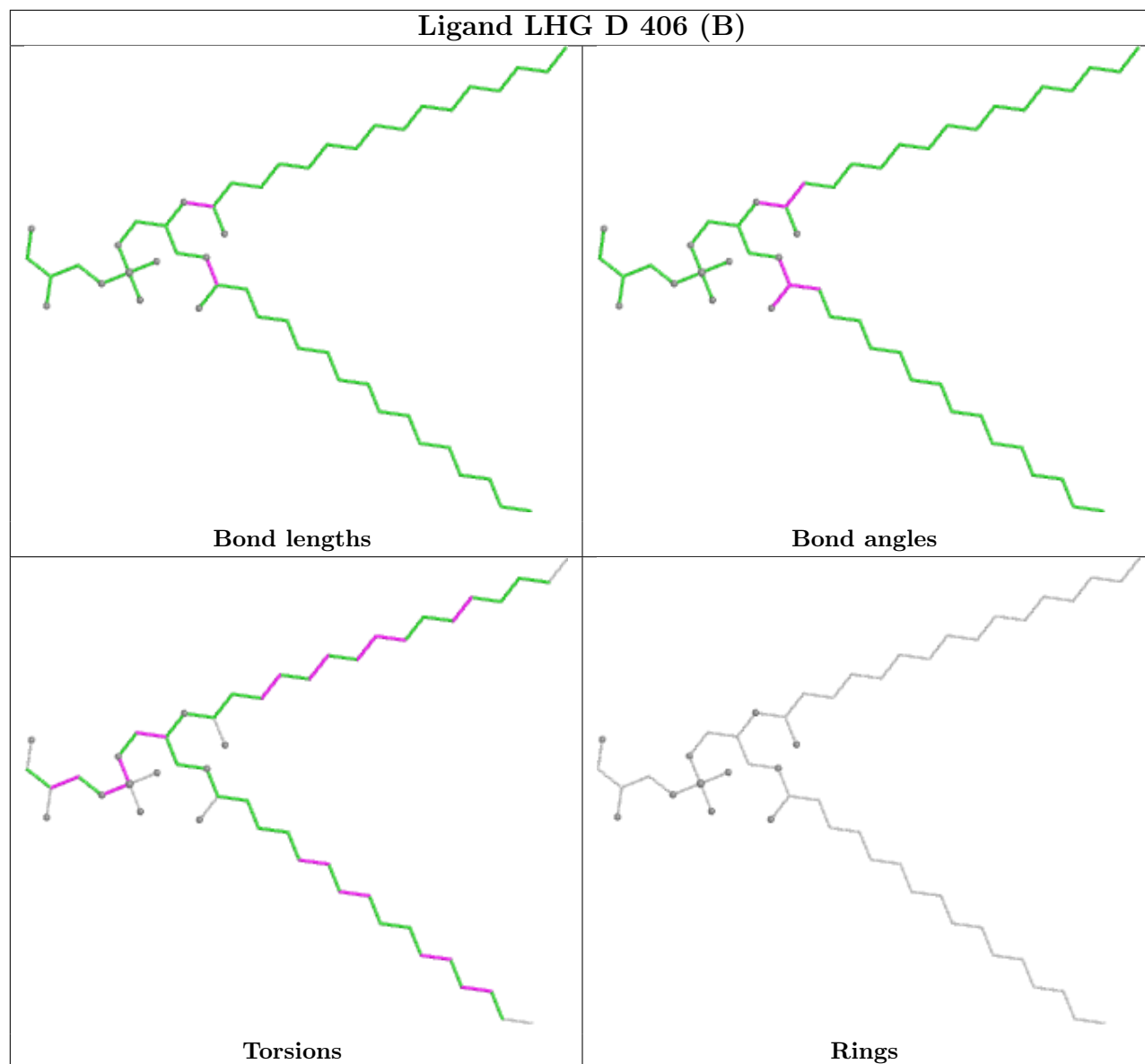
Ligand PL9 a 413 (B)	
	
Bond lengths	Bond angles
	
Torsions	Rings

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

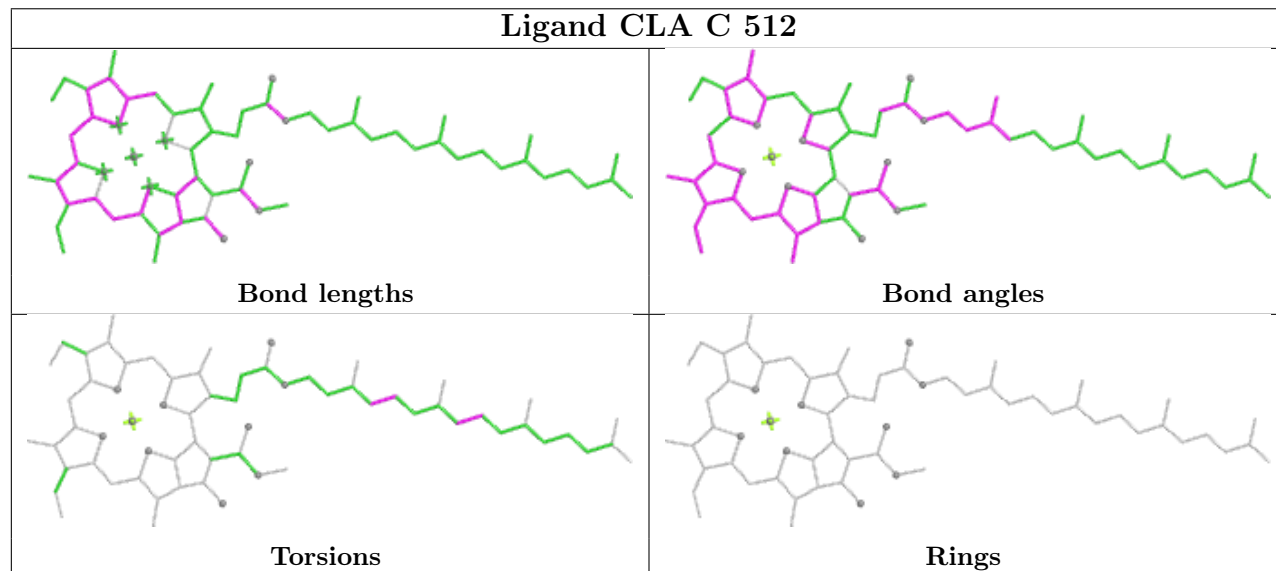
Ligand CLA B 602	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b 617	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG D 411	
 Bond lengths	 Bond angles
 Torsions	 Rings

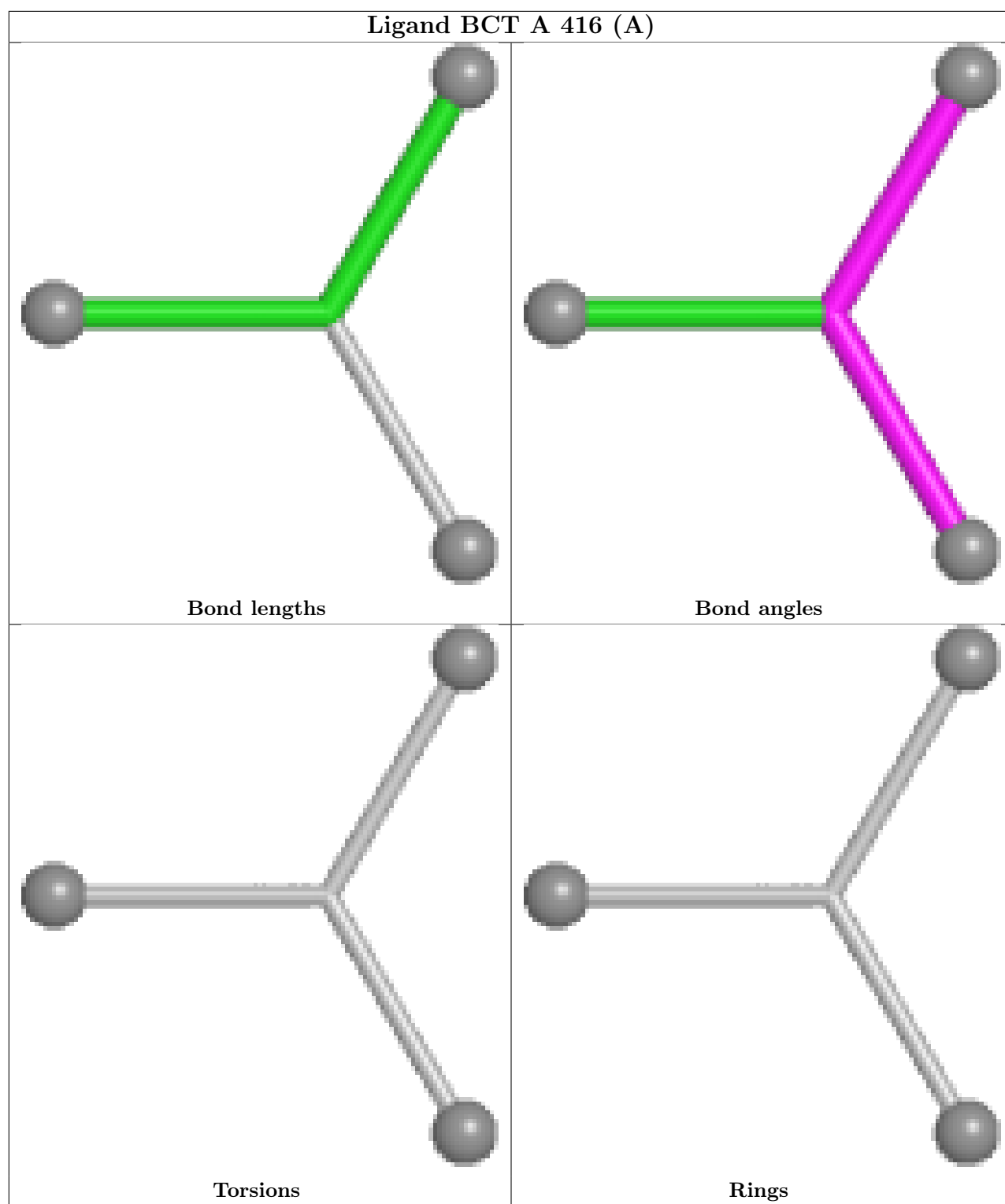


Ligand LHG D 406 (B)

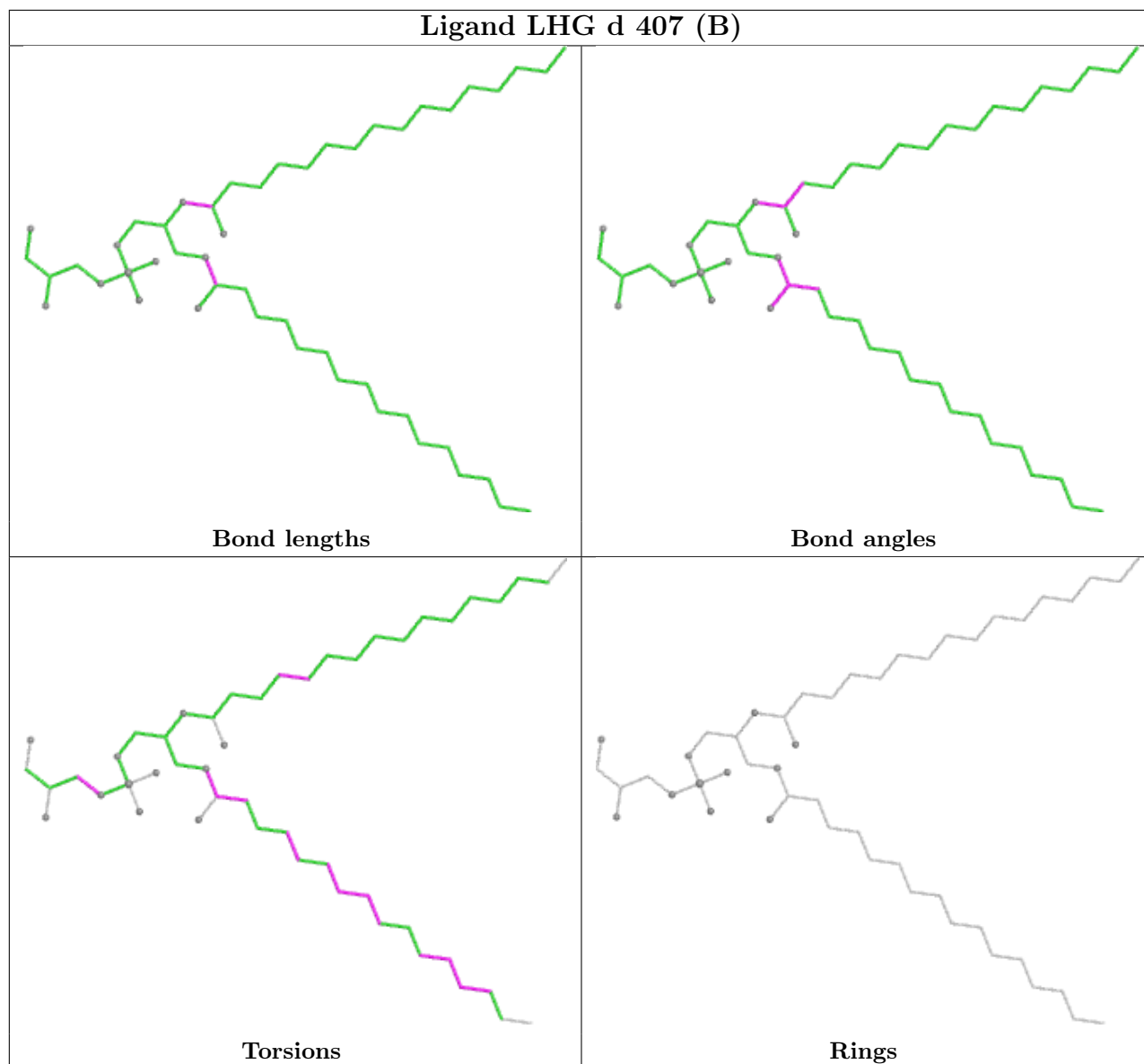


Ligand CLA C 512

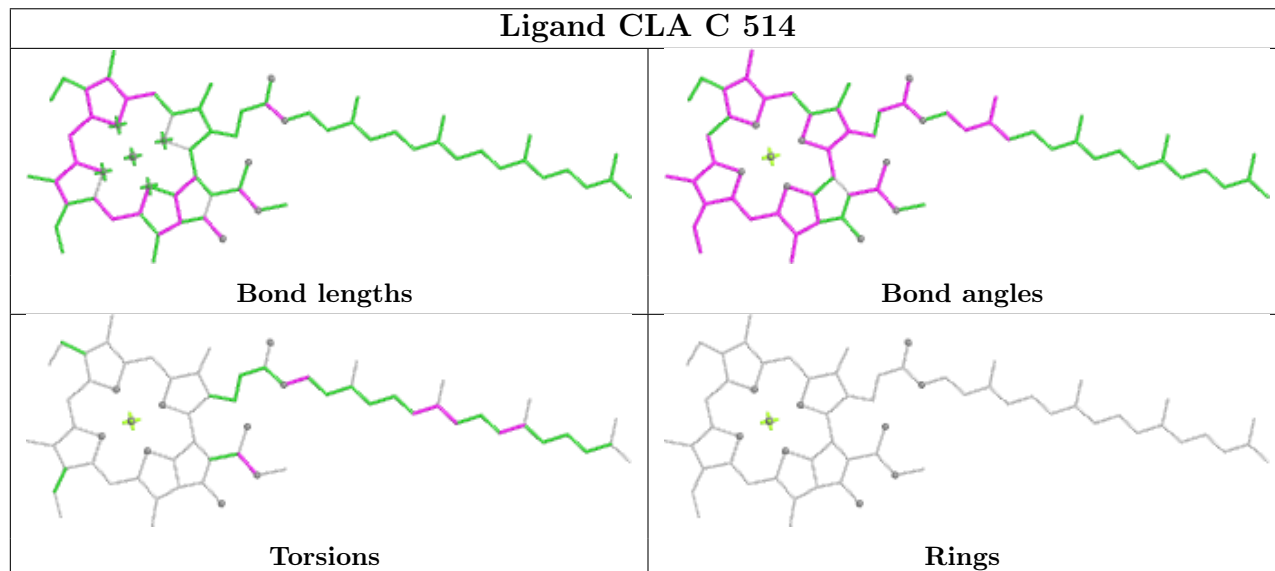


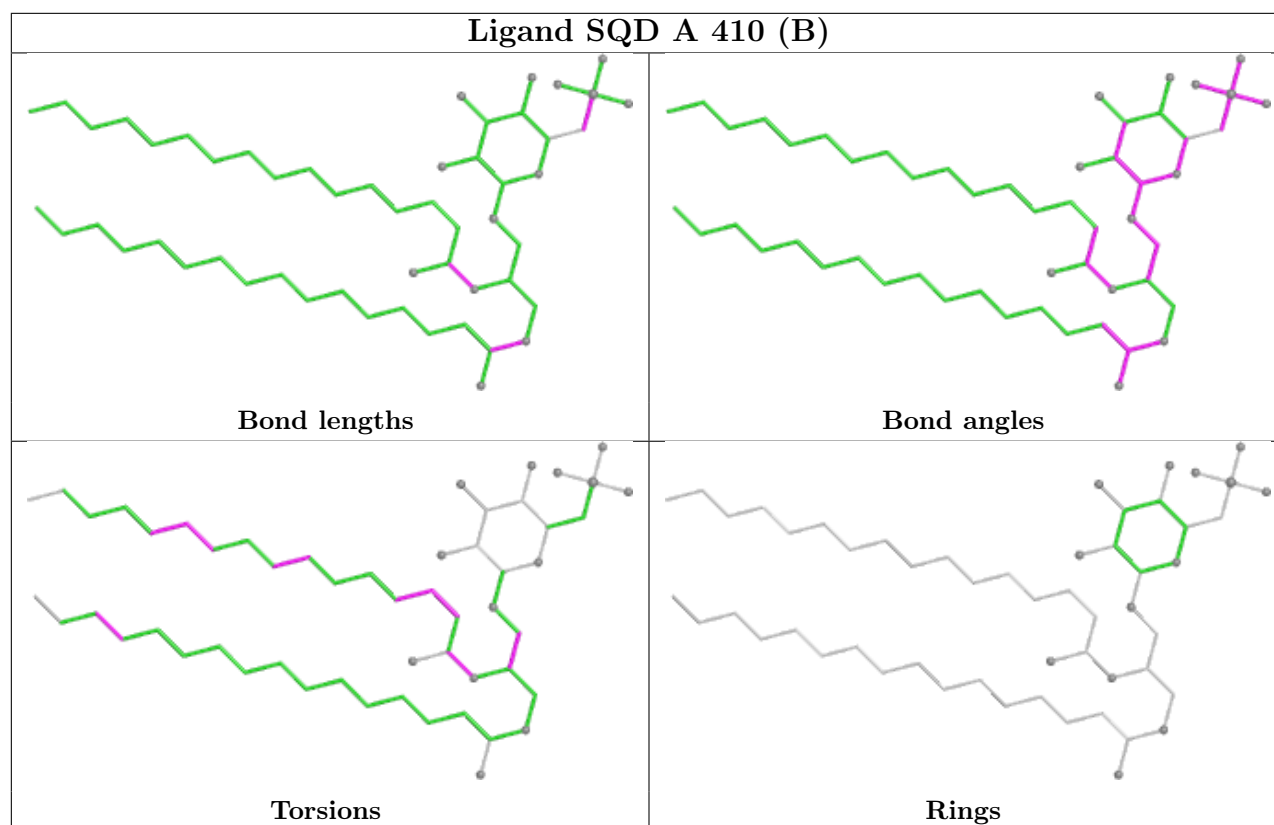
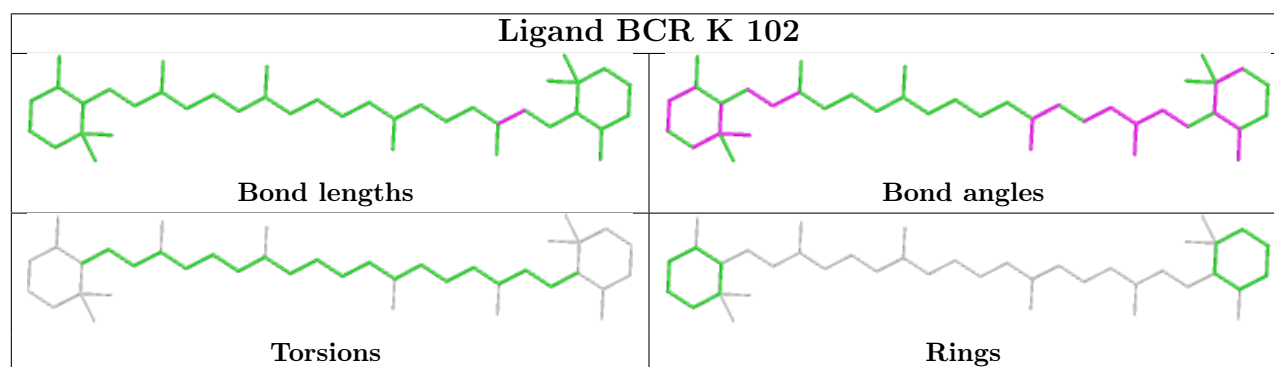
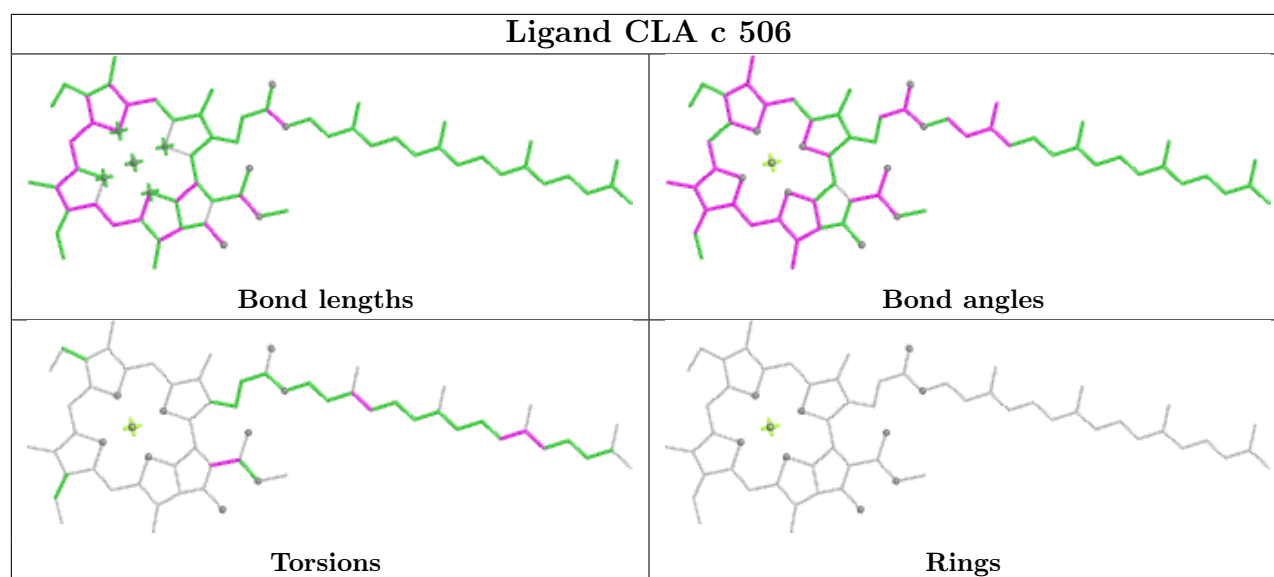


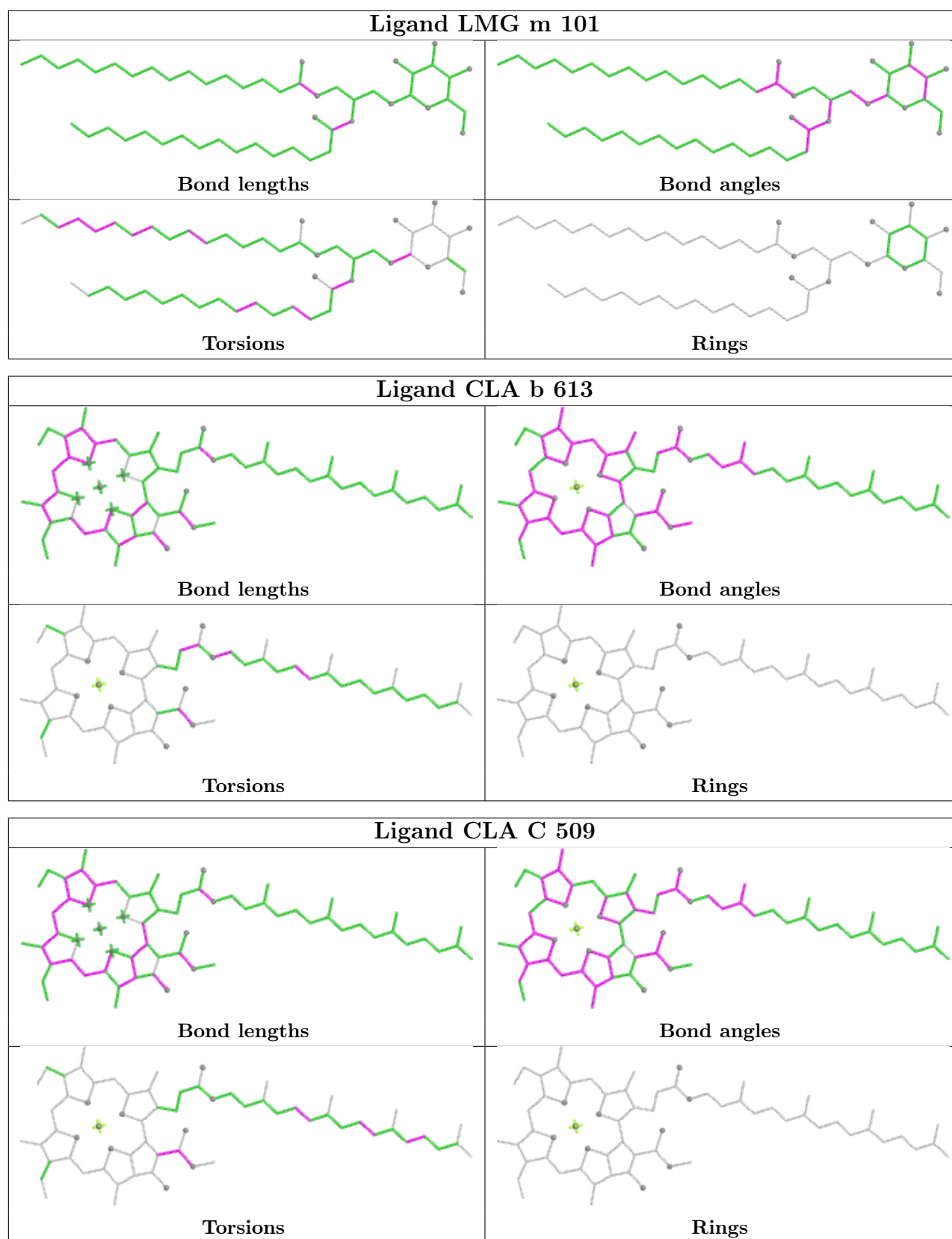
Ligand LHG d 407 (B)

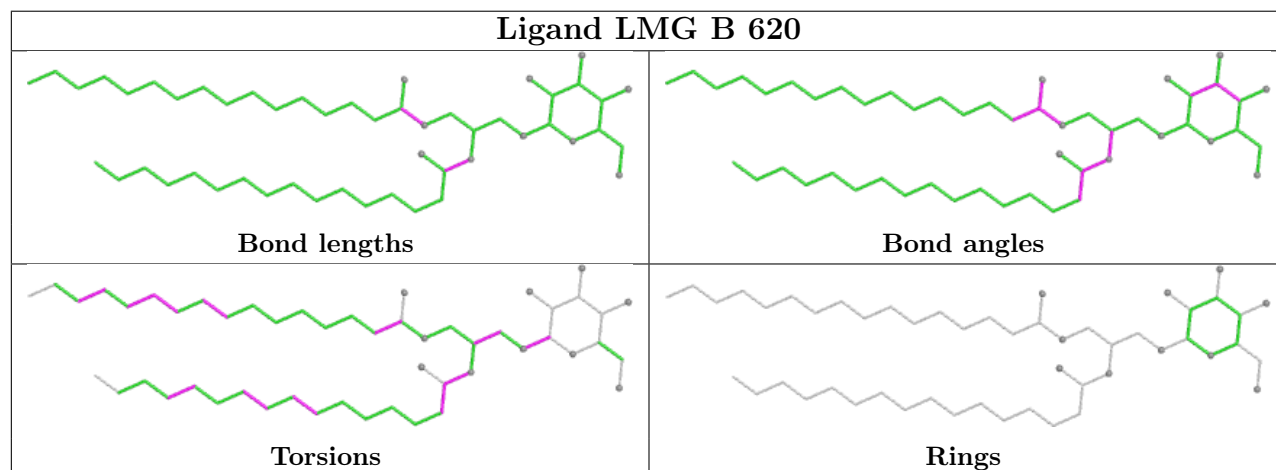
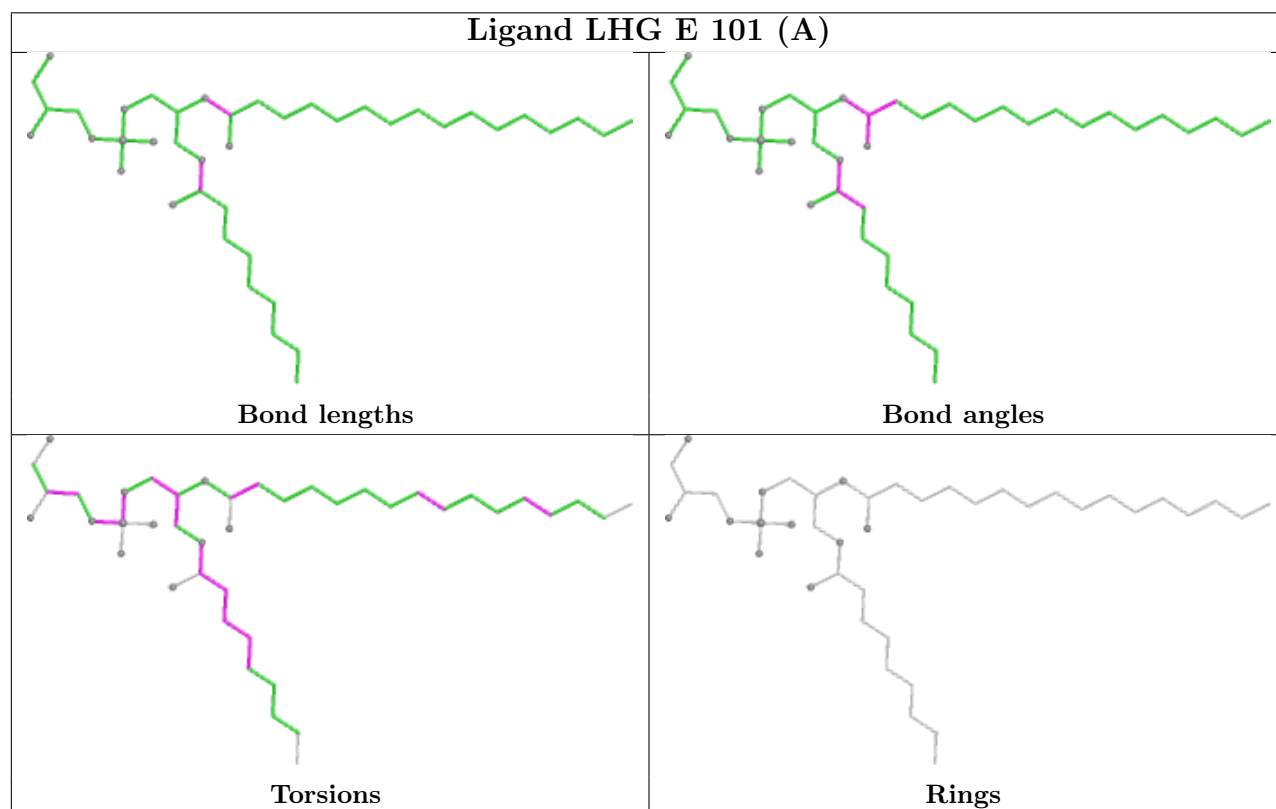
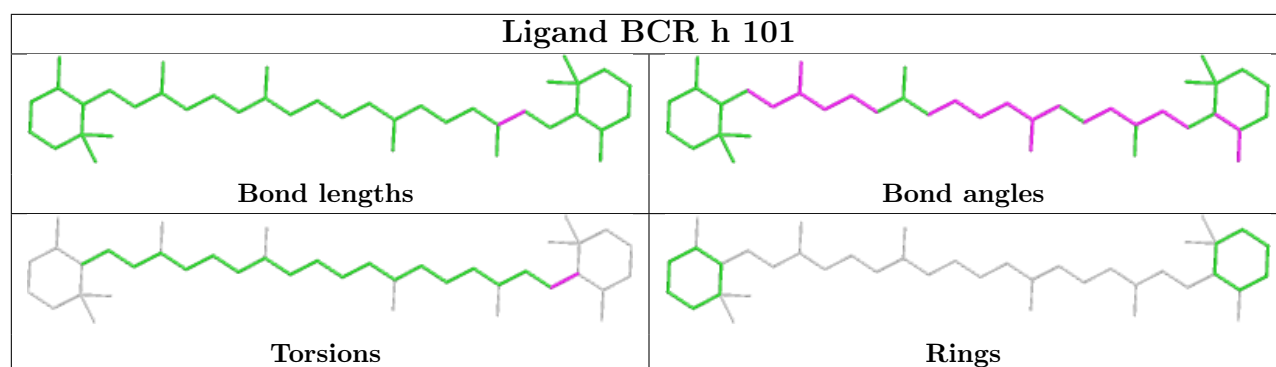


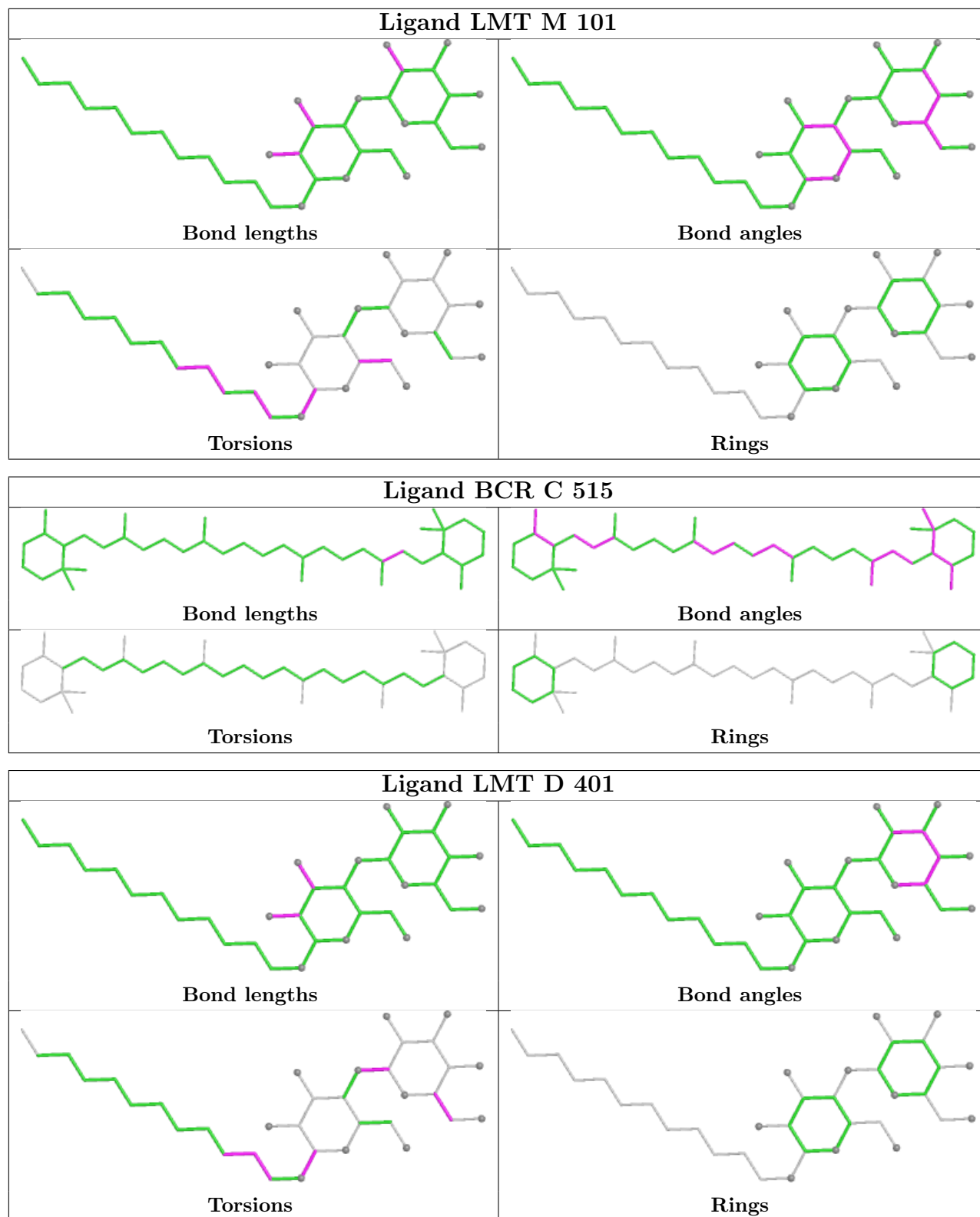
Ligand CLA C 514

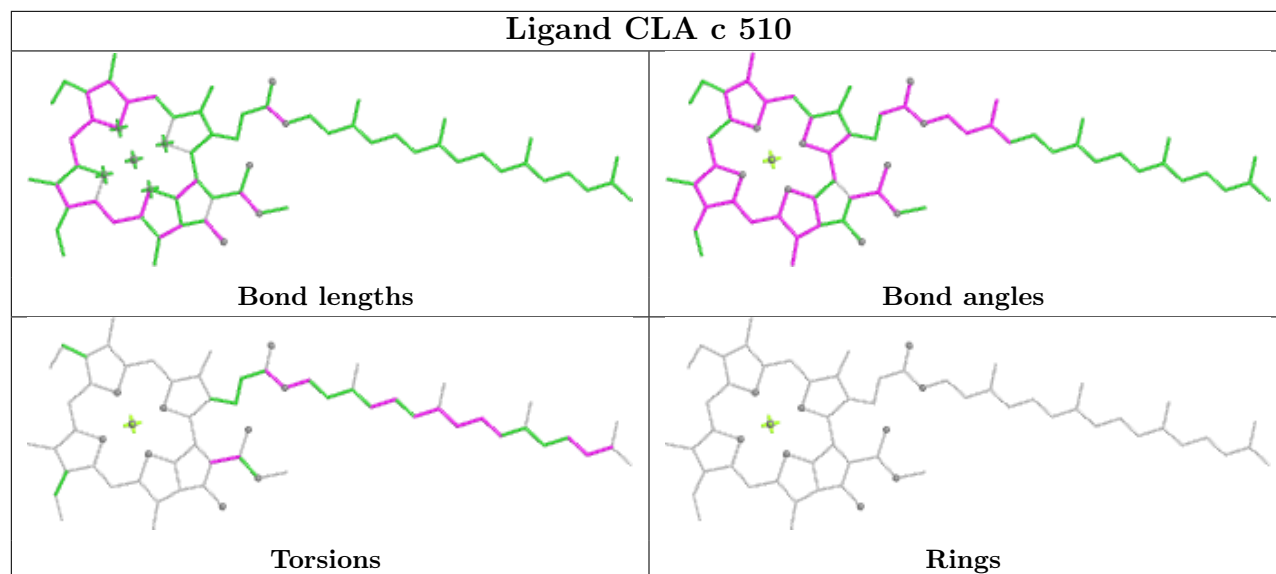
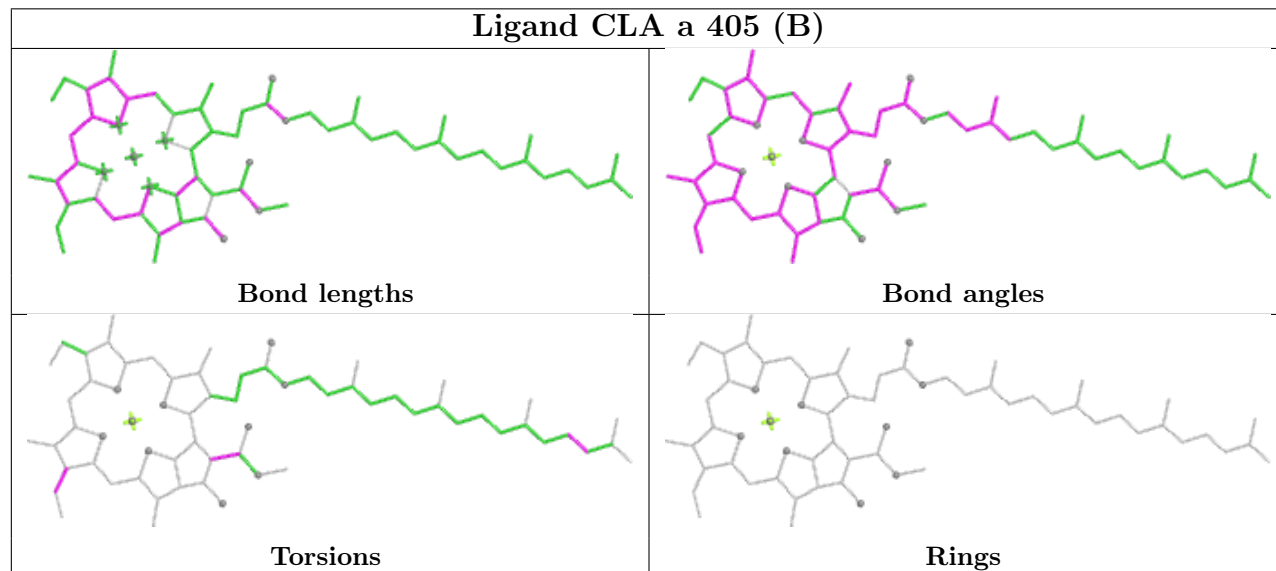


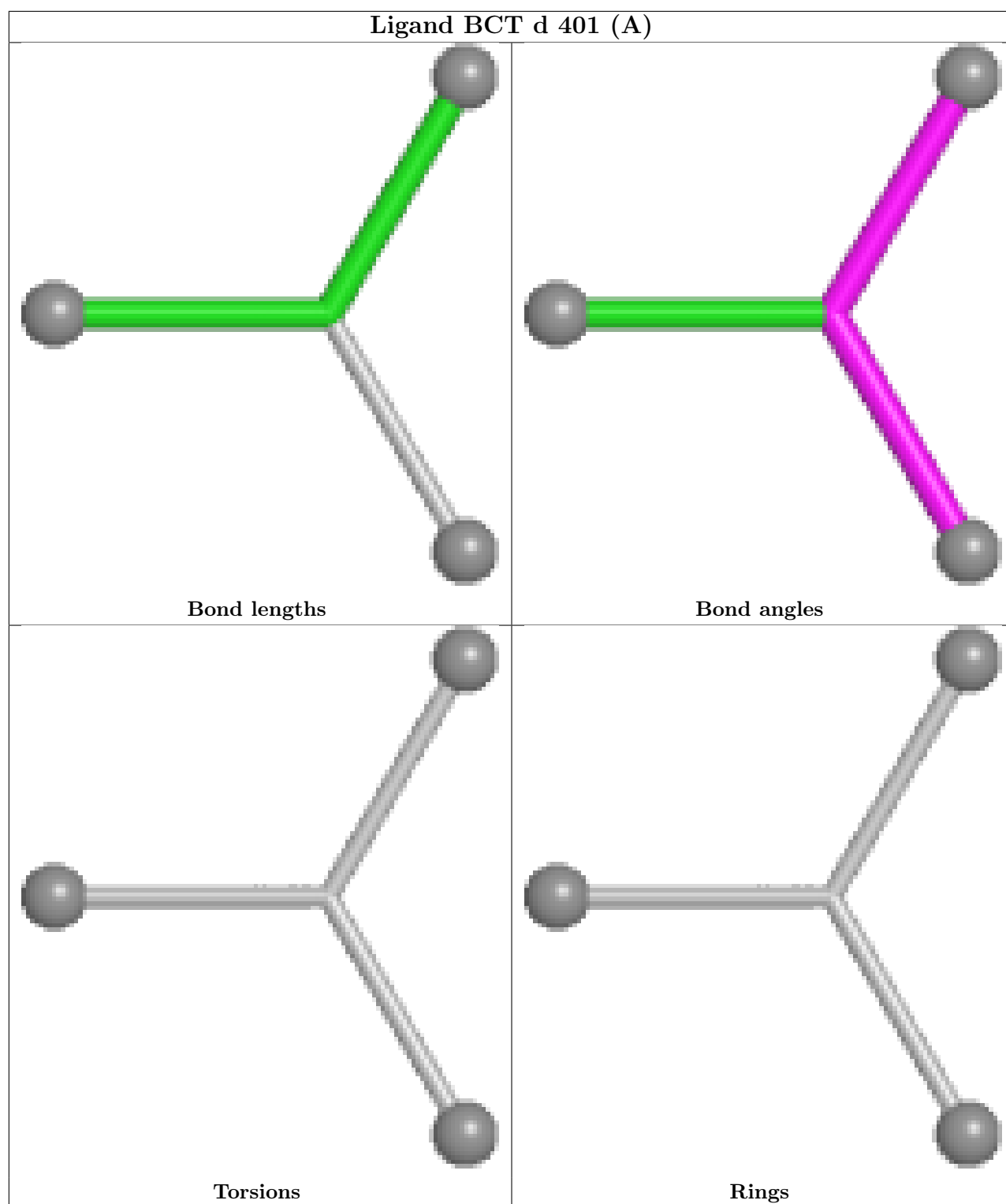


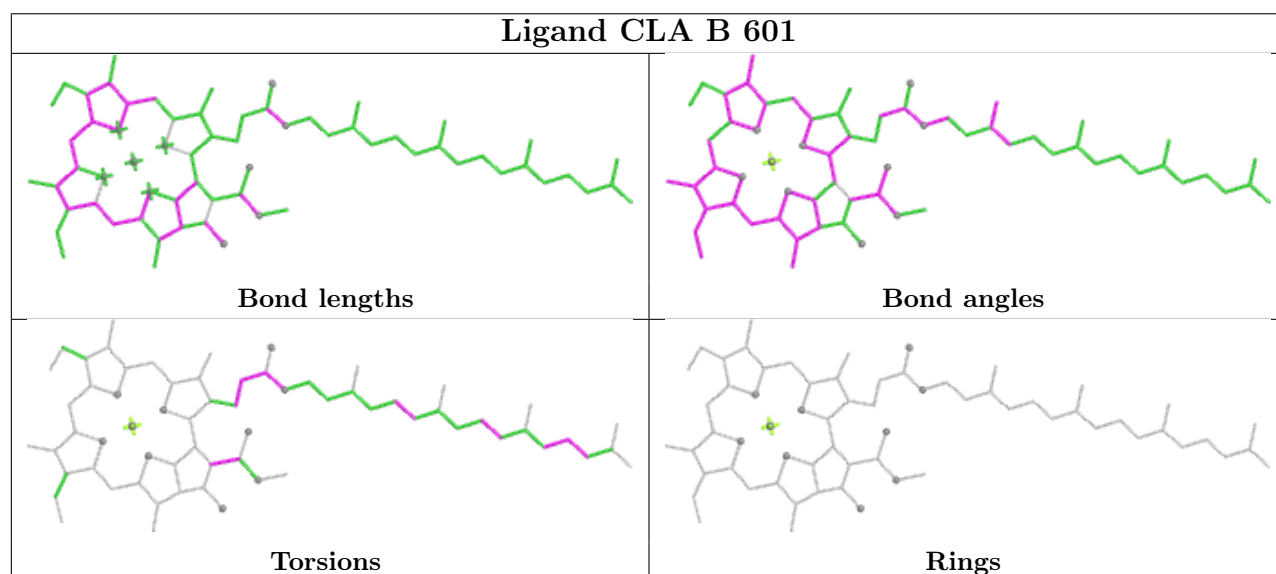
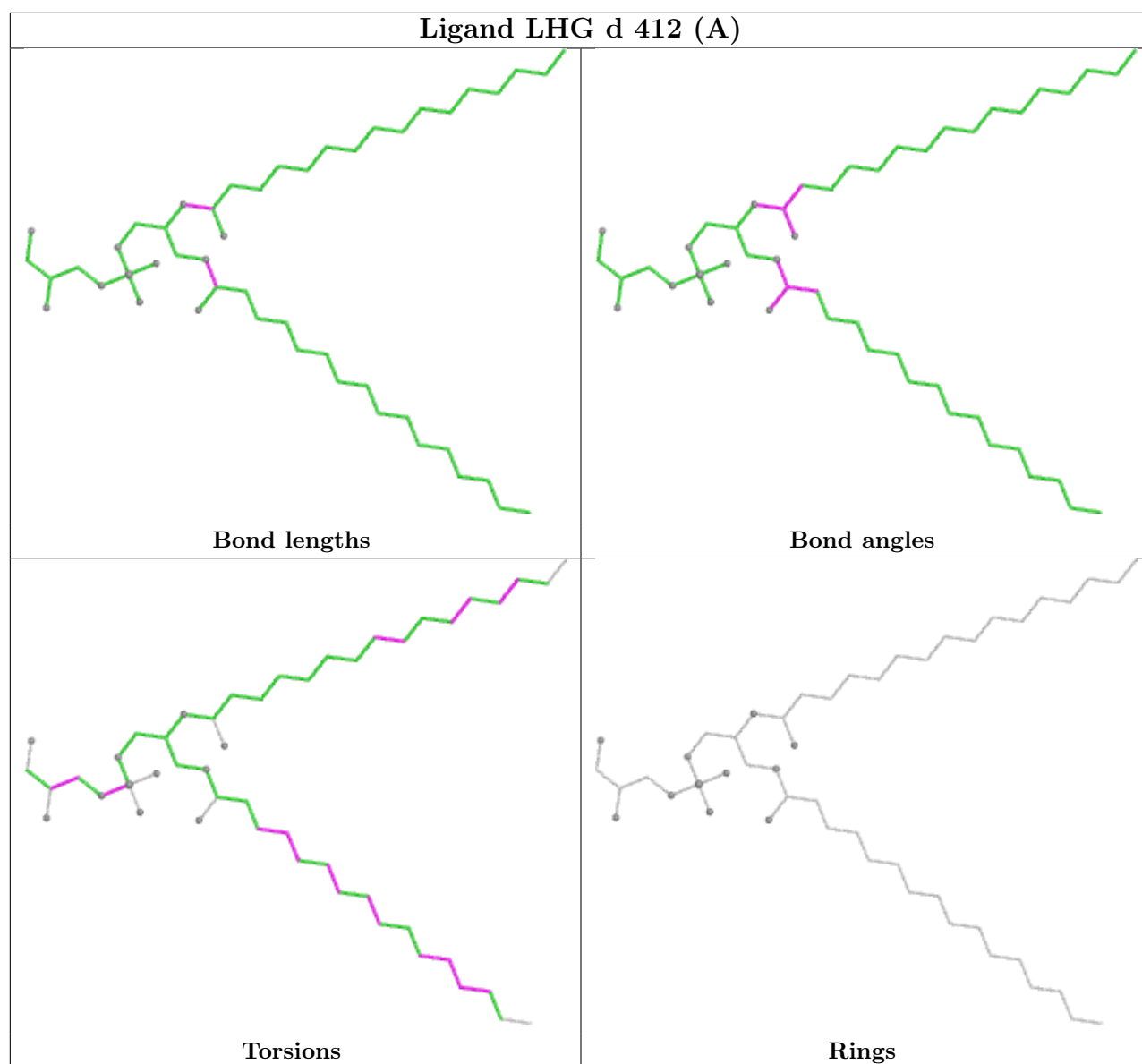


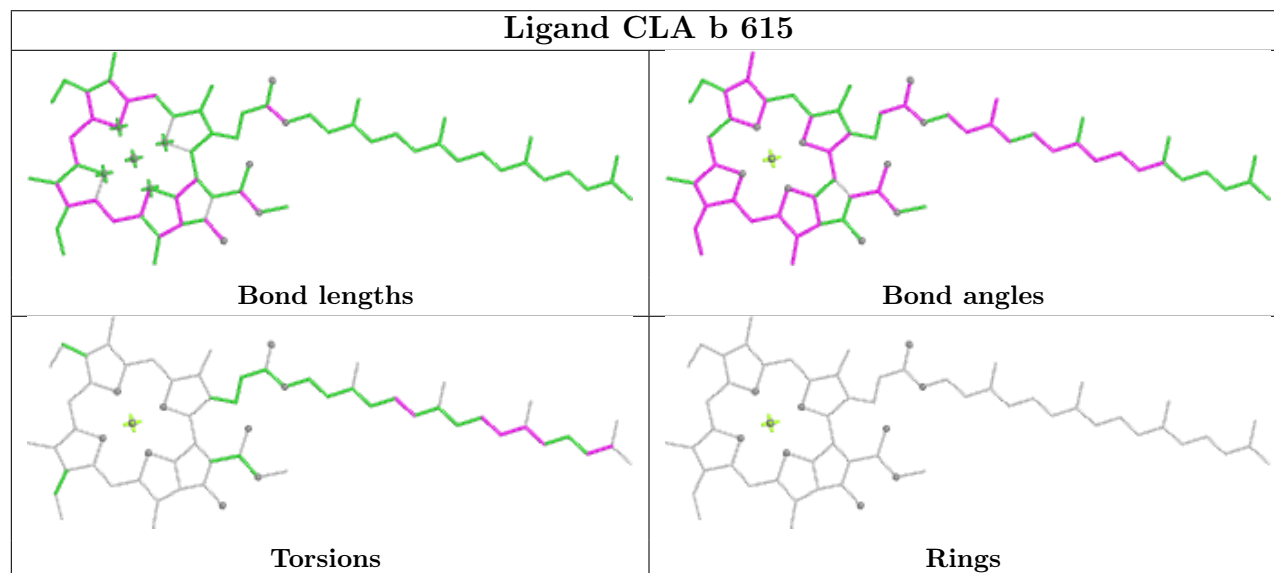
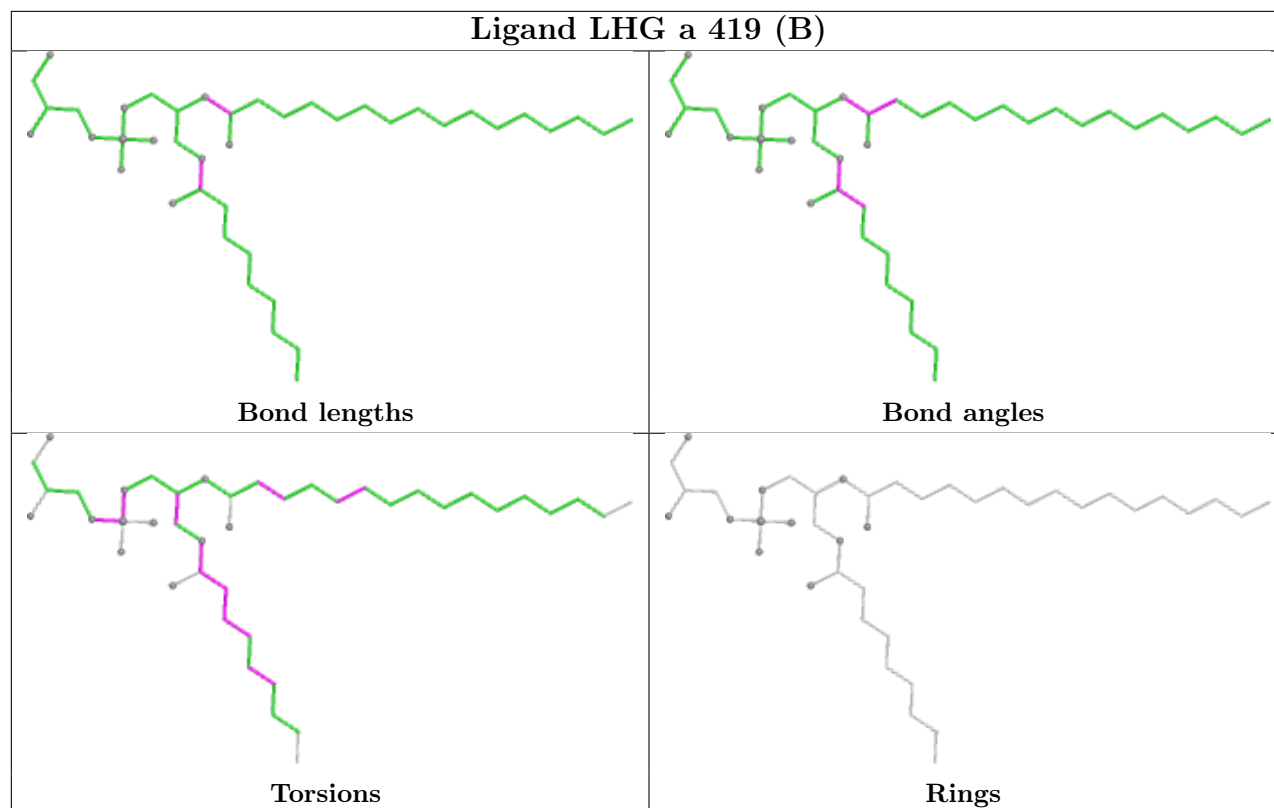


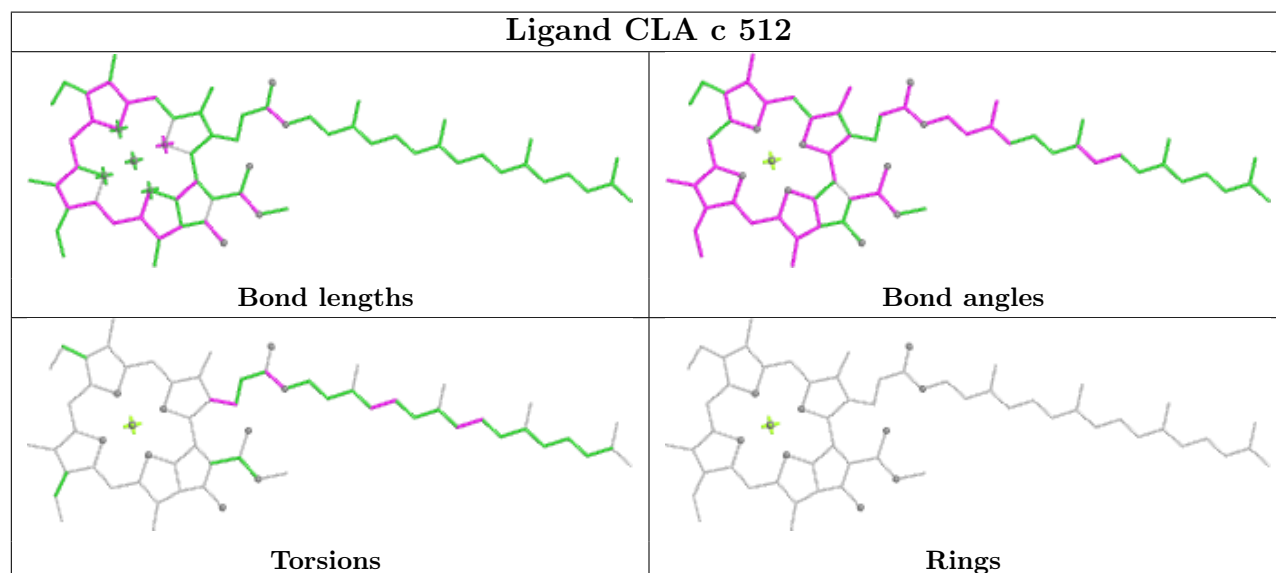
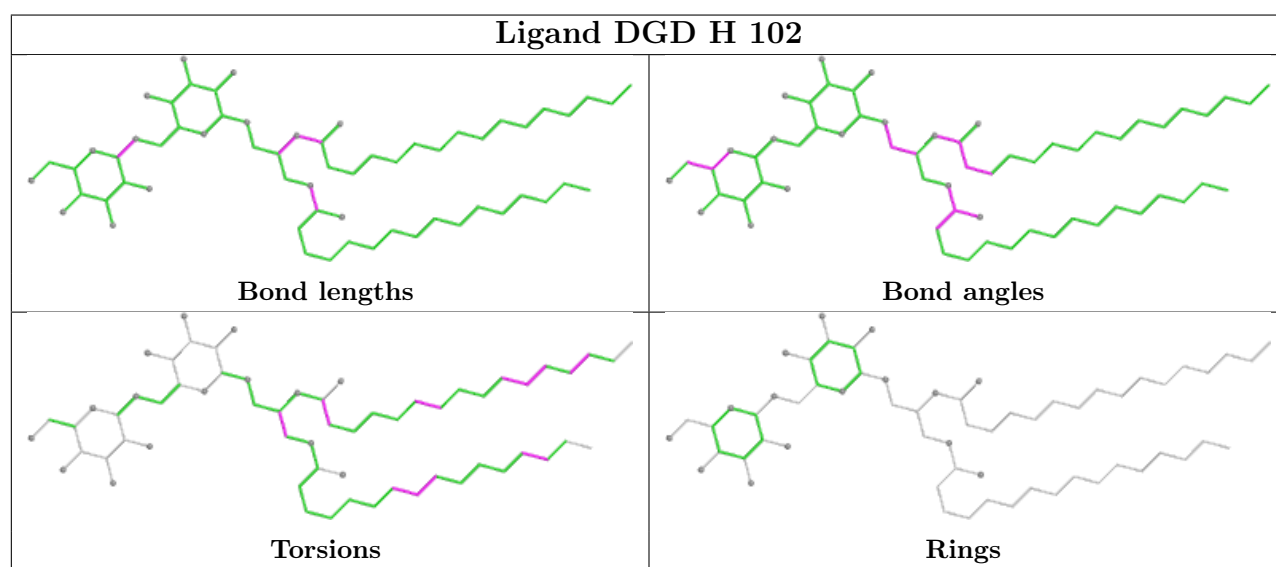
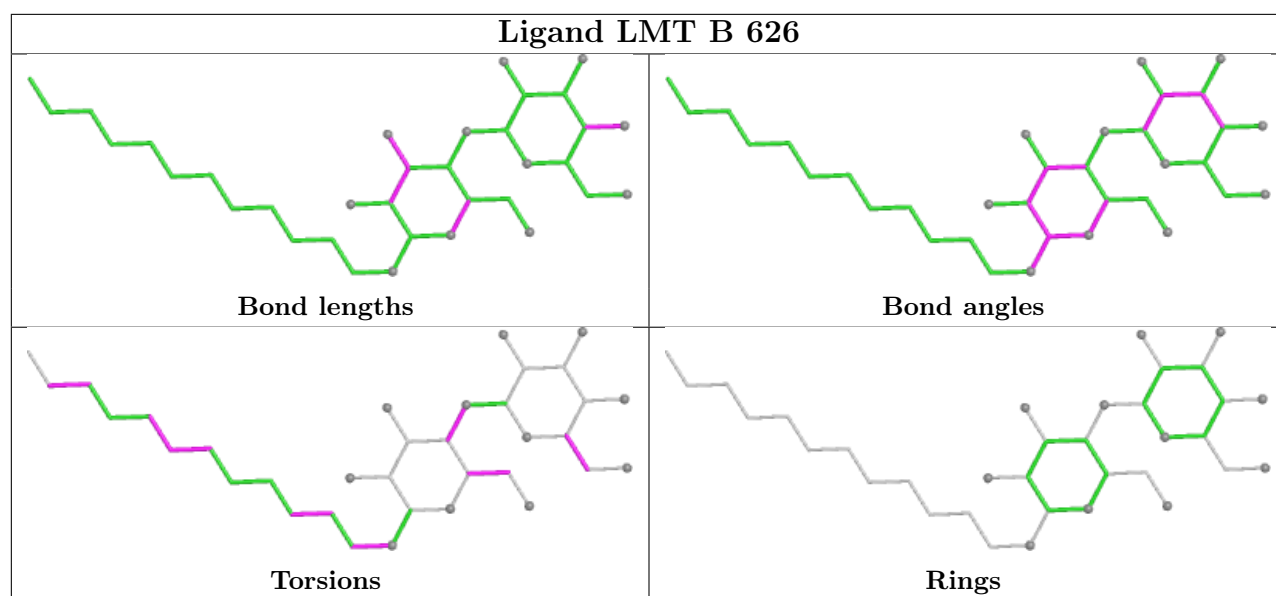


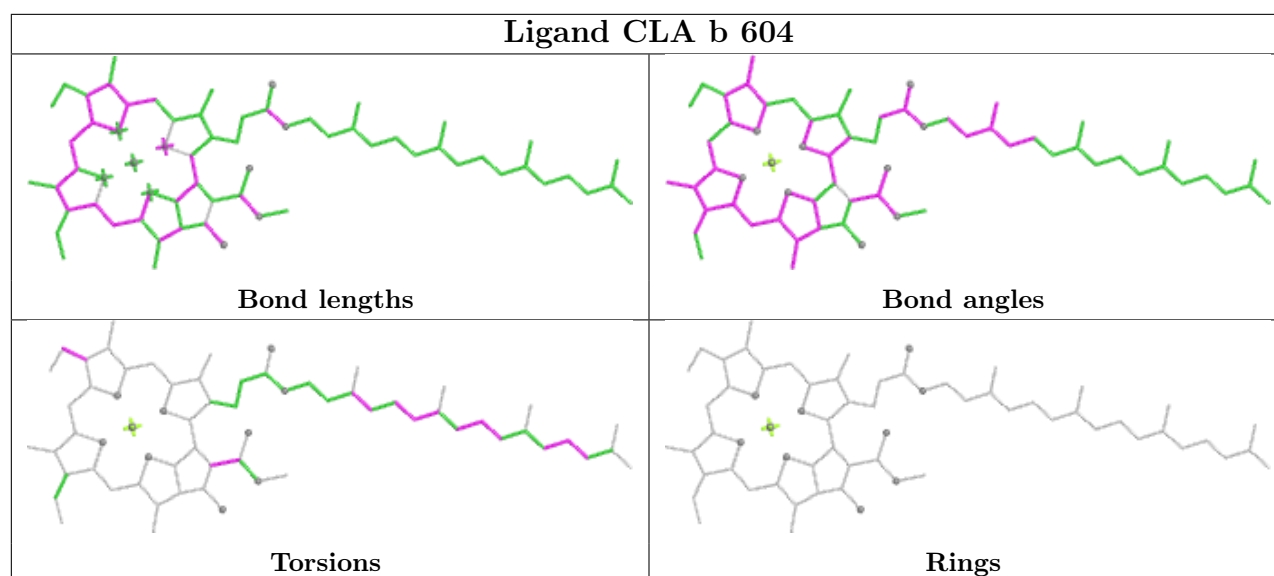
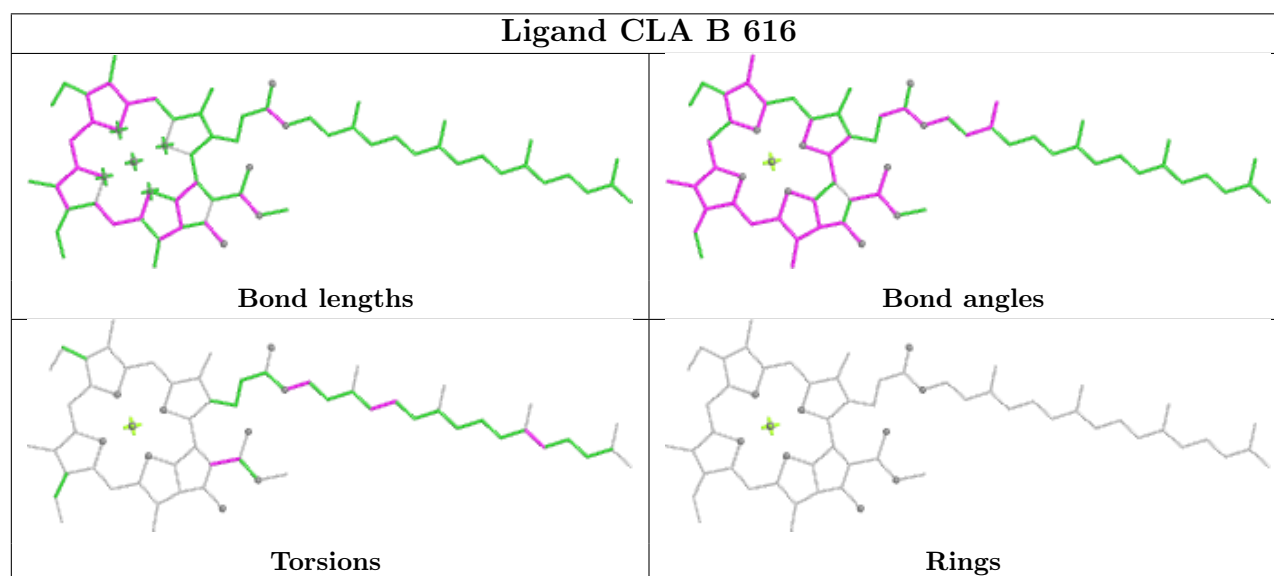
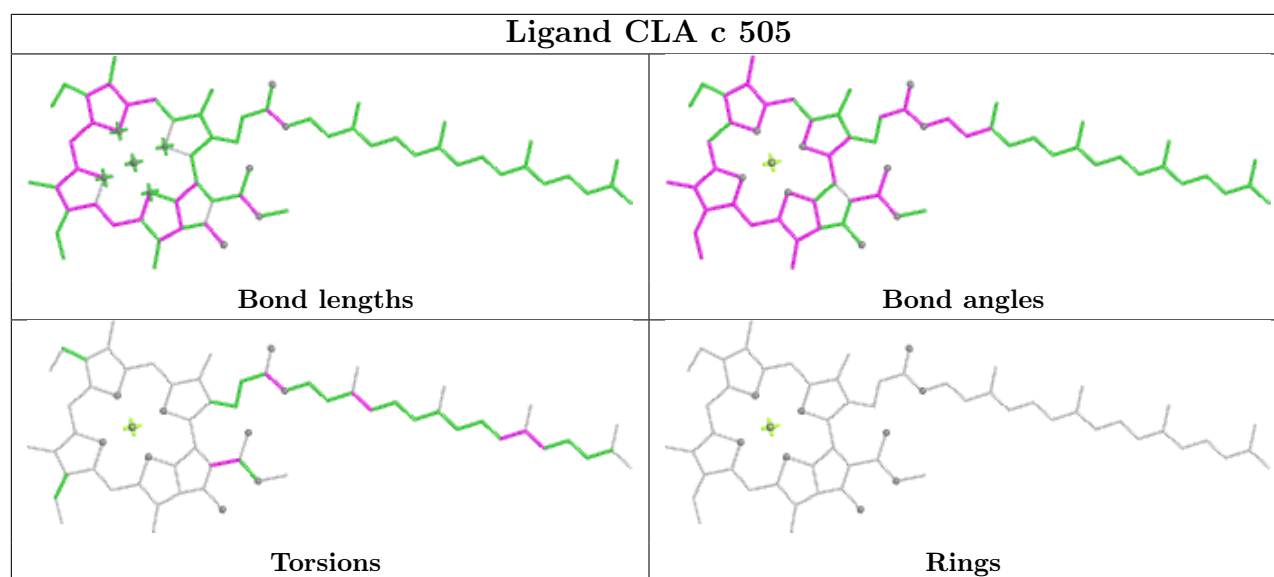
Ligand CLA c 510**Ligand CLA a 405 (B)**

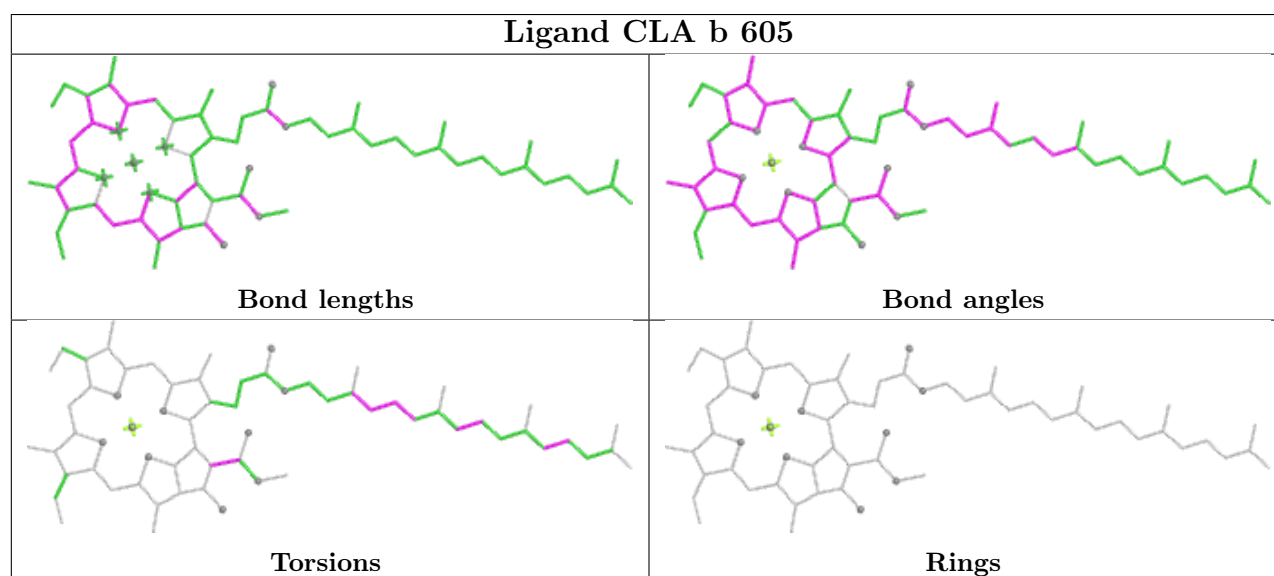
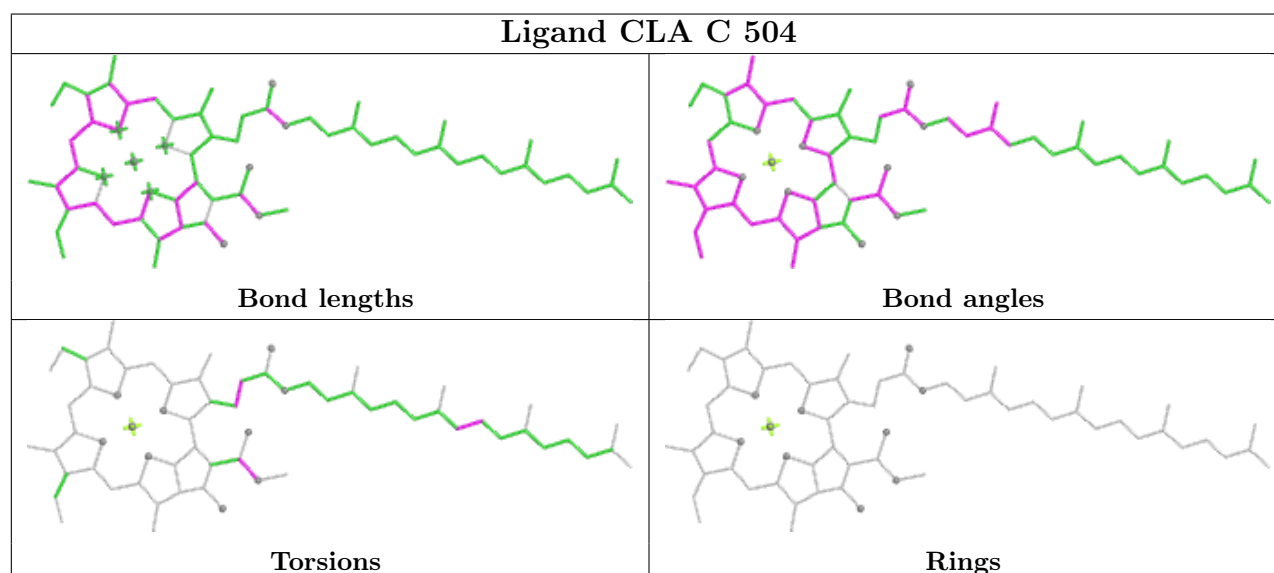
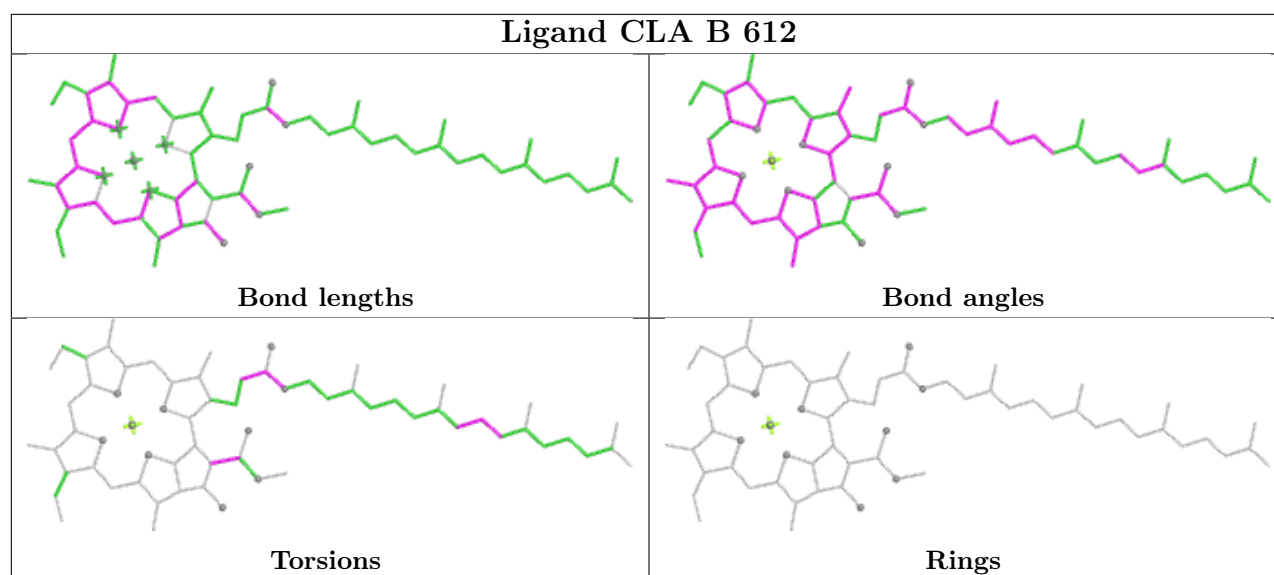


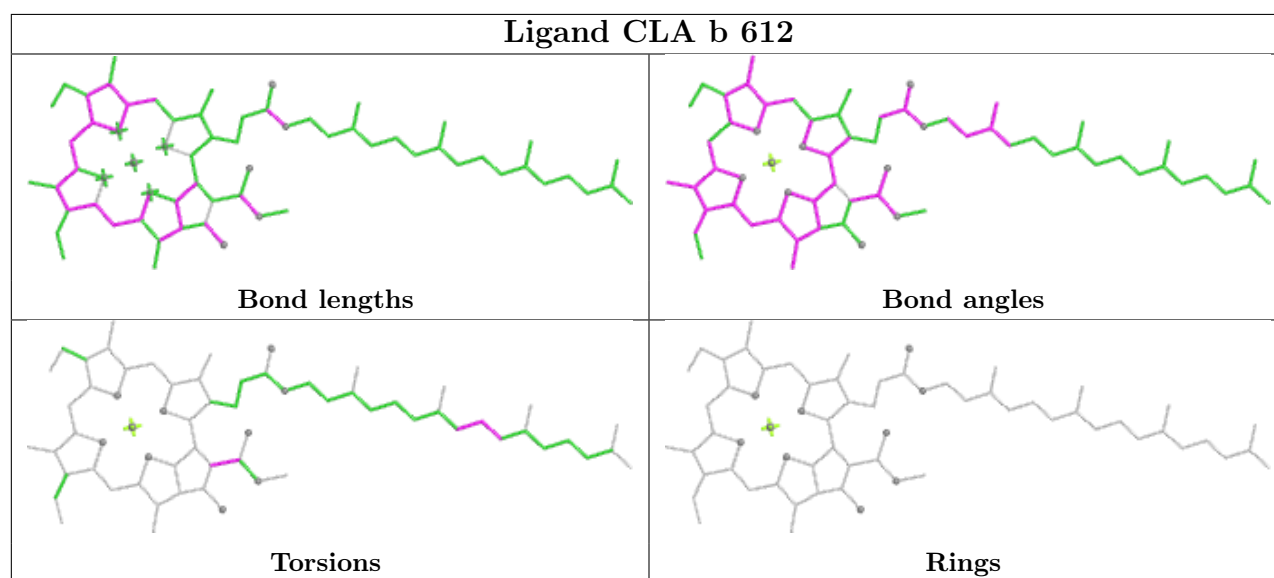
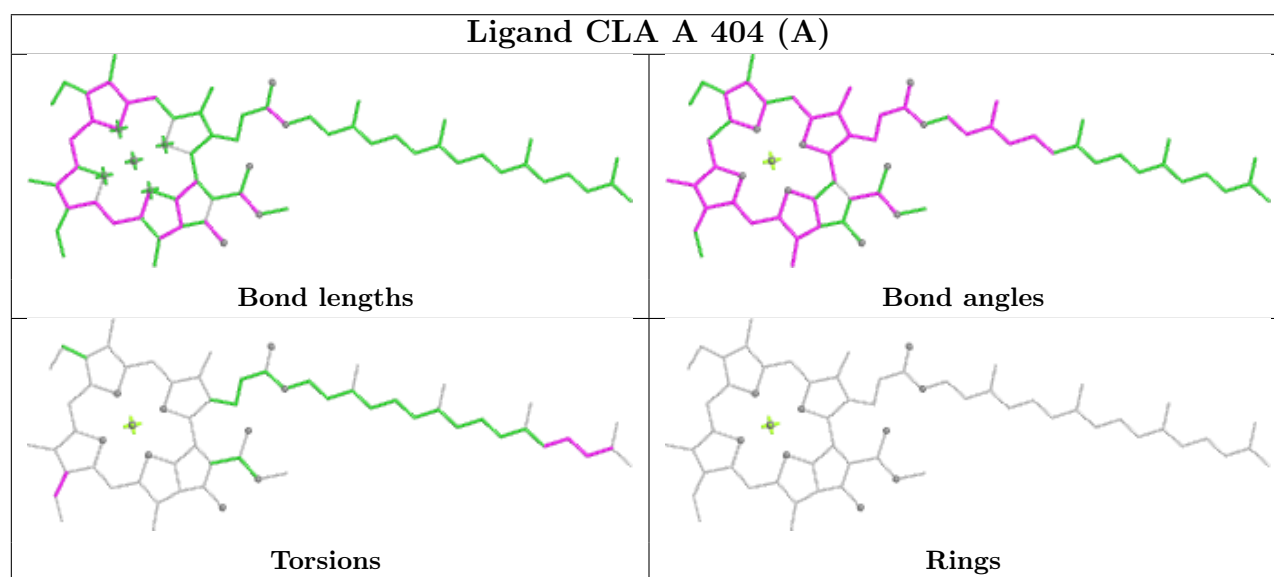
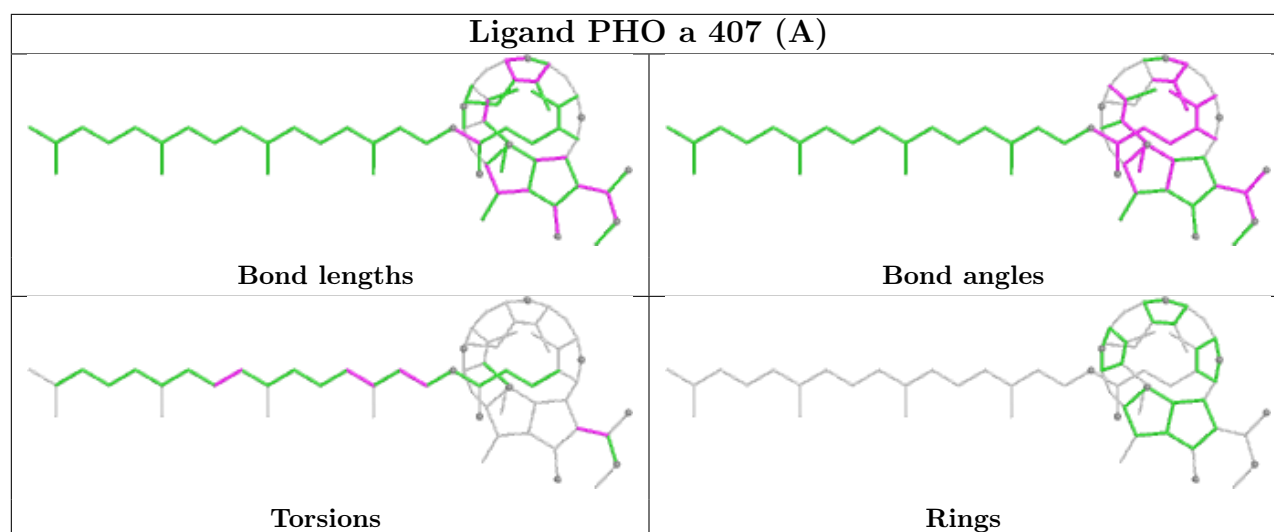


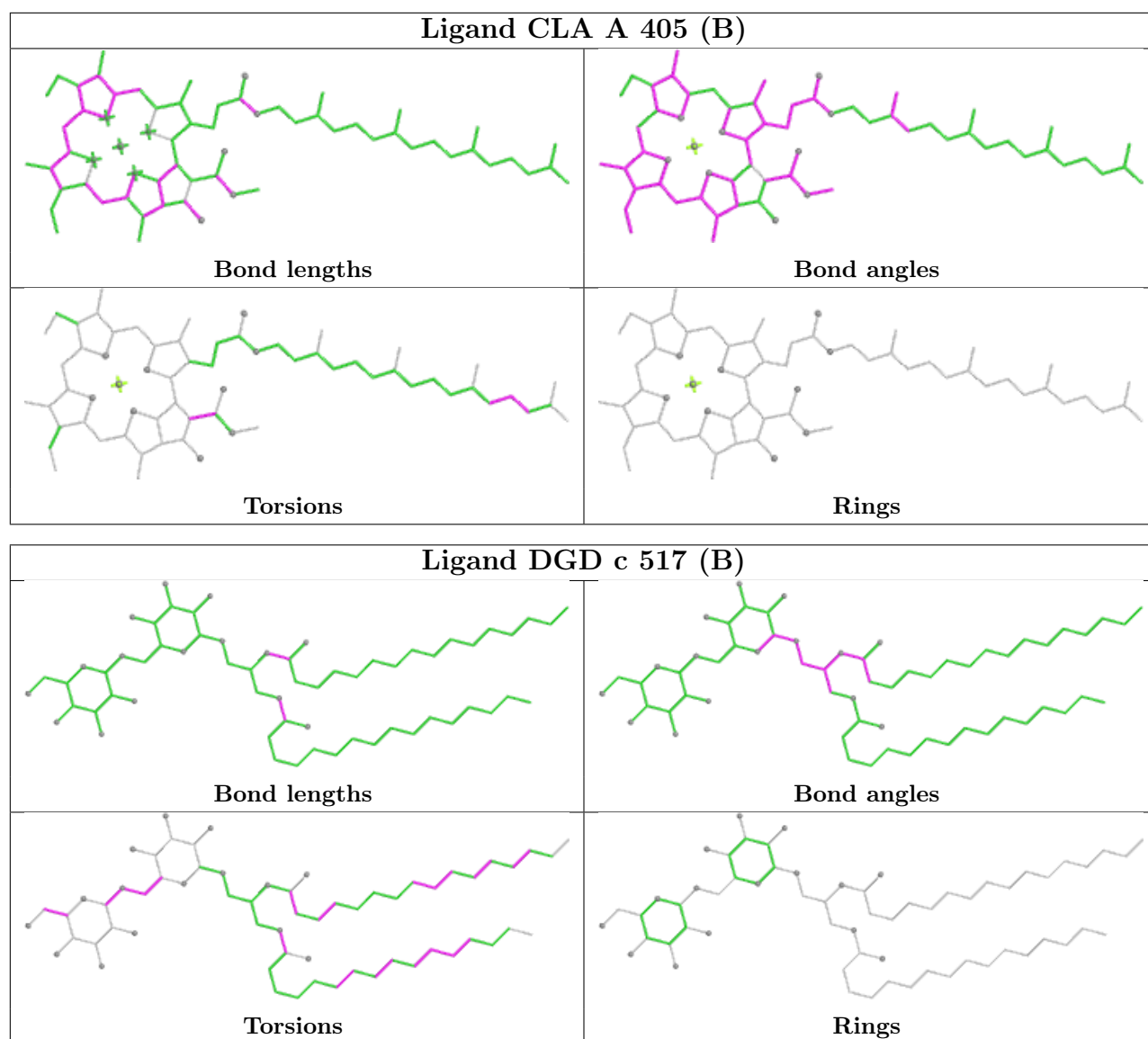












5.7 Other polymers [i](#)

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, 60, 128	222 (66%)
1	a	334/344 (97%)	-0.53	1 (0%) 90 88	22, 29, 66, 141	220 (65%)
2	B	504/505 (99%)	-0.47	1 (0%) 91 90	23, 54, 81, 119	22 (4%)
2	b	504/505 (99%)	-0.40	0 100 100	24, 57, 96, 162	19 (3%)
3	C	451/455 (99%)	-0.52	0 100 100	23, 59, 81, 162	99 (21%)
3	c	455/455 (100%)	-0.43	2 (0%) 88 87	25, 66, 86, 126	101 (22%)
4	D	342/342 (100%)	-0.58	0 100 100	21, 47, 65, 137	115 (33%)
4	d	341/342 (99%)	-0.57	0 100 100	22, 51, 73, 132	119 (34%)
5	E	81/84 (96%)	-0.30	1 (1%) 76 74	52, 69, 101, 170	0
5	e	79/84 (94%)	-0.27	1 (1%) 75 73	32, 77, 117, 152	2 (2%)
6	F	34/44 (77%)	-0.60	0 100 100	55, 61, 86, 108	0
6	f	31/44 (70%)	-0.40	1 (3%) 50 47	53, 66, 94, 148	1 (3%)
7	H	64/65 (98%)	-0.27	1 (1%) 70 67	52, 63, 84, 109	0
7	h	64/65 (98%)	-0.35	1 (1%) 70 67	39, 69, 93, 108	1 (1%)
8	I	37/38 (97%)	-0.18	0 100 100	57, 63, 124, 165	0
8	i	37/38 (97%)	-0.21	0 100 100	55, 64, 121, 139	0
9	J	38/39 (97%)	-0.31	0 100 100	51, 70, 118, 182	0
9	j	39/39 (100%)	-0.27	0 100 100	60, 76, 127, 174	0
10	K	37/37 (100%)	-0.59	0 100 100	59, 68, 86, 108	0
10	k	37/37 (100%)	-0.49	0 100 100	67, 74, 95, 113	0
11	L	36/37 (97%)	-0.55	0 100 100	24, 47, 104, 147	2 (5%)
11	l	36/37 (97%)	-0.54	0 100 100	25, 48, 104, 121	2 (5%)
12	M	32/36 (88%)	-0.50	0 100 100	27, 50, 79, 143	1 (3%)
12	m	33/36 (91%)	-0.44	0 100 100	24, 50, 74, 151	2 (6%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.47	0 100 100	22, 65, 121, 186	10 (4%)
13	o	243/244 (99%)	-0.42	0 100 100	22, 66, 125, 171	8 (3%)
14	T	29/32 (90%)	-0.58	0 100 100	27, 48, 57, 68	6 (20%)
14	t	29/32 (90%)	-0.57	1 (3%) 48 45	28, 49, 67, 75	5 (17%)
15	U	96/104 (92%)	-0.57	0 100 100	26, 60, 93, 101	4 (4%)
15	u	97/104 (93%)	-0.58	0 100 100	28, 62, 84, 139	5 (5%)
16	V	137/137 (100%)	-0.64	0 100 100	24, 58, 83, 107	6 (4%)
16	v	137/137 (100%)	-0.53	0 100 100	28, 71, 102, 136	6 (4%)
17	X	38/40 (95%)	-0.27	0 100 100	35, 71, 93, 113	1 (2%)
17	x	38/40 (95%)	0.01	0 100 100	63, 77, 123, 169	0
18	Y	29/30 (96%)	0.08	1 (3%) 48 45	68, 86, 120, 126	0
18	y	29/30 (96%)	-0.22	0 100 100	73, 90, 111, 118	0
19	Z	62/62 (100%)	-0.29	0 100 100	66, 81, 133, 169	0
19	z	62/62 (100%)	0.13	0 100 100	79, 95, 146, 202	0
20	R	34/34 (100%)	0.47	2 (5%) 28 25	75, 100, 130, 139	0
All	All	5283/5384 (98%)	-0.46	14 (0%) 90 88	20, 58, 99, 202	979 (18%)

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	e	79[A]	PHE	4.0
7	H	65	LEU	3.6
6	f	16[A]	PHE	2.9
14	t	30[A]	THR	2.7
1	a	11	ALA	2.5

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	T	1	10/11	0.93	0.09	46,60,72,76	0
8	FME	I	1	10/11	0.95	0.07	60,70,80,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	FME	i	1	10/11	0.96	0.07	57,69,76,89	0
14	FME	t	1	10/11	0.96	0.07	43,51,58,76	0
12	FME	m	1	10/11	0.97	0.07	55,64,93,112	0
12	FME	M	1	10/11	0.97	0.06	49,63,97,109	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	0.64	0.15	81,102,107,110	0
33	LMT	B	628	35/35	0.67	0.15	64,119,146,159	0
30	UNL	j	101	10/-	0.69	0.19	78,94,106,108	0
30	UNL	A	415	28/-	0.70	0.15	91,115,134,158	0
33	LMT	D	401	35/35	0.70	0.14	67,118,139,144	0
33	LMT	F	101	35/35	0.70	0.15	106,136,178,183	0
30	UNL	J	101	10/-	0.71	0.25	72,83,90,96	0
35	HTG	B	621	19/19	0.71	0.17	65,93,115,117	0
30	UNL	I	101	40/-	0.72	0.16	80,106,158,169	0
30	UNL	m	102	10/-	0.72	0.21	74,79,100,101	0
30	UNL	a	414	30/-	0.72	0.12	95,123,145,159	0
33	LMT	A	420	35/35	0.73	0.13	97,135,158,172	0
26	SQD	f	102	43/54	0.74	0.13	96,131,177,190	0
30	UNL	K	101[B]	34/-	0.75	0.14	89,113,127,128	34
27	GOL	o	303	6/6	0.75	0.18	80,102,112,119	0
33	LMT	a	416	35/35	0.75	0.13	108,138,156,164	0
33	LMT	e	101	35/35	0.75	0.13	113,151,189,195	0
30	UNL	K	101[A]	34/-	0.75	0.14	90,113,127,128	34
30	UNL	l	101	10/-	0.76	0.17	68,79,90,99	0
35	HTG	C	522	19/19	0.76	0.12	110,129,143,150	0
27	GOL	l	102[A]	6/6	0.77	0.20	67,100,107,110	6
27	GOL	l	102[B]	6/6	0.77	0.20	66,101,108,110	6
30	UNL	i	101	40/-	0.78	0.14	78,110,152,169	0
34	LMG	C	521	51/55	0.78	0.11	58,118,157,172	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	CA	F	104	1/1	0.78	0.23	131,131,131,131	0
27	GOL	O	303	6/6	0.79	0.15	84,101,109,113	0
30	UNL	b	626	33/-	0.80	0.12	67,100,154,165	0
30	UNL	b	629	36/-	0.80	0.12	71,98,130,143	0
33	LMT	b	621	25/35	0.80	0.13	83,115,157,170	0
35	HTG	D	410	16/19	0.80	0.12	90,106,132,143	0
30	UNL	D	409	40/-	0.80	0.13	67,96,135,148	0
30	UNL	c	525[A]	32/-	0.81	0.15	102,115,127,138	32
30	UNL	c	525[B]	32/-	0.81	0.15	102,115,127,139	32
27	GOL	o	304	6/6	0.82	0.15	82,93,102,108	0
27	GOL	B	625	6/6	0.82	0.13	69,87,98,117	0
27	GOL	b	624	6/6	0.82	0.15	91,98,104,106	0
27	GOL	d	411	6/6	0.82	0.14	53,74,81,90	0
32	LHG	a	419[A]	42/49	0.82	0.11	95,143,157,167	42
35	HTG	b	623	19/19	0.82	0.11	80,130,155,167	0
35	HTG	c	522	19/19	0.82	0.09	111,128,145,148	0
32	LHG	a	419[B]	42/49	0.82	0.11	95,143,157,168	42
27	GOL	O	302	6/6	0.83	0.10	79,86,105,110	0
26	SQD	a	411	54/54	0.83	0.10	69,97,137,153	0
33	LMT	B	626	35/35	0.83	0.11	70,98,140,150	0
30	UNL	B	624	33/-	0.83	0.14	57,106,145,153	0
35	HTG	V	202	11/19	0.84	0.09	82,114,126,133	0
27	GOL	a	418	6/6	0.84	0.14	58,83,85,95	0
27	GOL	A	411	6/6	0.84	0.13	69,78,88,94	0
33	LMT	B	629	25/35	0.84	0.12	65,91,149,165	0
40	HEC	V	201	43/43	0.84	0.10	38,52,72,137	0
29	PL9	A	414[A]	55/55	0.85	0.15	73,100,112,119	55
29	PL9	A	414[B]	55/55	0.85	0.15	73,100,112,120	55
33	LMT	T	101	35/35	0.85	0.11	75,127,183,186	0
27	GOL	A	418	6/6	0.85	0.16	54,76,86,91	0
26	SQD	A	412	54/54	0.85	0.11	70,92,134,155	0
27	GOL	v	202[A]	6/6	0.85	0.12	66,81,84,86	6
35	HTG	d	409	16/19	0.85	0.11	96,124,142,151	0
27	GOL	v	202[B]	6/6	0.85	0.12	66,81,85,86	6
34	LMG	Z	101	37/55	0.85	0.13	70,119,155,173	0
35	HTG	b	622	19/19	0.86	0.12	59,87,116,126	0
34	LMG	z	101	39/55	0.86	0.12	75,129,151,168	0
33	LMT	t	101	26/35	0.86	0.12	75,106,147,156	0
29	PL9	a	413[A]	55/55	0.86	0.15	90,109,123,132	55
34	LMG	c	521	51/55	0.86	0.10	75,136,166,190	0
29	PL9	a	413[B]	55/55	0.86	0.15	90,109,123,133	55
32	LHG	E	101[A]	42/49	0.87	0.12	79,104,116,124	42

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	LHG	E	101[B]	42/49	0.87	0.12	79,104,117,125	42
27	GOL	D	412	6/6	0.87	0.13	47,69,75,95	0
33	LMT	b	627	25/35	0.87	0.12	57,100,147,164	0
27	GOL	V	203[A]	6/6	0.87	0.14	60,72,77,80	6
35	HTG	o	301	19/19	0.87	0.12	61,88,118,123	0
33	LMT	m	103	35/35	0.87	0.10	60,91,109,119	0
27	GOL	V	203[B]	6/6	0.87	0.14	60,72,77,80	6
26	SQD	F	103	43/54	0.88	0.11	68,103,125,140	0
33	LMT	M	101	35/35	0.88	0.10	61,101,124,129	0
37	CA	f	103	1/1	0.88	0.11	125,125,125,125	0
27	GOL	c	527	6/6	0.88	0.17	104,117,125,127	0
26	SQD	b	620	54/54	0.89	0.10	66,97,127,132	0
26	SQD	L	101	54/54	0.89	0.10	66,95,137,148	0
23	CLA	b	601	65/65	0.89	0.10	59,90,127,159	0
37	CA	o	302	1/1	0.89	0.07	105,105,105,105	0
30	UNL	D	408	17/-	0.89	0.11	60,77,101,120	0
23	CLA	B	601	65/65	0.90	0.09	56,77,109,160	0
27	GOL	B	627	6/6	0.90	0.12	78,80,94,94	0
23	CLA	c	514	65/65	0.91	0.09	70,90,125,145	0
35	HTG	B	623	19/19	0.91	0.08	70,82,99,105	0
34	LMG	c	501	51/55	0.91	0.09	67,96,114,125	0
30	UNL	d	408	17/-	0.91	0.10	68,83,114,123	0
34	LMG	m	101	51/55	0.91	0.09	61,77,101,115	0
34	LMG	C	501	51/55	0.91	0.09	72,92,119,131	0
34	LMG	C	520	51/55	0.91	0.10	53,86,115,129	0
32	LHG	A	419[B]	49/49	0.92	0.10	52,66,87,90	49
34	LMG	B	620	51/55	0.92	0.09	58,73,95,116	0
34	LMG	c	520	51/55	0.92	0.09	60,94,129,159	0
25	BCR	T	102	40/40	0.92	0.07	46,58,74,84	0
35	HTG	b	625	19/19	0.92	0.08	66,81,97,116	0
32	LHG	A	419[A]	49/49	0.92	0.10	52,66,87,90	49
23	CLA	C	514	65/65	0.93	0.08	58,87,113,121	0
23	CLA	d	403	65/65	0.93	0.09	46,66,124,153	0
26	SQD	a	410[A]	54/54	0.93	0.09	62,83,118,122	54
32	LHG	D	407[A]	49/49	0.93	0.10	50,61,110,111	49
32	LHG	D	407[B]	49/49	0.93	0.10	50,61,110,112	49
26	SQD	a	410[B]	54/54	0.93	0.09	62,83,118,123	54
25	BCR	D	404	40/40	0.93	0.09	49,59,106,108	0
25	BCR	K	102	40/40	0.93	0.10	57,65,80,81	0
23	CLA	b	616	65/65	0.93	0.09	50,64,127,139	0
32	LHG	d	412[A]	49/49	0.93	0.09	55,69,84,93	49
32	LHG	d	412[B]	49/49	0.93	0.09	55,69,84,94	49

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	BCR	d	404	40/40	0.93	0.08	53,68,104,112	0
25	BCR	t	102	40/40	0.93	0.07	45,60,80,86	0
34	LMG	D	411	51/55	0.93	0.09	49,70,124,136	0
36	DGD	C	518[A]	62/66	0.93	0.08	51,64,111,116	62
36	DGD	C	518[B]	62/66	0.93	0.08	51,64,111,117	62
36	DGD	c	517[A]	62/66	0.93	0.08	48,65,100,106	62
36	DGD	c	517[B]	62/66	0.93	0.08	47,65,100,106	62
36	DGD	c	518[A]	62/66	0.93	0.08	56,69,117,131	62
36	DGD	c	518[B]	62/66	0.93	0.08	56,69,117,131	62
26	SQD	A	410[A]	54/54	0.93	0.09	56,80,114,116	54
37	CA	c	523	1/1	0.93	0.10	74,74,74,74	0
26	SQD	A	410[B]	54/54	0.93	0.09	56,81,114,117	54
23	CLA	c	513	65/65	0.93	0.09	62,81,130,136	0
34	LMG	d	410	51/55	0.93	0.08	54,71,117,148	0
23	CLA	c	508	65/65	0.94	0.09	50,68,85,90	0
23	CLA	C	505	65/65	0.94	0.08	40,58,106,138	0
23	CLA	C	507	65/65	0.94	0.08	51,70,120,142	0
23	CLA	C	513	65/65	0.94	0.08	56,73,115,137	0
25	BCR	A	409	40/40	0.94	0.07	42,52,68,69	0
25	BCR	B	619	40/40	0.94	0.08	48,60,96,97	0
25	BCR	C	515	40/40	0.94	0.08	53,75,88,91	0
23	CLA	A	408	65/65	0.94	0.09	45,53,130,148	0
25	BCR	H	101	40/40	0.94	0.08	51,67,85,88	0
31	BCT	d	401[A]	4/4	0.94	0.08	58,59,70,78	4
31	BCT	d	401[B]	4/4	0.94	0.08	58,60,70,80	4
27	GOL	B	622	6/6	0.94	0.08	72,82,89,91	0
23	CLA	a	408	65/65	0.94	0.10	43,56,141,159	0
23	CLA	B	606	65/65	0.94	0.08	39,56,110,130	0
36	DGD	C	519	62/66	0.94	0.08	45,63,102,116	0
36	DGD	H	102	62/66	0.94	0.09	47,63,75,84	0
25	BCR	b	618	40/40	0.94	0.07	46,58,82,94	0
25	BCR	c	515	40/40	0.94	0.08	68,84,93,98	0
23	CLA	b	606	65/65	0.94	0.08	44,60,114,128	0
25	BCR	h	101	40/40	0.94	0.09	53,69,93,101	0
36	DGD	c	519	62/66	0.94	0.08	51,68,108,132	0
36	DGD	h	102	62/66	0.94	0.09	53,66,79,85	0
23	CLA	b	614	65/65	0.94	0.07	42,53,103,117	0
23	CLA	B	614	65/65	0.94	0.08	39,50,105,124	0
23	CLA	c	505	65/65	0.94	0.08	52,66,110,134	0
23	CLA	c	507	65/65	0.94	0.09	50,70,121,138	0
27	GOL	b	628	6/6	0.94	0.07	83,90,91,96	0
31	BCT	A	416[A]	4/4	0.95	0.08	55,57,61,66	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	BCT	A	416[B]	4/4	0.95	0.08	54,56,62,72	4
23	CLA	C	509	65/65	0.95	0.07	45,57,119,142	0
23	CLA	c	502	65/65	0.95	0.08	55,68,80,95	0
23	CLA	B	603	65/65	0.95	0.08	40,54,72,91	0
25	BCR	Y	101	40/40	0.95	0.08	52,67,83,91	0
29	PL9	D	405[A]	55/55	0.95	0.07	38,50,61,70	55
29	PL9	D	405[B]	55/55	0.95	0.07	38,50,61,70	55
25	BCR	a	409	40/40	0.95	0.07	45,55,69,71	0
25	BCR	b	617	40/40	0.95	0.06	44,55,65,72	0
23	CLA	B	616	65/65	0.95	0.09	48,60,131,143	0
27	GOL	C	523[A]	6/6	0.95	0.09	59,64,68,70	6
32	LHG	b	630[A]	49/49	0.95	0.08	54,61,73,98	49
32	LHG	b	630[B]	49/49	0.95	0.08	53,61,73,98	49
32	LHG	d	406[A]	49/49	0.95	0.08	49,59,74,80	49
32	LHG	d	406[B]	49/49	0.95	0.08	48,59,74,80	49
32	LHG	d	407[A]	49/49	0.95	0.09	53,64,111,128	49
32	LHG	d	407[B]	49/49	0.95	0.09	53,65,111,129	49
27	GOL	C	523[B]	6/6	0.95	0.09	63,64,69,70	6
25	BCR	b	619	40/40	0.95	0.08	46,62,87,92	0
23	CLA	D	403	65/65	0.95	0.08	48,58,126,139	0
36	DGD	C	517[A]	62/66	0.95	0.07	47,58,101,106	62
36	DGD	C	517[B]	62/66	0.95	0.07	46,59,101,106	62
23	CLA	c	509	65/65	0.95	0.07	43,63,126,150	0
23	CLA	a	406[A]	65/65	0.95	0.07	42,54,123,132	65
25	BCR	k	101	40/40	0.95	0.09	57,73,84,88	0
30	UNL	X	101	18/-	0.95	0.10	61,78,111,113	0
23	CLA	a	406[B]	65/65	0.95	0.07	41,54,123,132	65
25	BCR	y	101	40/40	0.95	0.08	59,71,88,101	0
23	CLA	C	502	65/65	0.95	0.07	50,62,74,80	0
24	PHO	a	415[A]	64/64	0.95	0.07	44,56,62,69	64
24	PHO	a	415[B]	64/64	0.95	0.07	44,56,62,69	64
23	CLA	B	610	65/65	0.95	0.08	43,55,67,89	0
25	BCR	B	618	40/40	0.95	0.06	44,57,73,84	0
23	CLA	B	611	65/65	0.95	0.07	37,48,68,78	0
23	CLA	b	612	65/65	0.95	0.08	43,53,65,73	0
23	CLA	C	508	65/65	0.95	0.08	48,63,87,92	0
30	UNL	x	101	18/-	0.95	0.10	72,83,135,137	0
23	CLA	A	405[A]	65/65	0.96	0.06	37,44,58,69	65
23	CLA	b	607	65/65	0.96	0.07	39,50,84,97	0
23	CLA	b	609	65/65	0.96	0.07	46,65,79,89	0
23	CLA	b	611	65/65	0.96	0.07	40,51,73,84	0
23	CLA	C	506	65/65	0.96	0.07	48,61,96,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	b	613	65/65	0.96	0.06	41,50,86,107	0
27	GOL	c	526[A]	6/6	0.96	0.07	67,71,76,79	6
27	GOL	c	526[B]	6/6	0.96	0.07	67,73,77,80	6
23	CLA	A	405[B]	65/65	0.96	0.06	37,44,58,70	65
23	CLA	B	607	65/65	0.96	0.06	38,48,81,86	0
25	BCR	c	516	40/40	0.96	0.06	56,66,83,85	0
23	CLA	B	609	65/65	0.96	0.07	46,60,71,85	0
32	LHG	D	406[A]	49/49	0.96	0.08	49,56,70,78	49
32	LHG	D	406[B]	49/49	0.96	0.08	49,56,70,79	49
23	CLA	c	504	65/65	0.96	0.07	50,69,80,97	0
23	CLA	C	510	65/65	0.96	0.08	48,58,85,100	0
23	CLA	c	506	65/65	0.96	0.07	50,65,98,100	0
23	CLA	C	512	65/65	0.96	0.07	50,64,79,88	0
32	LHG	L	102[A]	49/49	0.96	0.07	50,59,69,95	49
32	LHG	L	102[B]	49/49	0.96	0.07	50,59,68,95	49
23	CLA	A	406[A]	65/65	0.96	0.06	41,49,115,126	65
23	CLA	A	406[B]	65/65	0.96	0.06	41,49,115,126	65
23	CLA	c	512	65/65	0.96	0.08	55,68,86,100	0
23	CLA	D	402[A]	65/65	0.96	0.07	33,44,69,79	65
23	CLA	D	402[B]	65/65	0.96	0.07	33,44,69,81	65
23	CLA	B	613	65/65	0.96	0.06	40,48,94,111	0
29	PL9	d	405[A]	55/55	0.96	0.07	41,52,63,72	55
29	PL9	d	405[B]	55/55	0.96	0.07	41,53,63,72	55
24	PHO	A	417[A]	64/64	0.96	0.06	40,51,58,65	64
24	PHO	A	417[B]	64/64	0.96	0.06	39,51,58,65	64
24	PHO	a	407[A]	64/64	0.96	0.06	44,50,56,61	64
24	PHO	a	407[B]	64/64	0.96	0.06	44,50,56,61	64
23	CLA	A	404[A]	65/65	0.96	0.07	37,44,64,71	65
23	CLA	A	404[B]	65/65	0.96	0.07	37,44,66,71	65
23	CLA	B	602	65/65	0.96	0.07	46,56,71,88	0
25	BCR	B	617	40/40	0.96	0.06	42,54,65,65	0
23	CLA	C	504	65/65	0.96	0.06	48,61,73,83	0
37	CA	C	524	1/1	0.96	0.05	74,74,74,74	0
23	CLA	b	602	65/65	0.96	0.07	48,60,82,91	0
23	CLA	b	603	65/65	0.96	0.07	46,57,82,94	0
25	BCR	C	516	40/40	0.96	0.06	51,64,76,88	0
23	CLA	b	604	65/65	0.96	0.07	39,51,100,123	0
23	CLA	b	605	65/65	0.96	0.07	39,52,73,84	0
23	CLA	d	402[B]	65/65	0.97	0.07	40,46,81,96	65
23	CLA	B	604	65/65	0.97	0.06	39,48,115,134	0
24	PHO	A	407[A]	64/64	0.97	0.05	39,47,55,58	64
24	PHO	A	407[B]	64/64	0.97	0.05	38,47,55,58	64

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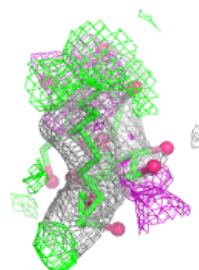
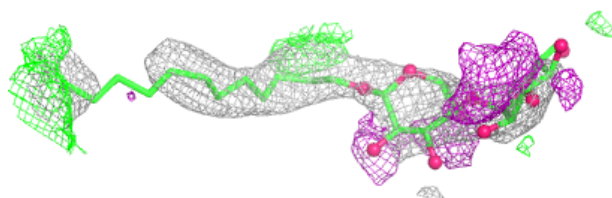
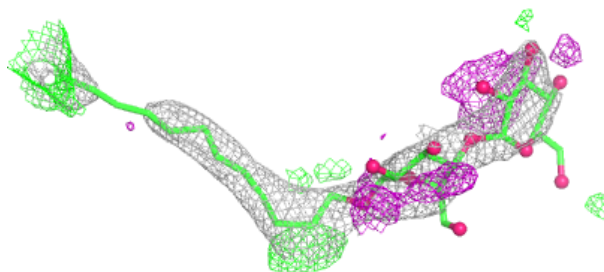
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	b	610	65/65	0.97	0.07	46,57,68,77	0
23	CLA	a	404[A]	65/65	0.97	0.06	41,47,67,78	65
23	CLA	a	404[B]	65/65	0.97	0.06	41,47,68,78	65
23	CLA	a	405[A]	65/65	0.97	0.05	40,46,68,74	65
23	CLA	a	405[B]	65/65	0.97	0.05	40,46,68,74	65
23	CLA	b	615	65/65	0.97	0.06	47,62,87,96	0
23	CLA	B	612	65/65	0.97	0.06	37,50,64,68	0
23	CLA	B	605	65/65	0.97	0.06	41,49,68,84	0
23	CLA	c	503	65/65	0.97	0.07	46,59,95,113	0
22	CL	a	402[A]	1/1	0.97	0.06	49,49,49,49	1
23	CLA	B	615	65/65	0.97	0.06	44,54,82,92	0
23	CLA	C	511	65/65	0.97	0.06	48,59,82,90	0
22	CL	a	402[B]	1/1	0.97	0.06	49,49,49,49	1
23	CLA	B	608	65/65	0.97	0.05	42,52,72,79	0
23	CLA	C	503	65/65	0.97	0.06	46,54,84,94	0
23	CLA	c	510	65/65	0.97	0.08	46,63,92,102	0
23	CLA	c	511	65/65	0.97	0.06	49,64,81,98	0
37	CA	O	301	1/1	0.97	0.04	105,105,105,105	0
22	CL	A	403[A]	1/1	0.97	0.04	47,47,47,47	1
22	CL	A	403[B]	1/1	0.97	0.04	47,47,47,47	1
23	CLA	b	608	65/65	0.97	0.06	43,58,85,97	0
23	CLA	d	402[A]	65/65	0.97	0.07	40,46,81,95	65
22	CL	A	402[A]	1/1	0.98	0.05	44,44,44,44	1
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	0.07	52,52,52,52	1
38	HEM	F	102	43/43	0.98	0.06	52,68,80,88	0
38	HEM	f	101	43/43	0.98	0.08	56,82,118,130	0
39	MG	J	102	1/1	0.98	0.03	60,60,60,60	0
39	MG	j	102	1/1	0.98	0.07	64,64,64,64	0
22	CL	a	403[B]	1/1	0.98	0.07	52,52,52,52	1
40	HEC	v	201	43/43	0.98	0.07	47,61,69,71	0
37	CA	c	524	1/1	0.99	0.03	77,77,77,77	0
21	FE2	A	401[B]	1/1	0.99	0.02	52,52,52,52	1
21	FE2	a	401[A]	1/1	0.99	0.03	54,54,54,54	1
21	FE2	a	401[B]	1/1	0.99	0.03	55,55,55,55	1
28	OEX	A	413[A]	10/10	0.99	0.03	40,45,49,49	10
28	OEX	A	413[B]	10/10	0.99	0.03	39,44,49,50	10
28	OEX	a	412[A]	10/10	0.99	0.03	46,49,51,55	10
28	OEX	a	412[B]	10/10	0.99	0.03	45,50,51,55	10
21	FE2	A	401[A]	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.

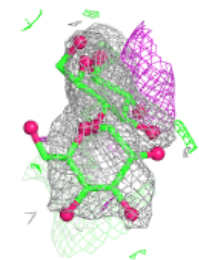
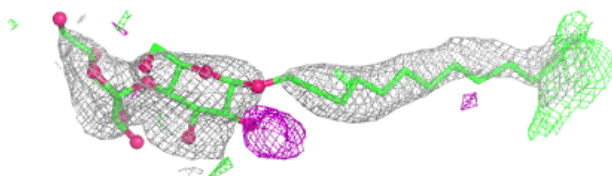
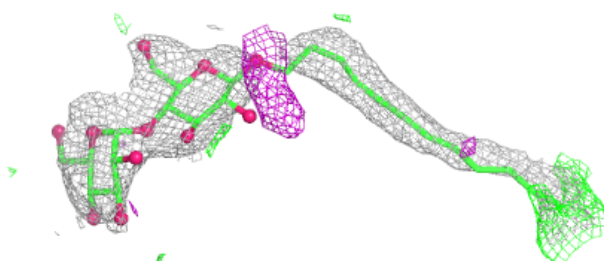
Electron density around LMT B 628:

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



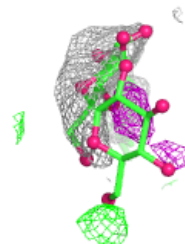
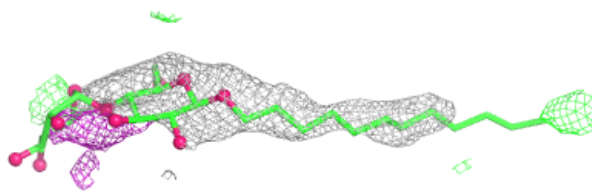
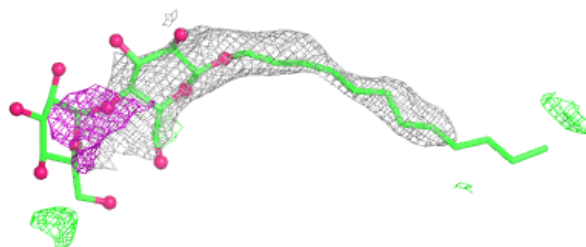
Electron density around LMT D 401:

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

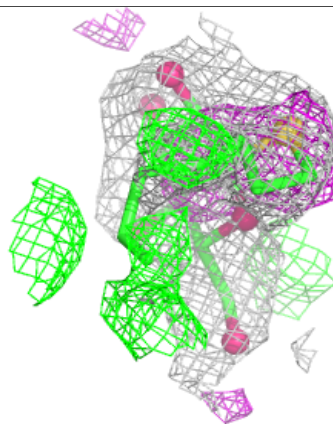
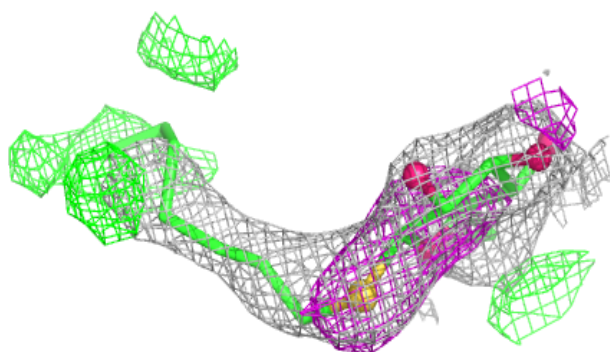
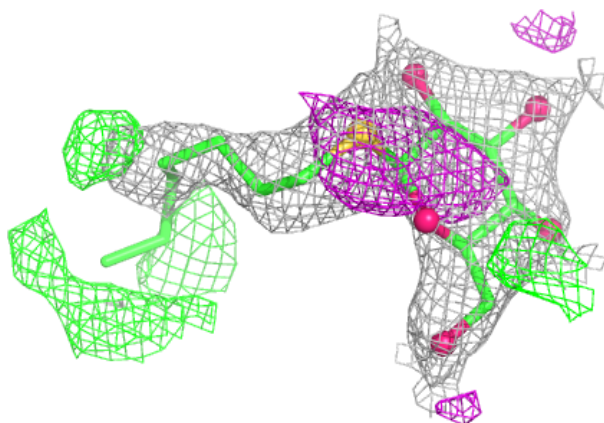


Electron density around LMT F 101:

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

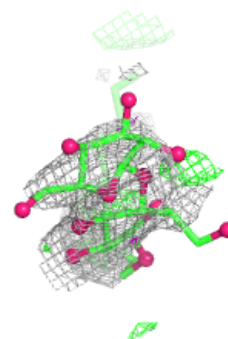
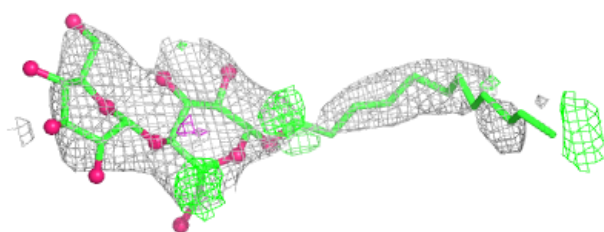
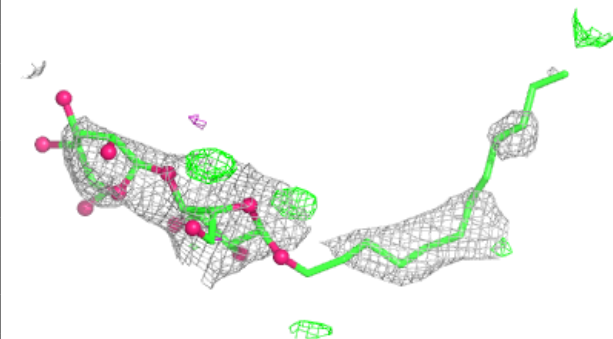
**Electron density around HTG B 621:**

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

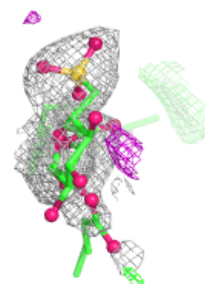
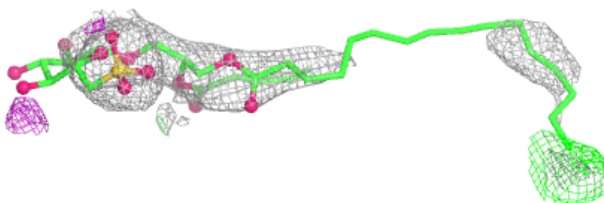
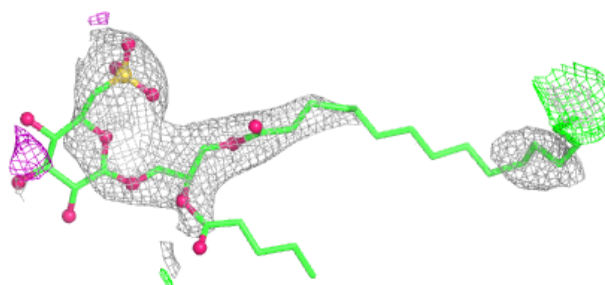


Electron density around LMT A 420:

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

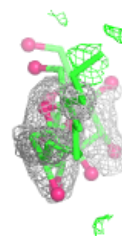
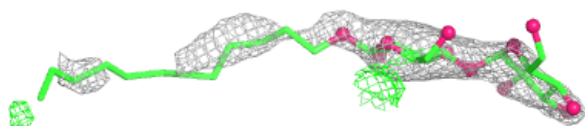
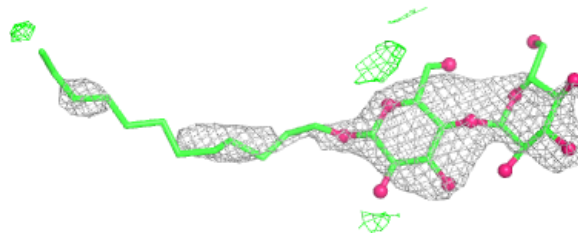
**Electron density around SQD f 102:**

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

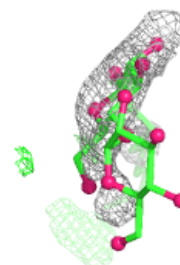
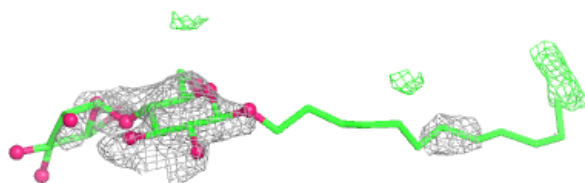
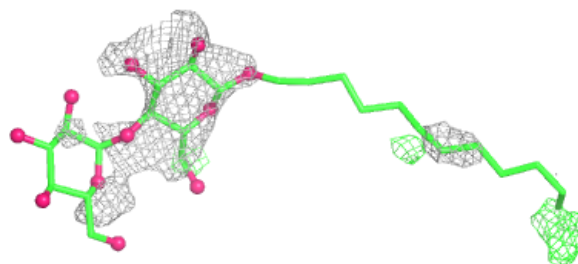


Electron density around LMT a 416:

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

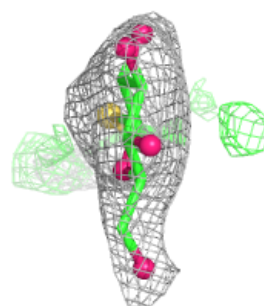
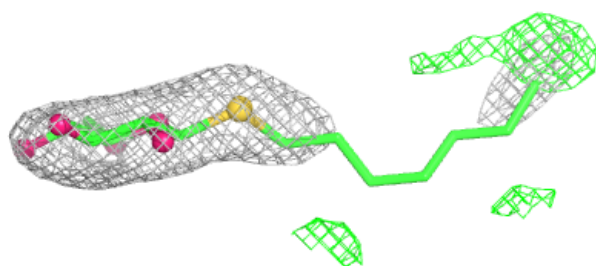
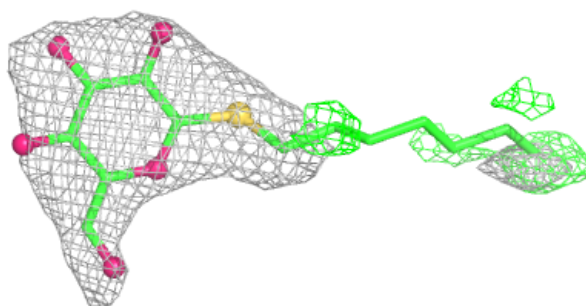
**Electron density around LMT e 101:**

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

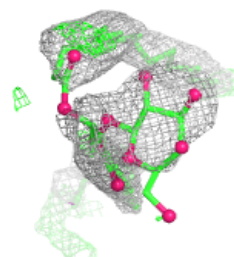
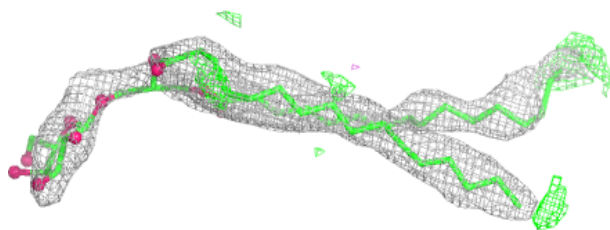
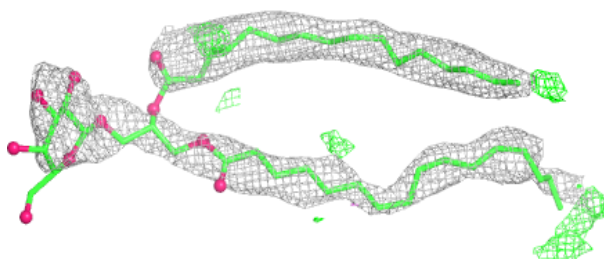


Electron density around HTG C 522:

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

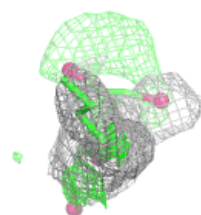
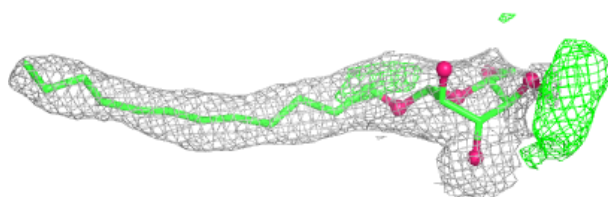
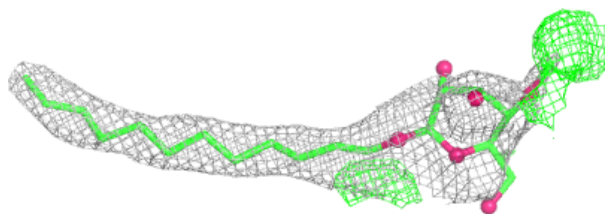
**Electron density around LMG C 521:**

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

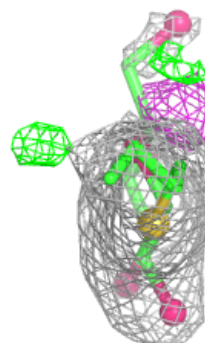
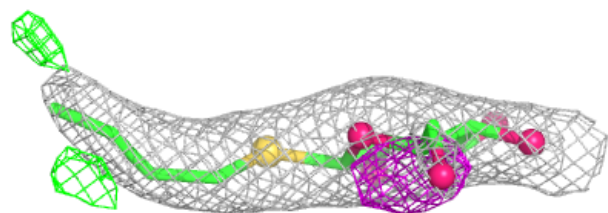
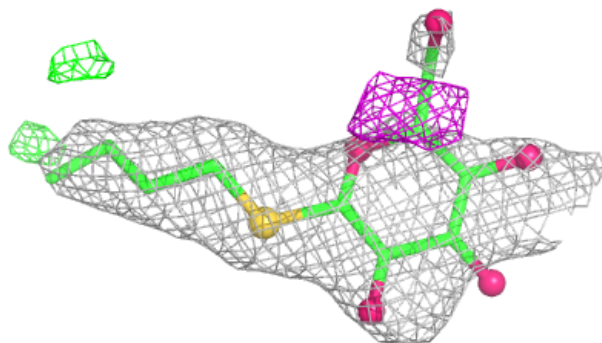


Electron density around LMT b 621:

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

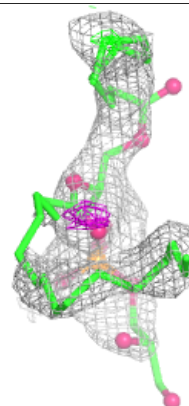
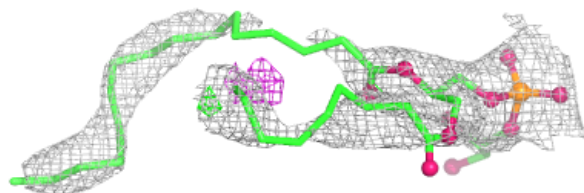
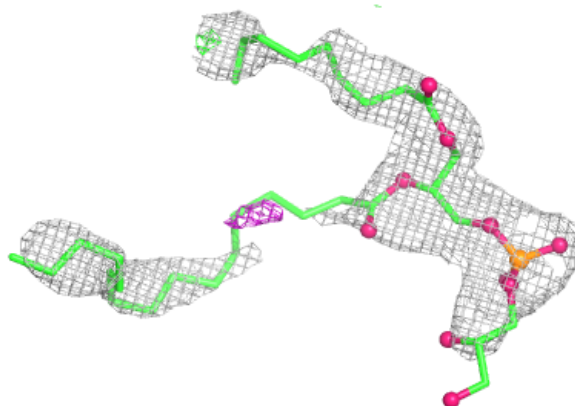
**Electron density around HTG D 410:**

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

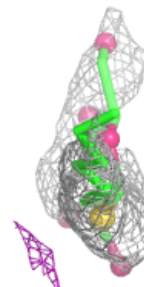
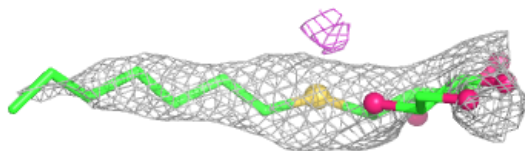
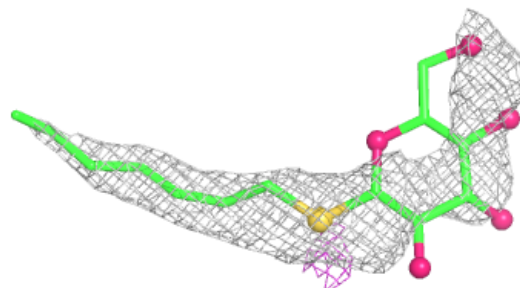


Electron density around LHG a 419 (A):

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

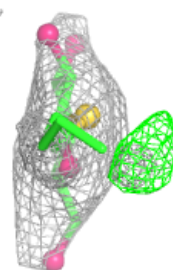
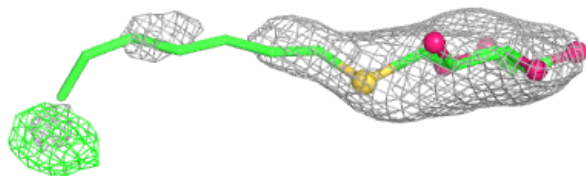
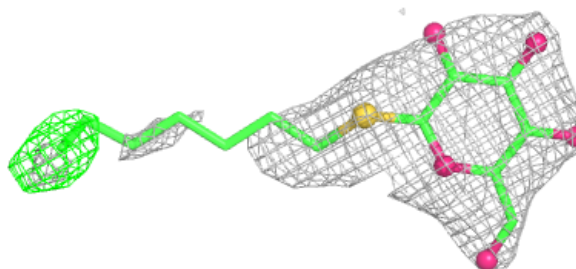
**Electron density around HTG b 623:**

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

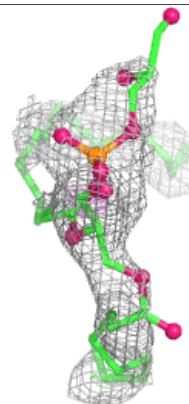
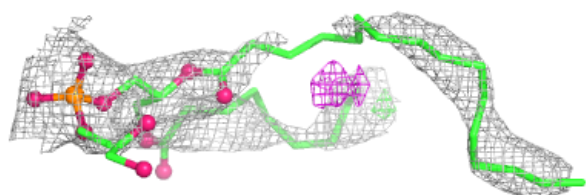
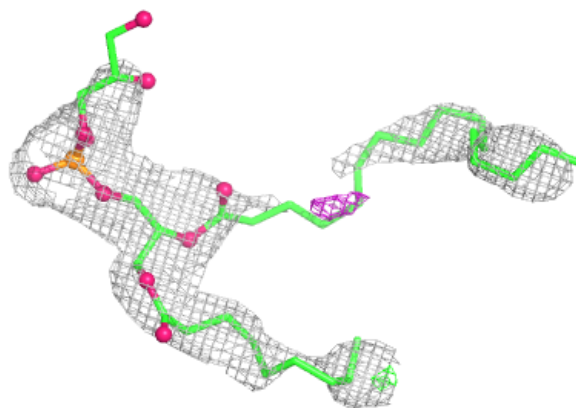


Electron density around HTG c 522:

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

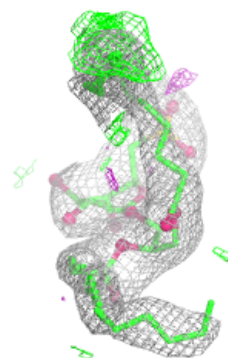
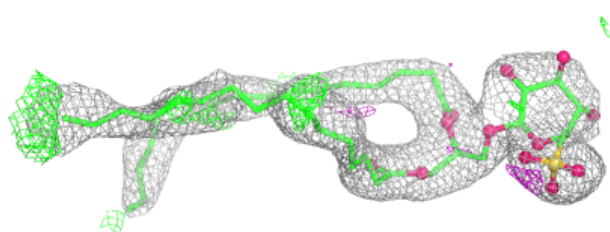
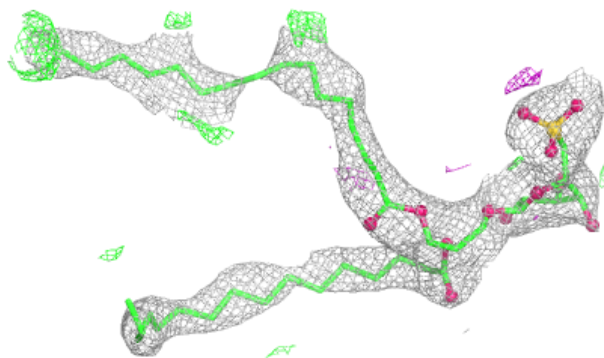
**Electron density around LHG a 419 (B):**

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

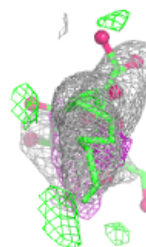
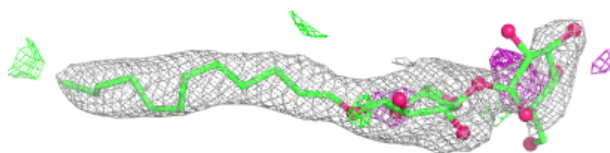
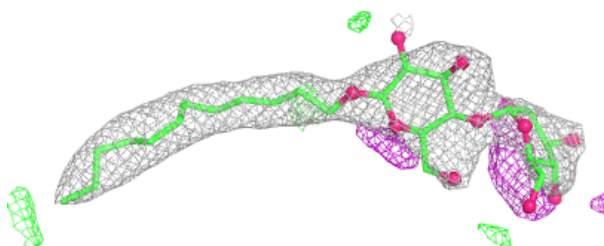


Electron density around SQD a 411:

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

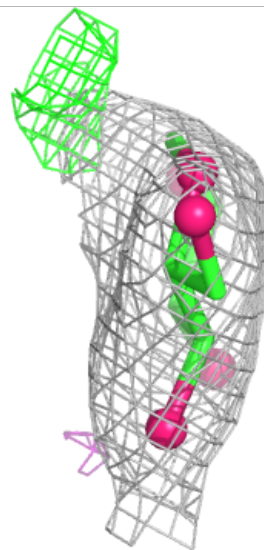
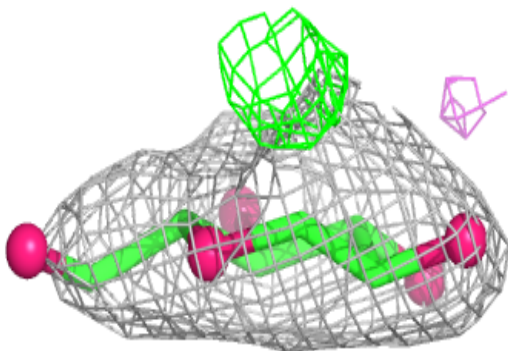
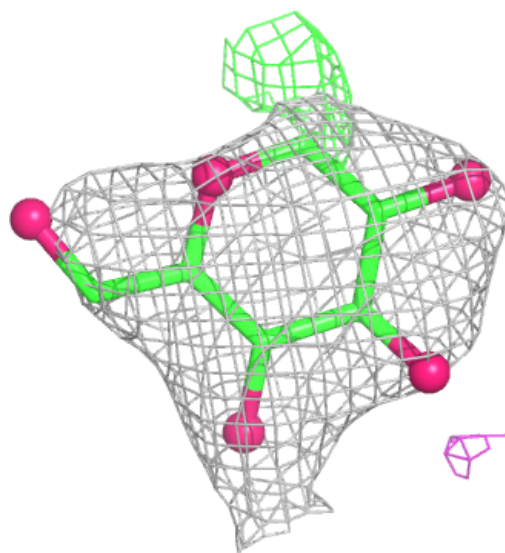
**Electron density around LMT B 626:**

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



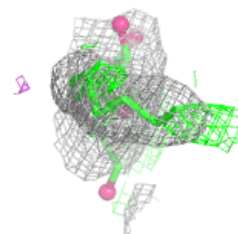
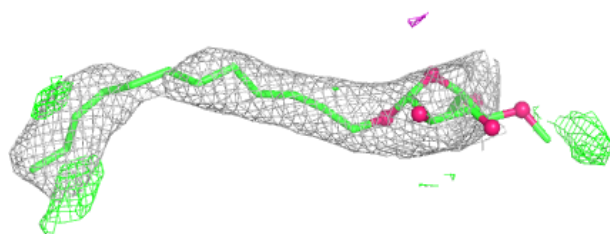
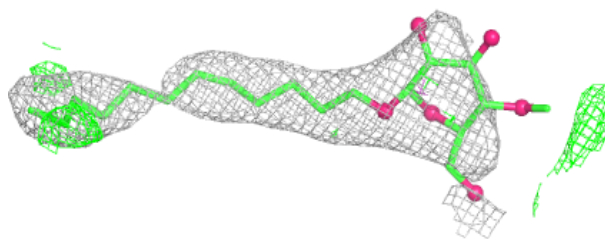
Electron density around HTG V 202:

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



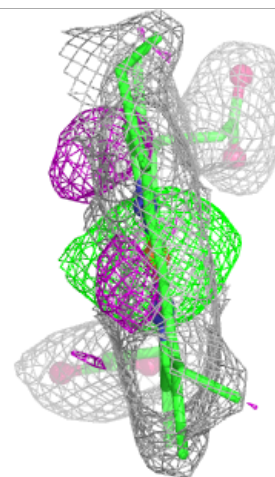
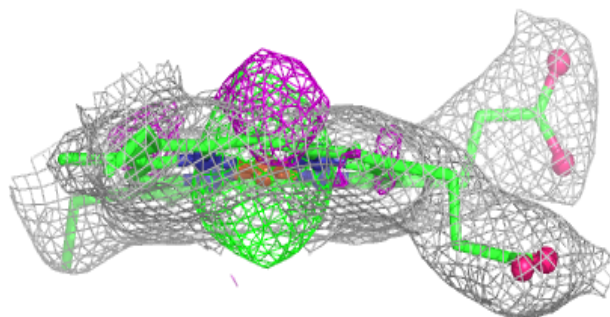
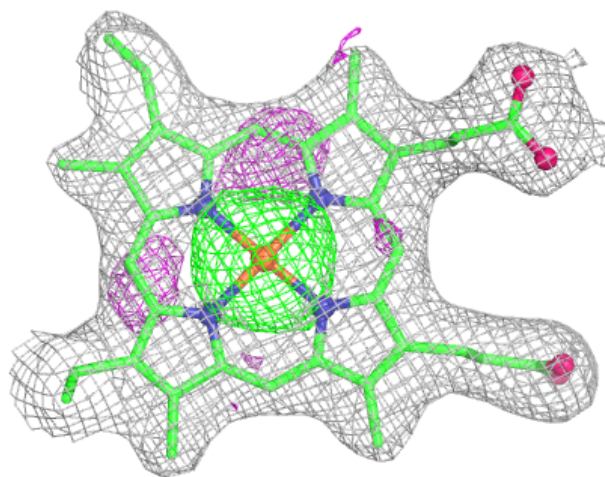
Electron density around LMT B 629:

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



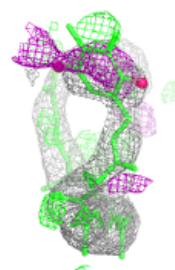
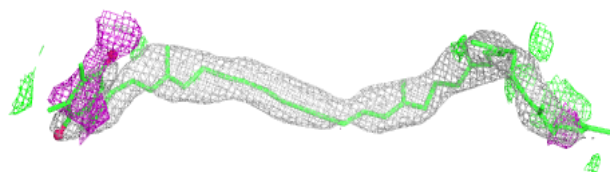
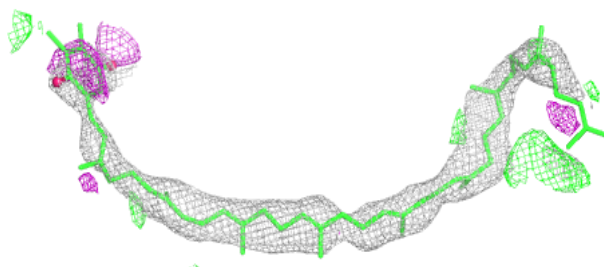
Electron density around HEC V 201:

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

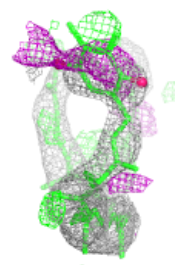
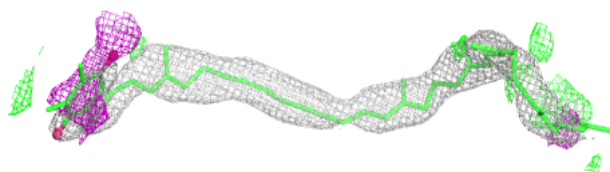
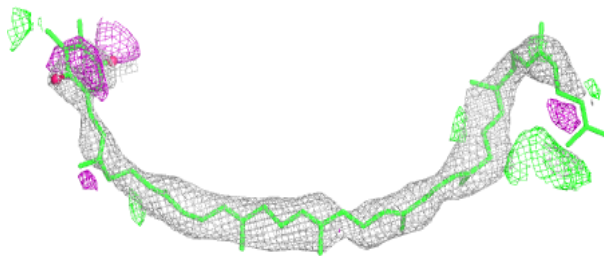


Electron density around PL9 A 414 (A):

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

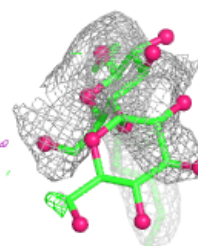
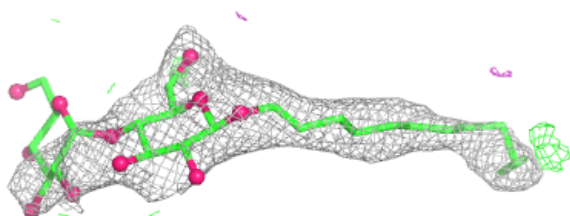
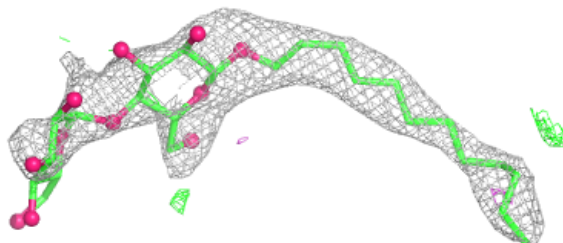
**Electron density around PL9 A 414 (B):**

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

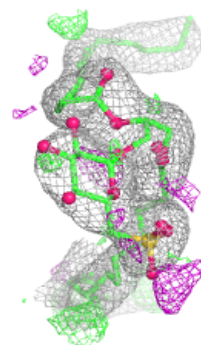
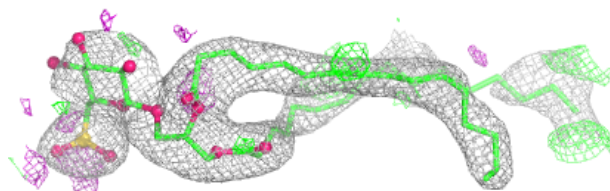
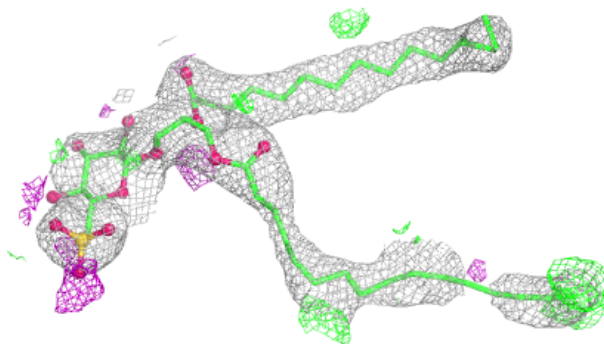


Electron density around LMT T 101:

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

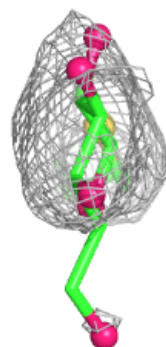
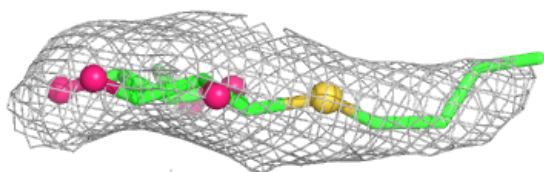
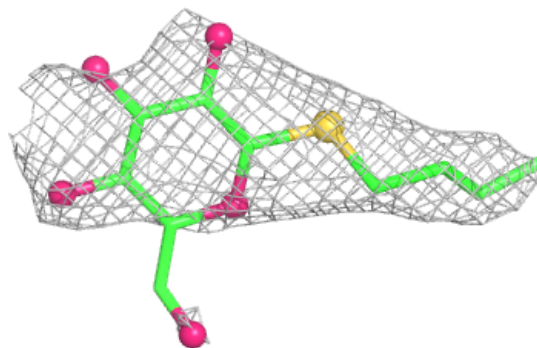
**Electron density around SQD A 412:**

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

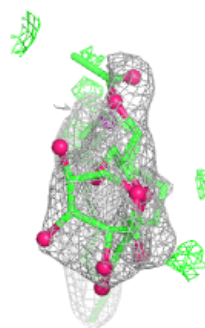
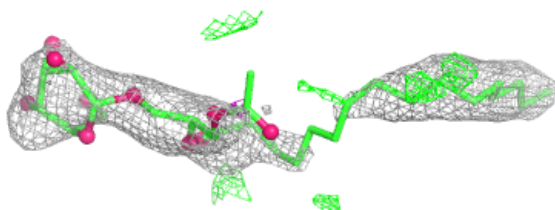
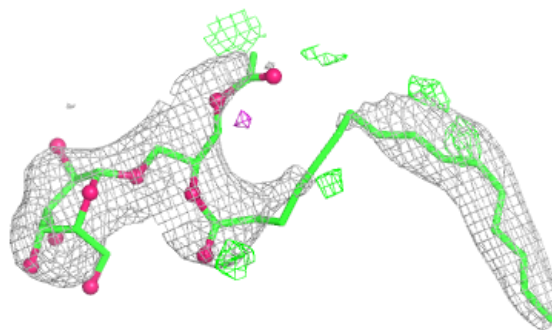


Electron density around HTG d 409:

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

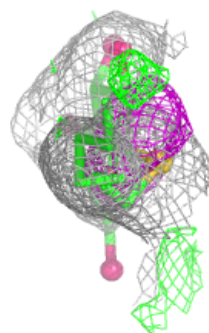
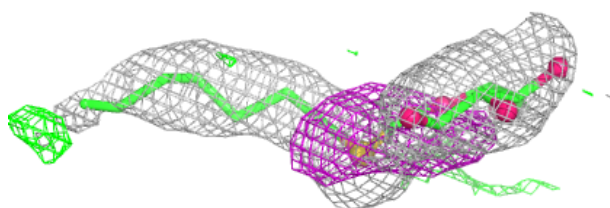
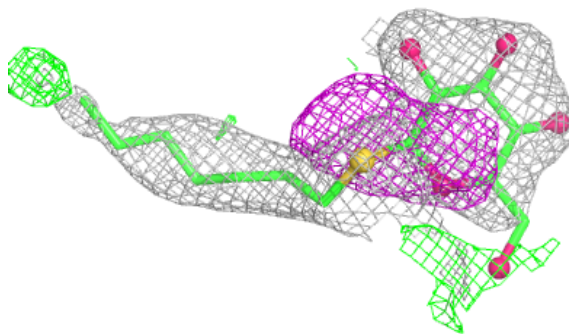
**Electron density around LMG Z 101:**

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

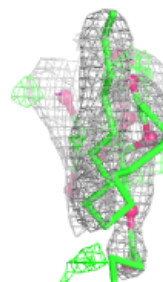
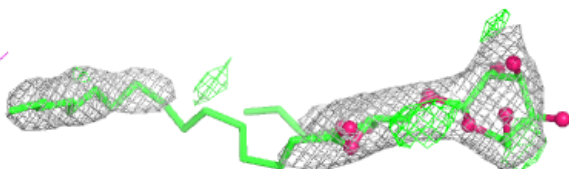
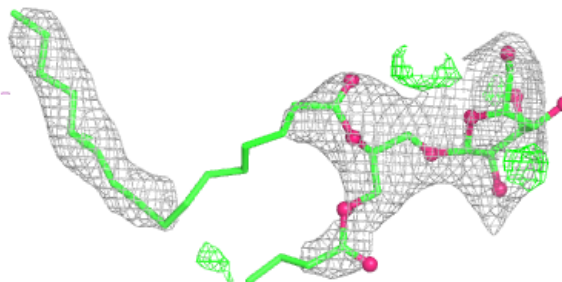


Electron density around HTG b 622:

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

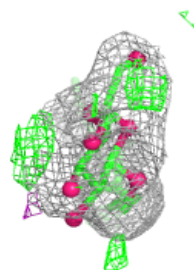
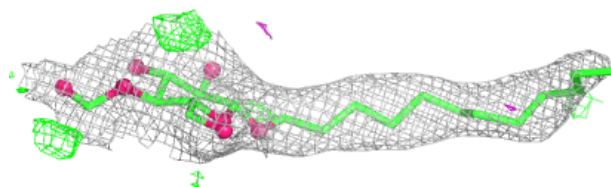
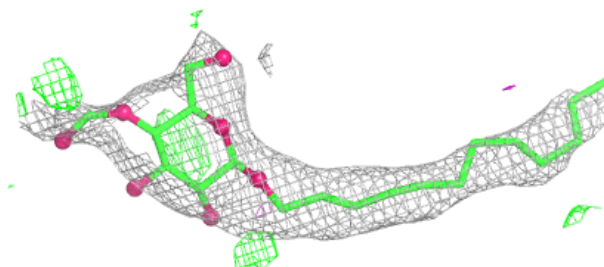
**Electron density around LMG z 101:**

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

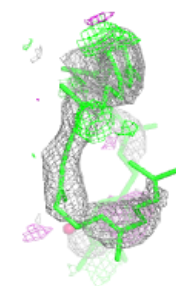
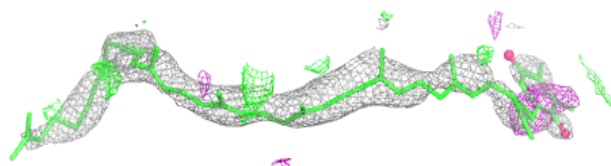
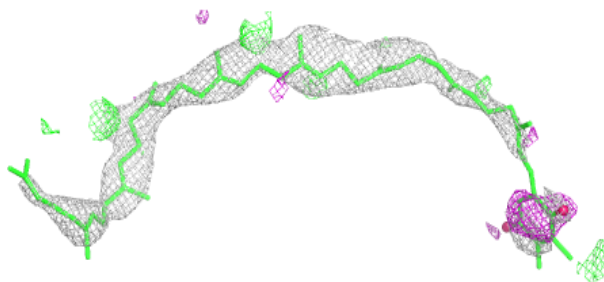


Electron density around LMT t 101:

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

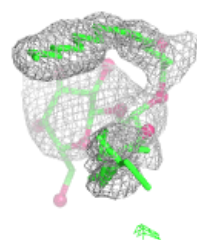
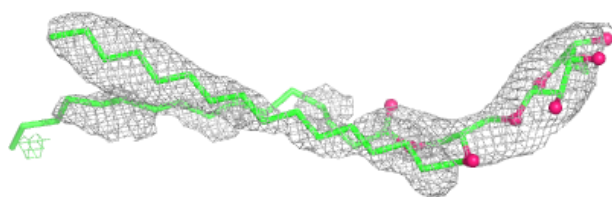
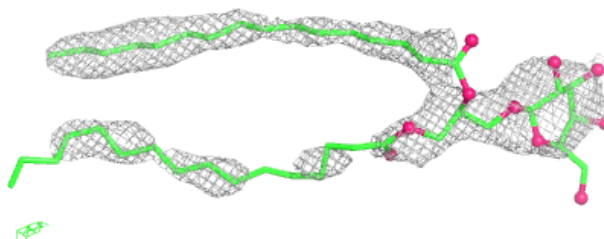
**Electron density around PL9 a 413 (A):**

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

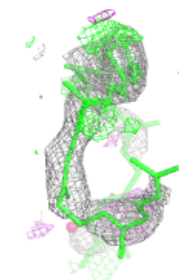
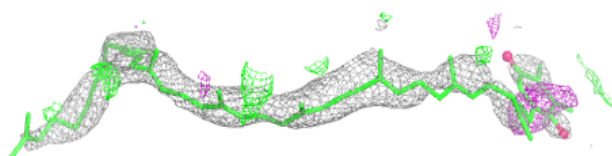
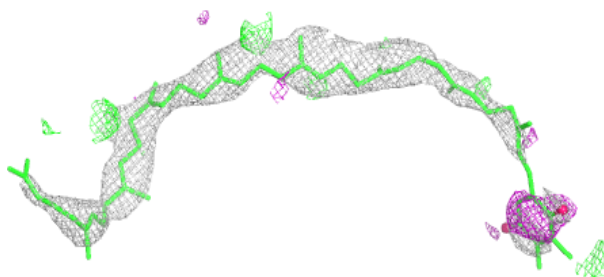


Electron density around LMG c 521:

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

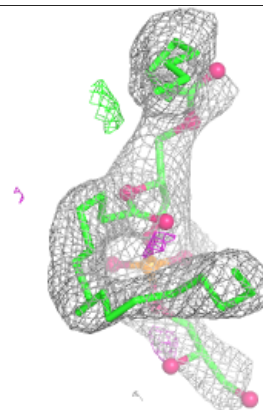
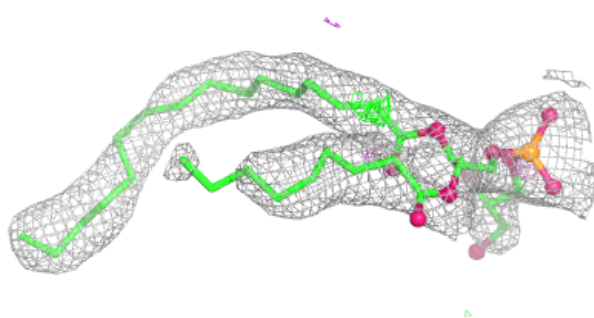
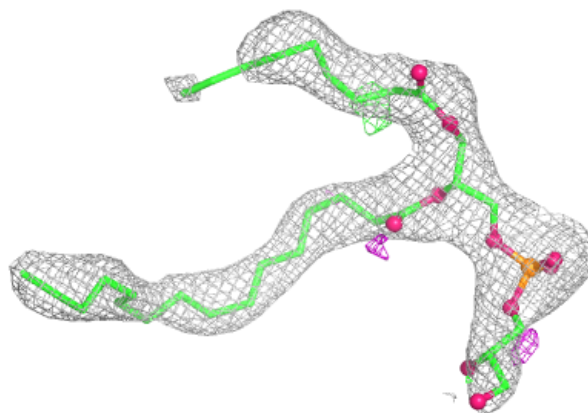
**Electron density around PL9 a 413 (B):**

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

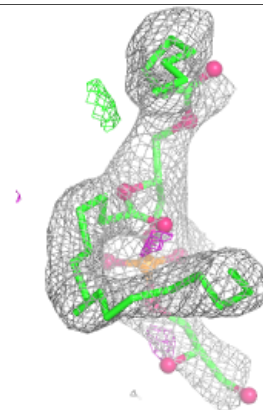
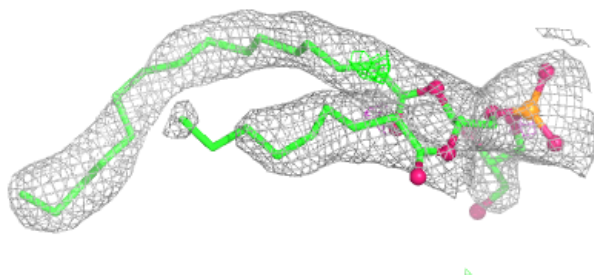
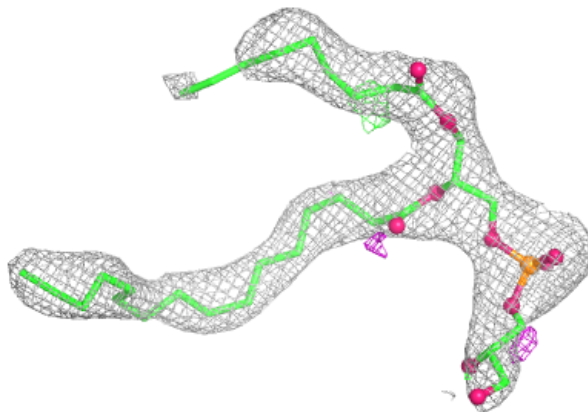


Electron density around LHG E 101 (A):

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

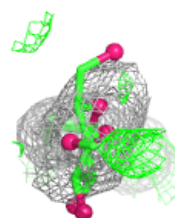
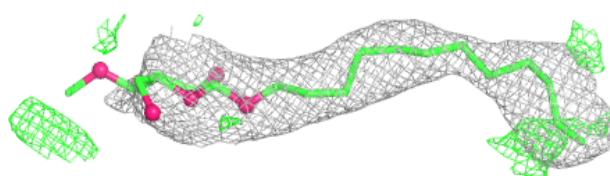
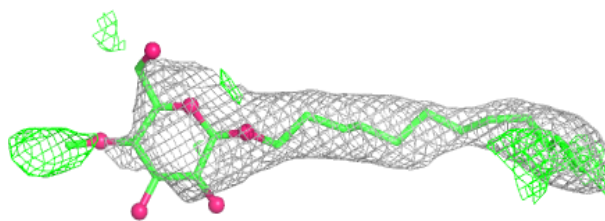
**Electron density around LHG E 101 (B):**

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

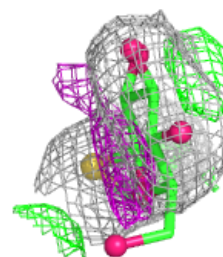
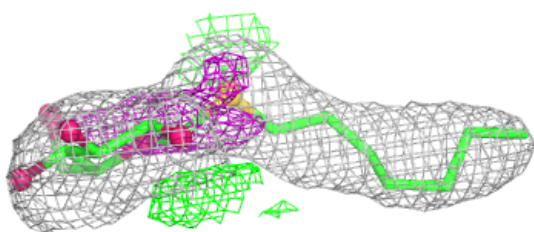
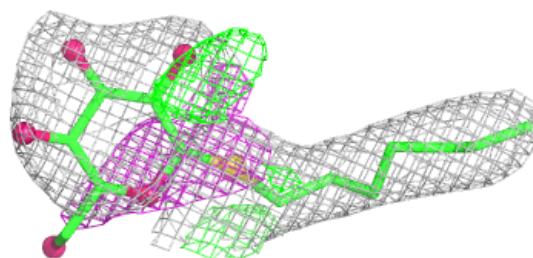


Electron density around LMT b 627:

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

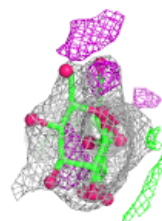
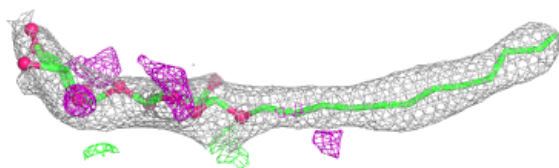
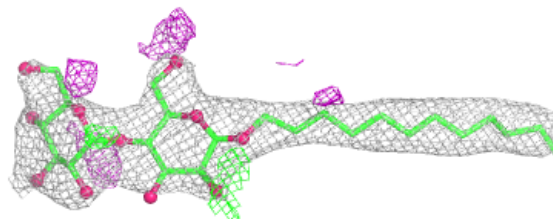
**Electron density around HTG o 301:**

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

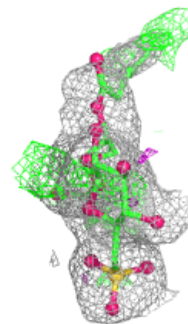
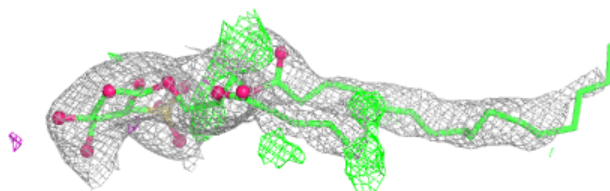
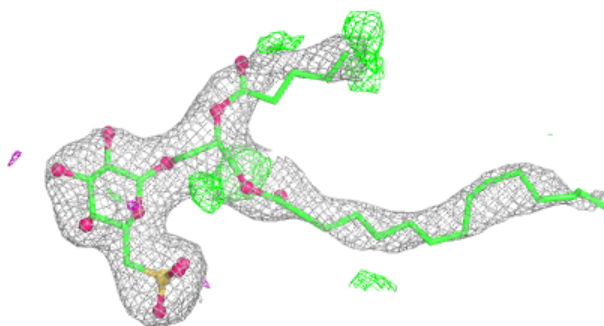


Electron density around LMT m 103:

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

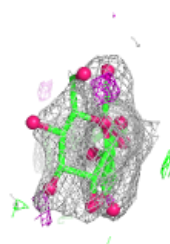
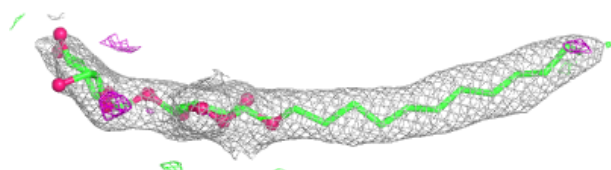
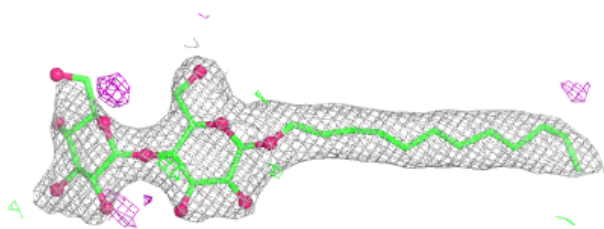
**Electron density around SQD F 103:**

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

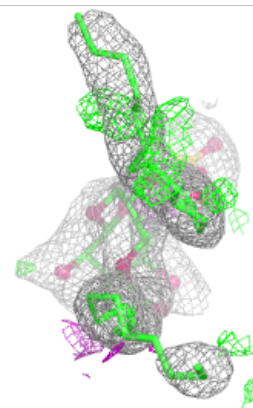
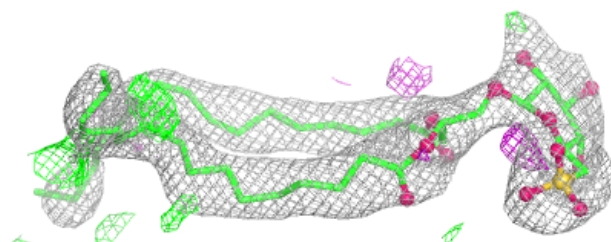
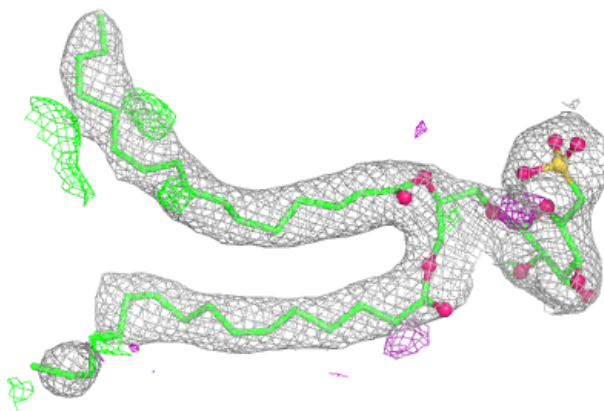


Electron density around LMT M 101:

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

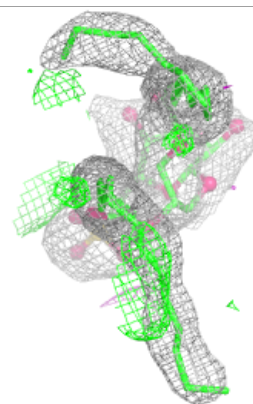
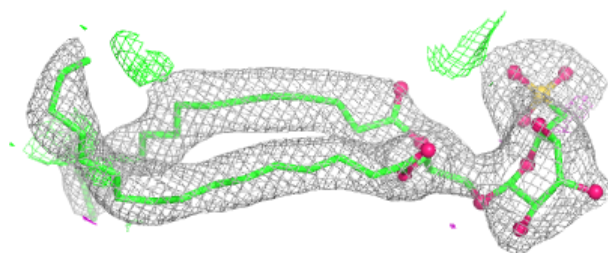
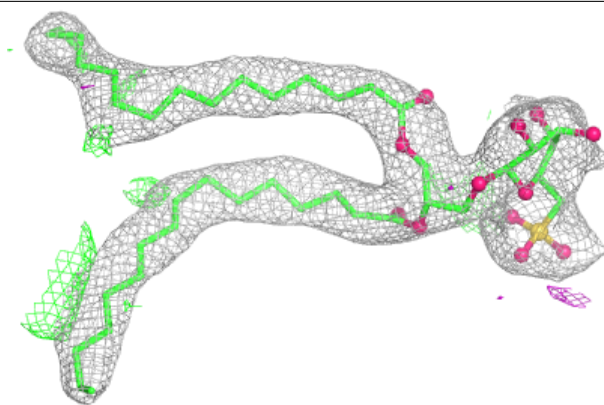
**Electron density around SQD b 620:**

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



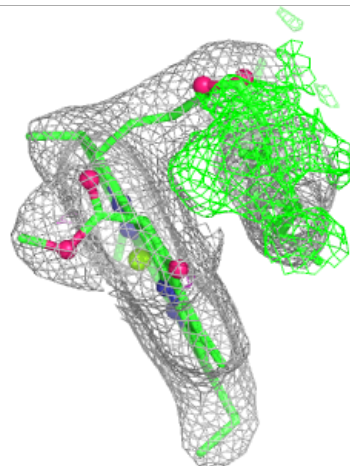
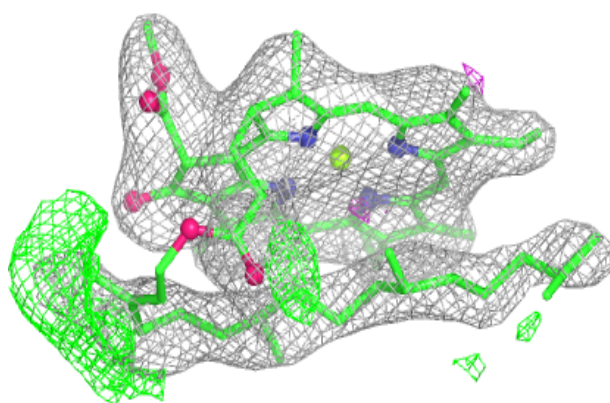
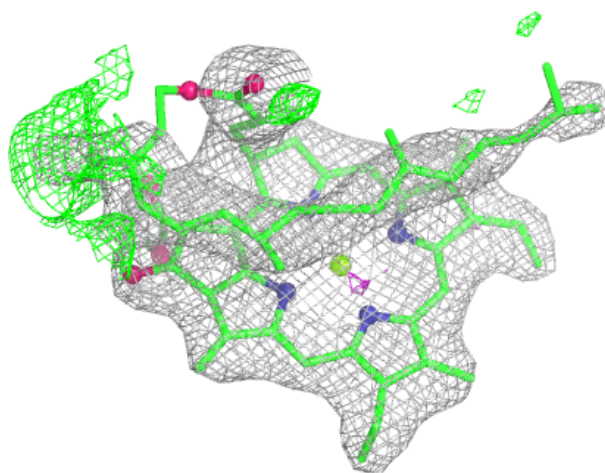
Electron density around SQD L 101:

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



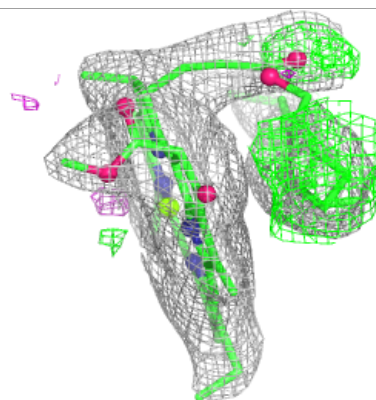
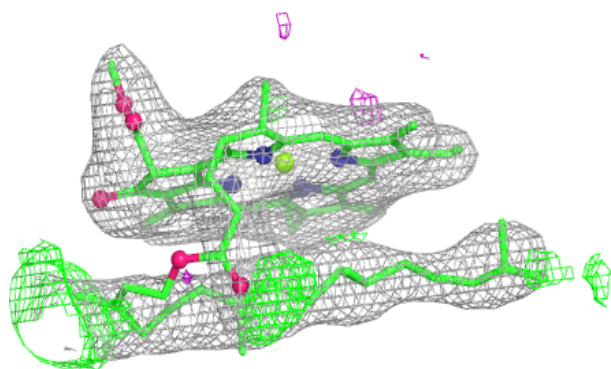
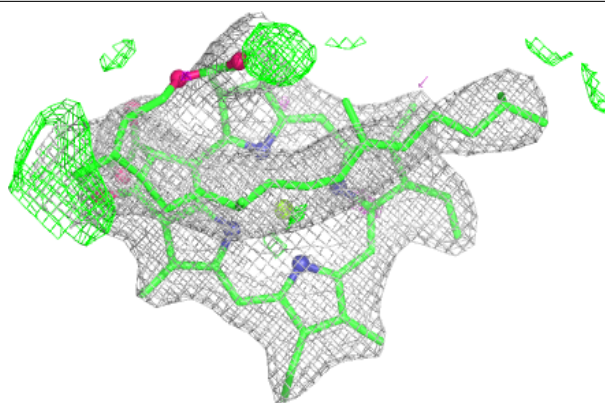
Electron density around CLA b 601:

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

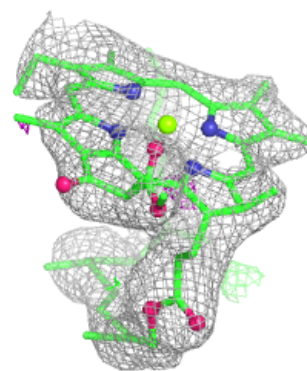
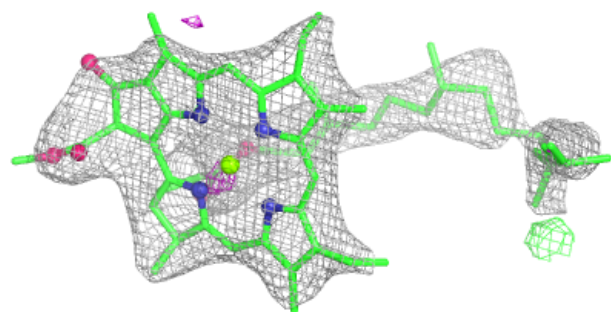
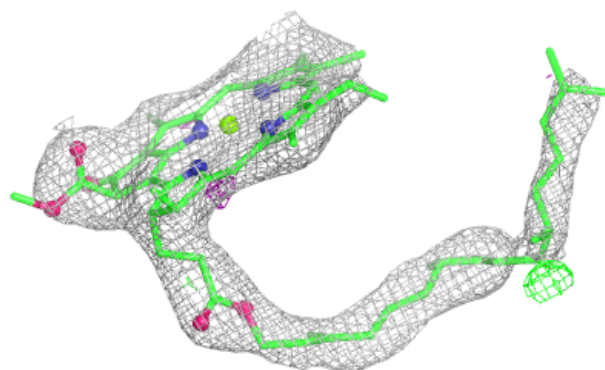


Electron density around CLA B 601:

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

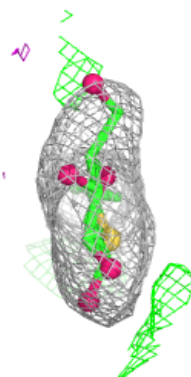
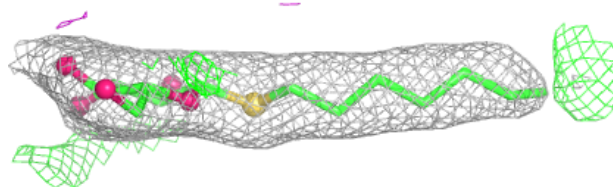
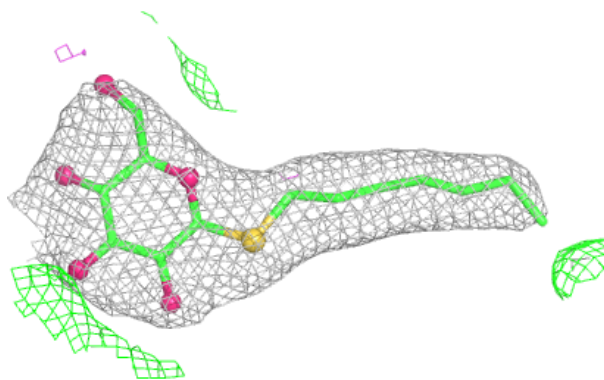
**Electron density around CLA c 514:**

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

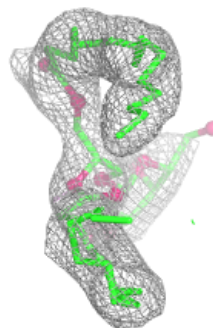
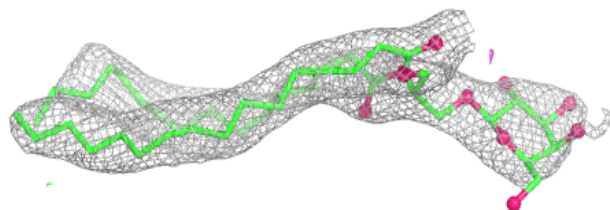
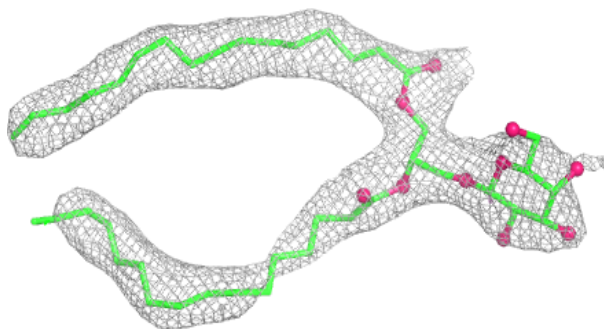


Electron density around HTG B 623:

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

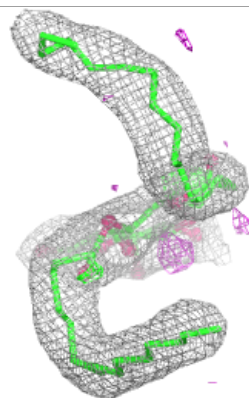
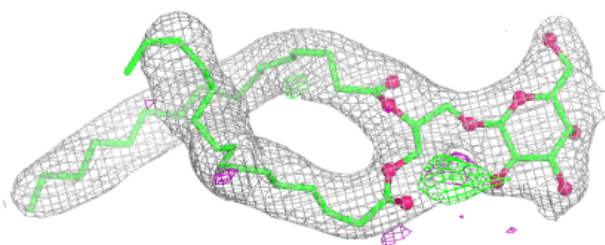
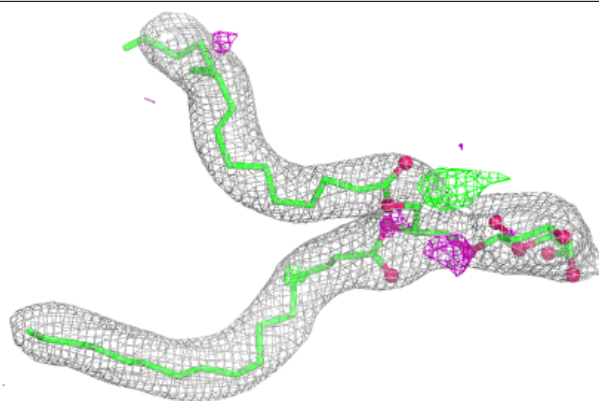
**Electron density around LMG c 501:**

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

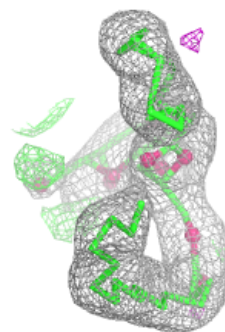
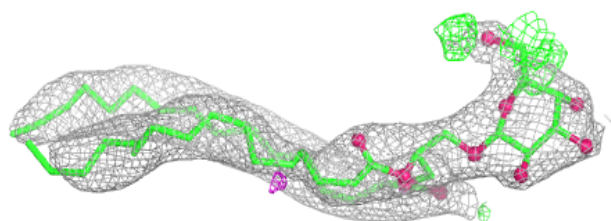
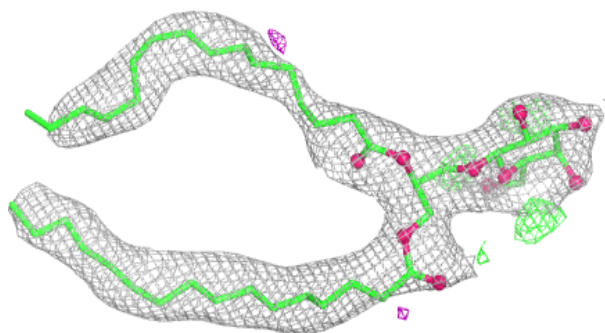


Electron density around LMG m 101:

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

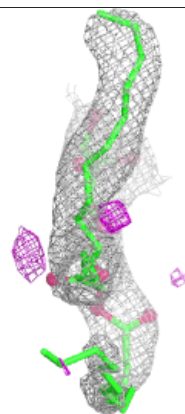
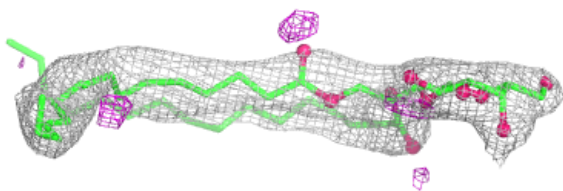
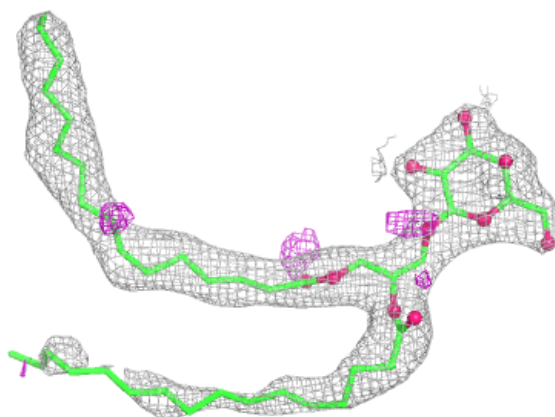
**Electron density around LMG C 501:**

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

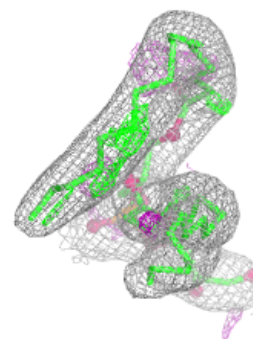
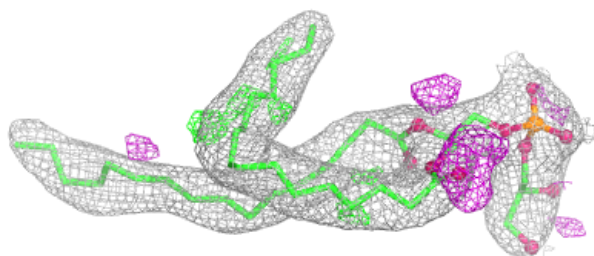
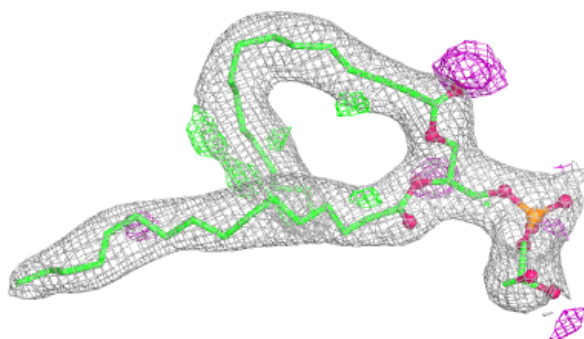


Electron density around LMG C 520:

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

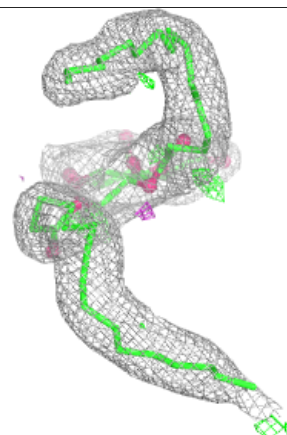
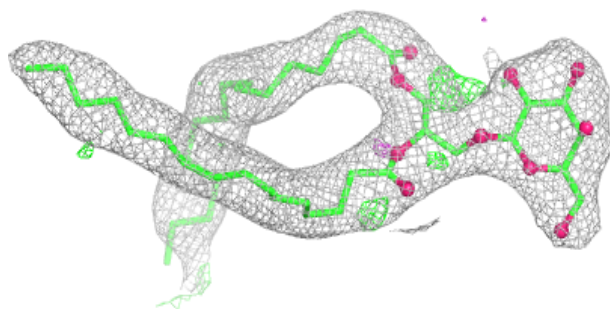
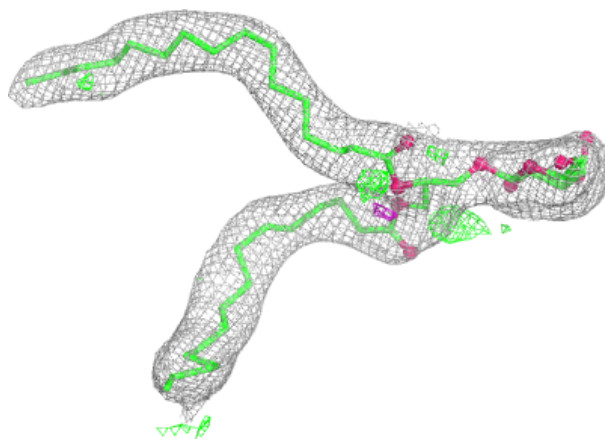
**Electron density around LHG A 419 (B):**

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



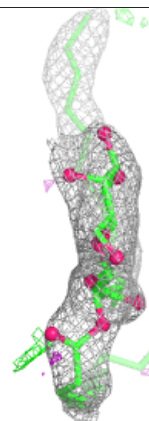
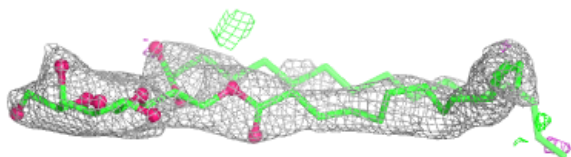
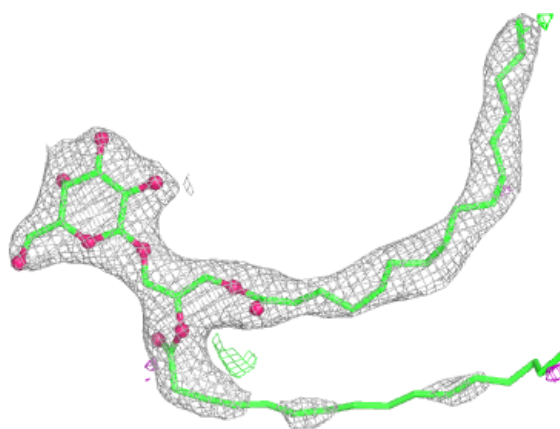
Electron density around LMG B 620:

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

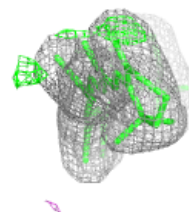
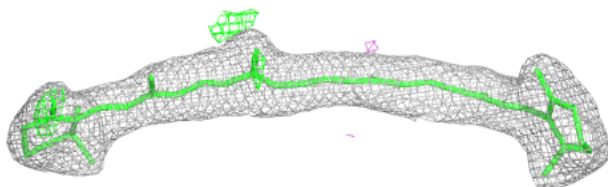
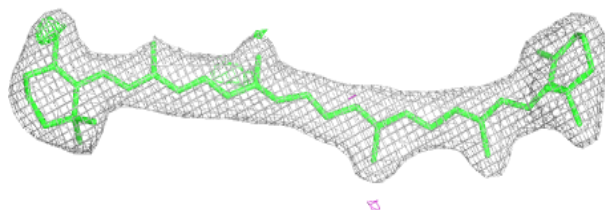


Electron density around LMG c 520:

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

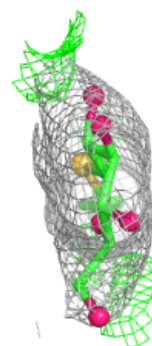
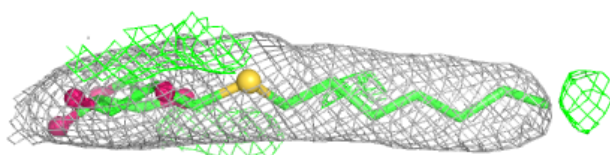
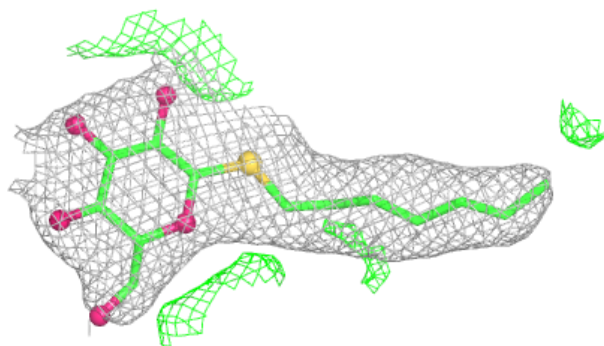
**Electron density around BCR T 102:**

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

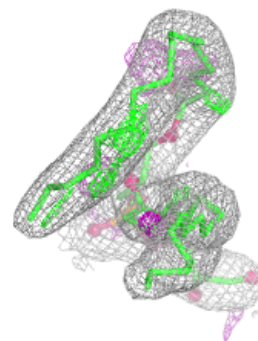
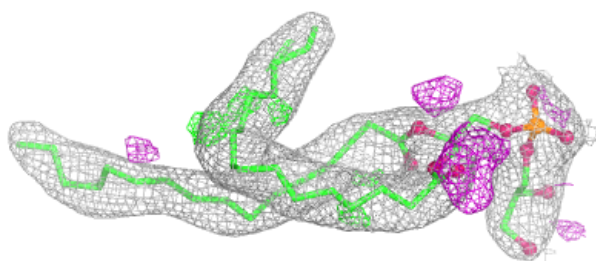
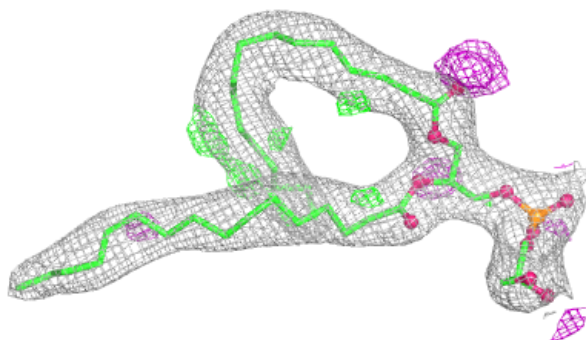


Electron density around HTG b 625:

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

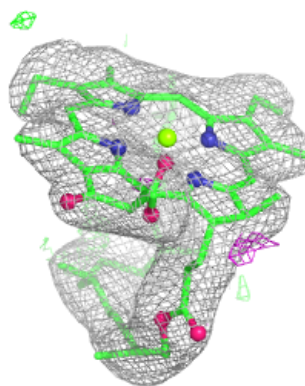
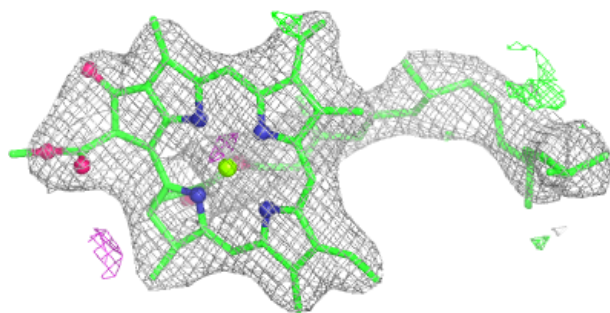
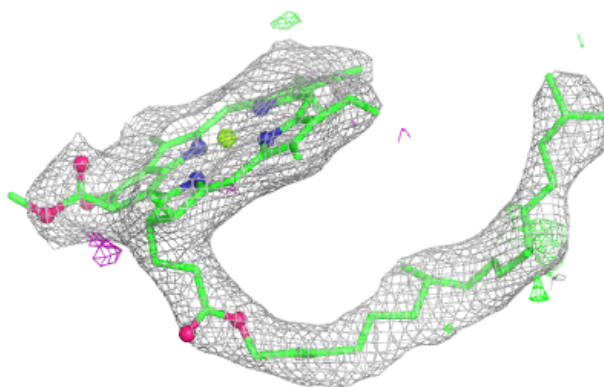
**Electron density around LHG A 419 (A):**

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

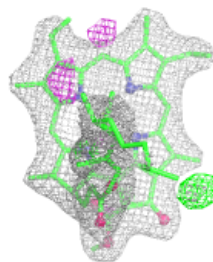
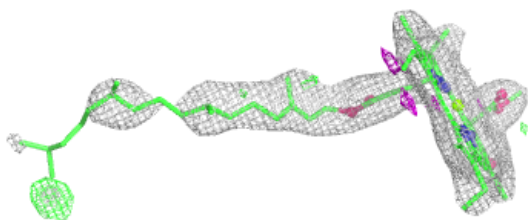
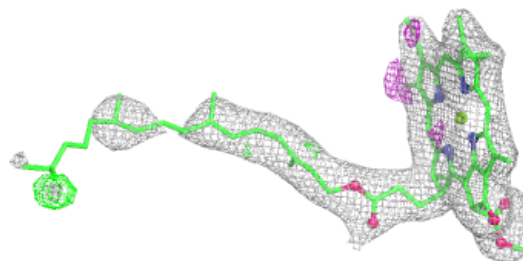


Electron density around CLA C 514:

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

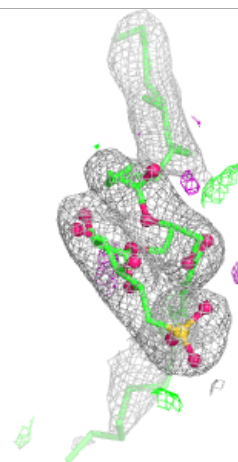
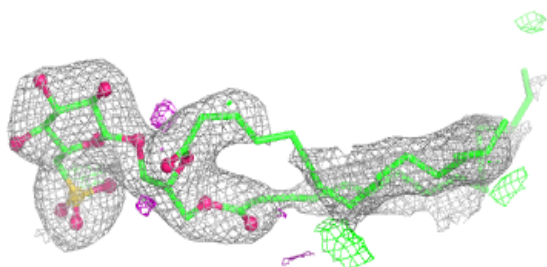
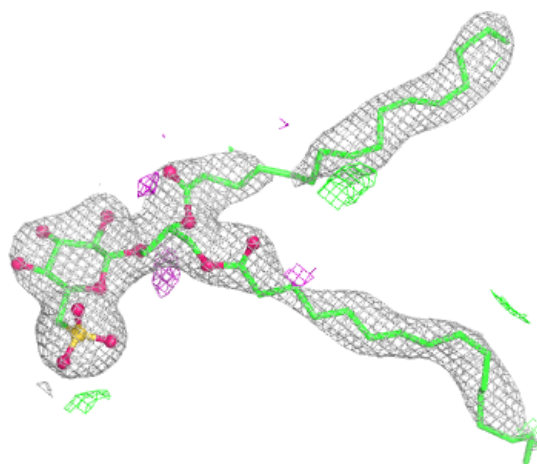
**Electron density around CLA d 403:**

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



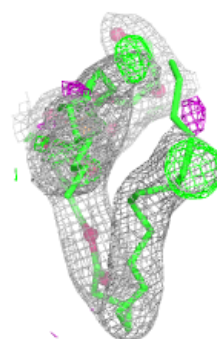
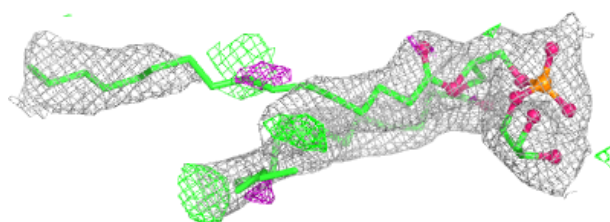
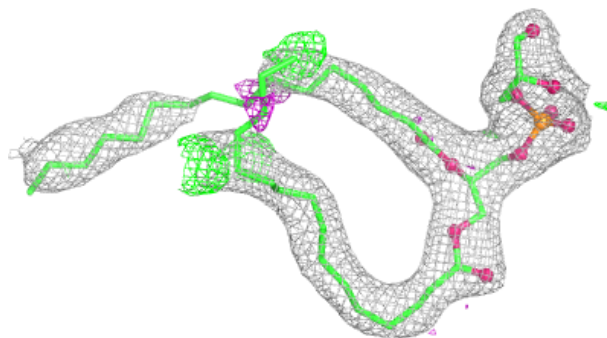
Electron density around SQD a 410 (A):

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

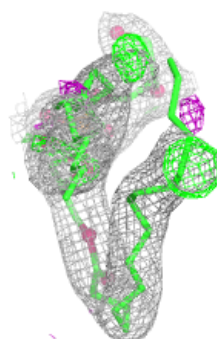
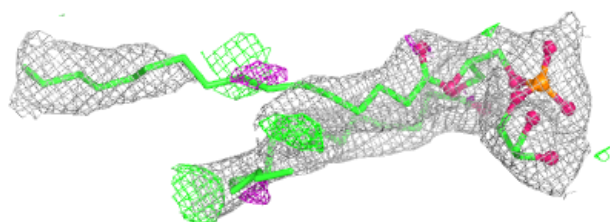
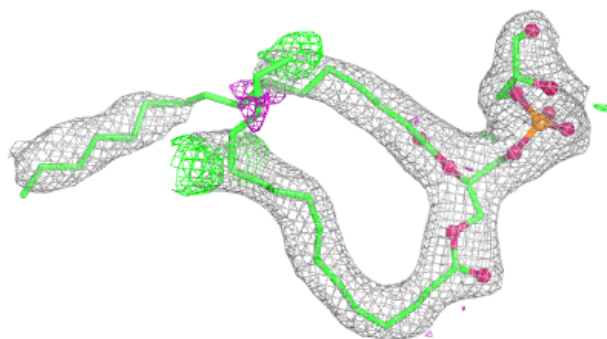


Electron density around LHG D 407 (A):

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

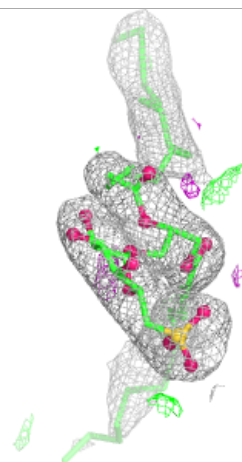
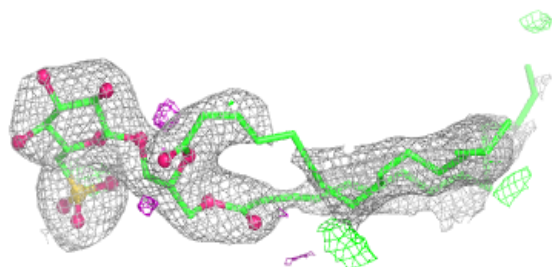
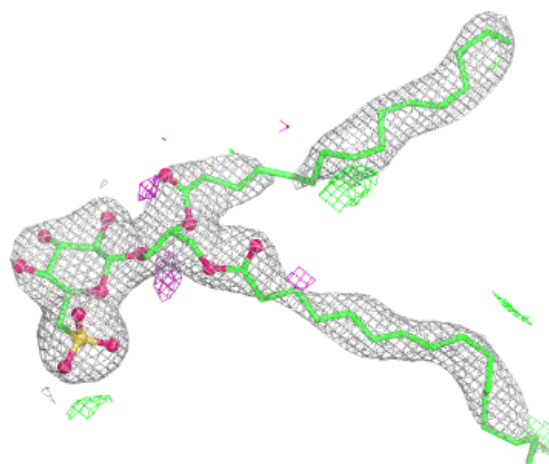
**Electron density around LHG D 407 (B):**

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



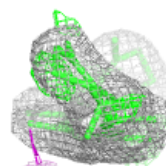
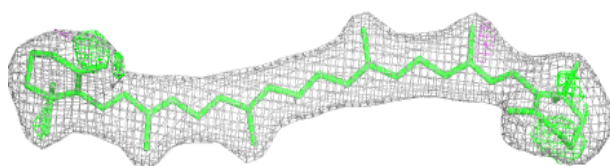
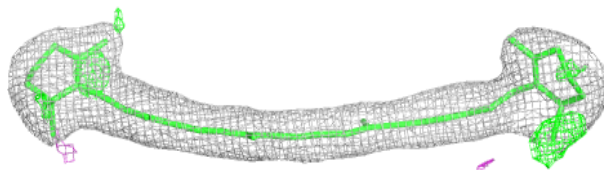
Electron density around SQD a 410 (B):

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

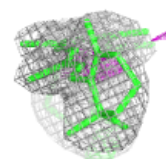
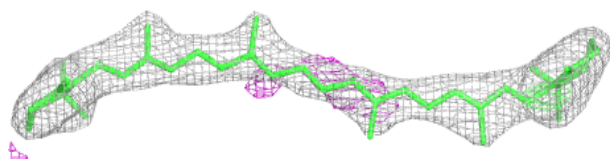
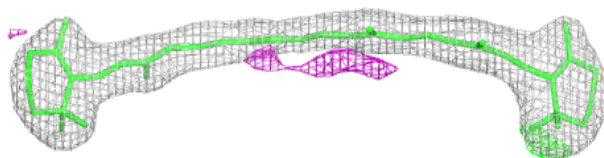


Electron density around BCR D 404:

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

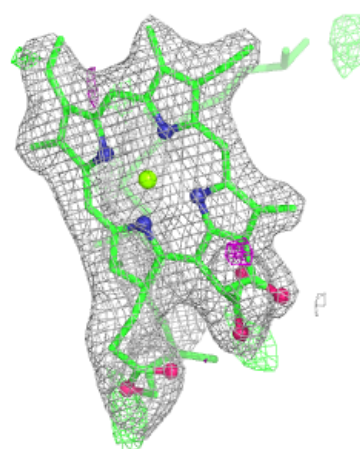
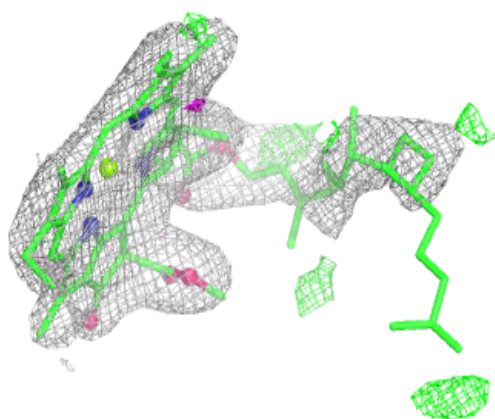
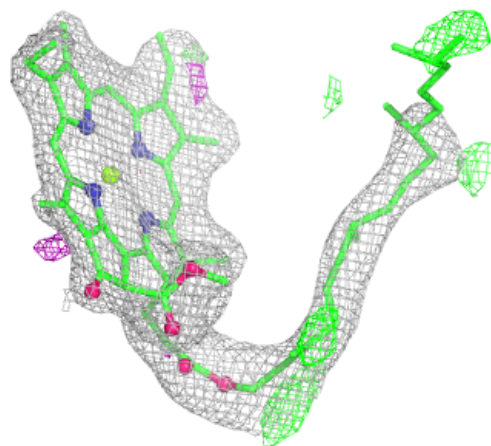
**Electron density around BCR K 102:**

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



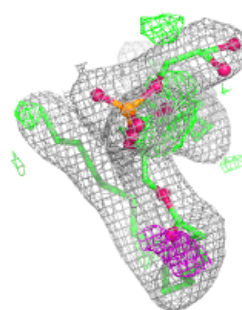
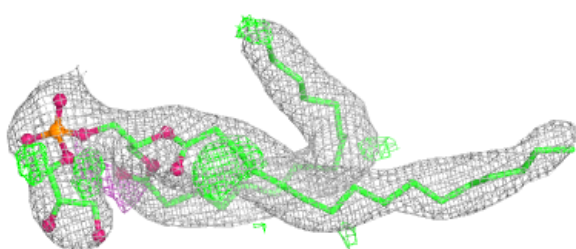
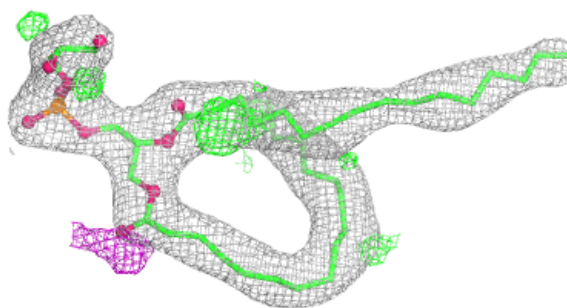
Electron density around CLA b 616:

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

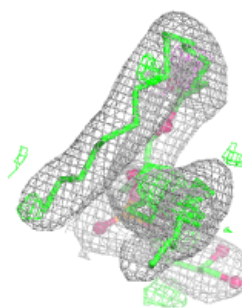
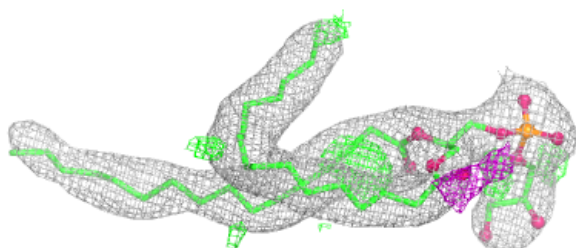
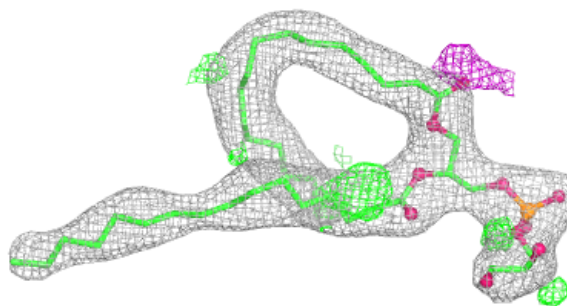


Electron density around LHG d 412 (A):

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

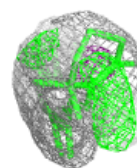
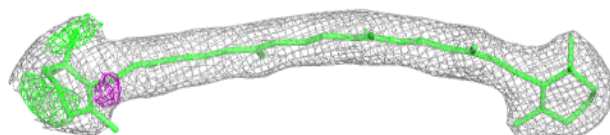
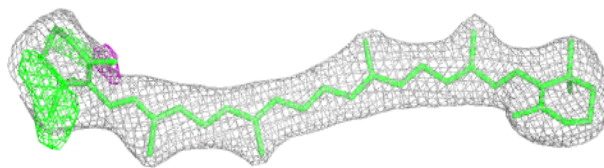
**Electron density around LHG d 412 (B):**

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

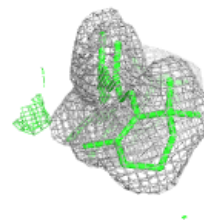
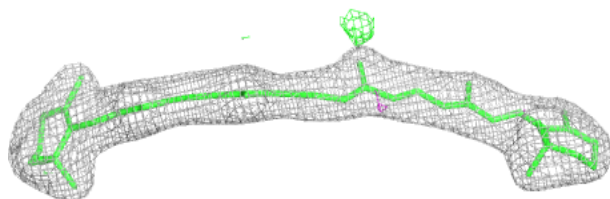
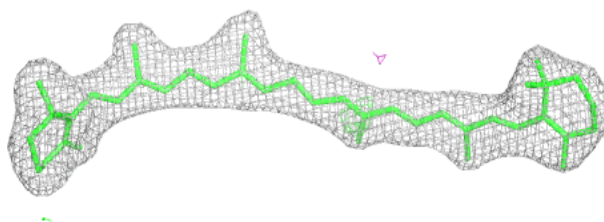


Electron density around BCR d 404:

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

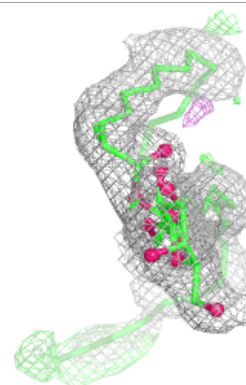
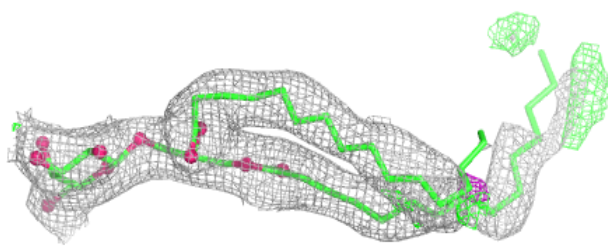
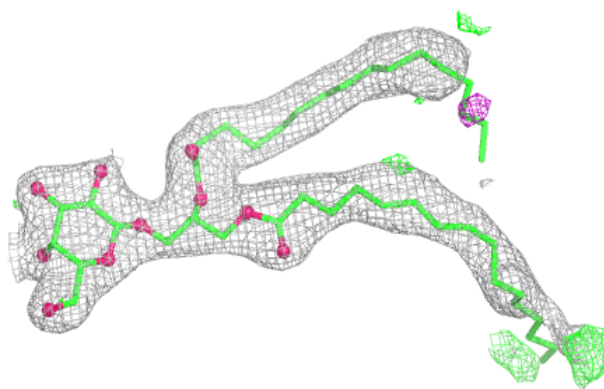
**Electron density around BCR t 102:**

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

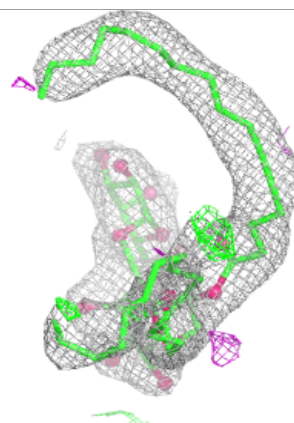
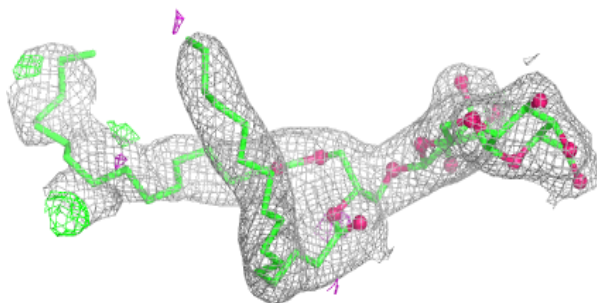
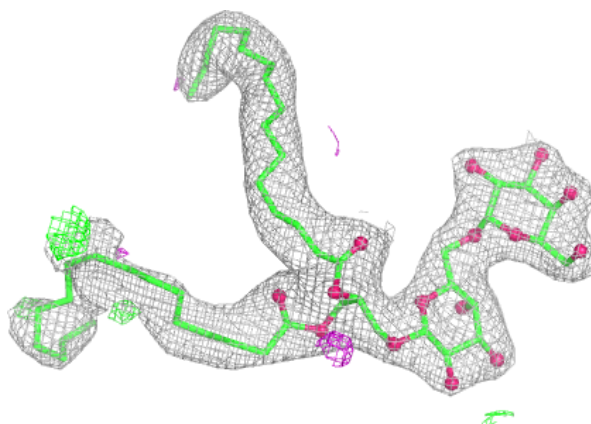


Electron density around LMG D 411:

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

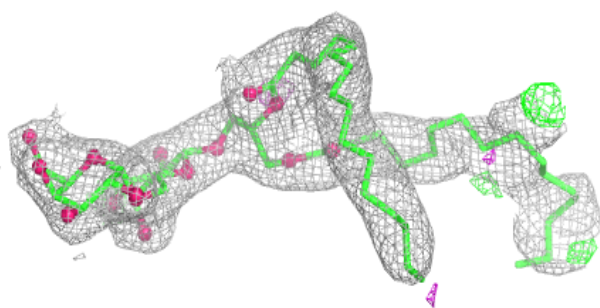
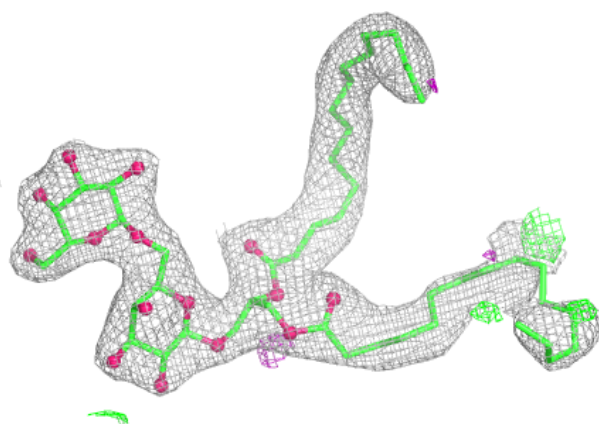
**Electron density around DGD C 518 (A):**

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

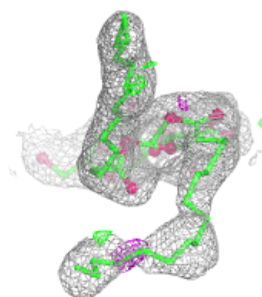
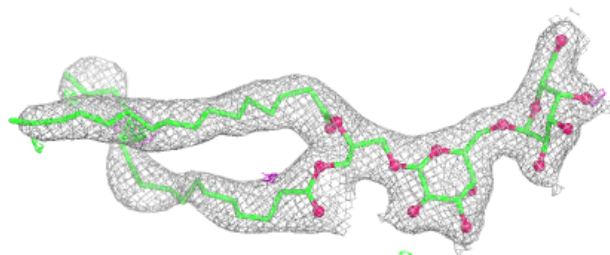
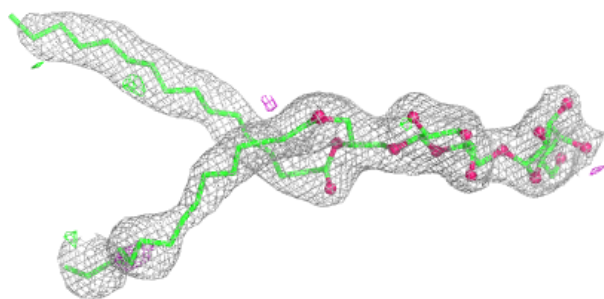


Electron density around DGD C 518 (B):

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

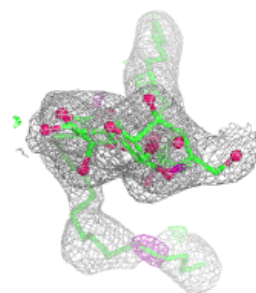
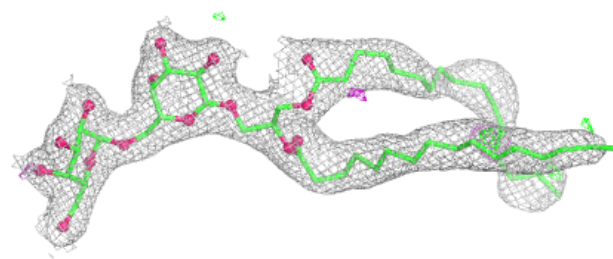
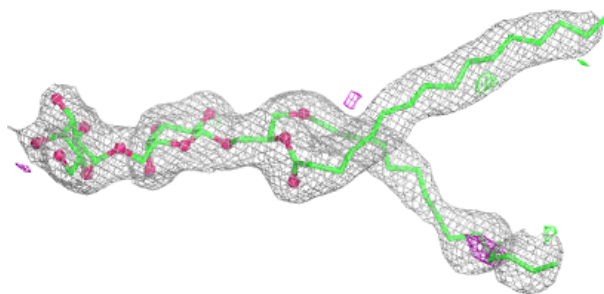
**Electron density around DGD c 517 (A):**

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

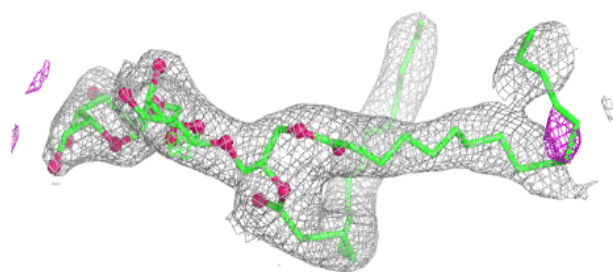
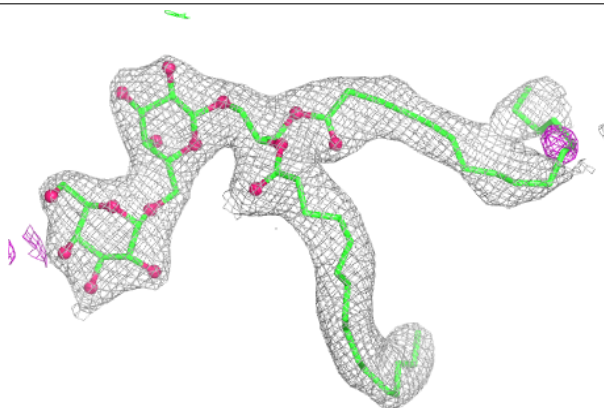


Electron density around DGD c 517 (B):

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

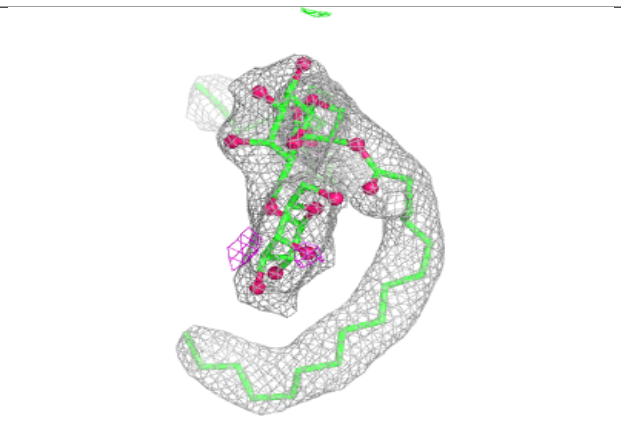
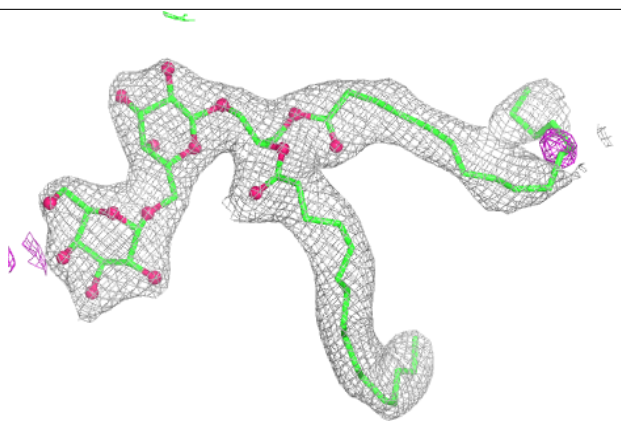
**Electron density around DGD c 518 (A):**

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



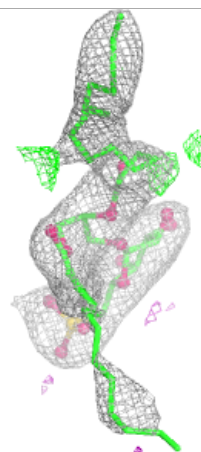
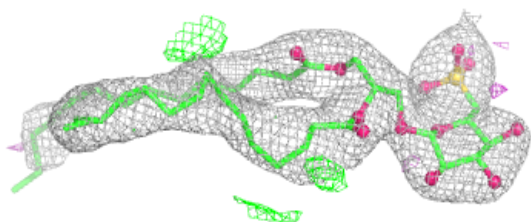
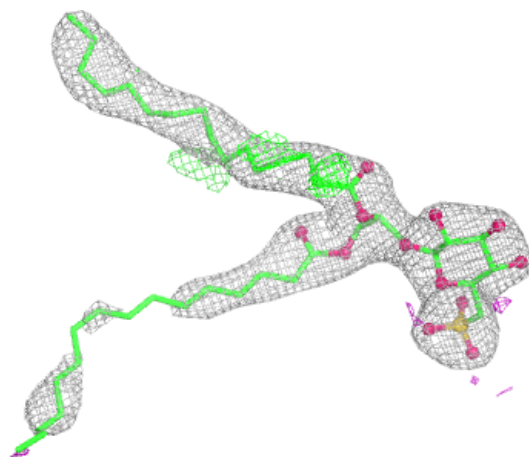
Electron density around DGD c 518 (B):

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



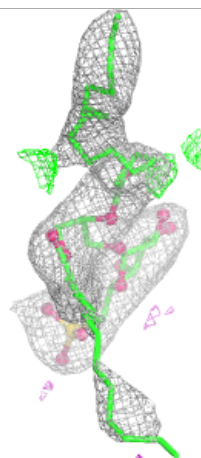
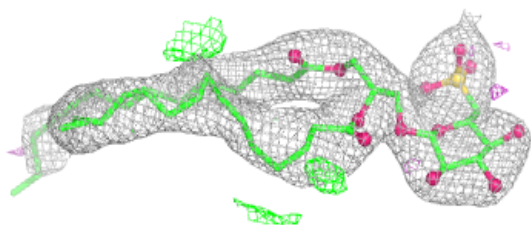
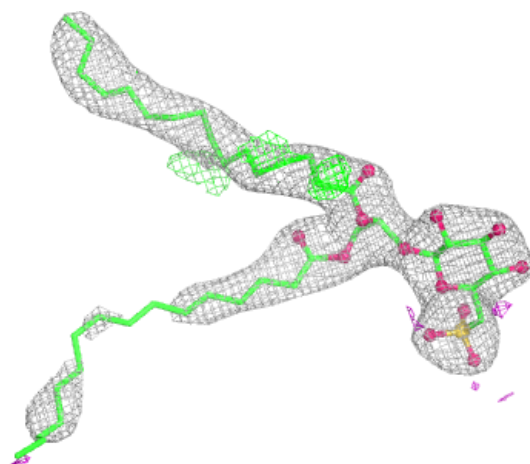
Electron density around SQD A 410 (A):

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



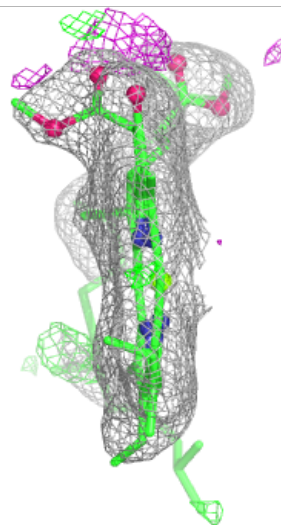
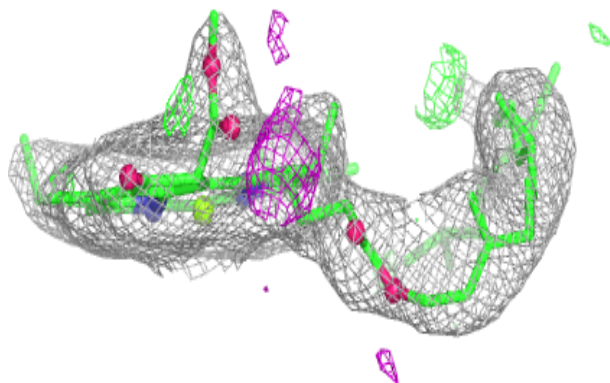
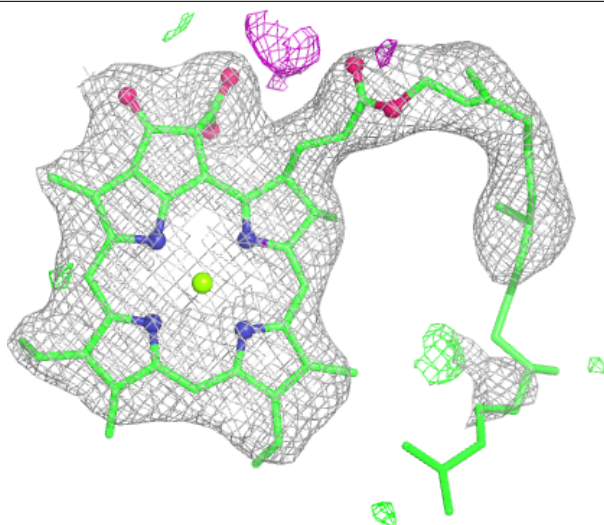
Electron density around SQD A 410 (B):

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



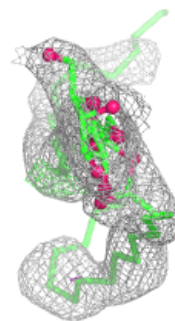
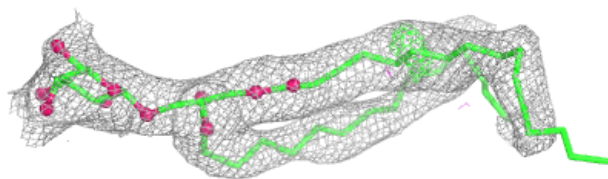
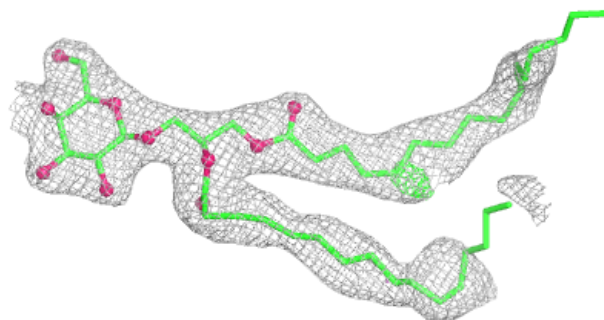
Electron density around CLA c 513:

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



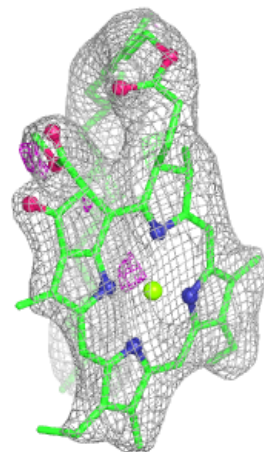
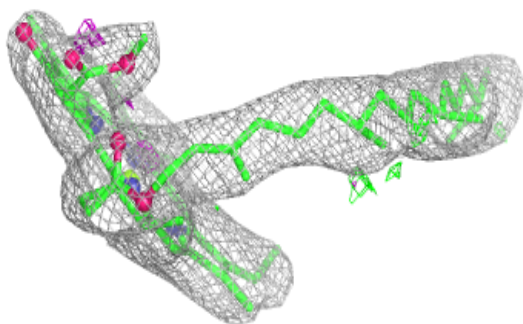
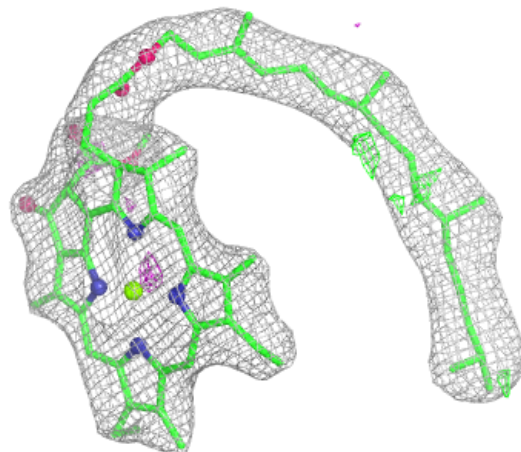
Electron density around LMG d 410:

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



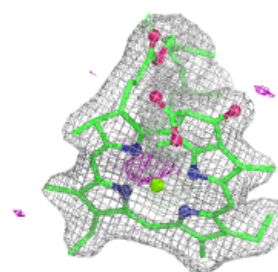
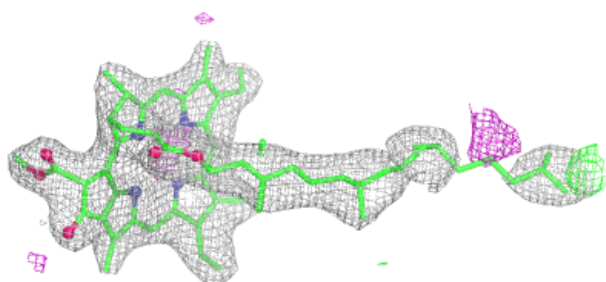
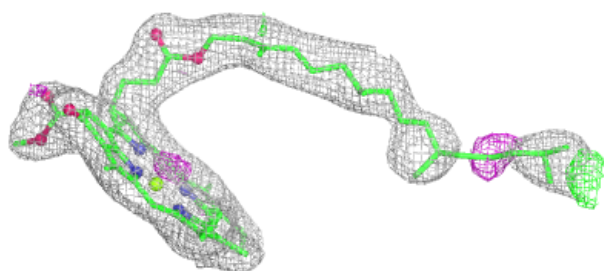
Electron density around CLA c 508:

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

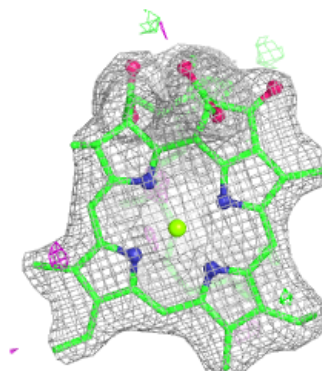
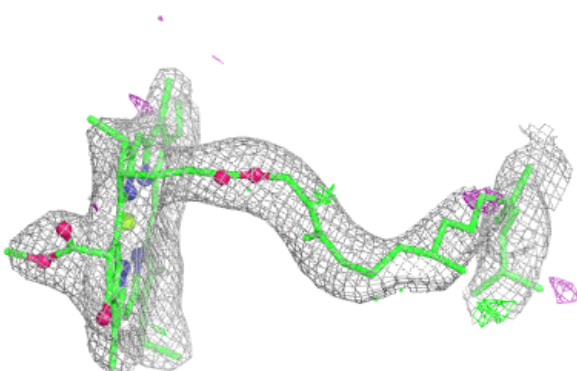
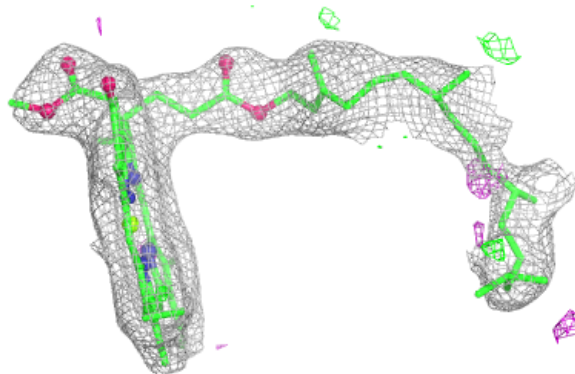


Electron density around CLA C 505:

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

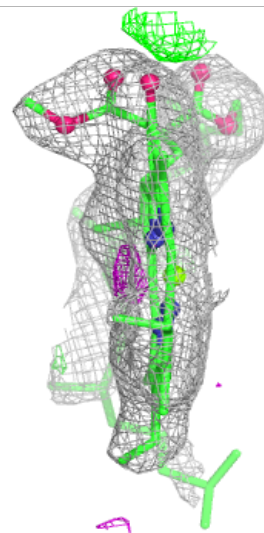
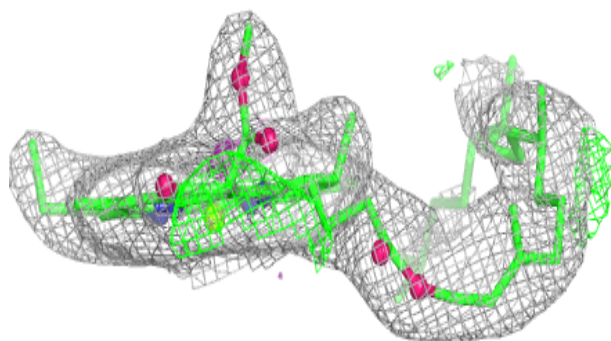
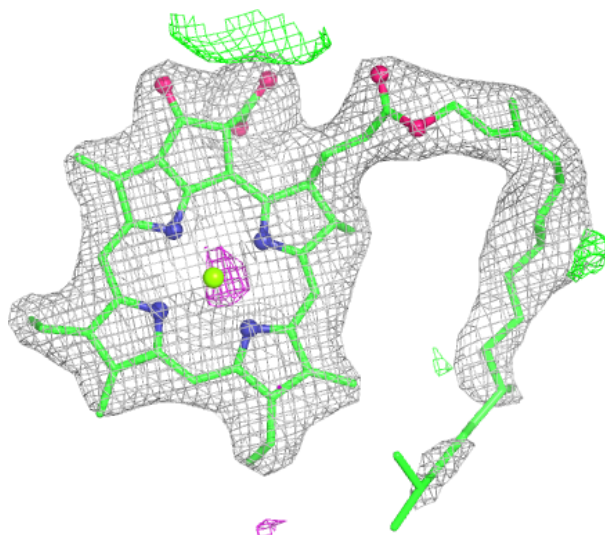
**Electron density around CLA C 507:**

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



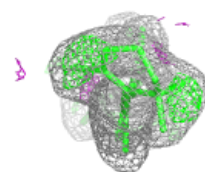
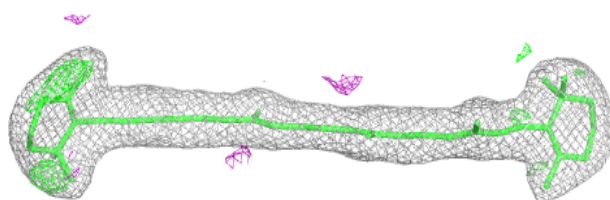
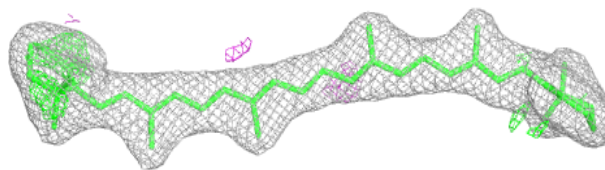
Electron density around CLA C 513:

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

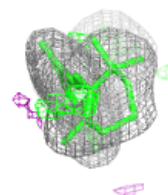
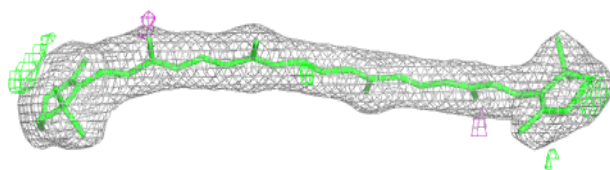
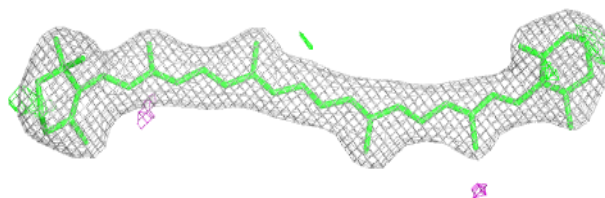


Electron density around BCR A 409:

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

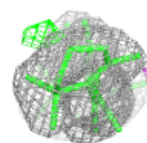
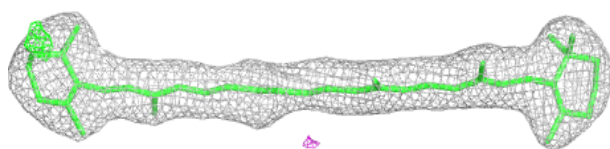
**Electron density around BCR B 619:**

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

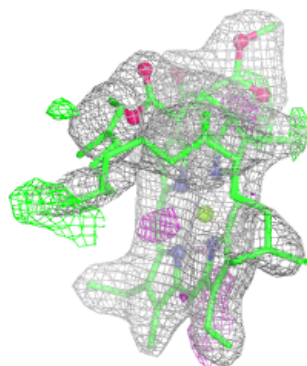
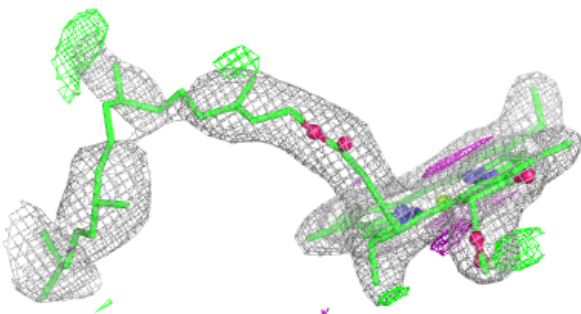
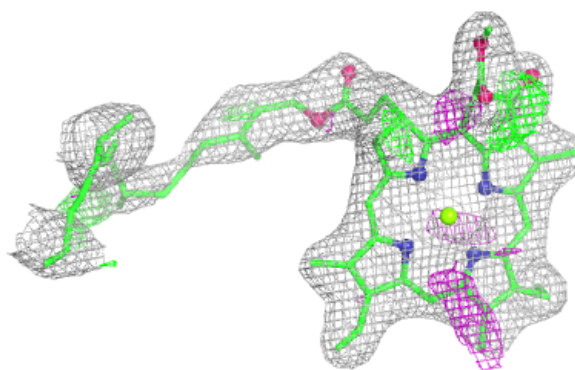


Electron density around BCR C 515:

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

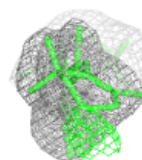
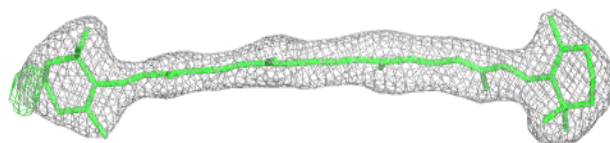
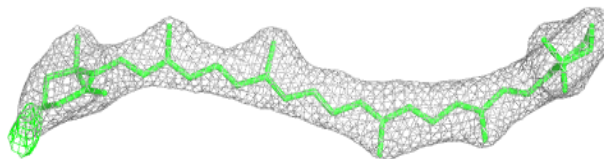
**Electron density around CLA A 408:**

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



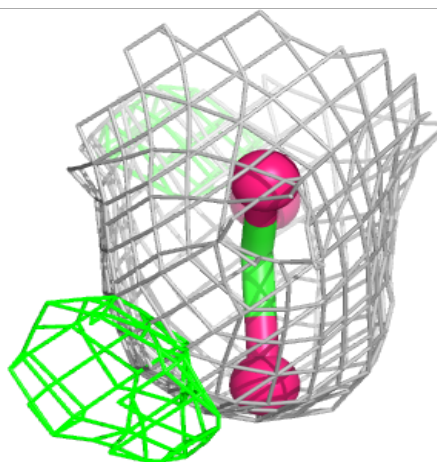
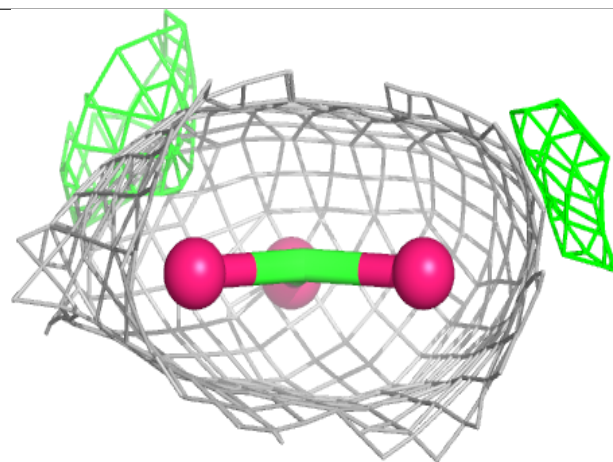
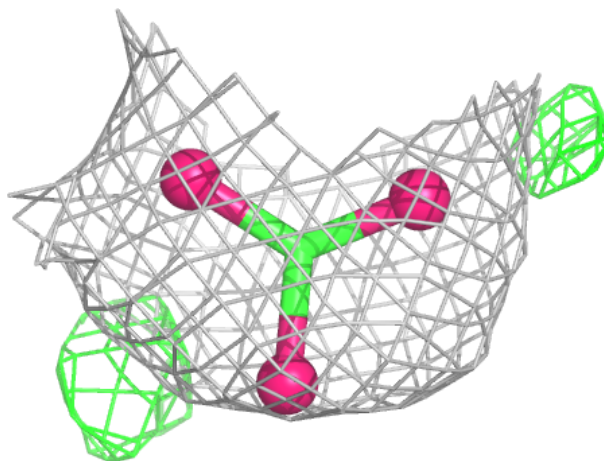
Electron density around BCR H 101:

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



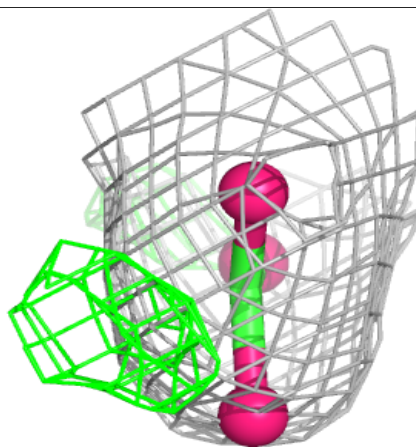
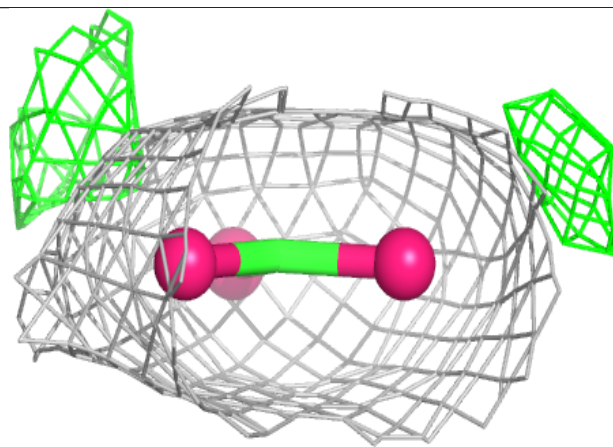
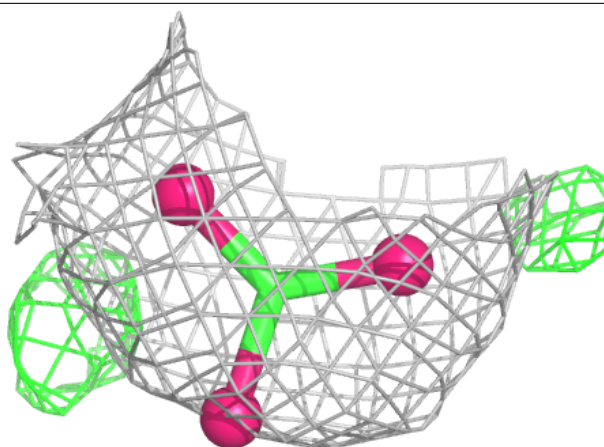
Electron density around BCT d 401 (A):

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



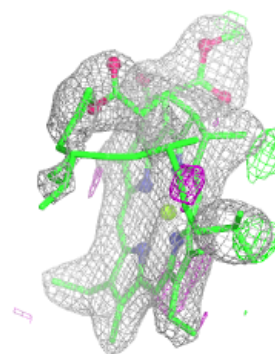
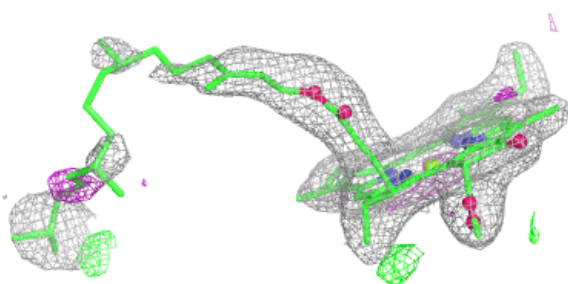
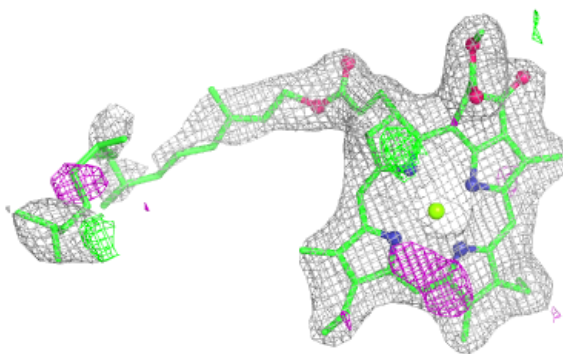
Electron density around BCT d 401 (B):

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

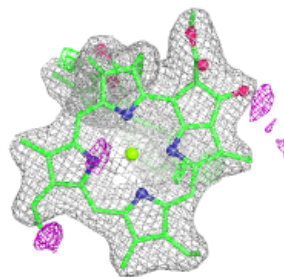
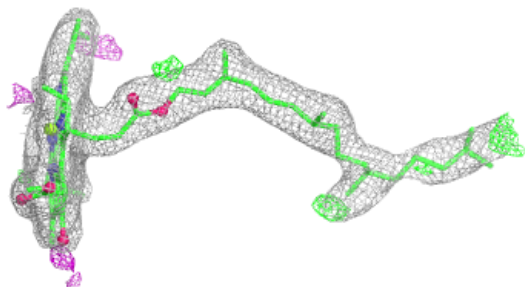
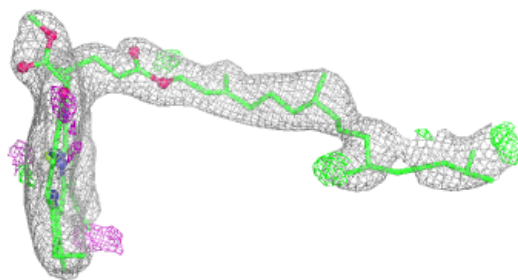


Electron density around CLA a 408:

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

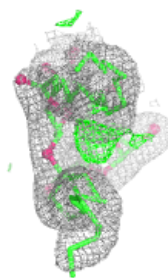
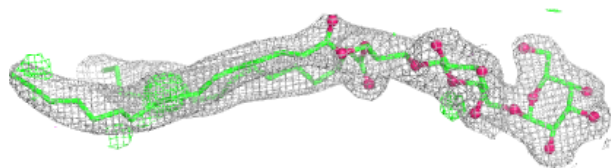
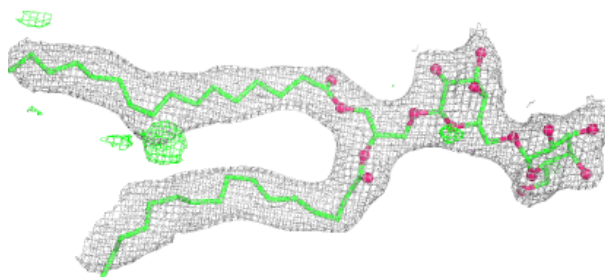
**Electron density around CLA B 606:**

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

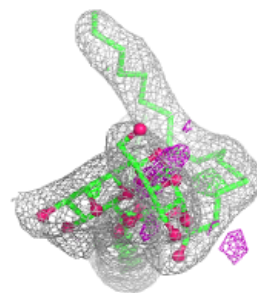
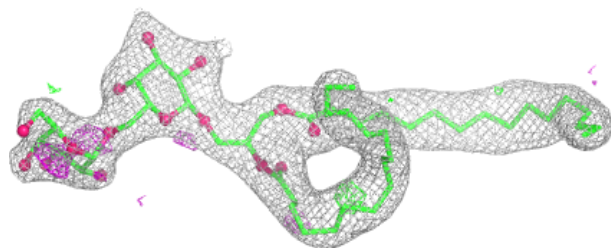
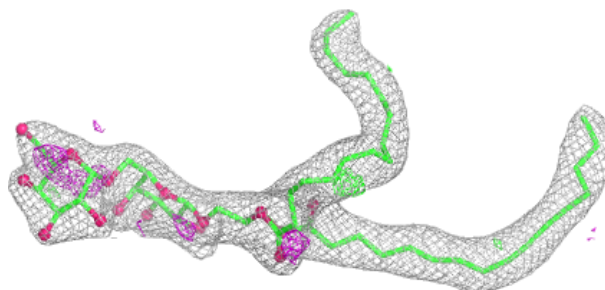


Electron density around DGD C 519:

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

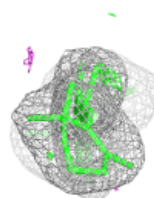
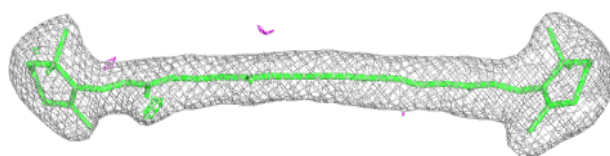
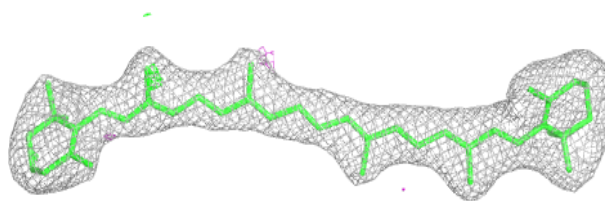
**Electron density around DGD H 102:**

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

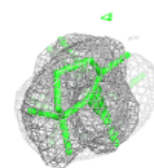
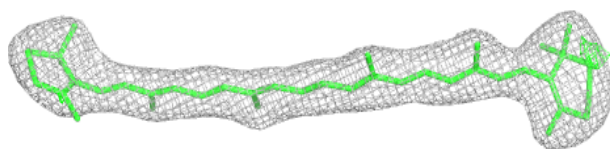
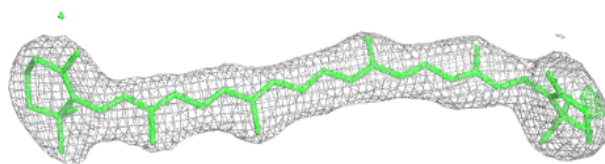


Electron density around BCR b 618:

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

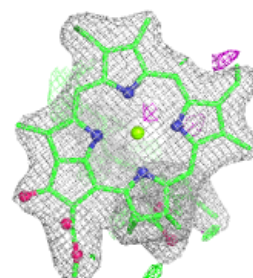
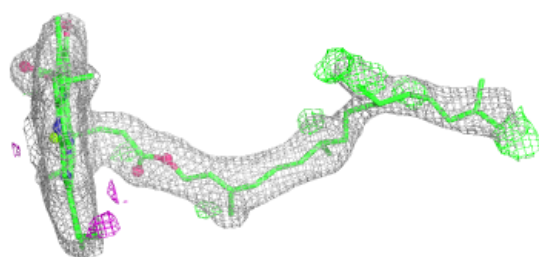
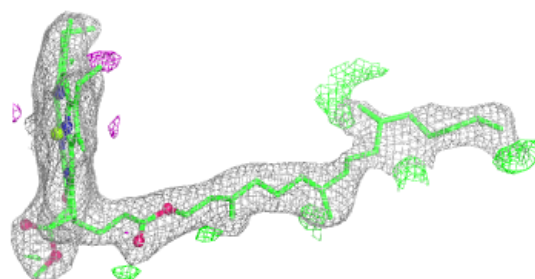
**Electron density around BCR c 515:**

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

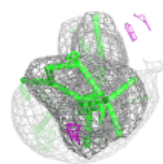
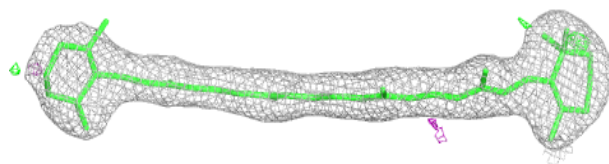
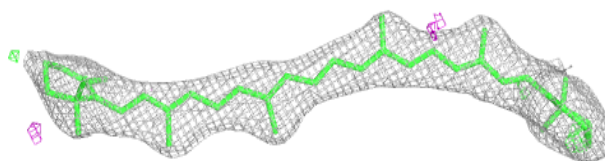


Electron density around CLA b 606:

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

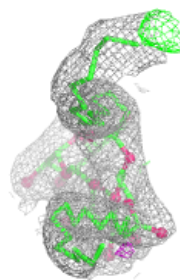
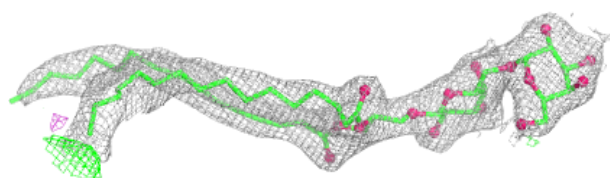
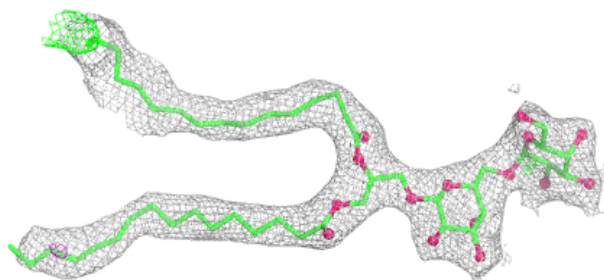
**Electron density around BCR h 101:**

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

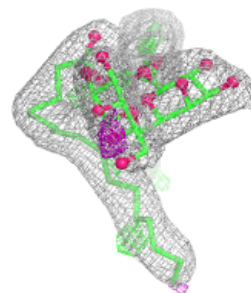
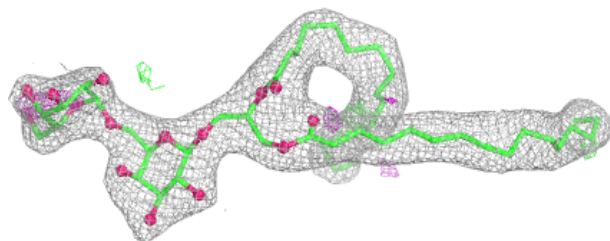
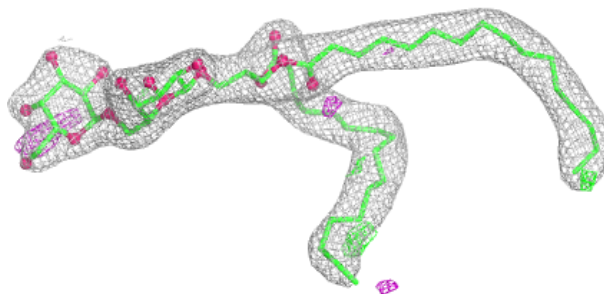


Electron density around DGD c 519:

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

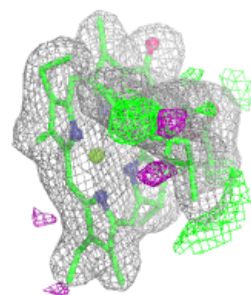
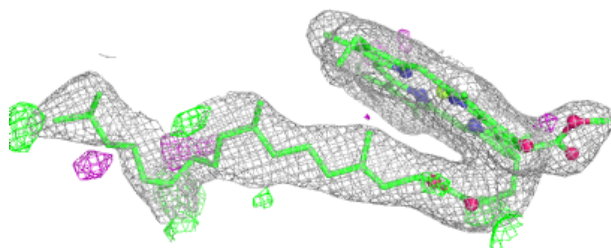
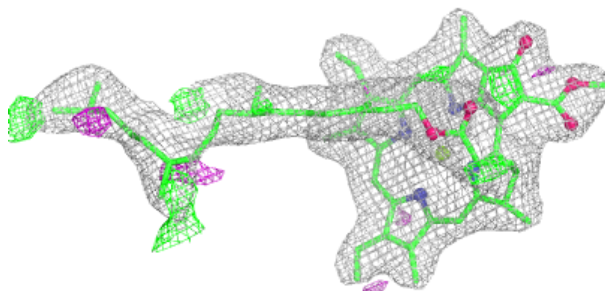
**Electron density around DGD h 102:**

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

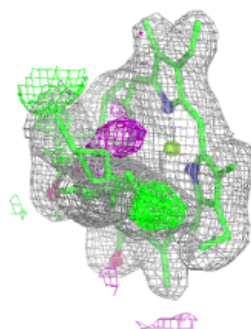
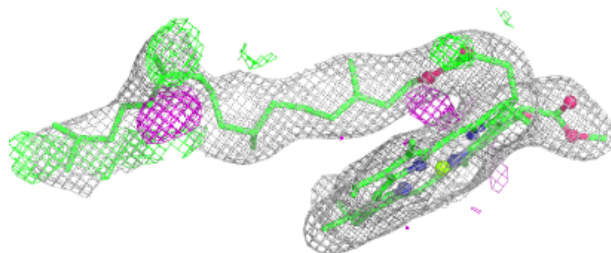
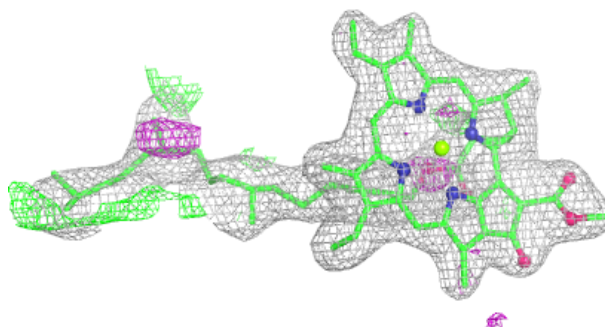


Electron density around CLA b 614:

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

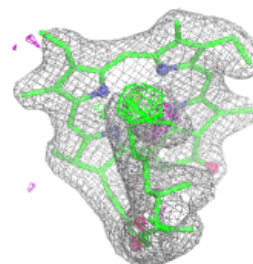
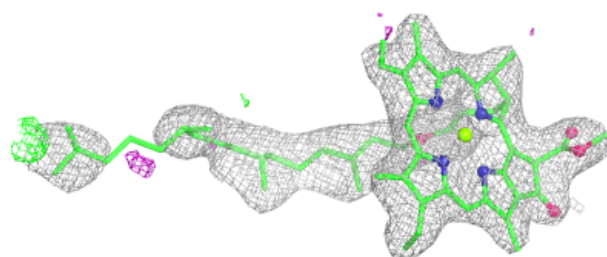
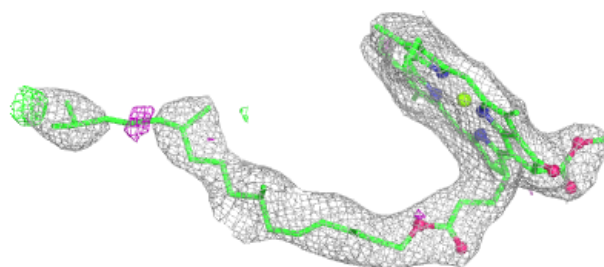
**Electron density around CLA B 614:**

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

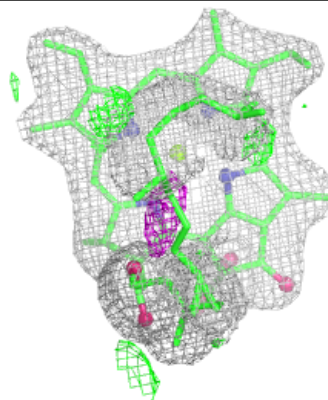
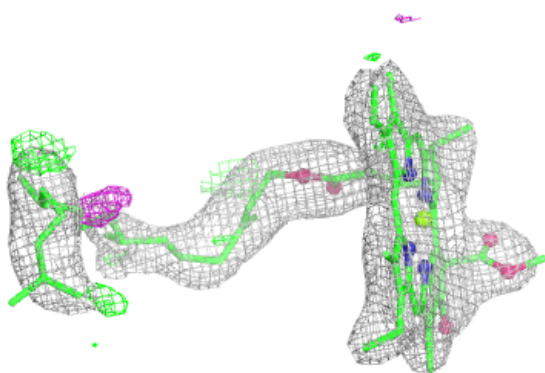
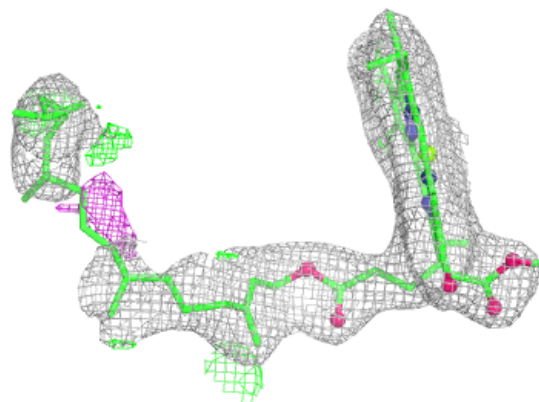


Electron density around CLA c 505:

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

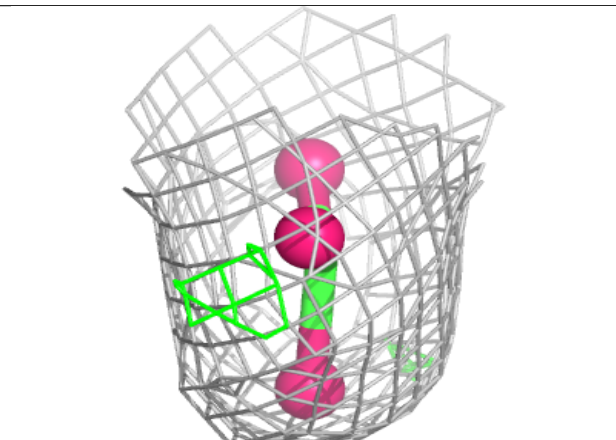
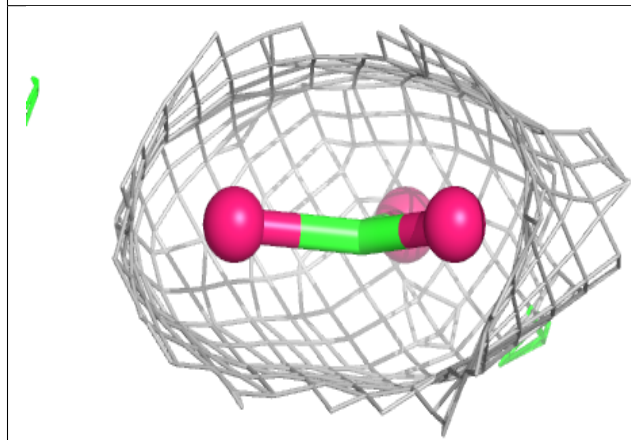
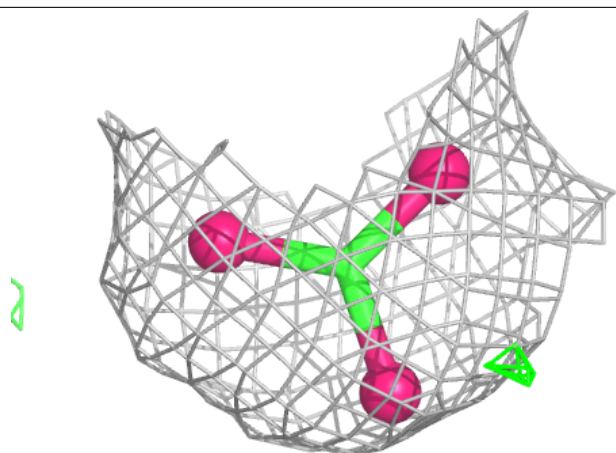
**Electron density around CLA c 507:**

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



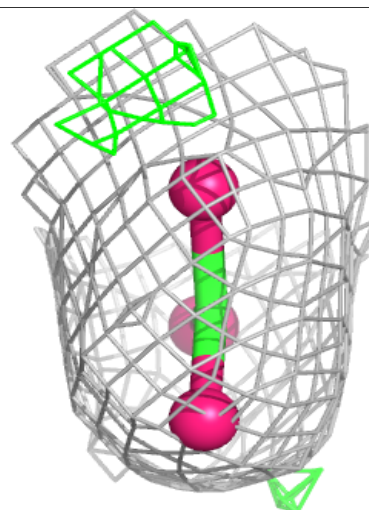
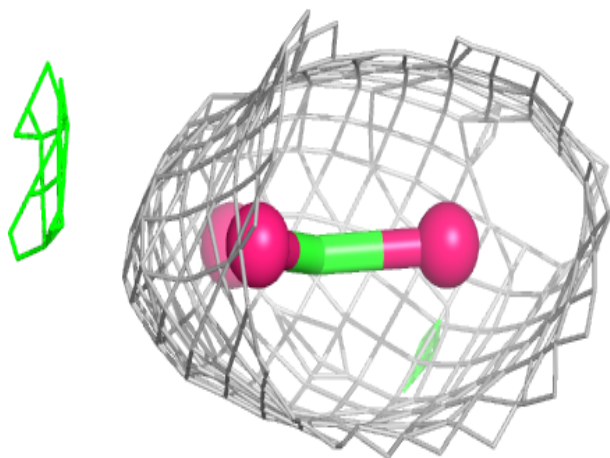
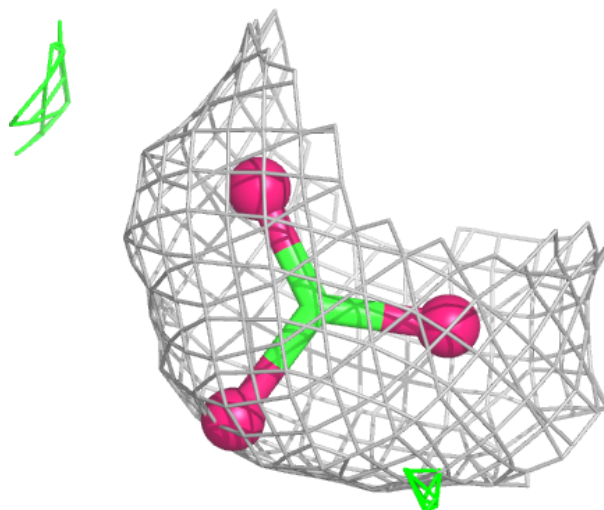
Electron density around BCT A 416 (A):

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



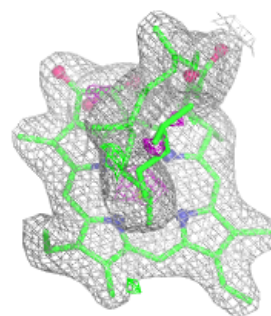
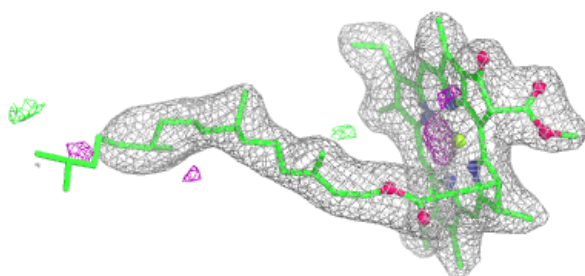
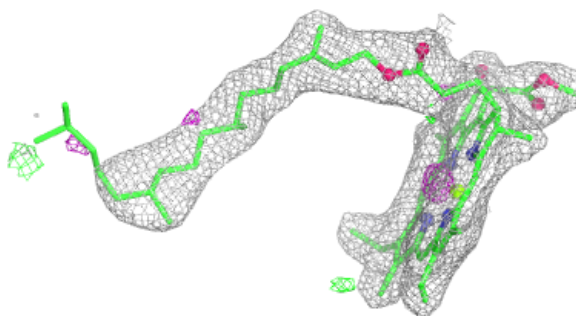
Electron density around BCT A 416 (B):

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

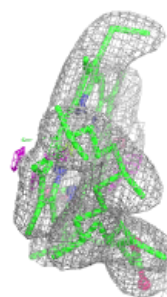
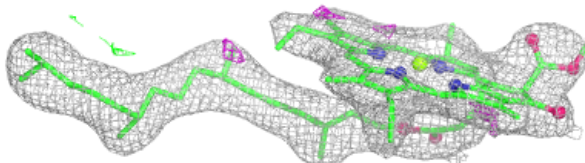
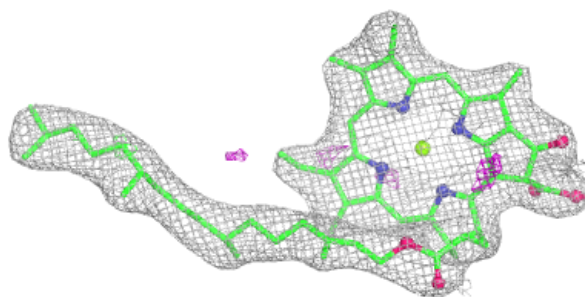


Electron density around CLA C 509:

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

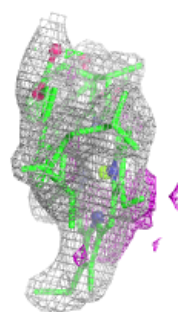
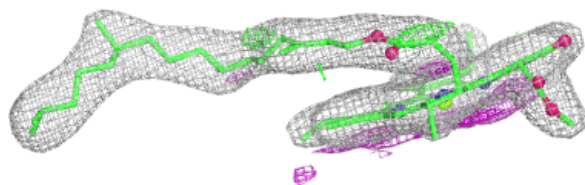
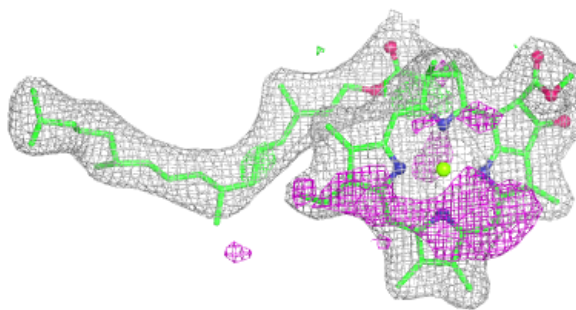
**Electron density around CLA c 502:**

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

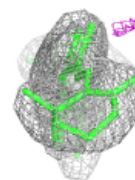
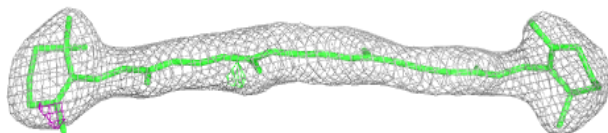
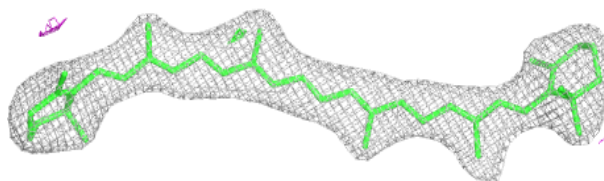


Electron density around CLA B 603:

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

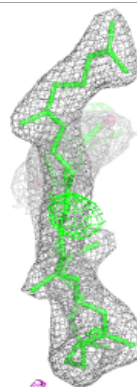
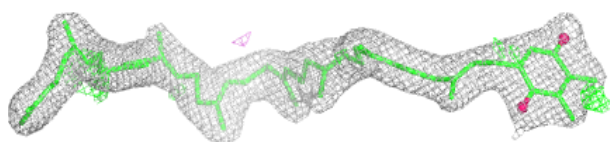
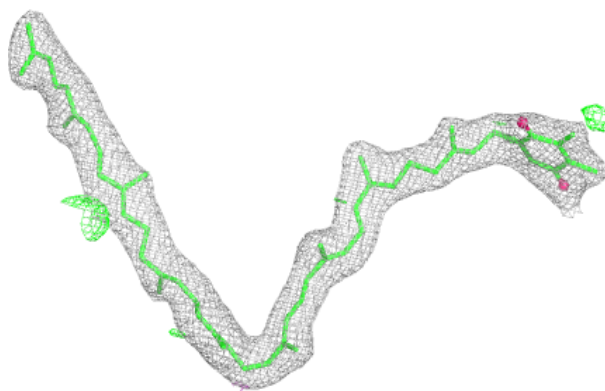
**Electron density around BCR Y 101:**

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

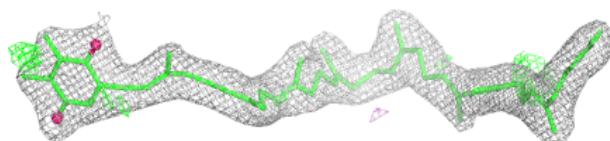
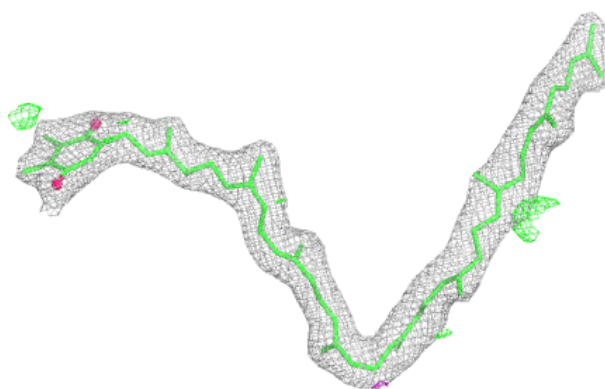


Electron density around PL9 D 405 (A):

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

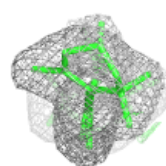
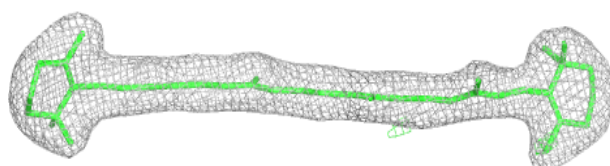
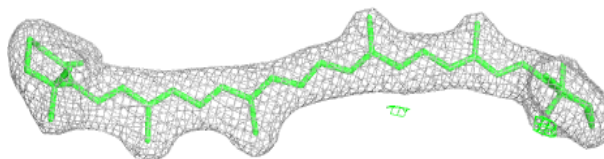
**Electron density around PL9 D 405 (B):**

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

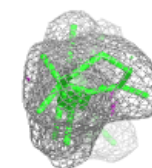
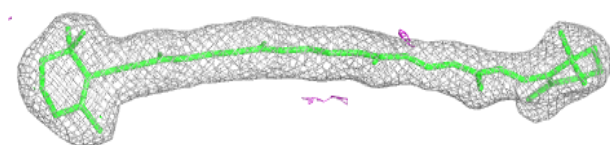
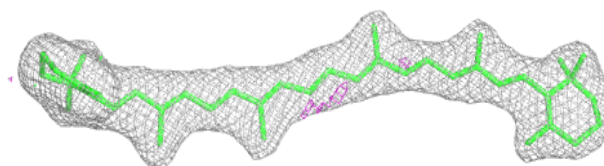


Electron density around BCR a 409:

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

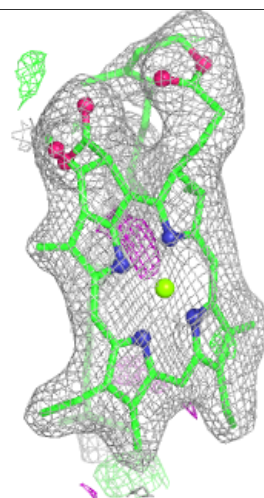
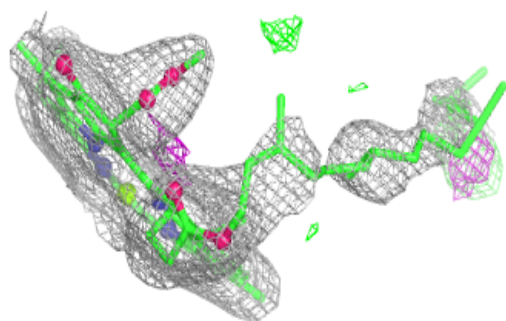
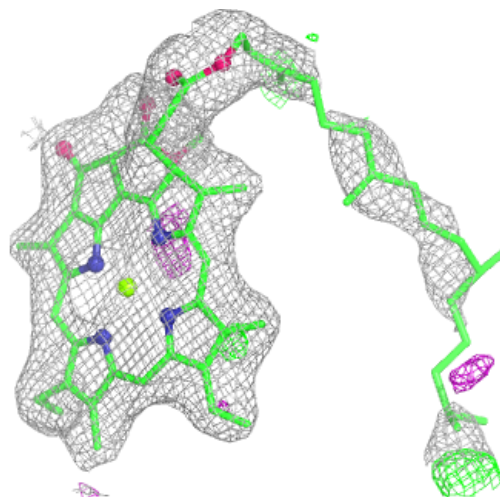
**Electron density around BCR b 617:**

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



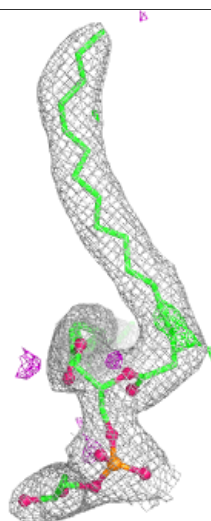
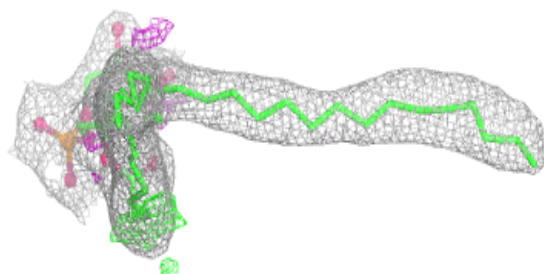
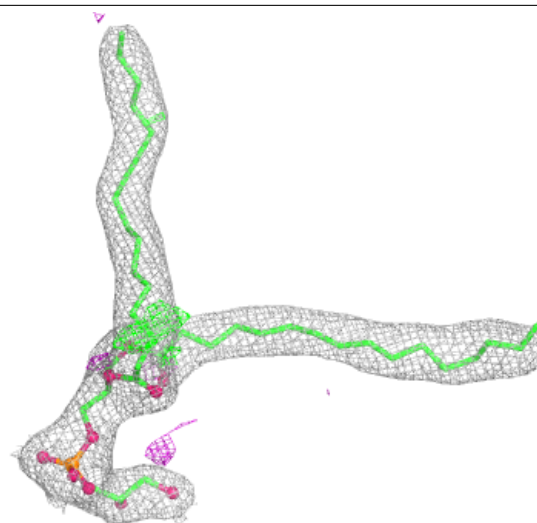
Electron density around CLA B 616:

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



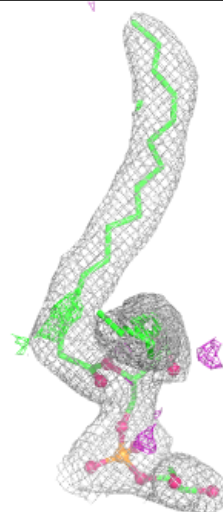
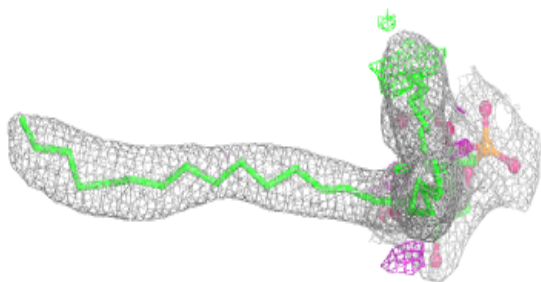
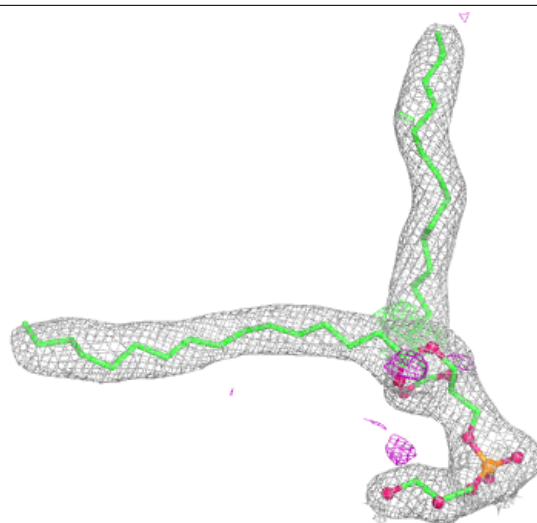
Electron density around LHG b 630 (A):

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



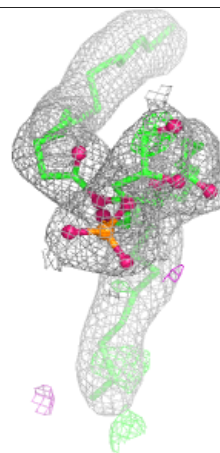
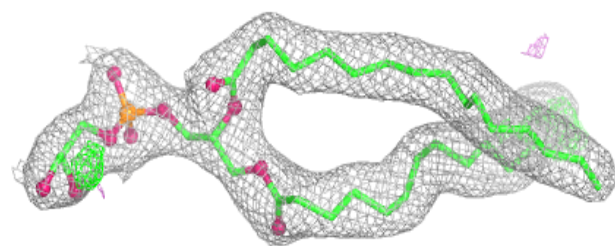
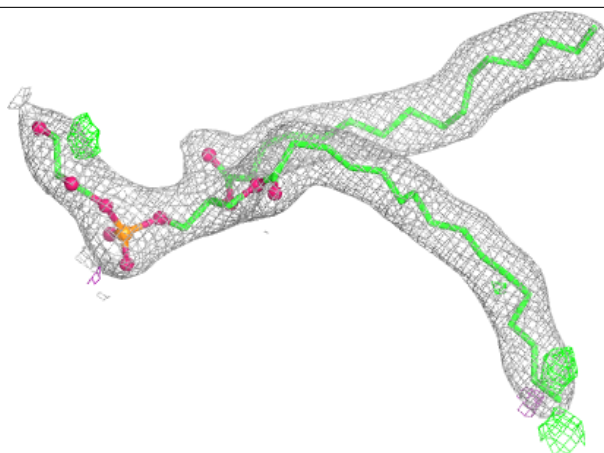
Electron density around LHG b 630 (B):

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



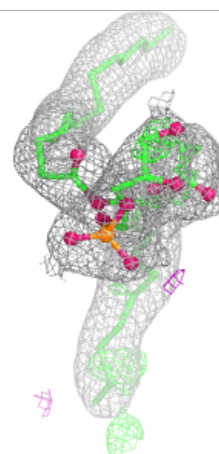
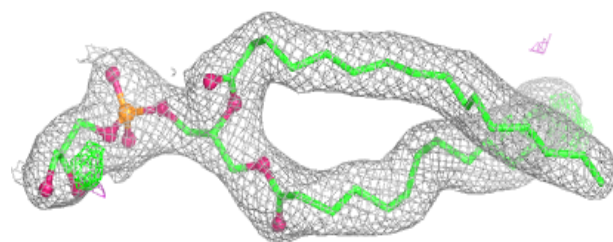
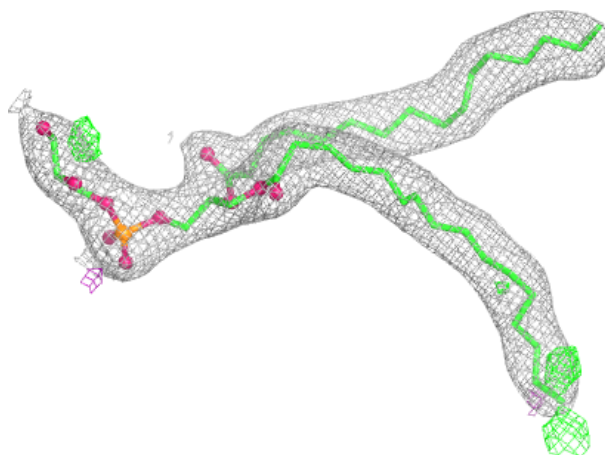
Electron density around LHG d 406 (A):

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



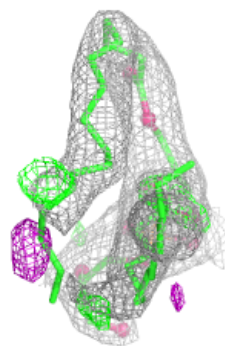
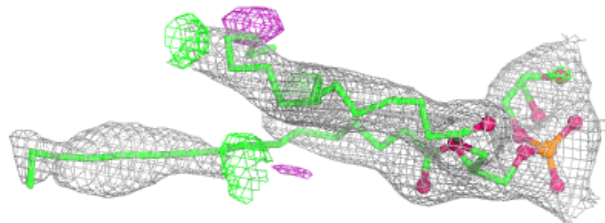
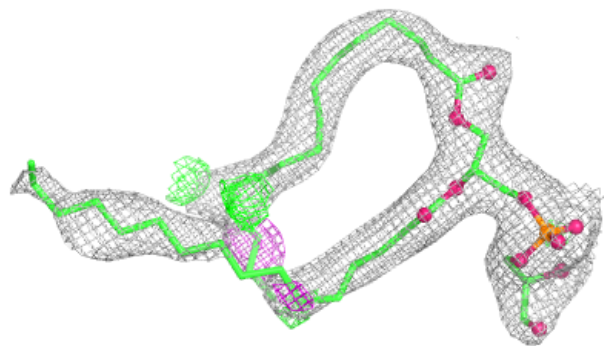
Electron density around LHG d 406 (B):

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

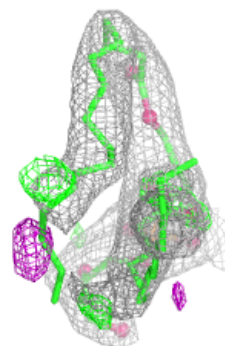
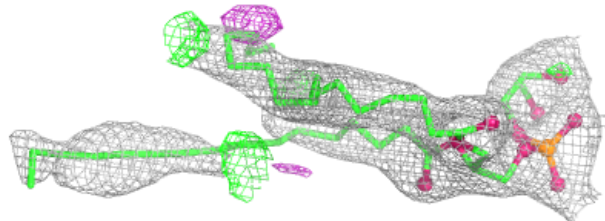
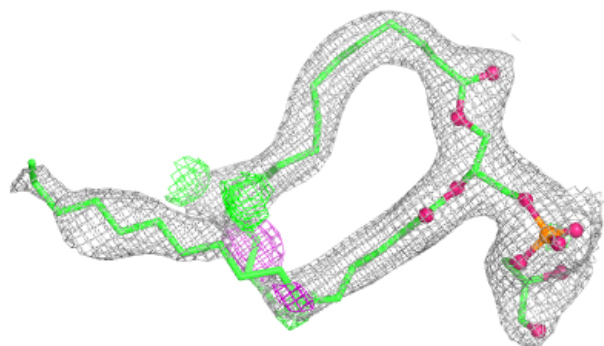


Electron density around LHG d 407 (A):

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

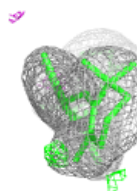
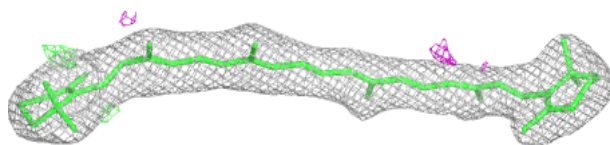
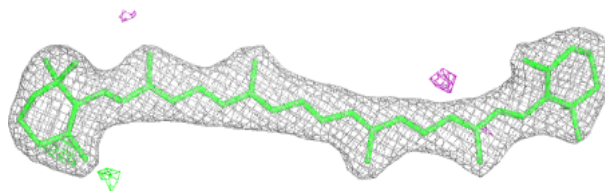
**Electron density around LHG d 407 (B):**

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

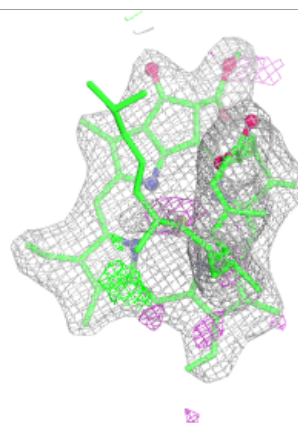
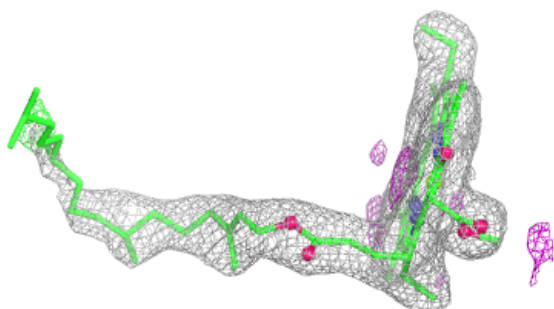
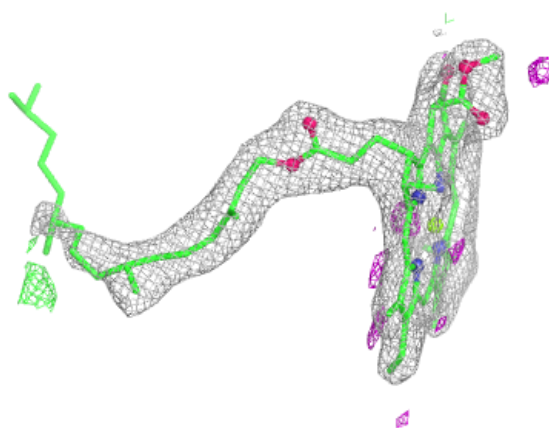


Electron density around BCR b 619:

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

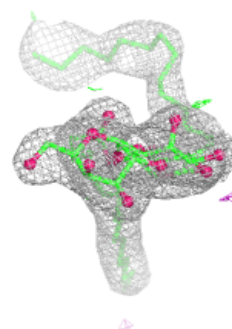
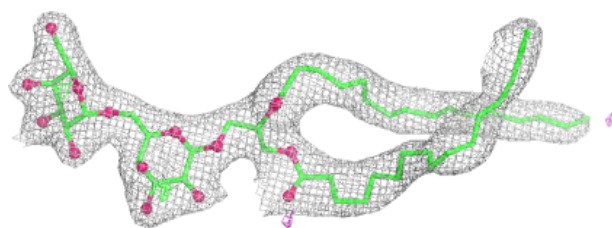
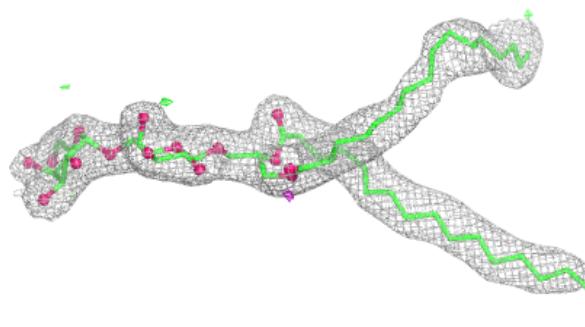
**Electron density around CLA D 403:**

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

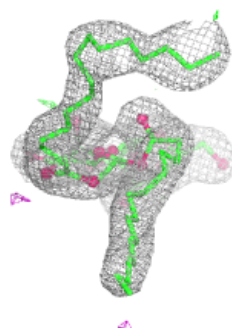
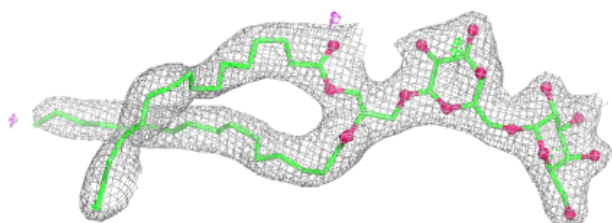
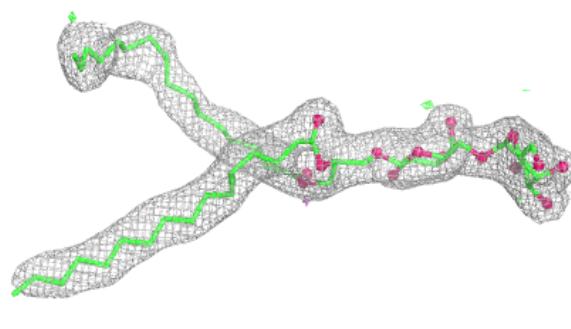


Electron density around DGD C 517 (A):

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

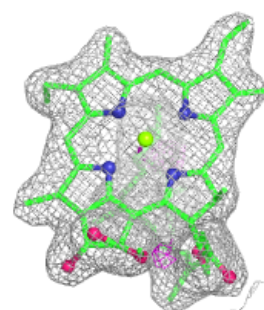
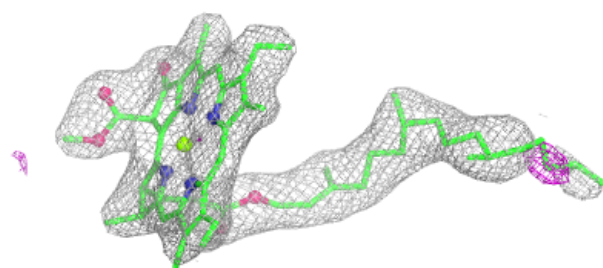
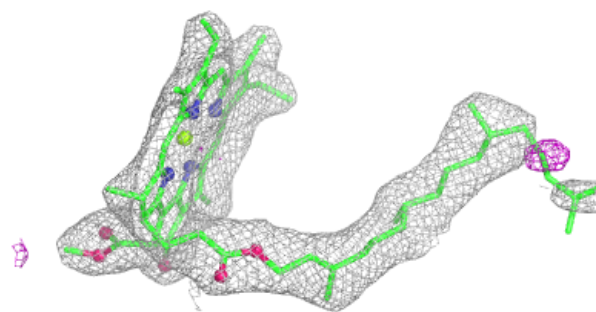
**Electron density around DGD C 517 (B):**

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

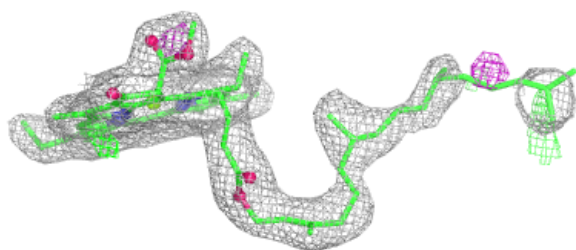
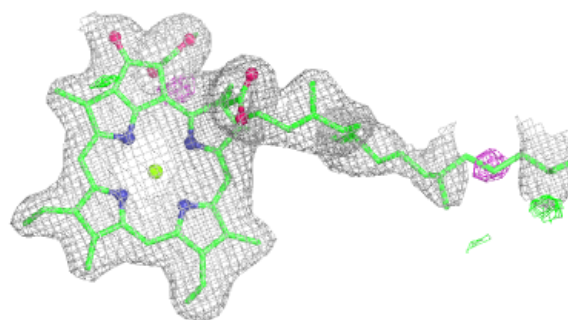


Electron density around CLA c 509:

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

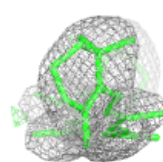
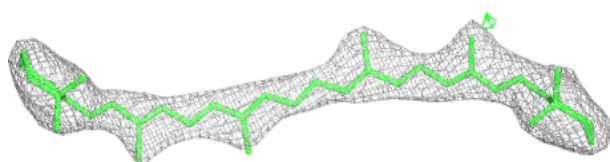
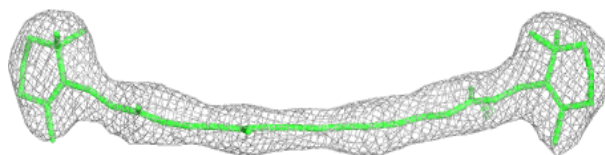
**Electron density around CLA a 406 (A):**

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

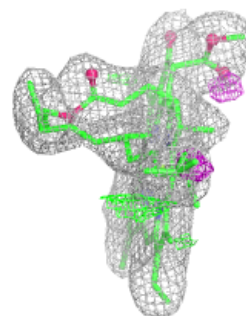
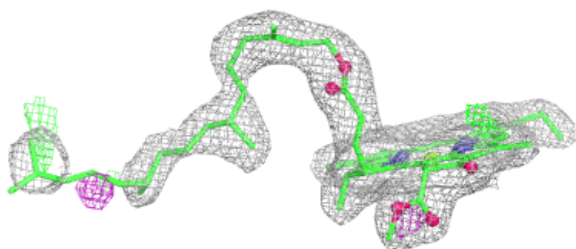
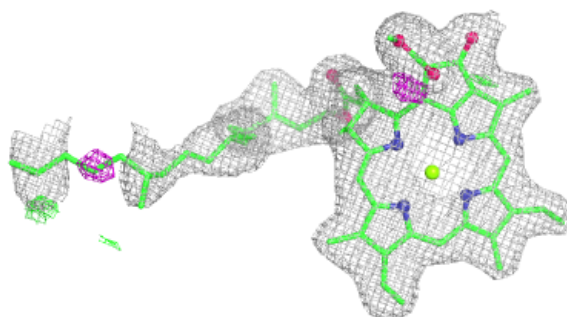


Electron density around BCR k 101:

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

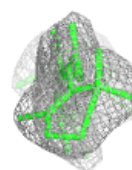
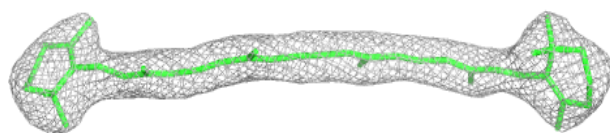
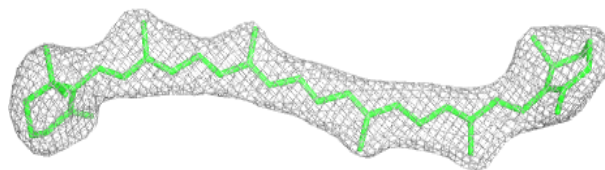
**Electron density around CLA a 406 (B):**

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

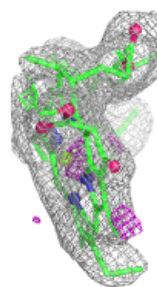
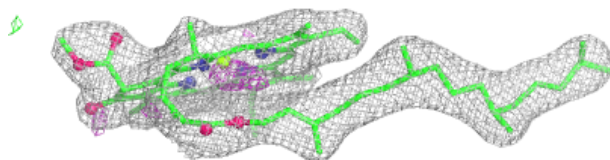
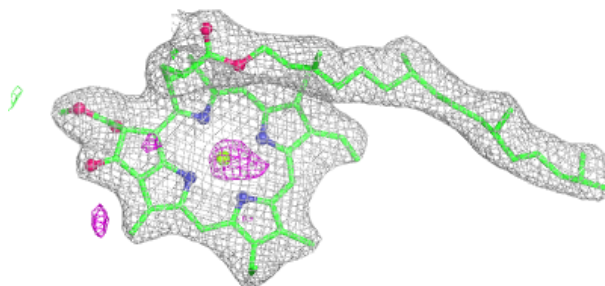


Electron density around BCR y 101:

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

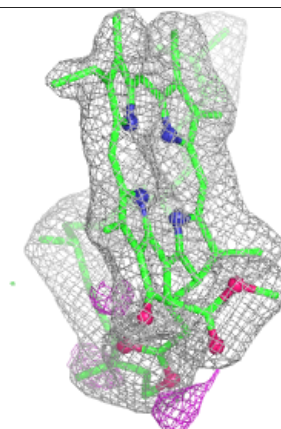
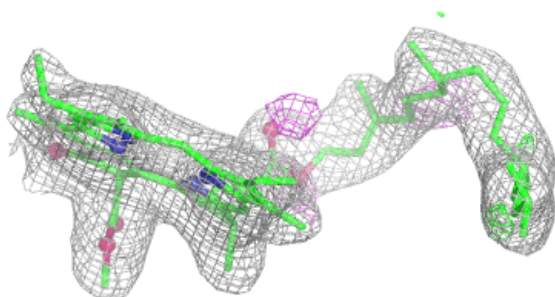
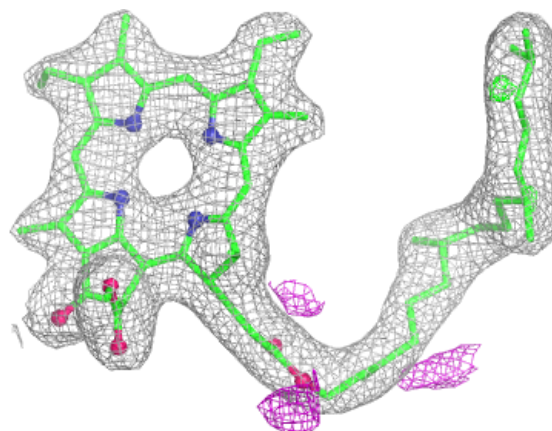
**Electron density around CLA C 502:**

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



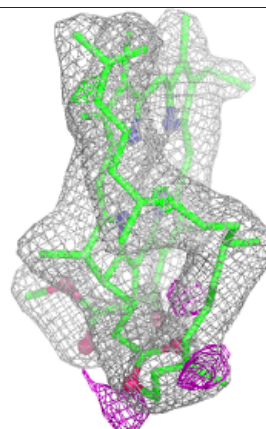
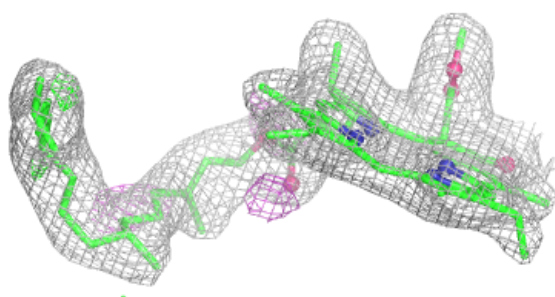
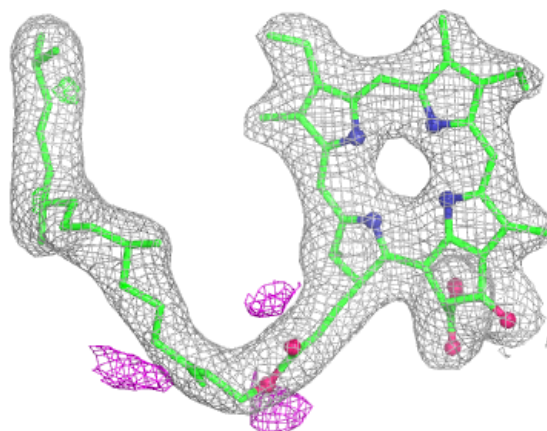
Electron density around PHO a 415 (A):

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



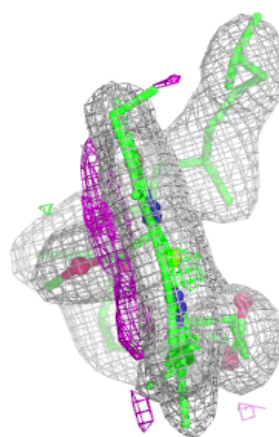
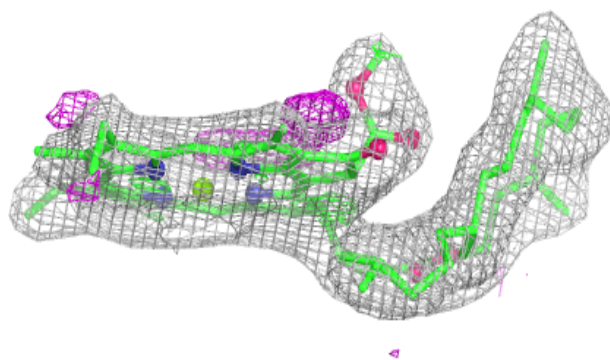
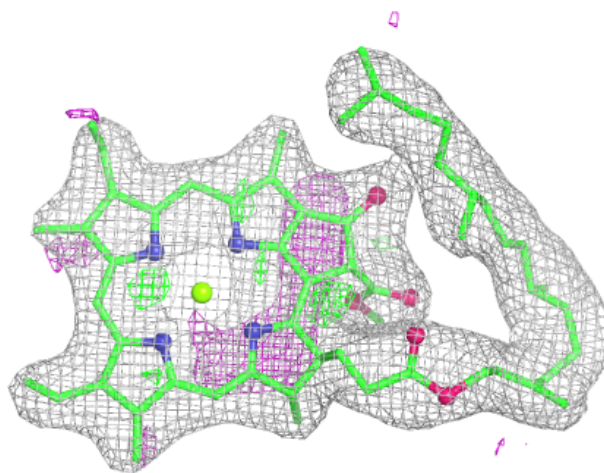
Electron density around PHO a 415 (B):

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



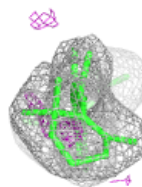
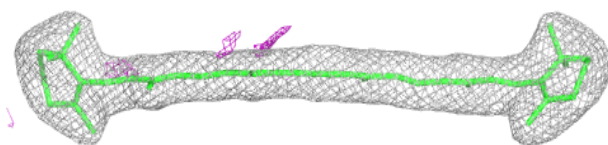
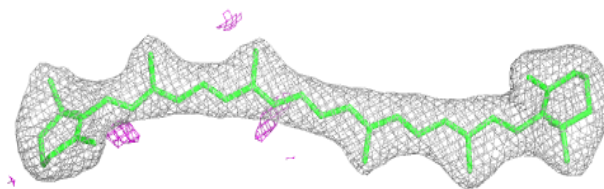
Electron density around CLA B 610:

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



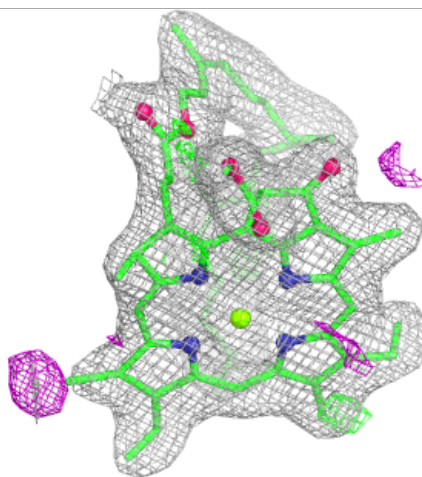
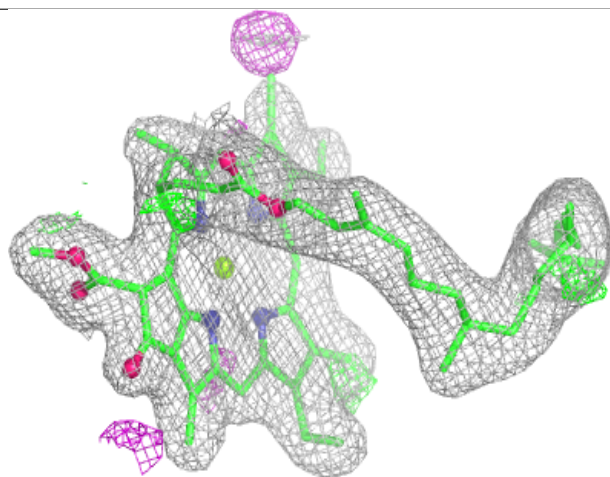
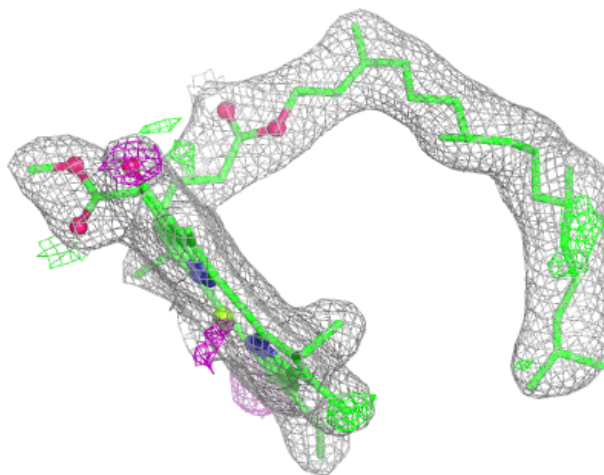
Electron density around BCR B 618:

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



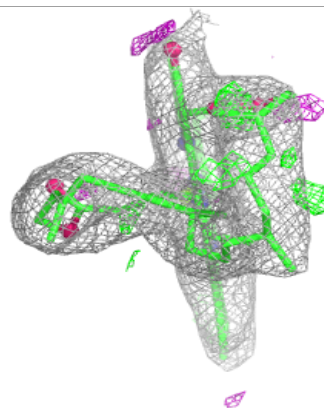
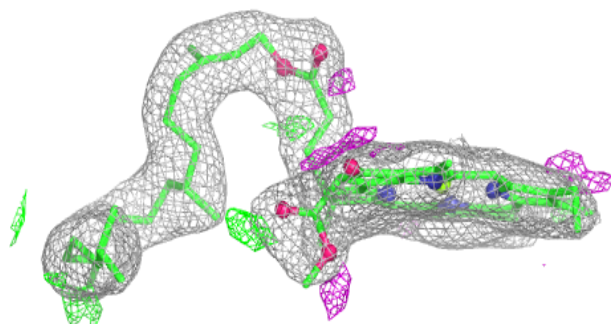
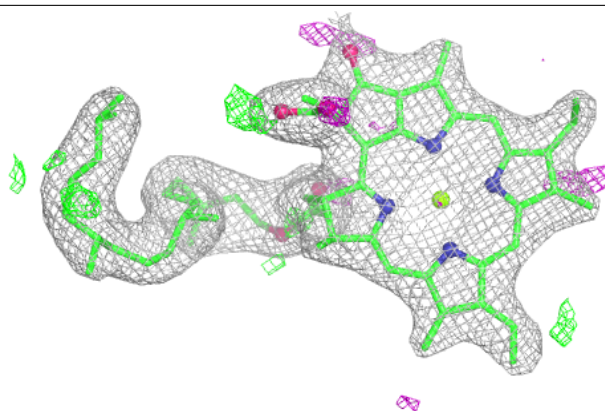
Electron density around CLA B 611:

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

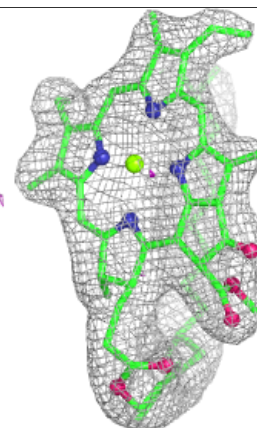
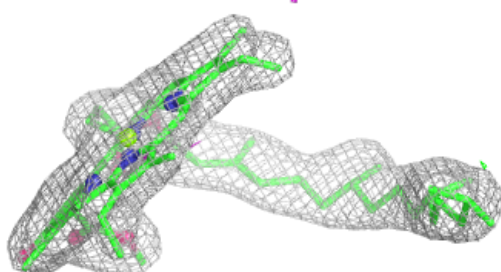
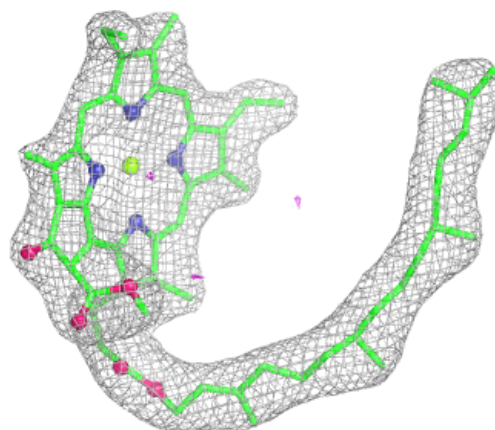


Electron density around CLA b 612:

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

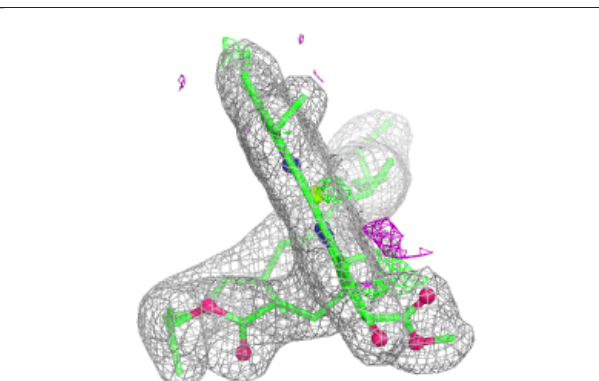
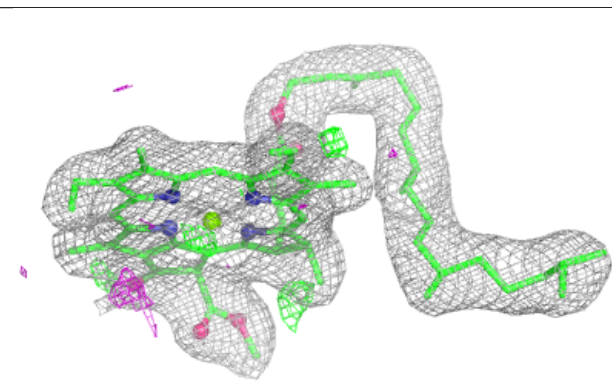
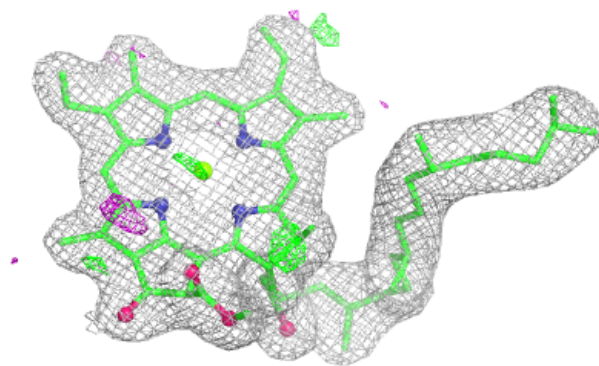
**Electron density around CLA C 508:**

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

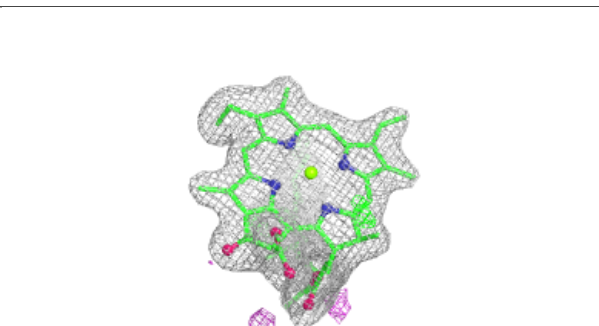
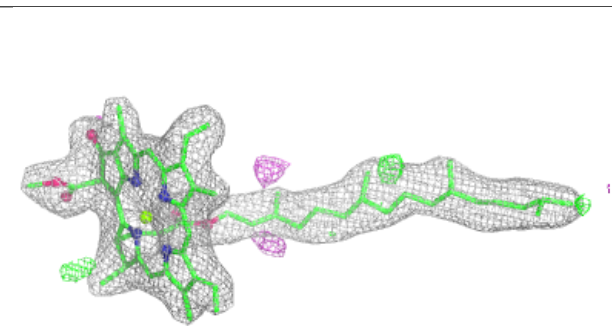
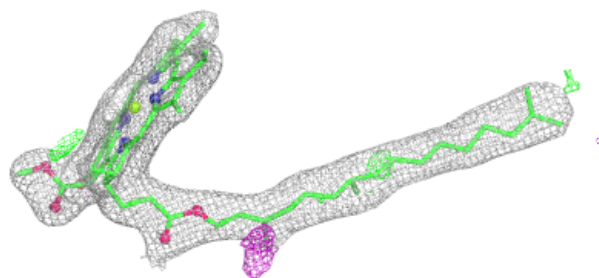


Electron density around CLA A 405 (A):

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

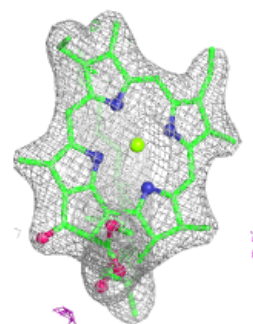
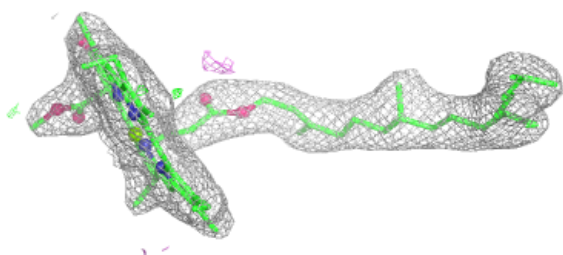
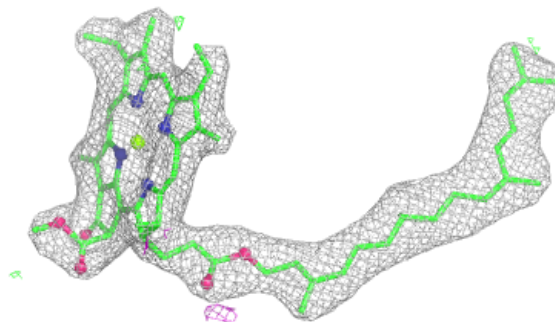
**Electron density around CLA b 607:**

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



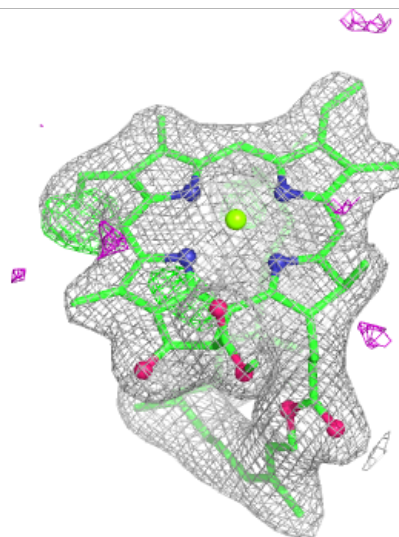
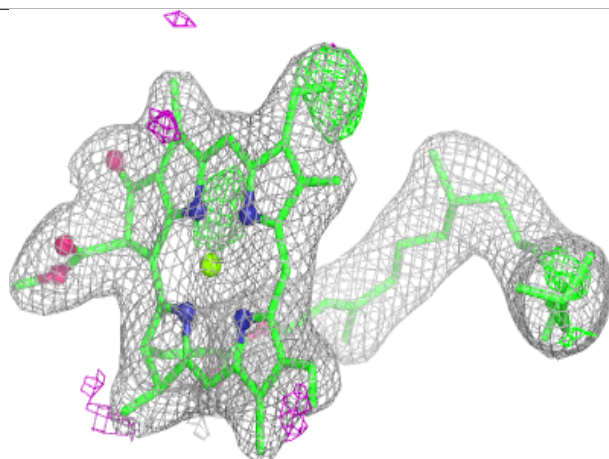
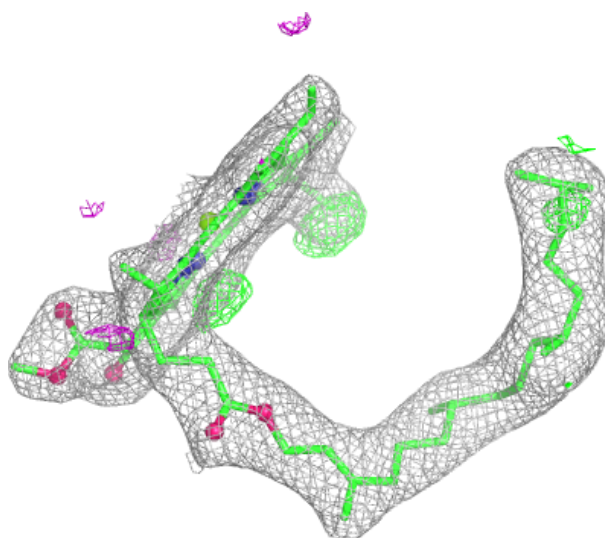
Electron density around CLA b 609:

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



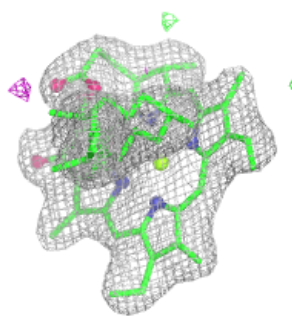
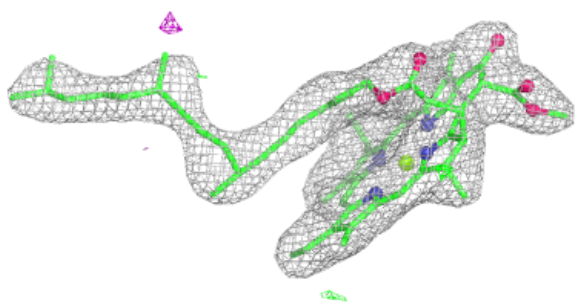
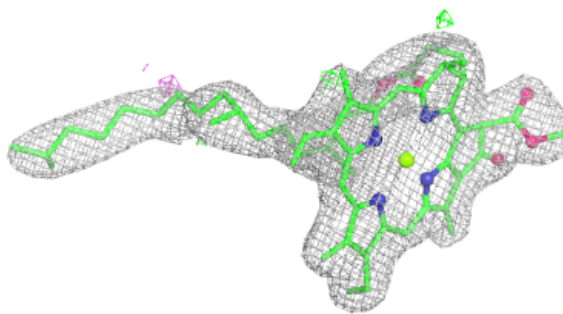
Electron density around CLA b 611:

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



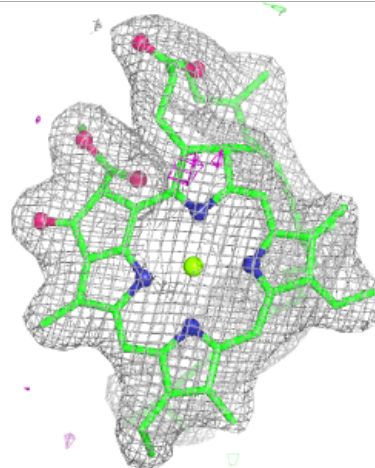
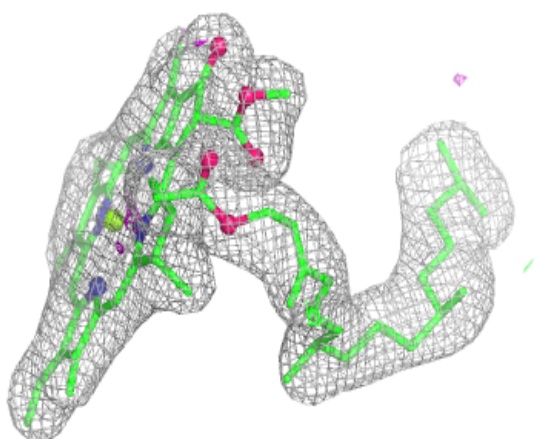
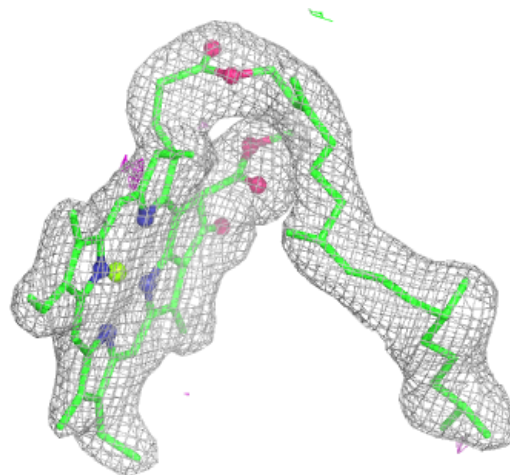
Electron density around CLA C 506:

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



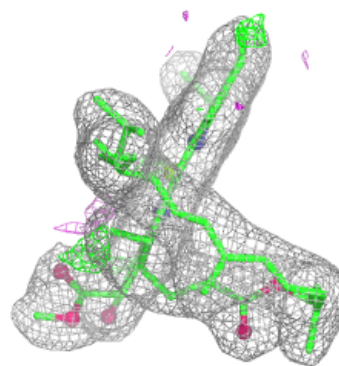
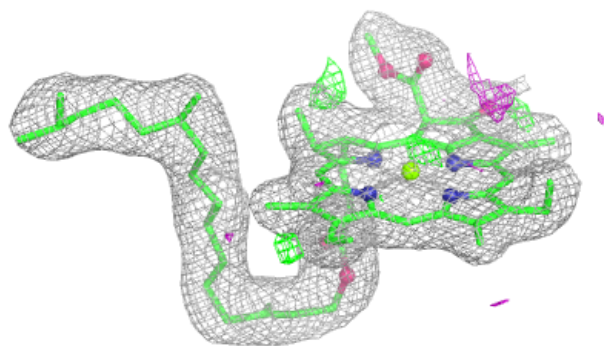
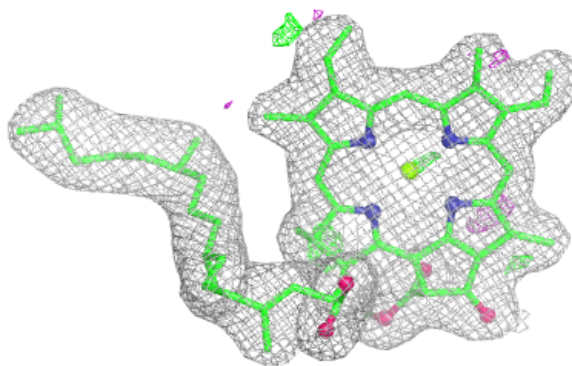
Electron density around CLA b 613:

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

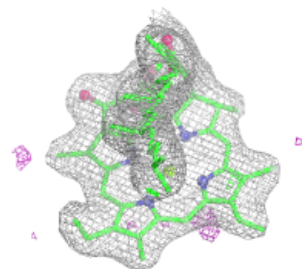
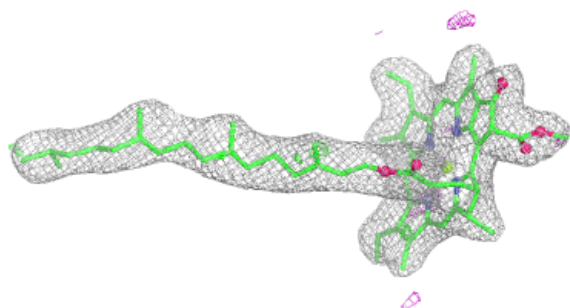
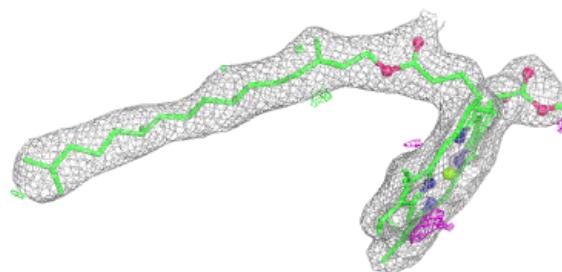


Electron density around CLA A 405 (B):

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

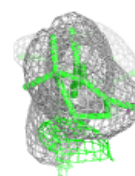
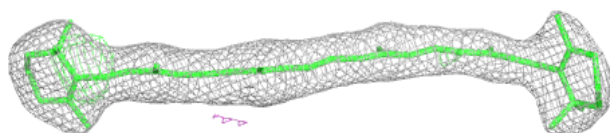
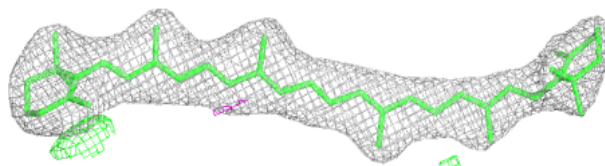
**Electron density around CLA B 607:**

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

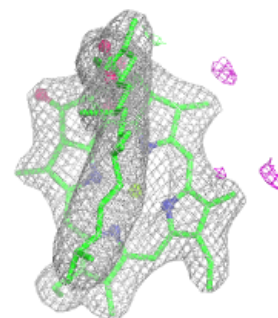
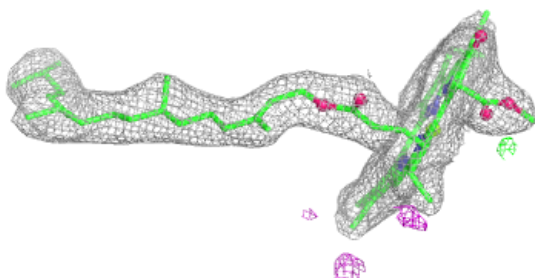
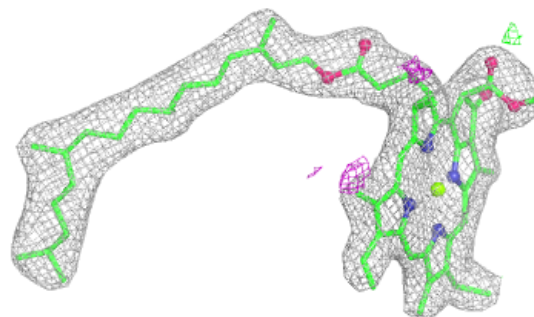


Electron density around BCR c 516:

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

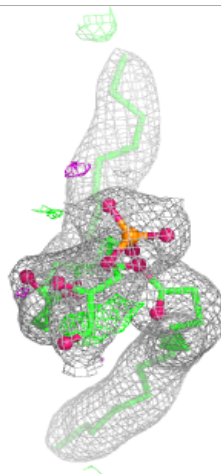
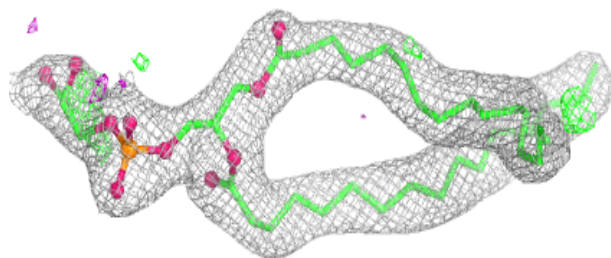
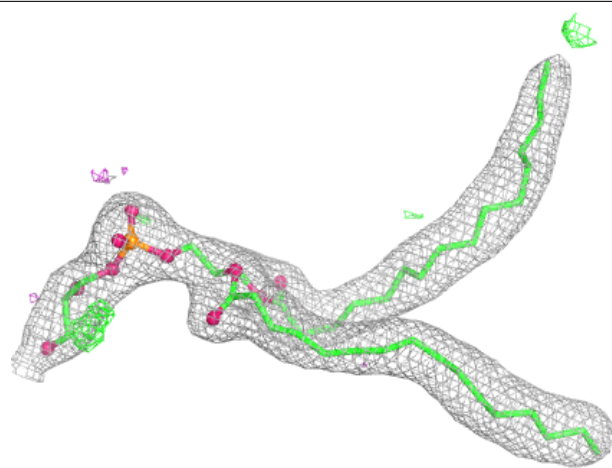
**Electron density around CLA B 609:**

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



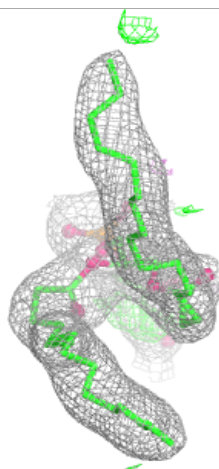
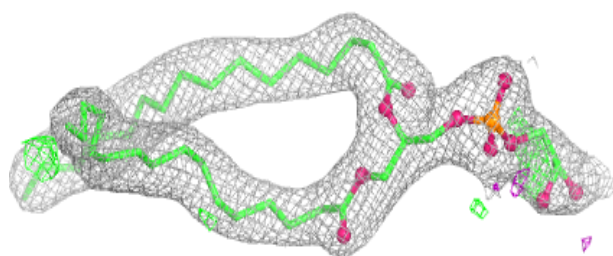
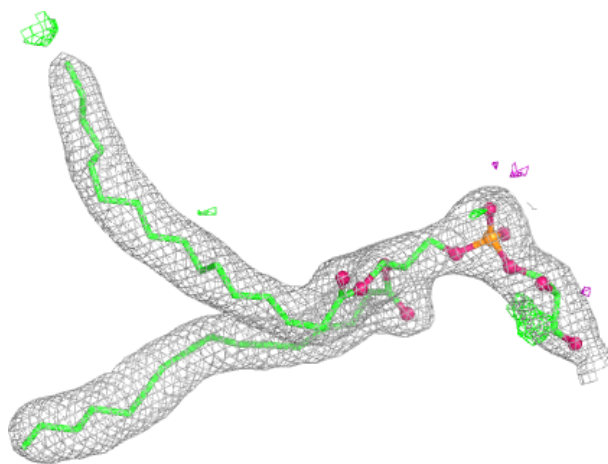
Electron density around LHG D 406 (A):

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



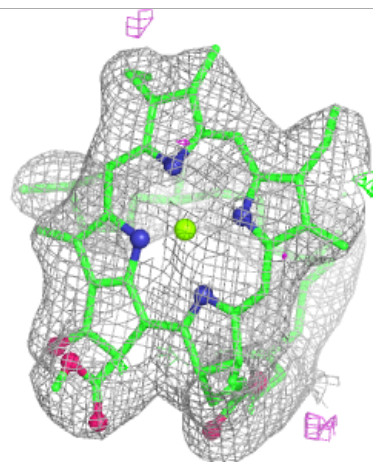
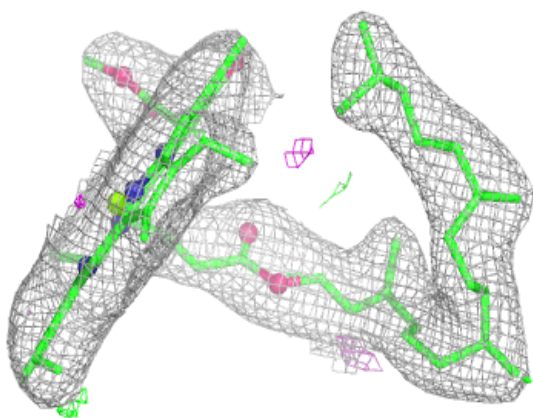
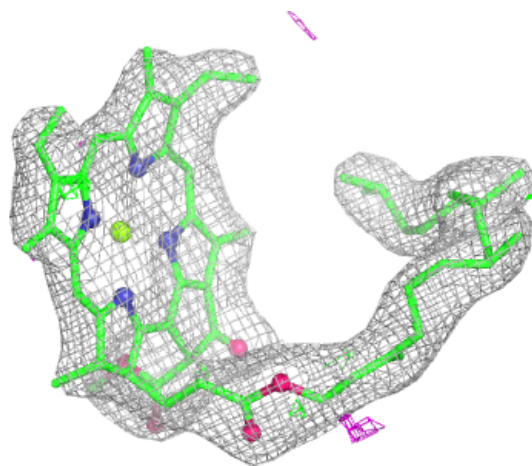
Electron density around LHG D 406 (B):

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



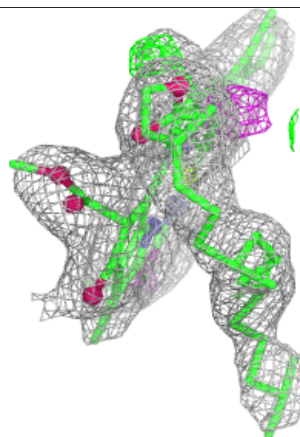
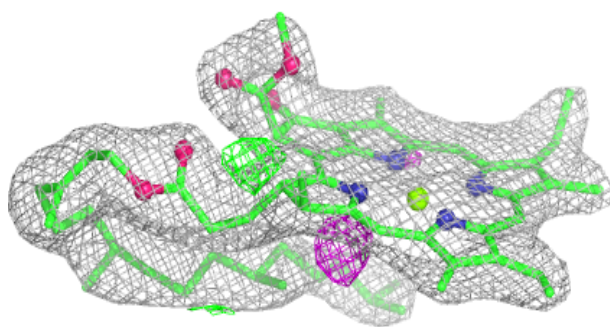
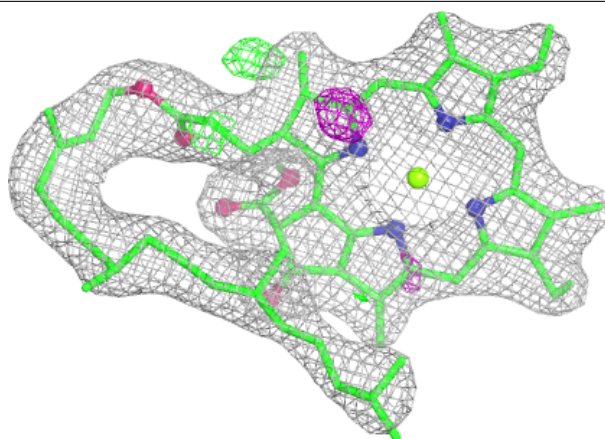
Electron density around CLA c 504:

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



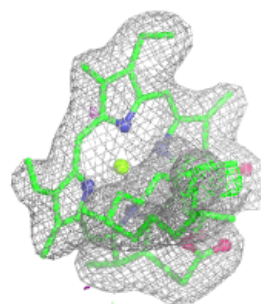
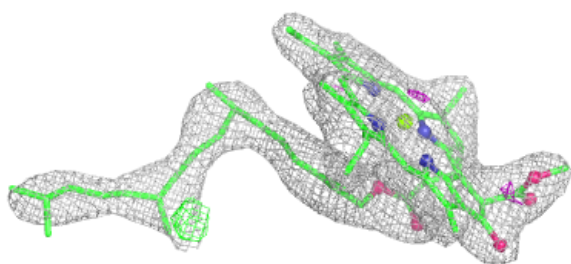
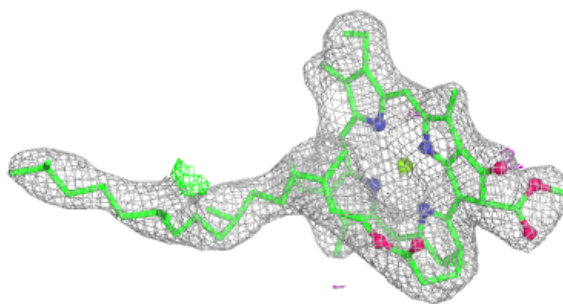
Electron density around CLA C 510:

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

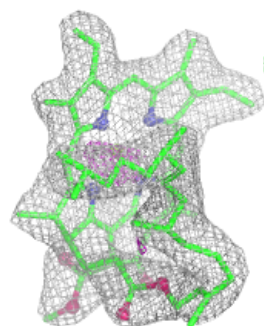
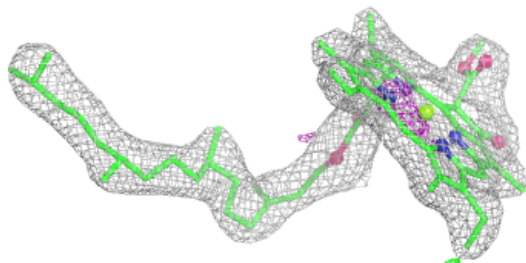
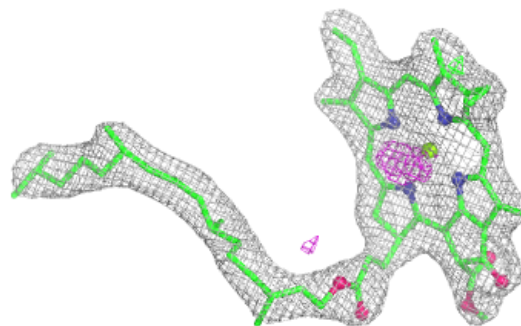


Electron density around CLA c 506:

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

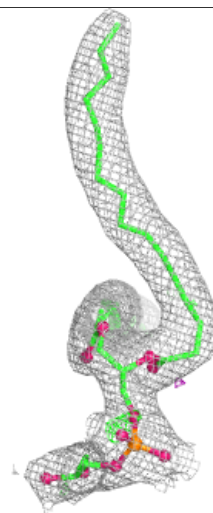
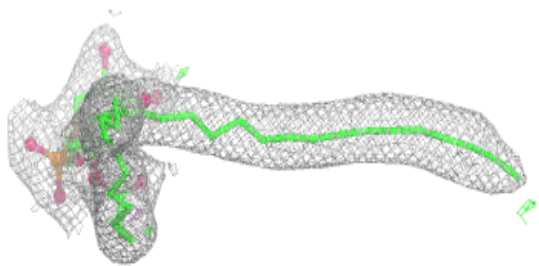
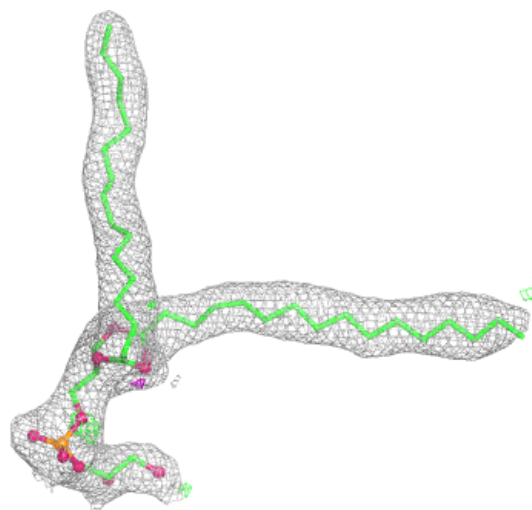
**Electron density around CLA C 512:**

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



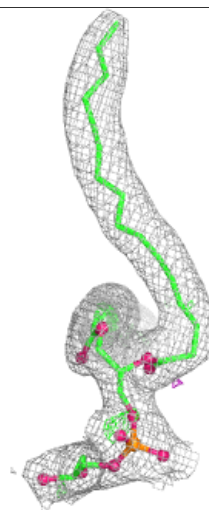
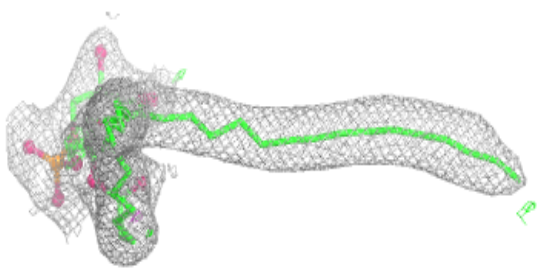
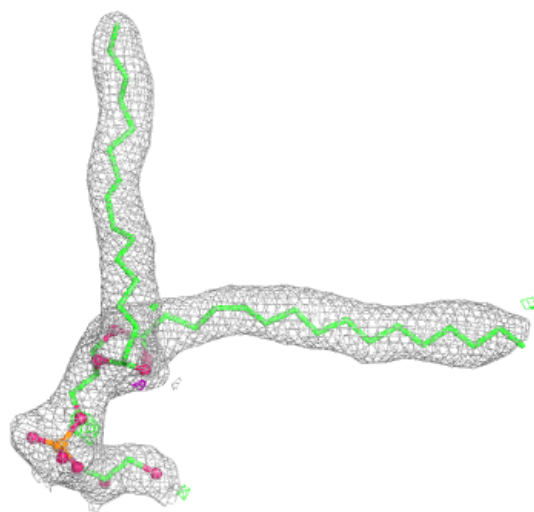
Electron density around LHG L 102 (A):

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



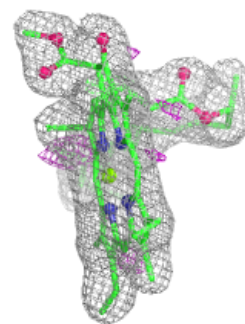
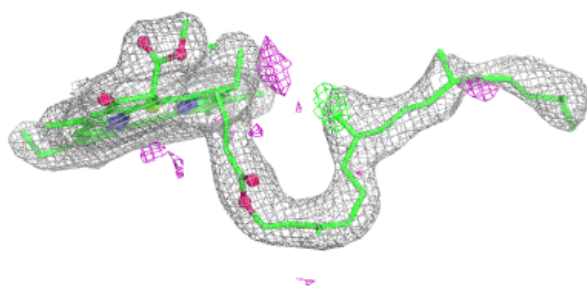
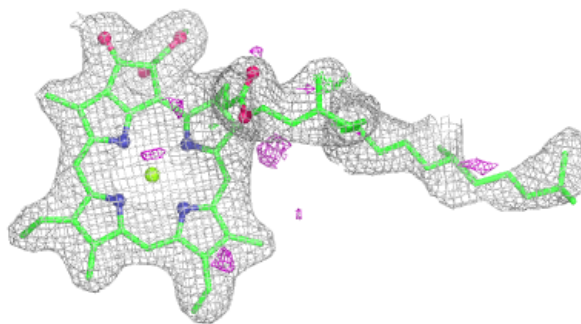
Electron density around LHG L 102 (B):

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

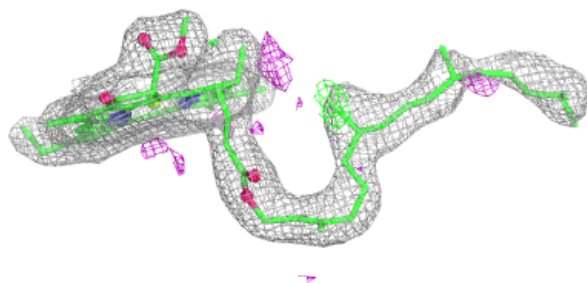
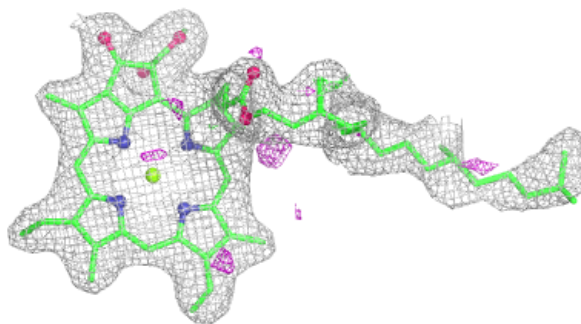


Electron density around CLA A 406 (A):

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

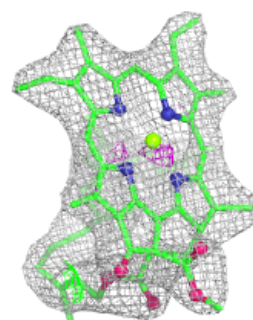
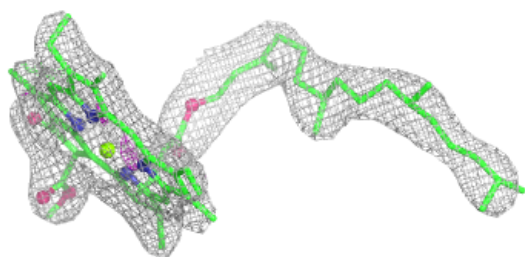
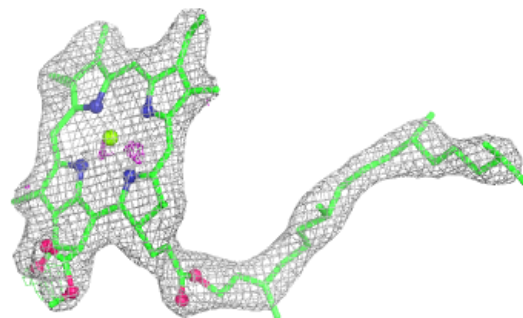
**Electron density around CLA A 406 (B):**

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

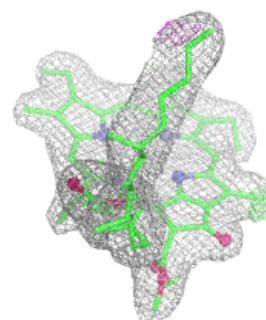
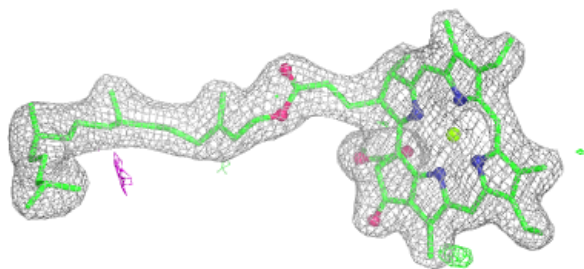
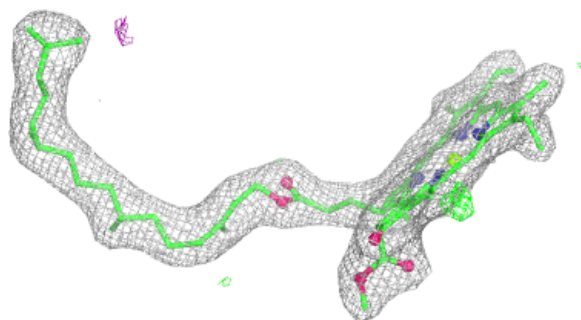


Electron density around CLA c 512:

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

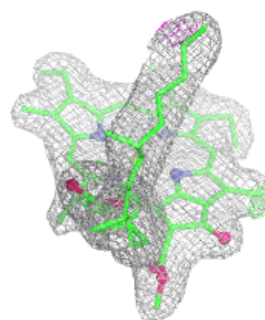
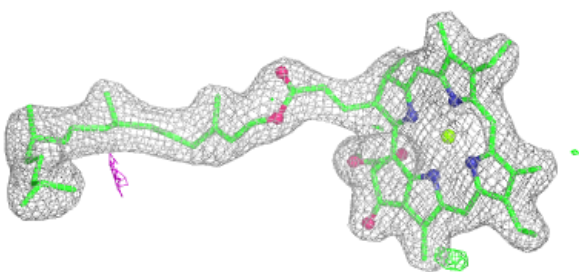
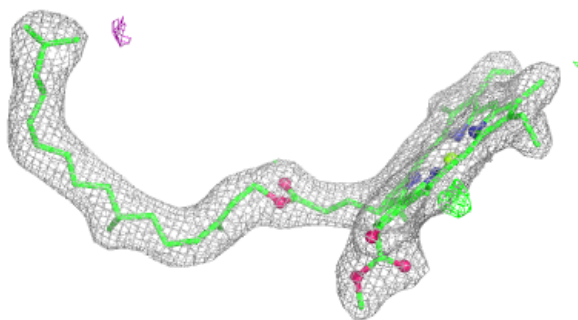
**Electron density around CLA D 402 (A):**

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



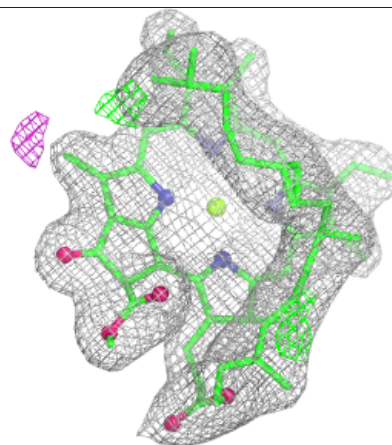
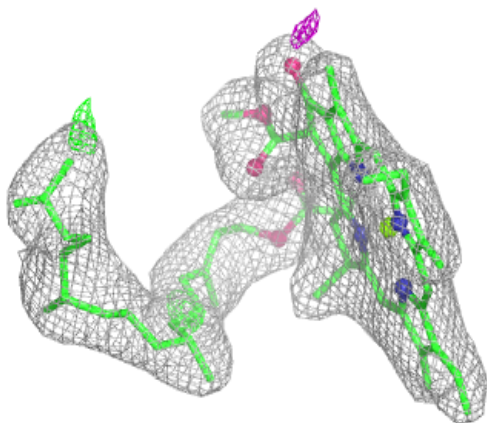
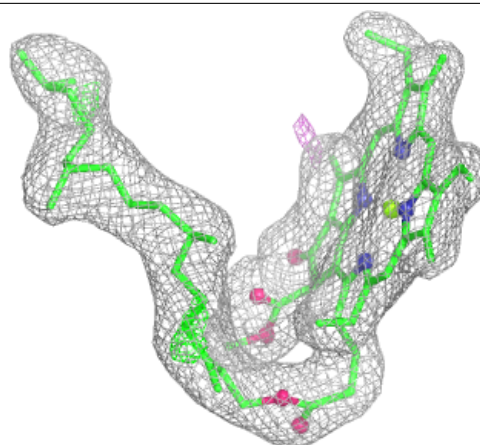
Electron density around CLA D 402 (B):

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

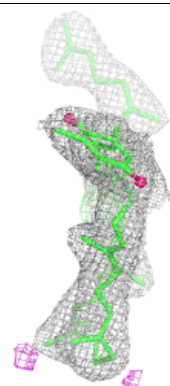
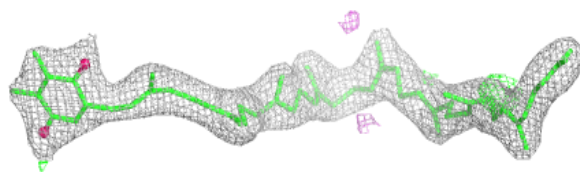
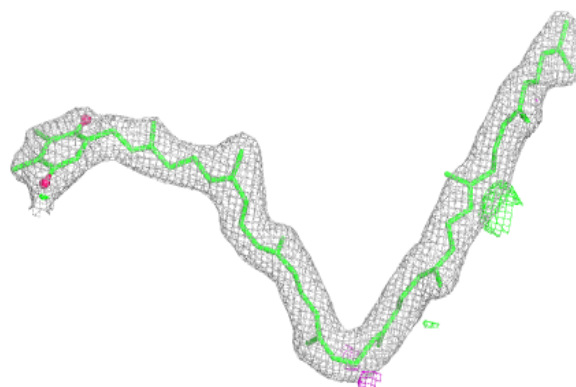


Electron density around CLA B 613:

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

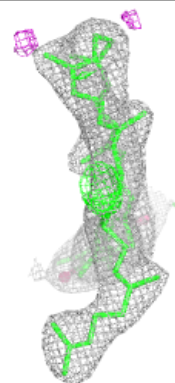
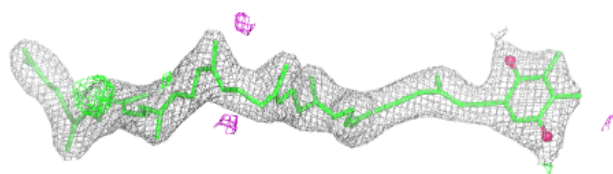
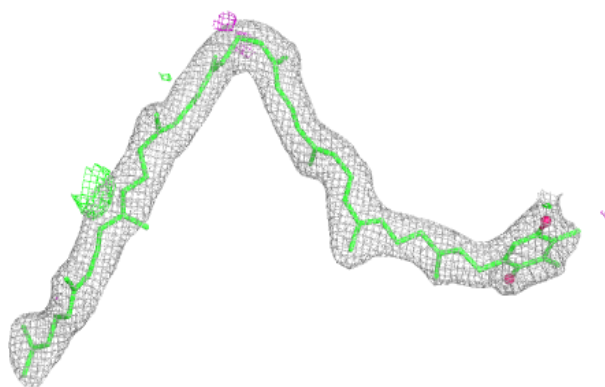
**Electron density around PL9 d 405 (A):**

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



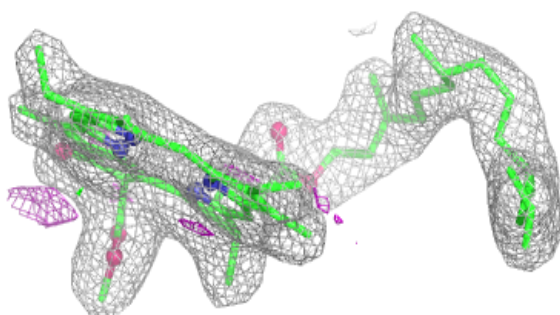
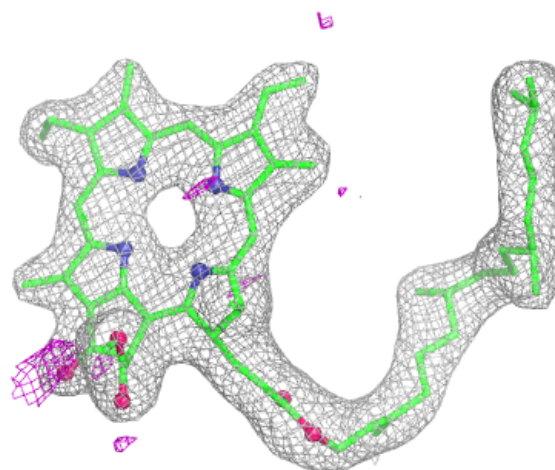
Electron density around PL9 d 405 (B):

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



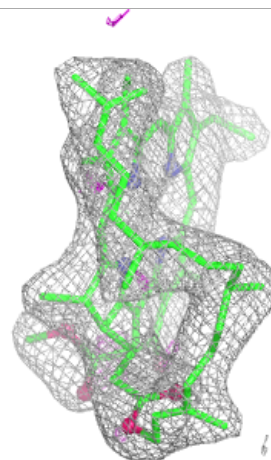
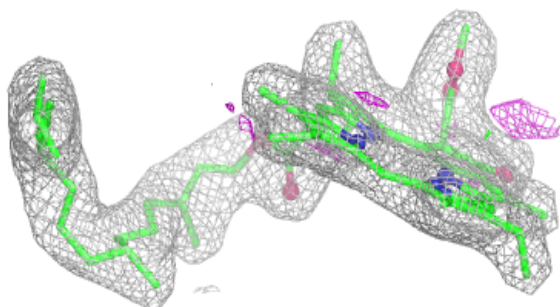
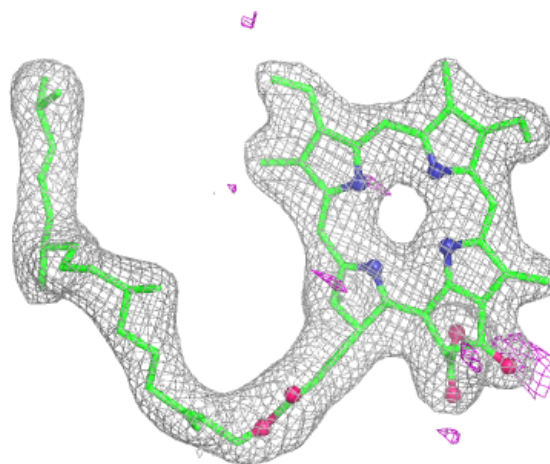
Electron density around PHO A 417 (A):

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



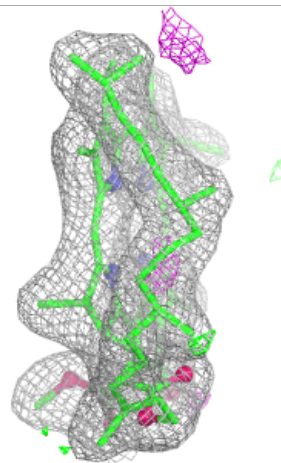
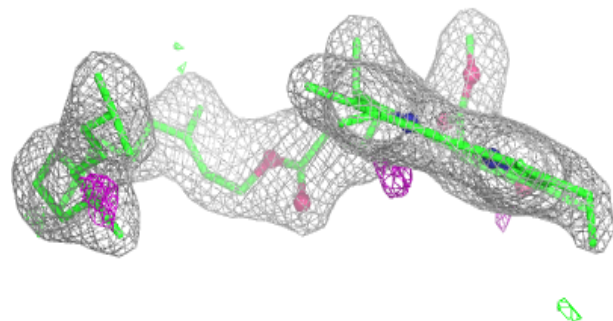
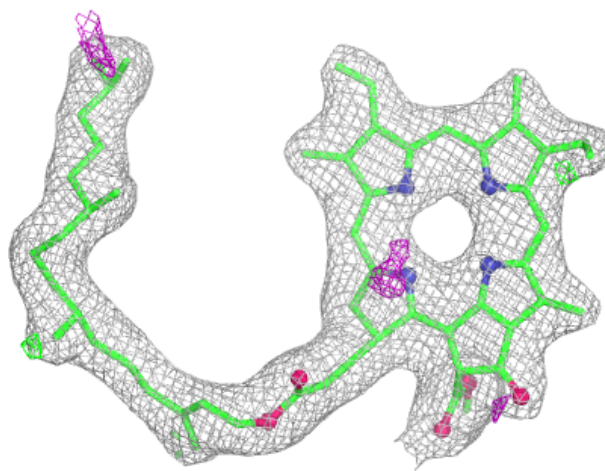
Electron density around PHO A 417 (B):

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



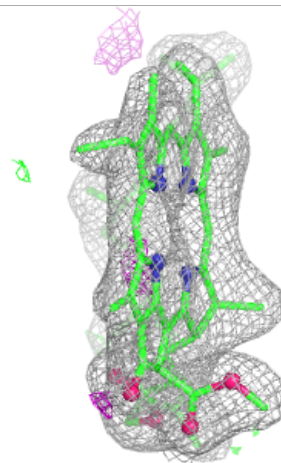
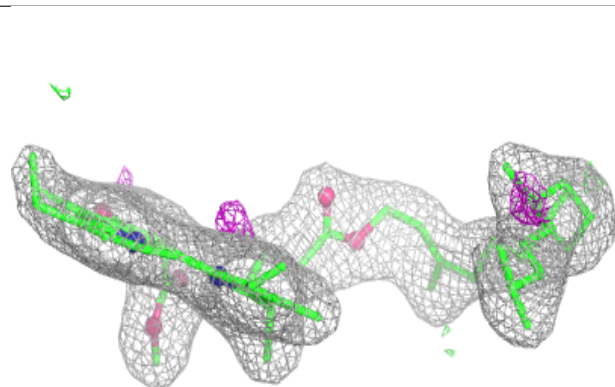
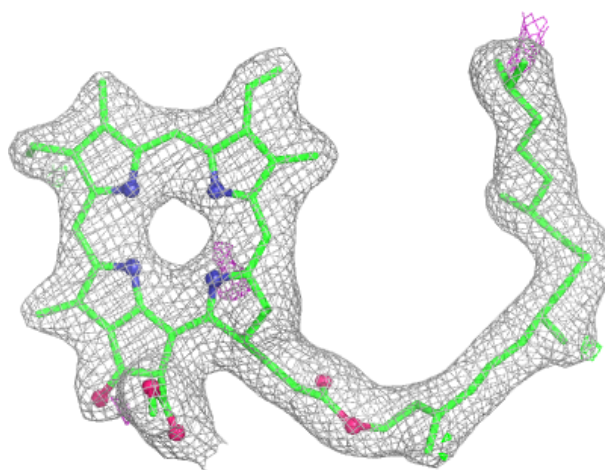
Electron density around PHO a 407 (A):

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



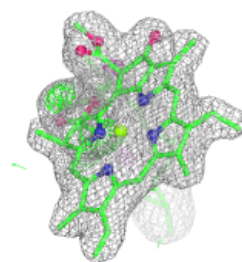
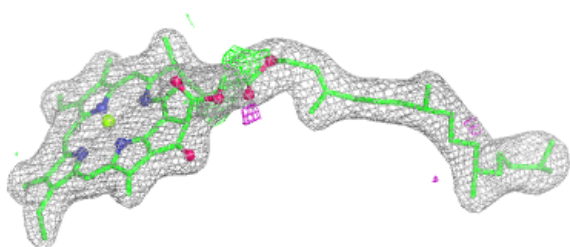
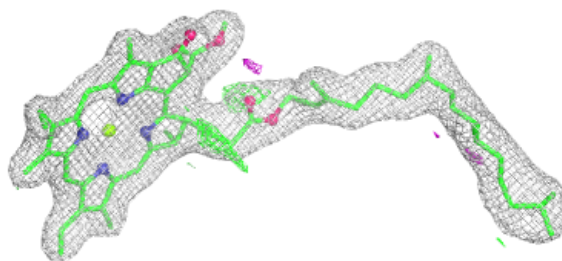
Electron density around PHO a 407 (B):

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

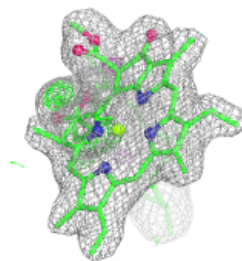
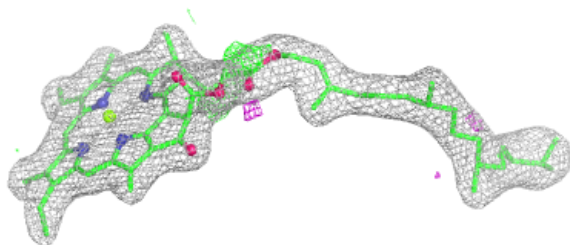
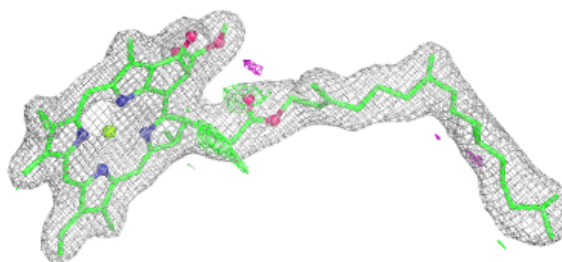


Electron density around CLA A 404 (A):

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

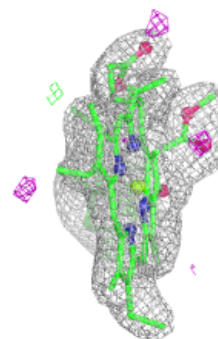
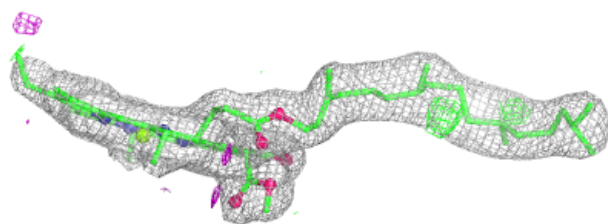
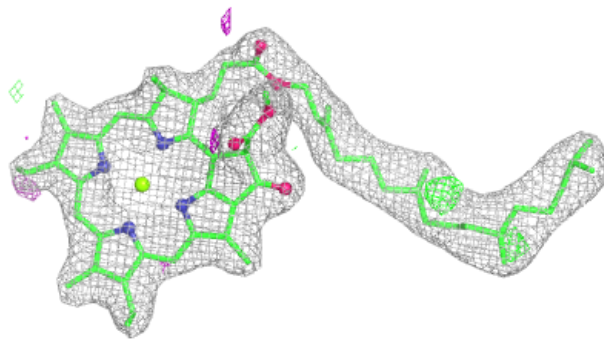
**Electron density around CLA A 404 (B):**

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

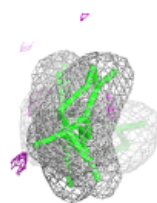
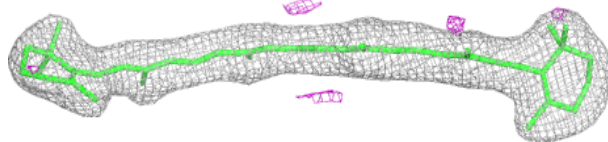
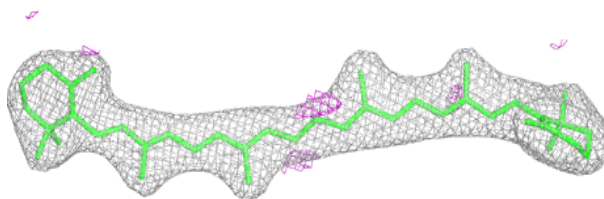


Electron density around CLA B 602:

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

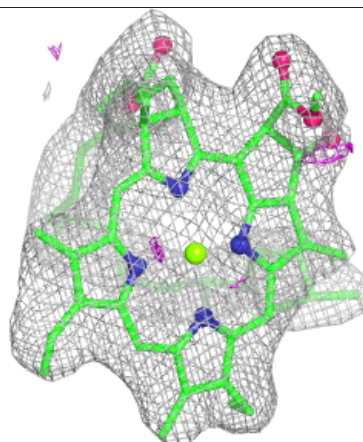
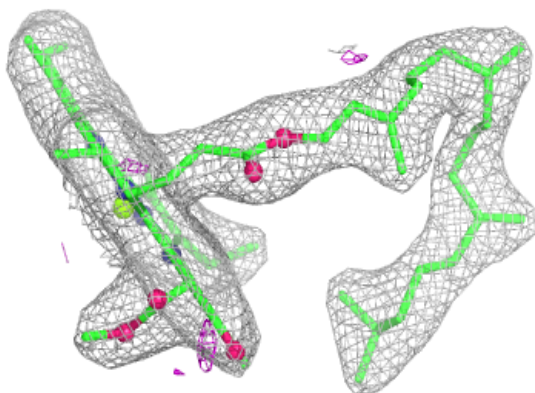
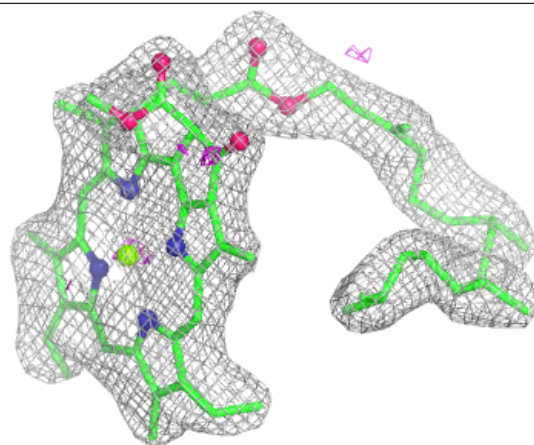
**Electron density around BCR B 617:**

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

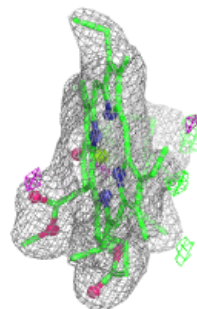
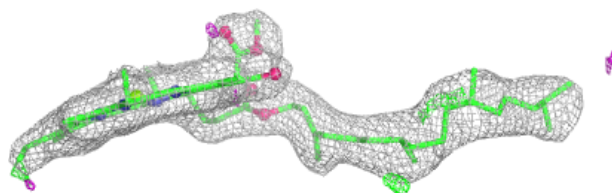
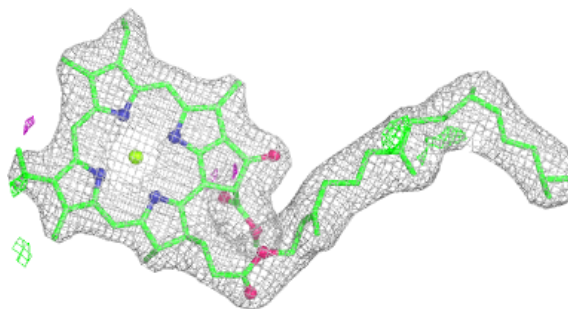


Electron density around CLA C 504:

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

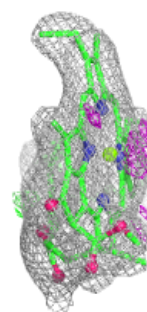
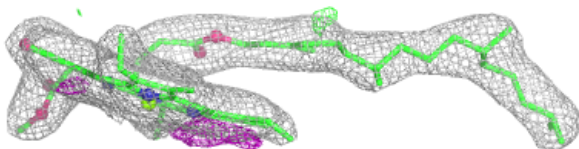
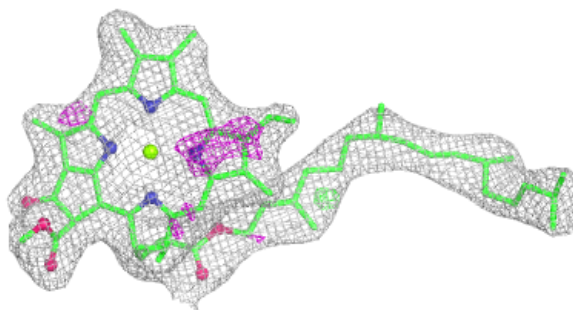
**Electron density around CLA b 602:**

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

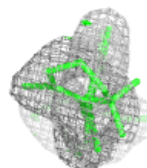
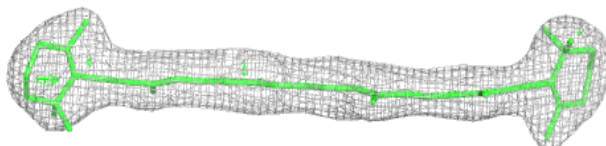
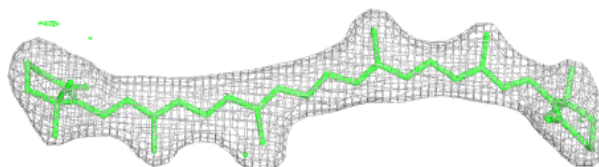


Electron density around CLA b 603:

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

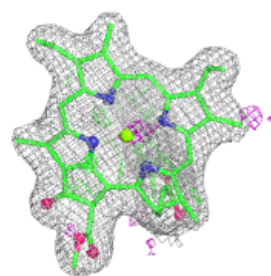
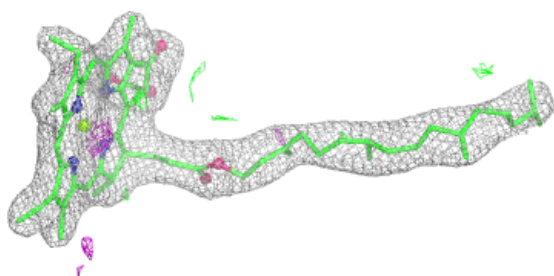
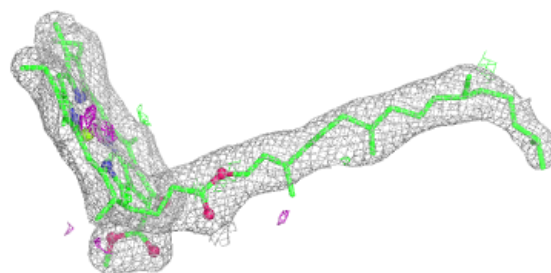
**Electron density around BCR C 516:**

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

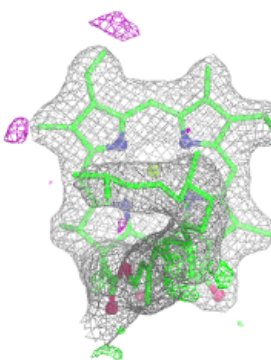
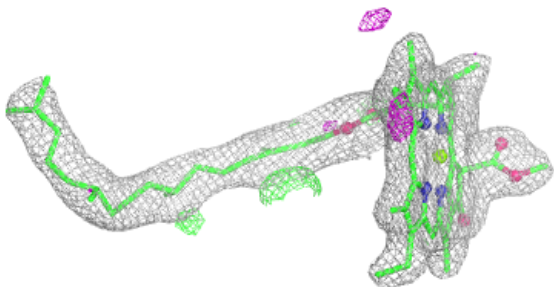
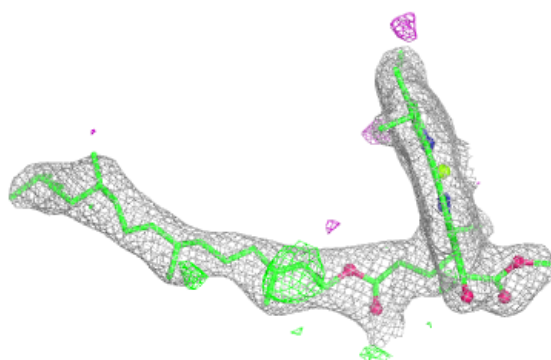


Electron density around CLA b 604:

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

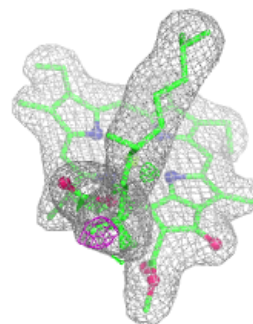
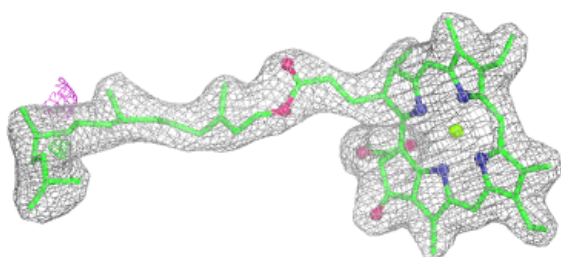
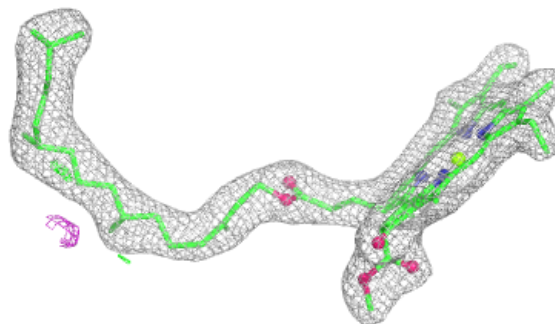
**Electron density around CLA b 605:**

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

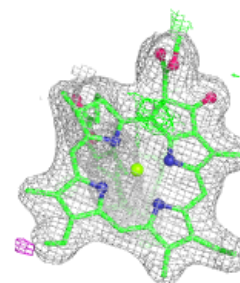
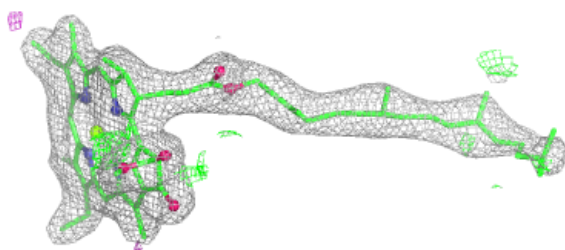
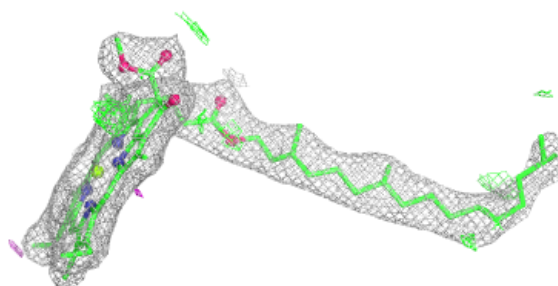


Electron density around CLA d 402 (B):

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

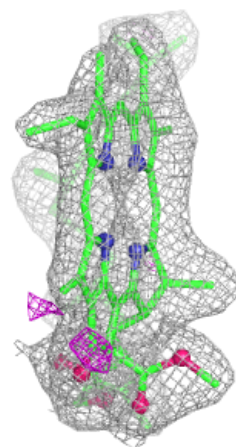
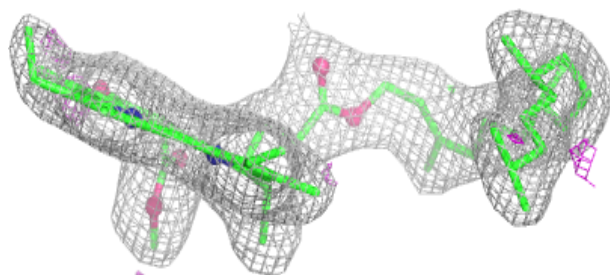
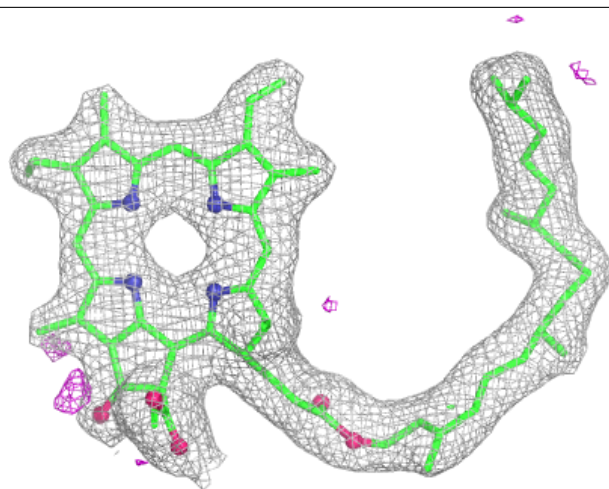
**Electron density around CLA B 604:**

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



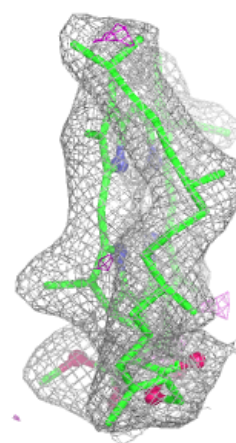
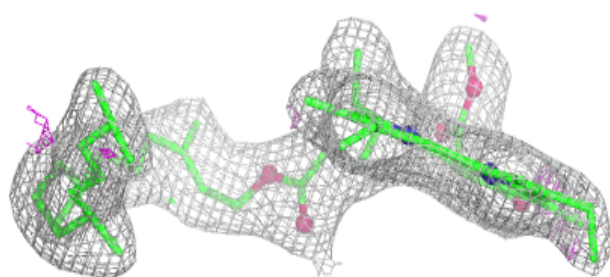
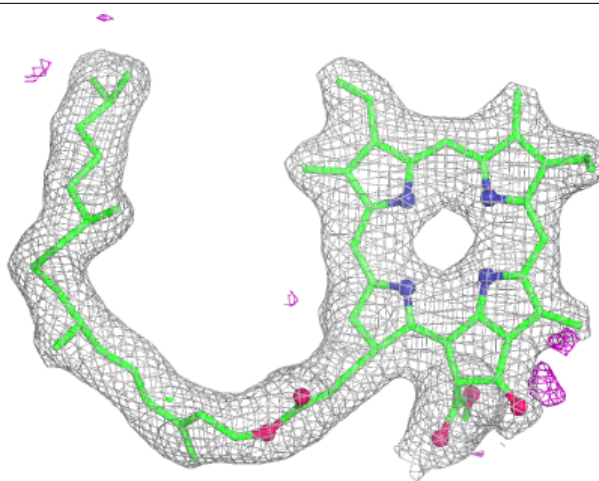
Electron density around PHO A 407 (A):

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



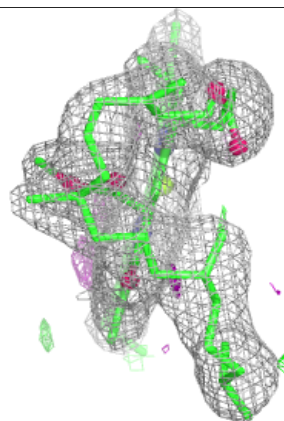
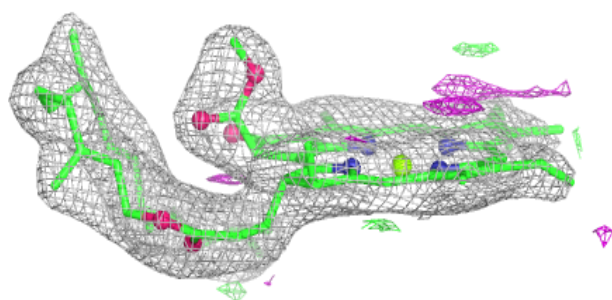
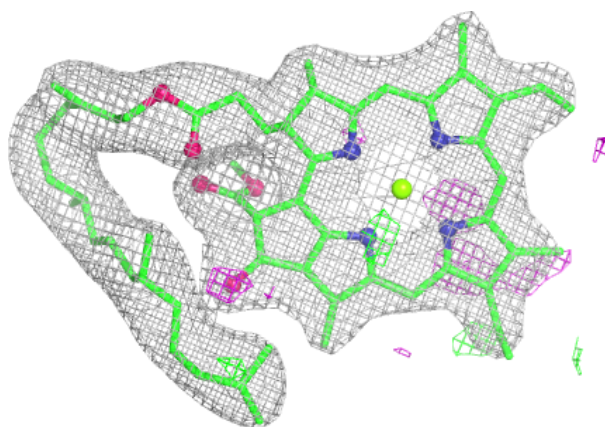
Electron density around PHO A 407 (B):

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

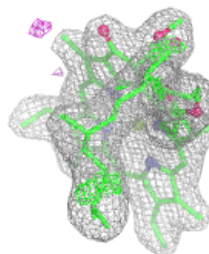
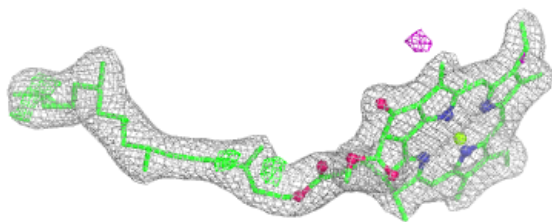
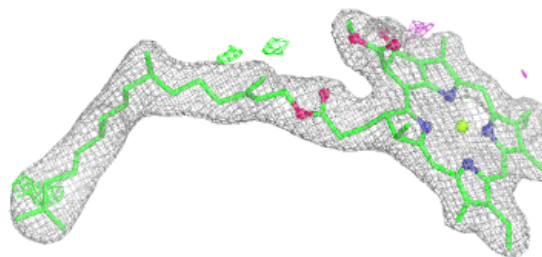


Electron density around CLA b 610:

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

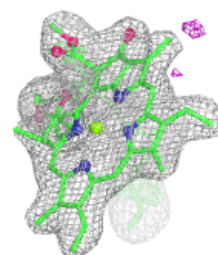
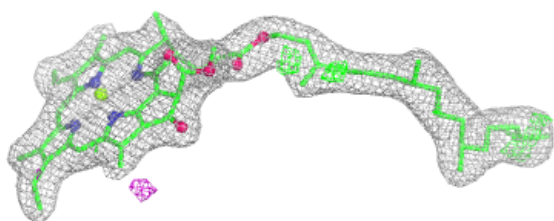
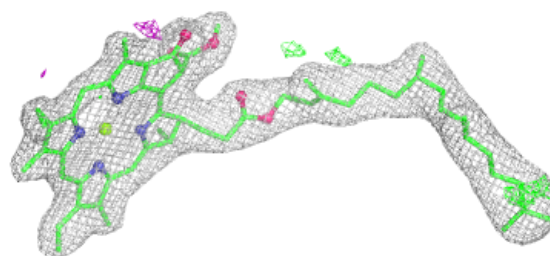
**Electron density around CLA a 404 (A):**

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

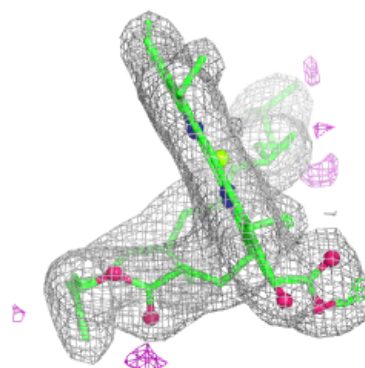
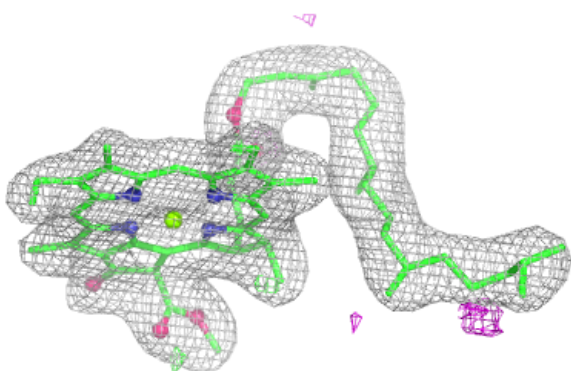
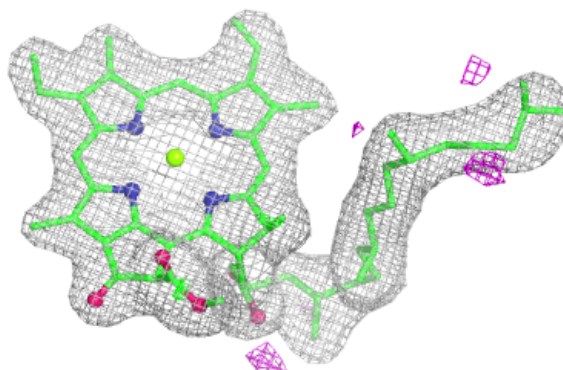


Electron density around CLA a 404 (B):

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

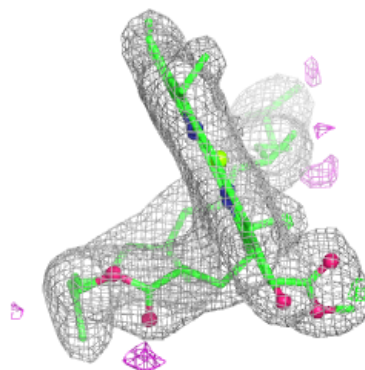
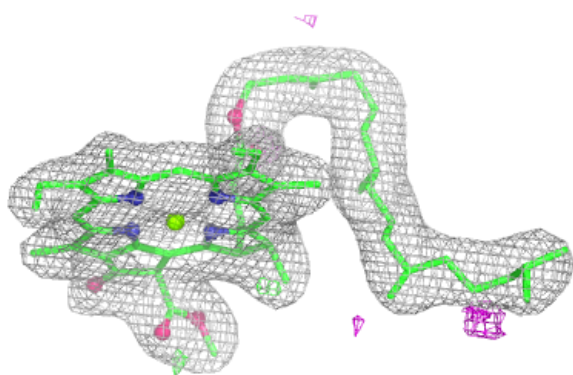
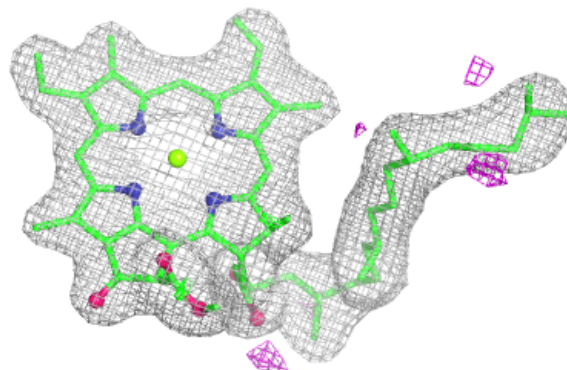
**Electron density around CLA a 405 (A):**

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



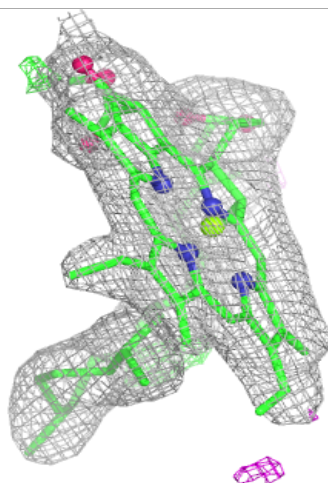
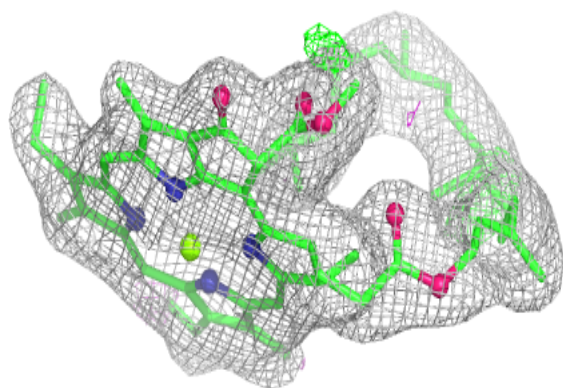
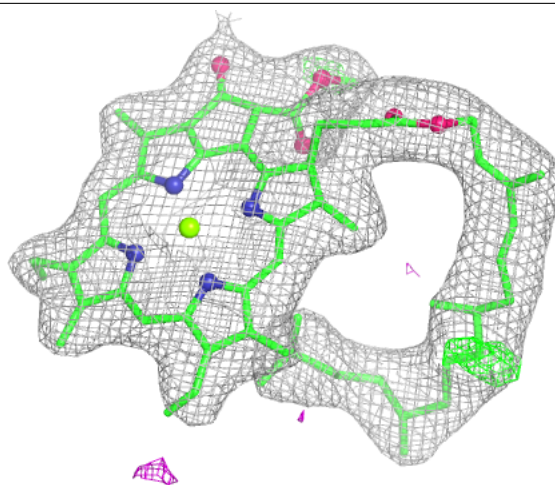
Electron density around CLA a 405 (B):

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



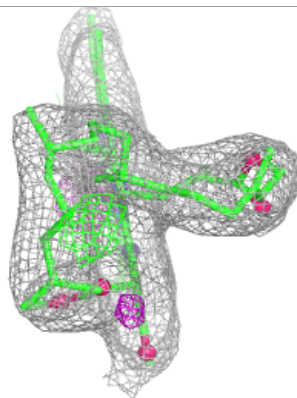
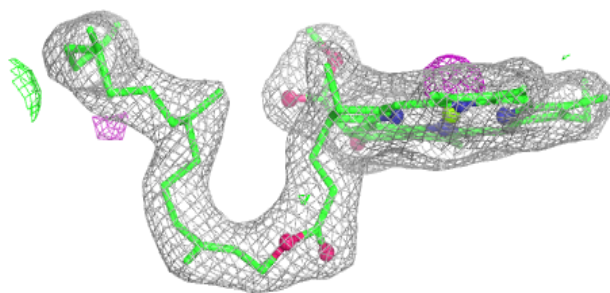
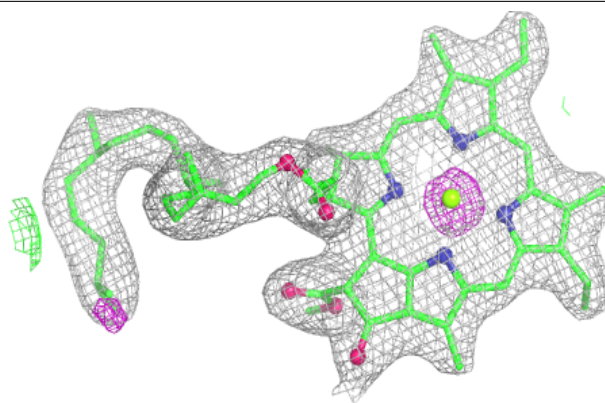
Electron density around CLA b 615:

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

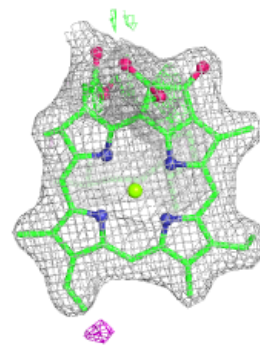
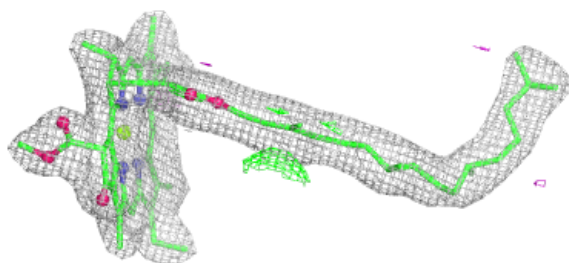
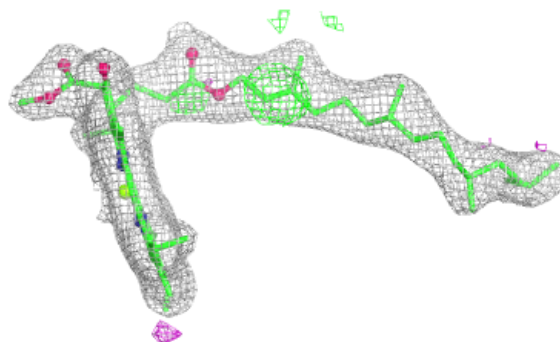


Electron density around CLA B 612:

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

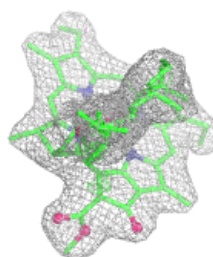
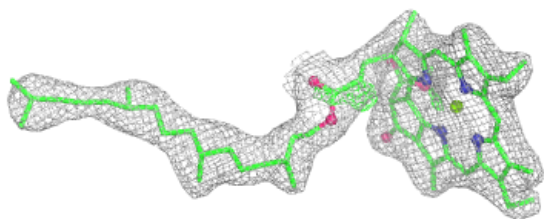
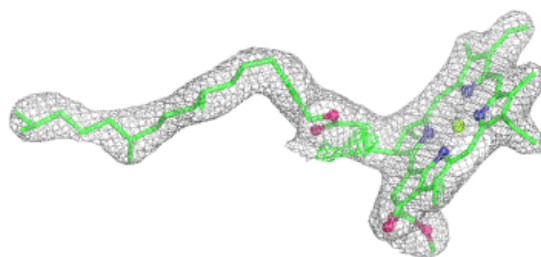
**Electron density around CLA B 605:**

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



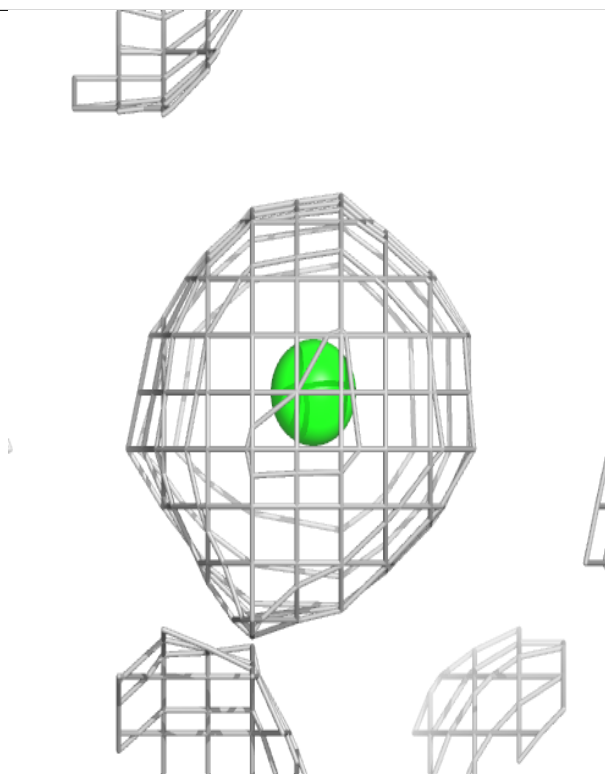
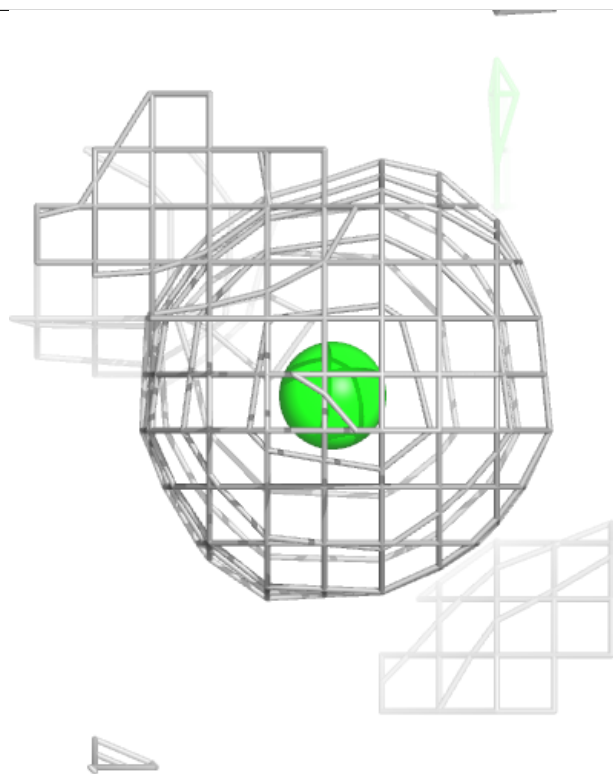
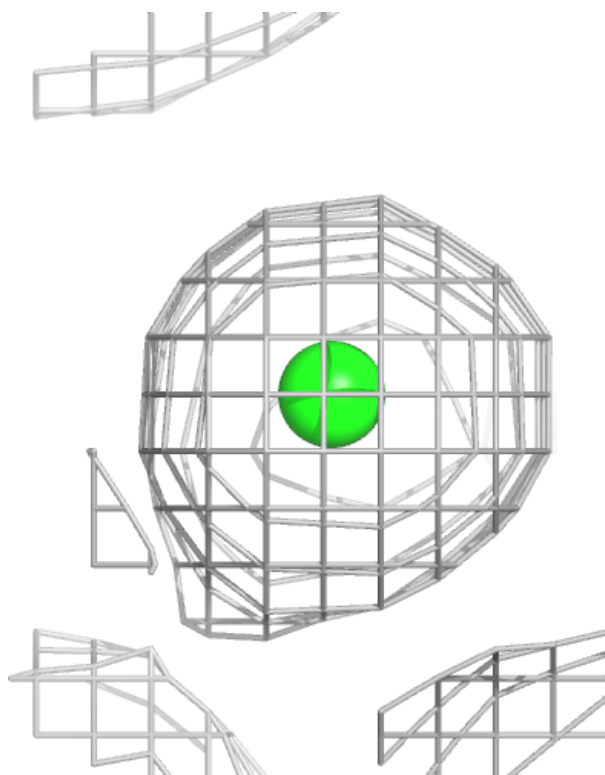
Electron density around CLA c 503:

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



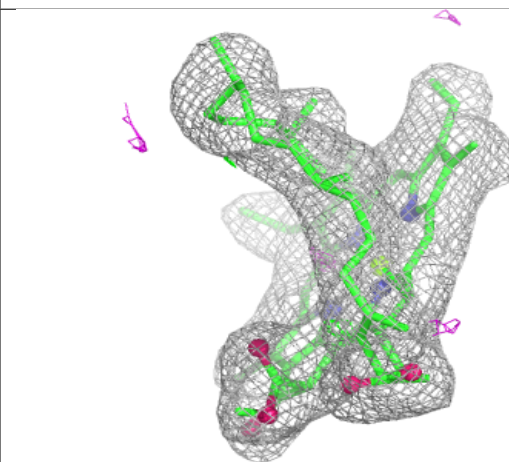
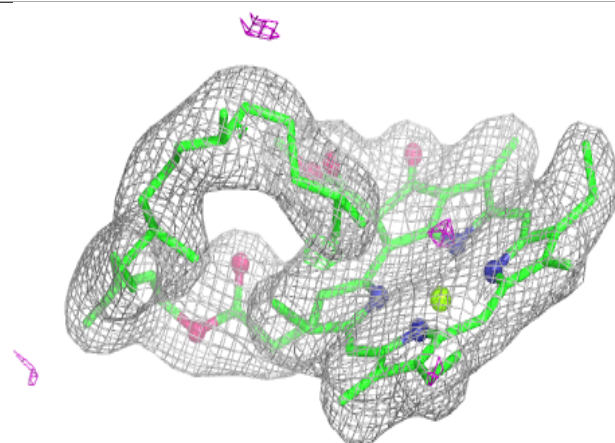
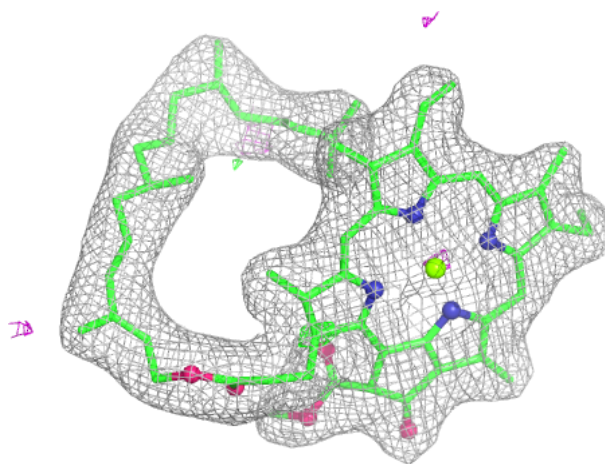
Electron density around CL a 402 (A):

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



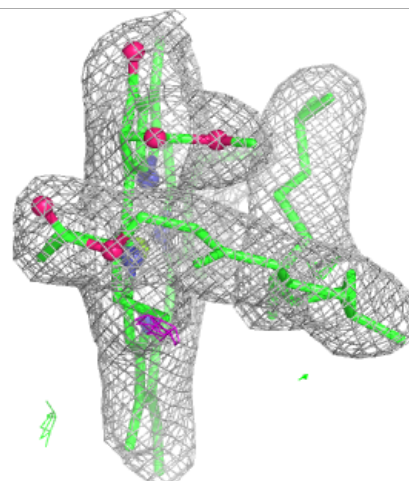
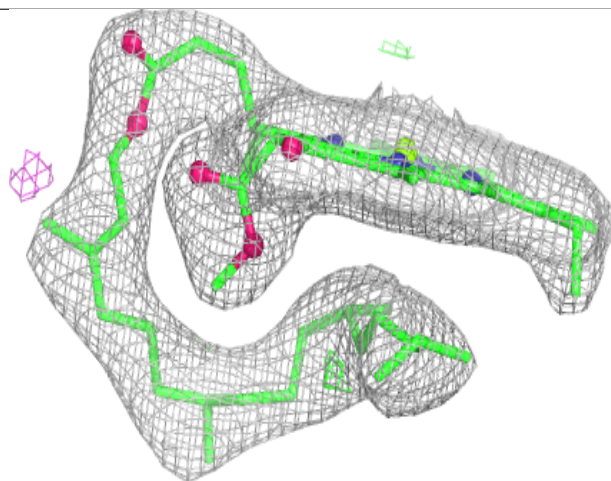
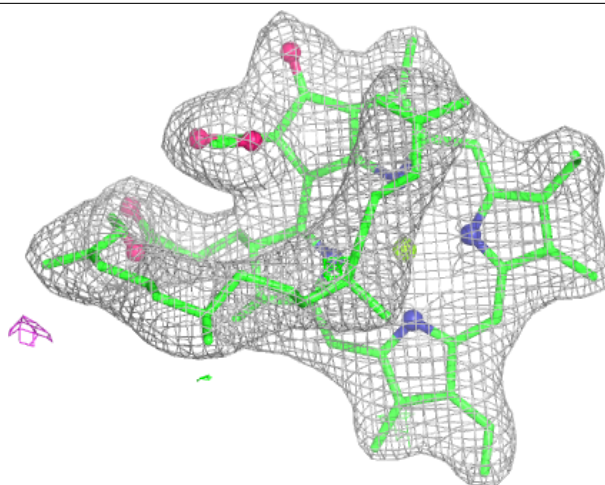
Electron density around CLA B 615:

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



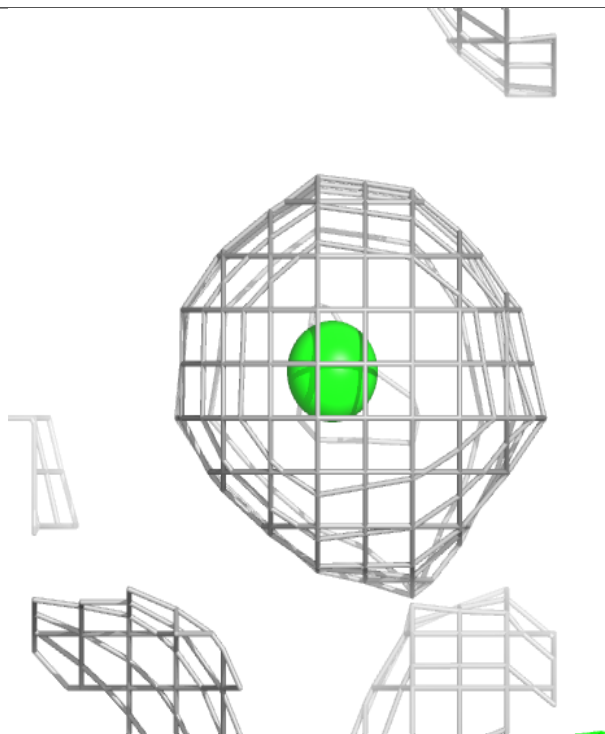
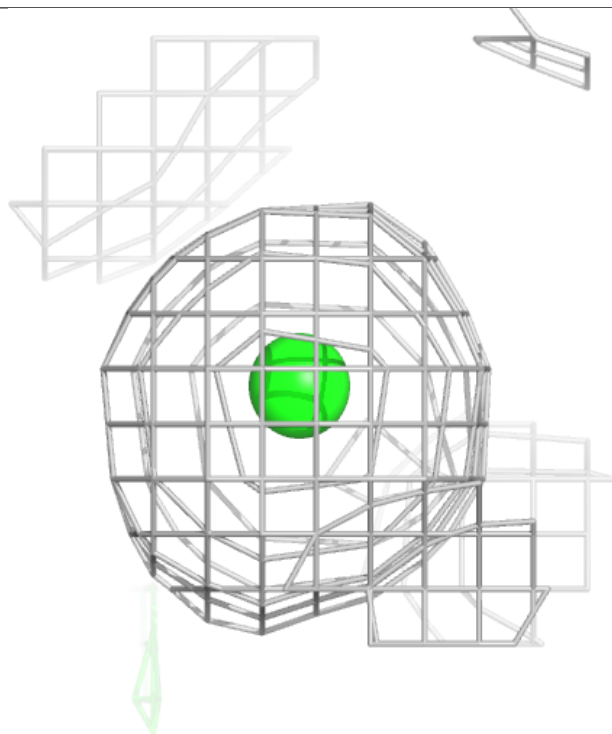
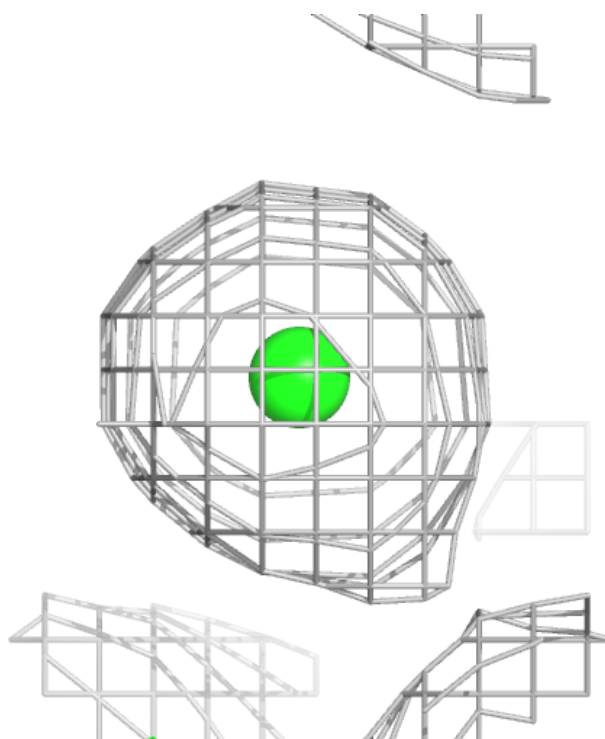
Electron density around CLA C 511:

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



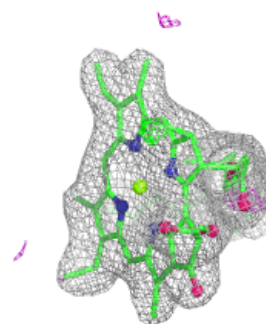
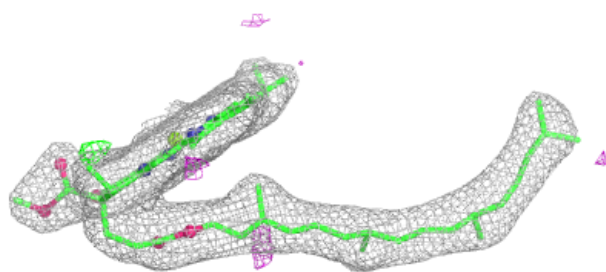
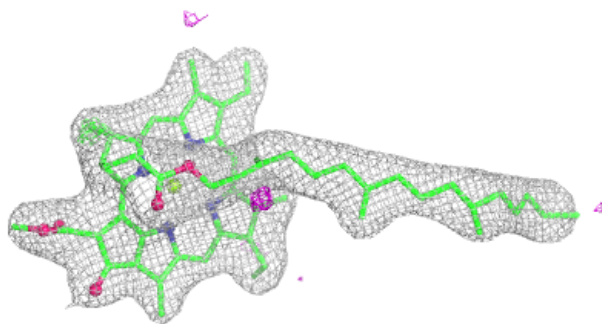
Electron density around CL a 402 (B):

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

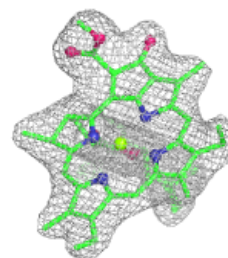
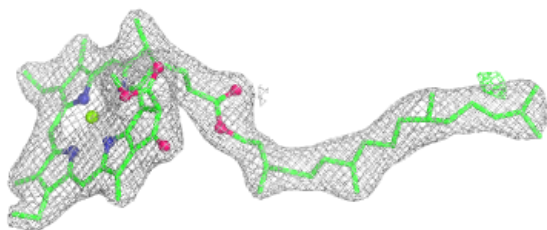
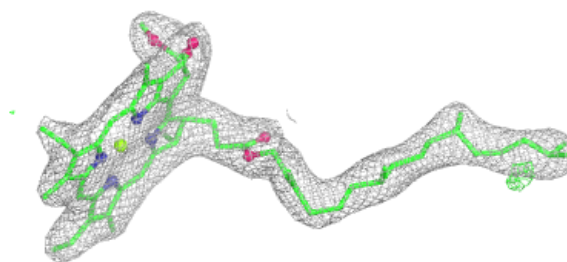


Electron density around CLA B 608:

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

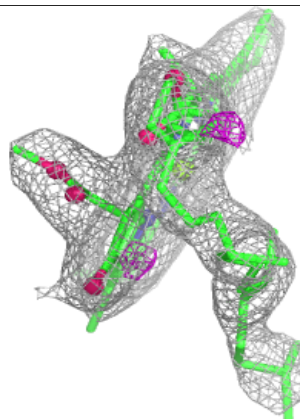
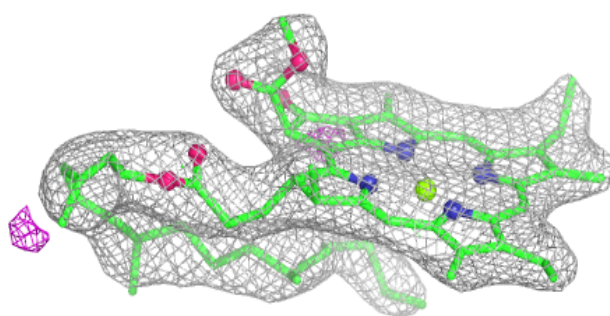
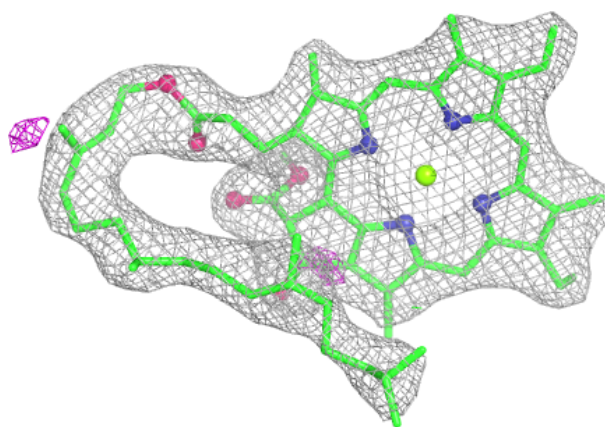
**Electron density around CLA C 503:**

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



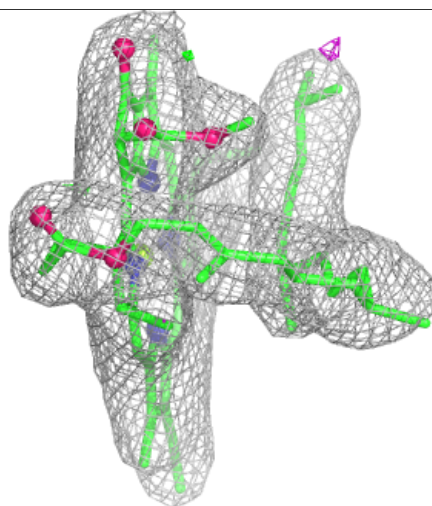
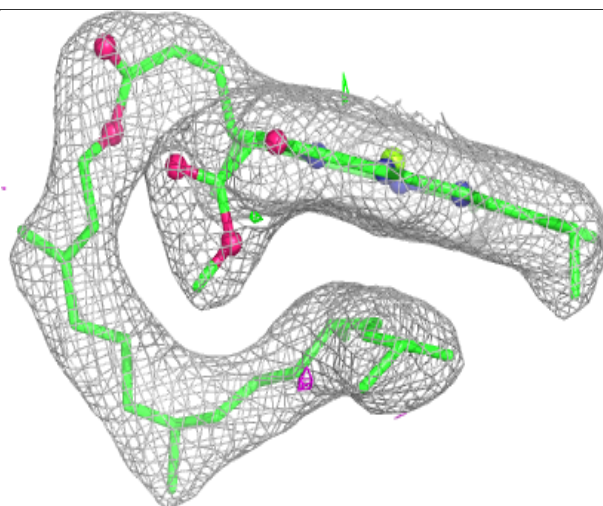
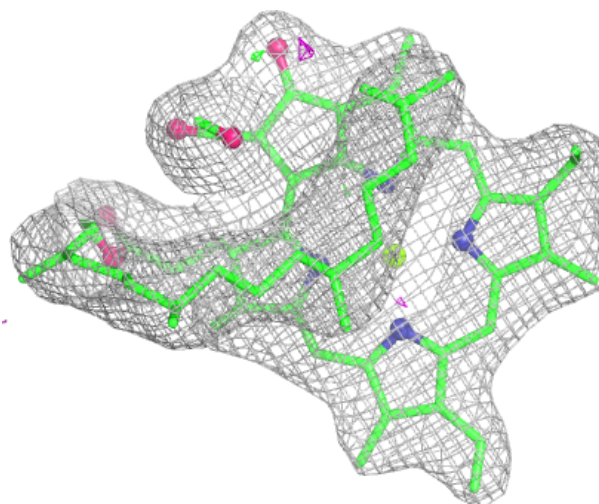
Electron density around CLA c 510:

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



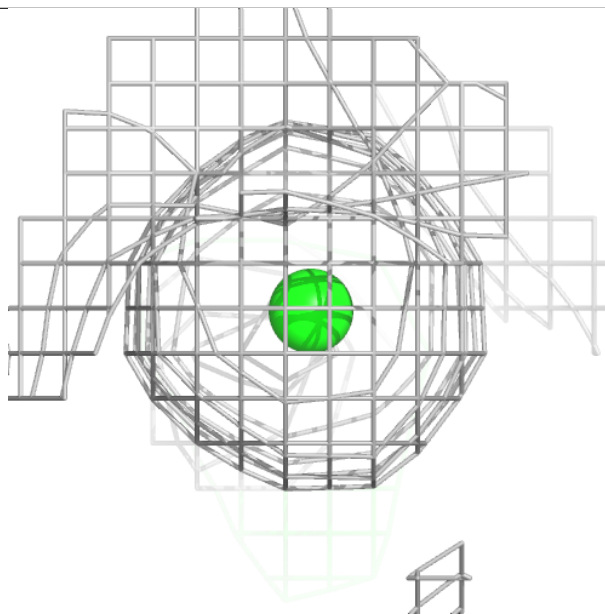
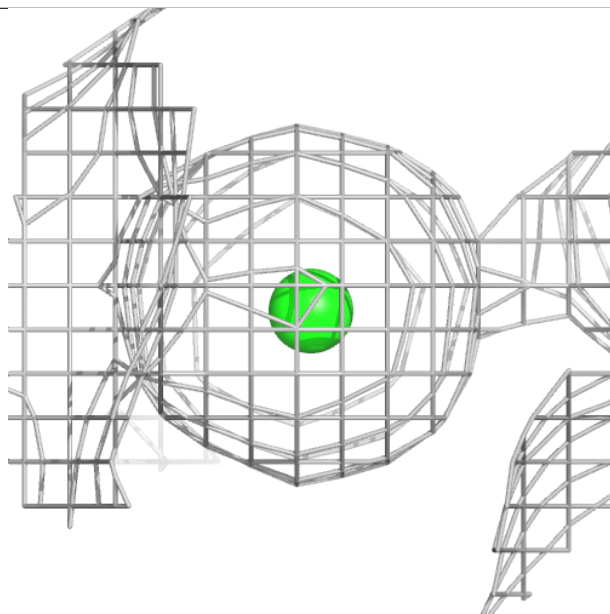
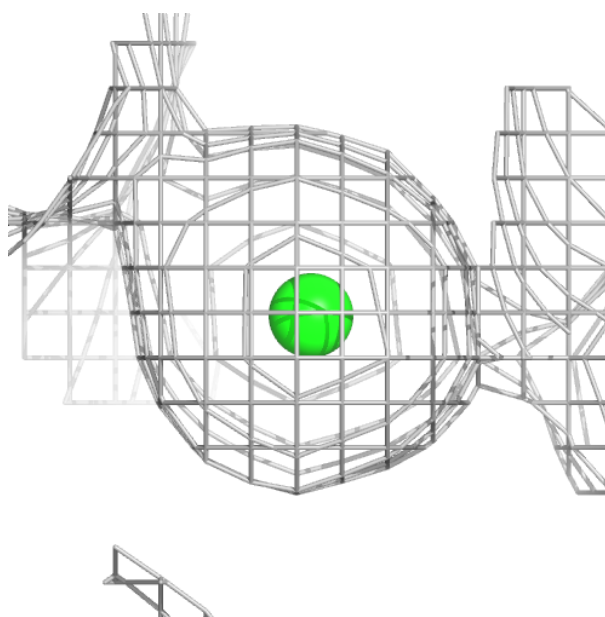
Electron density around CLA c 511:

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



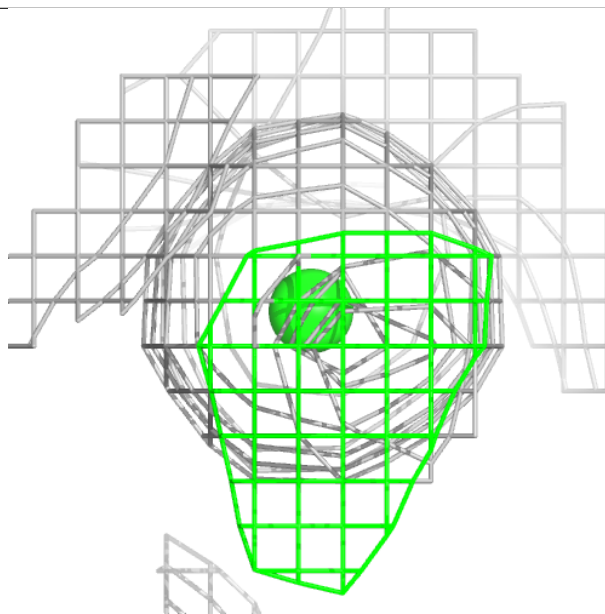
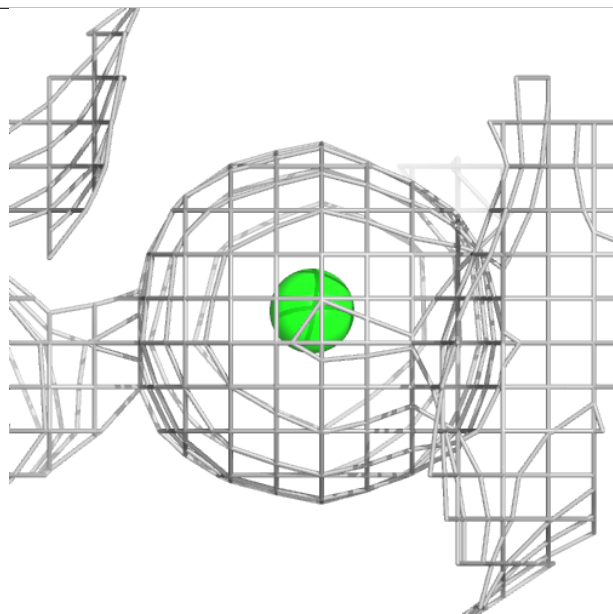
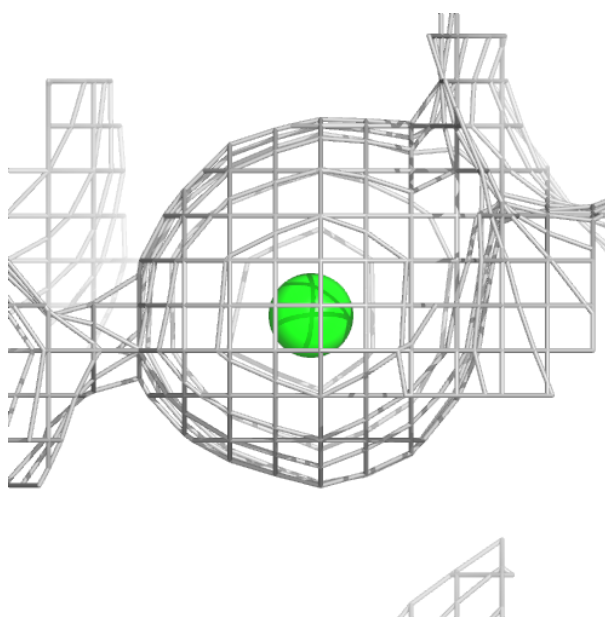
Electron density around CL A 403 (A):

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



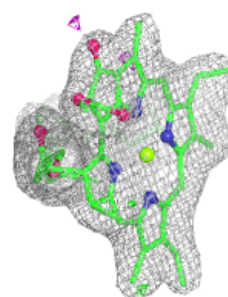
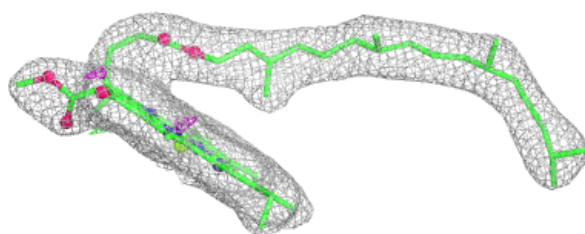
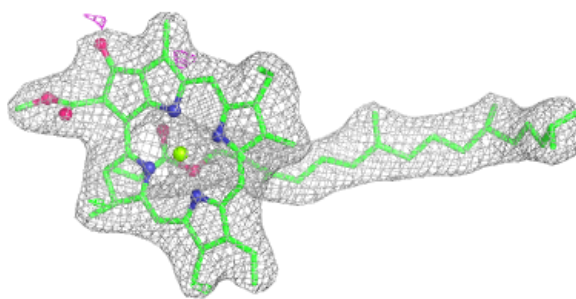
Electron density around CL A 403 (B):

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

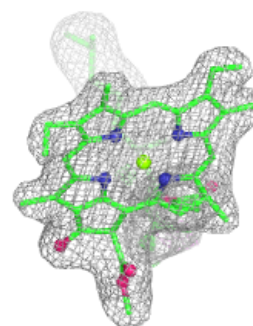
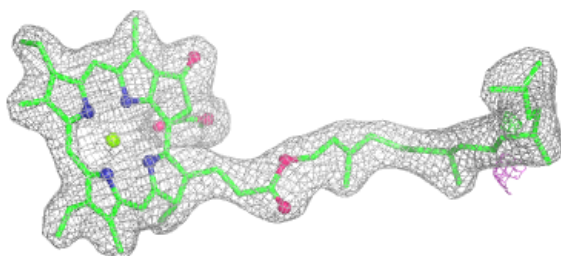
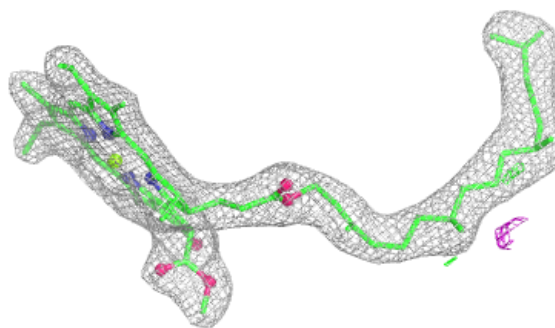


Electron density around CLA b 608:

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

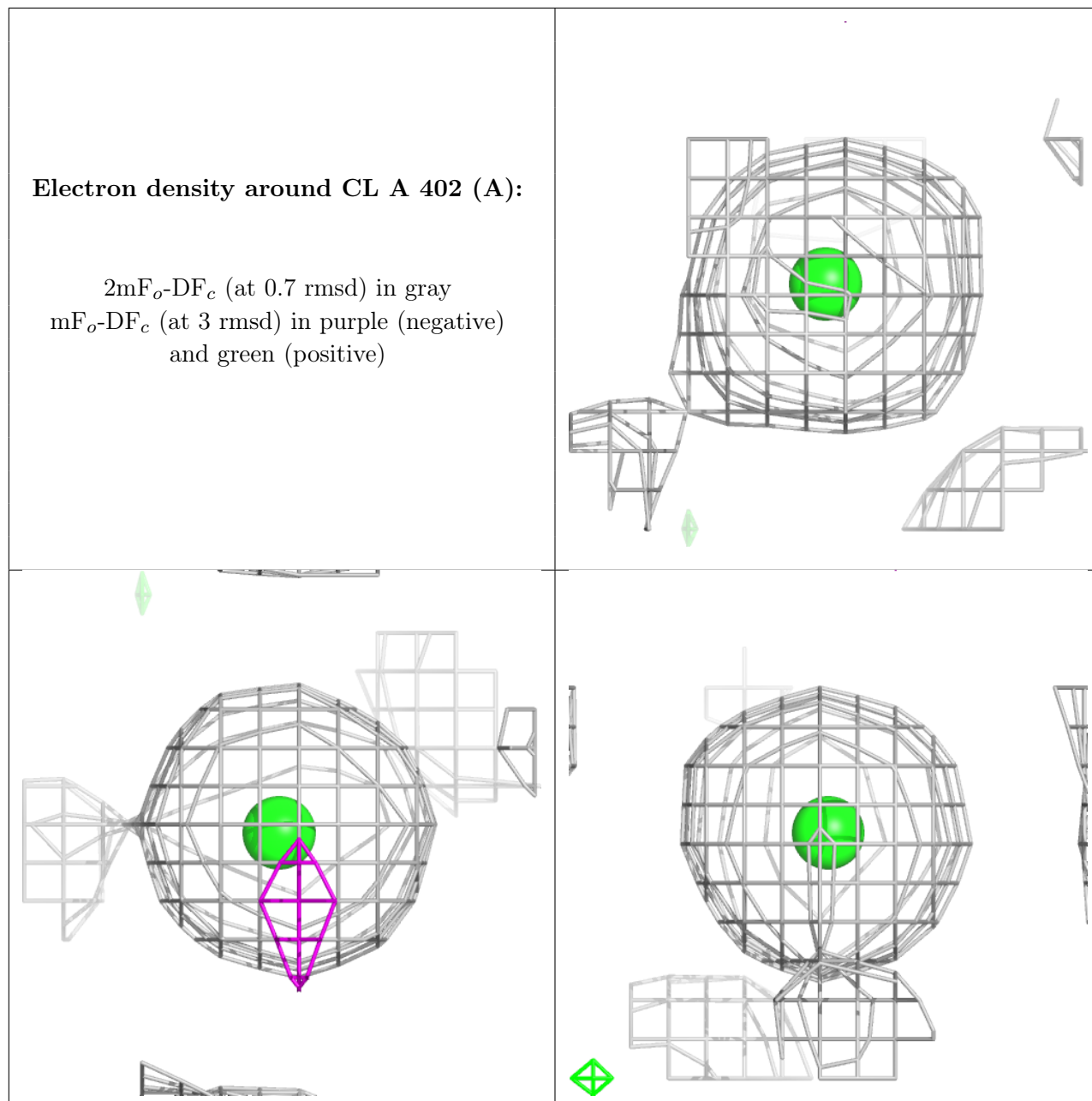
**Electron density around CLA d 402 (A):**

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



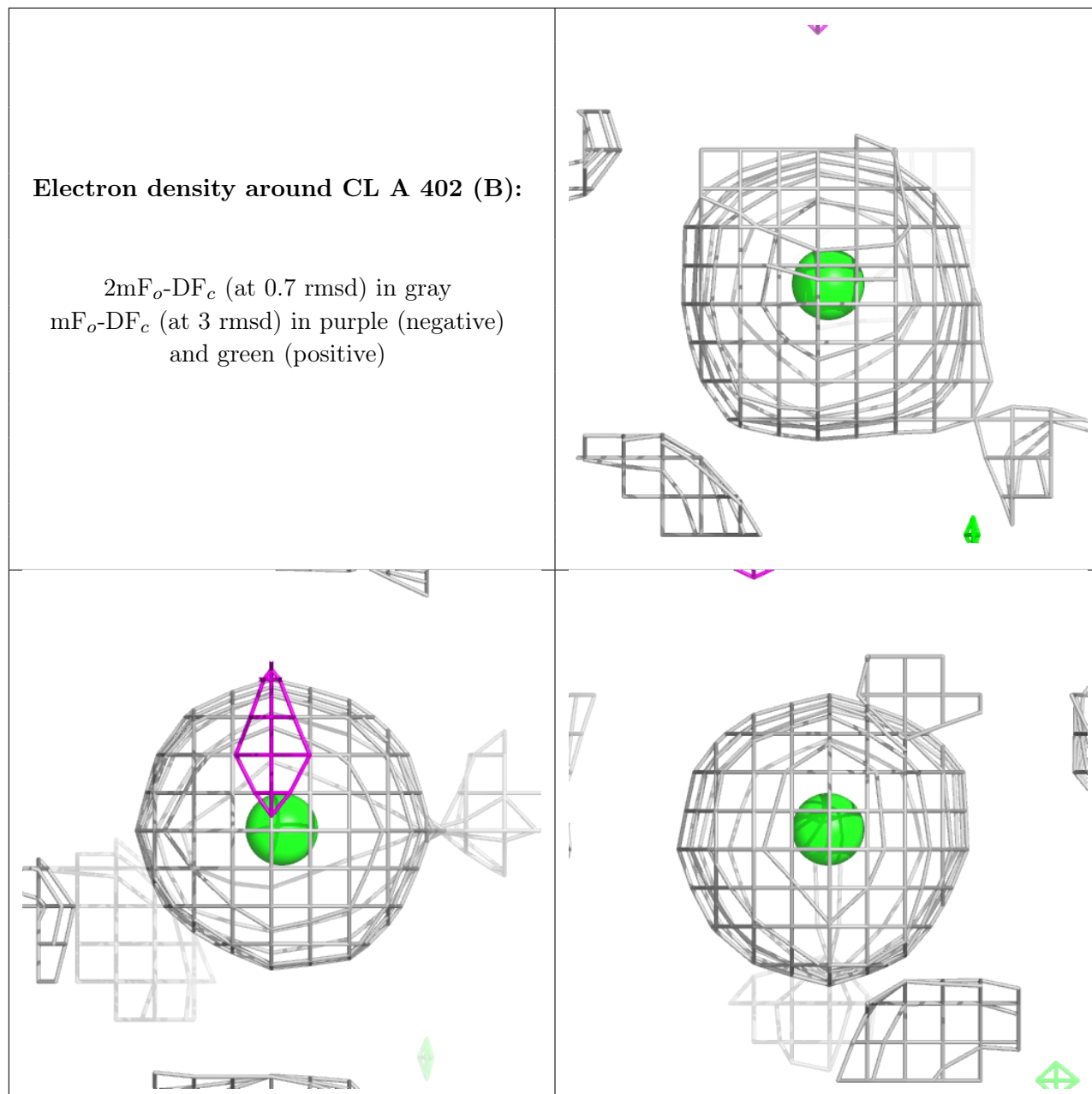
Electron density around CL A 402 (A):

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



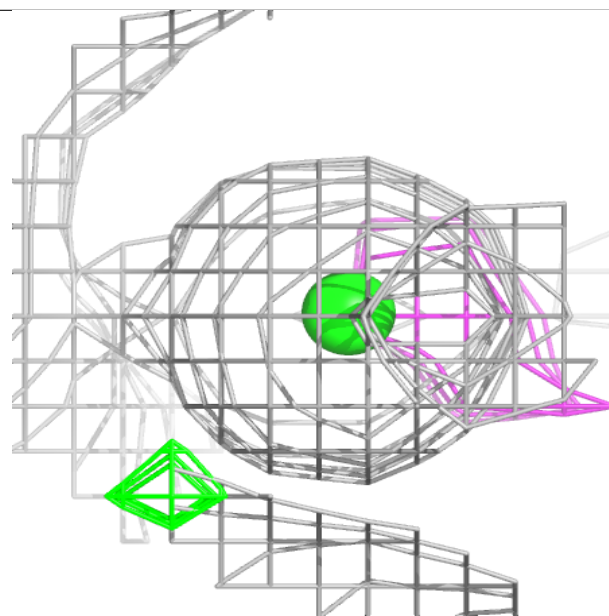
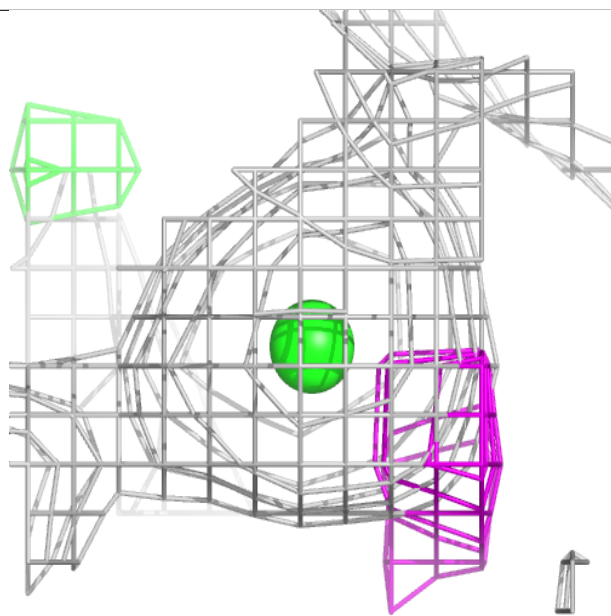
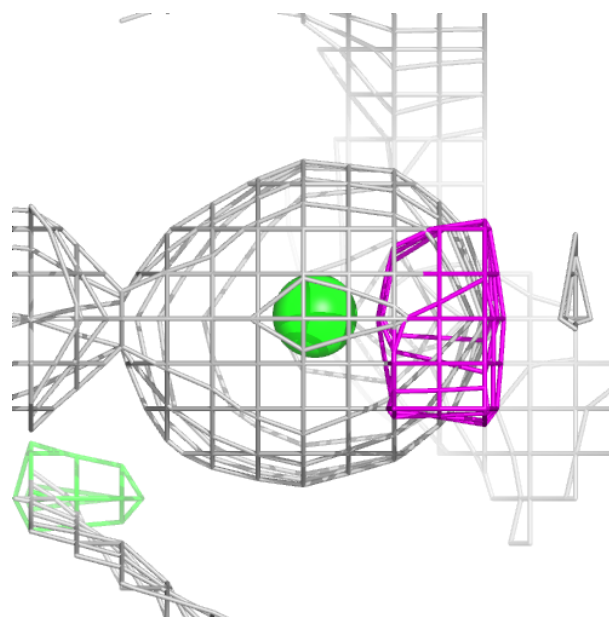
Electron density around CL A 402 (B):

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



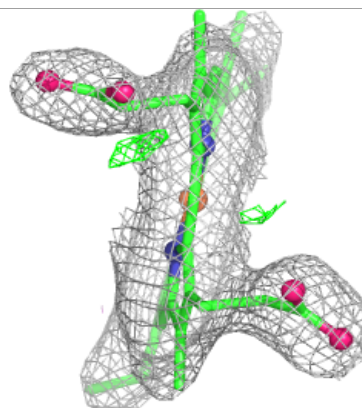
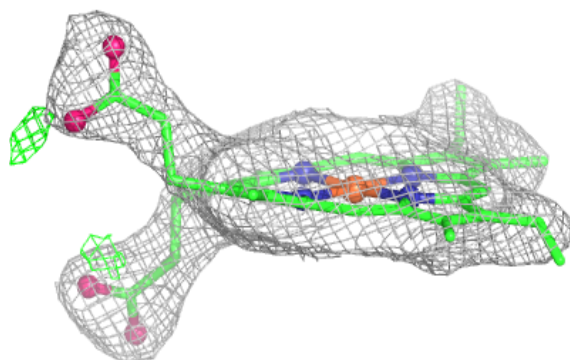
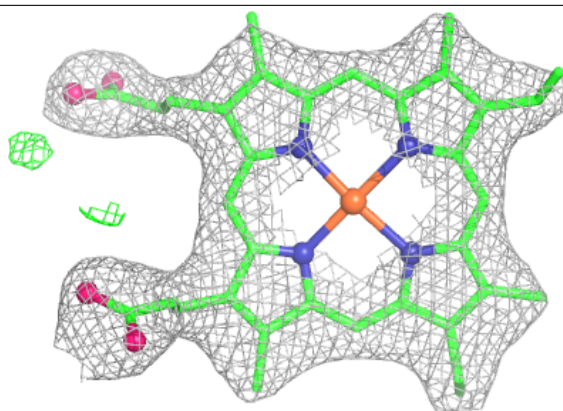
Electron density around CL a 403 (A):

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



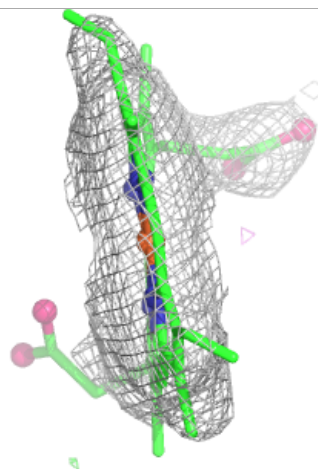
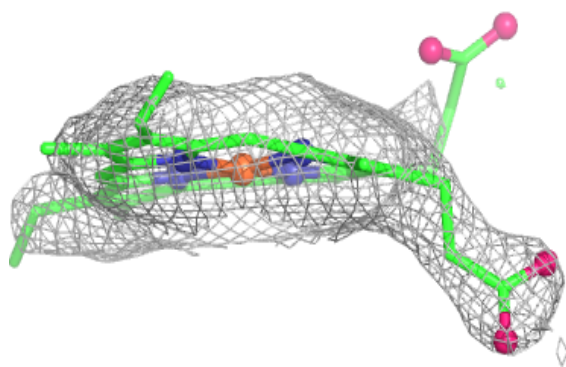
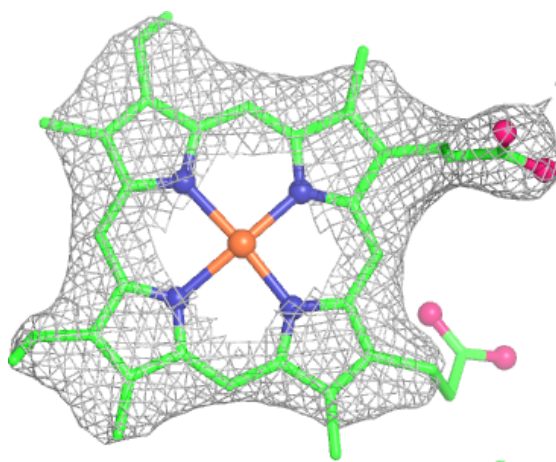
Electron density around HEM F 102:

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



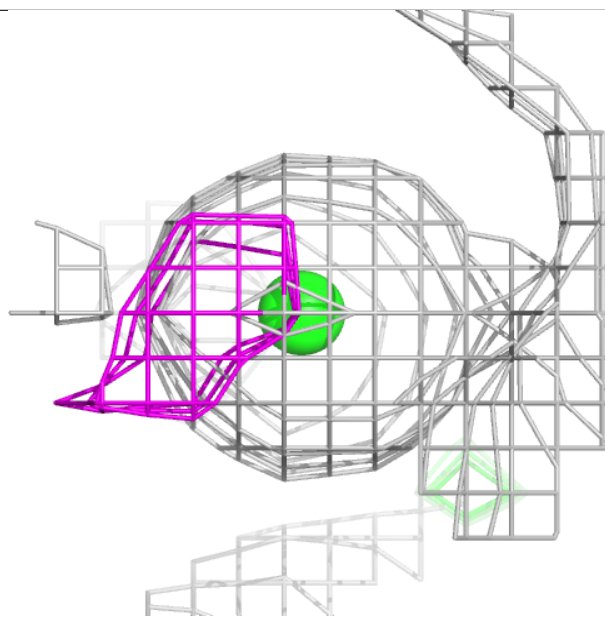
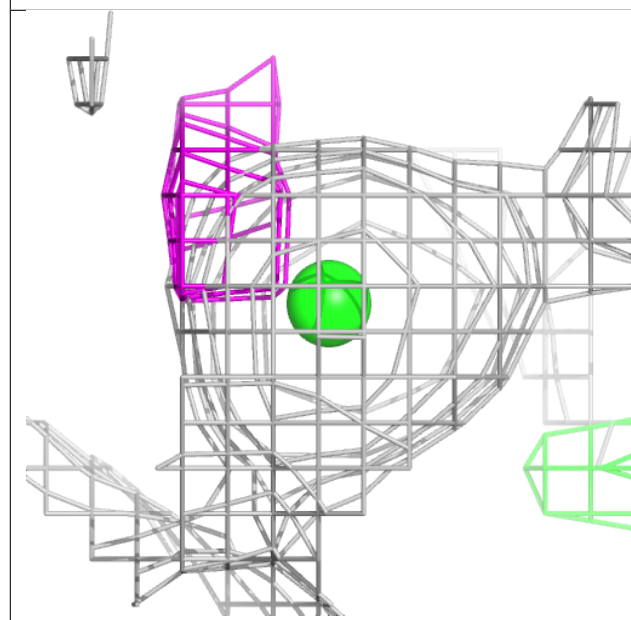
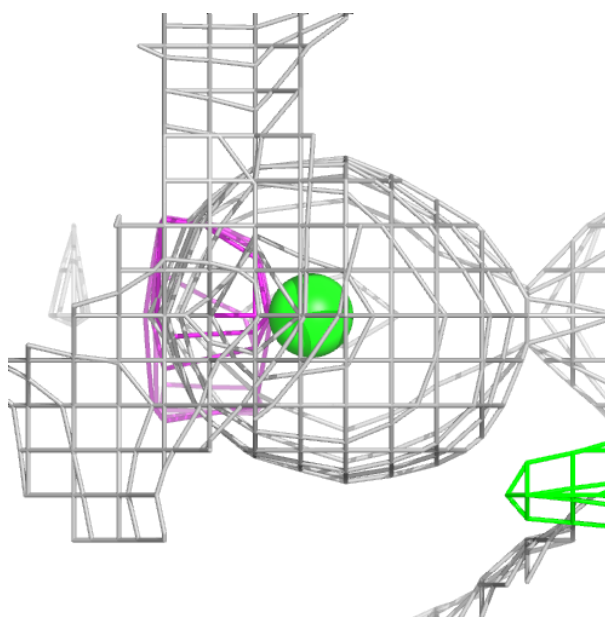
Electron density around HEM f 101:

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



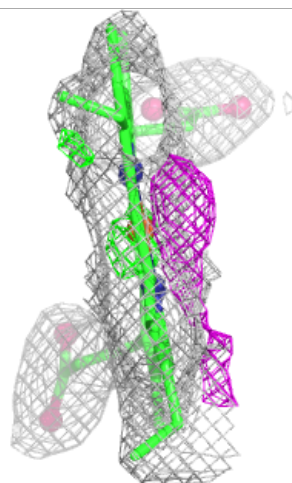
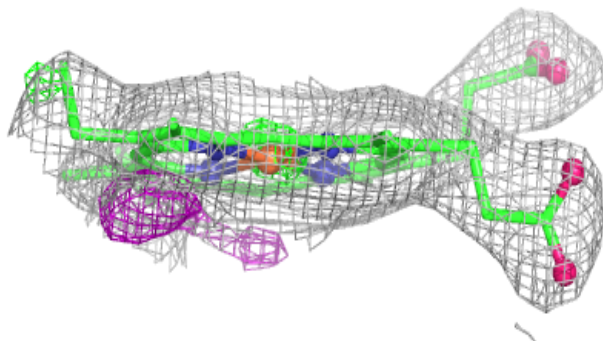
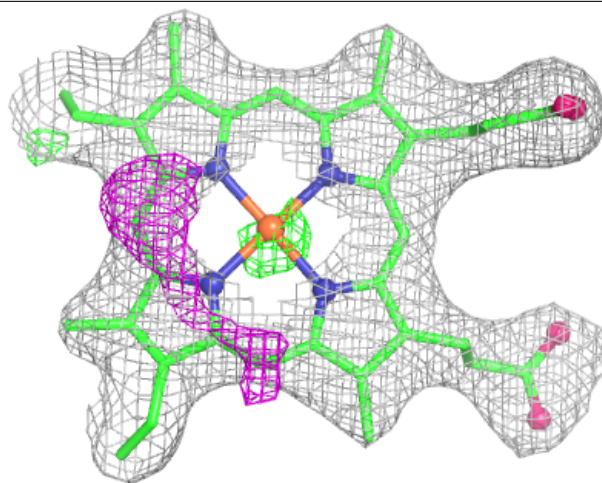
Electron density around CL a 403 (B):

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



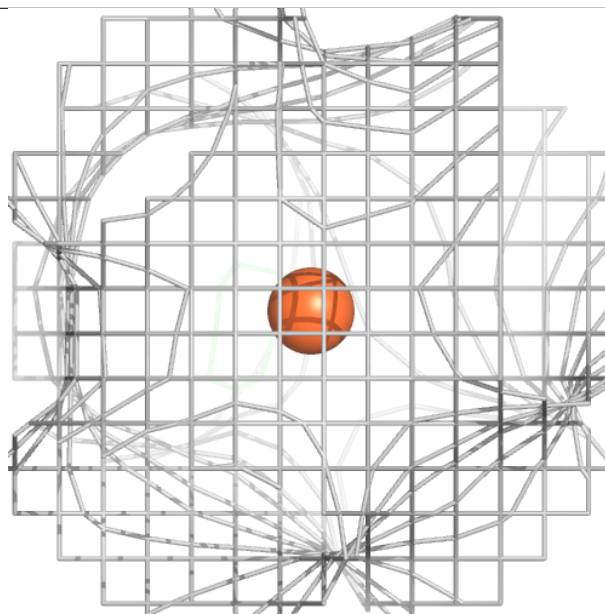
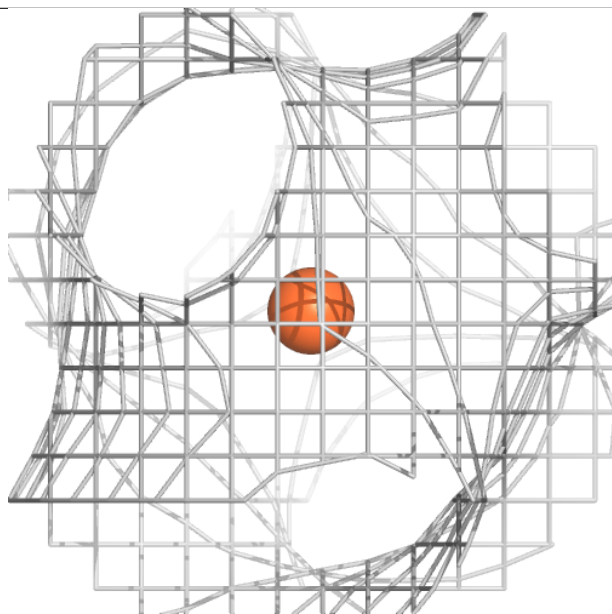
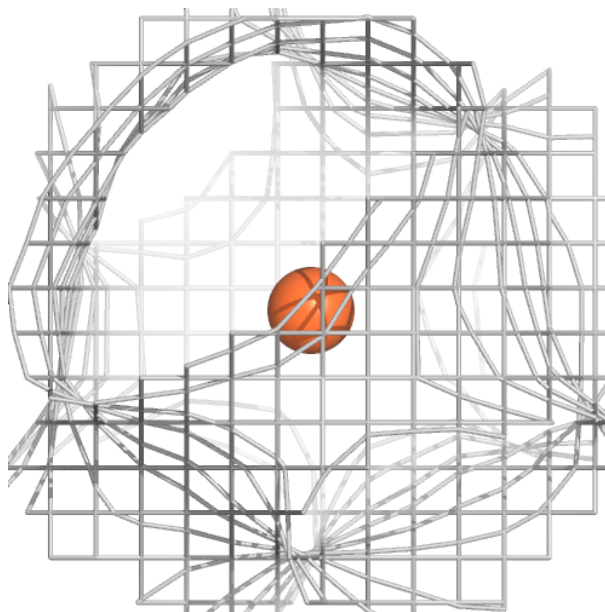
Electron density around HEC v 201:

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



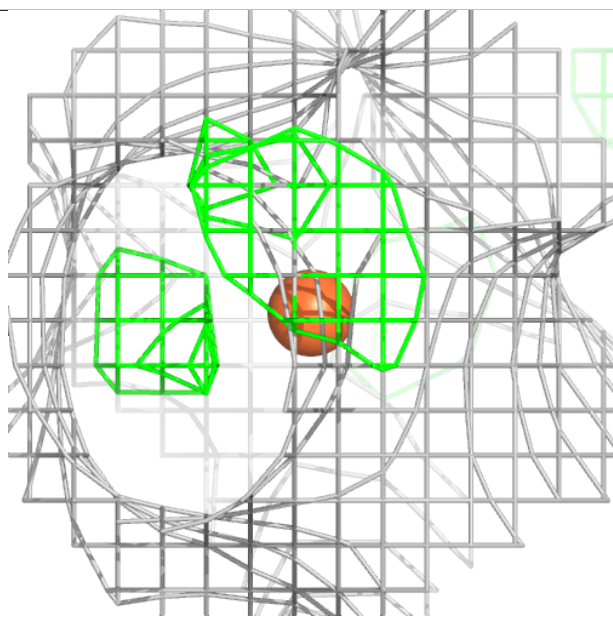
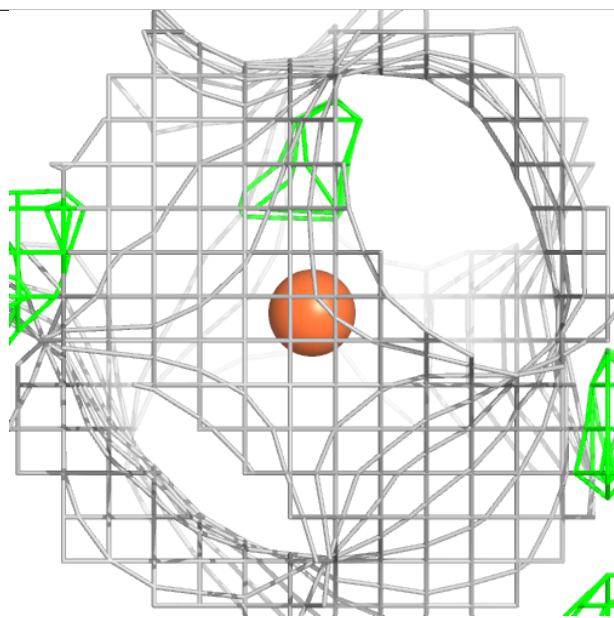
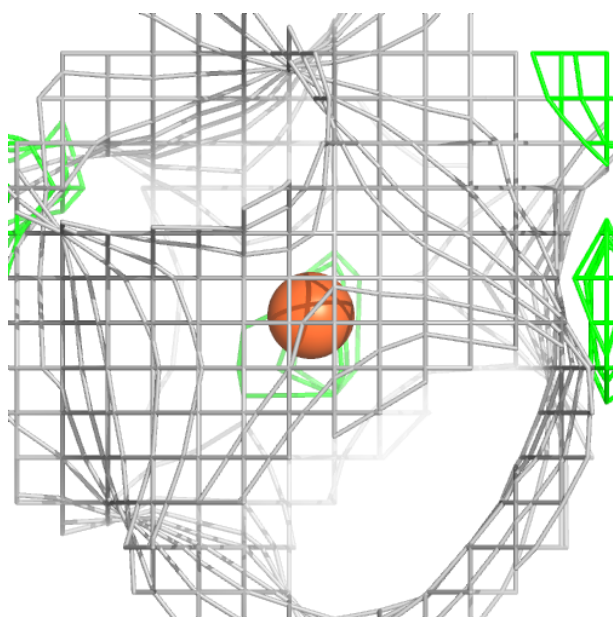
Electron density around FE2 A 401 (B):

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



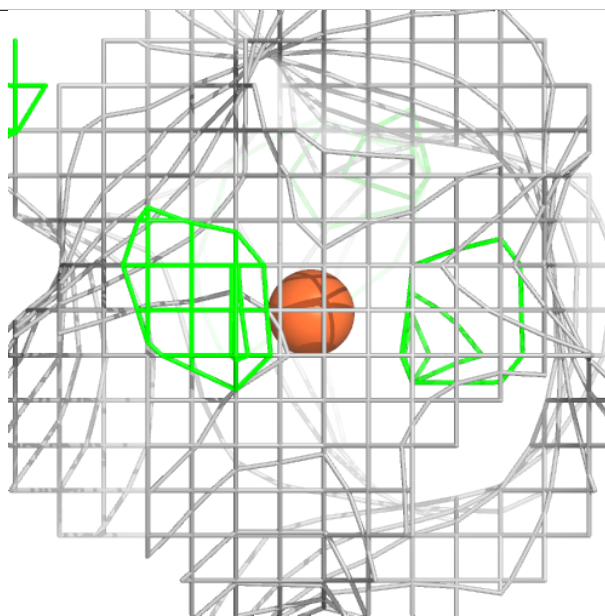
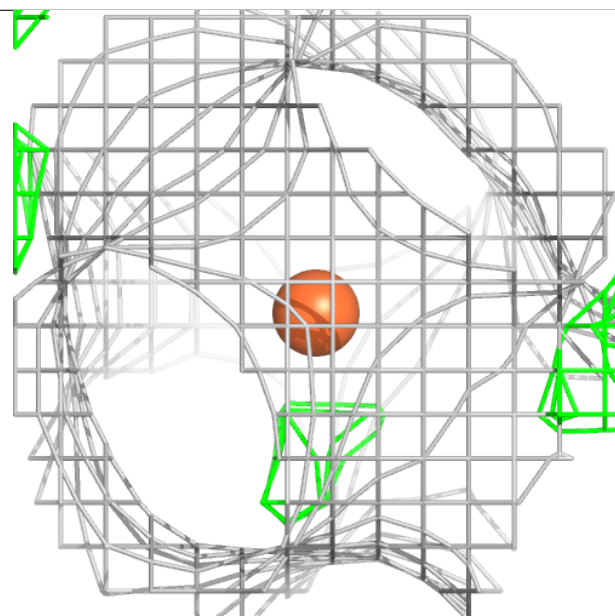
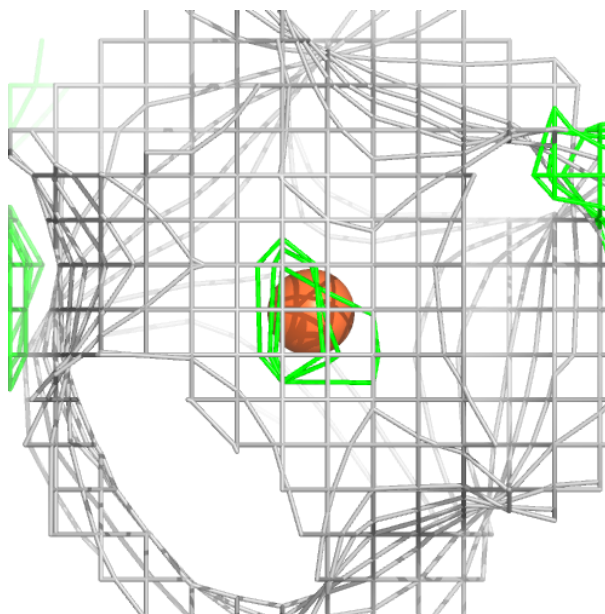
Electron density around FE2 a 401 (A):

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



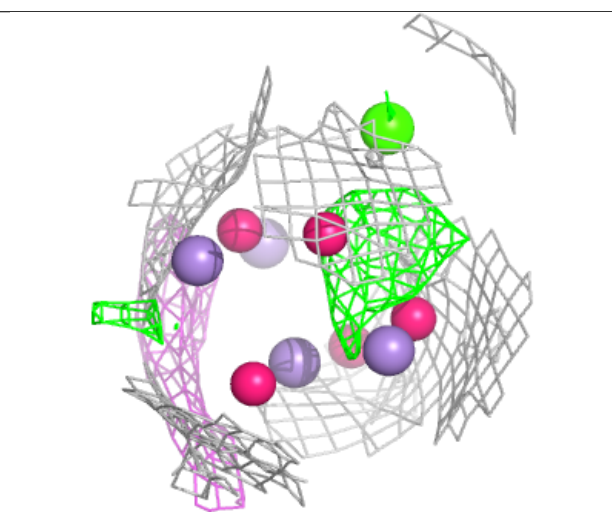
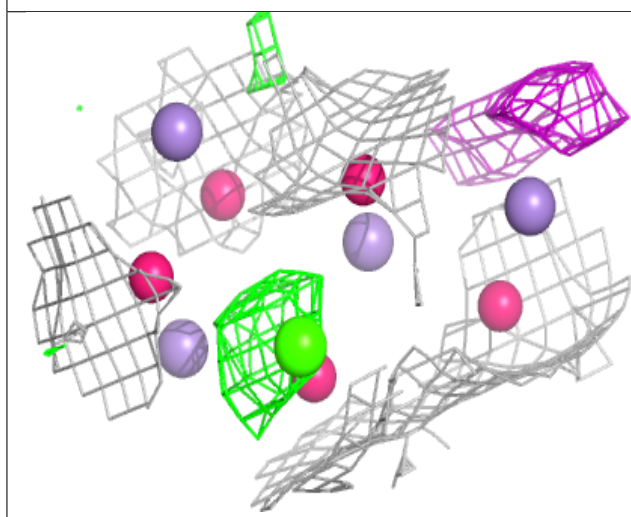
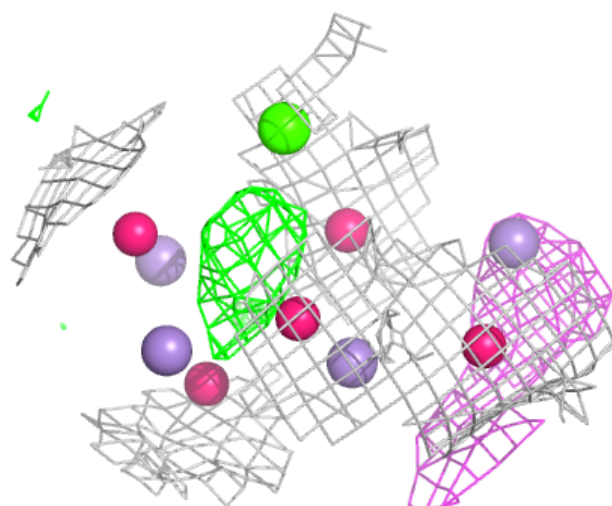
Electron density around FE2 a 401 (B):

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



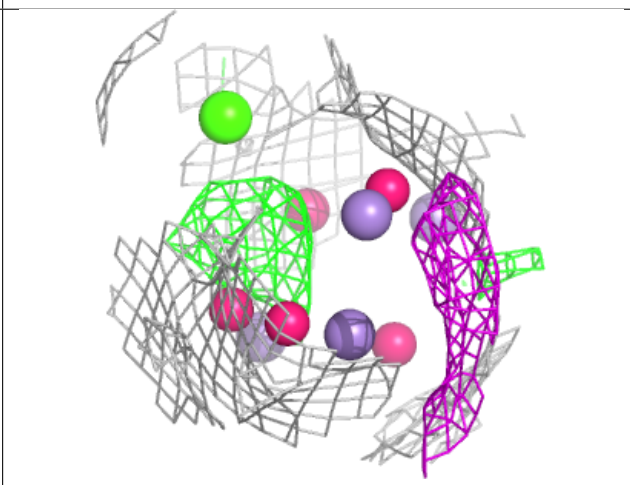
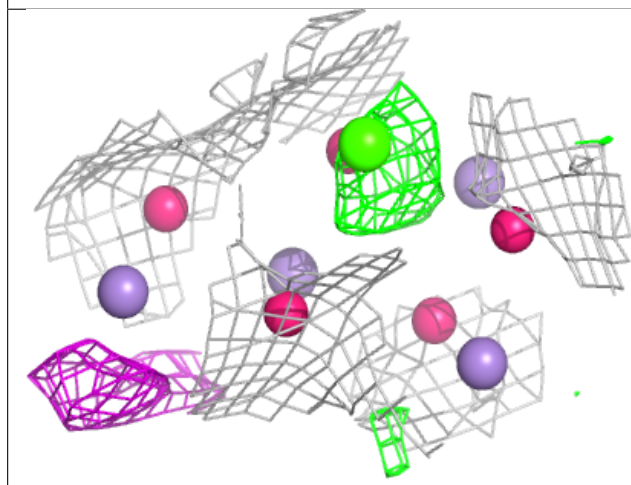
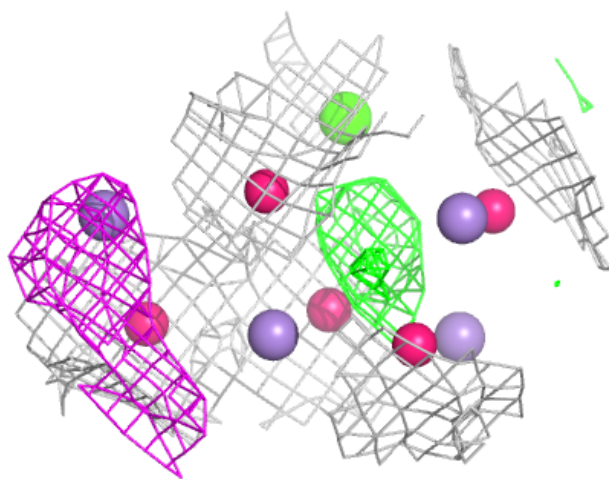
Electron density around OEX A 413 (A):

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



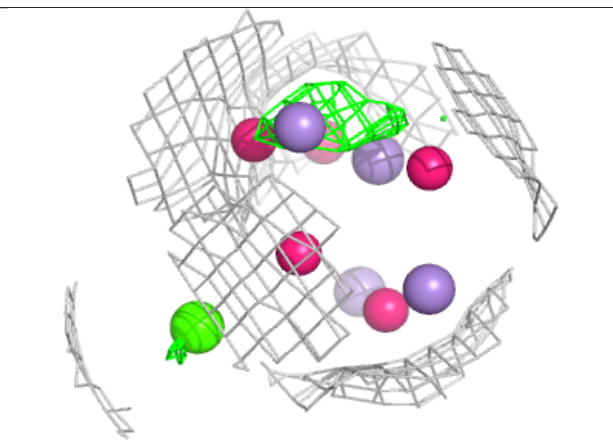
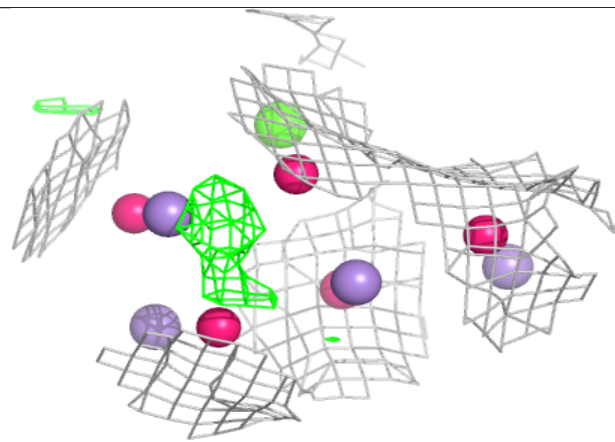
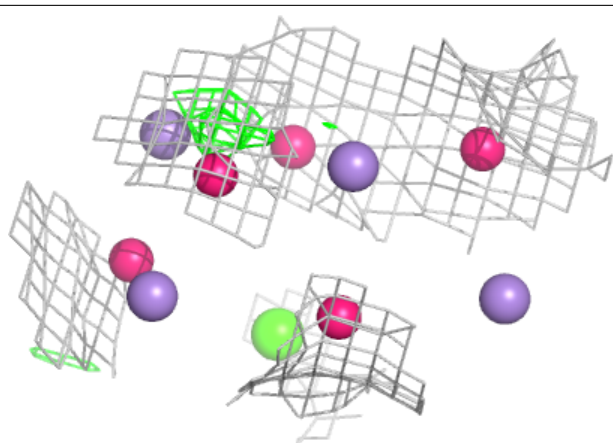
Electron density around OEX A 413 (B):

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



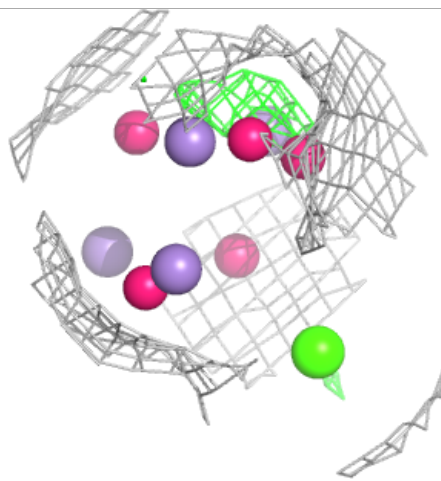
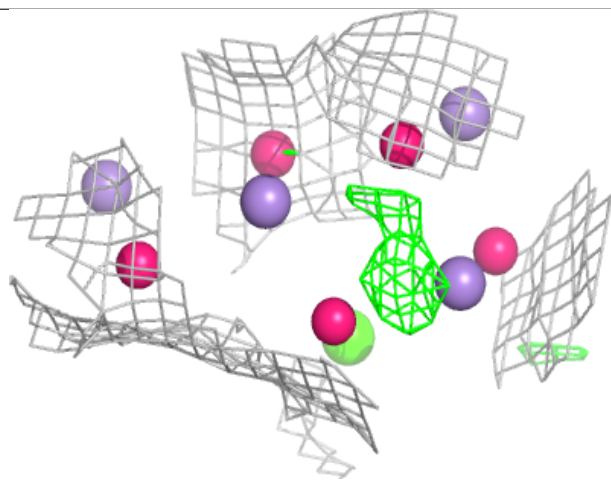
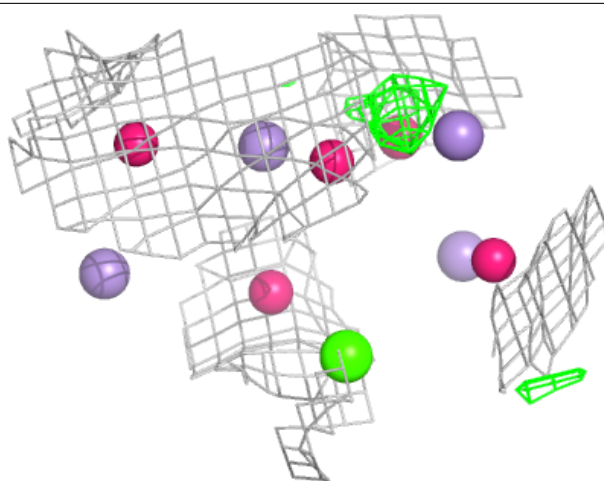
Electron density around OEX a 412 (A):

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



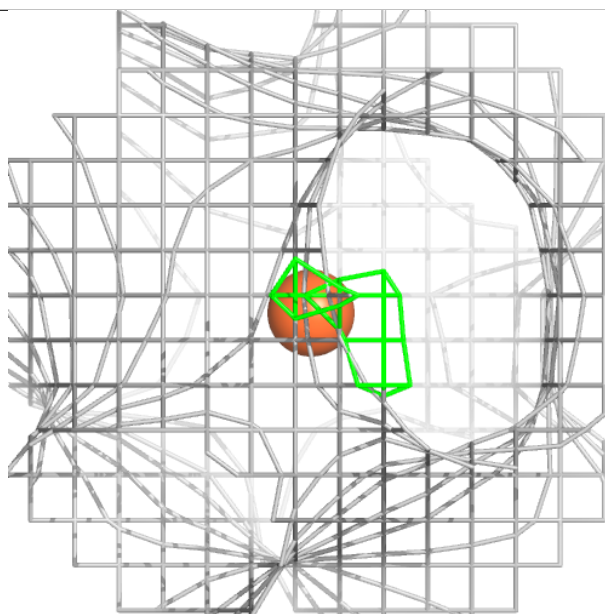
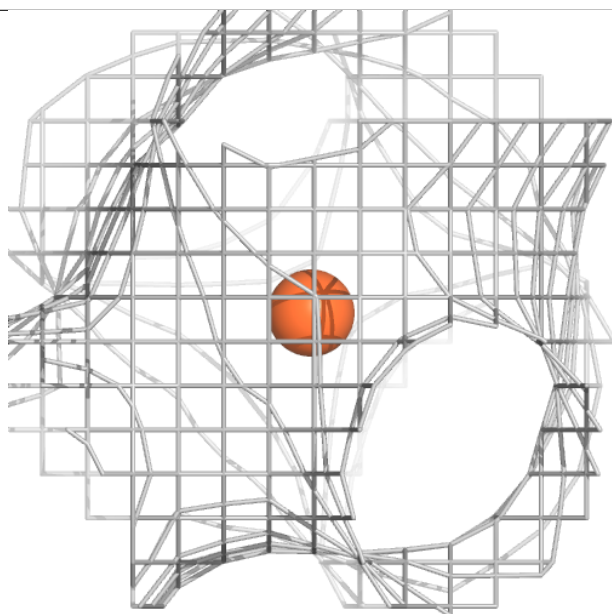
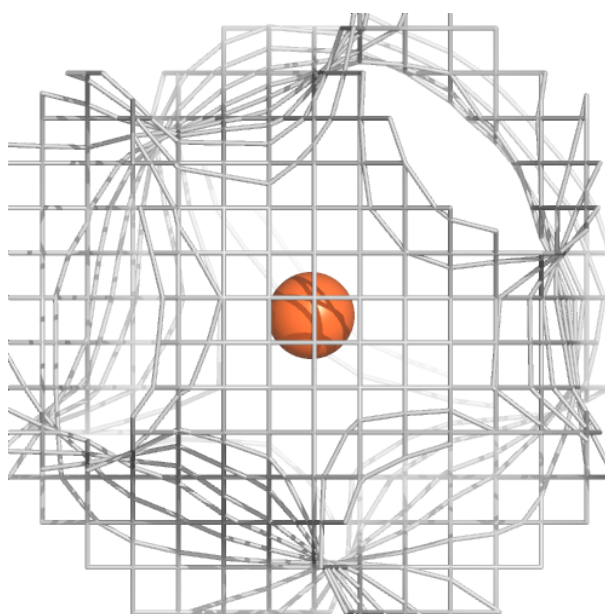
Electron density around OEX a 412 (B):

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



Electron density around 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.