



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 10:48 AM UTC

PDB ID : 6JLL / pdb_00006jll
Title : XFEL structure of cyanobacterial photosystem II (2F state, dataset1)
Authors : Suga, M.; Shen, J.R.
Deposited on : 2019-03-06
Resolution : 2.15 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 : 2022.3.0, CSD as543be (2022)
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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

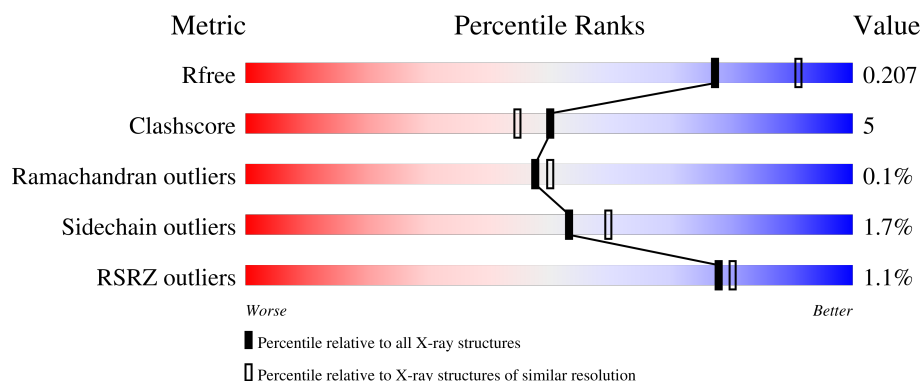
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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.



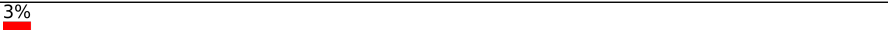
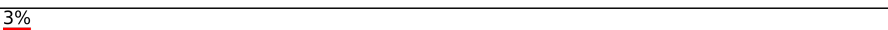
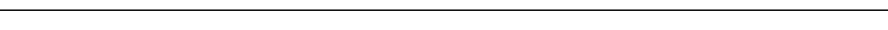
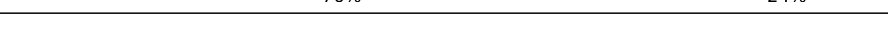
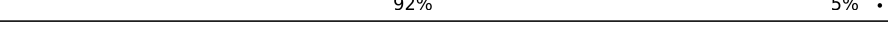
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	2% 88% 9% . .
2	B	505	89% 10% .
2	b	505	2% 90% 10%
3	C	455	91% 8% .

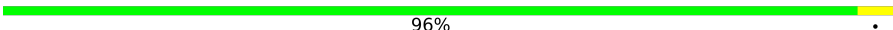
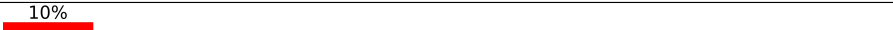
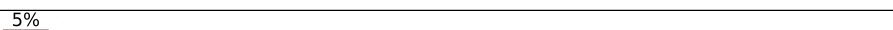
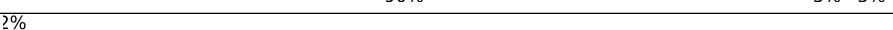
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Mol	Chain	Length	Quality of chain
3	c	455	
4	D	342	
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	

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Mol	Chain	Length	Quality of chain
16	V	137	 96% .
16	v	137	 86% 14%
17	Y	30	 10% 70% 27% .
17	y	30	 63% 33% .
18	X	40	 90% 8% .
18	x	40	 5% 90% 5% 5%
19	Z	62	 2% 87% 11% .
19	z	62	 5% 76% 24%
20	R	34	 44% 71% 15% . 12%

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
24	CLA	A	405	X	-	-	-
24	CLA	A	406	X	-	-	-
24	CLA	A	410	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	B	617	X	-	-	-
24	CLA	C	501	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	a	409	X	-	-	-
24	CLA	a	412	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	b	619	X	-	-	-
24	CLA	b	620	X	-	-	-
24	CLA	b	622	X	-	-	-
24	CLA	b	623	X	-	-	-
24	CLA	b	624	X	-	-	-
24	CLA	b	625	X	-	-	-
24	CLA	b	626	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	c	514	X	-	-	-
24	CLA	c	515	X	-	-	-
24	CLA	c	516	X	-	-	-
24	CLA	d	401	X	-	-	-
24	CLA	d	402	X	-	-	-
24	CLA	d	403	X	-	-	-

2 Entry composition

There are 42 unique types of molecules in this entry. The entry contains 55675 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	54	0
			3014	1963	496	537	18			
1	a	334	Total	C	N	O	S	0	56	0
			3010	1964	494	534	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	See sequence details	UNP P51765
a	279	PRO	ARG	See sequence details	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	10	0
			4021	2639	667	702	13			
2	b	503	Total	C	N	O	S	0	12	0
			4022	2644	664	701	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	14	0
			3553	2322	592	626	13			
3	c	455	Total	C	N	O	S	0	20	0
			3641	2382	606	639	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	See sequence details	UNP D0VWR7
C	20	SER	-	See sequence details	UNP D0VWR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	See sequence details	UNP D0VWR7
C	22	PHE	-	See sequence details	UNP D0VWR7
c	19	ASN	-	See sequence details	UNP D0VWR7
c	20	SER	-	See sequence details	UNP D0VWR7
c	21	ILE	-	See sequence details	UNP D0VWR7
c	22	PHE	-	See sequence details	UNP D0VWR7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	16	0
			2849	1884	469	483	13			
4	d	341	Total	C	N	O	S	0	16	0
			2849	1884	469	483	13			

- 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	2	0
			668	436	107	125			
5	e	81	Total	C	N	O	0	2	0
			670	439	107	124			

- 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	32	Total	C	N	O	S	0	0	0
			257	175	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	1	0
			519	346	85	86	2			
7	h	65	Total	C	N	O	S	0	0	0
			511	341	82	86	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	39	Total	C	N	O	S	0	0	0
			280	187	43	48	2			

- 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	See sequence details	UNP P19054
K	39	TRP	VAL	See sequence details	UNP P19054
k	33	LEU	PHE	See sequence details	UNP P19054
k	39	TRP	VAL	See sequence details	UNP P19054

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			
11	l	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	1	0
			274	184	40	49	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	0	0
			269	179	40	49	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	See sequence details	UNP P12312
m	8	LEU	PHE	See sequence details	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	8	0
			1903	1191	315	392	5			
13	o	243	Total	C	N	O	S	0	5	0
			1891	1183	315	388	5			

- 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	1	0
			264	185	36	41	2			
14	t	30	Total	C	N	O	S	0	1	0
			264	185	36	41	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O		0	0	0
			774	491	129	154				
15	u	97	Total	C	N	O		0	0	0
			774	491	129	154				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	2	0
			1085	689	181	211	4			
16	v	137	Total	C	N	O	S	0	1	0
			1077	684	178	211	4			

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	39	Total	C	N	O		0	0	0
			287	191	46	50				
18	x	38	Total	C	N	O		0	0	0
			281	188	45	48				

- 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	30	Total	C	N	O		98	0	0
			239	163	41	35				

- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 22 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

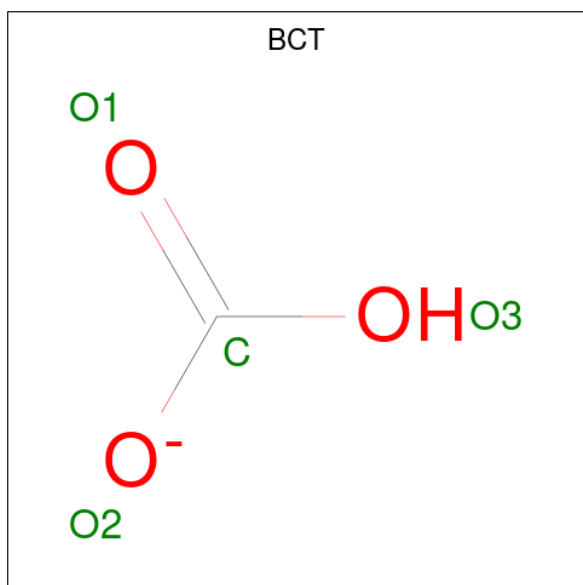
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	2
			4	4		
22	U	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	a	2	Total	Cl	0	2
			4	4		
22	v	1	Total	Cl	0	0
			1	1		

- Molecule 23 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	1
			8	2	6		
23	a	1	Total	C	O	0	1
			8	2	6		

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$).



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

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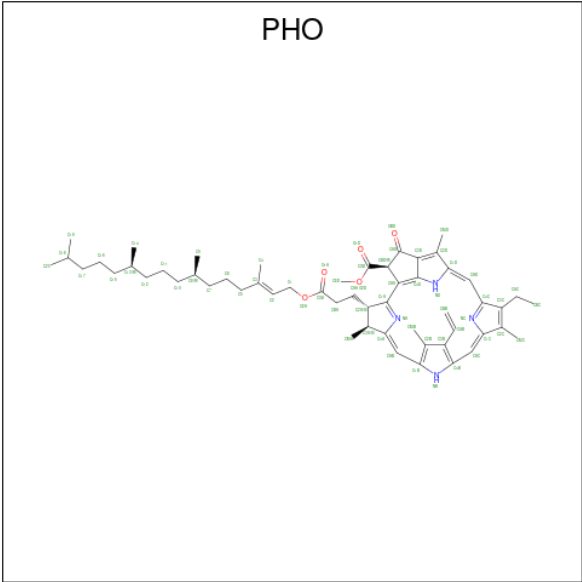
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24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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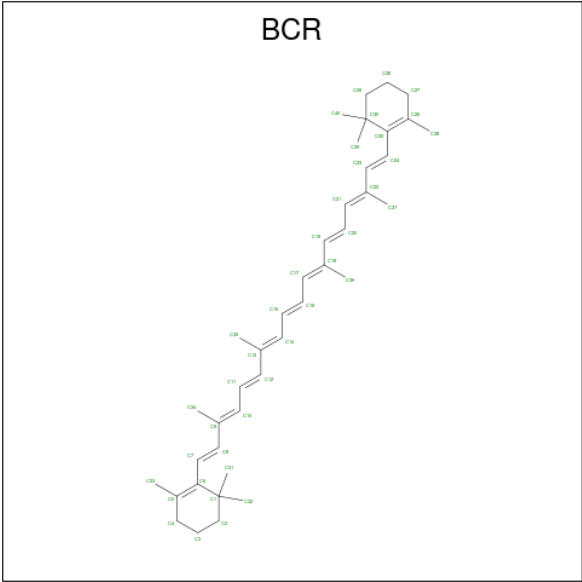
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total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

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



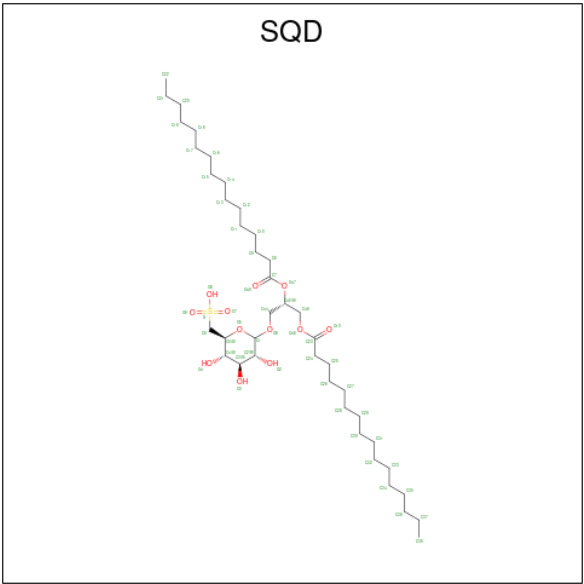
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	A	1	Total	C	N	O	0	1
			128	110	8	10		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	1
			128	110	8	10		

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



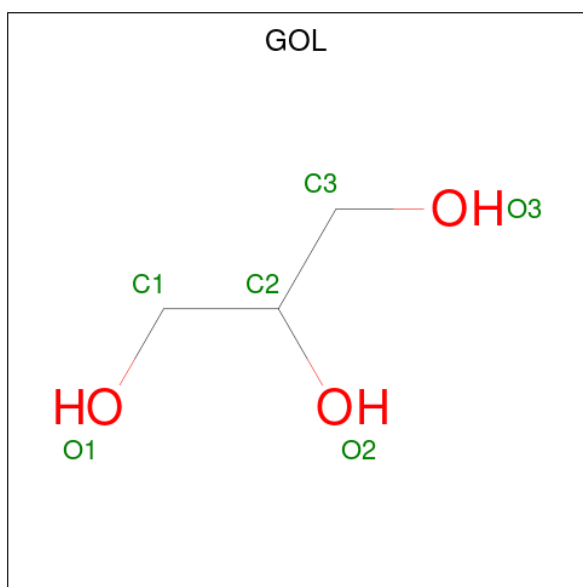
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Y	1	Total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

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	B	1	Total	C	O	S	0	0
			54	41	12	1		
27	F	1	Total	C	O	S	0	0
			43	30	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	b	1	Total	C	O	S	0	0
			54	41	12	1		
27	f	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 28 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



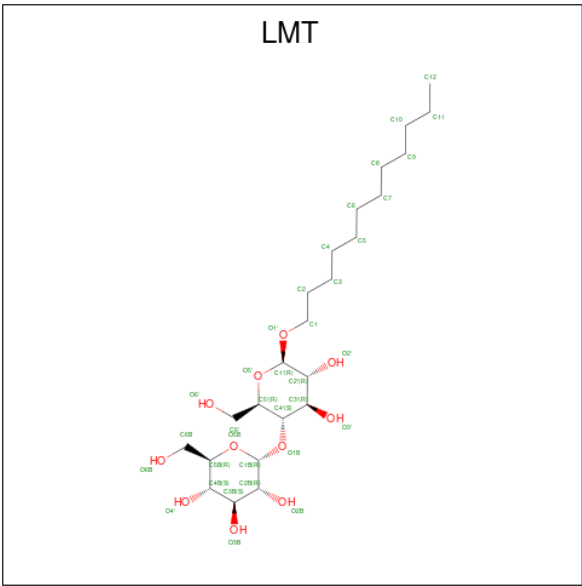
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			6	3	3		
28	A	1	Total	C	O	0	0
			6	3	3		
28	A	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	C	1	Total	C	O	0	0
			6	3	3		
28	C	1	Total	C	O	0	0
			6	3	3		
28	O	1	Total	C	O	0	0
			6	3	3		
28	T	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	T	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	c	1	Total	C	O	0	0
			6	3	3		
28	c	1	Total	C	O	0	0
			6	3	3		
28	f	1	Total	C	O	0	0
			6	3	3		
28	o	1	Total	C	O	0	0
			6	3	3		
28	t	1	Total	C	O	0	0
			6	3	3		
28	v	1	Total	C	O	0	0
			6	3	3		
28	v	1	Total	C	O	0	0
			6	3	3		
28	v	1	Total	C	O	0	0
			6	3	3		

- Molecule 29 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



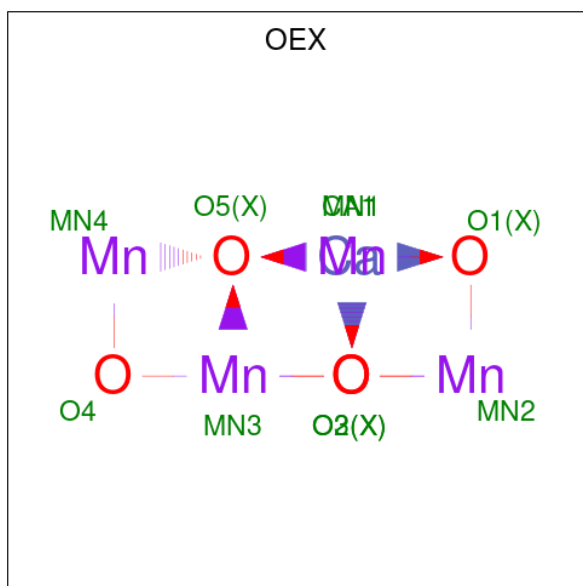
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			35	24	11		
29	B	1	Total	C	O	0	0
			25	19	6		
29	C	1	Total	C	O	0	0
			35	24	11		
29	D	1	Total	C	O	0	0
			35	24	11		
29	F	1	Total	C	O	0	0
			35	24	11		
29	M	1	Total	C	O	0	0
			35	24	11		
29	M	1	Total	C	O	0	0
			35	24	11		
29	M	1	Total	C	O	0	0
			35	24	11		
29	T	1	Total	C	O	0	0
			25	19	6		
29	a	1	Total	C	O	0	0
			35	24	11		
29	a	1	Total	C	O	0	0
			35	24	11		
29	b	1	Total	C	O	0	0
			25	19	6		
29	f	1	Total	C	O	0	0
			35	24	11		

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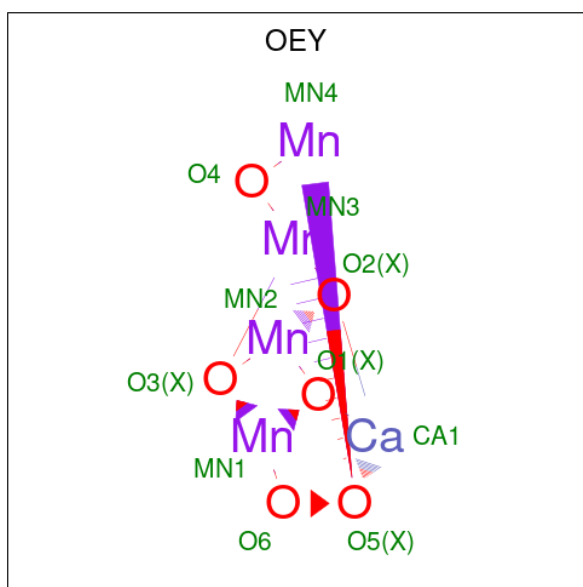
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	m	1	Total	C	O	0	0
			35	24	11		

- Molecule 30 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



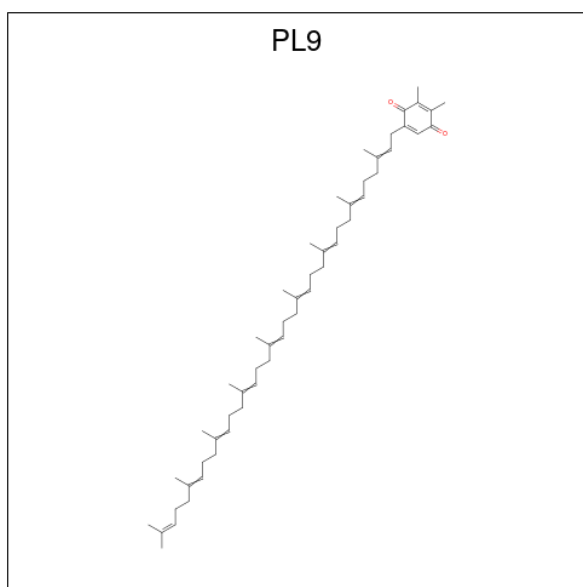
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
30	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 31 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: CaMn_4O_6).



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

- Molecule 32 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: C₅₃H₈₀O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	1
			110	106	4		

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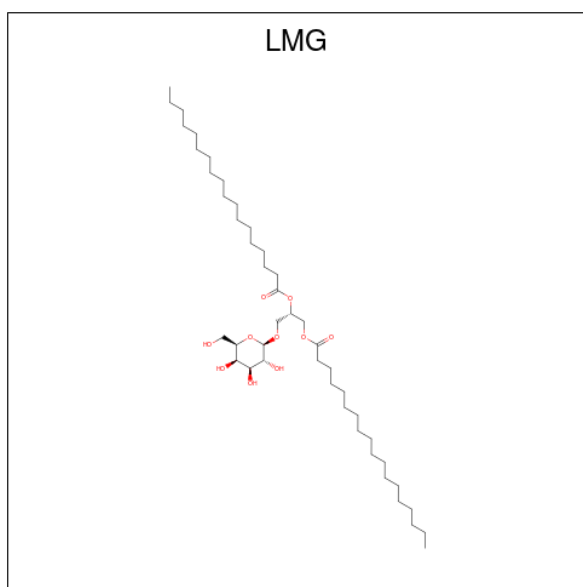
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	D	1	Total	C	O	0	1
			110	106	4		
32	a	1	Total	C	O	0	1
			110	106	4		
32	d	1	Total	C	O	0	1
			110	106	4		

- Molecule 33 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	A	1	Total	C	O	0	0
			28	23	5		
33	B	1	Total	C	O	0	0
			33	28	5		
33	C	1	Total	C	O	0	0
			34	29	5		
33	D	2	Total	C	O	0	0
			57	51	6		
33	I	1	Total	C	O	0	0
			40	35	5		
33	J	1	Total	C		0	0
			10	10			
33	M	1	Total	C		0	0
			10	10			
33	X	1	Total	C	O	0	0
			18	16	2		
33	a	1	Total	C	O	0	0
			30	25	5		
33	b	1	Total	C	O	0	0
			33	28	5		
33	c	1	Total	C	O	0	0
			32	27	5		
33	d	3	Total	C	O	0	0
			71	63	8		
33	i	1	Total	C	O	0	0
			40	35	5		
33	j	1	Total	C		0	0
			10	10			
33	m	1	Total	C		0	0
			10	10			

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).

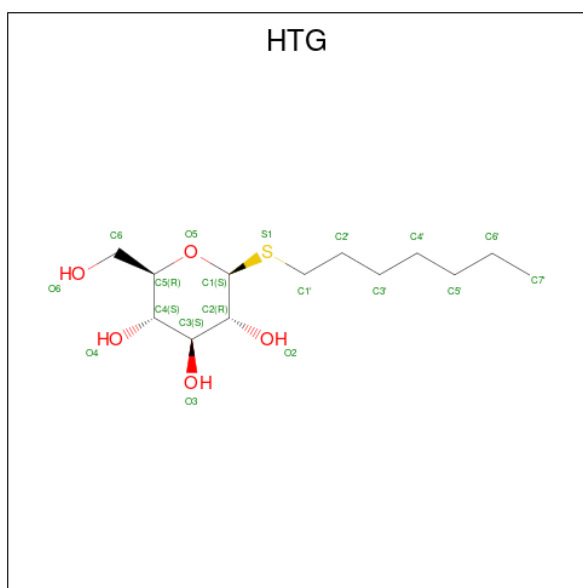


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	A	1	Total	C	O	0	0
			51	41	10		
34	B	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	D	1	Total	C	O	0	0
			51	41	10		
34	Z	1	Total	C	O	0	0
			37	27	10		
34	a	1	Total	C	O	0	0
			51	41	10		
34	b	1	Total	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	j	1	Total	C	O	0	0
			51	41	10		
34	z	1	Total	C	O	0	0
			39	29	10		

- Molecule 35 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 36 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: $C_{13}H_{26}O_5S$).



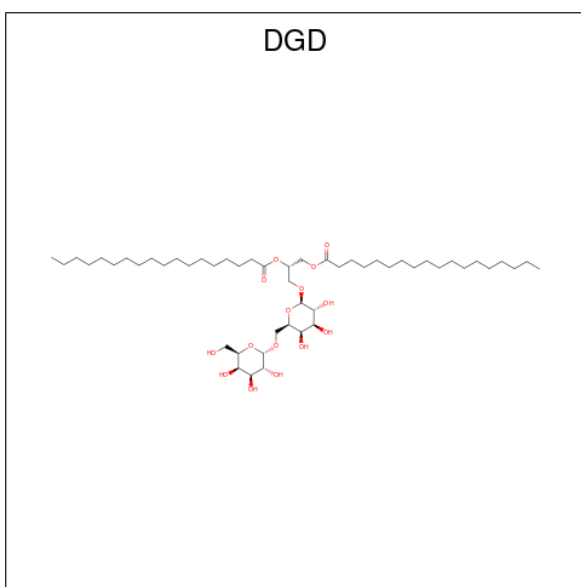
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	B	1	Total C O S 19 13 5 1	0	0
36	B	1	Total C O S 19 13 5 1	0	0
36	B	1	Total C O S 19 13 5 1	0	0
36	B	1	Total C O S 19 13 5 1	0	0

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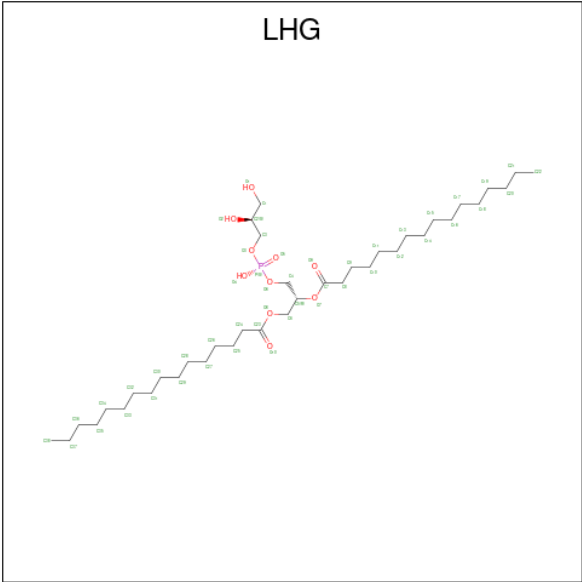
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	H	1	Total	C	O	S	0	0
			16	10	5	1		
36	V	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	d	1	Total	C	O	S	0	0
			16	10	5	1		

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



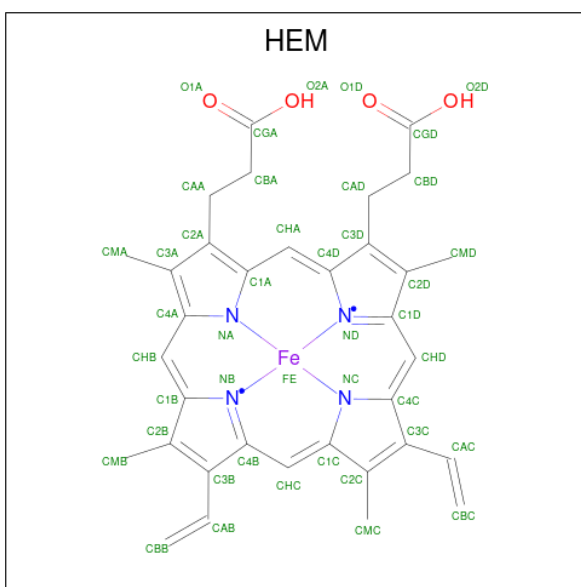
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	C	1	Total	C	O	0	0
			62	47	15		
37	C	1	Total	C	O	0	0
			62	47	15		
37	C	1	Total	C	O	0	0
			62	47	15		
37	D	1	Total	C	O	0	0
			52	42	10		
37	H	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	e	1	Total	C	O	0	0
			62	47	15		
37	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 38 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	D	1	Total	C	O	P	0	0
			49	38	10	1		
38	D	1	Total	C	O	P	0	0
			49	38	10	1		
38	D	1	Total	C	O	P	0	0
			49	38	10	1		
38	E	1	Total	C	O	P	0	0
			42	31	10	1		
38	L	1	Total	C	O	P	0	0
			49	38	10	1		
38	a	1	Total	C	O	P	0	0
			42	31	10	1		
38	d	1	Total	C	O	P	0	0
			49	38	10	1		
38	d	1	Total	C	O	P	0	0
			49	38	10	1		
38	d	1	Total	C	O	P	0	0
			49	38	10	1		
38	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 39 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).

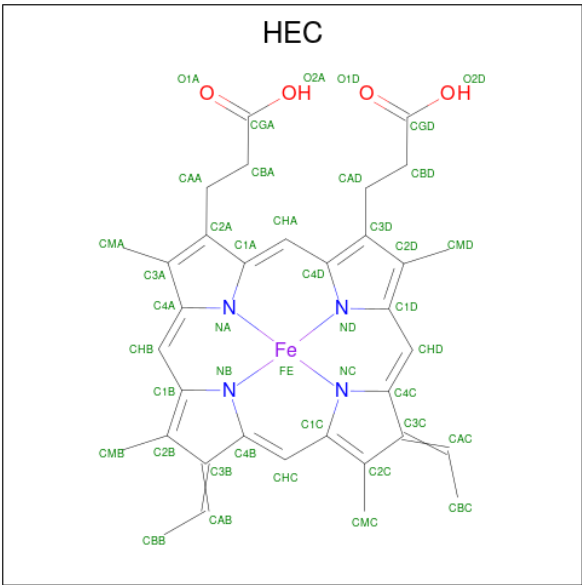


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
39	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
39	e	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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

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

- Molecule 41 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



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

- Molecule 42 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	A	161	Total	O	0	14
			173	173		
42	B	290	Total	O	0	4
			294	294		
42	C	228	Total	O	0	4
			232	232		
42	D	146	Total	O	0	5
			150	150		
42	E	30	Total	O	0	0
			30	30		
42	F	9	Total	O	0	0
			9	9		
42	H	48	Total	O	0	1
			49	49		
42	I	5	Total	O	0	0
			5	5		
42	J	10	Total	O	0	0
			10	10		
42	K	9	Total	O	0	0
			9	9		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
42	L	13	Total O 14 14	0	1
42	M	23	Total O 23 23	0	0
42	O	178	Total O 180 180	0	2
42	T	17	Total O 18 18	0	1
42	U	77	Total O 77 77	0	0
42	V	117	Total O 119 119	0	2
42	Y	4	Total O 4 4	0	0
42	X	6	Total O 6 6	0	0
42	Z	1	Total O 1 1	0	0
42	a	153	Total O 162 162	0	12
42	b	266	Total O 269 269	0	3
42	c	200	Total O 205 205	0	5
42	d	129	Total O 132 132	0	3
42	e	19	Total O 19 19	0	0
42	f	8	Total O 8 8	0	0
42	h	44	Total O 44 44	0	0
42	i	5	Total O 5 5	0	0
42	j	6	Total O 6 6	0	0
42	k	7	Total O 7 7	0	0
42	l	9	Total O 9 9	0	0
42	m	11	Total O 11 11	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	o	155	Total 155	O 155	0	0
42	t	11	Total 11	O 11	0	0
42	u	93	Total 93	O 93	0	0
42	v	81	Total 82	O 82	0	1
42	y	2	Total 2	O 2	0	0
42	x	6	Total 6	O 6	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.

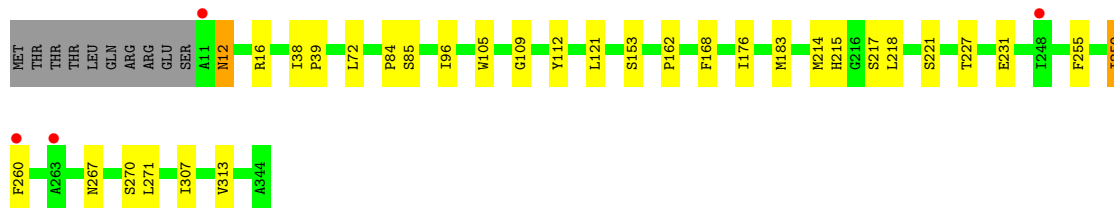
- Molecule 1: Photosystem II protein D1

Chain A: 



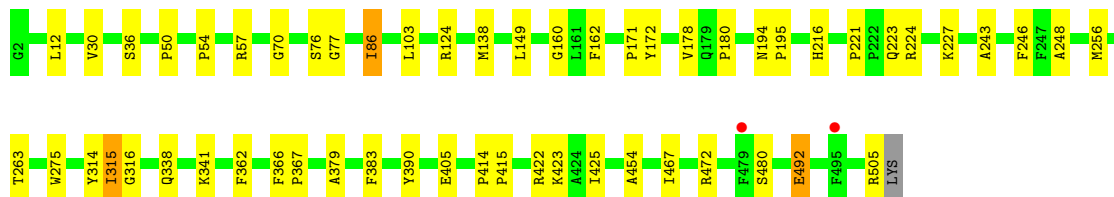
- Molecule 1: Photosystem II protein D1

Chain a: 



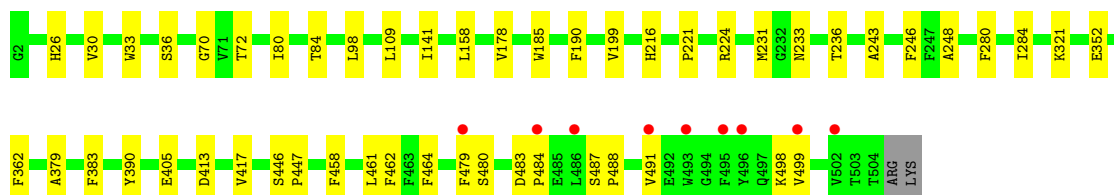
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B: 

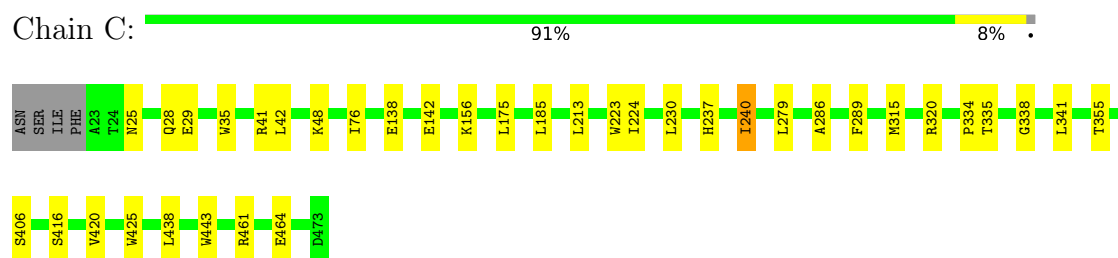


- Molecule 2: Photosystem II CP47 reaction center protein

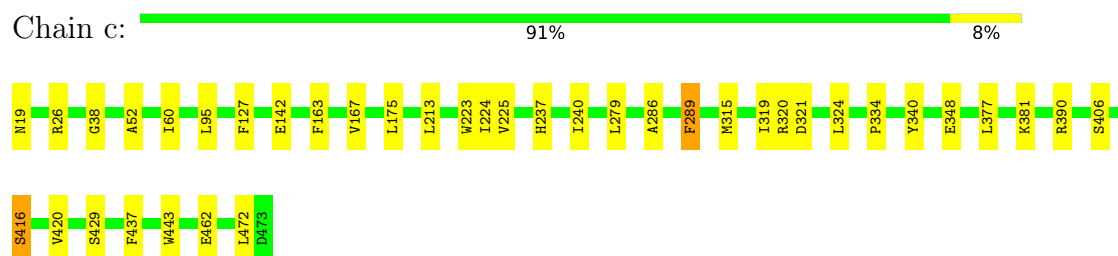
Chain b: 



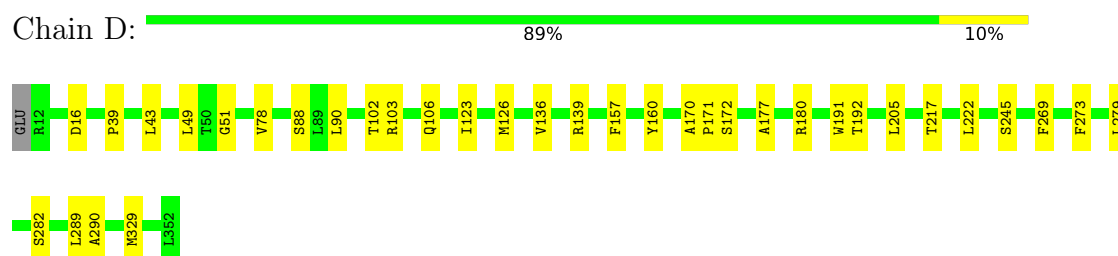
- Molecule 3: Photosystem II CP43 reaction center protein



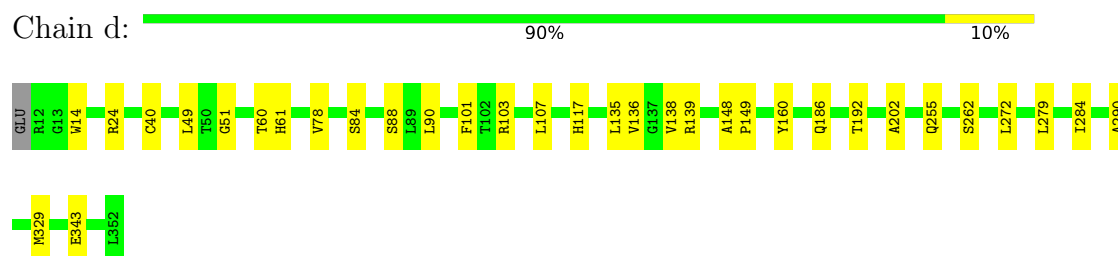
- Molecule 3: Photosystem II CP43 reaction center protein



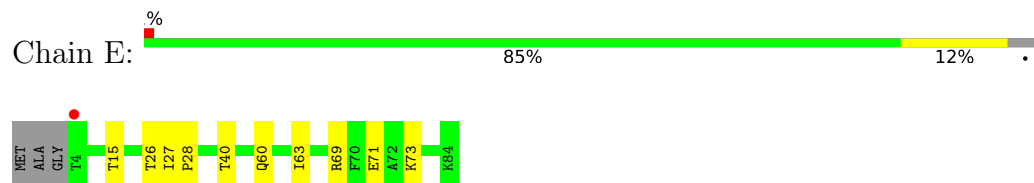
- Molecule 4: Photosystem II D2 protein



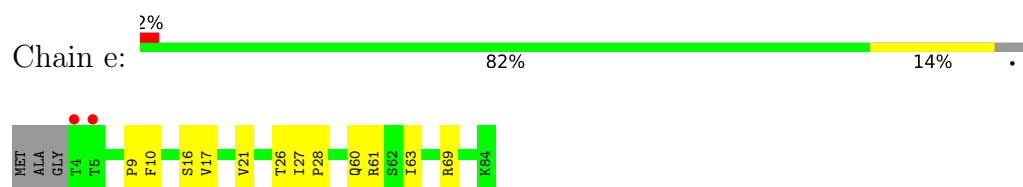
- Molecule 4: Photosystem II D2 protein



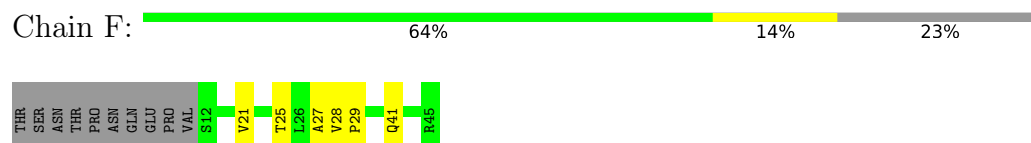
- Molecule 5: Cytochrome b559 subunit alpha



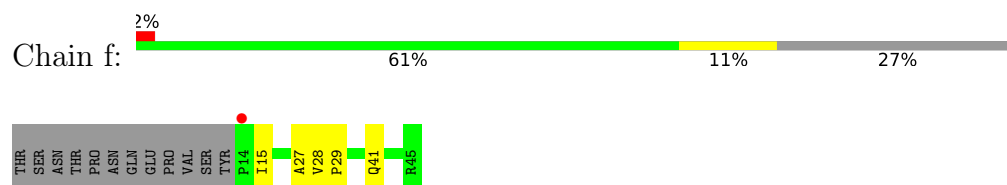
- Molecule 5: Cytochrome b559 subunit alpha



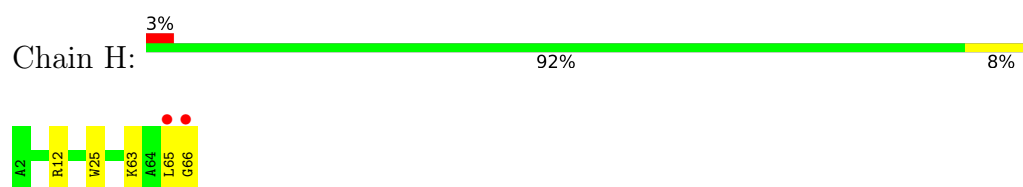
- Molecule 6: Cytochrome b559 subunit beta



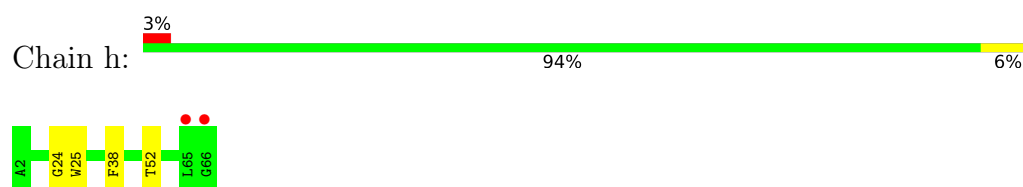
- Molecule 6: Cytochrome b559 subunit beta



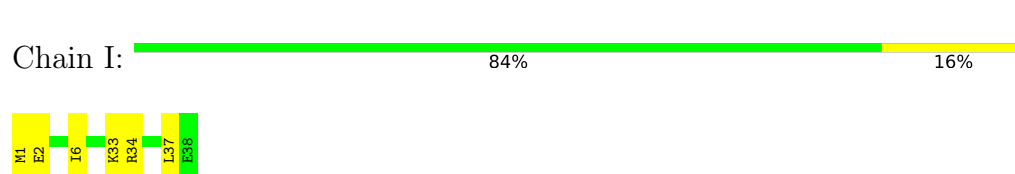
- Molecule 7: Photosystem II reaction center protein H



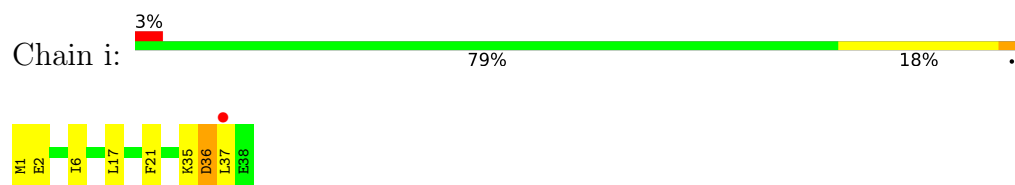
- Molecule 7: Photosystem II reaction center protein H



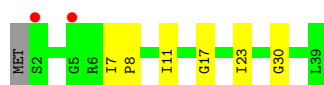
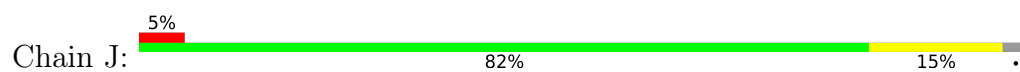
- Molecule 8: Photosystem II reaction center protein I



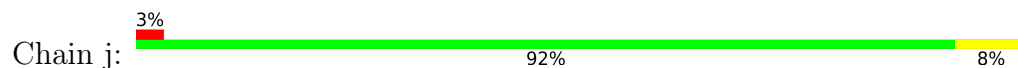
- Molecule 8: Photosystem II reaction center protein I



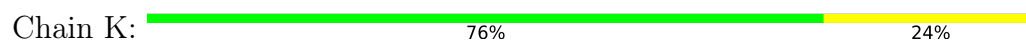
- Molecule 9: Photosystem II reaction center protein J



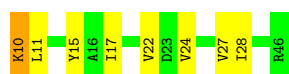
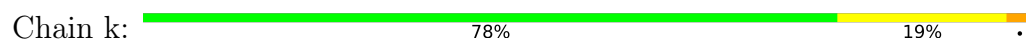
- Molecule 9: Photosystem II reaction center protein J



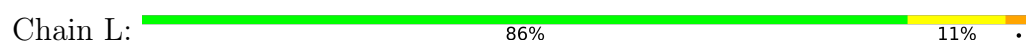
- Molecule 10: Photosystem II reaction center protein K



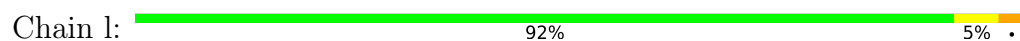
- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M



- Molecule 12: Photosystem II reaction center protein M

Chain m:  75% 17% 6%



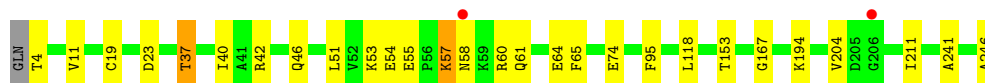
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  92% 8%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  88% 11% 1%



- Molecule 14: Photosystem II reaction center protein T

Chain T:  75% 16% 3% 6%



- Molecule 14: Photosystem II reaction center protein T

Chain t:  81% 12% 3% 6%



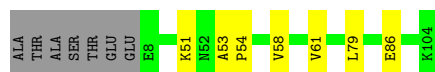
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  85% 9% 7%

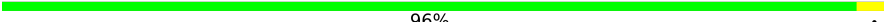


- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  87% 7% 7%



- Molecule 16: Cytochrome c-550

Chain V:  96% .



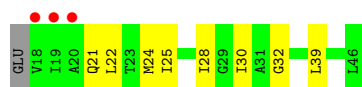
- Molecule 16: Cytochrome c-550

Chain v:  86% 14% .



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:  10% 70% 27% .



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:  63% 33% .



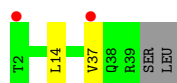
- Molecule 18: Photosystem II reaction center protein X

Chain X:  90% 8% .



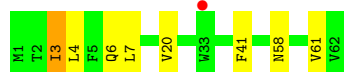
- Molecule 18: Photosystem II reaction center protein X

Chain x:  5% 90% 5% .

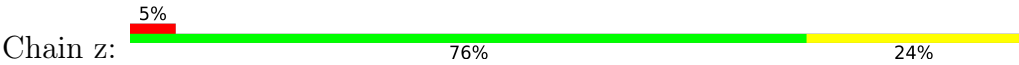


- Molecule 19: Photosystem II reaction center protein Z

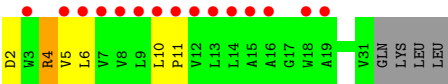
Chain Z:  2% 87% 11% .



- Molecule 19: Photosystem II reaction center protein Z



● Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.97Å 228.72Å 286.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.15 19.99 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.15) 99.8 (19.99-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.156 , 0.203 0.163 , 0.207	Depositor DCC
R_{free} test set	26822 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.670	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 74.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	55675	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.54	0/3115	0.82	0/4242
1	a	0.56	0/3117	0.79	1/4245 (0.0%)
2	B	0.54	0/4191	0.81	1/5709 (0.0%)
2	b	0.53	0/4198	0.82	1/5720 (0.0%)
3	C	0.48	0/3678	0.79	2/5007 (0.0%)
3	c	0.47	0/3774	0.78	0/5135
4	D	0.59	0/2952	0.81	2/4021 (0.0%)
4	d	0.54	0/2952	0.80	1/4021 (0.0%)
5	E	0.44	0/693	0.79	0/944
5	e	0.44	0/695	0.80	0/948
6	F	0.54	0/284	0.77	0/387
6	f	0.53	0/265	0.80	0/360
7	H	0.44	0/535	0.88	0/728
7	h	0.42	0/524	0.77	0/713
8	I	0.44	0/311	0.77	0/419
8	i	0.45	0/311	0.77	0/419
9	J	0.43	0/278	0.75	0/376
9	j	0.44	0/286	0.76	0/386
10	K	0.45	0/303	0.81	0/416
10	k	0.49	0/303	0.85	0/416
11	L	0.56	0/319	0.72	0/433
11	l	0.52	0/319	0.74	0/433
12	M	0.59	0/270	0.85	0/368
12	m	0.59	0/262	0.88	0/357
13	O	0.45	0/1958	0.78	1/2654 (0.0%)
13	o	0.45	0/1937	0.80	2/2625 (0.1%)
14	T	0.57	0/266	0.72	0/362
14	t	0.57	0/266	0.74	0/362
15	U	0.47	0/785	0.76	0/1064
15	u	0.47	0/785	0.74	0/1064
16	V	0.51	0/1109	0.72	0/1502

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.46	0/1098	0.77	0/1488
17	Y	0.48	0/216	0.83	0/289
17	y	0.42	0/216	0.74	0/289
18	X	0.43	0/290	0.76	0/392
18	x	0.42	0/284	0.76	0/384
19	Z	0.41	0/490	0.80	0/669
19	z	0.35	0/490	0.80	0/669
20	R	0.35	0/245	0.69	0/338
All	All	0.51	0/44370	0.79	11/60354 (0.0%)

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	170	ALA	CA-C-N	-6.09	113.67	119.76
4	D	170	ALA	C-N-CA	-6.09	113.67	119.76
3	C	76	ILE	CA-C-N	5.76	125.62	119.28
3	C	76	ILE	C-N-CA	5.76	125.62	119.28
2	b	221	PRO	O-C-N	5.67	123.81	121.15

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	3014	0	2870	23	0
1	a	3010	0	2876	28	0
2	B	4021	0	3898	45	0
2	b	4022	0	3908	42	0
3	C	3553	0	3473	25	0
3	c	3641	0	3569	27	0
4	D	2849	0	2741	30	0
4	d	2849	0	2741	27	0
5	E	668	0	658	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	e	670	0	664	10	0
6	F	275	0	282	4	0
6	f	257	0	269	3	0
7	H	519	0	545	7	0
7	h	511	0	532	6	0
8	I	314	0	328	3	0
8	i	314	0	328	3	0
9	J	272	0	279	5	0
9	j	280	0	291	2	0
10	K	293	0	305	5	0
10	k	293	0	305	6	0
11	L	309	0	327	6	0
11	l	309	0	327	4	0
12	M	274	0	299	9	0
12	m	269	0	288	6	0
13	O	1903	0	1886	9	0
13	o	1891	0	1870	15	0
14	T	264	0	267	4	0
14	t	264	0	267	2	0
15	U	774	0	773	4	0
15	u	774	0	773	3	0
16	V	1085	0	1095	3	0
16	v	1077	0	1082	14	0
17	Y	215	0	246	6	0
17	y	215	0	246	6	0
18	X	287	0	317	2	0
18	x	281	0	312	2	0
19	Z	479	0	516	3	0
19	z	479	0	516	8	0
20	R	239	0	262	4	0
21	A	2	0	0	0	0
21	a	1	0	0	0	0
22	A	4	0	0	0	0
22	U	1	0	0	1	0
22	a	4	0	0	0	0
22	v	1	0	0	0	0
23	A	8	0	0	0	0
23	a	8	0	0	0	0
24	A	260	0	288	11	0
24	B	1040	0	1152	30	0
24	C	845	0	936	29	0
24	D	130	0	144	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	195	0	216	6	0
24	b	1040	0	1152	29	0
24	c	845	0	936	34	0
24	d	195	0	216	7	0
25	A	192	0	222	7	0
25	a	192	0	222	5	0
26	A	40	0	56	1	0
26	B	120	0	168	8	0
26	C	80	0	112	4	0
26	D	40	0	56	2	0
26	H	40	0	56	3	0
26	K	40	0	56	2	0
26	T	40	0	56	4	0
26	Y	40	0	56	4	0
26	a	40	0	56	0	0
26	b	120	0	168	7	0
26	c	80	0	112	3	0
26	d	40	0	56	3	0
26	h	40	0	56	4	0
26	k	40	0	56	2	0
26	t	40	0	56	6	0
26	y	40	0	56	1	0
27	A	108	0	156	6	0
27	B	54	0	78	3	0
27	F	43	0	53	2	0
27	a	108	0	156	3	0
27	b	54	0	78	2	0
27	f	43	0	53	3	0
28	A	18	0	24	2	0
28	B	42	0	56	1	0
28	C	12	0	16	1	0
28	O	6	0	8	0	0
28	T	12	0	16	4	0
28	V	30	0	40	0	0
28	a	12	0	16	1	0
28	b	30	0	40	1	0
28	c	12	0	16	2	0
28	f	6	0	7	1	0
28	o	6	0	8	0	0
28	t	6	0	8	0	0
28	v	18	0	24	1	0
29	A	35	0	46	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	B	25	0	35	0	0
29	C	35	0	46	1	0
29	D	35	0	46	1	0
29	F	35	0	46	1	0
29	M	105	0	138	7	0
29	T	25	0	35	0	0
29	a	70	0	92	2	0
29	b	25	0	35	2	0
29	f	35	0	46	1	0
29	m	35	0	46	2	0
30	A	10	0	0	0	0
30	a	10	0	0	0	0
31	A	11	0	0	1	0
31	a	11	0	0	1	0
32	A	110	0	160	10	0
32	D	110	0	160	3	0
32	a	110	0	160	17	0
32	d	110	0	160	1	0
33	A	28	0	0	0	0
33	B	33	0	0	0	0
33	C	34	0	0	0	0
33	D	57	0	0	0	0
33	I	40	0	0	0	0
33	J	10	0	0	0	0
33	M	10	0	0	0	0
33	X	18	0	0	0	0
33	a	30	0	0	0	0
33	b	33	0	0	0	0
33	c	32	0	0	0	0
33	d	71	0	0	0	0
33	i	40	0	0	0	0
33	j	10	0	0	0	0
33	m	10	0	0	0	0
34	A	51	0	72	5	0
34	B	51	0	72	1	0
34	C	102	0	144	4	0
34	D	51	0	72	1	0
34	Z	37	0	44	2	0
34	a	51	0	72	3	0
34	b	51	0	72	2	0
34	c	102	0	144	3	0
34	j	51	0	72	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	z	39	0	48	4	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	F	1	0	0	0	0
35	O	1	0	0	0	0
35	b	1	0	0	0	0
35	c	2	0	0	0	0
35	f	1	0	0	0	0
35	o	1	0	0	0	0
36	B	95	0	130	2	0
36	C	38	0	52	0	0
36	H	16	0	17	2	0
36	V	19	0	26	3	0
36	b	95	0	130	3	0
36	c	38	0	52	0	0
36	d	16	0	17	3	0
37	C	186	0	246	7	0
37	D	52	0	71	3	0
37	H	62	0	82	1	0
37	c	186	0	246	3	0
37	e	62	0	82	6	0
37	h	62	0	82	1	0
38	D	147	0	222	9	0
38	E	42	0	57	2	0
38	L	49	0	74	3	0
38	a	42	0	57	5	0
38	d	147	0	222	7	0
38	l	49	0	74	2	0
39	F	43	0	30	3	0
39	e	43	0	30	3	0
40	J	1	0	0	0	0
40	j	1	0	0	0	0
41	V	43	0	30	0	0
41	v	43	0	30	0	0
42	A	173	0	0	2	0
42	B	294	0	0	4	0
42	C	232	0	0	4	0
42	D	150	0	0	0	0
42	E	30	0	0	0	0
42	F	9	0	0	0	0
42	H	49	0	0	0	0
42	I	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	J	10	0	0	0	0
42	K	9	0	0	1	0
42	L	14	0	0	0	0
42	M	23	0	0	0	0
42	O	180	0	0	2	0
42	T	18	0	0	2	0
42	U	77	0	0	1	0
42	V	119	0	0	2	0
42	X	6	0	0	0	0
42	Y	4	0	0	0	0
42	Z	1	0	0	0	0
42	a	162	0	0	0	0
42	b	269	0	0	3	0
42	c	205	0	0	2	0
42	d	132	0	0	1	0
42	e	19	0	0	0	0
42	f	8	0	0	0	0
42	h	44	0	0	0	0
42	i	5	0	0	0	0
42	j	6	0	0	0	0
42	k	7	0	0	0	0
42	l	9	0	0	1	0
42	m	11	0	0	0	0
42	o	155	0	0	2	0
42	t	11	0	0	0	0
42	u	93	0	0	0	0
42	v	82	0	0	3	0
42	x	6	0	0	0	0
42	y	2	0	0	0	0
All	All	55675	0	54222	563	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 563 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214[A]:MET:HG2	32:A:420[A]:PL9:H102	1.48	0.93
31:a:418[B]:OEY:O6	31:a:418[B]:OEY:O5	1.89	0.90
24:B:616:CLA:H71	24:B:617:CLA:H192	1.53	0.89
31:A:419[B]:OEY:O6	31:A:419[B]:OEY:O5	1.90	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:c:517:CLA:HHC	24:c:517:CLA:HBB1	1.56	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	384/344 (112%)	380 (99%)	3 (1%)	1 (0%)	36	34
1	a	384/344 (112%)	378 (98%)	5 (1%)	1 (0%)	36	34
2	B	512/505 (101%)	506 (99%)	6 (1%)	0	100	100
2	b	513/505 (102%)	503 (98%)	10 (2%)	0	100	100
3	C	461/455 (101%)	450 (98%)	9 (2%)	2 (0%)	30	26
3	c	473/455 (104%)	459 (97%)	12 (2%)	2 (0%)	30	26
4	D	355/342 (104%)	346 (98%)	9 (2%)	0	100	100
4	d	355/342 (104%)	345 (97%)	10 (3%)	0	100	100
5	E	81/84 (96%)	81 (100%)	0	0	100	100
5	e	81/84 (96%)	81 (100%)	0	0	100	100
6	F	32/44 (73%)	30 (94%)	2 (6%)	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	64/65 (98%)	61 (95%)	3 (5%)	0	100	100
7	h	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	4	1
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/36 (92%)	33 (100%)	0	0	100	100
12	m	32/36 (89%)	32 (100%)	0	0	100	100
13	O	249/244 (102%)	245 (98%)	4 (2%)	0	100	100
13	o	246/244 (101%)	240 (98%)	6 (2%)	0	100	100
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	29/32 (91%)	29 (100%)	0	0	100	100
15	U	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
16	V	136/137 (99%)	131 (96%)	5 (4%)	0	100	100
16	v	135/137 (98%)	129 (96%)	6 (4%)	0	100	100
17	Y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
17	y	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
18	X	37/40 (92%)	37 (100%)	0	0	100	100
18	x	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	2
19	z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	2
20	R	28/34 (82%)	27 (96%)	1 (4%)	0	100	100
All	All	5429/5384 (101%)	5309 (98%)	111 (2%)	9 (0%)	48	44

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
8	i	36	ASP

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	311/279 (112%)	311 (100%)	0	100	100
1	a	311/279 (112%)	310 (100%)	1 (0%)	86	91
2	B	412/403 (102%)	407 (99%)	5 (1%)	63	70
2	b	413/403 (102%)	409 (99%)	4 (1%)	68	75
3	C	361/356 (101%)	355 (98%)	6 (2%)	53	60
3	c	371/356 (104%)	364 (98%)	7 (2%)	50	56
4	D	290/277 (105%)	287 (99%)	3 (1%)	68	75
4	d	290/277 (105%)	288 (99%)	2 (1%)	76	82
5	E	74/73 (101%)	73 (99%)	1 (1%)	59	66
5	e	74/73 (101%)	73 (99%)	1 (1%)	59	66
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	26/38 (68%)	25 (96%)	1 (4%)	29	29
7	H	55/54 (102%)	54 (98%)	1 (2%)	51	58
7	h	54/54 (100%)	53 (98%)	1 (2%)	50	56
8	I	34/34 (100%)	34 (100%)	0	100	100
8	i	34/34 (100%)	33 (97%)	1 (3%)	37	39
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	27/27 (100%)	26 (96%)	1 (4%)	30	30
10	K	30/30 (100%)	27 (90%)	3 (10%)	7	3
10	k	30/30 (100%)	28 (93%)	2 (7%)	15	10
11	L	36/35 (103%)	35 (97%)	1 (3%)	38	40
11	l	36/35 (103%)	35 (97%)	1 (3%)	38	40
12	M	31/32 (97%)	31 (100%)	0	100	100
12	m	30/32 (94%)	29 (97%)	1 (3%)	33	34
13	O	214/207 (103%)	209 (98%)	5 (2%)	44	49
13	o	211/207 (102%)	205 (97%)	6 (3%)	38	40
14	T	27/28 (96%)	25 (93%)	2 (7%)	13	8
14	t	27/28 (96%)	25 (93%)	2 (7%)	13	8
15	U	84/89 (94%)	81 (96%)	3 (4%)	31	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	u	84/89 (94%)	82 (98%)	2 (2%)	43	47
16	V	119/117 (102%)	118 (99%)	1 (1%)	73	79
16	v	118/117 (101%)	117 (99%)	1 (1%)	73	79
17	Y	22/23 (96%)	21 (96%)	1 (4%)	24	22
17	y	22/23 (96%)	19 (86%)	3 (14%)	3	1
18	X	32/33 (97%)	32 (100%)	0	100	100
18	x	31/33 (94%)	31 (100%)	0	100	100
19	Z	52/52 (100%)	48 (92%)	4 (8%)	12	7
19	z	52/52 (100%)	48 (92%)	4 (8%)	12	7
20	R	25/29 (86%)	24 (96%)	1 (4%)	28	27
All	All	4504/4403 (102%)	4426 (98%)	78 (2%)	53	60

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	k	17	ILE
17	y	18	VAL
12	m	33	GLN
13	o	194	LYS
19	z	29	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
4	d	61	HIS
10	k	40	GLN
4	d	83	ASN
4	d	332	GLN
13	o	130	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
14	FME	t	1	14	8,9,10	0.81	0	8,9,11	2.19	4 (50%)
12	FME	M	1	12	8,9,10	0.71	0	8,9,11	1.33	2 (25%)
8	FME	i	1	8	8,9,10	0.64	0	8,9,11	1.15	1 (12%)
8	FME	I	1	8	8,9,10	0.66	0	8,9,11	1.19	1 (12%)
12	FME	m	1	12	8,9,10	0.69	0	8,9,11	1.25	1 (12%)
14	FME	T	1	14	8,9,10	0.74	0	8,9,11	1.24	1 (12%)

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
14	FME	t	1	14	-	1/7/9/11	-
12	FME	M	1	12	-	2/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
14	FME	T	1	14	-	1/7/9/11	-

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	CA-N-CN	-3.87	116.87	122.82
14	t	1	FME	C-CA-N	2.79	114.89	109.50
14	T	1	FME	O-C-CA	-2.55	118.22	124.77
14	t	1	FME	O-C-CA	-2.48	118.40	124.77
14	t	1	FME	O1-CN-N	-2.40	119.13	125.32

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O1-CN-N-CA
14	T	1	FME	O1-CN-N-CA
12	M	1	FME	CA-CB-CG-SD
12	M	1	FME	CB-CA-N-CN
14	t	1	FME	CB-CA-N-CN

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 266 ligands modelled in this entry, 24 are monoatomic and 18 are unknown - leaving 224 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	$\# Z > 2$
38	LHG	l	101	-	48,48,48	0.92	2 (4%)	51,54,54	1.12	6 (11%)
32	PL9	D	405[B]	-	55,55,55	0.66	2 (3%)	68,69,69	1.71	19 (27%)
24	CLA	C	503	-	69,73,73	2.04	19 (27%)	82,113,113	2.60	29 (35%)
37	DGD	h	102	-	63,63,67	0.92	3 (4%)	77,77,81	0.97	4 (5%)
24	CLA	B	602	42	69,73,73	2.04	19 (27%)	82,113,113	2.67	29 (35%)
24	CLA	b	619	-	69,73,73	2.01	19 (27%)	82,113,113	2.66	31 (37%)
24	CLA	B	616	-	69,73,73	1.99	19 (27%)	82,113,113	2.70	32 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PHO	a	411	-	58,69,69	2.76	14 (24%)	55,99,99	2.79	15 (27%)
26	BCR	h	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.39	8 (14%)
32	PL9	D	405[A]	-	55,55,55	0.65	2 (3%)	68,69,69	1.67	19 (27%)
25	PHO	A	409[B]	-	58,69,69	2.82	14 (24%)	55,99,99	2.89	15 (27%)
37	DGD	c	519	-	63,63,67	0.83	2 (3%)	77,77,81	1.10	5 (6%)
29	LMT	M	101	-	36,36,36	0.41	0	47,47,47	0.95	1 (2%)
24	CLA	B	610	-	69,73,73	2.05	19 (27%)	82,113,113	2.63	30 (36%)
32	PL9	a	416[B]	-	55,55,55	0.65	2 (3%)	68,69,69	1.87	21 (30%)
36	HTG	b	609	-	19,19,19	0.98	2 (10%)	23,24,24	1.13	3 (13%)
41	HEC	v	205	16	46,50,50	1.72	10 (21%)	58,82,82	1.65	13 (22%)
27	SQD	a	414	-	52,54,54	0.92	2 (3%)	62,65,65	1.50	12 (19%)
28	GOL	v	202	-	5,5,5	0.35	0	5,5,5	0.28	0
24	CLA	A	410	-	69,73,73	2.05	20 (28%)	82,113,113	2.65	35 (42%)
24	CLA	C	511	3	69,73,73	2.03	19 (27%)	82,113,113	2.63	31 (37%)
37	DGD	H	103	-	63,63,67	0.89	3 (4%)	77,77,81	1.05	7 (9%)
29	LMT	a	404	-	36,36,36	0.49	1 (2%)	47,47,47	1.23	3 (6%)
24	CLA	B	614	-	69,73,73	1.98	18 (26%)	82,113,113	2.53	33 (40%)
28	GOL	A	415	-	5,5,5	0.42	0	5,5,5	0.24	0
29	LMT	M	104	-	36,36,36	0.46	0	47,47,47	0.88	2 (4%)
26	BCR	Y	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.63	9 (16%)
29	LMT	T	104	-	25,25,36	0.50	0	30,30,47	0.94	1 (3%)
28	GOL	V	202	-	5,5,5	0.38	0	5,5,5	0.29	0
36	HTG	b	602	-	19,19,19	0.85	1 (5%)	23,24,24	1.07	2 (8%)
34	LMG	z	101	-	39,39,55	1.07	2 (5%)	47,47,63	1.14	4 (8%)
24	CLA	c	517	-	69,73,73	2.02	19 (27%)	82,113,113	2.69	33 (40%)
28	GOL	O	301	-	5,5,5	0.38	0	5,5,5	0.44	0
24	CLA	d	402	-	69,73,73	1.99	18 (26%)	82,113,113	2.66	31 (37%)
24	CLA	d	403	-	69,73,73	2.02	21 (30%)	82,113,113	2.71	31 (37%)
37	DGD	c	521	-	63,63,67	0.88	2 (3%)	77,77,81	1.09	6 (7%)
28	GOL	b	605	-	5,5,5	0.38	0	5,5,5	0.33	0
34	LMG	j	101	40	51,51,55	0.93	2 (3%)	59,59,63	0.94	4 (6%)
37	DGD	c	520	-	63,63,67	0.88	2 (3%)	77,77,81	0.96	2 (2%)
28	GOL	V	203	-	5,5,5	0.36	0	5,5,5	0.46	0
28	GOL	B	627	-	5,5,5	0.34	0	5,5,5	0.50	0
24	CLA	B	608	42	69,73,73	2.00	20 (28%)	82,113,113	2.63	33 (40%)
24	CLA	c	511	42	69,73,73	2.00	19 (27%)	82,113,113	2.63	28 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	b	620	42	69,73,73	2.05	20 (28%)	82,113,113	2.65	30 (36%)
32	PL9	d	405[B]	-	55,55,55	0.66	2 (3%)	68,69,69	1.61	17 (25%)
24	CLA	C	507	42	69,73,73	2.01	20 (28%)	82,113,113	2.63	31 (37%)
24	CLA	A	405	-	69,73,73	2.01	20 (28%)	82,113,113	2.62	30 (36%)
24	CLA	C	505	-	69,73,73	2.01	20 (28%)	82,113,113	2.61	29 (35%)
32	PL9	d	405[A]	-	55,55,55	0.67	2 (3%)	68,69,69	1.55	13 (19%)
34	LMG	a	415	-	51,51,55	0.91	2 (3%)	59,59,63	1.18	4 (6%)
38	LHG	L	101	-	48,48,48	0.92	2 (4%)	51,54,54	1.06	4 (7%)
24	CLA	a	412	-	69,73,73	2.03	19 (27%)	82,113,113	2.72	34 (41%)
24	CLA	C	504	42	69,73,73	2.00	19 (27%)	82,113,113	2.73	32 (39%)
26	BCR	b	628	-	41,41,41	0.98	1 (2%)	56,56,56	1.34	9 (16%)
36	HTG	B	623	-	19,19,19	0.95	1 (5%)	23,24,24	1.14	1 (4%)
24	CLA	b	617	42	69,73,73	1.96	18 (26%)	82,113,113	2.73	29 (35%)
24	CLA	c	507	-	69,73,73	2.03	20 (28%)	82,113,113	2.66	30 (36%)
26	BCR	k	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.47	11 (19%)
24	CLA	c	515	3	69,73,73	1.99	19 (27%)	82,113,113	2.59	29 (35%)
24	CLA	B	617	-	69,73,73	1.99	19 (27%)	82,113,113	2.63	30 (36%)
27	SQD	A	412	-	52,54,54	0.91	2 (3%)	62,65,65	1.50	11 (17%)
28	GOL	a	402	-	5,5,5	0.37	0	5,5,5	0.30	0
32	PL9	A	420[A]	-	55,55,55	0.64	2 (3%)	68,69,69	1.79	21 (30%)
36	HTG	B	633	-	19,19,19	0.93	1 (5%)	23,24,24	1.29	2 (8%)
24	CLA	b	612	-	69,73,73	2.03	21 (30%)	82,113,113	2.72	31 (37%)
24	CLA	C	508	-	69,73,73	2.05	20 (28%)	82,113,113	2.67	31 (37%)
24	CLA	b	624	-	69,73,73	1.97	18 (26%)	82,113,113	2.77	32 (39%)
24	CLA	B	605	-	69,73,73	1.96	19 (27%)	82,113,113	2.75	31 (37%)
26	BCR	b	629	-	41,41,41	1.10	1 (2%)	56,56,56	1.24	7 (12%)
26	BCR	d	404	-	41,41,41	1.14	1 (2%)	56,56,56	1.59	12 (21%)
26	BCR	a	413	-	41,41,41	1.05	1 (2%)	56,56,56	1.16	6 (10%)
37	DGD	D	406	-	52,52,67	1.01	3 (5%)	60,60,81	1.17	4 (6%)
25	PHO	A	409[A]	-	58,69,69	2.78	15 (25%)	55,99,99	2.92	15 (27%)
28	GOL	b	604	-	5,5,5	0.37	0	5,5,5	0.26	0
28	GOL	T	102	-	5,5,5	0.39	0	5,5,5	0.30	0
32	PL9	a	416[A]	-	55,55,55	0.64	2 (3%)	68,69,69	1.94	21 (30%)
31	OXY	a	418[B]	3,42,1	0,16,16	-	-	-	-	-
28	GOL	A	413	-	5,5,5	0.35	0	5,5,5	0.26	0
24	CLA	b	618	-	69,73,73	2.09	20 (28%)	82,113,113	2.56	34 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	HTG	b	608	-	19,19,19	0.94	2 (10%)	23,24,24	1.35	2 (8%)
28	GOL	c	502	-	5,5,5	0.42	0	5,5,5	0.54	0
24	CLA	b	622	-	69,73,73	2.02	19 (27%)	82,113,113	2.60	33 (40%)
24	CLA	c	506	-	69,73,73	2.02	21 (30%)	82,113,113	2.60	27 (32%)
26	BCR	A	411	-	41,41,41	1.05	1 (2%)	56,56,56	1.21	7 (12%)
24	CLA	C	509	-	69,73,73	2.08	20 (28%)	82,113,113	2.66	31 (37%)
27	SQD	a	405	-	52,54,54	1.00	2 (3%)	62,65,65	1.18	4 (6%)
34	LMG	b	630	-	51,51,55	0.91	2 (3%)	59,59,63	1.04	4 (6%)
26	BCR	B	618	-	41,41,41	1.01	1 (2%)	56,56,56	1.39	8 (14%)
41	HEC	V	206	16	46,50,50	1.78	11 (23%)	58,82,82	1.56	10 (17%)
38	LHG	D	409	-	48,48,48	0.95	2 (4%)	51,54,54	1.08	4 (7%)
28	GOL	B	631	-	5,5,5	0.38	0	5,5,5	0.34	0
24	CLA	d	401	42	69,73,73	2.03	20 (28%)	82,113,113	2.69	34 (41%)
28	GOL	C	524	-	5,5,5	0.39	0	5,5,5	0.81	0
34	LMG	C	520	-	51,51,55	0.96	2 (3%)	59,59,63	1.11	4 (6%)
24	CLA	C	510	-	69,73,73	2.05	20 (28%)	82,113,113	2.58	30 (36%)
29	LMT	f	103	-	36,36,36	0.47	0	47,47,47	0.84	1 (2%)
29	LMT	M	103	-	36,36,36	0.53	1 (2%)	47,47,47	1.00	3 (6%)
23	BCT	a	419[B]	21	3,3,3	0.53	0	2,3,3	0.73	0
36	HTG	H	101	-	16,16,19	1.03	2 (12%)	20,21,24	1.07	1 (5%)
24	CLA	A	406	42	69,73,73	1.98	18 (26%)	82,113,113	2.80	33 (40%)
37	DGD	e	101	-	63,63,67	0.93	2 (3%)	77,77,81	1.24	7 (9%)
28	GOL	B	630	-	5,5,5	0.40	0	5,5,5	0.13	0
24	CLA	c	514	-	69,73,73	2.03	19 (27%)	82,113,113	2.67	32 (39%)
24	CLA	B	612	-	69,73,73	1.97	20 (28%)	82,113,113	2.74	31 (37%)
26	BCR	B	619	-	41,41,41	1.07	1 (2%)	56,56,56	1.48	9 (16%)
26	BCR	D	404	-	41,41,41	1.03	1 (2%)	56,56,56	1.82	11 (19%)
26	BCR	y	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.57	10 (17%)
28	GOL	T	101	-	5,5,5	0.51	0	5,5,5	0.22	0
24	CLA	C	512	-	69,73,73	2.01	20 (28%)	82,113,113	2.68	31 (37%)
26	BCR	b	627	-	41,41,41	1.04	1 (2%)	56,56,56	1.35	6 (10%)
28	GOL	c	501	-	5,5,5	0.33	0	5,5,5	0.34	0
38	LHG	a	422	-	41,41,48	1.03	2 (4%)	44,47,54	0.96	3 (6%)
38	LHG	d	406	-	48,48,48	0.89	3 (6%)	51,54,54	1.07	5 (9%)
36	HTG	c	524	-	19,19,19	0.95	2 (10%)	23,24,24	1.37	1 (4%)
24	CLA	C	506	-	69,73,73	2.02	19 (27%)	82,113,113	2.59	31 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PHO	A	408	-	58,69,69	2.73	13 (22%)	55,99,99	3.00	15 (27%)
26	BCR	K	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.56	13 (23%)
24	CLA	C	513	-	69,73,73	2.03	20 (28%)	82,113,113	2.63	31 (37%)
28	GOL	B	628	-	5,5,5	0.36	0	5,5,5	0.59	0
28	GOL	V	205	-	5,5,5	0.35	0	5,5,5	0.41	0
39	HEM	F	102	6,5	50,50,50	1.53	7 (14%)	67,82,82	1.71	12 (17%)
24	CLA	D	402	-	69,73,73	1.94	19 (27%)	82,113,113	2.74	32 (39%)
24	CLA	D	403	-	69,73,73	2.02	21 (30%)	82,113,113	2.68	31 (37%)
30	OEX	a	417[A]	3,42,1	0,15,15	-	-	-	-	-
37	DGD	C	516	-	63,63,67	0.87	2 (3%)	77,77,81	1.09	6 (7%)
38	LHG	D	407	-	48,48,48	0.87	2 (4%)	51,54,54	1.11	5 (9%)
28	GOL	t	102	-	5,5,5	0.48	0	5,5,5	0.16	0
24	CLA	b	616	-	69,73,73	2.02	20 (28%)	82,113,113	2.68	29 (35%)
25	PHO	a	420[B]	-	58,69,69	2.79	13 (22%)	55,99,99	2.87	13 (23%)
26	BCR	T	103	-	41,41,41	1.07	1 (2%)	56,56,56	1.76	16 (28%)
26	BCR	C	515	-	41,41,41	1.00	1 (2%)	56,56,56	1.50	9 (16%)
36	HTG	b	633	-	19,19,19	1.06	2 (10%)	23,24,24	1.75	4 (17%)
24	CLA	b	625	-	69,73,73	2.01	20 (28%)	82,113,113	2.67	32 (39%)
29	LMT	F	101	-	36,36,36	0.48	0	47,47,47	0.93	1 (2%)
38	LHG	d	408	-	48,48,48	0.94	2 (4%)	51,54,54	0.99	2 (3%)
24	CLA	c	513	-	69,73,73	2.06	20 (28%)	82,113,113	2.64	30 (36%)
24	CLA	b	623	-	69,73,73	2.03	20 (28%)	82,113,113	2.60	30 (36%)
29	LMT	C	521	-	36,36,36	0.48	0	47,47,47	1.15	3 (6%)
29	LMT	a	421	-	36,36,36	0.46	0	47,47,47	0.84	1 (2%)
23	BCT	A	404[B]	21	3,3,3	0.51	0	2,3,3	1.01	0
24	CLA	a	409	-	69,73,73	2.02	19 (27%)	82,113,113	2.68	34 (41%)
36	HTG	B	625	-	19,19,19	0.99	1 (5%)	23,24,24	1.72	4 (17%)
36	HTG	B	632	-	19,19,19	1.00	2 (10%)	23,24,24	1.25	2 (8%)
24	CLA	b	614	-	69,73,73	2.01	19 (27%)	82,113,113	2.66	30 (36%)
27	SQD	B	621	-	52,54,54	0.97	2 (3%)	62,65,65	1.41	8 (12%)
26	BCR	B	620	-	41,41,41	1.07	1 (2%)	56,56,56	1.54	9 (16%)
29	LMT	A	417	-	36,36,36	0.62	1 (2%)	47,47,47	1.27	3 (6%)
29	LMT	m	102	-	36,36,36	0.45	0	47,47,47	1.03	3 (6%)
34	LMG	B	622	-	51,51,55	0.94	2 (3%)	59,59,63	1.08	4 (6%)
34	LMG	c	523	-	51,51,55	0.96	3 (5%)	59,59,63	1.23	8 (13%)
36	HTG	b	632	-	19,19,19	0.71	1 (5%)	23,24,24	1.17	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	c	510	-	69,73,73	2.00	20 (28%)	82,113,113	2.63	29 (35%)
28	GOL	o	301	-	5,5,5	0.38	0	5,5,5	0.29	0
24	CLA	C	502	-	69,73,73	2.00	20 (28%)	82,113,113	2.62	30 (36%)
34	LMG	c	522	-	51,51,55	0.91	2 (3%)	59,59,63	1.14	5 (8%)
28	GOL	B	629	-	5,5,5	0.36	0	5,5,5	0.37	0
26	BCR	C	514	-	41,41,41	1.05	1 (2%)	56,56,56	1.56	10 (17%)
24	CLA	B	607	-	69,73,73	2.01	20 (28%)	82,113,113	2.74	31 (37%)
39	HEM	e	102	6,5	50,50,50	1.54	8 (16%)	67,82,82	1.61	15 (22%)
28	GOL	b	603	-	5,5,5	0.43	0	5,5,5	0.53	0
24	CLA	c	516	-	69,73,73	2.02	20 (28%)	82,113,113	2.75	33 (40%)
23	BCT	a	419[A]	-	3,3,3	0.53	0	2,3,3	0.85	0
29	LMT	D	401	-	36,36,36	0.43	0	47,47,47	1.01	1 (2%)
24	CLA	b	615	-	69,73,73	2.00	19 (27%)	82,113,113	2.77	28 (34%)
36	HTG	c	525	-	19,19,19	0.93	2 (10%)	23,24,24	1.33	2 (8%)
31	OEY	A	419[B]	3,42,1	0,16,16	-	-	-	-	-
38	LHG	d	407	-	48,48,48	0.91	2 (4%)	51,54,54	1.03	4 (7%)
28	GOL	f	101	35	5,5,5	0.33	0	5,5,5	0.39	0
26	BCR	H	102	-	41,41,41	1.12	1 (2%)	56,56,56	1.44	9 (16%)
24	CLA	B	609	-	69,73,73	2.02	20 (28%)	82,113,113	2.63	32 (39%)
24	CLA	B	615	-	69,73,73	1.98	19 (27%)	82,113,113	2.75	31 (37%)
24	CLA	c	508	42	69,73,73	2.02	19 (27%)	82,113,113	2.74	34 (41%)
37	DGD	C	517	-	63,63,67	0.89	3 (4%)	77,77,81	0.99	5 (6%)
34	LMG	C	519	-	51,51,55	0.97	2 (3%)	59,59,63	0.99	3 (5%)
24	CLA	b	613	-	69,73,73	1.97	20 (28%)	82,113,113	2.67	32 (39%)
28	GOL	v	201	-	5,5,5	0.35	0	5,5,5	0.26	0
28	GOL	B	626	-	5,5,5	0.44	0	5,5,5	0.37	0
24	CLA	A	407	42	69,73,73	2.00	20 (28%)	82,113,113	2.68	34 (41%)
28	GOL	C	525	-	5,5,5	0.40	0	5,5,5	0.72	0
28	GOL	b	606	-	5,5,5	0.39	0	5,5,5	0.30	0
38	LHG	D	408	-	48,48,48	0.90	2 (4%)	51,54,54	0.86	3 (5%)
24	CLA	b	621	-	69,73,73	1.95	19 (27%)	82,113,113	2.67	31 (37%)
24	CLA	c	512	-	69,73,73	2.02	20 (28%)	82,113,113	2.61	32 (39%)
24	CLA	a	410	42	69,73,73	2.01	20 (28%)	82,113,113	2.69	33 (40%)
37	DGD	C	518	-	63,63,67	0.86	2 (3%)	77,77,81	0.92	4 (5%)
36	HTG	B	624	-	19,19,19	0.76	1 (5%)	23,24,24	1.38	2 (8%)
29	LMT	b	631	-	25,25,36	0.53	0	30,30,47	0.67	0
24	CLA	C	501	-	69,73,73	2.01	19 (27%)	82,113,113	2.65	29 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	LHG	E	101	-	41,41,48	1.04	2 (4%)	44,47,54	1.09	3 (6%)
34	LMG	D	412	40	51,51,55	0.90	2 (3%)	59,59,63	1.00	3 (5%)
25	PHO	a	420[A]	-	58,69,69	2.77	13 (22%)	55,99,99	3.03	15 (27%)
24	CLA	B	604	-	69,73,73	2.06	19 (27%)	82,113,113	2.69	29 (35%)
27	SQD	F	103	-	41,43,54	1.09	2 (4%)	51,54,65	1.61	11 (21%)
24	CLA	b	626	-	69,73,73	2.00	20 (28%)	82,113,113	2.66	31 (37%)
28	GOL	V	204	-	5,5,5	0.39	0	5,5,5	0.28	0
28	GOL	a	401	-	5,5,5	0.49	0	5,5,5	0.54	0
36	HTG	C	523	-	19,19,19	0.95	1 (5%)	23,24,24	1.70	4 (17%)
24	CLA	b	611	42	69,73,73	2.04	19 (27%)	82,113,113	2.67	27 (32%)
24	CLA	B	613	-	69,73,73	1.98	18 (26%)	82,113,113	2.75	31 (37%)
24	CLA	B	603	-	69,73,73	2.01	20 (28%)	82,113,113	2.74	33 (40%)
36	HTG	C	522	-	19,19,19	0.92	2 (10%)	23,24,24	1.39	2 (8%)
34	LMG	Z	101	-	37,37,55	0.96	2 (5%)	45,45,63	1.39	6 (13%)
28	GOL	b	607	-	5,5,5	0.37	0	5,5,5	0.33	0
28	GOL	A	414	-	5,5,5	0.47	0	5,5,5	0.59	0
27	SQD	f	102	-	41,43,54	1.11	2 (4%)	51,54,65	1.40	6 (11%)
24	CLA	B	611	42	69,73,73	2.09	19 (27%)	82,113,113	2.64	34 (41%)
36	HTG	V	207	-	19,19,19	0.96	2 (10%)	23,24,24	1.16	2 (8%)
23	BCT	A	404[A]	21	3,3,3	0.50	0	2,3,3	1.09	0
26	BCR	c	527	-	41,41,41	1.06	1 (2%)	56,56,56	1.56	7 (12%)
28	GOL	B	636	-	5,5,5	0.41	0	5,5,5	0.56	0
24	CLA	c	509	-	69,73,73	1.99	20 (28%)	82,113,113	2.58	30 (36%)
26	BCR	t	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.64	12 (21%)
24	CLA	B	606	-	69,73,73	1.99	18 (26%)	82,113,113	2.76	30 (36%)
30	OEX	A	418[A]	3,42,1	0,15,15	-	-	-	-	-
28	GOL	V	201	35	5,5,5	0.37	0	5,5,5	0.27	0
27	SQD	A	416	-	52,54,54	0.96	2 (3%)	62,65,65	1.16	5 (8%)
27	SQD	b	601	-	52,54,54	0.98	2 (3%)	62,65,65	1.53	9 (14%)
36	HTG	d	411	-	16,16,19	1.04	2 (12%)	20,21,24	1.70	2 (10%)
29	LMT	B	635	-	25,25,36	0.52	0	30,30,47	0.88	1 (3%)
28	GOL	v	203	-	5,5,5	0.41	0	5,5,5	0.26	0
32	PL9	A	420[B]	-	55,55,55	0.65	2 (3%)	68,69,69	1.78	22 (32%)
26	BCR	c	518	-	41,41,41	1.06	1 (2%)	56,56,56	1.51	10 (17%)
34	LMG	A	422	-	51,51,55	0.94	2 (3%)	59,59,63	1.14	5 (8%)
24	CLA	c	505	-	69,73,73	2.00	19 (27%)	82,113,113	2.58	30 (36%)

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
38	LHG	l	101	-	-	15/53/53/53	-
32	PL9	D	405[B]	-	-	8/53/73/73	0/1/1/1
24	CLA	C	503	-	1/1/15/20	1/39/115/115	-
37	DGD	h	102	-	-	11/51/91/95	0/2/2/2
24	CLA	B	602	42	1/1/15/20	13/39/115/115	-
24	CLA	b	619	-	1/1/15/20	5/39/115/115	-
24	CLA	B	616	-	1/1/15/20	12/39/115/115	-
25	PHO	a	411	-	-	3/37/103/103	0/5/6/6
26	BCR	h	101	-	-	1/29/63/63	0/2/2/2
32	PL9	D	405[A]	-	-	7/53/73/73	0/1/1/1
25	PHO	A	409[B]	-	-	1/37/103/103	0/5/6/6
37	DGD	c	519	-	-	14/51/91/95	0/2/2/2
29	LMT	M	101	-	-	4/21/61/61	0/2/2/2
24	CLA	B	610	-	1/1/15/20	6/39/115/115	-
32	PL9	a	416[B]	-	-	14/53/73/73	0/1/1/1
36	HTG	b	609	-	-	0/10/30/30	0/1/1/1
41	HEC	v	205	16	-	6/14/54/54	-
27	SQD	a	414	-	-	14/49/69/69	0/1/1/1
28	GOL	v	202	-	-	2/4/4/4	-
24	CLA	A	410	-	1/1/15/20	9/39/115/115	-
24	CLA	C	511	3	1/1/15/20	3/39/115/115	-
37	DGD	H	103	-	-	14/51/91/95	0/2/2/2
29	LMT	a	404	-	-	9/21/61/61	0/2/2/2
24	CLA	B	614	-	1/1/15/20	3/39/115/115	-
28	GOL	A	415	-	-	2/4/4/4	-
29	LMT	M	104	-	-	8/21/61/61	0/2/2/2
26	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
29	LMT	T	104	-	-	7/17/37/61	0/1/1/2
28	GOL	V	202	-	-	2/4/4/4	-
36	HTG	b	602	-	-	3/10/30/30	0/1/1/1
34	LMG	z	101	-	-	15/34/54/70	0/1/1/1
24	CLA	c	517	-	-	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	O	301	-	-	2/4/4/4	-
24	CLA	d	402	-	1/1/15/20	4/39/115/115	-
24	CLA	d	403	-	1/1/15/20	4/39/115/115	-
37	DGD	c	521	-	-	16/51/91/95	0/2/2/2
28	GOL	b	605	-	-	1/4/4/4	-
34	LMG	j	101	40	-	11/46/66/70	0/1/1/1
37	DGD	c	520	-	-	17/51/91/95	0/2/2/2
28	GOL	V	203	-	-	2/4/4/4	-
28	GOL	B	627	-	-	2/4/4/4	-
24	CLA	B	608	42	1/1/15/20	7/39/115/115	-
24	CLA	c	511	42	1/1/15/20	6/39/115/115	-
24	CLA	b	620	42	1/1/15/20	5/39/115/115	-
32	PL9	d	405[B]	-	-	5/53/73/73	0/1/1/1
24	CLA	C	507	42	1/1/15/20	8/39/115/115	-
24	CLA	A	405	-	1/1/15/20	7/39/115/115	-
24	CLA	C	505	-	1/1/15/20	4/39/115/115	-
32	PL9	d	405[A]	-	-	8/53/73/73	0/1/1/1
34	LMG	a	415	-	-	16/46/66/70	0/1/1/1
38	LHG	L	101	-	-	16/53/53/53	-
24	CLA	a	412	-	1/1/15/20	9/39/115/115	-
24	CLA	C	504	42	1/1/15/20	5/39/115/115	-
26	BCR	b	628	-	-	0/29/63/63	0/2/2/2
36	HTG	B	623	-	-	3/10/30/30	0/1/1/1
24	CLA	b	617	42	1/1/15/20	2/39/115/115	-
24	CLA	c	507	-	-	3/39/115/115	-
26	BCR	k	101	-	-	2/29/63/63	0/2/2/2
24	CLA	c	515	3	1/1/15/20	5/39/115/115	-
24	CLA	B	617	-	1/1/15/20	6/39/115/115	-
27	SQD	A	412	-	-	9/49/69/69	0/1/1/1
28	GOL	a	402	-	-	2/4/4/4	-
32	PL9	A	420[A]	-	-	10/53/73/73	0/1/1/1
36	HTG	B	633	-	-	0/10/30/30	0/1/1/1
24	CLA	b	612	-	1/1/15/20	5/39/115/115	-
24	CLA	C	508	-	1/1/15/20	3/39/115/115	-
24	CLA	b	624	-	1/1/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	605	-	1/1/15/20	5/39/115/115	-
26	BCR	b	629	-	-	0/29/63/63	0/2/2/2
26	BCR	d	404	-	-	3/29/63/63	0/2/2/2
26	BCR	a	413	-	-	0/29/63/63	0/2/2/2
37	DGD	D	406	-	-	22/47/67/95	0/1/1/2
25	PHO	A	409[A]	-	-	0/37/103/103	0/5/6/6
28	GOL	b	604	-	-	0/4/4/4	-
28	GOL	T	102	-	-	2/4/4/4	-
32	PL9	a	416[A]	-	-	14/53/73/73	0/1/1/1
28	GOL	A	413	-	-	1/4/4/4	-
24	CLA	b	618	-	-	1/39/115/115	-
36	HTG	b	608	-	-	1/10/30/30	0/1/1/1
28	GOL	c	502	-	-	1/4/4/4	-
24	CLA	b	622	-	1/1/15/20	1/39/115/115	-
24	CLA	c	506	-	-	6/39/115/115	-
26	BCR	A	411	-	-	0/29/63/63	0/2/2/2
24	CLA	C	509	-	1/1/15/20	14/39/115/115	-
27	SQD	a	405	-	-	17/49/69/69	0/1/1/1
34	LMG	b	630	-	-	10/46/66/70	0/1/1/1
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
41	HEC	V	206	16	-	6/14/54/54	-
38	LHG	D	409	-	-	11/53/53/53	-
28	GOL	B	631	-	-	1/4/4/4	-
24	CLA	d	401	42	1/1/15/20	4/39/115/115	-
28	GOL	C	524	-	-	2/4/4/4	-
34	LMG	C	520	-	-	12/46/66/70	0/1/1/1
24	CLA	C	510	-	1/1/15/20	6/39/115/115	-
29	LMT	f	103	-	-	9/21/61/61	0/2/2/2
29	LMT	M	103	-	-	9/21/61/61	0/2/2/2
36	HTG	H	101	-	-	0/7/27/30	0/1/1/1
24	CLA	A	406	42	1/1/15/20	4/39/115/115	-
37	DGD	e	101	-	-	27/51/91/95	0/2/2/2
28	GOL	B	630	-	-	4/4/4/4	-
24	CLA	c	514	-	1/1/15/20	9/39/115/115	-
24	CLA	B	612	-	1/1/15/20	0/39/115/115	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
26	BCR	D	404	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	y	101	-	-	4/29/63/63	0/2/2/2
28	GOL	T	101	-	-	1/4/4/4	-
24	CLA	C	512	-	1/1/15/20	9/39/115/115	-
26	BCR	b	627	-	-	2/29/63/63	0/2/2/2
28	GOL	c	501	-	-	0/4/4/4	-
38	LHG	a	422	-	-	18/46/46/53	-
38	LHG	d	406	-	-	10/53/53/53	-
36	HTG	c	524	-	-	3/10/30/30	0/1/1/1
24	CLA	C	506	-	1/1/15/20	8/39/115/115	-
25	PHO	A	408	-	-	2/37/103/103	0/5/6/6
26	BCR	K	101	-	-	1/29/63/63	0/2/2/2
24	CLA	C	513	-	1/1/15/20	7/39/115/115	-
28	GOL	B	628	-	-	2/4/4/4	-
28	GOL	V	205	-	-	2/4/4/4	-
39	HEM	F	102	6,5	-	8/14/54/54	-
24	CLA	D	402	-	1/1/15/20	3/39/115/115	-
24	CLA	D	403	-	1/1/15/20	3/39/115/115	-
37	DGD	C	516	-	-	16/51/91/95	0/2/2/2
38	LHG	D	407	-	-	13/53/53/53	-
28	GOL	t	102	-	-	0/4/4/4	-
24	CLA	b	616	-	1/1/15/20	5/39/115/115	-
25	PHO	a	420[B]	-	-	3/37/103/103	0/5/6/6
26	BCR	T	103	-	-	3/29/63/63	0/2/2/2
26	BCR	C	515	-	-	2/29/63/63	0/2/2/2
36	HTG	b	633	-	-	5/10/30/30	0/1/1/1
24	CLA	b	625	-	1/1/15/20	5/39/115/115	-
29	LMT	F	101	-	-	3/21/61/61	0/2/2/2
38	LHG	d	408	-	-	11/53/53/53	-
24	CLA	c	513	-	1/1/15/20	13/39/115/115	-
24	CLA	b	623	-	1/1/15/20	3/39/115/115	-
29	LMT	C	521	-	-	11/21/61/61	0/2/2/2
29	LMT	a	421	-	-	4/21/61/61	0/2/2/2
24	CLA	a	409	-	1/1/15/20	4/39/115/115	-
36	HTG	B	625	-	-	4/10/30/30	0/1/1/1
36	HTG	B	632	-	-	3/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	614	-	1/1/15/20	5/39/115/115	-
27	SQD	B	621	-	-	20/49/69/69	0/1/1/1
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
29	LMT	A	417	-	-	5/21/61/61	0/2/2/2
29	LMT	m	102	-	-	7/21/61/61	0/2/2/2
34	LMG	B	622	-	-	9/46/66/70	0/1/1/1
34	LMG	c	523	-	-	3/46/66/70	0/1/1/1
36	HTG	b	632	-	-	3/10/30/30	0/1/1/1
24	CLA	c	510	-	1/1/15/20	14/39/115/115	-
28	GOL	o	301	-	-	0/4/4/4	-
24	CLA	C	502	-	1/1/15/20	7/39/115/115	-
34	LMG	c	522	-	-	14/46/66/70	0/1/1/1
28	GOL	B	629	-	-	1/4/4/4	-
26	BCR	C	514	-	-	2/29/63/63	0/2/2/2
24	CLA	B	607	-	1/1/15/20	3/39/115/115	-
39	HEM	e	102	6,5	-	9/14/54/54	-
28	GOL	b	603	-	-	1/4/4/4	-
24	CLA	c	516	-	1/1/15/20	10/39/115/115	-
29	LMT	D	401	-	-	8/21/61/61	0/2/2/2
36	HTG	c	525	-	-	0/10/30/30	0/1/1/1
24	CLA	b	615	-	1/1/15/20	4/39/115/115	-
38	LHG	d	407	-	-	10/53/53/53	-
28	GOL	f	101	35	-	3/4/4/4	-
26	BCR	H	102	-	-	1/29/63/63	0/2/2/2
24	CLA	B	615	-	1/1/15/20	14/39/115/115	-
24	CLA	B	609	-	-	1/39/115/115	-
24	CLA	c	508	42	1/1/15/20	4/39/115/115	-
37	DGD	C	517	-	-	16/51/91/95	0/2/2/2
34	LMG	C	519	-	-	13/46/66/70	0/1/1/1
24	CLA	b	613	-	1/1/15/20	4/39/115/115	-
28	GOL	v	201	-	-	2/4/4/4	-
28	GOL	B	626	-	-	2/4/4/4	-
24	CLA	A	407	42	-	2/39/115/115	-
28	GOL	C	525	-	-	0/4/4/4	-
28	GOL	b	606	-	-	2/4/4/4	-
38	LHG	D	408	-	-	11/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	621	-	-	3/39/115/115	-
24	CLA	c	512	-	1/1/15/20	2/39/115/115	-
24	CLA	a	410	42	-	6/39/115/115	-
37	DGD	C	518	-	-	11/51/91/95	0/2/2/2
36	HTG	B	624	-	-	2/10/30/30	0/1/1/1
29	LMT	b	631	-	-	4/17/37/61	0/1/1/2
24	CLA	C	501	-	1/1/15/20	3/39/115/115	-
38	LHG	E	101	-	-	19/46/46/53	-
34	LMG	D	412	40	-	6/46/66/70	0/1/1/1
25	PHO	a	420[A]	-	-	1/37/103/103	0/5/6/6
24	CLA	B	604	-	1/1/15/20	7/39/115/115	-
27	SQD	F	103	-	-	16/38/58/69	0/1/1/1
24	CLA	b	626	-	1/1/15/20	8/39/115/115	-
28	GOL	V	204	-	-	1/4/4/4	-
28	GOL	a	401	-	-	0/4/4/4	-
36	HTG	C	523	-	-	3/10/30/30	0/1/1/1
24	CLA	b	611	42	1/1/15/20	15/39/115/115	-
24	CLA	B	613	-	1/1/15/20	3/39/115/115	-
24	CLA	B	603	-	1/1/15/20	3/39/115/115	-
36	HTG	C	522	-	-	0/10/30/30	0/1/1/1
34	LMG	Z	101	-	-	14/31/51/70	0/1/1/1
28	GOL	b	607	-	-	3/4/4/4	-
28	GOL	A	414	-	-	2/4/4/4	-
27	SQD	f	102	-	-	14/38/58/69	0/1/1/1
24	CLA	B	611	42	1/1/15/20	3/39/115/115	-
36	HTG	V	207	-	-	1/10/30/30	0/1/1/1
26	BCR	c	527	-	-	0/29/63/63	0/2/2/2
28	GOL	B	636	-	-	0/4/4/4	-
24	CLA	c	509	-	1/1/15/20	1/39/115/115	-
26	BCR	t	101	-	-	2/29/63/63	0/2/2/2
24	CLA	B	606	-	1/1/15/20	5/39/115/115	-
28	GOL	V	201	35	-	2/4/4/4	-
27	SQD	A	416	-	-	15/49/69/69	0/1/1/1
27	SQD	b	601	-	-	22/49/69/69	0/1/1/1
36	HTG	d	411	-	-	1/7/27/30	0/1/1/1
29	LMT	B	635	-	-	7/17/37/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	v	203	-	-	2/4/4/4	-
32	PL9	A	420[B]	-	-	11/53/73/73	0/1/1/1
26	BCR	c	518	-	-	2/29/63/63	0/2/2/2
34	LMG	A	422	-	-	19/46/66/70	0/1/1/1
24	CLA	c	505	-	1/1/15/20	4/39/115/115	-

The worst 5 of 1634 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	408	PHO	C1B-C2B	9.39	1.49	1.39
25	a	411	PHO	C1D-C2D	9.35	1.49	1.39
25	a	420[B]	PHO	C1B-C2B	9.28	1.49	1.39
25	A	409[B]	PHO	C1B-C2B	9.16	1.49	1.39
25	a	420[A]	PHO	C1D-C2D	8.87	1.49	1.39

The worst 5 of 2945 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	408	PHO	C2D-C1D-ND	11.62	117.83	109.43
25	A	409[B]	PHO	C2D-C1D-ND	11.53	117.76	109.43
25	A	409[A]	PHO	C2D-C1D-ND	11.23	117.55	109.43
25	a	420[B]	PHO	C2D-C1D-ND	10.95	117.34	109.43
25	a	420[A]	PHO	C2D-C1D-ND	10.80	117.24	109.43

5 of 62 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	405	CLA	ND
24	A	406	CLA	ND
24	A	410	CLA	ND
24	B	602	CLA	ND
24	B	603	CLA	ND

5 of 1298 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	602	CLA	CAD-CBD-CGD-O2D
24	B	615	CLA	CAD-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O2D
24	B	615	CLA	C2-C3-C5-C6
24	B	615	CLA	C4-C3-C5-C6

There are no ring outliers.

169 monomers are involved in 335 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	l	101	LHG	2	0
32	D	405[B]	PL9	2	0
24	C	503	CLA	4	0
37	h	102	DGD	1	0
24	B	602	CLA	1	0
24	b	619	CLA	3	0
24	B	616	CLA	5	0
25	a	411	PHO	1	0
26	h	101	BCR	4	0
32	D	405[A]	PL9	1	0
25	A	409[B]	PHO	3	0
37	c	519	DGD	1	0
29	M	101	LMT	3	0
24	B	610	CLA	4	0
32	a	416[B]	PL9	8	0
27	a	414	SQD	1	0
24	A	410	CLA	1	0
24	C	511	CLA	3	0
37	H	103	DGD	1	0
29	a	404	LMT	2	0
24	B	614	CLA	2	0
28	A	415	GOL	1	0
29	M	104	LMT	3	0
26	Y	101	BCR	4	0
36	b	602	HTG	2	0
34	z	101	LMG	4	0
24	c	517	CLA	5	0
24	d	402	CLA	3	0
24	d	403	CLA	1	0
28	b	605	GOL	1	0
34	j	101	LMG	2	0
37	c	520	DGD	2	0
24	B	608	CLA	1	0
24	c	511	CLA	2	0
24	b	620	CLA	1	0
32	d	405[B]	PL9	1	0
24	C	507	CLA	4	0
24	A	405	CLA	3	0
24	C	505	CLA	6	0
34	a	415	LMG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	L	101	LHG	3	0
24	a	412	CLA	1	0
24	C	504	CLA	1	0
26	b	628	BCR	3	0
36	B	623	HTG	2	0
24	c	507	CLA	3	0
26	k	101	BCR	2	0
24	c	515	CLA	2	0
24	B	617	CLA	5	0
27	A	412	SQD	5	0
28	a	402	GOL	1	0
32	A	420[A]	PL9	5	0
24	b	612	CLA	4	0
24	C	508	CLA	2	0
24	b	624	CLA	1	0
24	B	605	CLA	2	0
26	b	629	BCR	2	0
26	d	404	BCR	3	0
37	D	406	DGD	3	0
25	A	409[A]	PHO	2	0
28	T	102	GOL	2	0
32	a	416[A]	PL9	9	0
31	a	418[B]	OEY	1	0
28	c	502	GOL	2	0
24	b	622	CLA	1	0
24	c	506	CLA	3	0
26	A	411	BCR	1	0
24	C	509	CLA	2	0
27	a	405	SQD	2	0
34	b	630	LMG	2	0
26	B	618	BCR	1	0
38	D	409	LHG	7	0
24	d	401	CLA	3	0
28	C	524	GOL	1	0
34	C	520	LMG	2	0
24	C	510	CLA	2	0
29	f	103	LMT	1	0
29	M	103	LMT	1	0
36	H	101	HTG	2	0
24	A	406	CLA	4	0
37	e	101	DGD	6	0
28	B	630	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	c	514	CLA	4	0
26	B	619	BCR	3	0
26	D	404	BCR	2	0
26	y	101	BCR	1	0
28	T	101	GOL	2	0
24	C	512	CLA	5	0
26	b	627	BCR	2	0
38	a	422	LHG	5	0
38	d	406	LHG	1	0
24	C	506	CLA	1	0
25	A	408	PHO	2	0
26	K	101	BCR	2	0
24	C	513	CLA	6	0
39	F	102	HEM	3	0
24	D	402	CLA	3	0
24	D	403	CLA	1	0
37	C	516	DGD	3	0
38	D	407	LHG	1	0
25	a	420[B]	PHO	3	0
26	T	103	BCR	4	0
26	C	515	BCR	2	0
36	b	633	HTG	1	0
24	b	625	CLA	5	0
29	F	101	LMT	1	0
38	d	408	LHG	5	0
24	c	513	CLA	2	0
24	b	623	CLA	1	0
29	C	521	LMT	1	0
24	a	409	CLA	3	0
24	b	614	CLA	3	0
27	B	621	SQD	3	0
26	B	620	BCR	4	0
29	A	417	LMT	3	0
29	m	102	LMT	2	0
34	B	622	LMG	1	0
34	c	523	LMG	1	0
24	c	510	CLA	3	0
24	C	502	CLA	2	0
34	c	522	LMG	2	0
26	C	514	BCR	2	0
24	B	607	CLA	4	0
39	e	102	HEM	3	0

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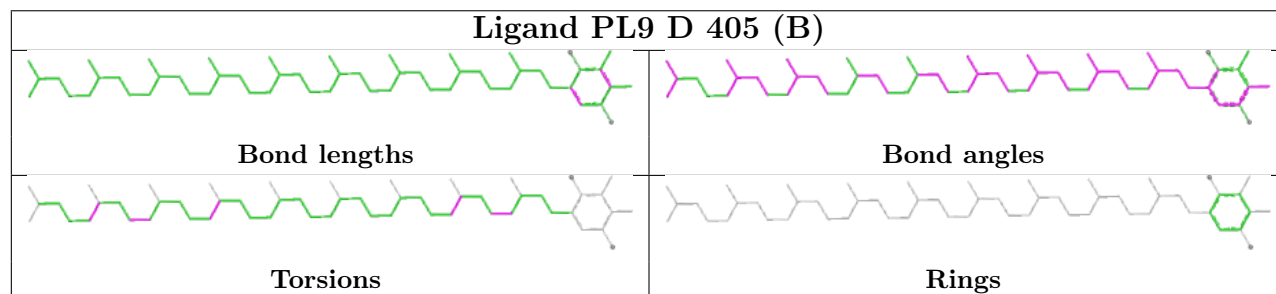
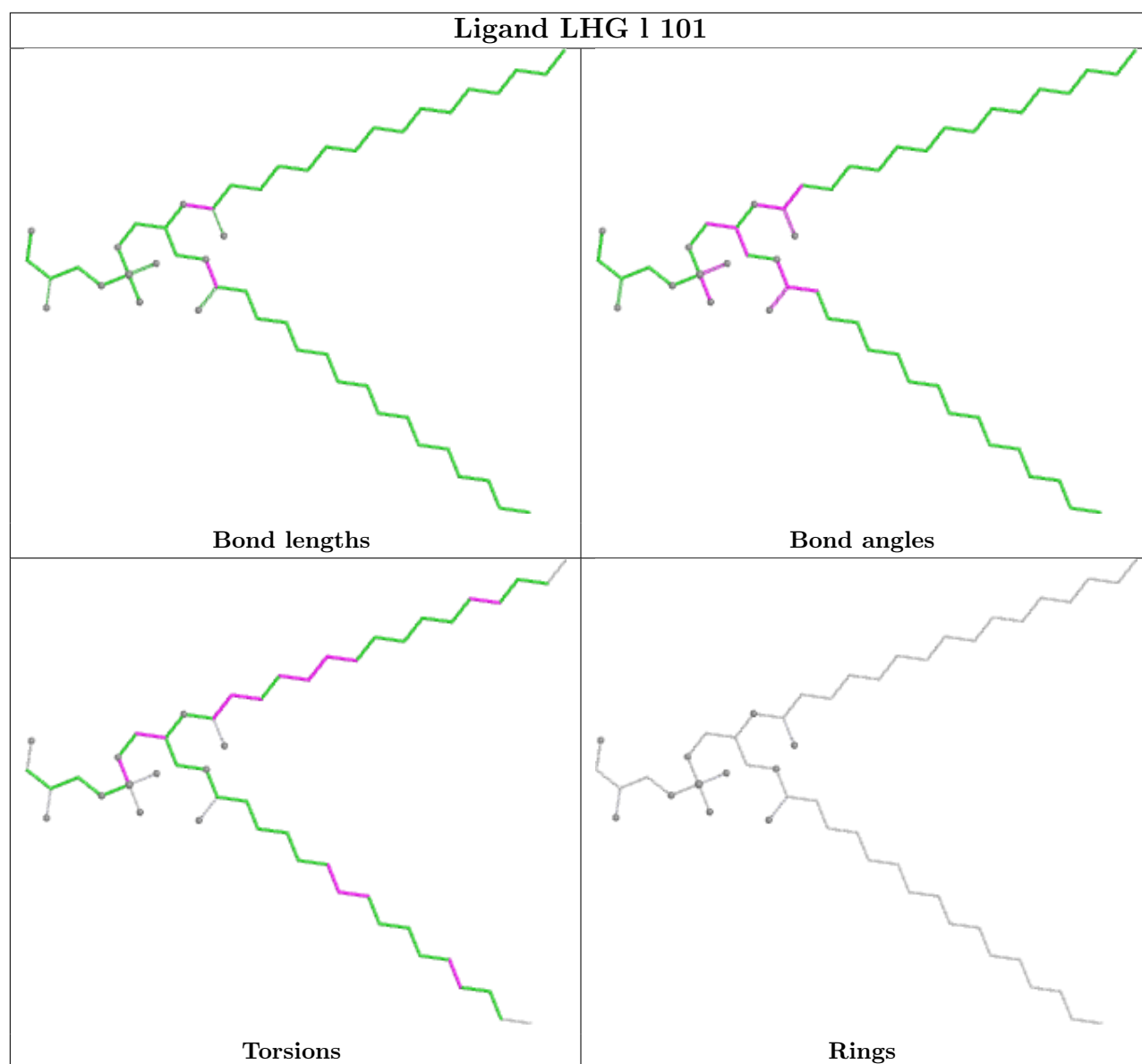
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	c	516	CLA	3	0
29	D	401	LMT	1	0
24	b	615	CLA	5	0
31	A	419[B]	OEY	1	0
38	d	407	LHG	1	0
28	f	101	GOL	1	0
26	H	102	BCR	3	0
24	B	615	CLA	4	0
24	c	508	CLA	1	0
37	C	517	DGD	3	0
34	C	519	LMG	2	0
24	b	613	CLA	2	0
28	v	201	GOL	1	0
24	A	407	CLA	4	0
38	D	408	LHG	1	0
24	b	621	CLA	2	0
24	c	512	CLA	6	0
24	a	410	CLA	2	0
37	C	518	DGD	2	0
29	b	631	LMT	2	0
24	C	501	CLA	1	0
38	E	101	LHG	2	0
34	D	412	LMG	1	0
25	a	420[A]	PHO	1	0
24	B	604	CLA	2	0
27	F	103	SQD	2	0
24	b	626	CLA	2	0
24	b	611	CLA	2	0
24	B	613	CLA	1	0
34	Z	101	LMG	2	0
28	A	414	GOL	1	0
27	f	102	SQD	3	0
24	B	611	CLA	1	0
36	V	207	HTG	3	0
26	c	527	BCR	2	0
24	c	509	CLA	4	0
26	t	101	BCR	6	0
24	B	606	CLA	2	0
27	A	416	SQD	1	0
27	b	601	SQD	2	0
36	d	411	HTG	3	0
32	A	420[B]	PL9	5	0

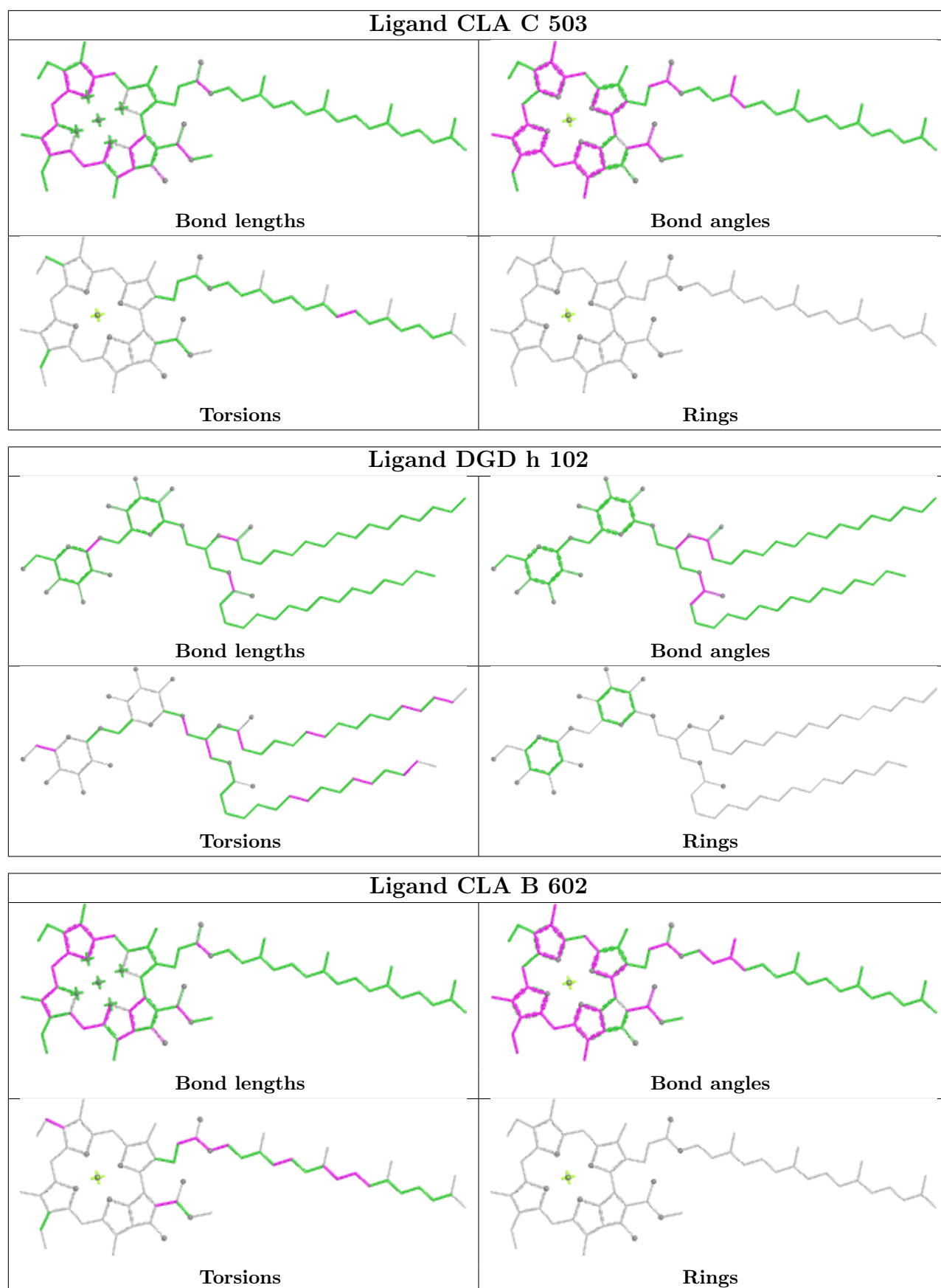
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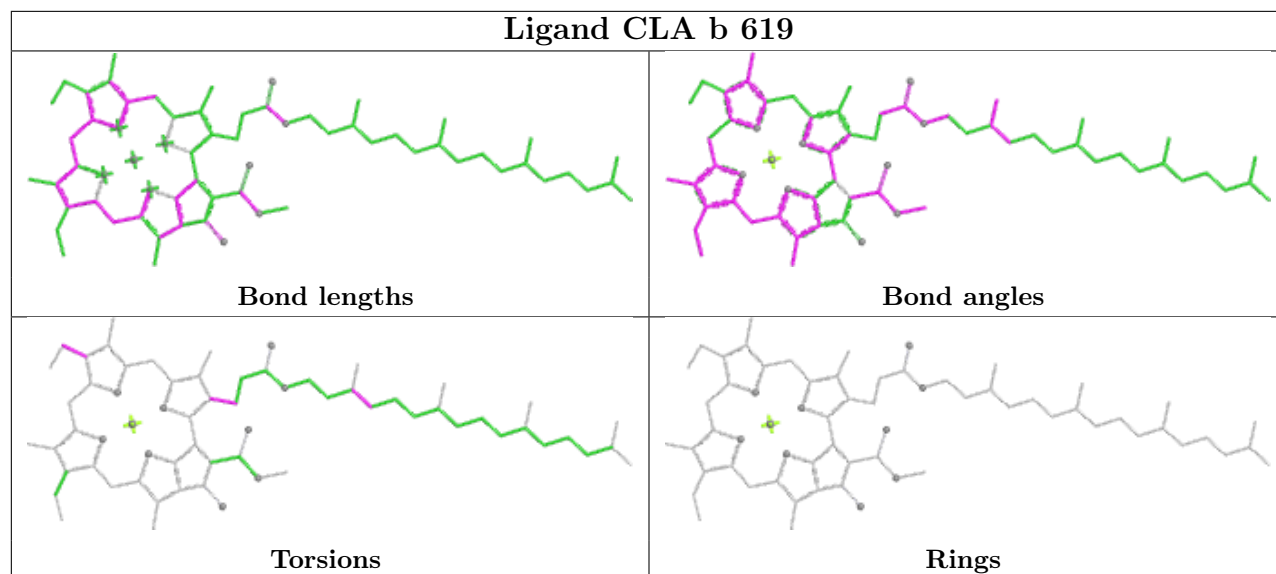
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	c	518	BCR	1	0
34	A	422	LMG	5	0
24	c	505	CLA	3	0

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

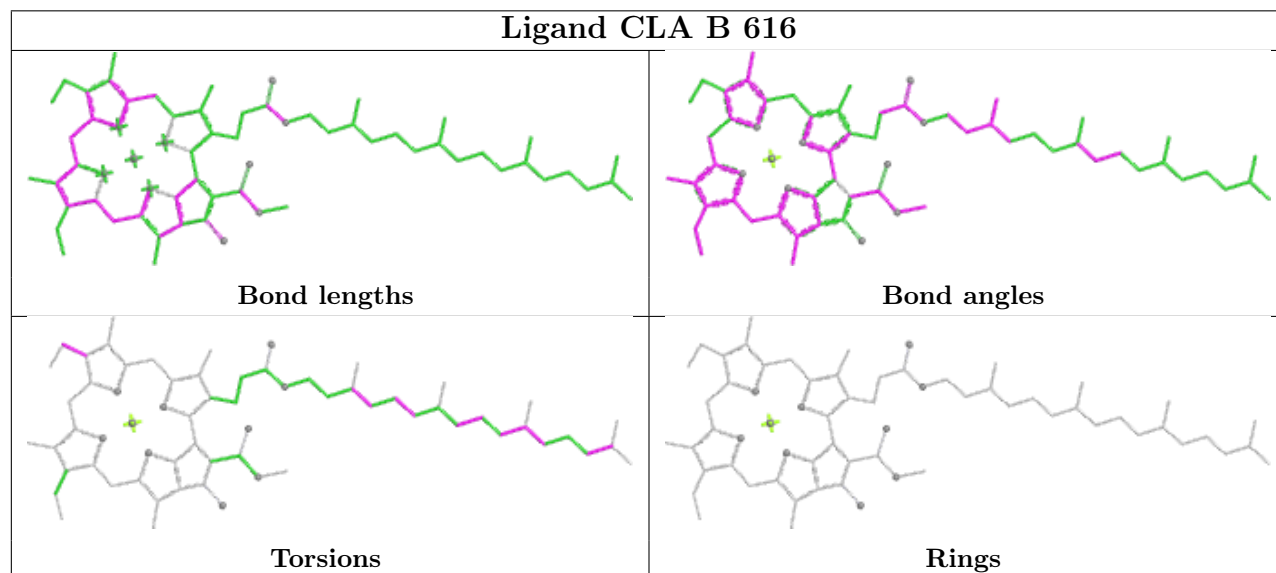




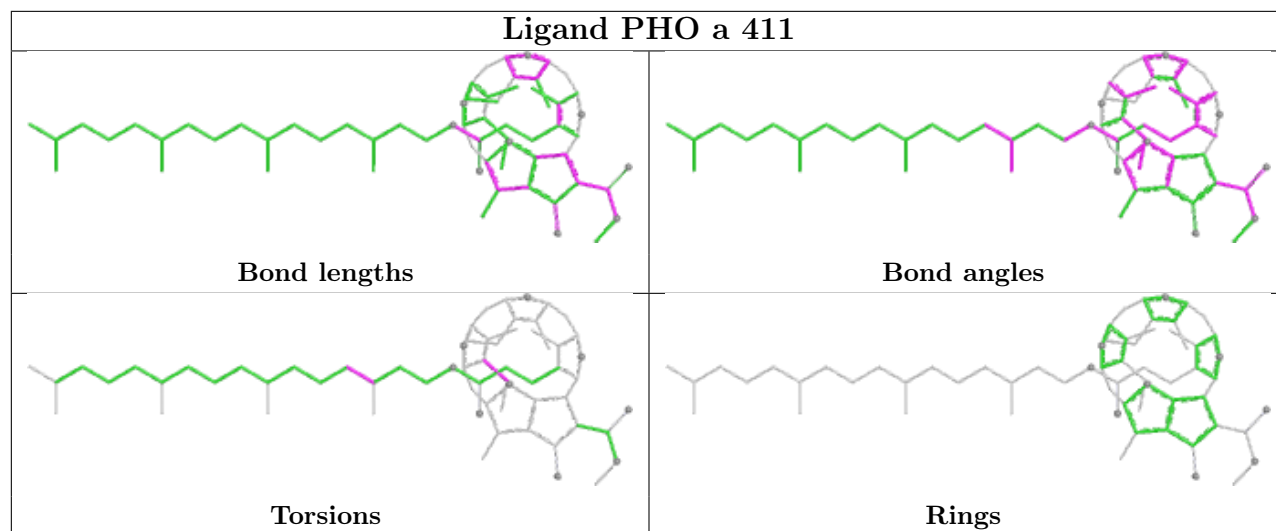
Ligand CLA b 619

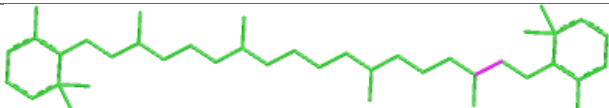
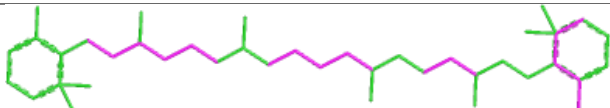
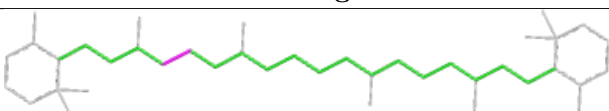
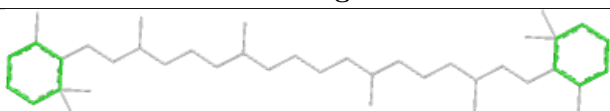


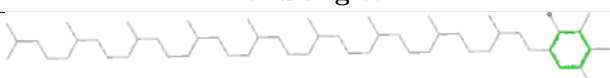
Ligand CLA B 616

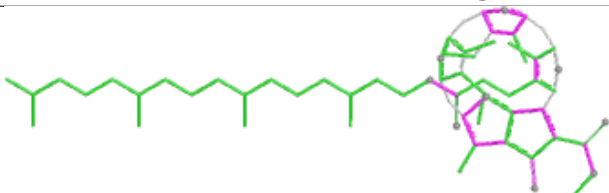
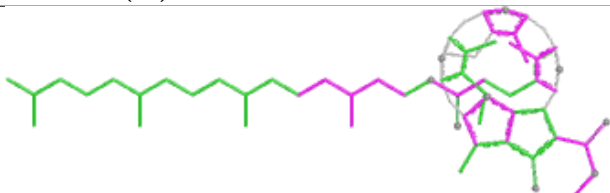
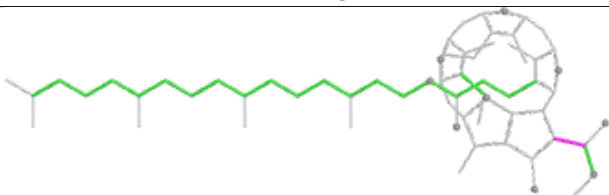
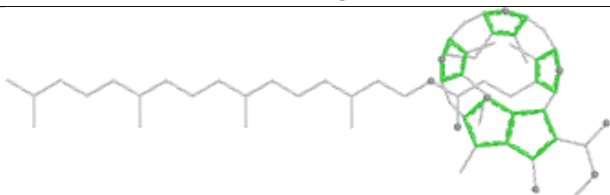


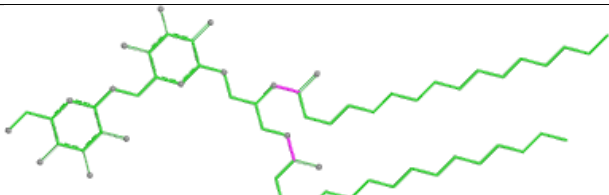
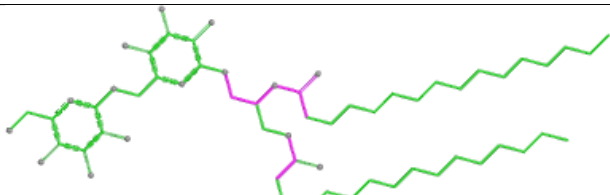
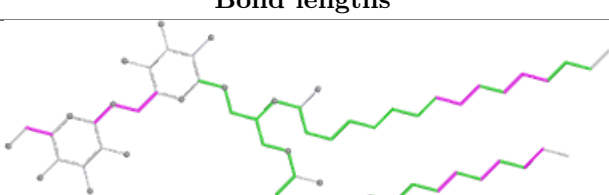
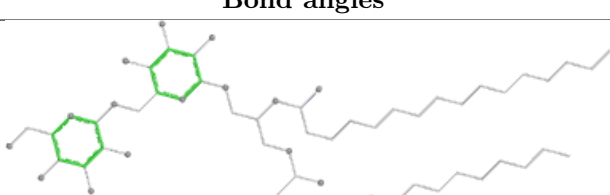
Ligand PHO a 411

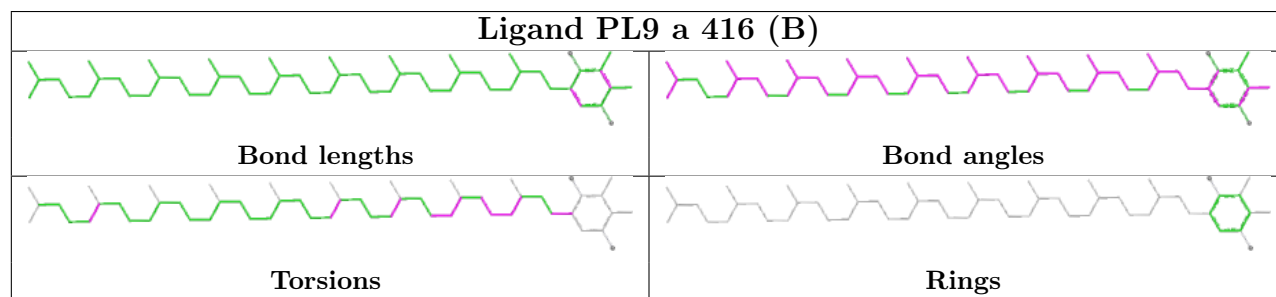
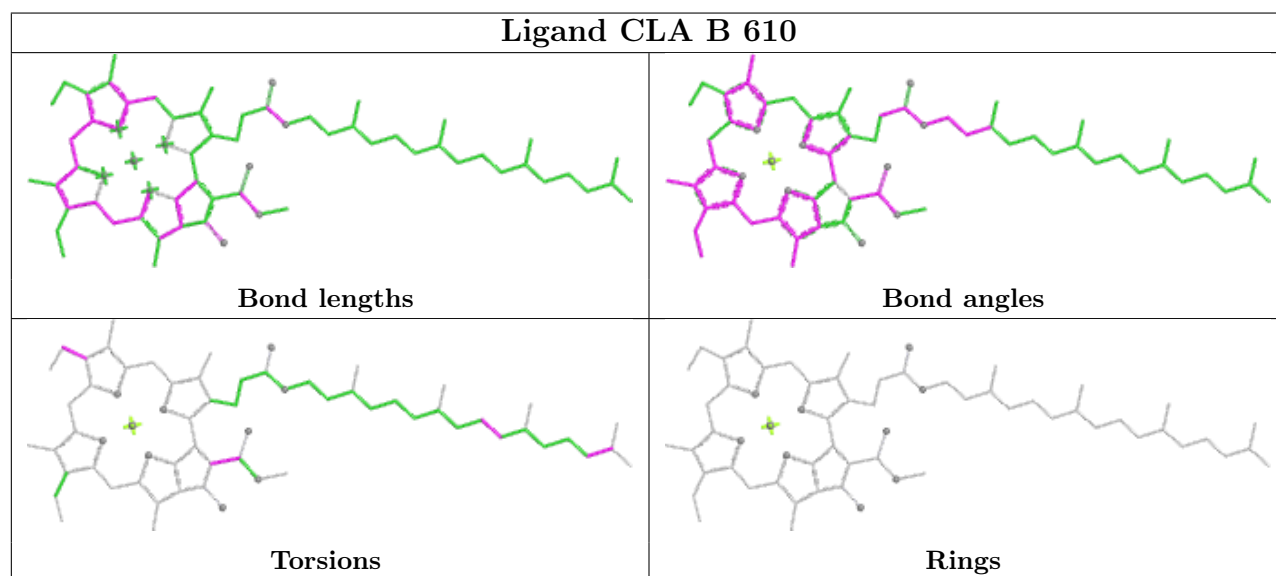
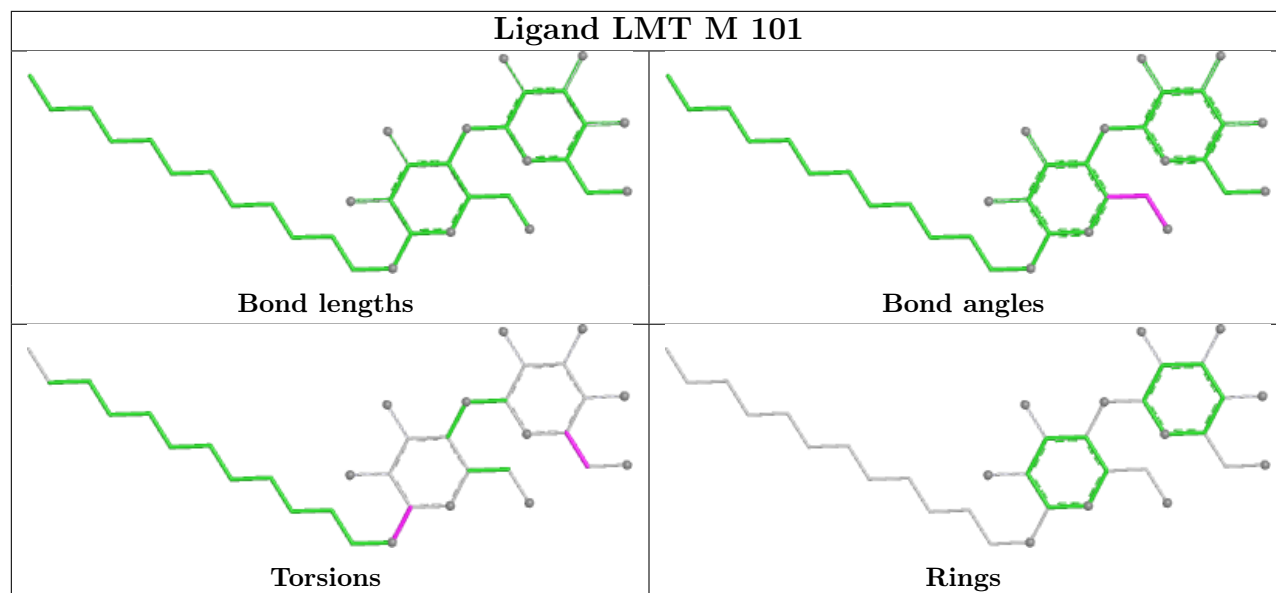


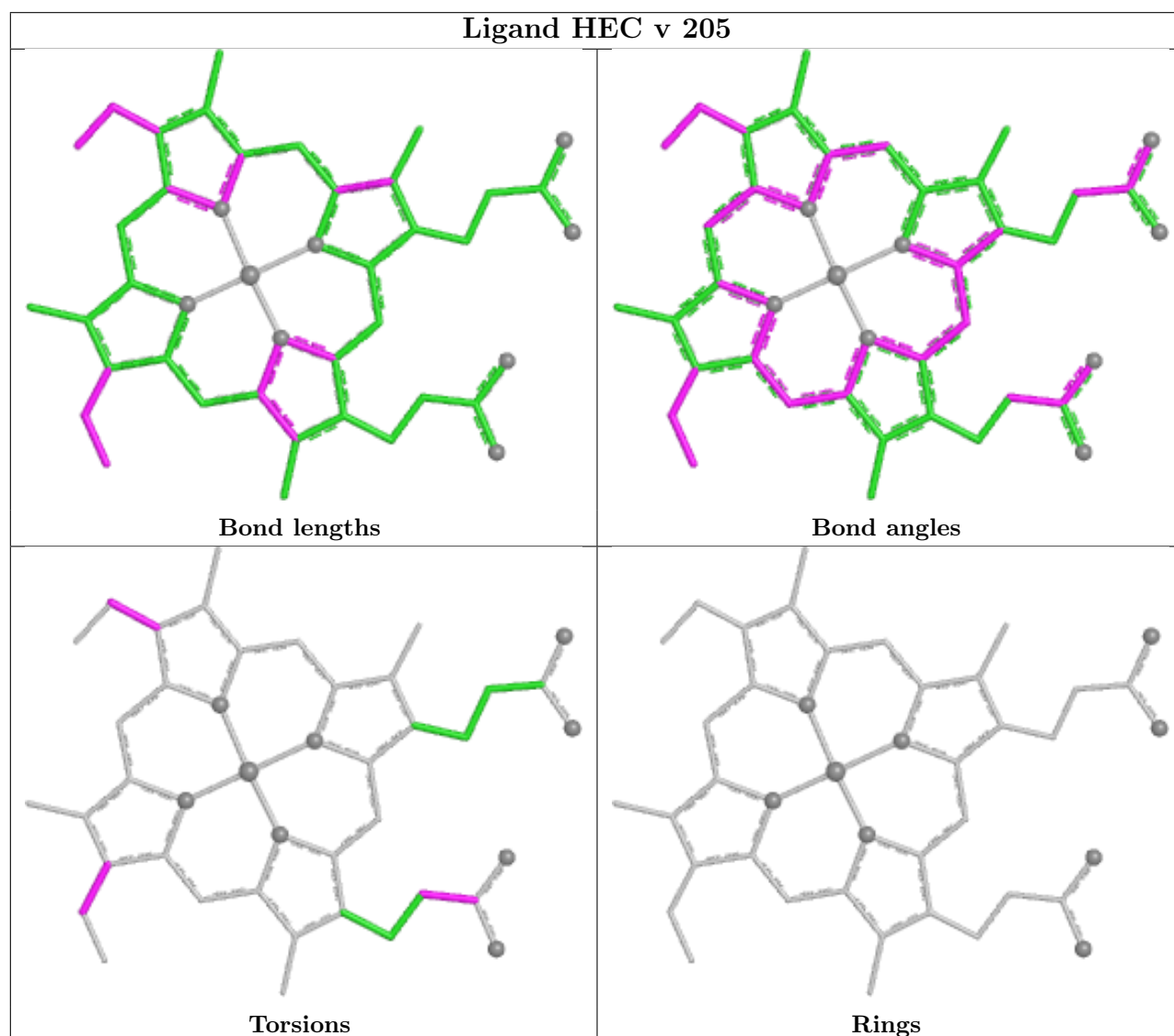
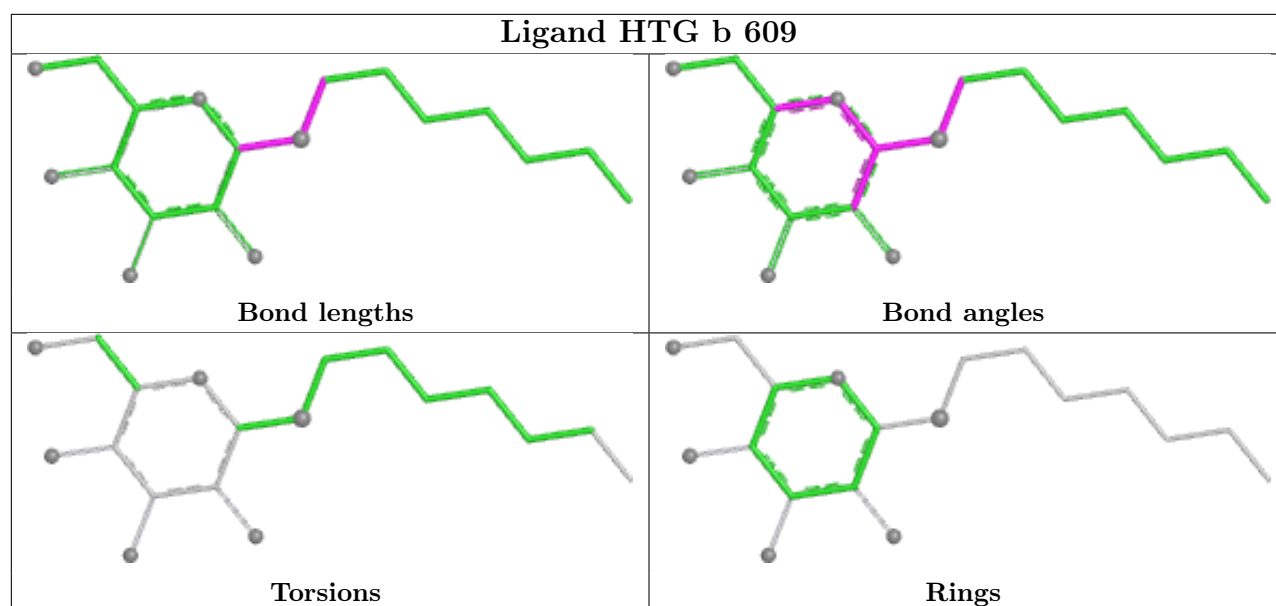
Ligand BCR h 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

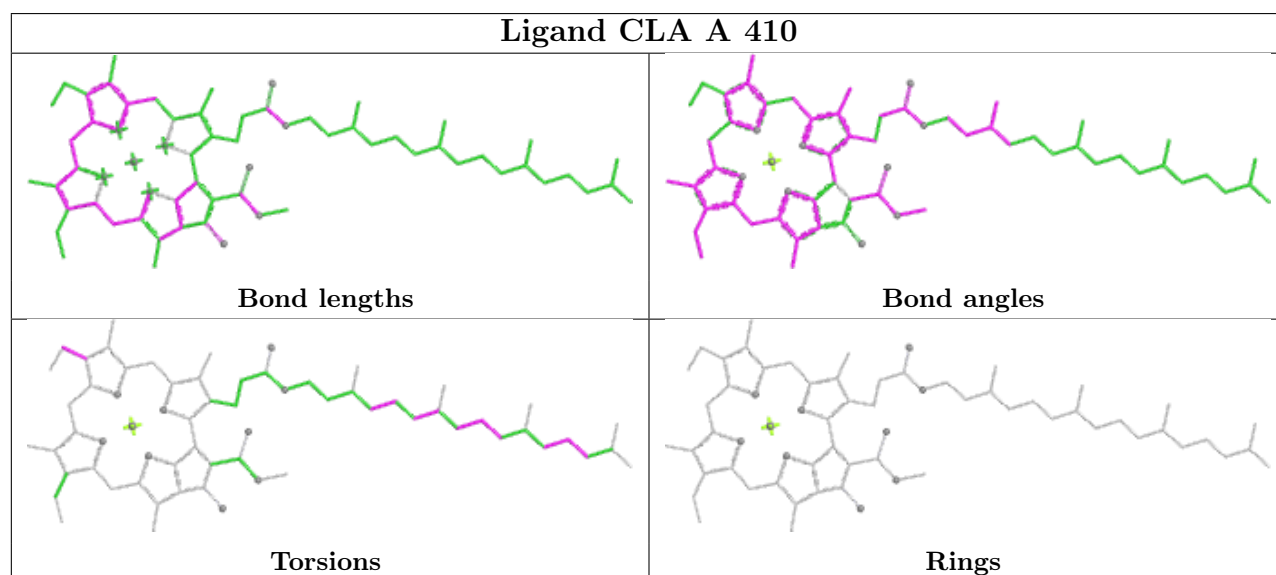
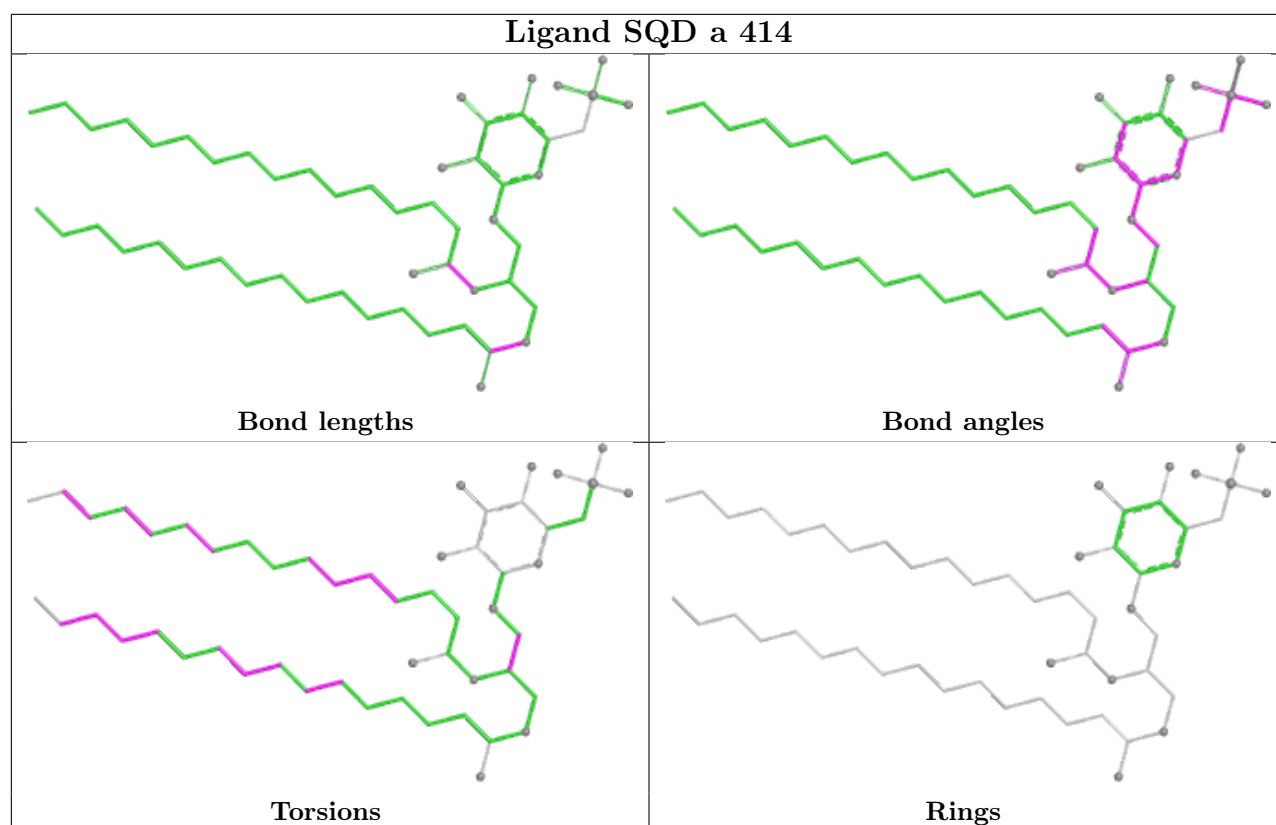
Ligand PL9 D 405 (A)	
	
Bond lengths	Bond angles
	
Torsions	Rings

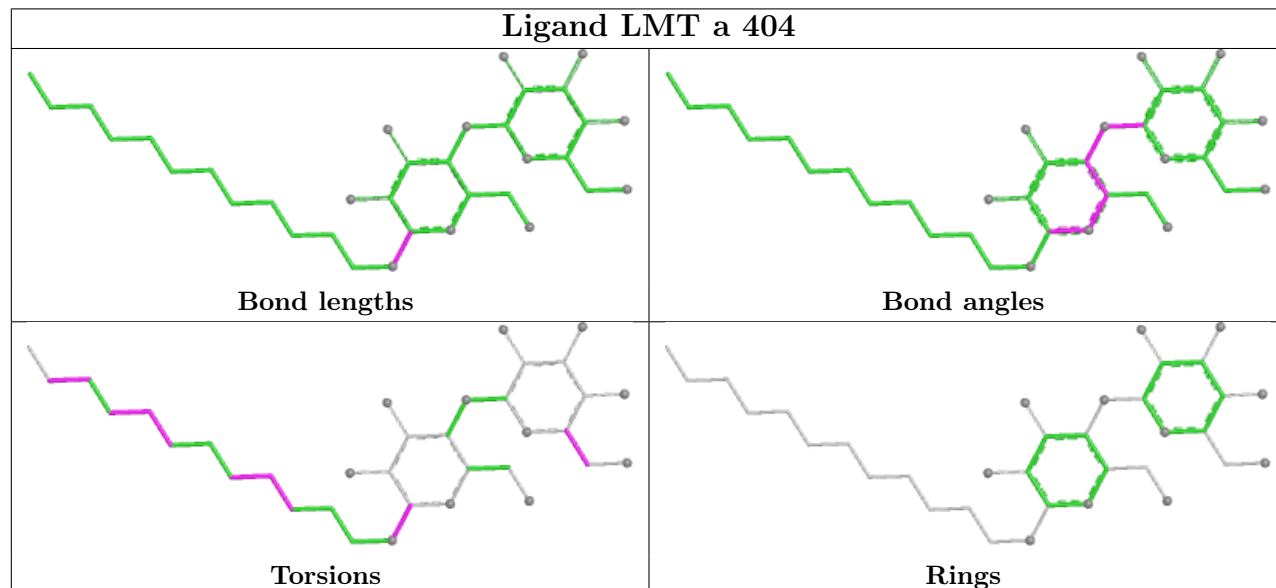
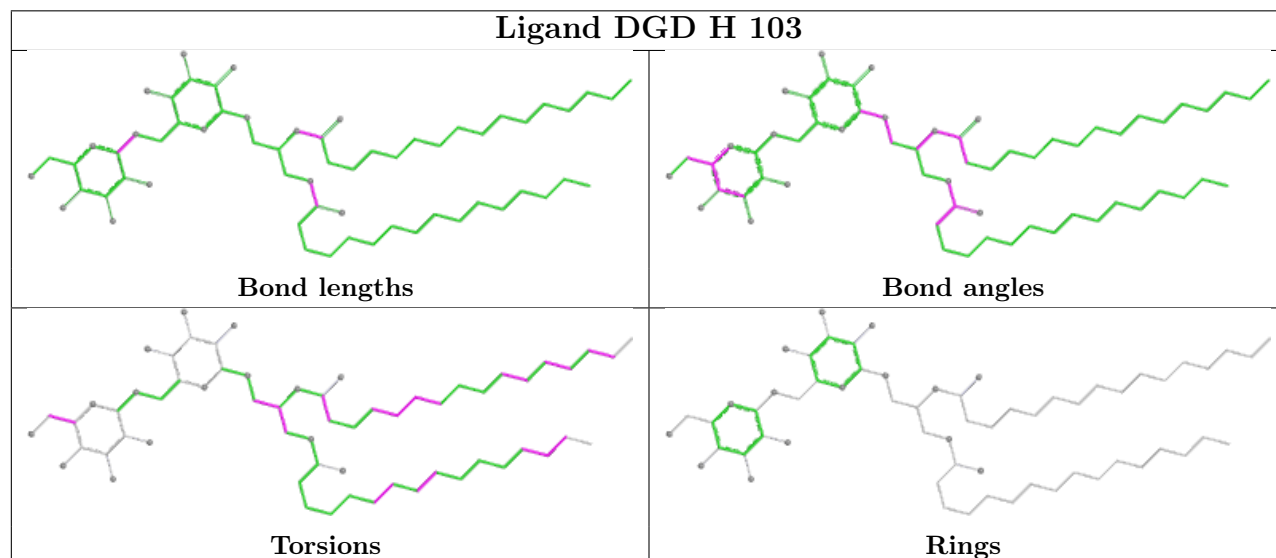
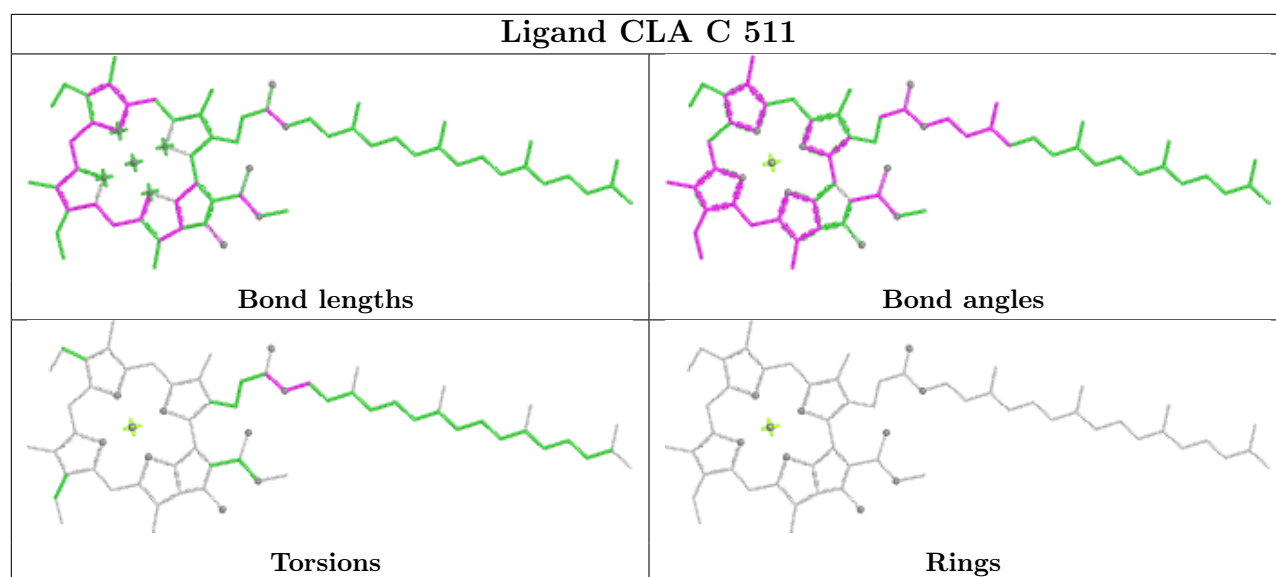
Ligand PHO A 409 (B)	
	
Bond lengths	Bond angles
	
Torsions	Rings

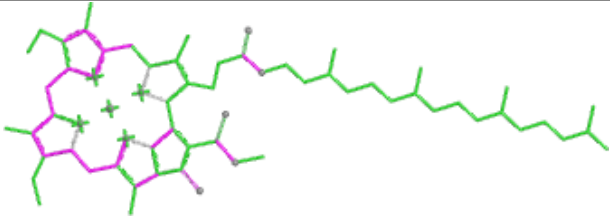
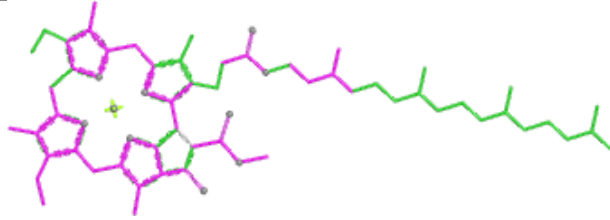
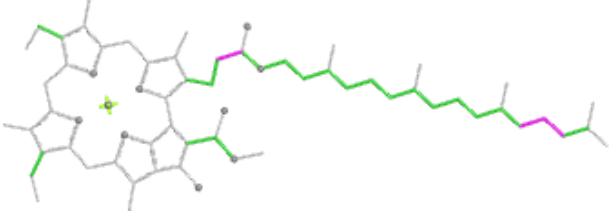
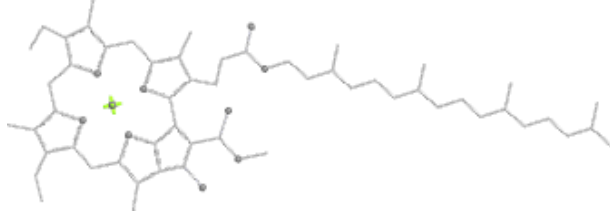
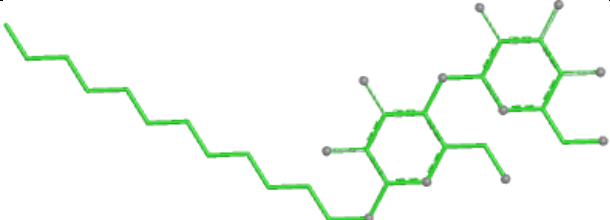
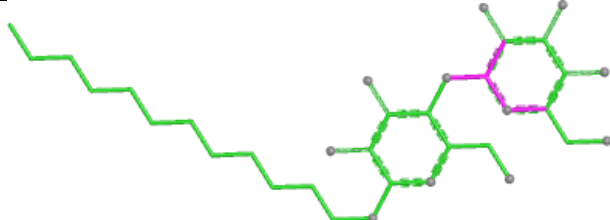
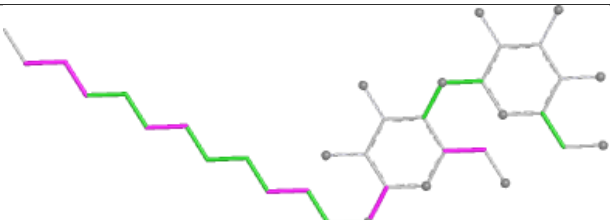
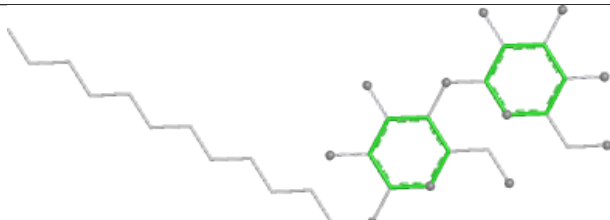
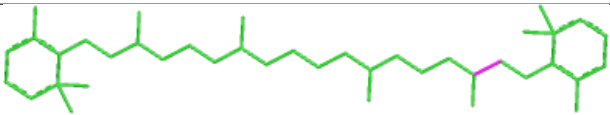
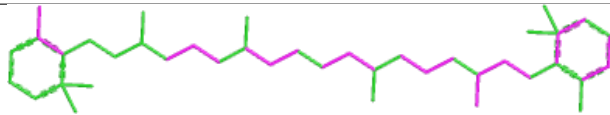
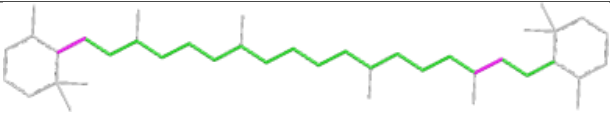
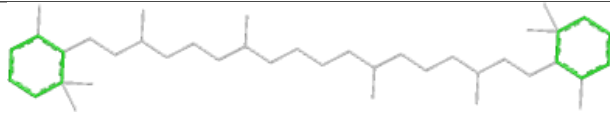
Ligand DGD c 519	
	
Bond lengths	Bond angles
	
Torsions	Rings

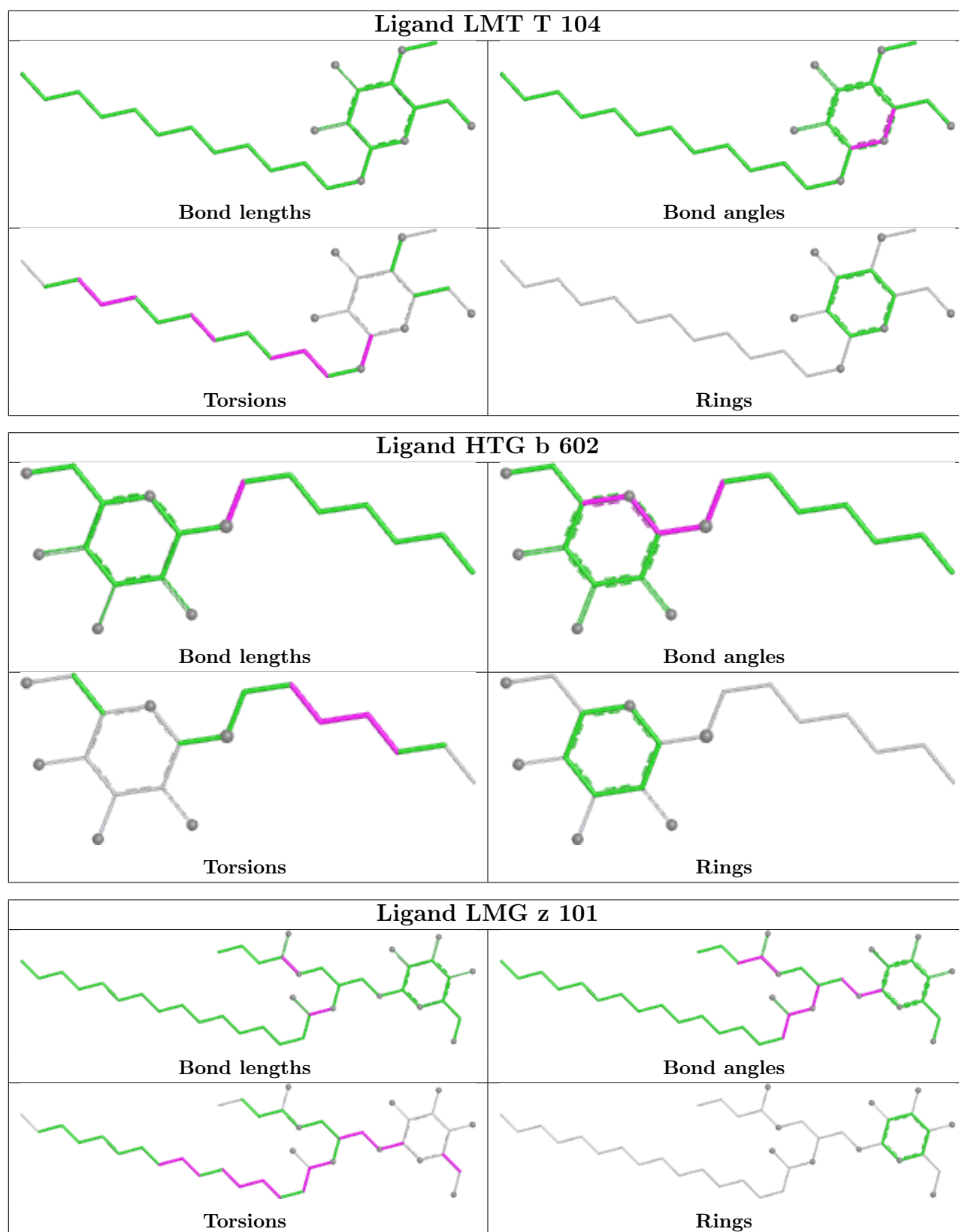




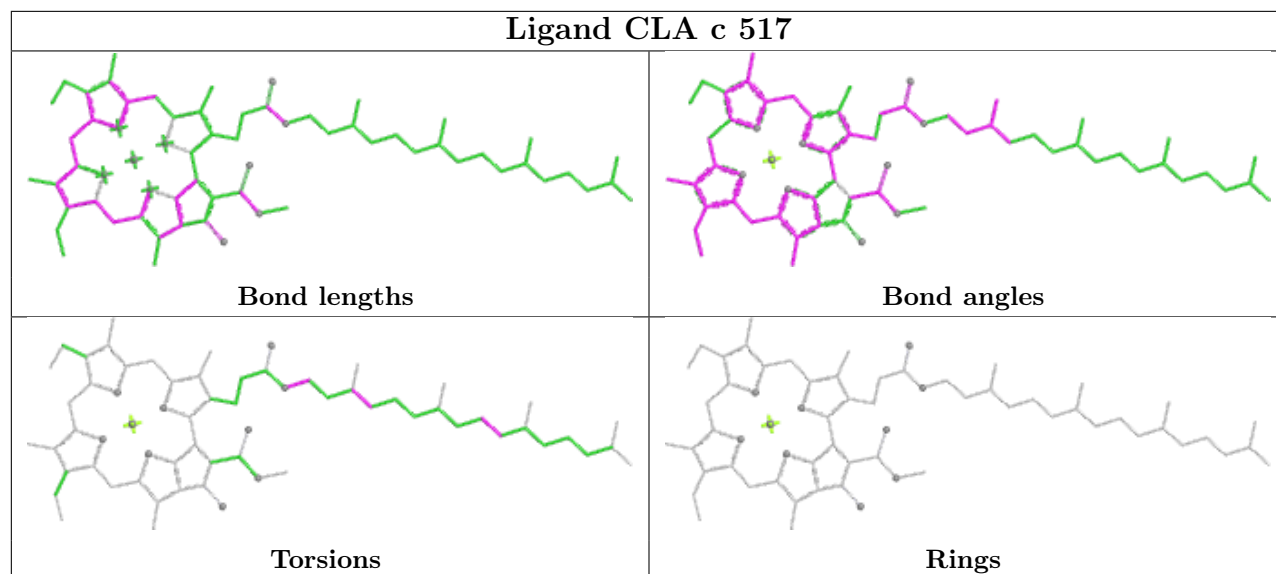




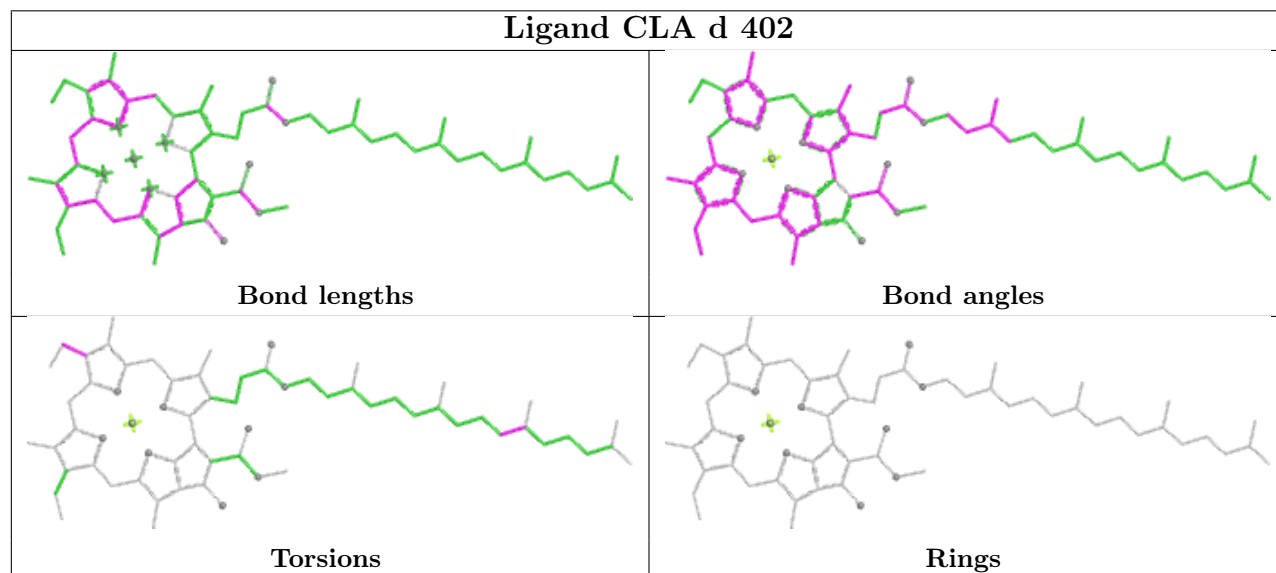
Ligand CLA B 614	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMT M 104	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR Y 101	
 Bond lengths	 Bond angles
 Torsions	 Rings



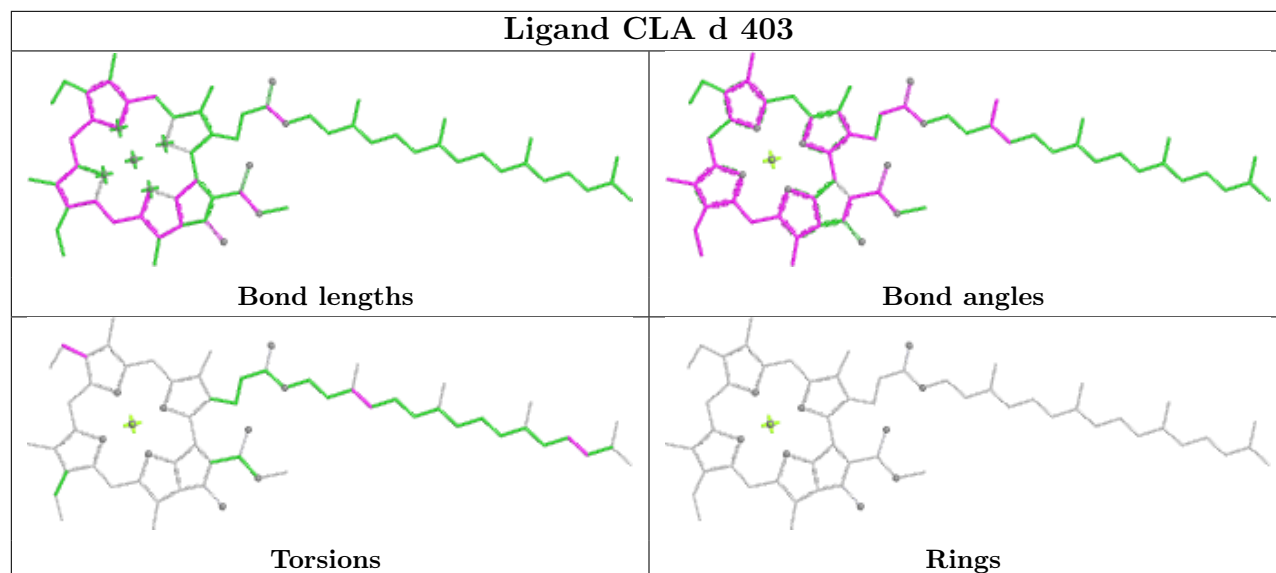
Ligand CLA c 517

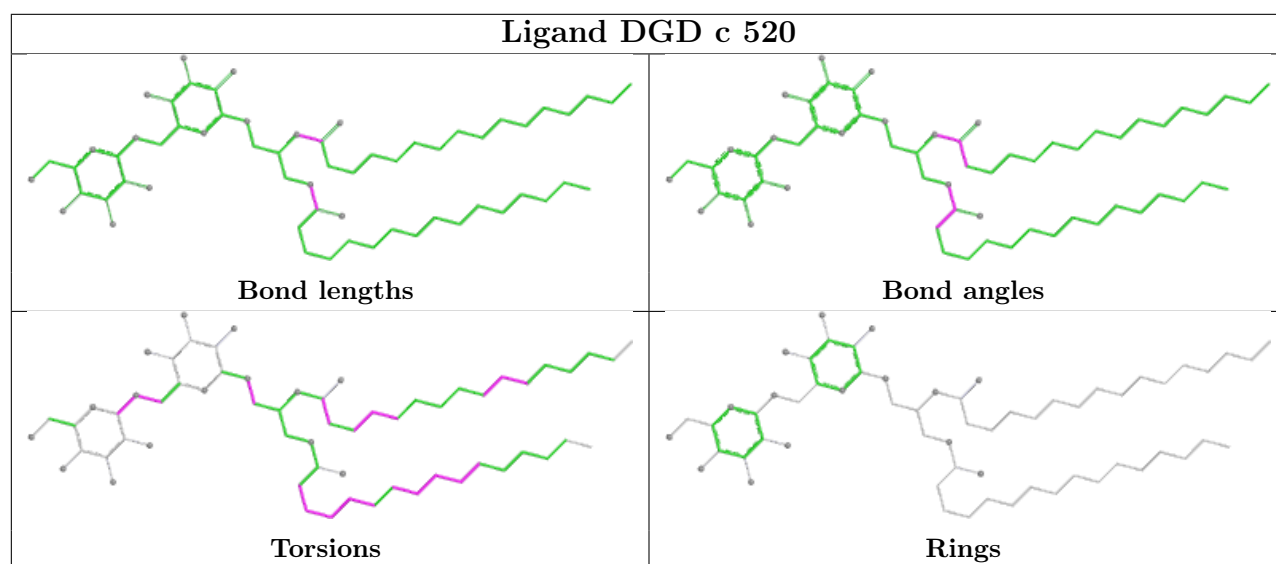
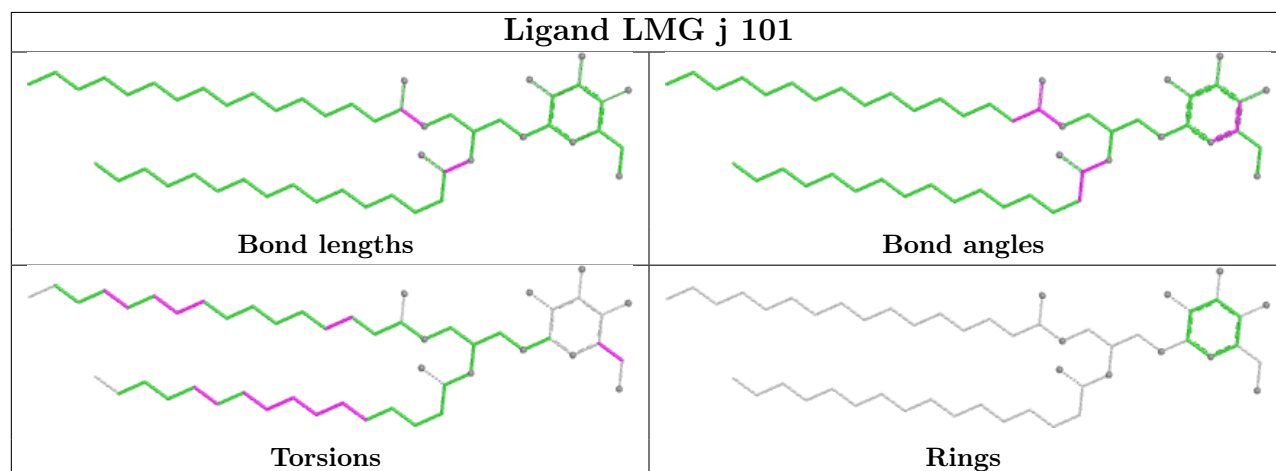
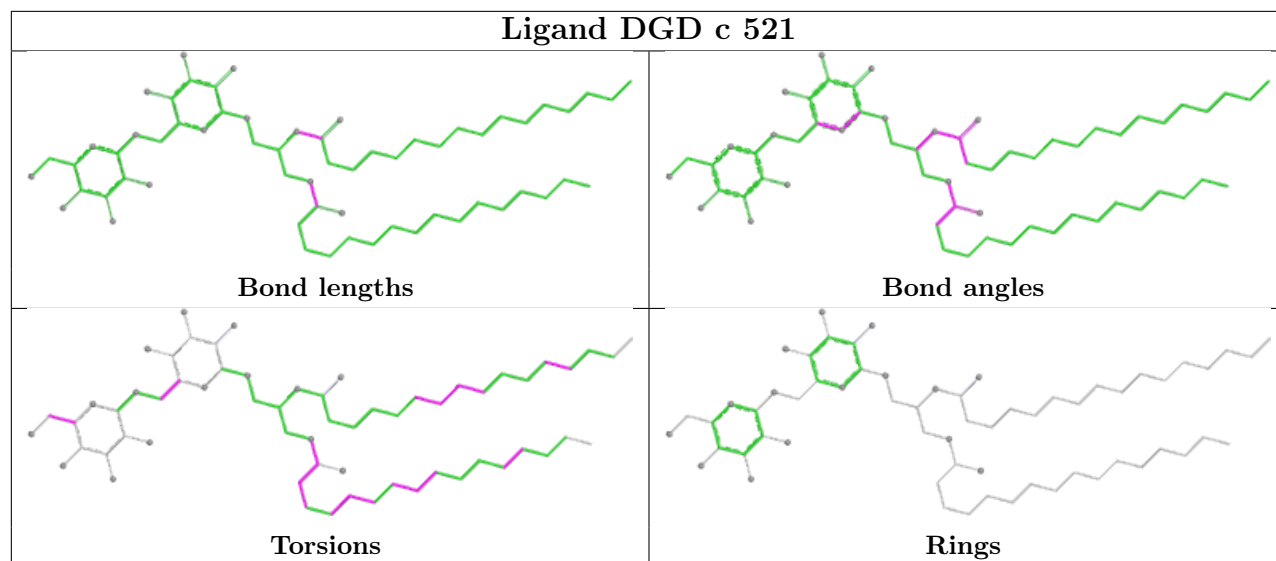


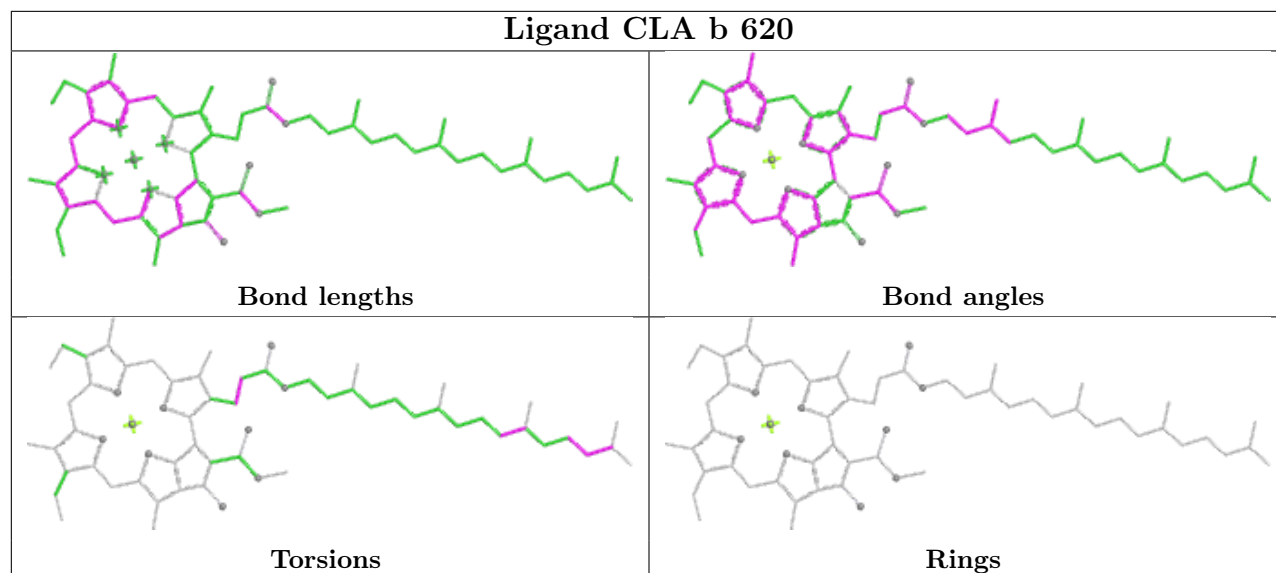
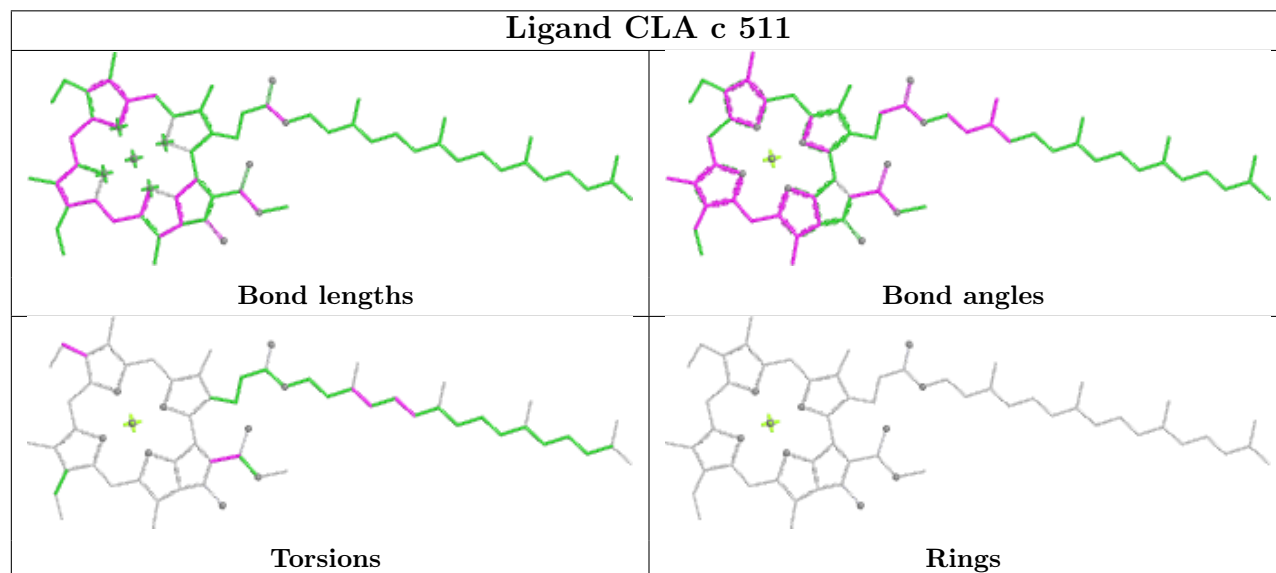
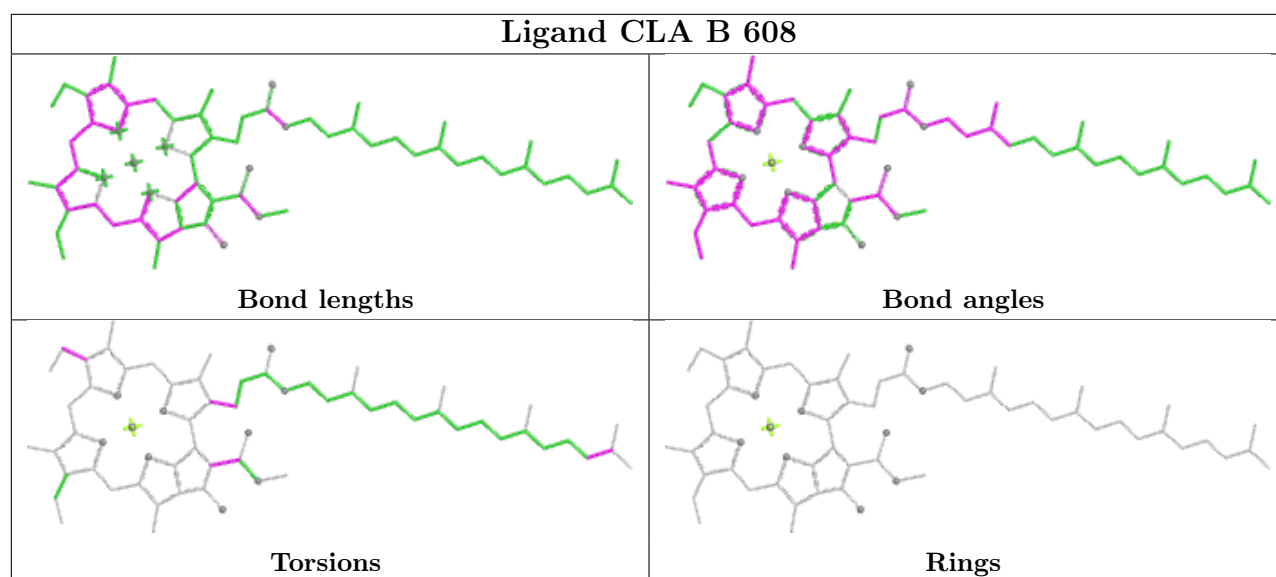
Ligand CLA d 402

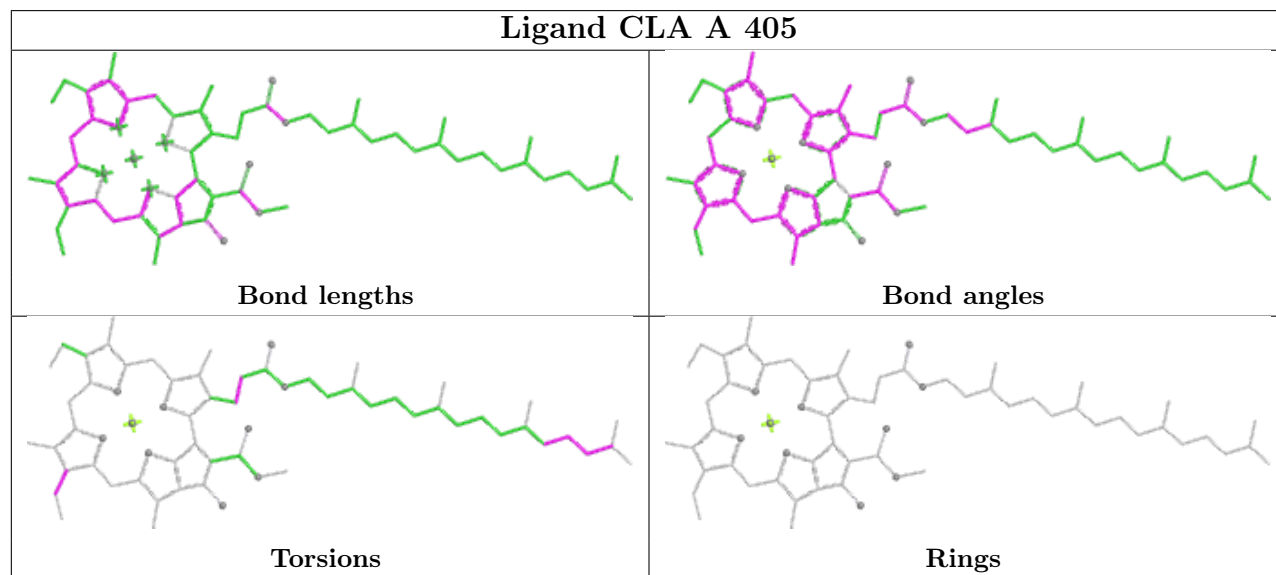
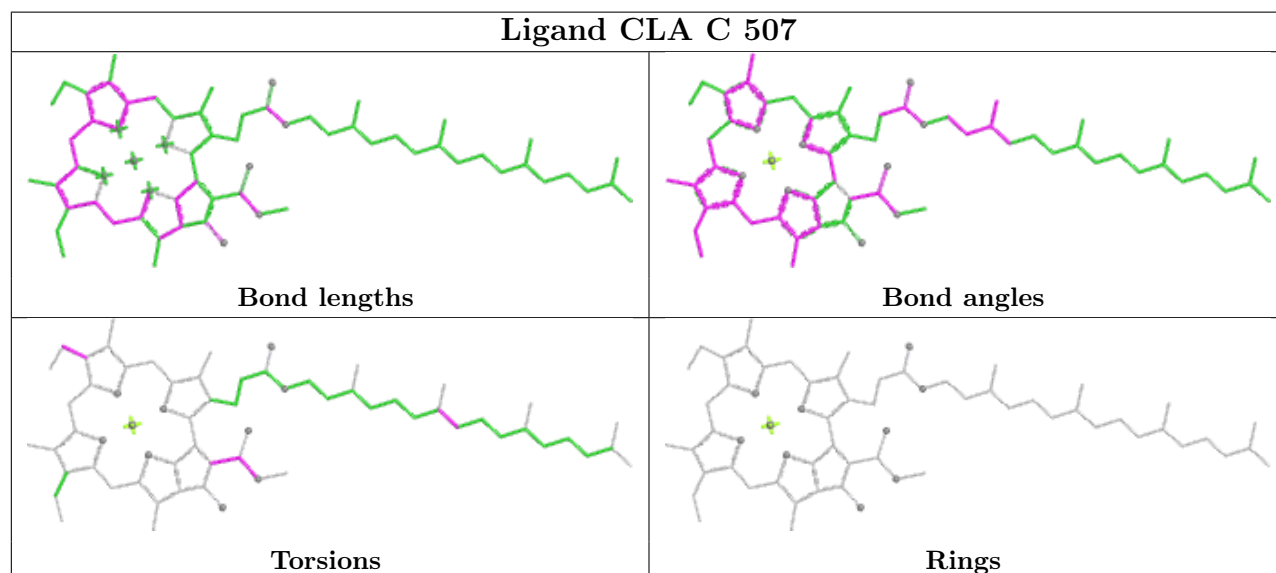
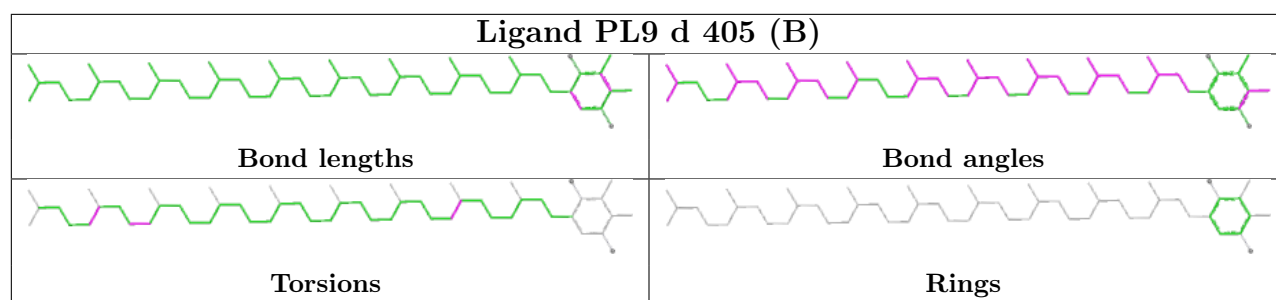


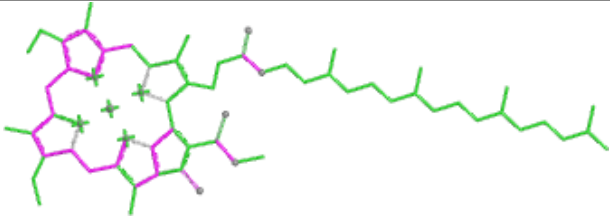
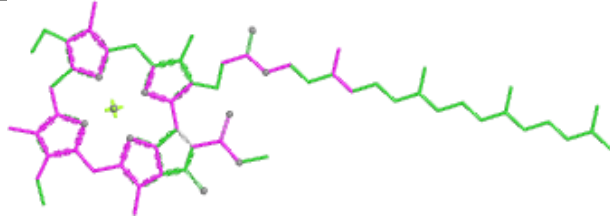
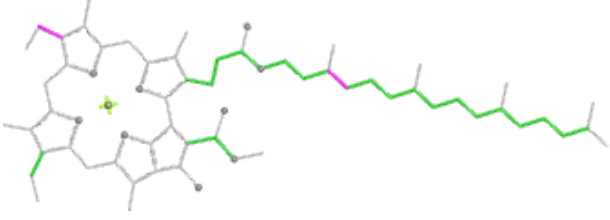
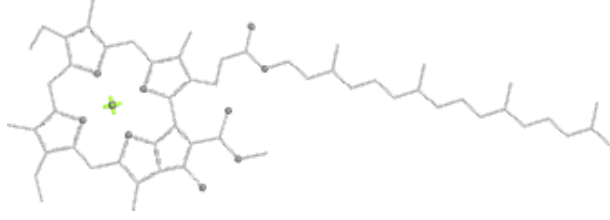
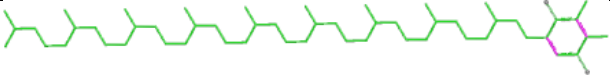
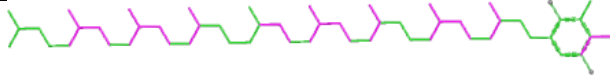
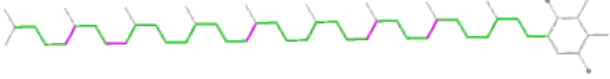
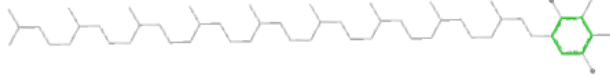
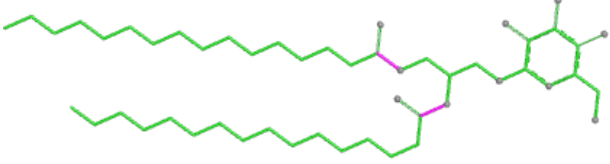
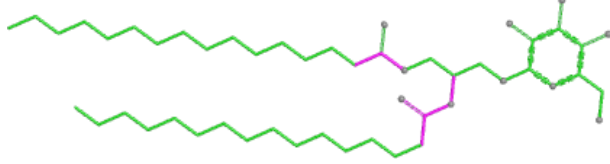
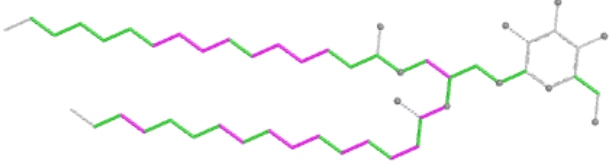
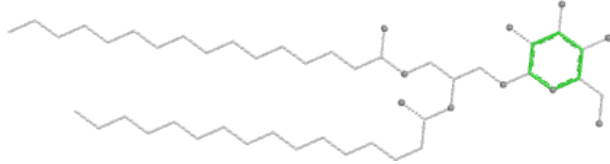
Ligand CLA d 403

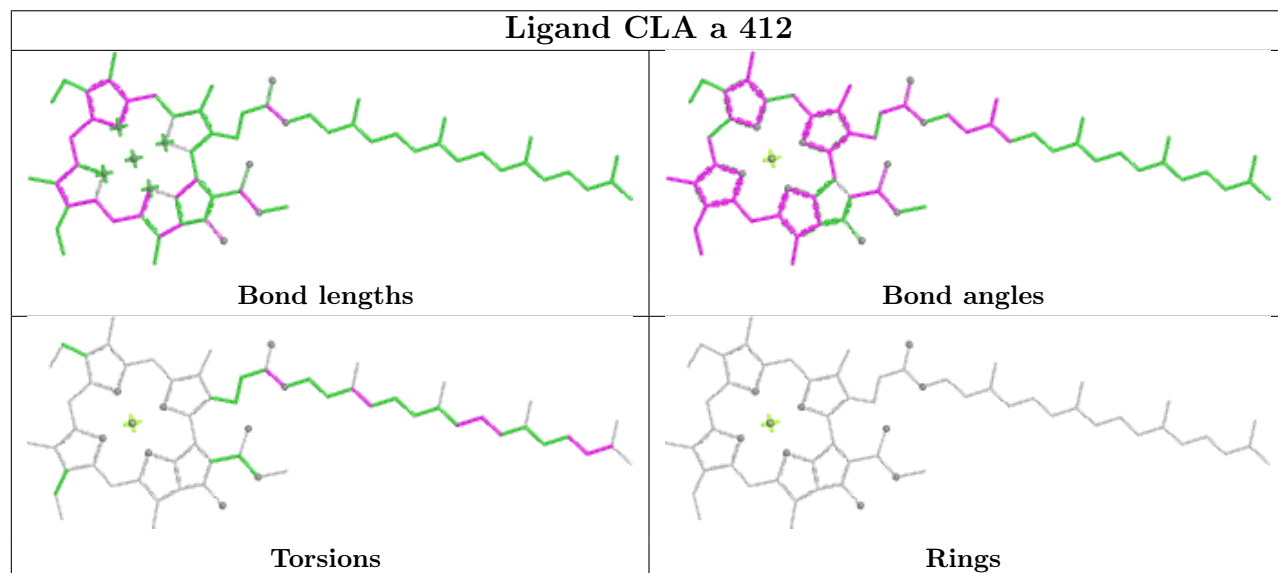
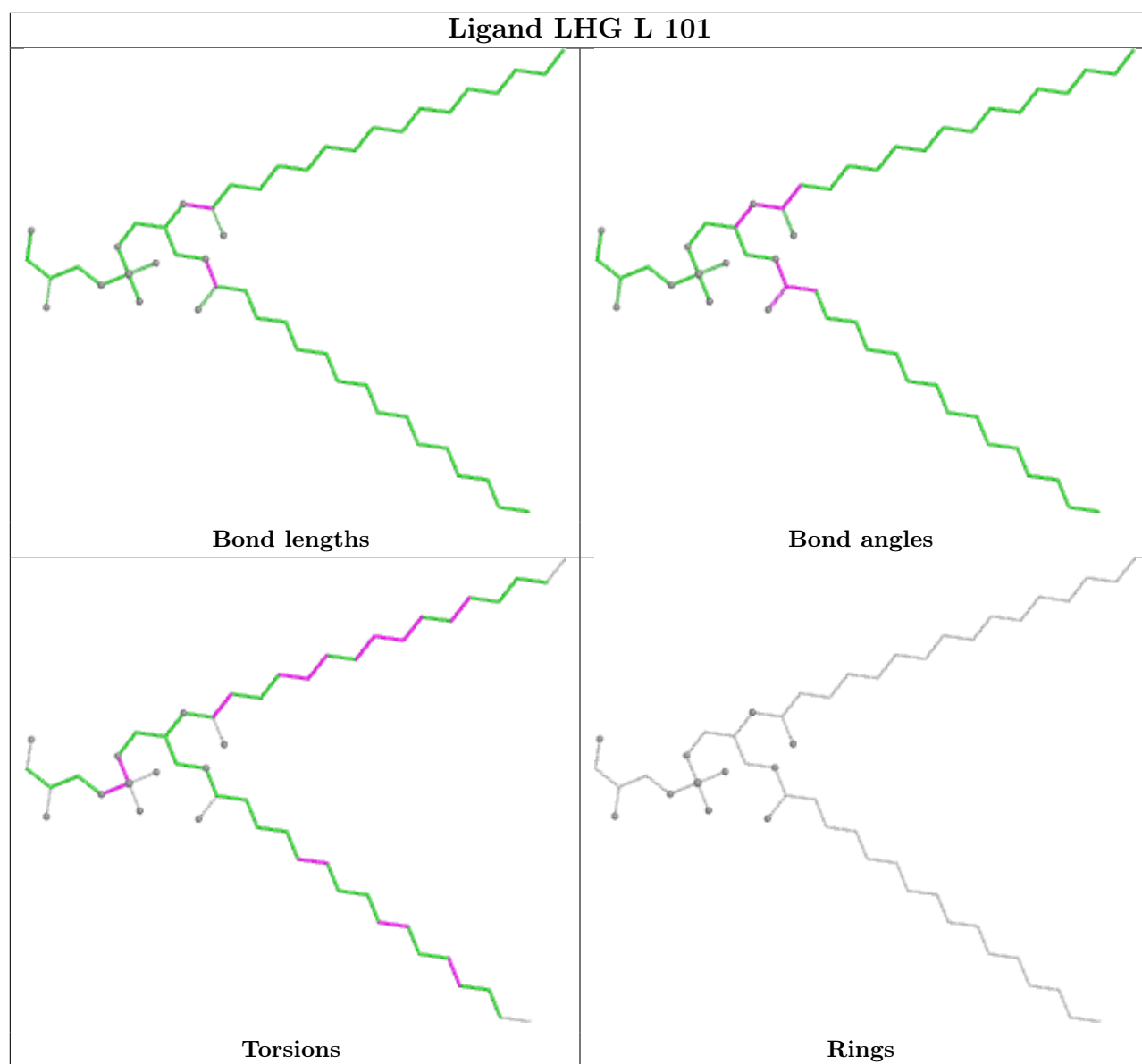


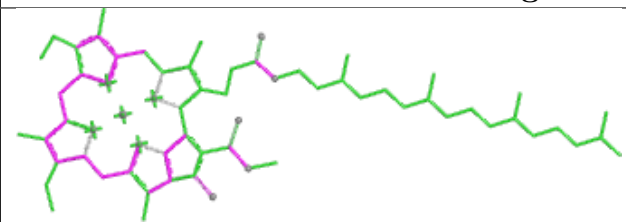
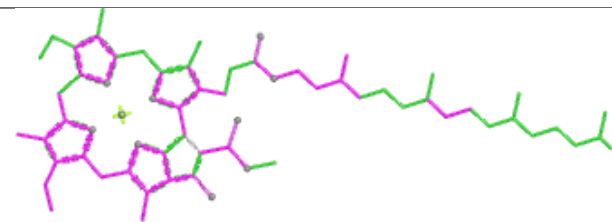
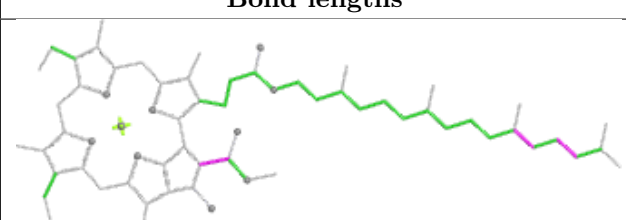
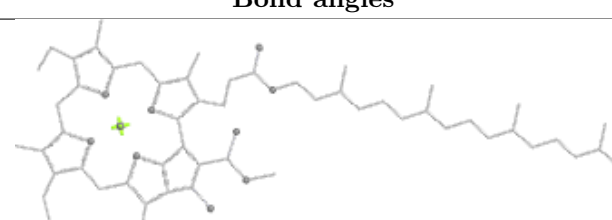


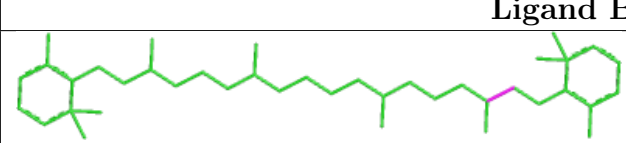
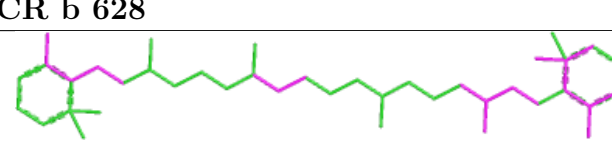
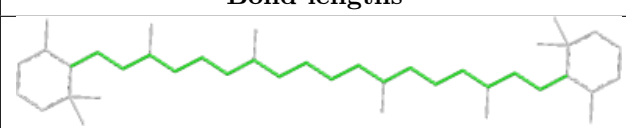
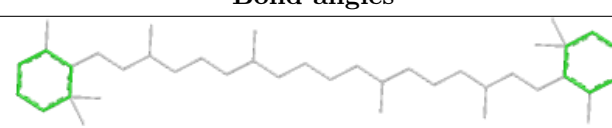


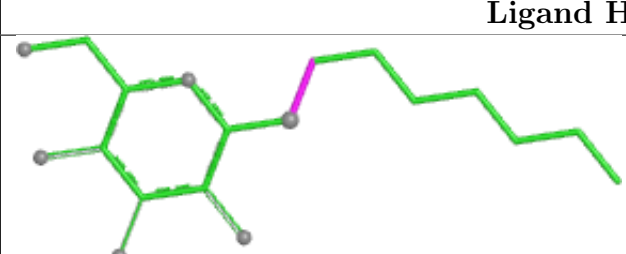
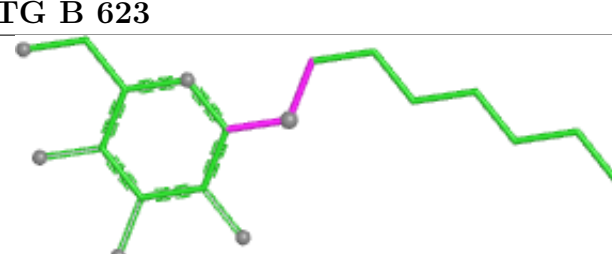
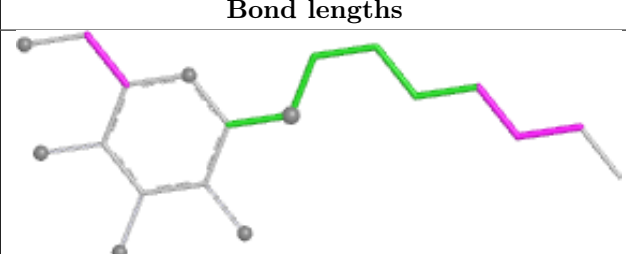
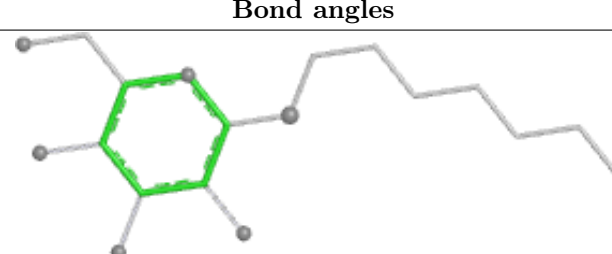


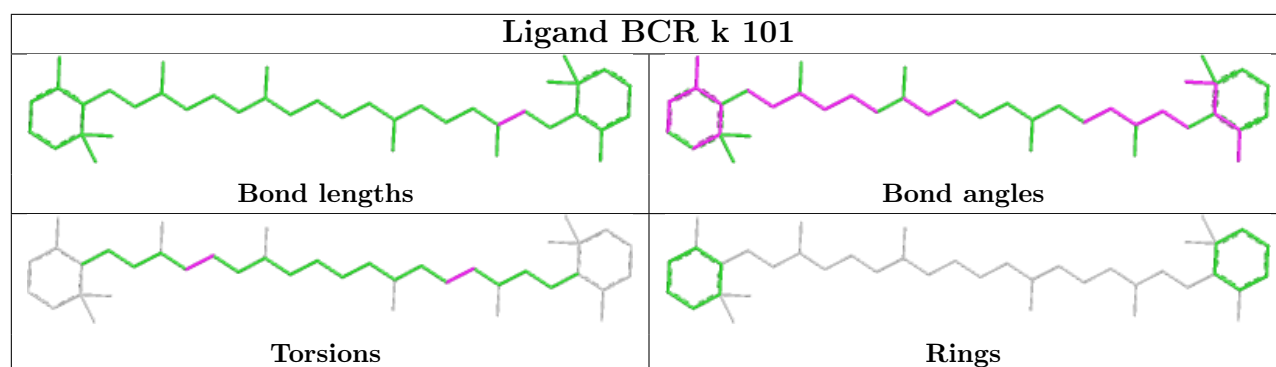
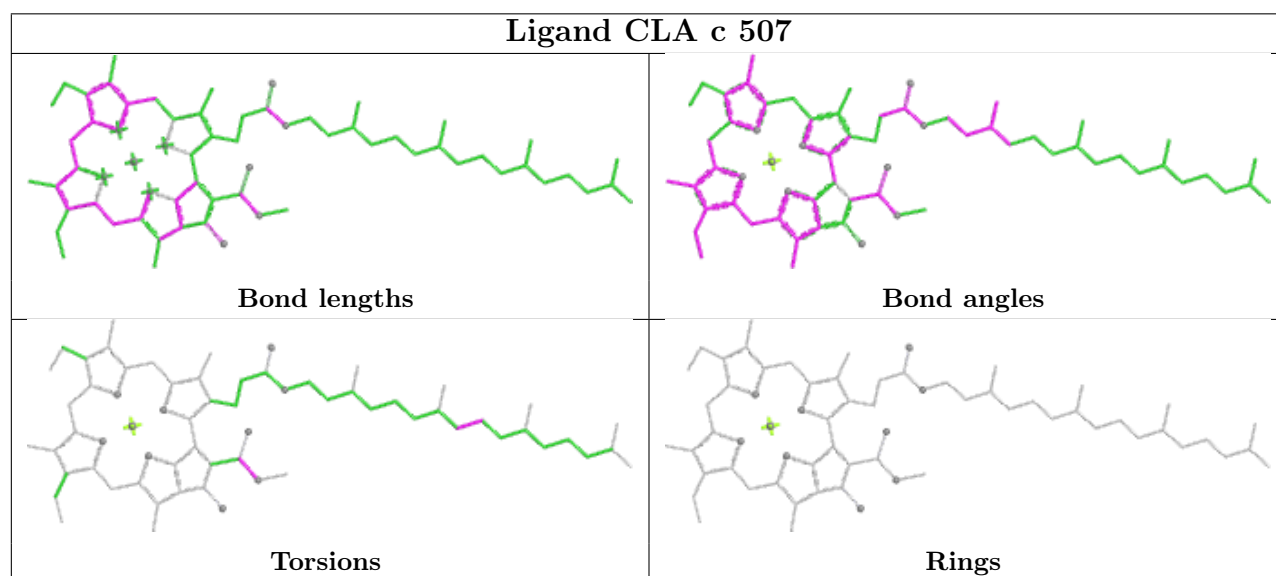
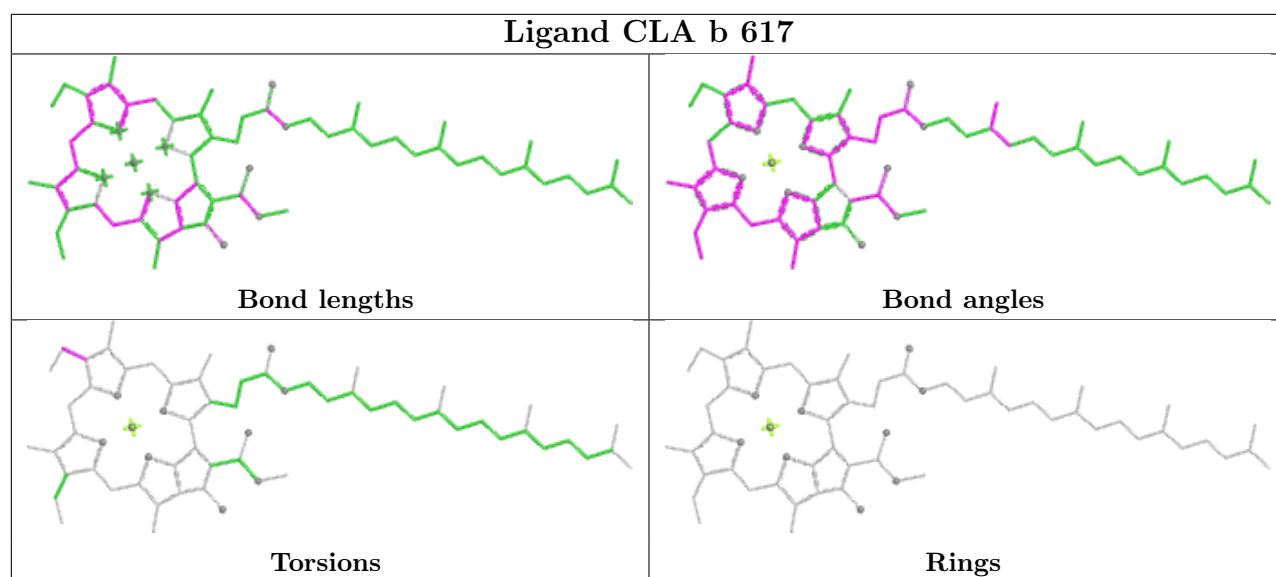
Ligand CLA C 505	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 d 405 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG a 415	
 Bond lengths	 Bond angles
 Torsions	 Rings

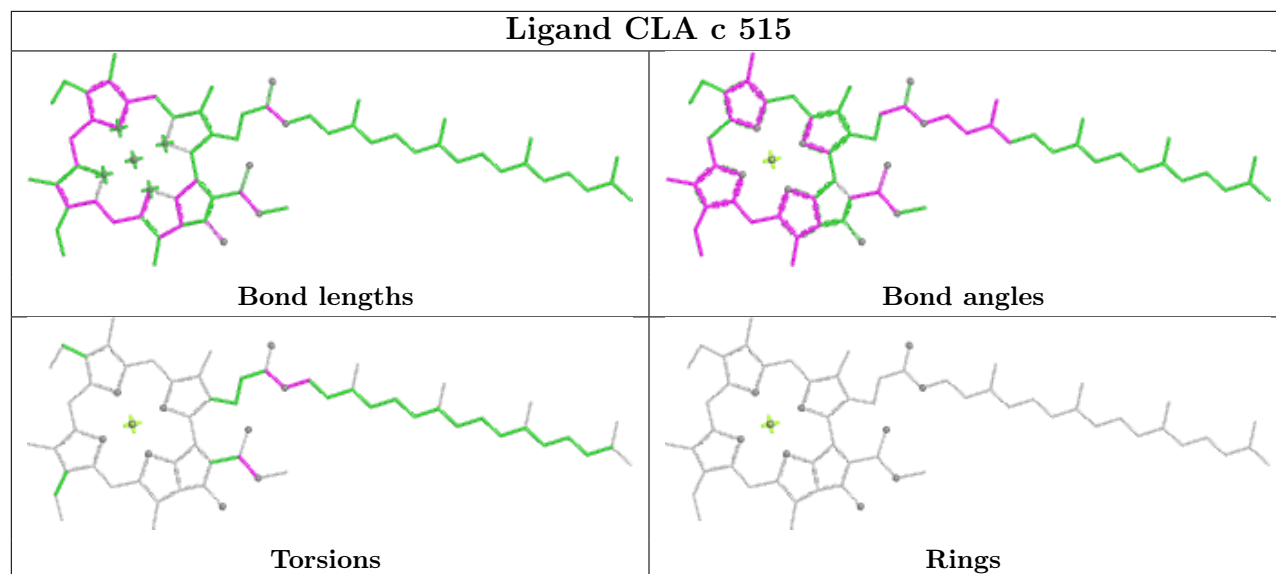
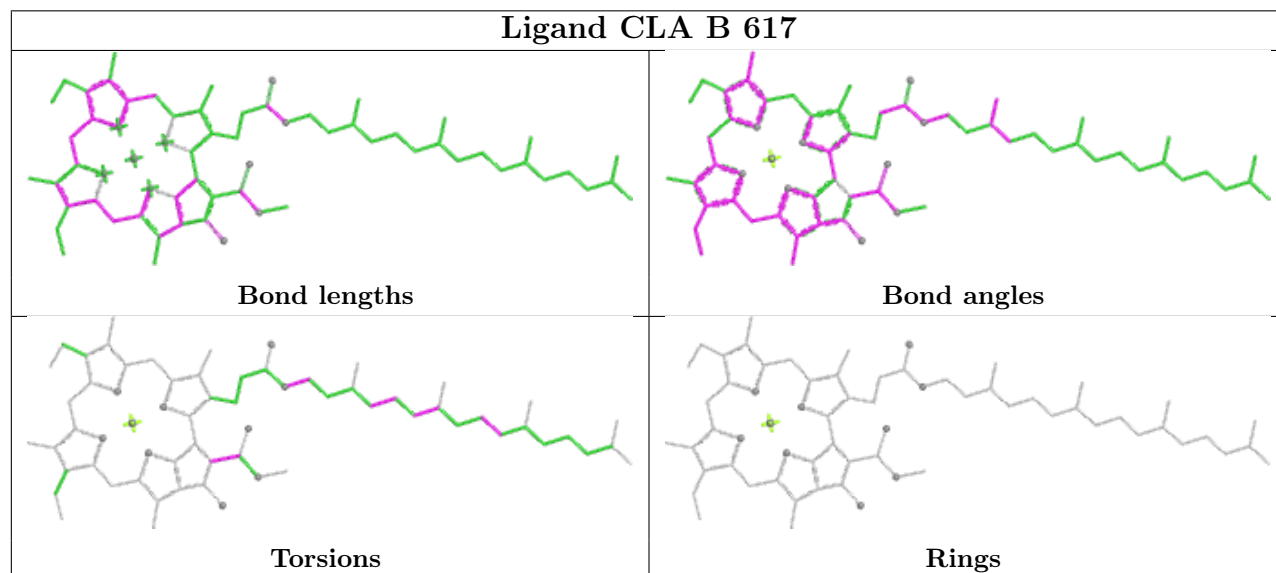


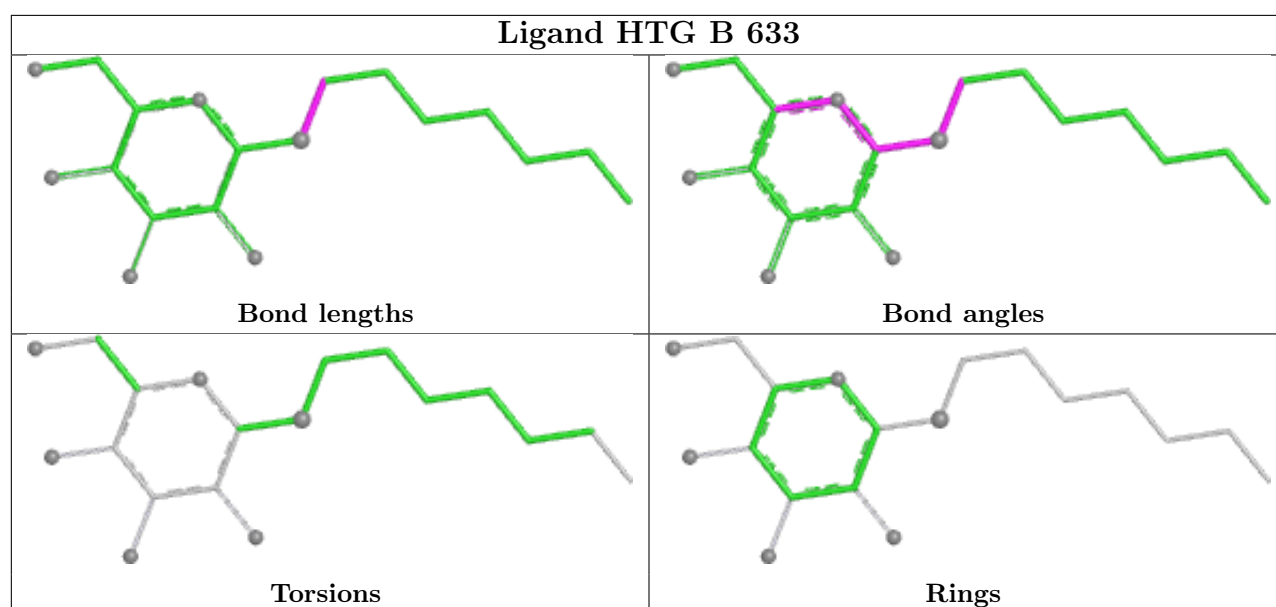
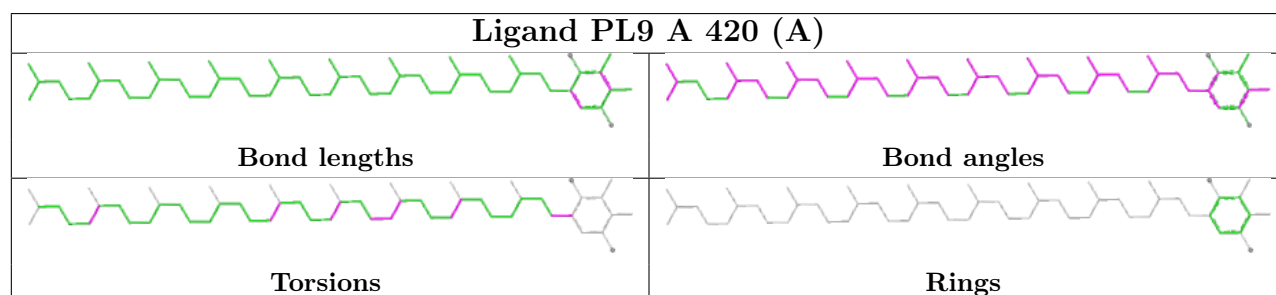
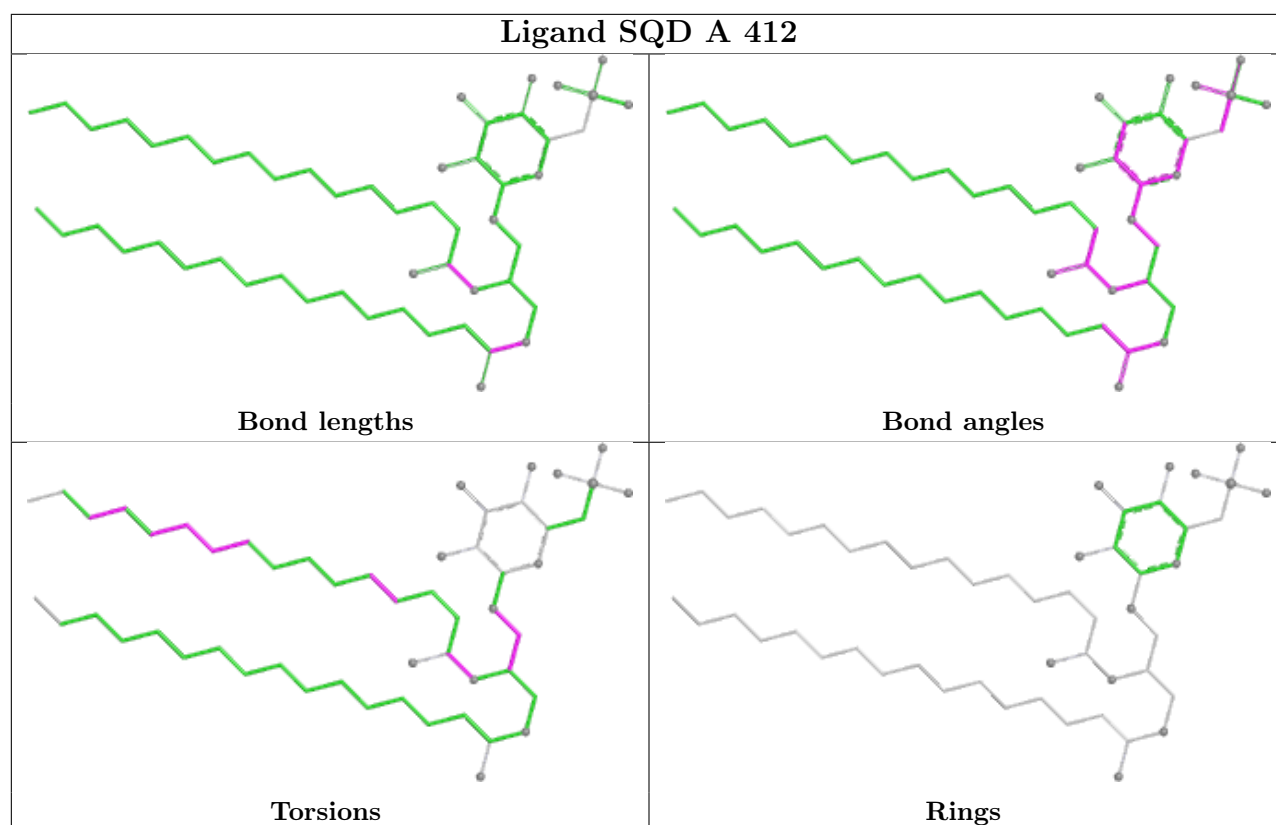
Ligand CLA C 504	
	
Bond lengths	Bond angles
	
Torsions	Rings

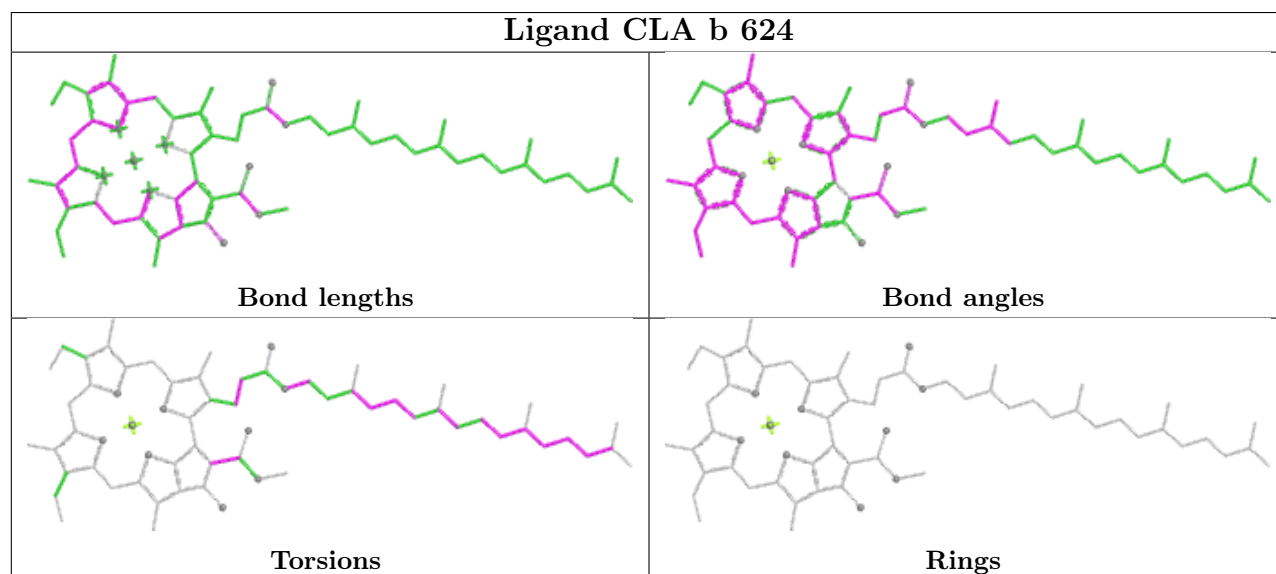
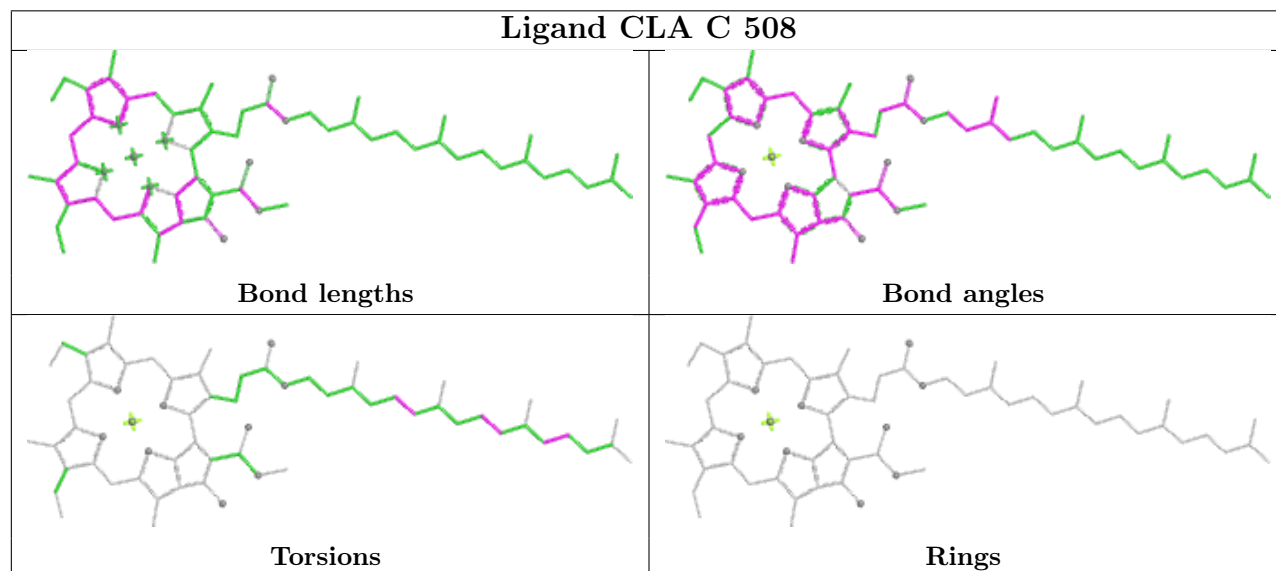
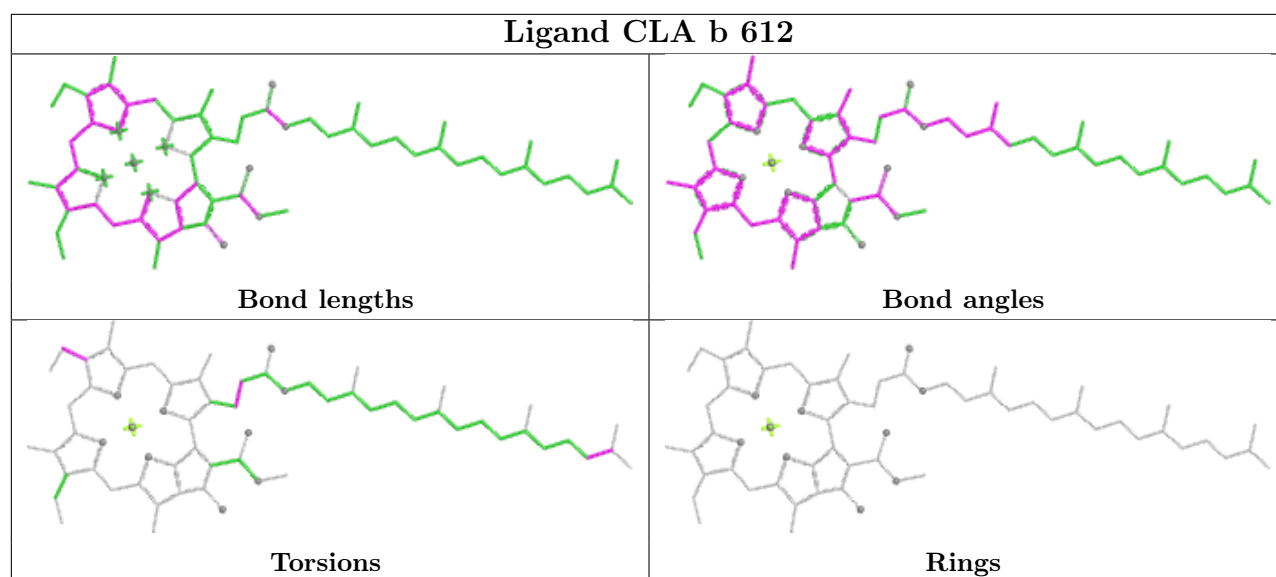
Ligand BCR b 628	
	
Bond lengths	Bond angles
	
Torsions	Rings

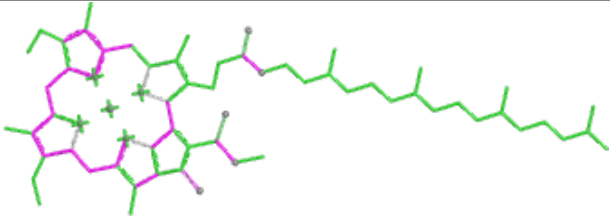
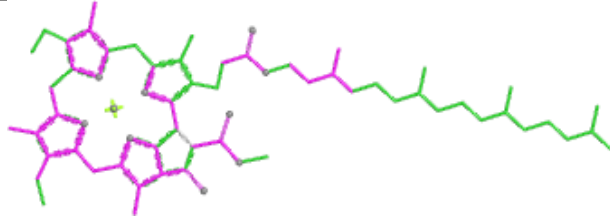
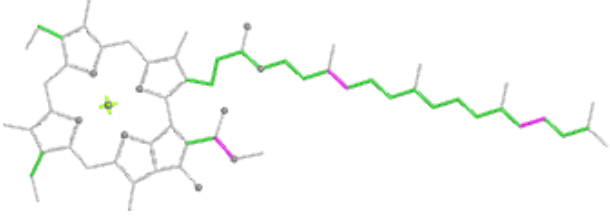
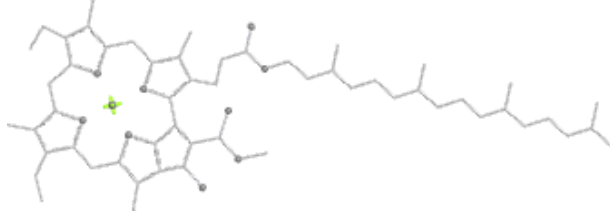
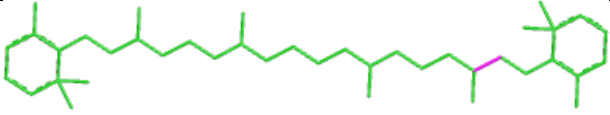
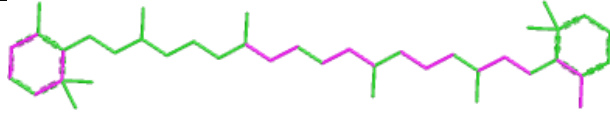
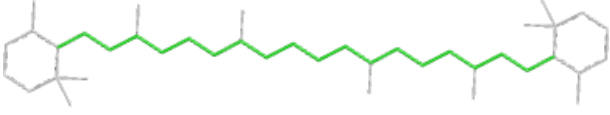
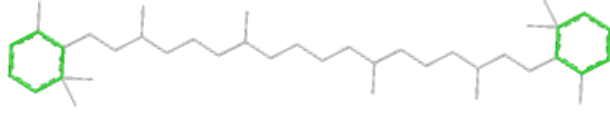
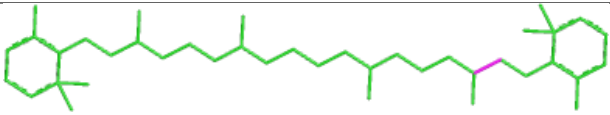
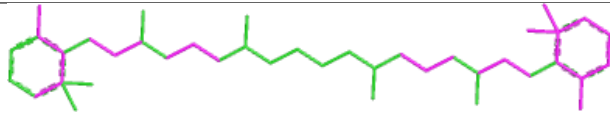
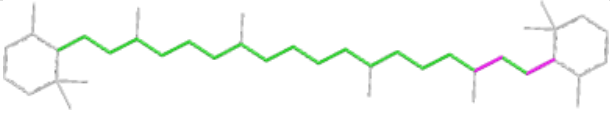
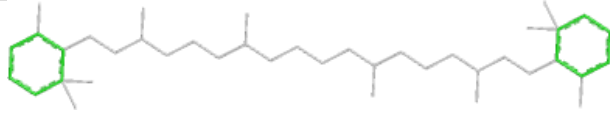
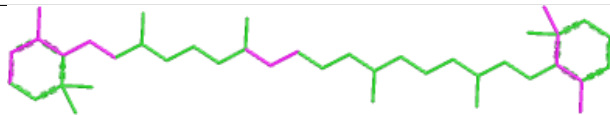
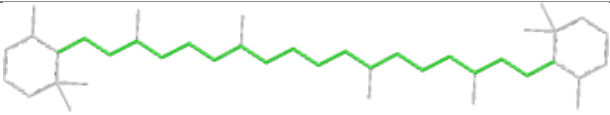
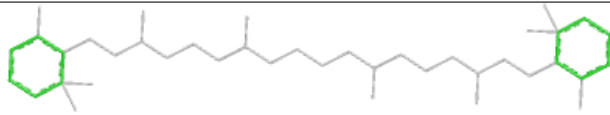
Ligand HTG B 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

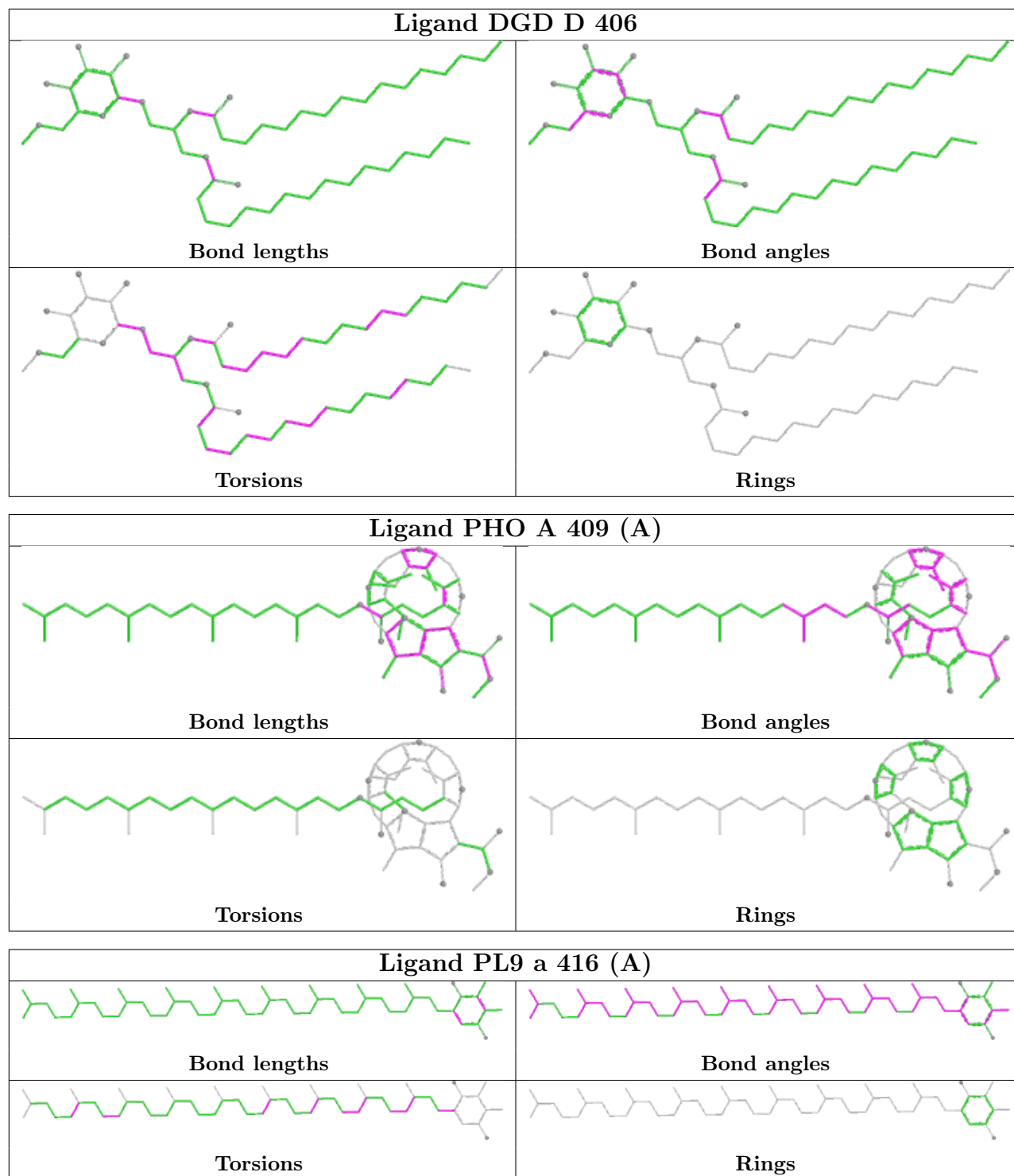


Ligand CLA c 515**Ligand CLA B 617**

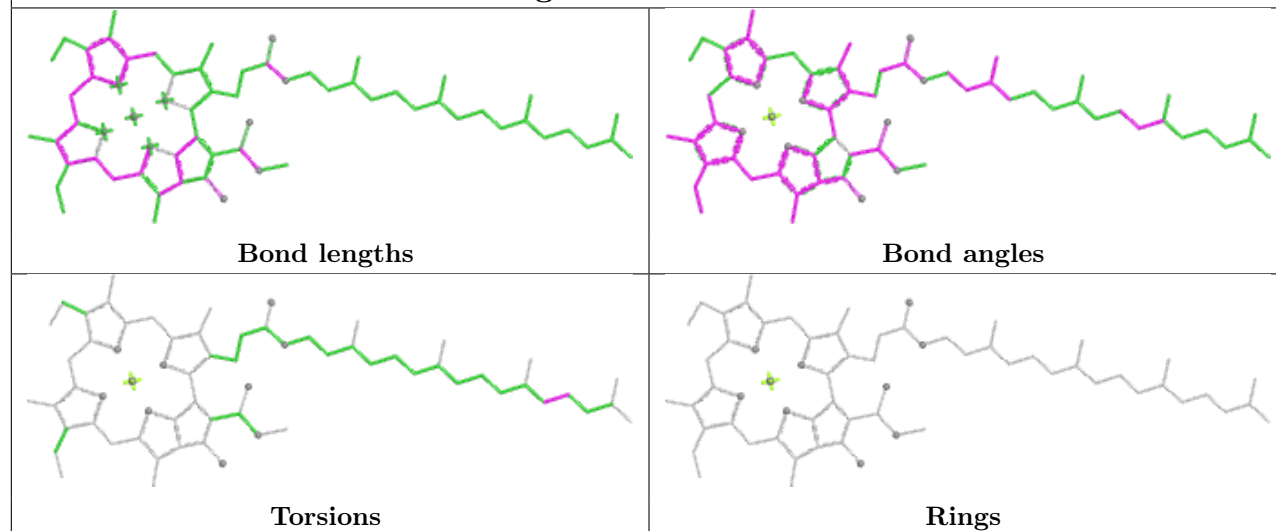




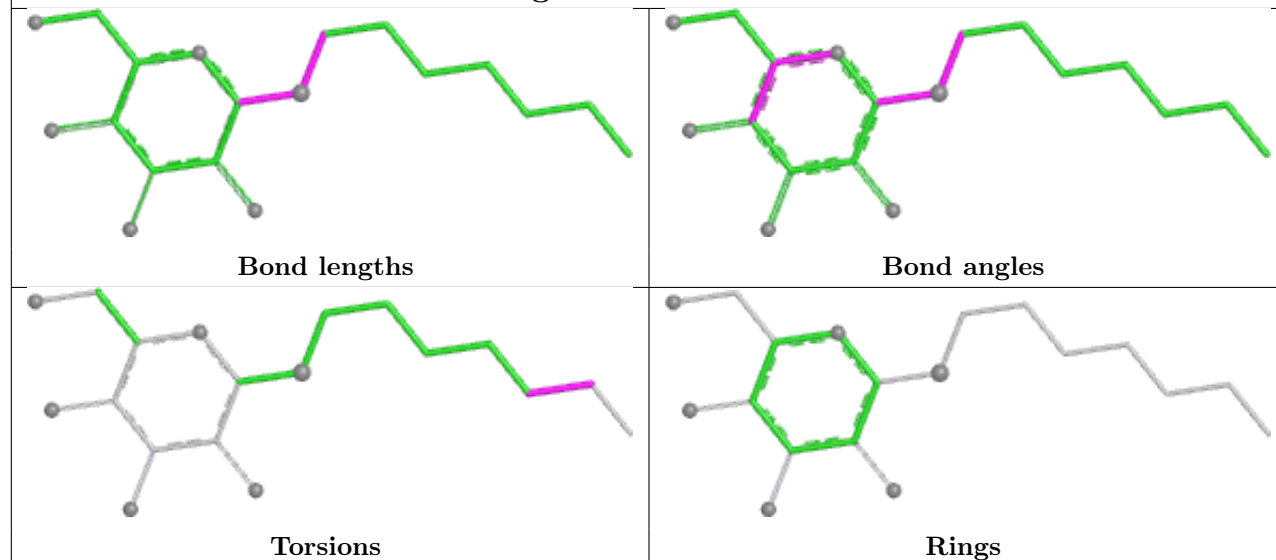
Ligand CLA B 605	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b 629	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR d 404	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR a 413	
 Bond lengths	 Bond angles
 Torsions	 Rings



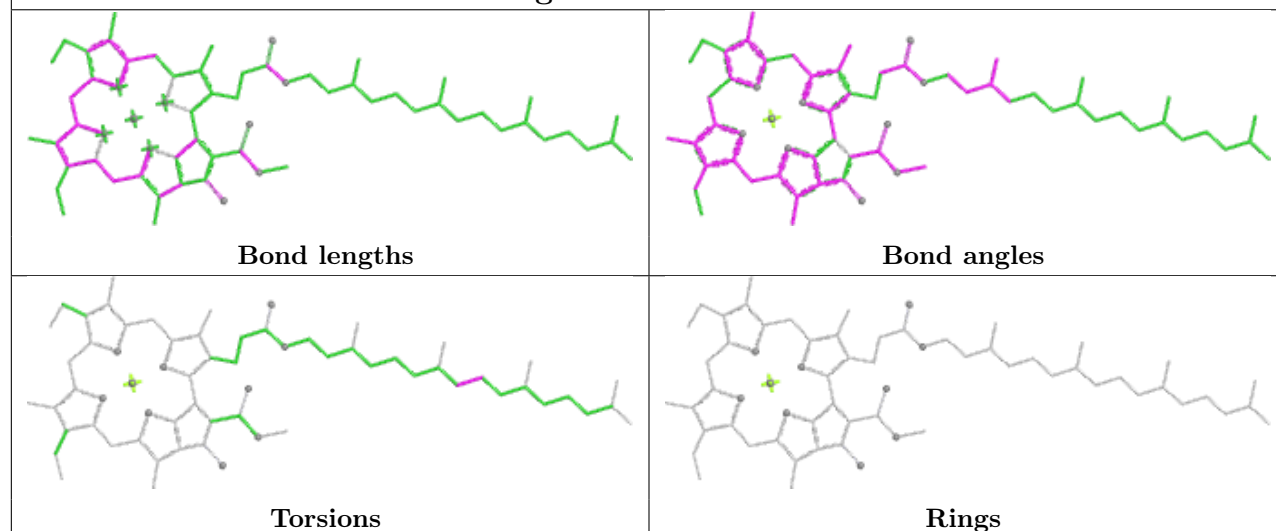
Ligand CLA b 618

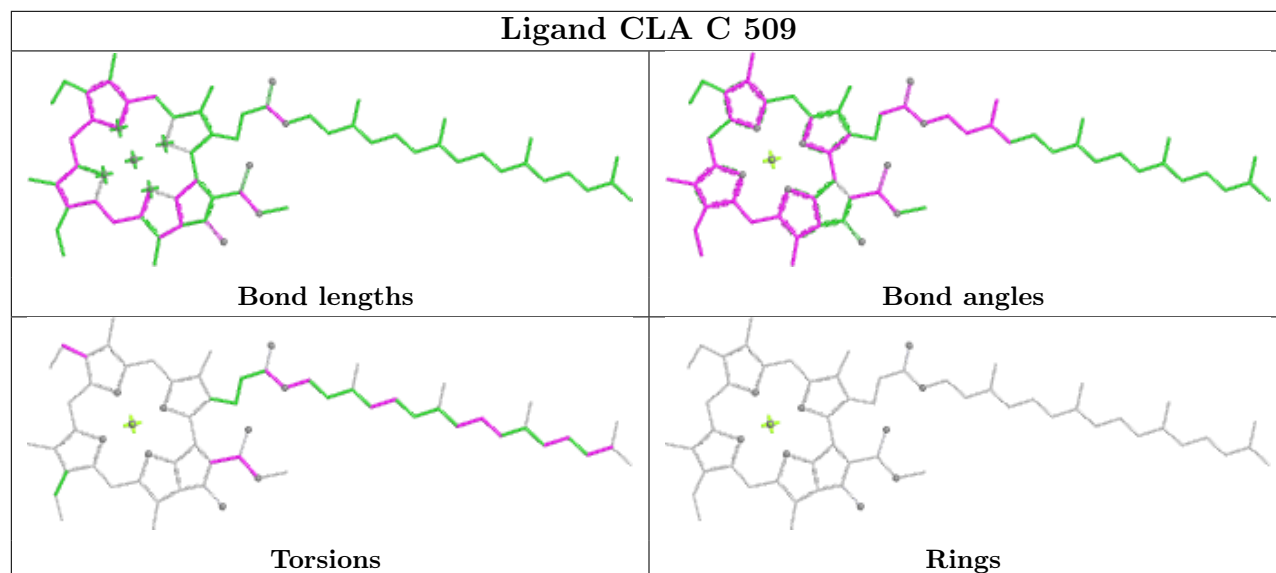
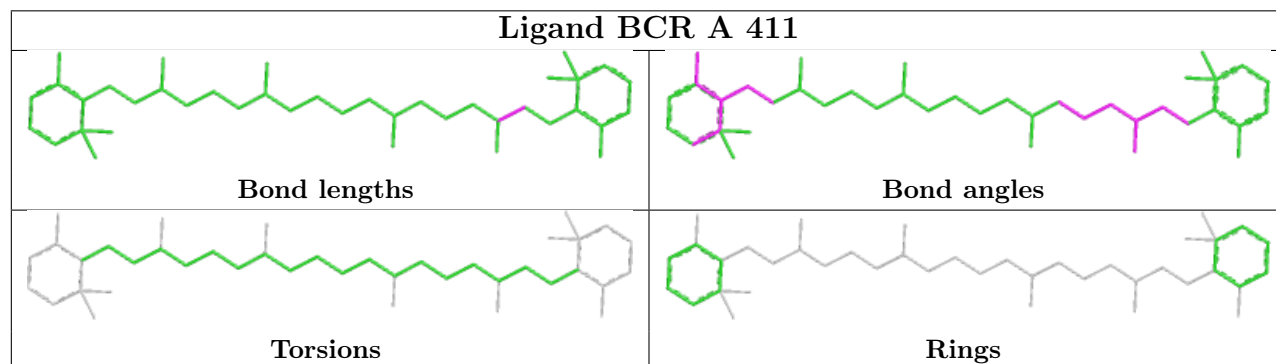
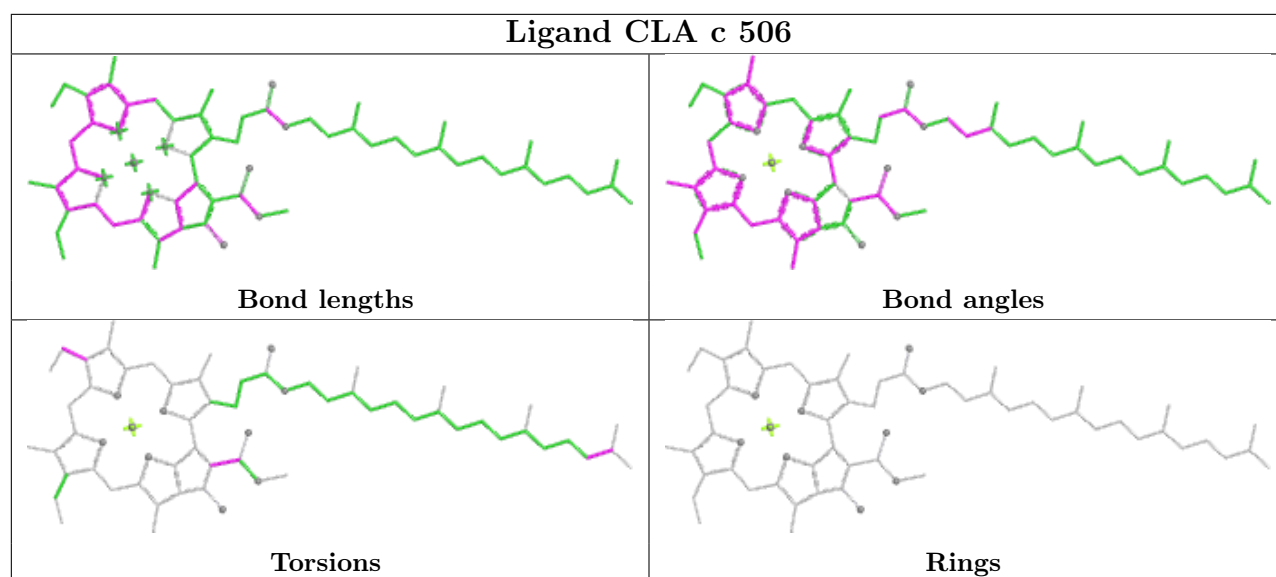


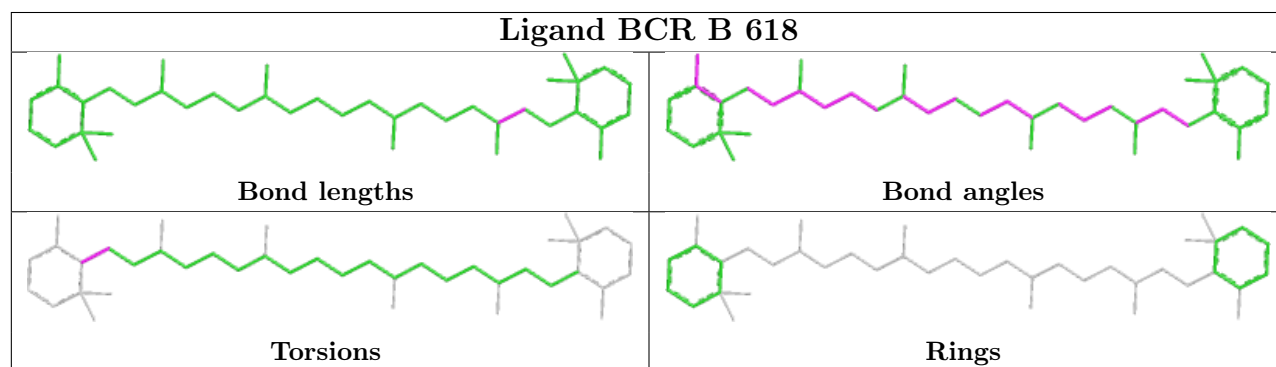
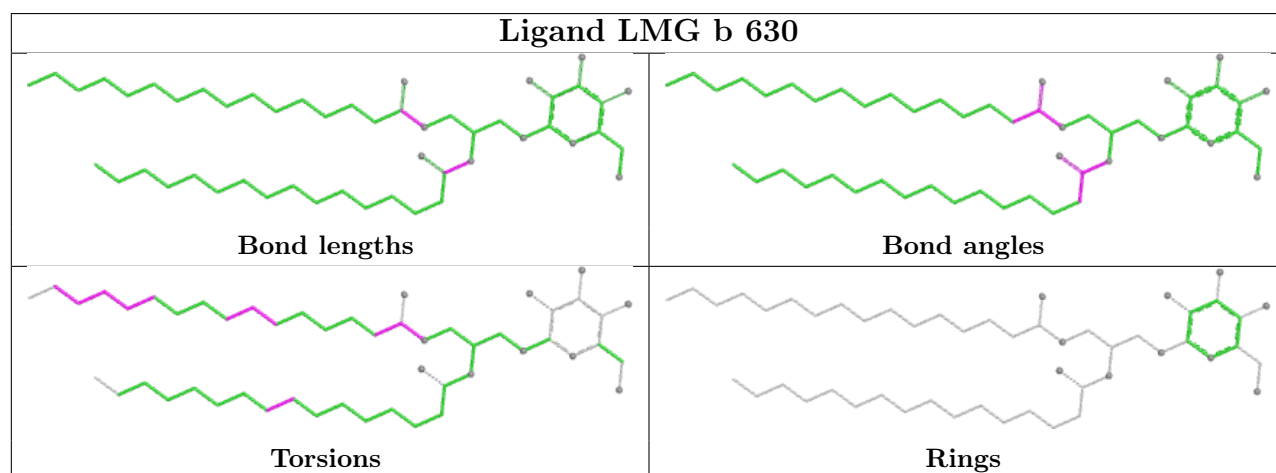
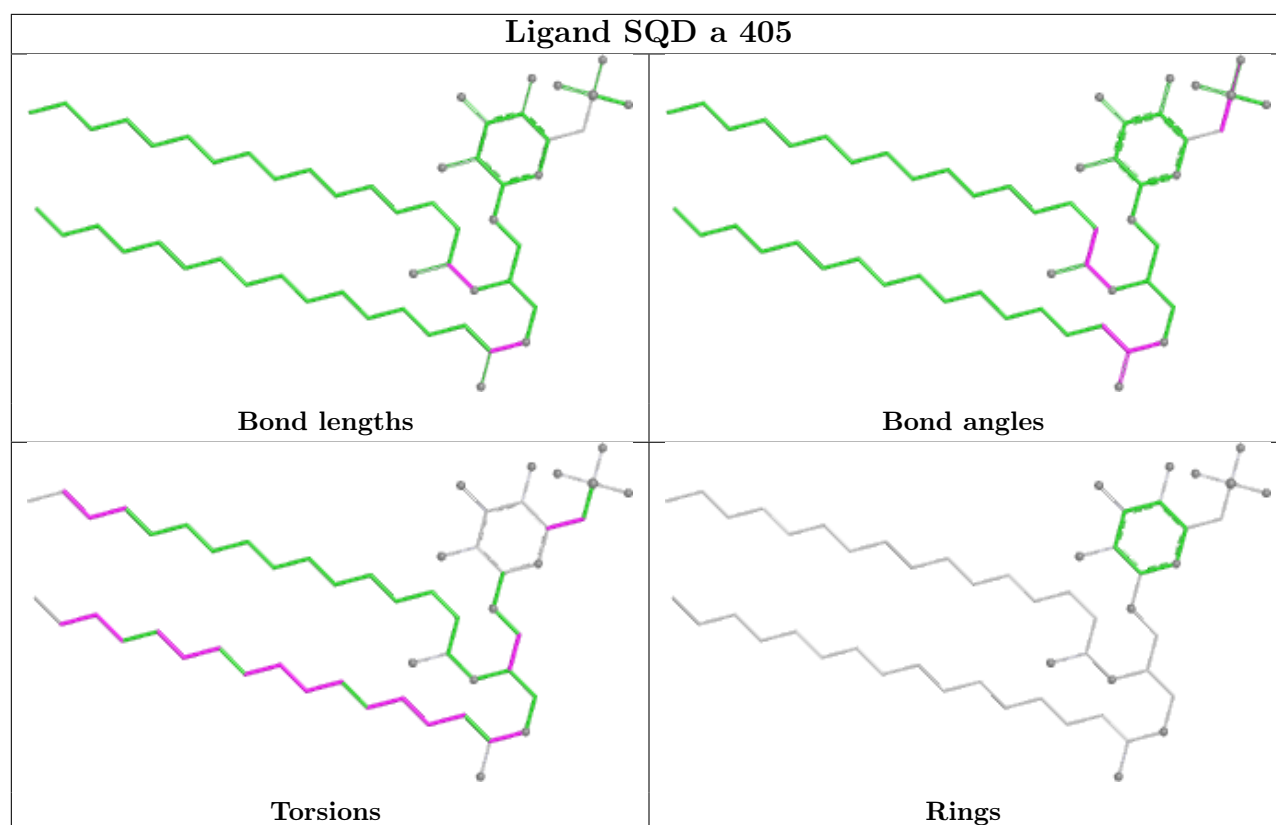
Ligand HTG b 608

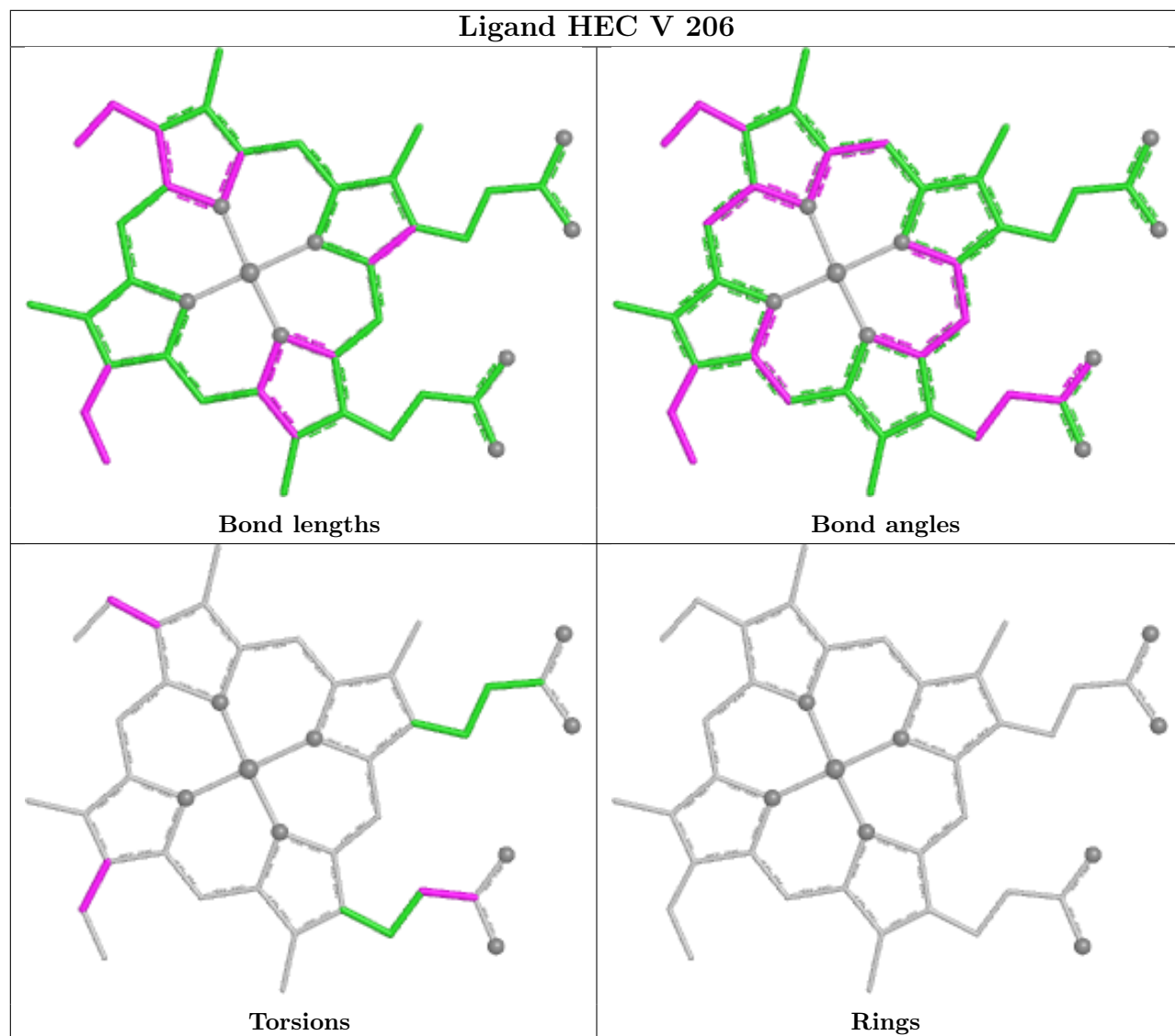


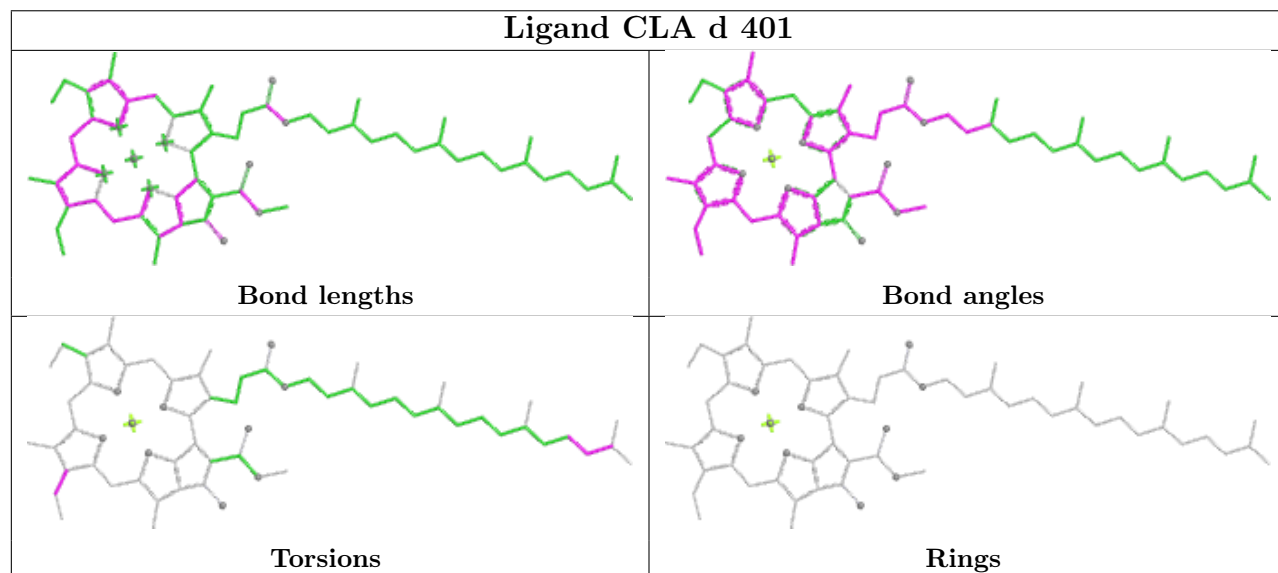
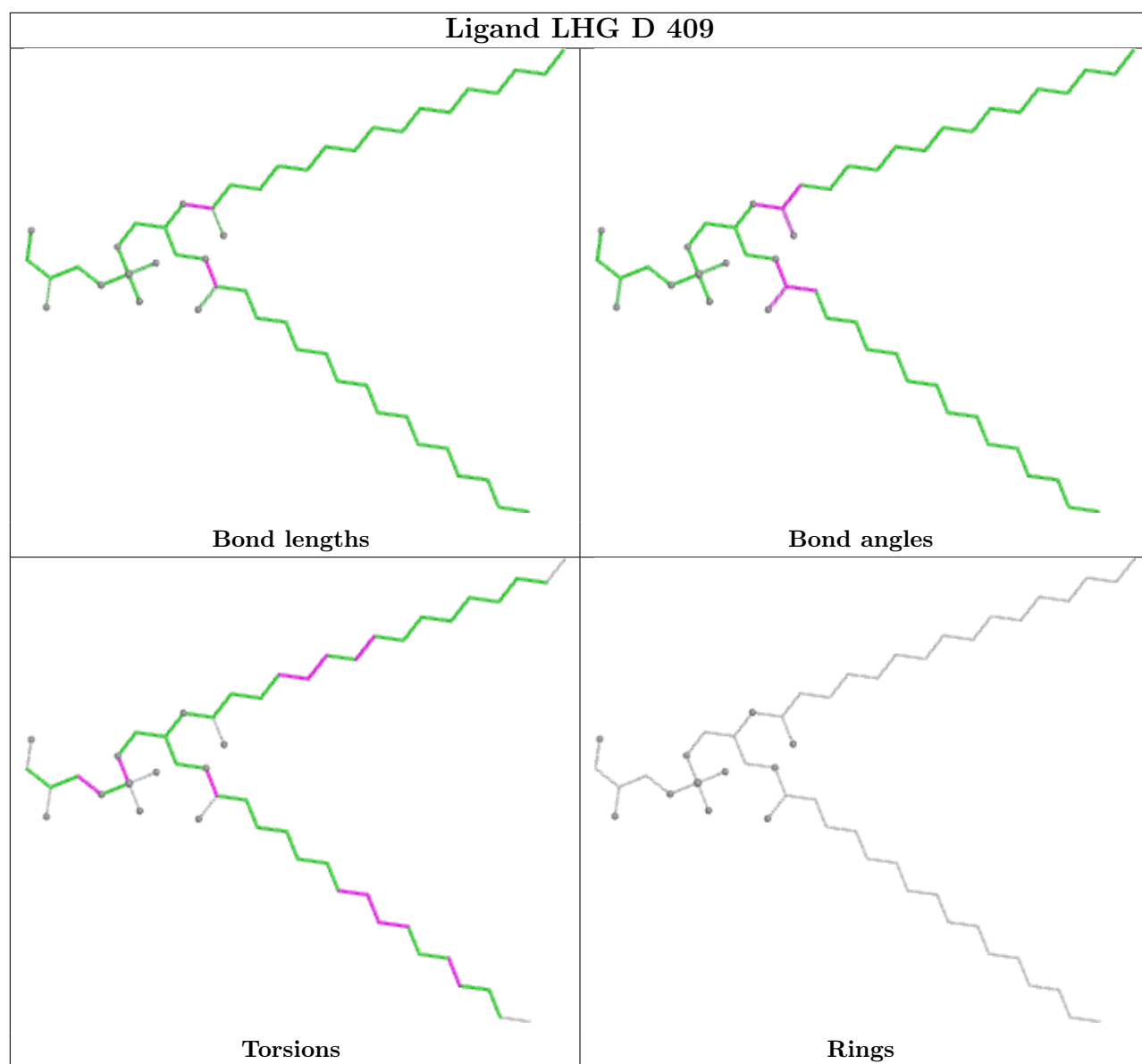
Ligand CLA b 622

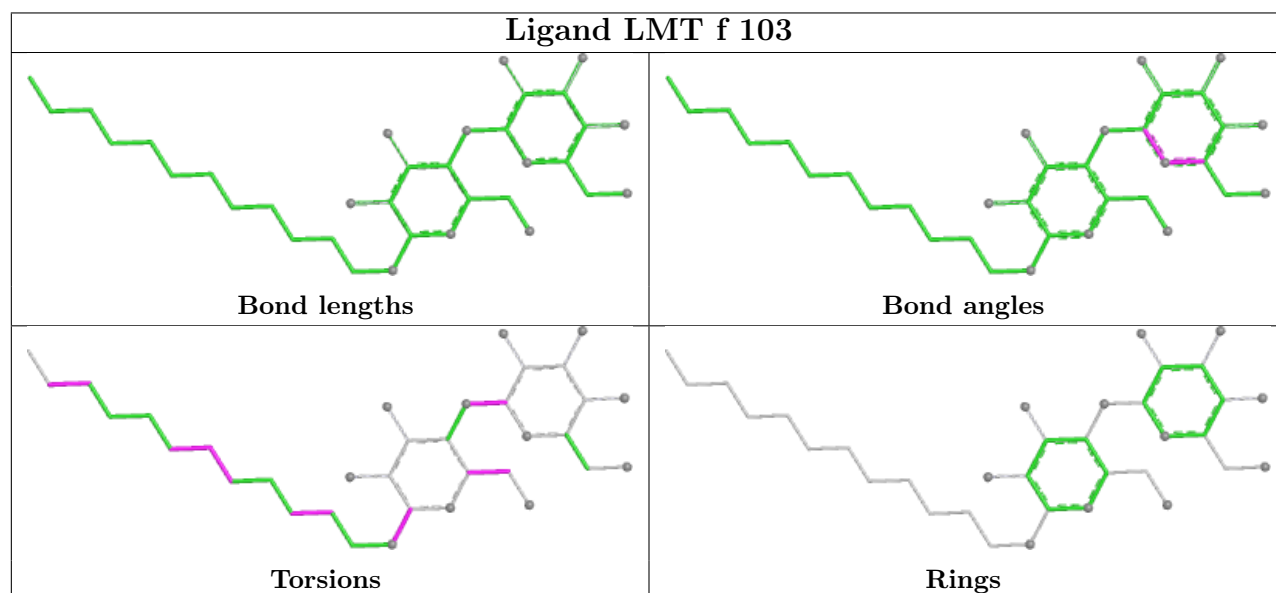
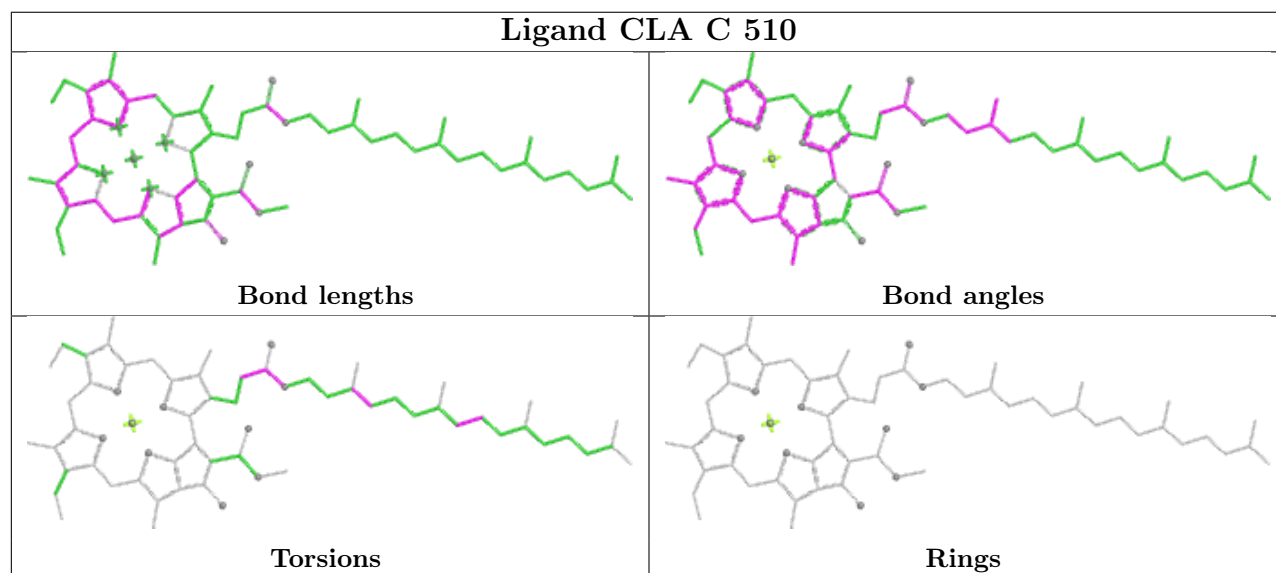
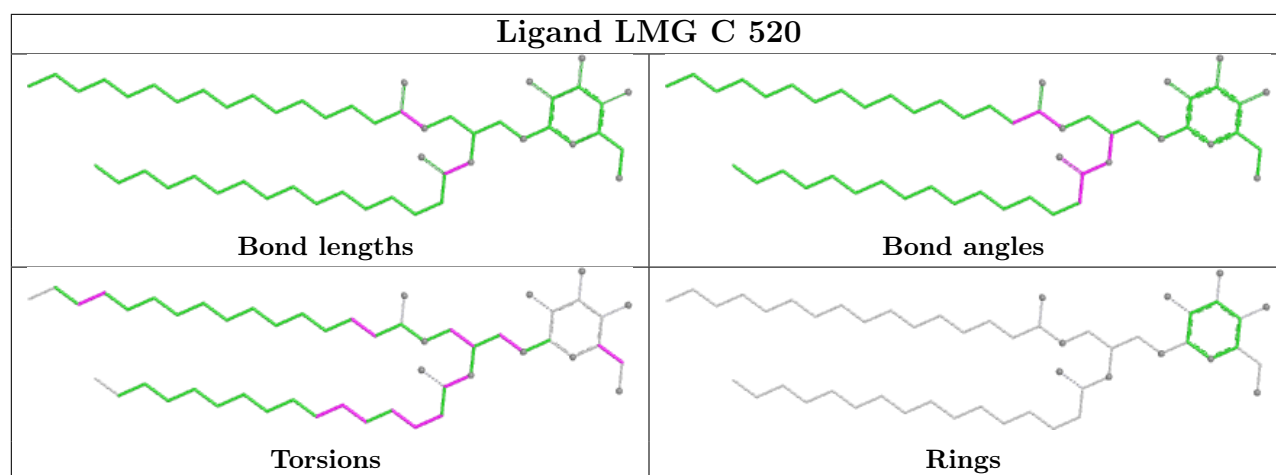


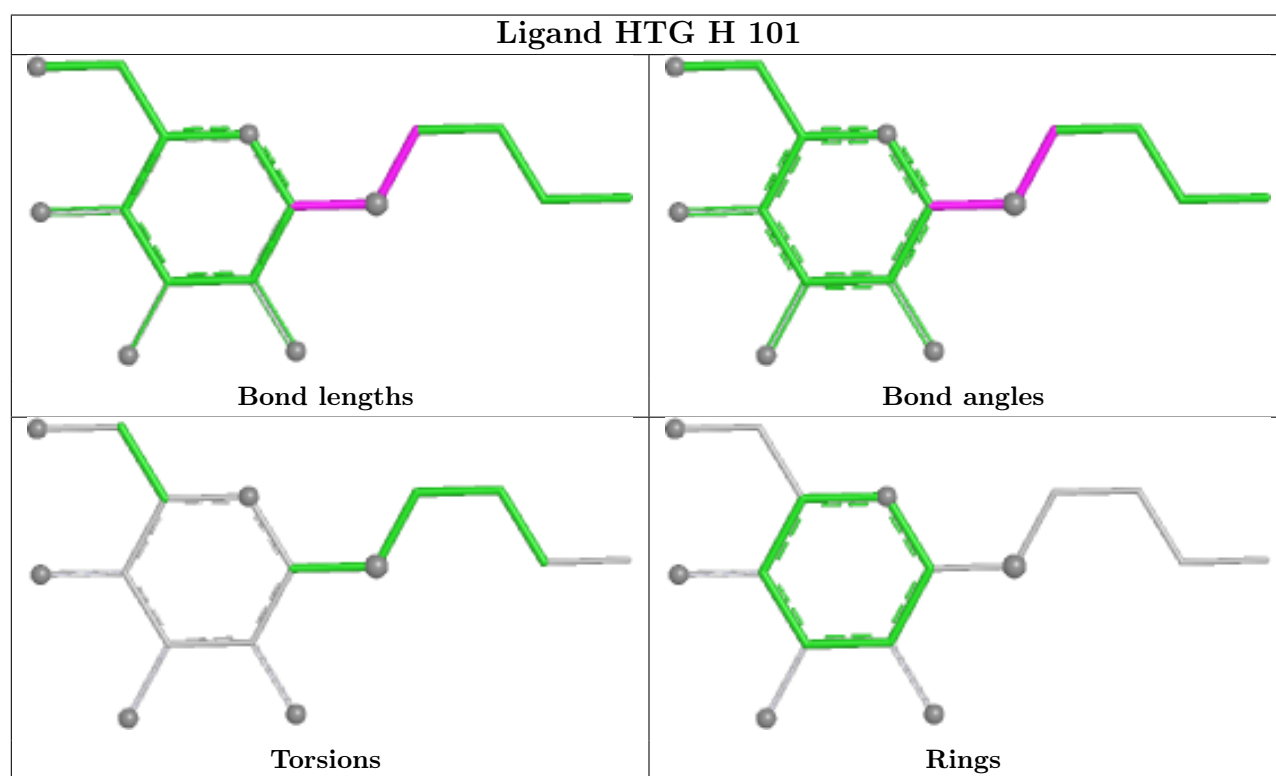
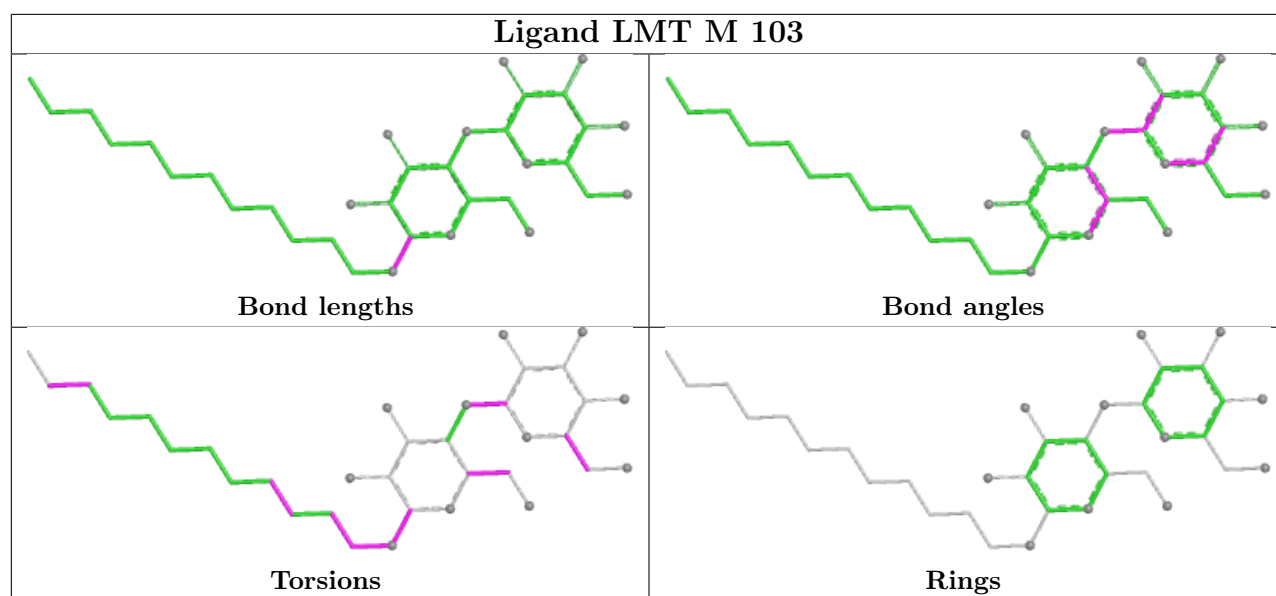


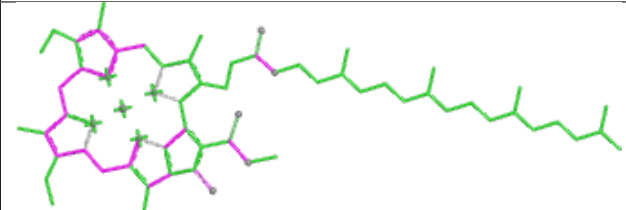
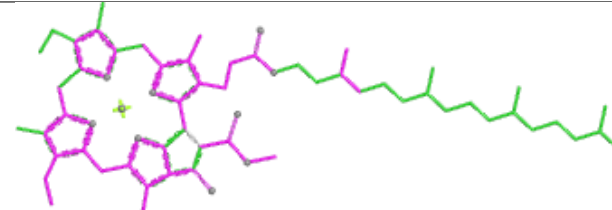
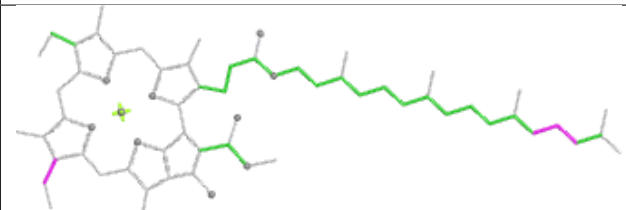
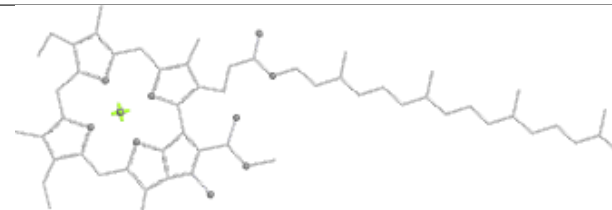


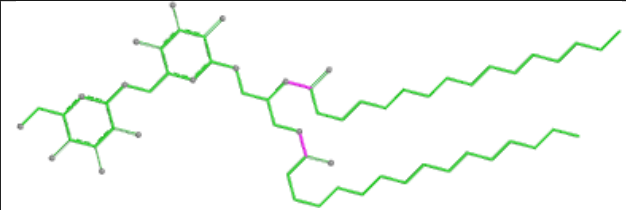
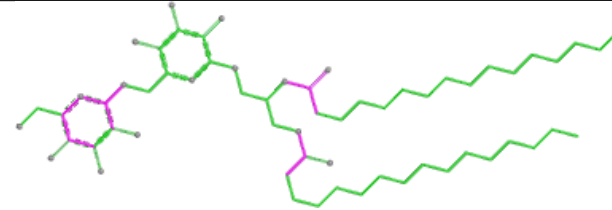
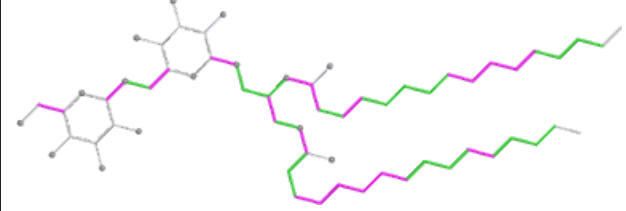
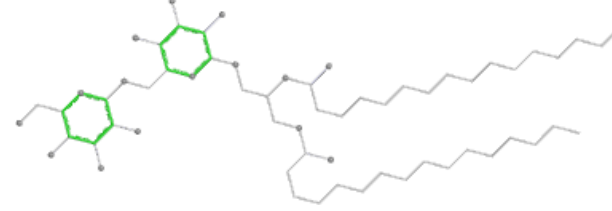


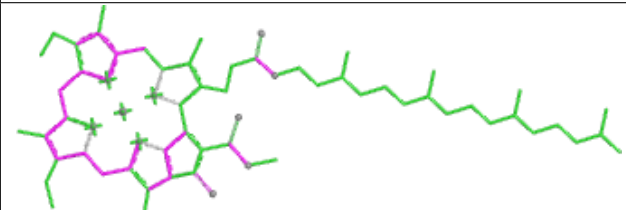
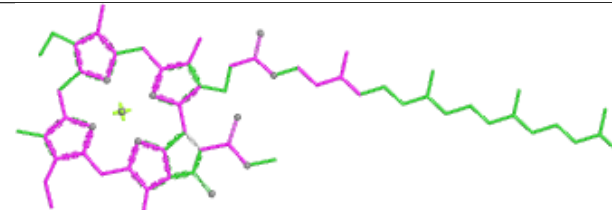
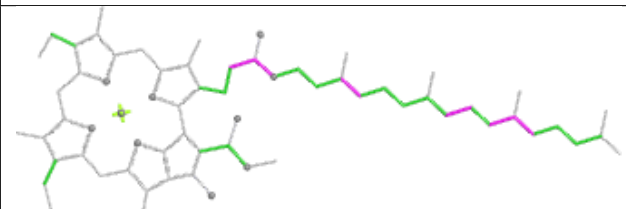
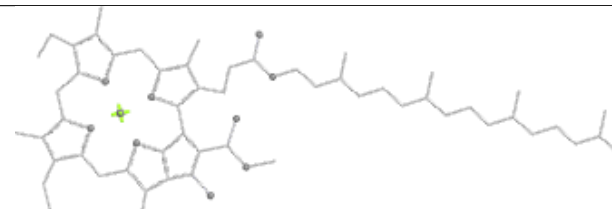


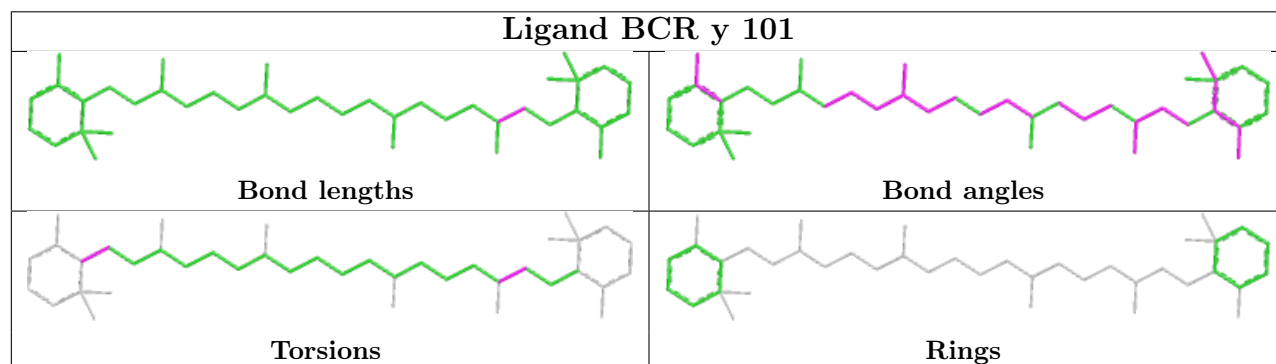
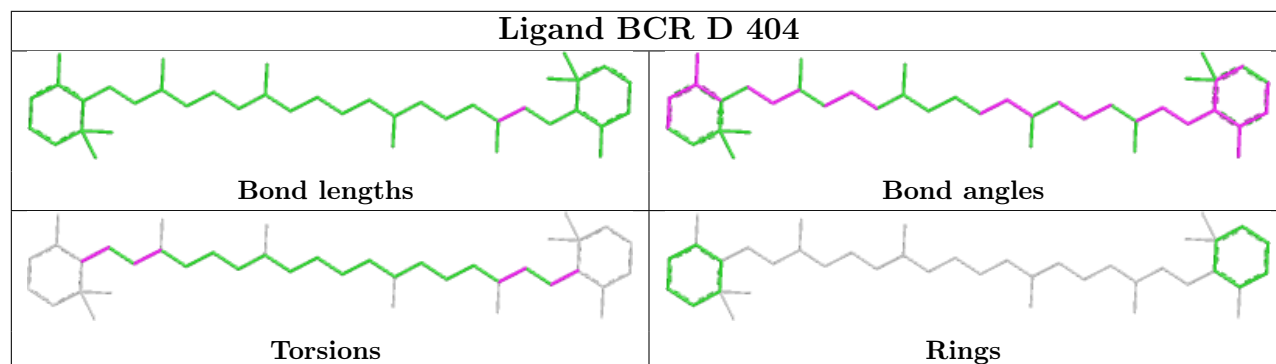
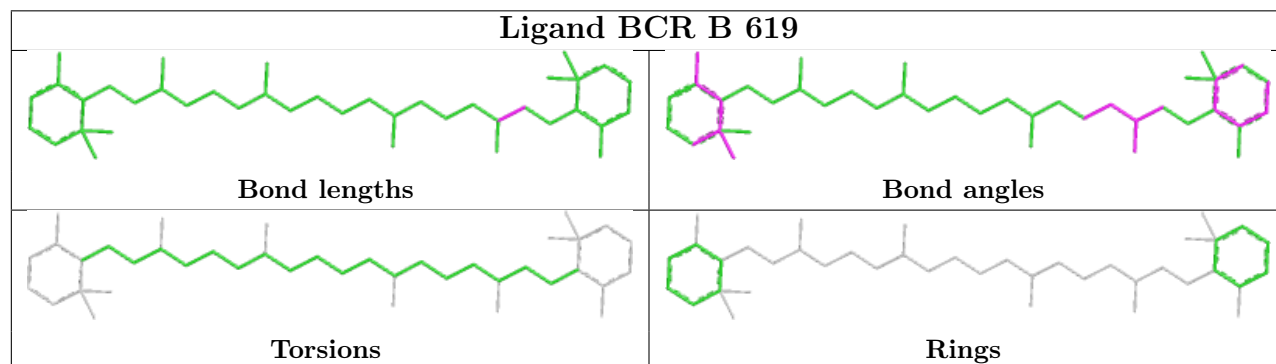
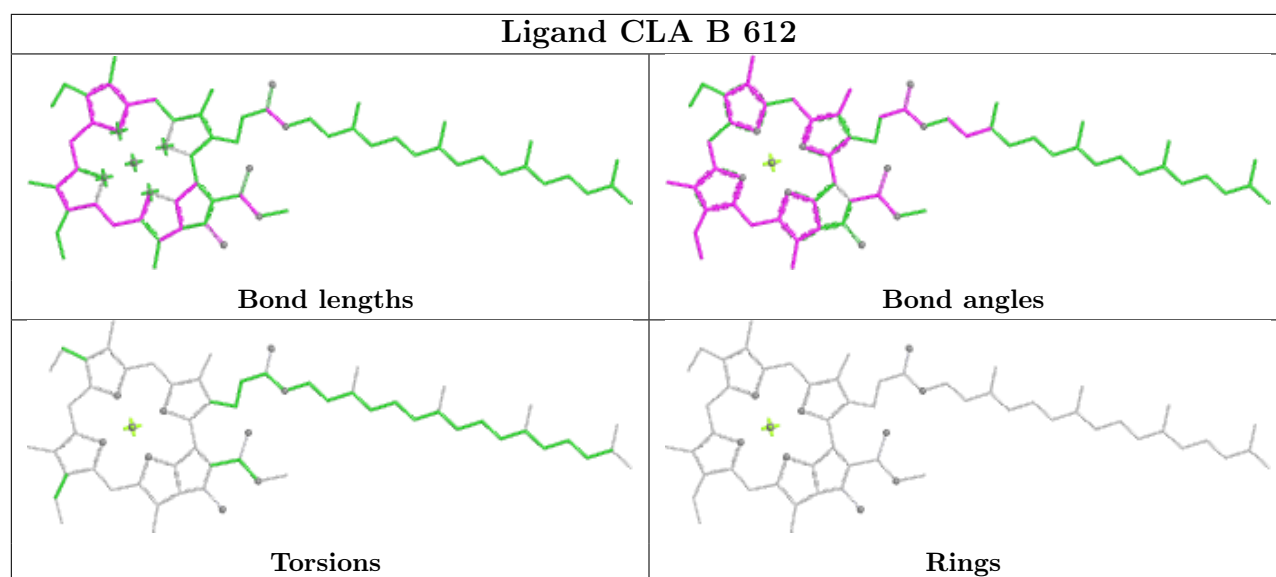


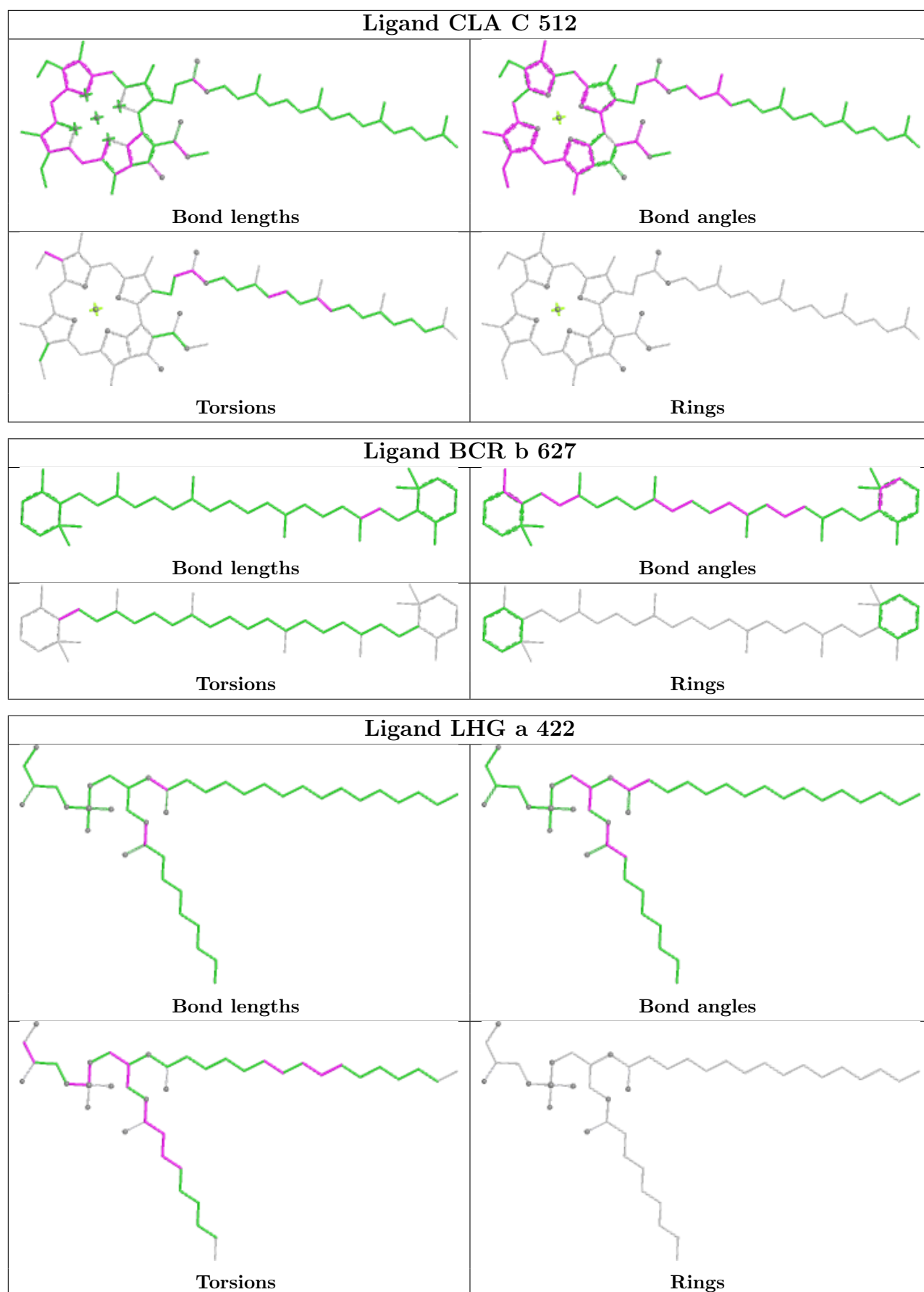


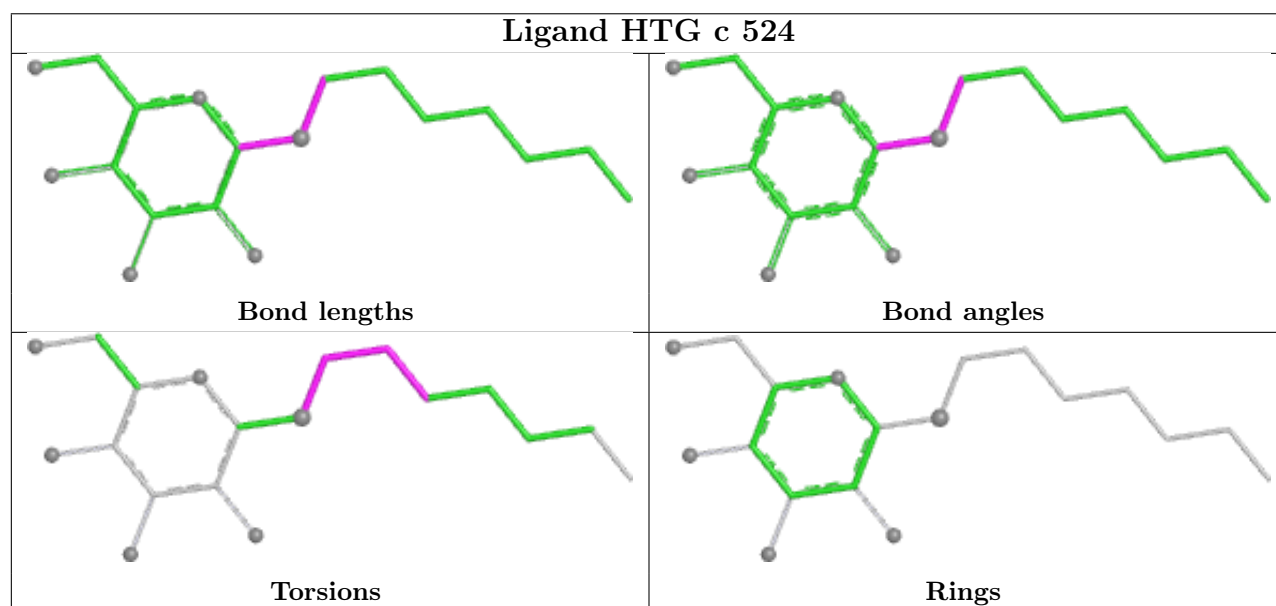
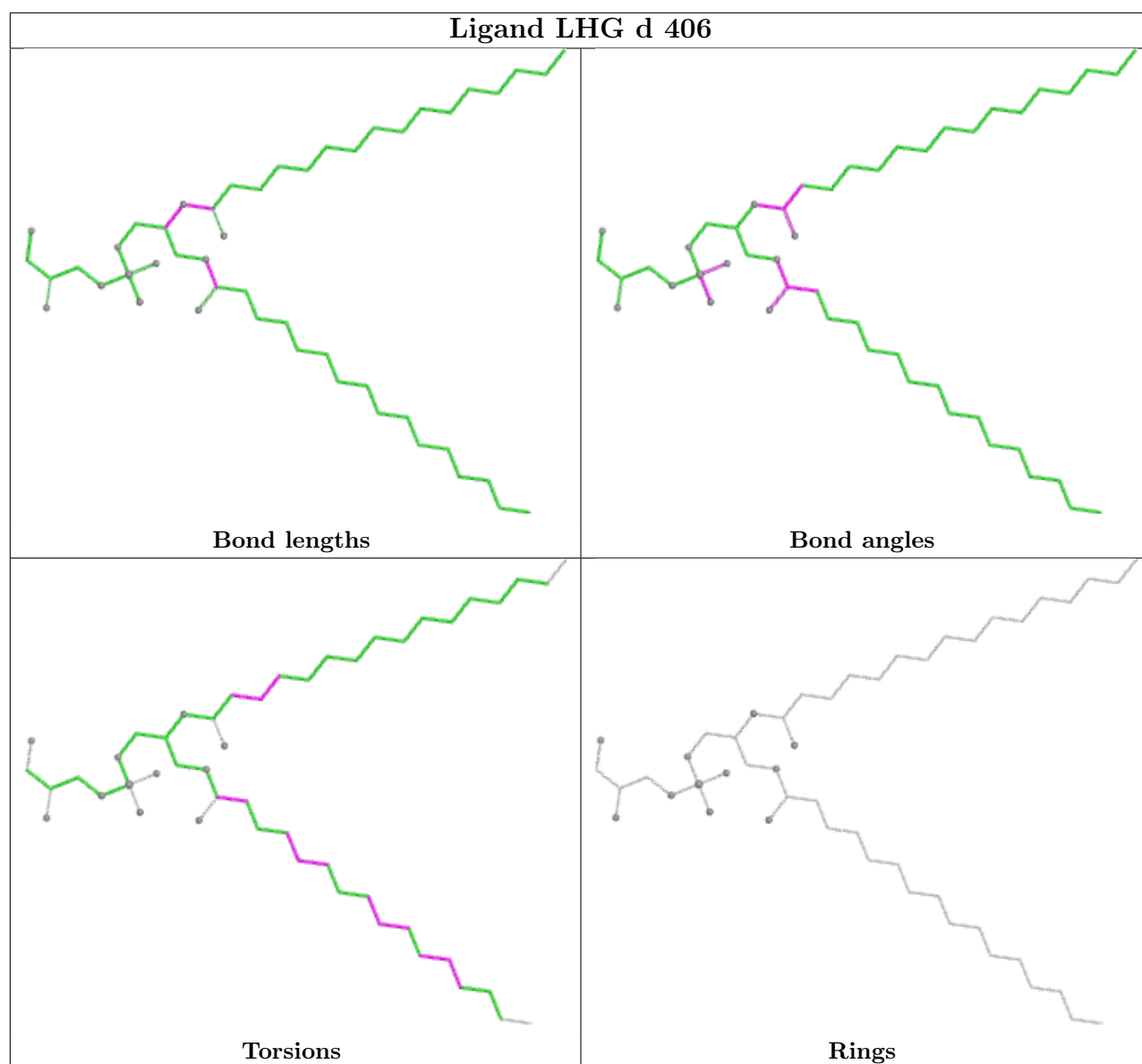
Ligand CLA A 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

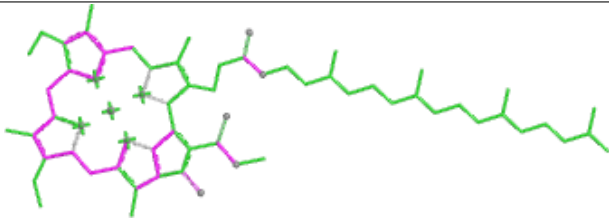
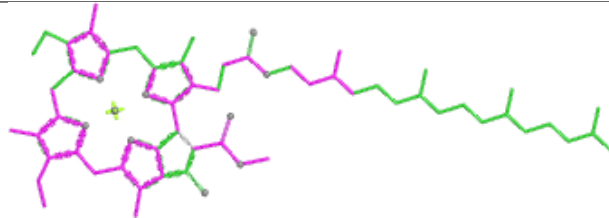
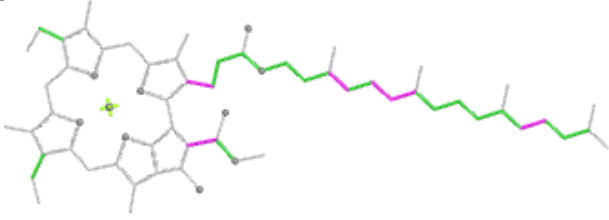
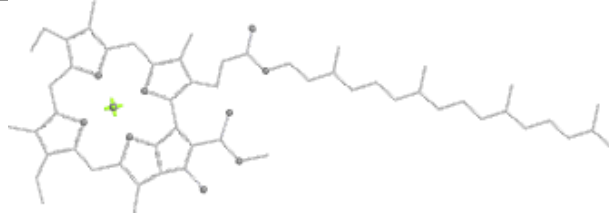
Ligand DGD e 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

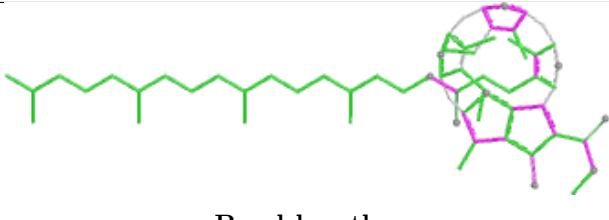
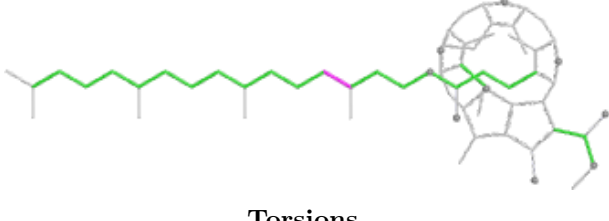
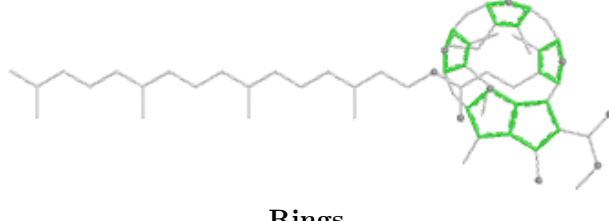
Ligand CLA c 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

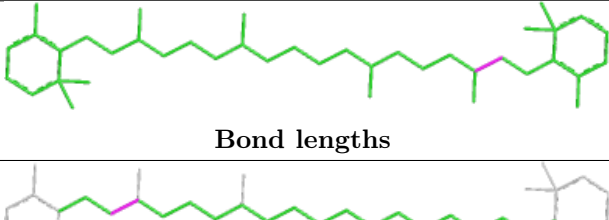
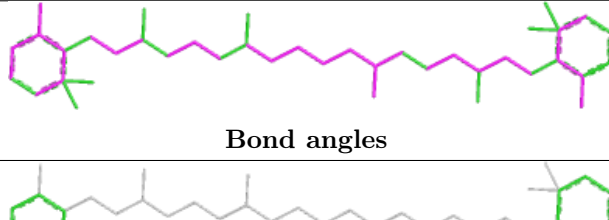




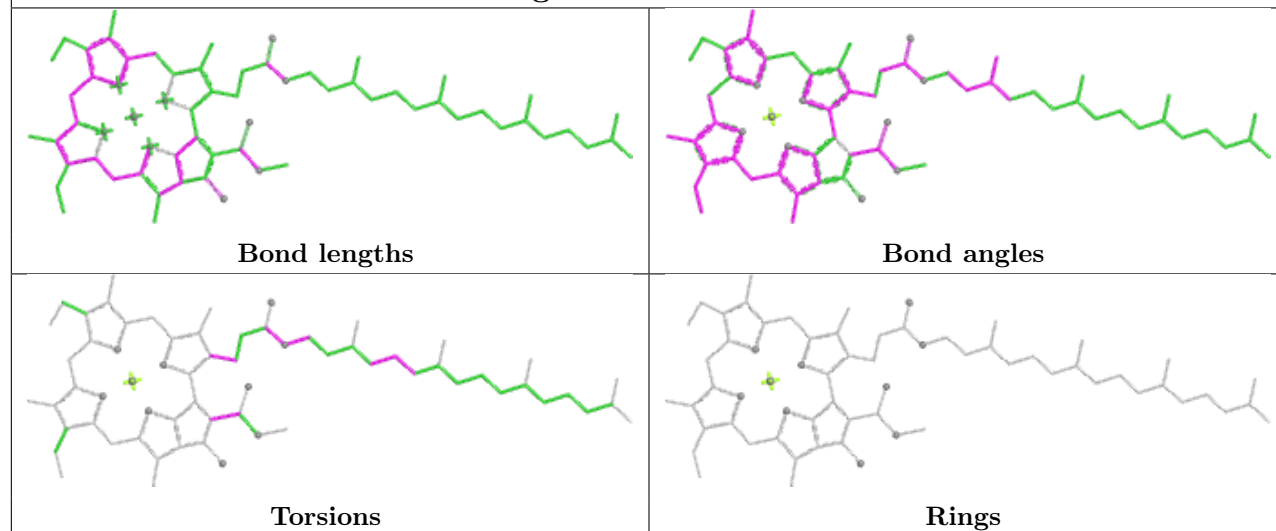


Ligand CLA C 506	
	
Bond lengths	Bond angles
	
Torsions	Rings

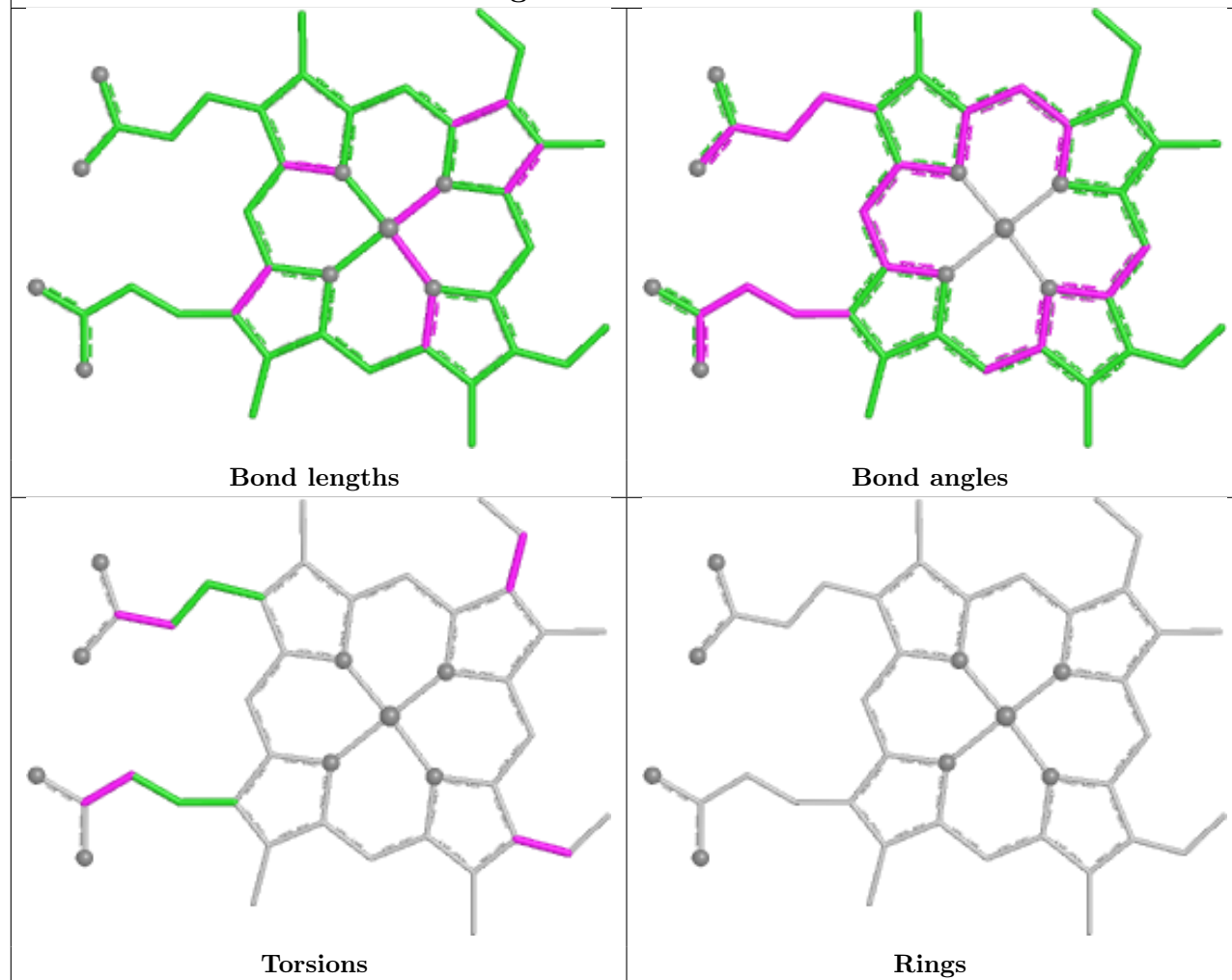
Ligand PHO A 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

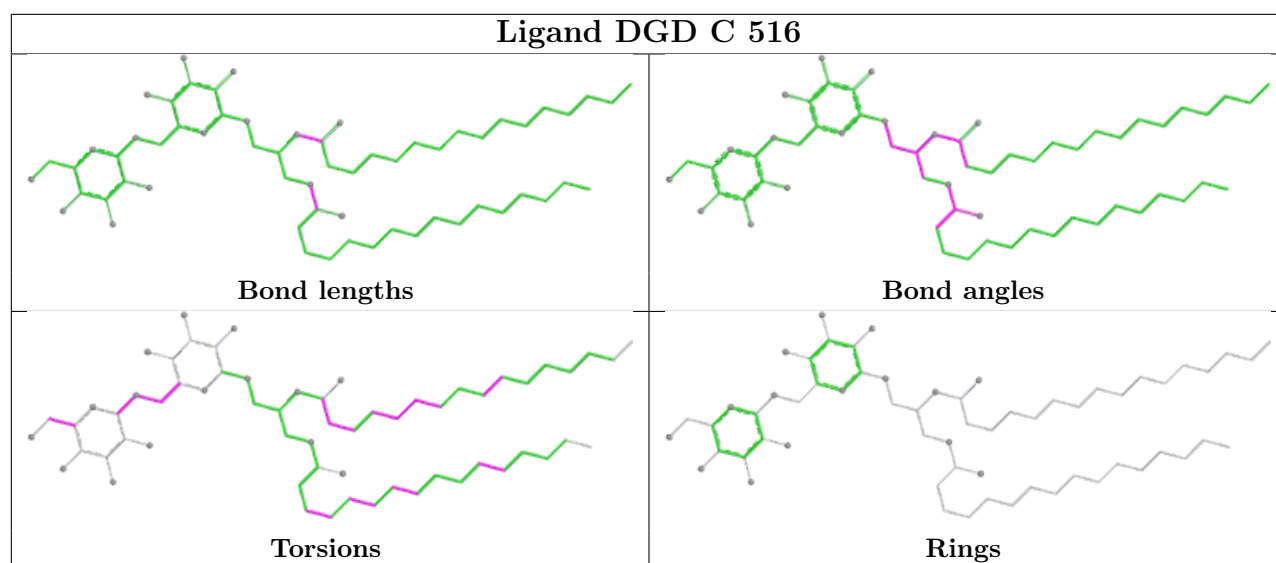
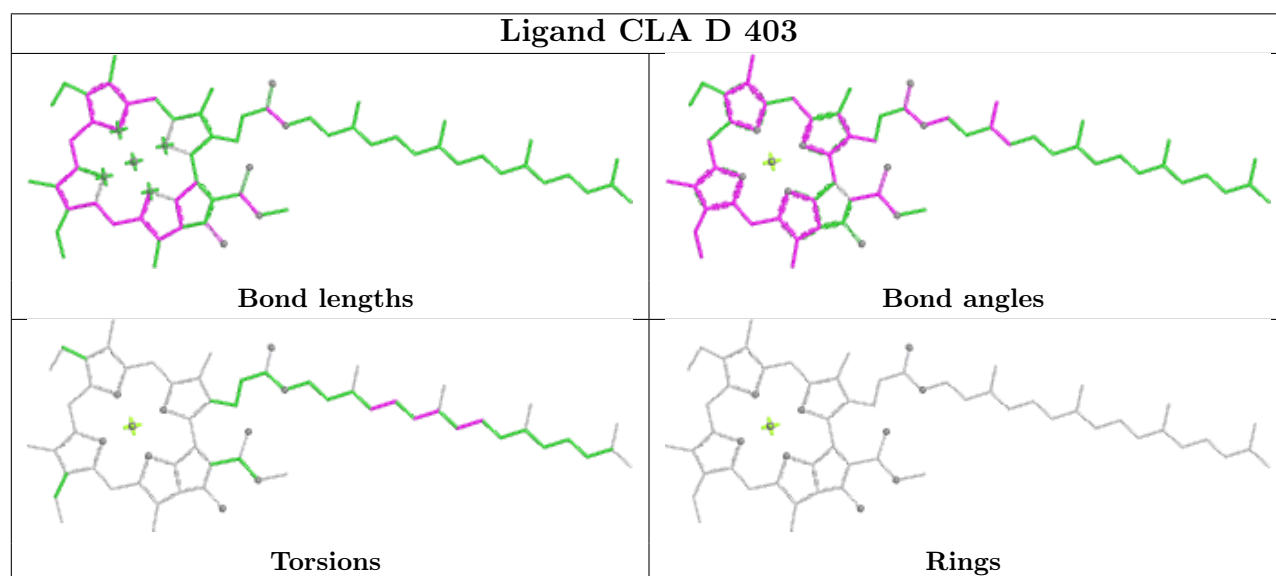
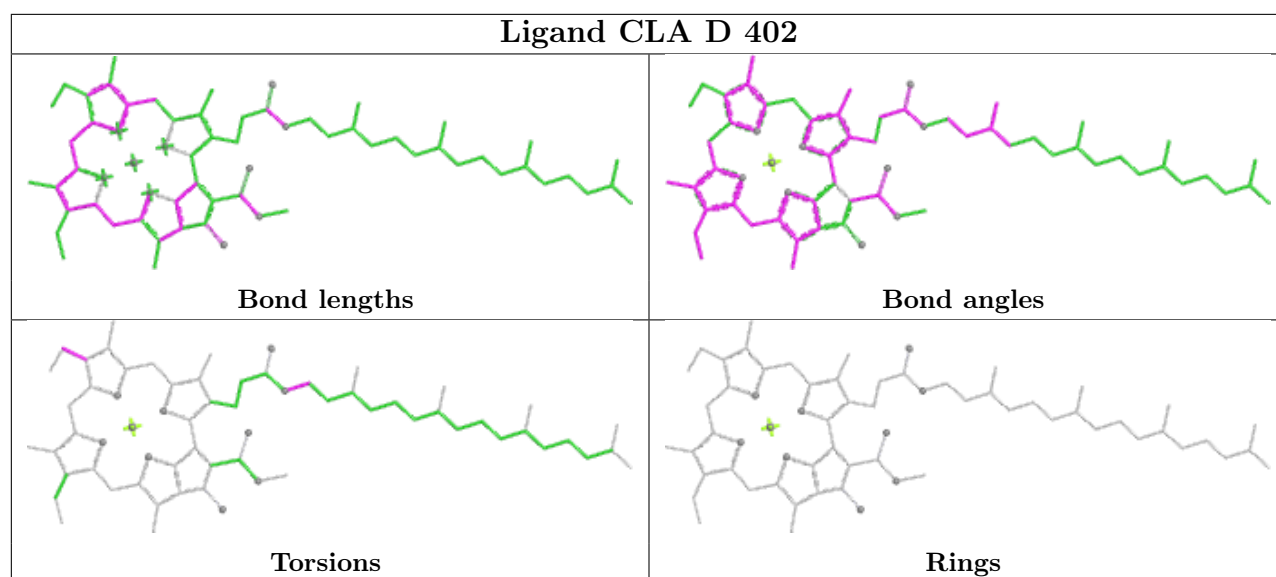
Ligand BCR K 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

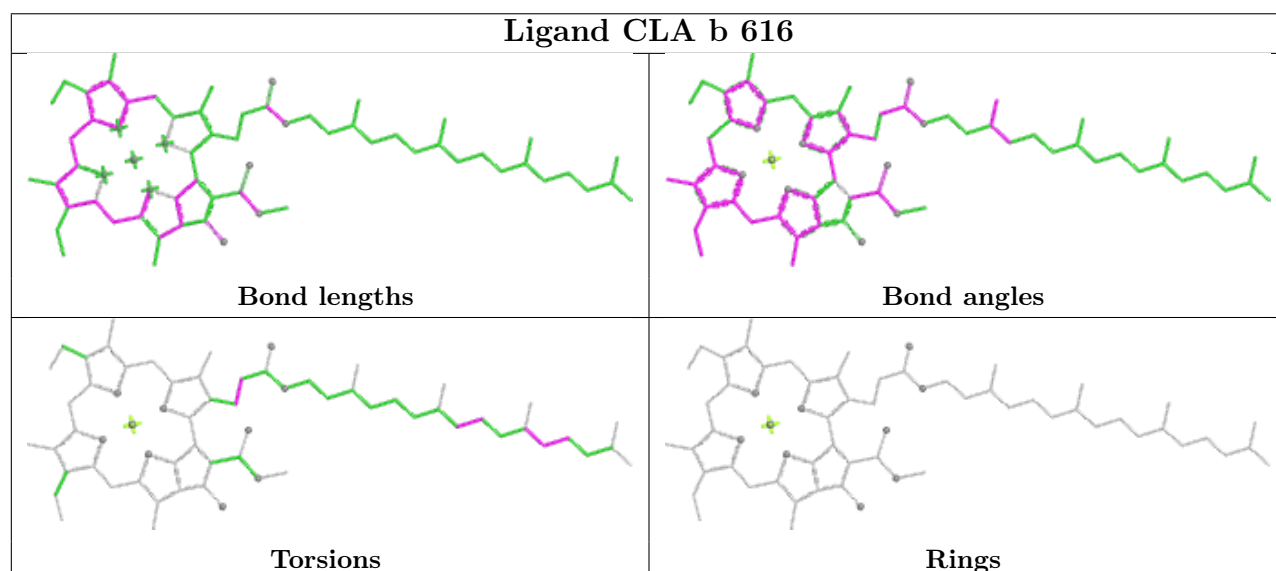
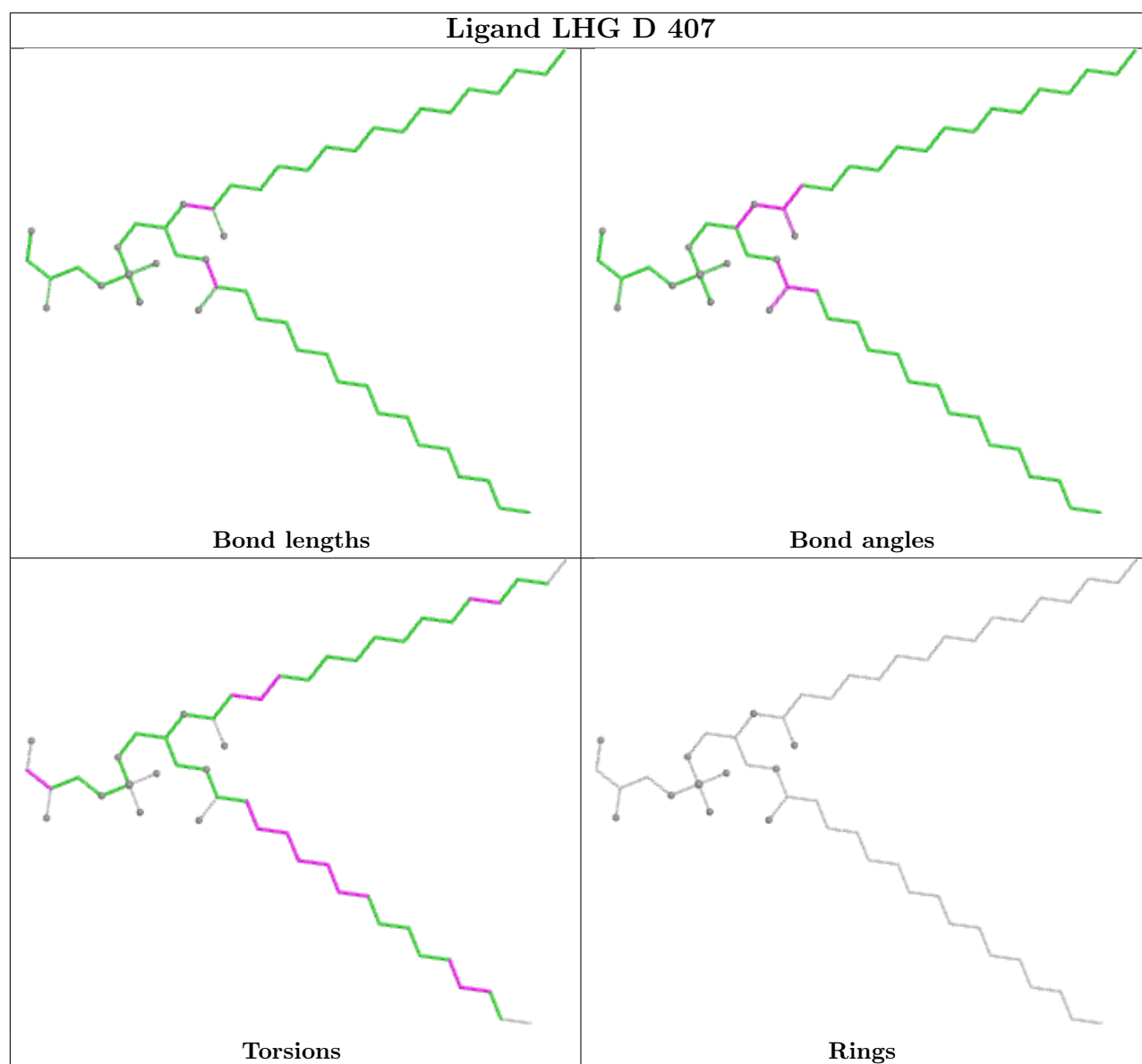
Ligand CLA C 513



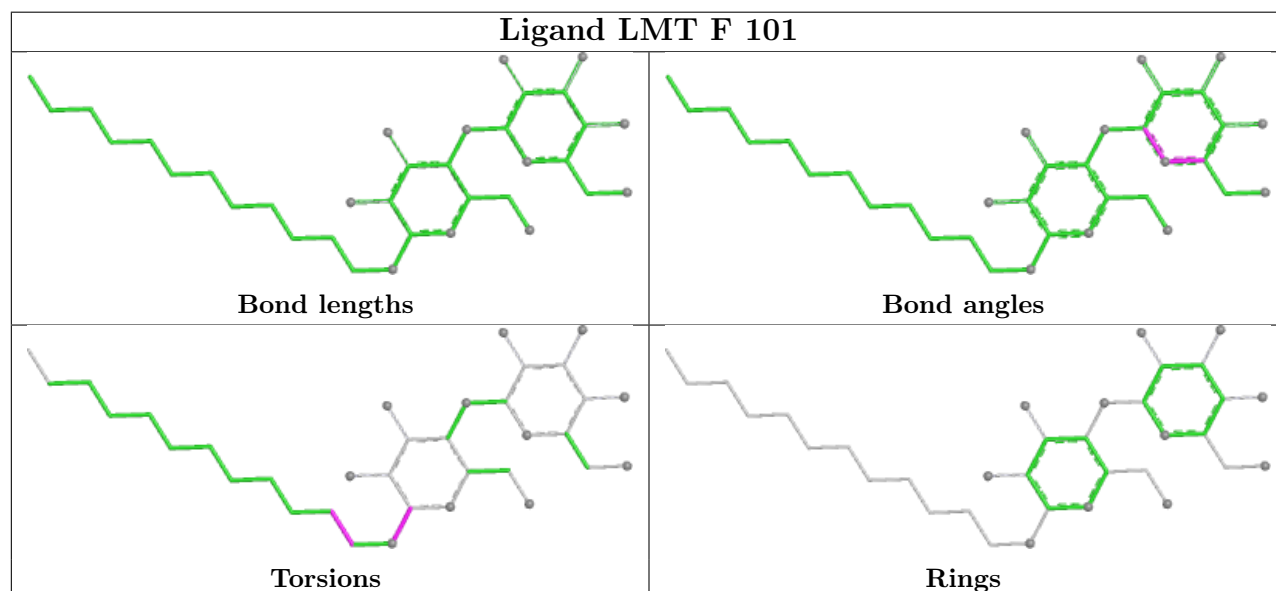
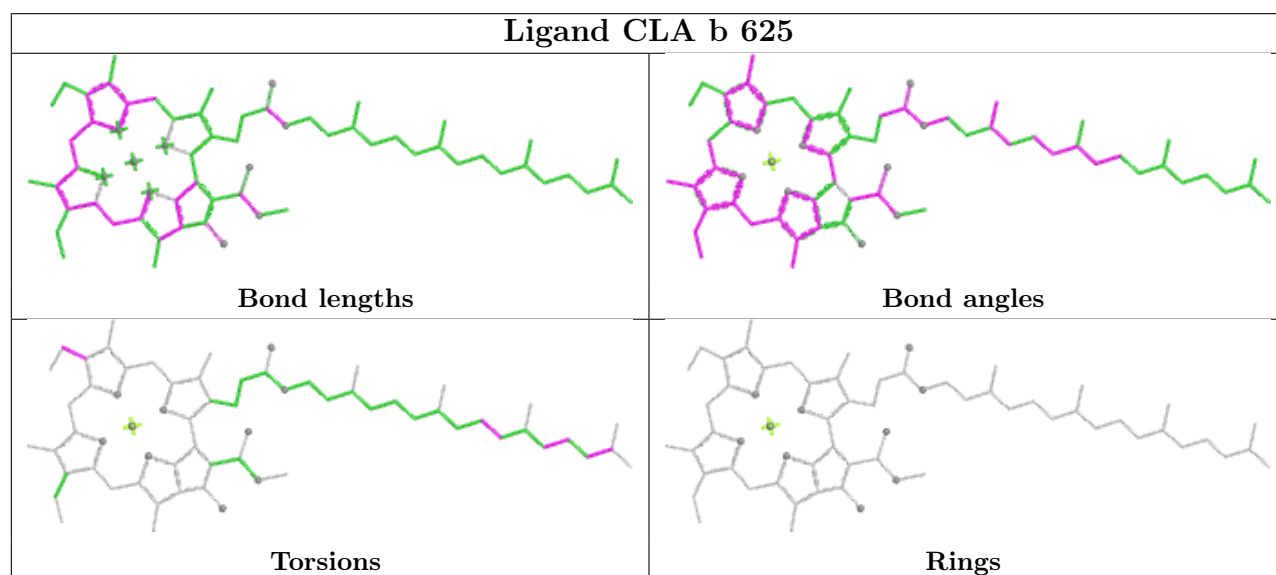
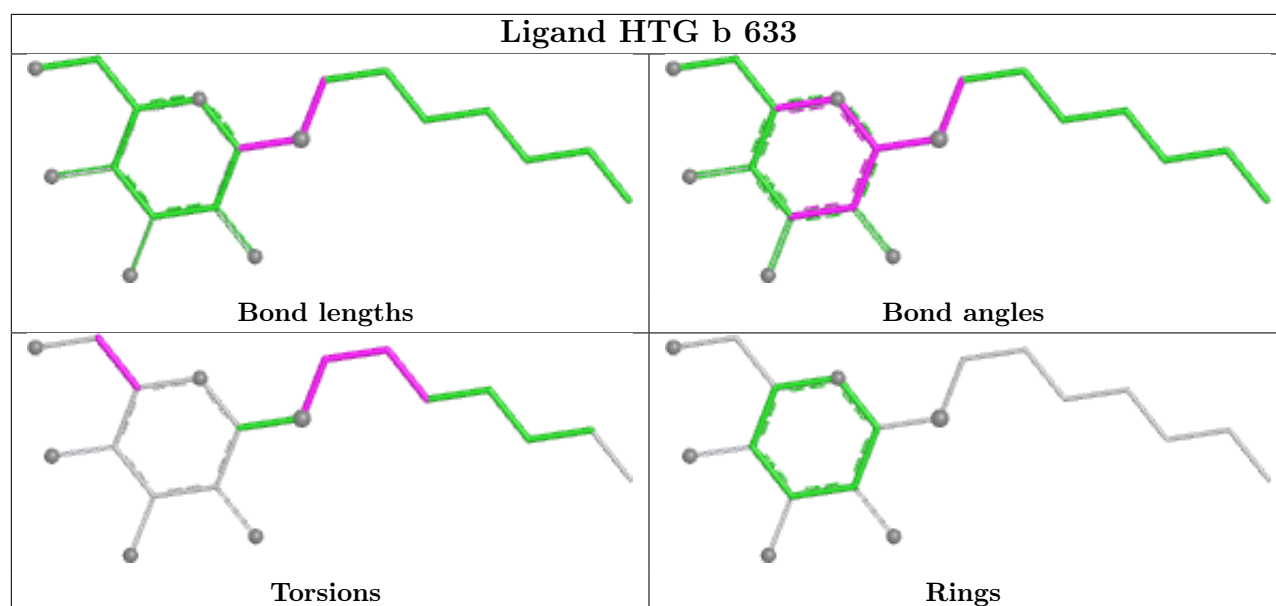
Ligand HEM F 102

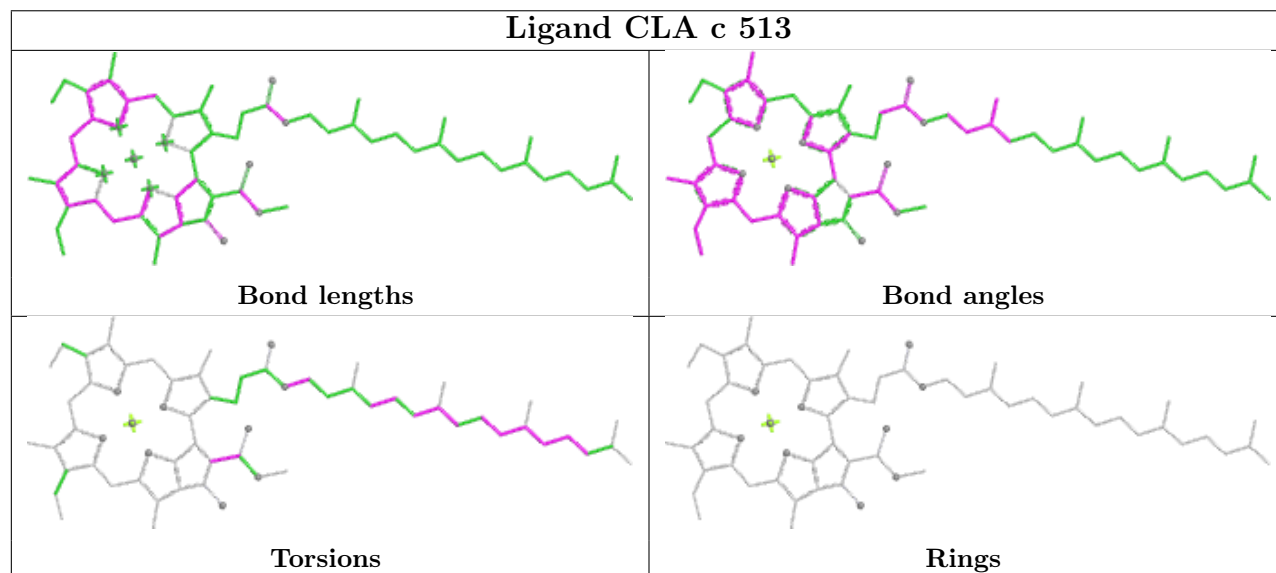
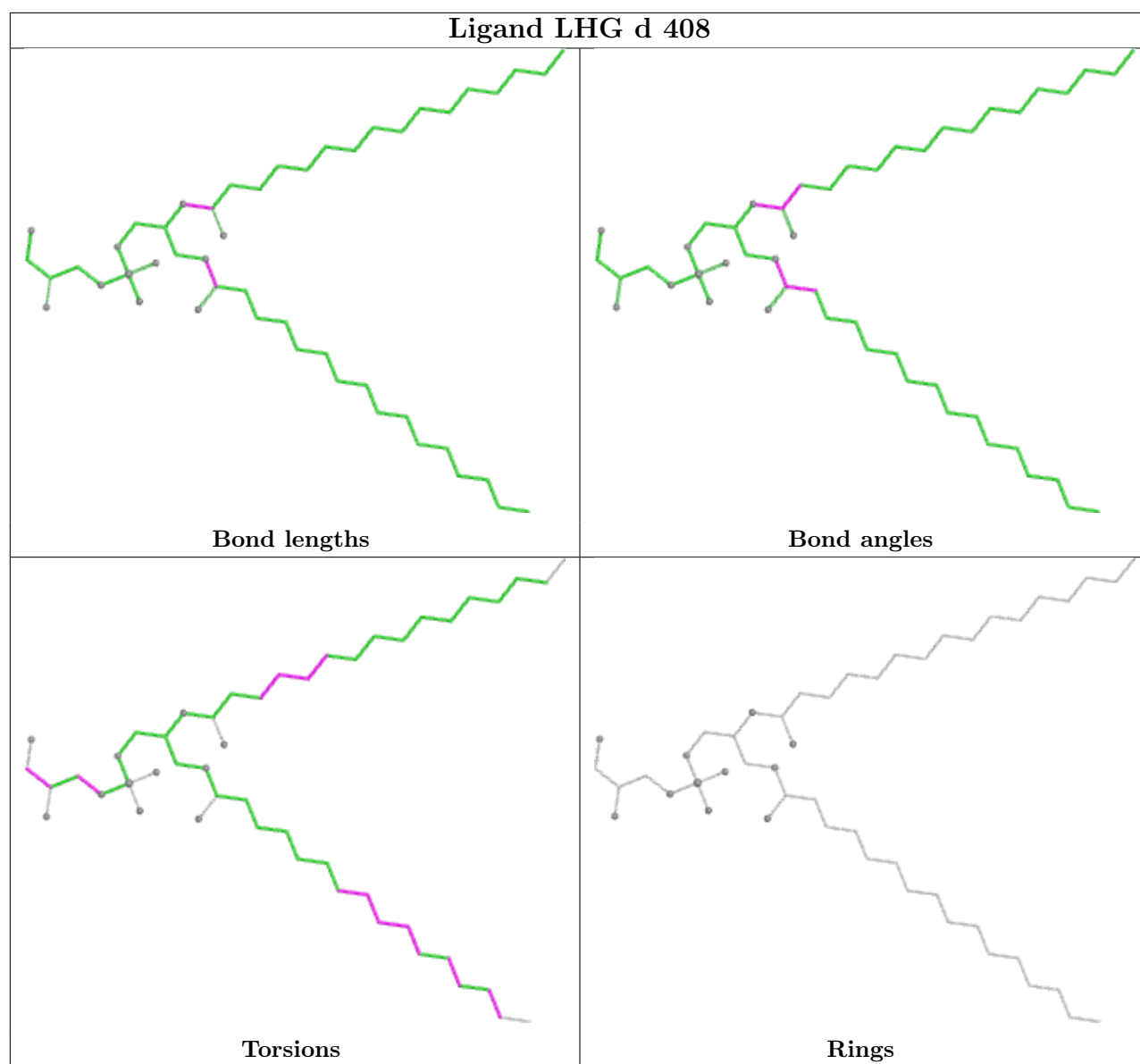


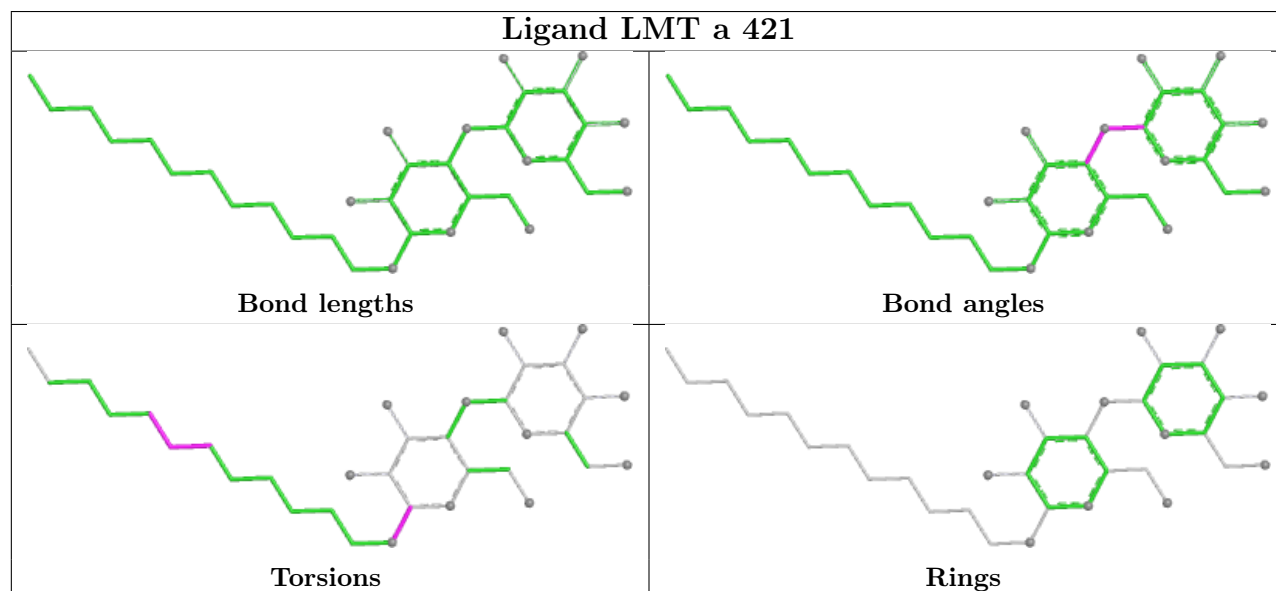
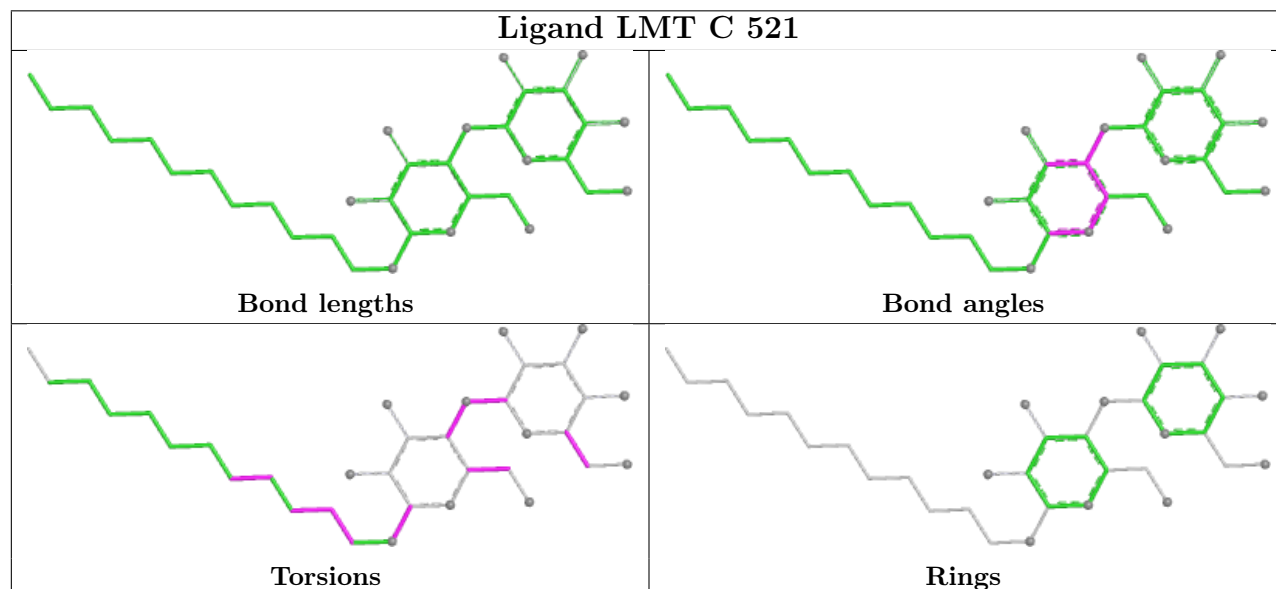
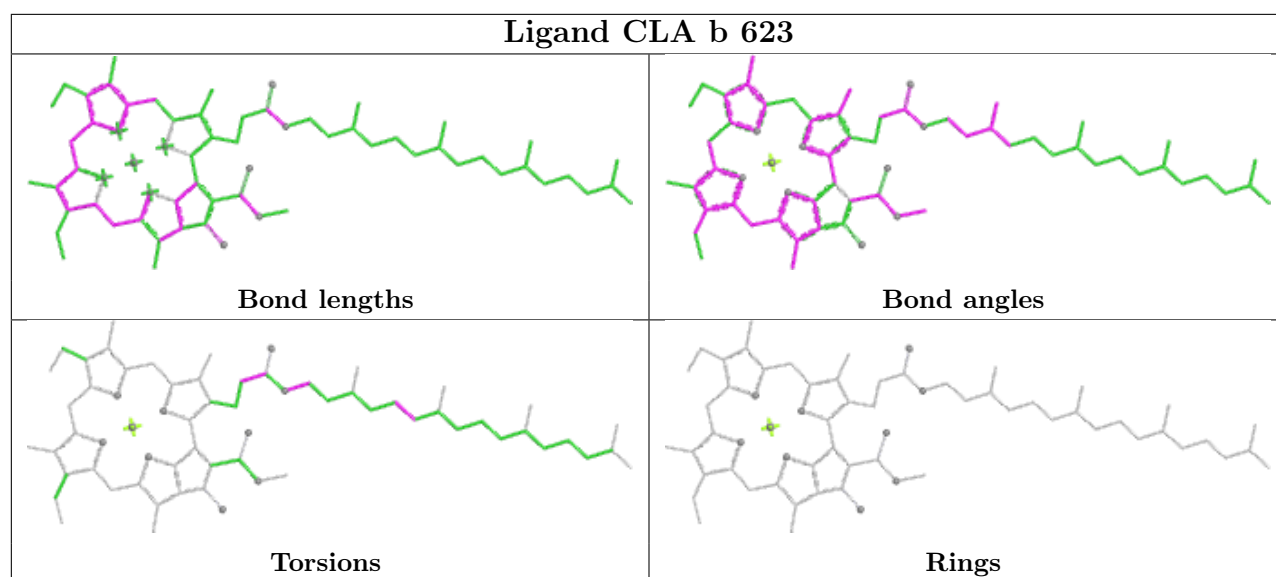


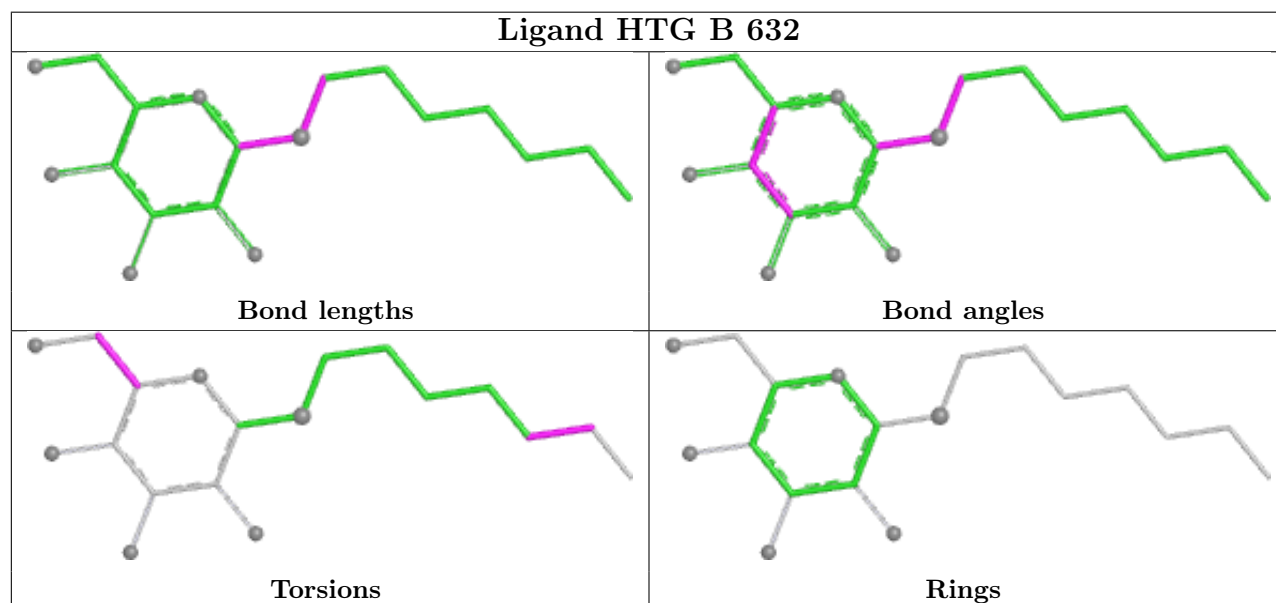
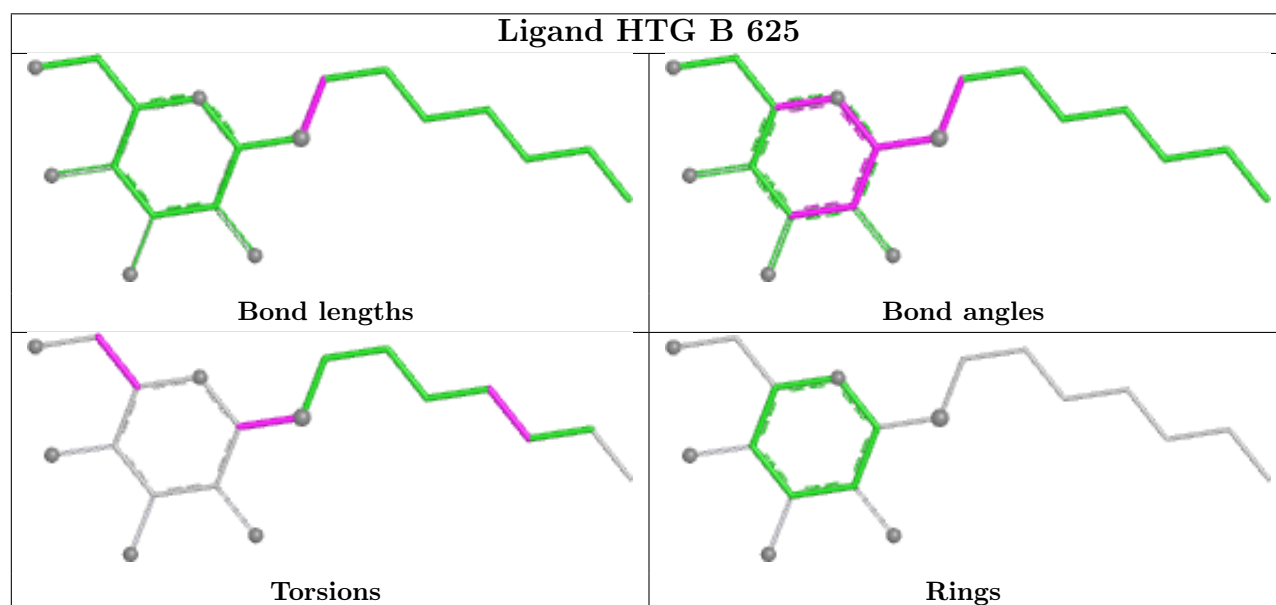
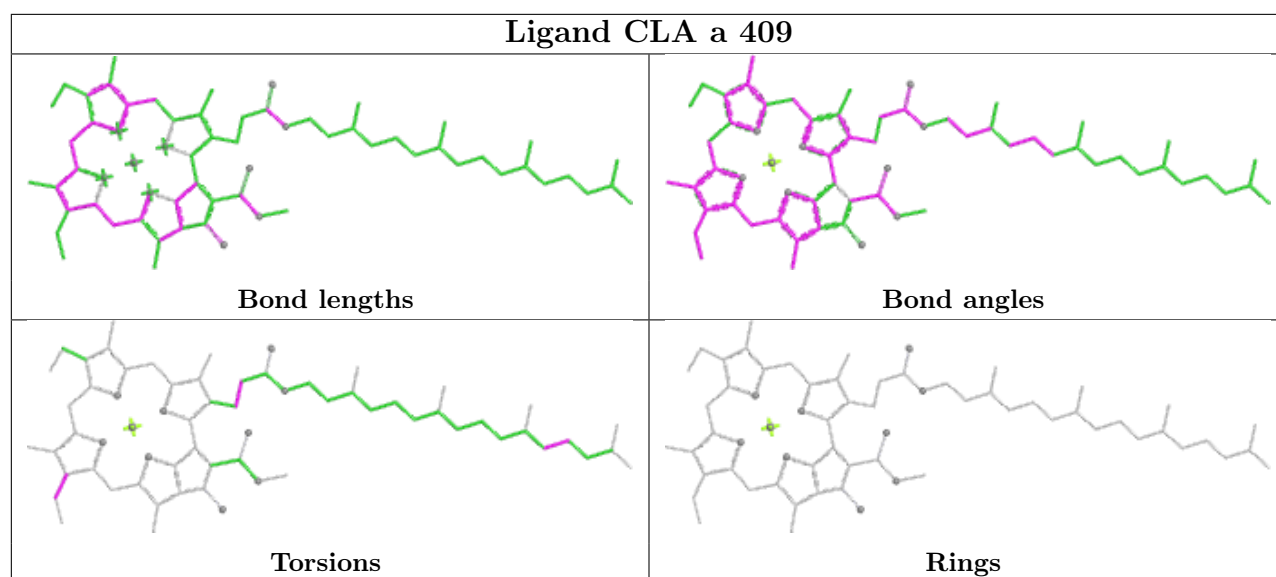


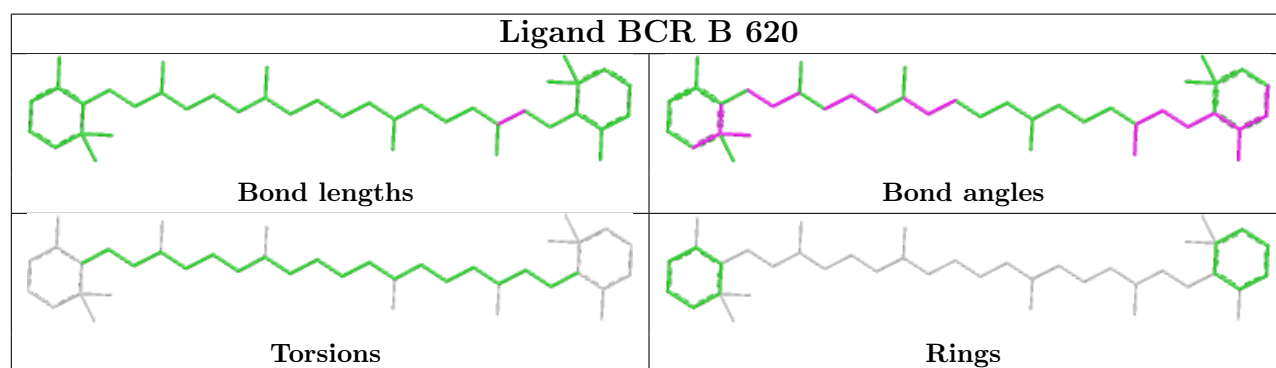
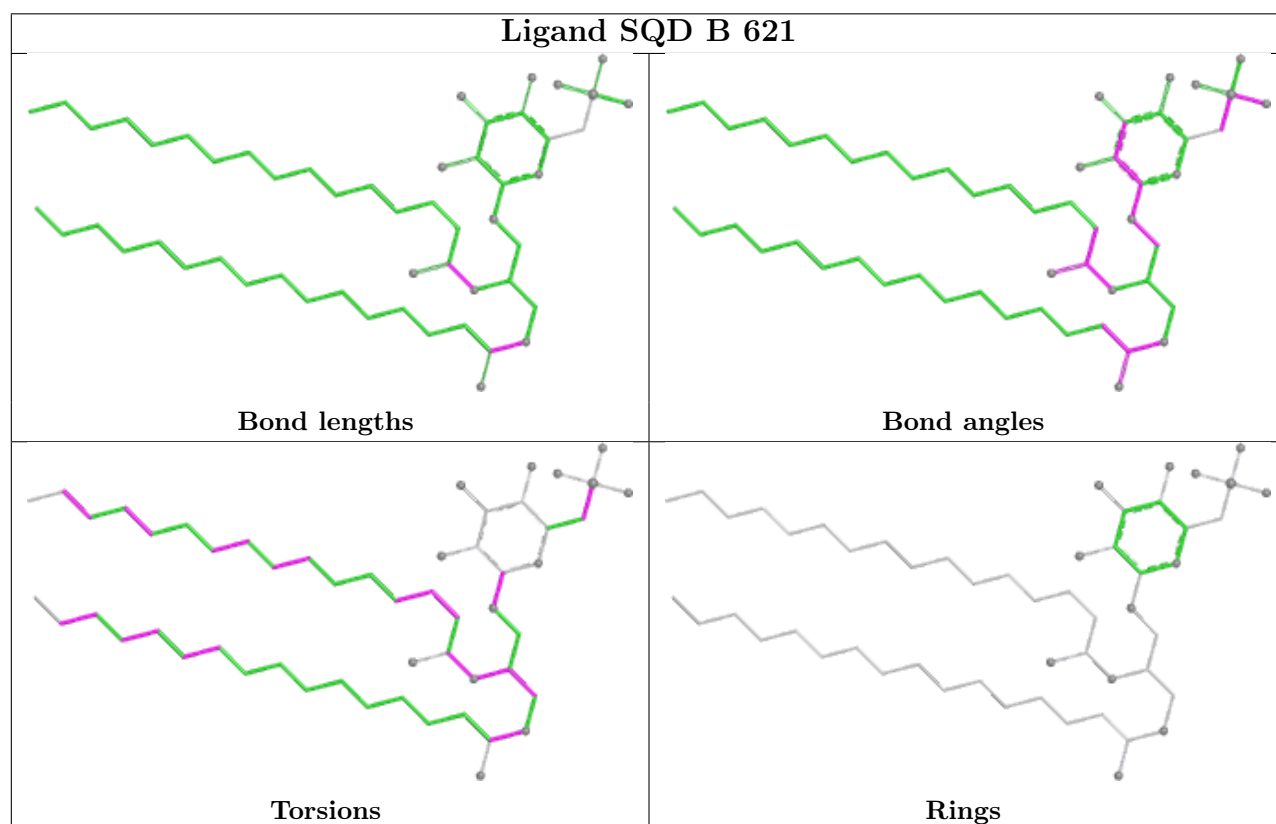
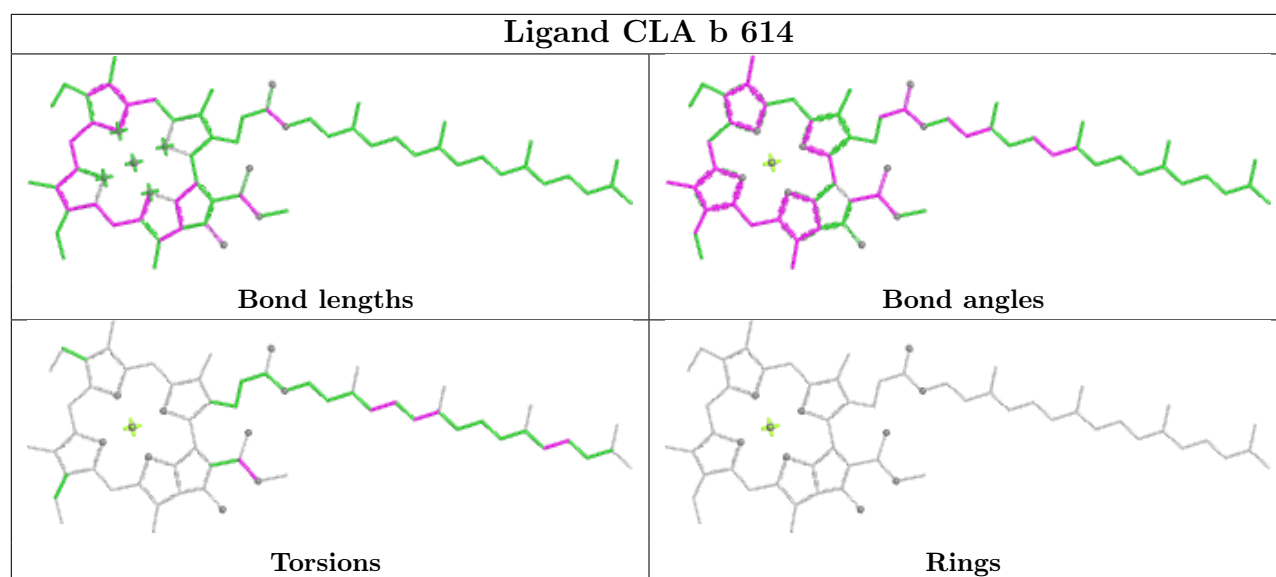
Ligand PHO a 420 (B)	
Bond lengths	Bond angles
Torsions	Rings
Ligand BCR T 103	
Bond lengths	Bond angles
Torsions	Rings
Ligand BCR C 515	
Bond lengths	Bond angles
Torsions	Rings

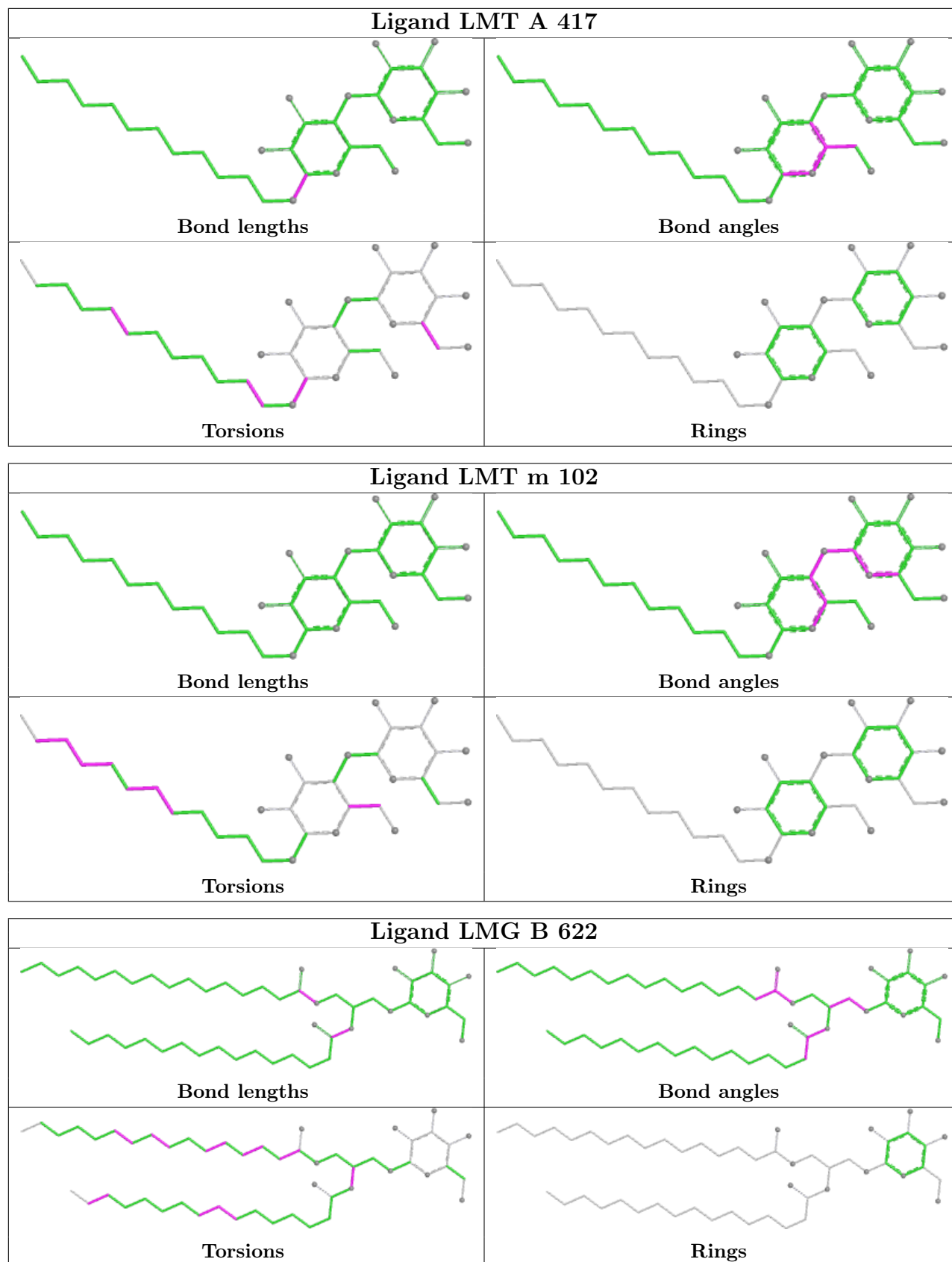


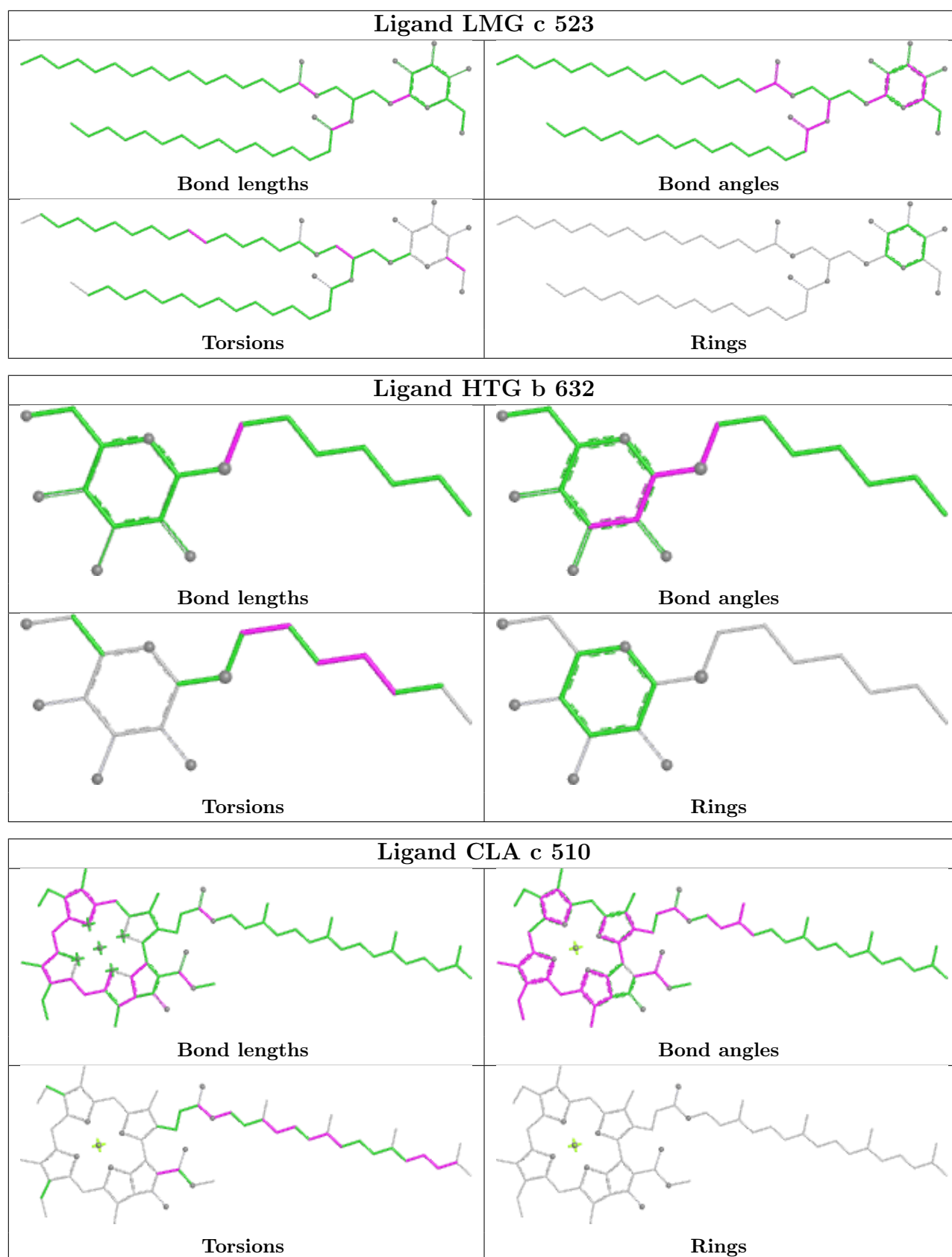


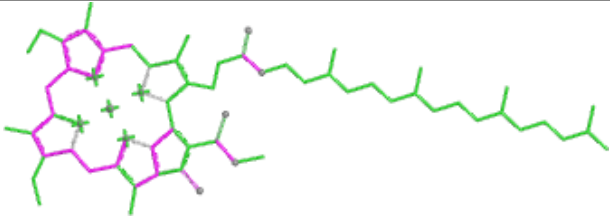
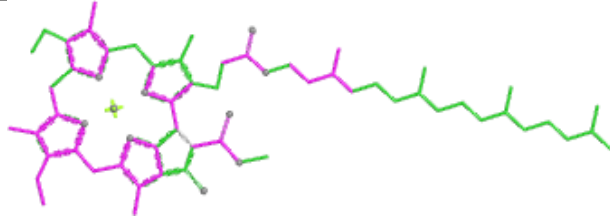
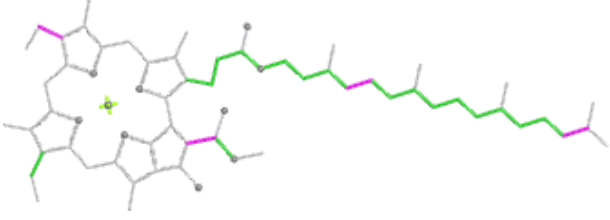
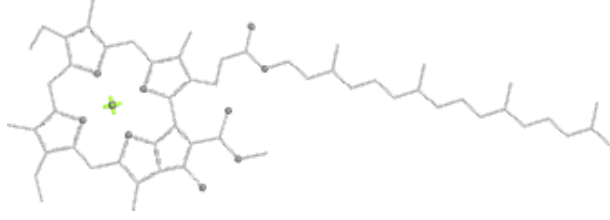
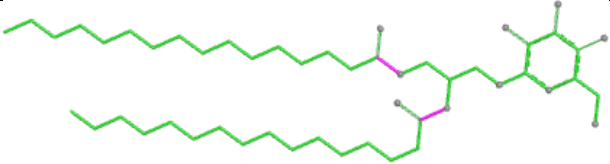
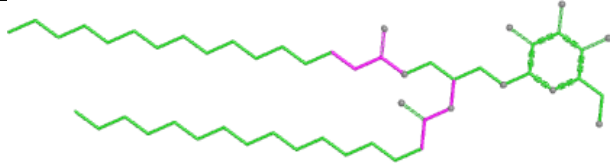
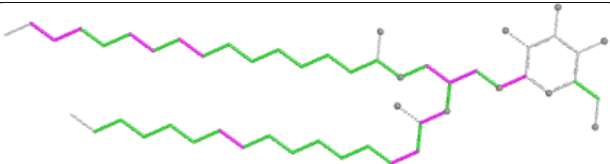
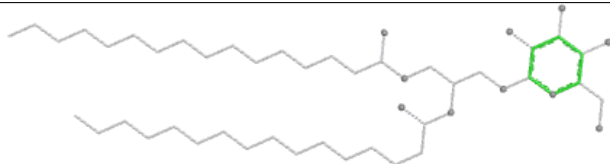
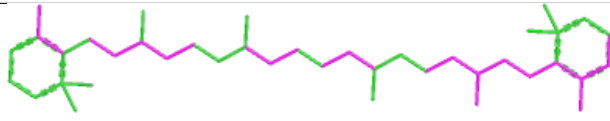
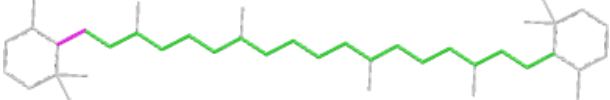
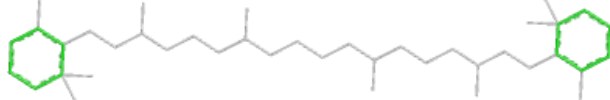




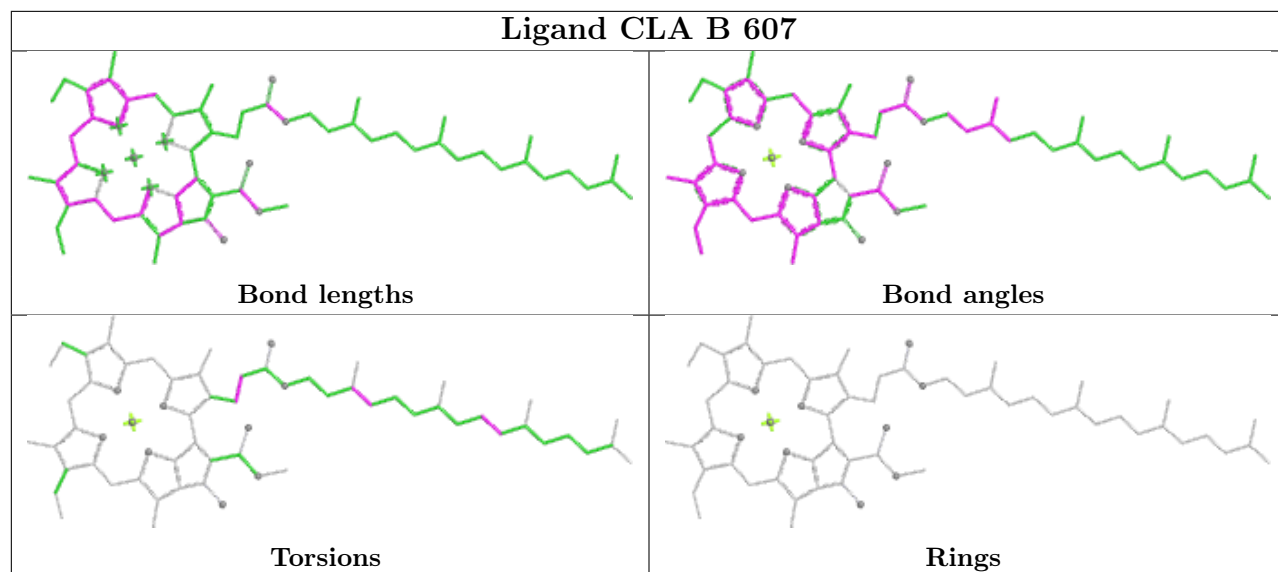




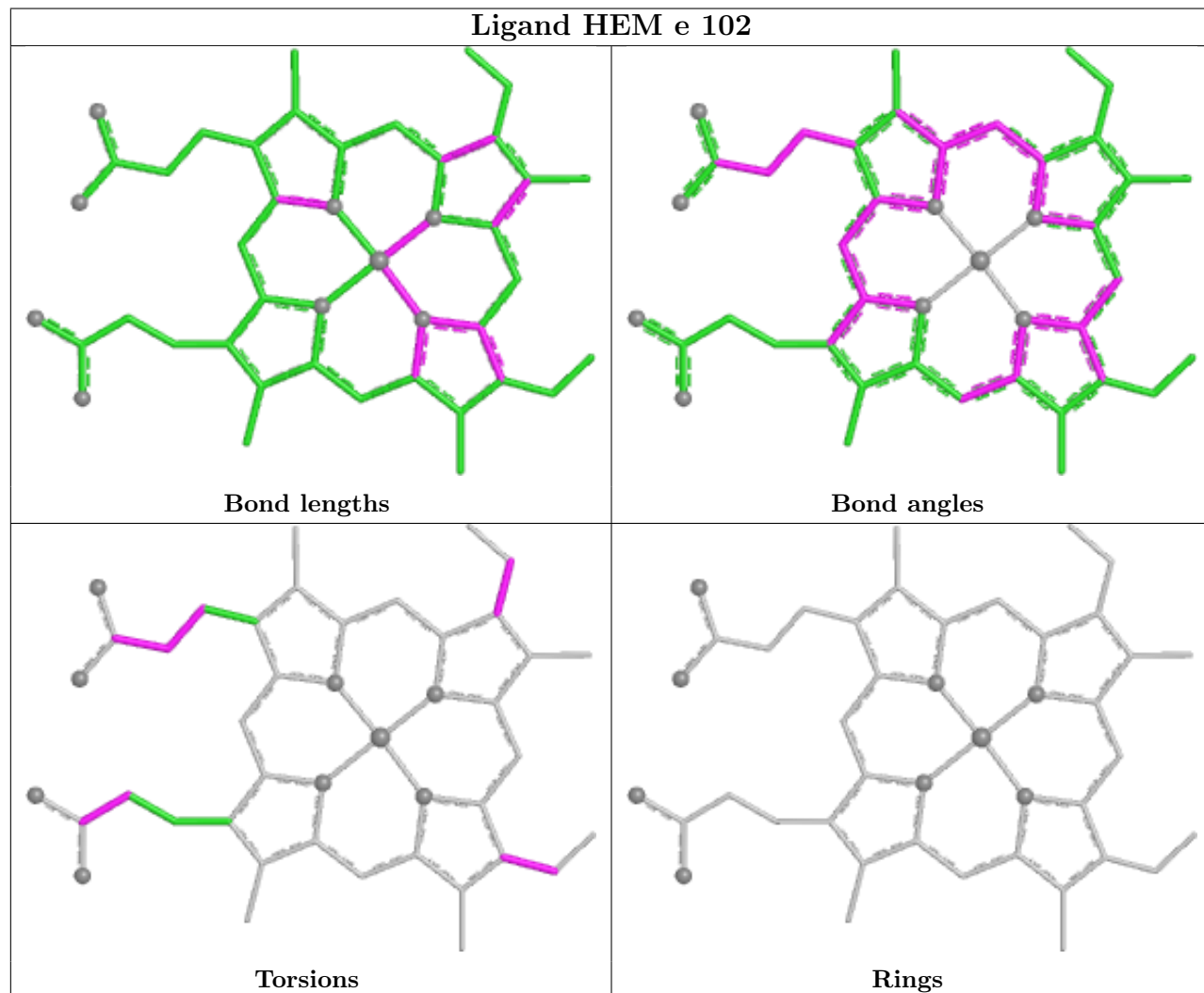


Ligand CLA C 502	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG c 522	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR C 514	
 Bond lengths	 Bond angles
 Torsions	 Rings

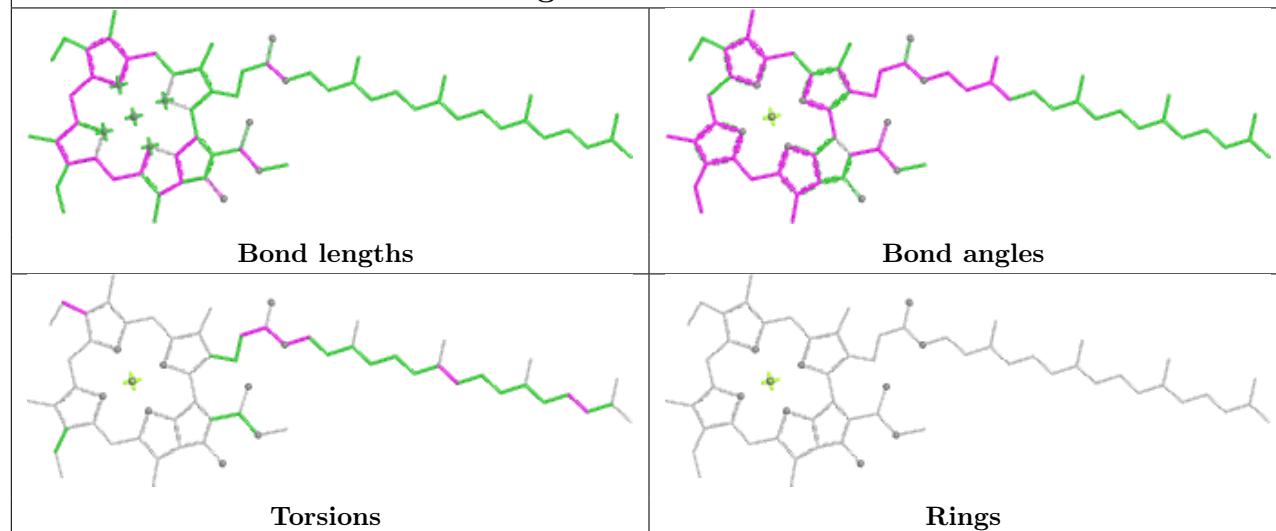
Ligand CLA B 607



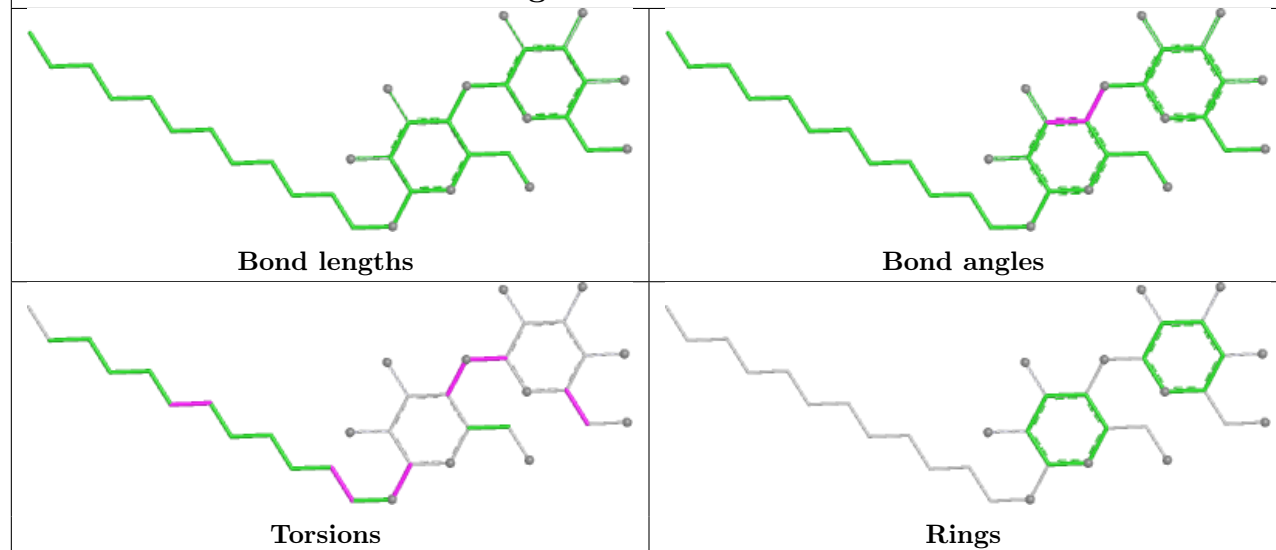
Ligand HEM e 102



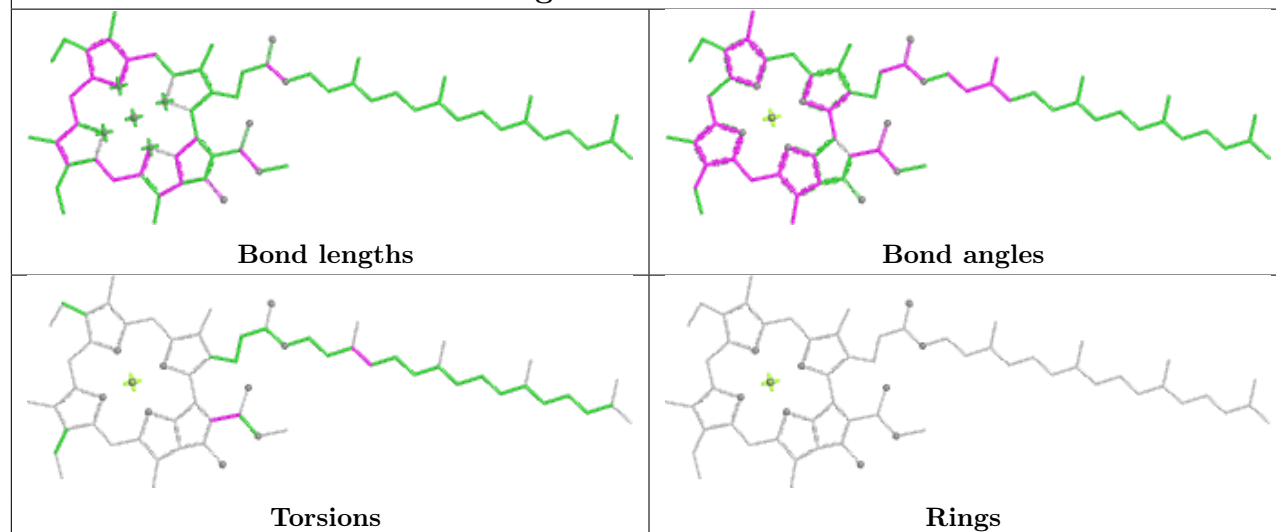
Ligand CLA c 516

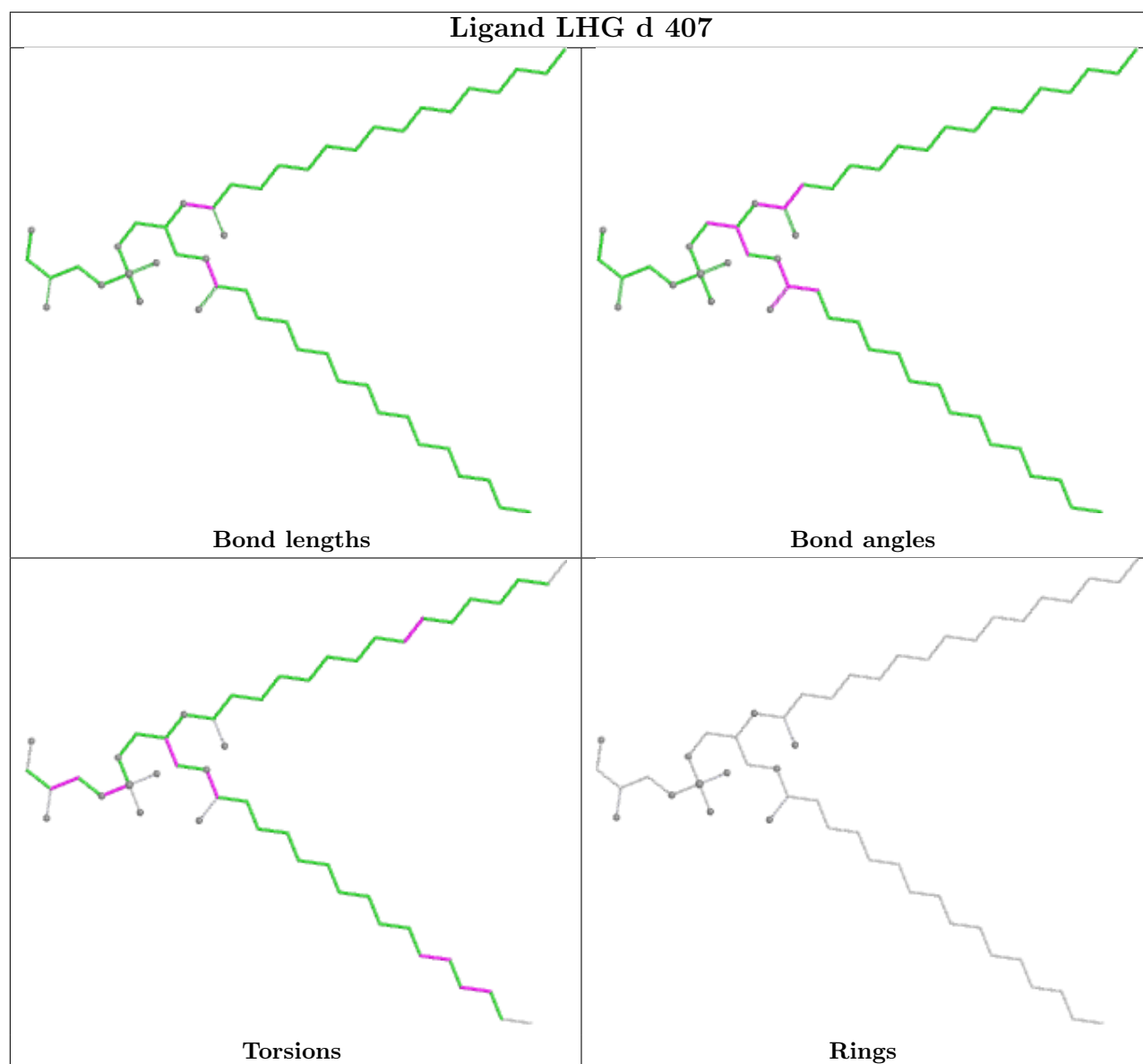
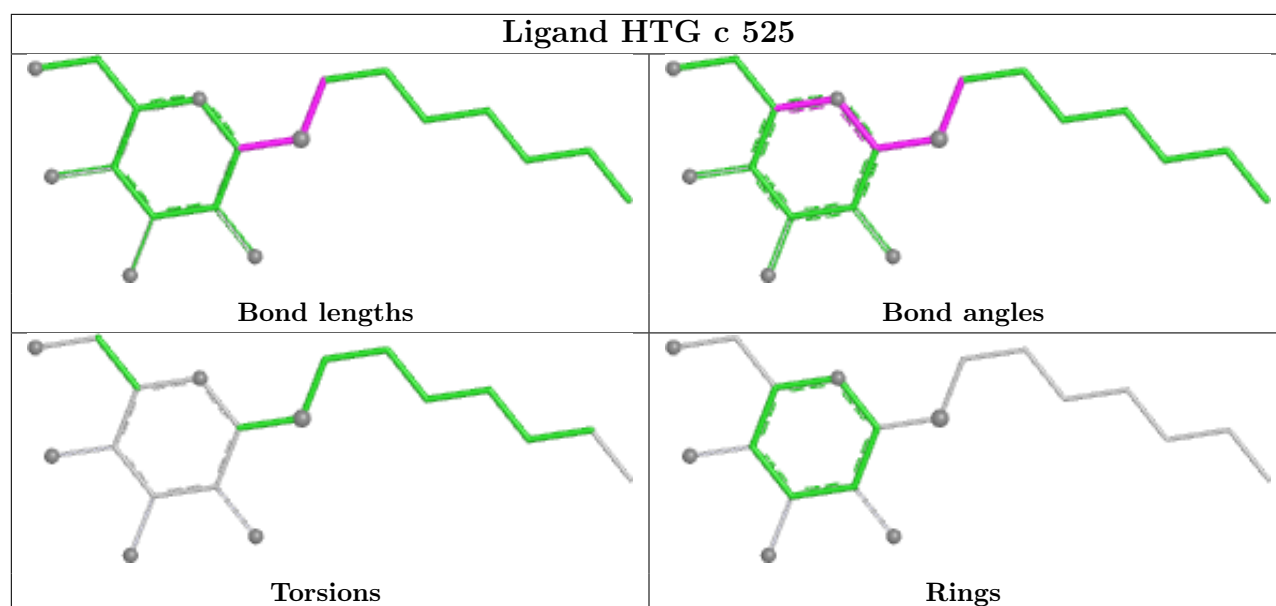


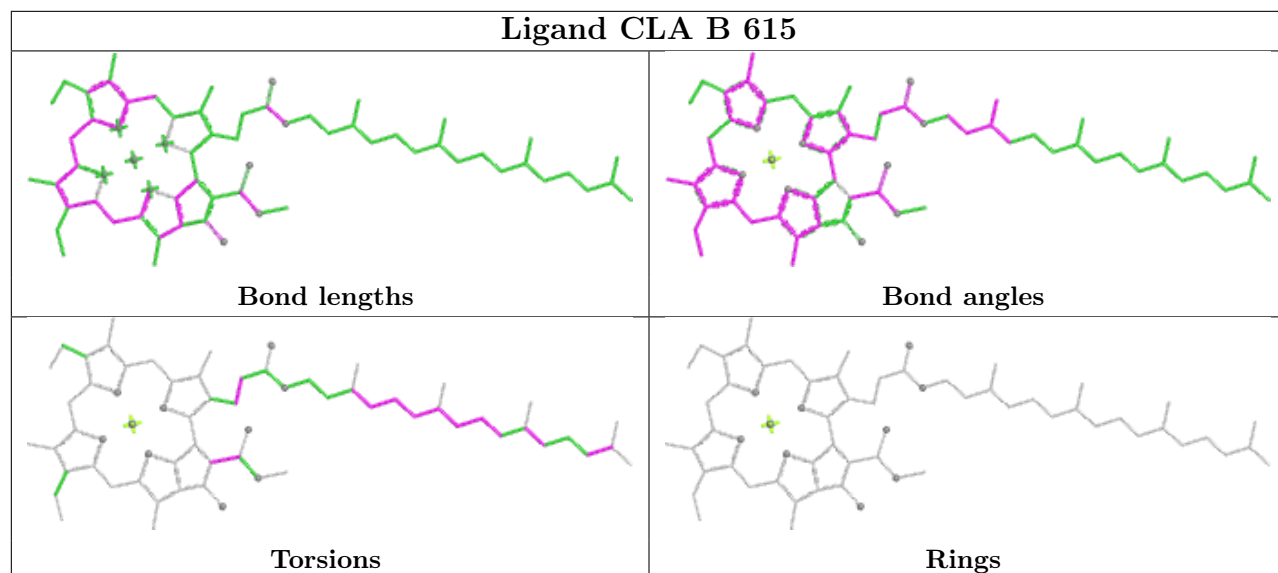
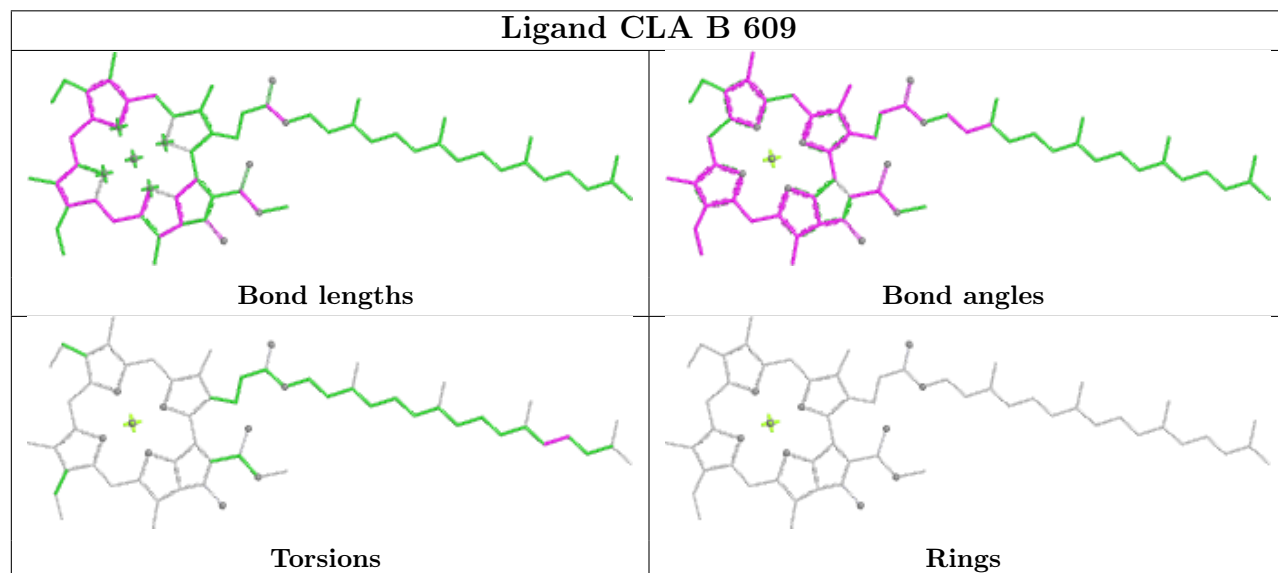
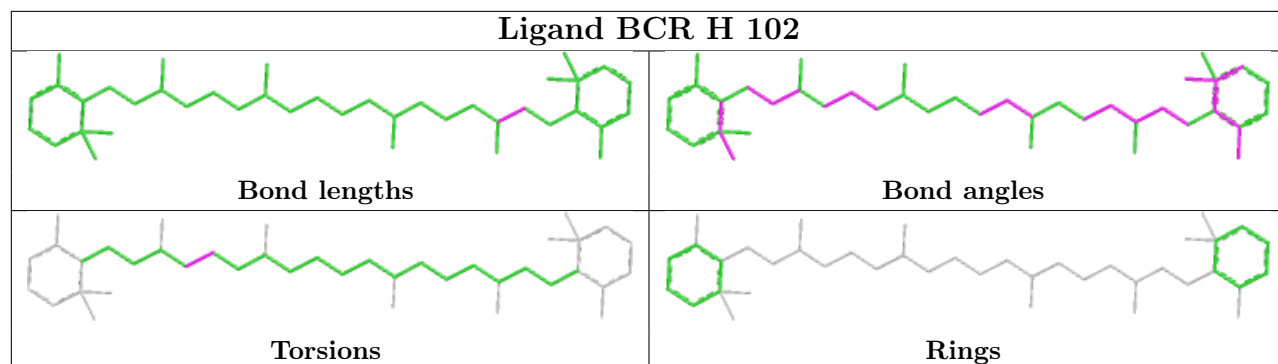
Ligand LMT D 401

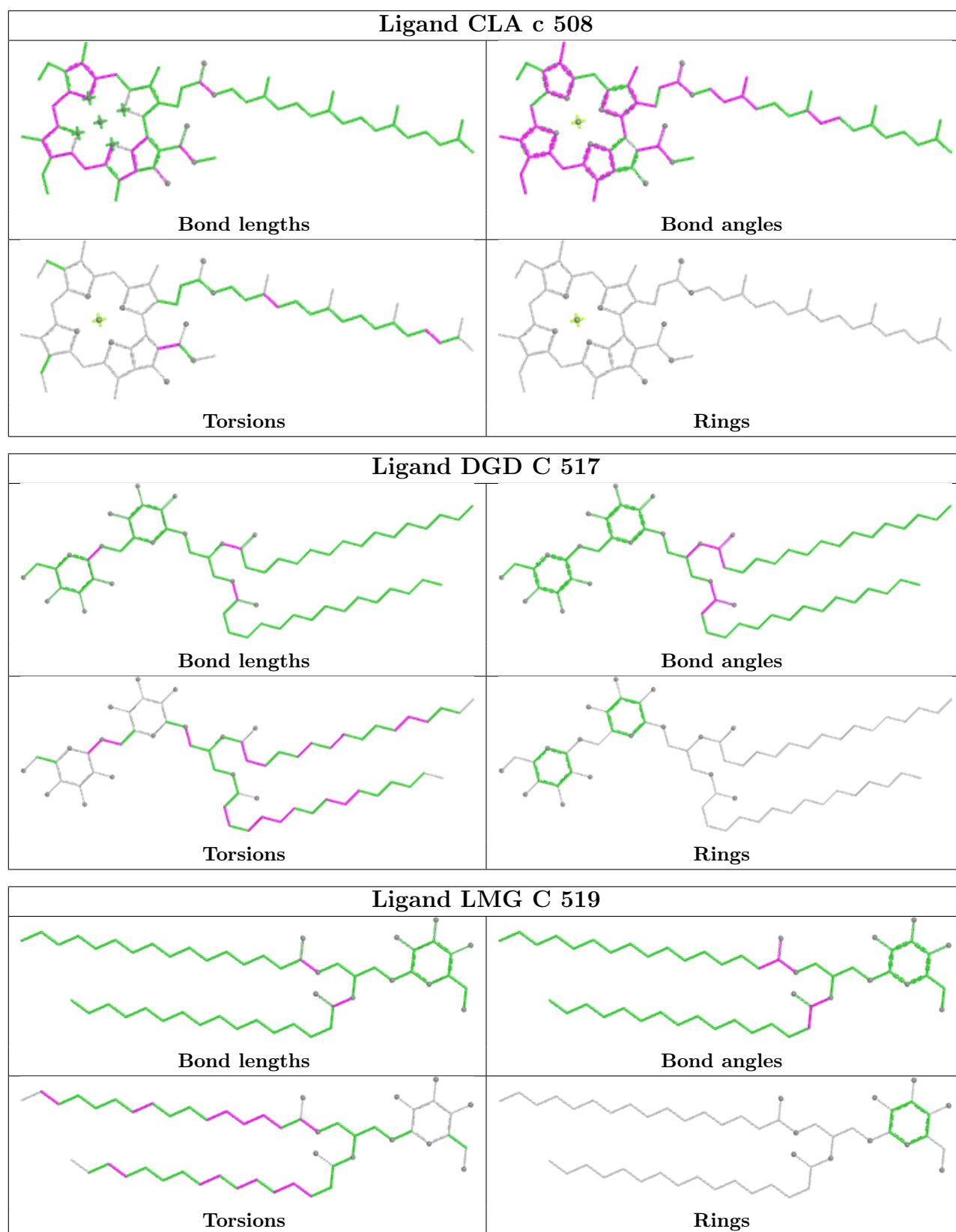


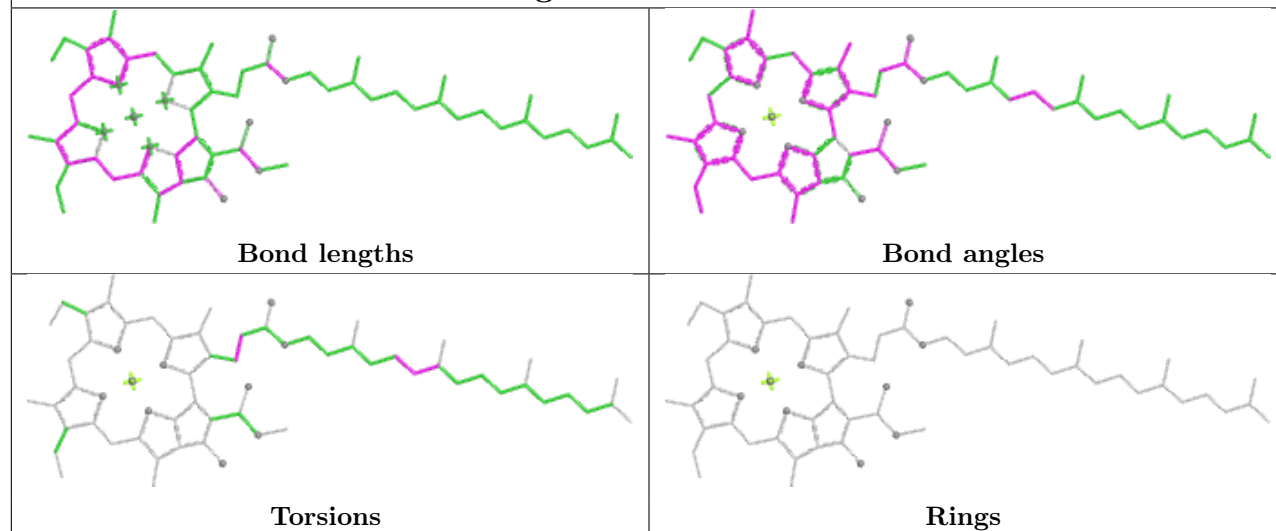
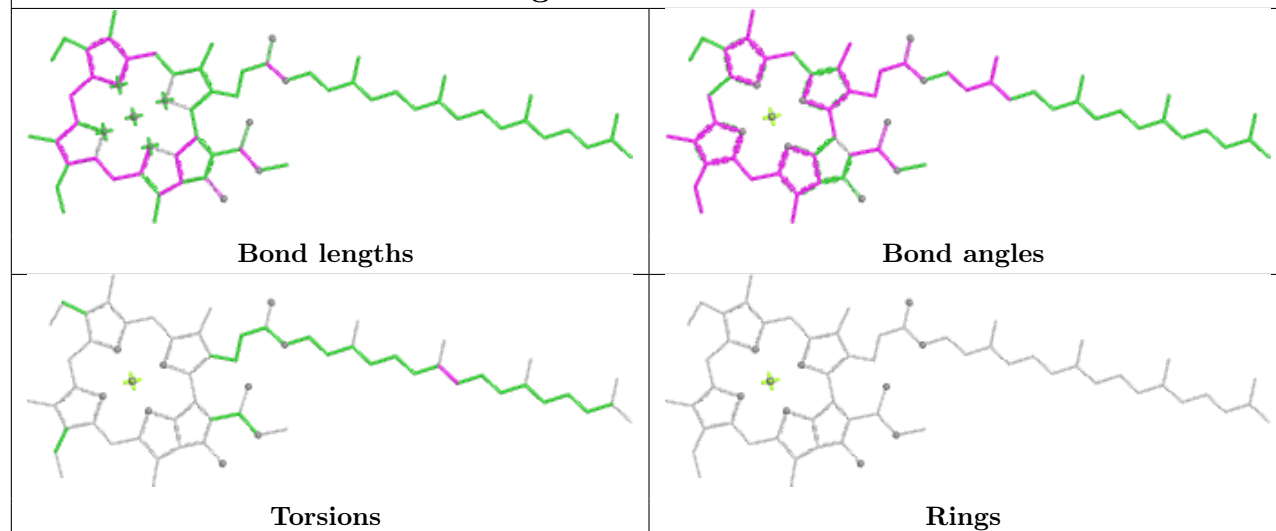
Ligand CLA b 615

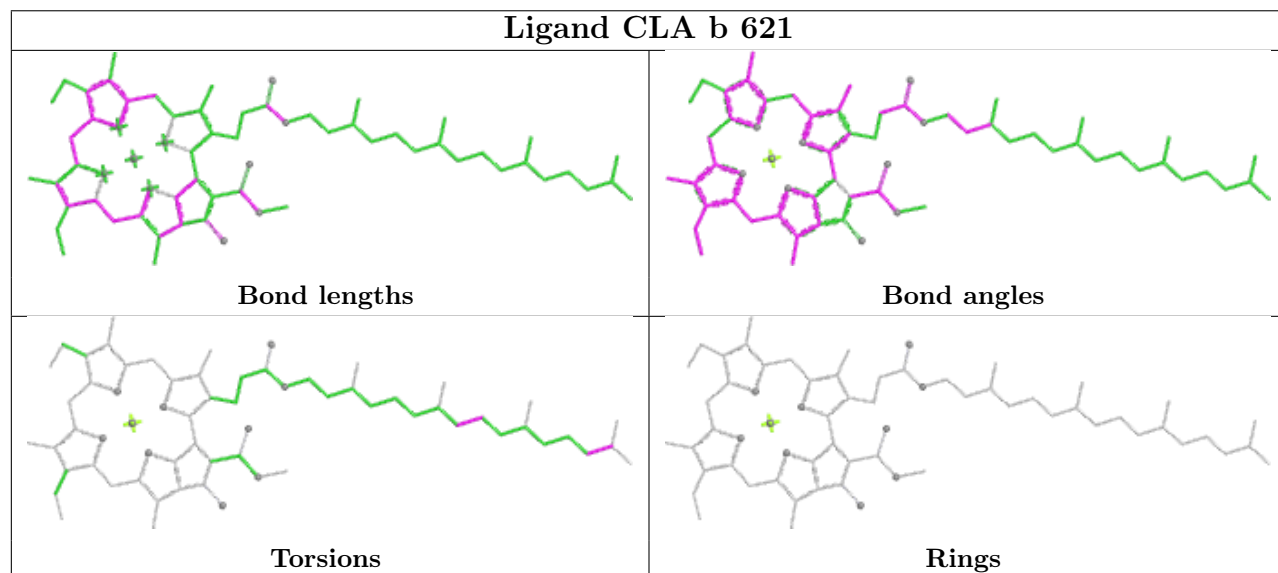
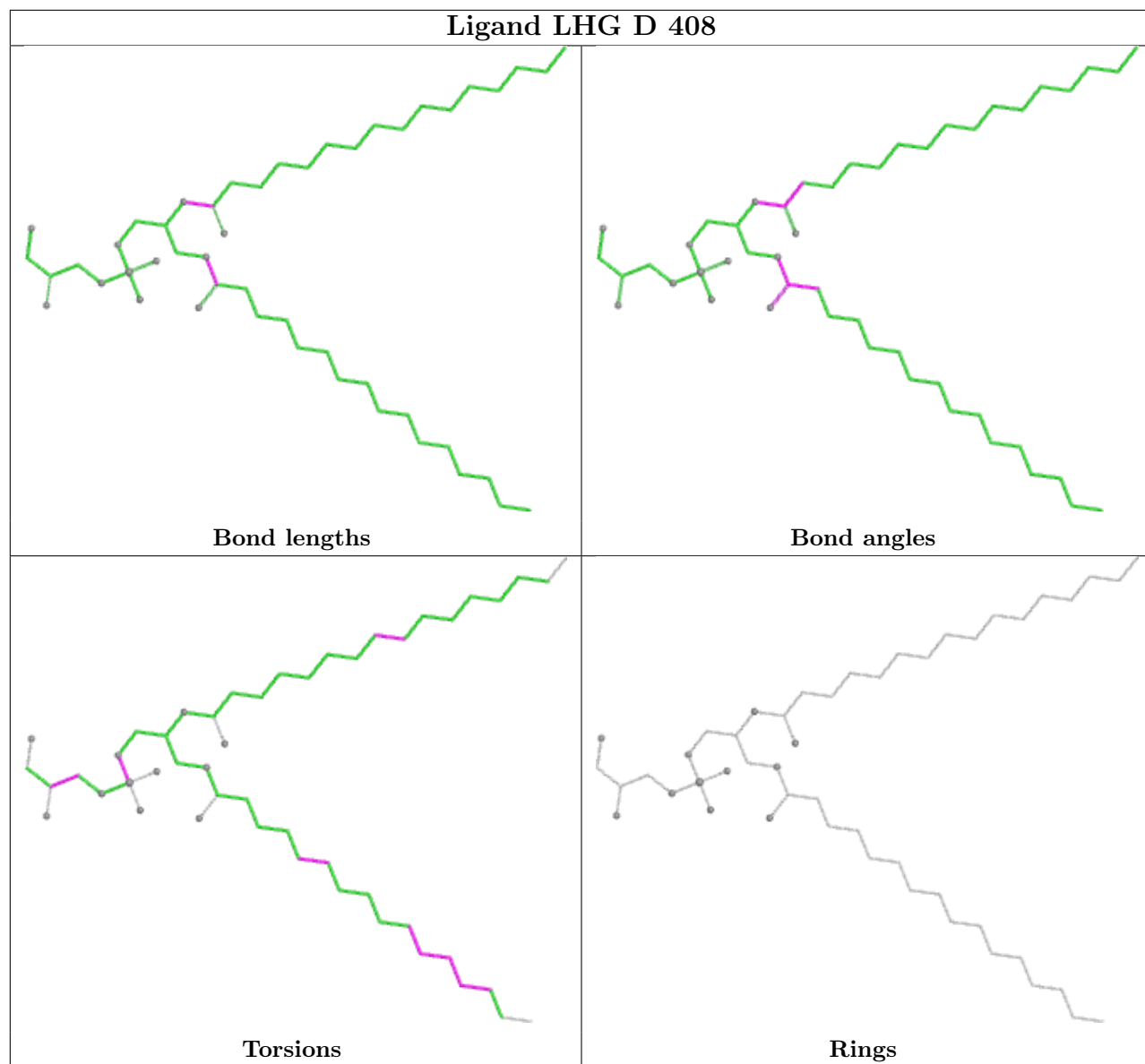




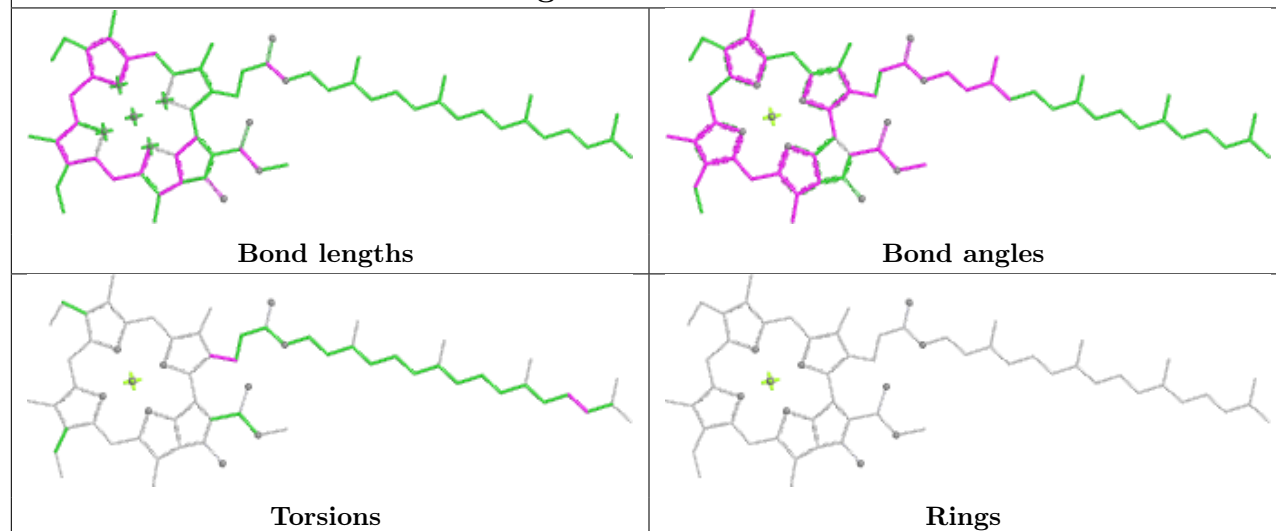




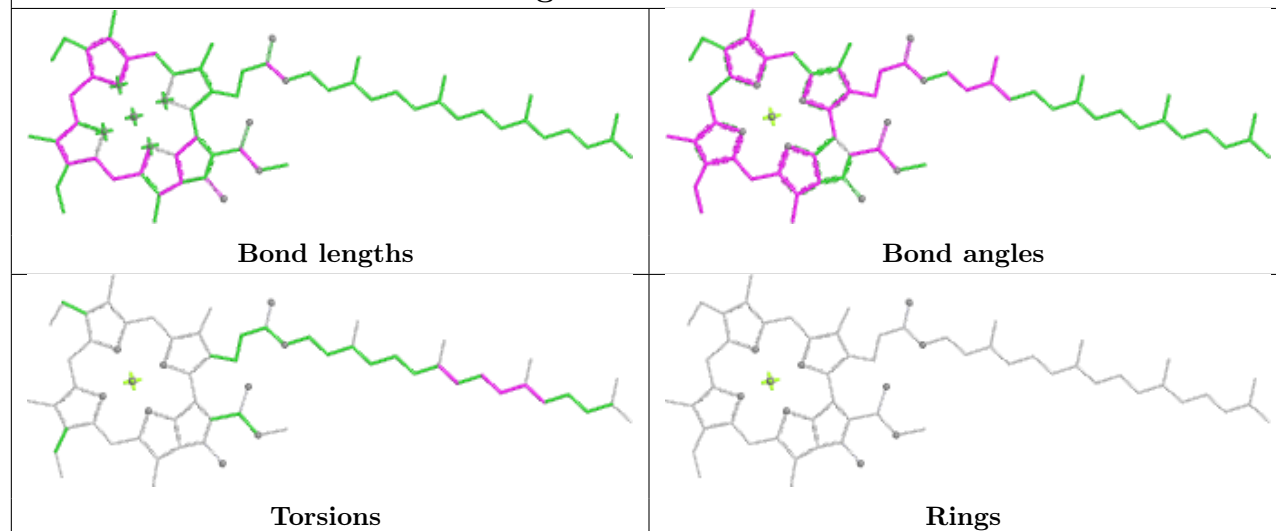
Ligand CLA b 613**Ligand CLA A 407**



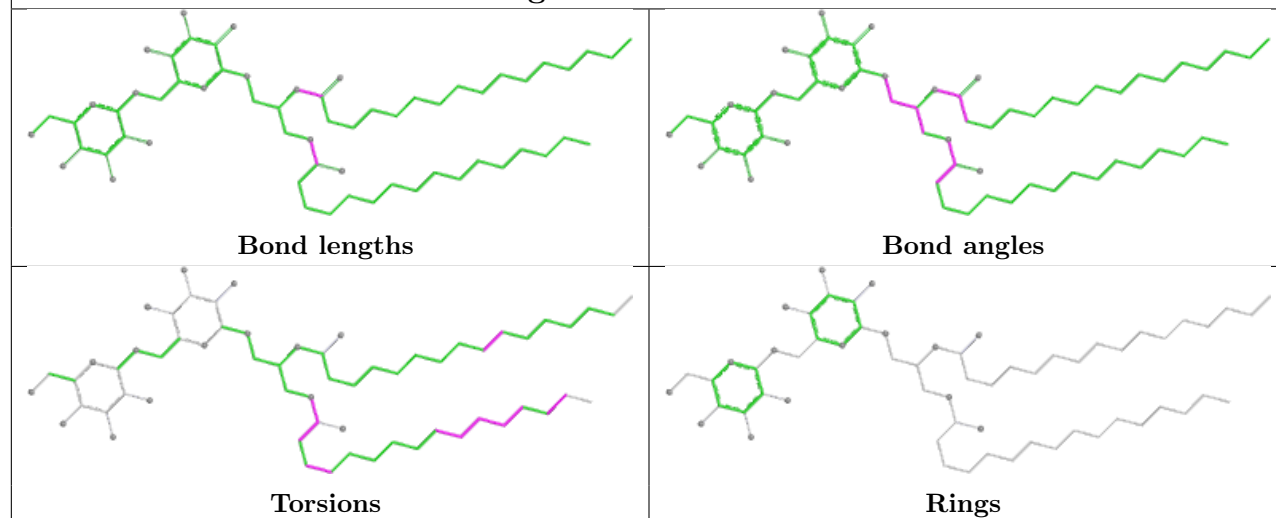
Ligand CLA c 512

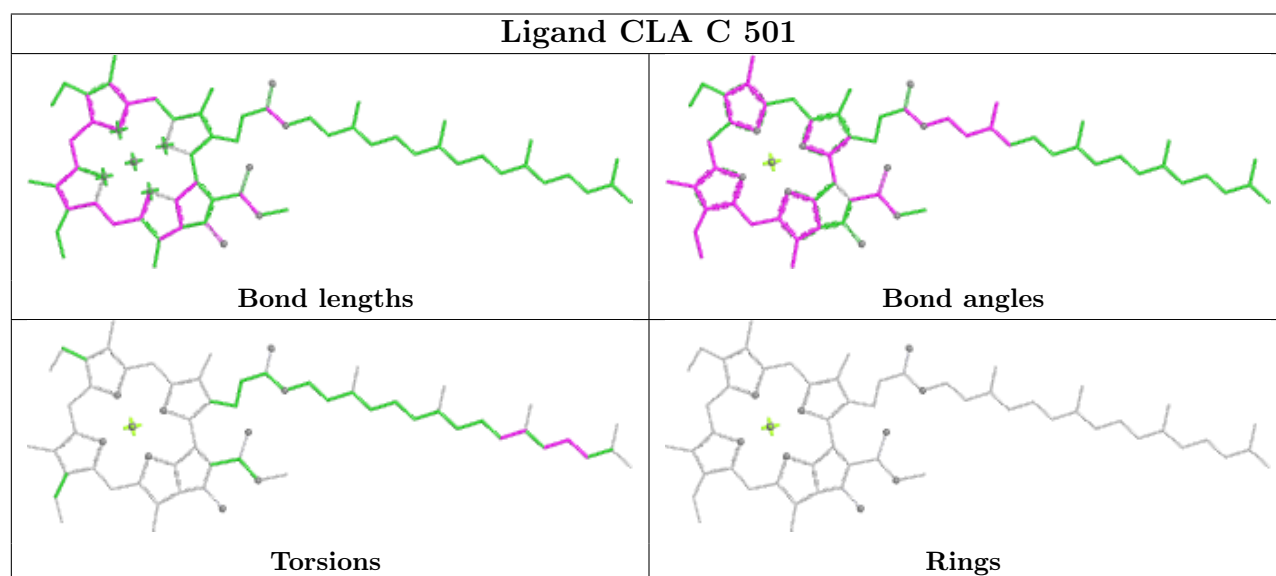
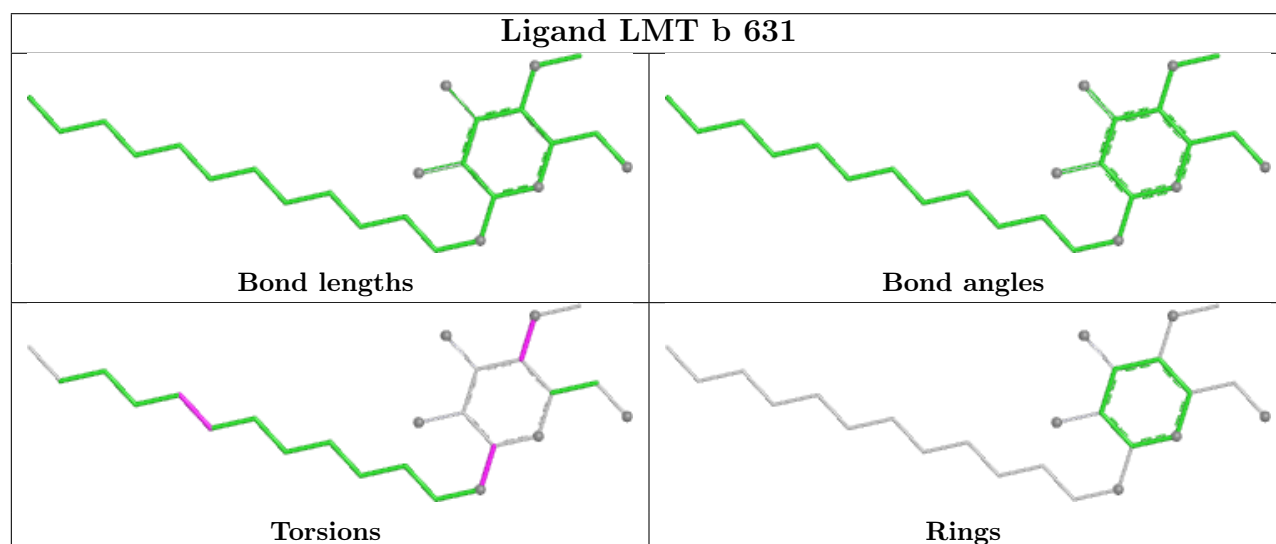
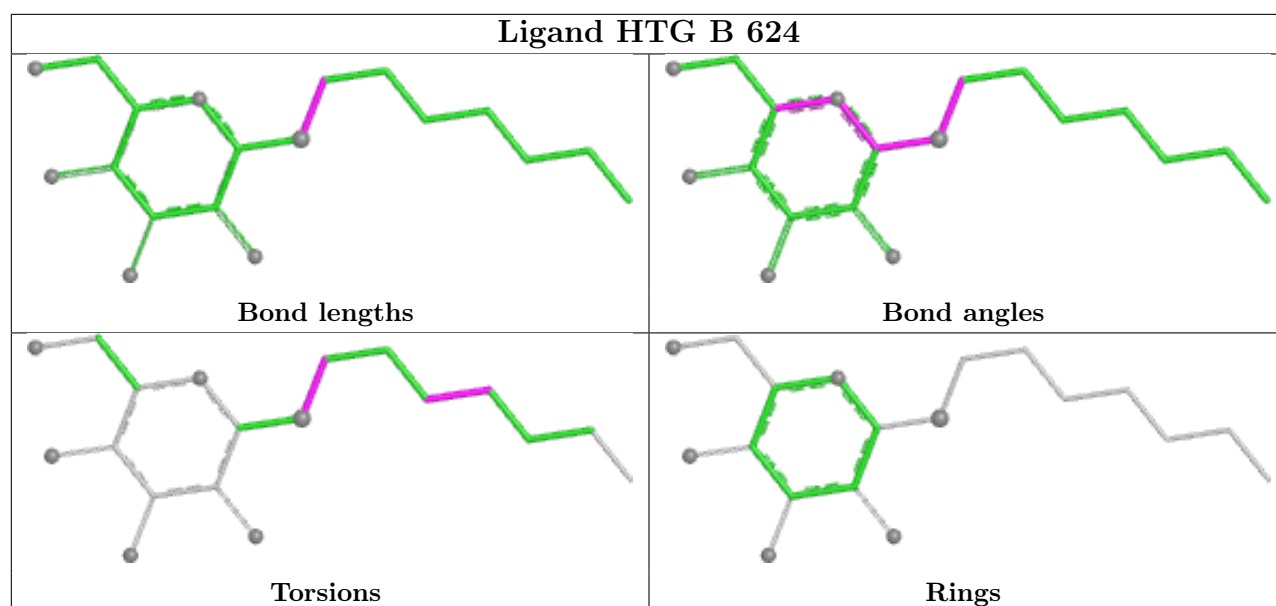


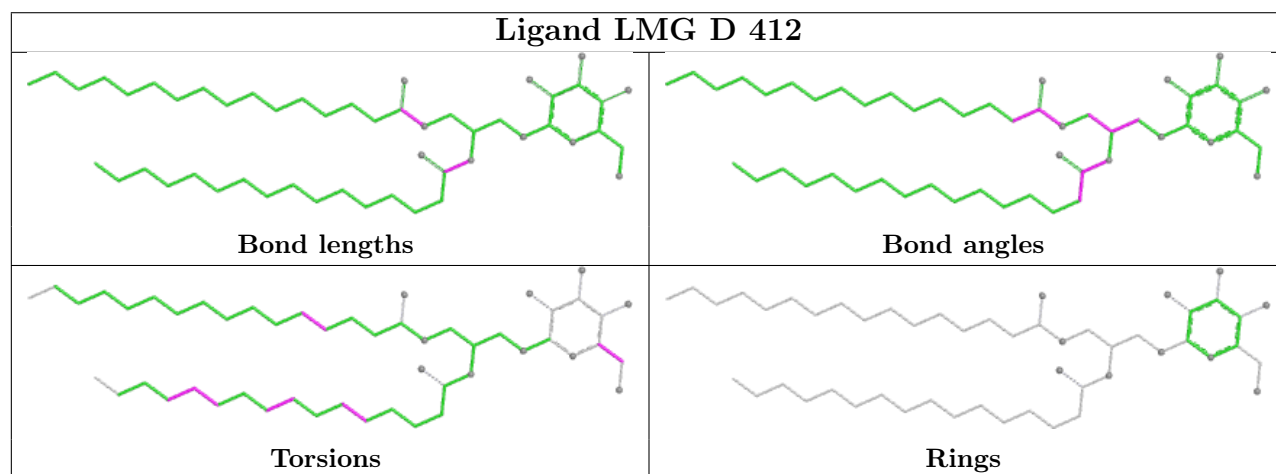
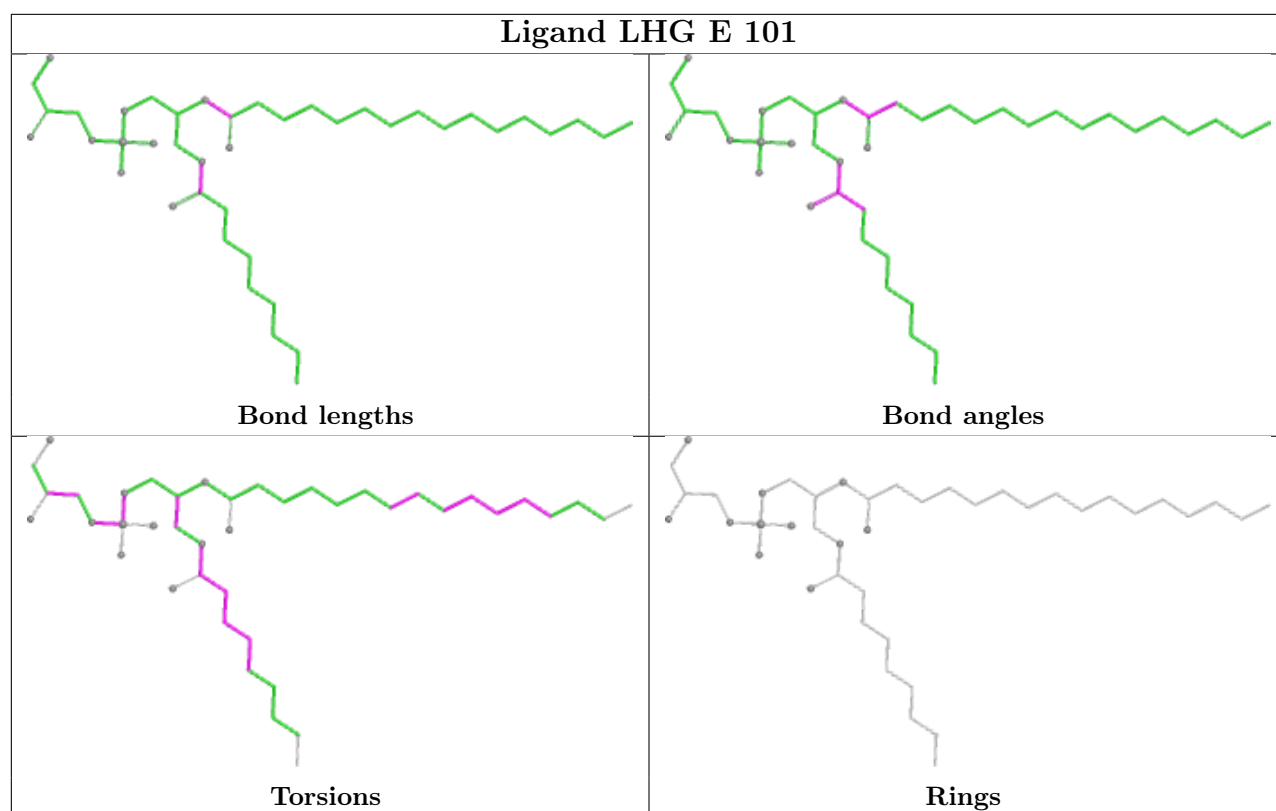
Ligand CLA a 410

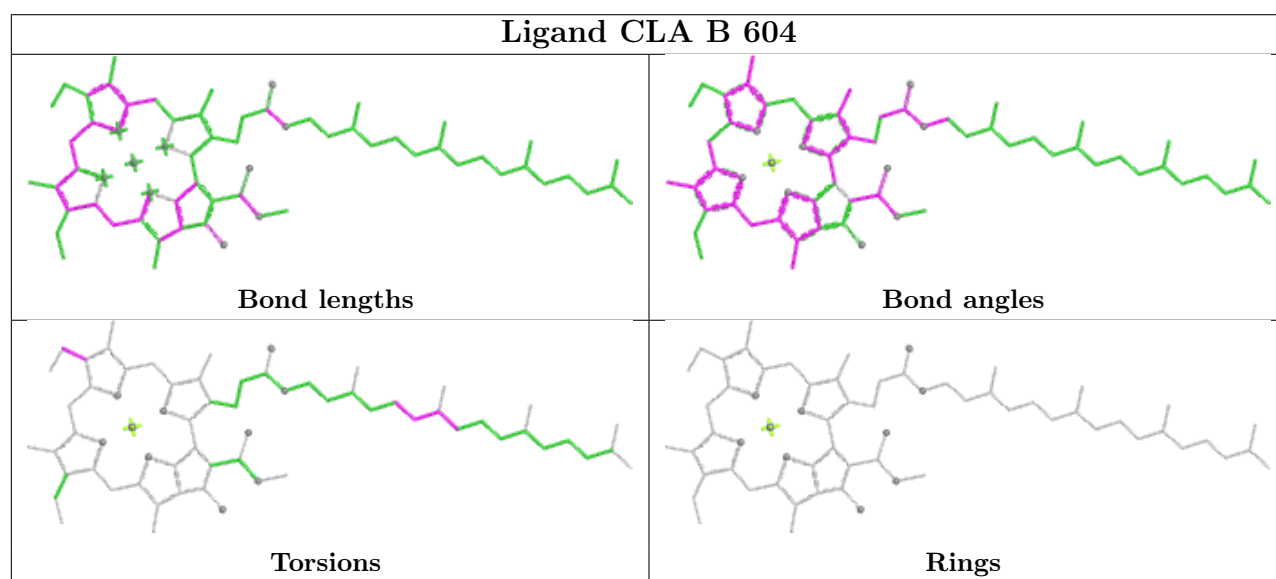
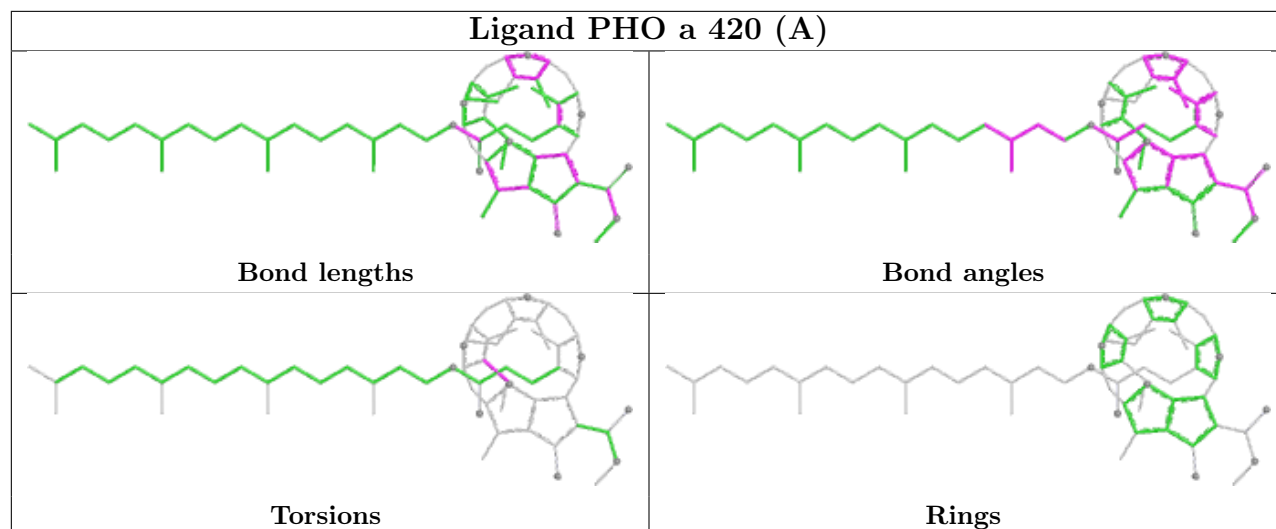


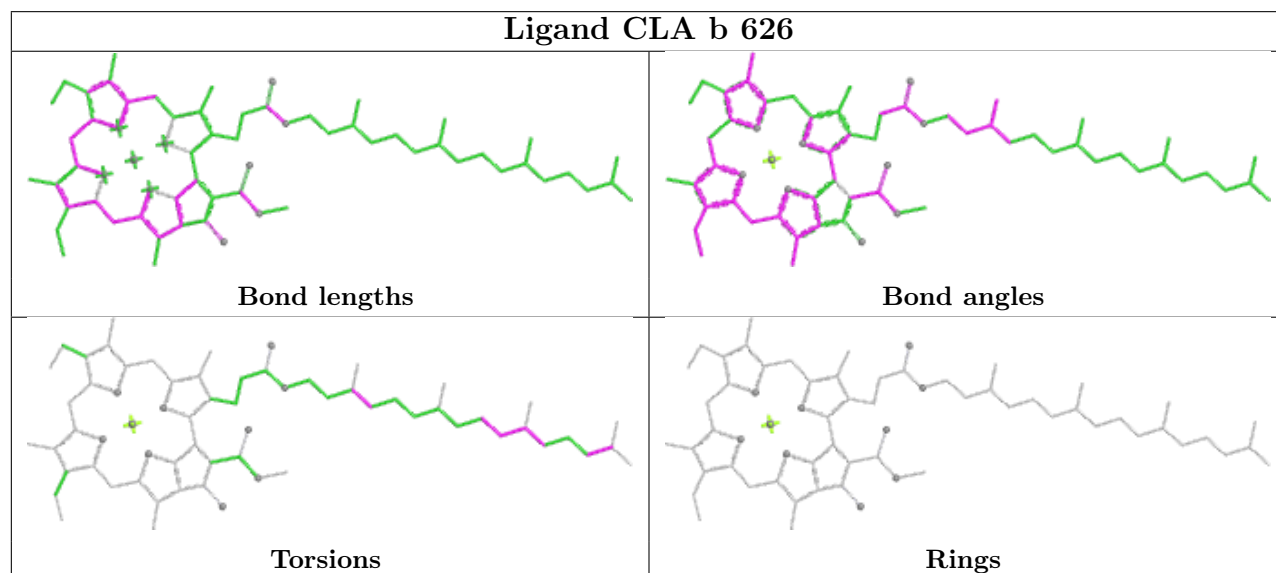
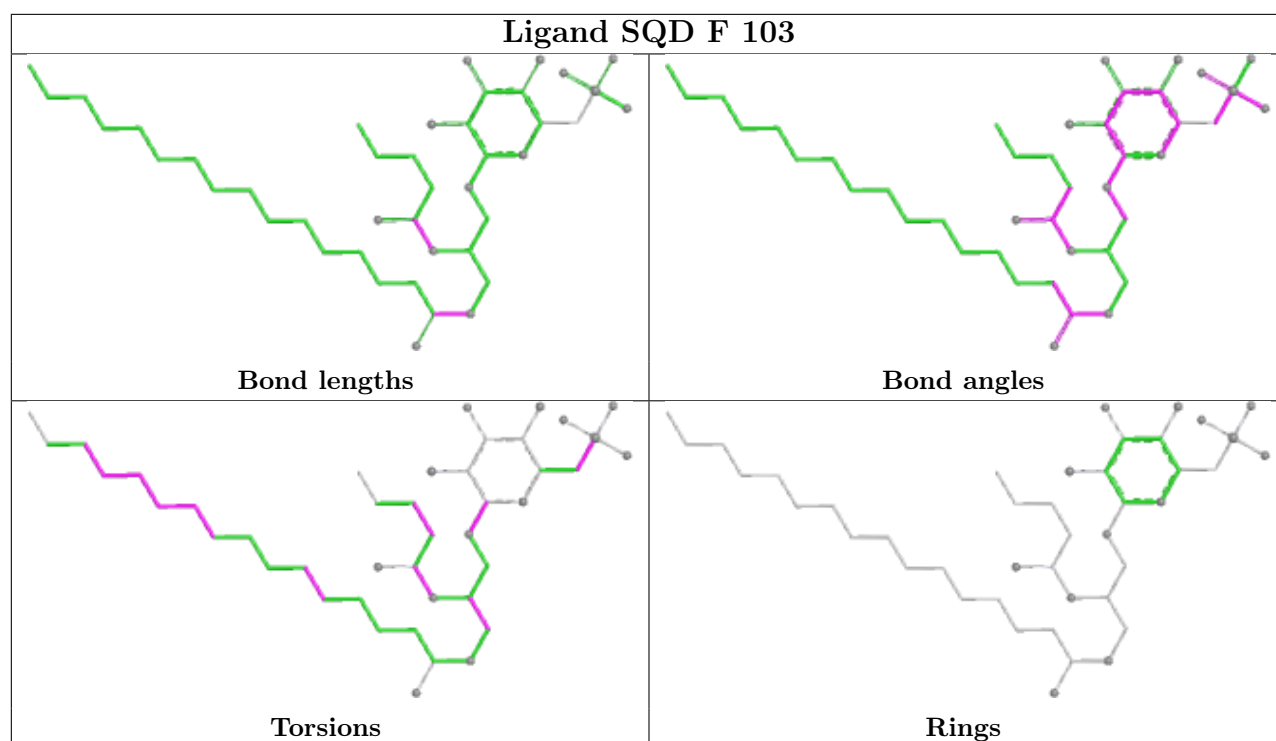
Ligand DGD C 518

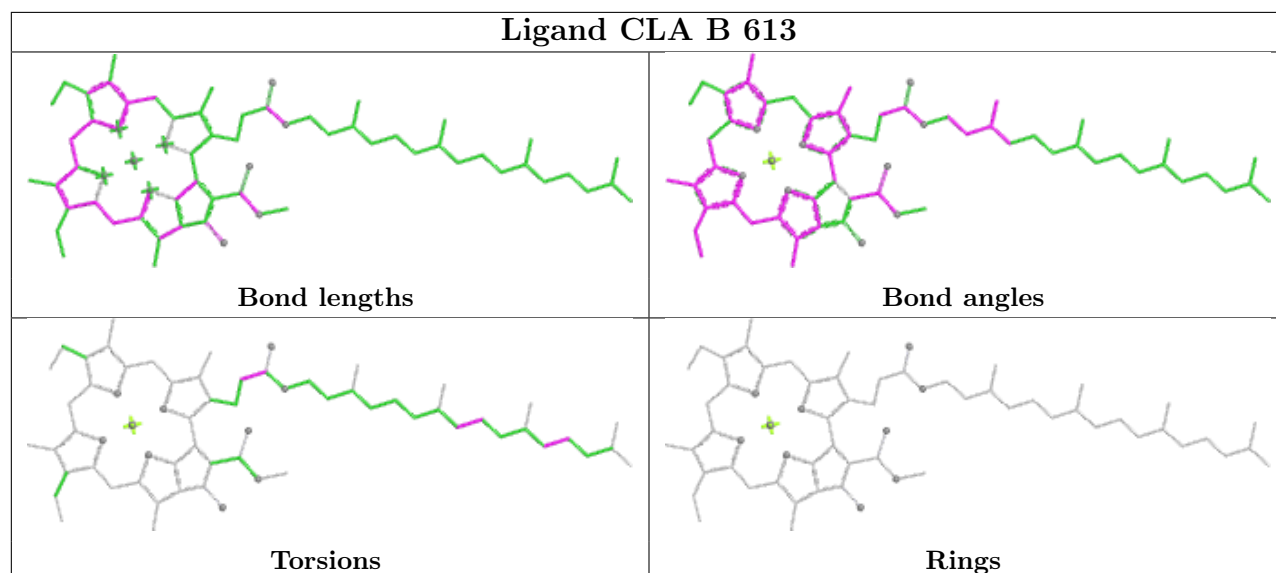
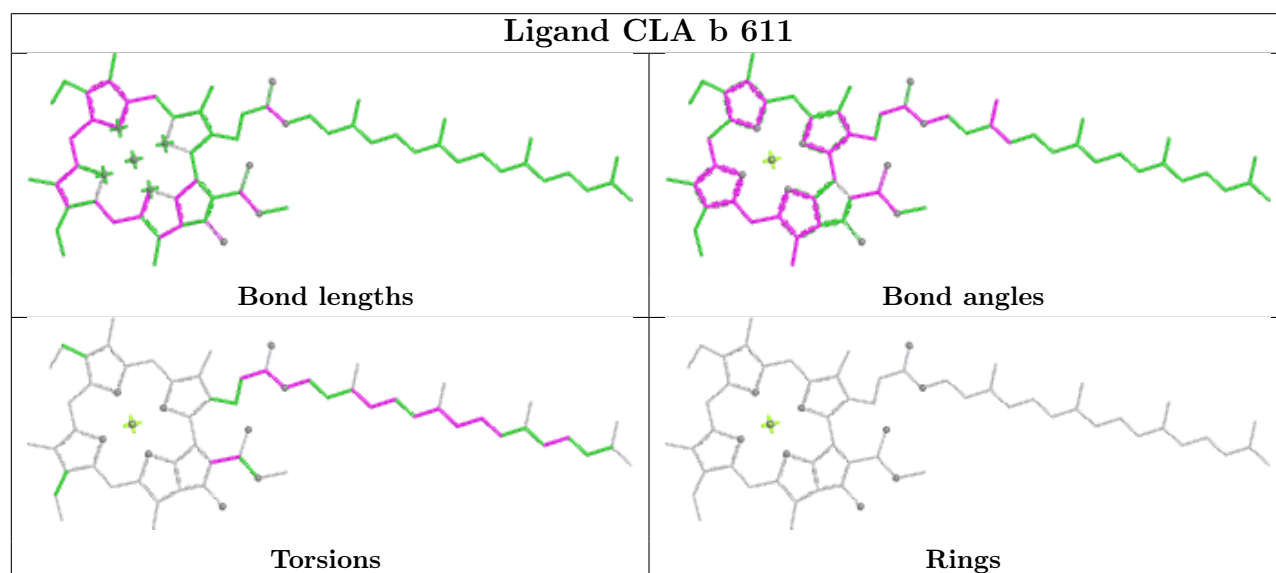
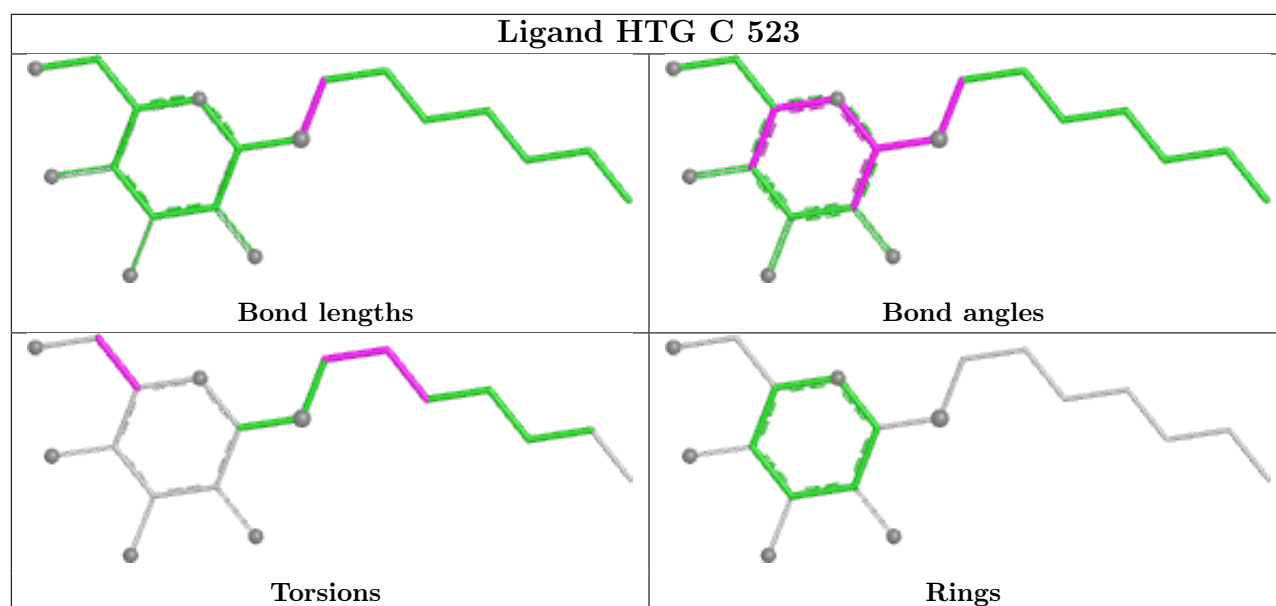


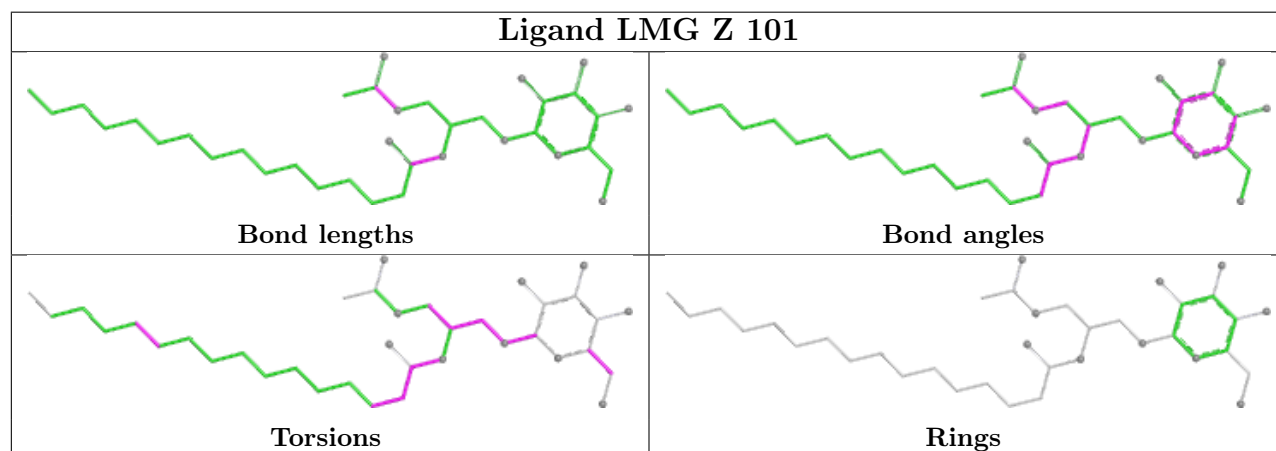
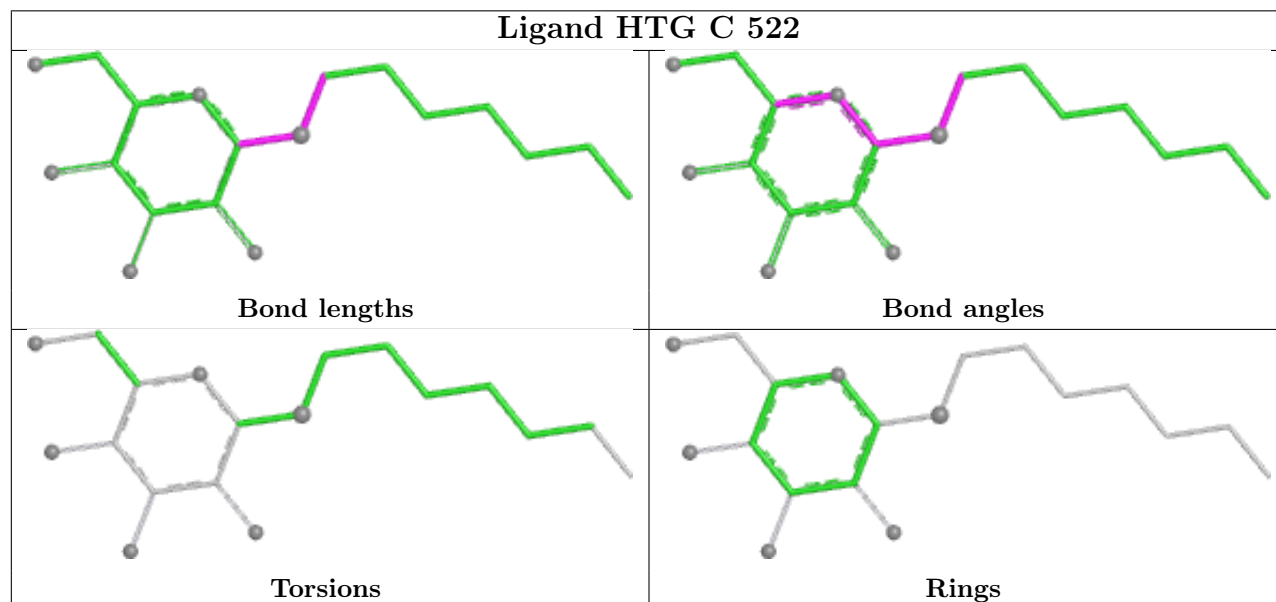
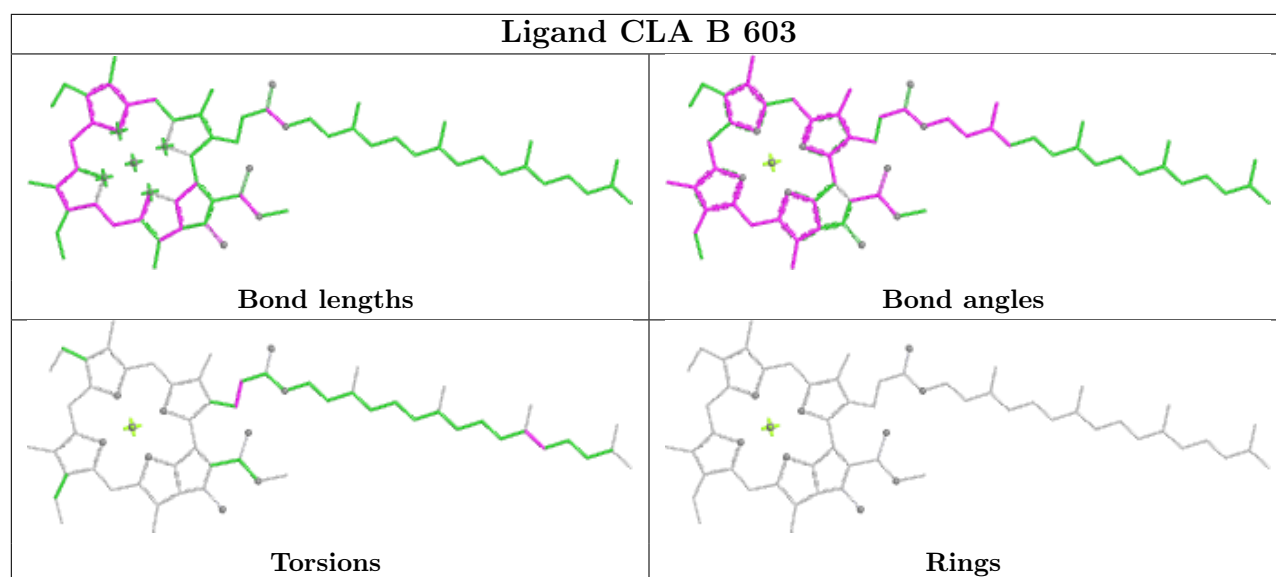


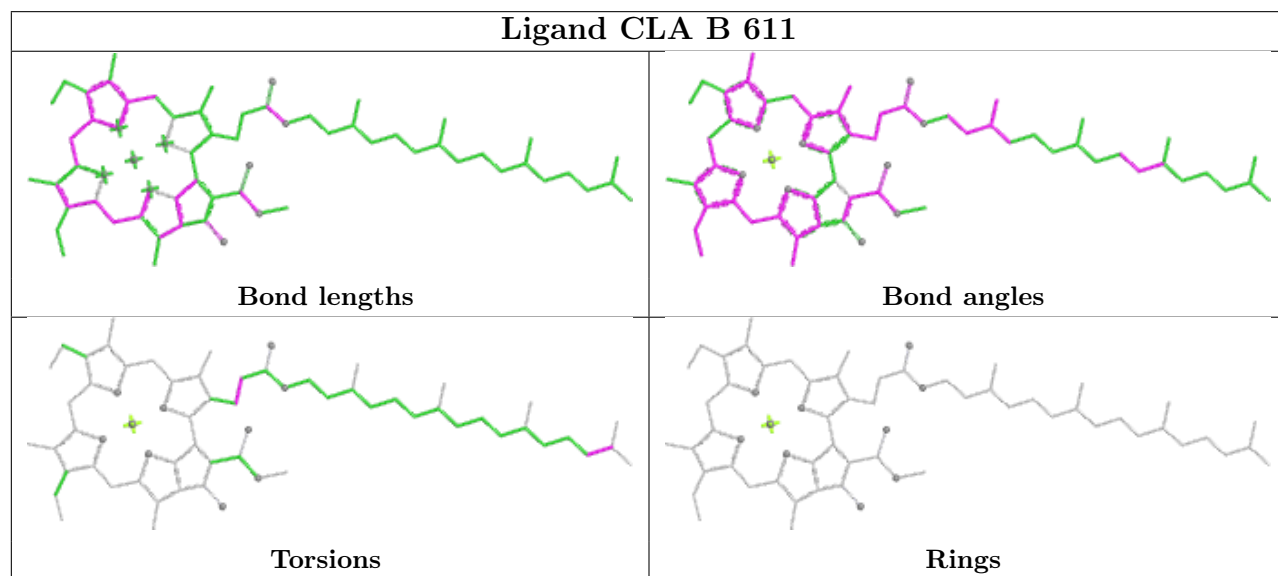
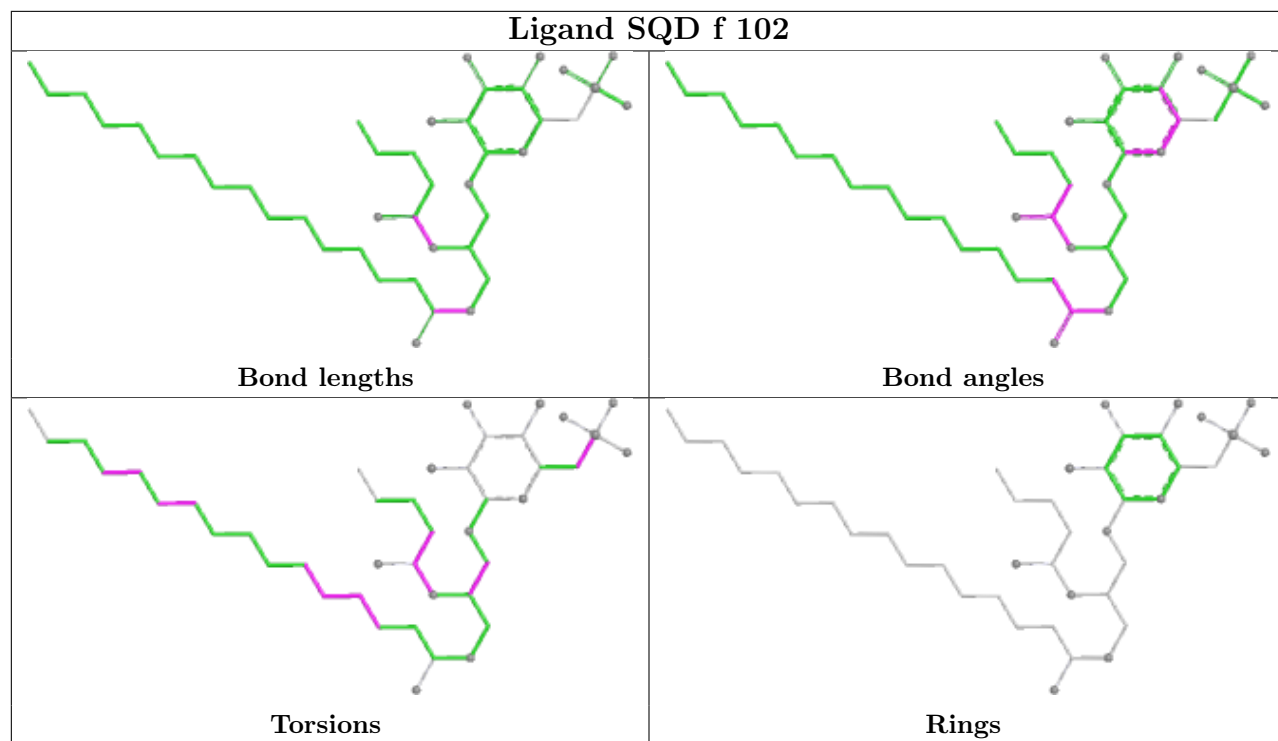


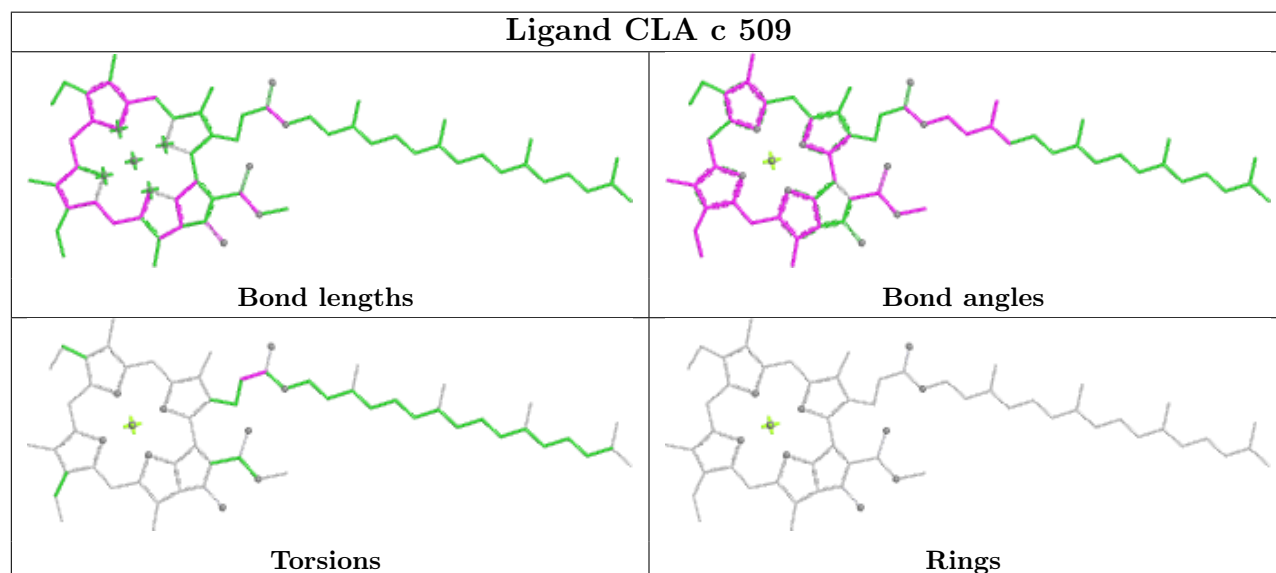
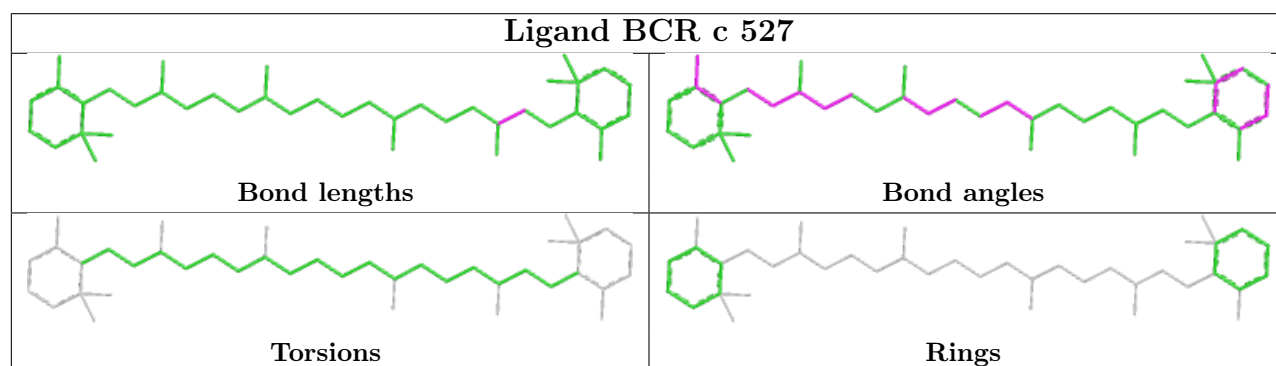
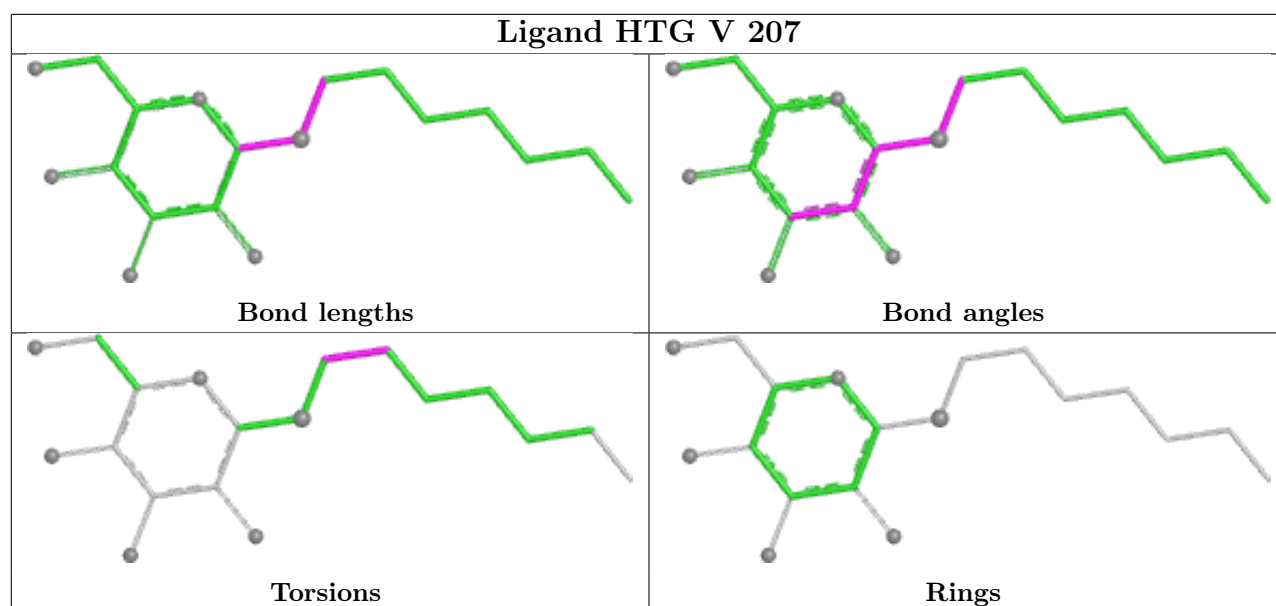


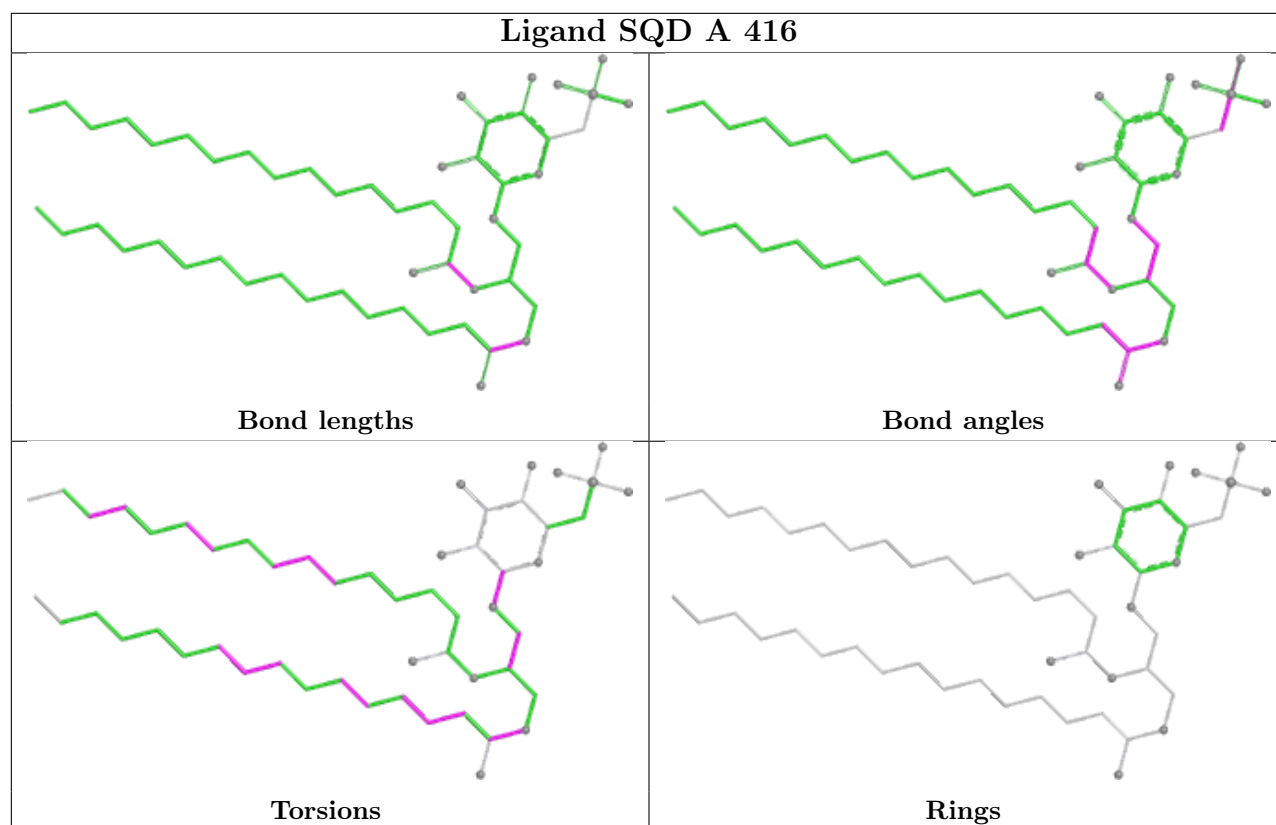
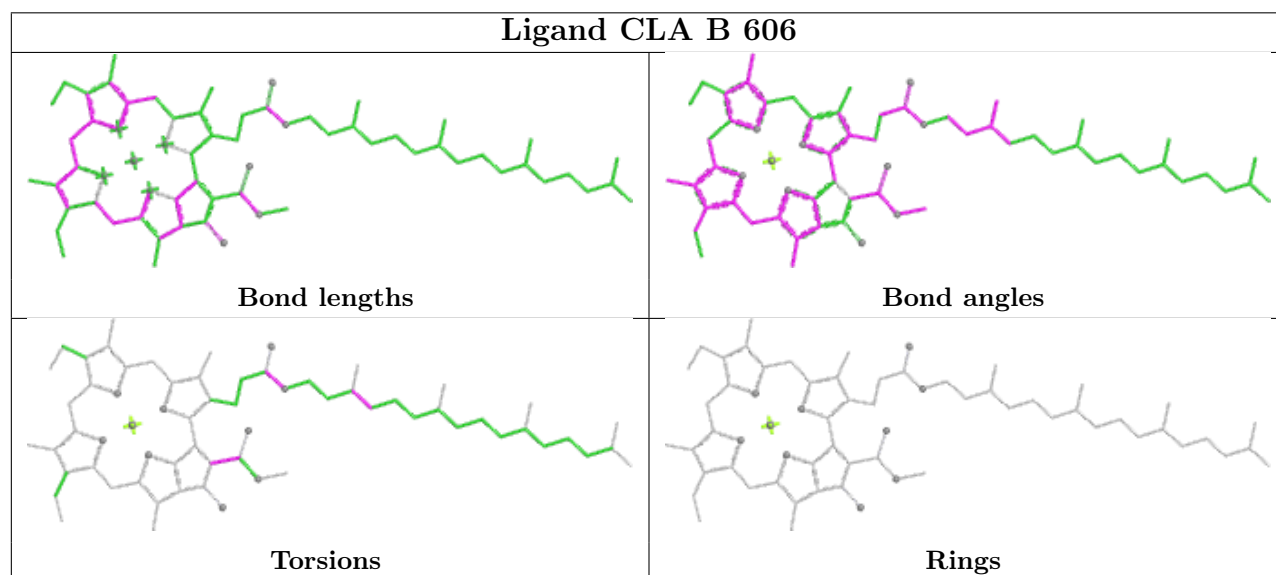
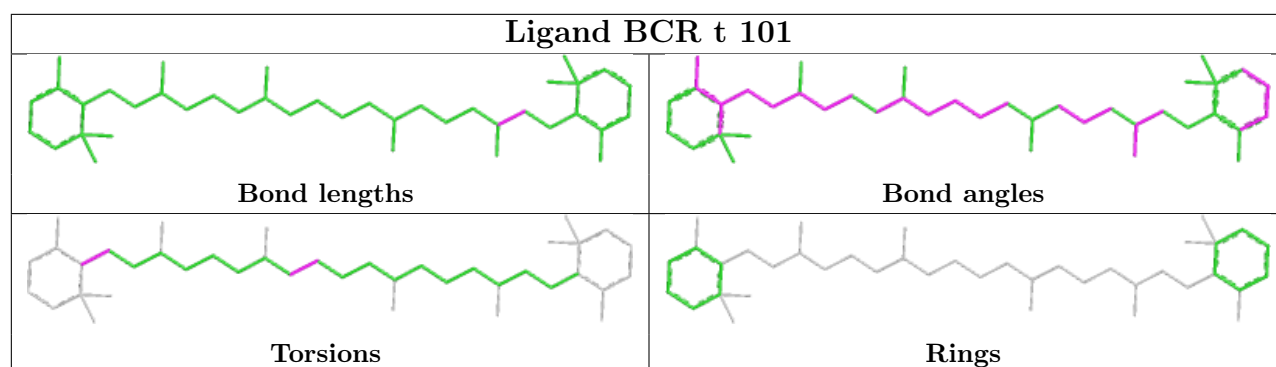


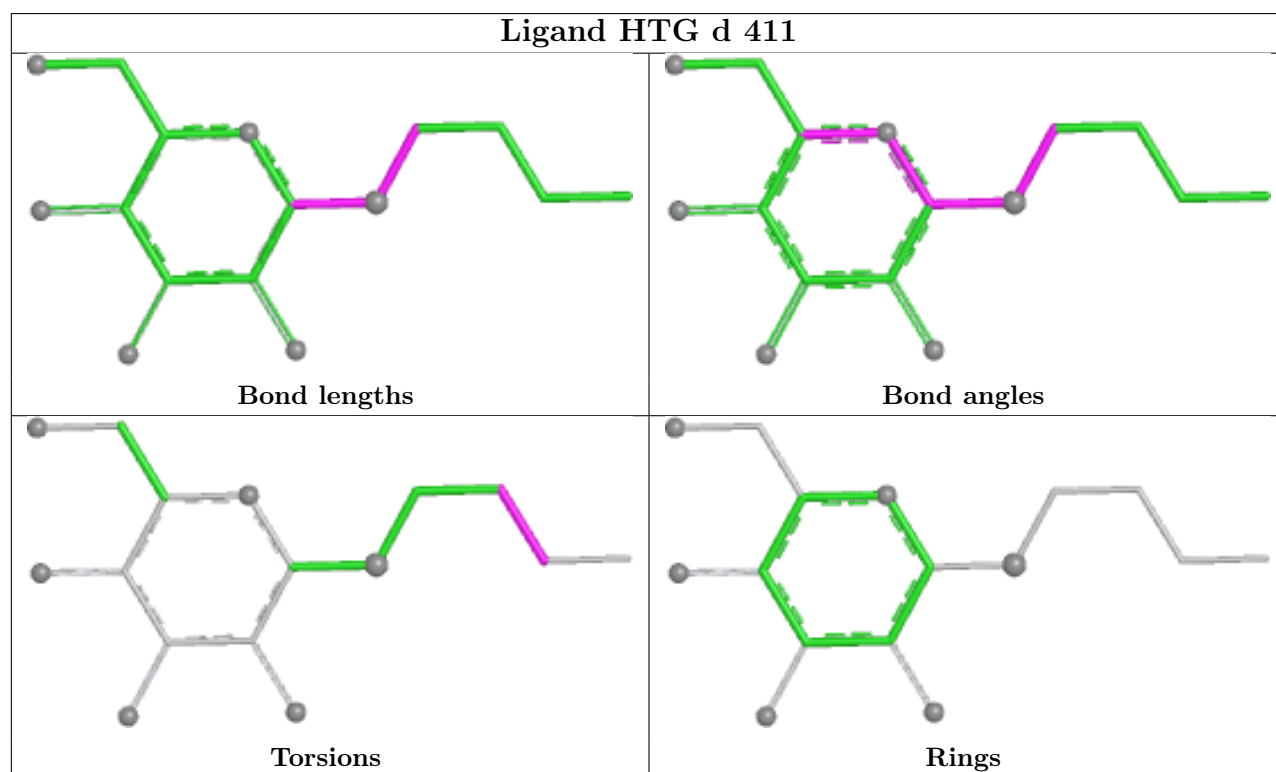
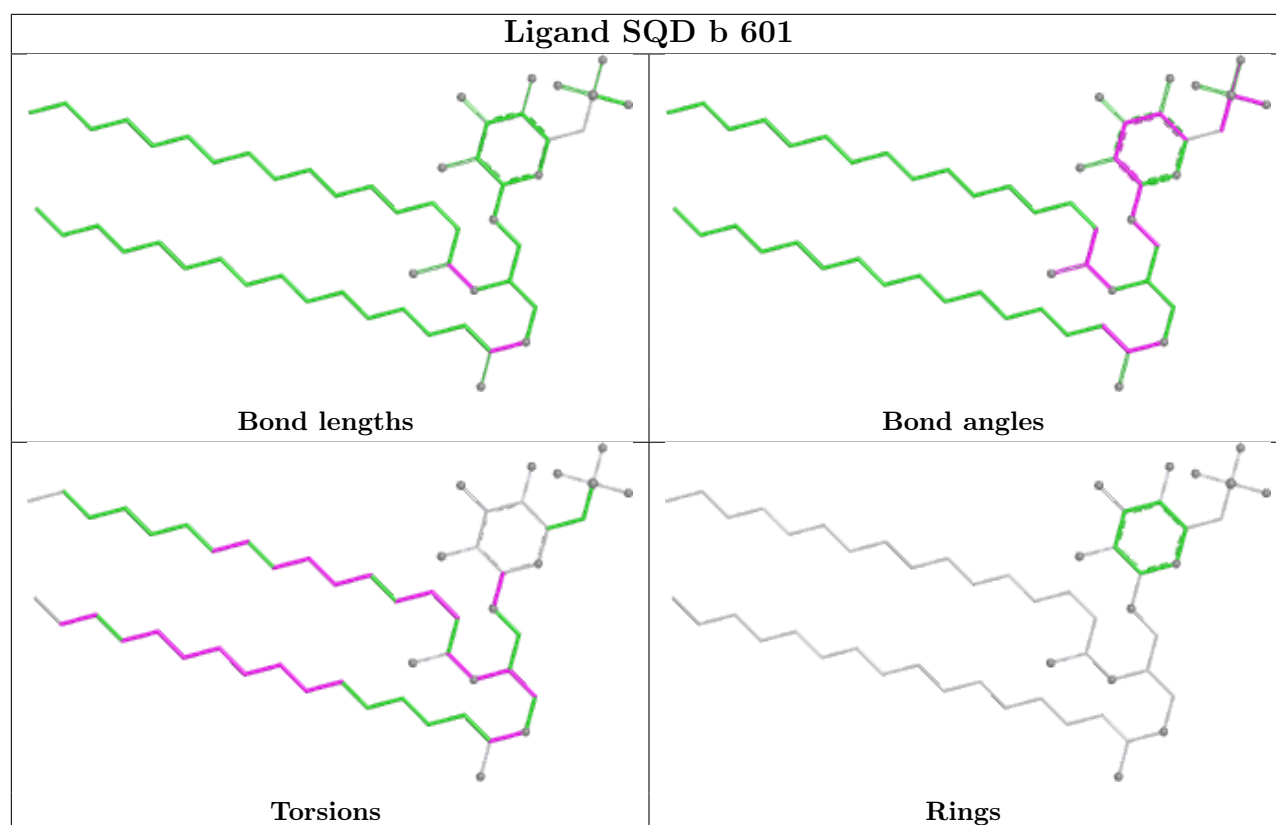


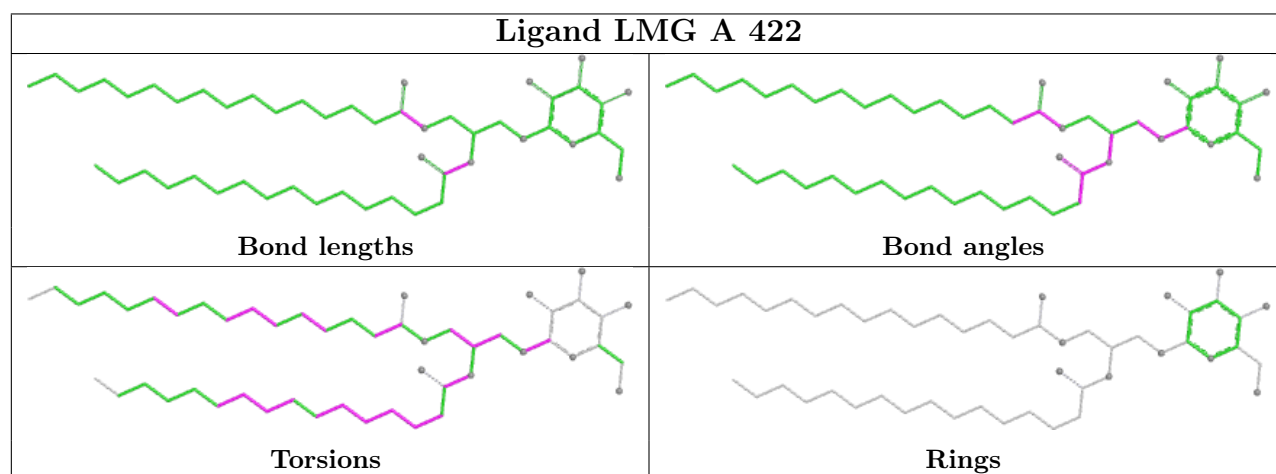
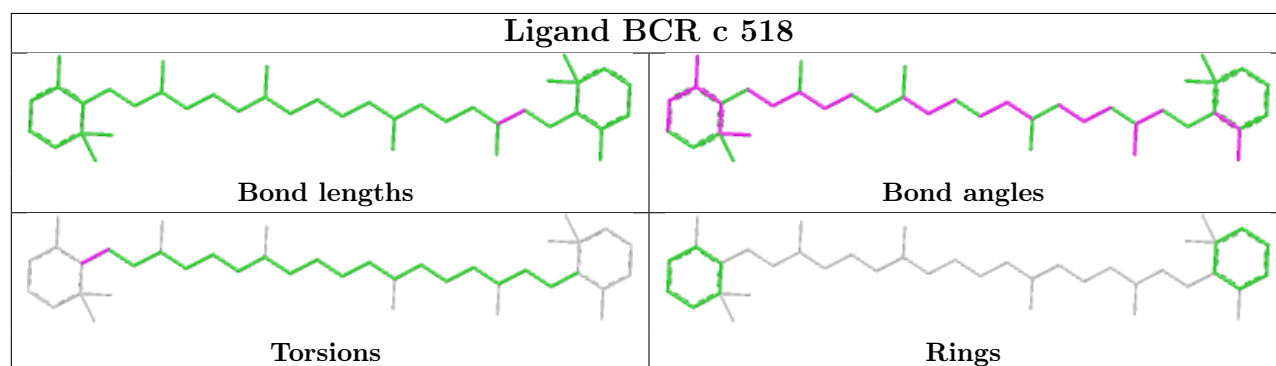
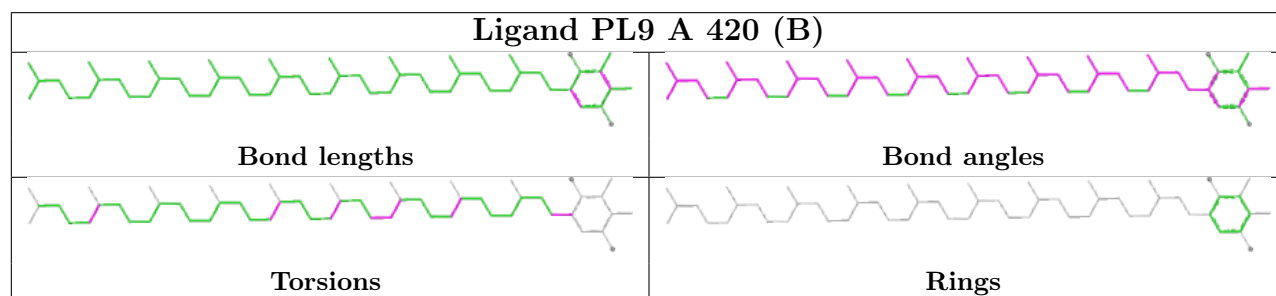
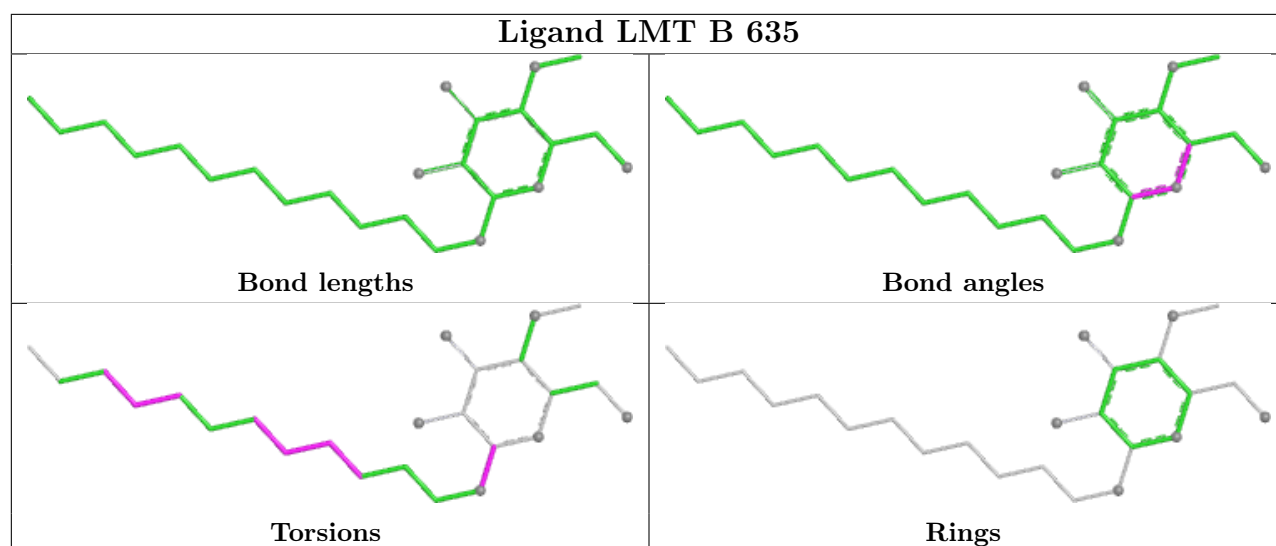


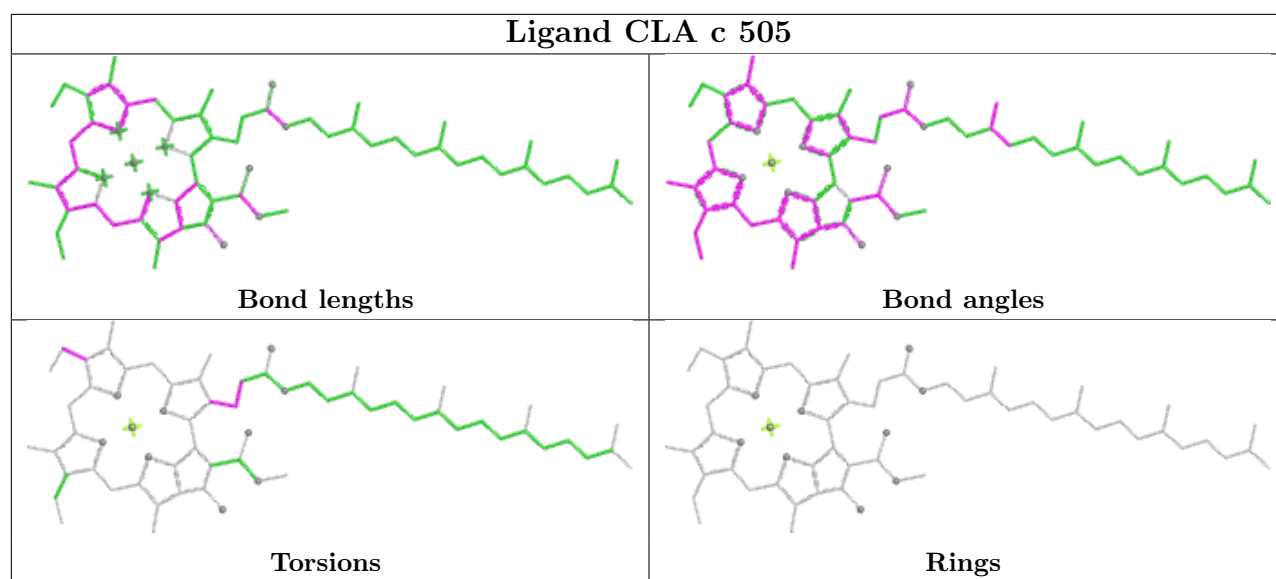












5.7 Other polymers [i](#)

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%)	-0.67	0 100 100	16, 36, 59, 107	53 (15%)
1	a	334/344 (97%)	-0.63	4 (1%) 76 79	16, 37, 71, 150	53 (15%)
2	B	504/505 (99%)	-0.61	2 (0%) 88 90	21, 42, 76, 120	10 (1%)
2	b	503/505 (99%)	-0.49	9 (1%) 67 71	26, 43, 75, 162	12 (2%)
3	C	451/455 (99%)	-0.55	0 100 100	18, 49, 68, 110	12 (2%)
3	c	455/455 (100%)	-0.51	0 100 100	18, 52, 70, 121	20 (4%)
4	D	341/342 (99%)	-0.73	0 100 100	18, 38, 59, 134	16 (4%)
4	d	341/342 (99%)	-0.71	0 100 100	19, 40, 58, 112	16 (4%)
5	E	81/84 (96%)	-0.09	1 (1%) 76 79	30, 62, 92, 139	2 (2%)
5	e	81/84 (96%)	-0.00	2 (2%) 58 62	36, 64, 110, 167	2 (2%)
6	F	34/44 (77%)	-0.25	0 100 100	45, 54, 92, 96	0
6	f	32/44 (72%)	-0.16	1 (3%) 51 55	45, 54, 112, 130	0
7	H	65/65 (100%)	-0.37	2 (3%) 51 55	33, 52, 68, 144	1 (1%)
7	h	65/65 (100%)	-0.37	2 (3%) 51 55	40, 54, 74, 162	0
8	I	37/38 (97%)	-0.21	0 100 100	44, 52, 104, 148	0
8	i	37/38 (97%)	-0.27	1 (2%) 56 60	41, 50, 97, 126	0
9	J	38/39 (97%)	-0.02	2 (5%) 32 36	42, 58, 135, 165	0
9	j	39/39 (100%)	-0.09	1 (2%) 57 61	46, 59, 130, 162	0
10	K	37/37 (100%)	-0.38	0 100 100	50, 58, 72, 91	0
10	k	37/37 (100%)	-0.27	0 100 100	50, 63, 79, 98	0
11	L	37/37 (100%)	-0.68	0 100 100	18, 34, 94, 106	1 (2%)
11	l	37/37 (100%)	-0.63	0 100 100	22, 35, 90, 121	1 (2%)
12	M	33/36 (91%)	-0.73	0 100 100	22, 36, 61, 112	1 (3%)
12	m	33/36 (91%)	-0.64	0 100 100	30, 37, 66, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.60	1 (0%) 88 90	24, 47, 91, 130	8 (3%)
13	o	243/244 (99%)	-0.44	2 (0%) 82 84	26, 49, 103, 167	5 (2%)
14	T	29/32 (90%)	-0.74	1 (3%) 48 52	30, 36, 62, 135	1 (3%)
14	t	29/32 (90%)	-0.64	1 (3%) 48 52	27, 36, 64, 128	1 (3%)
15	U	97/104 (93%)	-0.63	0 100 100	35, 46, 75, 109	0
15	u	97/104 (93%)	-0.60	0 100 100	37, 49, 68, 117	0
16	V	137/137 (100%)	-0.67	0 100 100	19, 45, 65, 84	2 (1%)
16	v	137/137 (100%)	-0.51	0 100 100	22, 56, 82, 129	1 (0%)
17	Y	29/30 (96%)	0.60	3 (10%) 12 13	60, 71, 151, 153	0
17	y	29/30 (96%)	0.36	0 100 100	68, 80, 106, 124	0
18	X	39/40 (97%)	-0.04	0 100 100	47, 60, 112, 132	0
18	x	38/40 (95%)	0.18	2 (5%) 32 36	52, 61, 113, 134	0
19	Z	62/62 (100%)	0.09	1 (1%) 70 74	56, 72, 108, 126	0
19	z	62/62 (100%)	0.43	3 (4%) 35 40	70, 83, 128, 175	0
20	R	18/34 (52%)	3.00	15 (83%) 0 0	111, 142, 168, 174	0
All	All	5275/5384 (97%)	-0.50	56 (1%) 78 80	16, 46, 88, 175	218 (4%)

The worst 5 of 56 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	R	15	ALA	5.2
20	R	13	LEU	4.6
20	R	3	TRP	4.1
20	R	9	LEU	4.0
2	b	486	LEU	3.8

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	T	1	10/11	0.94	0.07	37,40,54,78	0
12	FME	m	1	10/11	0.96	0.07	34,45,87,98	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	0.97	0.07	39,48,57,57	0
12	FME	M	1	10/11	0.97	0.07	26,45,71,76	0
14	FME	t	1	10/11	0.97	0.05	28,35,39,84	0
8	FME	I	1	10/11	0.98	0.06	36,46,51,55	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
37	DGD	e	101	62/66	0.66	0.17	66,114,163,166	0
37	DGD	D	406	52/66	0.69	0.15	67,101,132,138	0
38	LHG	a	422	42/49	0.70	0.13	78,125,159,162	0
33	UNL	m	101	10/-	0.71	0.16	50,57,79,81	0
29	LMT	F	101	35/35	0.73	0.16	97,128,145,146	0
29	LMT	b	631	25/35	0.73	0.15	72,95,139,144	0
28	GOL	V	202	6/6	0.74	0.15	62,77,81,82	0
33	UNL	a	403	30/-	0.74	0.15	77,91,116,118	0
33	UNL	M	102	10/-	0.75	0.12	50,64,69,73	0
29	LMT	a	421	35/35	0.75	0.15	94,110,132,135	0
36	HTG	c	525	19/19	0.76	0.13	68,104,113,143	0
33	UNL	j	102	10/-	0.76	0.14	70,80,90,91	0
29	LMT	C	521	35/35	0.77	0.14	94,119,146,148	0
27	SQD	f	102	43/54	0.77	0.15	97,116,146,147	0
33	UNL	C	527	34/-	0.78	0.14	76,103,111,117	0
33	UNL	A	421	28/-	0.79	0.14	68,84,98,99	0
29	LMT	A	417	35/35	0.79	0.12	41,79,99,112	0
36	HTG	B	625	19/19	0.79	0.12	64,120,133,158	0
36	HTG	H	101	16/19	0.79	0.13	70,131,138,139	0
33	UNL	I	101	40/-	0.79	0.15	43,83,129,135	0
29	LMT	M	103	35/35	0.79	0.14	45,92,128,137	0
29	LMT	f	103	35/35	0.79	0.12	72,117,137,137	0
33	UNL	i	101	40/-	0.79	0.14	50,74,125,128	0
29	LMT	D	401	35/35	0.80	0.13	75,118,137,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	CA	b	610	1/1	0.80	0.13	130,130,130,130	0
38	LHG	E	101	42/49	0.81	0.12	69,98,119,122	0
33	UNL	D	411	40/-	0.81	0.12	57,79,113,123	0
29	LMT	a	404	35/35	0.82	0.12	47,86,111,123	0
34	LMG	C	520	51/55	0.82	0.12	53,105,116,119	0
36	HTG	B	633	19/19	0.82	0.12	53,110,132,175	0
34	LMG	z	101	39/55	0.82	0.14	69,112,127,136	0
36	HTG	b	609	19/19	0.82	0.12	62,113,140,141	0
33	UNL	d	410	36/-	0.83	0.12	53,77,122,126	0
33	UNL	J	101	10/-	0.83	0.13	46,70,80,85	0
36	HTG	d	411	16/19	0.83	0.12	70,111,121,126	0
33	UNL	B	634	33/-	0.83	0.14	54,88,123,126	0
27	SQD	F	103	43/54	0.83	0.12	74,97,116,118	0
33	UNL	c	526	32/-	0.83	0.13	77,98,122,128	0
36	HTG	V	207	19/19	0.83	0.12	63,87,104,205	0
33	UNL	b	634	33/-	0.84	0.14	48,98,141,142	0
27	SQD	B	621	54/54	0.84	0.12	48,81,143,146	0
28	GOL	C	524	6/6	0.84	0.14	63,65,79,82	0
28	GOL	O	301	6/6	0.84	0.09	68,76,77,77	0
32	PL9	A	420[B]	55/55	0.85	0.14	71,87,101,101	55
36	HTG	b	633	19/19	0.85	0.12	70,120,135,135	0
27	SQD	a	405	54/54	0.85	0.10	45,76,111,114	0
29	LMT	B	635	25/35	0.85	0.13	38,73,124,127	0
32	PL9	A	420[A]	55/55	0.85	0.14	70,87,101,101	55
36	HTG	C	523	19/19	0.85	0.10	75,95,121,124	0
34	LMG	Z	101	37/55	0.85	0.14	57,108,124,127	0
34	LMG	c	523	51/55	0.85	0.11	49,106,118,120	0
29	LMT	m	102	35/35	0.86	0.11	47,95,121,125	0
27	SQD	b	601	54/54	0.86	0.10	52,72,120,129	0
28	GOL	c	502	6/6	0.86	0.15	70,79,91,98	0
32	PL9	a	416[A]	55/55	0.86	0.14	83,102,111,114	55
32	PL9	a	416[B]	55/55	0.86	0.14	84,102,111,114	55
27	SQD	A	416	54/54	0.86	0.10	47,73,104,112	0
36	HTG	b	632	19/19	0.86	0.13	51,67,77,78	0
36	HTG	B	624	19/19	0.88	0.11	54,64,74,81	0
29	LMT	M	104	35/35	0.88	0.10	46,79,89,95	0
36	HTG	c	524	19/19	0.88	0.10	81,89,96,118	0
29	LMT	T	104	25/35	0.88	0.13	38,71,116,121	0
36	HTG	C	522	19/19	0.88	0.09	72,80,91,95	0
28	GOL	T	102	6/6	0.88	0.13	103,114,116,120	0
28	GOL	v	201	6/6	0.88	0.13	78,85,89,90	0
28	GOL	A	415	6/6	0.88	0.11	54,73,76,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	GOL	b	607	6/6	0.88	0.11	64,77,80,80	0
34	LMG	c	522	51/55	0.89	0.10	52,86,107,110	0
28	GOL	T	101	6/6	0.89	0.14	55,69,88,96	0
28	GOL	t	102	6/6	0.89	0.14	49,76,86,89	0
34	LMG	C	519	51/55	0.90	0.10	50,78,102,103	0
28	GOL	b	606	6/6	0.90	0.15	75,79,94,95	0
28	GOL	B	630	6/6	0.90	0.11	50,66,68,71	0
28	GOL	a	402	6/6	0.90	0.11	76,90,92,92	0
33	UNL	X	101	18/-	0.91	0.10	58,70,93,100	0
33	UNL	d	412	18/-	0.91	0.11	61,68,102,107	0
34	LMG	a	415	51/55	0.91	0.09	58,75,96,97	0
28	GOL	B	636	6/6	0.91	0.09	48,51,55,55	0
29	LMT	M	101	35/35	0.91	0.09	39,82,98,103	0
28	GOL	o	301	6/6	0.91	0.10	64,70,80,88	0
34	LMG	A	422	51/55	0.91	0.09	56,79,99,104	0
33	UNL	d	409	17/-	0.91	0.10	46,63,91,92	0
24	CLA	b	611	65/65	0.92	0.09	46,69,101,116	0
28	GOL	B	626	6/6	0.92	0.10	39,52,57,71	0
28	GOL	v	202	6/6	0.92	0.10	72,79,89,99	0
28	GOL	B	628	6/6	0.92	0.10	52,70,78,85	0
28	GOL	f	101	6/6	0.93	0.08	74,84,86,89	0
23	BCT	a	419[A]	4/4	0.93	0.07	53,54,57,63	4
36	HTG	B	632	19/19	0.93	0.07	41,75,91,92	0
33	UNL	D	410	17/-	0.93	0.08	39,67,83,87	0
23	BCT	a	419[B]	4/4	0.93	0.07	53,53,57,64	4
24	CLA	B	602	65/65	0.93	0.09	44,61,94,111	0
24	CLA	C	506	65/65	0.93	0.08	44,60,101,105	0
24	CLA	C	513	65/65	0.93	0.08	50,64,93,98	0
22	CL	U	201	1/1	0.93	0.11	93,93,93,93	0
28	GOL	A	414	6/6	0.93	0.13	52,54,57,60	0
34	LMG	b	630	51/55	0.93	0.08	39,48,68,82	0
24	CLA	c	517	65/65	0.93	0.08	61,77,92,94	0
26	BCR	y	101	40/40	0.93	0.07	43,60,68,76	0
34	LMG	j	101	51/55	0.93	0.08	46,56,92,106	0
28	GOL	B	627	6/6	0.93	0.11	56,65,80,92	0
35	CA	B	601	1/1	0.93	0.06	118,118,118,118	0
38	LHG	D	409	49/49	0.93	0.10	37,54,105,113	0
27	SQD	A	412	54/54	0.93	0.09	43,76,91,94	0
35	CA	f	104	1/1	0.93	0.06	97,97,97,97	0
32	PL9	D	405[B]	55/55	0.94	0.06	27,35,43,47	55
26	BCR	K	101	40/40	0.94	0.08	43,55,62,63	0
27	SQD	a	414	54/54	0.94	0.09	54,77,98,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	BCR	T	103	40/40	0.94	0.06	28,45,55,58	0
26	BCR	b	628	40/40	0.94	0.07	31,43,54,61	0
34	LMG	B	622	51/55	0.94	0.07	32,49,69,85	0
26	BCR	c	527	40/40	0.94	0.08	56,72,78,81	0
28	GOL	b	603	6/6	0.94	0.09	53,57,64,80	0
36	HTG	b	608	19/19	0.94	0.07	48,68,78,79	0
34	LMG	D	412	51/55	0.94	0.09	35,55,100,106	0
26	BCR	d	404	40/40	0.94	0.07	38,50,73,79	0
26	BCR	k	101	40/40	0.94	0.07	44,60,70,74	0
24	CLA	b	616	65/65	0.94	0.08	30,43,84,96	0
24	CLA	b	626	65/65	0.94	0.08	35,50,97,100	0
28	GOL	B	629	6/6	0.94	0.10	43,47,50,52	0
37	DGD	C	517	62/66	0.94	0.07	37,52,86,94	0
24	CLA	C	504	65/65	0.94	0.07	35,46,77,83	0
26	BCR	C	514	40/40	0.94	0.07	49,65,73,78	0
26	BCR	D	404	40/40	0.94	0.07	36,49,79,88	0
28	GOL	C	525	6/6	0.94	0.08	39,48,50,51	0
32	PL9	D	405[A]	55/55	0.94	0.06	28,35,45,49	55
24	CLA	C	512	65/65	0.95	0.07	46,64,76,80	0
24	CLA	B	615	65/65	0.95	0.07	27,38,82,86	0
26	BCR	Y	101	40/40	0.95	0.07	48,59,67,72	0
24	CLA	a	412	65/65	0.95	0.09	32,45,111,115	0
24	CLA	B	617	65/65	0.95	0.09	31,50,107,110	0
24	CLA	C	501	65/65	0.95	0.07	38,47,69,78	0
28	GOL	V	201	6/6	0.95	0.07	68,75,76,79	0
26	BCR	h	101	40/40	0.95	0.06	39,54,64,66	0
28	GOL	V	203	6/6	0.95	0.09	39,50,64,67	0
28	GOL	V	205	6/6	0.95	0.08	71,75,81,91	0
28	GOL	a	401	6/6	0.95	0.10	50,61,66,76	0
24	CLA	b	619	65/65	0.95	0.07	35,49,56,65	0
26	BCR	t	101	40/40	0.95	0.06	30,43,60,68	0
24	CLA	b	624	65/65	0.95	0.07	27,39,83,97	0
23	BCT	A	404[B]	4/4	0.95	0.07	51,52,57,63	4
24	CLA	c	505	65/65	0.95	0.07	40,54,62,66	0
24	CLA	c	507	65/65	0.95	0.07	41,51,60,77	0
24	CLA	c	508	65/65	0.95	0.06	38,50,71,75	0
24	CLA	c	510	65/65	0.95	0.07	44,62,87,95	0
24	CLA	c	511	65/65	0.95	0.07	43,54,62,67	0
24	CLA	c	516	65/65	0.95	0.07	51,62,77,83	0
28	GOL	v	203	6/6	0.95	0.10	46,50,57,61	0
24	CLA	C	505	65/65	0.95	0.07	32,47,66,74	0
28	GOL	A	413	6/6	0.95	0.07	43,44,56,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	PHO	a	420[A]	64/64	0.95	0.06	31,41,46,49	64
25	PHO	a	420[B]	64/64	0.95	0.06	31,40,46,50	64
26	BCR	A	411	40/40	0.95	0.06	29,37,44,45	0
37	DGD	C	518	62/66	0.95	0.06	37,47,75,87	0
26	BCR	B	620	40/40	0.95	0.06	31,43,57,59	0
37	DGD	H	103	62/66	0.95	0.07	32,47,70,74	0
37	DGD	c	520	62/66	0.95	0.07	38,51,100,112	0
37	DGD	c	521	62/66	0.95	0.07	39,51,82,89	0
23	BCT	A	404[A]	4/4	0.95	0.07	51,52,57,63	4
37	DGD	h	102	62/66	0.95	0.07	35,48,63,73	0
38	LHG	D	407	49/49	0.95	0.07	35,47,59,64	0
24	CLA	C	507	65/65	0.95	0.07	40,52,67,72	0
26	BCR	H	102	40/40	0.95	0.06	36,52,65,68	0
28	GOL	B	631	6/6	0.95	0.15	48,62,69,70	0
38	LHG	d	406	49/49	0.95	0.07	41,49,58,63	0
38	LHG	d	408	49/49	0.95	0.09	34,52,103,105	0
24	CLA	b	620	65/65	0.96	0.06	33,44,51,57	0
24	CLA	b	621	65/65	0.96	0.06	26,38,48,55	0
24	CLA	b	622	65/65	0.96	0.06	29,39,47,49	0
24	CLA	b	623	65/65	0.96	0.05	28,39,55,57	0
26	BCR	b	627	40/40	0.96	0.05	30,39,47,47	0
24	CLA	A	410	65/65	0.96	0.07	29,47,108,113	0
26	BCR	c	518	40/40	0.96	0.06	39,55,64,64	0
24	CLA	b	625	65/65	0.96	0.05	34,44,62,67	0
32	PL9	d	405[A]	55/55	0.96	0.06	25,35,44,49	55
32	PL9	d	405[B]	55/55	0.96	0.06	25,35,43,49	55
24	CLA	C	508	65/65	0.96	0.07	35,48,107,117	0
24	CLA	C	509	65/65	0.96	0.07	41,52,73,76	0
24	CLA	c	506	65/65	0.96	0.07	38,50,63,69	0
28	GOL	b	604	6/6	0.96	0.08	41,56,70,75	0
28	GOL	b	605	6/6	0.96	0.07	53,64,74,84	0
36	HTG	b	602	19/19	0.96	0.07	35,49,65,66	0
24	CLA	C	510	65/65	0.96	0.06	39,51,60,69	0
24	CLA	C	511	65/65	0.96	0.07	42,56,67,78	0
24	CLA	A	407	65/65	0.96	0.06	27,37,90,96	0
24	CLA	B	603	65/65	0.96	0.05	33,42,47,53	0
24	CLA	c	512	65/65	0.96	0.07	36,46,109,121	0
24	CLA	c	513	65/65	0.96	0.07	43,54,67,82	0
24	CLA	c	514	65/65	0.96	0.06	38,50,60,68	0
37	DGD	C	516	62/66	0.96	0.06	33,44,85,86	0
24	CLA	c	515	65/65	0.96	0.07	43,55,73,80	0
24	CLA	D	403	65/65	0.96	0.07	39,49,99,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	a	410	65/65	0.96	0.07	29,40,99,105	0
24	CLA	d	403	65/65	0.96	0.07	39,49,98,106	0
37	DGD	c	519	62/66	0.96	0.07	37,46,91,95	0
25	PHO	A	409[A]	64/64	0.96	0.05	29,40,44,47	64
25	PHO	A	409[B]	64/64	0.96	0.05	30,39,44,49	64
24	CLA	C	503	65/65	0.96	0.06	39,50,59,65	0
24	CLA	B	607	65/65	0.96	0.07	31,43,85,91	0
24	CLA	B	611	65/65	0.96	0.06	35,44,50,57	0
26	BCR	B	619	40/40	0.96	0.05	26,36,55,58	0
24	CLA	b	617	65/65	0.96	0.05	26,34,42,50	0
24	CLA	b	618	65/65	0.96	0.05	32,42,51,56	0
26	BCR	C	515	40/40	0.96	0.06	39,53,60,63	0
24	CLA	B	614	65/65	0.96	0.06	25,35,63,75	0
39	HEM	e	102	43/43	0.96	0.10	53,76,114,130	0
25	PHO	a	411	64/64	0.97	0.05	26,34,40,45	0
28	GOL	V	204	6/6	0.97	0.07	55,61,65,65	0
24	CLA	B	605	65/65	0.97	0.05	25,35,67,69	0
24	CLA	B	606	65/65	0.97	0.05	28,37,50,52	0
24	CLA	a	409	65/65	0.97	0.05	27,32,48,57	0
26	BCR	B	618	40/40	0.97	0.04	28,37,45,45	0
24	CLA	C	502	65/65	0.97	0.05	36,44,55,70	0
24	CLA	A	405	65/65	0.97	0.05	25,32,41,57	0
24	CLA	B	608	65/65	0.97	0.05	24,33,44,53	0
24	CLA	b	612	65/65	0.97	0.06	33,44,51,57	0
24	CLA	c	509	65/65	0.97	0.06	34,45,64,72	0
24	CLA	b	613	65/65	0.97	0.06	34,43,52,58	0
24	CLA	b	614	65/65	0.97	0.06	26,39,70,74	0
24	CLA	b	615	65/65	0.97	0.06	28,38,50,52	0
24	CLA	B	609	65/65	0.97	0.05	32,42,52,54	0
26	BCR	a	413	40/40	0.97	0.04	28,38,46,47	0
24	CLA	B	610	65/65	0.97	0.05	35,46,55,71	0
24	CLA	A	406	65/65	0.97	0.05	24,32,38,45	0
26	BCR	b	629	40/40	0.97	0.05	37,48,60,64	0
24	CLA	B	612	65/65	0.97	0.05	26,35,47,53	0
36	HTG	B	623	19/19	0.97	0.06	37,51,65,70	0
38	LHG	D	408	49/49	0.97	0.06	30,41,62,74	0
24	CLA	B	613	65/65	0.97	0.05	27,36,45,47	0
24	CLA	d	401	65/65	0.97	0.04	26,32,41,51	0
38	LHG	L	101	49/49	0.97	0.05	31,43,54,61	0
22	CL	v	204	1/1	0.97	0.07	88,88,88,88	0
25	PHO	A	408	64/64	0.97	0.04	26,32,38,43	0
38	LHG	d	407	49/49	0.97	0.06	30,39,57,75	0

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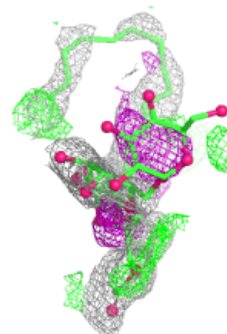
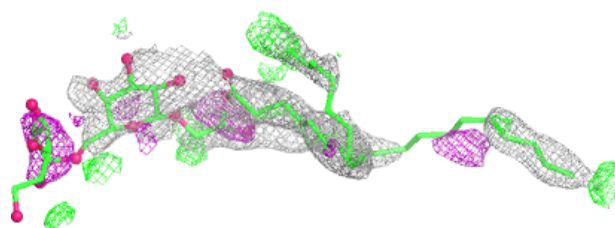
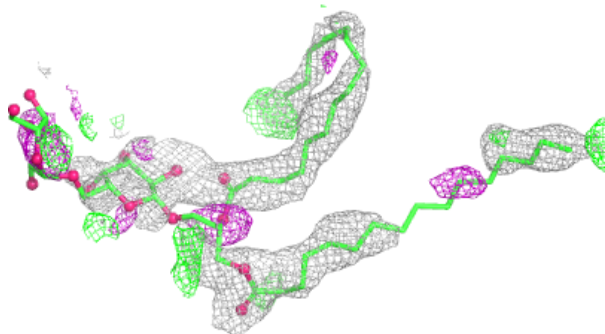
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	B	604	65/65	0.97	0.05	33,43,50,53	0
38	LHG	l	101	49/49	0.97	0.06	33,44,53,59	0
24	CLA	B	616	65/65	0.97	0.06	33,44,60,68	0
40	MG	j	103	1/1	0.97	0.07	55,55,55,55	0
22	CL	A	403[B]	1/1	0.98	0.08	33,33,33,33	1
28	GOL	c	501	6/6	0.98	0.07	43,46,52,53	0
22	CL	A	403[A]	1/1	0.98	0.08	33,33,33,33	1
24	CLA	d	402	65/65	0.98	0.05	26,35,54,64	0
24	CLA	D	402	65/65	0.98	0.05	24,33,52,57	0
22	CL	a	408[A]	1/1	0.98	0.03	40,40,40,40	1
39	HEM	F	102	43/43	0.98	0.06	46,64,75,83	0
35	CA	F	104	1/1	0.98	0.04	82,82,82,82	0
40	MG	J	102	1/1	0.98	0.04	50,50,50,50	0
22	CL	a	408[B]	1/1	0.98	0.03	38,38,38,38	1
41	HEC	V	206	43/43	0.98	0.05	34,39,47,50	0
41	HEC	v	205	43/43	0.98	0.05	41,49,55,57	0
22	CL	a	407[B]	1/1	0.99	0.04	33,33,33,33	1
35	CA	c	503	1/1	0.99	0.09	63,63,63,63	0
35	CA	c	504	1/1	0.99	0.03	73,73,73,73	0
31	OEY	A	419[B]	11/11	0.99	0.03	31,36,42,47	11
35	CA	o	302	1/1	0.99	0.03	86,86,86,86	0
35	CA	C	526	1/1	0.99	0.06	67,67,67,67	0
22	CL	a	407[A]	1/1	0.99	0.04	34,34,34,34	1
35	CA	O	302	1/1	0.99	0.02	80,80,80,80	0
21	FE2	A	401[A]	1/1	1.00	0.01	45,45,45,45	1
21	FE2	A	401[B]	1/1	1.00	0.01	47,47,47,47	1
30	OEX	A	418[A]	10/10	1.00	0.02	31,35,38,46	10
30	OEX	a	417[A]	10/10	1.00	0.02	31,37,39,45	10
21	FE2	a	406[B]	1/1	1.00	0.01	46,46,46,46	0
31	OEY	a	418[B]	11/11	1.00	0.02	32,37,44,57	11
22	CL	A	402[A]	1/1	1.00	0.02	30,30,30,30	1
22	CL	A	402[B]	1/1	1.00	0.02	31,31,31,31	1

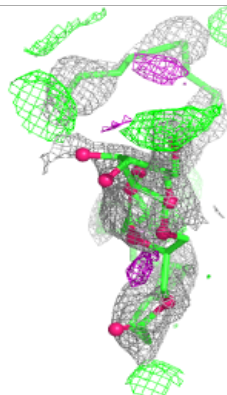
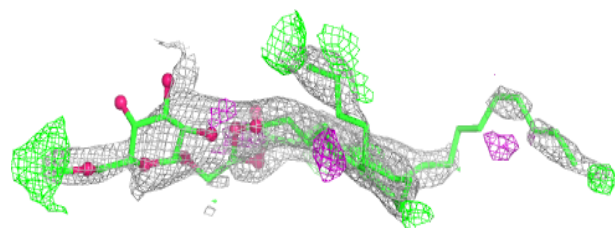
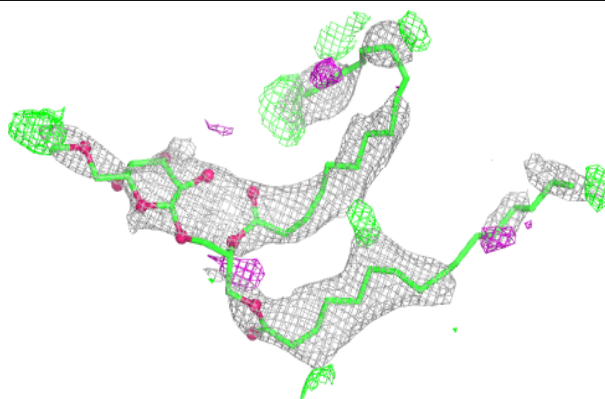
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DGD 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)

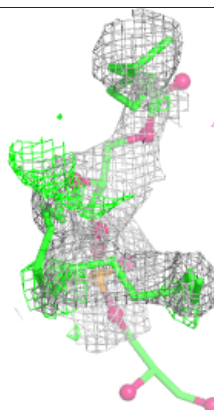
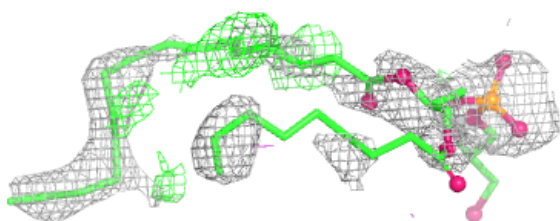
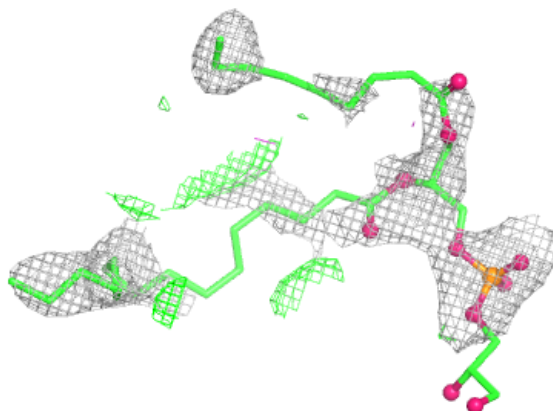
**Electron density around DGD D 406:**

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

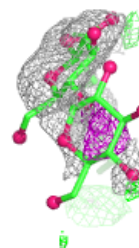
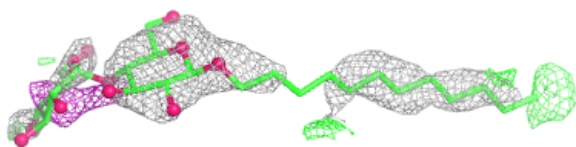
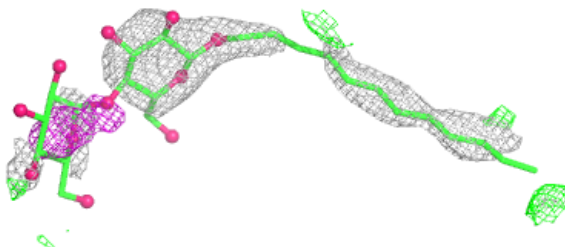


Electron density around LHG a 422:

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

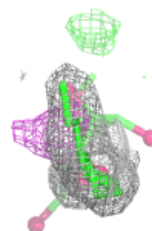
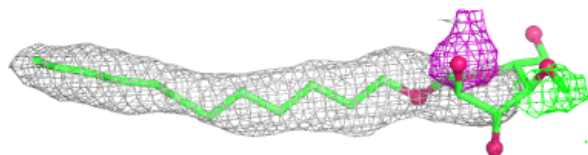
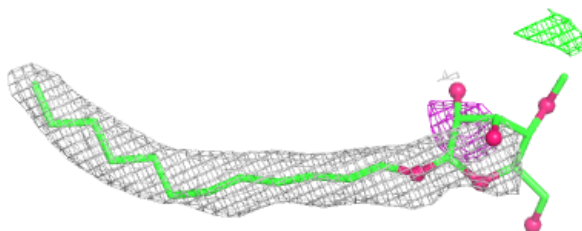
**Electron density around LMT F 101:**

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

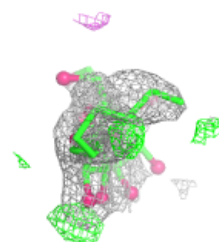
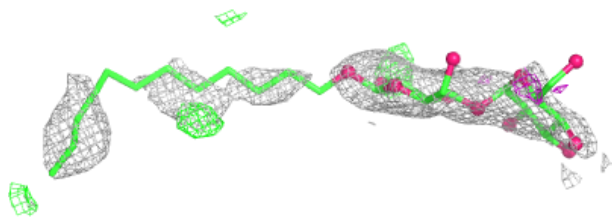
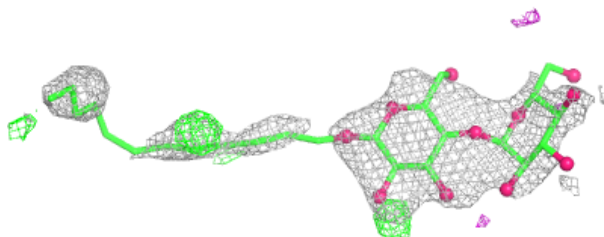


Electron density around LMT b 631:

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

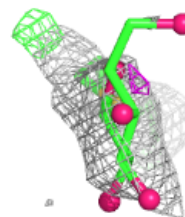
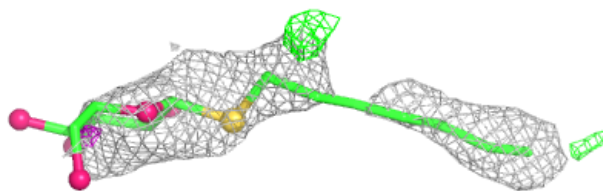
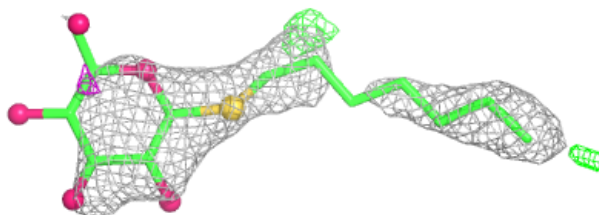
**Electron density around LMT a 421:**

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

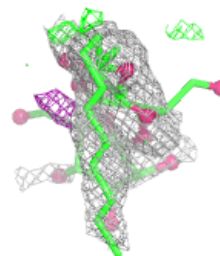
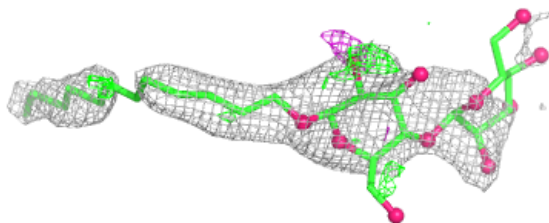
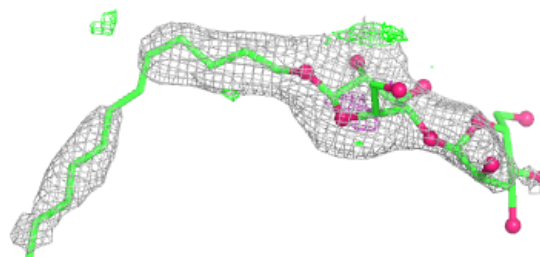


Electron density around HTG c 525:

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

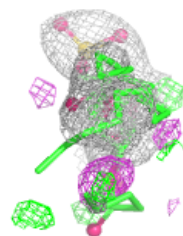
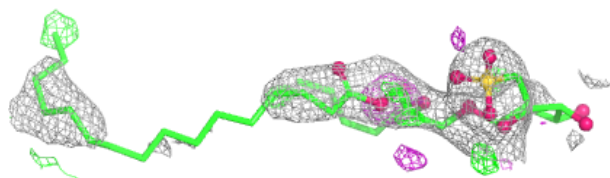
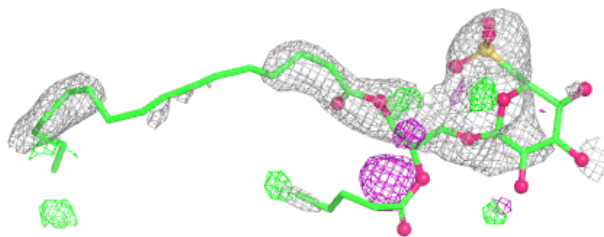
**Electron density around LMT C 521:**

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

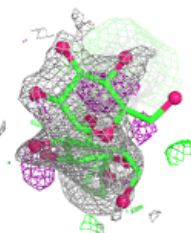
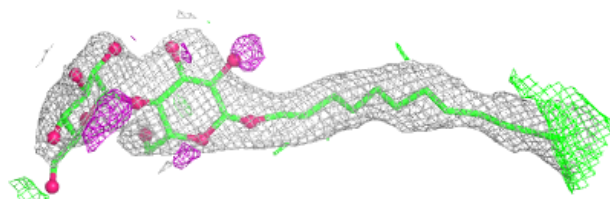
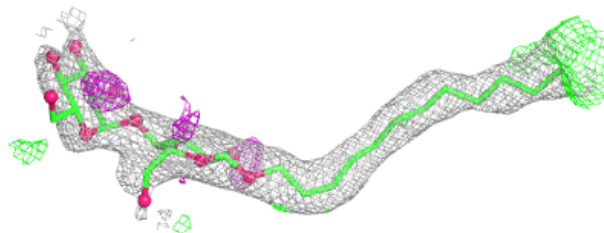


Electron density around SQD f 102:

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

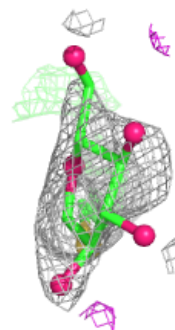
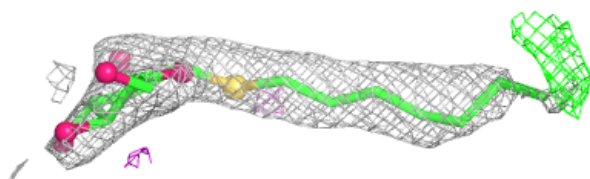
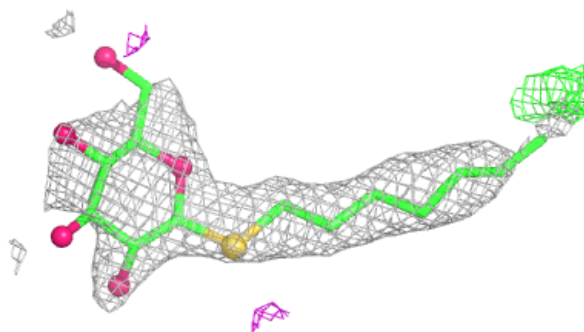
**Electron density around LMT A 417:**

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

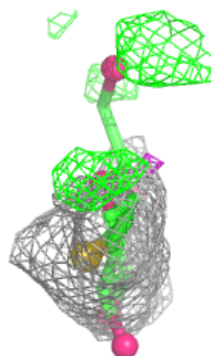
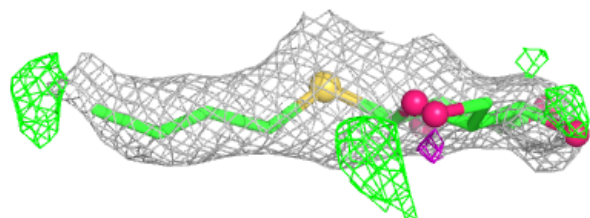
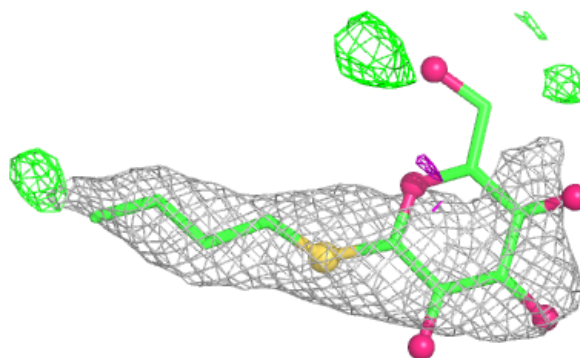


Electron density around HTG B 625:

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

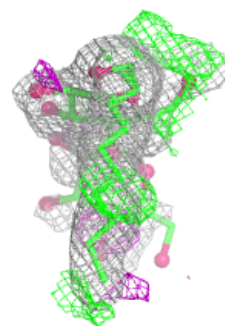
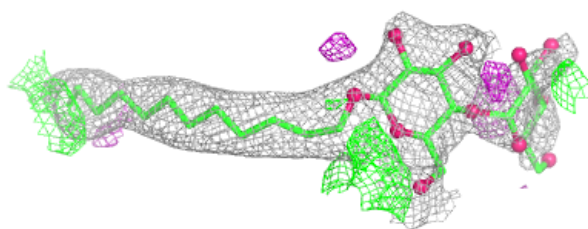
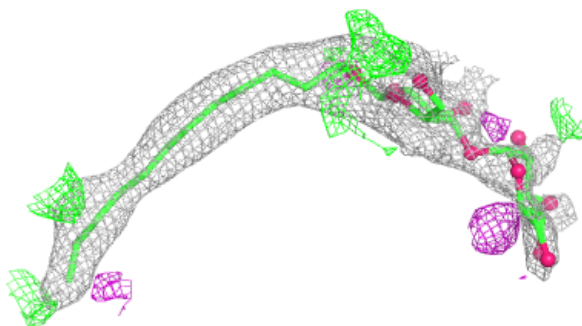
**Electron density around HTG H 101:**

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

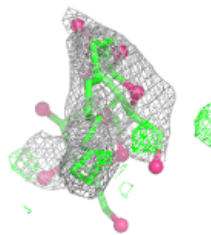
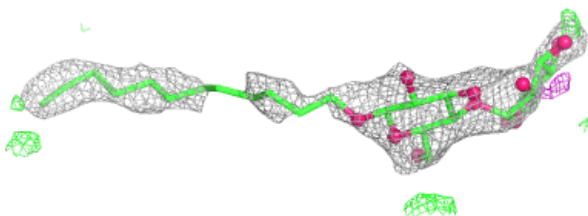
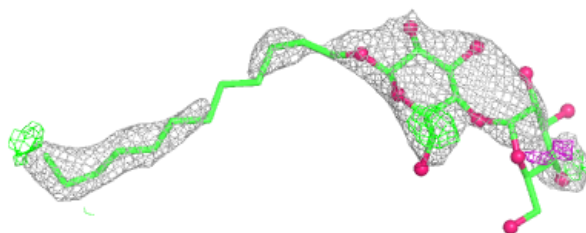


Electron density around LMT M 103:

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

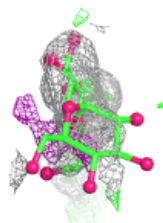
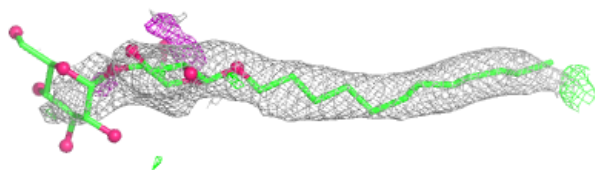
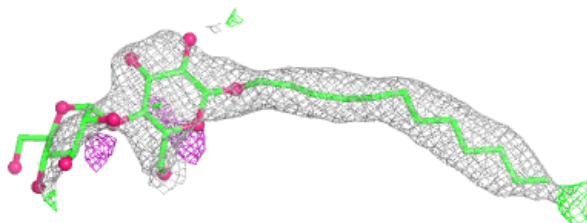
**Electron density around LMT f 103:**

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



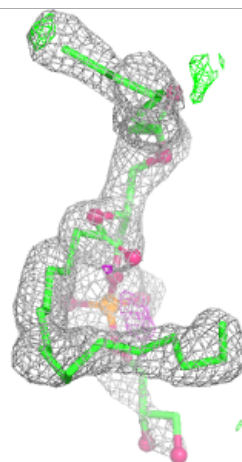
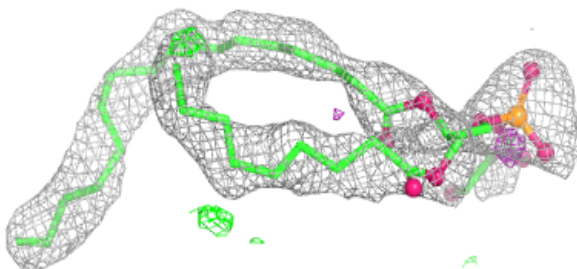
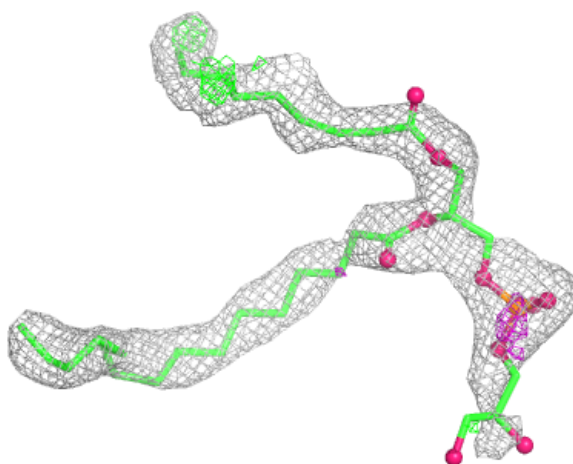
Electron density around LMT D 401:

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



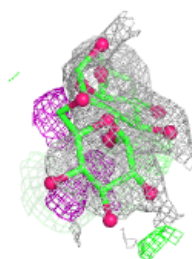
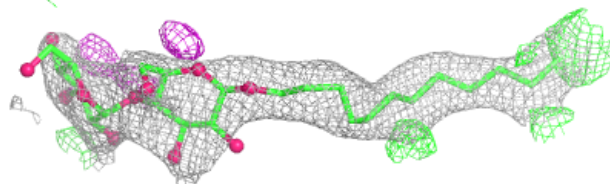
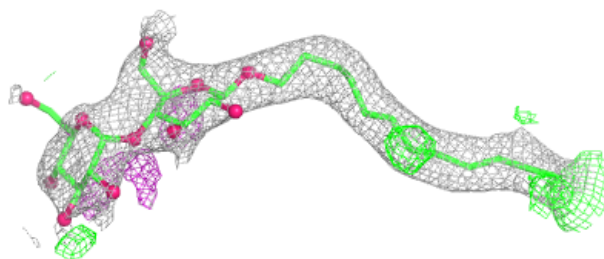
Electron density around LHG E 101:

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

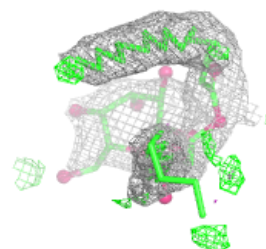
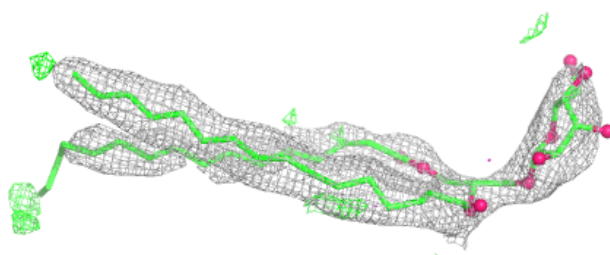
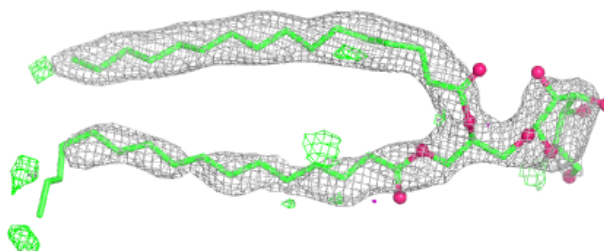


Electron density around LMT a 404:

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

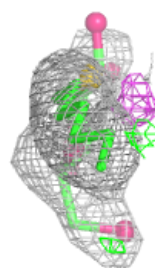
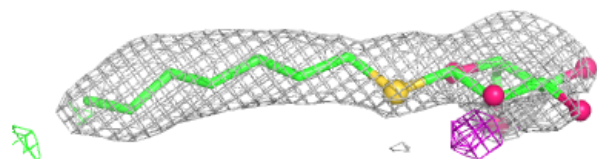
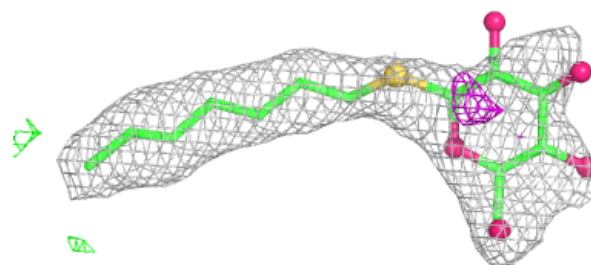
**Electron density around LMG C 520:**

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

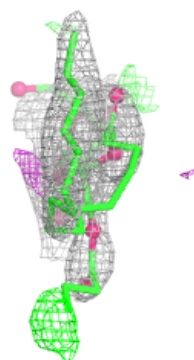
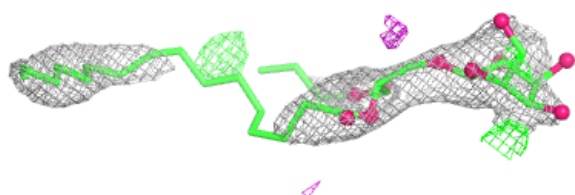
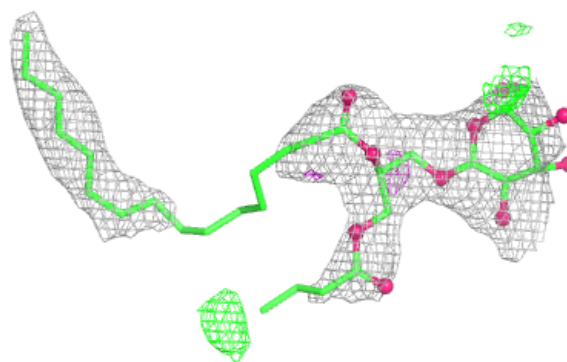


Electron density around HTG B 633:

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

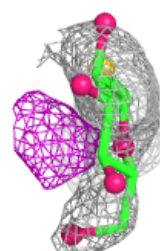
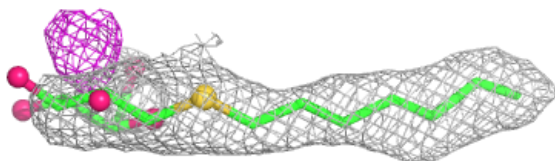
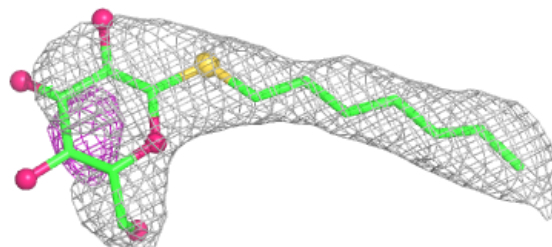
**Electron density around LMG z 101:**

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

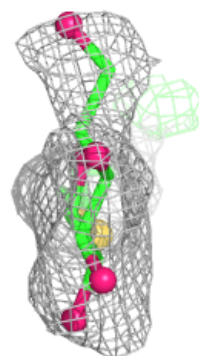
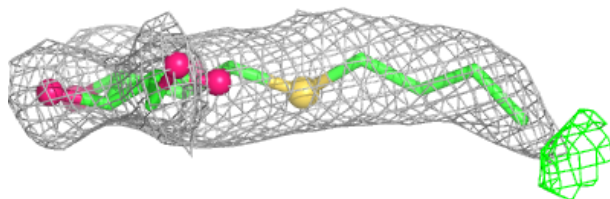
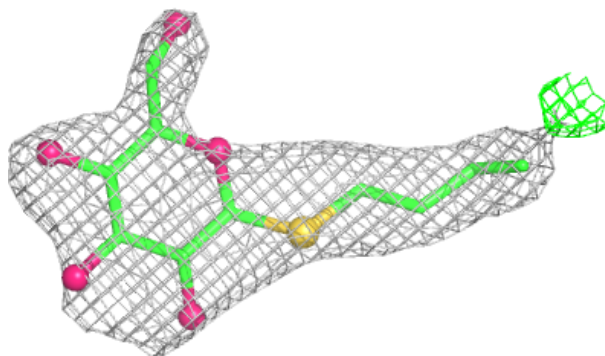


Electron density around HTG b 609:

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

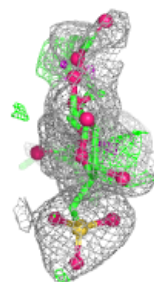
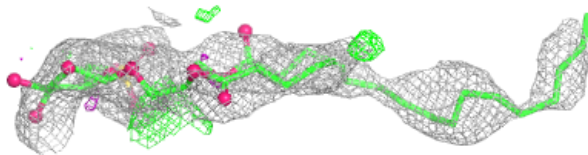
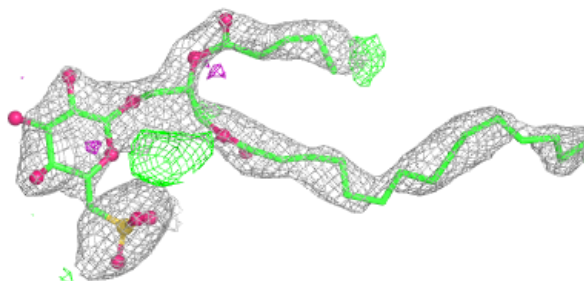
**Electron density around HTG d 411:**

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

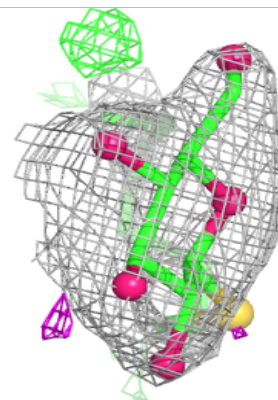
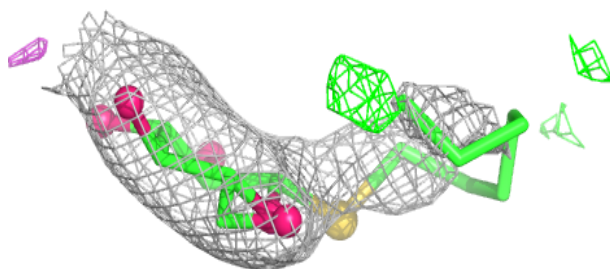
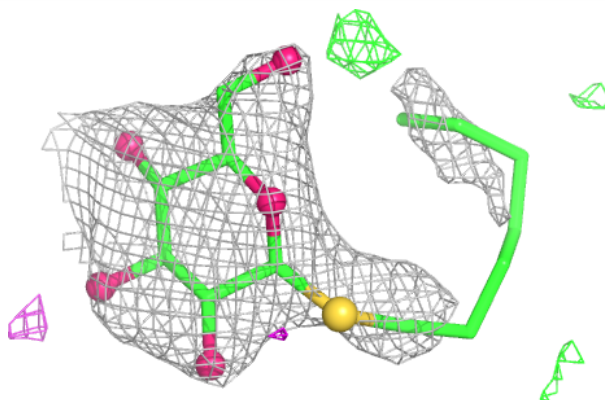


Electron density around SQD F 103:

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

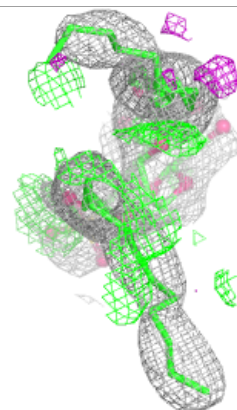
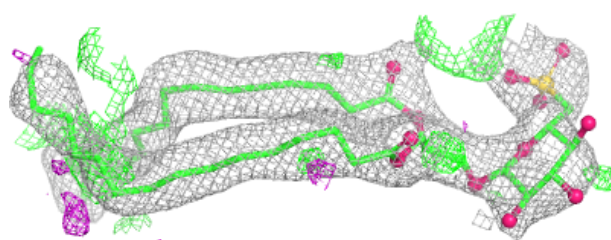
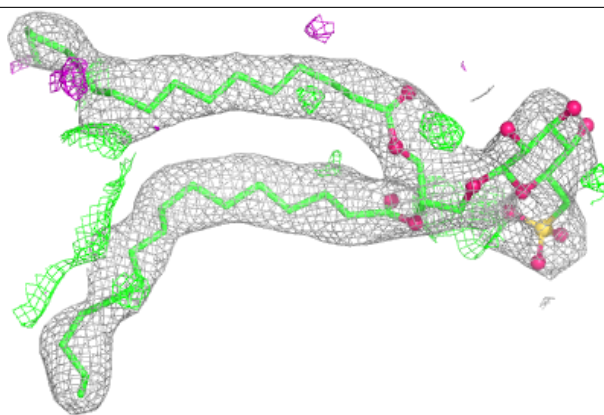
**Electron density around HTG V 207:**

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

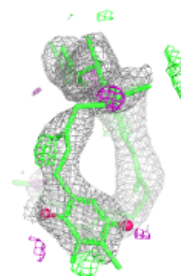
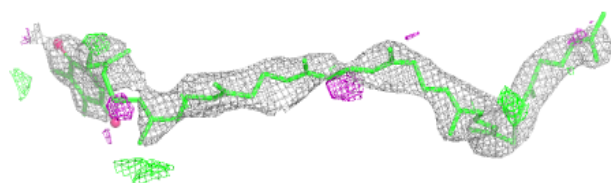
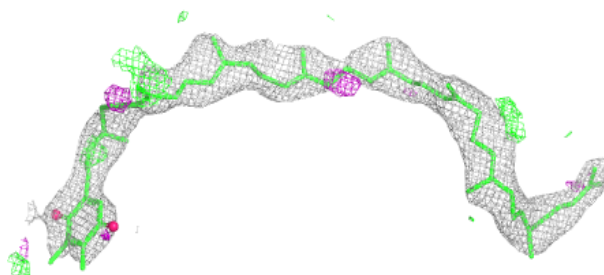


Electron density around SQD B 621:

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

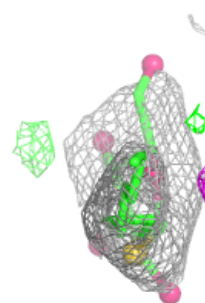
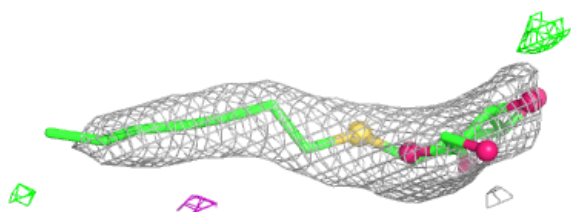
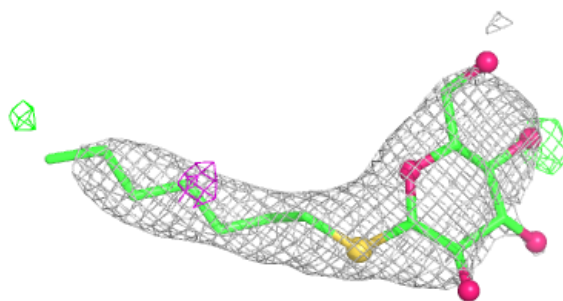
**Electron density around PL9 A 420 (B):**

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

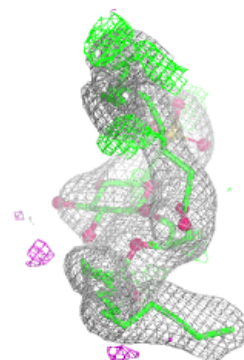
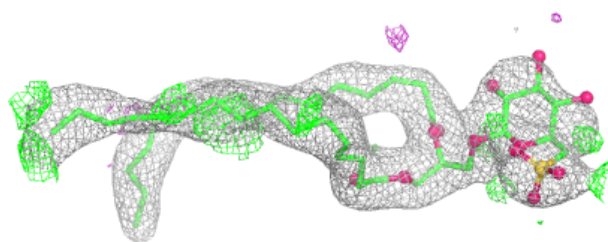
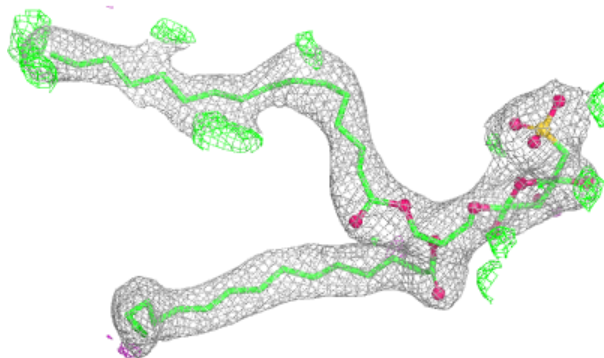


Electron density around HTG b 633:

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

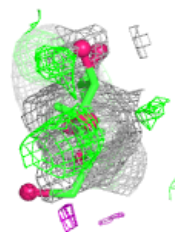
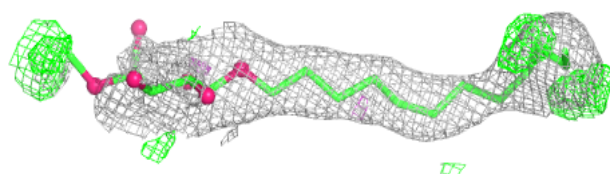
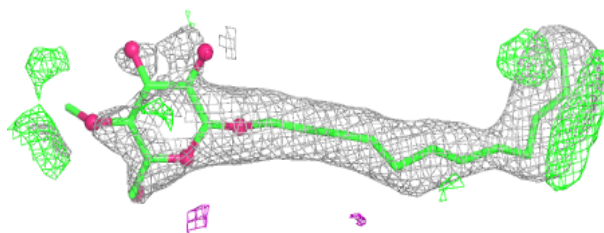
**Electron density around SQD a 405:**

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

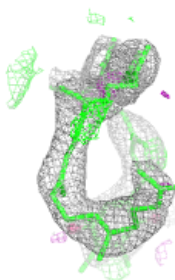
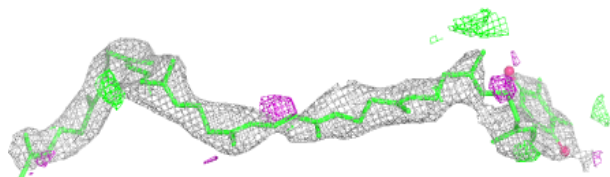
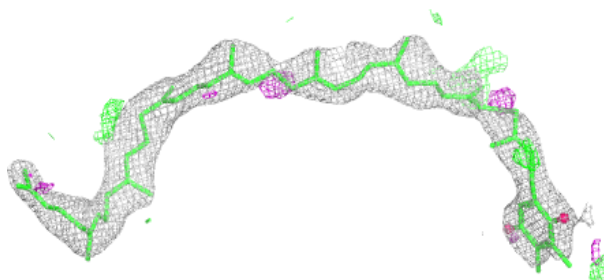


Electron density around LMT B 635:

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

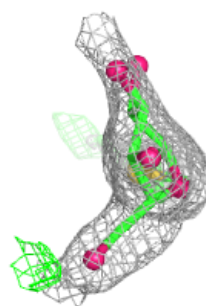
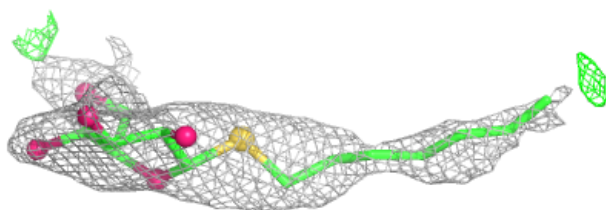
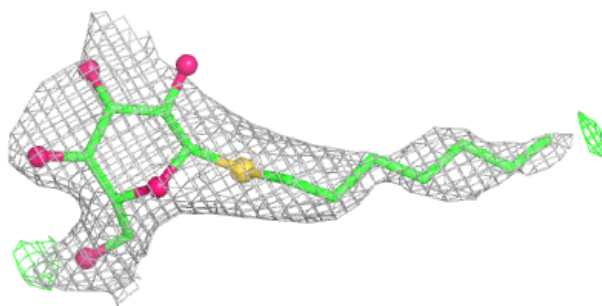
**Electron density around PL9 A 420 (A):**

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

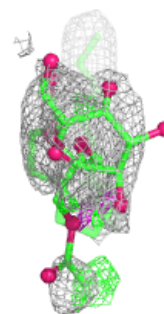
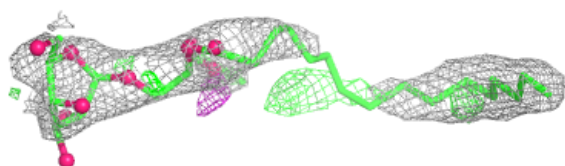
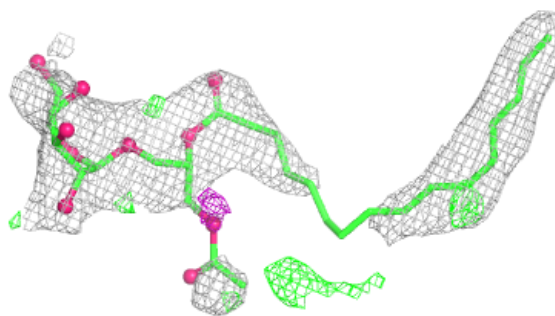


Electron density around HTG C 523:

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

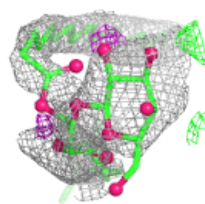
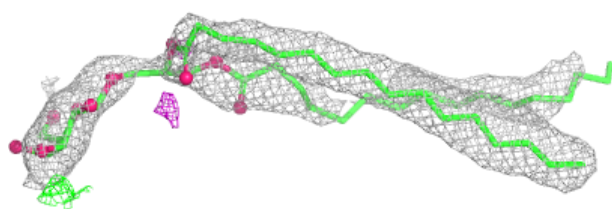
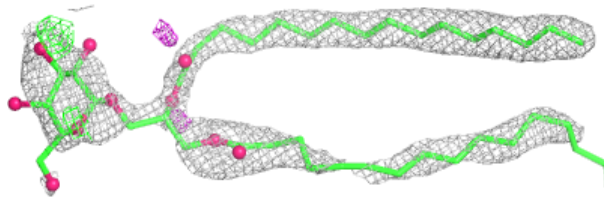
**Electron density around LMG Z 101:**

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

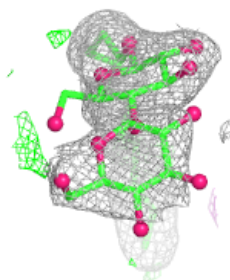
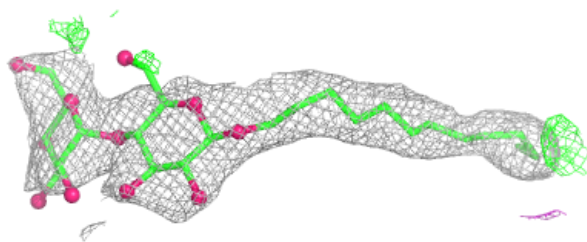
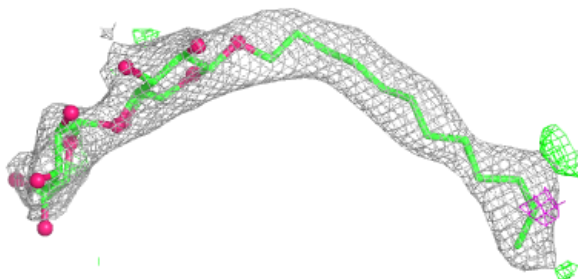


Electron density around LMG c 523:

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

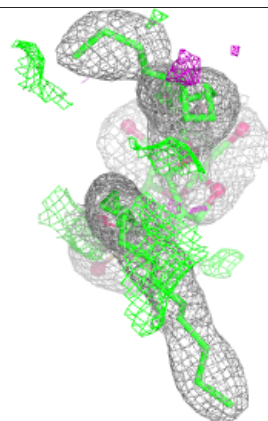
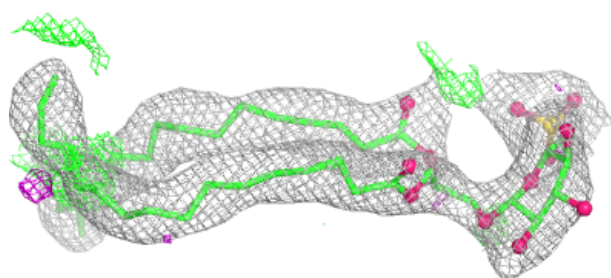
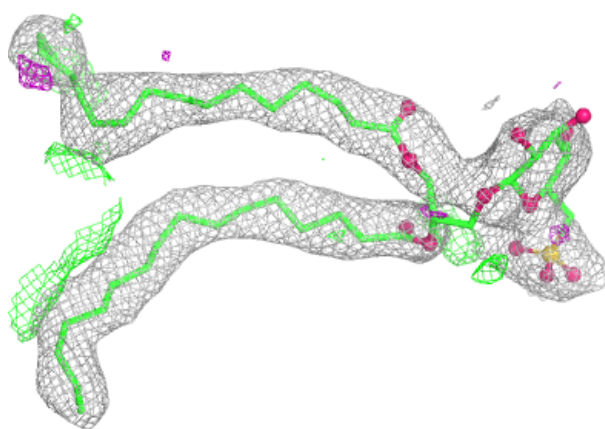
**Electron density around LMT m 102:**

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

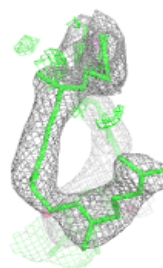
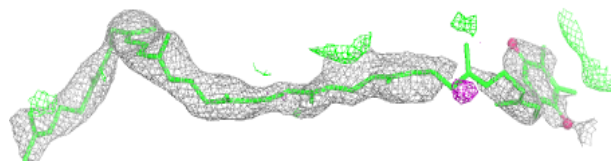
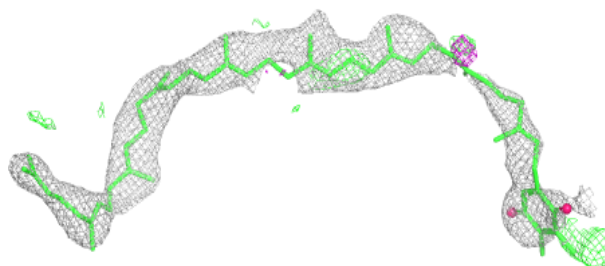


Electron density around SQD b 601:

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

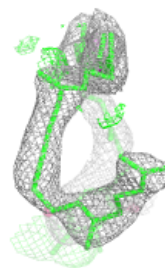
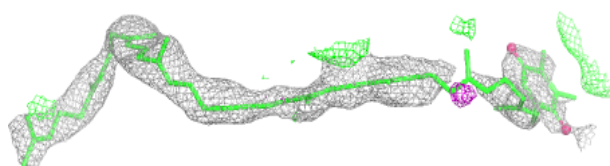
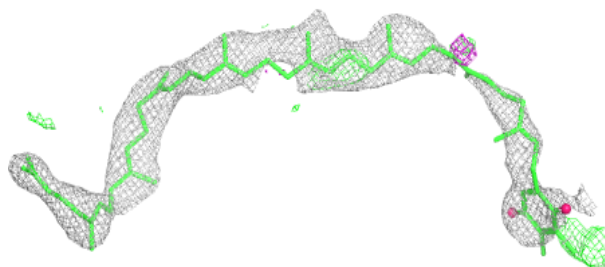
**Electron density around PL9 a 416 (A):**

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

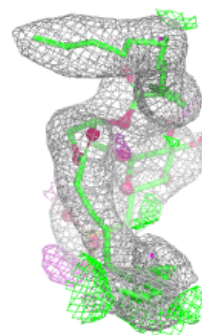
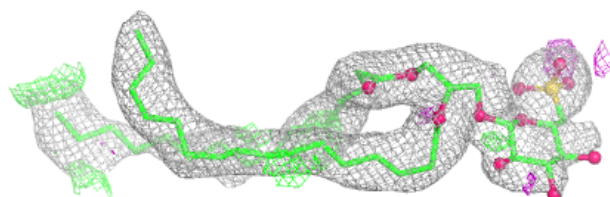
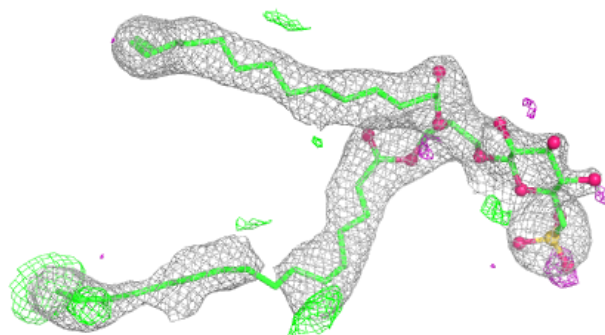


Electron density around PL9 a 416 (B):

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

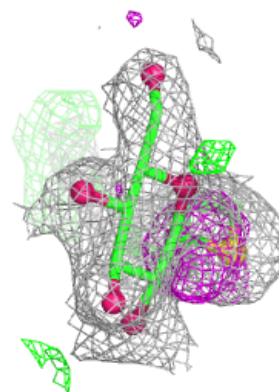
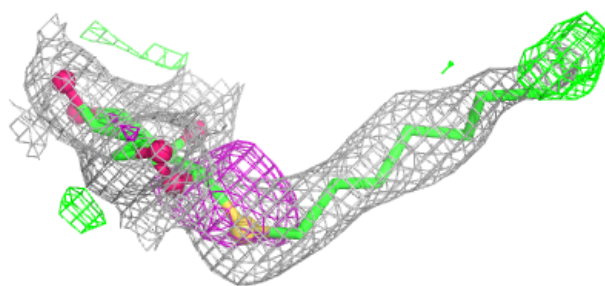
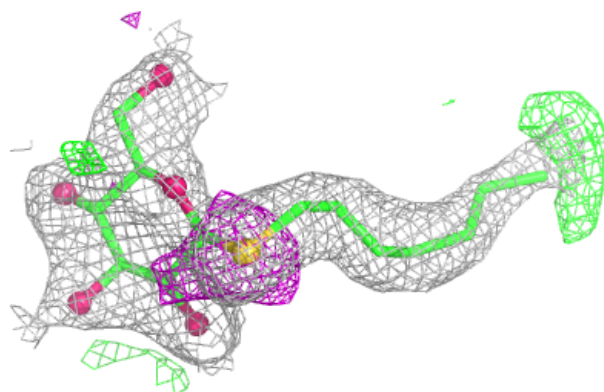
**Electron density around SQD A 416:**

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

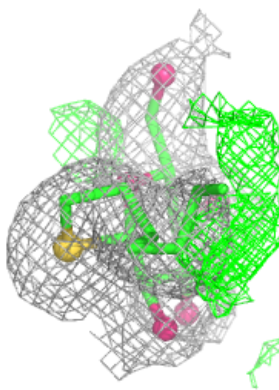
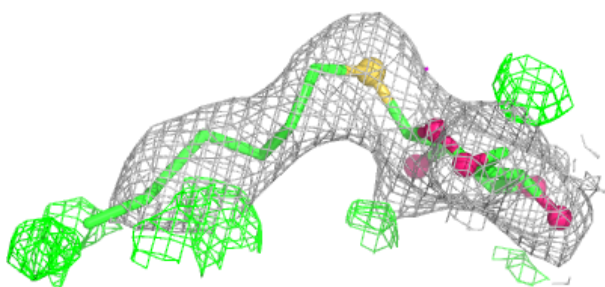
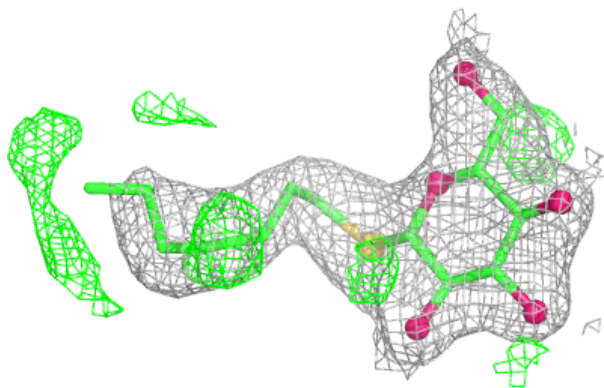


Electron density around HTG b 632:

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

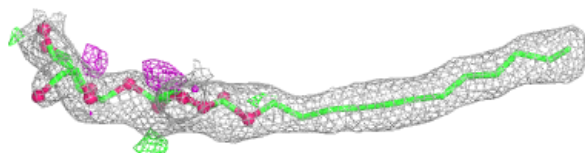
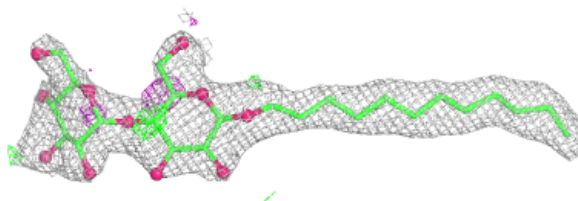
**Electron density around HTG B 624:**

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

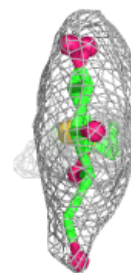
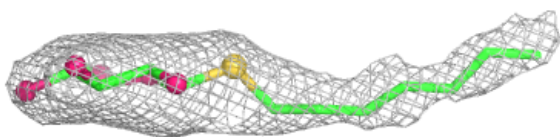
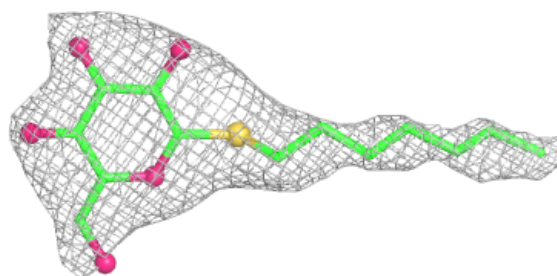


Electron density around LMT M 104:

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

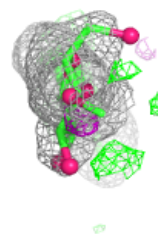
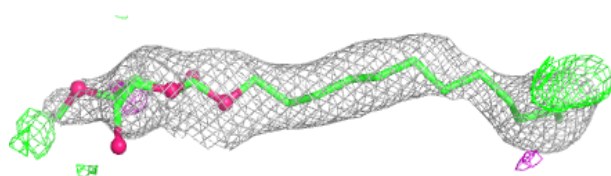
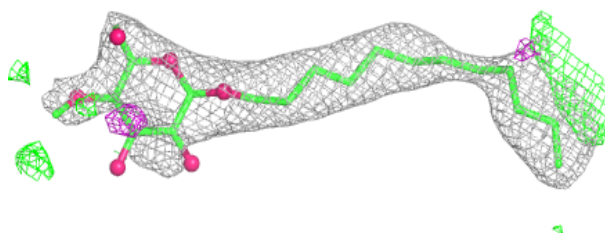
**Electron density around HTG c 524:**

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

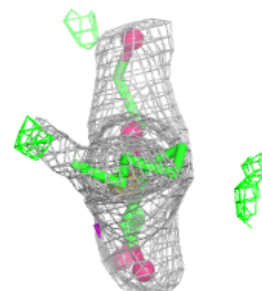
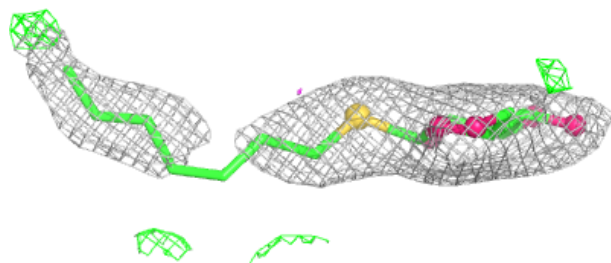
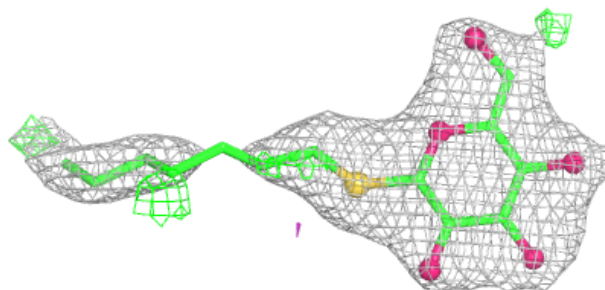


Electron density around LMT T 104:

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

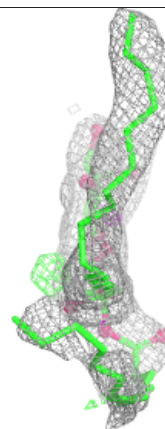
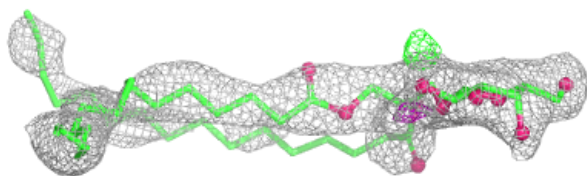
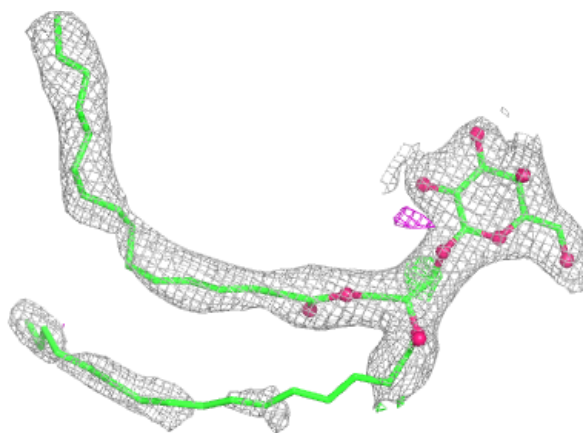
**Electron density around HTG C 522:**

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

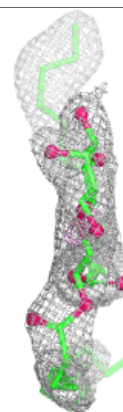
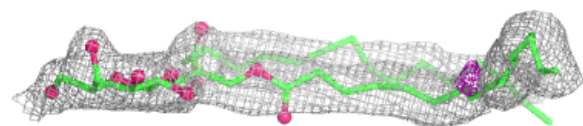
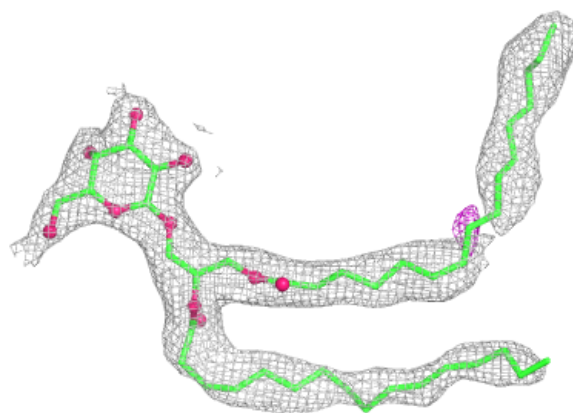


Electron density around LMG c 522:

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

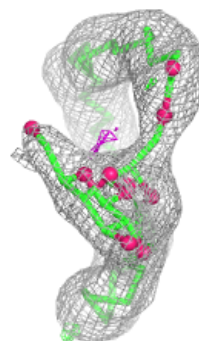
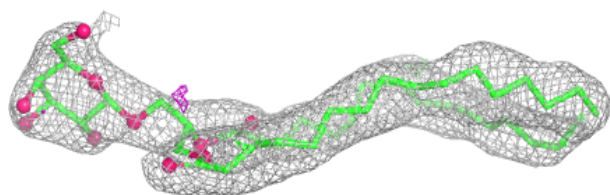
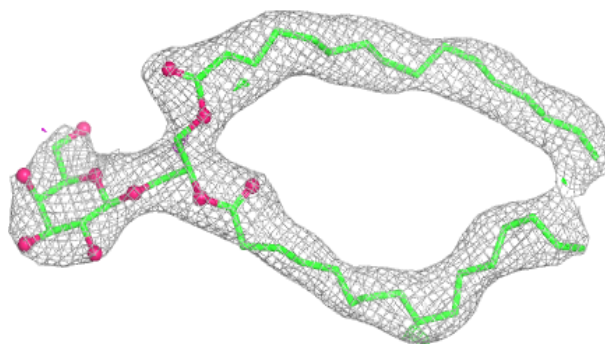
**Electron density around LMG C 519:**

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

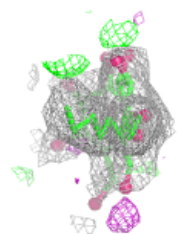
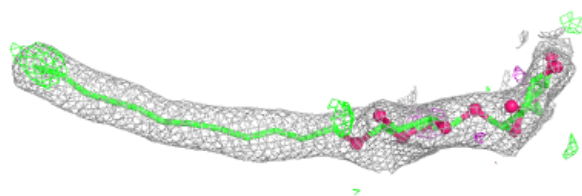
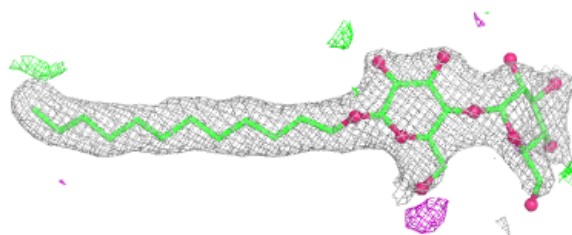


Electron density around LMG a 415:

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

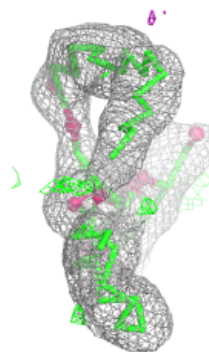
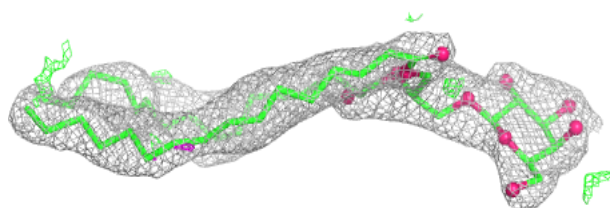
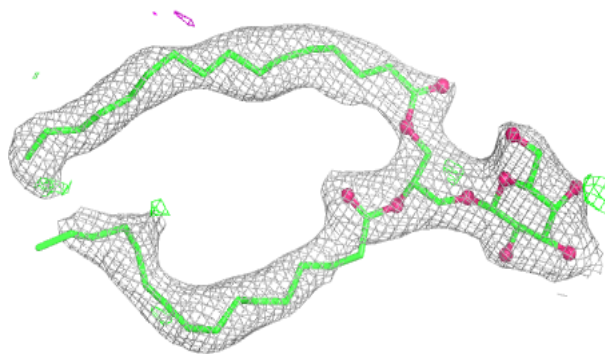
**Electron density around LMT M 101:**

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

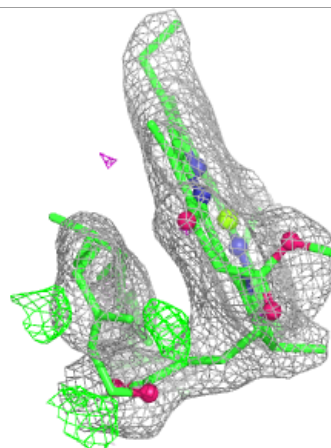
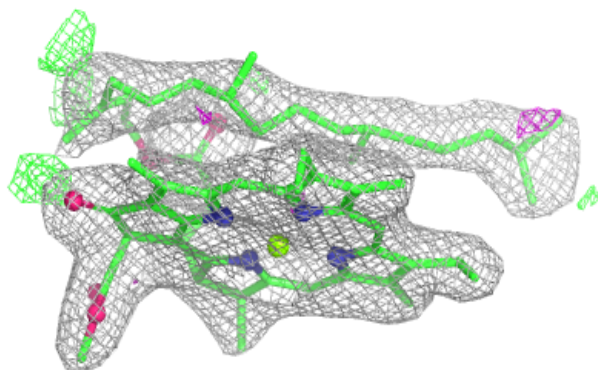
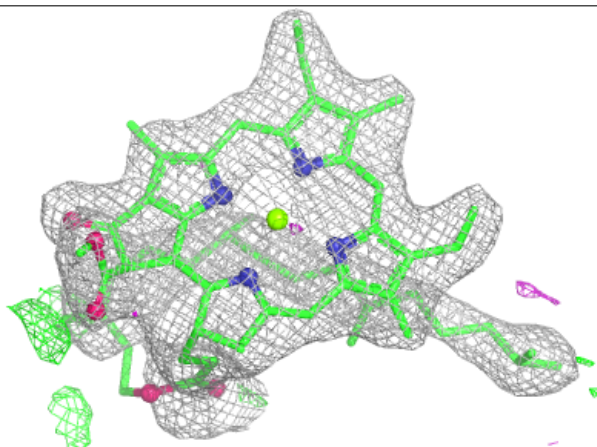


Electron density around LMG A 422:

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

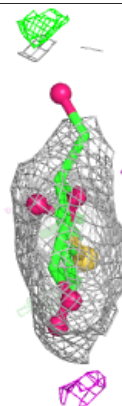
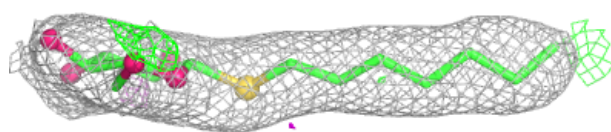
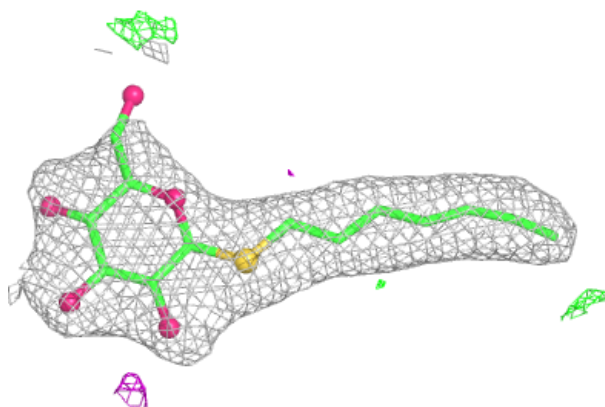
**Electron density around CLA b 611:**

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

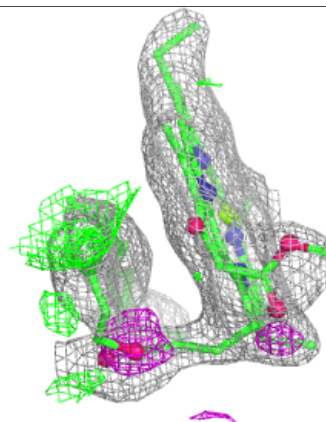
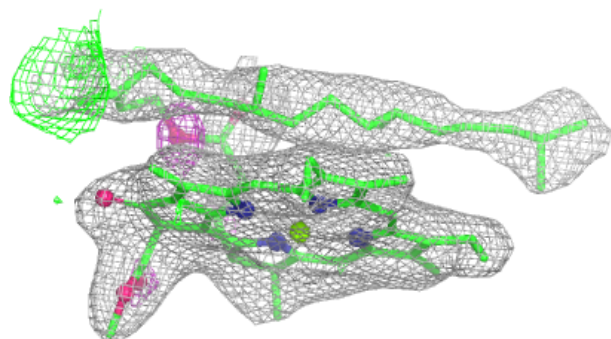
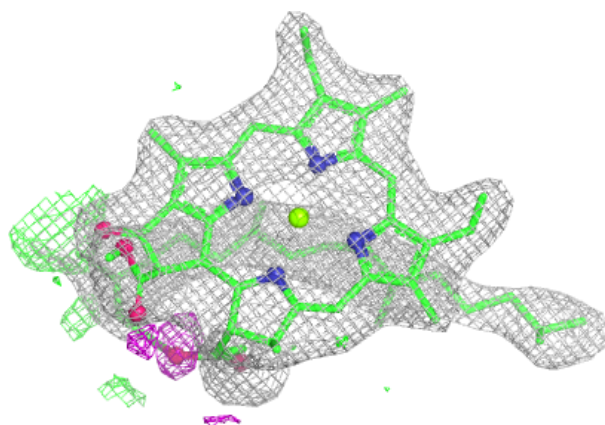


Electron density around HTG B 632:

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

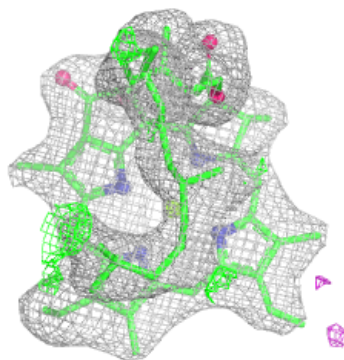
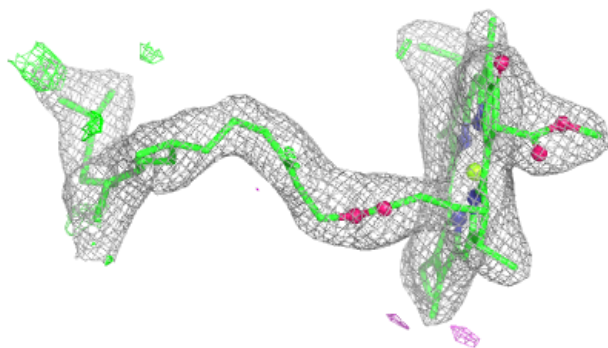
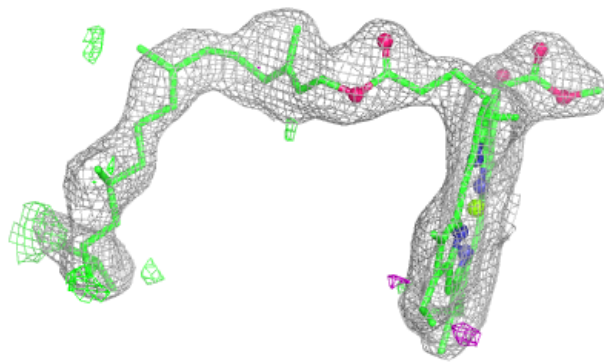
**Electron density around CLA B 602:**

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

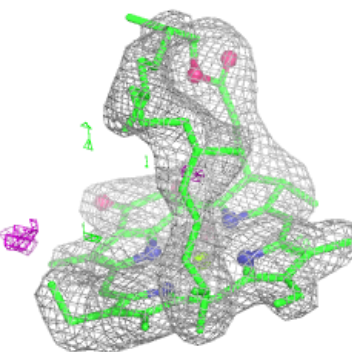
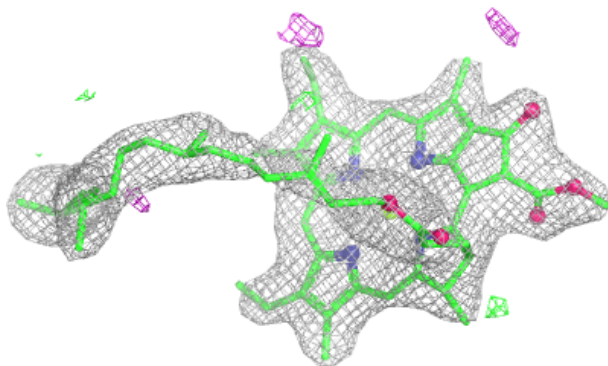
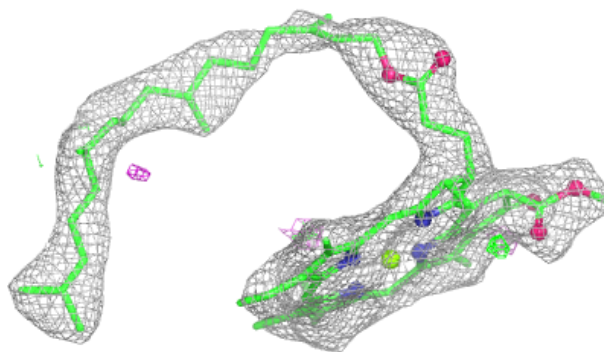


Electron density around CLA C 506:

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

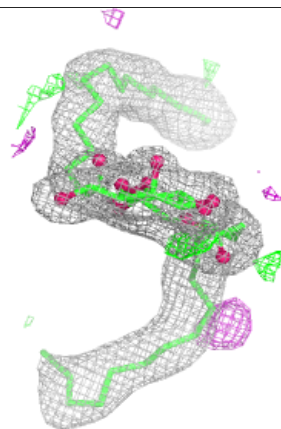
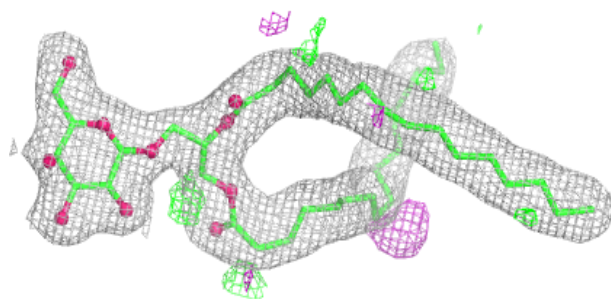
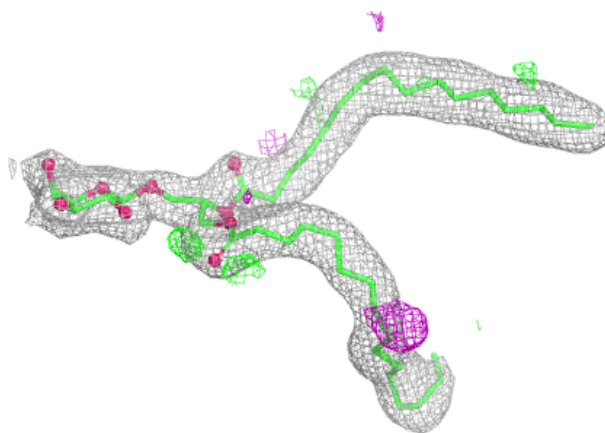
**Electron density around CLA C 513:**

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

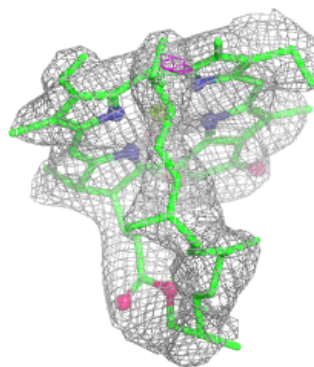
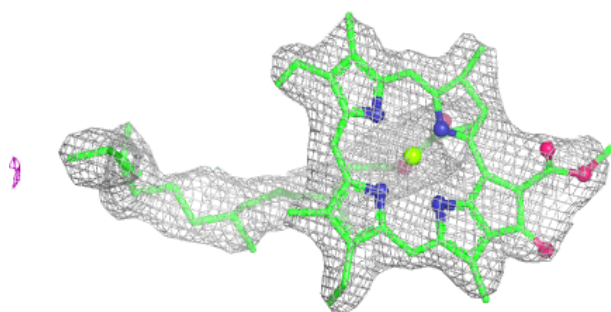
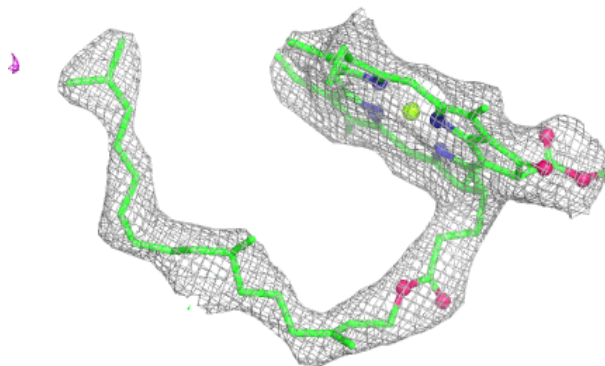


Electron density around LMG b 630:

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

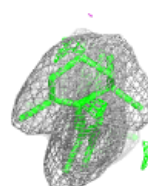
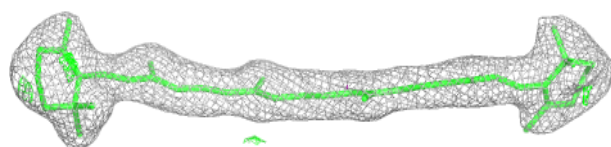
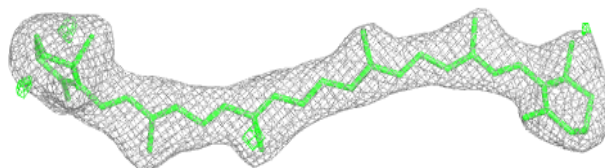
**Electron density around CLA c 517:**

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

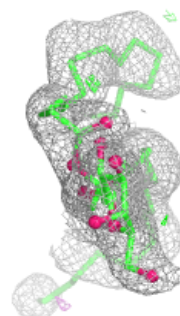
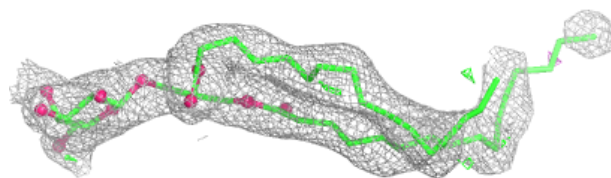
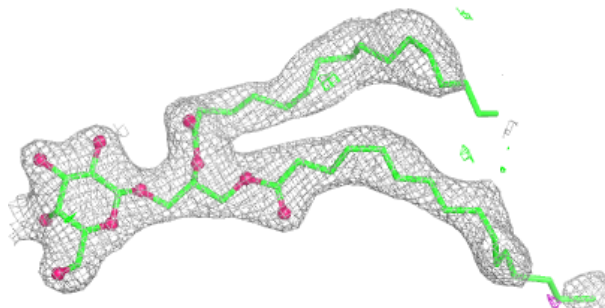


Electron density around BCR y 101:

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

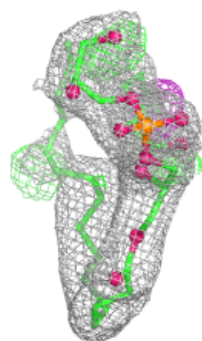
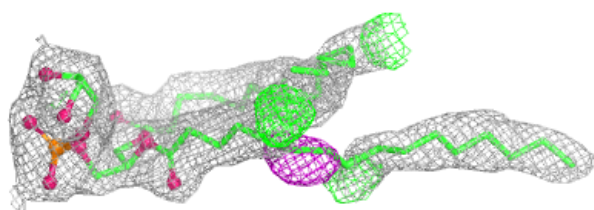
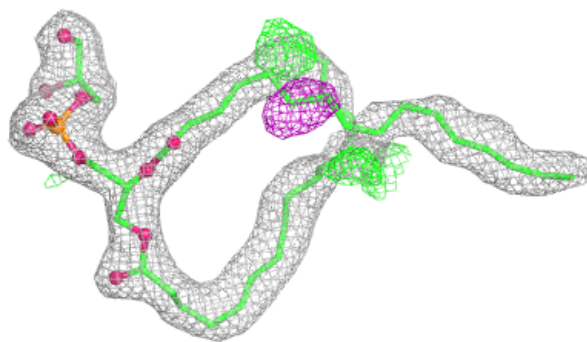
**Electron density around LMG j 101:**

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



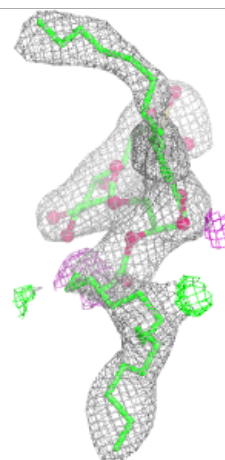
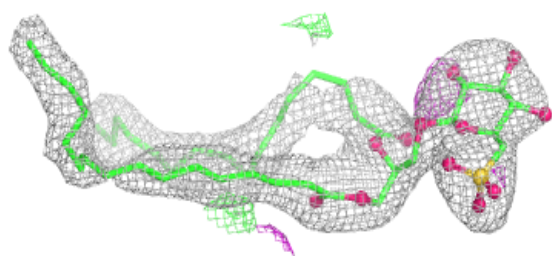
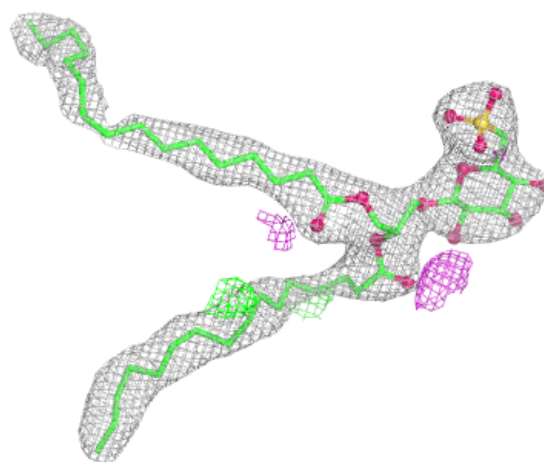
Electron density around LHG D 409:

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



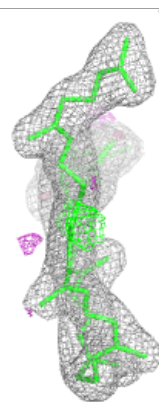
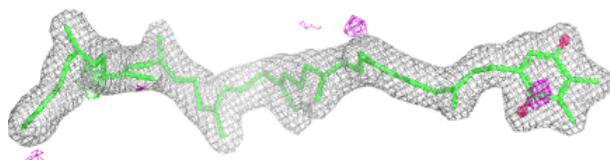
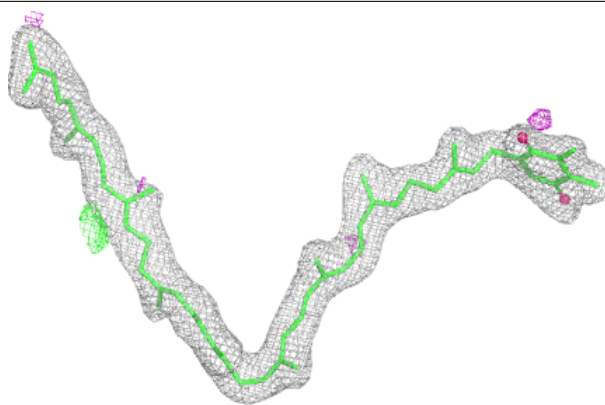
Electron density around SQD A 412:

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

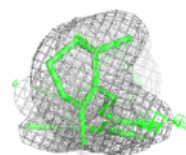
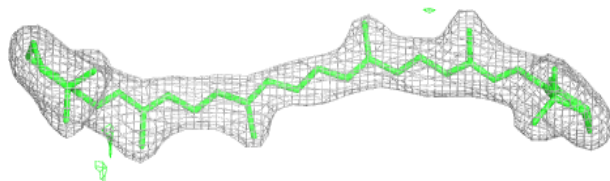
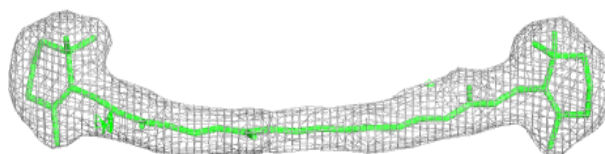


Electron density around PL9 D 405 (B):

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

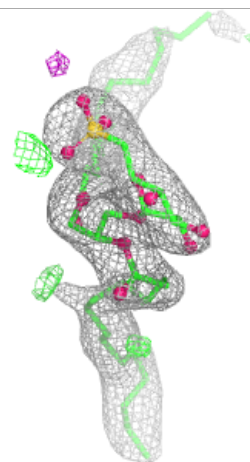
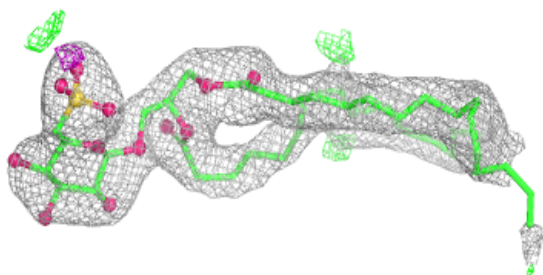
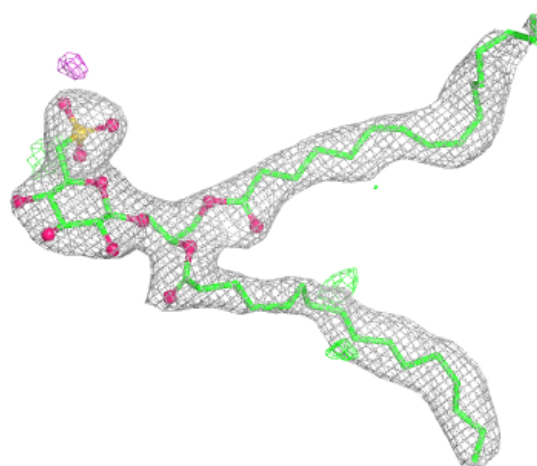
**Electron density around BCR K 101:**

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



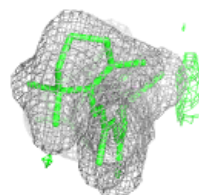
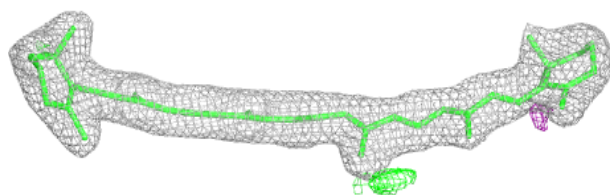
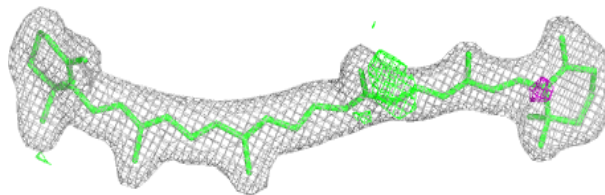
Electron density around SQD a 414:

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

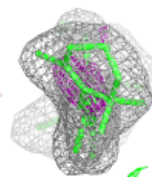
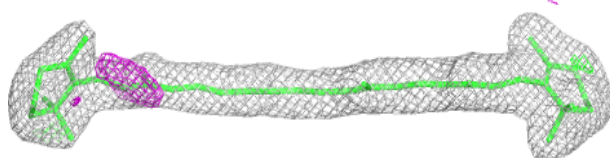
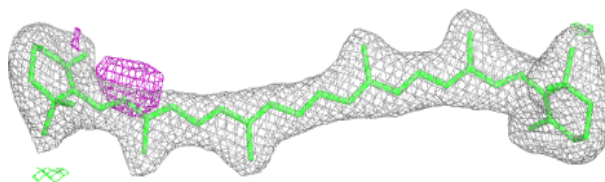


Electron density around BCR T 103:

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

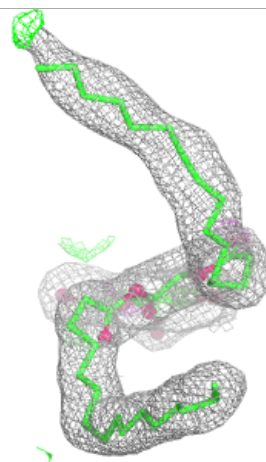
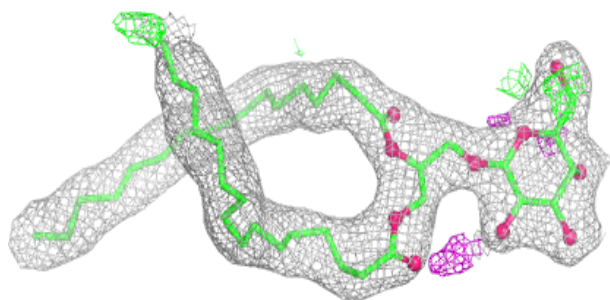
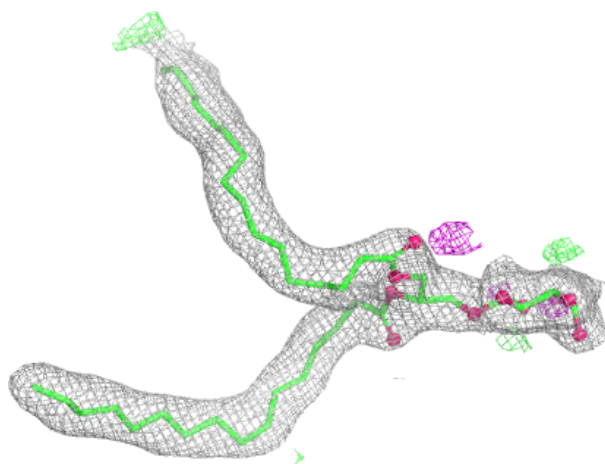
**Electron density around BCR b 628:**

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



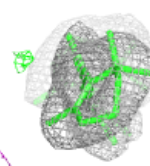
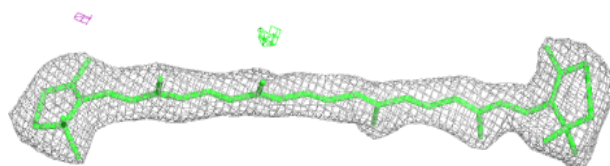
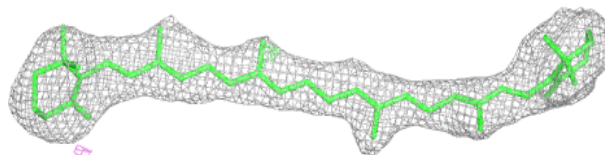
Electron density around LMG B 622:

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

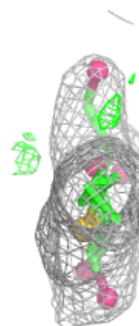
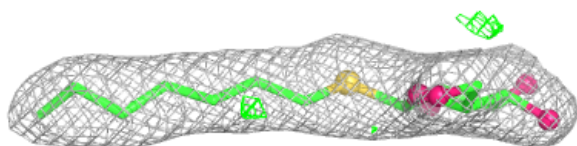
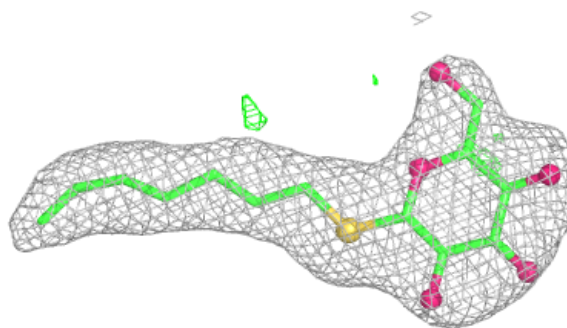


Electron density around BCR c 527:

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

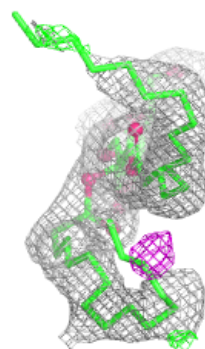
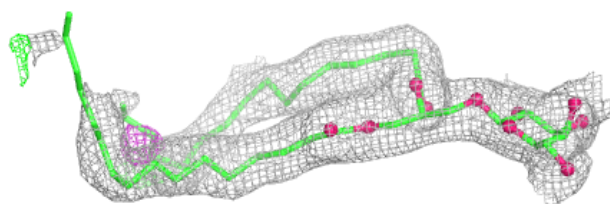
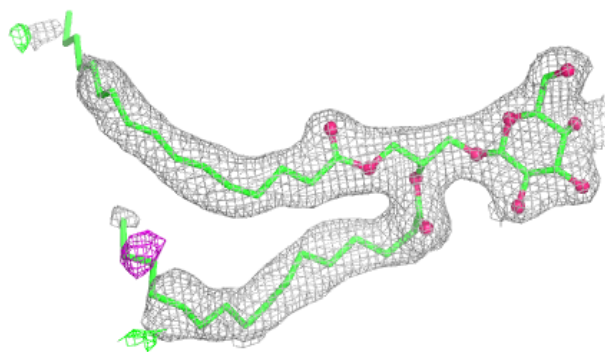
**Electron density around HTG b 608:**

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

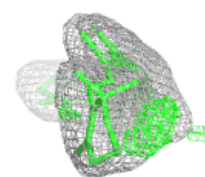
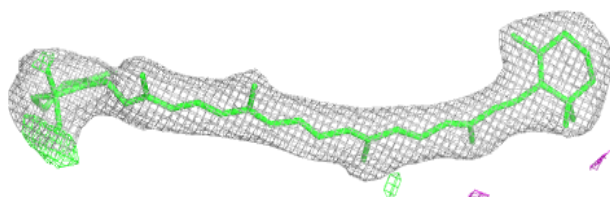
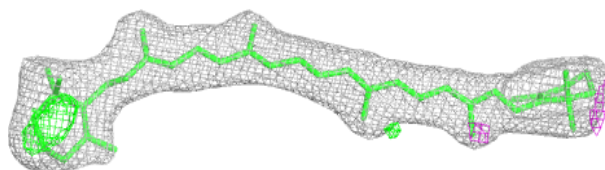


Electron density around LMG D 412:

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

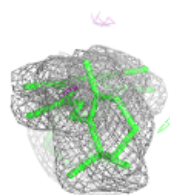
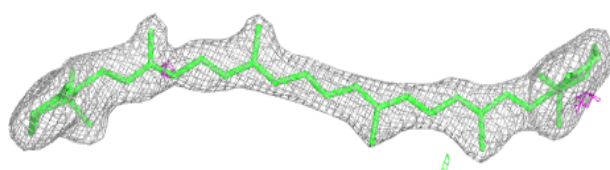
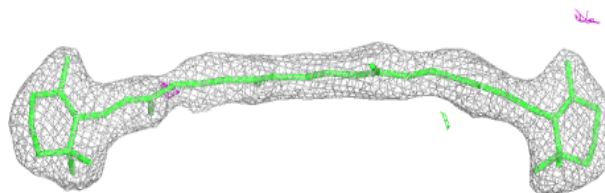
**Electron density around BCR d 404:**

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

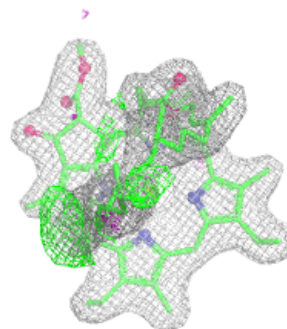
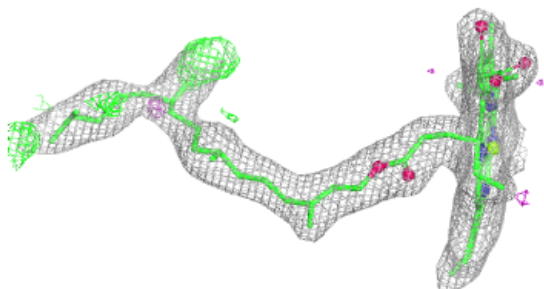
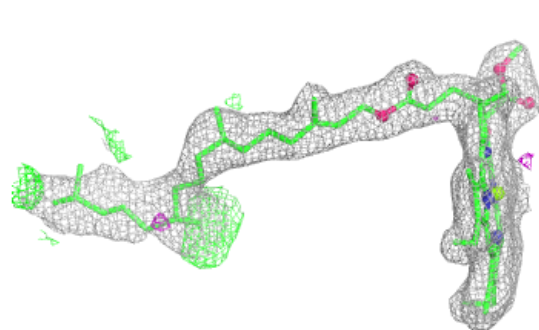


Electron density around BCR k 101:

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

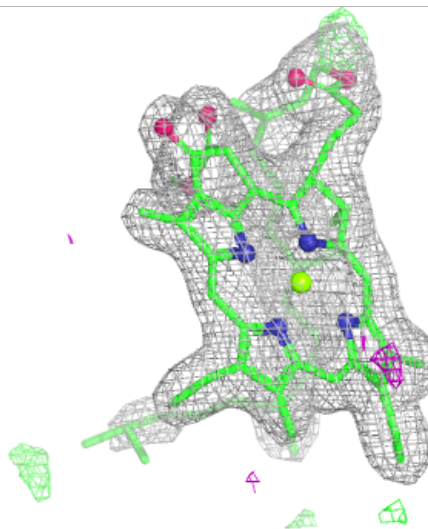
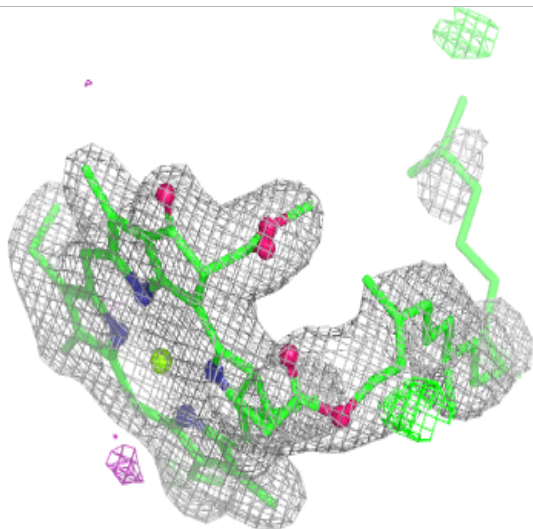
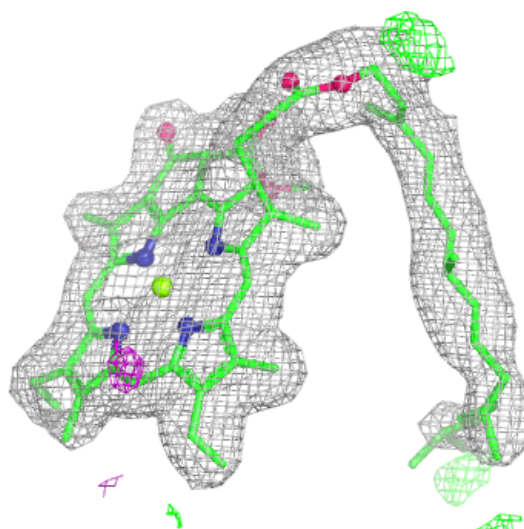
**Electron density around CLA b 616:**

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



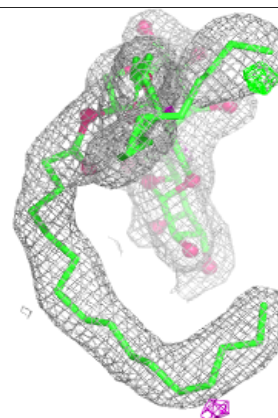
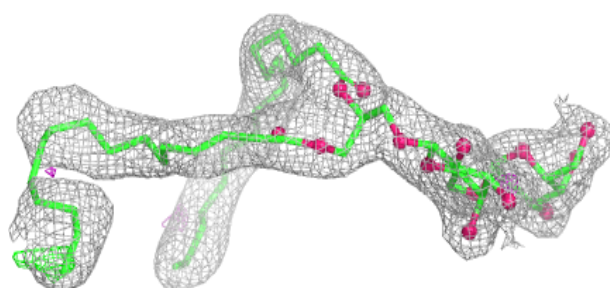
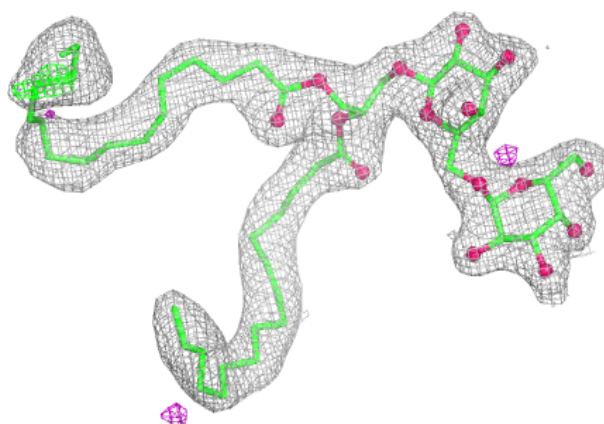
Electron density around CLA b 626:

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

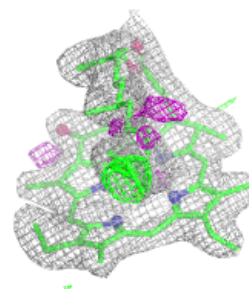
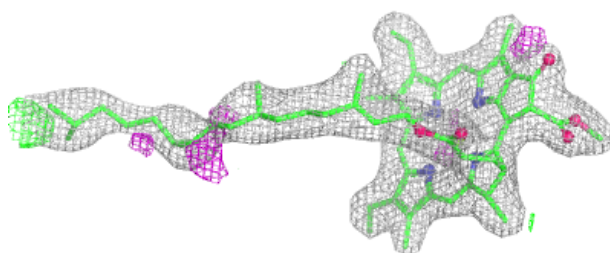
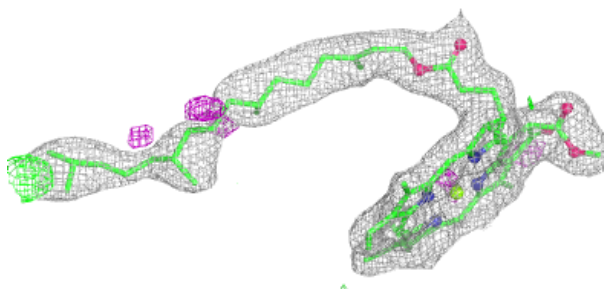


Electron density around DGD C 517:

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

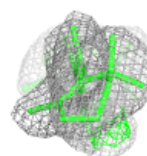
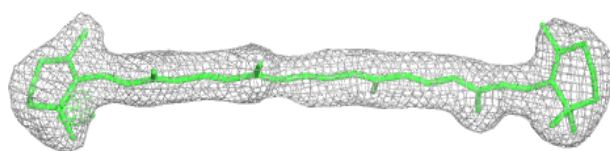
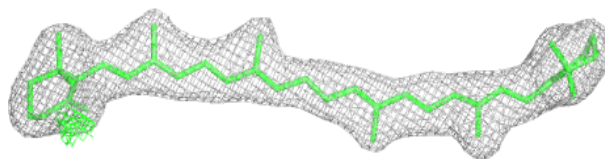
**Electron density around CLA C 504:**

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

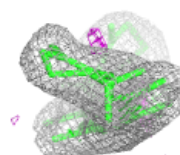
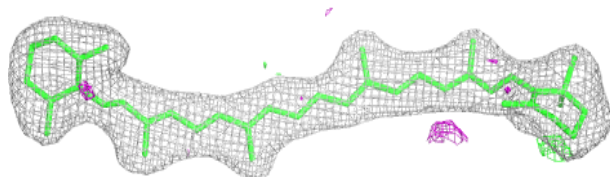
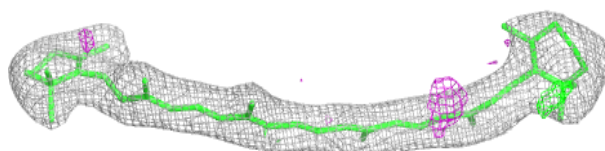


Electron density around BCR C 514:

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

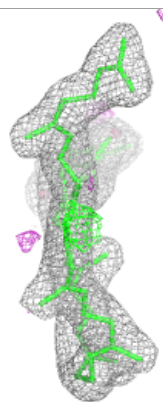
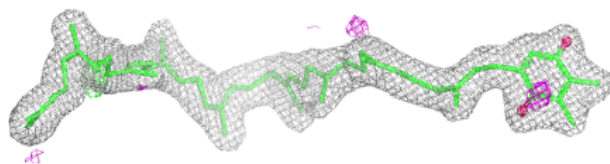
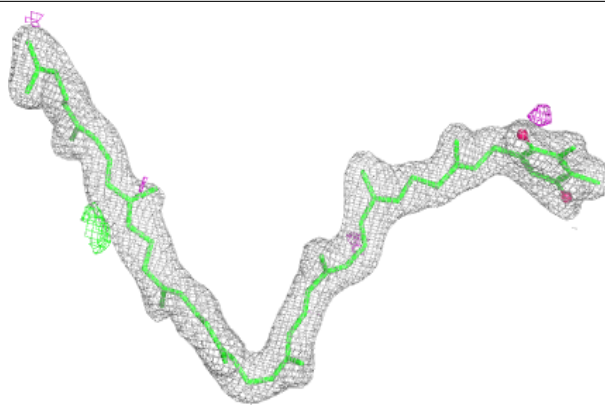
**Electron density around BCR D 404:**

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



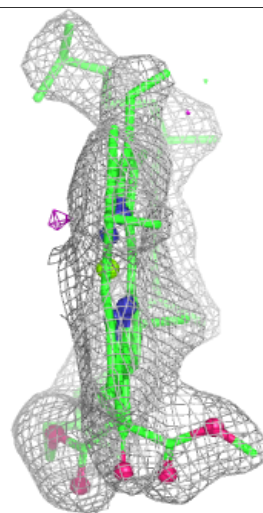
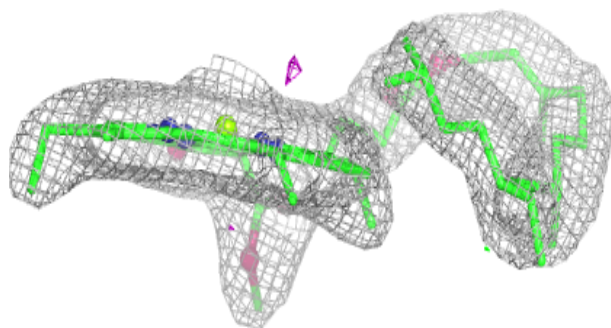
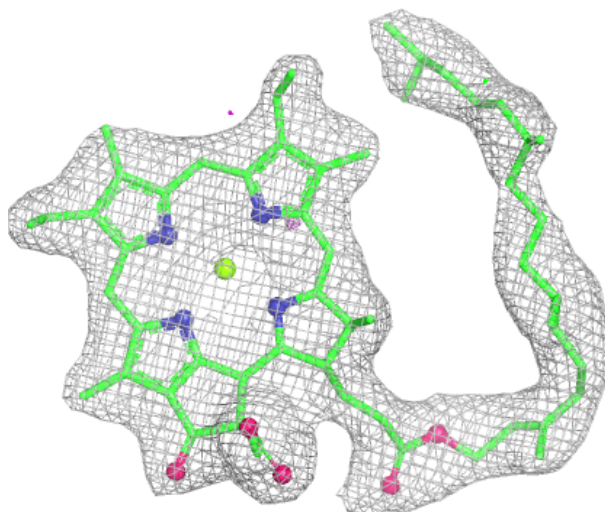
Electron density around PL9 D 405 (A):

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



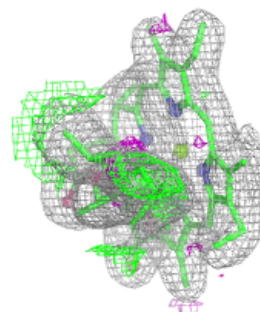
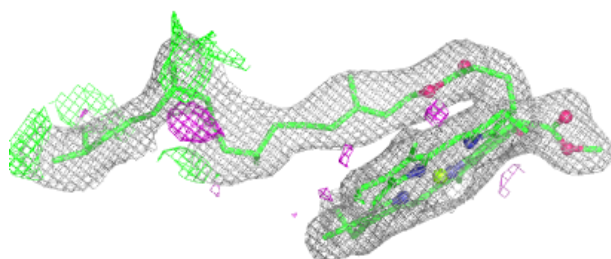
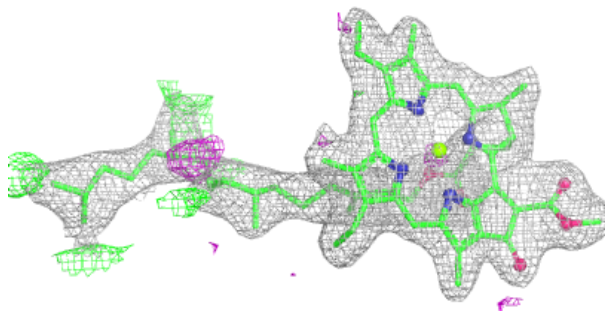
Electron density around CLA C 512:

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

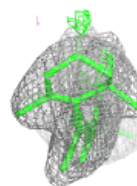
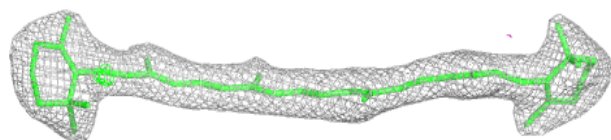
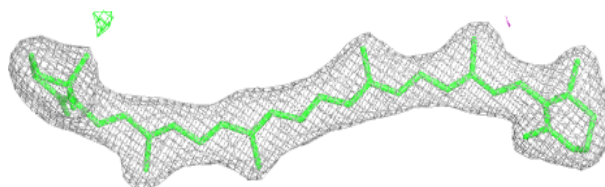


Electron density around CLA B 615:

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

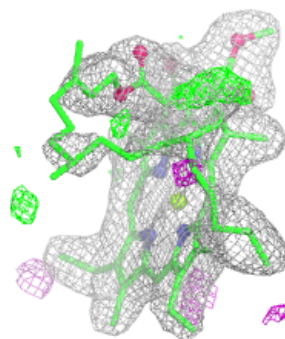
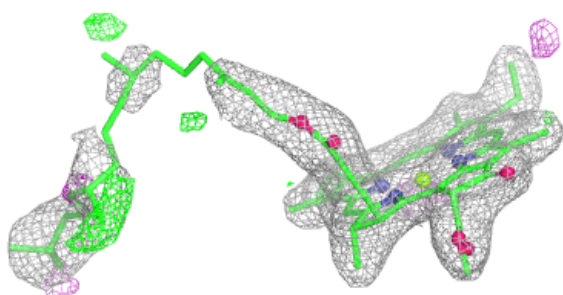
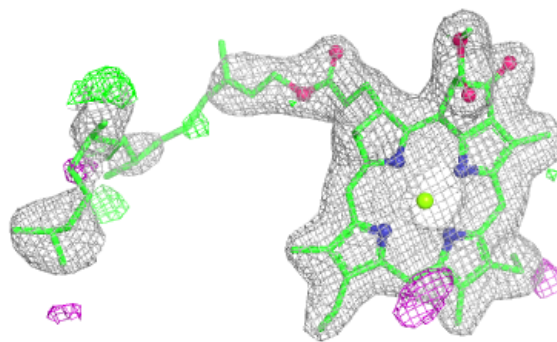
**Electron density around BCR Y 101:**

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



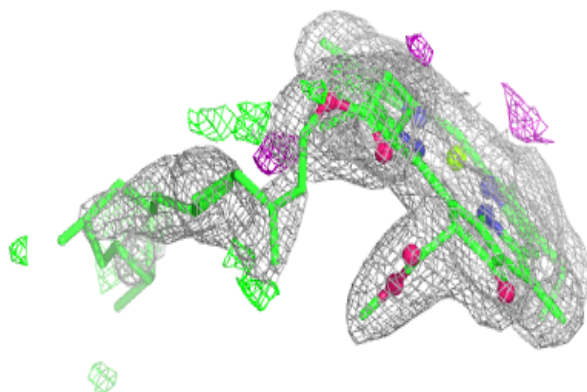
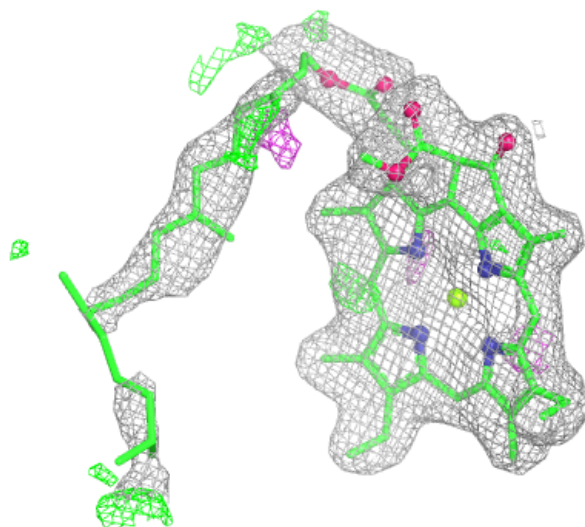
Electron density around CLA a 412:

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



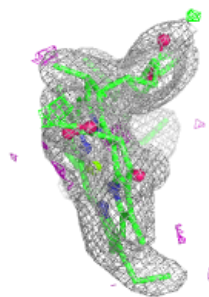
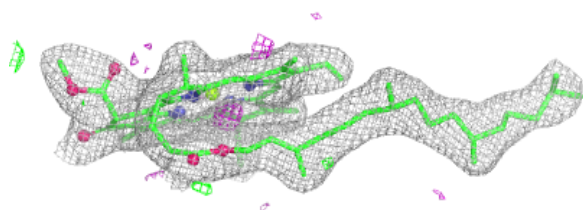
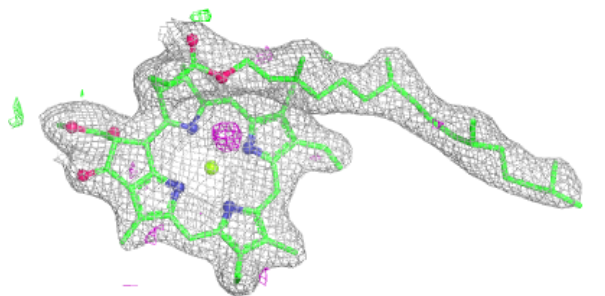
Electron density around CLA B 617:

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

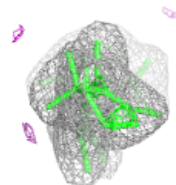
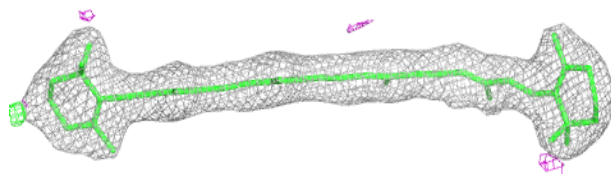
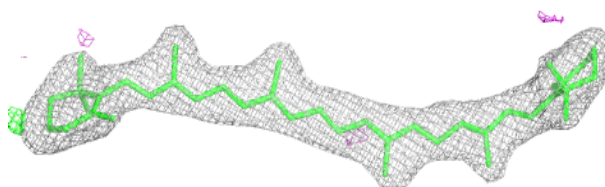


Electron density around CLA C 501:

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

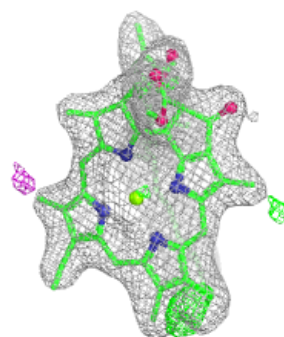
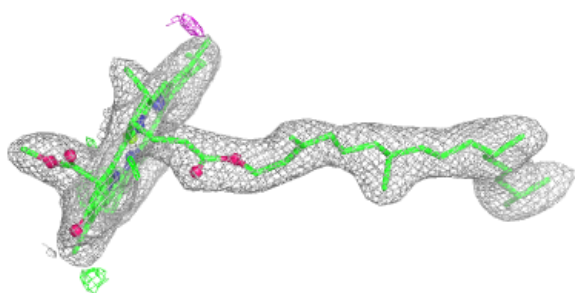
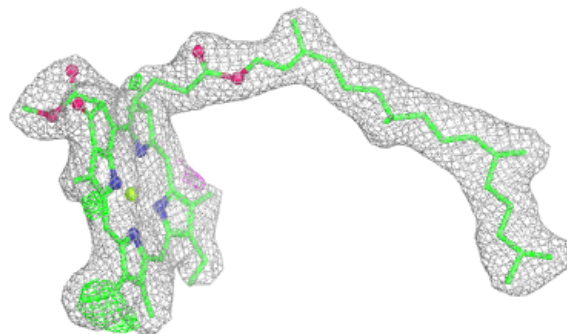
**Electron density around BCR h 101:**

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

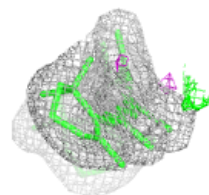
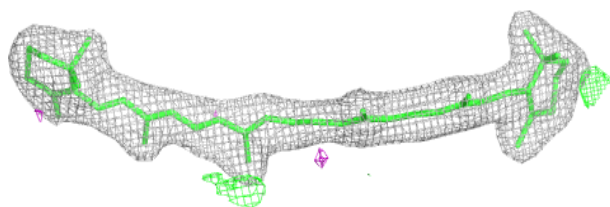
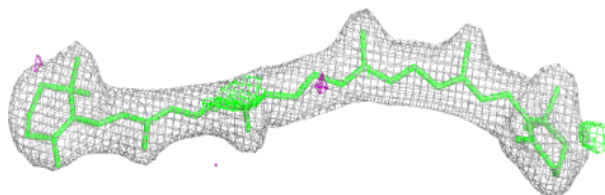


Electron density around CLA b 619:

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

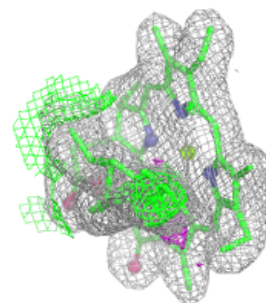
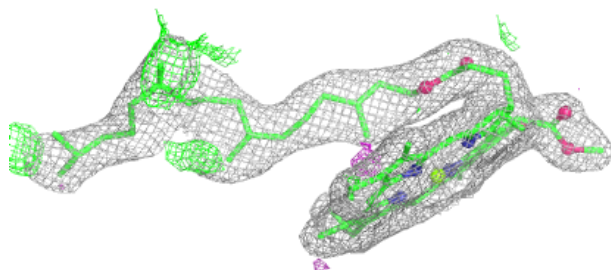
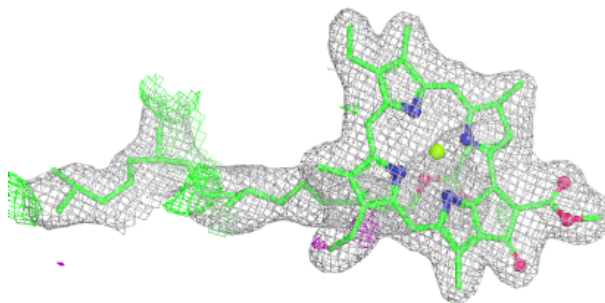
**Electron density around BCR t 101:**

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

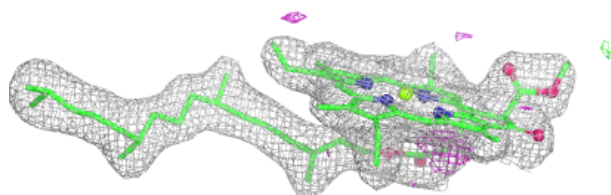
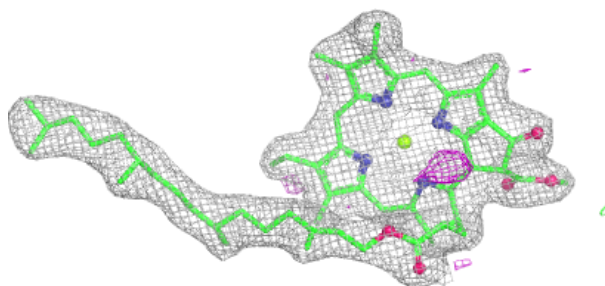


Electron density around CLA b 624:

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

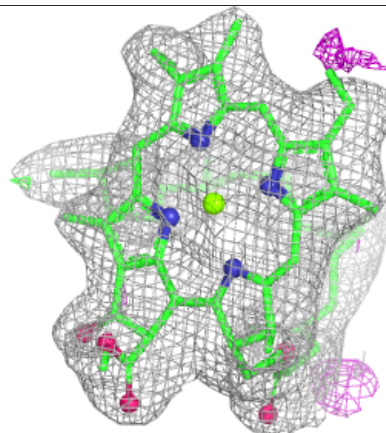
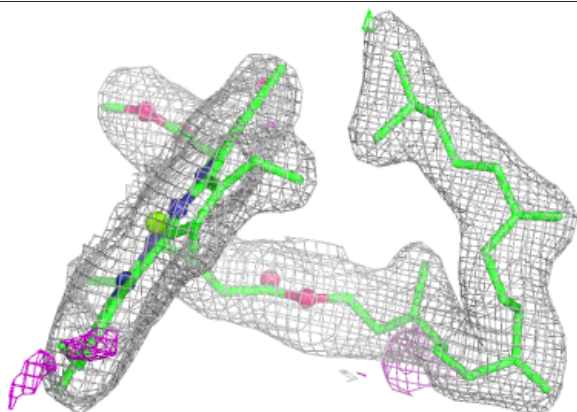
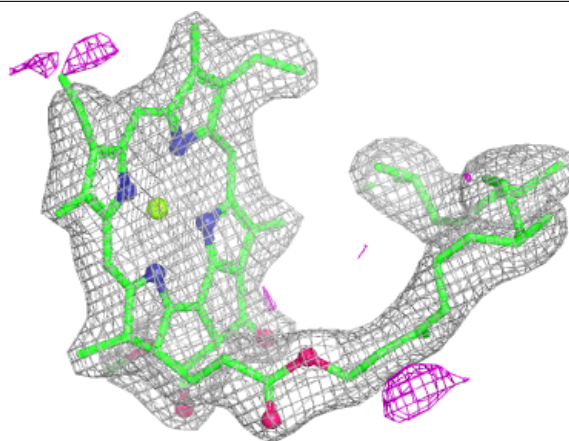
**Electron density around CLA c 505:**

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

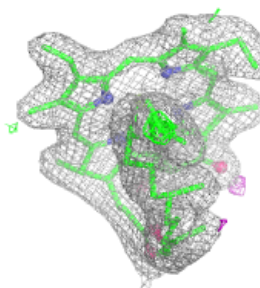
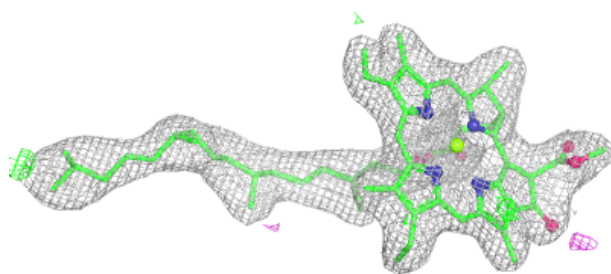
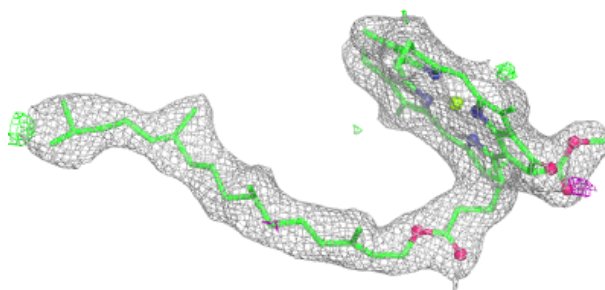


Electron density around CLA c 507:

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

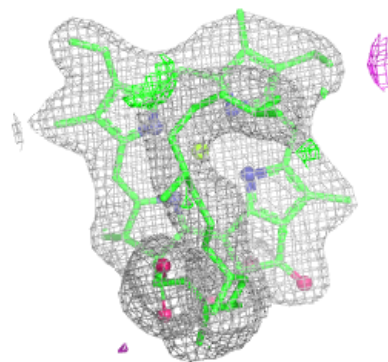
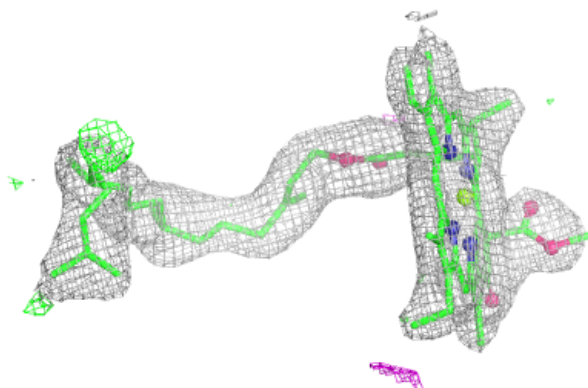
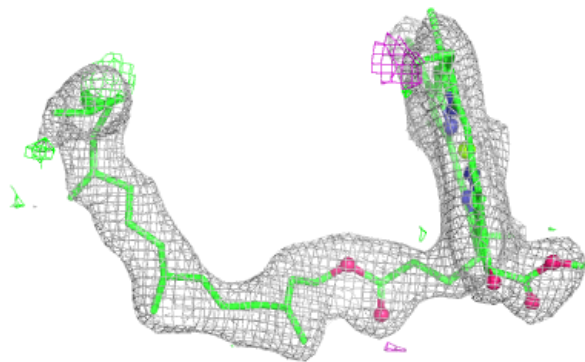
**Electron density around CLA c 508:**

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



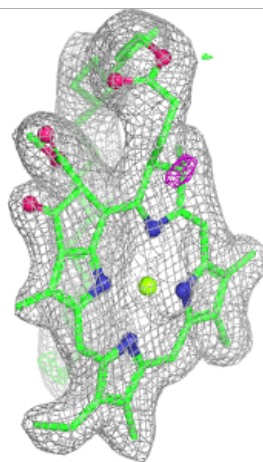
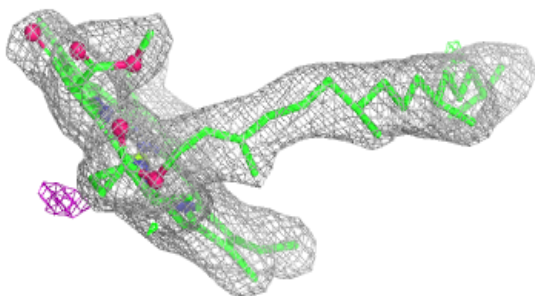
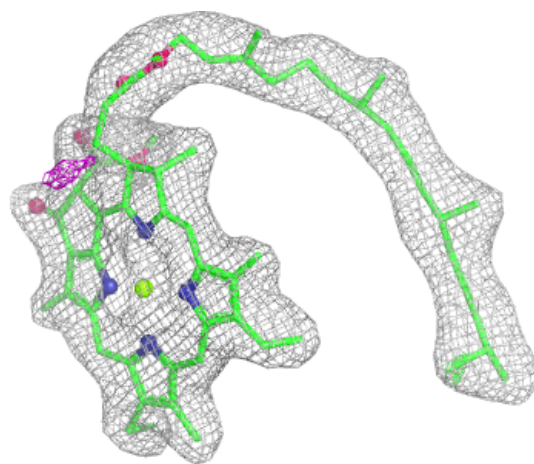
Electron density around CLA c 510:

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



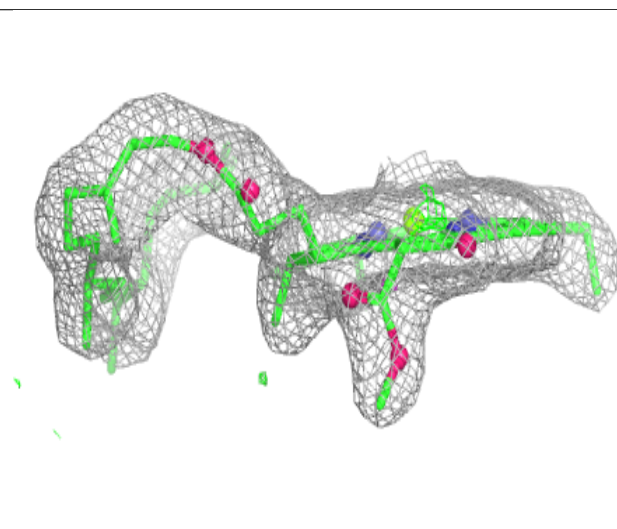
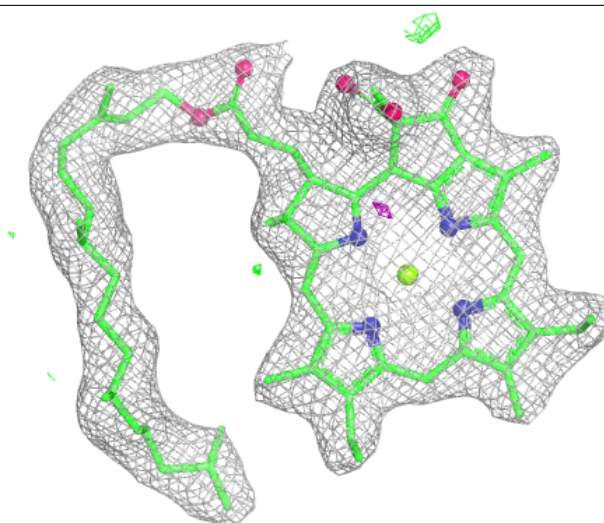
Electron density around CLA c 511:

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



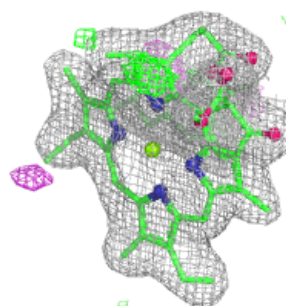
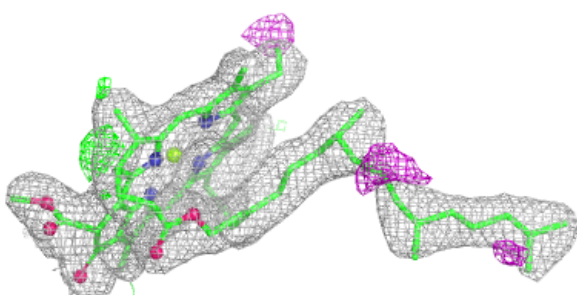
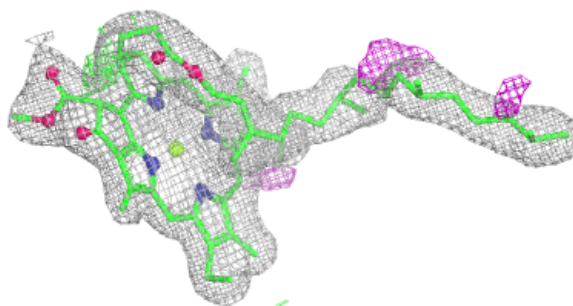
Electron density around CLA c 516:

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



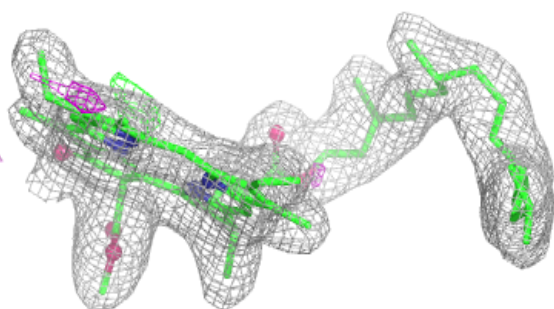
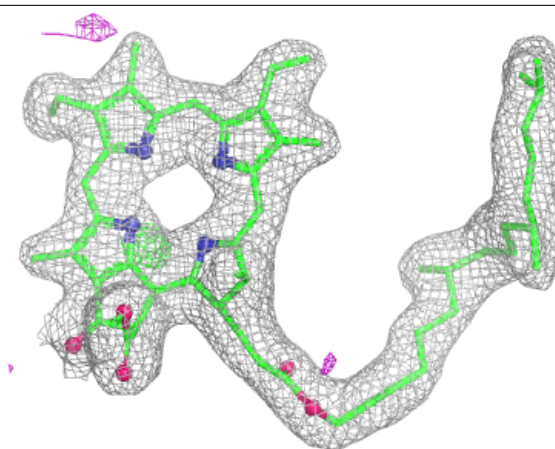
Electron density around CLA C 505:

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



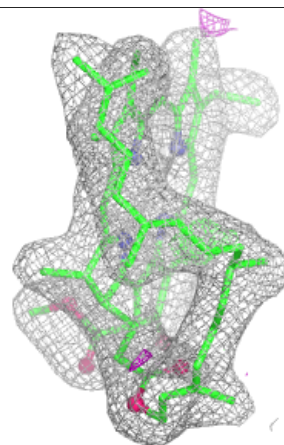
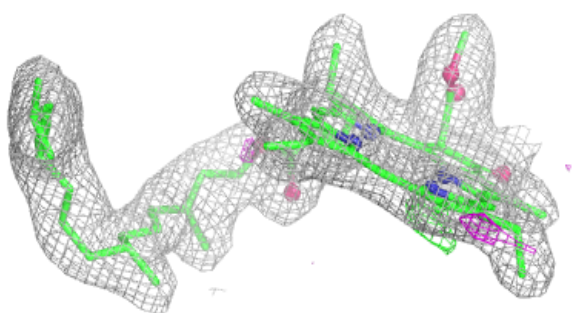
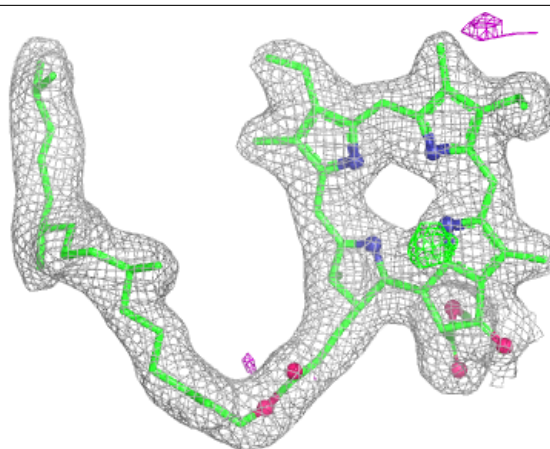
Electron density around PHO a 420 (A):

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

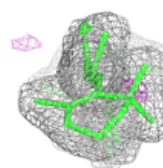
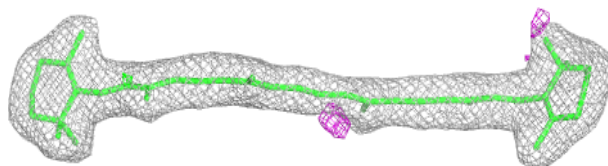
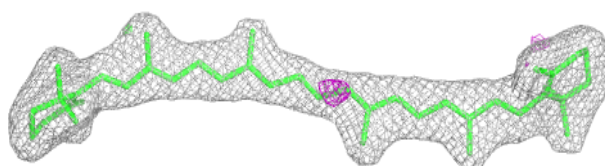


Electron density around PHO a 420 (B):

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

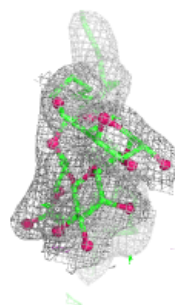
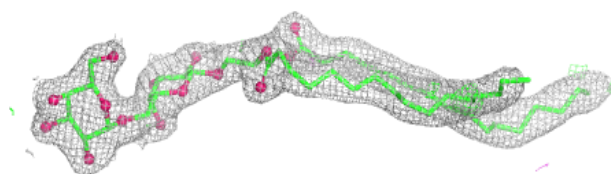
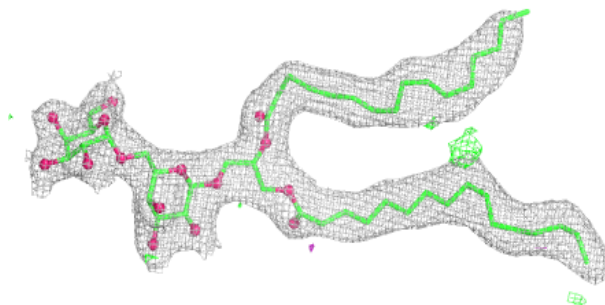
**Electron density around BCR A 411:**

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

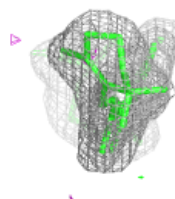
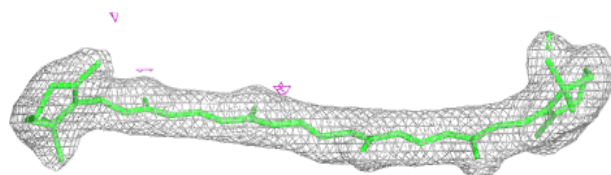
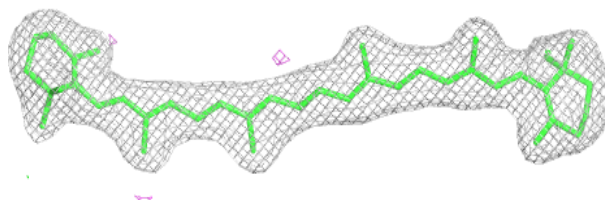


Electron density around DGD C 518:

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

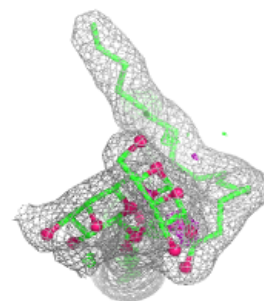
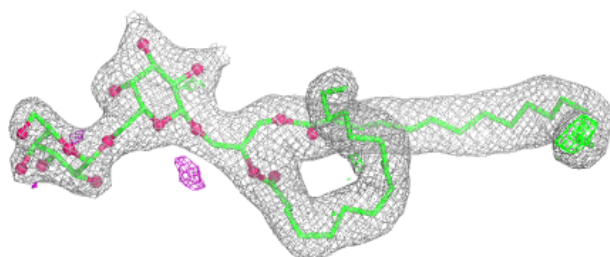
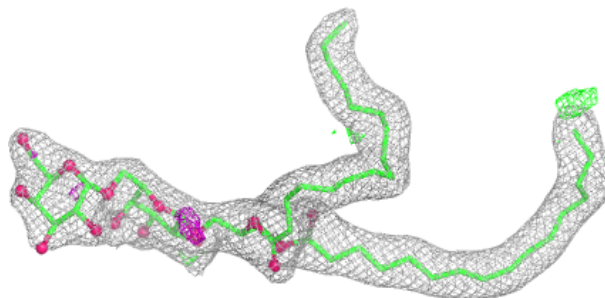
**Electron density around BCR B 620:**

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

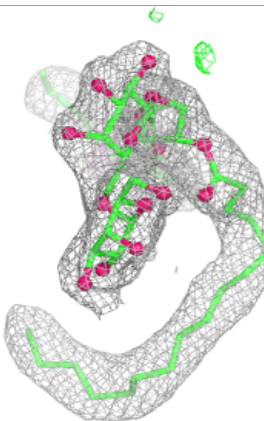
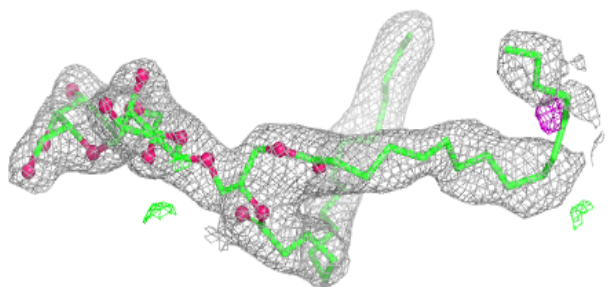
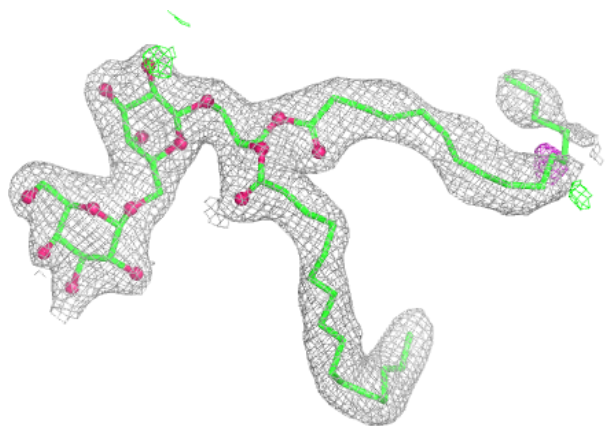


Electron density around DGD H 103:

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

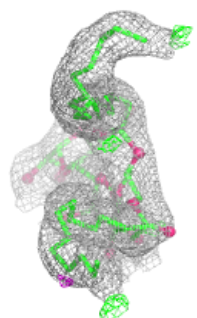
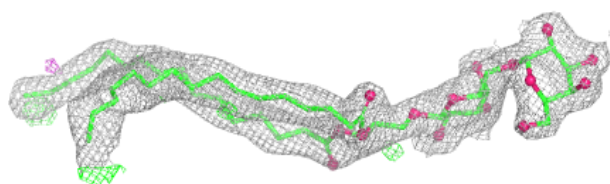
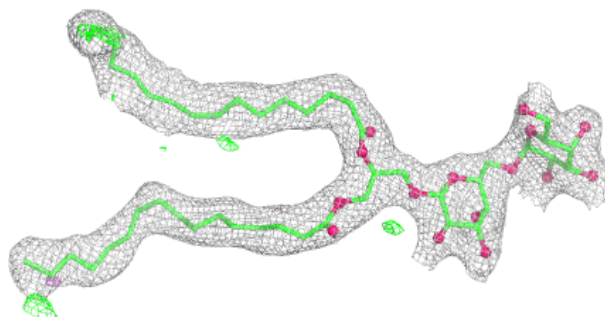
**Electron density around DGD c 520:**

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

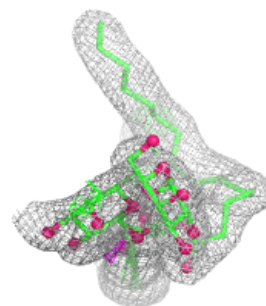
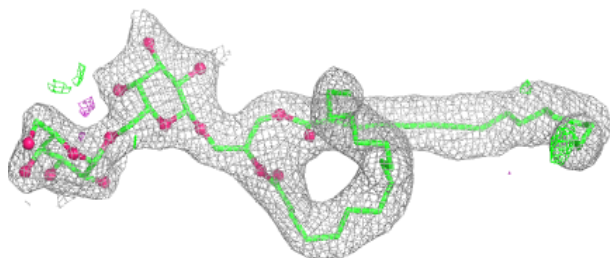
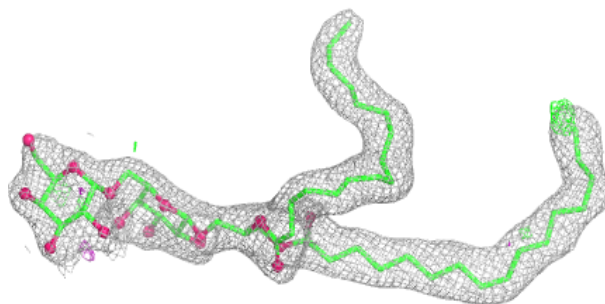


Electron density around DGD c 521:

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

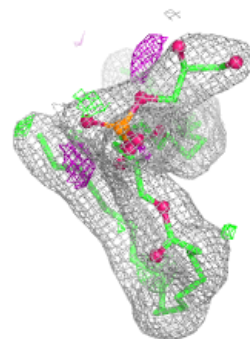
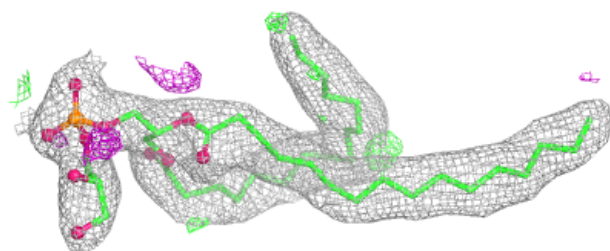
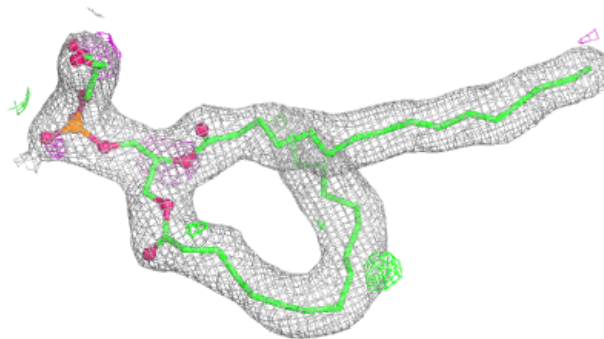
**Electron density around DGD h 102:**

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



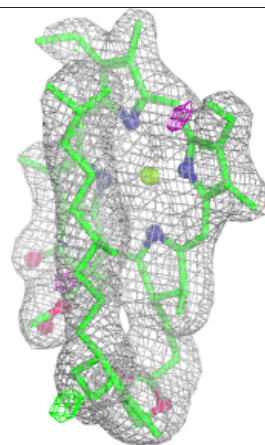
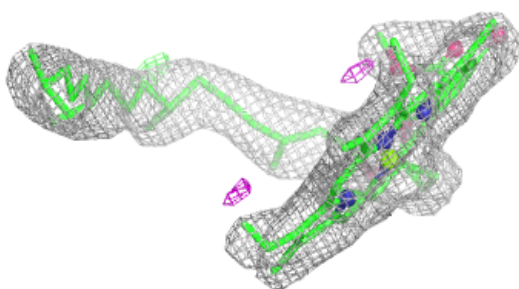
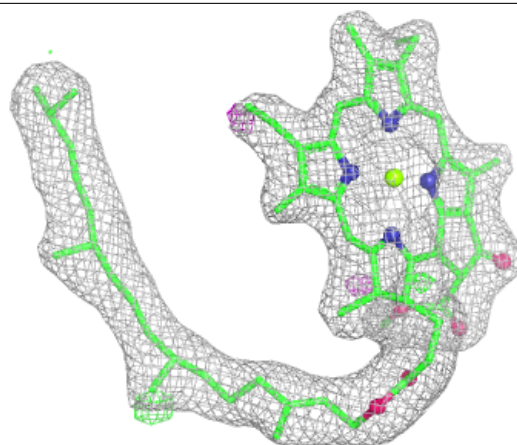
Electron density around LHG D 407:

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

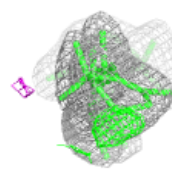
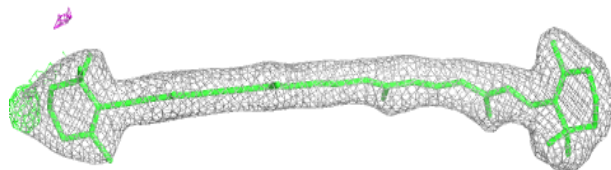
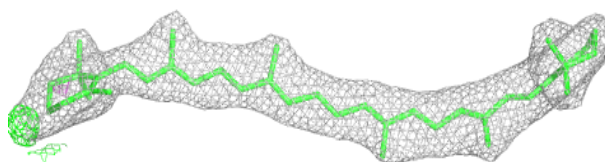


Electron density around CLA C 507:

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

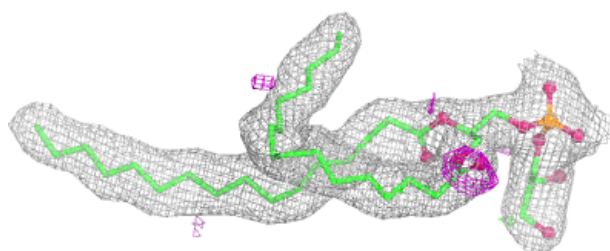
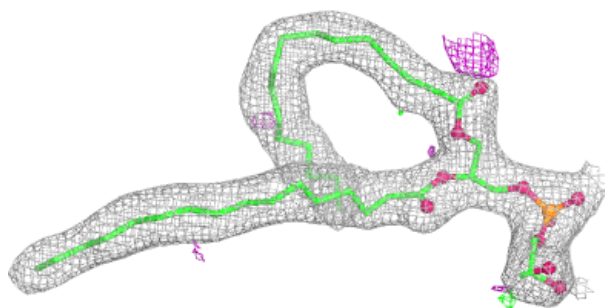
**Electron density around BCR H 102:**

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

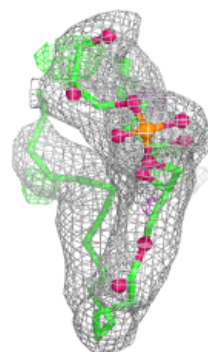
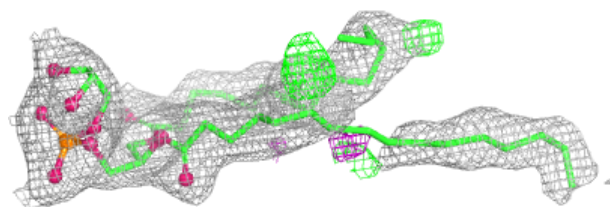
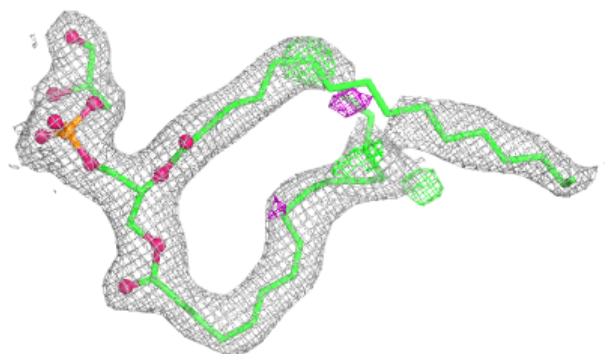


Electron density around LHG d 406:

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

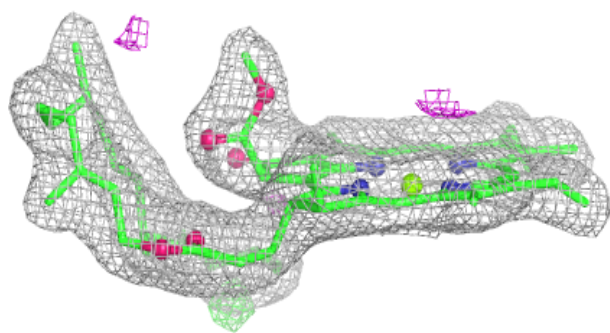
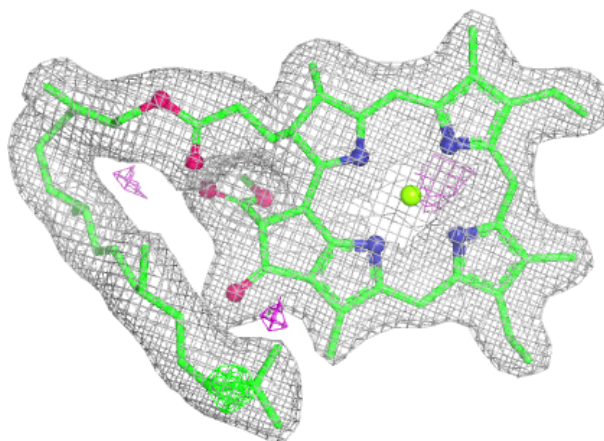
**Electron density around LHG d 408:**

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



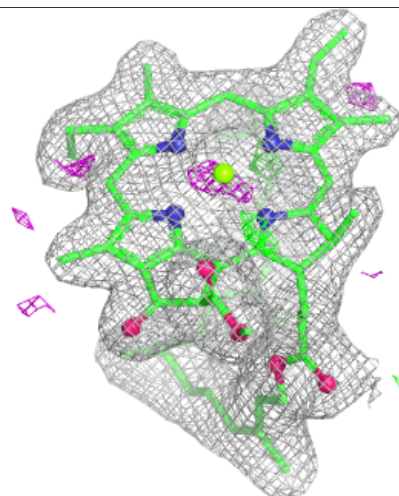
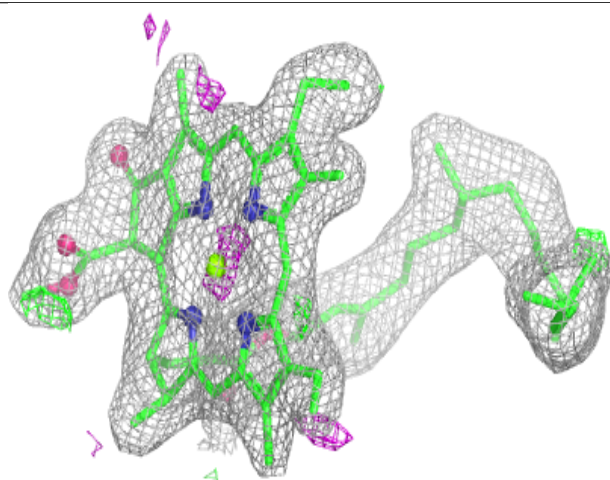
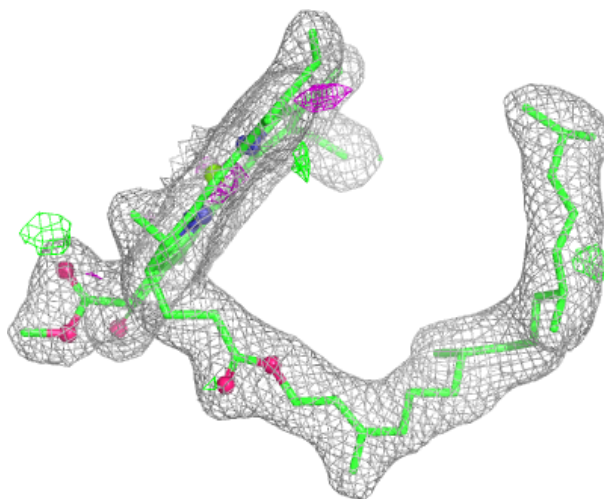
Electron density around CLA b 620:

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



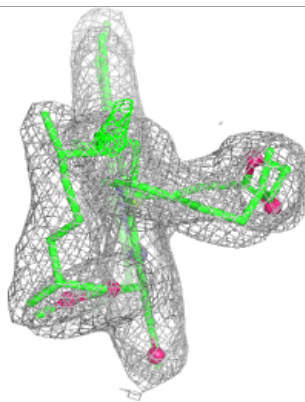
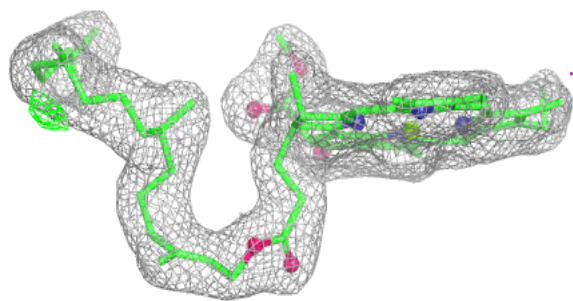
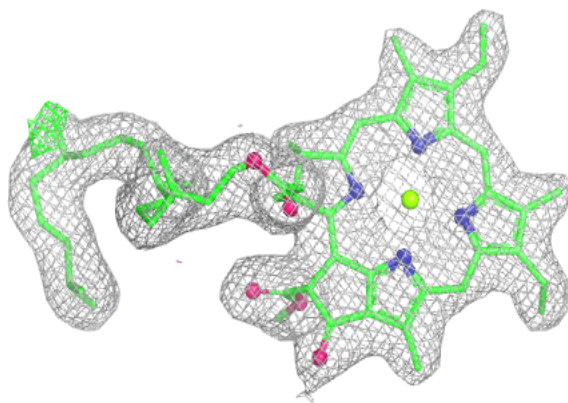
Electron density around CLA b 621:

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



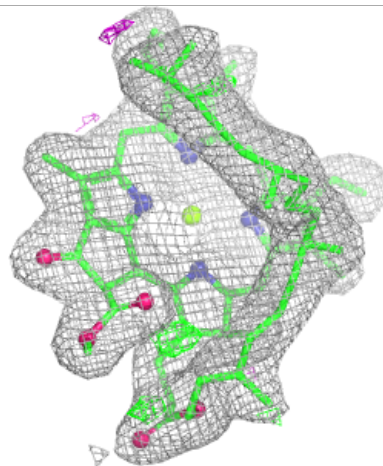
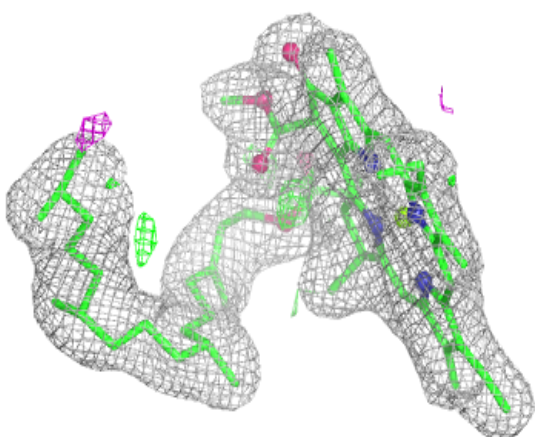
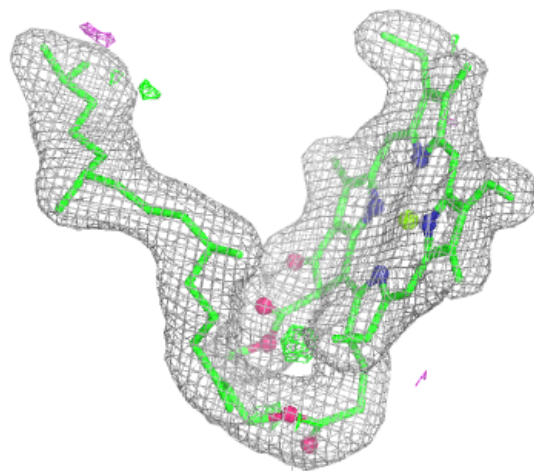
Electron density around CLA b 622:

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



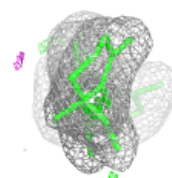
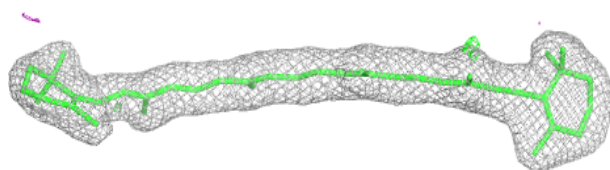
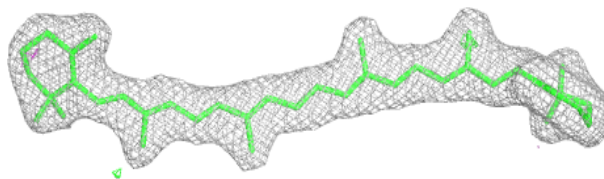
Electron density around CLA b 623:

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

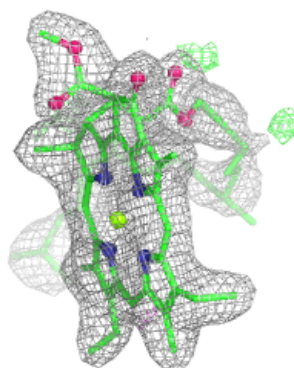
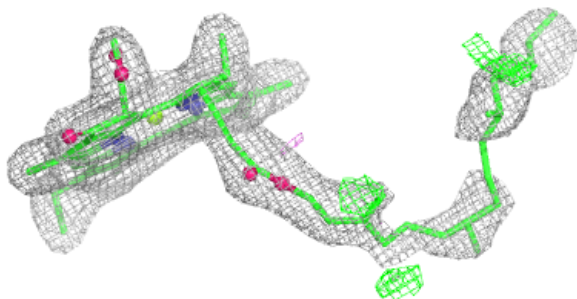
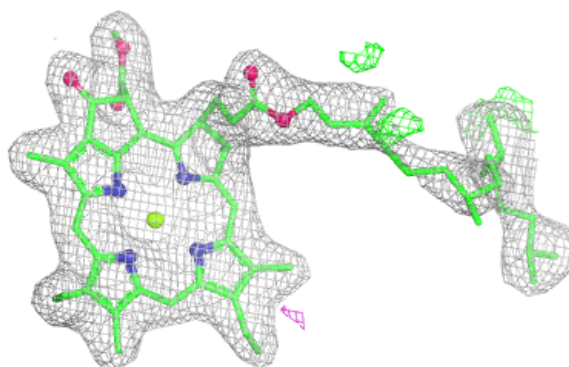


Electron density around BCR b 627:

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

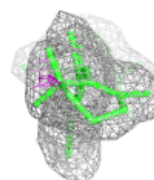
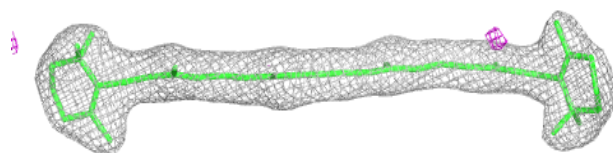
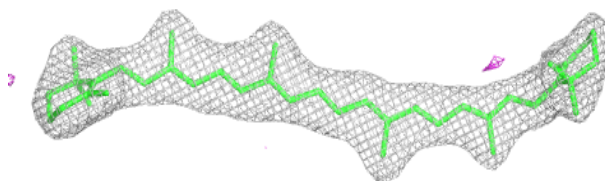
**Electron density around CLA A 410:**

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



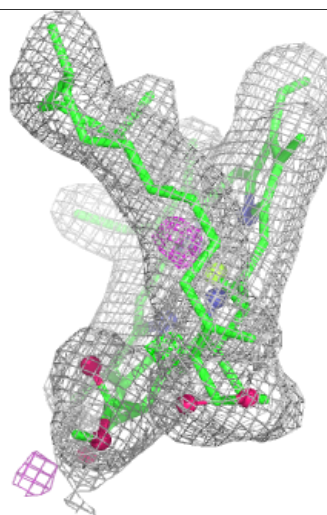
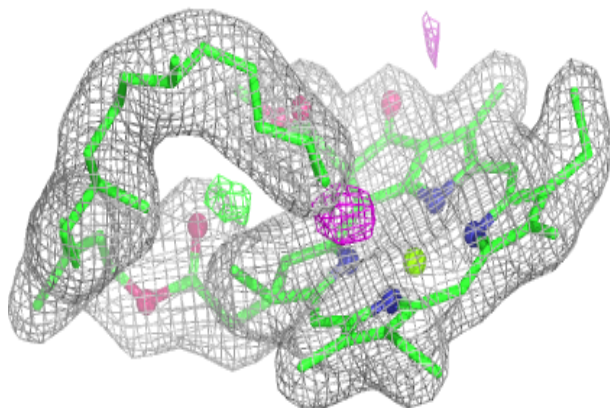
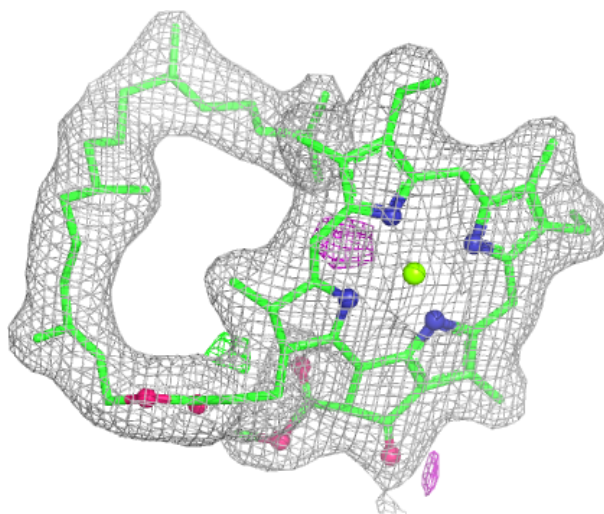
Electron density around BCR c 518:

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



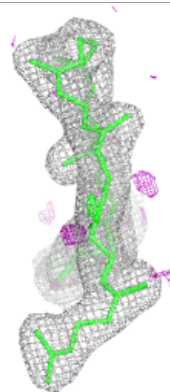
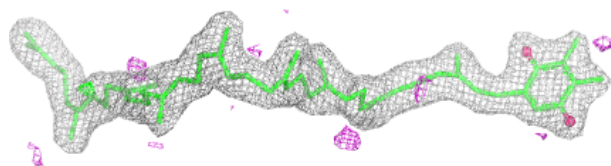
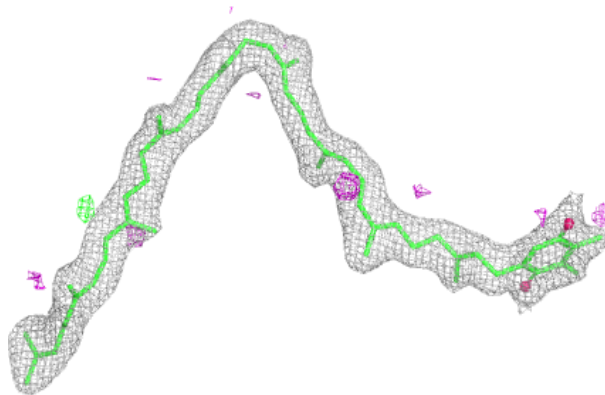
Electron density around CLA b 625:

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

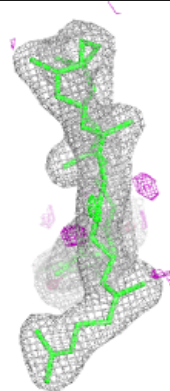
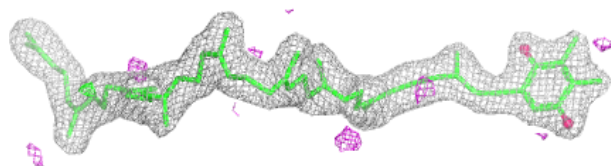
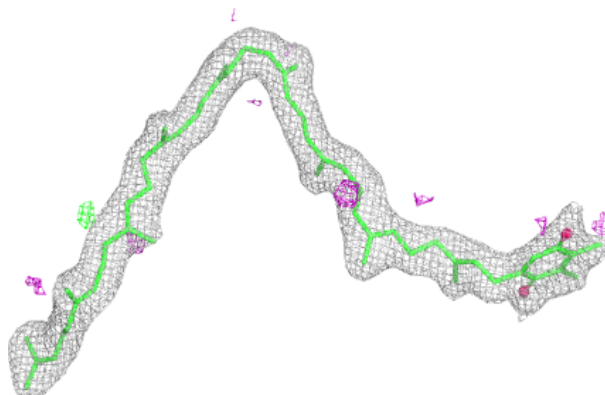


Electron density around PL9 d 405 (A):

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

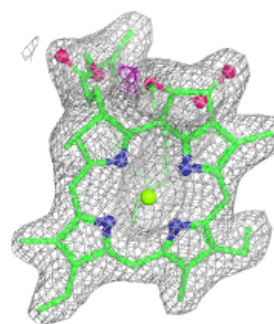
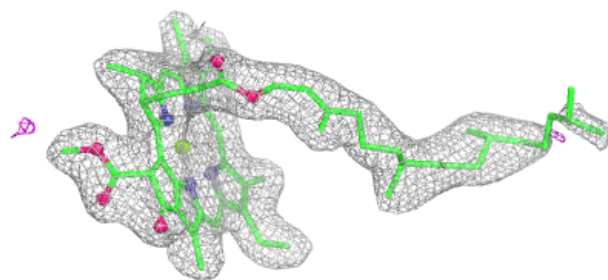
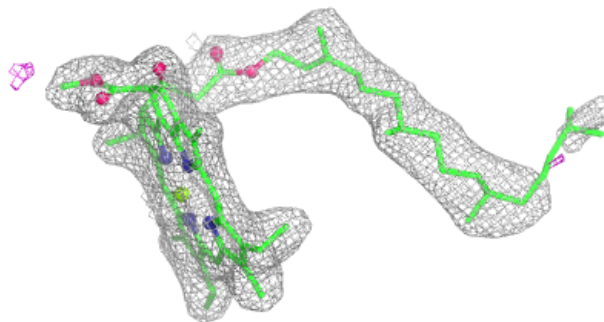
**Electron density around PL9 d 405 (B):**

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



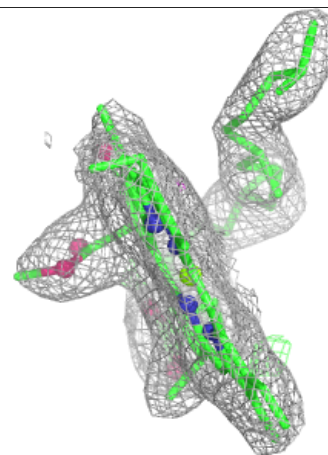
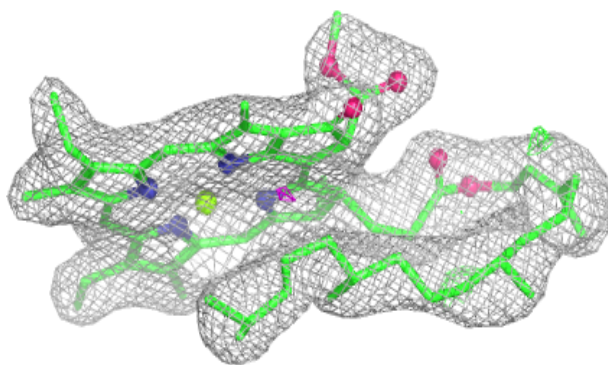
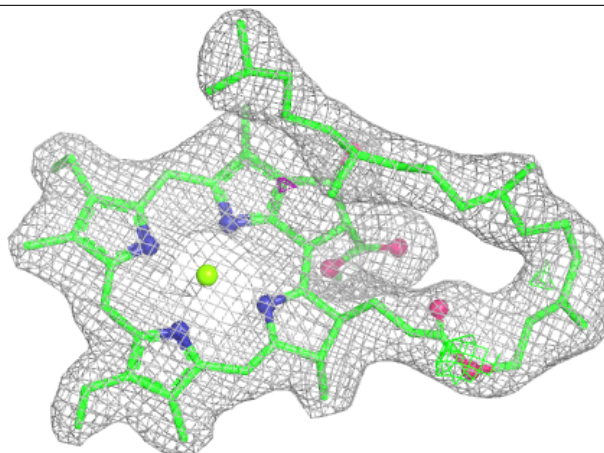
Electron density around CLA C 508:

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



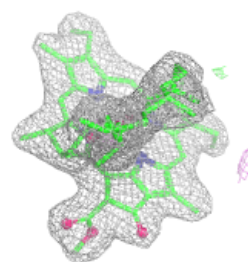
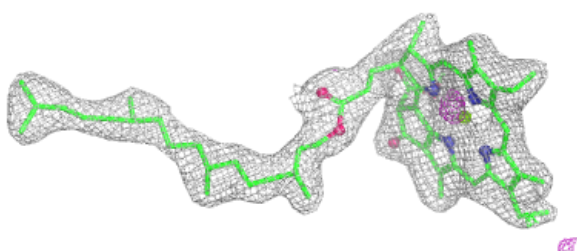
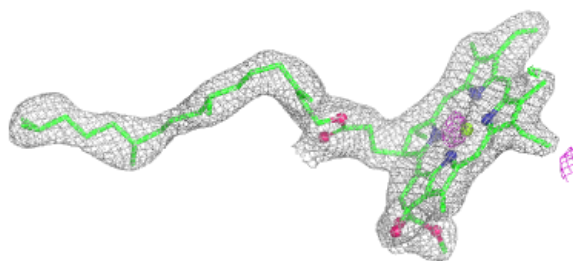
Electron density around CLA C 509:

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

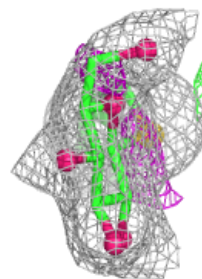
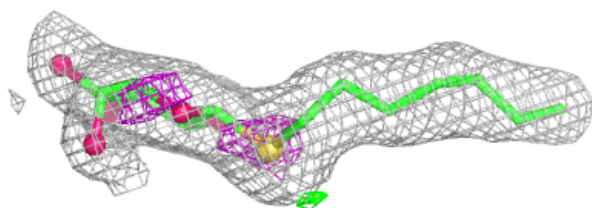
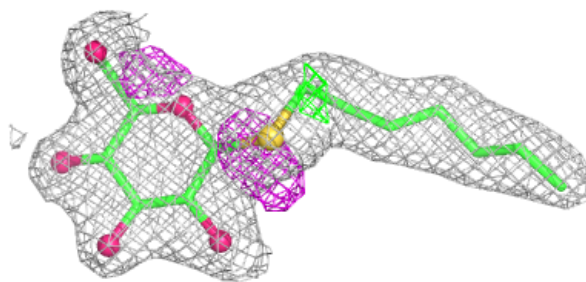


Electron density around CLA c 506:

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

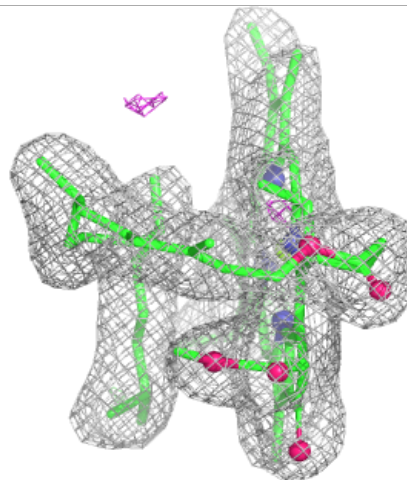
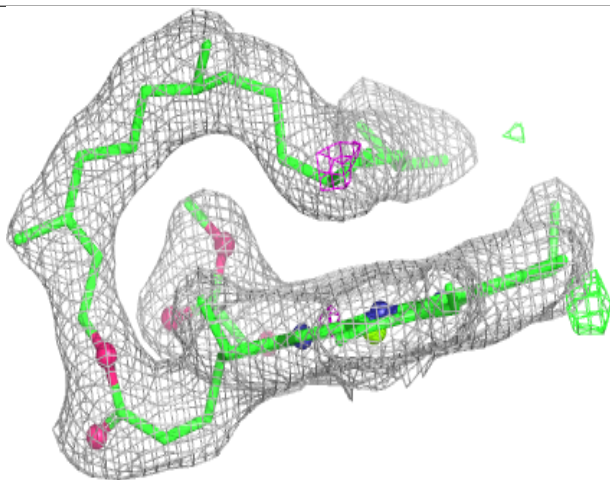
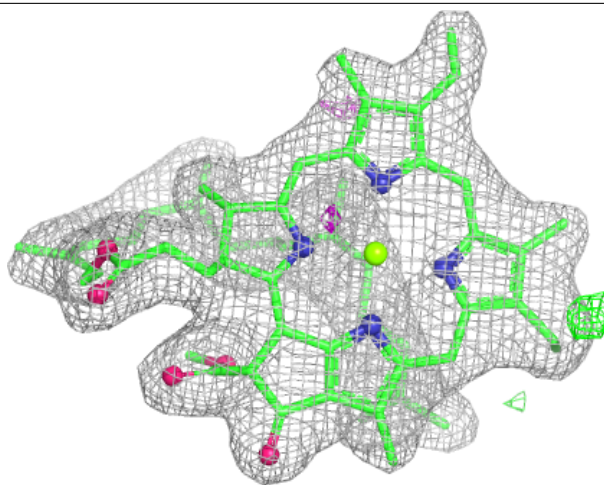
**Electron density around HTG b 602:**

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



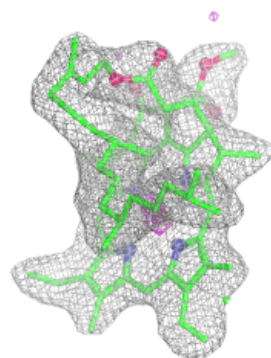
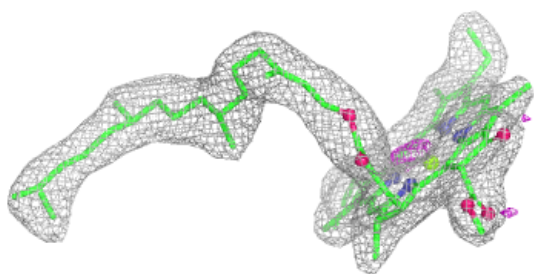
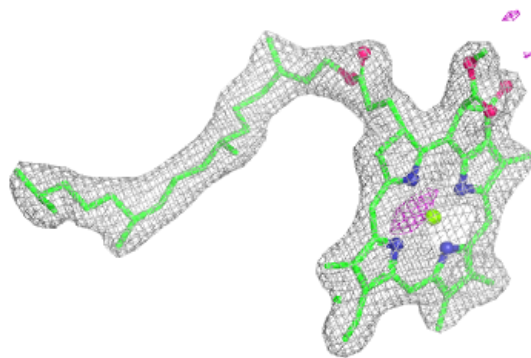
Electron density around CLA C 510:

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

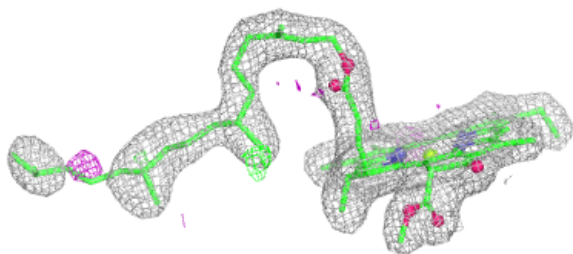
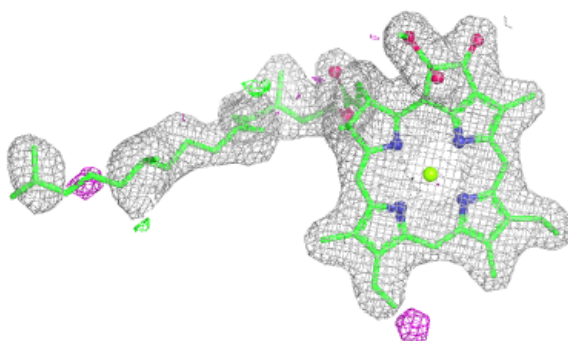


Electron density around CLA C 511:

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

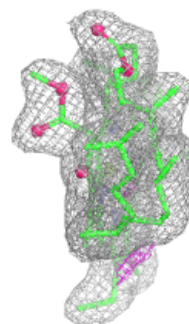
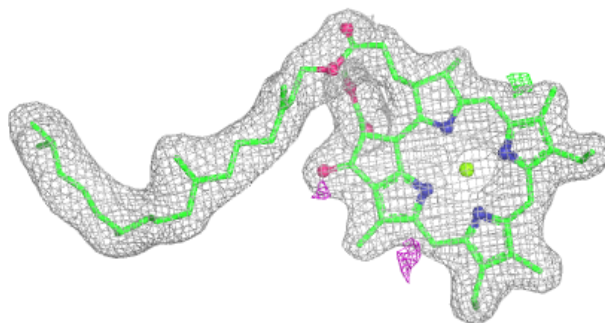
**Electron density around CLA A 407:**

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

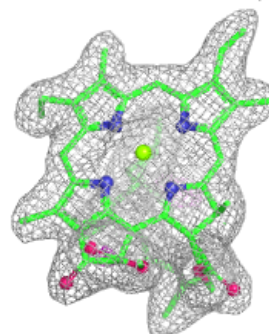
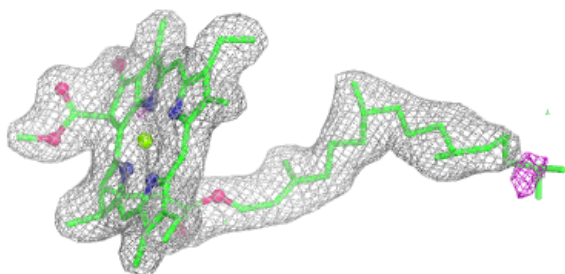
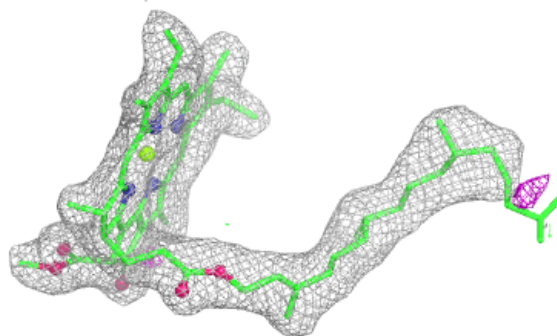


Electron density around CLA B 603:

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

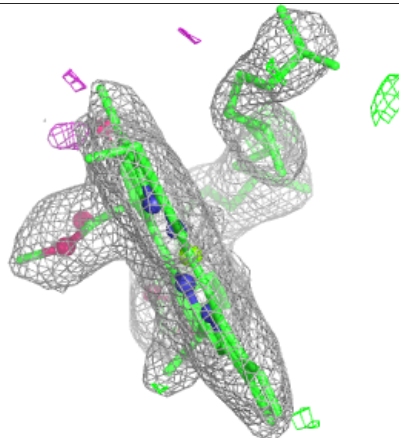
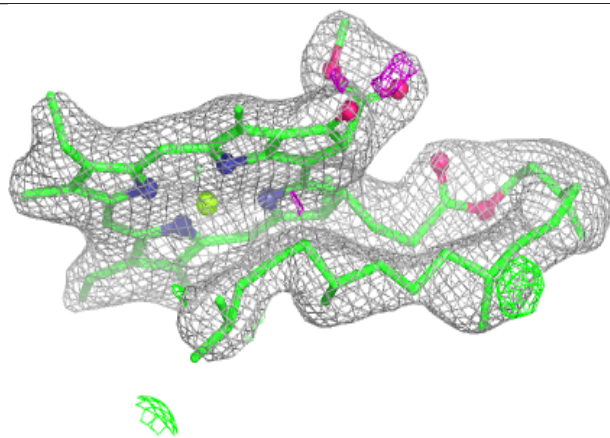
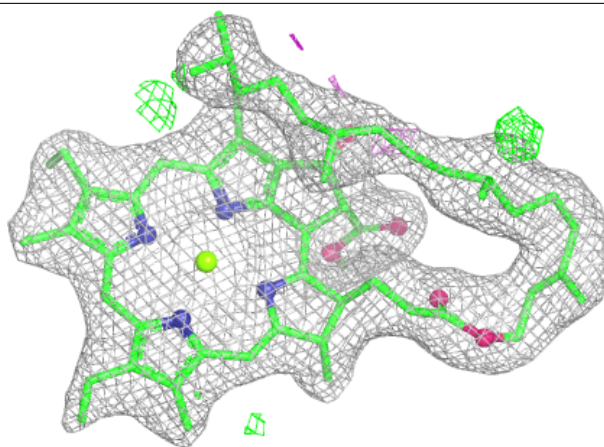
**Electron density around CLA c 512:**

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



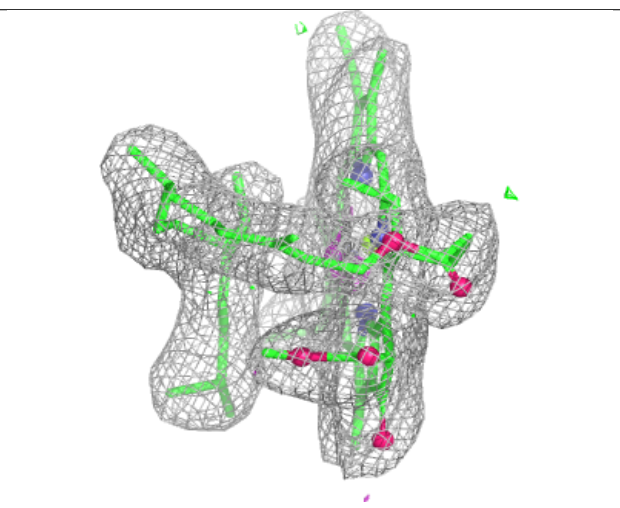
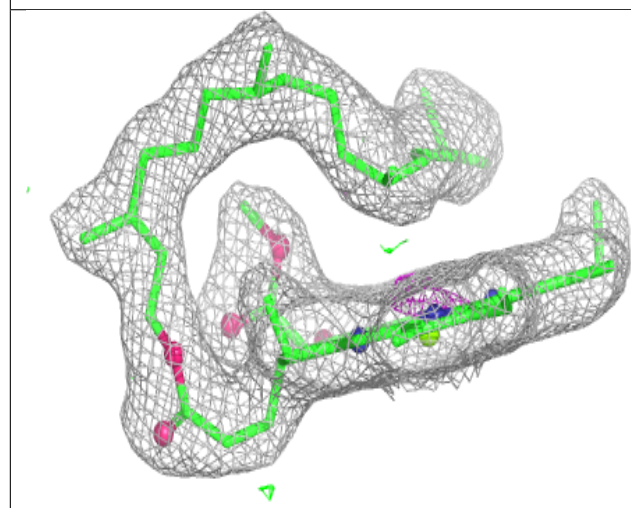
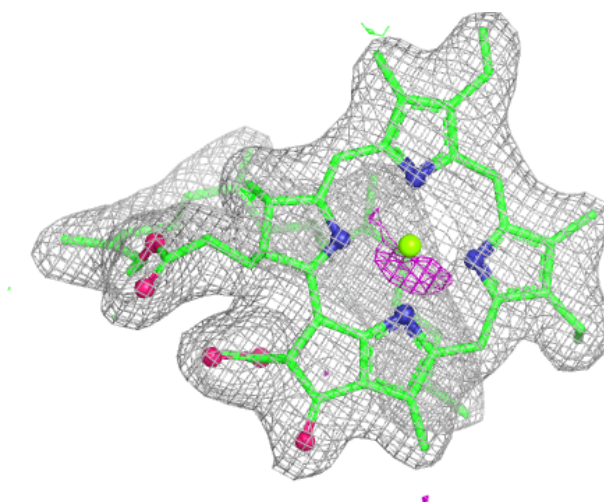
Electron density around CLA c 513:

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



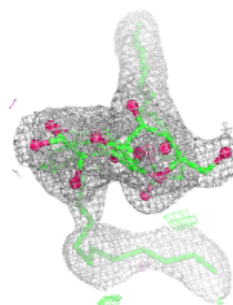
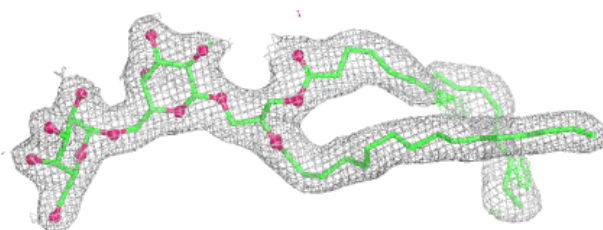
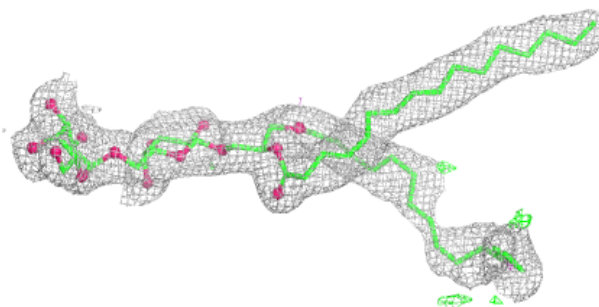
Electron density around CLA c 514:

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

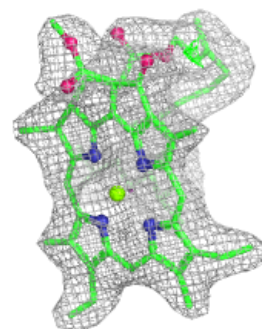
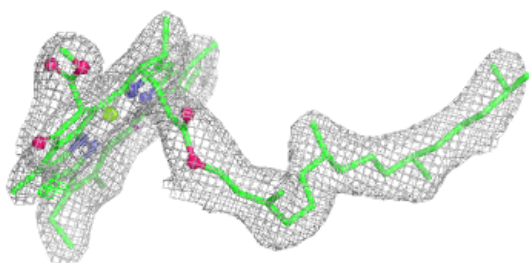
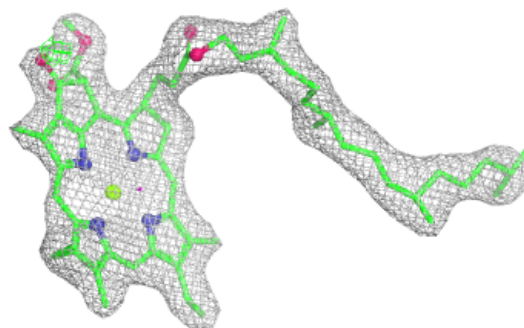


Electron density around DGD C 516:

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

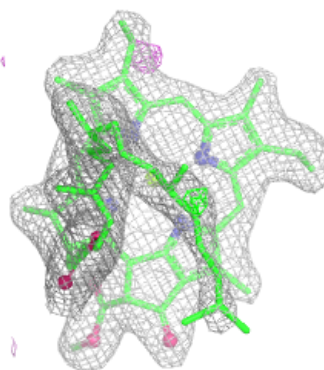
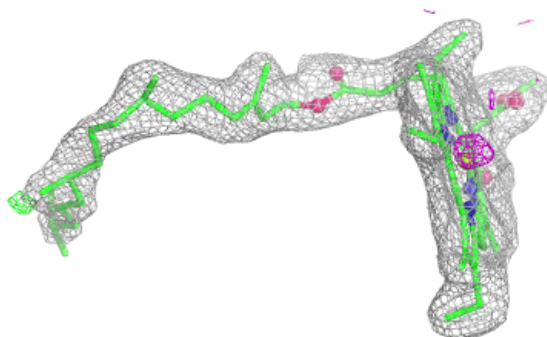
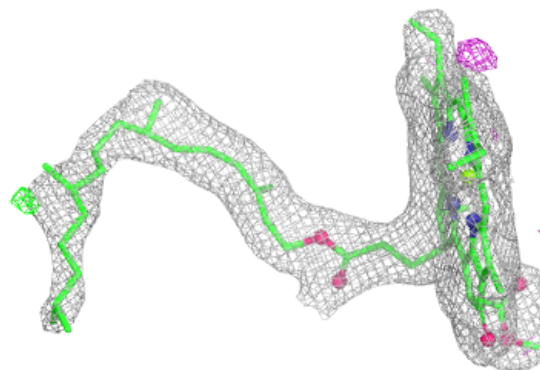
**Electron density around CLA c 515:**

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

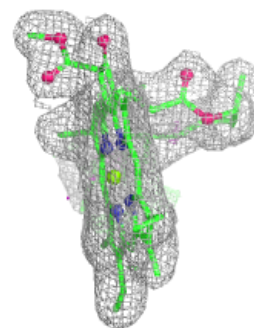
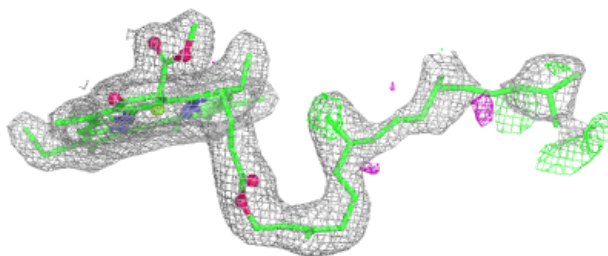
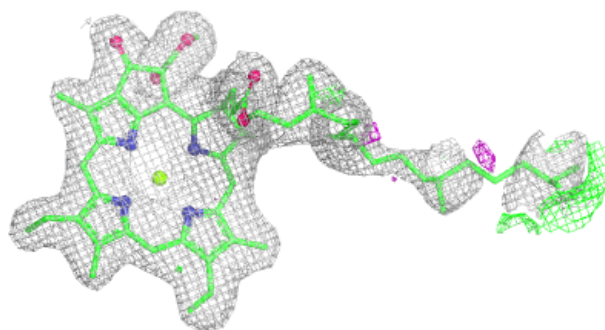


Electron density around CLA D 403:

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

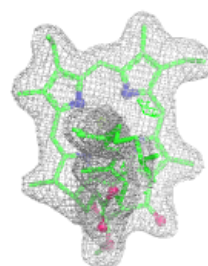
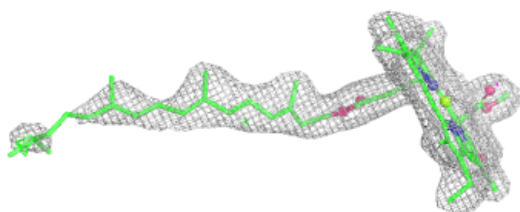
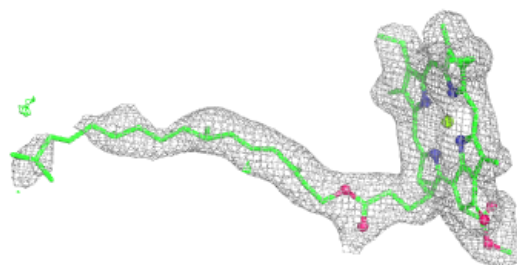
**Electron density around CLA a 410:**

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

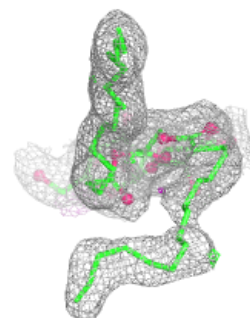
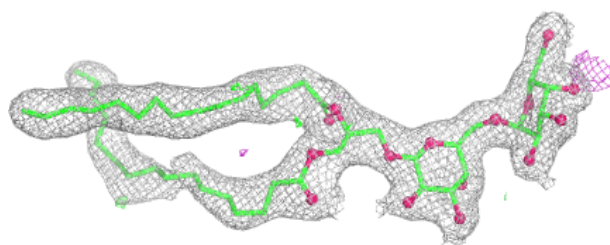
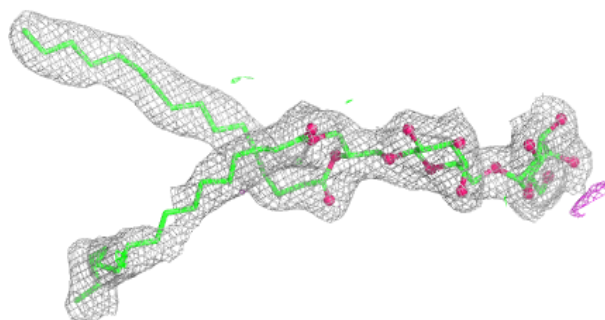


Electron density around CLA d 403:

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

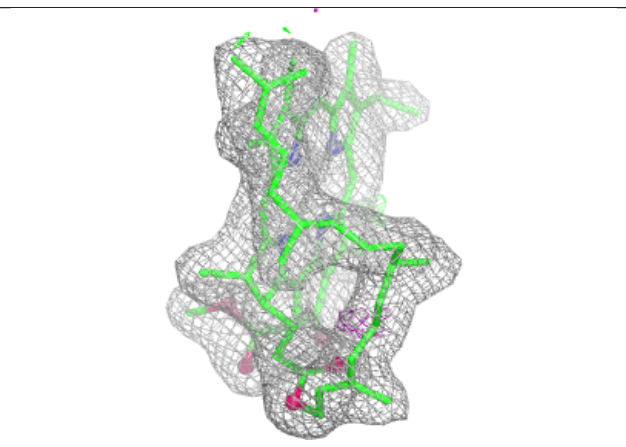
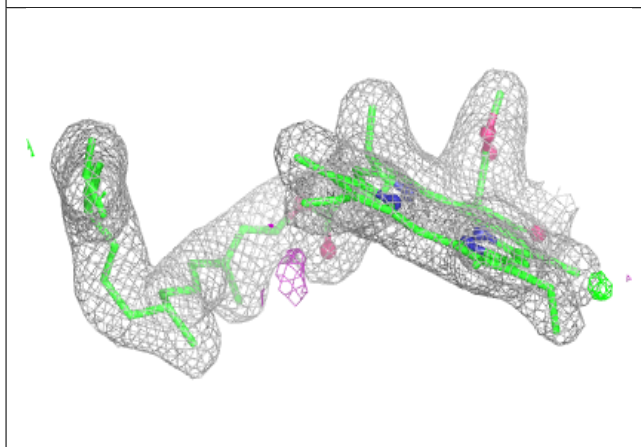
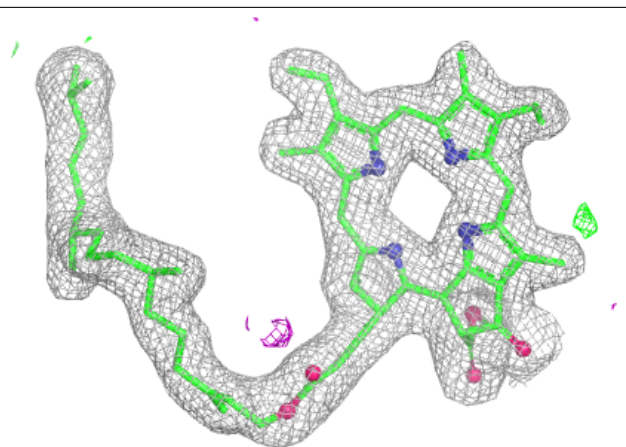
**Electron density around DGD c 519:**

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



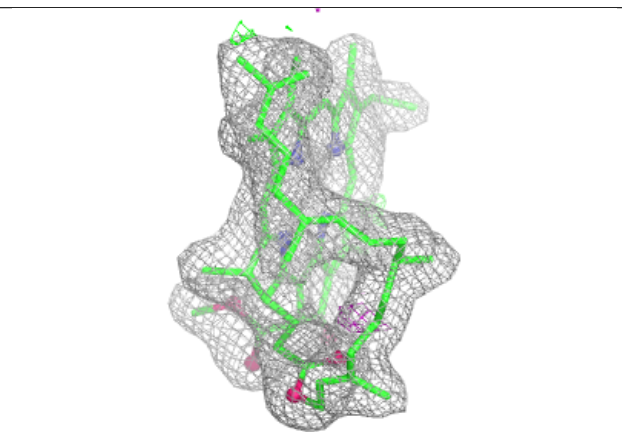
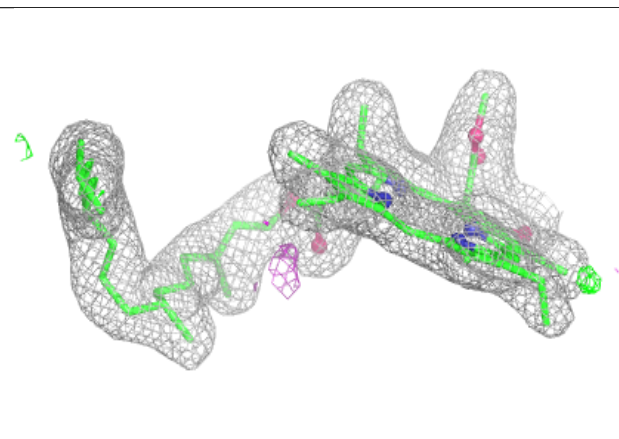
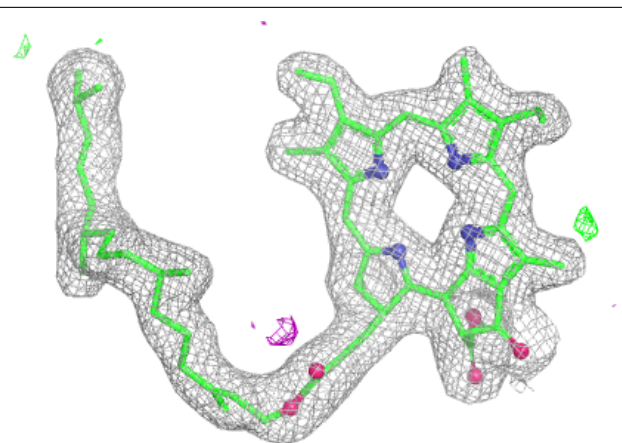
Electron density around PHO A 409 (A):

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



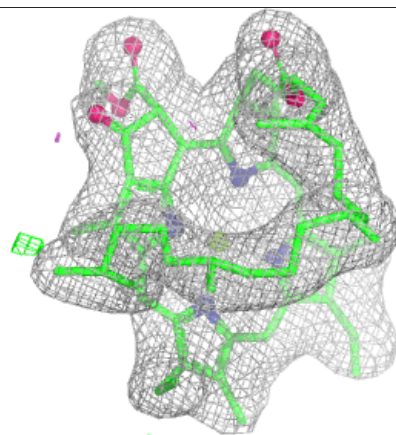
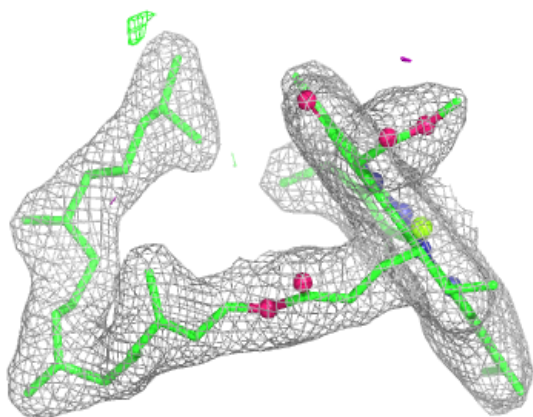
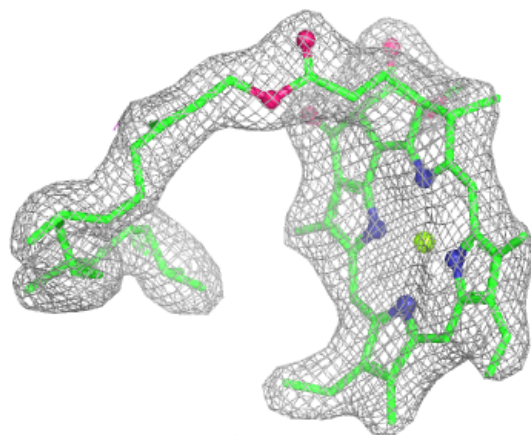
Electron density around PHO A 409 (B):

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



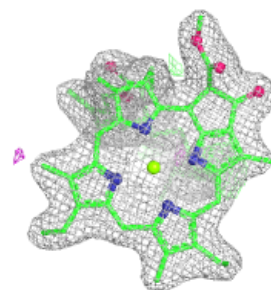
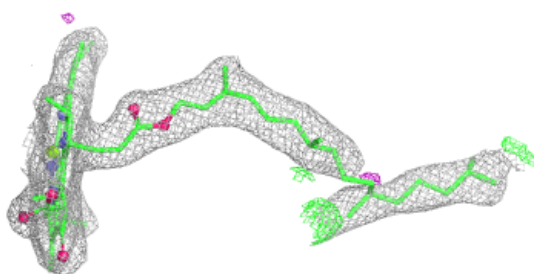
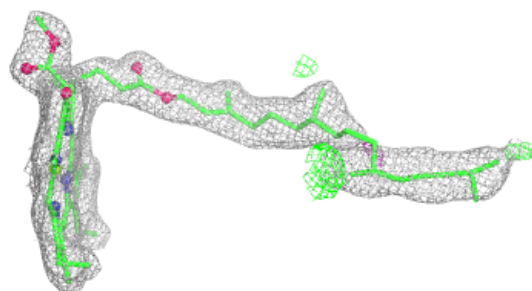
Electron density around CLA C 503:

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



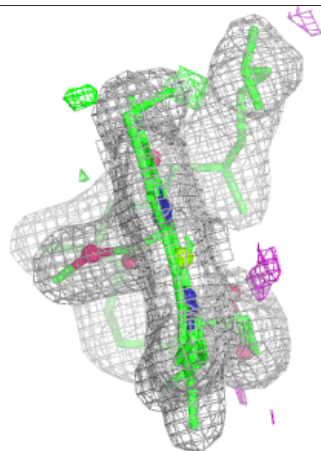
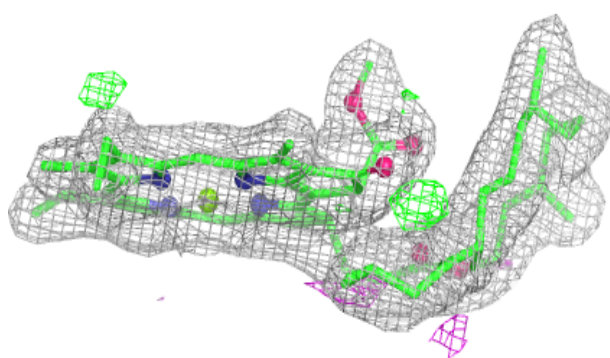
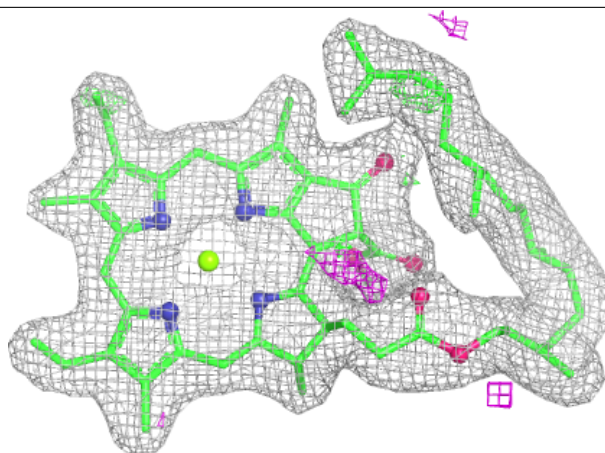
Electron density around CLA B 607:

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

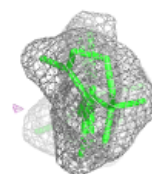
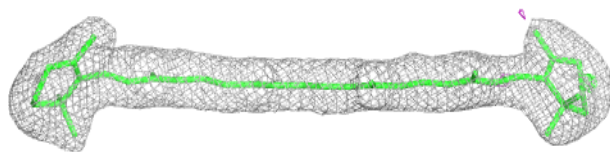
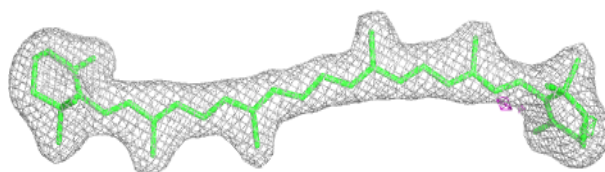


Electron density around CLA B 611:

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

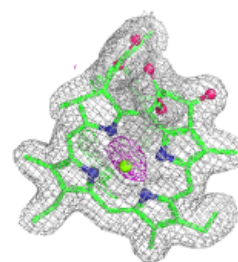
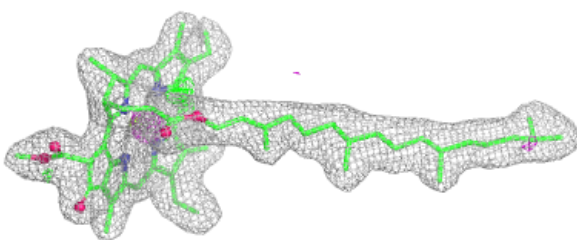
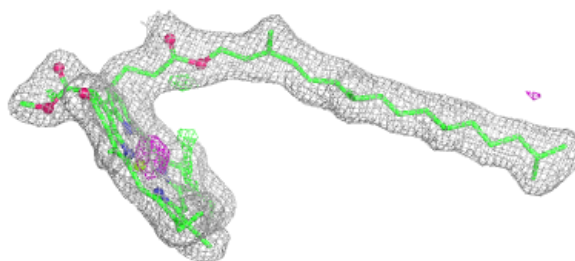
**Electron density around BCR B 619:**

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

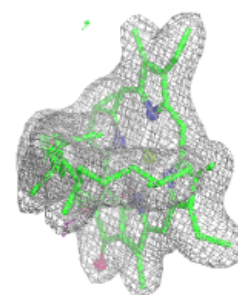
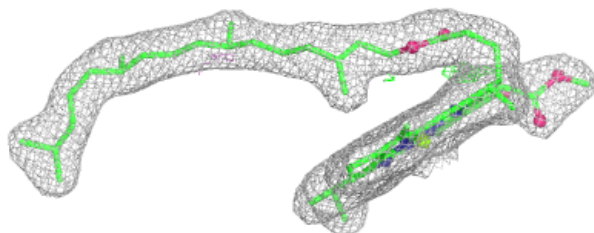
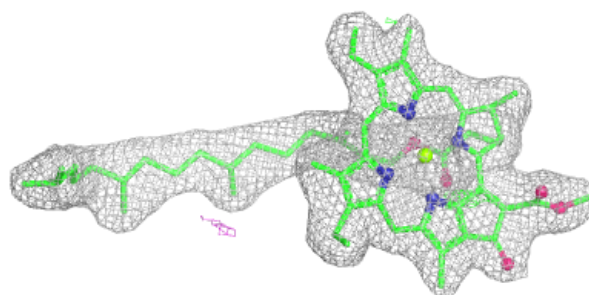


Electron density around CLA b 617:

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

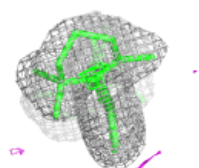
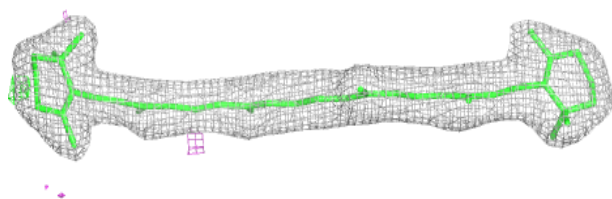
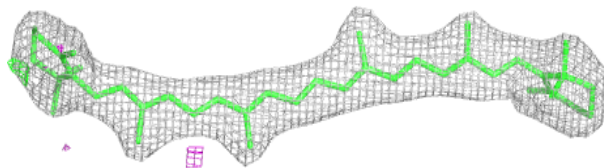
**Electron density around CLA b 618:**

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



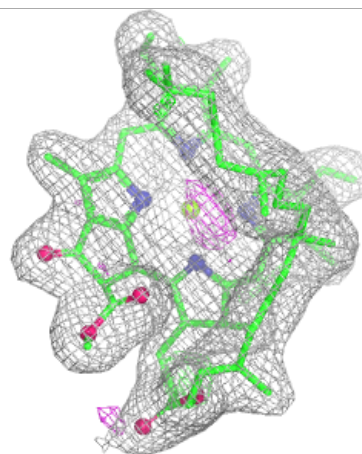
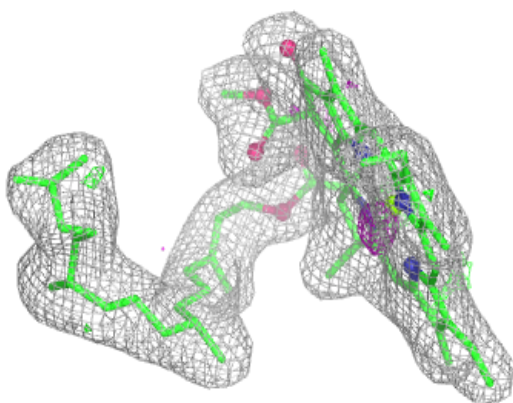
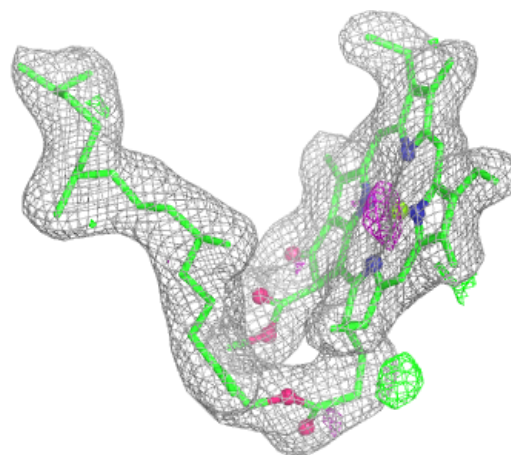
Electron density around BCR C 515:

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



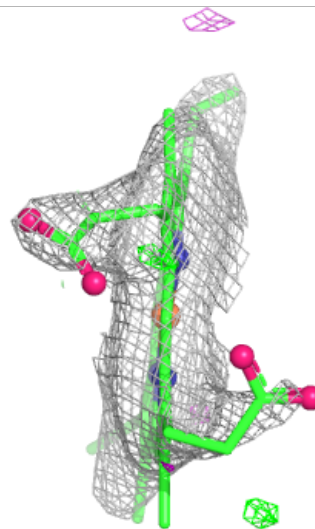
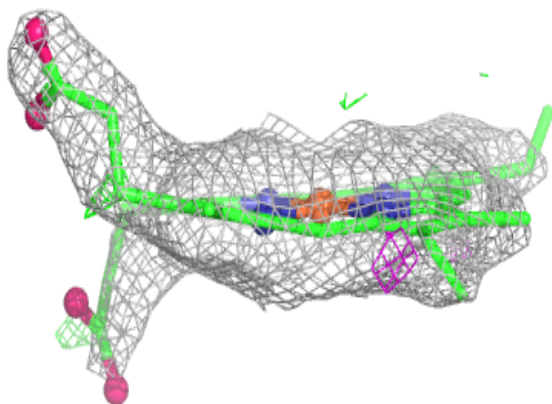
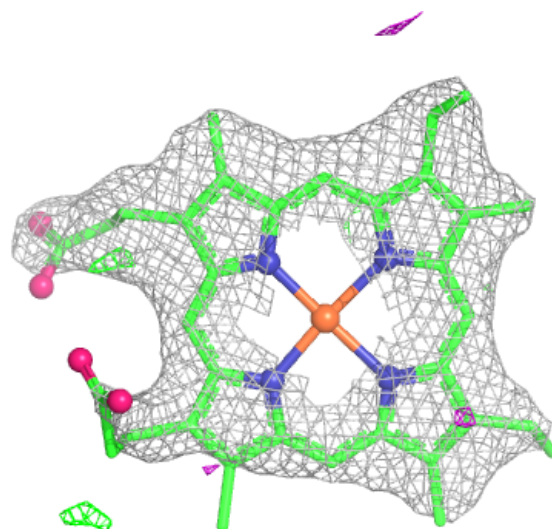
Electron density around CLA B 614:

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



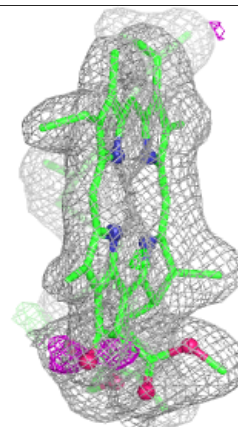
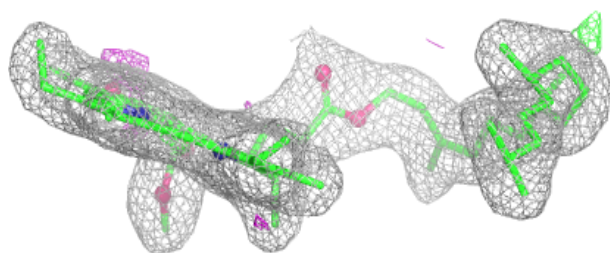
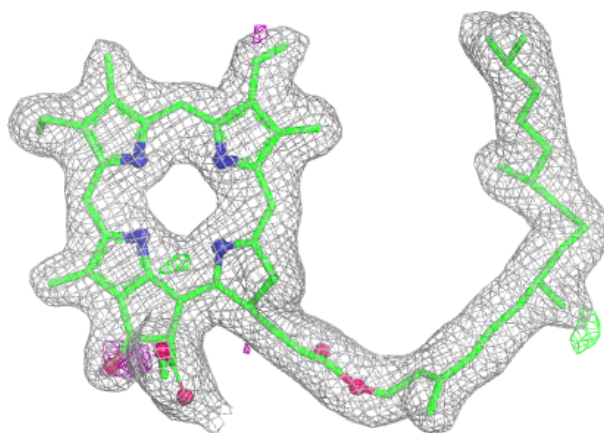
Electron density around HEM e 102:

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

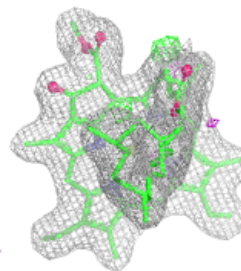
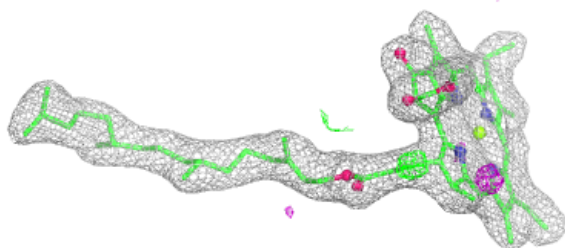
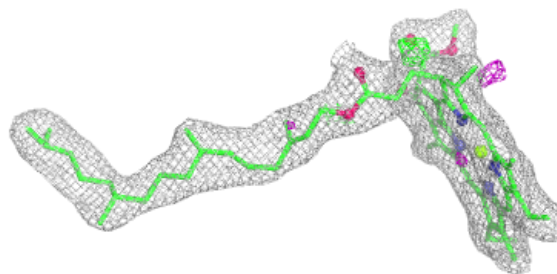


Electron density around PHO a 411:

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

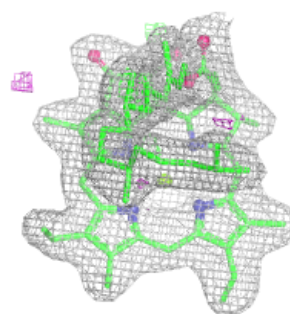
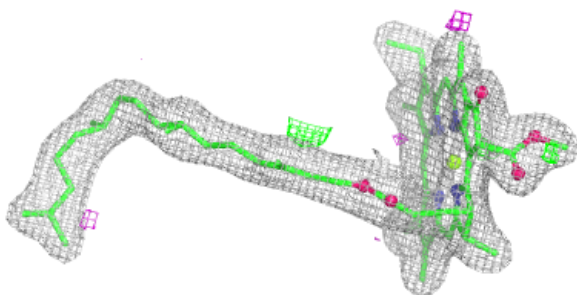
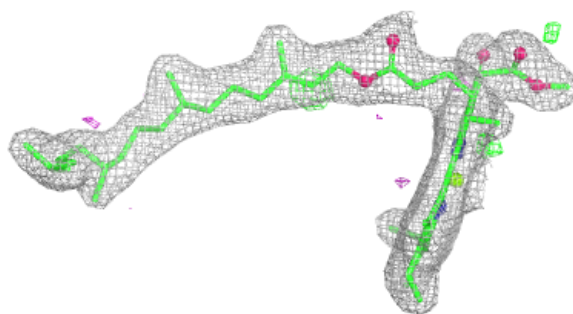
**Electron density around CLA B 605:**

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

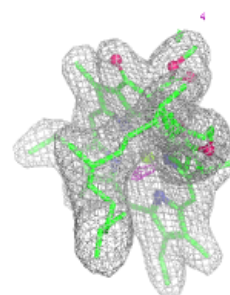
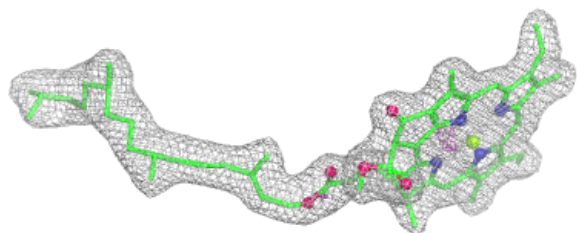
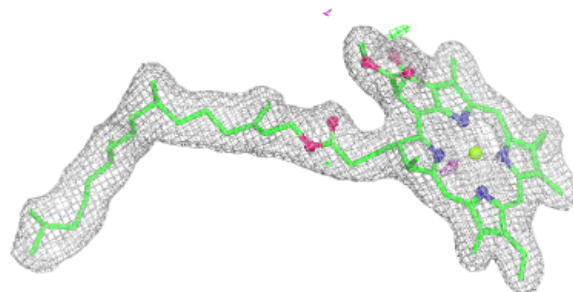


Electron density around CLA B 606:

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

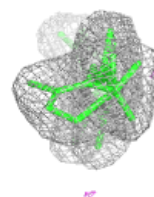
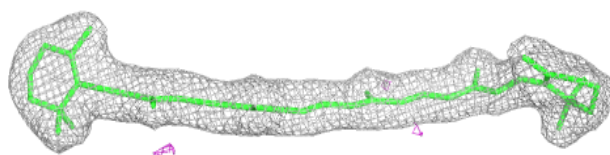
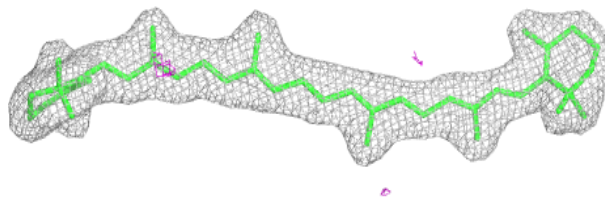
**Electron density around CLA a 409:**

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

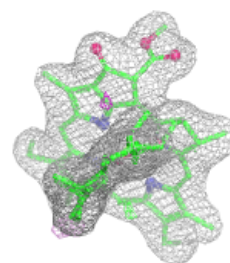
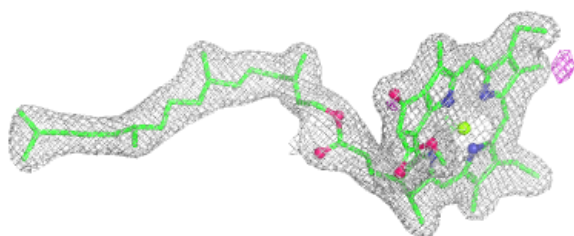
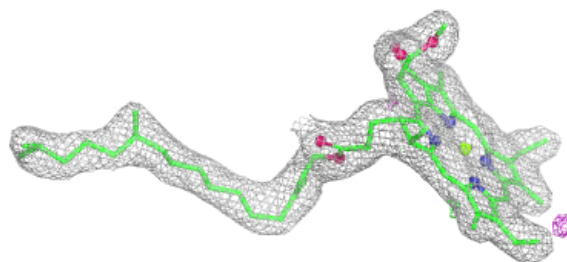


Electron density around BCR B 618:

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

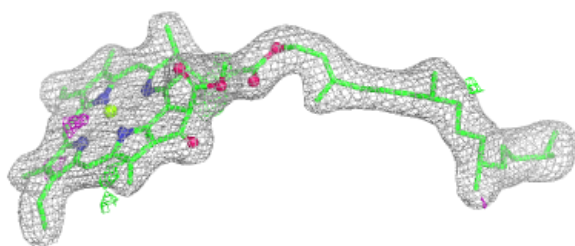
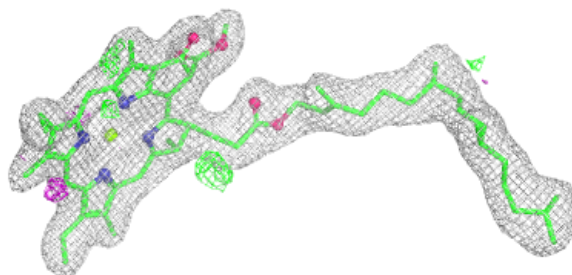
**Electron density around CLA C 502:**

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

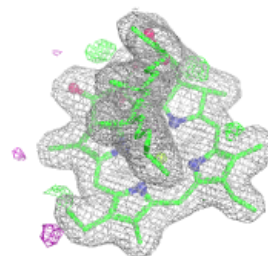
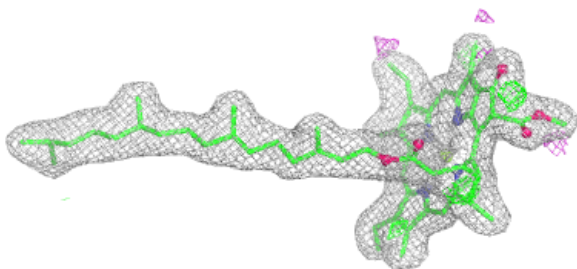
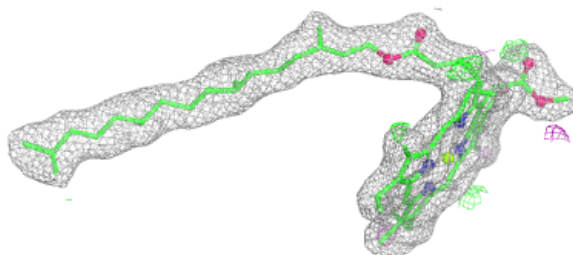


Electron density around CLA A 405:

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

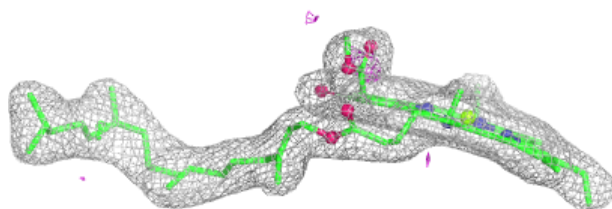
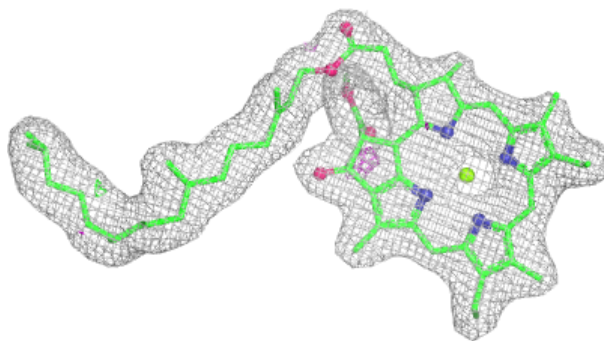
**Electron density around CLA B 608:**

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

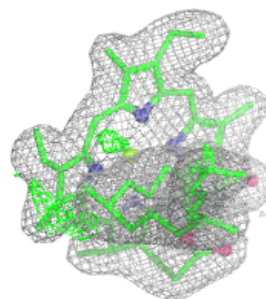
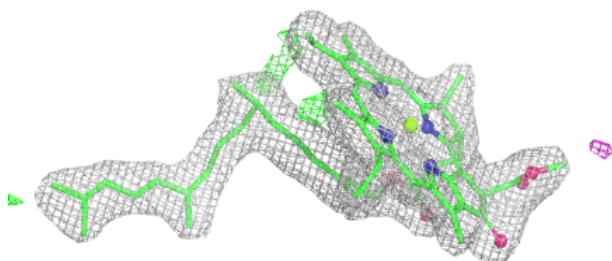
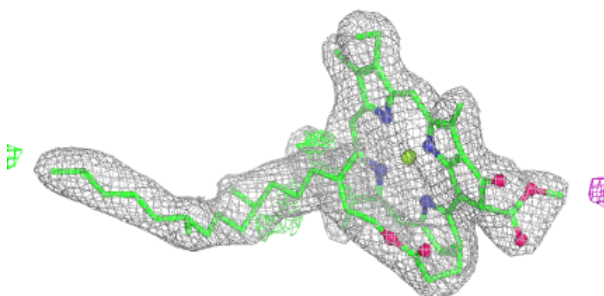


Electron density around CLA b 612:

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

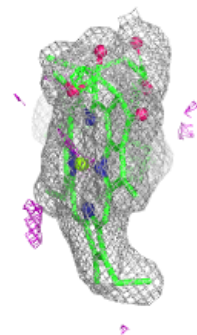
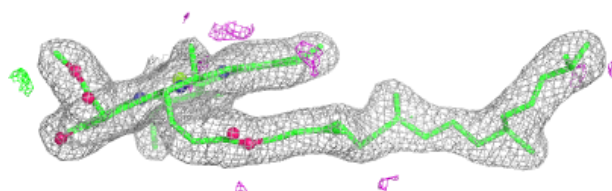
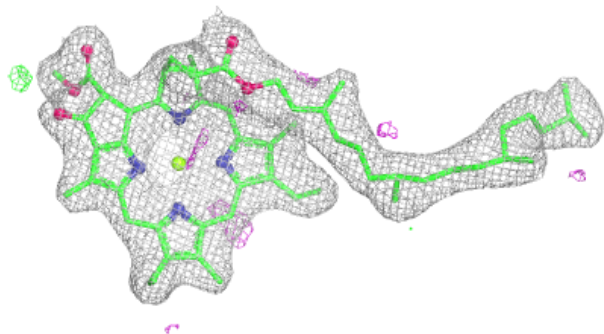
**Electron density around CLA c 509:**

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

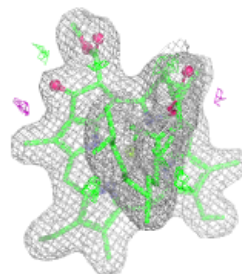
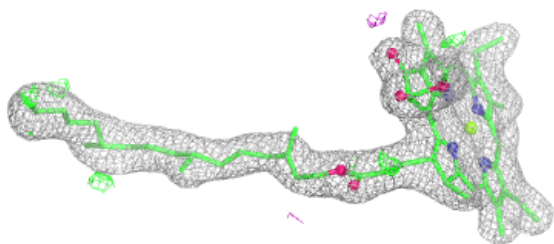
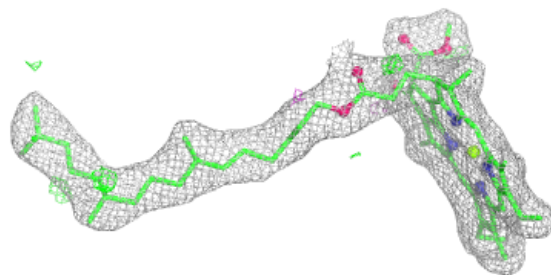


Electron density around CLA b 613:

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

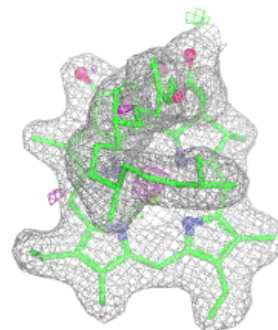
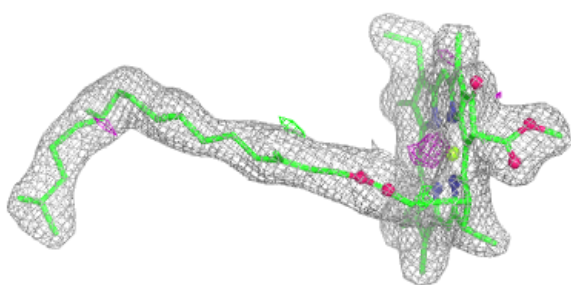
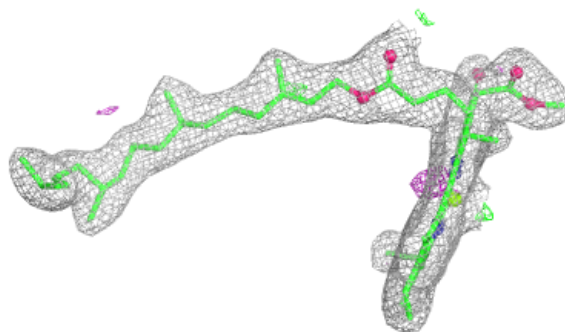
**Electron density around CLA b 614:**

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

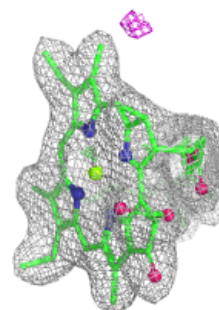
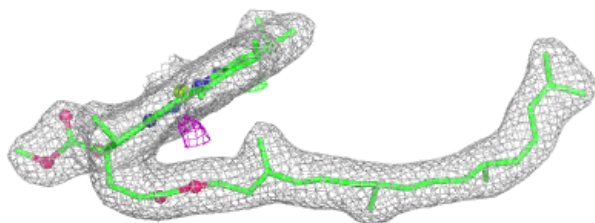
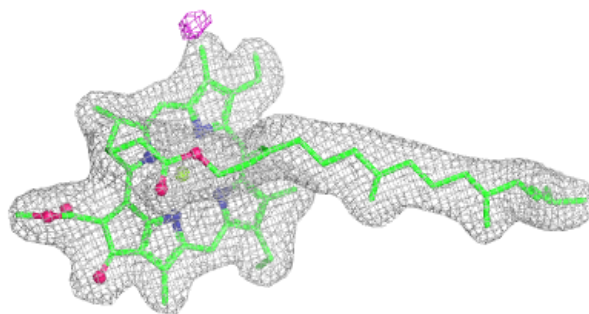


Electron density around CLA b 615:

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

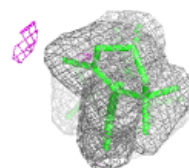
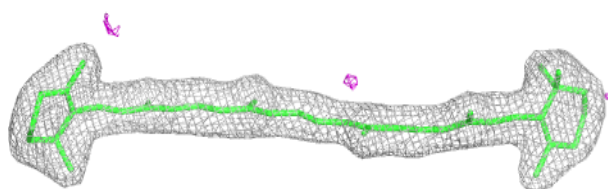
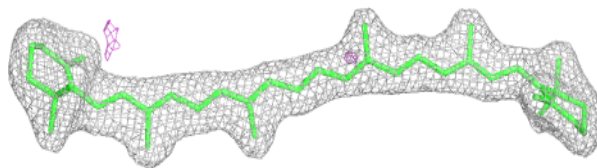
**Electron density around CLA B 609:**

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

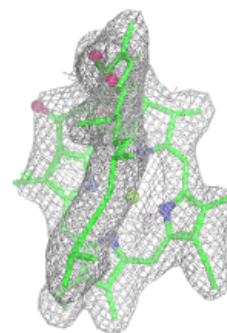
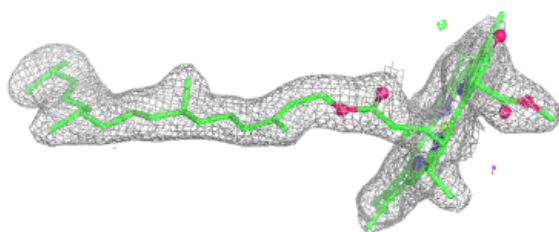
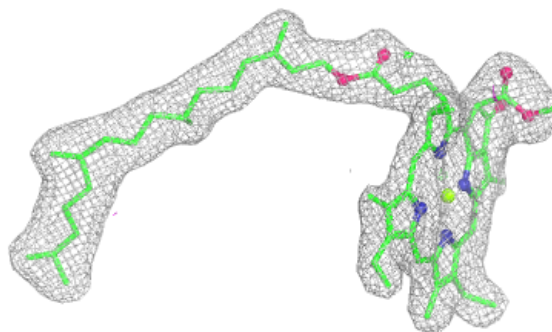


Electron density around BCR a 413:

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

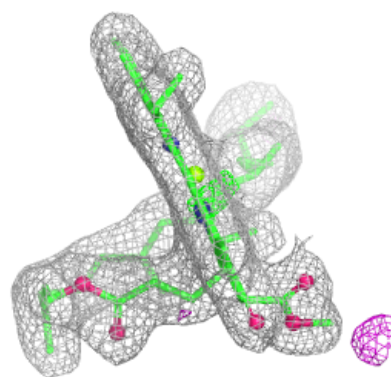
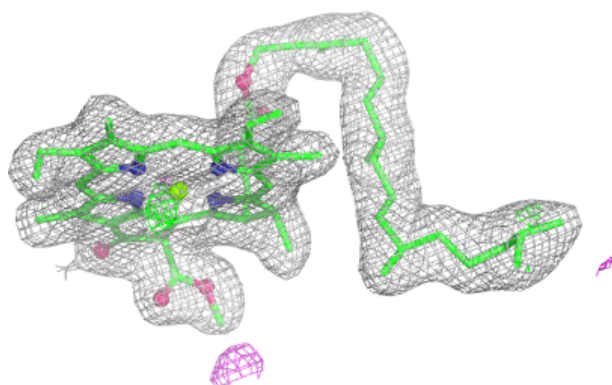
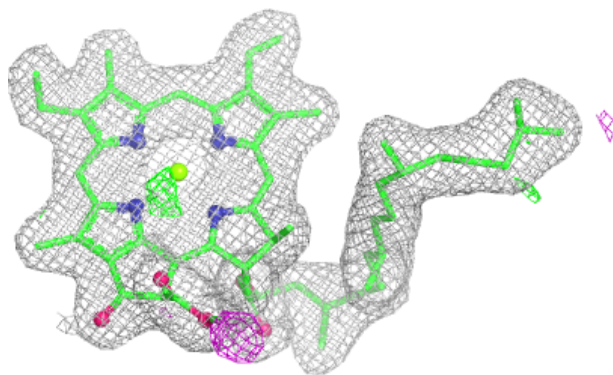
**Electron density around CLA B 610:**

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

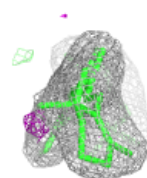
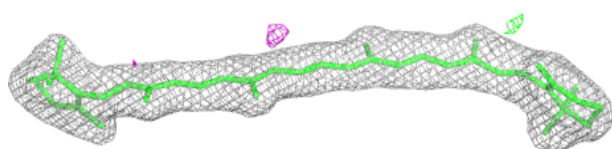
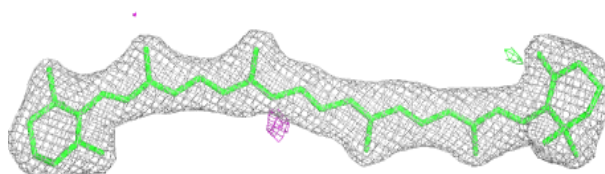


Electron density around CLA A 406:

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

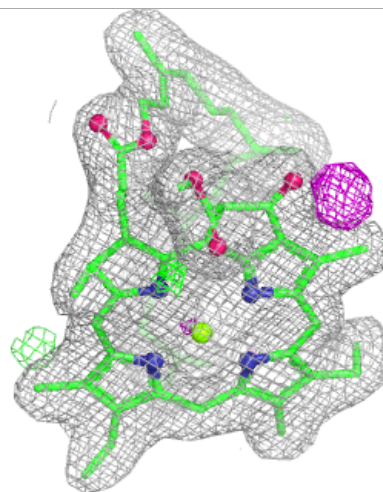
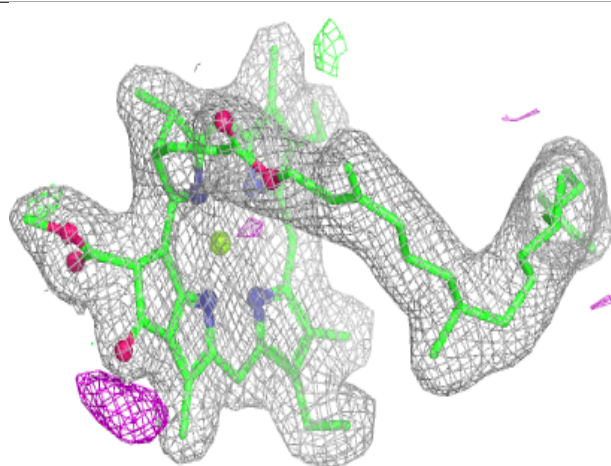
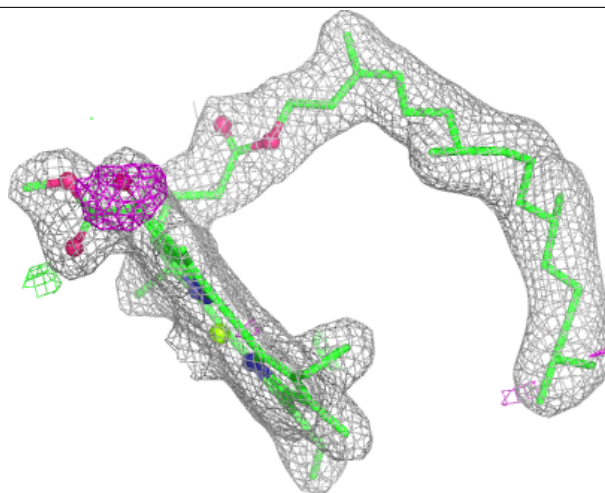
**Electron density around BCR b 629:**

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



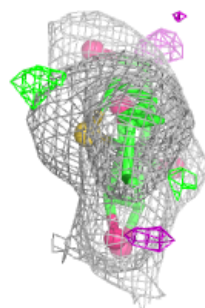
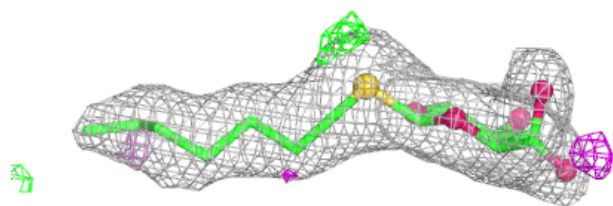
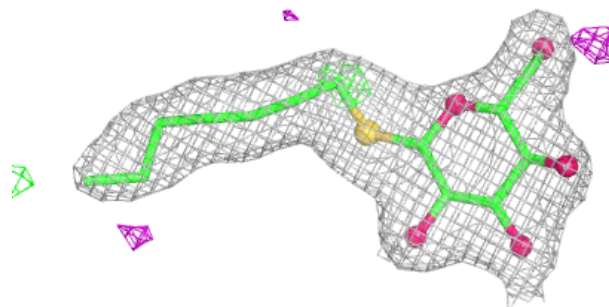
Electron density around CLA B 612:

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



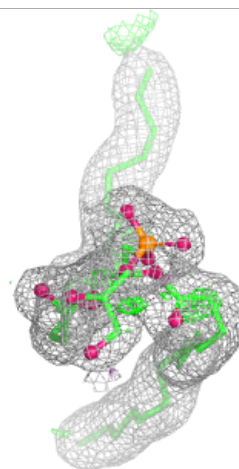
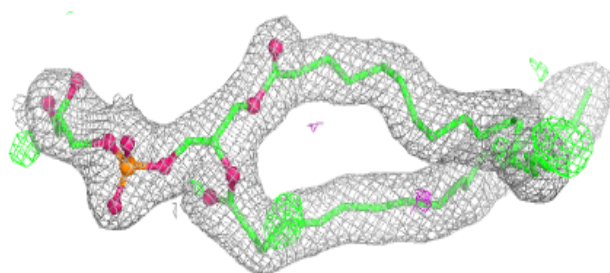
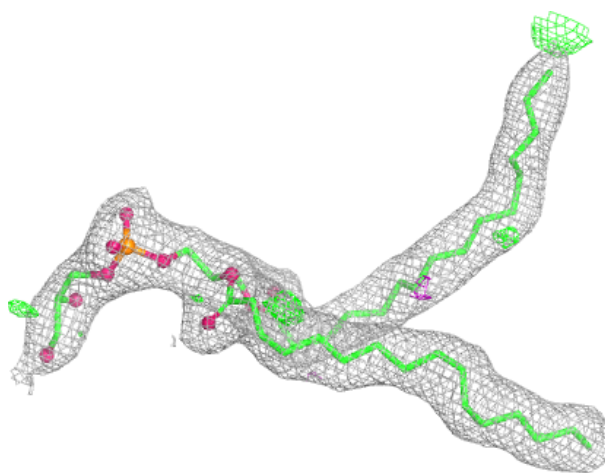
Electron density around HTG B 623:

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



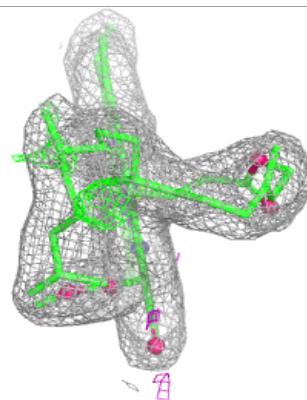
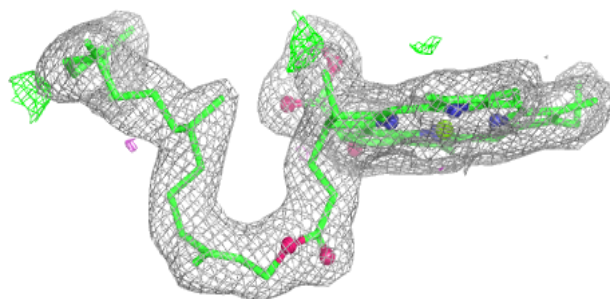
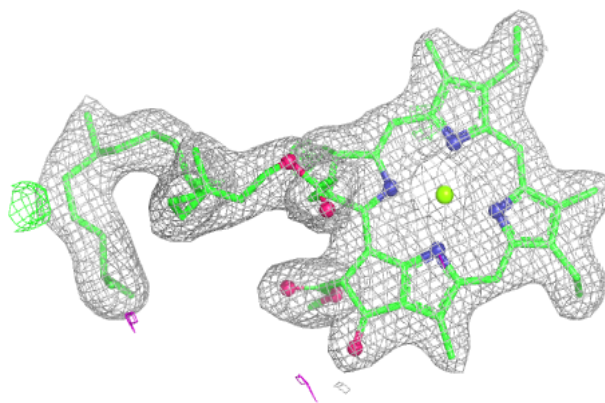
Electron density around LHG D 408:

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

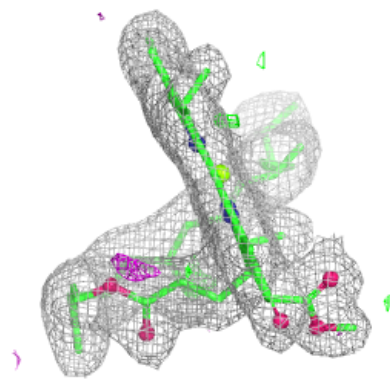
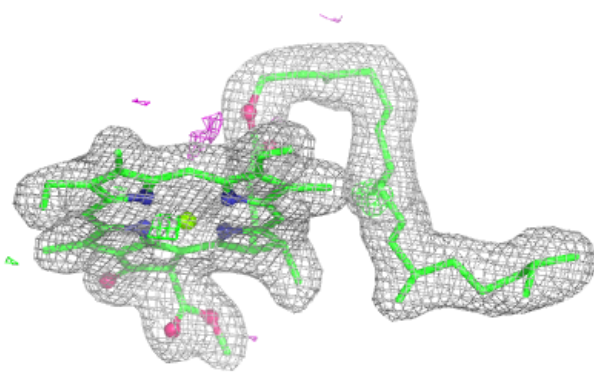
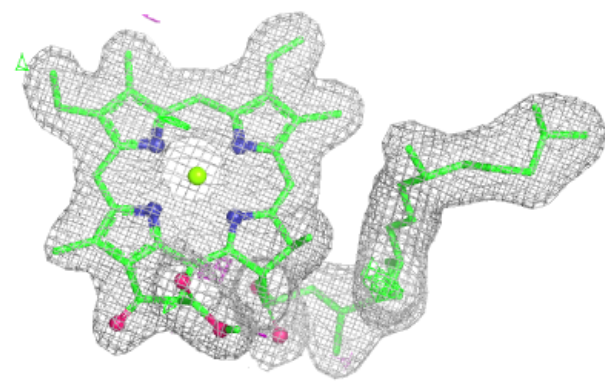


Electron density around CLA B 613:

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

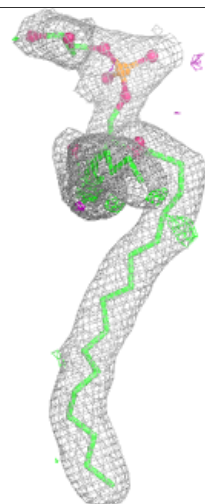
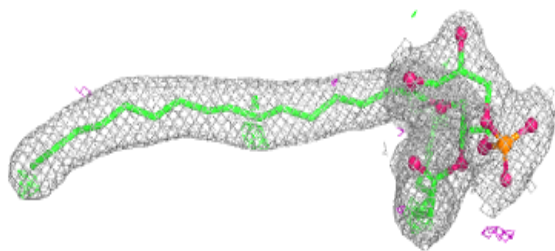
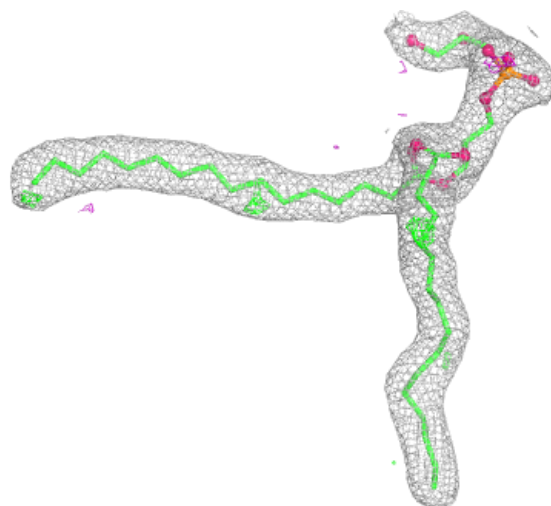
**Electron density around CLA d 401:**

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



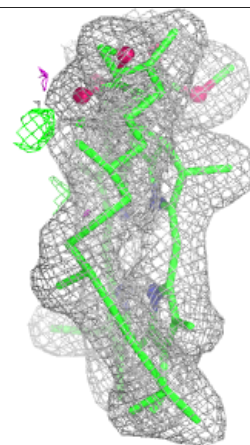
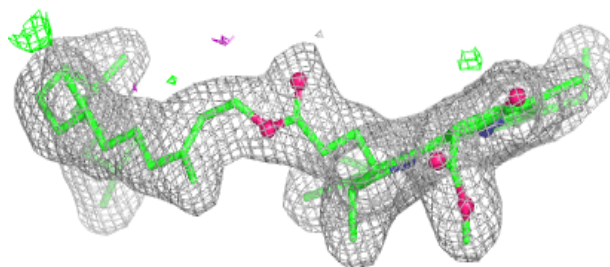
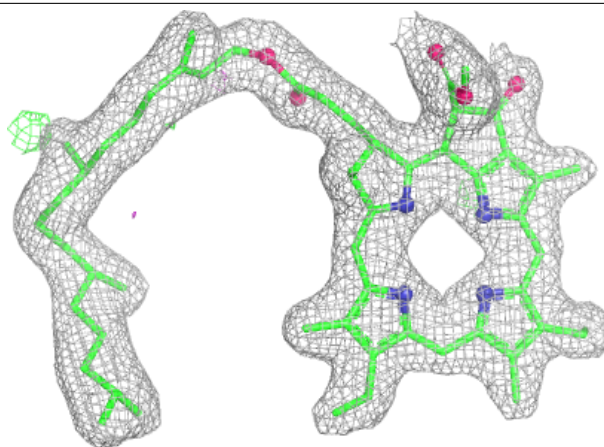
Electron density around LHG L 101:

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



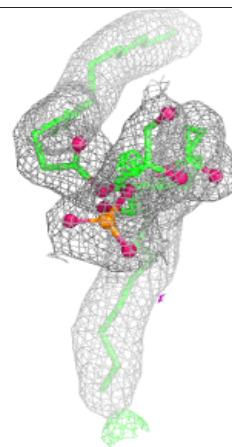
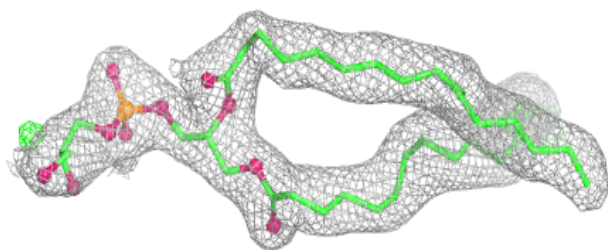
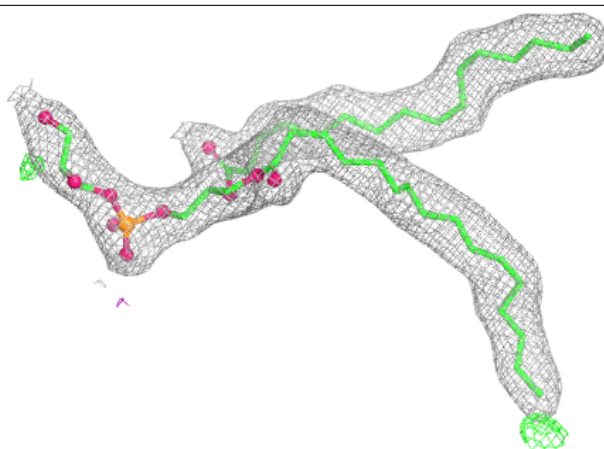
Electron density around PHO A 408:

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



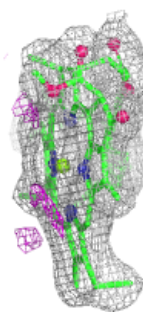
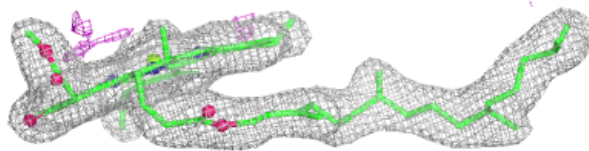
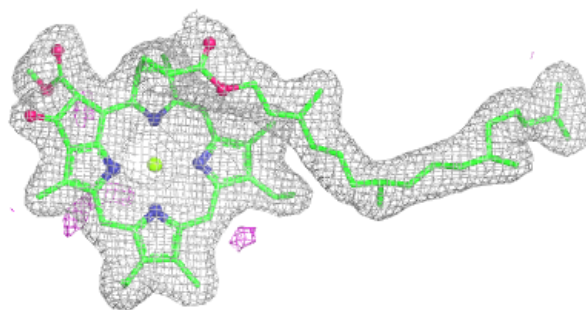
Electron density around LHG d 407:

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



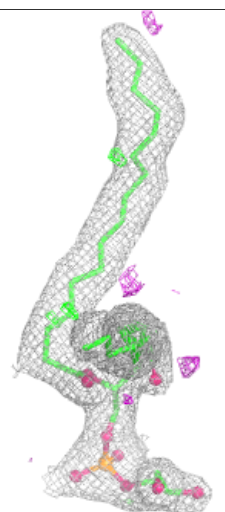
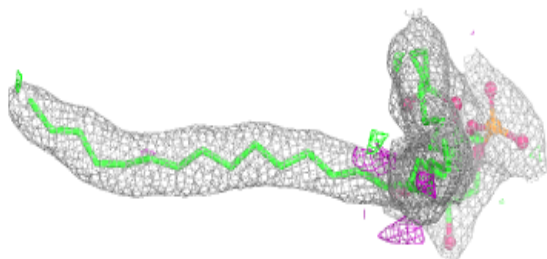
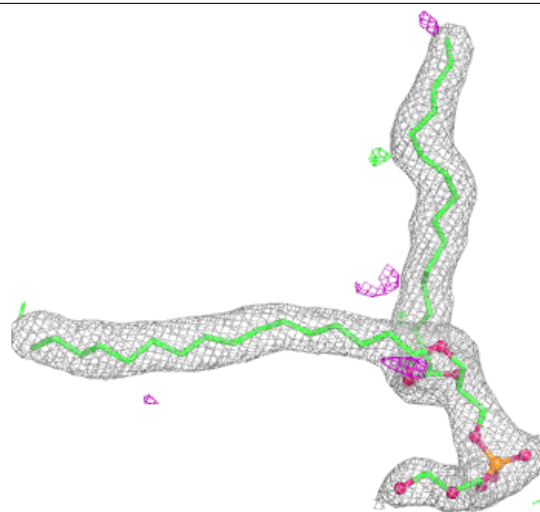
Electron density around CLA B 604:

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



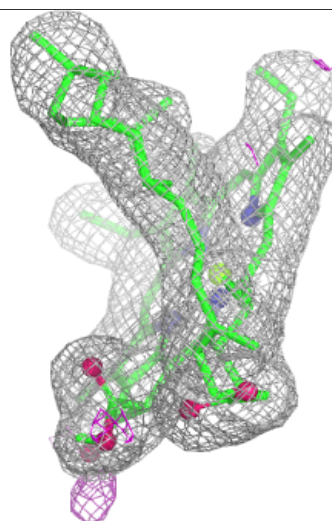
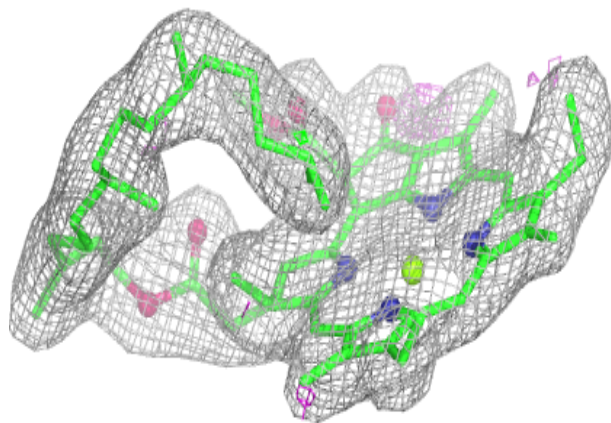
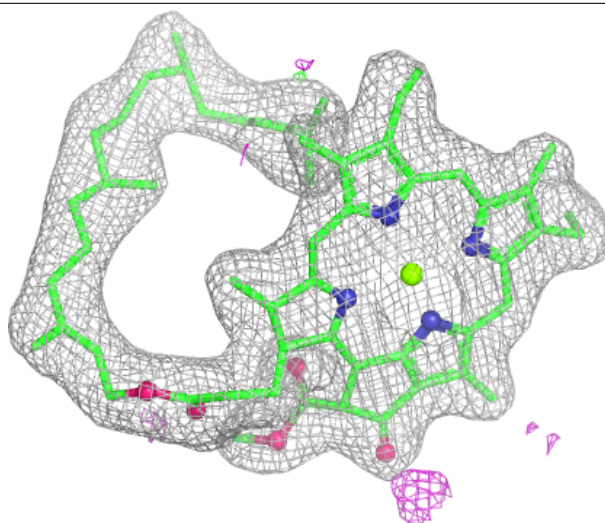
Electron density around LHG 1 101:

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



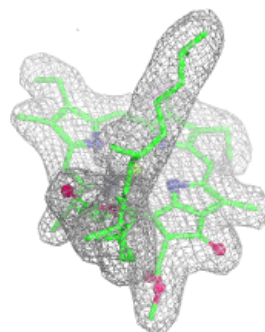
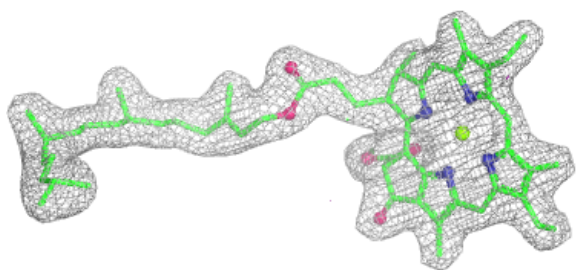
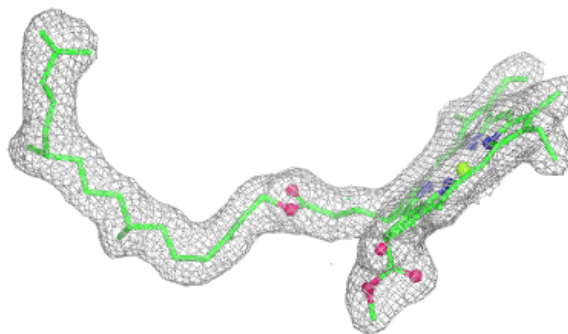
Electron density around CLA B 616:

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

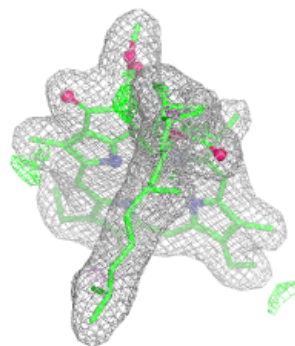
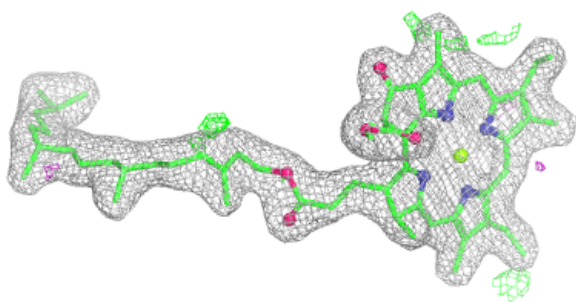
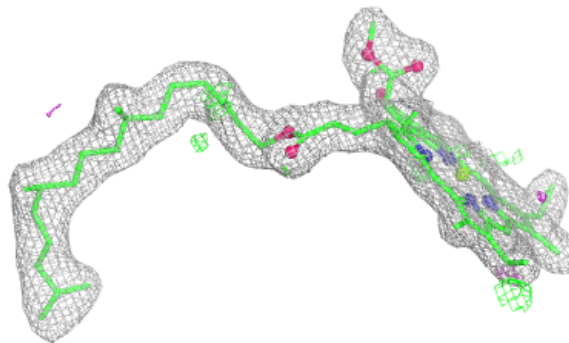


Electron density around CLA d 402:

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

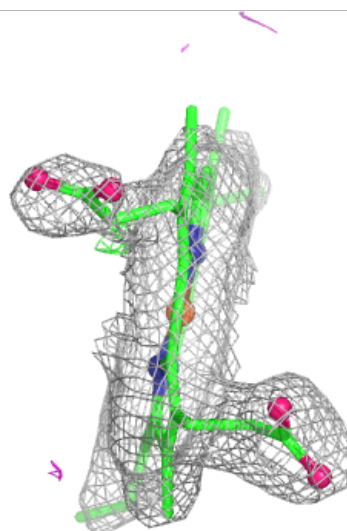
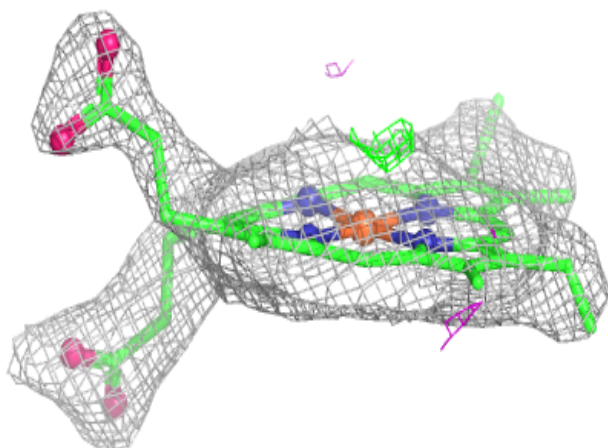
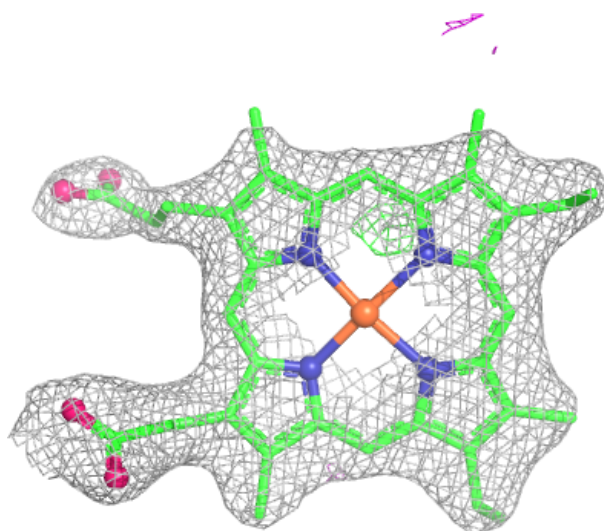
**Electron density around CLA D 402:**

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



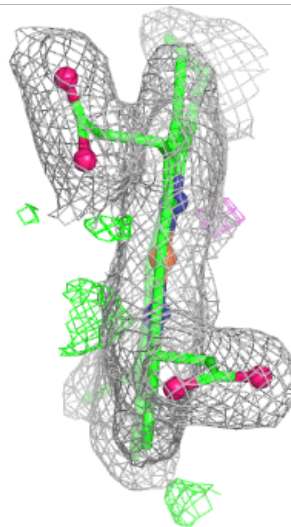
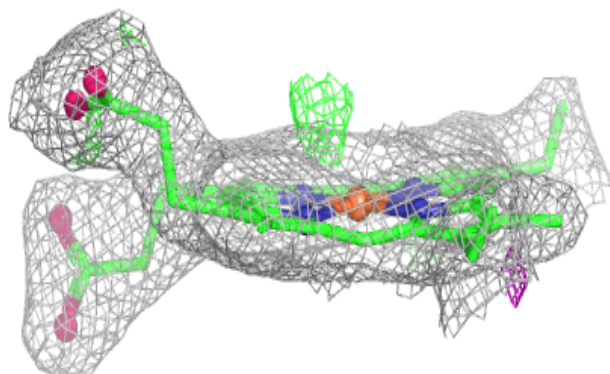
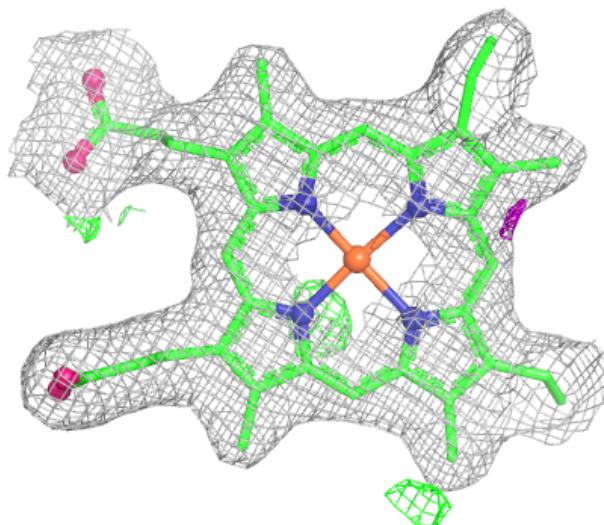
Electron density around HEM F 102:

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



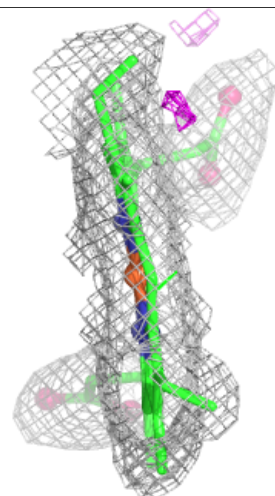
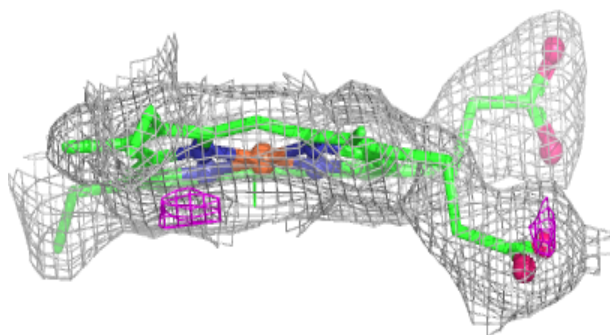
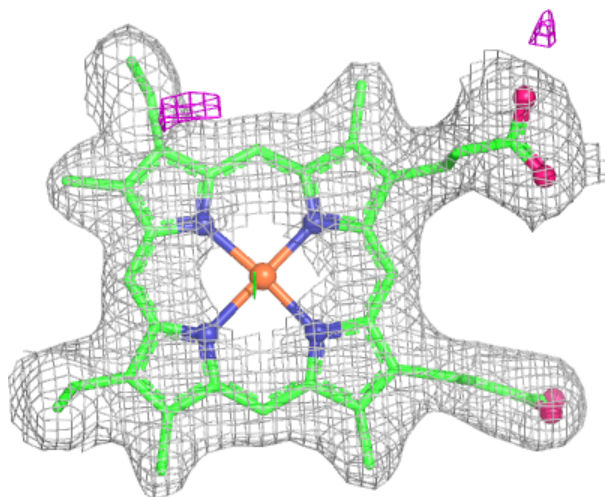
Electron density around HEC V 206:

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



Electron density around HEC v 205:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.