



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 11:12 PM UTC

PDB ID : 8IR5 / pdb_00008ir5
Title : XFEL structure of cyanobacterial photosystem II under dark conditions
Authors : Li, H.; Suga, M.; Shen, J.R.
Deposited on : 2023-03-17
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

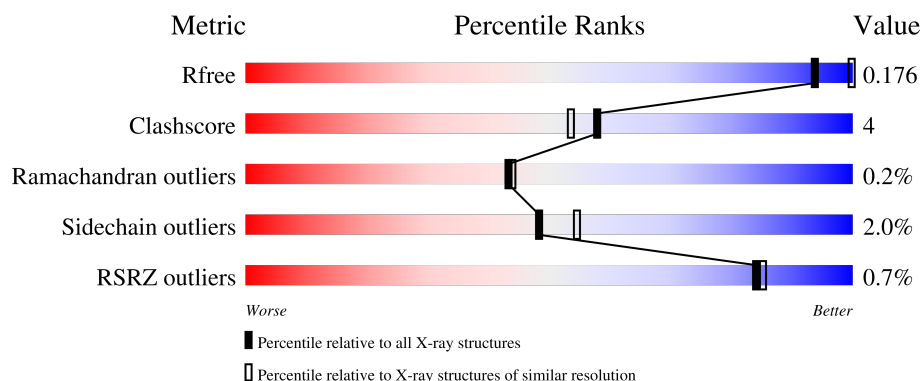
1 Overall quality at a glance

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.



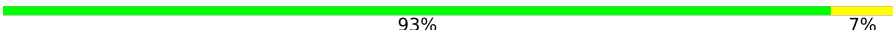
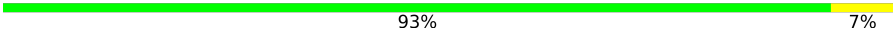
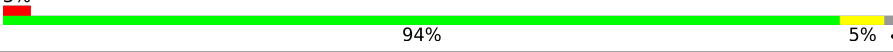
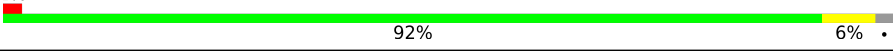
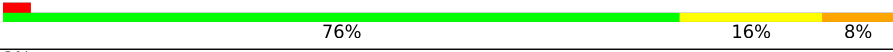
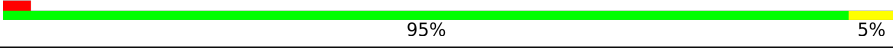
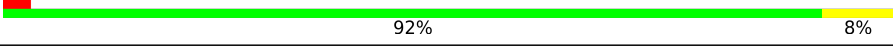
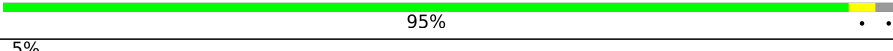
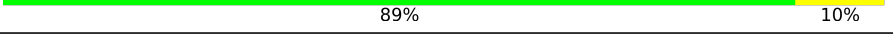
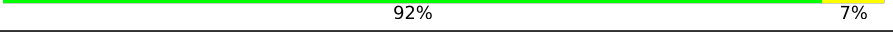
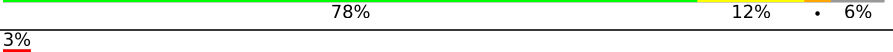
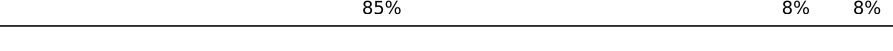
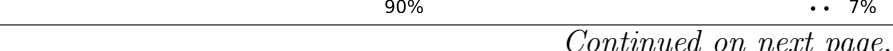
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	92%
1	a	344	2% 90% 7%
2	B	505	93% 6%
2	b	505	2% 93% 7%
3	C	455	91% 8%

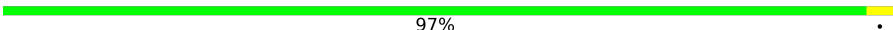
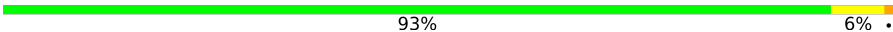
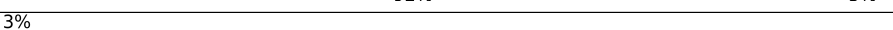
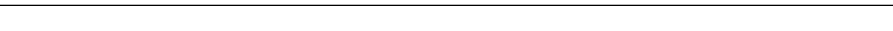
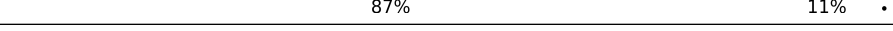
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Mol	Chain	Length	Quality of chain
3	c	455	 93% 7%
4	D	342	 92% 8%
4	d	342	 93% 7%
5	E	84	 2% 86% 11% .
5	e	84	 1% 86% 8% 6%
6	F	44	 64% 14% 23%
6	f	44	 5% 61% 9% 30%
7	H	65	 3% 94% 5% .
7	h	65	 2% 92% 6% .
8	I	38	 3% 76% 16% 8%
8	i	38	 3% 95% 5%
9	J	39	 87% 10% .
9	j	39	 3% 92% 8%
10	K	37	 70% 24% 5%
10	k	37	 78% 16% 5%
11	L	37	 95% . .
11	l	37	 5% 86% 11% .
12	M	36	 78% 11% . 8%
12	m	36	 81% 11% . 6%
13	O	244	 89% 10%
13	o	244	 92% 7%
14	T	32	 78% 12% . 6%
14	t	32	 3% 81% 12% 6%
15	U	104	 85% 8% 8%
15	u	104	 90% . . 7%

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Mol	Chain	Length	Quality of chain
16	V	137	 97% .
16	v	137	 93% 6% .
17	X	40	 85% 10% 5%
17	x	40	 2% 92% . 5%
18	Y	30	 3% 83% 13% .
18	y	30	 70% 27% .
19	Z	62	 87% 11% .
19	z	62	 76% 24%
20	R	34	 9% 71% 29%

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
23	CLA	A	404	X	-	-	-
23	CLA	A	408	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	501	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	507	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	D	402	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	406	X	-	-	-
23	CLA	a	409	X	-	-	-
23	CLA	b	601	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
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23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	c	514	X	-	-	-
23	CLA	d	401	X	-	-	-
23	CLA	d	402	X	-	-	-
27	GOL	a	420	-	-	X	-

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 52978 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	1	0
			2628	1722	432	459	15			
1	a	334	Total	C	N	O	S	0	2	0
			2629	1721	432	461	15			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	7	0
			4029	2639	674	703	13			
2	b	504	Total	C	N	O	S	0	6	0
			4017	2636	669	699	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	1	0
			3497	2287	588	609	13			
3	c	455	Total	C	N	O	S	0	5	0
			3555	2327	595	620	13			

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	1	0
			2732	1808	446	466	12			
4	d	341	Total	C	N	O	S	0	2	0
			2732	1808	447	465	12			

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

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

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

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

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

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

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	36	Total	C	N	O	0	0	0
			296	197	47	52			
11	l	36	Total	C	N	O	0	0	0
			296	197	47	52			

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	3	0
			1894	1181	321	388	4			
13	o	243	Total	C	N	O	S	0	0	0
			1865	1165	315	381	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	1	0
			267	186	37	42	2			
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	96	Total	C	N	O		0	1	0
			774	491	129	154				
15	u	97	Total	C	N	O		0	1	0
			781	496	130	155				

- 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
			1082	685	179	214	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

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

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

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

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

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

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

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

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

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

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

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

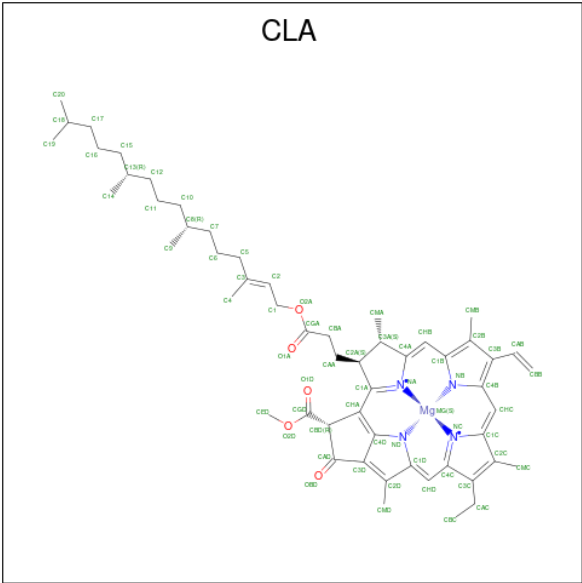
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		

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

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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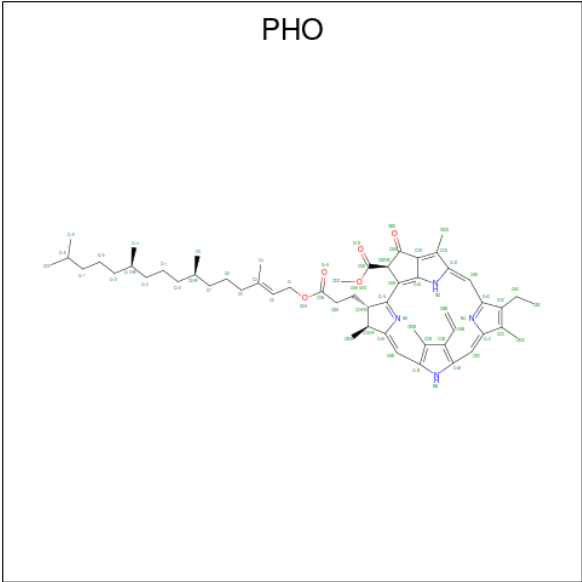
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N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

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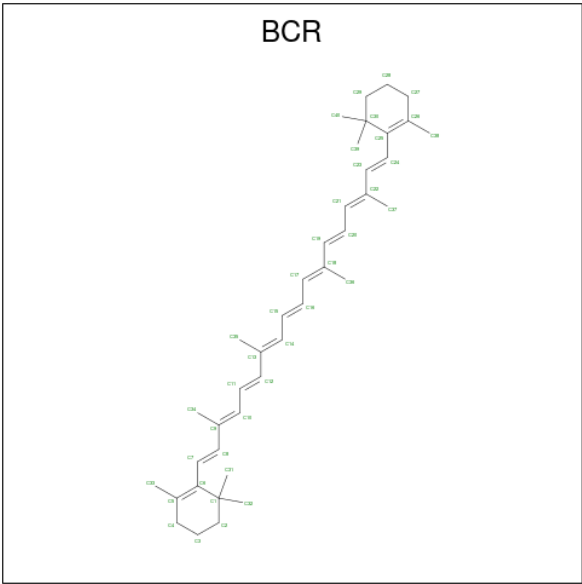
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 24 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



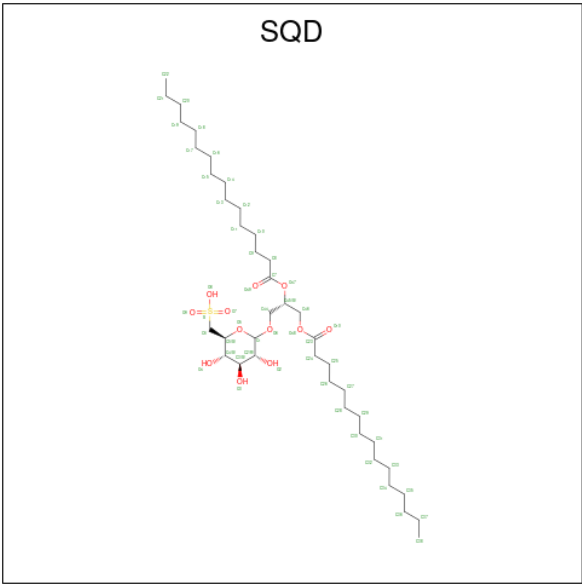
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		

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



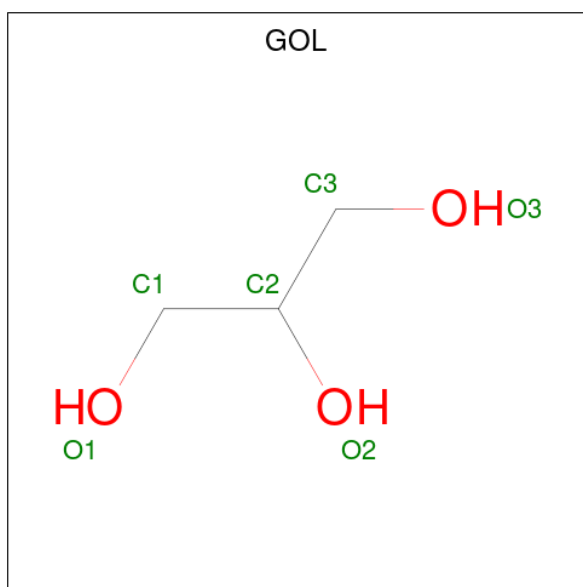
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total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

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



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

- Molecule 27 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



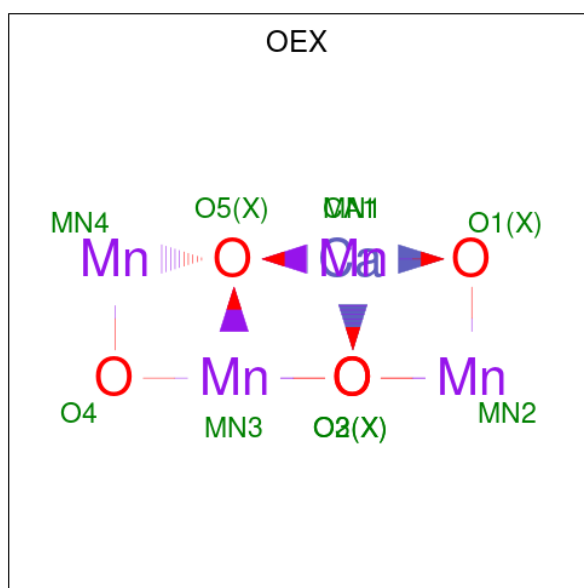
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			6	3	3		
27	A	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	0
			6	3	3		
27	O	1	Total	C	O	0	0
			6	3	3		
27	O	1	Total	C	O	0	0
			6	3	3		
27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

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

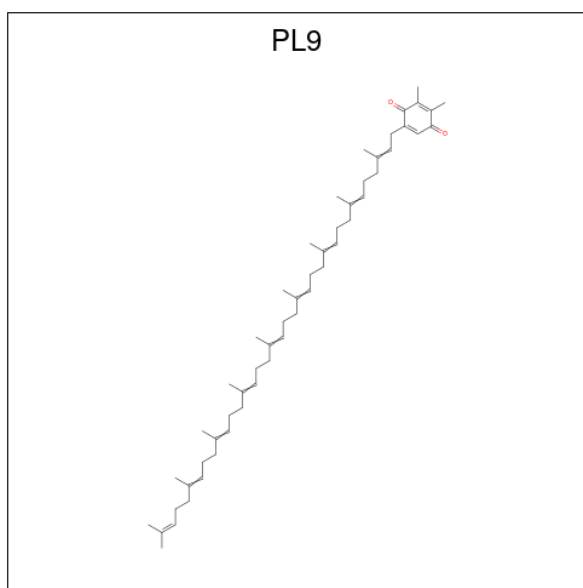
- Molecule 28 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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

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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			55	53	2		
29	D	1	Total	C	O	0	0
			55	53	2		
29	a	1	Total	C	O	0	0
			55	53	2		
29	d	1	Total	C	O	0	0
			55	53	2		

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

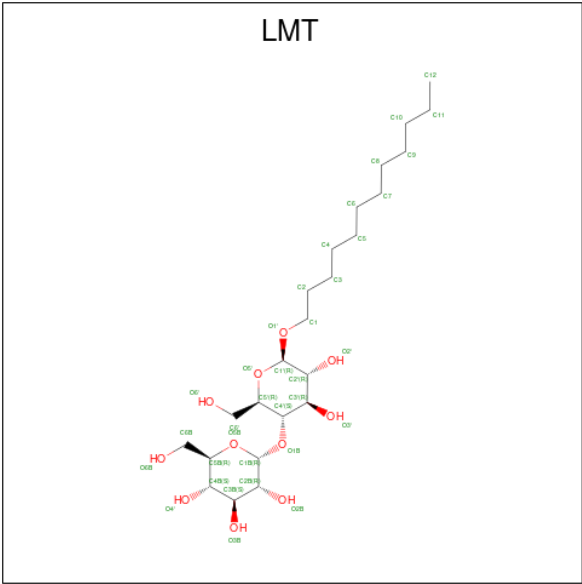
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			28	23	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	I	1	Total	C	O	0	0
			40	35	5		
30	J	1	Total	C		0	0
			10	10			
30	K	1	Total	C	O	0	0
			34	29	5		
30	X	1	Total	C	O	0	0
			18	16	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	a	1	Total	C	O	0	0
			30	25	5		
30	b	1	Total	C	O	0	0
			33	28	5		
30	c	1	Total	C	O	0	0
			32	27	5		
30	d	2	Total	C	O	0	0
			53	47	6		
30	i	1	Total	C	O	0	0
			40	35	5		
30	j	1	Total	C		0	0
			10	10			
30	l	1	Total	C		0	0
			10	10			
30	m	1	Total	C		0	0
			10	10			
30	x	1	Total	C	O	0	0
			18	16	2		

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



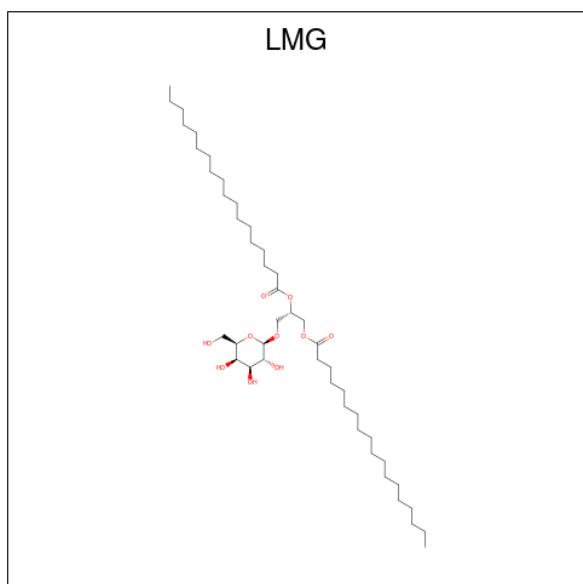
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			35	24	11		
31	A	1	Total	C	O	0	0
			35	24	11		

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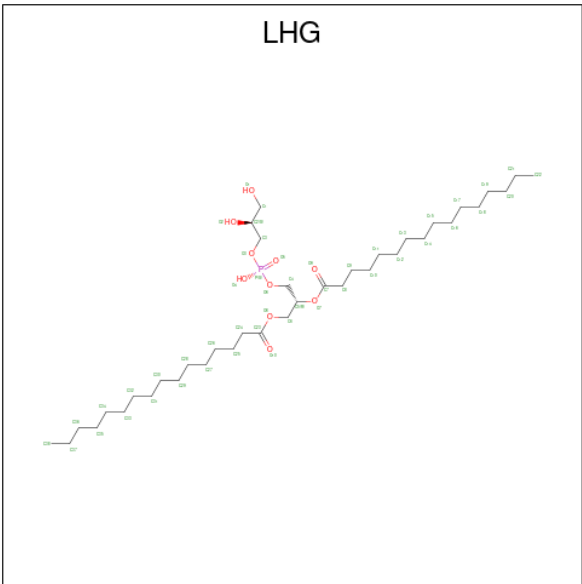
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			25	19	6		
31	F	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total	C	O	0	0
			35	24	11		
31	T	1	Total	C	O	0	0
			35	24	11		
31	b	1	Total	C	O	0	0
			25	19	6		
31	b	1	Total	C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

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



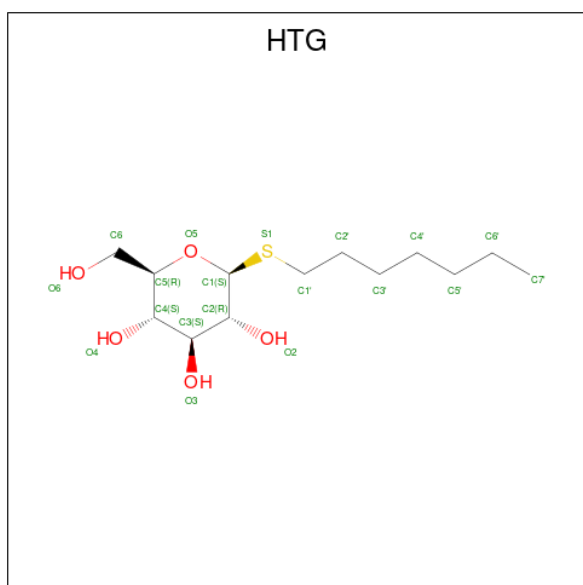
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			51	41	10		
32	B	1	Total	C	O	0	0
			51	41	10		
32	C	1	Total	C	O	0	0
			51	41	10		
32	C	1	Total	C	O	0	0
			51	41	10		
32	D	1	Total	C	O	0	0
			51	41	10		
32	a	1	Total	C	O	0	0
			51	41	10		
32	c	1	Total	C	O	0	0
			51	41	10		
32	c	1	Total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

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



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

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



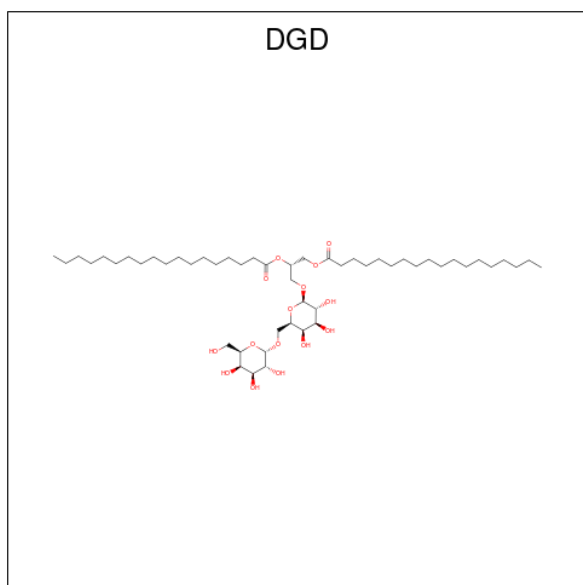
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		

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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	C	1	Total	C	O	0	0
			62	47	15		
35	C	1	Total	C	O	0	0
			62	47	15		

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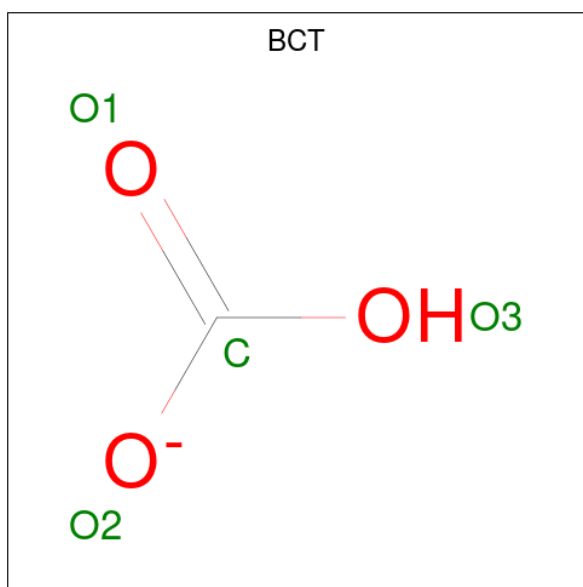
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	C	1	Total	C	O	0	0
			62	47	15		
35	H	1	Total	C	O	0	0
			62	47	15		
35	c	1	Total	C	O	0	0
			62	47	15		
35	c	1	Total	C	O	0	0
			62	47	15		
35	c	1	Total	C	O	0	0
			62	47	15		
35	h	1	Total	C	O	0	0
			62	47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

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

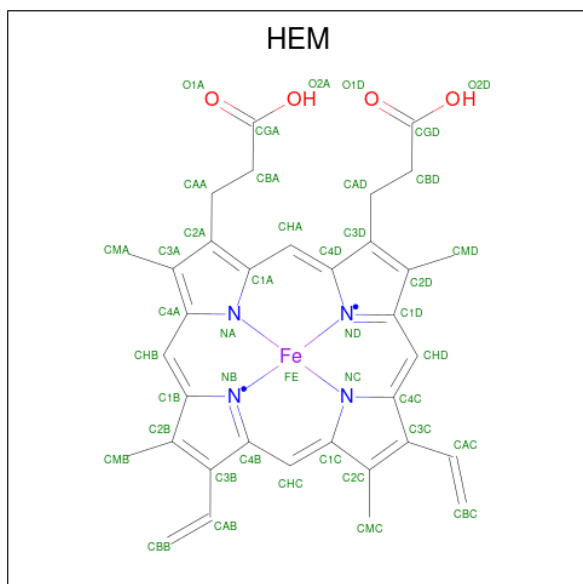
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	C	1	Total	Ca	0	0
			1	1		
36	F	1	Total	Ca	0	0
			1	1		
36	O	1	Total	Ca	0	0
			1	1		
36	c	2	Total	Ca	0	0
			2	2		
36	f	1	Total	Ca	0	0
			1	1		
36	o	1	Total	Ca	0	0
			1	1		

- Molecule 37 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	D	1	Total	C	O	0	0
			4	1	3		
37	a	1	Total	C	O	0	0
			4	1	3		

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



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

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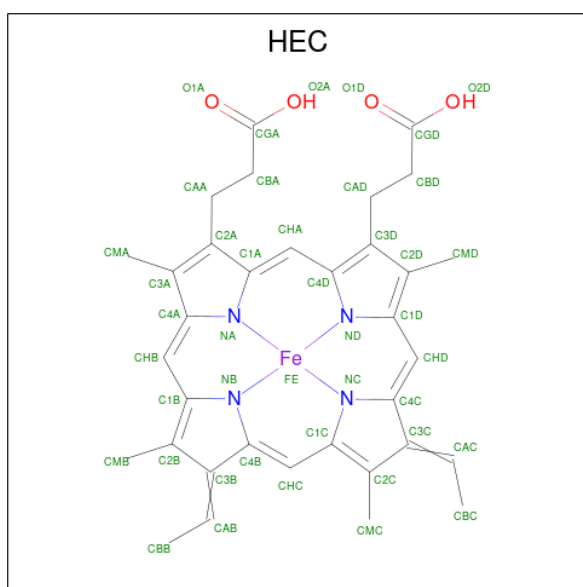
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
38	f	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

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

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



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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	C	167	Total 167	O 167	0	0
41	D	123	Total 123	O 123	0	0
41	E	13	Total 13	O 13	0	0
41	F	7	Total 7	O 7	0	0
41	H	21	Total 21	O 21	0	0
41	I	5	Total 5	O 5	0	0
41	J	8	Total 8	O 8	0	0
41	K	5	Total 5	O 5	0	0
41	L	9	Total 9	O 9	0	0
41	M	5	Total 5	O 5	0	0
41	O	105	Total 105	O 105	0	0
41	T	10	Total 10	O 10	0	0
41	U	44	Total 44	O 44	0	0
41	V	82	Total 82	O 82	0	0
41	X	7	Total 7	O 7	0	0
41	a	130	Total 130	O 130	0	0
41	b	202	Total 202	O 202	0	0
41	c	161	Total 161	O 161	0	0
41	d	111	Total 111	O 111	0	0
41	e	9	Total 9	O 9	0	0
41	f	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	h	17	Total 17	O 17	0	0
41	i	2	Total 2	O 2	0	0
41	j	2	Total 2	O 2	0	0
41	k	3	Total 3	O 3	0	0
41	l	8	Total 8	O 8	0	0
41	m	13	Total 13	O 13	0	0
41	o	103	Total 103	O 103	0	0
41	t	7	Total 7	O 7	0	0
41	u	49	Total 49	O 49	0	0
41	v	57	Total 57	O 57	0	0
41	x	8	Total 8	O 8	0	0
41	y	2	Total 2	O 2	0	0

3 Residue-property plots [i](#)

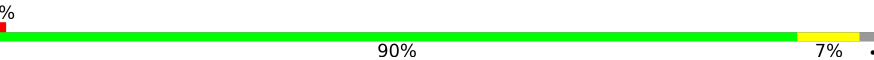
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

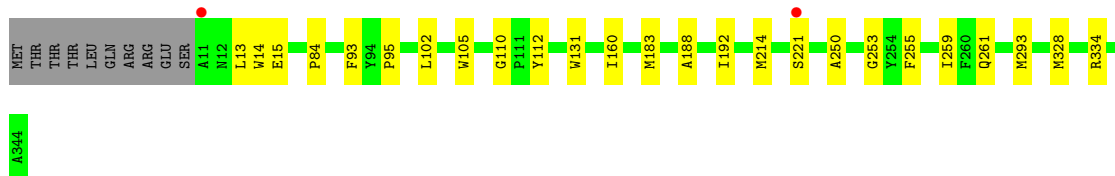
- Molecule 1: Photosystem II protein D1

Chain A:  92% 7% 1%



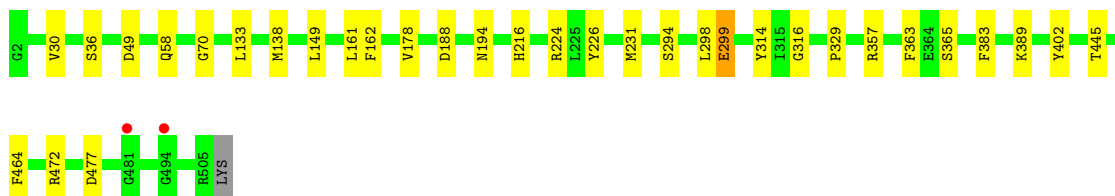
- Molecule 1: Photosystem II protein D1

Chain a:  90% 7% 3%

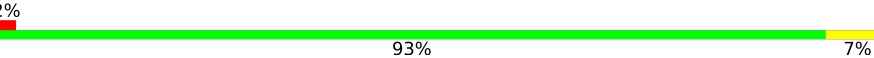


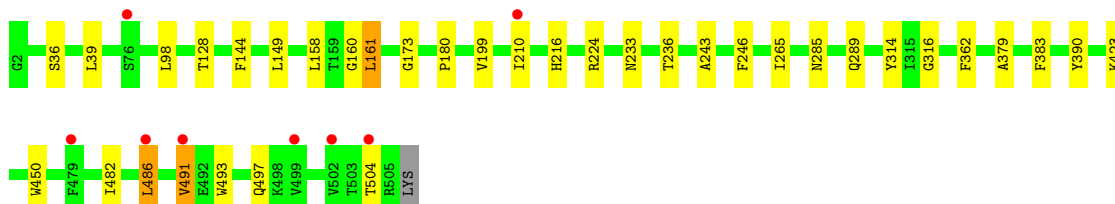
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  93% 6% 1%

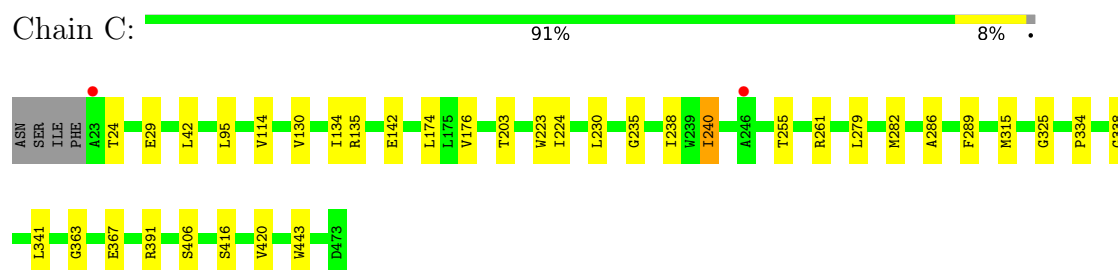


- Molecule 2: Photosystem II CP47 reaction center protein

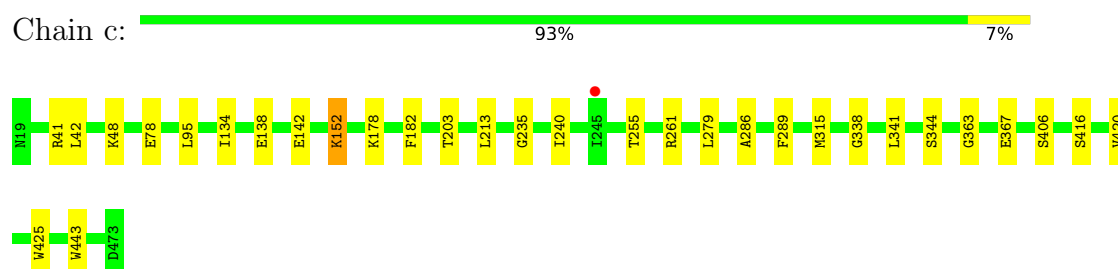
Chain b:  93% 7% 2%



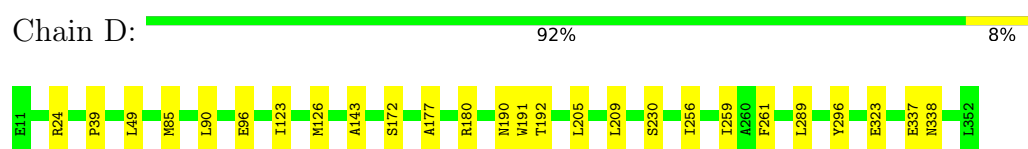
- Molecule 3: Photosystem II CP43 reaction center protein



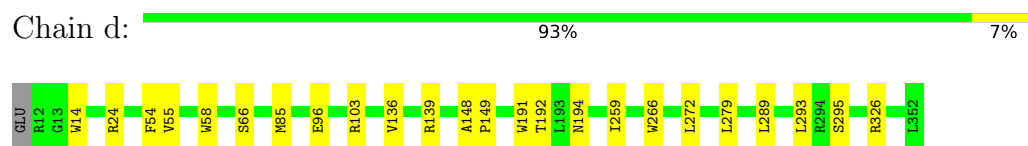
- Molecule 3: Photosystem II CP43 reaction center protein



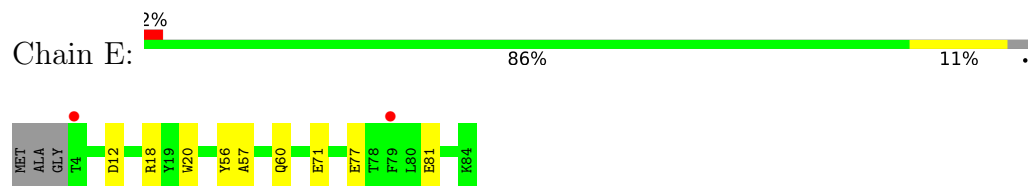
- Molecule 4: Photosystem II D2 protein



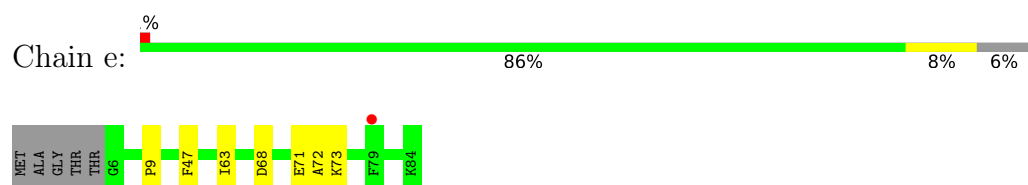
- Molecule 4: Photosystem II D2 protein



- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha



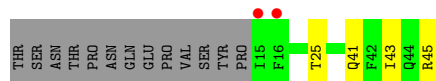
- Molecule 6: Cytochrome b559 subunit beta

Chain F:  64% 14% 23%

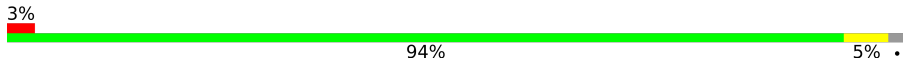


- Molecule 6: Cytochrome b559 subunit beta

Chain f:  5% 61% 9% 30%

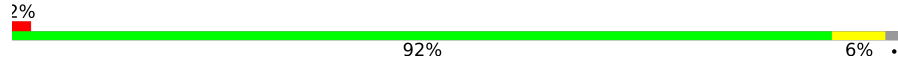


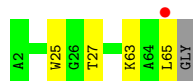
- Molecule 7: Photosystem II reaction center protein H

Chain H:  3% 94% 5%



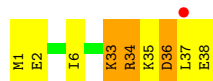
- Molecule 7: Photosystem II reaction center protein H

Chain h:  2% 92% 6%

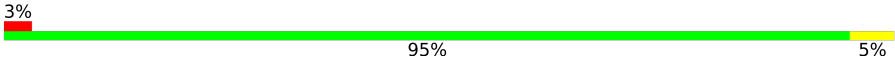


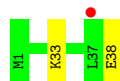
- Molecule 8: Photosystem II reaction center protein I

Chain I:  3% 76% 16% 8%



- Molecule 8: Photosystem II reaction center protein I

Chain i:  3% 95% 5%

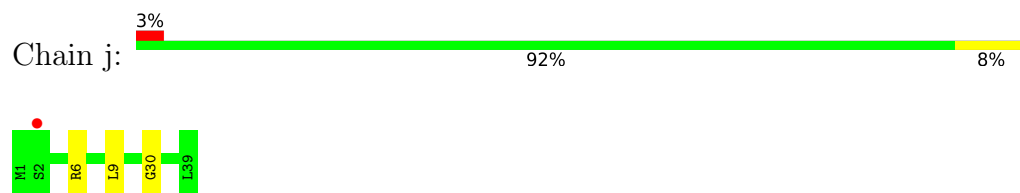


- Molecule 9: Photosystem II reaction center protein J

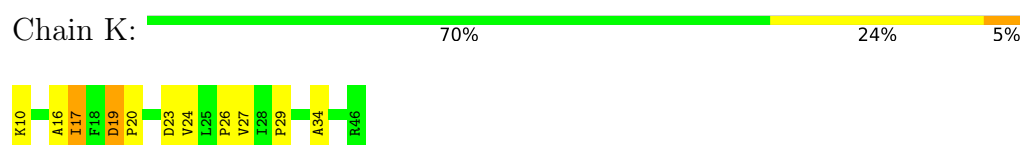
Chain J:  87% 10%



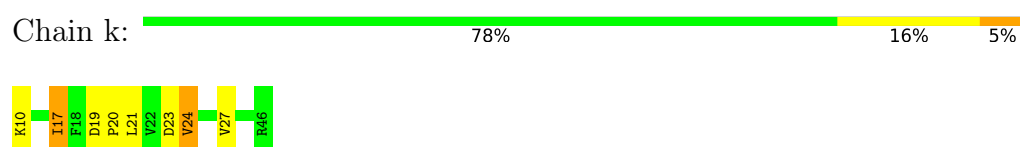
- Molecule 9: Photosystem II reaction center protein J



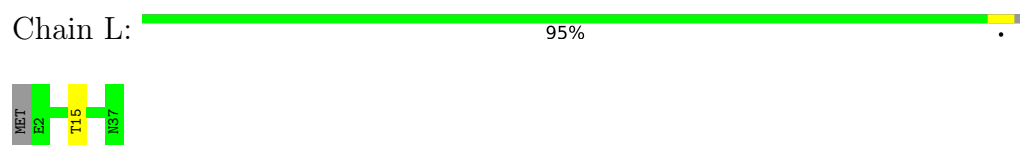
- Molecule 10: Photosystem II reaction center protein K



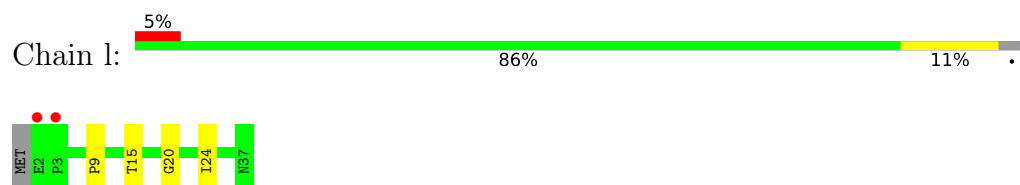
- Molecule 10: Photosystem II reaction center protein K



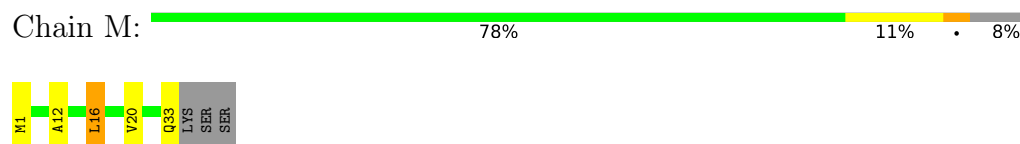
- Molecule 11: Photosystem II reaction center protein L



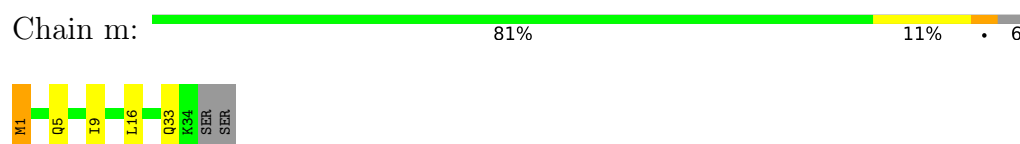
- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M

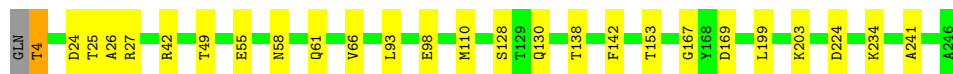


- Molecule 12: Photosystem II reaction center protein M



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  89% 10%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  92% 7%



- Molecule 14: Photosystem II reaction center protein T

Chain T:  78% 12% 6%



- Molecule 14: Photosystem II reaction center protein T

Chain t:  81% 12% 6% 3%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  85% 8% 8%

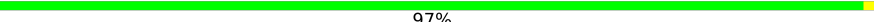


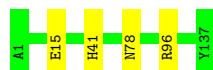
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  90% 7%



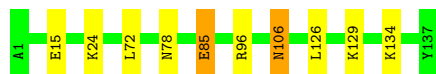
- Molecule 16: Cytochrome c-550

Chain V:  97%



- Molecule 16: Cytochrome c-550

Chain v:  93% 6%

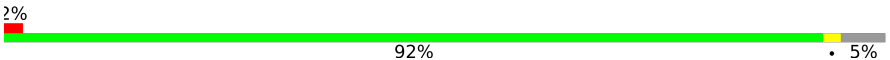


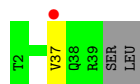
- Molecule 17: Photosystem II reaction center protein X

Chain X:  85% 10% 5%



- Molecule 17: Photosystem II reaction center protein X

Chain x:  2% 92% 5%



- Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:  3% 83% 13%



- Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:  70% 27%



- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  87% 11%



- Molecule 19: Photosystem II reaction center protein Z

Chain z:  76% 24%



- Molecule 20: Photosystem II protein Y

Chain R:  9% 71% 29%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	125.75Å 231.60Å 288.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.15 19.98 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.98-2.15) 99.7 (19.98-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.15Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.144 , 0.175 0.146 , 0.176	Depositor DCC
R_{free} test set	22666 reflections (2.78%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 67.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	52978	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.36	0/2713	0.53	0/3700
1	a	0.33	0/2717	0.49	0/3705
2	B	0.32	0/4169	0.47	0/5679
2	b	0.29	0/4161	0.47	0/5669
3	C	0.29	0/3610	0.45	0/4914
3	c	0.28	0/3675	0.43	0/5002
4	D	0.35	0/2827	0.50	0/3852
4	d	0.34	0/2827	0.48	0/3852
5	E	0.27	0/681	0.46	0/928
5	e	0.25	0/690	0.42	0/939
6	F	0.27	0/284	0.41	0/387
6	f	0.23	0/269	0.40	0/365
7	H	0.26	0/519	0.43	0/708
7	h	0.25	0/530	0.44	0/722
8	I	0.25	0/311	0.40	0/419
8	i	0.29	0/311	0.44	0/419
9	J	0.25	0/278	0.34	0/376
9	j	0.23	0/283	0.38	0/383
10	K	0.28	0/303	0.43	0/416
10	k	0.27	0/303	0.41	0/416
11	L	0.31	0/303	0.44	0/412
11	l	0.33	0/303	0.46	0/412
12	M	0.32	0/261	0.48	0/357
12	m	0.30	0/279	0.43	0/380
13	O	0.30	0/1925	0.47	0/2609
13	o	0.28	0/1896	0.46	0/2571
14	T	0.32	0/266	0.40	0/362
14	t	0.31	0/257	0.40	0/349
15	U	0.32	0/785	0.52	0/1064
15	u	0.31	0/792	0.51	0/1074
16	V	0.32	0/1103	0.46	0/1497

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.27	0/1085	0.42	0/1473
17	X	0.21	0/292	0.31	0/395
17	x	0.20	0/284	0.33	0/384
18	Y	0.23	0/216	0.40	0/289
18	y	0.19	0/216	0.35	0/289
19	Z	0.18	0/490	0.33	0/669
19	z	0.19	0/490	0.35	0/669
20	R	0.21	0/279	0.34	0/383
All	All	0.30	0/42983	0.46	0/58489

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2628	0	2527	10	0
1	a	2629	0	2526	18	0
2	B	4029	0	3880	26	0
2	b	4017	0	3872	29	0
3	C	3497	0	3419	21	0
3	c	3555	0	3480	21	0
4	D	2732	0	2631	20	0
4	d	2732	0	2632	18	0
5	E	662	0	648	6	0
5	e	670	0	655	5	0
6	F	275	0	282	4	0
6	f	261	0	269	4	0
7	H	506	0	529	3	0
7	h	517	0	541	2	0
8	I	314	0	328	5	0
8	i	314	0	328	1	0
9	J	272	0	279	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	277	0	284	2	0
10	K	293	0	305	7	0
10	k	293	0	305	7	0
11	L	296	0	304	1	0
11	l	296	0	304	3	0
12	M	268	0	285	3	0
12	m	286	0	305	7	0
13	O	1894	0	1860	15	0
13	o	1865	0	1838	9	0
14	T	267	0	267	3	0
14	t	258	0	261	3	0
15	U	774	0	772	5	0
15	u	781	0	781	2	0
16	V	1082	0	1083	2	0
16	v	1064	0	1073	6	0
17	X	289	0	322	3	0
17	x	281	0	312	1	0
18	Y	215	0	246	3	0
18	y	215	0	246	6	0
19	Z	479	0	516	3	0
19	z	479	0	516	5	0
20	R	273	0	305	4	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0
23	A	260	0	288	13	0
23	B	1040	0	1152	29	0
23	C	845	0	936	28	0
23	D	130	0	144	3	0
23	a	260	0	288	9	0
23	b	1040	0	1152	21	0
23	c	845	0	936	33	0
23	d	130	0	144	3	0
24	A	128	0	148	3	0
24	a	128	0	148	2	0
25	A	40	0	56	2	0
25	B	120	0	168	5	0
25	C	40	0	56	1	0
25	D	40	0	56	3	0
25	H	40	0	56	2	0
25	K	80	0	112	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	T	40	0	56	7	0
25	Y	40	0	56	2	0
25	a	40	0	56	2	0
25	b	120	0	168	7	0
25	c	80	0	112	6	0
25	d	40	0	56	2	0
25	h	40	0	56	3	0
25	k	40	0	56	0	0
25	t	40	0	56	5	0
25	y	40	0	56	2	0
26	A	108	0	155	3	0
26	B	54	0	78	1	0
26	F	43	0	53	2	0
26	a	108	0	155	5	0
26	b	54	0	78	2	0
26	f	43	0	53	1	0
27	A	12	0	15	3	0
27	B	18	0	24	5	0
27	C	6	0	8	0	0
27	O	12	0	16	3	0
27	V	6	0	8	0	0
27	a	18	0	24	6	0
27	b	18	0	24	3	0
27	c	12	0	16	0	0
27	l	6	0	8	1	0
27	o	12	0	16	0	0
27	v	6	0	8	1	0
28	A	10	0	0	0	0
28	a	10	0	0	0	0
29	A	55	0	80	10	0
29	D	55	0	80	0	0
29	a	55	0	80	4	0
29	d	55	0	80	0	0
30	A	28	0	0	0	0
30	B	33	0	0	0	0
30	D	57	0	0	0	0
30	I	40	0	0	0	0
30	J	10	0	0	0	0
30	K	34	0	0	0	0
30	X	18	0	0	0	0
30	a	30	0	0	0	0
30	b	33	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	c	32	0	0	0	0
30	d	53	0	0	0	0
30	i	40	0	0	0	0
30	j	10	0	0	0	0
30	l	10	0	0	0	0
30	m	10	0	0	0	0
30	x	18	0	0	0	0
31	A	70	0	92	2	0
31	B	95	0	127	3	0
31	F	35	0	46	0	0
31	M	35	0	46	1	0
31	T	35	0	46	0	0
31	b	50	0	70	1	0
31	c	35	0	46	2	0
31	e	35	0	46	1	0
31	m	35	0	45	0	0
31	t	26	0	33	2	0
32	A	51	0	72	0	0
32	B	51	0	72	1	0
32	C	102	0	144	4	0
32	D	51	0	72	0	0
32	Z	37	0	44	2	0
32	a	51	0	72	0	0
32	c	102	0	144	2	0
32	d	51	0	72	2	0
32	m	51	0	72	0	0
32	z	39	0	48	2	0
33	A	49	0	74	2	0
33	D	98	0	148	7	0
33	E	42	0	57	4	0
33	L	49	0	74	0	0
33	a	42	0	57	4	0
33	b	49	0	74	0	0
33	d	147	0	222	12	0
34	B	57	0	78	3	0
34	C	19	0	26	0	0
34	D	16	0	17	1	0
34	V	11	0	10	0	0
34	b	57	0	78	3	0
34	c	19	0	26	1	0
34	d	16	0	17	1	0
35	C	186	0	246	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	H	62	0	82	1	0
35	c	186	0	246	4	0
35	h	62	0	82	1	0
36	C	1	0	0	0	0
36	F	1	0	0	0	0
36	O	1	0	0	0	0
36	c	2	0	0	0	0
36	f	1	0	0	0	0
36	o	1	0	0	0	0
37	D	4	0	0	0	0
37	a	4	0	0	0	0
38	F	43	0	30	1	0
38	f	43	0	30	0	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	V	43	0	30	1	0
40	v	43	0	30	0	0
41	A	140	0	0	1	0
41	B	188	0	0	1	0
41	C	167	0	0	1	0
41	D	123	0	0	1	0
41	E	13	0	0	0	0
41	F	7	0	0	0	0
41	H	21	0	0	0	0
41	I	5	0	0	0	0
41	J	8	0	0	1	0
41	K	5	0	0	1	0
41	L	9	0	0	1	0
41	M	5	0	0	0	0
41	O	105	0	0	2	0
41	T	10	0	0	0	0
41	U	44	0	0	0	0
41	V	82	0	0	0	0
41	X	7	0	0	0	0
41	a	130	0	0	2	0
41	b	202	0	0	0	0
41	c	161	0	0	2	0
41	d	111	0	0	1	0
41	e	9	0	0	0	0
41	f	3	0	0	1	0
41	h	17	0	0	0	0
41	i	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	j	2	0	0	0	0
41	k	3	0	0	0	0
41	l	8	0	0	0	0
41	m	13	0	0	0	0
41	o	103	0	0	0	0
41	t	7	0	0	1	0
41	u	49	0	0	1	0
41	v	57	0	0	1	0
41	x	8	0	0	0	0
41	y	2	0	0	0	0
All	All	52978	0	52086	462	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 4.

The worst 5 of 462 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:418:GOL:H11	12:M:1:FME:HG2	1.44	0.99
23:B:604:CLA:H42	23:B:605:CLA:H2	1.53	0.91
1:a:250:ALA:HA	2:b:491:VAL:HG11	1.53	0.88
23:c:504:CLA:HBB1	23:c:513:CLA:H41	1.62	0.82
23:b:605:CLA:HHC	23:b:605:CLA:HBB1	1.62	0.81

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	333/344 (97%)	328 (98%)	4 (1%)	1 (0%)	36 34
1	a	334/344 (97%)	327 (98%)	6 (2%)	1 (0%)	36 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	509/505 (101%)	501 (98%)	8 (2%)	0	100	100
2	b	508/505 (101%)	496 (98%)	12 (2%)	0	100	100
3	C	450/455 (99%)	443 (98%)	6 (1%)	1 (0%)	43	44
3	c	458/455 (101%)	449 (98%)	8 (2%)	1 (0%)	43	44
4	D	341/342 (100%)	327 (96%)	14 (4%)	0	100	100
4	d	341/342 (100%)	334 (98%)	7 (2%)	0	100	100
5	E	79/84 (94%)	78 (99%)	1 (1%)	0	100	100
5	e	79/84 (94%)	79 (100%)	0	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
7	h	63/65 (97%)	60 (95%)	2 (3%)	1 (2%)	7	3
8	I	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	4	1
8	i	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	37 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	34/37 (92%)	34 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	34/36 (94%)	34 (100%)	0	0	100	100
13	O	244/244 (100%)	237 (97%)	5 (2%)	2 (1%)	16	10
13	o	241/244 (99%)	237 (98%)	4 (2%)	0	100	100
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
15	u	96/104 (92%)	94 (98%)	2 (2%)	0	100	100
16	V	137/137 (100%)	133 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
17	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	x	36/40 (90%)	36 (100%)	0	0	100	100
18	Y	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
18	y	27/30 (90%)	27 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	2
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	7	2
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	5252/5384 (98%)	5138 (98%)	104 (2%)	10 (0%)	43	44

5 of 10 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/279 (97%)	268 (99%)	2 (1%)	76	82
1	a	271/279 (97%)	270 (100%)	1 (0%)	84	89
2	B	409/403 (102%)	404 (99%)	5 (1%)	63	70
2	b	408/403 (101%)	403 (99%)	5 (1%)	63	70
3	C	353/356 (99%)	346 (98%)	7 (2%)	48	54
3	c	361/356 (101%)	355 (98%)	6 (2%)	53	60
4	D	278/277 (100%)	276 (99%)	2 (1%)	76	82
4	d	278/277 (100%)	276 (99%)	2 (1%)	76	82
5	E	72/73 (99%)	71 (99%)	1 (1%)	59	66
5	e	72/73 (99%)	71 (99%)	1 (1%)	59	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	26/38 (68%)	26 (100%)	0	100	100
7	H	54/54 (100%)	52 (96%)	2 (4%)	30	30
7	h	55/54 (102%)	54 (98%)	1 (2%)	51	58
8	I	34/34 (100%)	32 (94%)	2 (6%)	18	13
8	i	34/34 (100%)	33 (97%)	1 (3%)	37	39
9	J	26/27 (96%)	25 (96%)	1 (4%)	29	29
9	j	26/27 (96%)	25 (96%)	1 (4%)	29	29
10	K	30/30 (100%)	26 (87%)	4 (13%)	4	1
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	3
11	L	34/35 (97%)	34 (100%)	0	100	100
11	l	34/35 (97%)	34 (100%)	0	100	100
12	M	30/32 (94%)	27 (90%)	3 (10%)	7	3
12	m	32/32 (100%)	29 (91%)	3 (9%)	8	4
13	O	209/207 (101%)	203 (97%)	6 (3%)	37	39
13	o	206/207 (100%)	200 (97%)	6 (3%)	37	39
14	T	27/28 (96%)	24 (89%)	3 (11%)	6	3
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	84/89 (94%)	82 (98%)	2 (2%)	43	47
15	u	85/89 (96%)	83 (98%)	2 (2%)	43	47
16	V	119/117 (102%)	118 (99%)	1 (1%)	73	79
16	v	117/117 (100%)	113 (97%)	4 (3%)	32	33
17	X	32/33 (97%)	32 (100%)	0	100	100
17	x	31/33 (94%)	31 (100%)	0	100	100
18	Y	22/23 (96%)	22 (100%)	0	100	100
18	y	22/23 (96%)	19 (86%)	3 (14%)	3	1
19	Z	52/52 (100%)	49 (94%)	3 (6%)	18	14
19	z	52/52 (100%)	46 (88%)	6 (12%)	5	2
20	R	29/29 (100%)	27 (93%)	2 (7%)	14	9
All	All	4358/4403 (99%)	4267 (98%)	91 (2%)	48	52

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	i	33	LYS
15	u	10[A]	VAL
10	k	10	LYS
13	o	25	THR
16	v	85	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	14	ASN
4	d	186	GLN
3	c	201	ASN
11	l	8	GLN
5	E	60	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	I	1	8	8,9,10	0.59	0	8,9,11	1.18	1 (12%)
14	FME	t	1	14	8,9,10	0.67	0	8,9,11	1.55	2 (25%)
14	FME	T	1	14	8,9,10	0.72	0	8,9,11	1.84	3 (37%)
8	FME	i	1	8	8,9,10	0.66	0	8,9,11	1.21	0
12	FME	M	1	12	8,9,10	0.69	0	8,9,11	1.14	0
12	FME	m	1	12	8,9,10	0.58	0	8,9,11	1.32	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
8	FME	I	1	8	-	0/7/9/11	-
14	FME	t	1	14	-	0/7/9/11	-
14	FME	T	1	14	-	0/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
12	FME	m	1	12	-	1/7/9/11	-

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	CB-CA-N	-2.92	105.19	110.52
14	t	1	FME	CA-N-CN	-2.69	118.69	122.82
14	t	1	FME	O-C-CA	-2.47	118.42	124.77
14	T	1	FME	CA-N-CN	2.43	126.55	122.82
12	m	1	FME	O1-CN-N	-2.32	119.31	125.32

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 5 short contacts:

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 225 ligands modelled in this entry, 15 are monoatomic and 18 are unknown - leaving 192 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$
27	GOL	V	203	-	5,5,5	1.29	1 (20%)	5,5,5	0.97	0
27	GOL	a	412	-	5,5,5	0.93	0	5,5,5	1.10	0
25	BCR	K	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.40	6 (10%)
23	CLA	C	505	-	69,73,73	1.99	19 (27%)	82,113,113	2.67	31 (37%)
24	PHO	A	416	-	58,69,69	2.74	14 (24%)	55,99,99	2.91	17 (30%)
23	CLA	b	609	-	69,73,73	1.99	19 (27%)	82,113,113	2.63	33 (40%)
31	LMT	A	417	-	36,36,36	0.92	3 (8%)	47,47,47	1.02	1 (2%)
23	CLA	b	602	-	69,73,73	2.04	19 (27%)	82,113,113	2.78	36 (43%)
35	DGD	c	517	-	63,63,67	0.85	2 (3%)	77,77,81	1.12	6 (7%)
31	LMT	t	101	-	26,26,36	0.91	2 (7%)	31,31,47	1.33	2 (6%)
24	PHO	a	408	-	58,69,69	2.73	11 (18%)	55,99,99	2.83	15 (27%)
29	PL9	d	404	-	55,55,55	0.67	1 (1%)	68,69,69	1.62	15 (22%)
34	HTG	V	202	-	11,11,19	0.23	0	15,15,24	1.07	1 (6%)
23	CLA	b	610	41	69,73,73	1.98	20 (28%)	82,113,113	2.71	31 (37%)
37	BCT	a	404	21	3,3,3	0.46	0	2,3,3	1.59	0
31	LMT	F	101	-	36,36,36	1.05	1 (2%)	47,47,47	1.03	2 (4%)
27	GOL	b	624	-	5,5,5	1.22	1 (20%)	5,5,5	0.87	0
32	LMG	Z	101	-	37,37,55	1.00	2 (5%)	45,45,63	1.43	5 (11%)
25	BCR	H	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.35	7 (12%)
23	CLA	B	601	41	69,73,73	2.05	20 (28%)	82,113,113	2.67	31 (37%)
23	CLA	B	604	-	69,73,73	1.96	22 (31%)	82,113,113	2.63	32 (39%)
23	CLA	B	613	-	69,73,73	1.97	18 (26%)	82,113,113	2.66	31 (37%)
23	CLA	A	405	41	69,73,73	1.91	18 (26%)	82,113,113	2.74	36 (43%)
25	BCR	d	403	-	41,41,41	1.13	2 (4%)	56,56,56	1.91	17 (30%)
26	SQD	a	411	-	52,54,54	0.89	2 (3%)	62,65,65	1.74	12 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LHG	A	420	-	48,48,48	0.84	2 (4%)	51,54,54	1.33	6 (11%)
23	CLA	C	503	-	69,73,73	1.98	19 (27%)	82,113,113	2.71	31 (37%)
23	CLA	b	608	-	69,73,73	1.94	19 (27%)	82,113,113	2.73	34 (41%)
23	CLA	c	508	41	69,73,73	2.01	18 (26%)	82,113,113	2.69	29 (35%)
28	OEX	a	414	41,1,3	0,15,15	-	-	-	-	-
27	GOL	a	420	-	5,5,5	1.33	1 (20%)	5,5,5	0.94	0
31	LMT	A	421	-	36,36,36	1.03	2 (5%)	47,47,47	1.15	4 (8%)
23	CLA	A	408	-	69,73,73	1.95	18 (26%)	82,113,113	2.77	36 (43%)
32	LMG	d	410	39	51,51,55	0.91	2 (3%)	59,59,63	1.10	5 (8%)
23	CLA	b	607	41	69,73,73	1.94	20 (28%)	82,113,113	2.64	31 (37%)
25	BCR	t	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.60	11 (19%)
23	CLA	D	402	-	69,73,73	1.96	18 (26%)	82,113,113	2.75	33 (40%)
33	LHG	d	405	-	48,48,48	0.87	2 (4%)	51,54,54	1.09	4 (7%)
23	CLA	c	505	41	69,73,73	2.03	20 (28%)	82,113,113	2.66	31 (37%)
23	CLA	C	506	-	69,73,73	2.01	21 (30%)	82,113,113	2.64	32 (39%)
27	GOL	A	418	-	5,5,5	1.65	2 (40%)	5,5,5	1.08	1 (20%)
40	HEC	V	201	16	46,50,50	1.91	6 (13%)	58,82,82	1.76	5 (8%)
40	HEC	v	201	16	46,50,50	1.90	5 (10%)	58,82,82	1.95	6 (10%)
27	GOL	o	302	-	5,5,5	0.98	0	5,5,5	1.02	0
32	LMG	C	518	-	51,51,55	0.93	2 (3%)	59,59,63	1.12	4 (6%)
32	LMG	c	521	-	51,51,55	0.99	2 (3%)	59,59,63	1.36	7 (11%)
34	HTG	B	623	-	19,19,19	0.74	1 (5%)	23,24,24	1.33	1 (4%)
34	HTG	b	623	-	19,19,19	0.96	1 (5%)	23,24,24	1.66	2 (8%)
31	LMT	c	501	-	36,36,36	1.00	1 (2%)	47,47,47	1.03	1 (2%)
32	LMG	B	621	-	51,51,55	0.92	2 (3%)	59,59,63	1.28	4 (6%)
23	CLA	B	605	-	69,73,73	1.98	18 (26%)	82,113,113	2.79	31 (37%)
23	CLA	C	502	-	69,73,73	2.00	20 (28%)	82,113,113	2.58	29 (35%)
27	GOL	l	102	-	5,5,5	1.01	0	5,5,5	1.04	0
27	GOL	O	302	-	5,5,5	0.95	0	5,5,5	1.02	0
27	GOL	O	303	-	5,5,5	0.88	0	5,5,5	1.23	1 (20%)
31	LMT	B	628	-	36,36,36	1.15	4 (11%)	47,47,47	1.31	5 (10%)
31	LMT	B	630	-	36,36,36	0.97	3 (8%)	47,47,47	1.15	3 (6%)
33	LHG	E	101	-	41,41,48	1.07	2 (4%)	44,47,54	1.12	3 (6%)
33	LHG	D	407	-	48,48,48	0.92	2 (4%)	51,54,54	1.01	4 (7%)
34	HTG	B	625	-	19,19,19	0.95	2 (10%)	23,24,24	1.16	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	603	-	69,73,73	1.98	20 (28%)	82,113,113	2.83	30 (36%)
23	CLA	C	509	-	69,73,73	2.03	20 (28%)	82,113,113	2.77	30 (36%)
27	GOL	b	628	-	5,5,5	0.41	0	5,5,5	1.48	1 (20%)
23	CLA	C	501	-	69,73,73	1.96	20 (28%)	82,113,113	2.68	31 (37%)
23	CLA	c	509	-	69,73,73	2.06	20 (28%)	82,113,113	2.64	29 (35%)
31	LMT	e	101	-	36,36,36	1.01	2 (5%)	47,47,47	0.98	1 (2%)
23	CLA	b	615	-	69,73,73	1.97	18 (26%)	82,113,113	2.67	34 (41%)
29	PL9	A	414	-	55,55,55	0.70	3 (5%)	68,69,69	2.11	27 (39%)
23	CLA	B	607	41	69,73,73	1.93	19 (27%)	82,113,113	2.68	31 (37%)
23	CLA	B	606	-	69,73,73	1.96	20 (28%)	82,113,113	2.79	33 (40%)
34	HTG	b	625	-	19,19,19	0.92	2 (10%)	23,24,24	1.57	4 (17%)
23	CLA	C	512	-	69,73,73	2.03	20 (28%)	82,113,113	2.72	36 (43%)
23	CLA	b	603	-	69,73,73	1.94	19 (27%)	82,113,113	2.74	31 (37%)
26	SQD	A	410	-	52,54,54	0.86	2 (3%)	62,65,65	1.79	9 (14%)
23	CLA	C	511	3	69,73,73	1.99	21 (30%)	82,113,113	2.64	29 (35%)
23	CLA	B	615	-	69,73,73	2.02	19 (27%)	82,113,113	2.68	30 (36%)
25	BCR	c	516	-	41,41,41	1.05	1 (2%)	56,56,56	1.35	10 (17%)
33	LHG	d	411	-	48,48,48	0.90	2 (4%)	51,54,54	1.14	5 (9%)
32	LMG	z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.08	3 (6%)
32	LMG	A	419	-	51,51,55	0.92	2 (3%)	59,59,63	1.41	8 (13%)
33	LHG	d	406	-	48,48,48	0.92	2 (4%)	51,54,54	1.00	3 (5%)
23	CLA	b	605	-	69,73,73	1.94	19 (27%)	82,113,113	2.86	28 (34%)
25	BCR	h	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.32	7 (12%)
25	BCR	K	103	-	41,41,41	1.05	1 (2%)	56,56,56	1.44	9 (16%)
33	LHG	b	630	-	48,48,48	0.86	3 (6%)	51,54,54	1.05	4 (7%)
27	GOL	a	419	-	5,5,5	1.08	0	5,5,5	1.03	0
33	LHG	D	406	-	48,48,48	0.86	3 (6%)	51,54,54	1.00	4 (7%)
27	GOL	o	303	-	5,5,5	1.11	1 (20%)	5,5,5	1.12	0
23	CLA	B	612	-	69,73,73	1.98	18 (26%)	82,113,113	2.69	33 (40%)
34	HTG	c	522	-	19,19,19	0.89	1 (5%)	23,24,24	1.36	2 (8%)
33	LHG	L	101	-	48,48,48	0.89	2 (4%)	51,54,54	1.16	3 (5%)
37	BCT	D	401	21	3,3,3	0.43	0	2,3,3	1.83	0
25	BCR	k	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.55	13 (23%)
26	SQD	A	412	-	52,54,54	0.99	2 (3%)	62,65,65	1.13	5 (8%)
34	HTG	d	409	-	16,16,19	0.90	1 (6%)	20,21,24	1.41	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	GOL	v	202	-	5,5,5	1.35	1 (20%)	5,5,5	0.77	0
23	CLA	c	510	-	69,73,73	2.02	19 (27%)	82,113,113	2.72	30 (36%)
32	LMG	c	520	-	51,51,55	0.91	2 (3%)	59,59,63	1.13	6 (10%)
35	DGD	C	515	-	63,63,67	0.82	2 (3%)	77,77,81	1.21	9 (11%)
26	SQD	f	102	-	41,43,54	1.12	2 (4%)	51,54,65	1.55	9 (17%)
25	BCR	D	404	-	41,41,41	1.09	1 (2%)	56,56,56	1.83	14 (25%)
23	CLA	a	406	41	69,73,73	1.98	17 (24%)	82,113,113	2.66	30 (36%)
32	LMG	C	519	-	51,51,55	1.05	3 (5%)	59,59,63	1.32	6 (10%)
31	LMT	m	103	-	36,36,36	1.07	3 (8%)	47,47,47	1.07	3 (6%)
23	CLA	d	402	-	69,73,73	2.01	20 (28%)	82,113,113	2.71	33 (40%)
23	CLA	B	602	-	69,73,73	2.00	20 (28%)	82,113,113	2.73	31 (37%)
35	DGD	C	517	-	63,63,67	0.88	3 (4%)	77,77,81	0.93	2 (2%)
23	CLA	D	403	-	69,73,73	2.06	18 (26%)	82,113,113	2.67	33 (40%)
23	CLA	A	406	41	69,73,73	1.97	18 (26%)	82,113,113	2.71	33 (40%)
23	CLA	b	612	-	69,73,73	1.95	20 (28%)	82,113,113	2.69	30 (36%)
23	CLA	b	601	41	69,73,73	2.08	20 (28%)	82,113,113	2.66	32 (39%)
23	CLA	b	613	-	69,73,73	1.92	18 (26%)	82,113,113	2.66	32 (39%)
25	BCR	b	617	-	41,41,41	1.07	1 (2%)	56,56,56	1.35	5 (8%)
23	CLA	B	616	-	69,73,73	1.96	20 (28%)	82,113,113	2.73	27 (32%)
23	CLA	c	507	-	69,73,73	2.01	20 (28%)	82,113,113	2.66	31 (37%)
23	CLA	b	606	-	69,73,73	1.97	19 (27%)	82,113,113	2.74	33 (40%)
23	CLA	c	513	-	69,73,73	2.03	20 (28%)	82,113,113	2.68	34 (41%)
23	CLA	b	611	-	69,73,73	1.92	20 (28%)	82,113,113	2.75	31 (37%)
25	BCR	y	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.67	10 (17%)
26	SQD	a	413	-	52,54,54	1.00	2 (3%)	62,65,65	1.16	7 (11%)
25	BCR	T	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.58	12 (21%)
32	LMG	m	101	-	51,51,55	0.87	2 (3%)	59,59,63	1.23	5 (8%)
34	HTG	B	622	-	19,19,19	1.08	2 (10%)	23,24,24	1.43	4 (17%)
26	SQD	F	103	-	41,43,54	1.15	3 (7%)	51,54,65	2.00	12 (23%)
23	CLA	A	404	-	69,73,73	1.97	19 (27%)	82,113,113	2.69	33 (40%)
33	LHG	a	421	-	41,41,48	1.04	2 (4%)	44,47,54	0.94	2 (4%)
23	CLA	B	611	-	69,73,73	2.49	20 (28%)	82,113,113	3.59	31 (37%)
35	DGD	c	519	-	63,63,67	0.88	3 (4%)	77,77,81	1.00	5 (6%)
32	LMG	a	418	-	51,51,55	0.92	2 (3%)	59,59,63	1.17	5 (8%)
25	BCR	c	515	-	41,41,41	1.02	1 (2%)	56,56,56	1.60	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	d	401	-	69,73,73	1.92	19 (27%)	82,113,113	2.67	30 (36%)
25	BCR	B	618	-	41,41,41	0.99	1 (2%)	56,56,56	1.34	8 (14%)
23	CLA	C	507	41	69,73,73	1.97	18 (26%)	82,113,113	2.67	29 (35%)
23	CLA	c	506	-	69,73,73	1.98	19 (27%)	82,113,113	2.62	30 (36%)
23	CLA	c	503	-	69,73,73	1.96	18 (26%)	82,113,113	2.64	28 (34%)
27	GOL	b	629	-	5,5,5	1.11	0	5,5,5	0.99	0
23	CLA	C	513	-	69,73,73	2.02	20 (28%)	82,113,113	2.66	31 (37%)
27	GOL	A	411	-	5,5,5	1.19	0	5,5,5	0.78	0
23	CLA	B	614	-	69,73,73	2.00	19 (27%)	82,113,113	2.82	33 (40%)
32	LMG	D	411	39	51,51,55	0.84	2 (3%)	59,59,63	1.02	3 (5%)
29	PL9	D	405	-	55,55,55	0.64	2 (3%)	68,69,69	1.64	18 (26%)
23	CLA	B	608	-	69,73,73	1.89	19 (27%)	82,113,113	2.70	34 (41%)
24	PHO	A	407	-	58,69,69	2.70	13 (22%)	55,99,99	2.89	15 (27%)
34	HTG	C	520	-	19,19,19	0.82	1 (5%)	23,24,24	1.20	2 (8%)
31	LMT	b	627	-	25,25,36	0.88	1 (4%)	30,30,47	1.12	1 (3%)
23	CLA	c	514	-	69,73,73	2.08	21 (30%)	82,113,113	2.68	31 (37%)
23	CLA	c	512	3	69,73,73	2.05	19 (27%)	82,113,113	2.66	33 (40%)
26	SQD	b	620	-	52,54,54	0.99	2 (3%)	62,65,65	1.59	11 (17%)
23	CLA	a	407	41	69,73,73	1.94	19 (27%)	82,113,113	2.70	33 (40%)
23	CLA	c	511	-	69,73,73	1.97	20 (28%)	82,113,113	2.72	32 (39%)
25	BCR	B	617	-	41,41,41	1.06	1 (2%)	56,56,56	1.26	4 (7%)
27	GOL	B	627	-	5,5,5	0.99	0	5,5,5	1.07	1 (20%)
34	HTG	b	622	-	19,19,19	1.13	2 (10%)	23,24,24	1.90	7 (30%)
31	LMT	M	101	-	36,36,36	1.12	3 (8%)	47,47,47	1.22	4 (8%)
23	CLA	b	604	-	69,73,73	1.99	20 (28%)	82,113,113	2.65	29 (35%)
27	GOL	B	624	-	5,5,5	0.90	0	5,5,5	1.22	1 (20%)
23	CLA	B	609	-	69,73,73	2.00	18 (26%)	82,113,113	2.65	31 (37%)
23	CLA	c	502	-	69,73,73	1.98	21 (30%)	82,113,113	2.68	30 (36%)
25	BCR	C	514	-	41,41,41	1.05	1 (2%)	56,56,56	1.39	8 (14%)
23	CLA	a	405	-	69,73,73	1.94	19 (27%)	82,113,113	2.76	34 (41%)
31	LMT	T	101	-	36,36,36	1.07	4 (11%)	47,47,47	1.07	2 (4%)
27	GOL	c	526	-	5,5,5	0.99	0	5,5,5	1.02	0
29	PL9	a	415	-	55,55,55	0.67	2 (3%)	68,69,69	2.01	21 (30%)
23	CLA	b	614	-	69,73,73	1.98	20 (28%)	82,113,113	2.78	31 (37%)
25	BCR	Y	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.74	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	GOL	B	629	-	5,5,5	1.37	1 (20%)	5,5,5	0.96	0
25	BCR	b	619	-	41,41,41	1.09	1 (2%)	56,56,56	1.29	7 (12%)
31	LMT	B	631	-	25,25,36	0.89	2 (8%)	30,30,47	1.14	3 (10%)
35	DGD	C	516	-	63,63,67	0.89	3 (4%)	77,77,81	1.03	5 (6%)
23	CLA	C	504	41	69,73,73	1.97	19 (27%)	82,113,113	2.61	31 (37%)
31	LMT	b	621	-	25,25,36	0.96	2 (8%)	30,30,47	1.19	2 (6%)
23	CLA	B	610	41	69,73,73	2.04	19 (27%)	82,113,113	2.79	34 (41%)
23	CLA	C	508	-	69,73,73	2.04	20 (28%)	82,113,113	2.64	29 (35%)
28	OEX	A	413	41,1,3	0,15,15	-	-	-	-	-
25	BCR	A	409	-	41,41,41	1.03	1 (2%)	56,56,56	1.41	9 (16%)
34	HTG	D	410	-	16,16,19	1.00	2 (12%)	20,21,24	1.28	1 (5%)
23	CLA	a	409	-	69,73,73	1.95	20 (28%)	82,113,113	2.72	31 (37%)
35	DGD	c	518	-	63,63,67	0.84	3 (4%)	77,77,81	0.98	5 (6%)
25	BCR	B	619	-	41,41,41	1.07	2 (4%)	56,56,56	1.32	7 (12%)
38	HEM	f	101	5,6	50,50,50	1.51	7 (14%)	67,82,82	1.58	11 (16%)
23	CLA	b	616	-	69,73,73	1.98	18 (26%)	82,113,113	2.82	33 (40%)
23	CLA	C	510	-	69,73,73	2.04	19 (27%)	82,113,113	2.78	33 (40%)
35	DGD	H	102	-	63,63,67	0.86	4 (6%)	77,77,81	0.97	6 (7%)
35	DGD	h	102	-	63,63,67	0.87	3 (4%)	77,77,81	1.08	6 (7%)
25	BCR	a	410	-	41,41,41	1.05	1 (2%)	56,56,56	1.40	8 (14%)
27	GOL	c	527	-	5,5,5	1.03	0	5,5,5	1.06	0
26	SQD	B	620	-	52,54,54	1.02	3 (5%)	62,65,65	1.73	13 (20%)
27	GOL	C	521	-	5,5,5	1.24	0	5,5,5	0.89	0
25	BCR	b	618	-	41,41,41	1.01	1 (2%)	56,56,56	1.22	7 (12%)
23	CLA	c	504	-	69,73,73	2.02	19 (27%)	82,113,113	2.70	29 (35%)
24	PHO	a	417	-	58,69,69	2.76	13 (22%)	55,99,99	3.06	17 (30%)
38	HEM	F	102	5,6	50,50,50	1.54	7 (14%)	67,82,82	1.73	15 (22%)

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
27	GOL	V	203	-	-	2/4/4/4	-
27	GOL	a	412	-	-	4/4/4/4	-
25	BCR	K	101	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	505	-	1/1/15/20	6/39/115/115	-
24	PHO	A	416	-	-	1/37/103/103	0/5/6/6
23	CLA	b	609	-	1/1/15/20	1/39/115/115	-
31	LMT	A	417	-	-	8/21/61/61	0/2/2/2
23	CLA	b	602	-	1/1/15/20	5/39/115/115	-
35	DGD	c	517	-	-	20/51/91/95	0/2/2/2
31	LMT	t	101	-	-	8/17/38/61	0/1/1/2
24	PHO	a	408	-	-	5/37/103/103	0/5/6/6
29	PL9	d	404	-	-	6/53/73/73	0/1/1/1
34	HTG	V	202	-	-	0/2/19/30	0/1/1/1
23	CLA	b	610	41	1/1/15/20	6/39/115/115	-
31	LMT	F	101	-	-	9/21/61/61	0/2/2/2
27	GOL	b	624	-	-	2/4/4/4	-
32	LMG	Z	101	-	-	10/31/51/70	0/1/1/1
25	BCR	H	101	-	-	2/29/63/63	0/2/2/2
23	CLA	B	601	41	1/1/15/20	11/39/115/115	-
23	CLA	B	604	-	1/1/15/20	1/39/115/115	-
23	CLA	B	613	-	1/1/15/20	8/39/115/115	-
23	CLA	A	405	41	-	2/39/115/115	-
25	BCR	d	403	-	-	4/29/63/63	0/2/2/2
26	SQD	a	411	-	-	9/49/69/69	0/1/1/1
33	LHG	A	420	-	-	10/53/53/53	-
23	CLA	C	503	-	-	2/39/115/115	-
23	CLA	b	608	-	-	5/39/115/115	-
23	CLA	c	508	41	1/1/15/20	9/39/115/115	-
27	GOL	a	420	-	-	0/4/4/4	-
31	LMT	A	421	-	-	15/21/61/61	0/2/2/2
23	CLA	A	408	-	1/1/15/20	8/39/115/115	-
32	LMG	d	410	39	-	11/46/66/70	0/1/1/1
23	CLA	b	607	41	1/1/15/20	1/39/115/115	-
25	BCR	t	102	-	-	1/29/63/63	0/2/2/2
23	CLA	D	402	-	1/1/15/20	0/39/115/115	-
33	LHG	d	405	-	-	12/53/53/53	-
23	CLA	c	505	41	1/1/15/20	9/39/115/115	-
23	CLA	C	506	-	1/1/15/20	12/39/115/115	-
27	GOL	A	418	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	HEC	V	201	16	-	6/14/54/54	-
40	HEC	v	201	16	-	6/14/54/54	-
27	GOL	o	302	-	-	2/4/4/4	-
32	LMG	C	518	-	-	8/46/66/70	0/1/1/1
32	LMG	c	521	-	-	7/46/66/70	0/1/1/1
34	HTG	B	623	-	-	1/10/30/30	0/1/1/1
34	HTG	b	623	-	-	4/10/30/30	0/1/1/1
31	LMT	c	501	-	-	12/21/61/61	0/2/2/2
32	LMG	B	621	-	-	18/46/66/70	0/1/1/1
23	CLA	B	605	-	1/1/15/20	3/39/115/115	-
23	CLA	C	502	-	1/1/15/20	8/39/115/115	-
27	GOL	l	102	-	-	1/4/4/4	-
27	GOL	O	302	-	-	2/4/4/4	-
27	GOL	O	303	-	-	2/4/4/4	-
31	LMT	B	628	-	-	10/21/61/61	0/2/2/2
31	LMT	B	630	-	-	11/21/61/61	0/2/2/2
33	LHG	E	101	-	-	21/46/46/53	-
33	LHG	D	407	-	-	13/53/53/53	-
34	HTG	B	625	-	-	4/10/30/30	0/1/1/1
23	CLA	B	603	-	1/1/15/20	5/39/115/115	-
23	CLA	C	509	-	1/1/15/20	4/39/115/115	-
27	GOL	b	628	-	-	0/4/4/4	-
23	CLA	C	501	-	1/1/15/20	6/39/115/115	-
23	CLA	c	509	-	1/1/15/20	3/39/115/115	-
31	LMT	e	101	-	-	14/21/61/61	0/2/2/2
23	CLA	b	615	-	1/1/15/20	7/39/115/115	-
29	PL9	A	414	-	-	15/53/73/73	0/1/1/1
23	CLA	B	607	41	1/1/15/20	2/39/115/115	-
23	CLA	B	606	-	1/1/15/20	8/39/115/115	-
34	HTG	b	625	-	-	3/10/30/30	0/1/1/1
23	CLA	C	512	-	1/1/15/20	11/39/115/115	-
23	CLA	b	603	-	1/1/15/20	5/39/115/115	-
26	SQD	A	410	-	-	12/49/69/69	0/1/1/1
23	CLA	C	511	3	1/1/15/20	2/39/115/115	-
23	CLA	B	615	-	1/1/15/20	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	c	516	-	-	0/29/63/63	0/2/2/2
33	LHG	d	411	-	-	12/53/53/53	-
32	LMG	z	101	-	-	9/34/54/70	0/1/1/1
32	LMG	A	419	-	-	13/46/66/70	0/1/1/1
33	LHG	d	406	-	-	11/53/53/53	-
23	CLA	b	605	-	1/1/15/20	6/39/115/115	-
25	BCR	h	101	-	-	0/29/63/63	0/2/2/2
25	BCR	K	103	-	-	3/29/63/63	0/2/2/2
33	LHG	b	630	-	-	20/53/53/53	-
27	GOL	a	419	-	-	2/4/4/4	-
33	LHG	D	406	-	-	16/53/53/53	-
27	GOL	o	303	-	-	4/4/4/4	-
23	CLA	B	612	-	1/1/15/20	4/39/115/115	-
34	HTG	c	522	-	-	2/10/30/30	0/1/1/1
33	LHG	L	101	-	-	19/53/53/53	-
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2
26	SQD	A	412	-	-	12/49/69/69	0/1/1/1
34	HTG	d	409	-	-	1/7/27/30	0/1/1/1
27	GOL	v	202	-	-	1/4/4/4	-
23	CLA	c	510	-	1/1/15/20	15/39/115/115	-
32	LMG	c	520	-	-	11/46/66/70	0/1/1/1
35	DGD	C	515	-	-	12/51/91/95	0/2/2/2
26	SQD	f	102	-	-	12/38/58/69	0/1/1/1
25	BCR	D	404	-	-	4/29/63/63	0/2/2/2
23	CLA	a	406	41	1/1/15/20	4/39/115/115	-
32	LMG	C	519	-	-	12/46/66/70	0/1/1/1
31	LMT	m	103	-	-	4/21/61/61	0/2/2/2
23	CLA	d	402	-	1/1/15/20	8/39/115/115	-
23	CLA	B	602	-	1/1/15/20	9/39/115/115	-
35	DGD	C	517	-	-	16/51/91/95	0/2/2/2
23	CLA	D	403	-	1/1/15/20	14/39/115/115	-
23	CLA	b	613	-	1/1/15/20	3/39/115/115	-
23	CLA	b	612	-	1/1/15/20	2/39/115/115	-
23	CLA	b	601	41	1/1/15/20	17/39/115/115	-
23	CLA	A	406	41	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
23	CLA	B	616	-	1/1/15/20	5/39/115/115	-
23	CLA	c	507	-	1/1/15/20	6/39/115/115	-
23	CLA	b	606	-	1/1/15/20	11/39/115/115	-
23	CLA	c	513	-	1/1/15/20	12/39/115/115	-
23	CLA	b	611	-	1/1/15/20	3/39/115/115	-
25	BCR	y	101	-	-	3/29/63/63	0/2/2/2
26	SQD	a	413	-	-	14/49/69/69	0/1/1/1
25	BCR	T	102	-	-	1/29/63/63	0/2/2/2
32	LMG	m	101	-	-	8/46/66/70	0/1/1/1
34	HTG	B	622	-	-	4/10/30/30	0/1/1/1
26	SQD	F	103	-	-	15/38/58/69	0/1/1/1
23	CLA	A	404	-	1/1/15/20	5/39/115/115	-
33	LHG	a	421	-	-	16/46/46/53	-
23	CLA	B	611	-	1/1/15/20	3/39/115/115	-
35	DGD	c	519	-	-	8/51/91/95	0/2/2/2
32	LMG	a	418	-	-	13/46/66/70	0/1/1/1
25	BCR	c	515	-	-	0/29/63/63	0/2/2/2
23	CLA	d	401	-	1/1/15/20	2/39/115/115	-
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
23	CLA	C	507	41	1/1/15/20	8/39/115/115	-
23	CLA	c	506	-	1/1/15/20	7/39/115/115	-
23	CLA	c	503	-	1/1/15/20	5/39/115/115	-
27	GOL	b	629	-	-	0/4/4/4	-
23	CLA	C	513	-	1/1/15/20	7/39/115/115	-
27	GOL	A	411	-	-	2/4/4/4	-
23	CLA	B	614	-	1/1/15/20	13/39/115/115	-
32	LMG	D	411	39	-	9/46/66/70	0/1/1/1
29	PL9	D	405	-	-	7/53/73/73	0/1/1/1
23	CLA	B	608	-	-	4/39/115/115	-
24	PHO	A	407	-	-	1/37/103/103	0/5/6/6
34	HTG	C	520	-	-	0/10/30/30	0/1/1/1
31	LMT	b	627	-	-	11/17/37/61	0/1/1/2
23	CLA	c	514	-	1/1/15/20	10/39/115/115	-
23	CLA	c	512	3	1/1/15/20	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	SQD	b	620	-	-	18/49/69/69	0/1/1/1
23	CLA	a	407	41	-	5/39/115/115	-
23	CLA	c	511	-	1/1/15/20	9/39/115/115	-
25	BCR	B	617	-	-	2/29/63/63	0/2/2/2
27	GOL	B	627	-	-	1/4/4/4	-
34	HTG	b	622	-	-	5/10/30/30	0/1/1/1
31	LMT	M	101	-	-	4/21/61/61	0/2/2/2
23	CLA	b	604	-	1/1/15/20	9/39/115/115	-
27	GOL	B	624	-	-	4/4/4/4	-
23	CLA	B	609	-	1/1/15/20	0/39/115/115	-
23	CLA	c	502	-	1/1/15/20	2/39/115/115	-
25	BCR	C	514	-	-	0/29/63/63	0/2/2/2
23	CLA	a	405	-	1/1/15/20	3/39/115/115	-
31	LMT	T	101	-	-	8/21/61/61	0/2/2/2
27	GOL	c	526	-	-	0/4/4/4	-
29	PL9	a	415	-	-	14/53/73/73	0/1/1/1
23	CLA	b	614	-	1/1/15/20	12/39/115/115	-
25	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
27	GOL	B	629	-	-	4/4/4/4	-
25	BCR	b	619	-	-	3/29/63/63	0/2/2/2
31	LMT	B	631	-	-	10/17/37/61	0/1/1/2
35	DGD	C	516	-	-	14/51/91/95	0/2/2/2
23	CLA	C	504	41	1/1/15/20	8/39/115/115	-
31	LMT	b	621	-	-	8/17/37/61	0/1/1/2
23	CLA	B	610	41	1/1/15/20	6/39/115/115	-
23	CLA	C	508	-	-	2/39/115/115	-
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
34	HTG	D	410	-	-	3/7/27/30	0/1/1/1
23	CLA	a	409	-	1/1/15/20	9/39/115/115	-
35	DGD	c	518	-	-	17/51/91/95	0/2/2/2
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
38	HEM	f	101	5,6	-	6/14/54/54	-
23	CLA	b	616	-	1/1/15/20	9/39/115/115	-
23	CLA	C	510	-	1/1/15/20	12/39/115/115	-
35	DGD	H	102	-	-	9/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	DGD	h	102	-	-	15/51/91/95	0/2/2/2
25	BCR	a	410	-	-	1/29/63/63	0/2/2/2
27	GOL	c	527	-	-	3/4/4/4	-
26	SQD	B	620	-	-	13/49/69/69	0/1/1/1
27	GOL	C	521	-	-	0/4/4/4	-
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
23	CLA	c	504	-	1/1/15/20	1/39/115/115	-
24	PHO	a	417	-	-	0/37/103/103	0/5/6/6
38	HEM	F	102	5,6	-	6/14/54/54	-

The worst 5 of 1602 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407	PHO	C1D-C2D	9.27	1.49	1.39
24	a	408	PHO	C1B-C2B	9.11	1.49	1.39
24	a	417	PHO	C1B-C2B	8.92	1.49	1.39
24	A	416	PHO	C1D-C2D	8.86	1.49	1.39
24	a	417	PHO	C1D-C2D	8.73	1.49	1.39

The worst 5 of 2880 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	C3B-C2B-C1B	-13.61	91.13	107.17
23	B	611	CLA	C1D-ND-C4D	-11.78	98.05	106.31
24	a	417	PHO	C2D-C1D-ND	11.51	117.75	109.43
24	A	407	PHO	C2D-C1D-ND	11.05	117.42	109.43
24	a	408	PHO	C2D-C1D-ND	10.84	117.26	109.43

5 of 63 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404	CLA	ND
23	A	408	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND

5 of 1230 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	614	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	B	614	CLA	CAD-CBD-CGD-O2D
23	C	507	CLA	C2B-C3B-CAB-CBB
23	C	507	CLA	C4B-C3B-CAB-CBB
23	C	507	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

147 monomers are involved in 285 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	K	101	BCR	3	0
23	C	505	CLA	5	0
24	A	416	PHO	1	0
23	b	609	CLA	3	0
31	A	417	LMT	1	0
23	b	602	CLA	1	0
35	c	517	DGD	2	0
31	t	101	LMT	2	0
32	Z	101	LMG	2	0
25	H	101	BCR	2	0
23	B	601	CLA	2	0
23	B	604	CLA	2	0
23	B	613	CLA	3	0
23	A	405	CLA	4	0
25	d	403	BCR	2	0
26	a	411	SQD	4	0
33	A	420	LHG	2	0
23	C	503	CLA	3	0
23	c	508	CLA	3	0
27	a	420	GOL	5	0
31	A	421	LMT	1	0
23	A	408	CLA	4	0
32	d	410	LMG	2	0
23	b	607	CLA	2	0
25	t	102	BCR	5	0
23	D	402	CLA	3	0
33	d	405	LHG	3	0
23	c	505	CLA	3	0
23	C	506	CLA	4	0
27	A	418	GOL	3	0
40	V	201	HEC	1	0
32	c	521	LMG	1	0
31	c	501	LMT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	B	621	LMG	1	0
23	B	605	CLA	5	0
23	C	502	CLA	2	0
27	l	102	GOL	1	0
27	O	302	GOL	1	0
27	O	303	GOL	2	0
31	B	628	LMT	1	0
31	B	630	LMT	1	0
33	E	101	LHG	4	0
33	D	407	LHG	5	0
34	B	625	HTG	1	0
23	B	603	CLA	1	0
23	C	509	CLA	1	0
27	b	628	GOL	2	0
23	C	501	CLA	5	0
23	c	509	CLA	4	0
31	e	101	LMT	1	0
23	b	615	CLA	2	0
29	A	414	PL9	10	0
23	B	606	CLA	4	0
34	b	625	HTG	1	0
23	C	512	CLA	1	0
26	A	410	SQD	2	0
23	C	511	CLA	1	0
23	B	615	CLA	5	0
25	c	516	BCR	2	0
32	z	101	LMG	2	0
33	d	406	LHG	9	0
23	b	605	CLA	3	0
25	h	101	BCR	3	0
25	K	103	BCR	1	0
27	a	419	GOL	1	0
33	D	406	LHG	2	0
23	B	612	CLA	4	0
34	c	522	HTG	1	0
26	A	412	SQD	1	0
34	d	409	HTG	1	0
27	v	202	GOL	1	0
23	c	510	CLA	2	0
32	c	520	LMG	1	0
35	C	515	DGD	2	0
26	f	102	SQD	1	0

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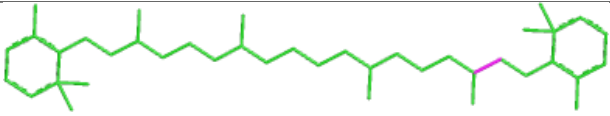
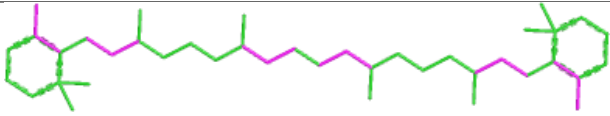
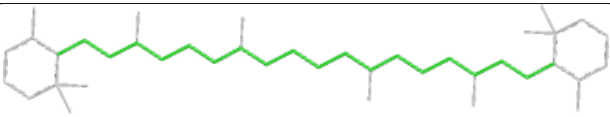
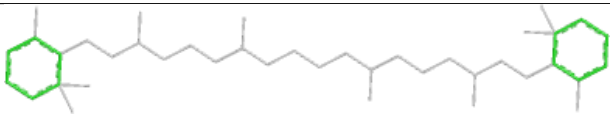
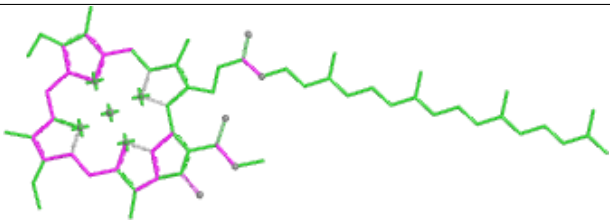
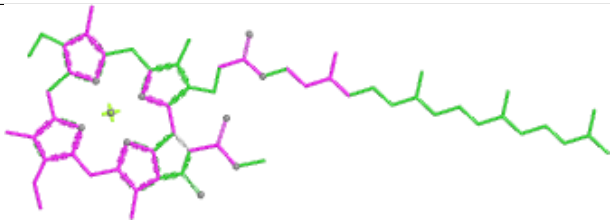
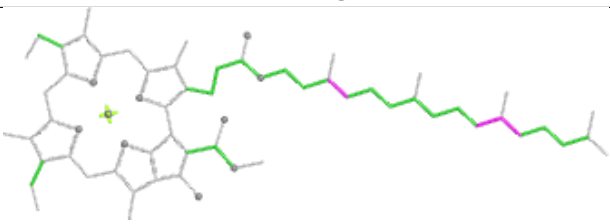
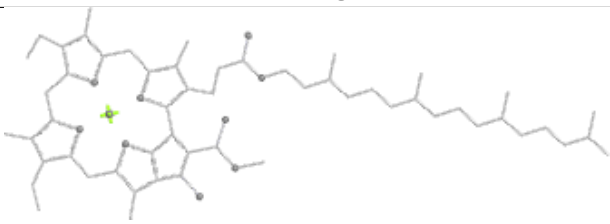
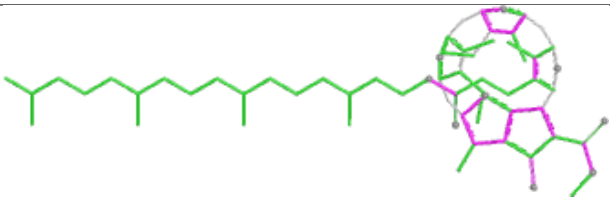
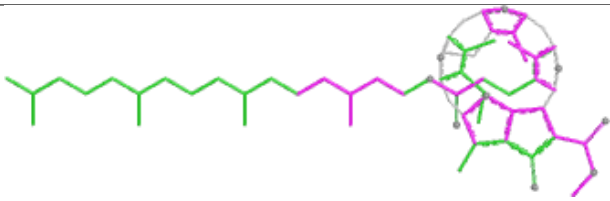
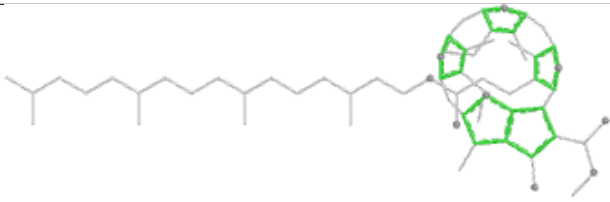
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25	D	404	BCR	3	0
23	a	406	CLA	2	0
32	C	519	LMG	4	0
23	d	402	CLA	1	0
23	B	602	CLA	1	0
35	C	517	DGD	2	0
23	A	406	CLA	1	0
23	b	601	CLA	3	0
23	b	613	CLA	1	0
25	b	617	BCR	1	0
23	B	616	CLA	4	0
23	c	507	CLA	2	0
23	b	606	CLA	2	0
23	c	513	CLA	5	0
25	y	101	BCR	2	0
26	a	413	SQD	1	0
25	T	102	BCR	7	0
34	B	622	HTG	2	0
26	F	103	SQD	2	0
23	A	404	CLA	5	0
33	a	421	LHG	4	0
35	c	519	DGD	2	0
25	c	515	BCR	4	0
23	d	401	CLA	2	0
25	B	618	BCR	2	0
23	C	507	CLA	2	0
23	c	506	CLA	6	0
23	c	503	CLA	2	0
27	b	629	GOL	1	0
23	C	513	CLA	2	0
23	B	614	CLA	1	0
24	A	407	PHO	2	0
23	c	514	CLA	3	0
23	c	512	CLA	5	0
26	b	620	SQD	2	0
23	a	407	CLA	2	0
25	B	617	BCR	2	0
27	B	627	GOL	1	0
34	b	622	HTG	2	0
31	M	101	LMT	1	0
23	b	604	CLA	2	0
27	B	624	GOL	2	0

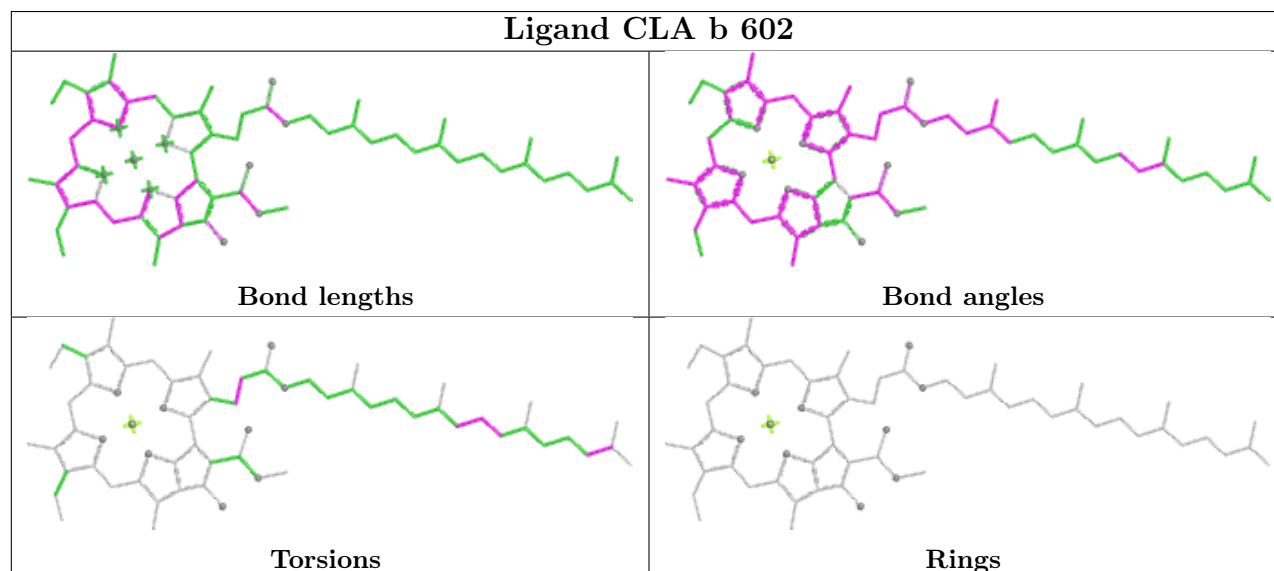
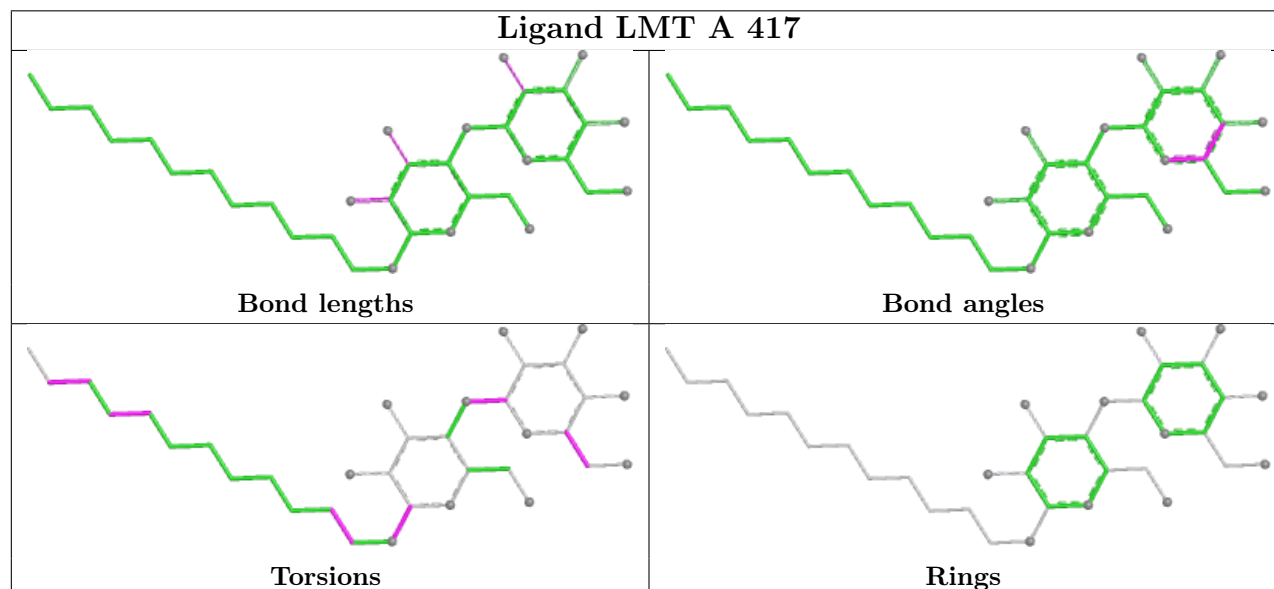
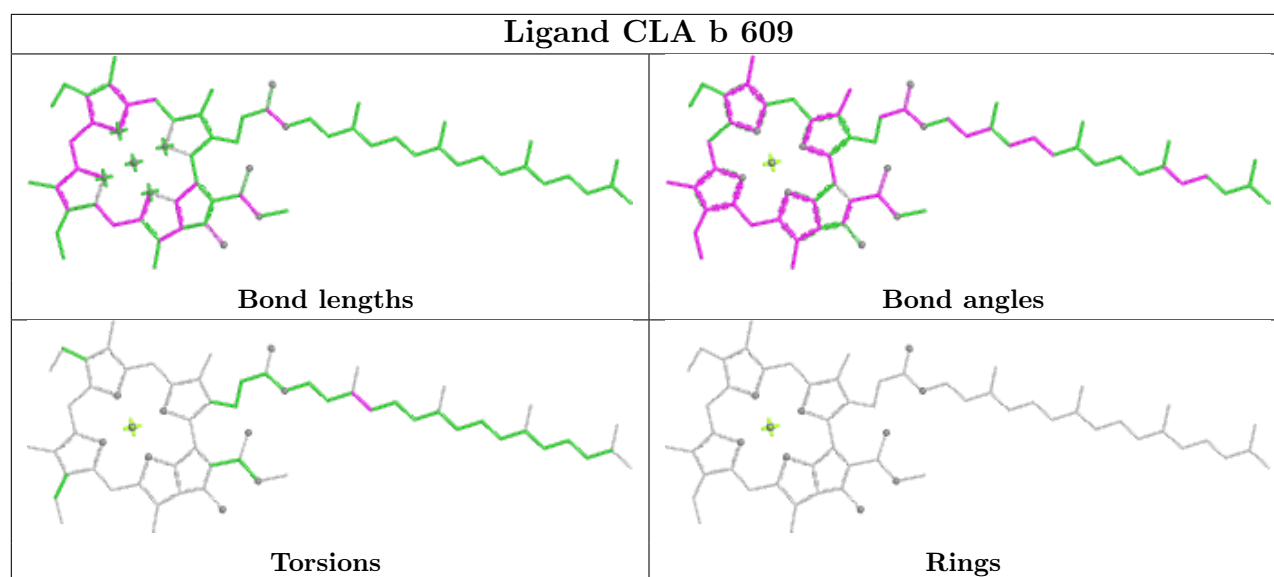
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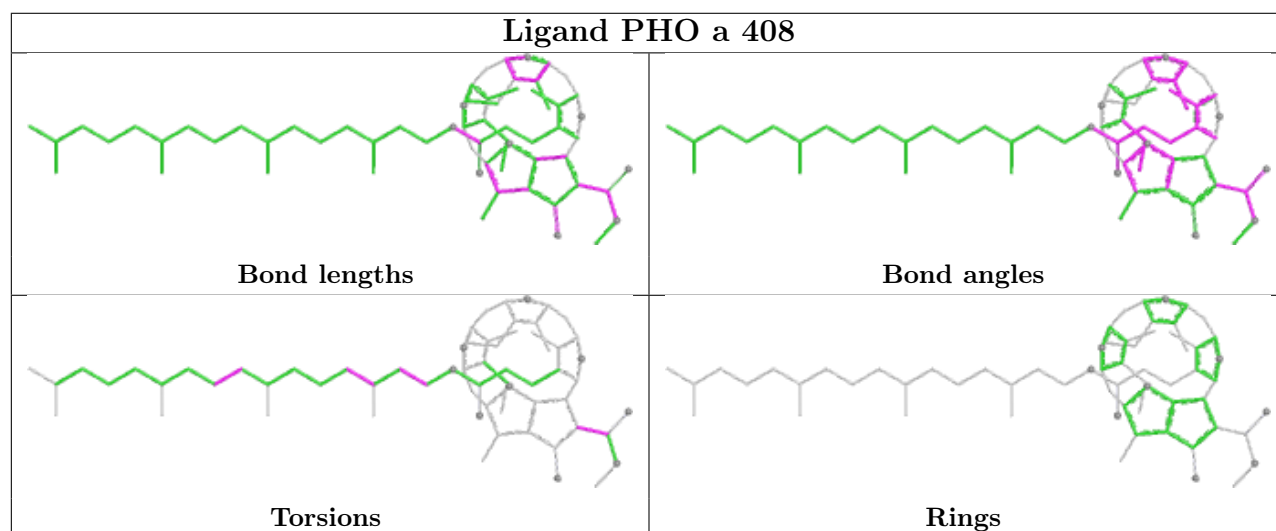
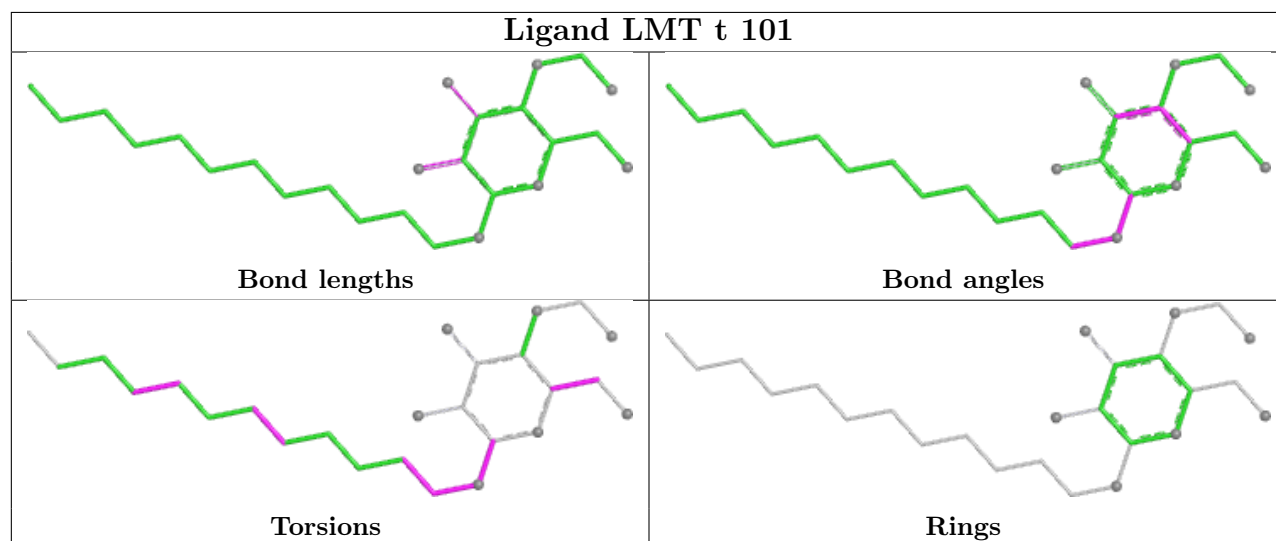
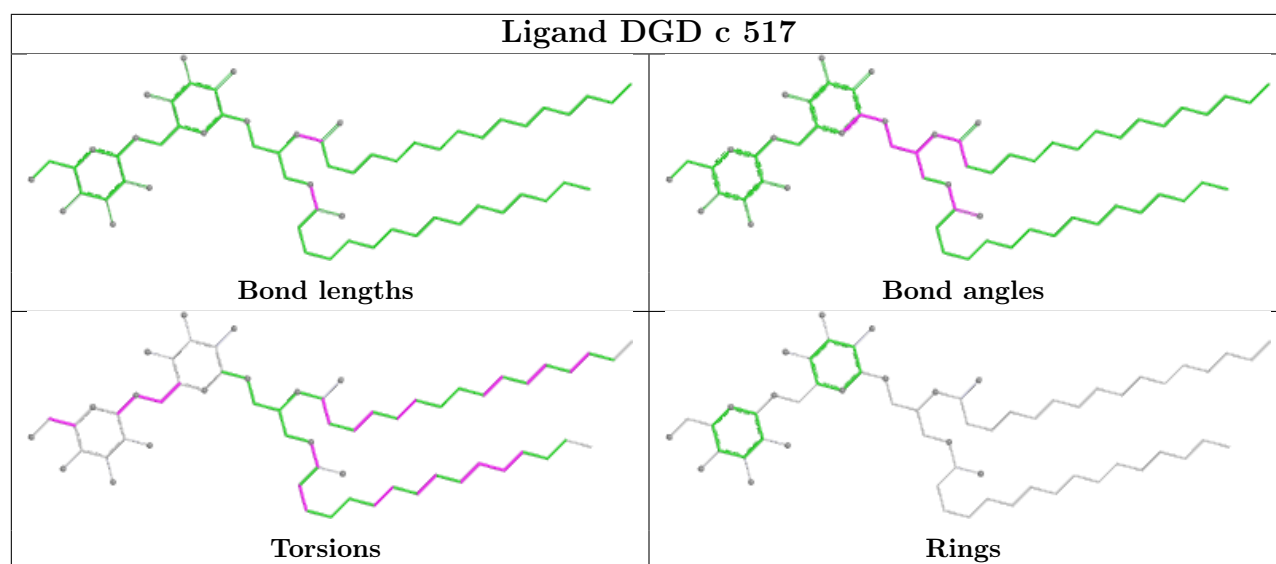
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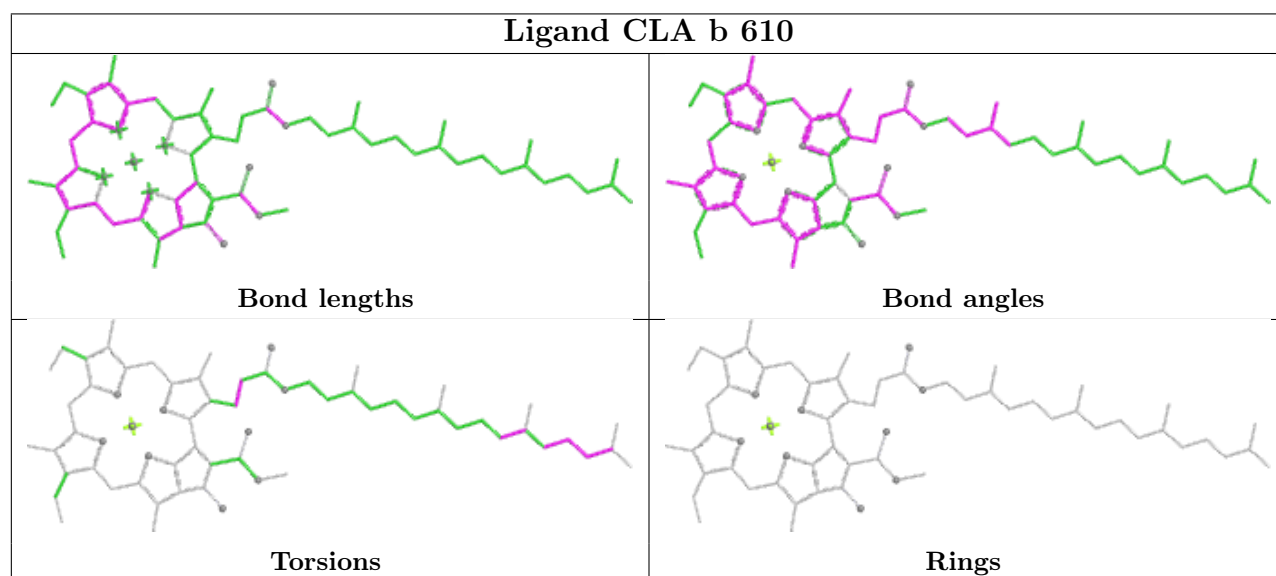
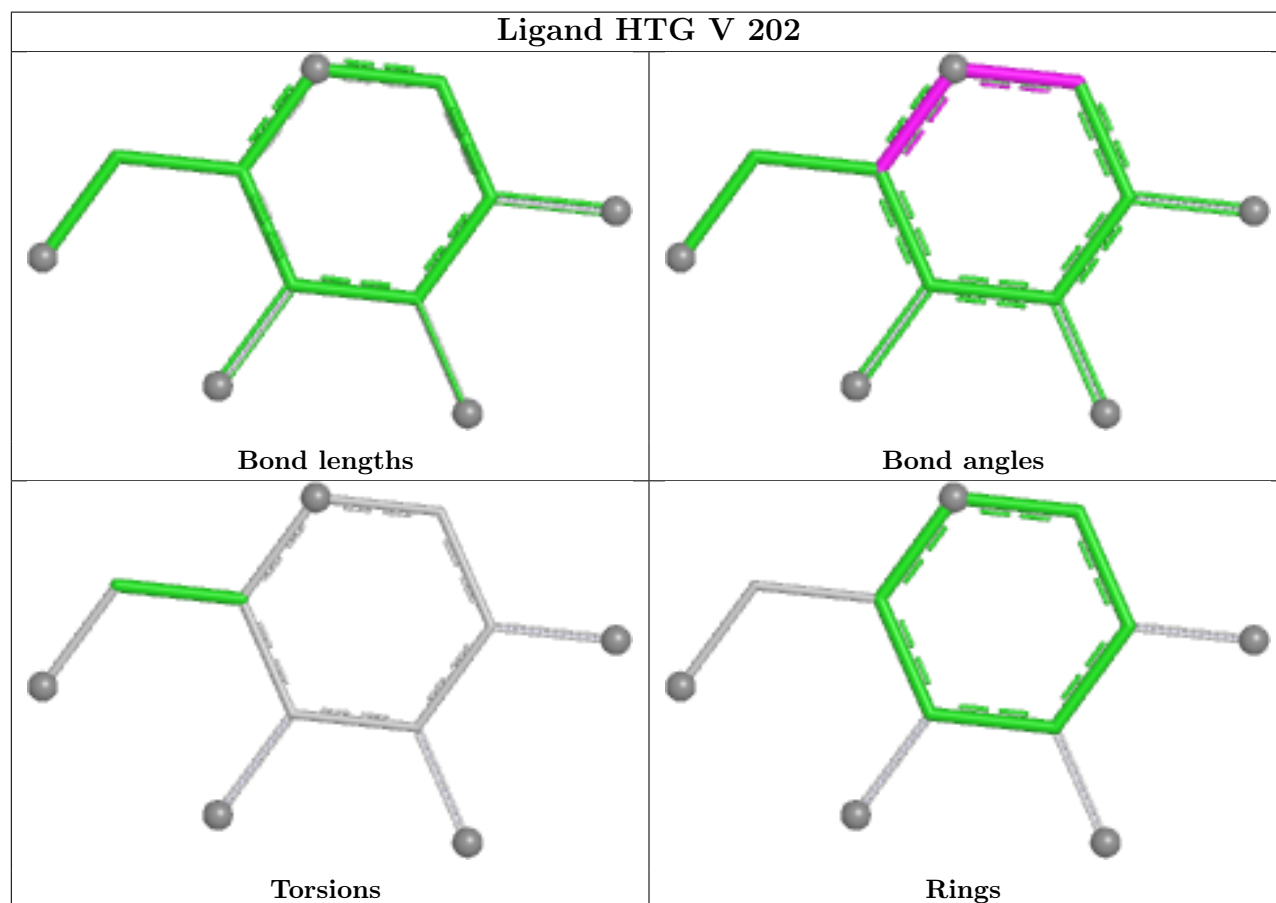
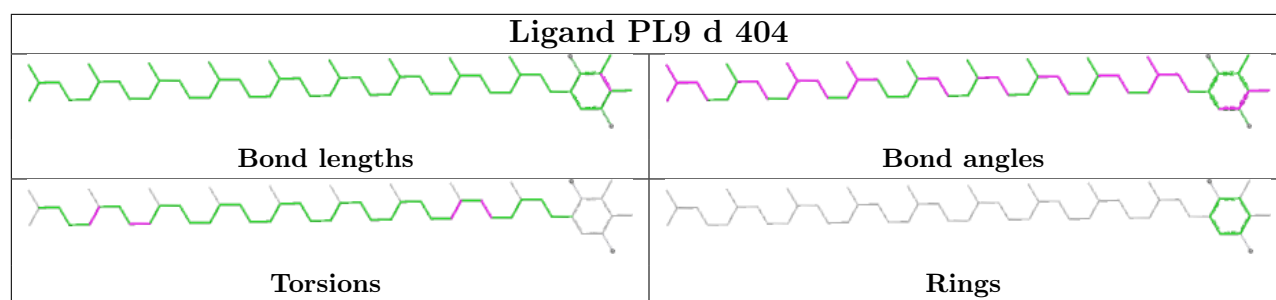
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	609	CLA	2	0
23	c	502	CLA	3	0
25	C	514	BCR	1	0
23	a	405	CLA	3	0
29	a	415	PL9	4	0
23	b	614	CLA	2	0
25	Y	101	BCR	2	0
27	B	629	GOL	2	0
25	b	619	BCR	3	0
31	B	631	LMT	1	0
35	C	516	DGD	2	0
23	C	504	CLA	1	0
31	b	621	LMT	1	0
23	B	610	CLA	2	0
23	C	508	CLA	4	0
25	A	409	BCR	2	0
34	D	410	HTG	1	0
23	a	409	CLA	2	0
35	c	518	DGD	1	0
25	B	619	BCR	1	0
23	b	616	CLA	1	0
23	C	510	CLA	3	0
35	H	102	DGD	1	0
35	h	102	DGD	1	0
25	a	410	BCR	2	0
26	B	620	SQD	1	0
25	b	618	BCR	3	0
23	c	504	CLA	3	0
24	a	417	PHO	2	0
38	F	102	HEM	1	0

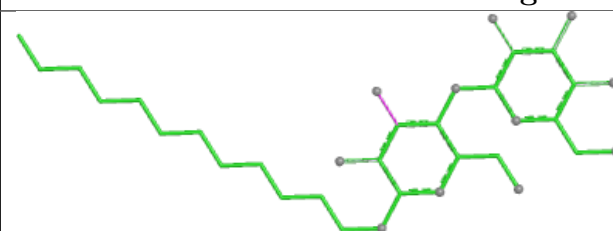
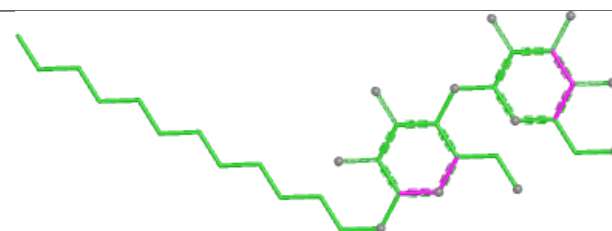
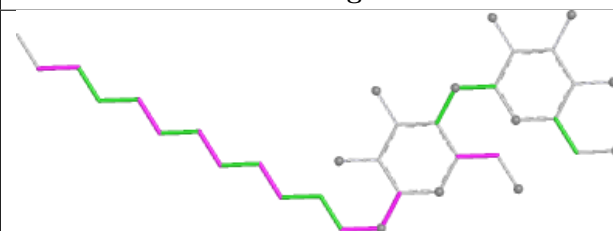
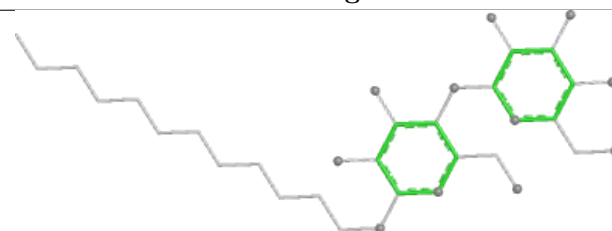
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

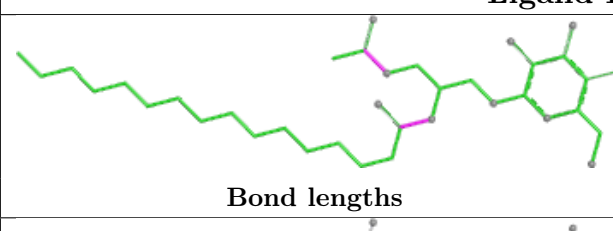
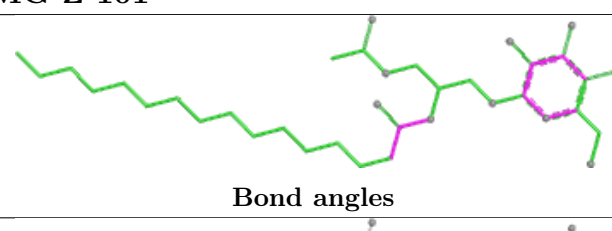
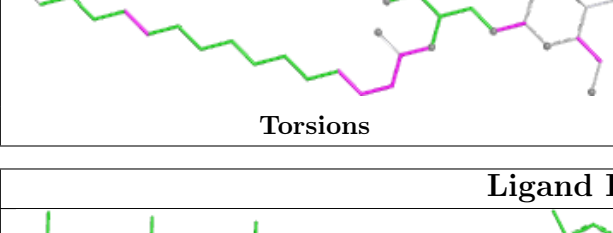
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 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA C 505	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PHO A 416	
 Bond lengths	 Bond angles
 Torsions	 Rings

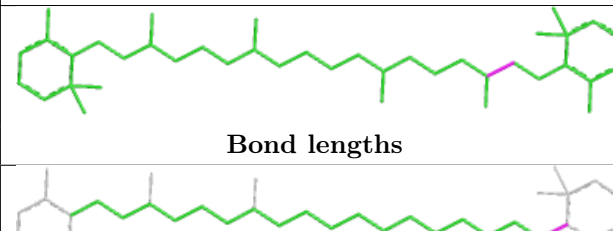
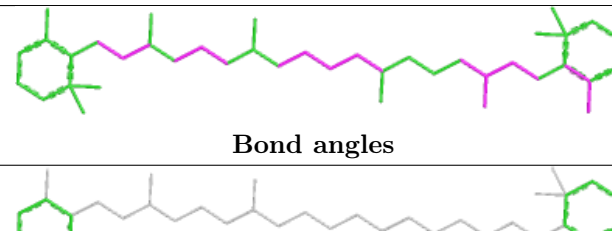
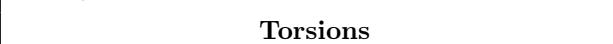


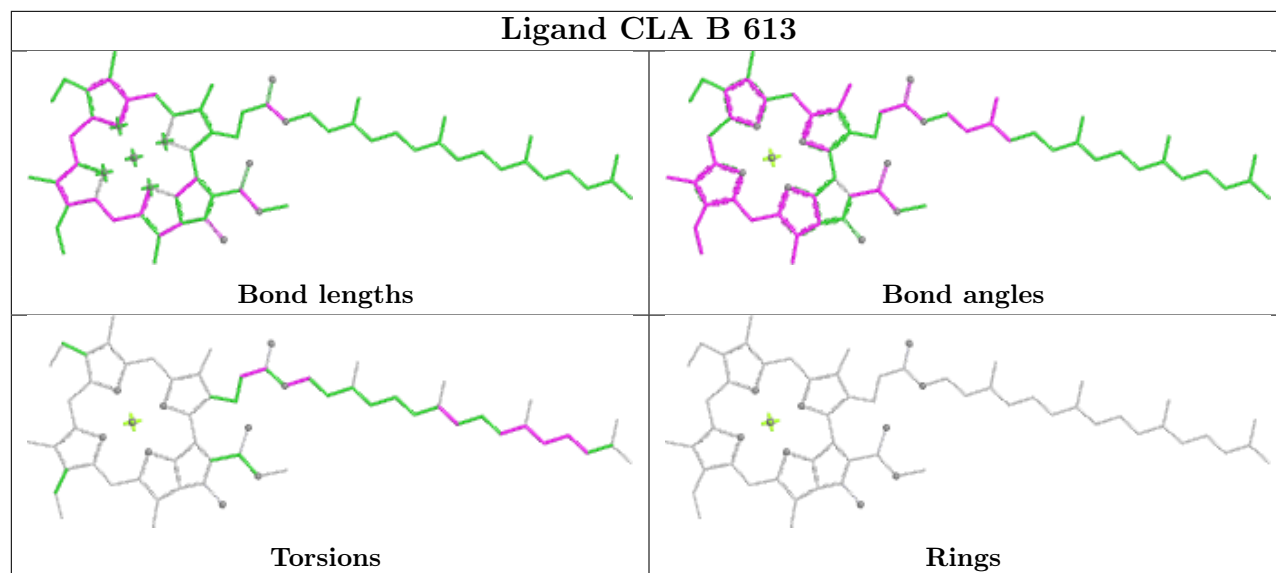
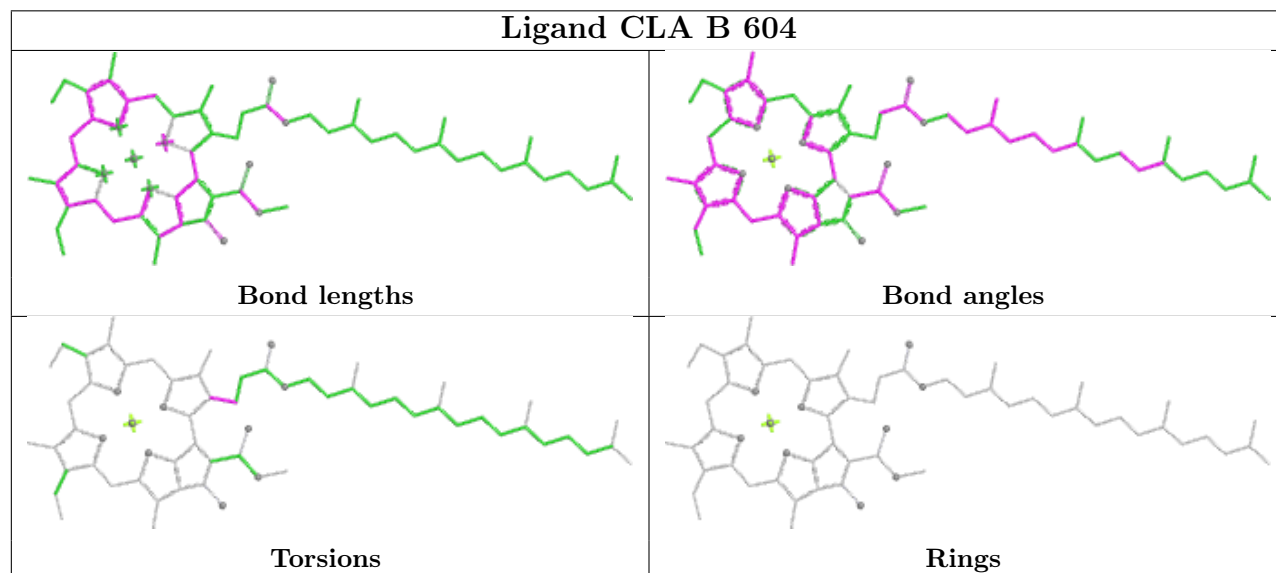
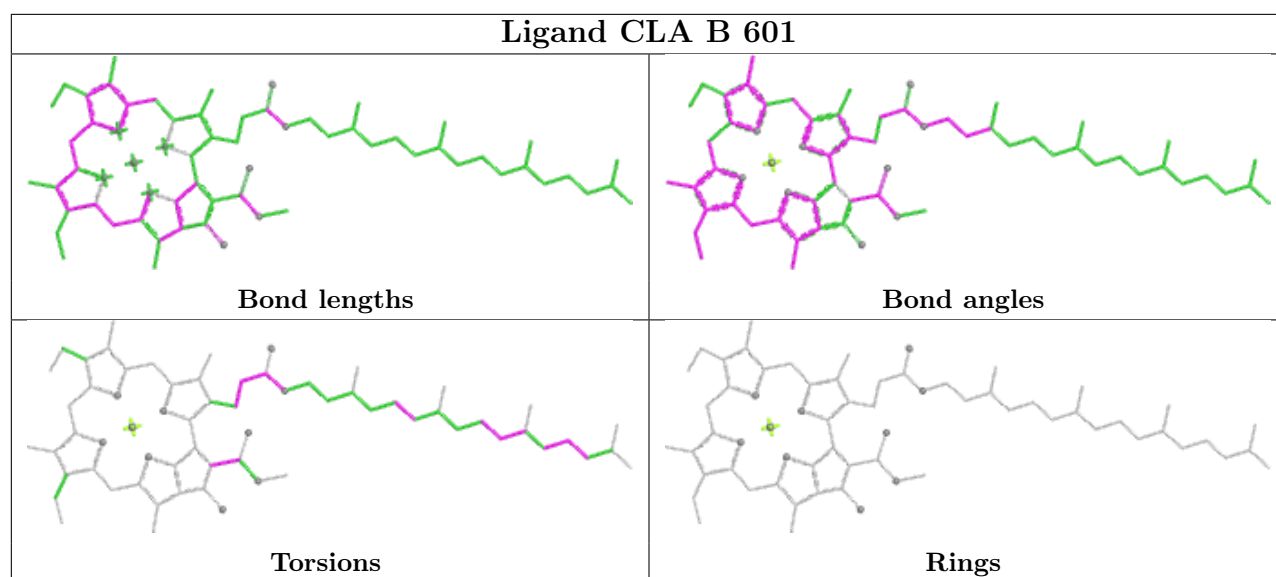


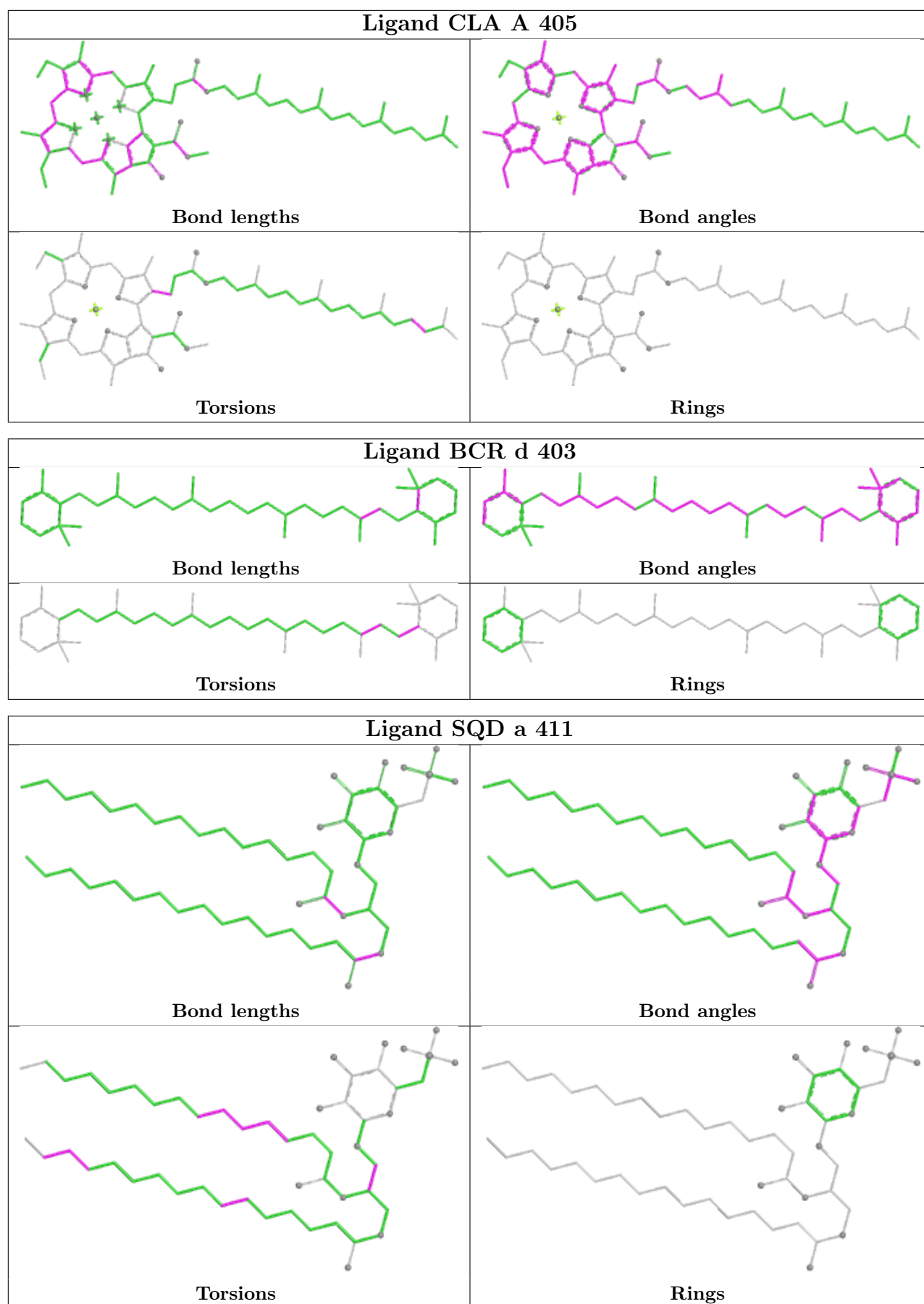


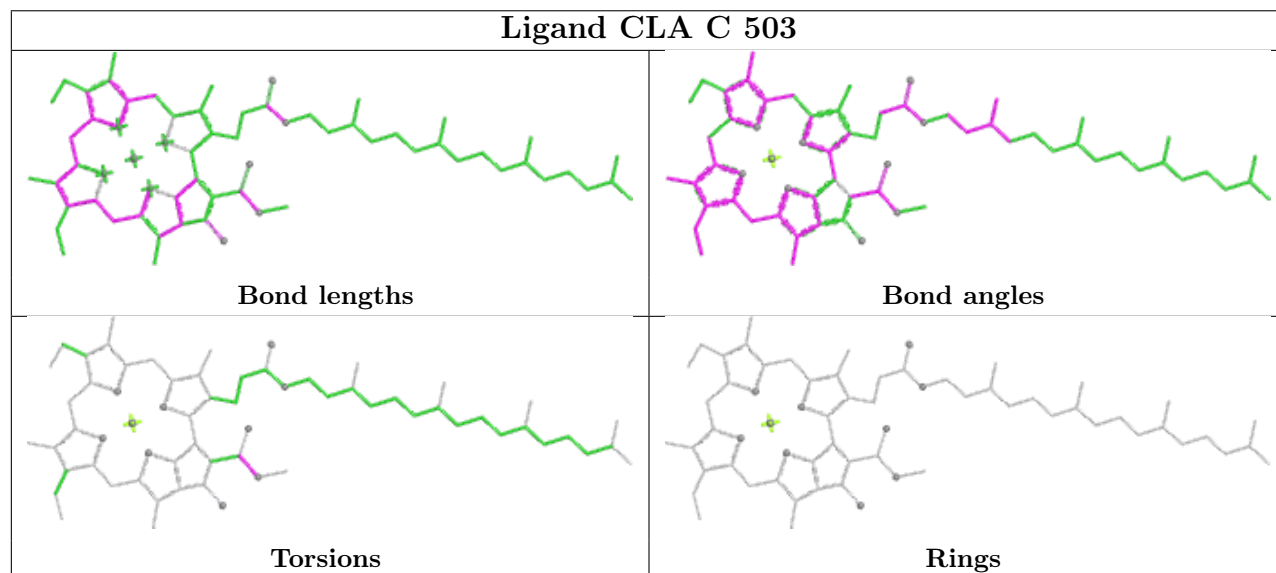
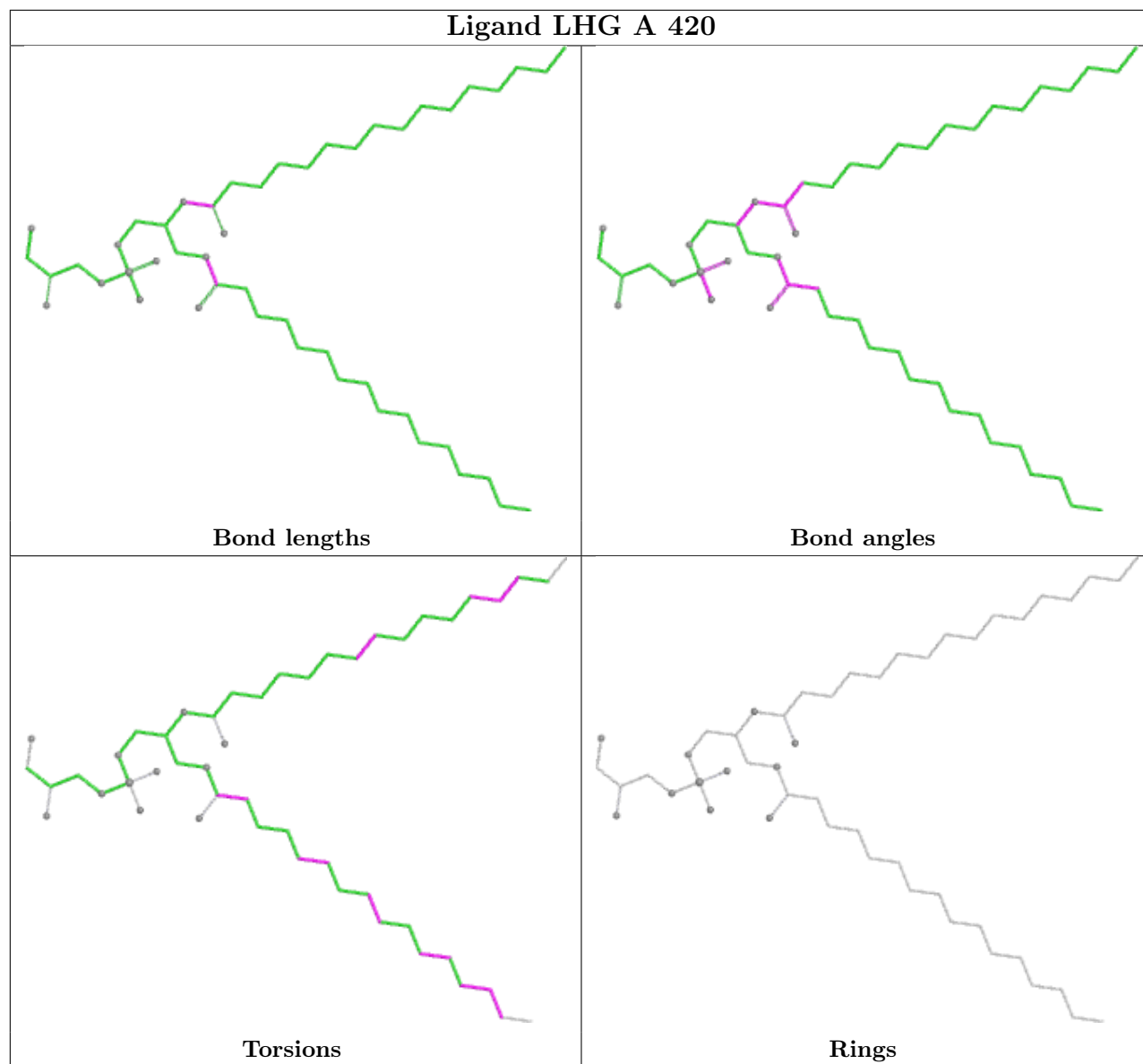
Ligand LMT F 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

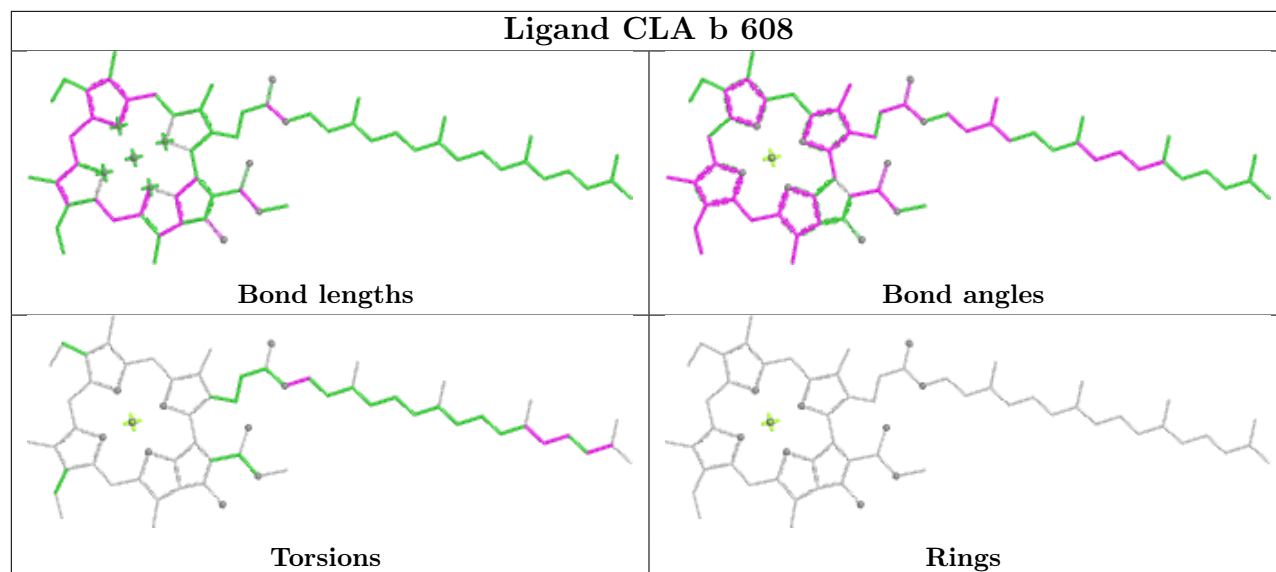
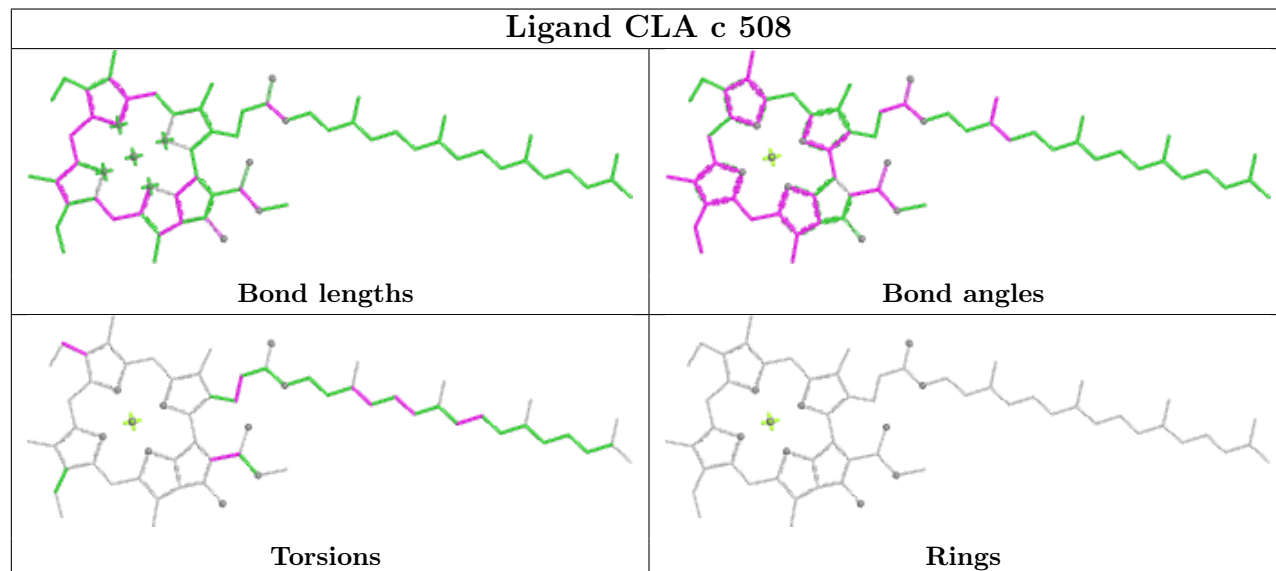
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Bond lengths	Bond angles
	
Torsions	Rings

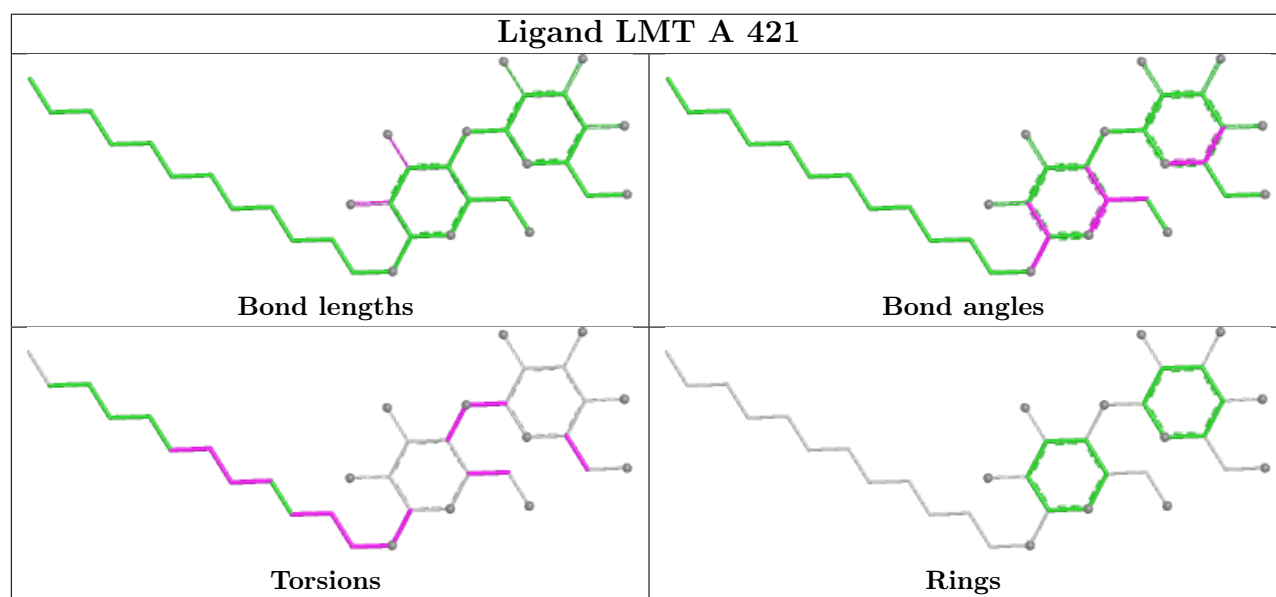
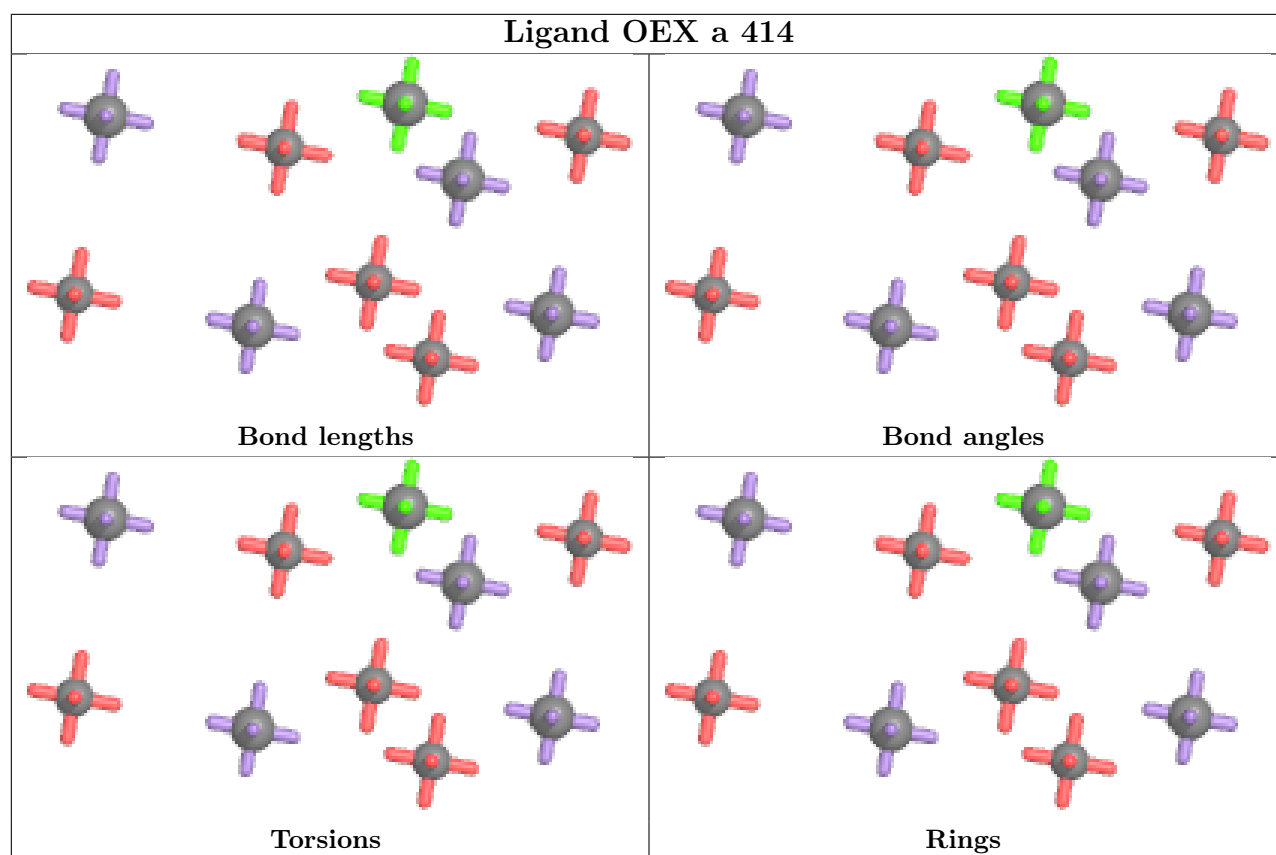
Ligand BCR H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

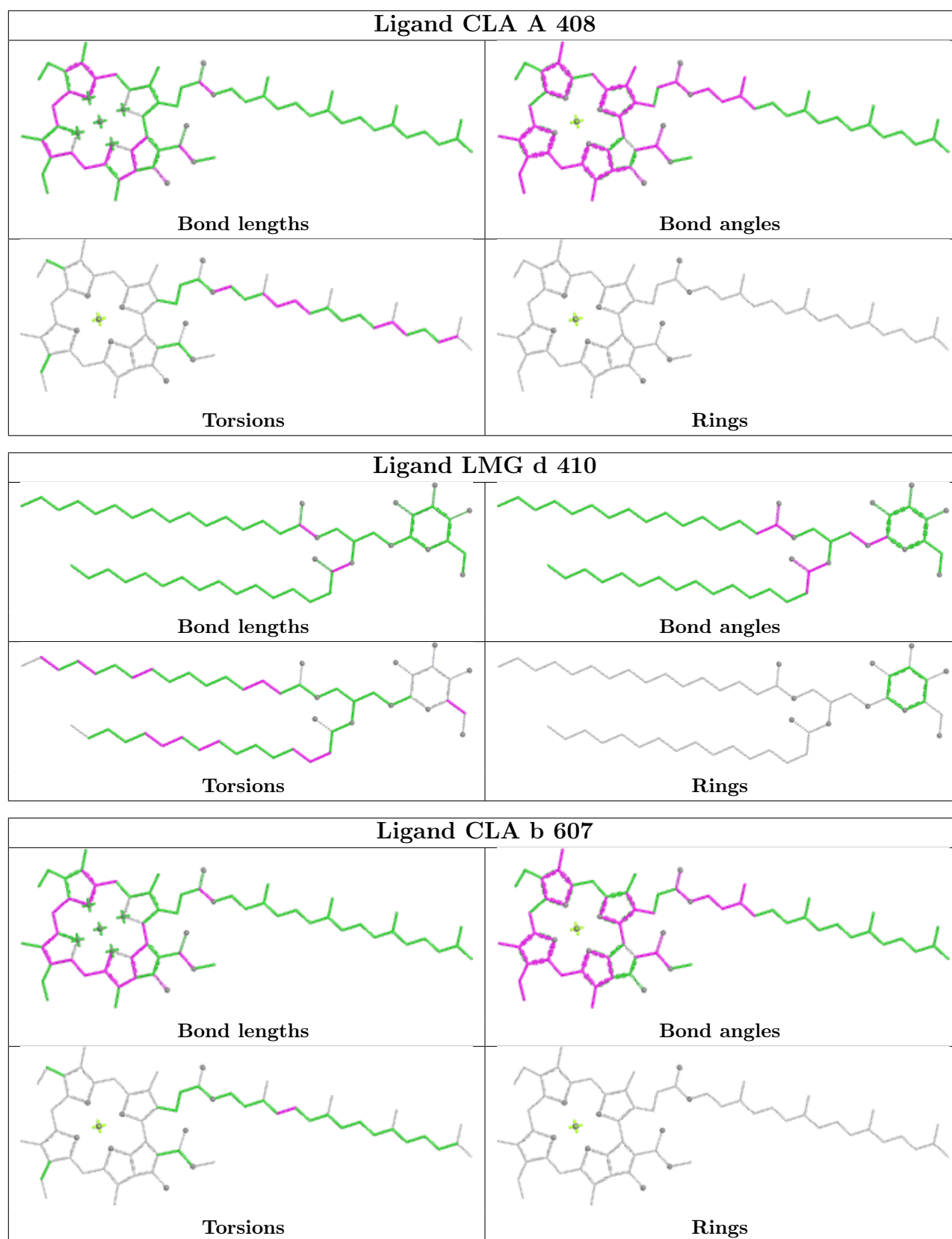


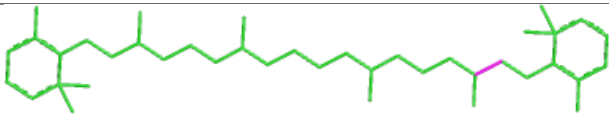
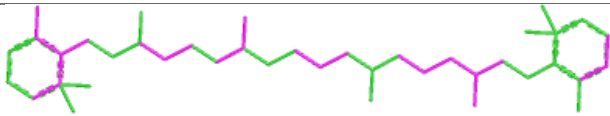
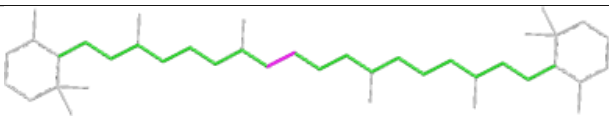
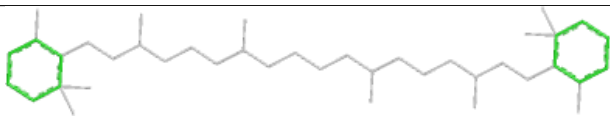


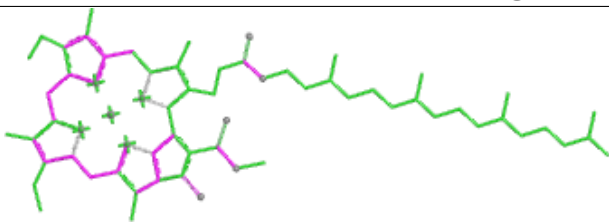
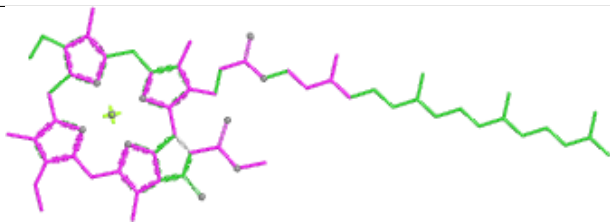
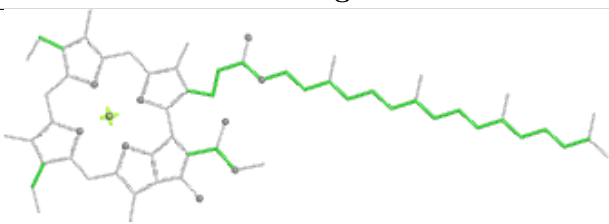
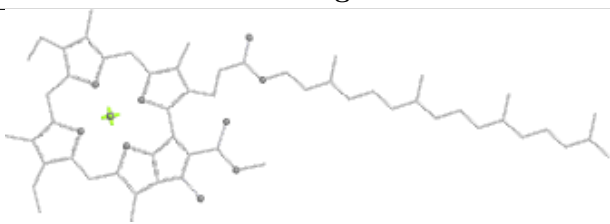


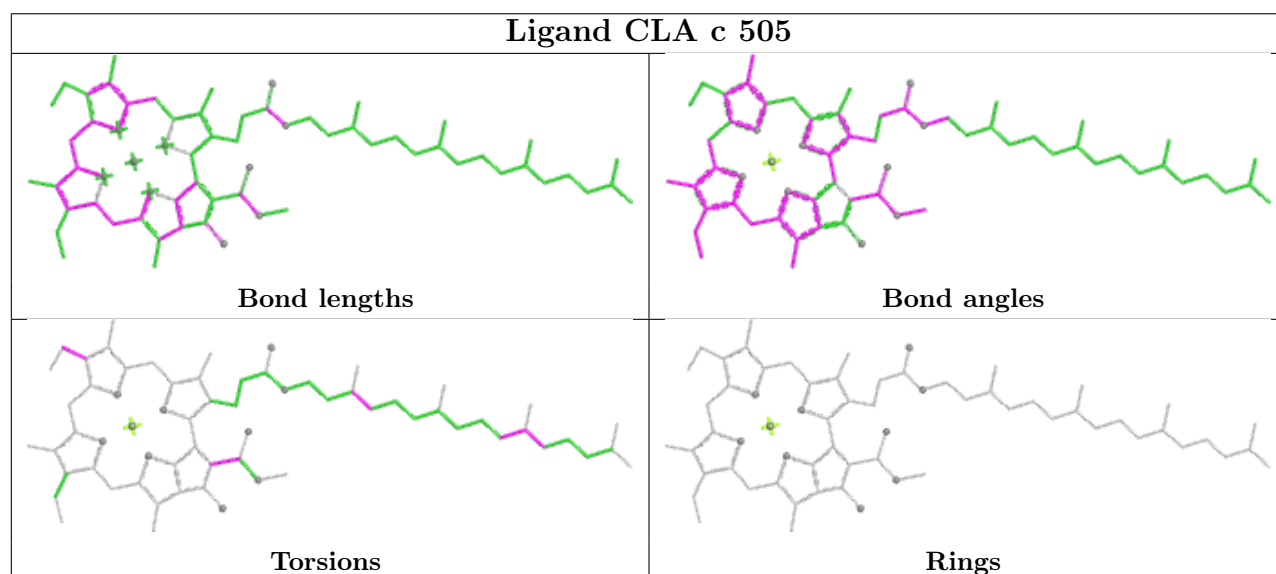
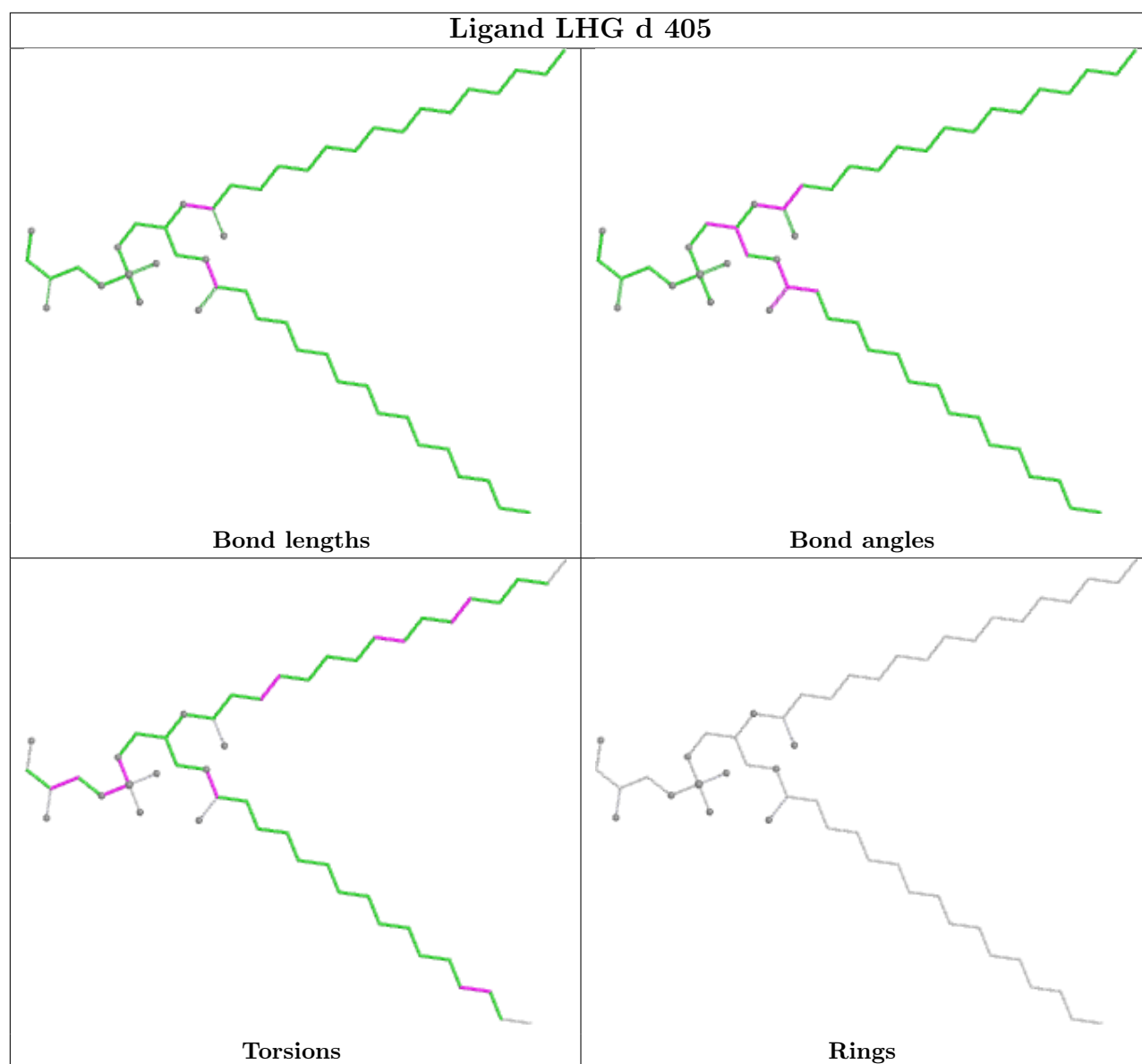
Ligand CLA b 608**Ligand CLA c 508**



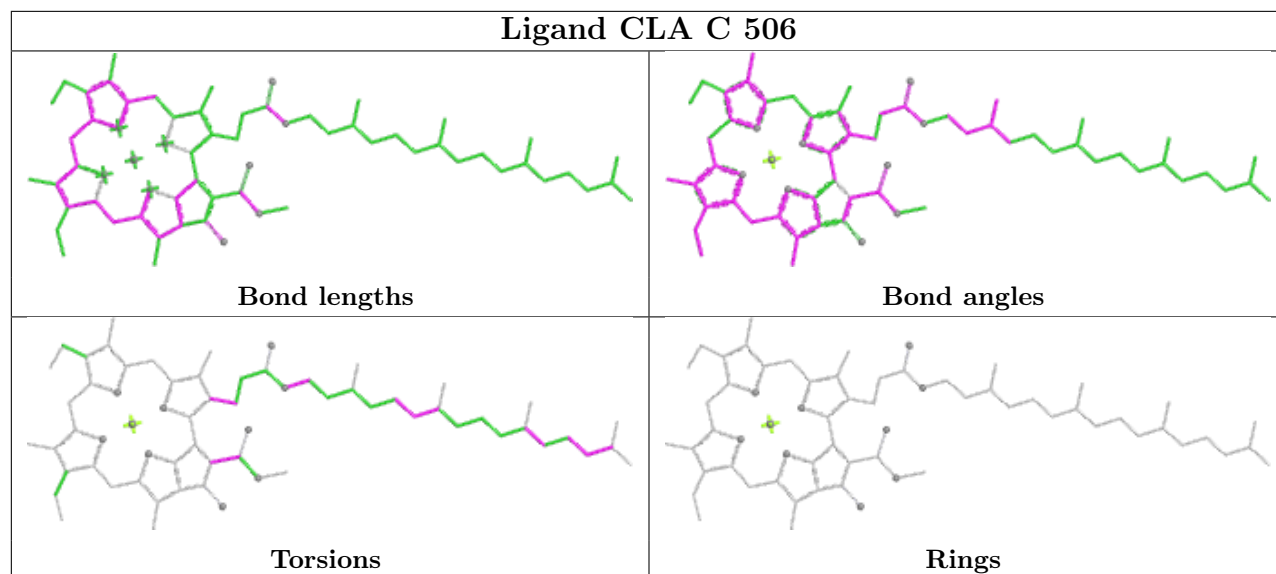


Ligand BCR t 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

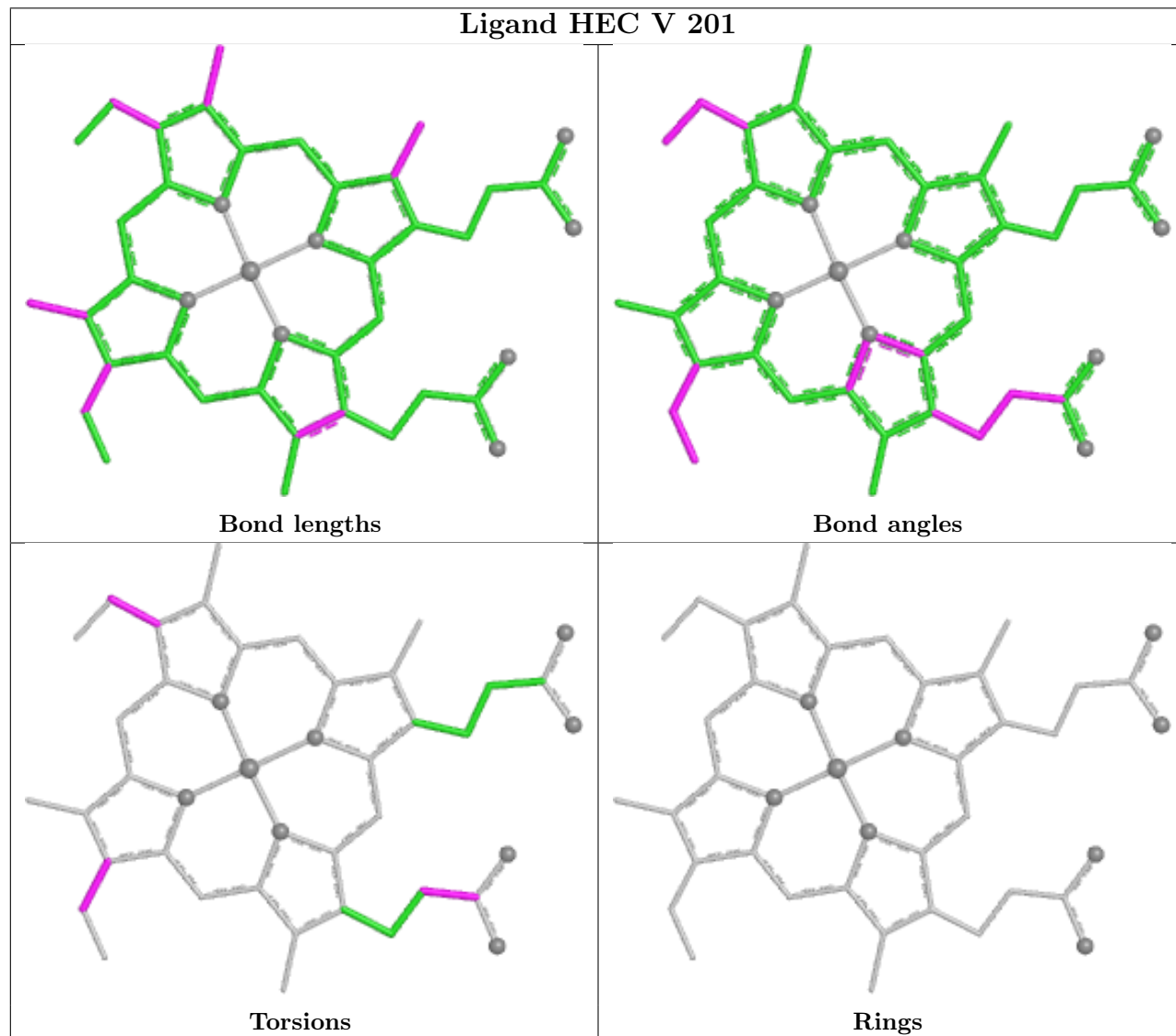
Ligand CLA D 402	
	
Bond lengths	Bond angles
	
Torsions	Rings



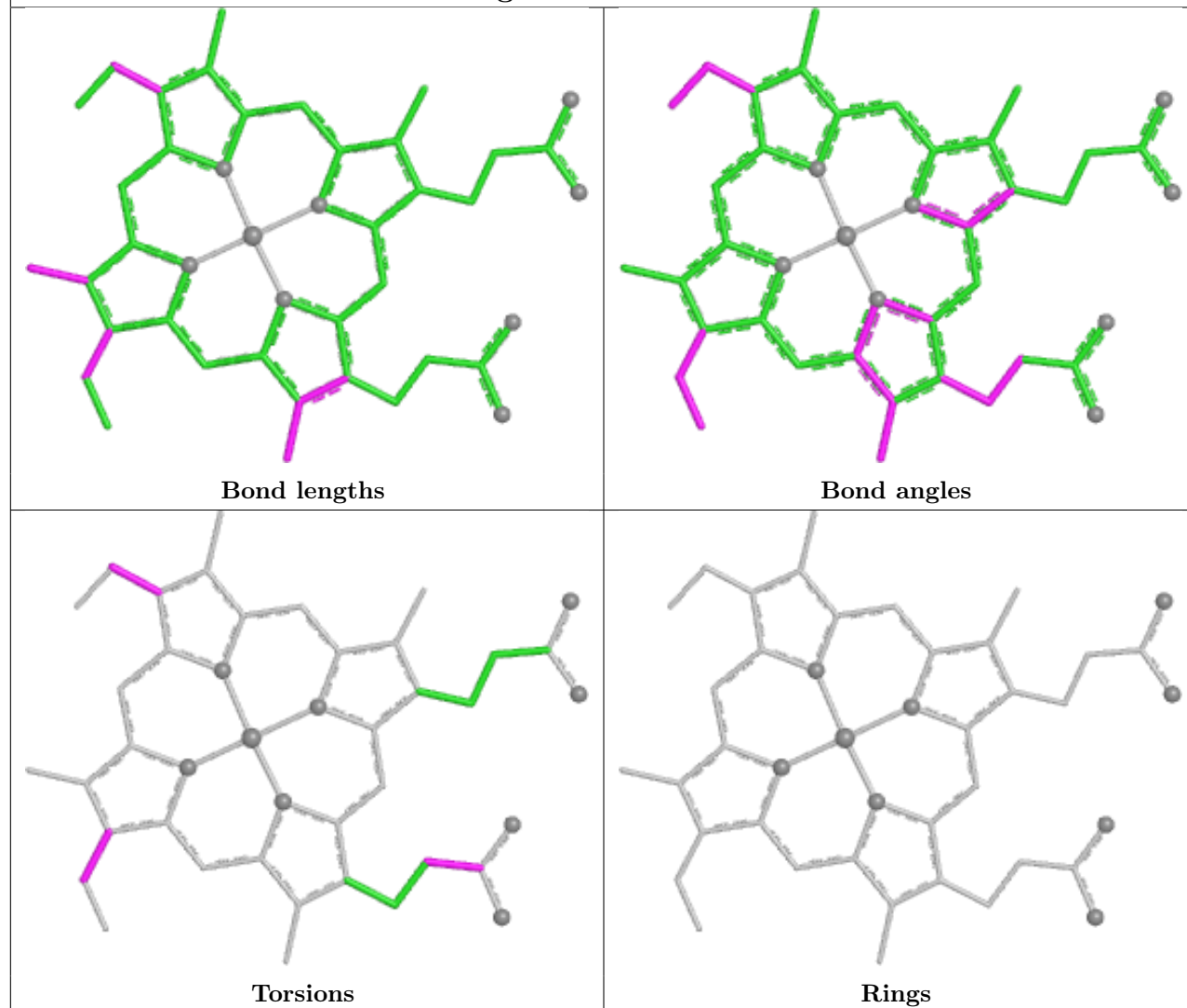
Ligand CLA C 506



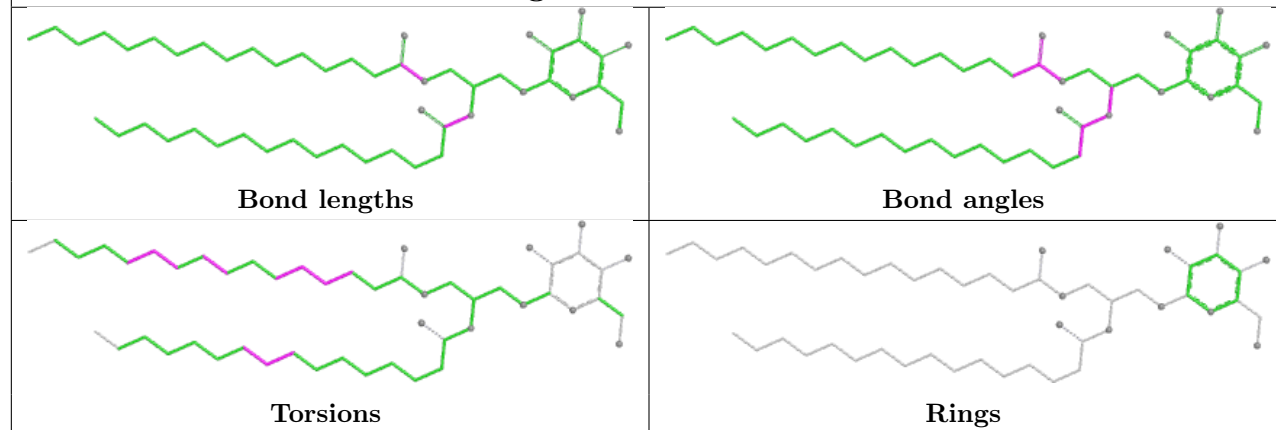
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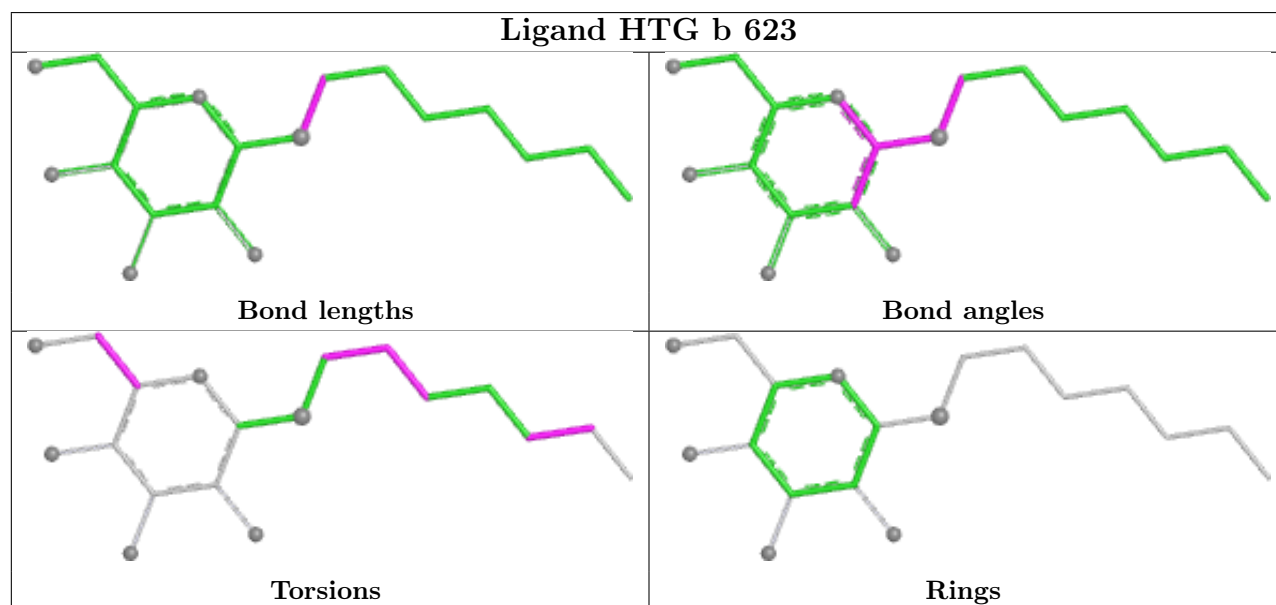
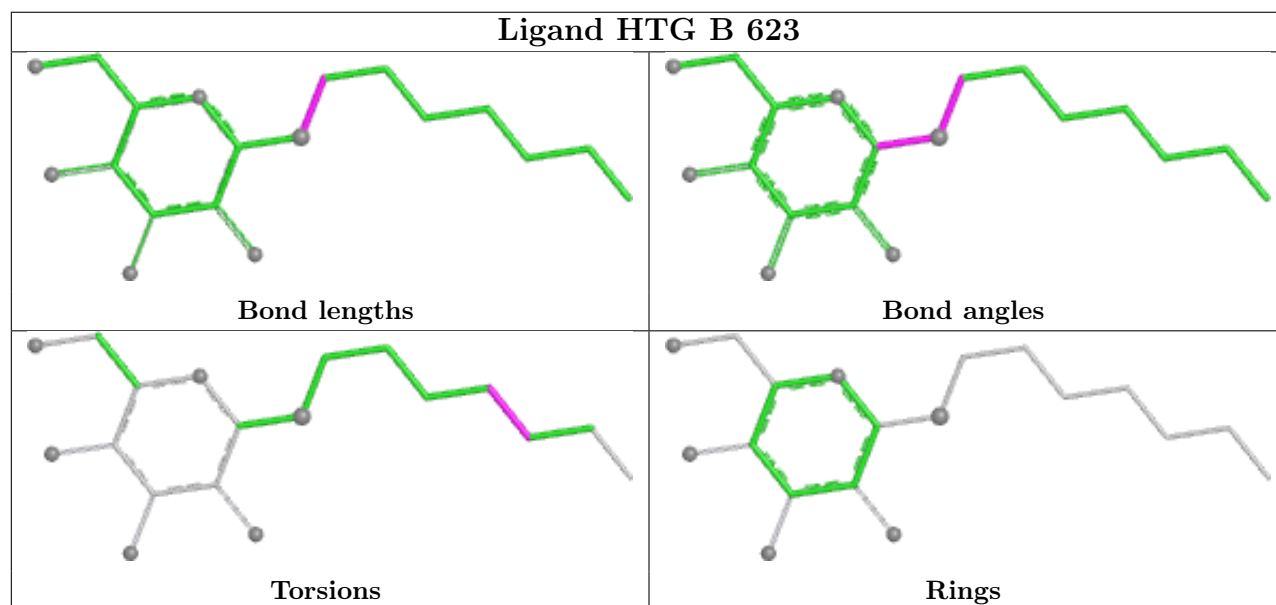
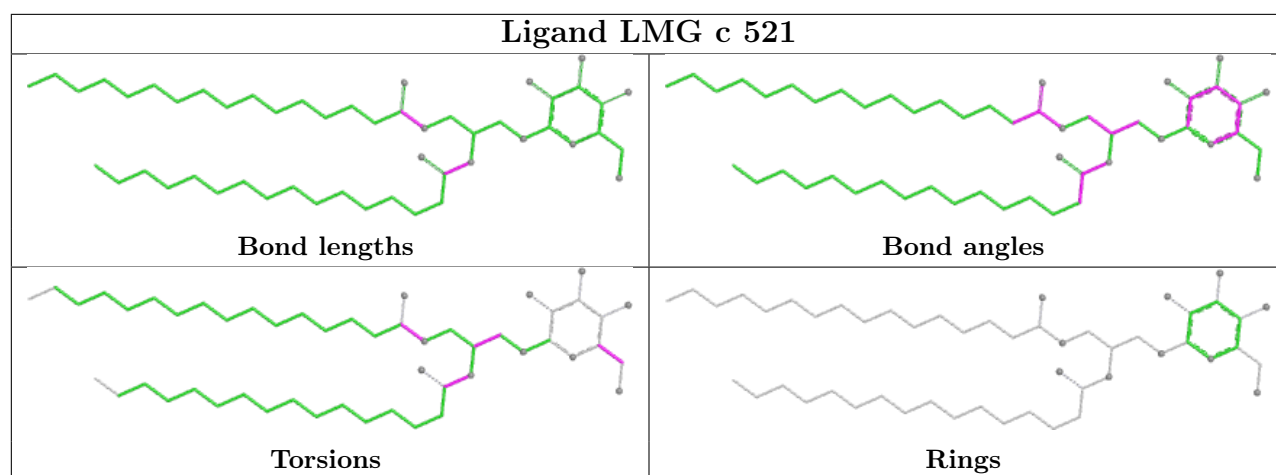


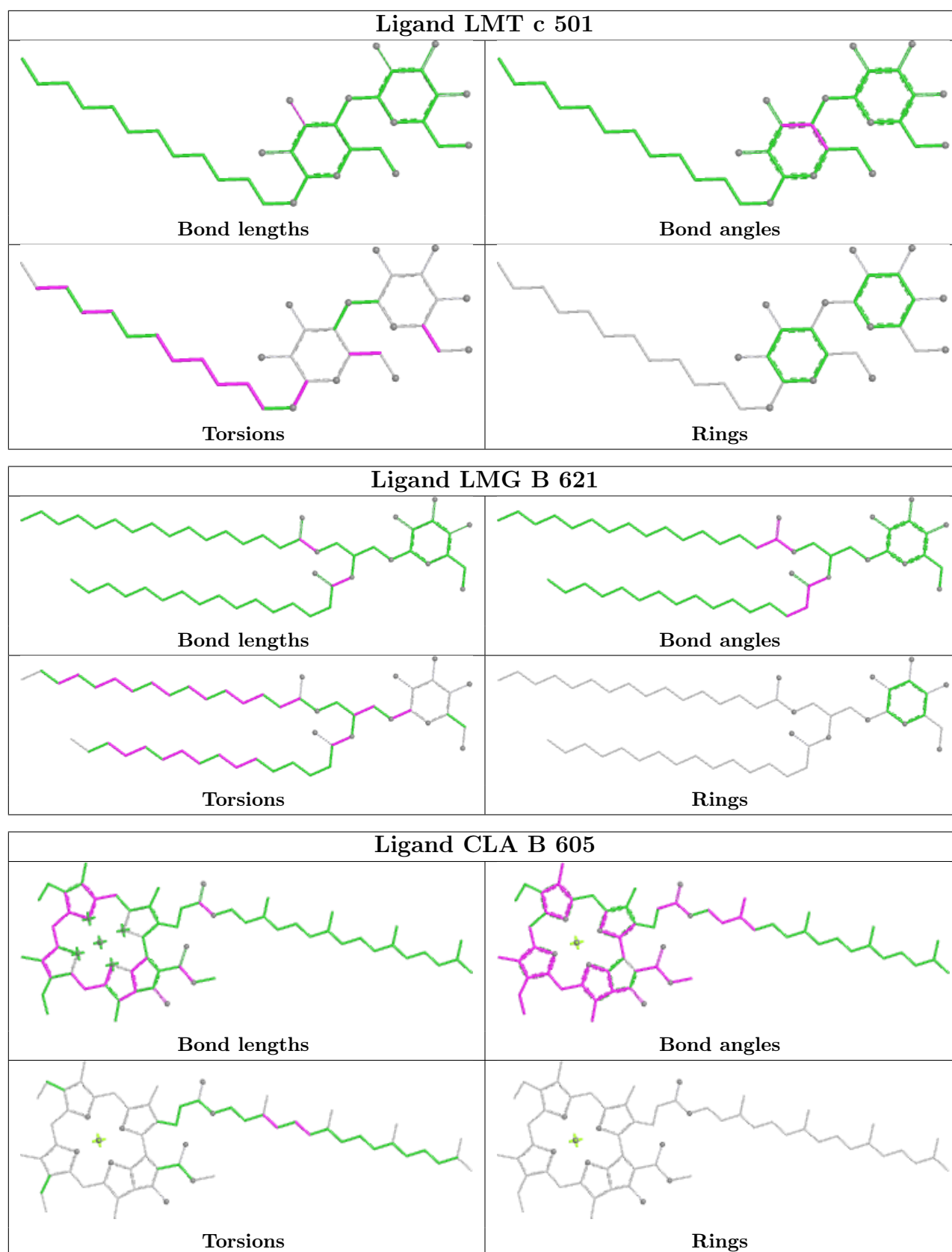
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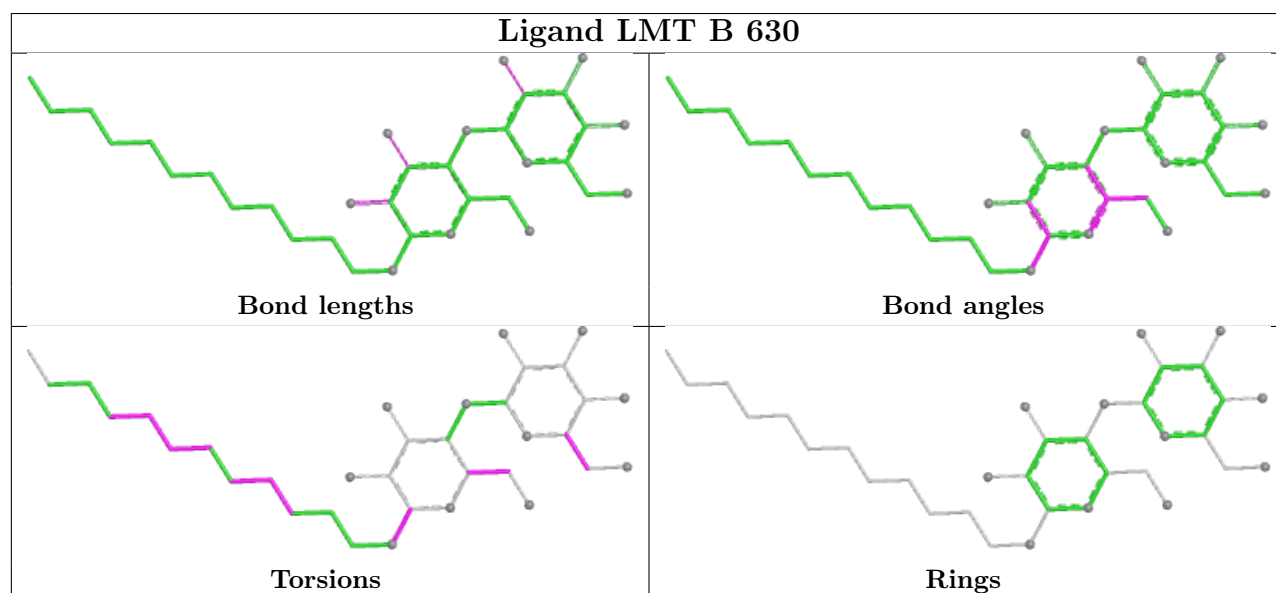
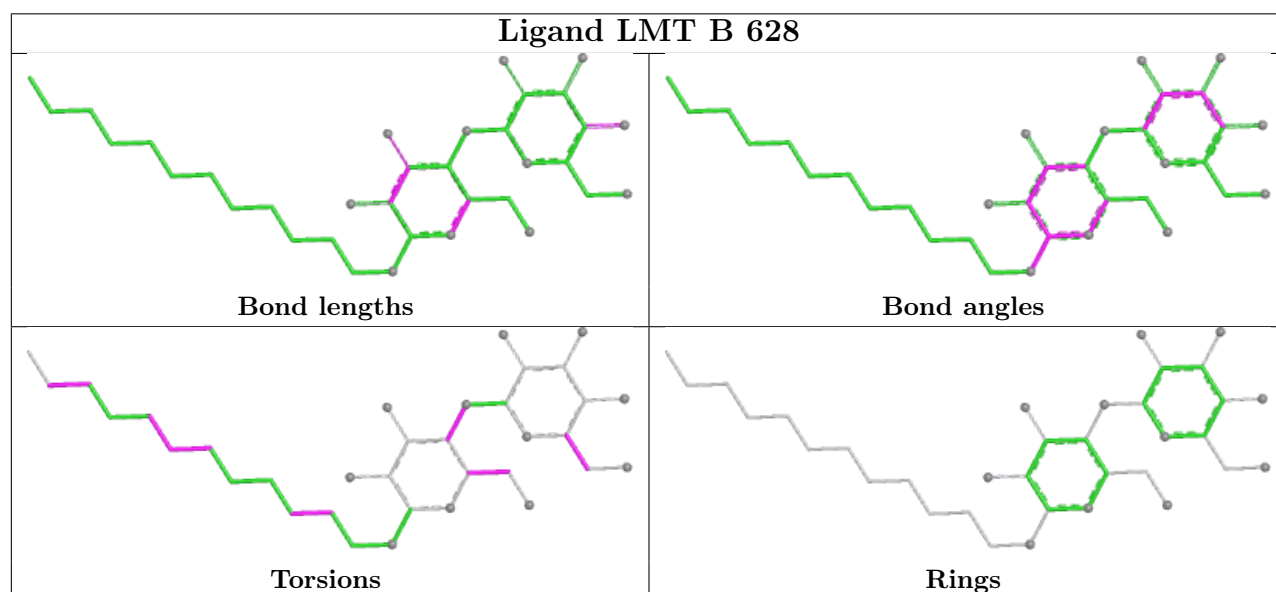
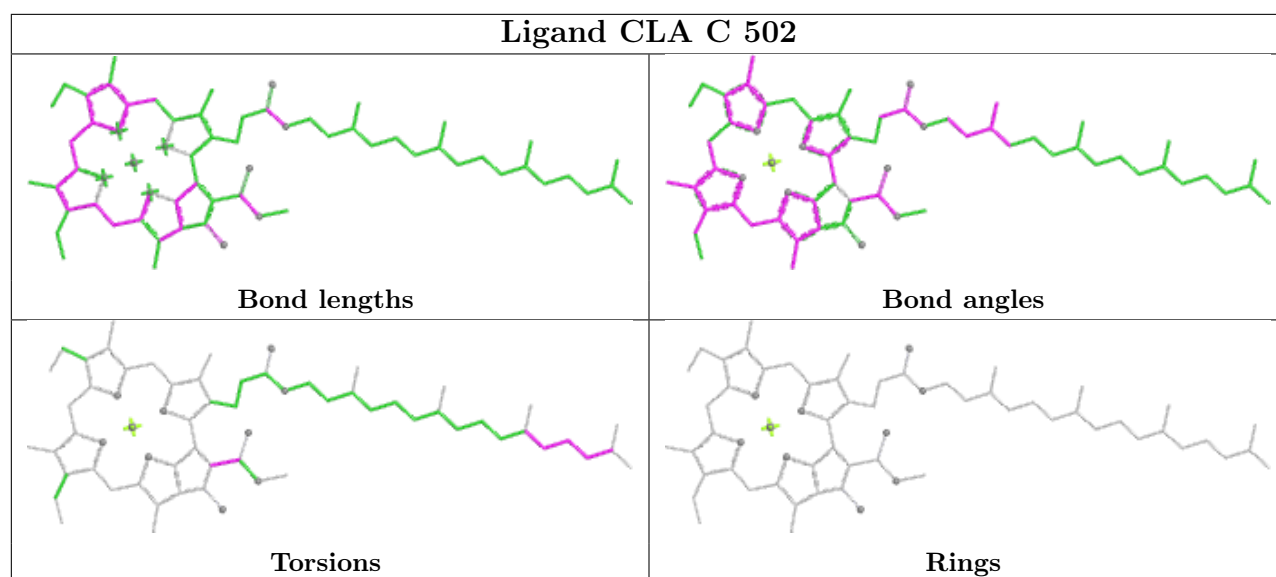


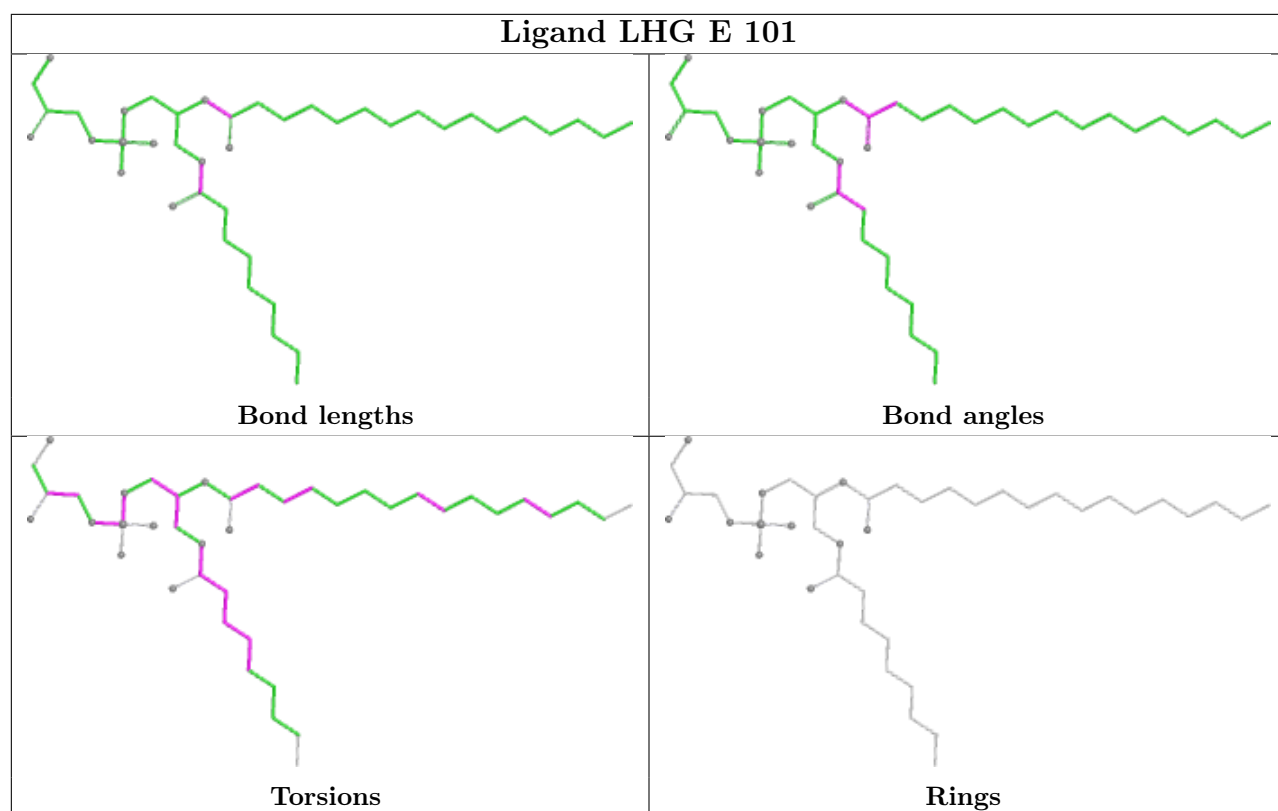
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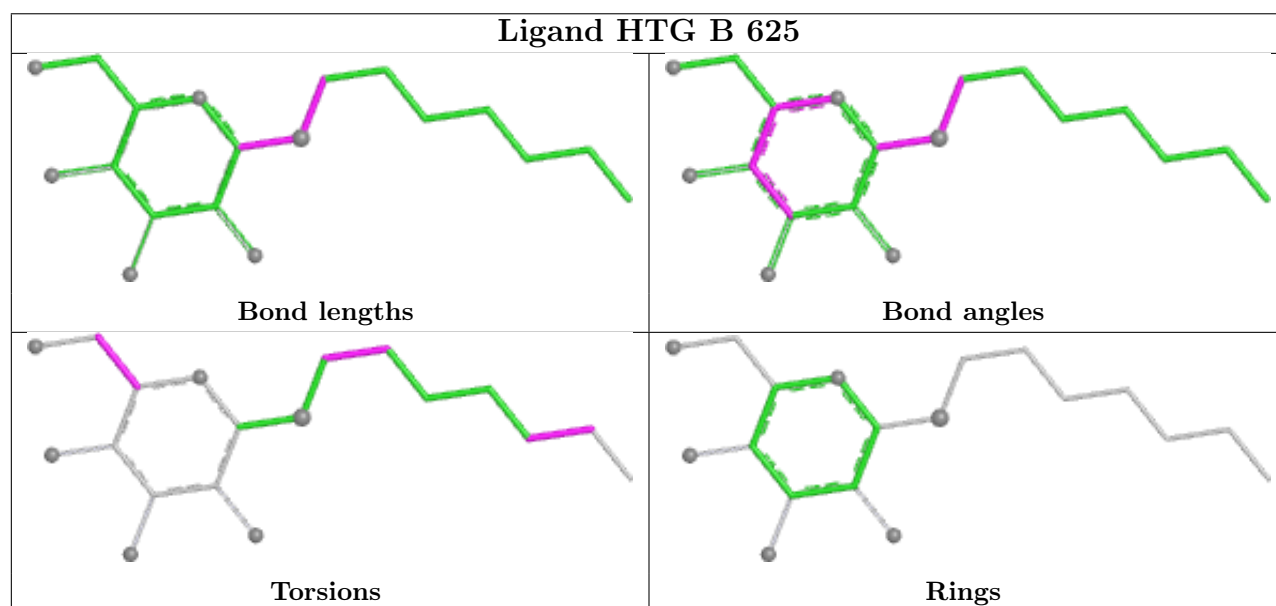
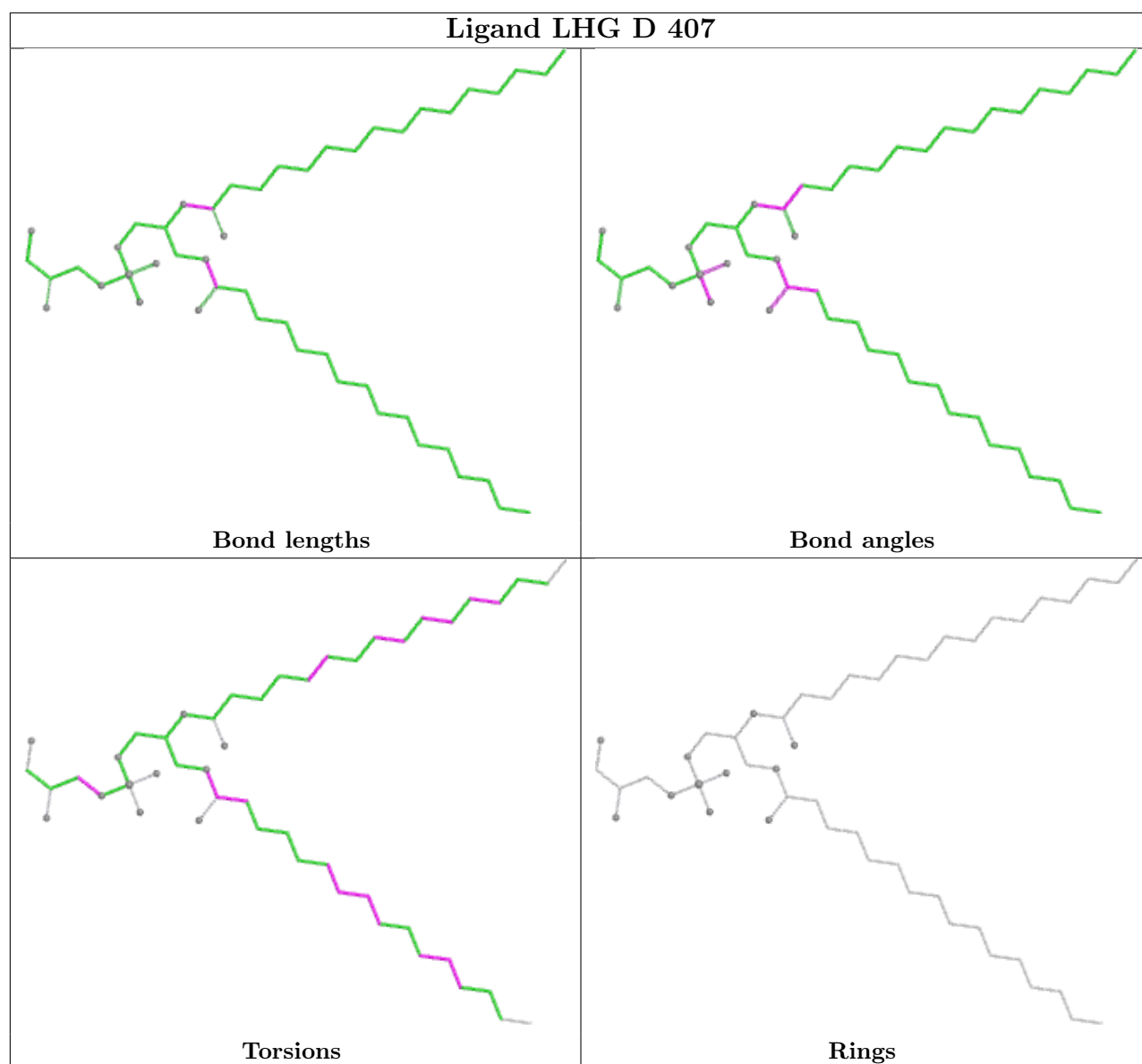


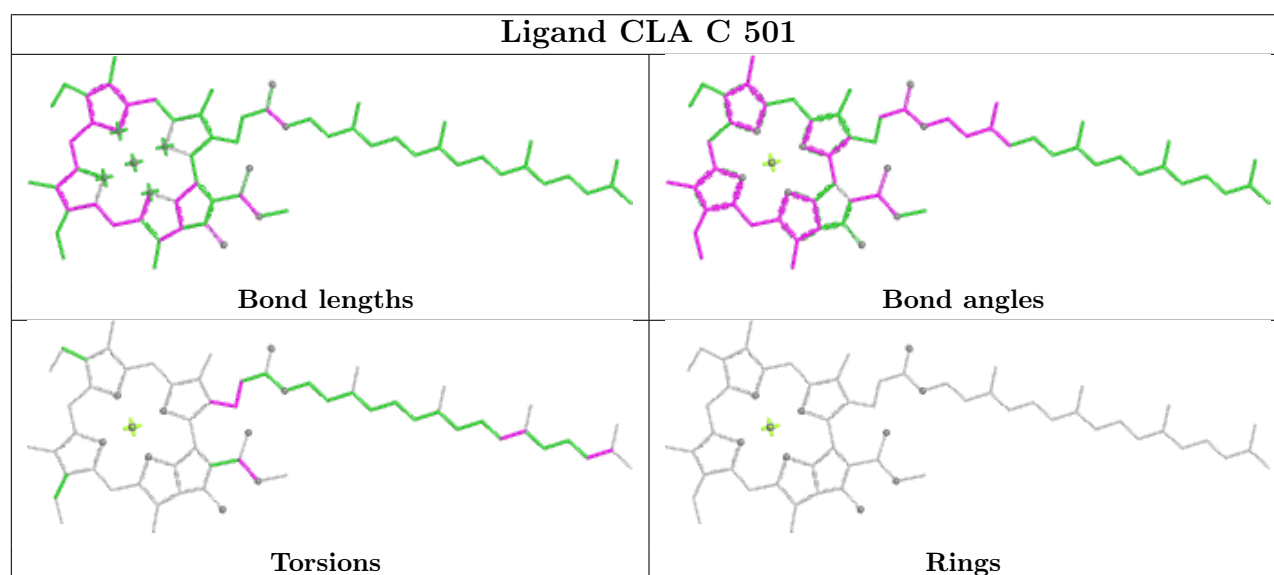
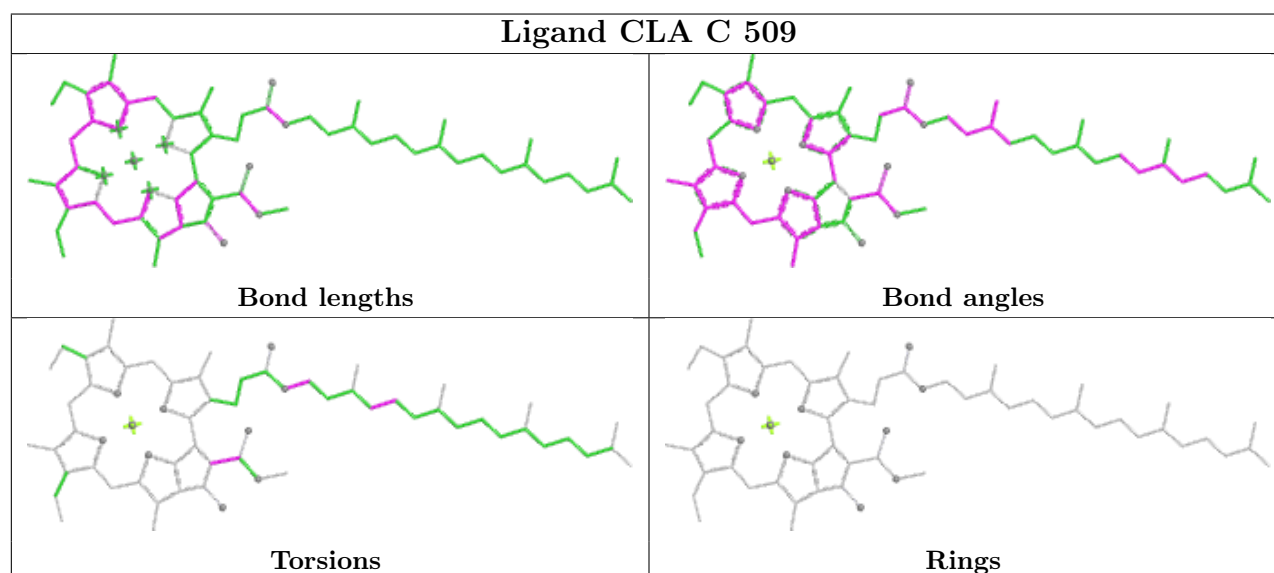
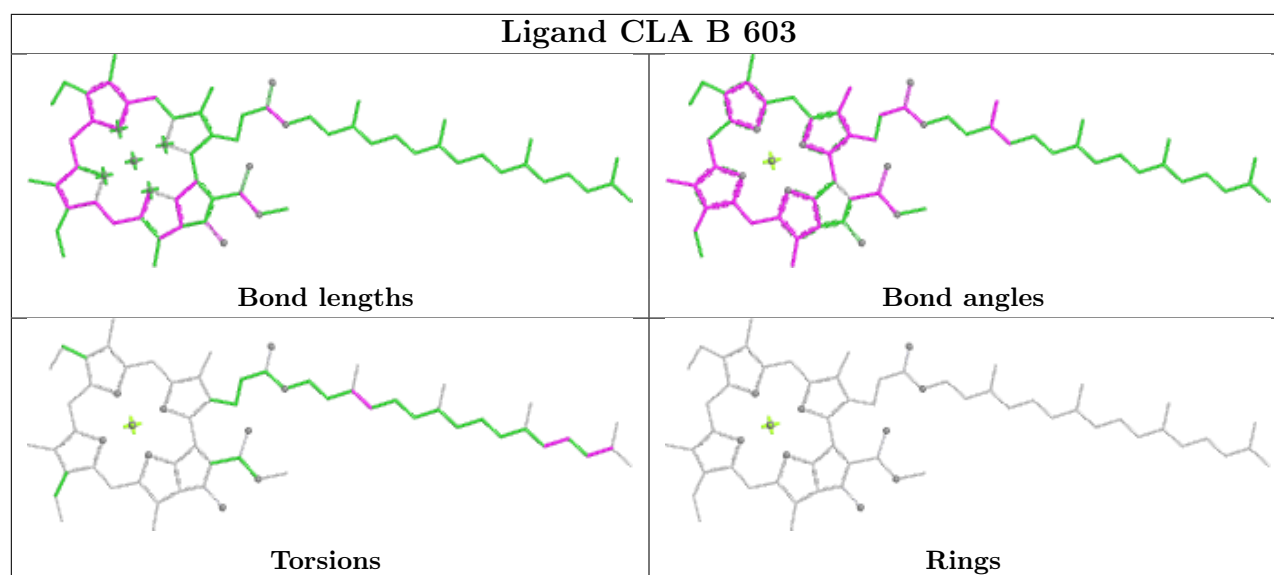


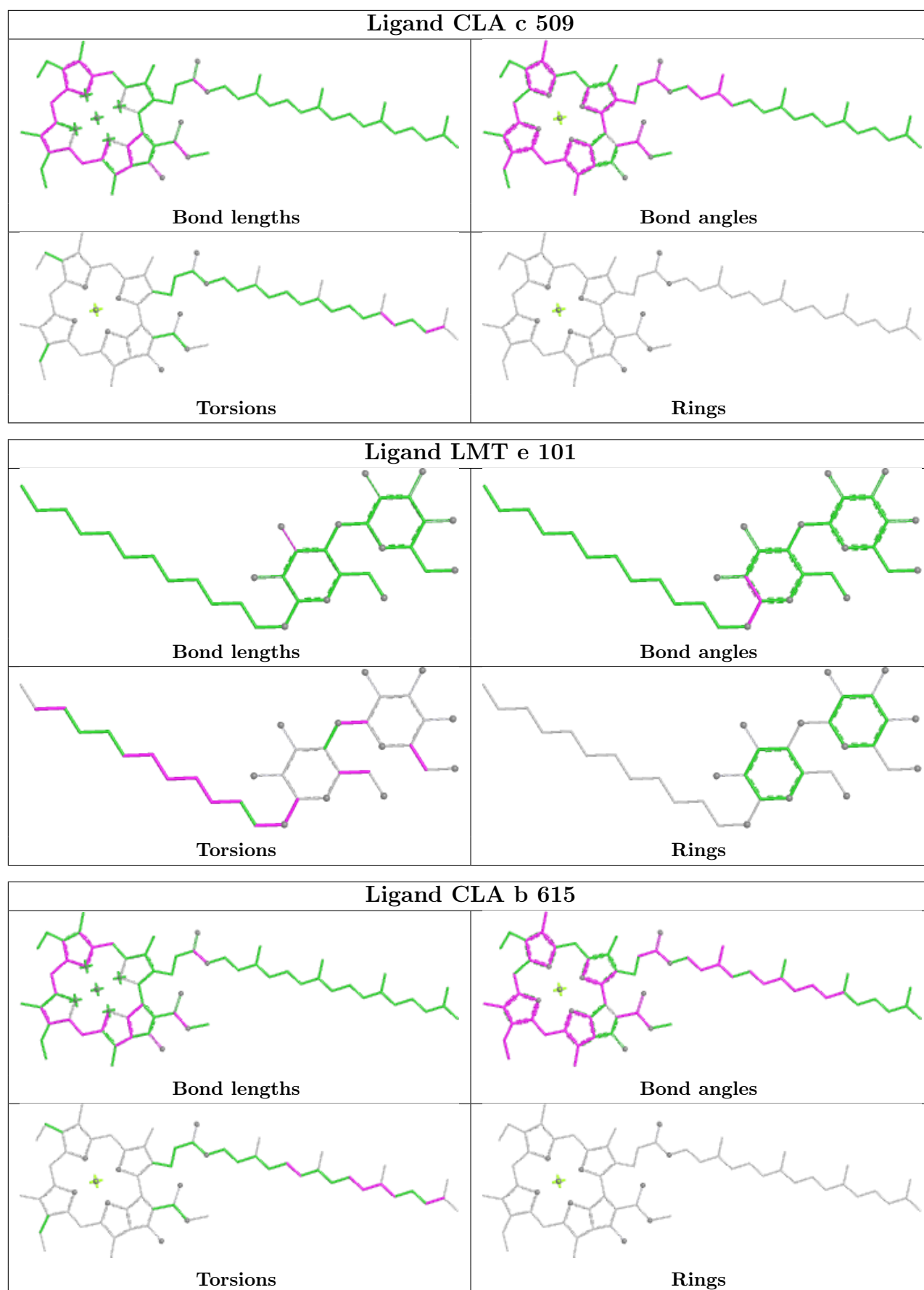


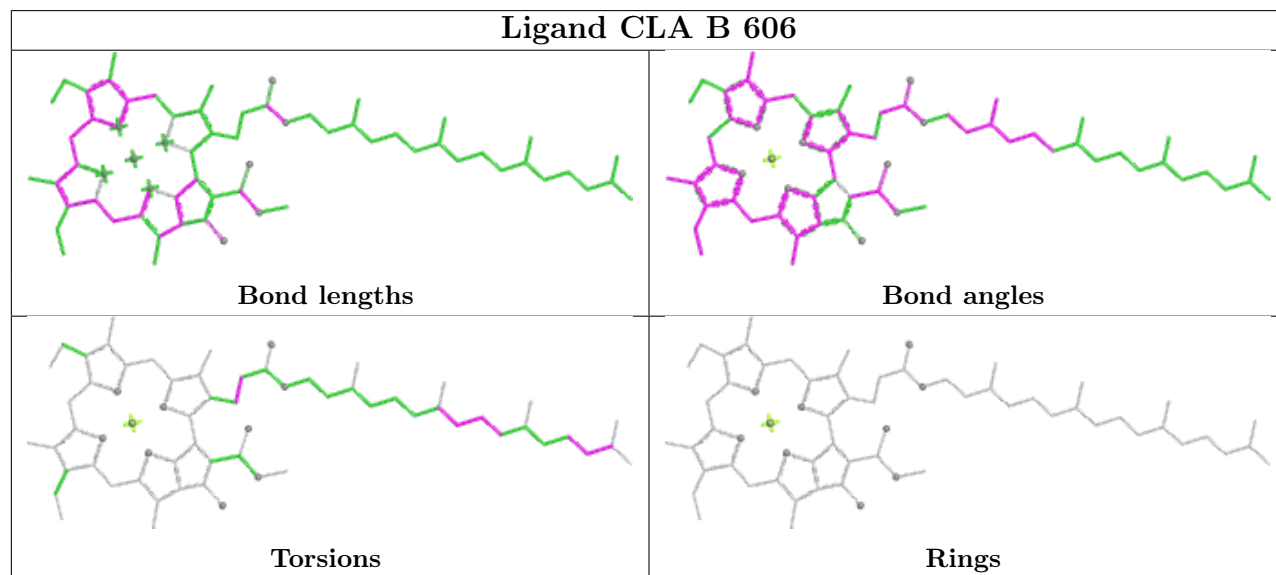
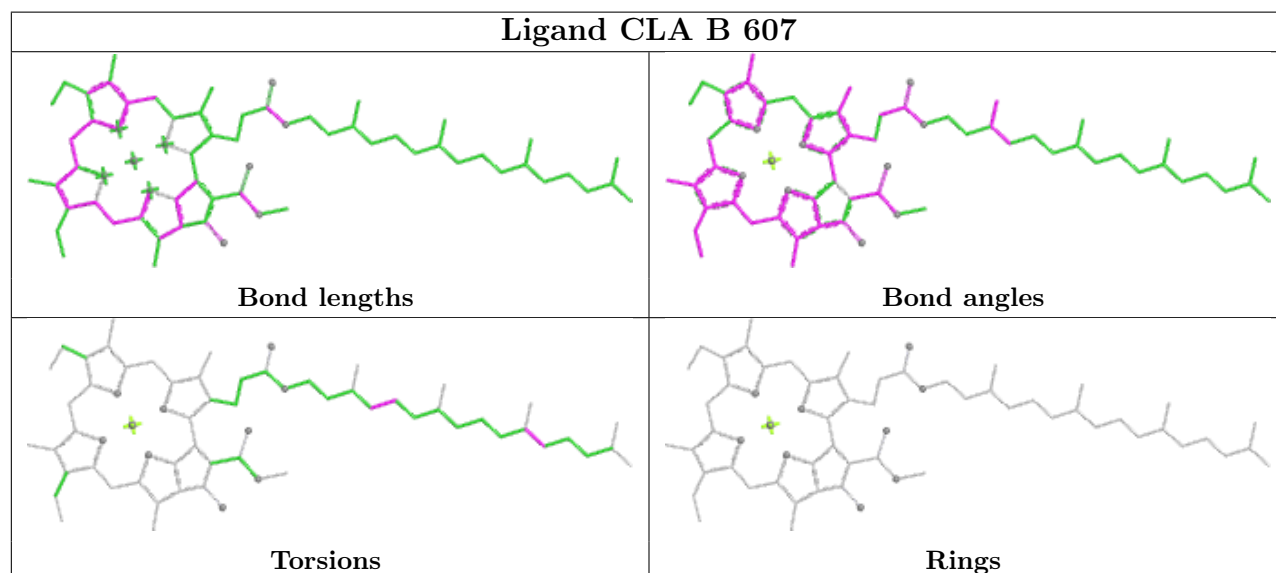
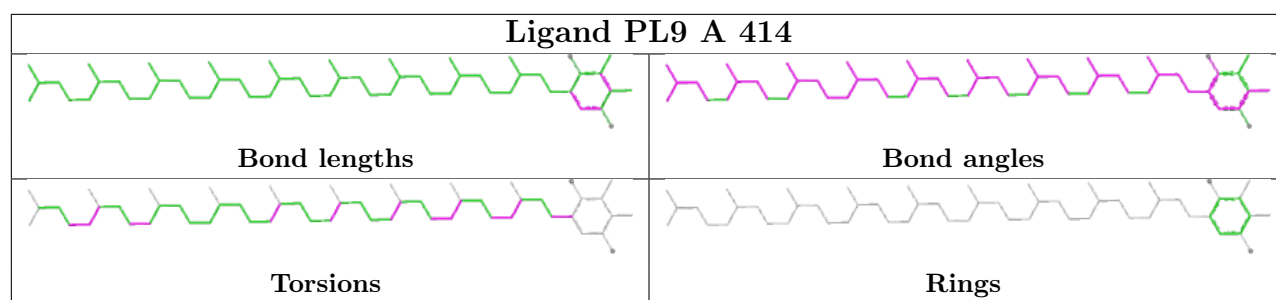


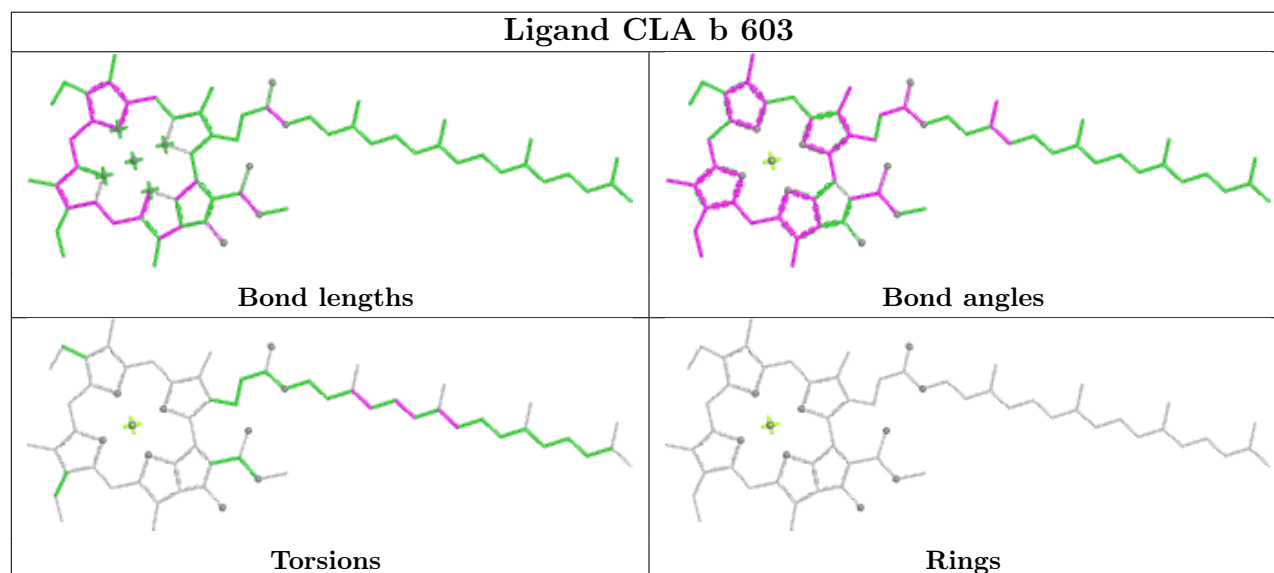
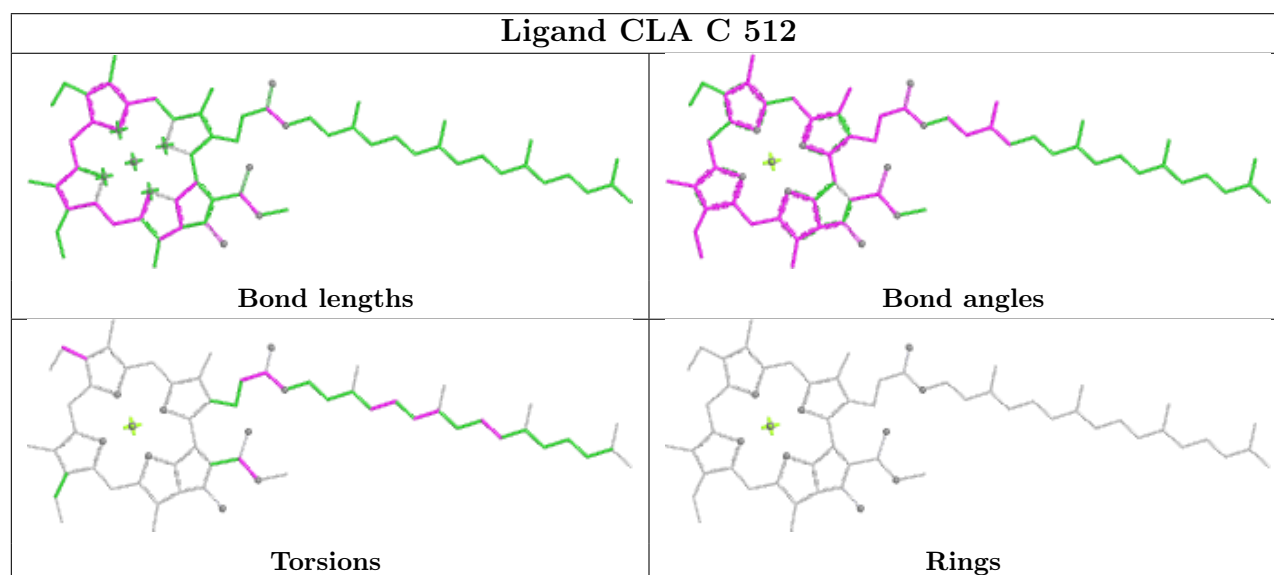
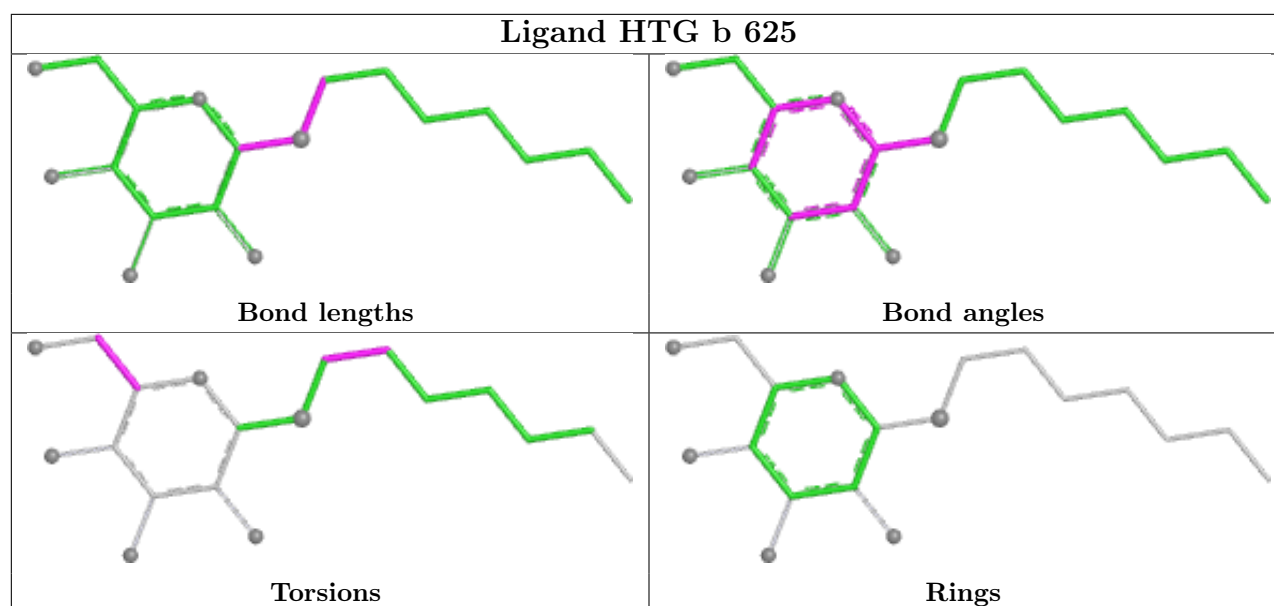


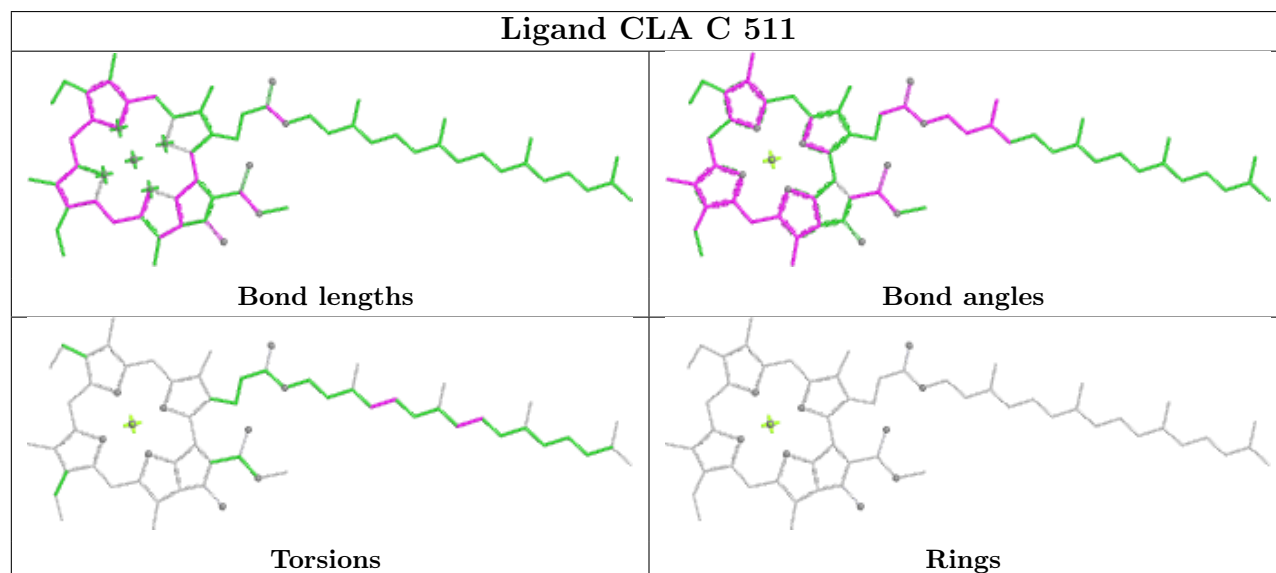
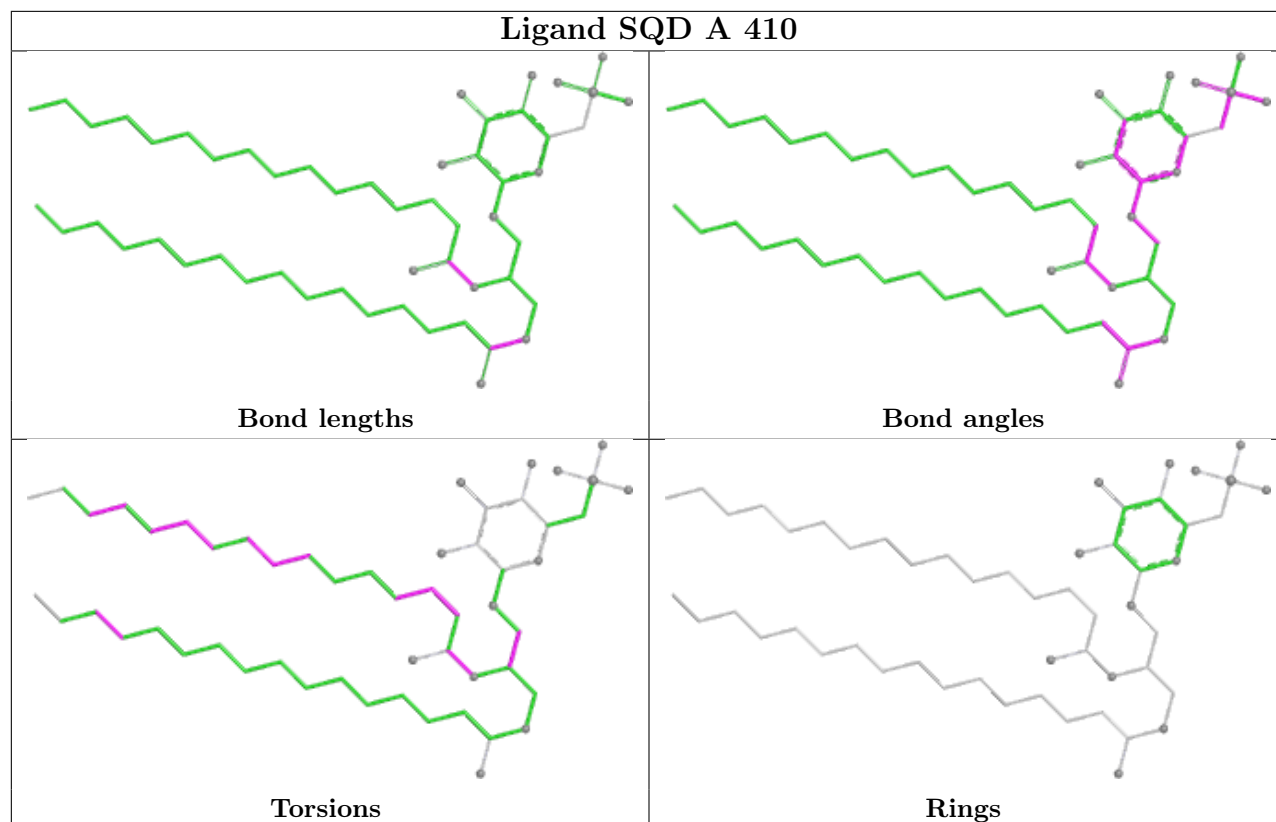


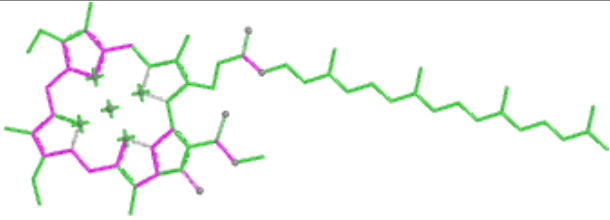
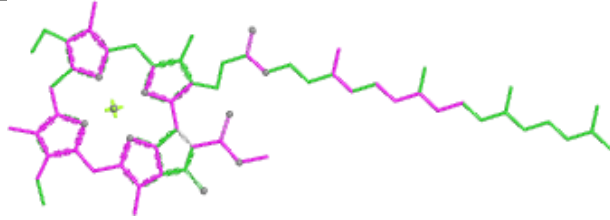
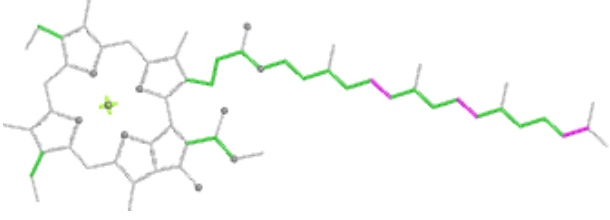
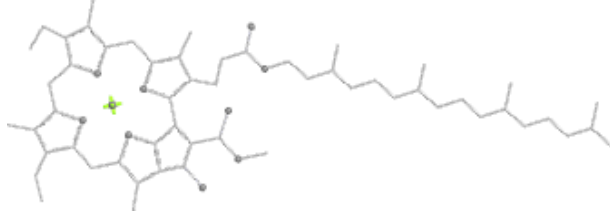


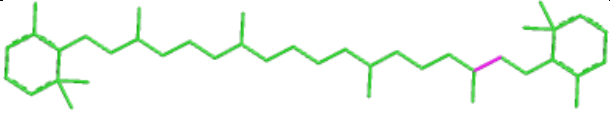
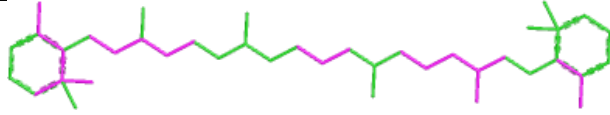
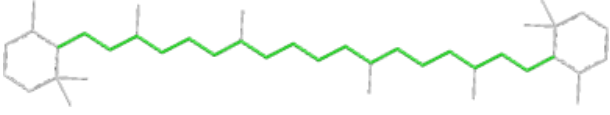
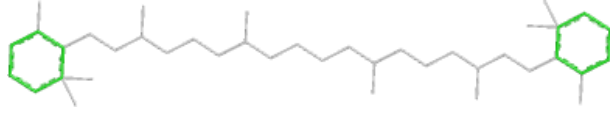


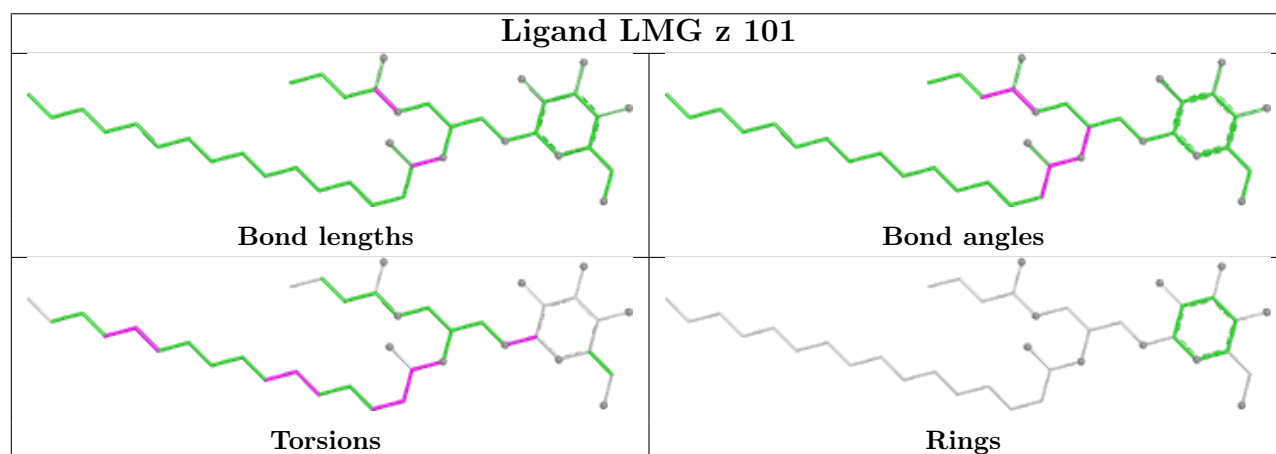
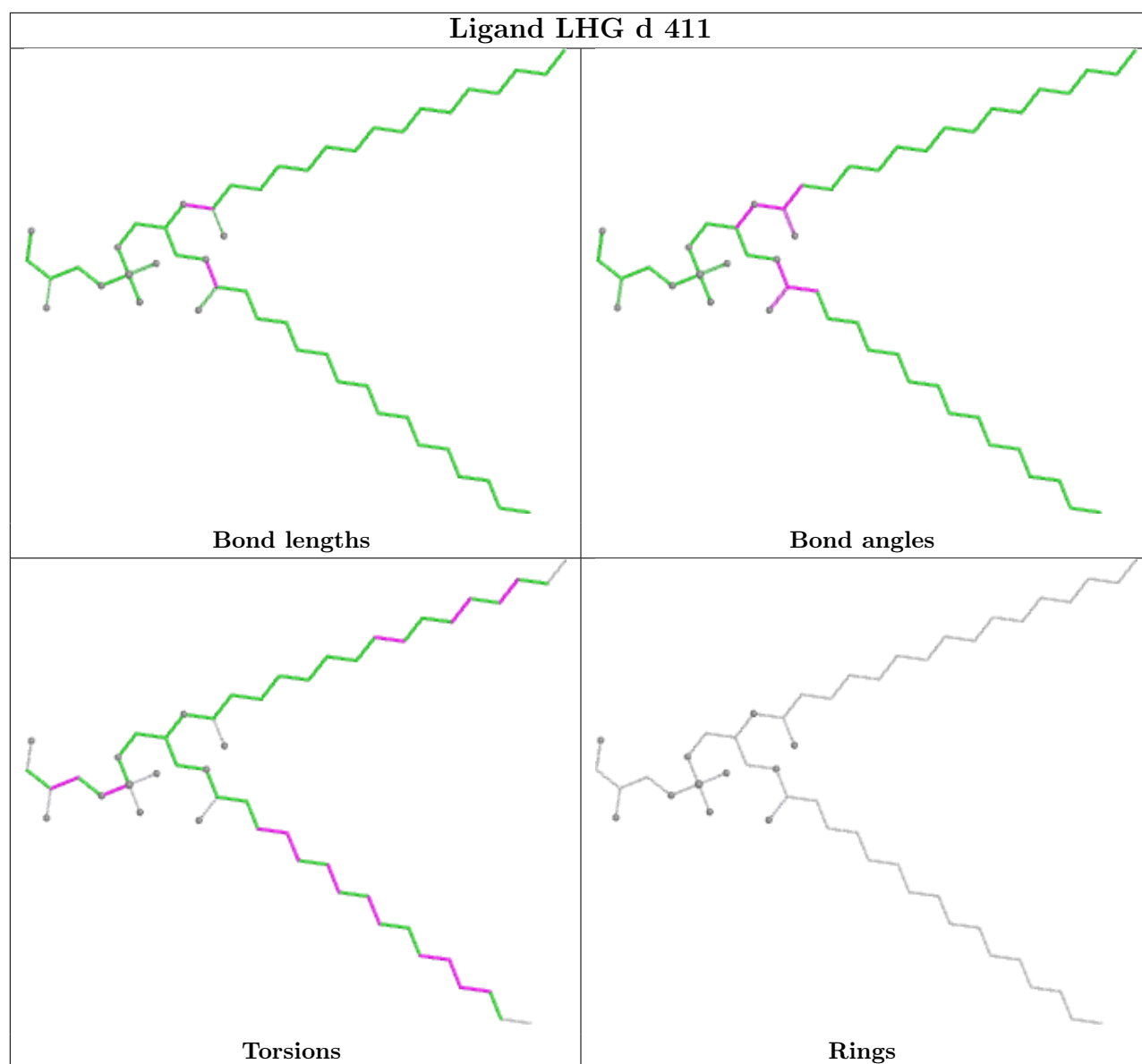


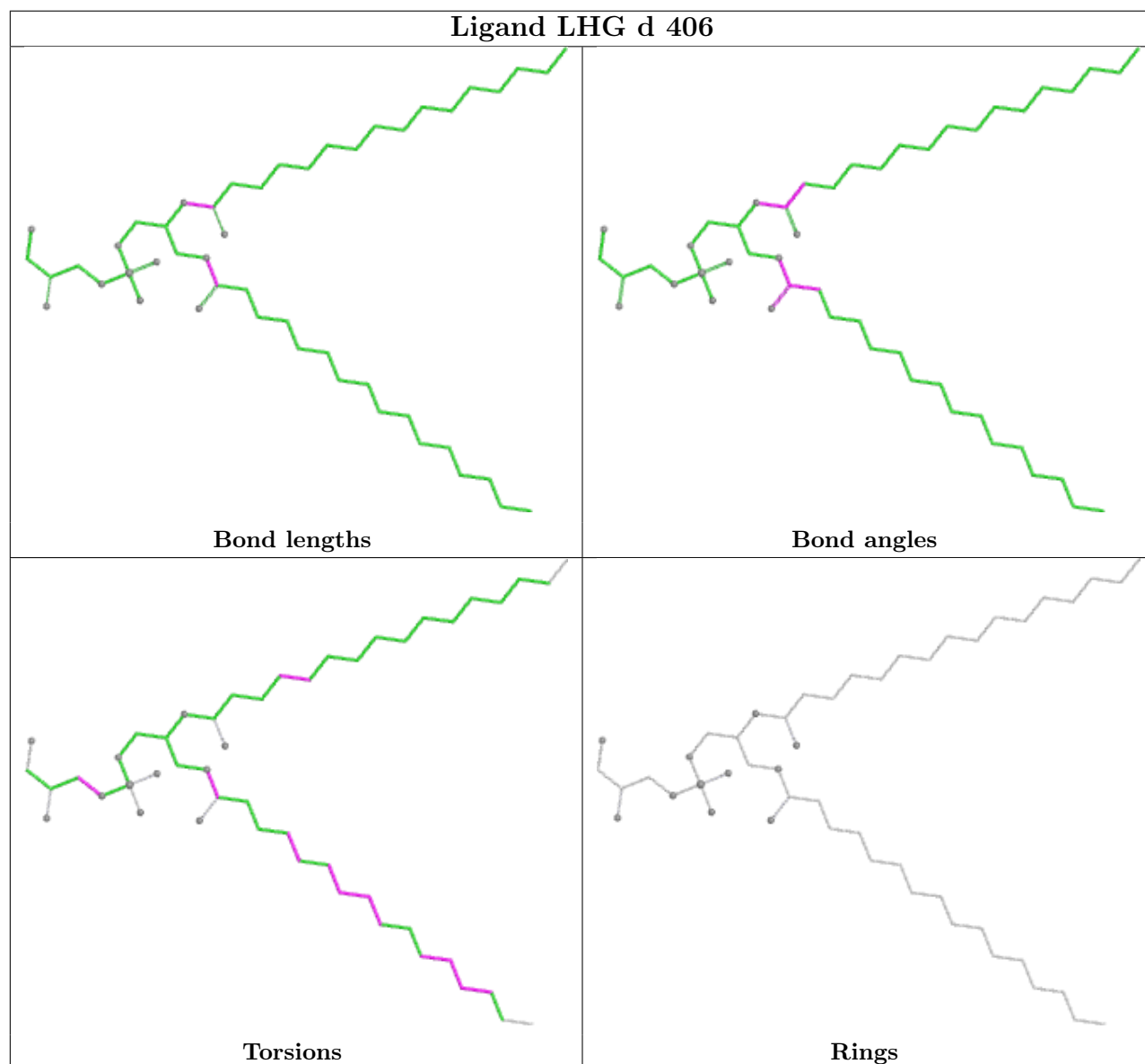
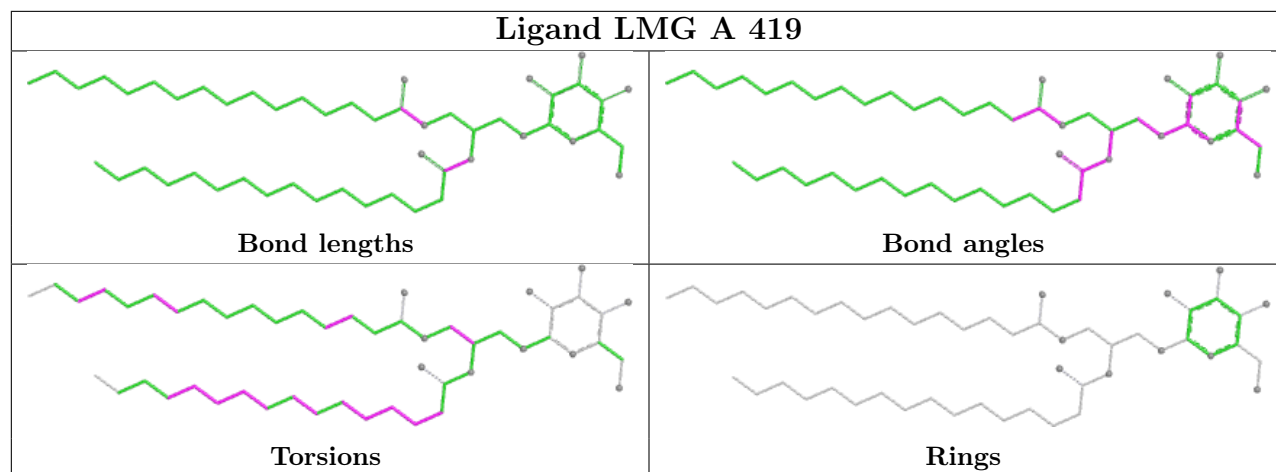


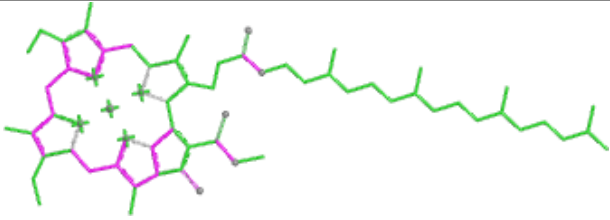
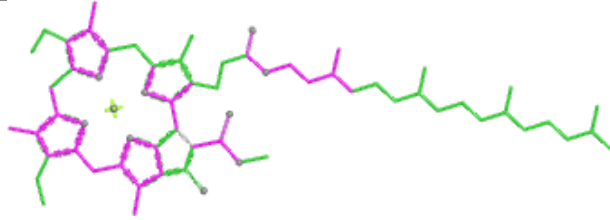
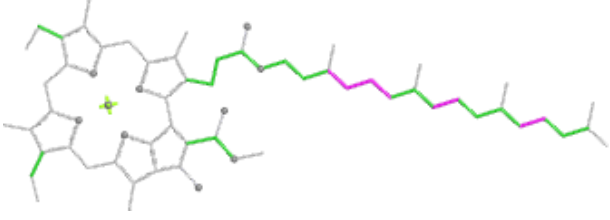
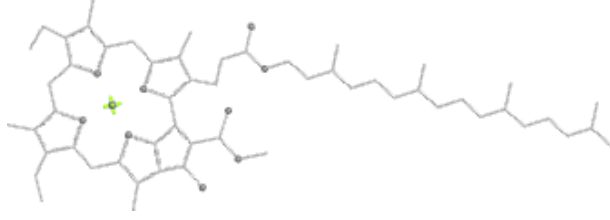
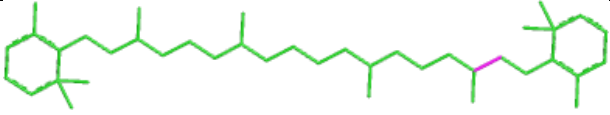
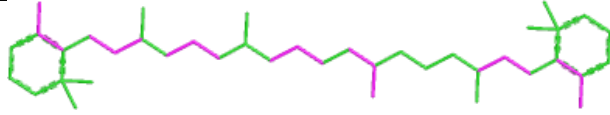
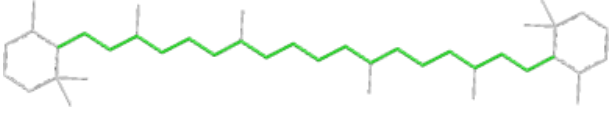
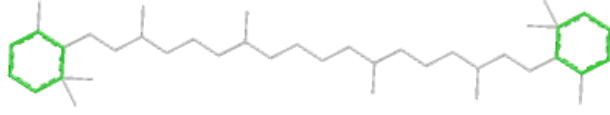
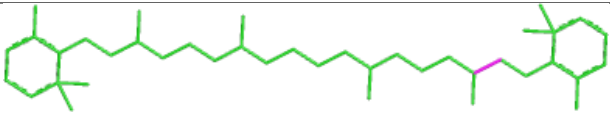
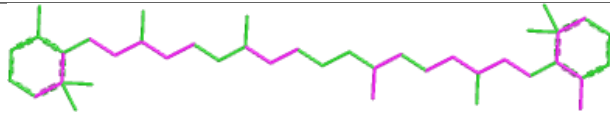
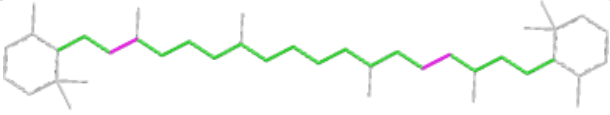
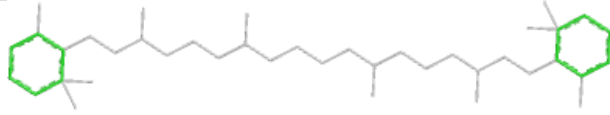


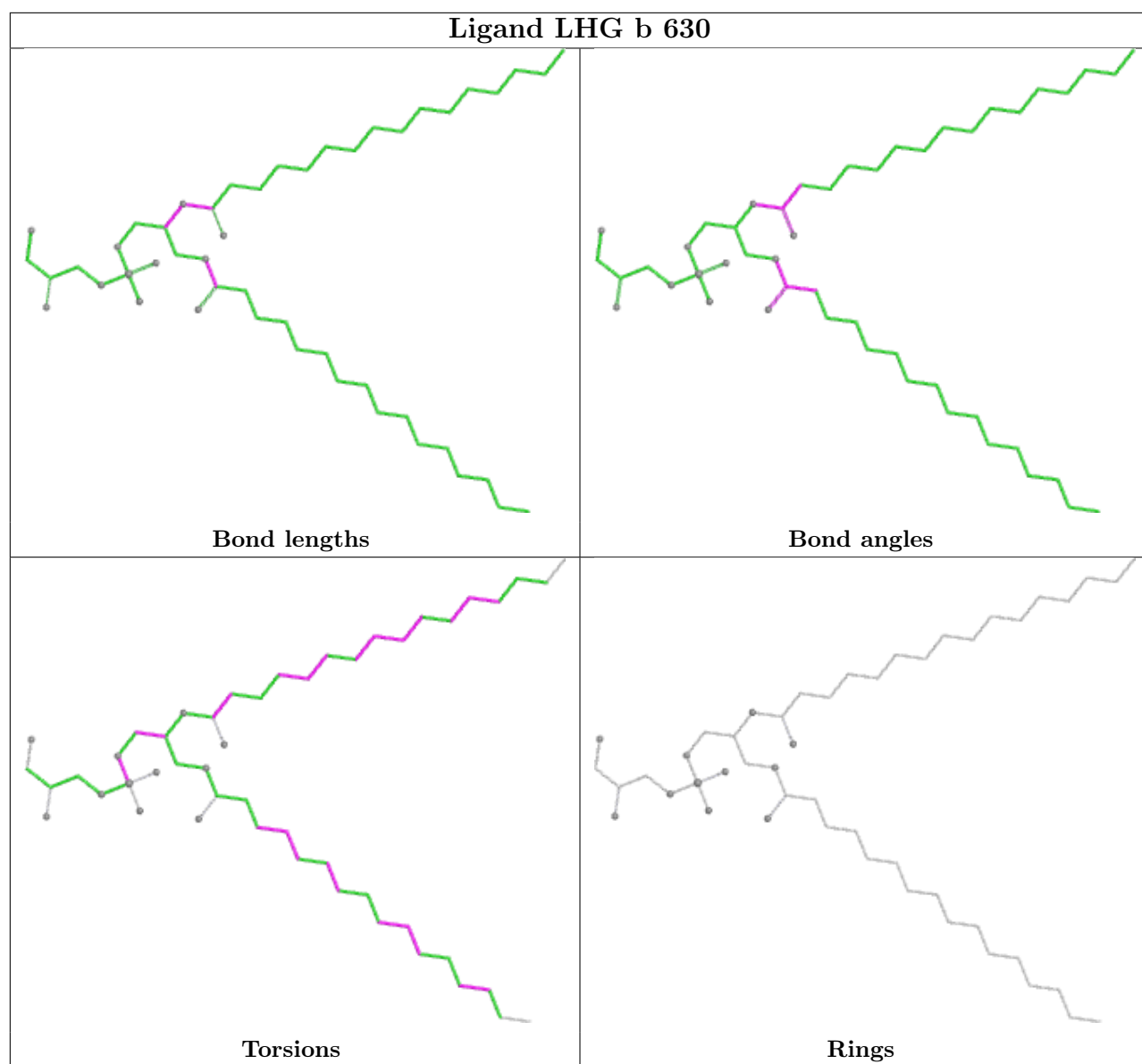
Ligand CLA B 615			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

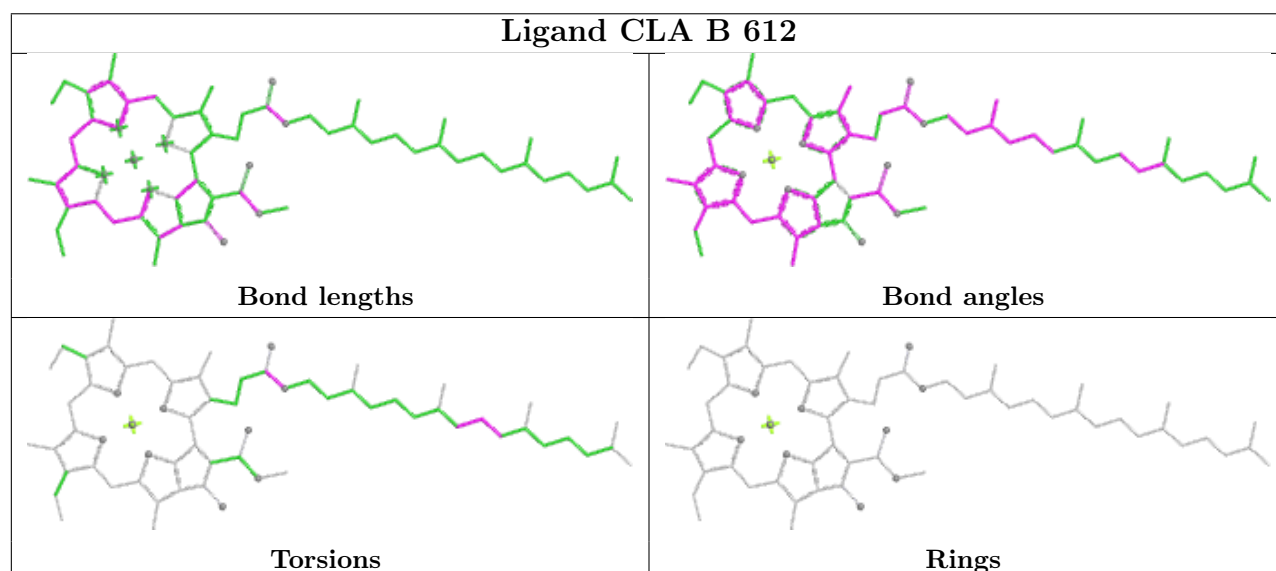
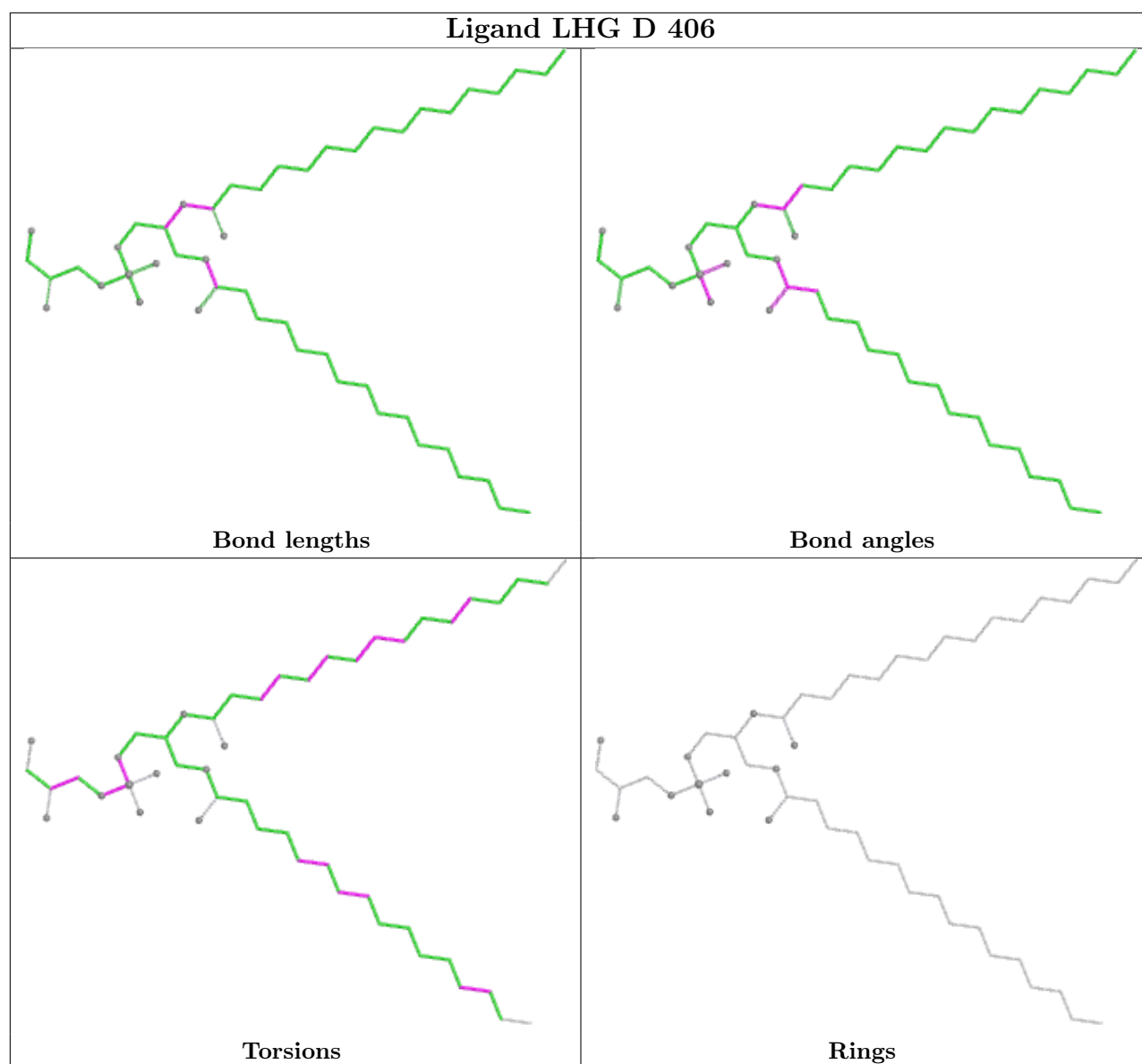
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Bond lengths	Bond angles		
			
Torsions	Rings		

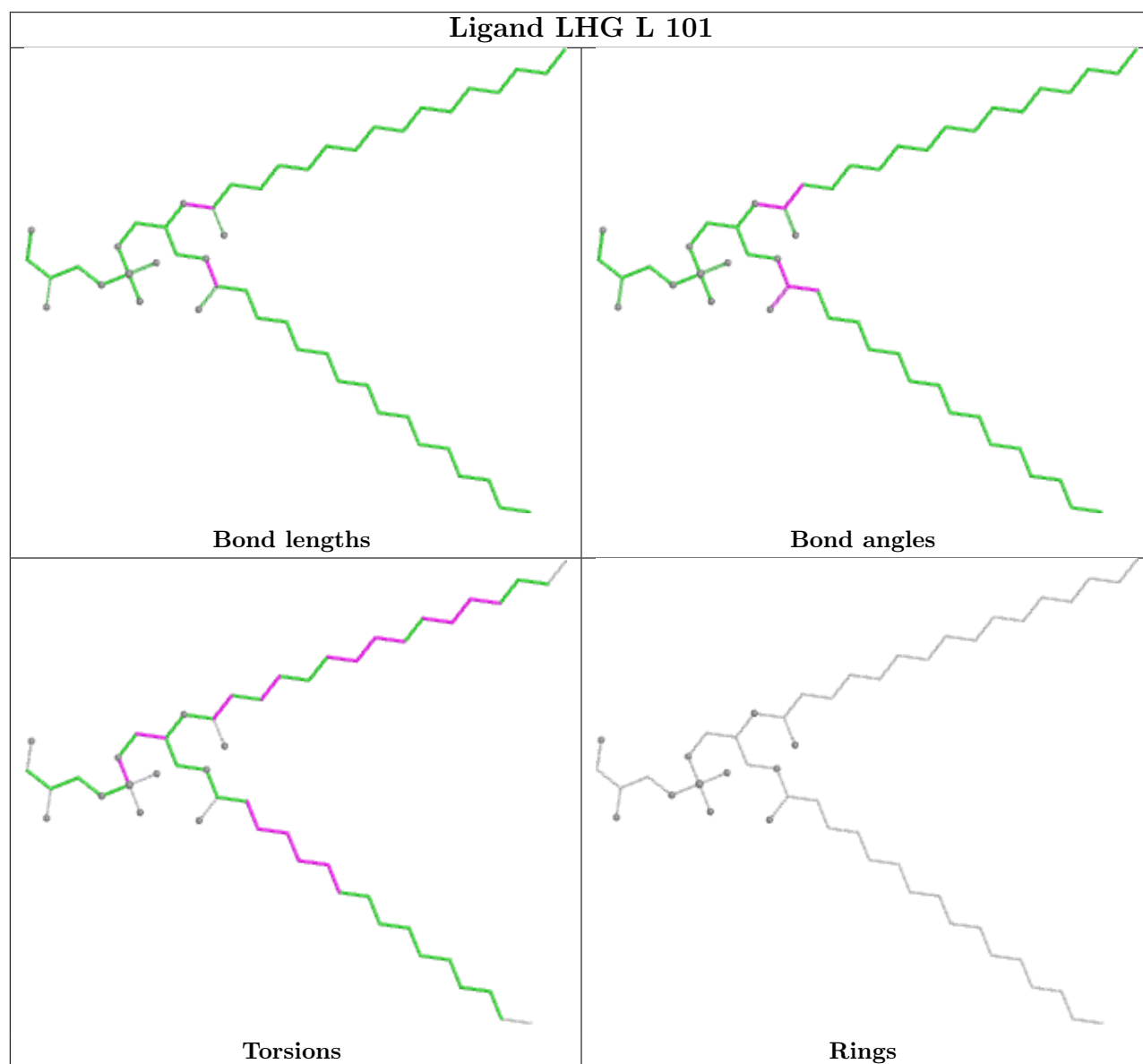
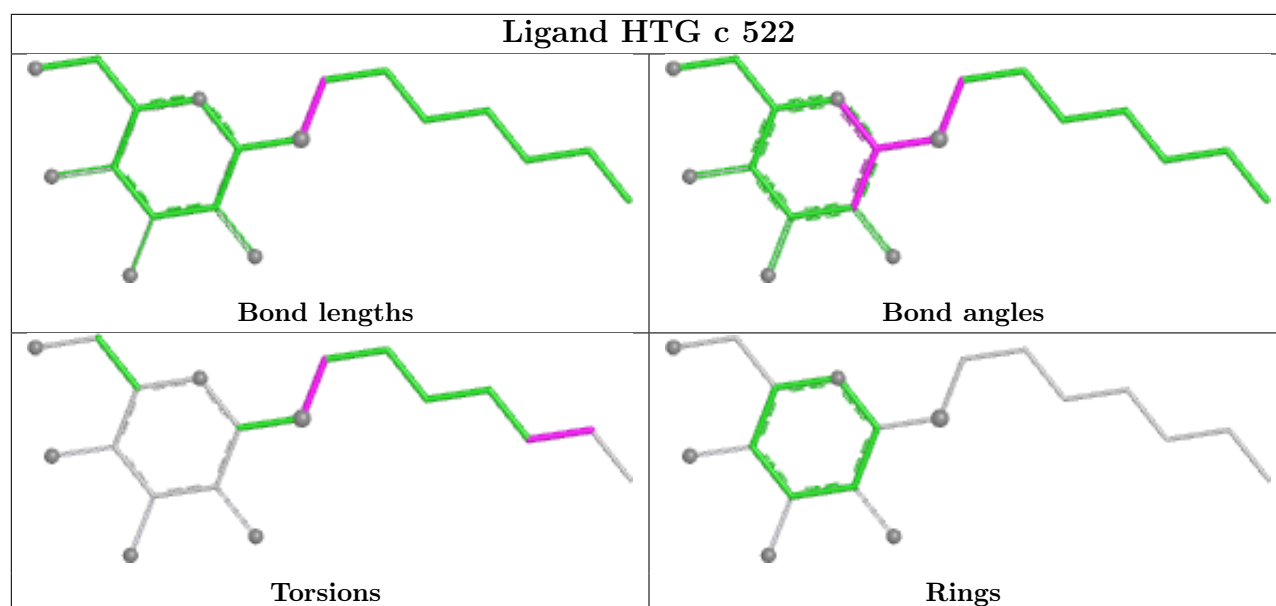


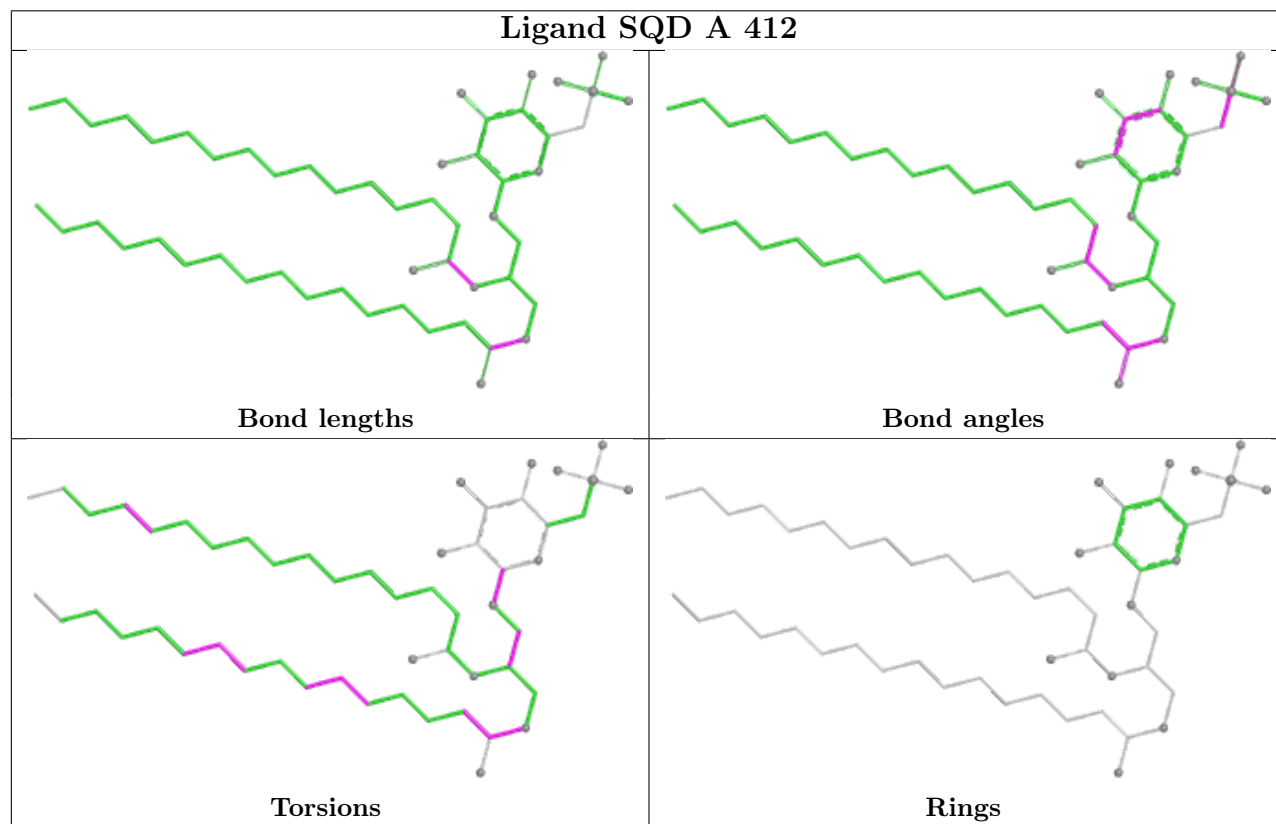
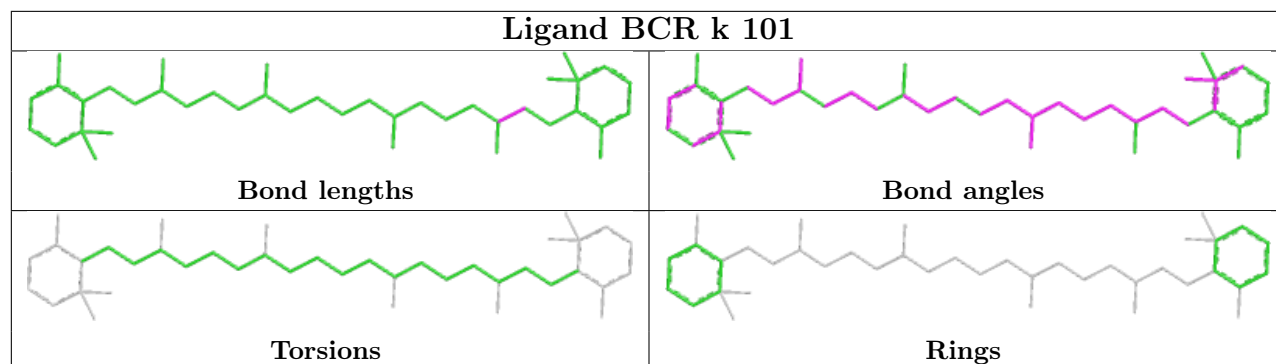


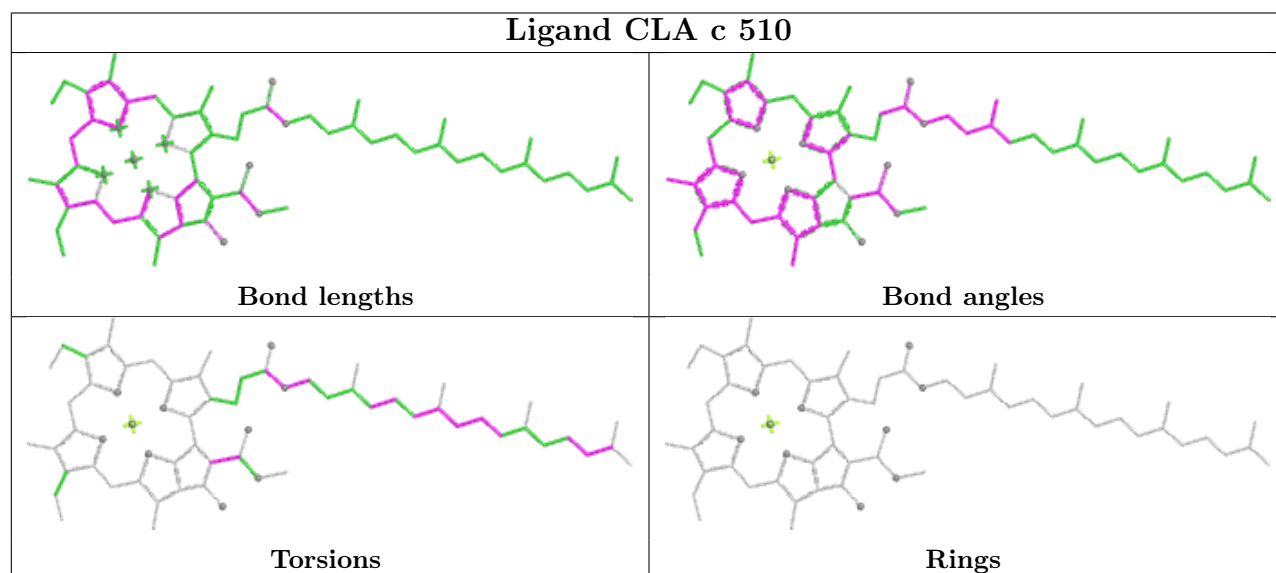
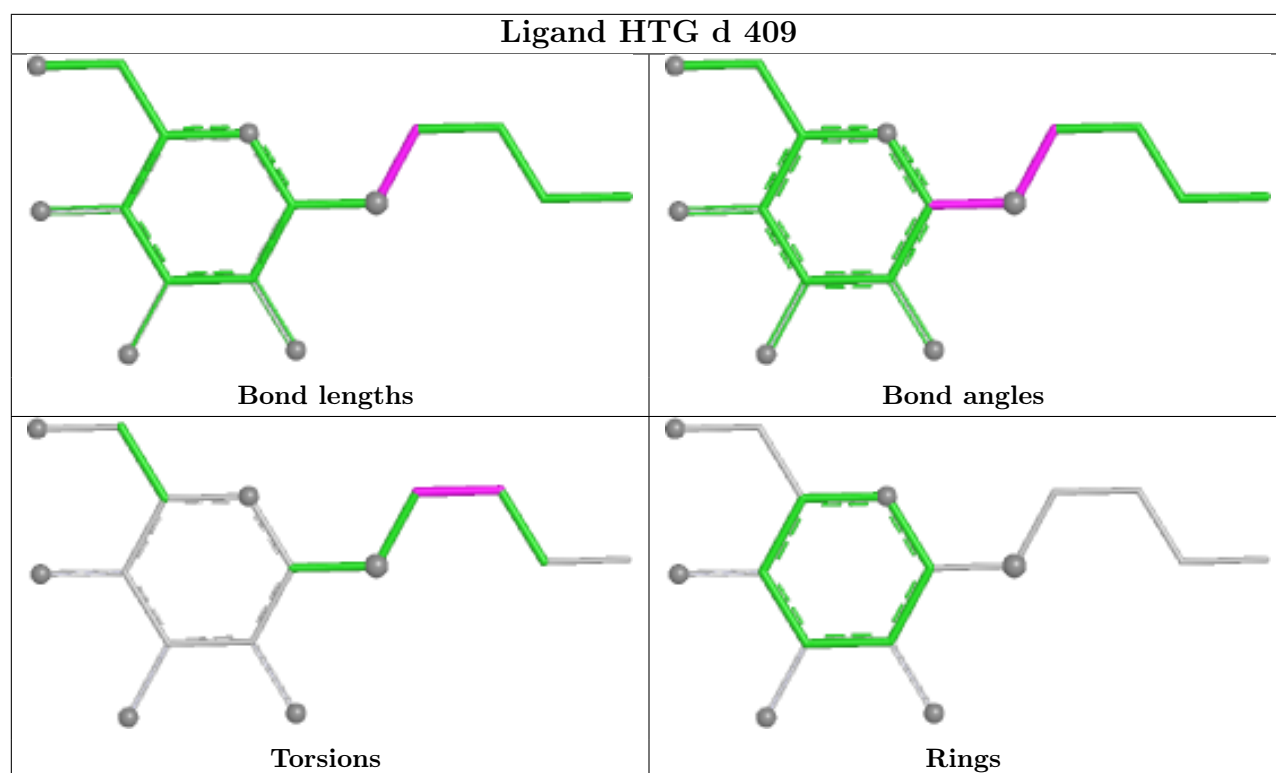
Ligand CLA b 605	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR h 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
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 Bond lengths	 Bond angles
 Torsions	 Rings

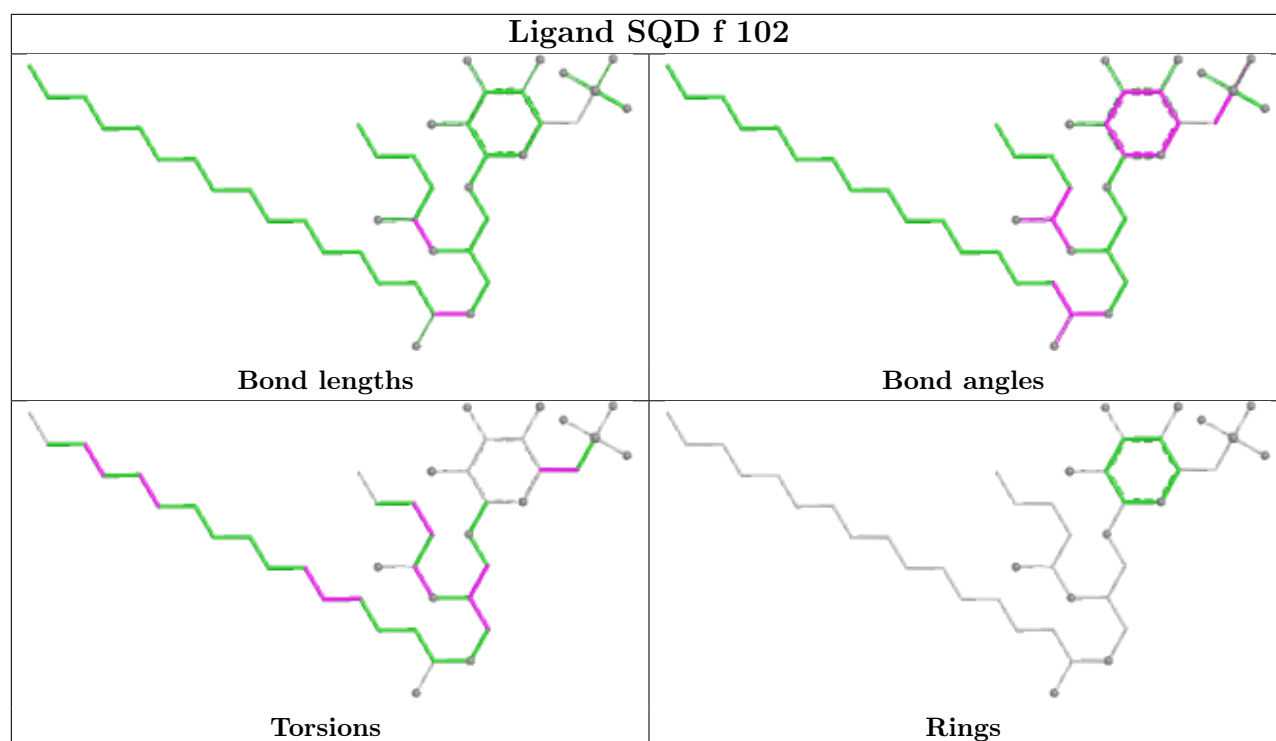
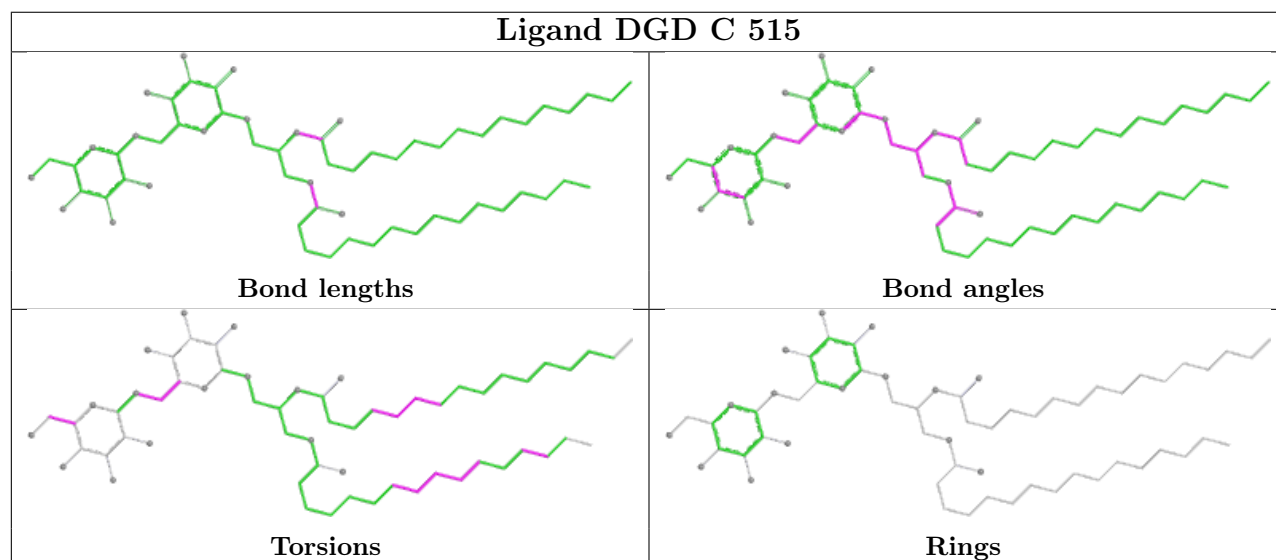
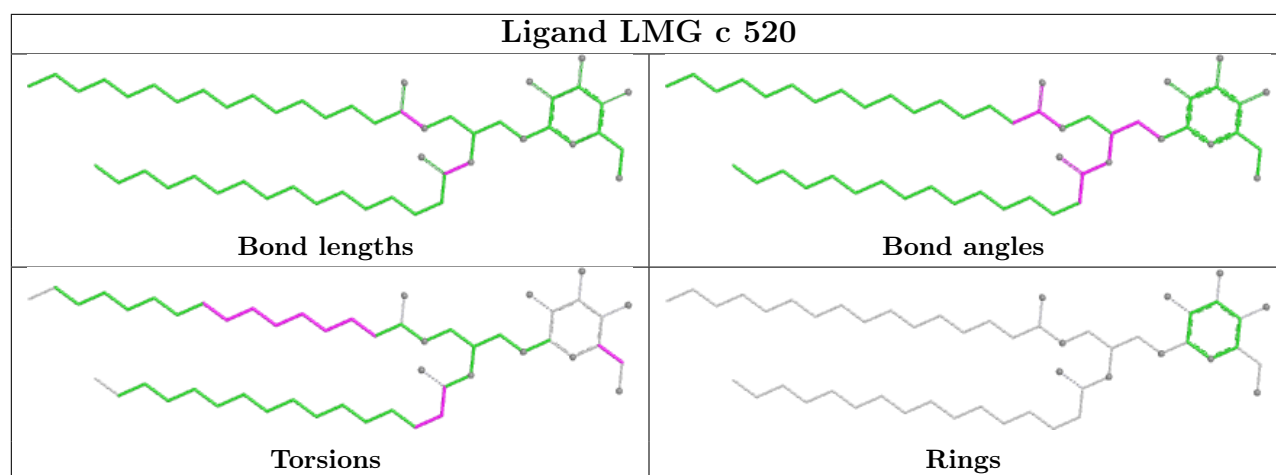


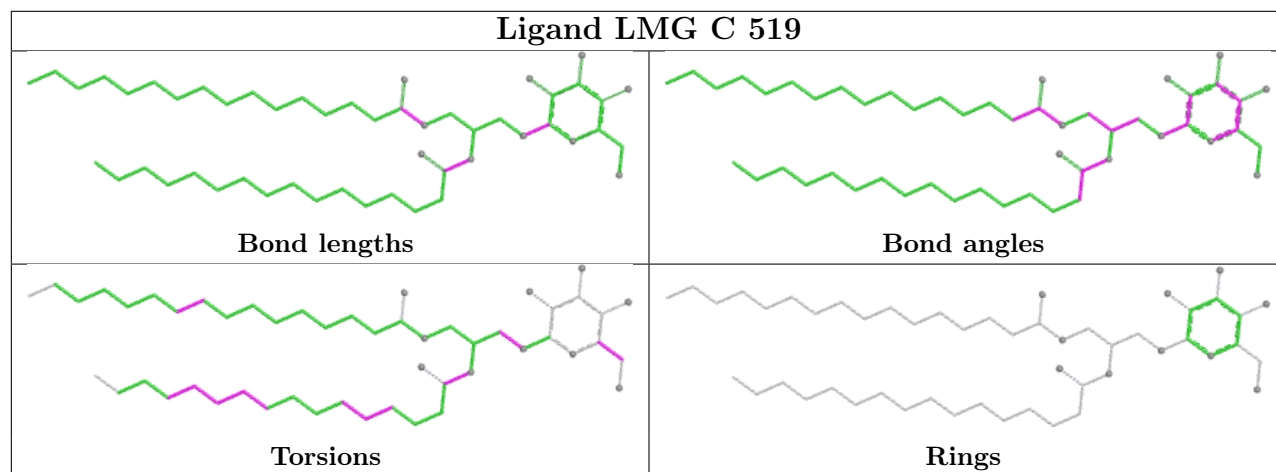
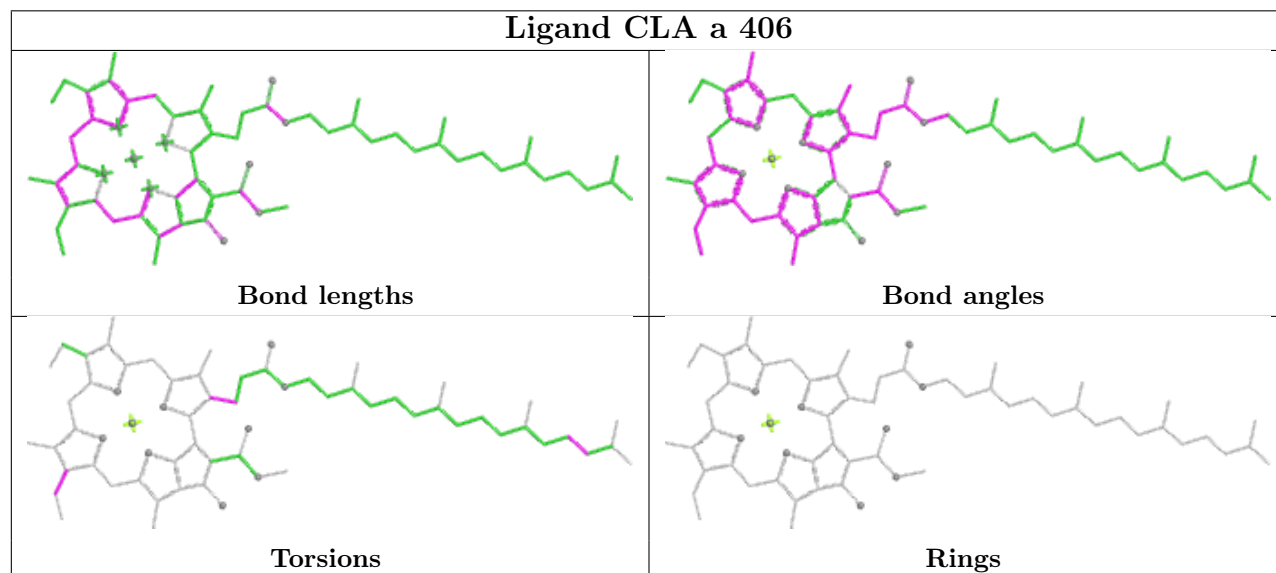
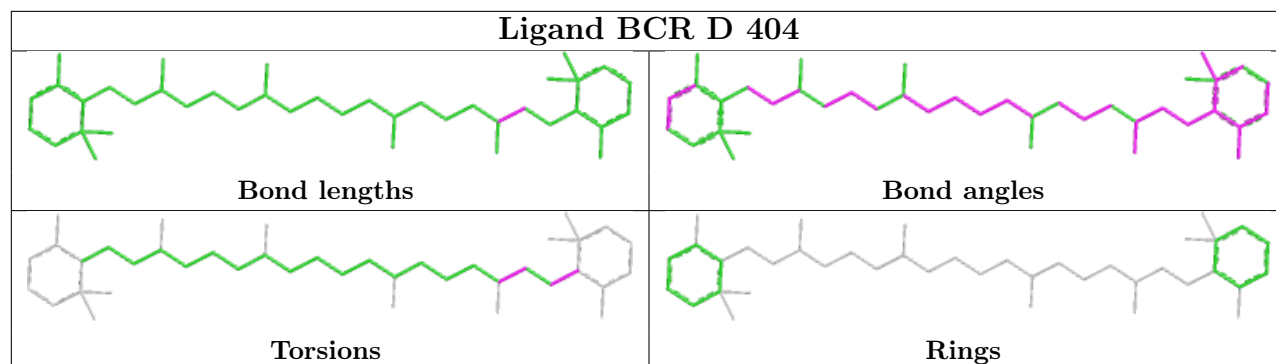


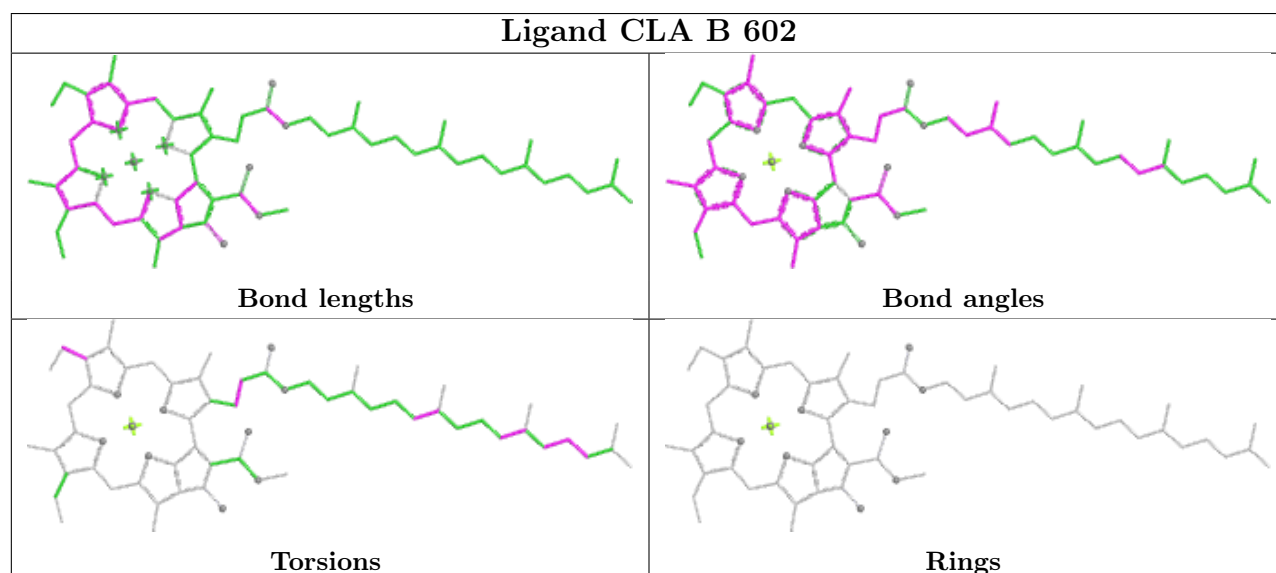
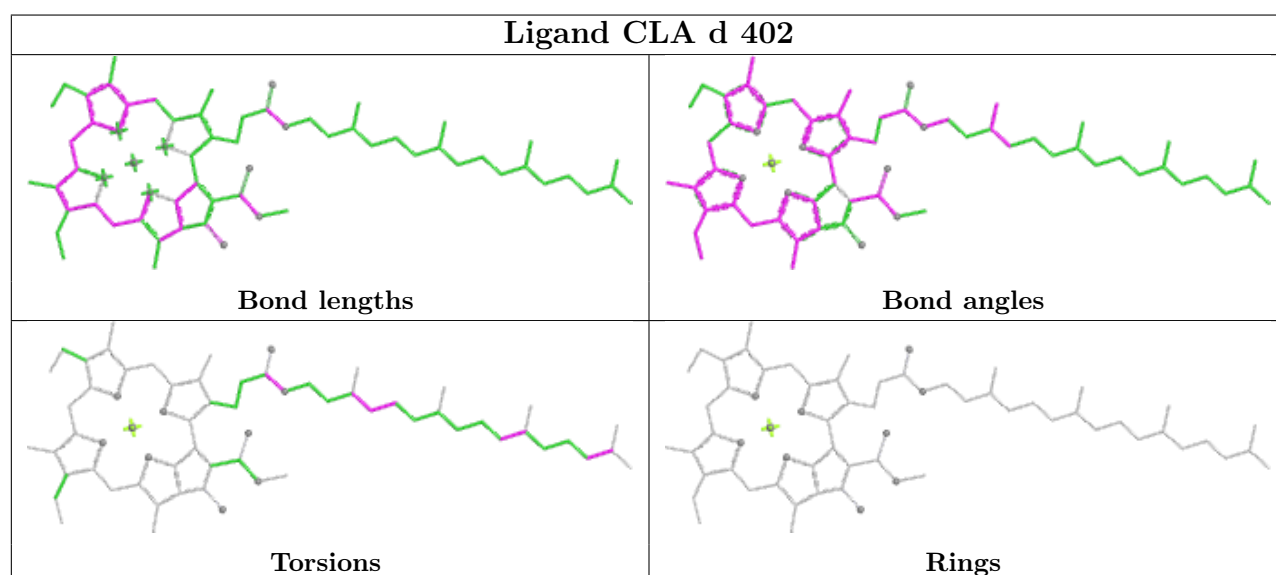
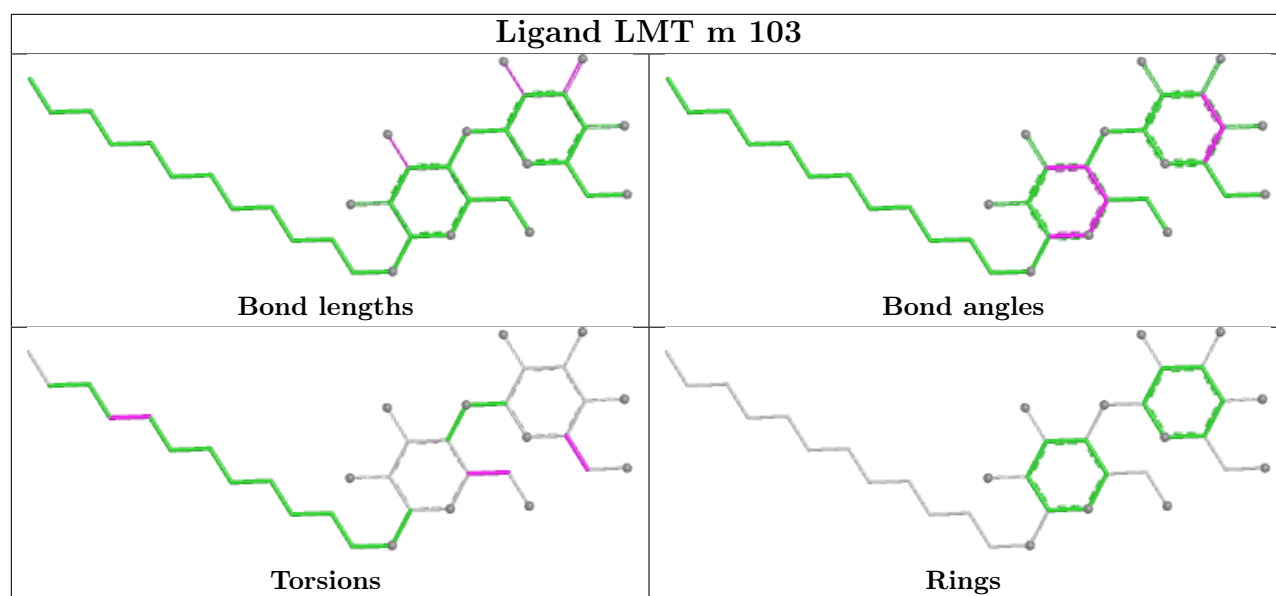


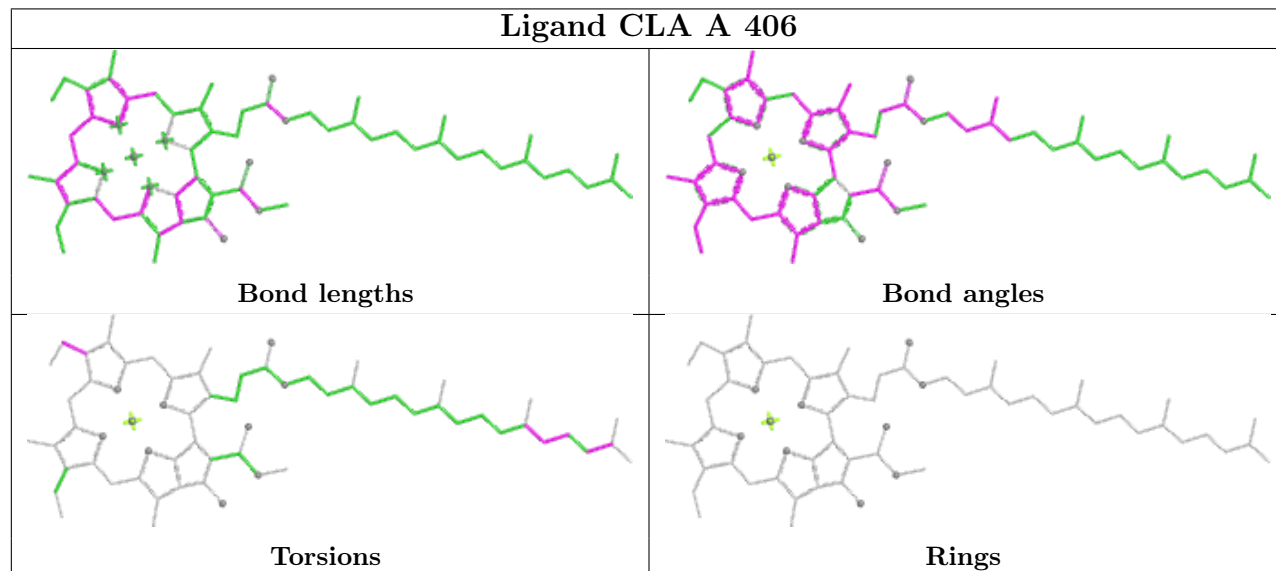
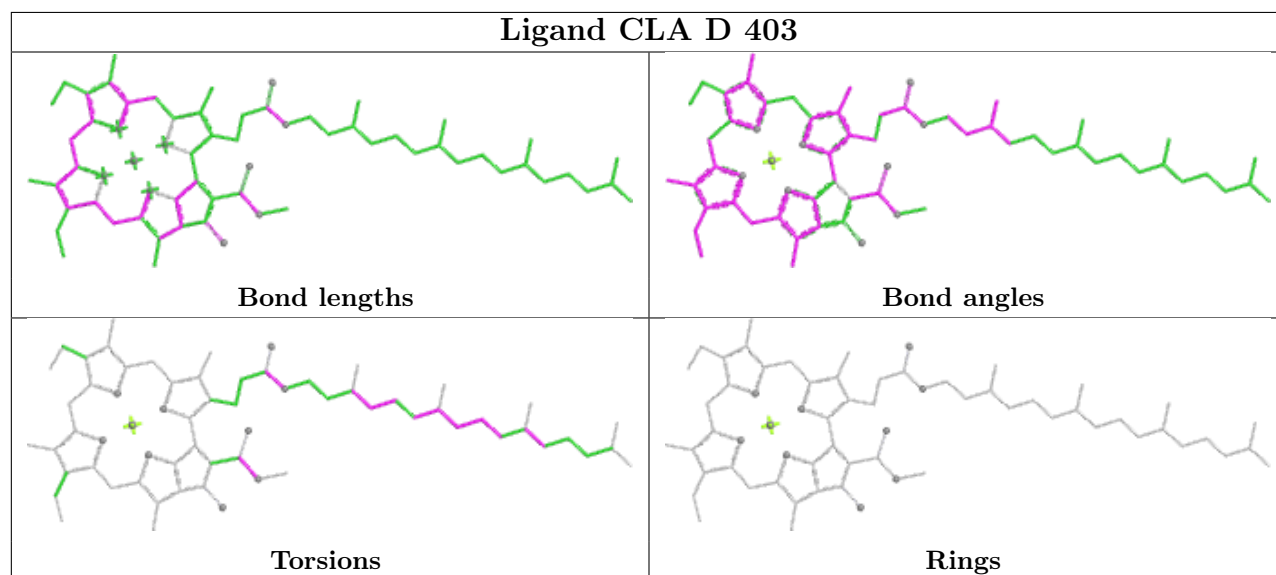
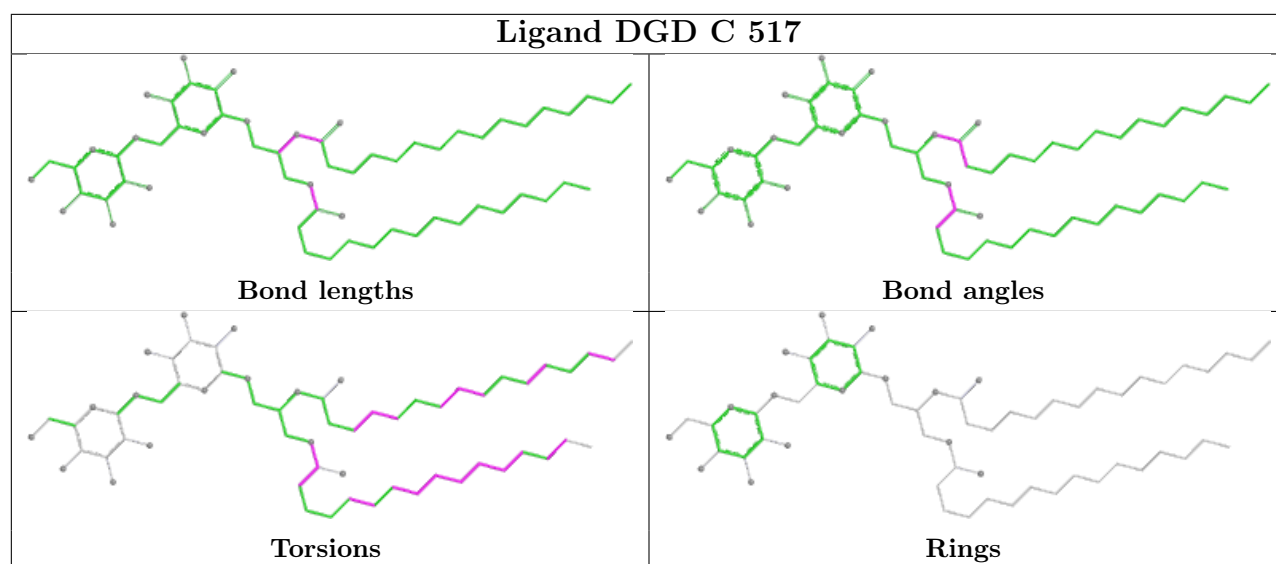


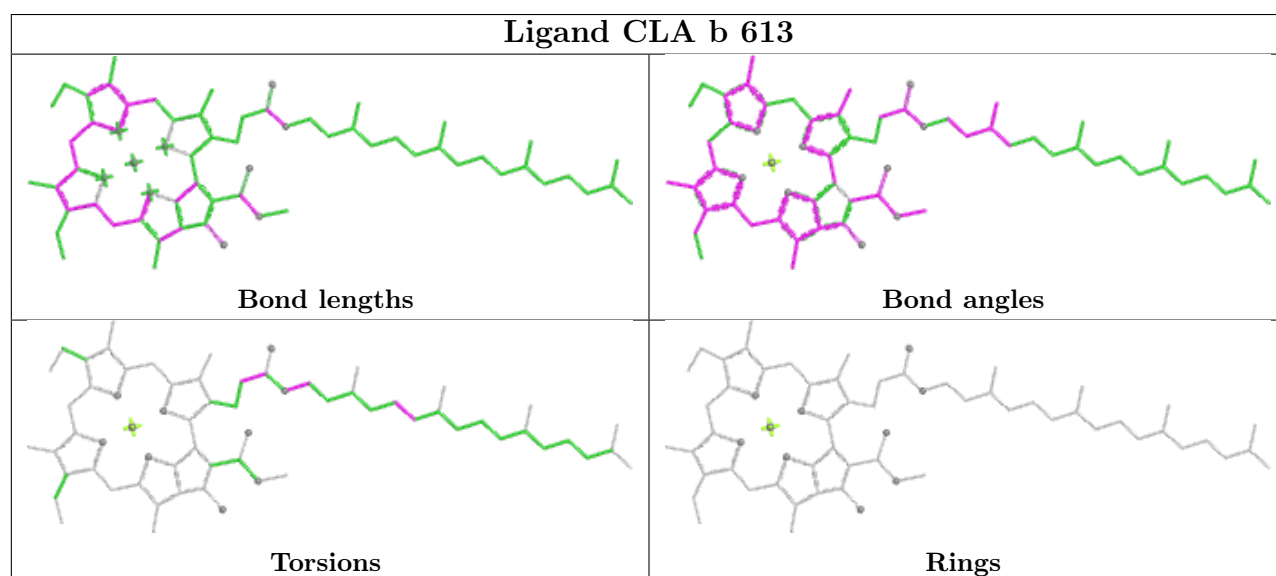
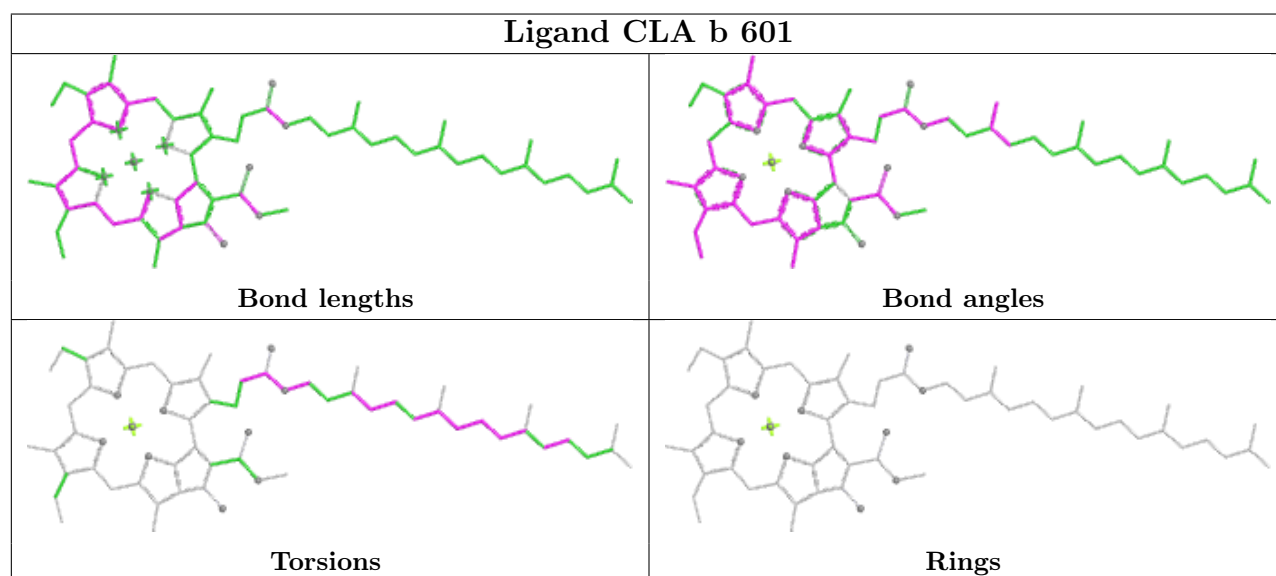
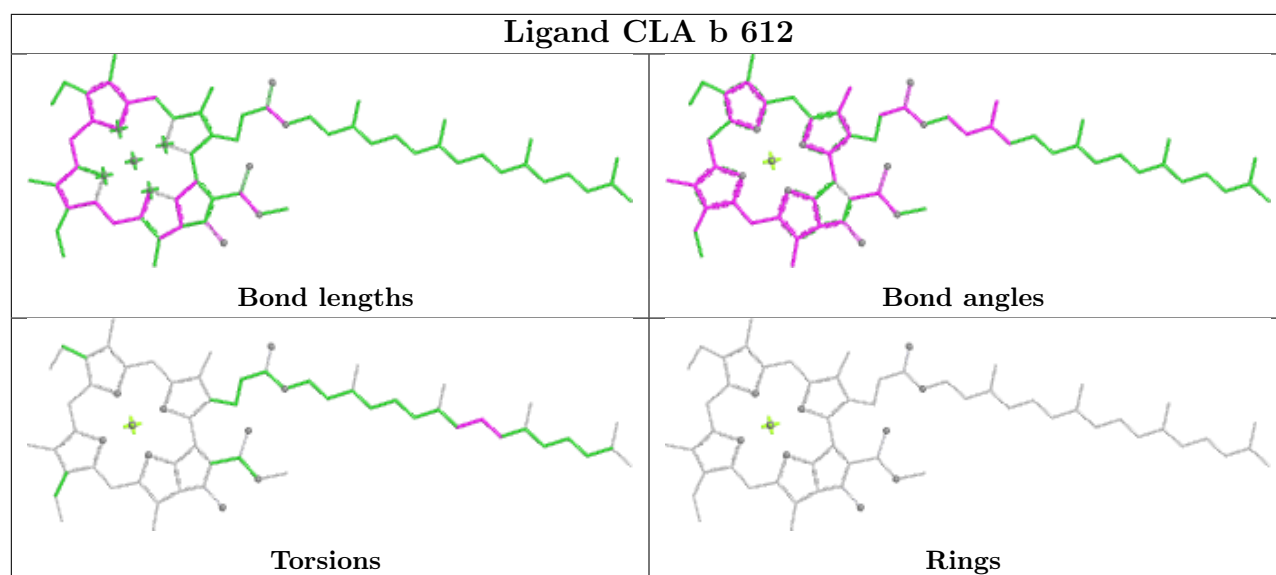


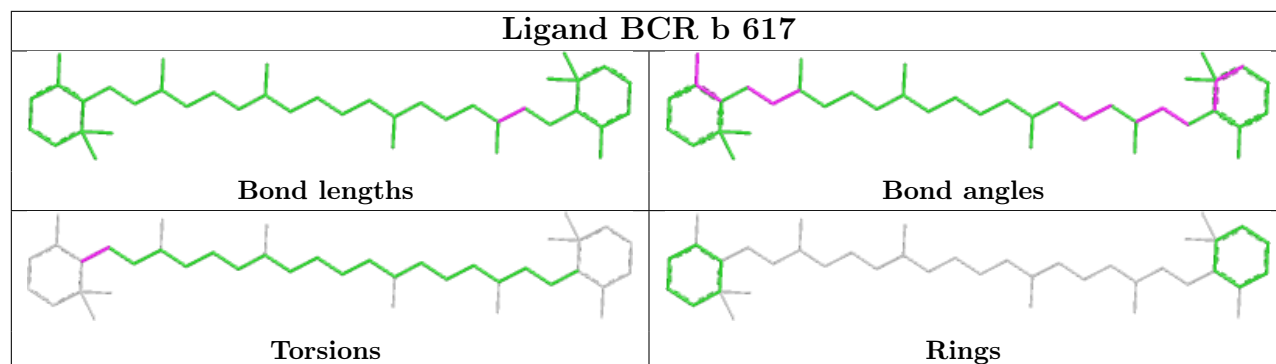
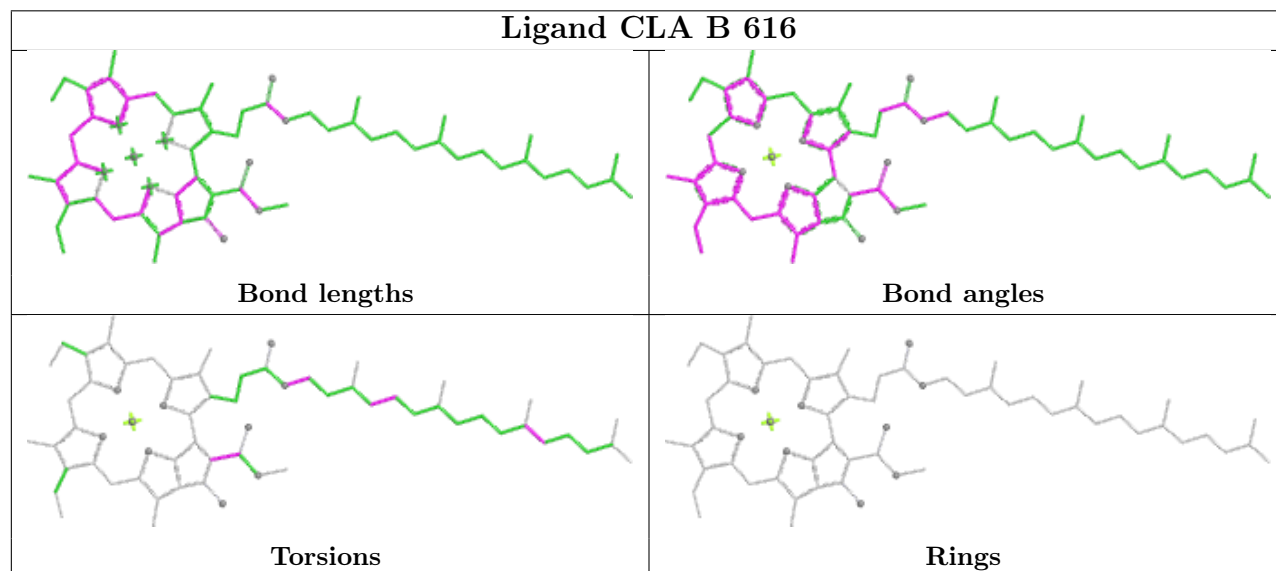
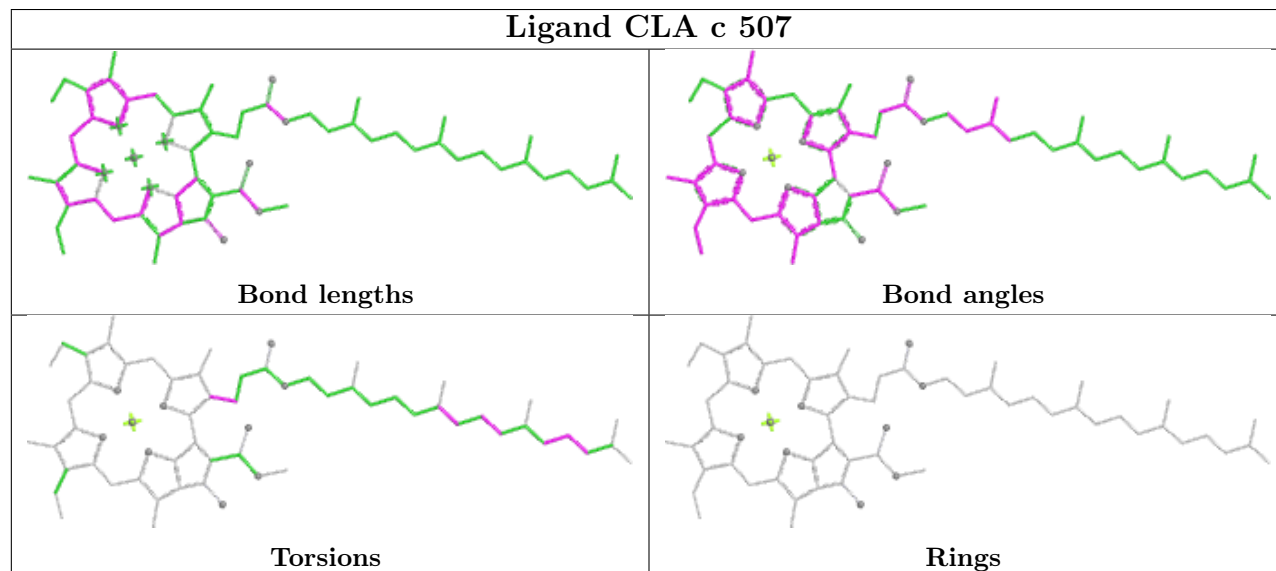




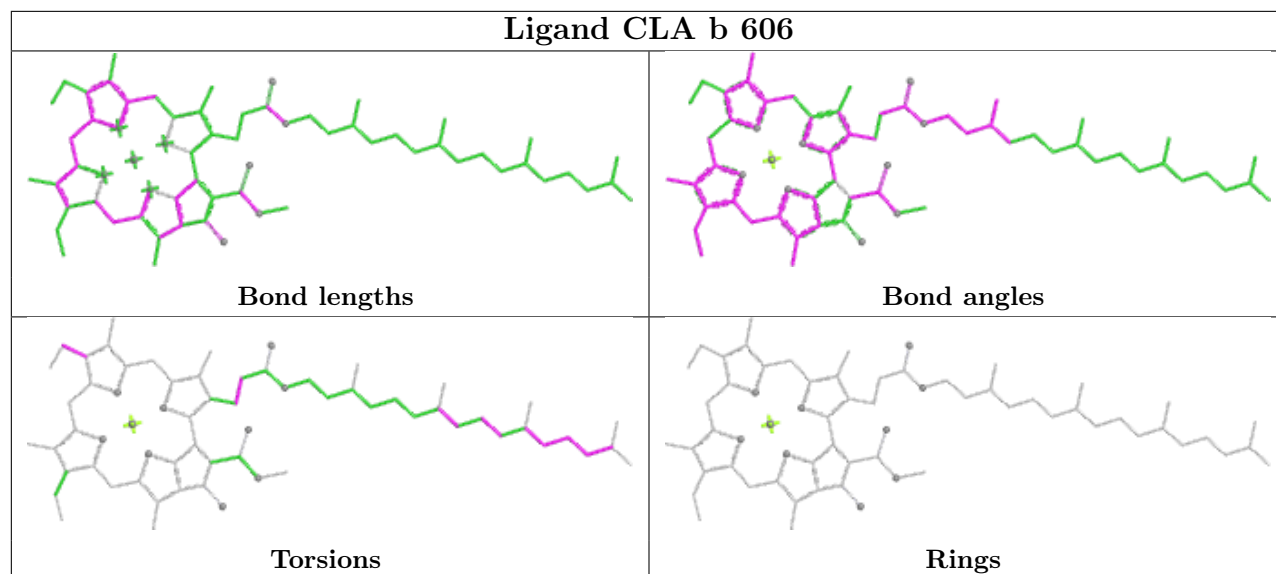




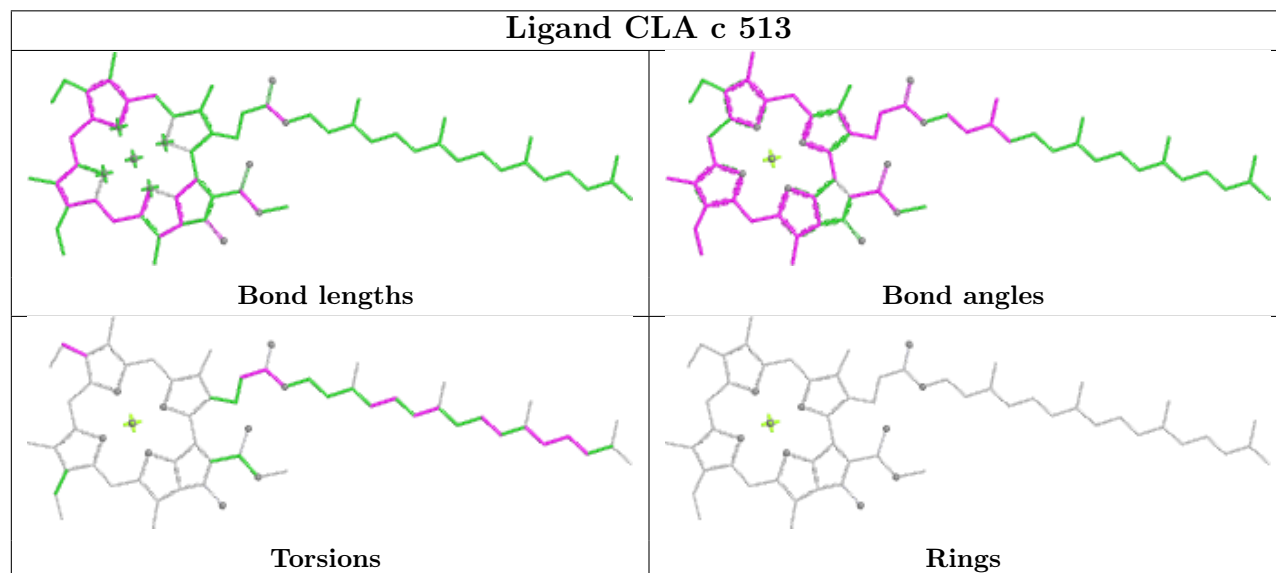


Ligand BCR b 617**Ligand CLA B 616****Ligand CLA c 507**

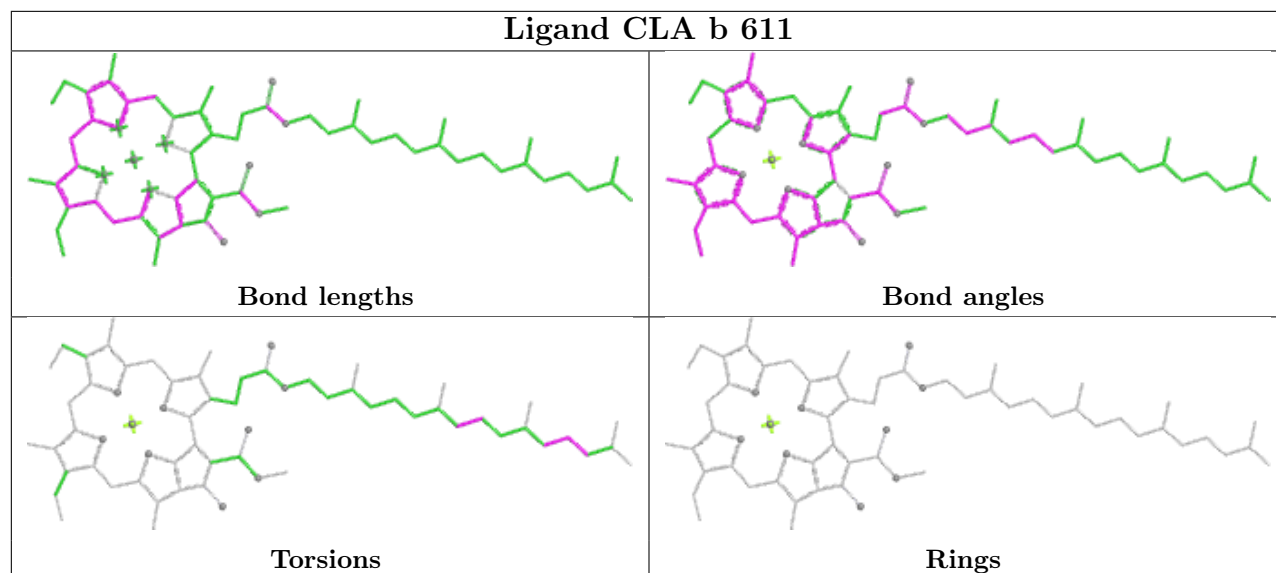
Ligand CLA b 606

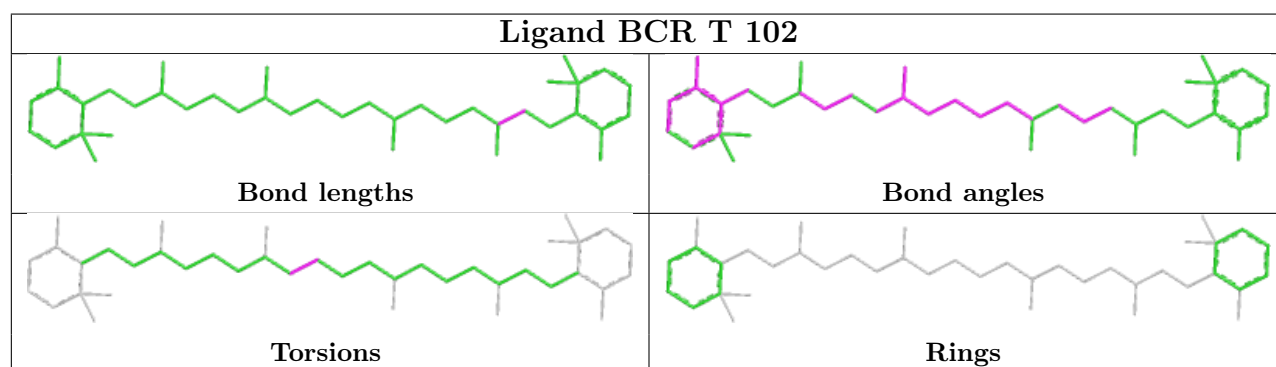
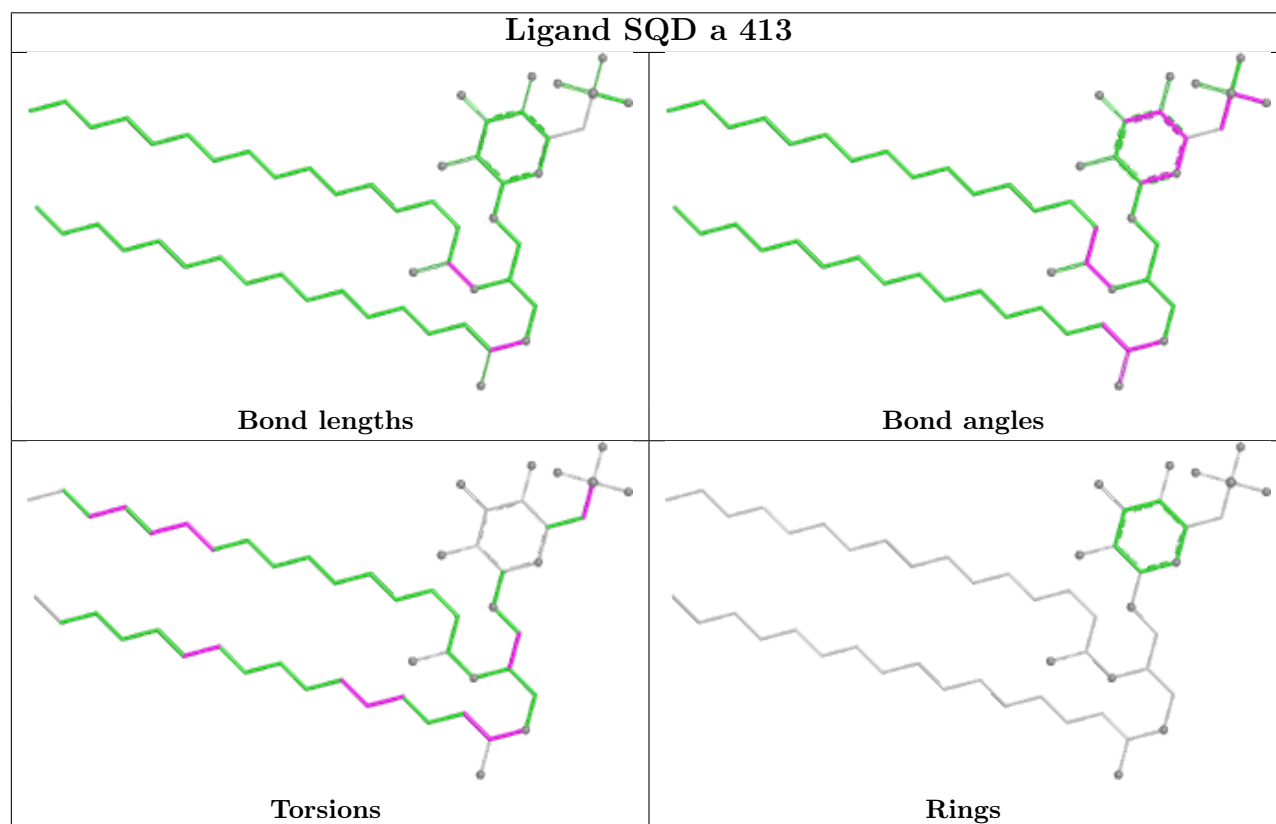
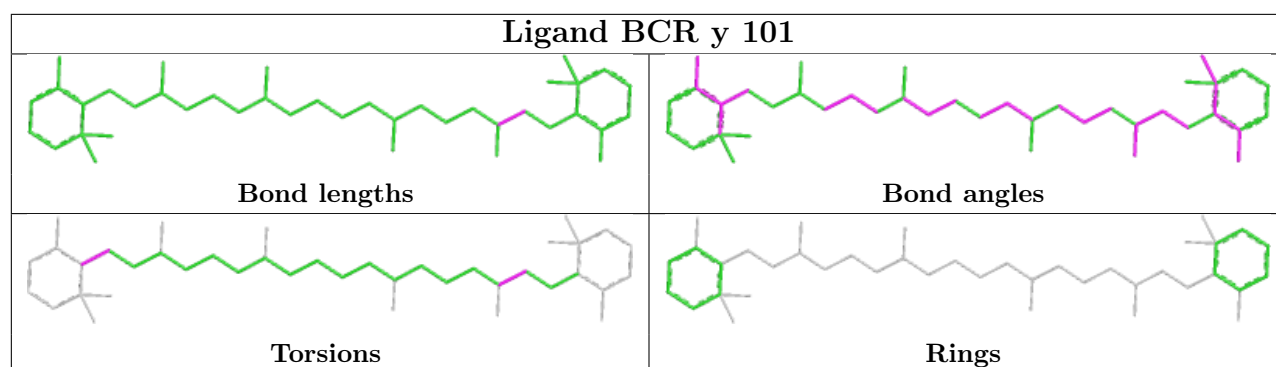


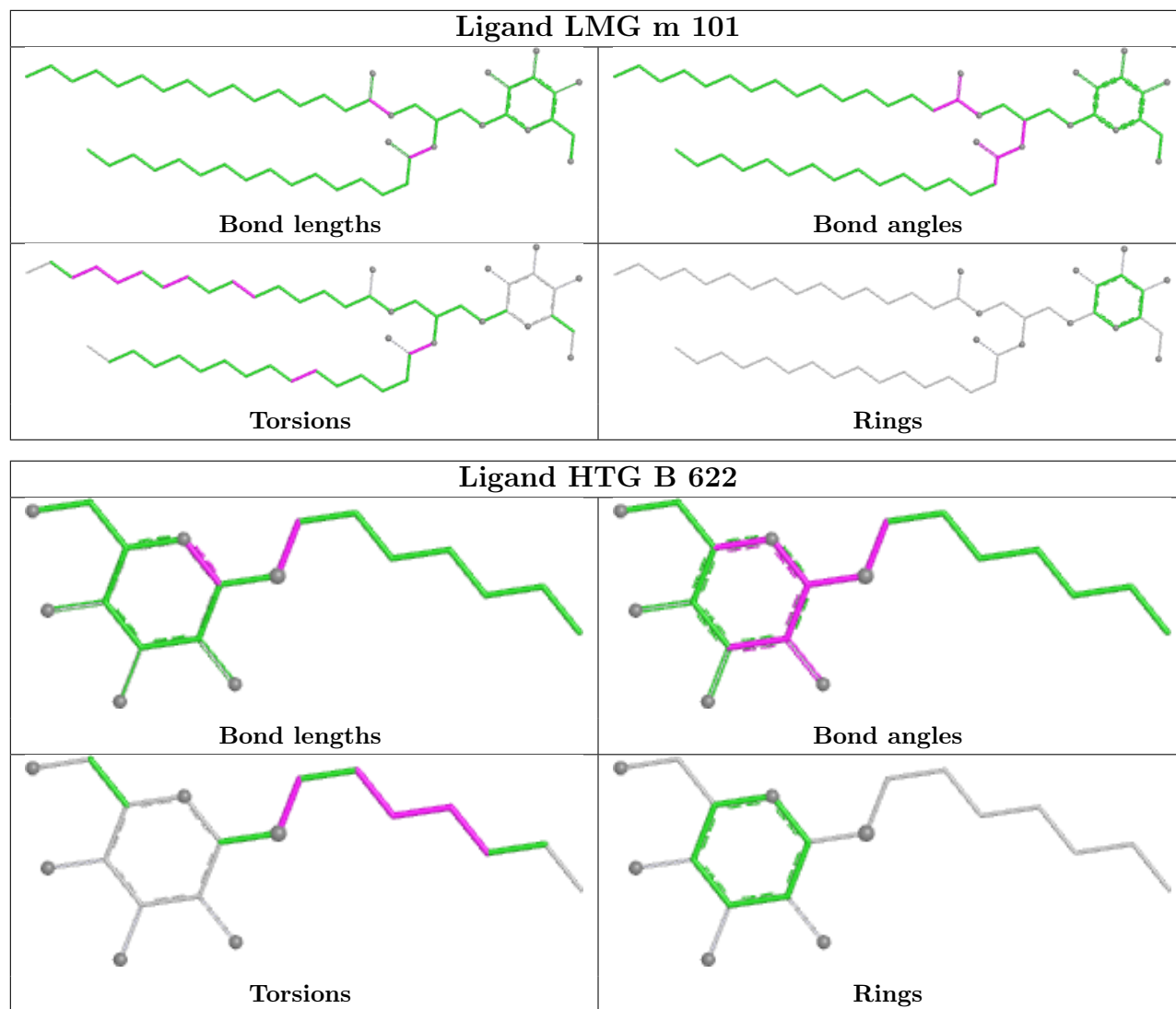
Ligand CLA c 513

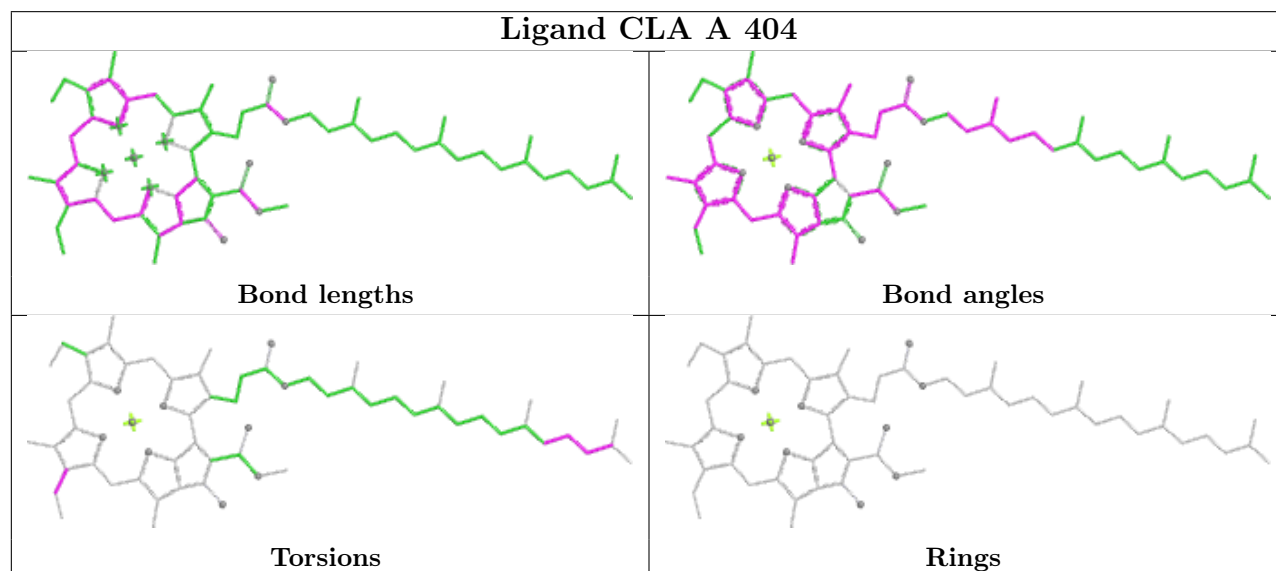
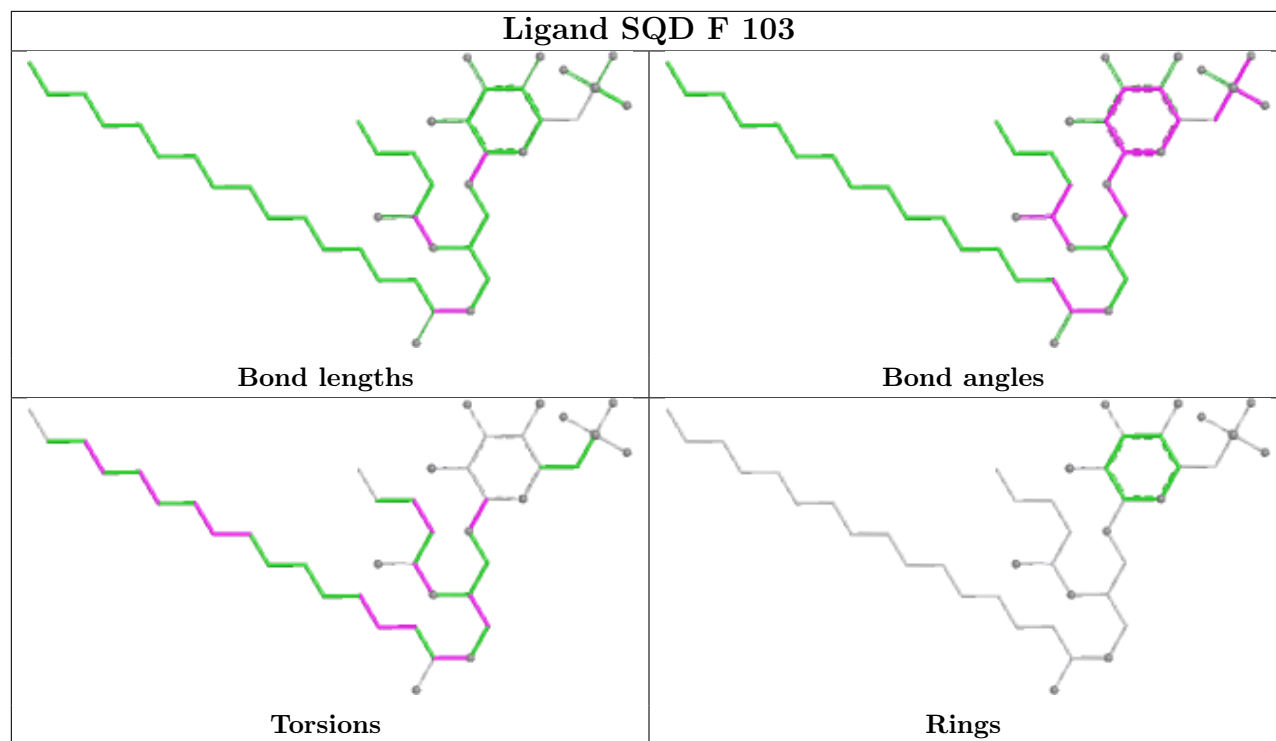


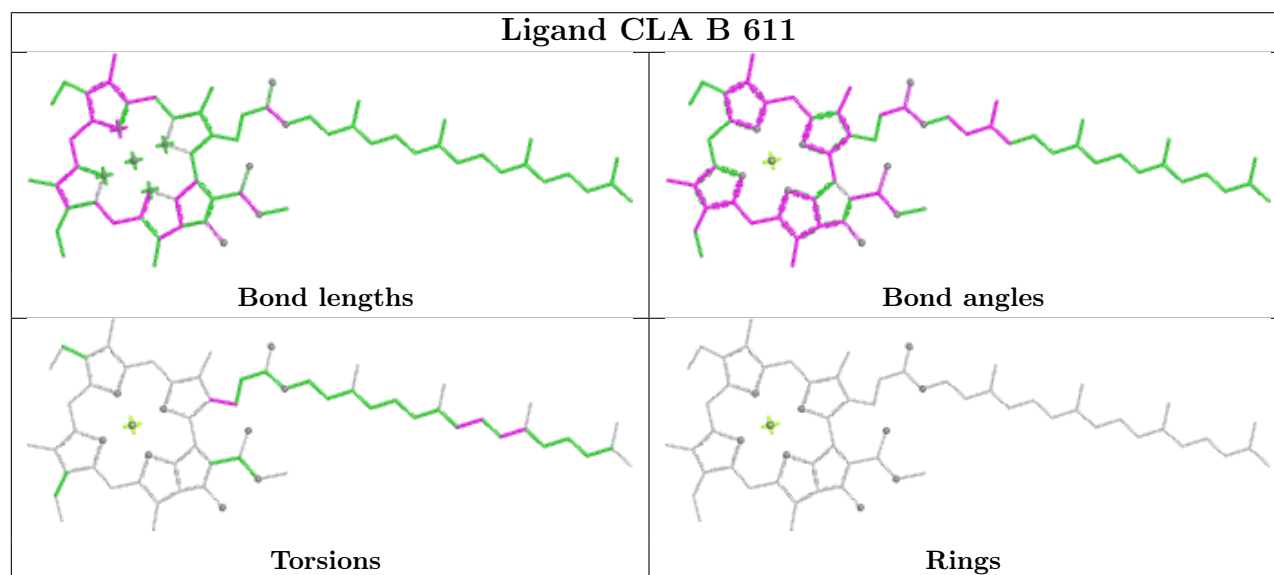
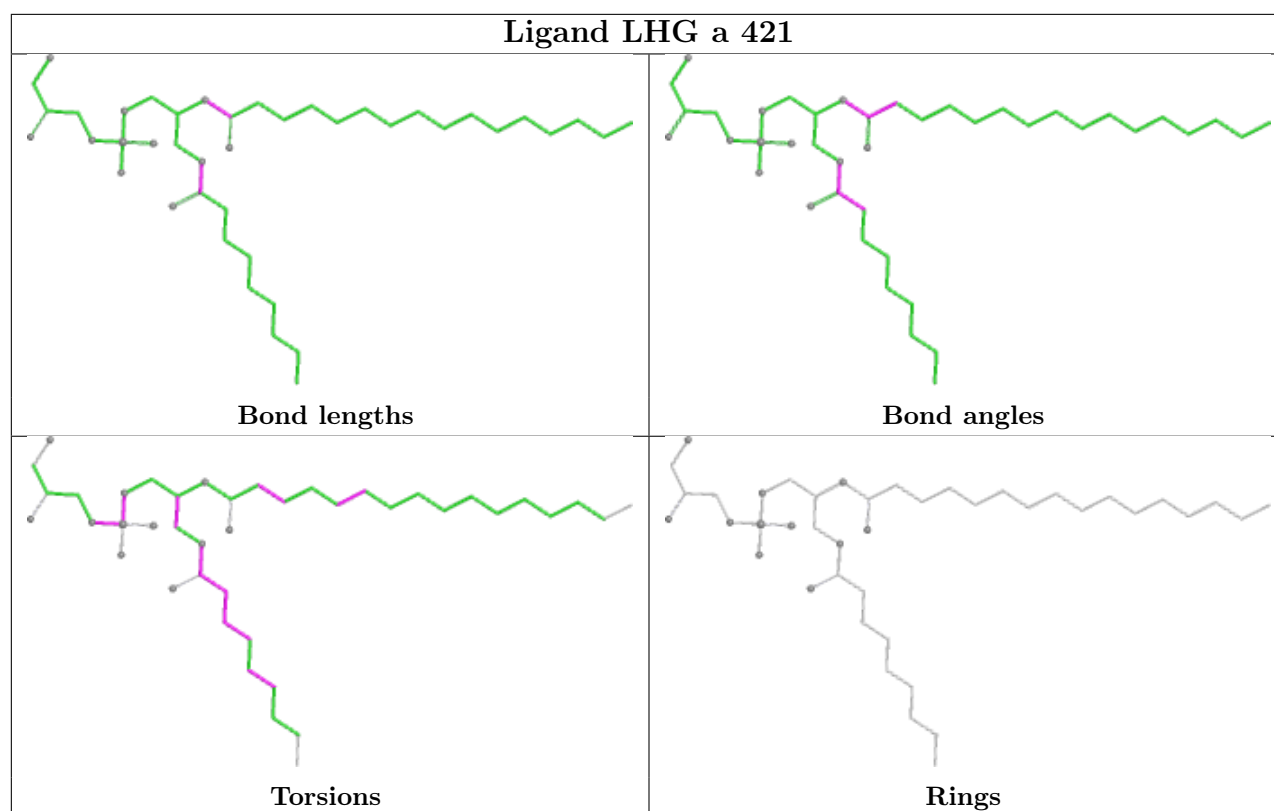
Ligand CLA b 611

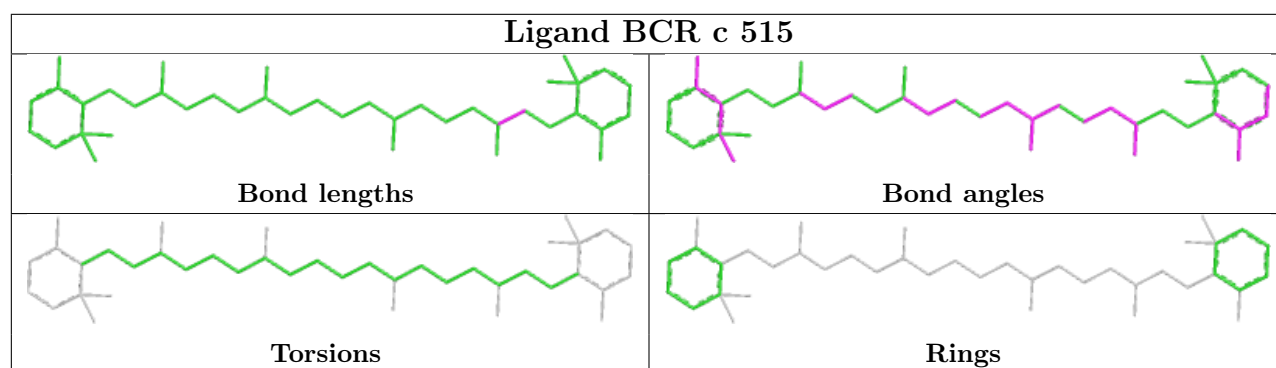
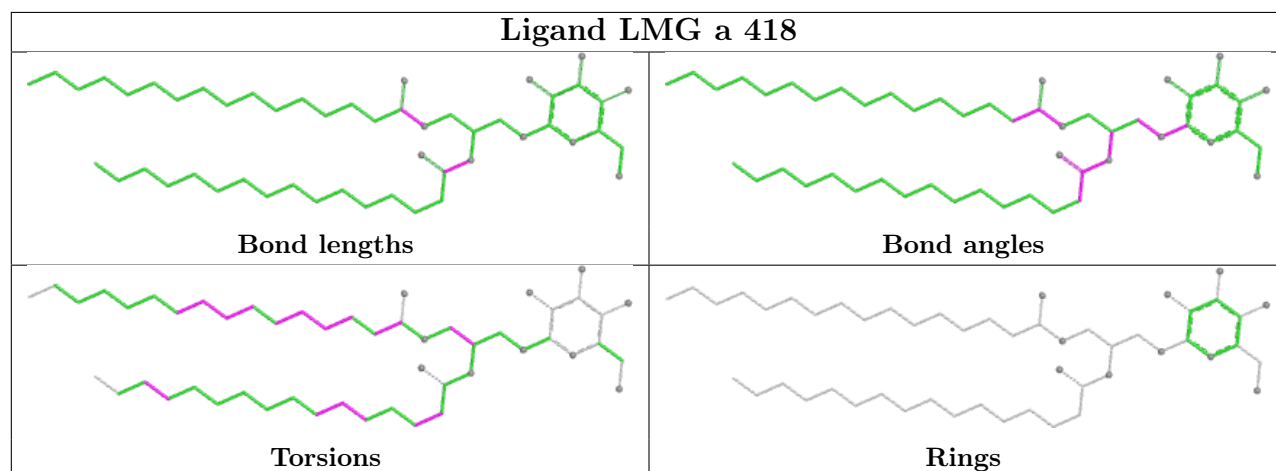
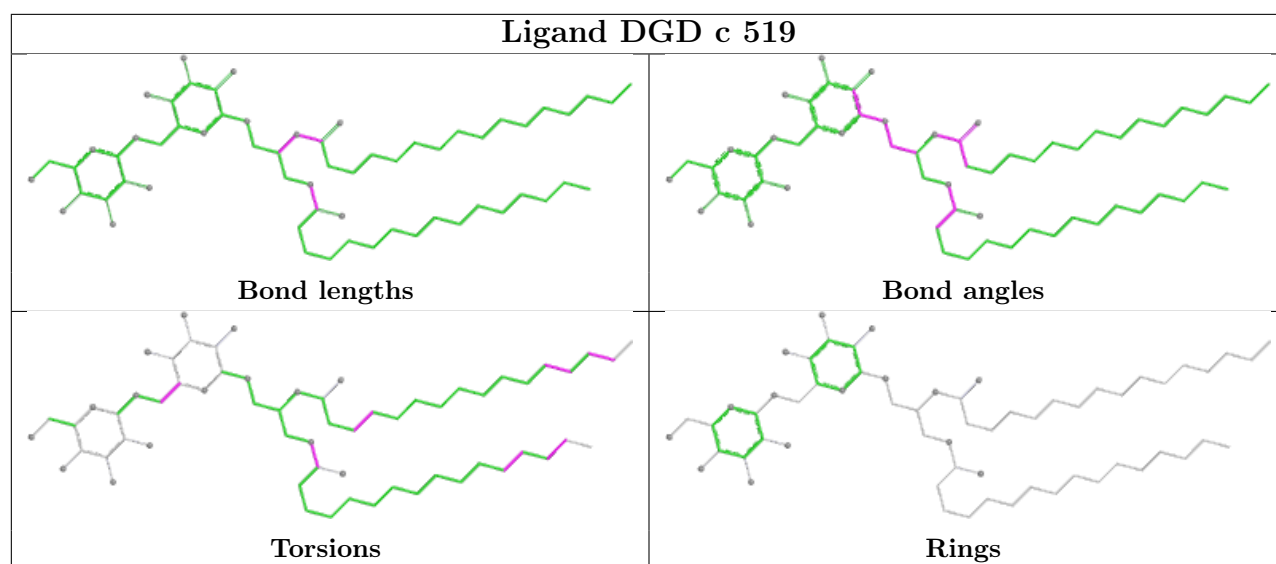


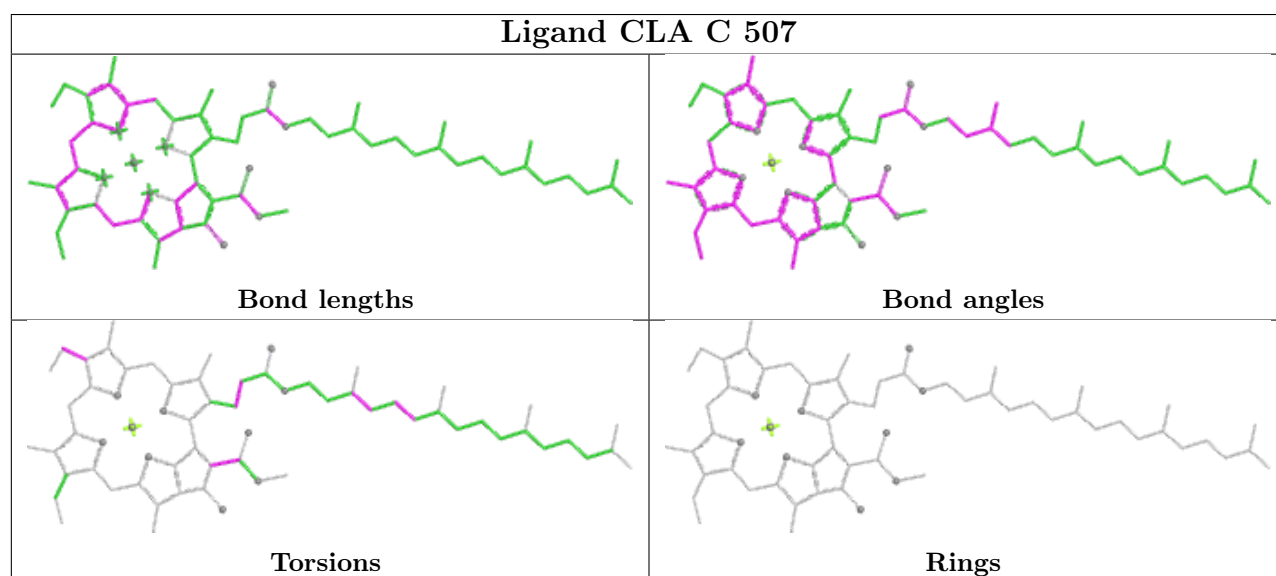
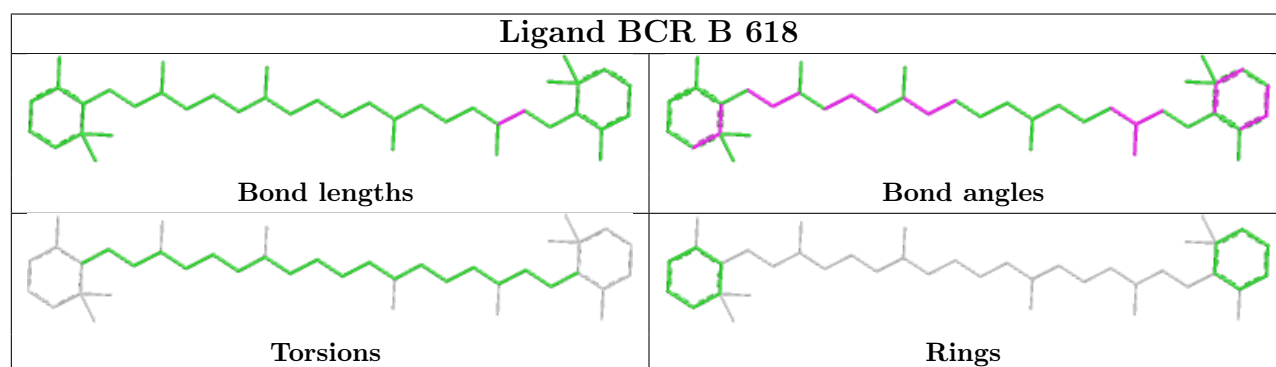
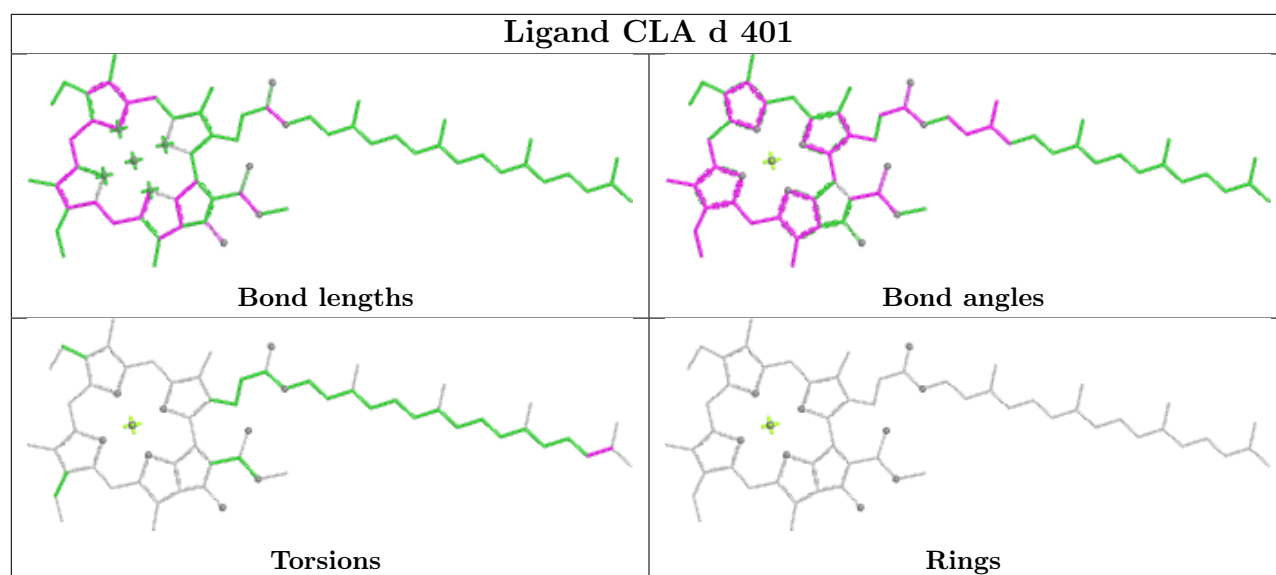


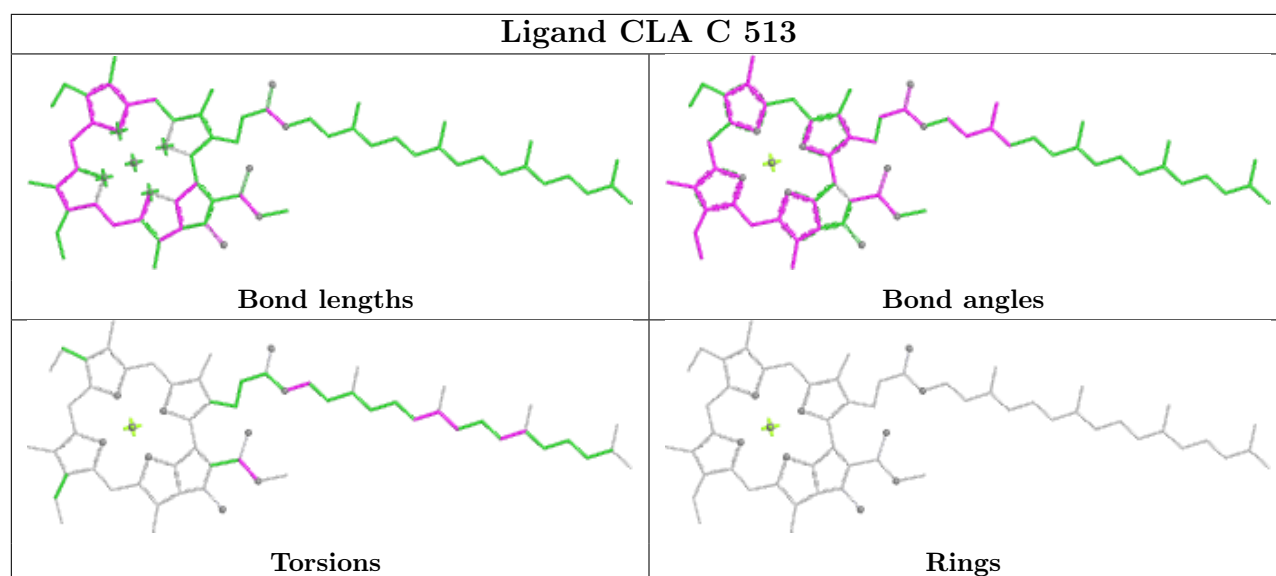
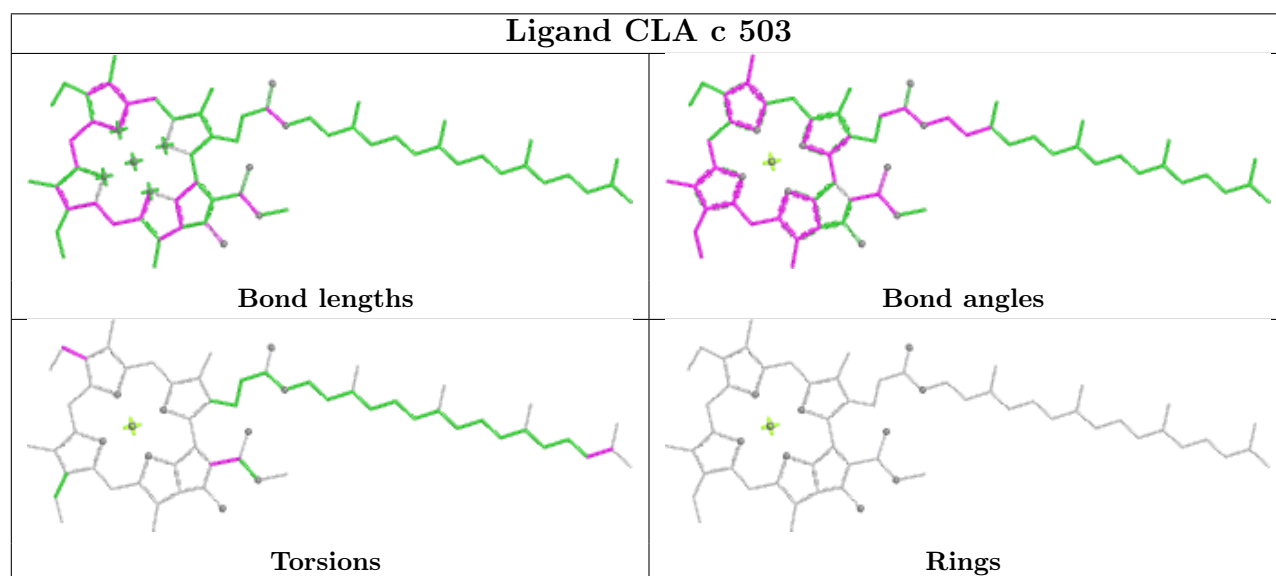
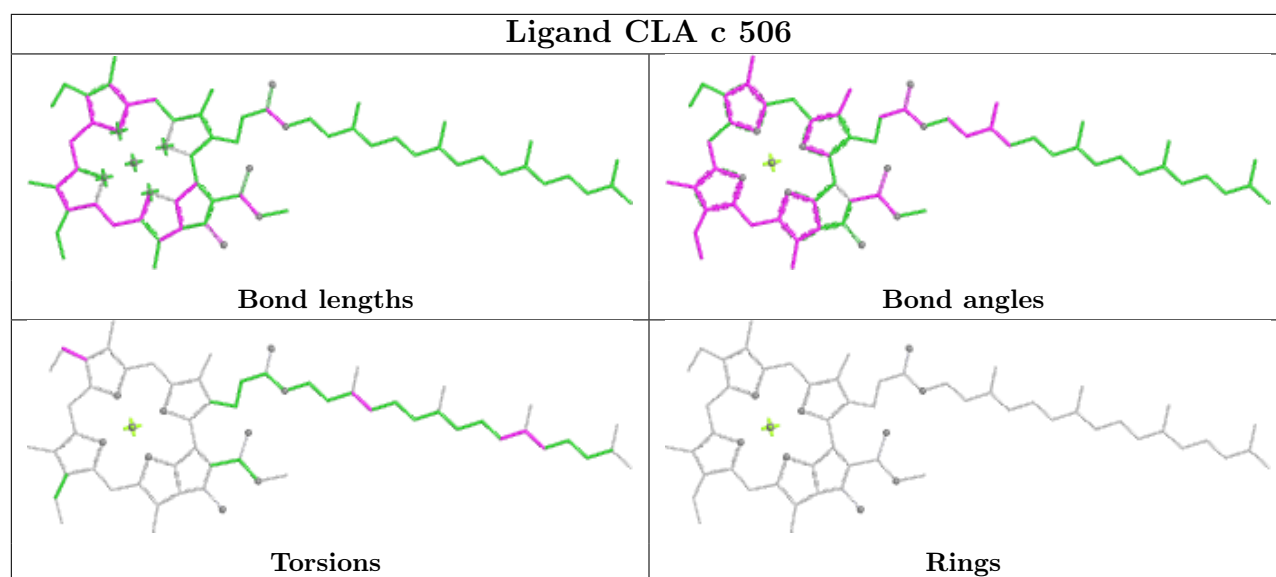


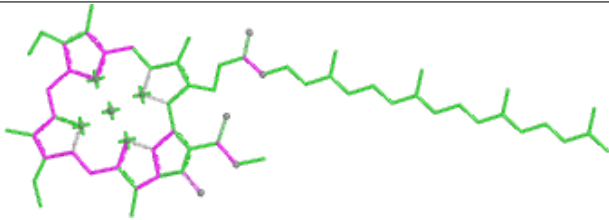
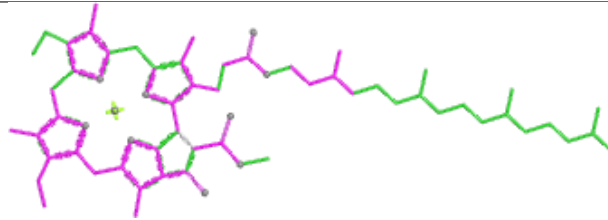
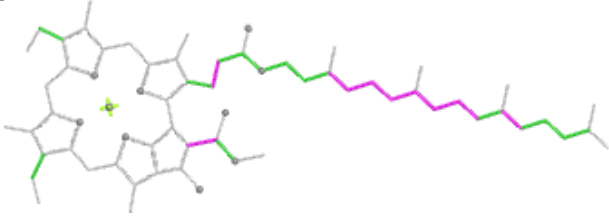
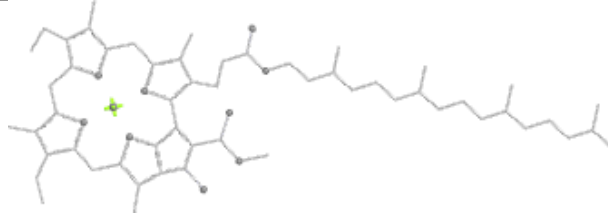


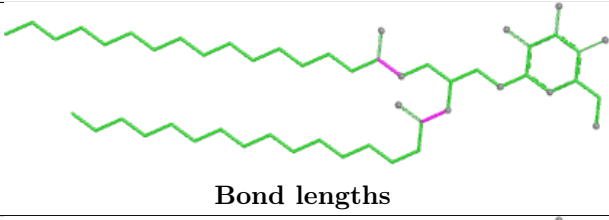
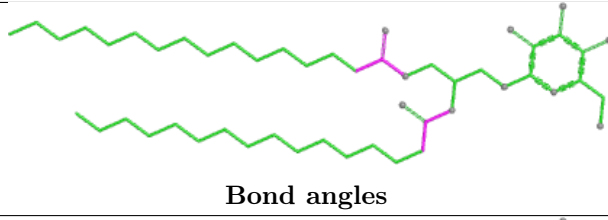
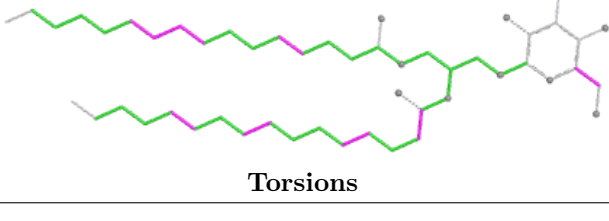
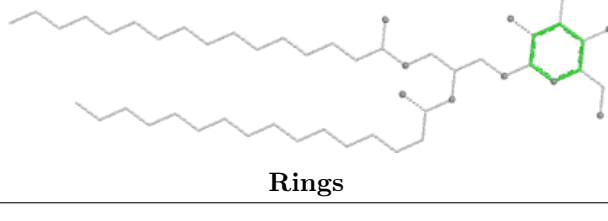


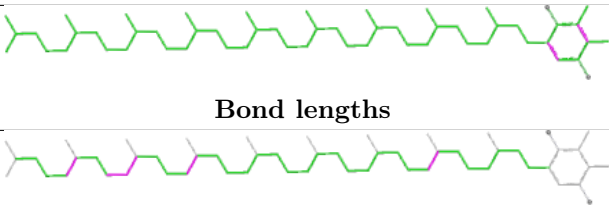
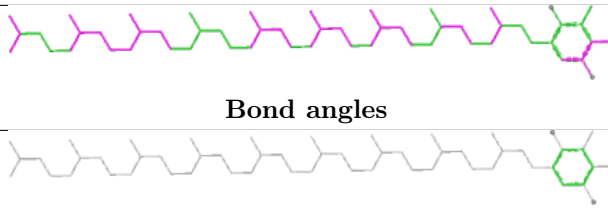
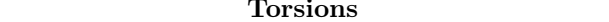
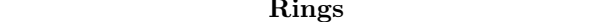


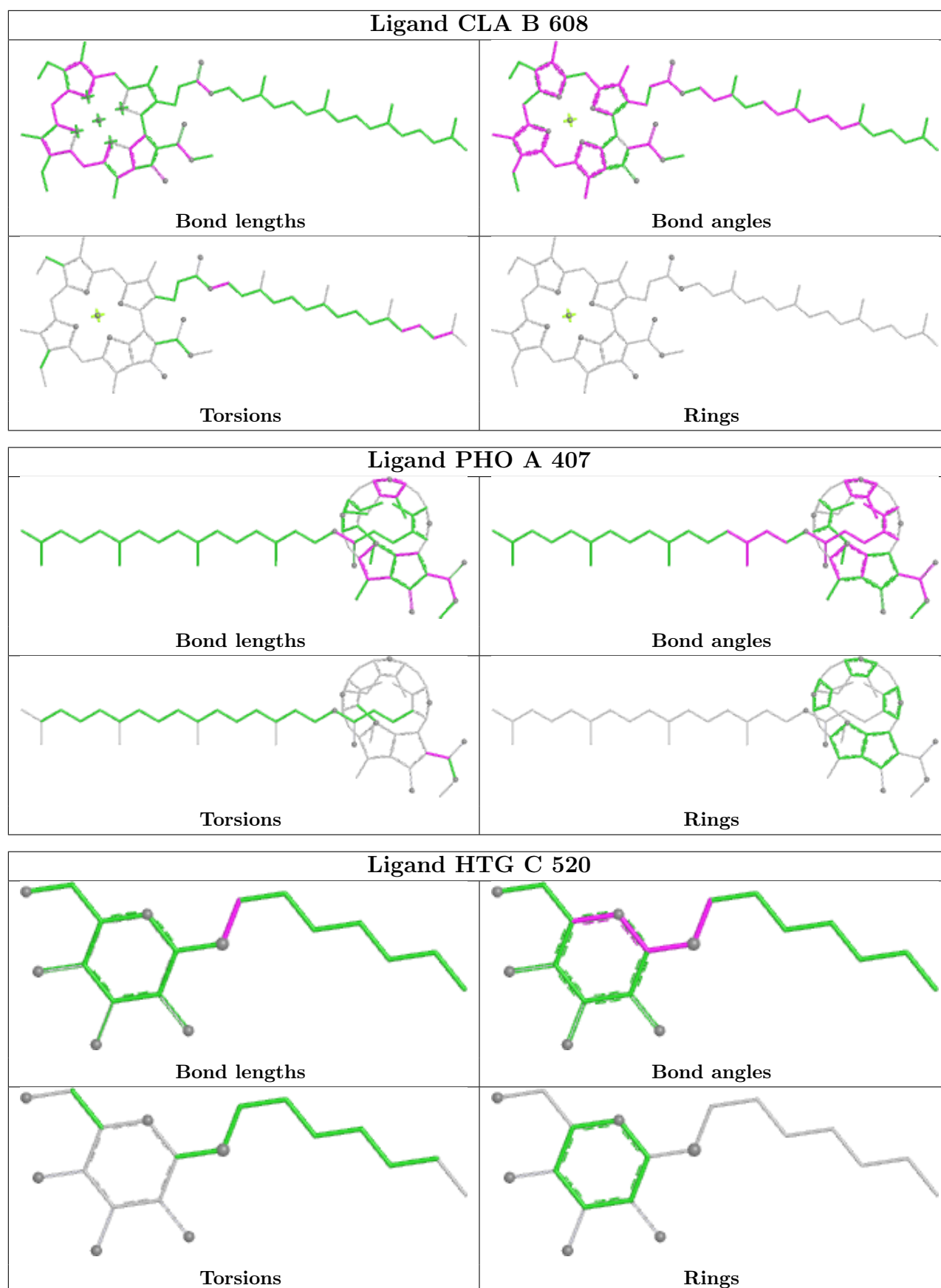


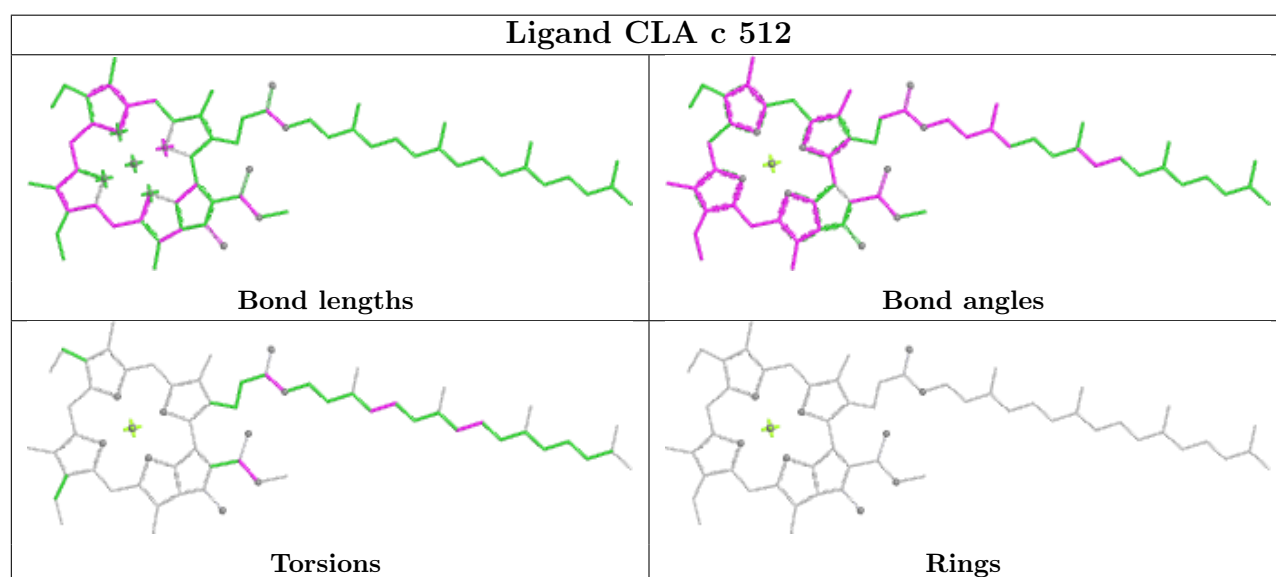
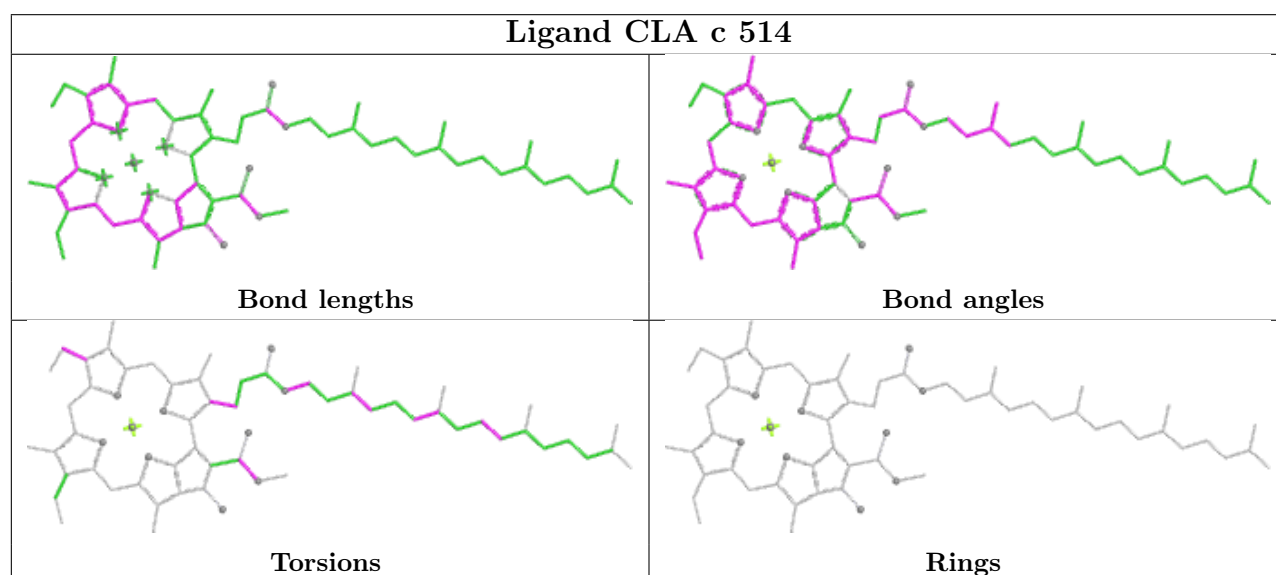
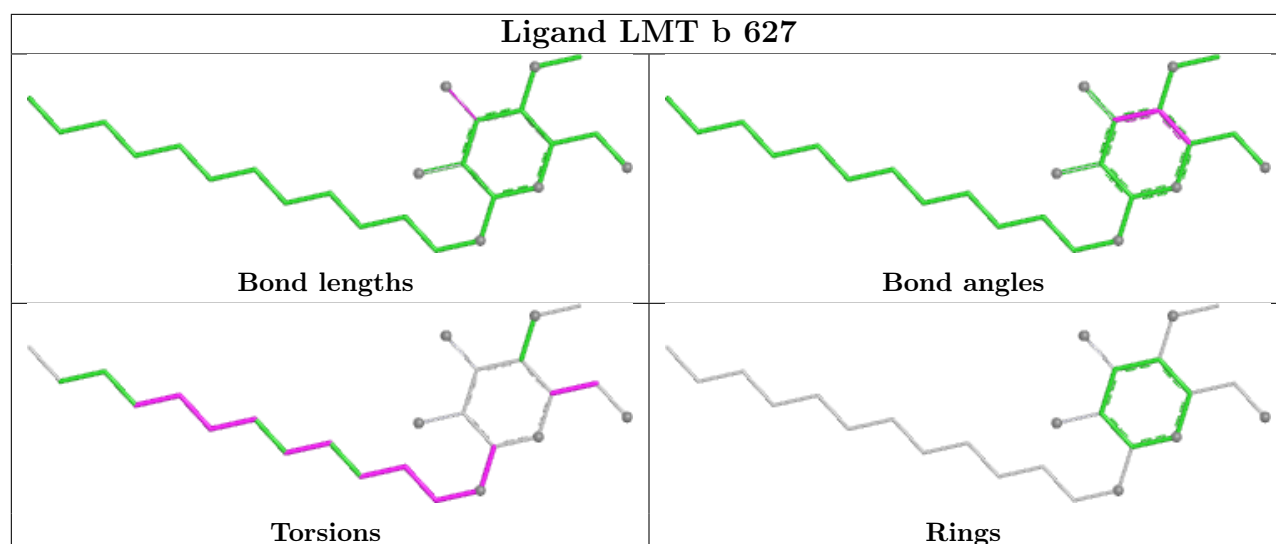


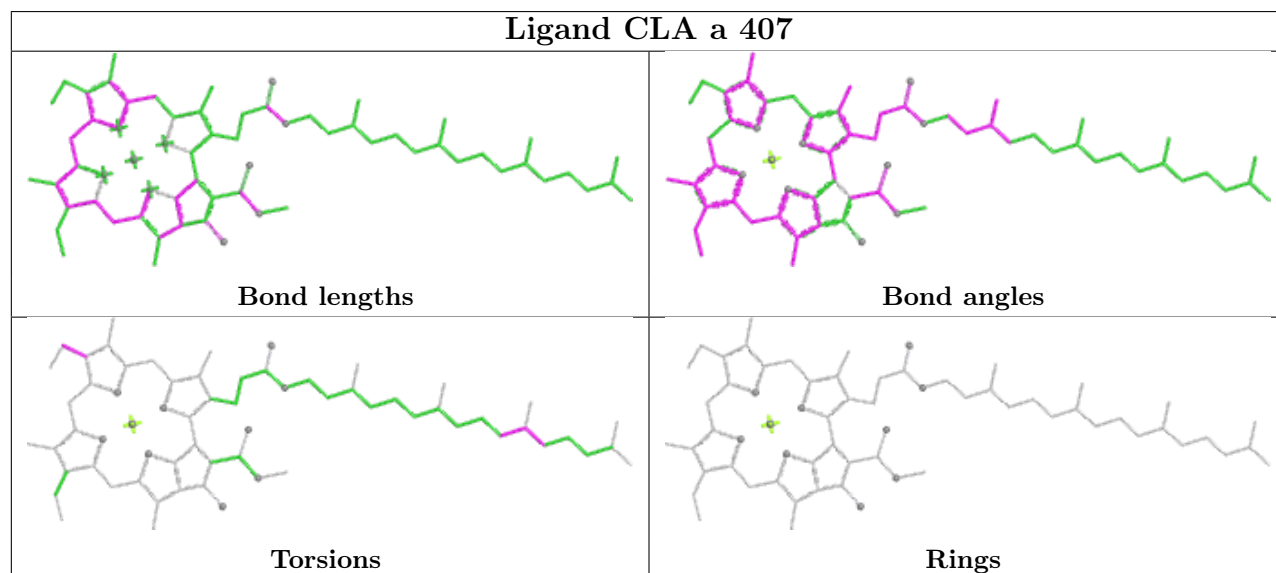
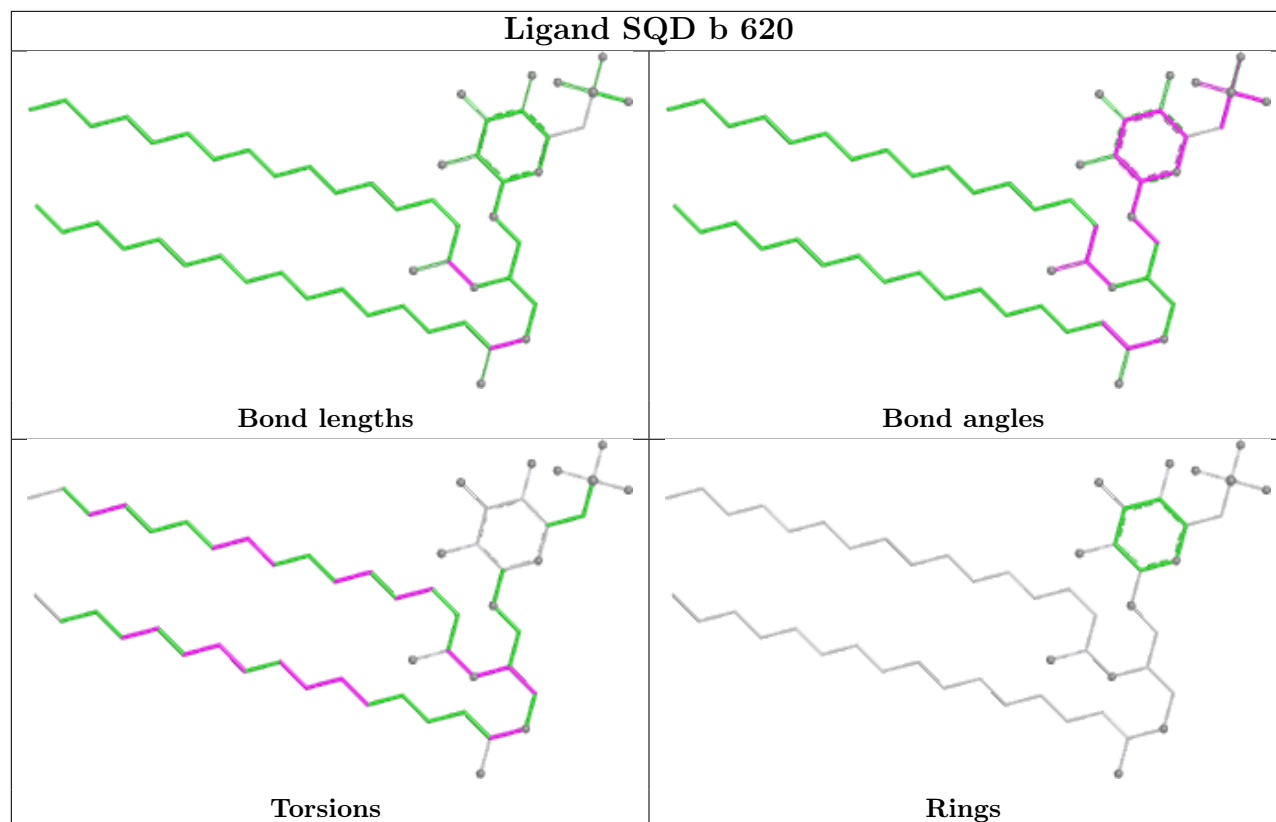
Ligand CLA B 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

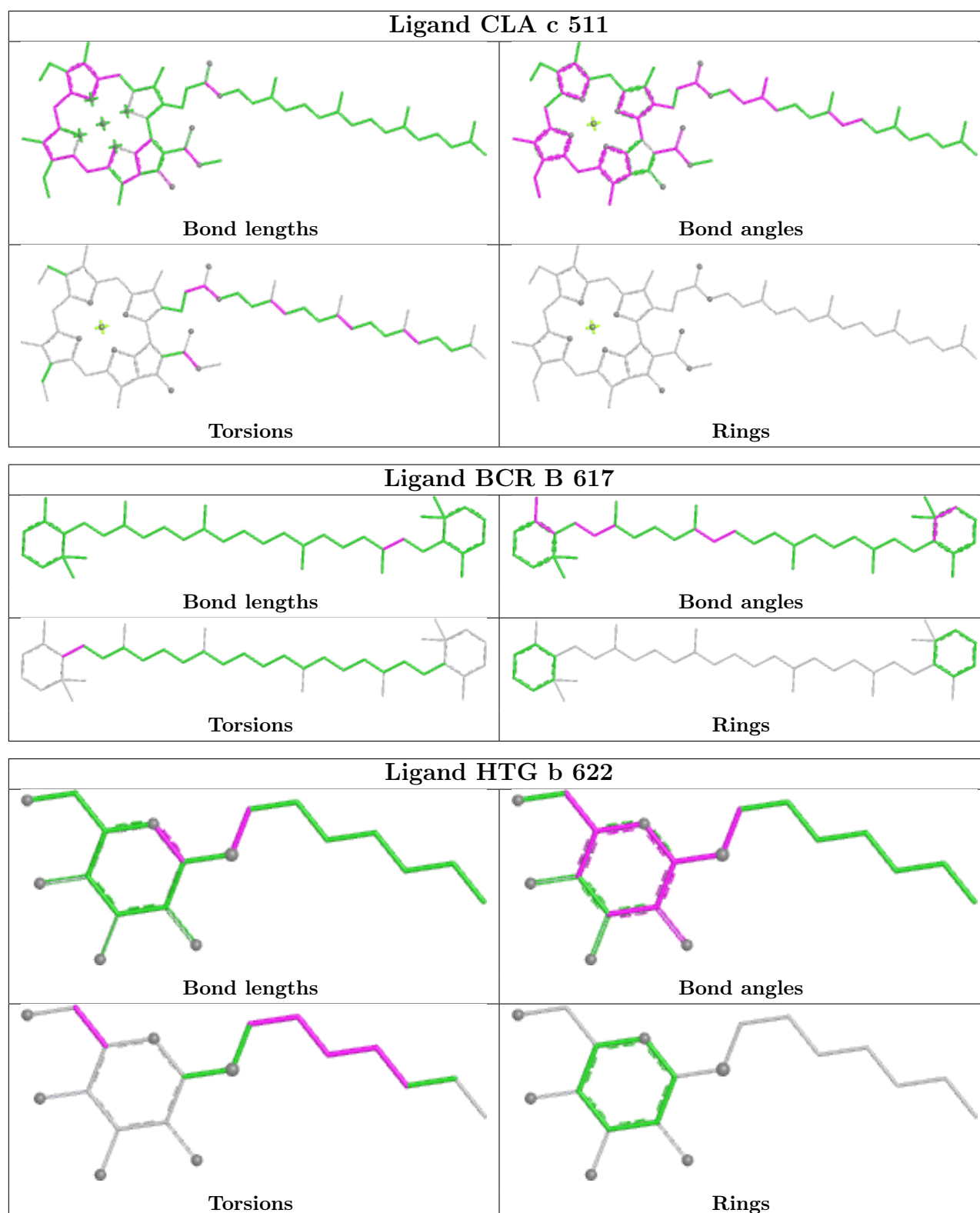
Ligand LMG D 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

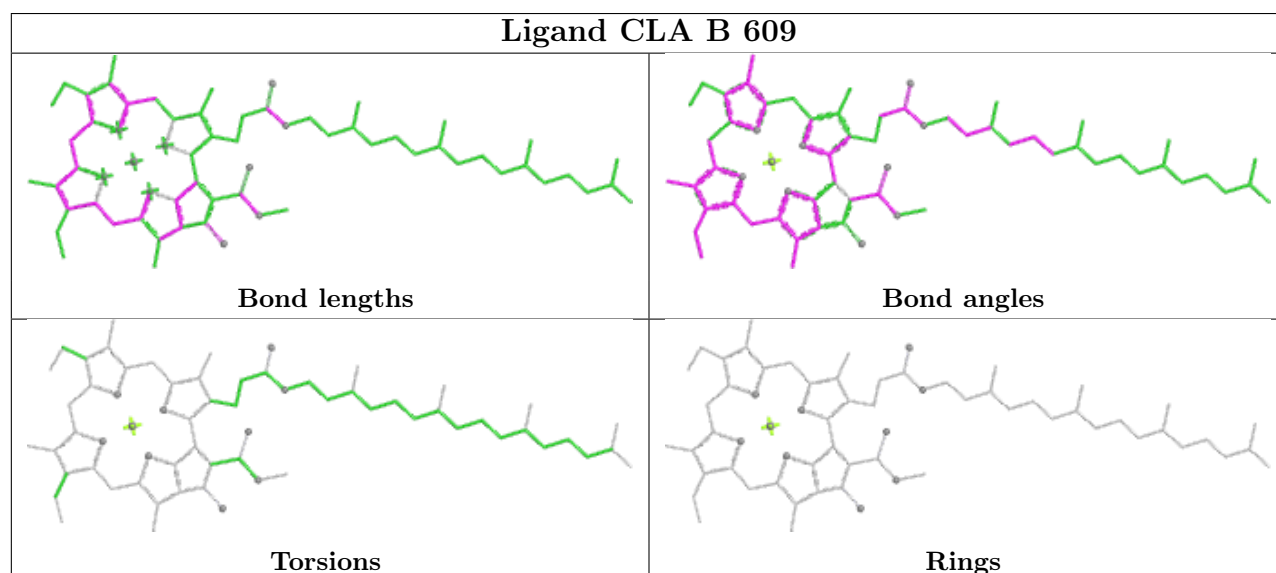
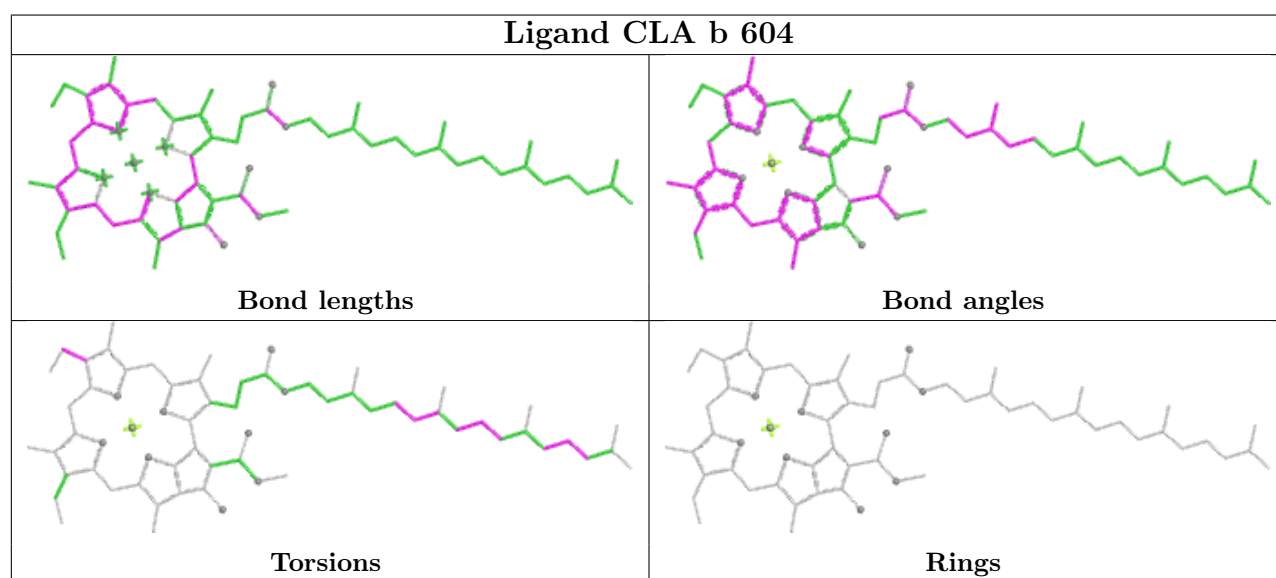
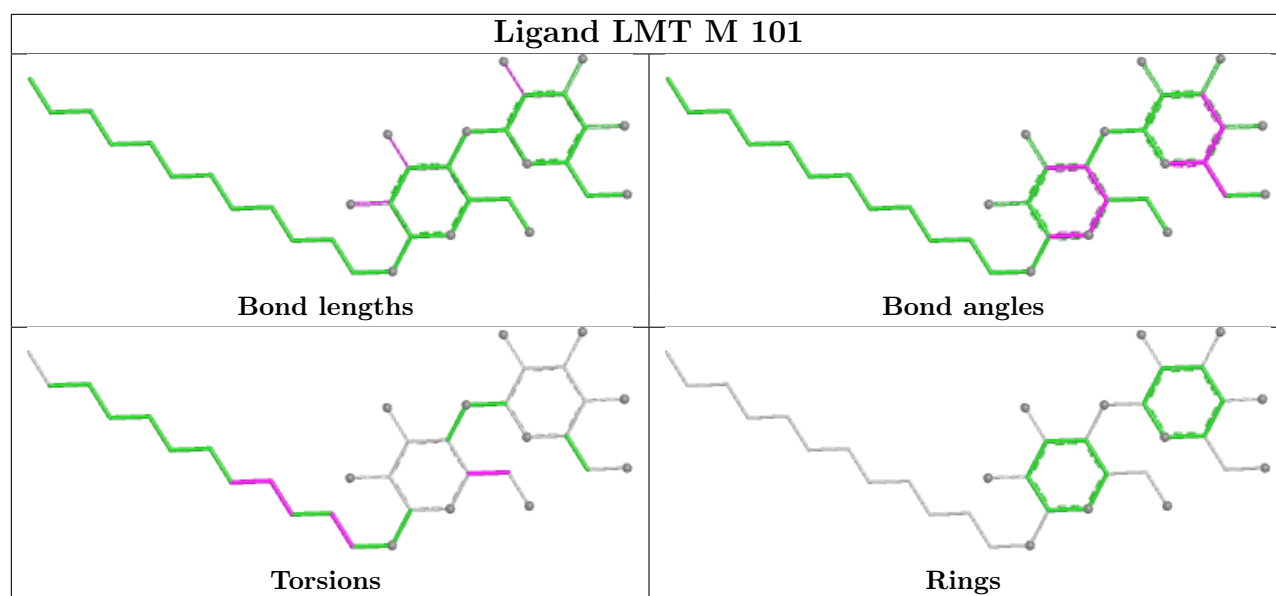
Ligand PL9 D 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

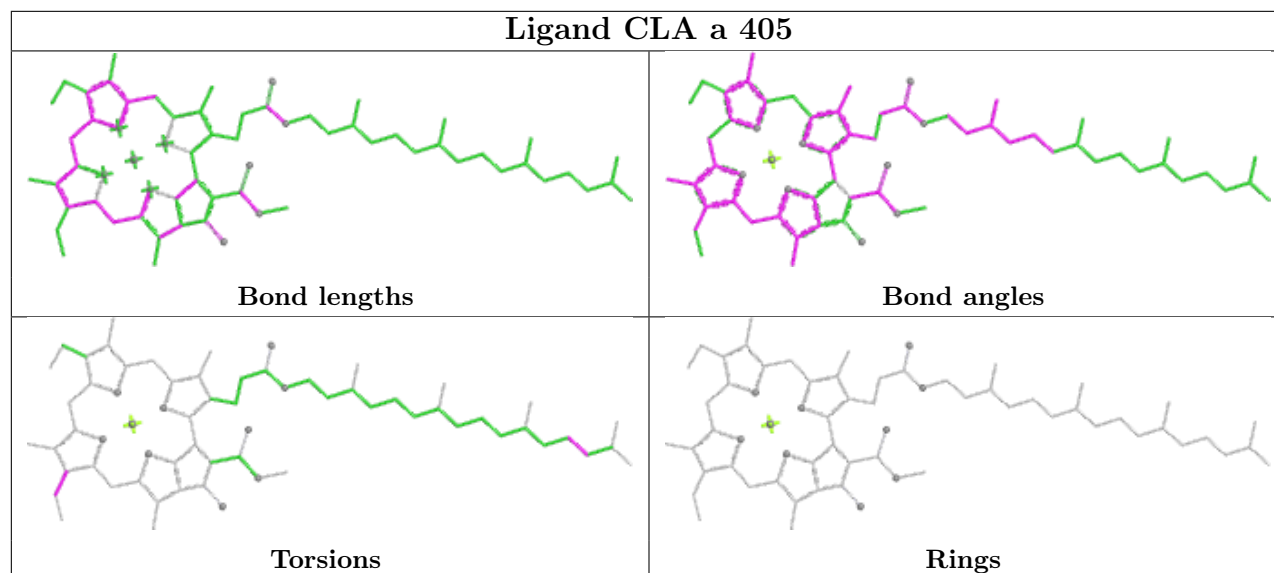
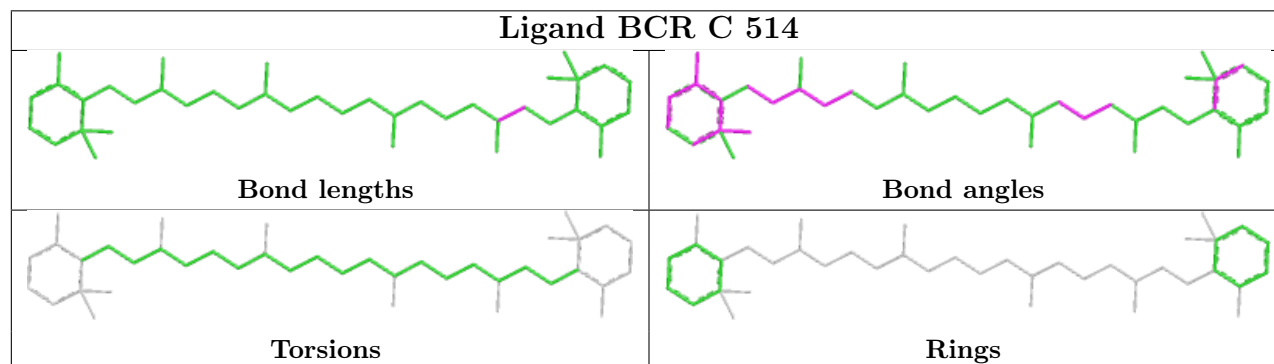
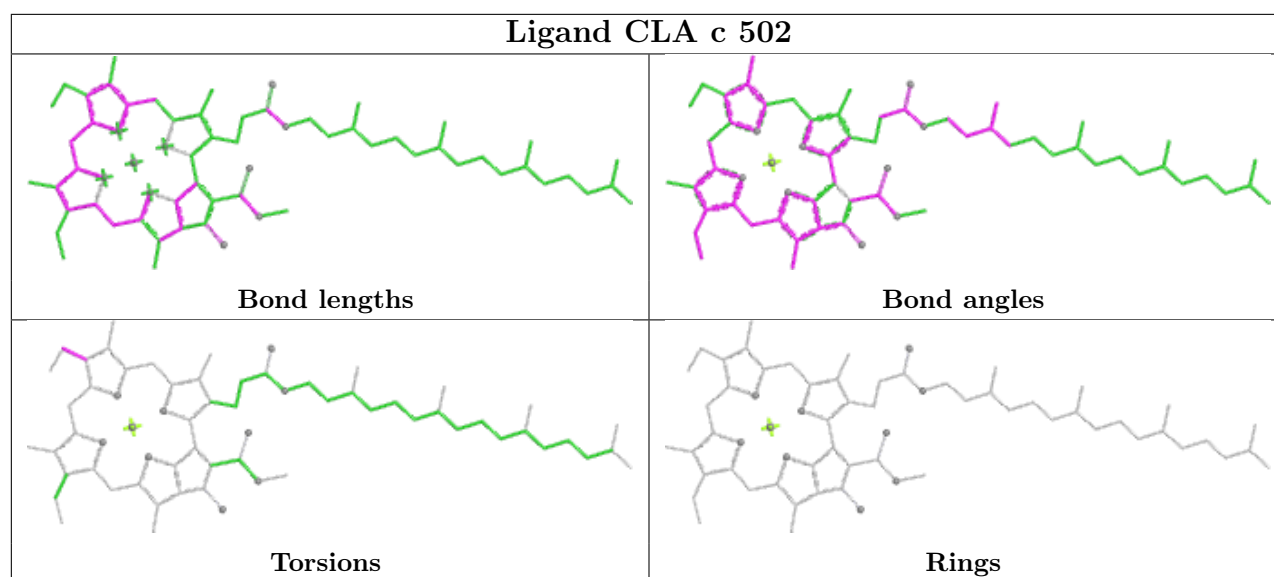


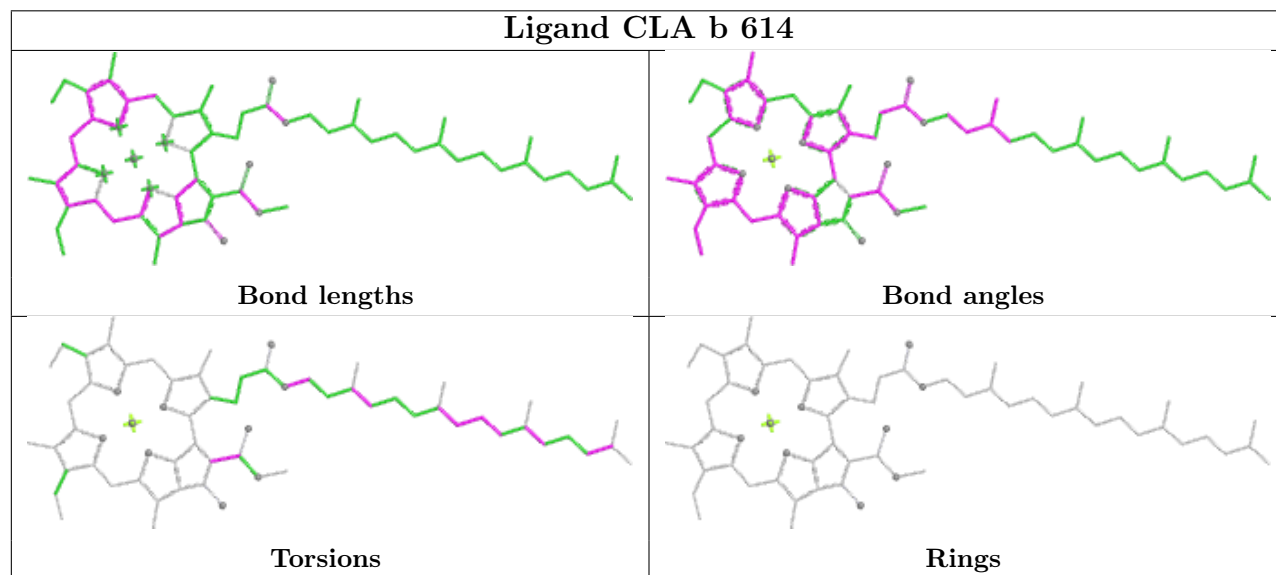
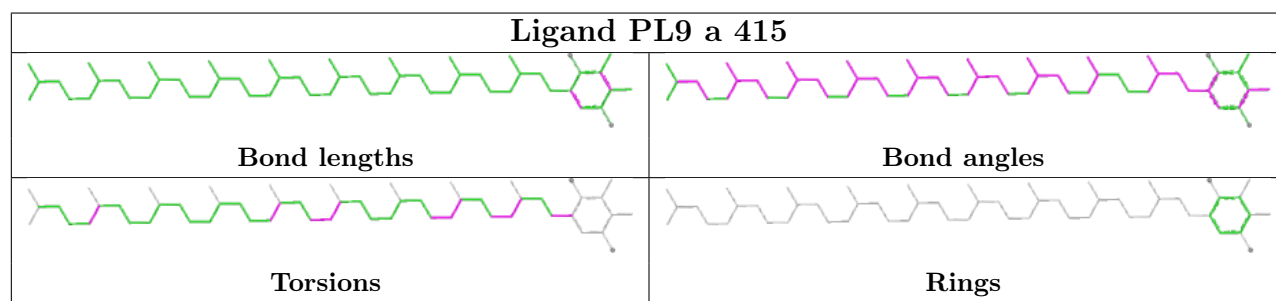
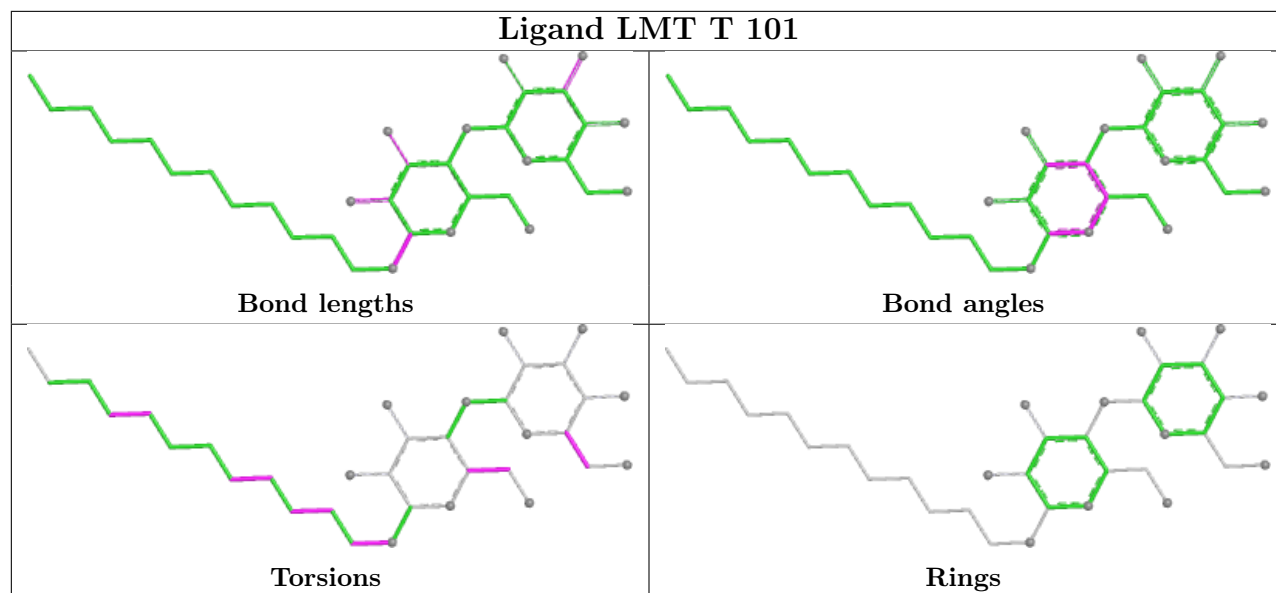


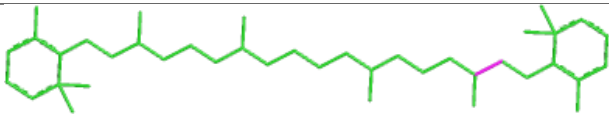
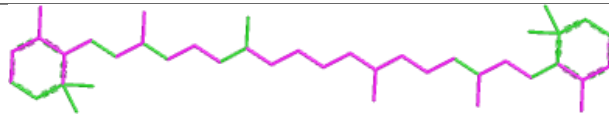
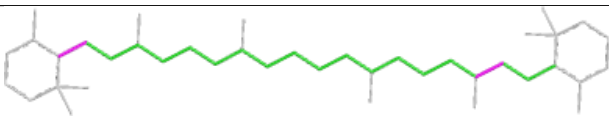
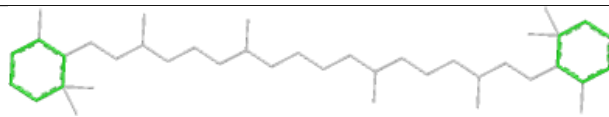


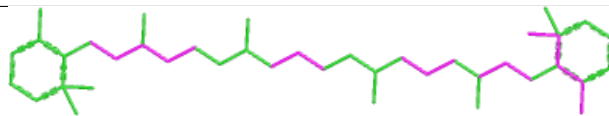
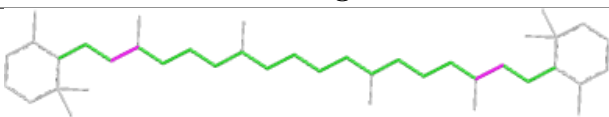
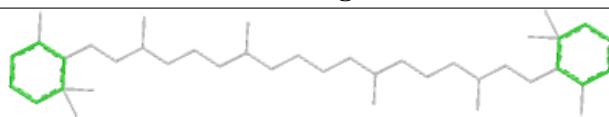


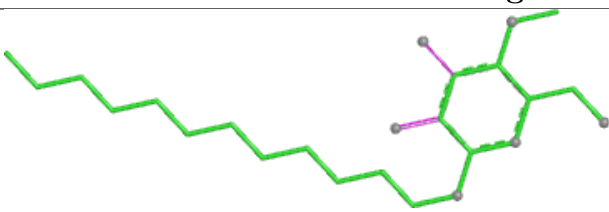
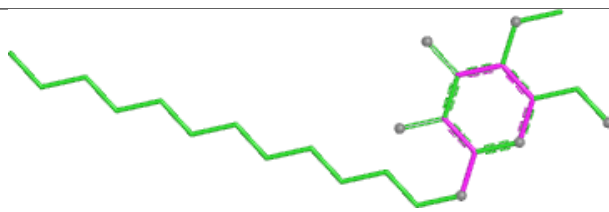
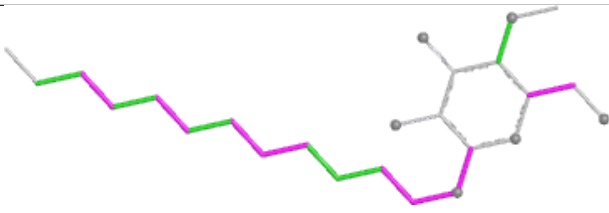
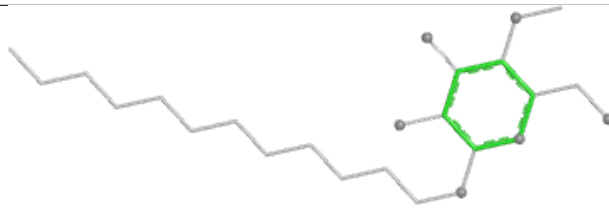


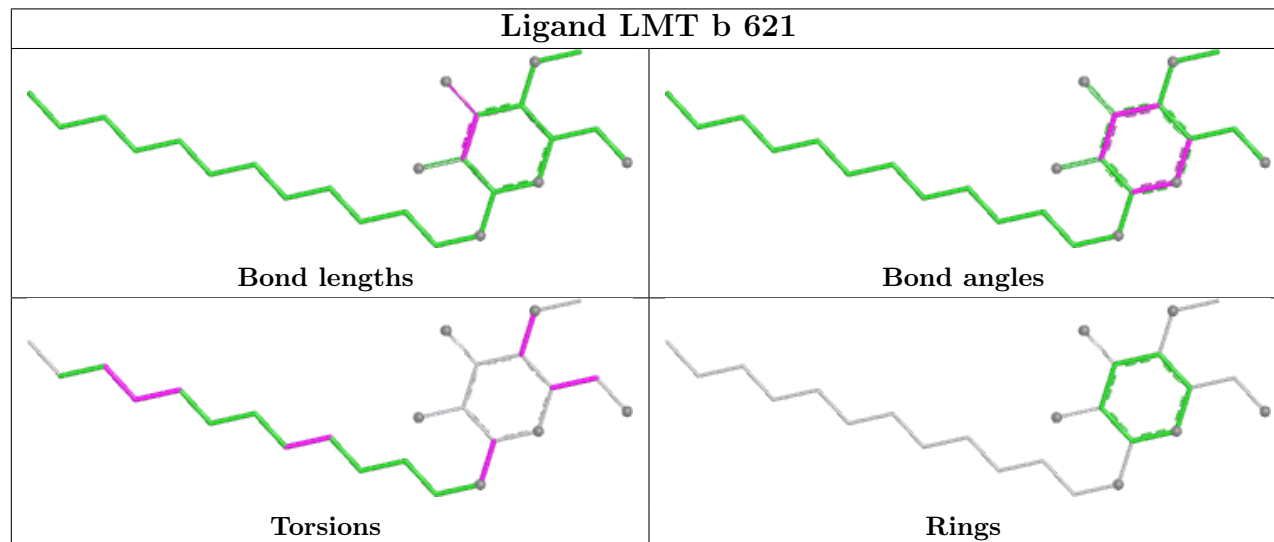
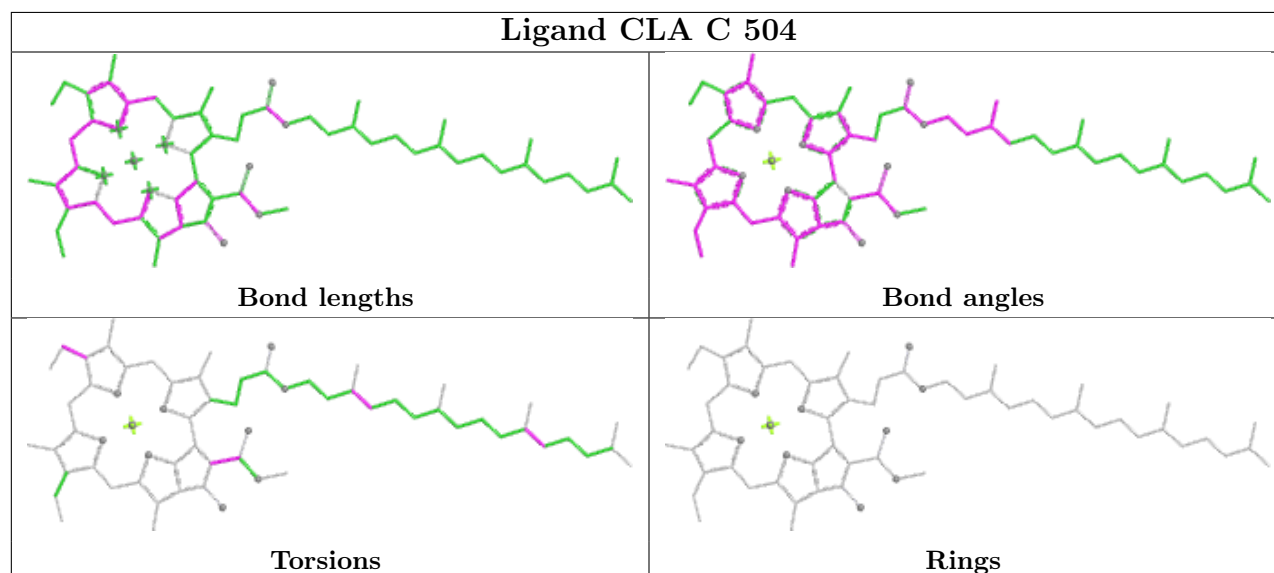
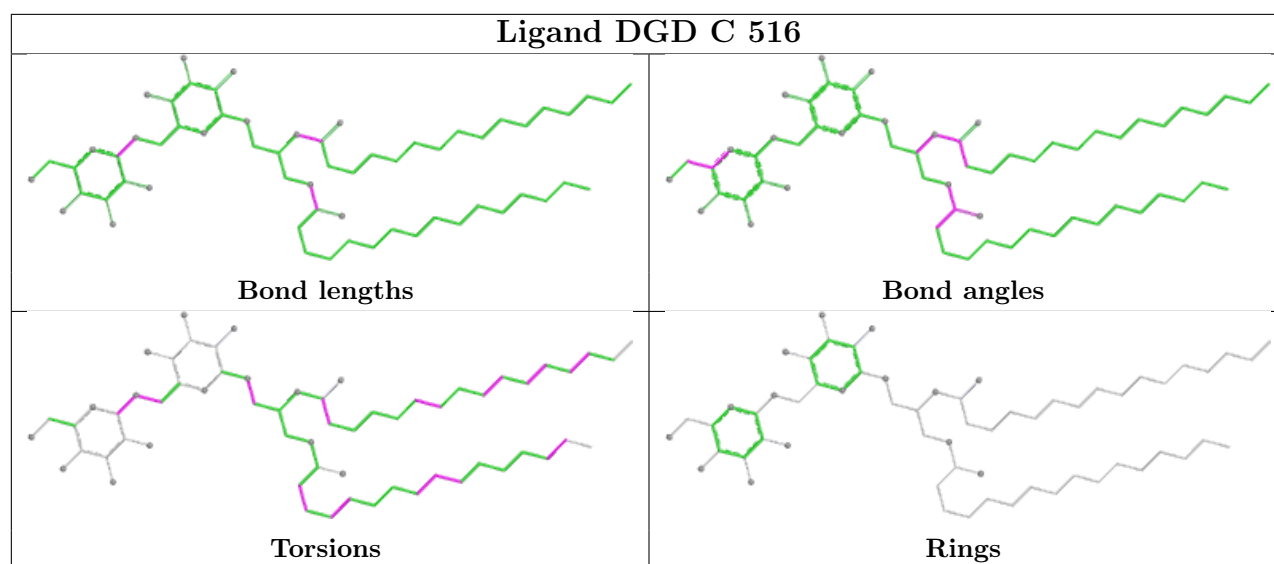


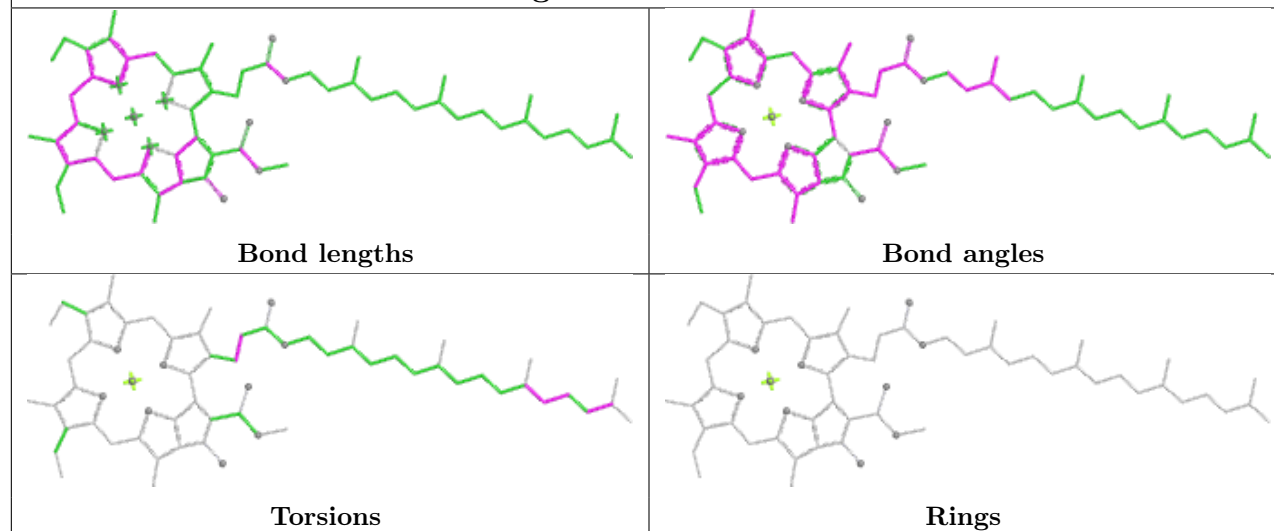
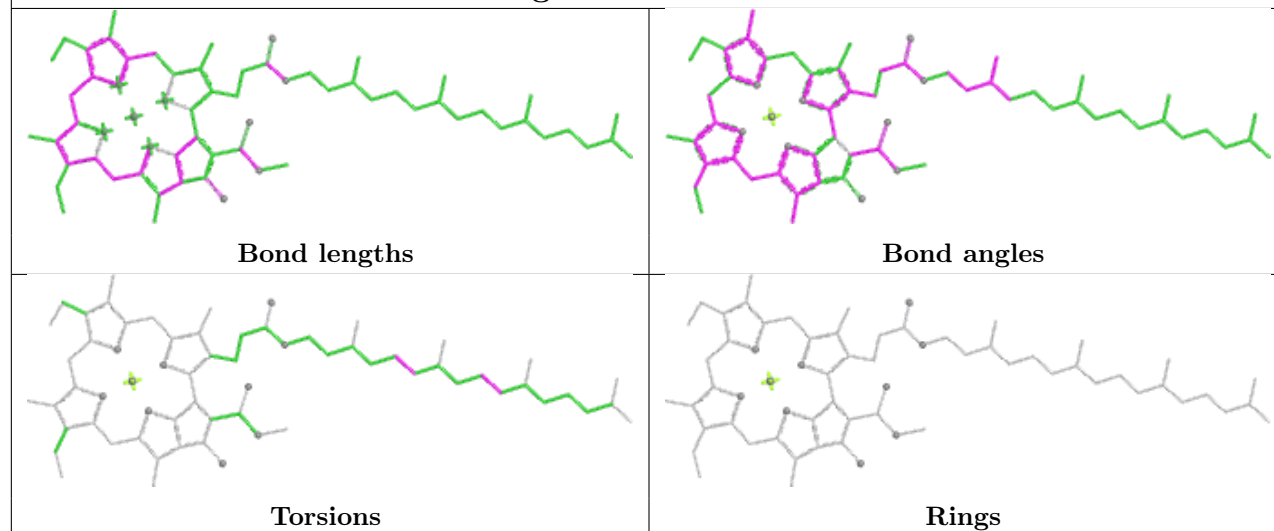


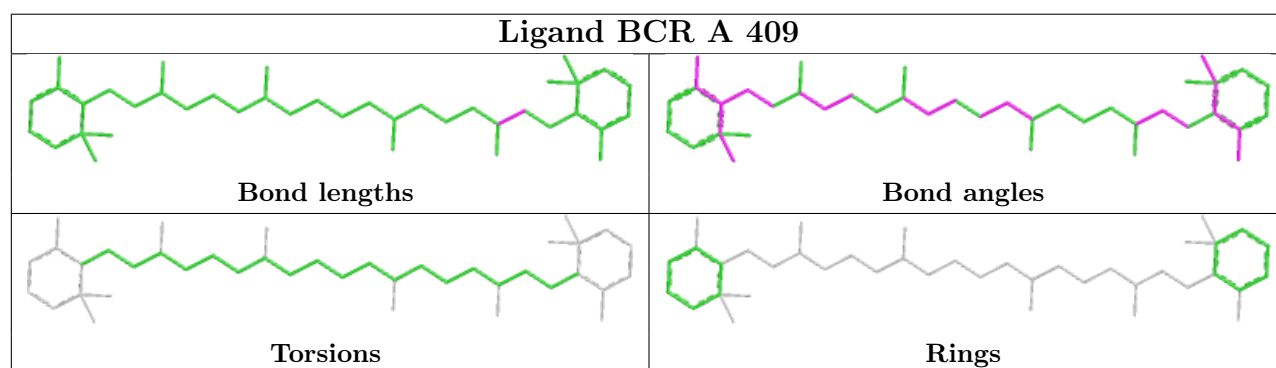
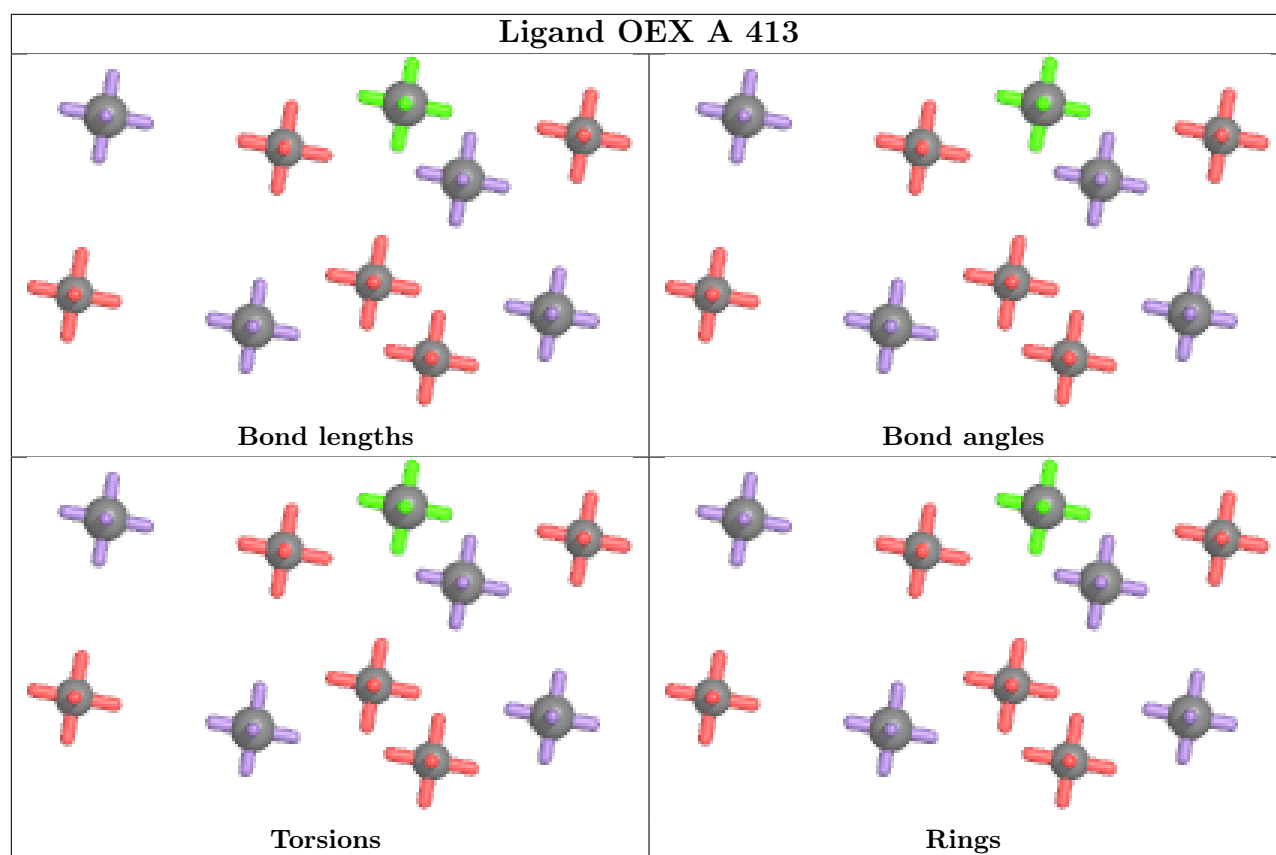
Ligand BCR Y 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

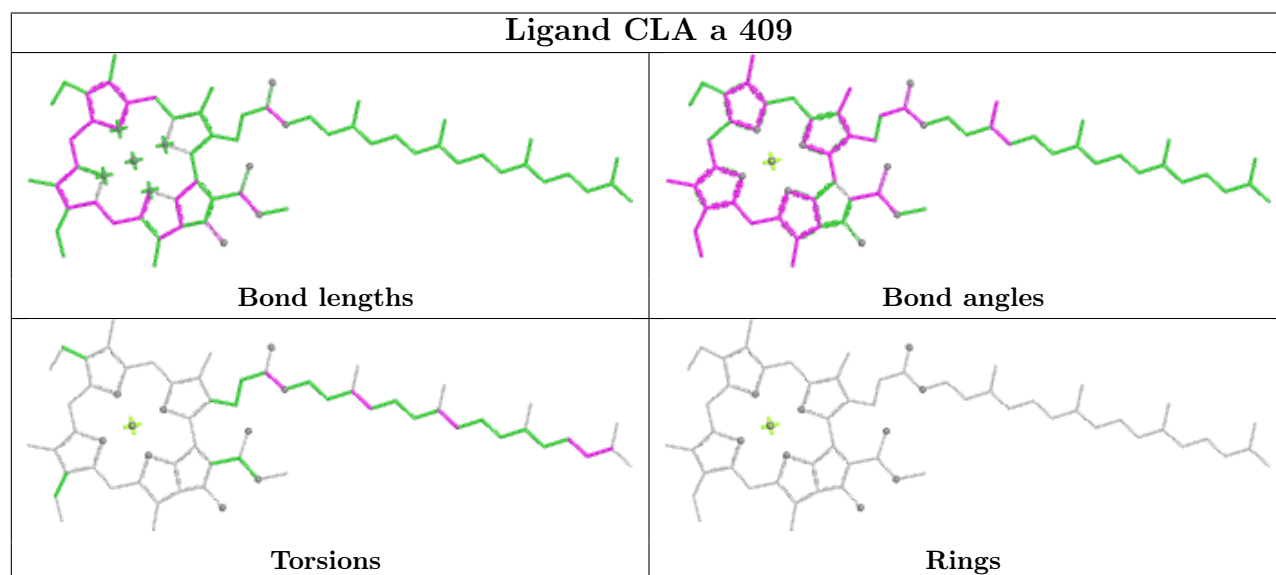
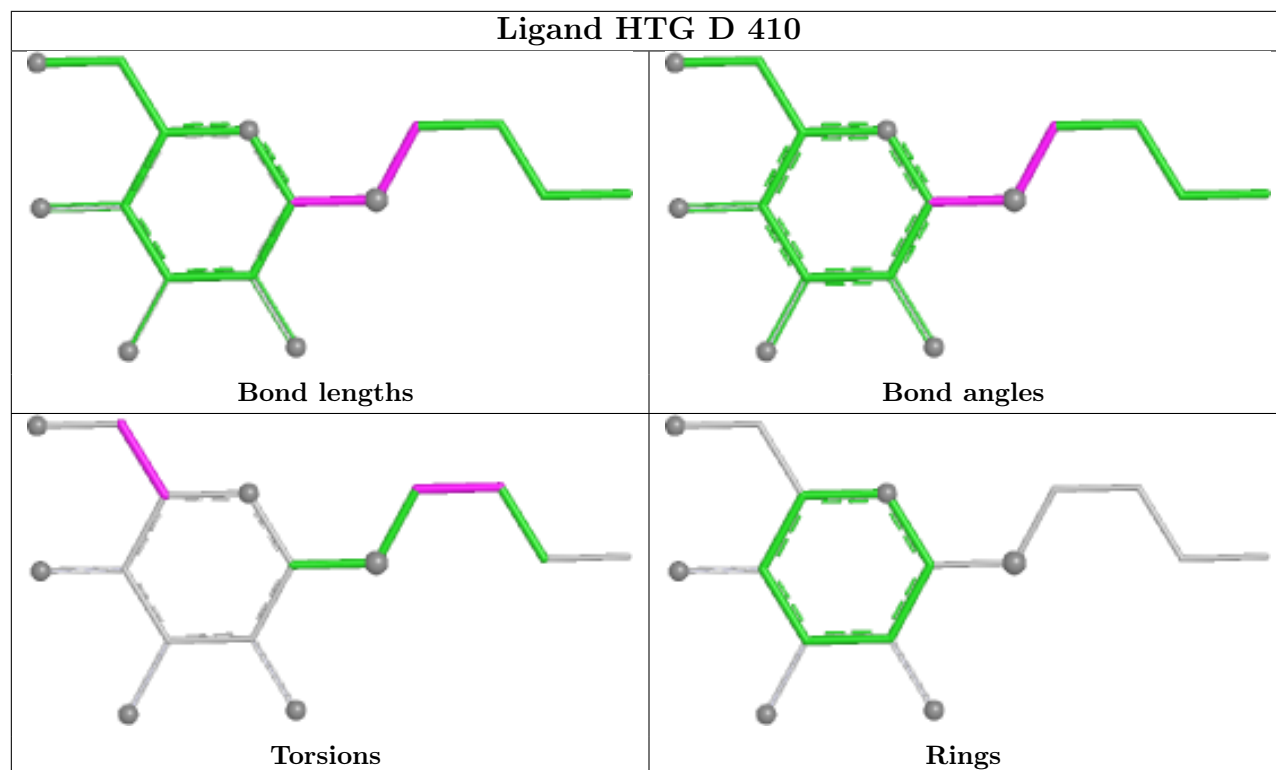
Ligand BCR b 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

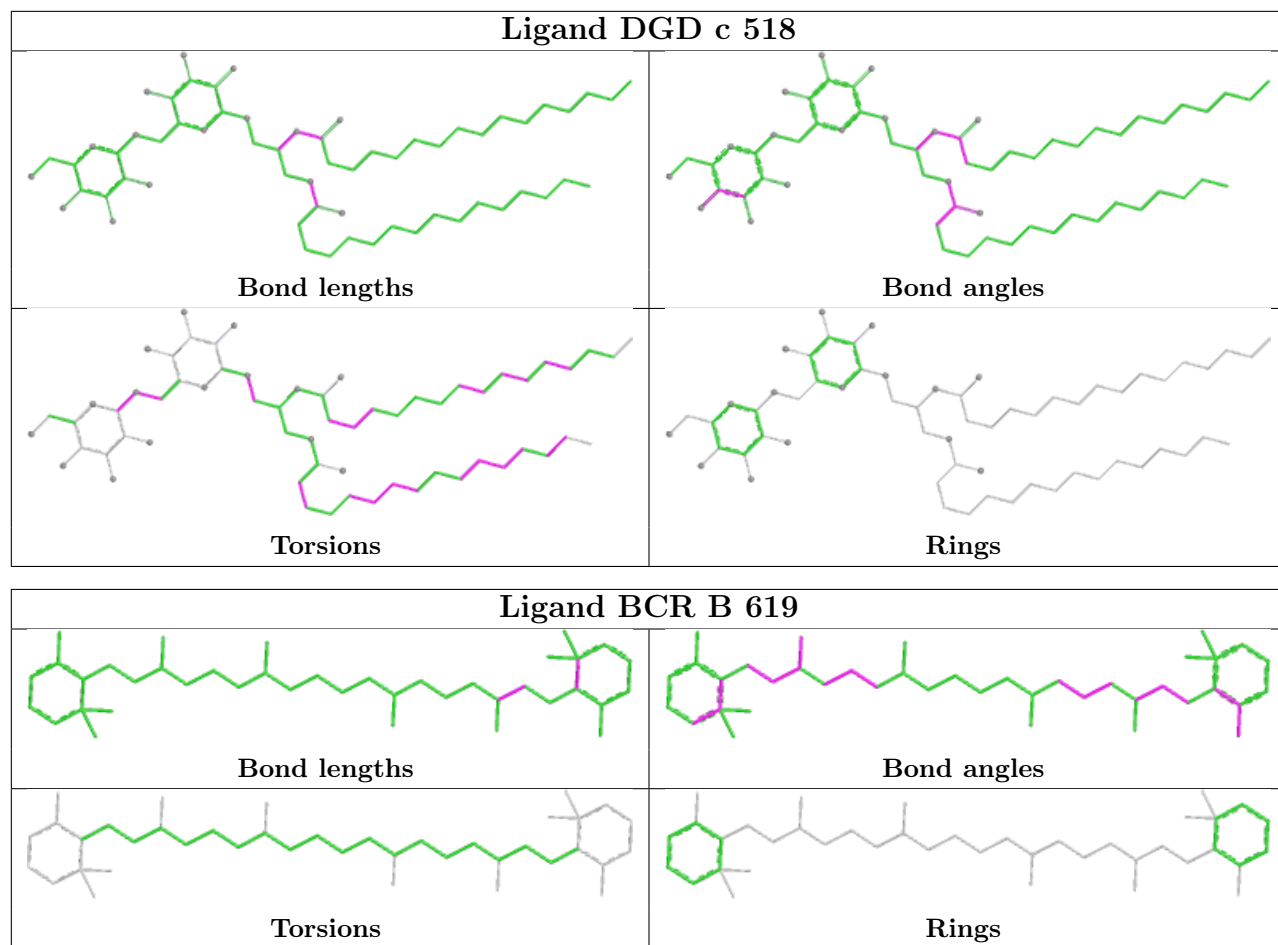
Ligand LMT B 631	
	
Bond lengths	Bond angles
	
Torsions	Rings



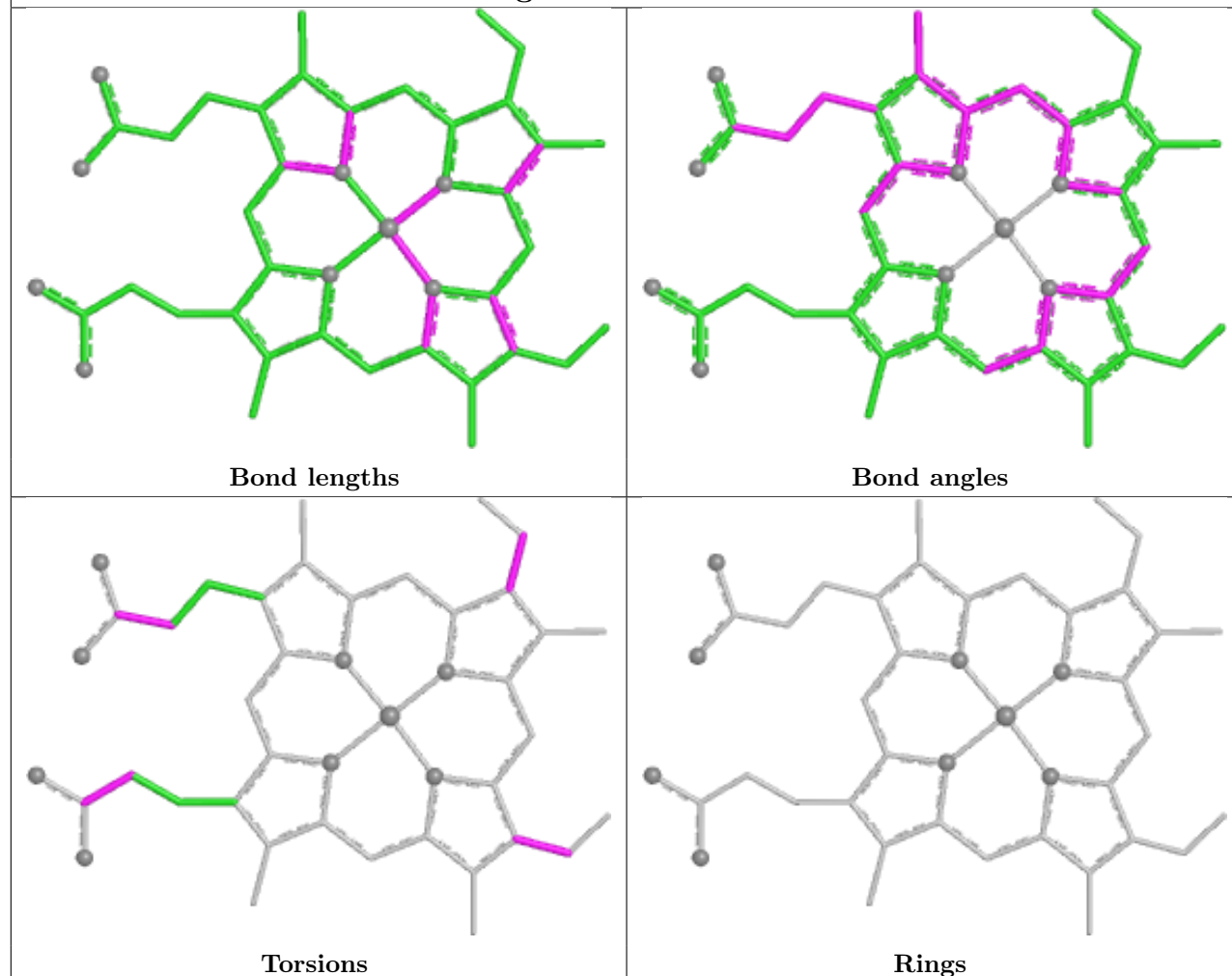
Ligand CLA B 610**Ligand CLA C 508**



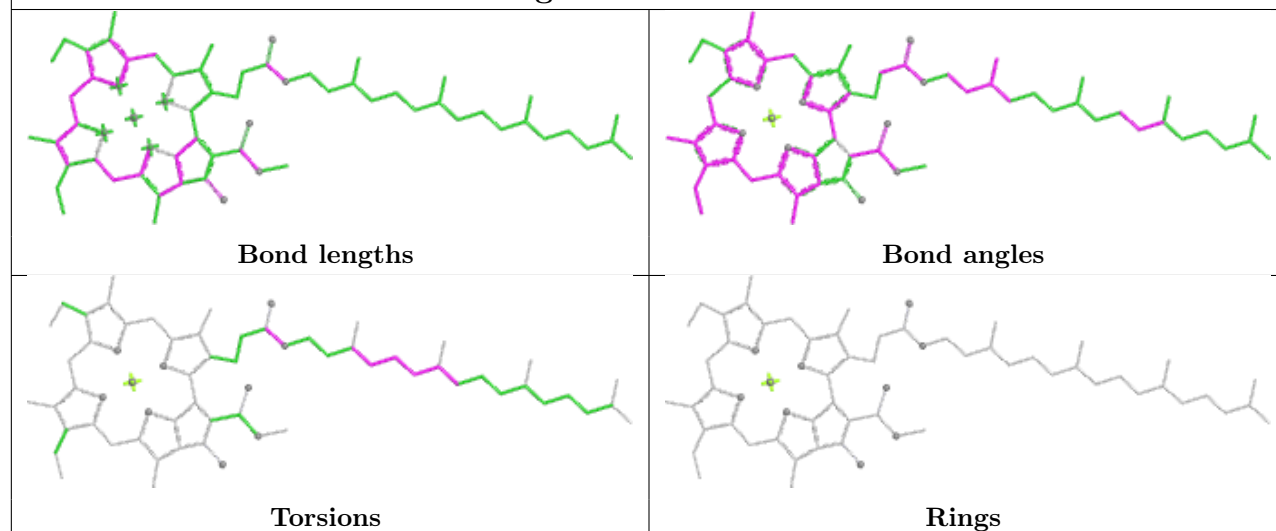


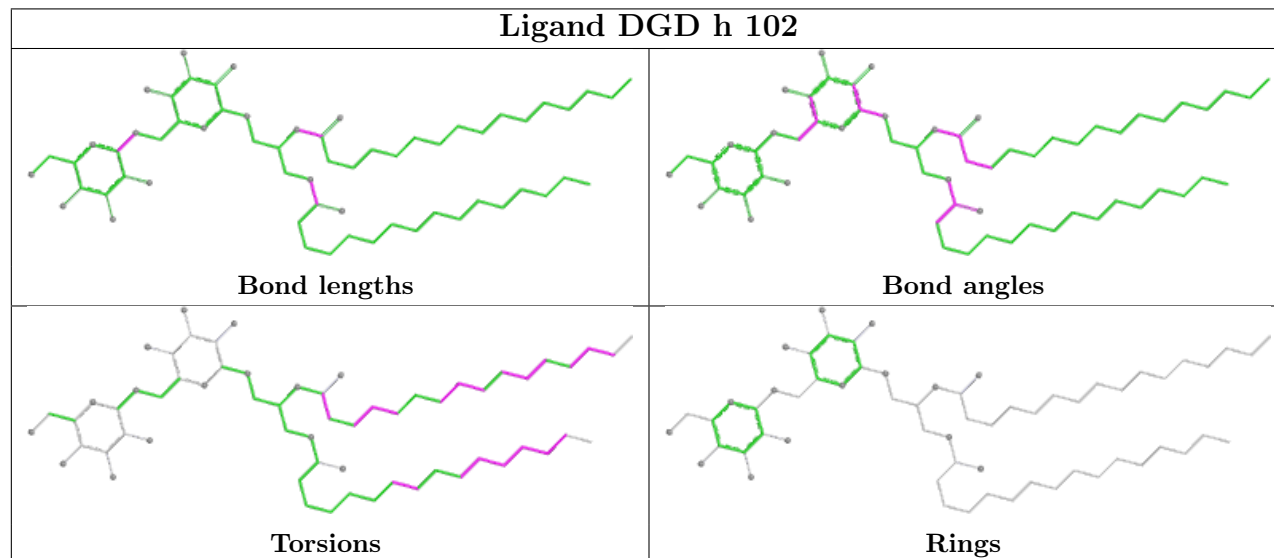
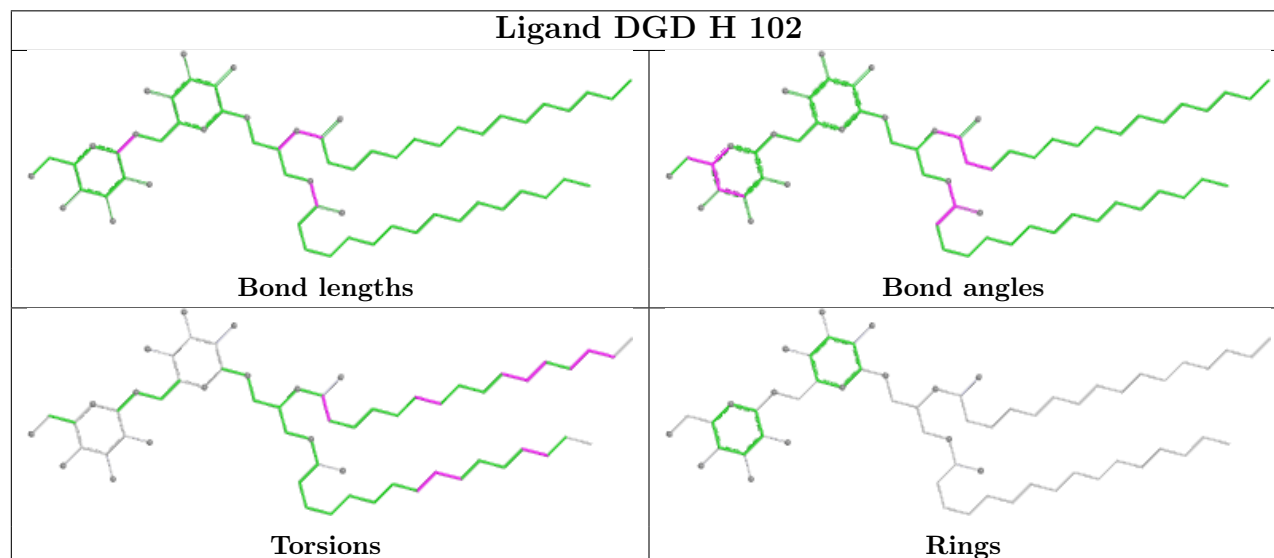
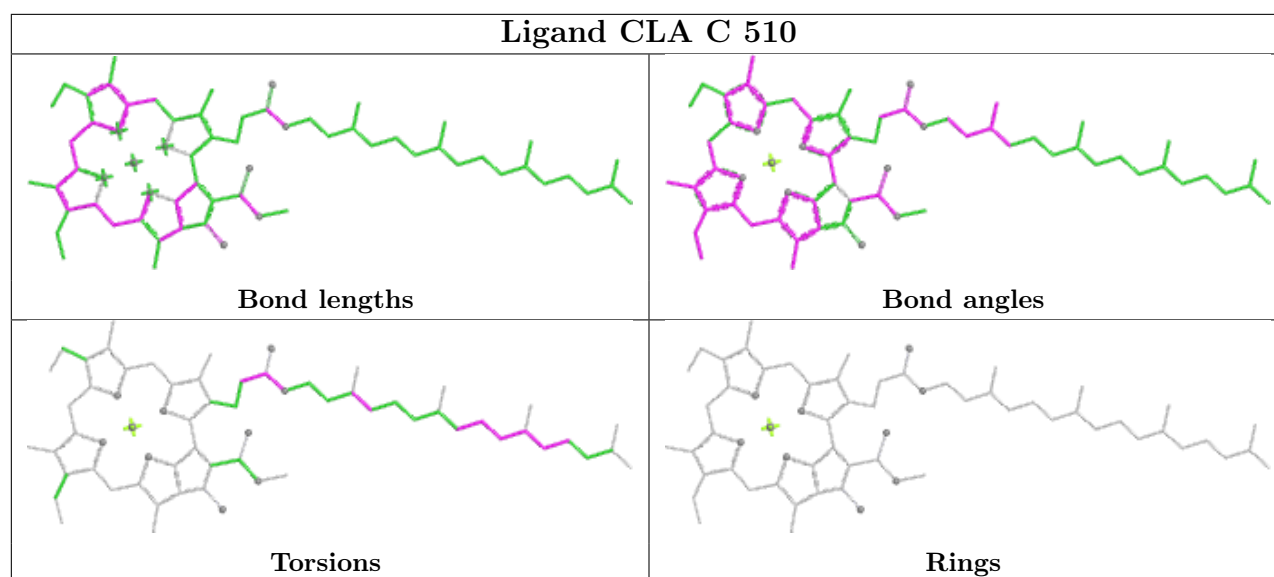


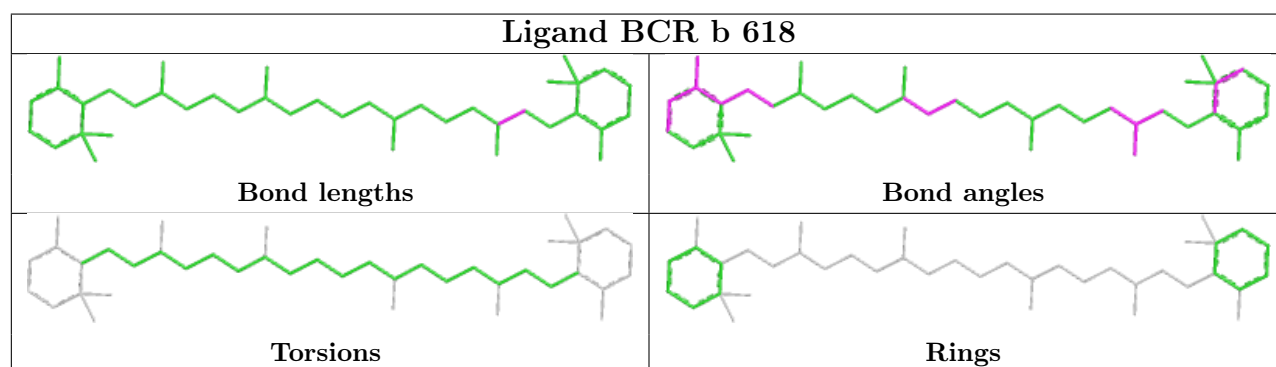
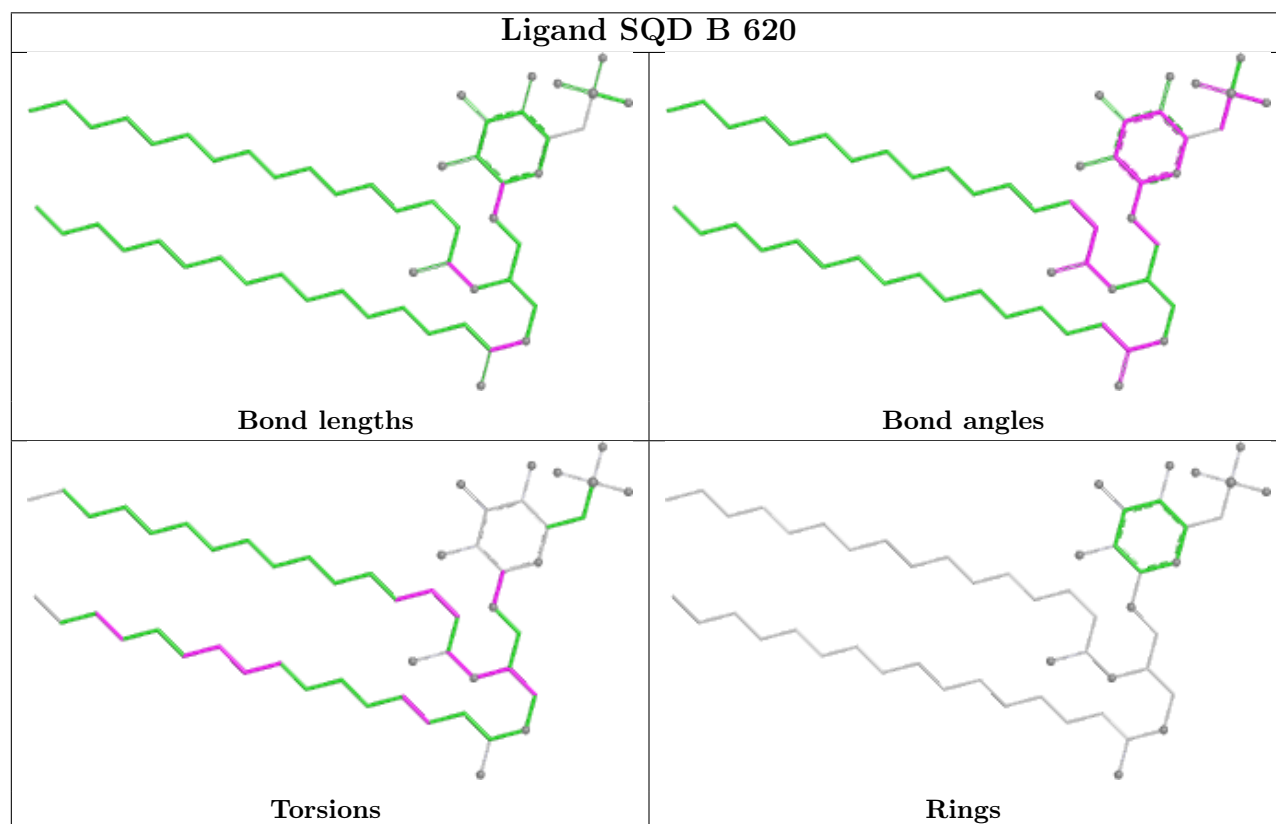
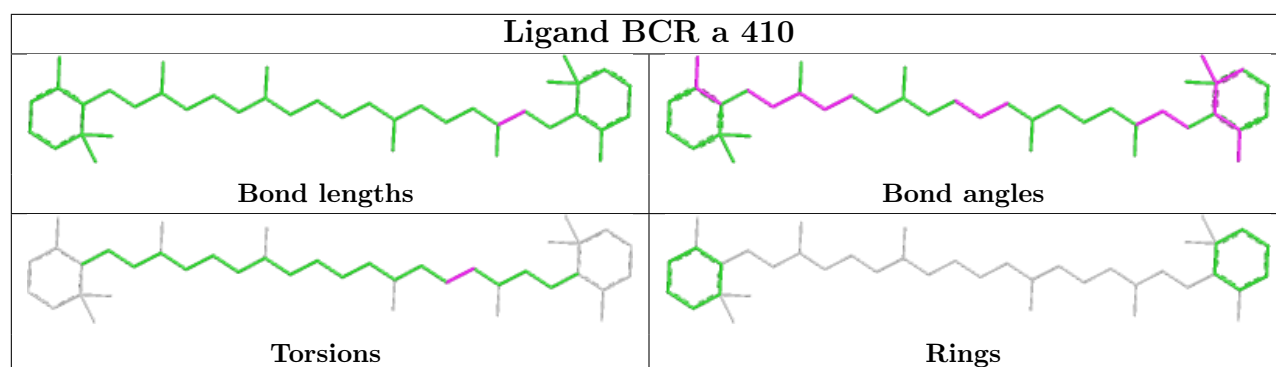
Ligand HEM f 101



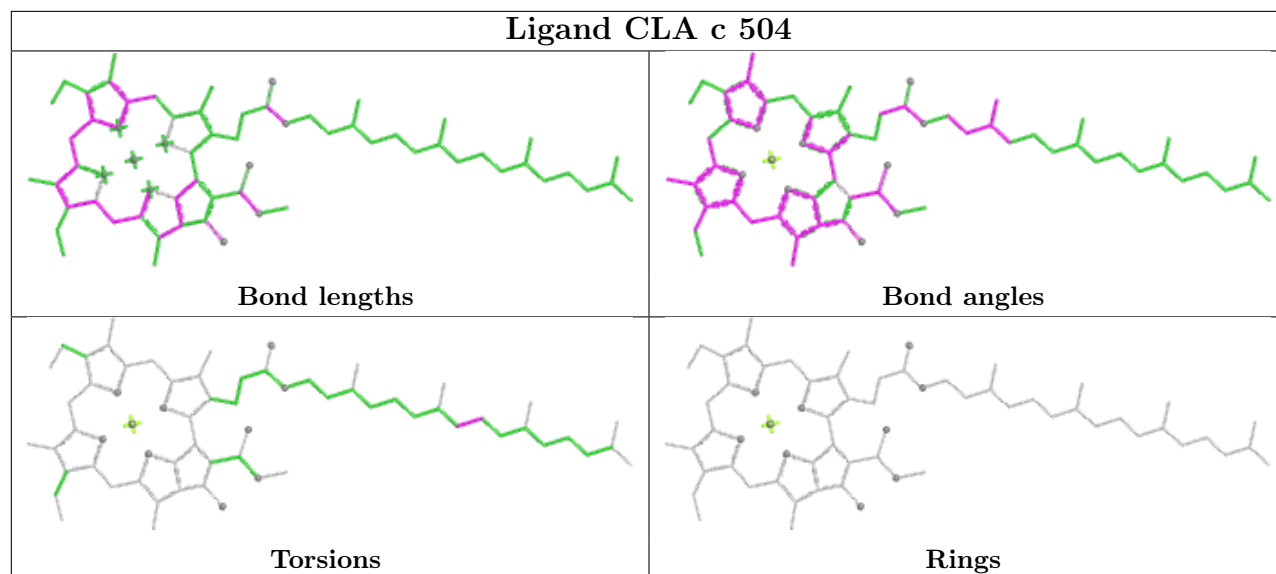
Ligand CLA b 616



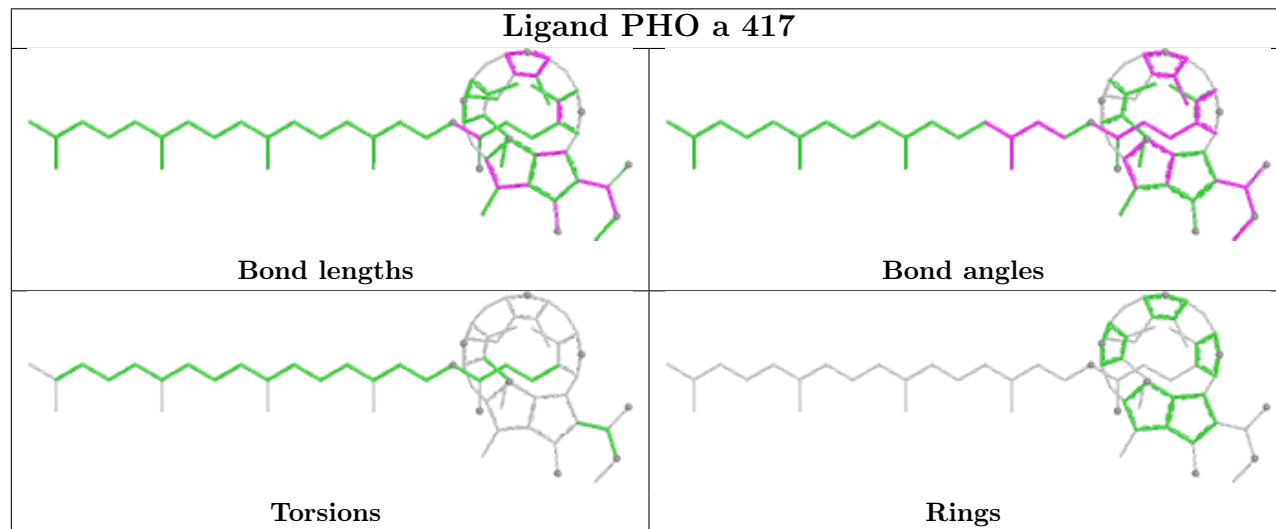


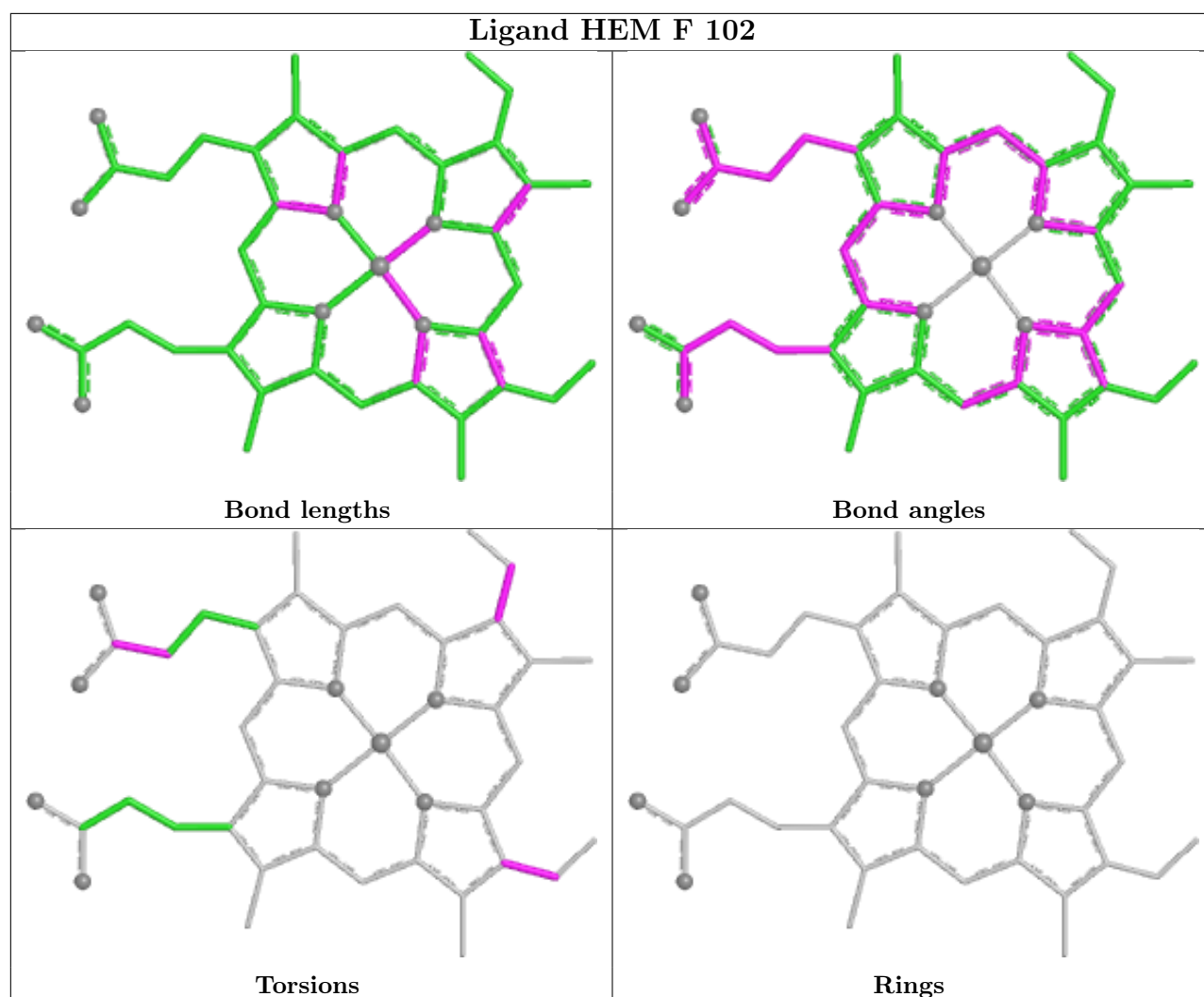


Ligand CLA c 504



Ligand PHO a 417





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%)	-0.43	1 (0%) 90 91	24, 48, 69, 119	1 (0%)
1	a	334/344 (97%)	-0.43	2 (0%) 85 87	26, 52, 79, 125	2 (0%)
2	B	504/505 (99%)	-0.32	2 (0%) 88 90	22, 54, 79, 111	7 (1%)
2	b	504/505 (99%)	-0.25	8 (1%) 70 74	24, 58, 95, 164	6 (1%)
3	C	451/455 (99%)	-0.39	2 (0%) 88 90	30, 59, 79, 159	1 (0%)
3	c	455/455 (100%)	-0.38	1 (0%) 91 92	29, 66, 85, 128	5 (1%)
4	D	342/342 (100%)	-0.46	0 100 100	23, 50, 67, 137	1 (0%)
4	d	341/342 (99%)	-0.49	0 100 100	24, 54, 75, 131	2 (0%)
5	E	81/84 (96%)	-0.18	2 (2%) 58 62	53, 68, 94, 167	0
5	e	79/84 (94%)	-0.15	1 (1%) 75 78	33, 75, 110, 146	2 (2%)
6	F	34/44 (77%)	-0.43	0 100 100	54, 62, 83, 114	0
6	f	31/44 (70%)	-0.17	2 (6%) 25 28	55, 66, 89, 155	1 (3%)
7	H	64/65 (98%)	-0.10	2 (3%) 51 55	52, 61, 78, 106	0
7	h	64/65 (98%)	-0.21	1 (1%) 70 74	37, 69, 88, 110	1 (1%)
8	I	37/38 (97%)	0.05	1 (2%) 56 60	55, 63, 122, 168	0
8	i	37/38 (97%)	-0.09	1 (2%) 56 60	56, 64, 116, 142	0
9	J	38/39 (97%)	-0.17	0 100 100	52, 70, 117, 179	0
9	j	39/39 (100%)	-0.13	1 (2%) 57 61	59, 77, 125, 170	0
10	K	37/37 (100%)	-0.55	0 100 100	60, 68, 88, 102	0
10	k	37/37 (100%)	-0.41	0 100 100	65, 74, 95, 105	0
11	L	36/37 (97%)	-0.37	0 100 100	42, 47, 90, 145	0
11	l	36/37 (97%)	-0.36	2 (5%) 30 34	43, 49, 99, 122	0
12	M	32/36 (88%)	-0.36	0 100 100	26, 50, 70, 139	1 (3%)
12	m	33/36 (91%)	-0.28	0 100 100	24, 50, 70, 151	2 (6%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.36	0 100 100	35, 64, 113, 181	3 (1%)
13	o	243/244 (99%)	-0.29	0 100 100	45, 66, 117, 166	0
14	T	29/32 (90%)	-0.40	0 100 100	30, 48, 75, 116	1 (3%)
14	t	29/32 (90%)	-0.42	1 (3%) 48 52	45, 51, 77, 126	0
15	U	96/104 (92%)	-0.41	0 100 100	34, 59, 85, 91	1 (1%)
15	u	97/104 (93%)	-0.45	0 100 100	31, 63, 79, 135	1 (1%)
16	V	137/137 (100%)	-0.51	0 100 100	32, 57, 77, 101	2 (1%)
16	v	137/137 (100%)	-0.47	0 100 100	54, 71, 98, 133	0
17	X	38/40 (95%)	-0.10	0 100 100	35, 71, 89, 113	1 (2%)
17	x	38/40 (95%)	0.17	1 (2%) 57 61	63, 77, 117, 164	0
18	Y	29/30 (96%)	0.21	1 (3%) 48 52	68, 84, 120, 129	0
18	y	29/30 (96%)	-0.08	0 100 100	74, 90, 107, 113	0
19	Z	62/62 (100%)	-0.20	0 100 100	67, 80, 136, 162	0
19	z	62/62 (100%)	0.29	0 100 100	80, 92, 140, 192	0
20	R	34/34 (100%)	0.78	3 (8%) 15 17	79, 101, 126, 136	0
All	All	5283/5384 (98%)	-0.33	35 (0%) 84 85	22, 59, 97, 192	41 (0%)

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	4.8
5	e	79[A]	PHE	4.7
2	b	479[A]	PHE	4.6
6	f	16[A]	PHE	4.2
8	i	37	LEU	3.5

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	T	1	10/11	0.94	0.08	47,54,66,71	0
8	FME	I	1	10/11	0.95	0.07	61,69,78,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	FME	t	1	10/11	0.95	0.07	47,51,60,72	0
12	FME	m	1	10/11	0.96	0.07	54,64,82,94	0
12	FME	M	1	10/11	0.97	0.07	48,62,84,86	0
8	FME	i	1	10/11	0.97	0.07	59,69,77,78	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
27	GOL	a	419	6/6	0.50	0.18	80,92,94,96	0
31	LMT	B	630	35/35	0.61	0.17	82,106,122,128	0
31	LMT	A	417	35/35	0.64	0.16	86,110,122,126	0
30	UNL	j	101	10/-	0.64	0.22	86,95,100,102	0
30	UNL	A	415	28/-	0.66	0.16	103,117,125,134	0
30	UNL	J	101	10/-	0.68	0.27	80,86,89,96	0
30	UNL	m	102	10/-	0.68	0.22	80,83,89,95	0
31	LMT	F	101	35/35	0.68	0.17	115,135,160,163	0
30	UNL	a	416	30/-	0.69	0.14	107,122,136,137	0
31	LMT	e	101	35/35	0.69	0.16	124,145,169,174	0
30	UNL	I	101	40/-	0.70	0.17	85,110,133,135	0
31	LMT	c	501	35/35	0.72	0.15	122,132,145,151	0
31	LMT	A	421	35/35	0.72	0.14	121,134,154,156	0
34	HTG	B	623	19/19	0.72	0.17	71,85,102,104	0
34	HTG	C	520	19/19	0.73	0.14	121,127,141,144	0
30	UNL	K	102	34/-	0.74	0.14	94,112,126,126	0
26	SQD	f	102	43/54	0.74	0.14	115,129,152,155	0
30	UNL	i	101	40/-	0.75	0.15	82,104,130,136	0
27	GOL	o	302	6/6	0.75	0.18	88,101,106,109	0
30	UNL	l	101	10/-	0.75	0.17	73,79,91,91	0
32	LMG	C	519	51/55	0.76	0.13	69,116,136,139	0
30	UNL	D	409	40/-	0.76	0.14	74,93,114,120	0
31	LMT	b	621	25/35	0.76	0.14	94,115,138,141	0
36	CA	F	104	1/1	0.76	0.25	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	UNL	d	408	36/-	0.77	0.13	73,97,115,119	0
27	GOL	b	629	6/6	0.77	0.14	58,69,75,76	0
27	GOL	B	627	6/6	0.77	0.13	73,76,85,102	0
34	HTG	D	410	16/19	0.77	0.13	94,109,119,129	0
27	GOL	o	303	6/6	0.77	0.16	86,90,93,96	0
33	LHG	a	421	42/49	0.78	0.12	99,144,155,158	0
27	GOL	l	102	6/6	0.78	0.18	71,97,99,101	0
31	LMT	B	628	35/35	0.78	0.13	79,103,120,123	0
30	UNL	b	626	33/-	0.78	0.14	72,99,138,140	0
30	UNL	c	525	32/-	0.78	0.15	100,115,126,133	0
30	UNL	B	626	33/-	0.79	0.16	67,102,124,131	0
27	GOL	a	420	6/6	0.80	0.16	64,71,78,79	0
31	LMT	T	101	35/35	0.80	0.12	85,118,145,149	0
27	GOL	b	624	6/6	0.80	0.17	93,95,96,107	0
31	LMT	b	627	25/35	0.80	0.15	69,89,123,125	0
27	GOL	O	302	6/6	0.80	0.10	86,95,97,100	0
27	GOL	A	411	6/6	0.80	0.14	69,77,81,82	0
27	GOL	A	418	6/6	0.81	0.17	57,75,75,77	0
27	GOL	O	303	6/6	0.81	0.13	86,95,97,100	0
26	SQD	A	412	54/54	0.81	0.12	73,92,117,124	0
26	SQD	a	413	54/54	0.82	0.10	76,95,120,124	0
31	LMT	M	101	35/35	0.82	0.12	67,90,98,103	0
32	LMG	Z	101	37/55	0.82	0.15	77,118,134,143	0
34	HTG	c	522	19/19	0.82	0.10	123,132,138,140	0
29	PL9	A	414	55/55	0.82	0.15	76,100,113,116	0
36	CA	f	103	1/1	0.82	0.13	125,125,125,125	0
34	HTG	V	202	11/19	0.83	0.10	92,107,115,116	0
34	HTG	b	622	19/19	0.83	0.13	70,80,87,96	0
34	HTG	b	623	19/19	0.83	0.12	93,129,136,139	0
31	LMT	B	631	25/35	0.83	0.14	70,91,121,130	0
31	LMT	m	103	35/35	0.83	0.12	69,89,99,104	0
31	LMT	t	101	26/35	0.83	0.14	89,110,127,136	0
27	GOL	a	412	6/6	0.84	0.14	75,79,87,88	0
34	HTG	d	409	16/19	0.84	0.11	99,117,124,135	0
32	LMG	c	521	51/55	0.84	0.11	80,125,148,151	0
34	HTG	B	622	19/19	0.84	0.13	66,83,92,93	0
29	PL9	a	415	55/55	0.85	0.15	88,111,123,129	0
26	SQD	B	620	54/54	0.85	0.12	75,96,117,127	0
27	GOL	v	202	6/6	0.86	0.11	66,78,83,85	0
27	GOL	c	527	6/6	0.86	0.18	107,114,117,121	0
32	LMG	z	101	39/55	0.87	0.12	81,123,136,146	0
33	LHG	E	101	42/49	0.87	0.12	79,104,117,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	UNL	D	408	17/-	0.87	0.12	66,75,99,104	0
26	SQD	b	620	54/54	0.87	0.10	69,92,107,117	0
27	GOL	V	203	6/6	0.87	0.13	60,68,74,76	0
26	SQD	F	103	43/54	0.87	0.11	70,95,116,122	0
23	CLA	b	601	65/65	0.87	0.10	66,85,114,125	0
34	HTG	B	625	19/19	0.89	0.09	77,81,92,95	0
32	LMG	A	419	51/55	0.89	0.10	79,91,102,109	0
23	CLA	B	601	65/65	0.90	0.09	57,77,100,115	0
32	LMG	B	621	51/55	0.90	0.10	61,74,87,95	0
32	LMG	C	518	51/55	0.90	0.10	58,84,102,108	0
30	UNL	d	407	17/-	0.90	0.10	74,83,97,98	0
32	LMG	a	418	51/55	0.90	0.09	74,92,100,113	0
32	LMG	c	520	51/55	0.90	0.09	63,91,116,123	0
27	GOL	B	629	6/6	0.90	0.16	53,63,68,74	0
32	LMG	m	101	51/55	0.90	0.10	62,77,90,99	0
36	CA	o	301	1/1	0.90	0.07	102,102,102,102	0
27	GOL	C	521	6/6	0.91	0.14	57,60,65,66	0
25	BCR	T	102	40/40	0.91	0.07	47,58,68,69	0
32	LMG	D	411	51/55	0.91	0.10	51,67,103,106	0
23	CLA	b	616	65/65	0.92	0.09	54,62,117,125	0
34	HTG	b	625	19/19	0.92	0.08	71,82,88,96	0
23	CLA	c	514	65/65	0.92	0.09	71,89,112,120	0
33	LHG	A	420	49/49	0.92	0.10	52,65,81,84	0
27	GOL	B	624	6/6	0.92	0.08	73,77,85,86	0
32	LMG	d	410	51/55	0.92	0.09	58,71,102,107	0
23	CLA	C	513	65/65	0.92	0.08	65,83,103,109	0
23	CLA	C	506	65/65	0.93	0.09	59,69,103,104	0
25	BCR	d	403	40/40	0.93	0.08	53,67,92,95	0
33	LHG	d	411	49/49	0.93	0.09	57,68,77,81	0
25	BCR	t	102	40/40	0.93	0.07	48,57,75,79	0
26	SQD	A	410	54/54	0.93	0.09	59,81,104,109	0
23	CLA	A	408	65/65	0.93	0.09	45,53,110,114	0
23	CLA	B	614	65/65	0.93	0.08	43,51,85,92	0
23	CLA	b	614	65/65	0.93	0.07	45,52,84,88	0
26	SQD	a	411	54/54	0.93	0.09	64,84,111,117	0
23	CLA	B	616	65/65	0.93	0.10	49,59,106,115	0
23	CLA	c	507	65/65	0.93	0.08	58,69,100,105	0
23	CLA	c	513	65/65	0.93	0.09	66,80,114,117	0
23	CLA	C	504	65/65	0.93	0.08	47,56,89,99	0
23	CLA	d	402	65/65	0.93	0.09	55,65,113,123	0
35	DGD	C	516	62/66	0.93	0.08	51,64,102,106	0
25	BCR	D	404	40/40	0.93	0.09	50,60,92,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	BCR	K	101	40/40	0.93	0.08	62,76,85,89	0
33	LHG	D	407	49/49	0.93	0.09	52,61,99,105	0
27	GOL	c	526	6/6	0.94	0.07	65,65,71,74	0
25	BCR	h	101	40/40	0.94	0.09	57,68,87,93	0
30	UNL	X	101	18/-	0.94	0.12	66,74,99,102	0
23	CLA	b	606	65/65	0.94	0.08	48,60,97,106	0
23	CLA	C	512	65/65	0.94	0.08	63,72,101,106	0
23	CLA	B	606	65/65	0.94	0.08	44,57,97,104	0
25	BCR	H	101	40/40	0.94	0.08	53,65,85,87	0
23	CLA	c	505	65/65	0.94	0.07	56,63,97,100	0
25	BCR	K	103	40/40	0.94	0.09	57,64,72,74	0
23	CLA	a	409	65/65	0.94	0.10	47,55,113,119	0
25	BCR	Y	101	40/40	0.94	0.08	57,65,78,80	0
25	BCR	b	618	40/40	0.94	0.07	49,59,74,77	0
25	BCR	c	515	40/40	0.94	0.08	73,83,89,90	0
35	DGD	C	517	62/66	0.94	0.07	48,61,89,100	0
35	DGD	H	102	62/66	0.94	0.09	51,62,72,74	0
35	DGD	c	517	62/66	0.94	0.07	48,62,97,101	0
35	DGD	c	518	62/66	0.94	0.07	54,68,111,123	0
35	DGD	c	519	62/66	0.94	0.07	53,67,100,116	0
23	CLA	C	508	65/65	0.94	0.07	48,56,105,113	0
33	LHG	b	630	49/49	0.94	0.08	54,59,69,83	0
33	LHG	d	406	49/49	0.94	0.09	55,65,109,123	0
23	CLA	C	501	65/65	0.95	0.06	52,61,70,76	0
29	PL9	D	405	55/55	0.95	0.07	39,51,57,66	0
23	CLA	A	406	65/65	0.95	0.06	40,49,109,115	0
29	PL9	d	404	55/55	0.95	0.07	43,52,60,65	0
23	CLA	b	607	65/65	0.95	0.07	40,49,72,77	0
23	CLA	b	609	65/65	0.95	0.07	51,64,72,80	0
23	CLA	b	612	65/65	0.95	0.08	43,52,61,66	0
23	CLA	B	609	65/65	0.95	0.07	49,59,69,74	0
25	BCR	a	410	40/40	0.95	0.07	46,55,62,64	0
23	CLA	B	610	65/65	0.95	0.09	46,56,61,75	0
25	BCR	b	619	40/40	0.95	0.07	52,62,82,86	0
23	CLA	B	611	65/65	0.95	0.07	41,47,64,67	0
23	CLA	B	602	65/65	0.95	0.07	48,56,67,77	0
23	CLA	c	508	65/65	0.95	0.08	56,68,79,83	0
23	CLA	c	509	65/65	0.95	0.07	51,62,115,121	0
25	BCR	y	101	40/40	0.95	0.07	62,71,80,86	0
27	GOL	b	628	6/6	0.95	0.07	79,84,94,95	0
23	CLA	D	403	65/65	0.95	0.08	51,59,104,108	0
23	CLA	a	407	65/65	0.95	0.07	43,54,120,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	B	603	65/65	0.95	0.08	44,52,70,74	0
25	BCR	A	409	40/40	0.95	0.07	42,53,65,66	0
30	UNL	x	101	18/-	0.95	0.11	75,83,119,121	0
35	DGD	h	102	62/66	0.95	0.08	57,65,74,79	0
25	BCR	B	618	40/40	0.95	0.06	47,56,69,74	0
36	CA	O	301	1/1	0.95	0.04	100,100,100,100	0
25	BCR	B	619	40/40	0.95	0.07	51,60,83,88	0
25	BCR	C	514	40/40	0.95	0.06	55,64,71,80	0
37	BCT	a	404	4/4	0.95	0.07	58,60,68,77	0
24	PHO	A	416	64/64	0.96	0.06	39,51,58,64	0
24	PHO	a	417	64/64	0.96	0.06	46,54,62,68	0
33	LHG	d	405	49/49	0.96	0.07	49,58,72,76	0
23	CLA	b	604	65/65	0.96	0.07	42,52,87,99	0
25	BCR	B	617	40/40	0.96	0.06	45,53,61,64	0
23	CLA	b	605	65/65	0.96	0.07	43,51,71,77	0
23	CLA	B	612	65/65	0.96	0.06	39,49,59,63	0
23	CLA	C	507	65/65	0.96	0.07	52,62,78,87	0
23	CLA	B	613	65/65	0.96	0.06	41,47,84,90	0
23	CLA	b	611	65/65	0.96	0.06	43,51,66,70	0
23	CLA	C	509	65/65	0.96	0.07	52,58,77,80	0
23	CLA	b	613	65/65	0.96	0.06	43,50,81,87	0
23	CLA	C	510	65/65	0.96	0.06	52,60,75,76	0
23	CLA	B	607	65/65	0.96	0.07	40,47,68,73	0
23	CLA	c	502	65/65	0.96	0.07	59,66,75,78	0
25	BCR	b	617	40/40	0.96	0.05	48,54,61,61	0
35	DGD	C	515	62/66	0.96	0.07	48,56,95,100	0
23	CLA	c	504	65/65	0.96	0.06	53,69,78,88	0
23	CLA	A	404	65/65	0.96	0.06	38,45,62,66	0
23	CLA	c	506	65/65	0.96	0.07	52,63,84,92	0
25	BCR	c	516	40/40	0.96	0.06	60,66,73,78	0
23	CLA	B	605	65/65	0.96	0.07	43,49,66,73	0
23	CLA	C	503	65/65	0.96	0.06	49,61,68,77	0
25	BCR	k	101	40/40	0.96	0.08	60,74,81,82	0
23	CLA	A	405	65/65	0.96	0.06	37,44,58,70	0
23	CLA	C	505	65/65	0.96	0.07	51,59,83,90	0
36	CA	c	523	1/1	0.96	0.08	75,75,75,75	0
33	LHG	D	406	49/49	0.96	0.07	48,56,68,73	0
23	CLA	b	602	65/65	0.96	0.07	52,60,72,76	0
23	CLA	b	603	65/65	0.96	0.07	47,58,78,84	0
23	CLA	B	604	65/65	0.97	0.06	41,47,97,103	0
23	CLA	c	510	65/65	0.97	0.07	49,64,83,85	0
23	CLA	c	511	65/65	0.97	0.06	53,63,74,89	0

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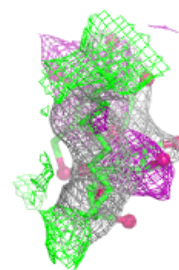
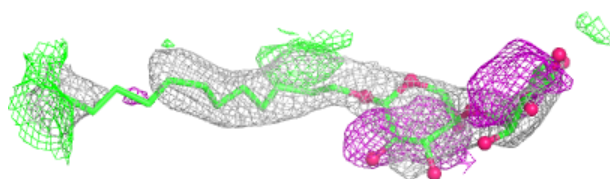
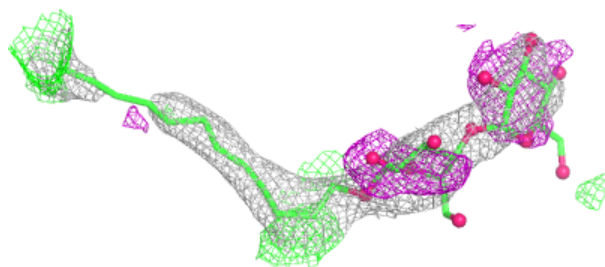
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	c	512	65/65	0.97	0.07	59,67,83,93	0
23	CLA	D	402	65/65	0.97	0.06	36,44,69,76	0
23	CLA	B	608	65/65	0.97	0.06	44,51,69,77	0
23	CLA	d	401	65/65	0.97	0.06	41,47,77,91	0
33	LHG	L	101	49/49	0.97	0.06	52,58,70,87	0
23	CLA	b	615	65/65	0.97	0.06	51,59,77,78	0
24	PHO	A	407	64/64	0.97	0.05	37,46,54,59	0
23	CLA	a	405	65/65	0.97	0.06	42,48,63,74	0
24	PHO	a	408	64/64	0.97	0.05	43,49,54,56	0
23	CLA	a	406	65/65	0.97	0.05	41,46,63,69	0
36	CA	C	522	1/1	0.97	0.05	73,73,73,73	0
23	CLA	c	503	65/65	0.97	0.07	49,60,89,107	0
23	CLA	C	502	65/65	0.97	0.06	48,56,78,85	0
23	CLA	b	608	65/65	0.97	0.05	46,56,78,86	0
23	CLA	C	511	65/65	0.97	0.07	52,64,77,80	0
23	CLA	b	610	65/65	0.97	0.07	51,58,64,69	0
37	BCT	D	401	4/4	0.97	0.06	54,58,61,66	0
23	CLA	B	615	65/65	0.97	0.06	46,54,74,80	0
38	HEM	f	101	43/43	0.97	0.09	67,81,101,109	0
22	CL	A	403	1/1	0.98	0.04	47,47,47,47	0
22	CL	a	403	1/1	0.98	0.08	52,52,52,52	0
38	HEM	F	102	43/43	0.98	0.06	60,68,75,85	0
22	CL	A	402	1/1	0.98	0.07	43,43,43,43	0
39	MG	J	102	1/1	0.98	0.03	59,59,59,59	0
40	HEC	V	201	43/43	0.98	0.06	44,51,56,57	0
40	HEC	v	201	43/43	0.98	0.07	55,61,67,69	0
36	CA	c	524	1/1	0.99	0.04	76,76,76,76	0
22	CL	a	402	1/1	0.99	0.05	50,50,50,50	0
28	OEX	A	413	10/10	0.99	0.03	41,44,48,50	0
39	MG	j	102	1/1	0.99	0.06	63,63,63,63	0
28	OEX	a	414	10/10	0.99	0.03	47,50,51,55	0
21	FE2	a	401	1/1	0.99	0.02	55,55,55,55	0
21	FE2	A	401	1/1	1.00	0.02	52,52,52,52	0

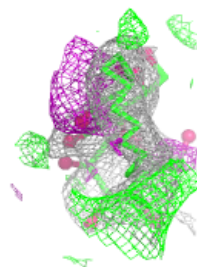
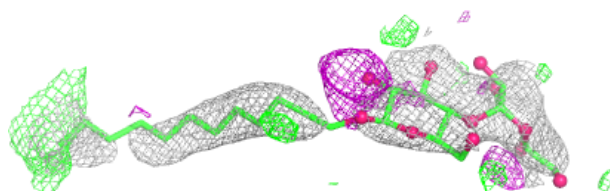
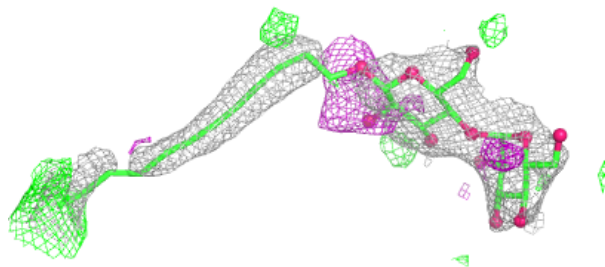
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT B 630:

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

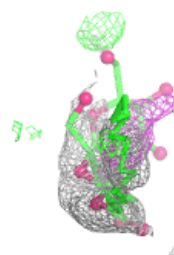
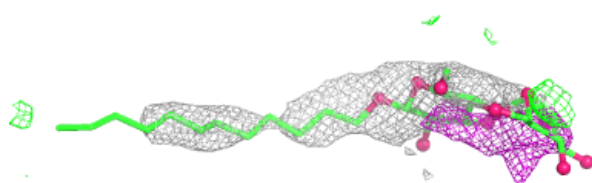
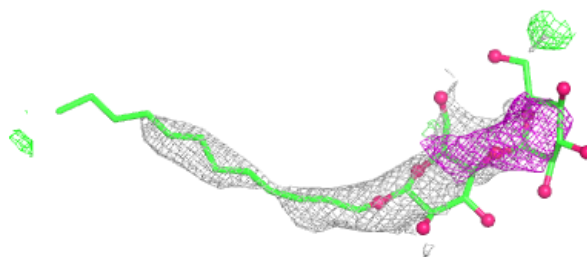
**Electron density around LMT A 417:**

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

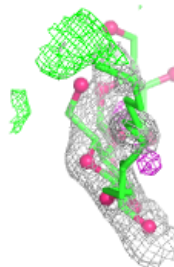
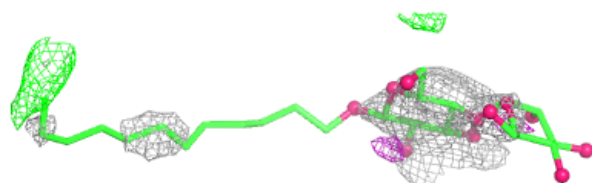
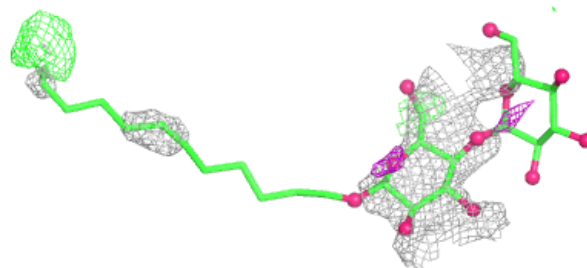


Electron density around LMT F 101:

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

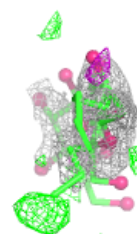
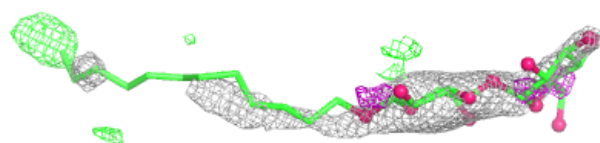
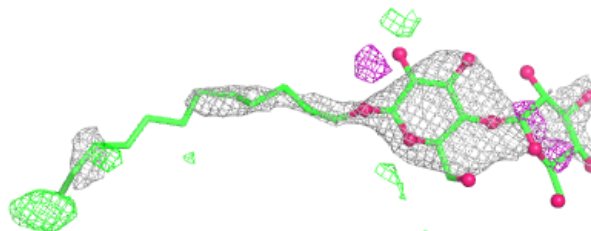
**Electron density around LMT e 101:**

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

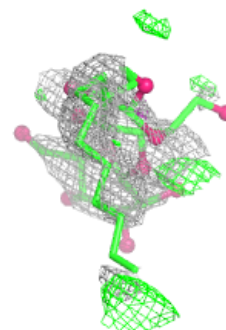
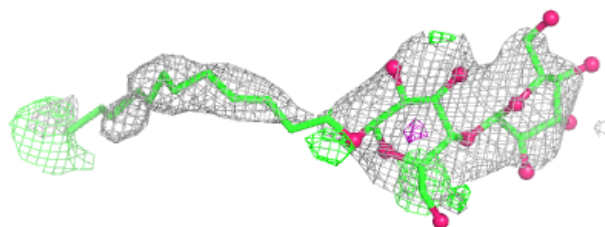
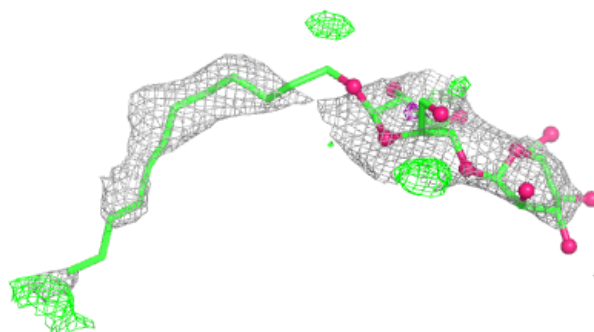


Electron density around LMT c 501:

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

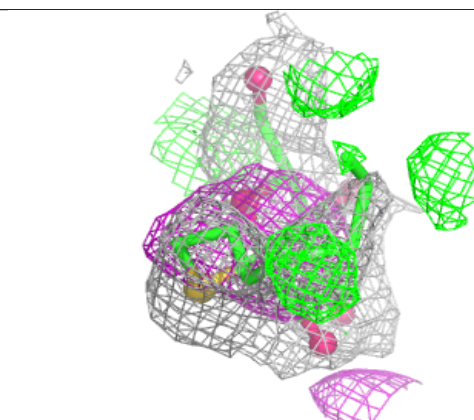
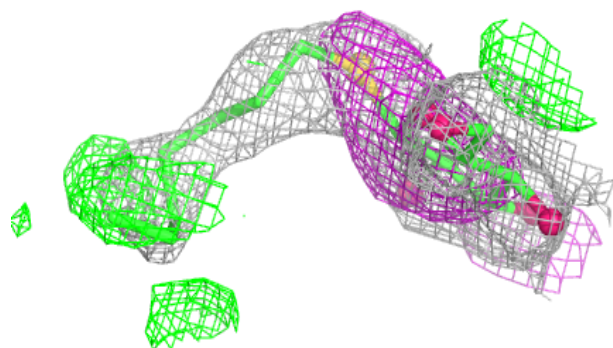
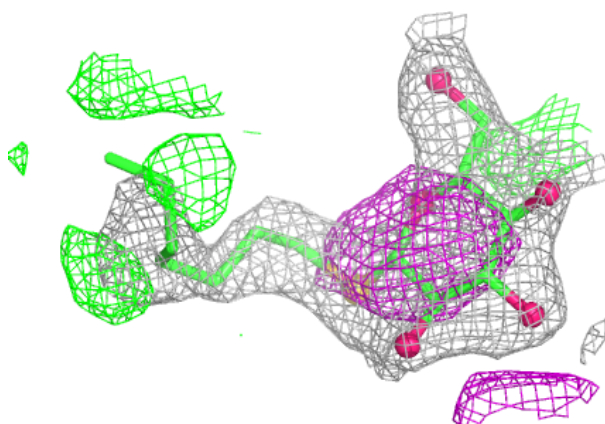
**Electron density around LMT A 421:**

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

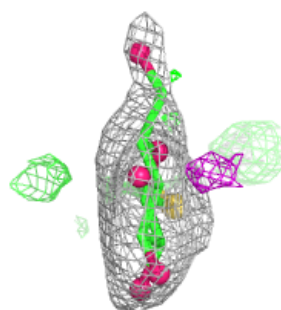
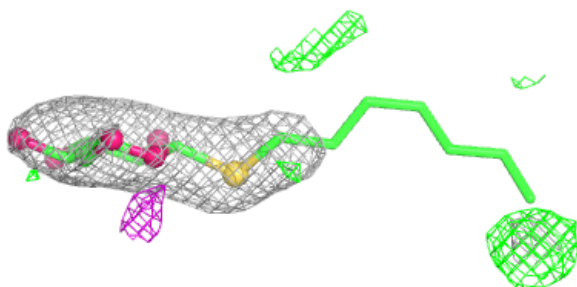
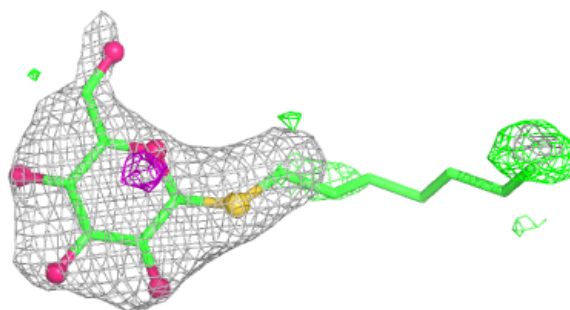


Electron density around HTG B 623:

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

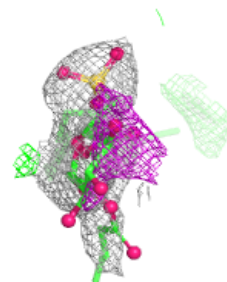
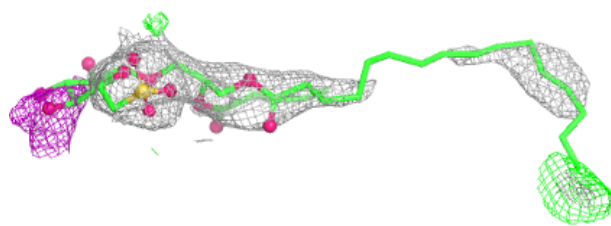
**Electron density around HTG C 520:**

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

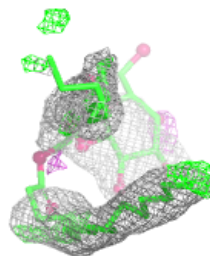
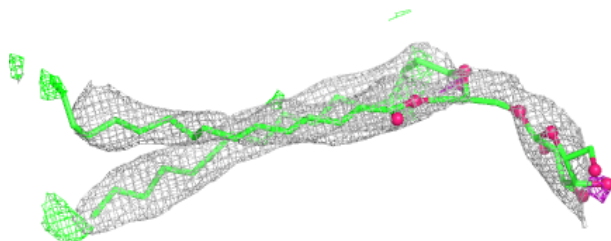
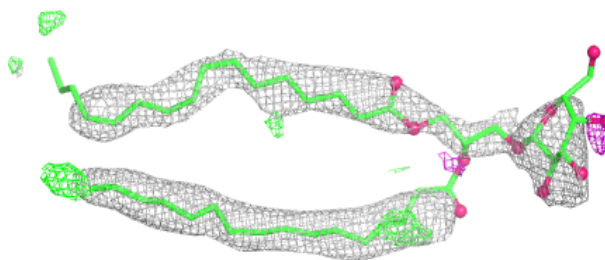


Electron density around SQD f 102:

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

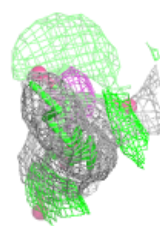
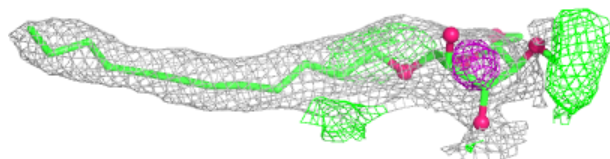
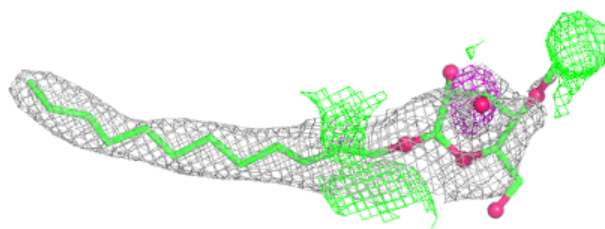
**Electron density around LMG C 519:**

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

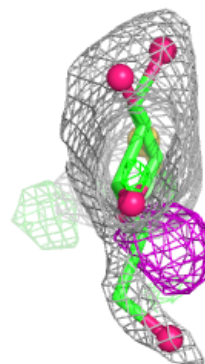
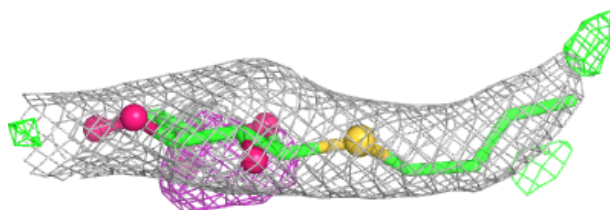
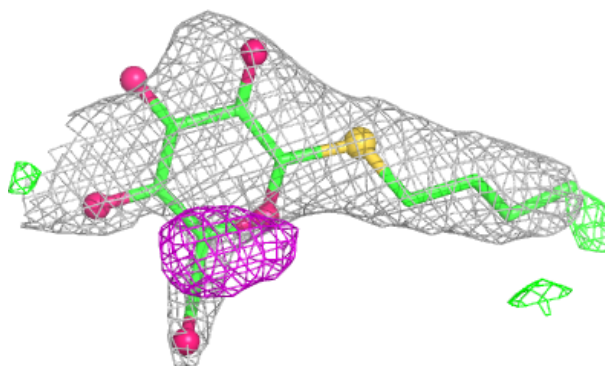


Electron density around LMT b 621:

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

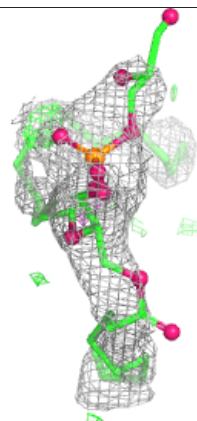
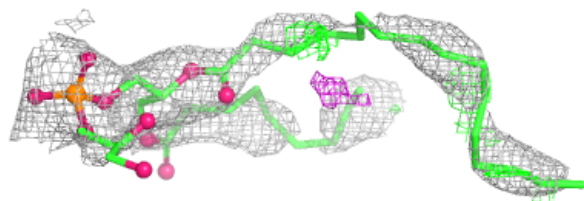
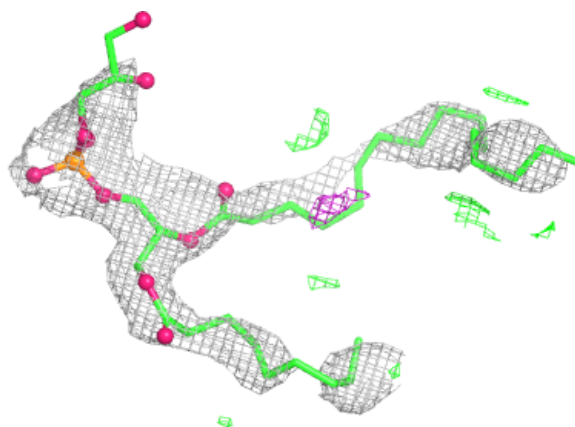
**Electron density around HTG D 410:**

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

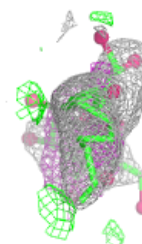
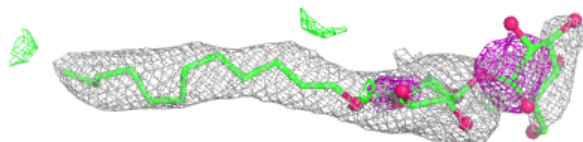
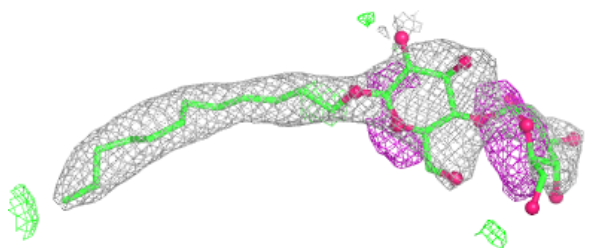


Electron density around LHG a 421:

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

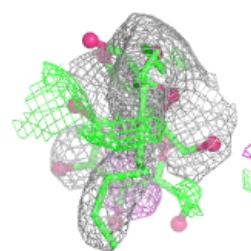
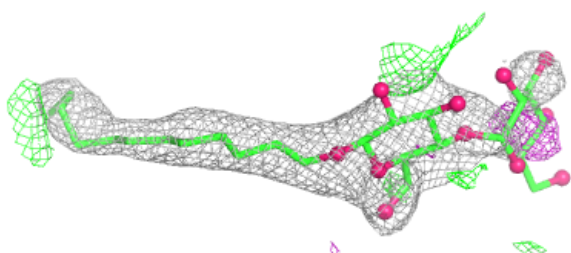
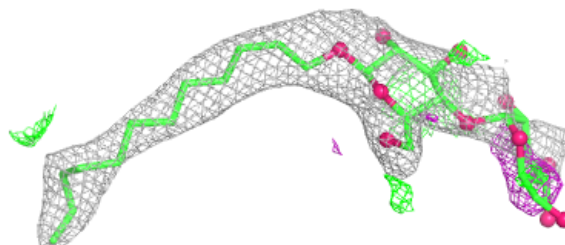
**Electron density around LMT B 628:**

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

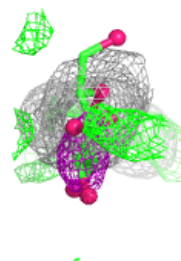
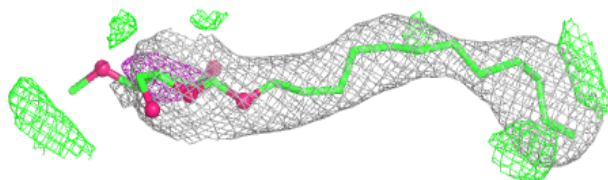
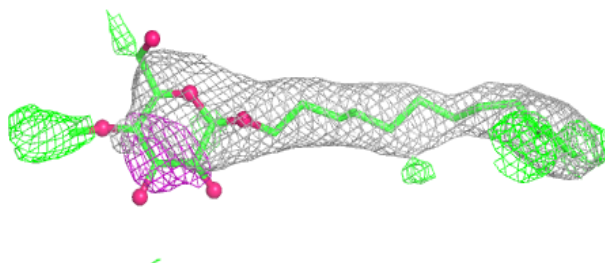


Electron density around LMT T 101:

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

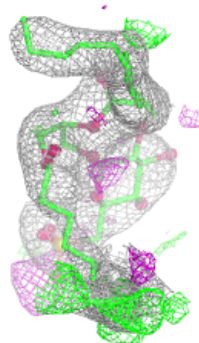
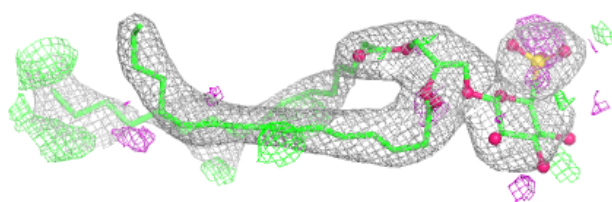
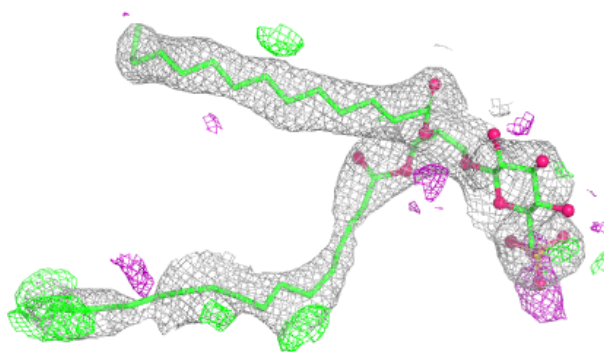
**Electron density around LMT b 627:**

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

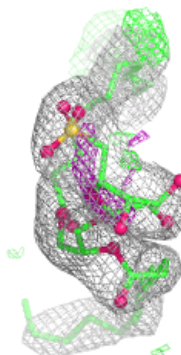
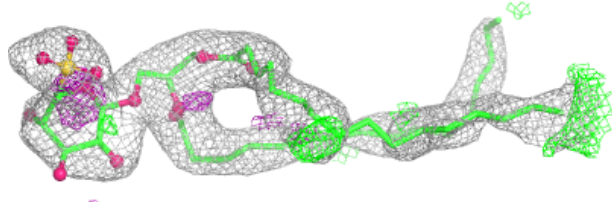
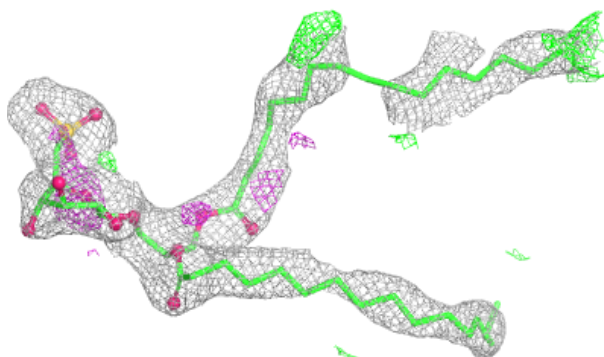


Electron density around SQD A 412:

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

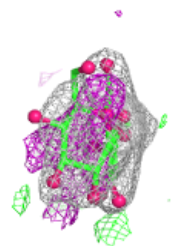
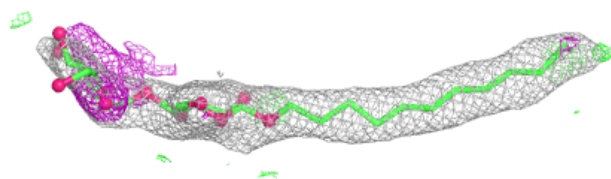
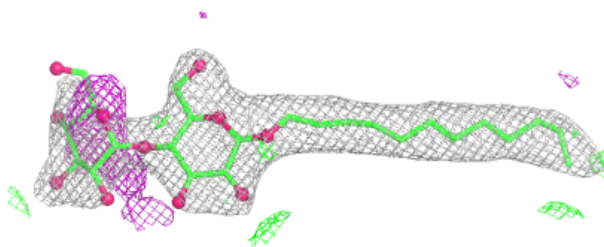
**Electron density around SQD a 413:**

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

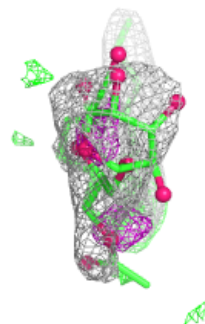
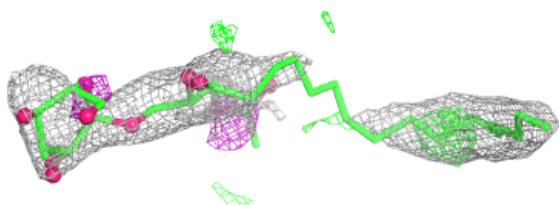
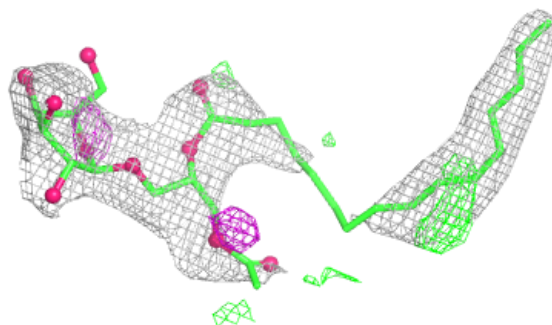


Electron density around LMT M 101:

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

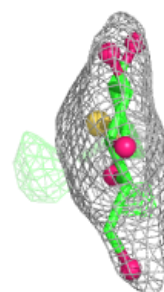
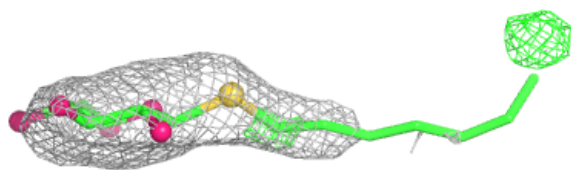
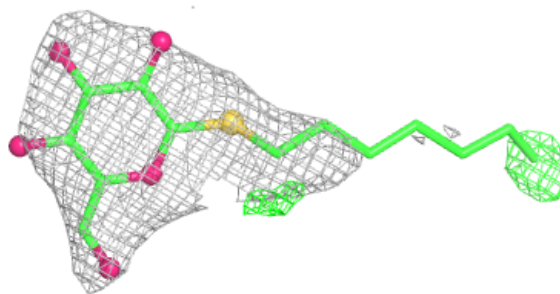
**Electron density around LMG Z 101:**

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

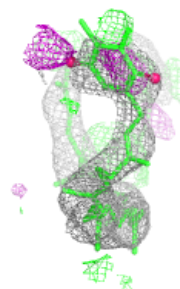
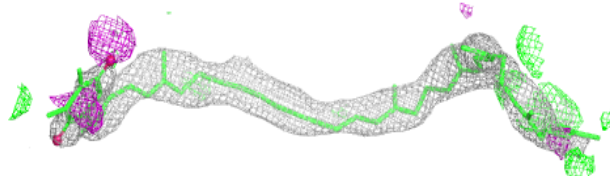
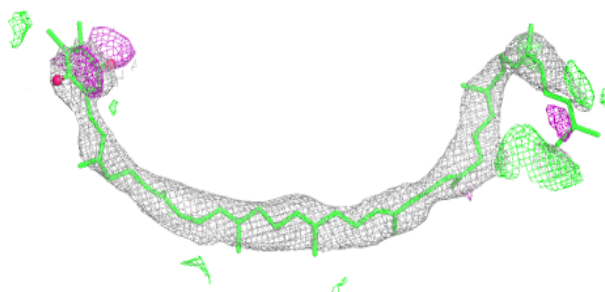


Electron density around HTG c 522:

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

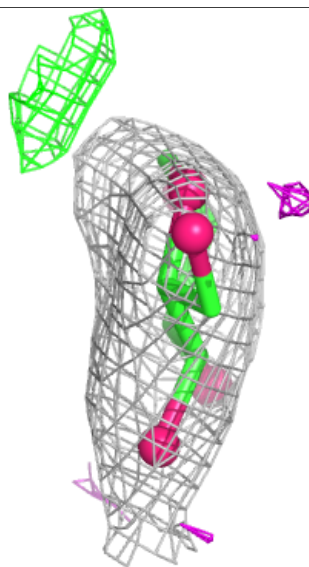
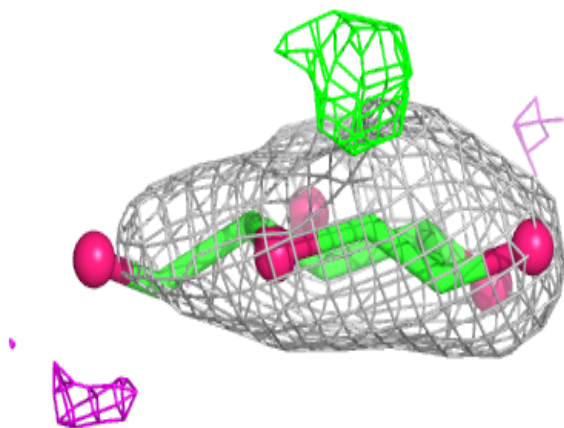
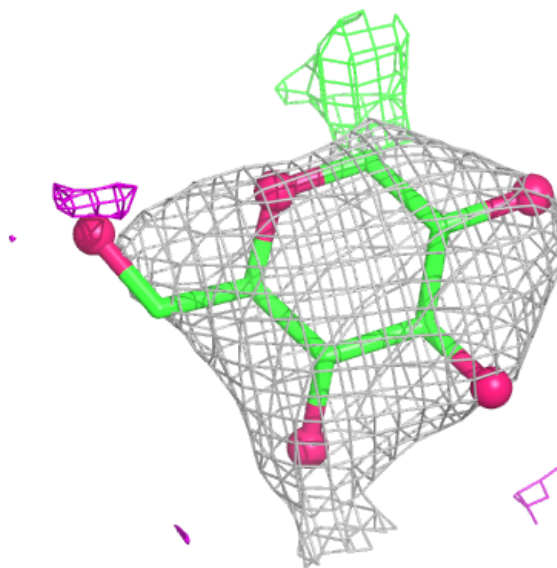
**Electron density around PL9 A 414:**

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



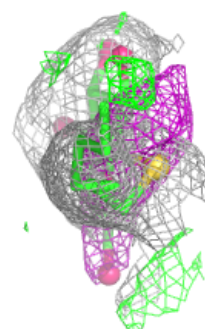
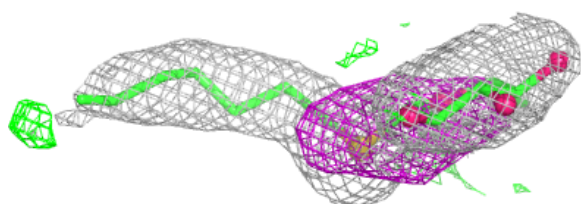
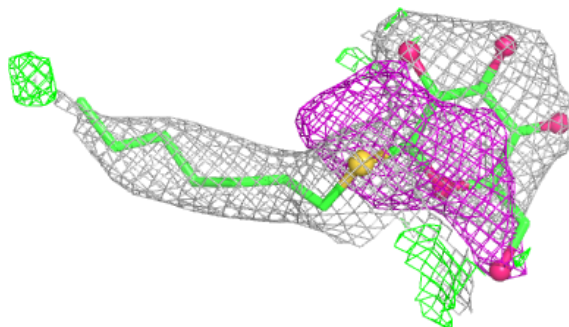
Electron density around HTG V 202:

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

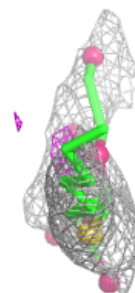
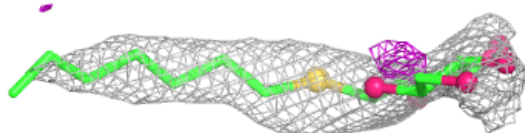
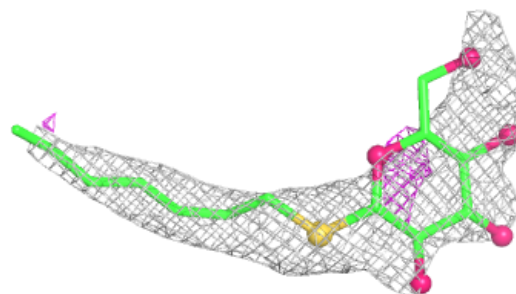


Electron density around HTG b 622:

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

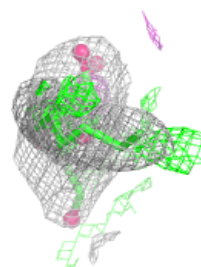
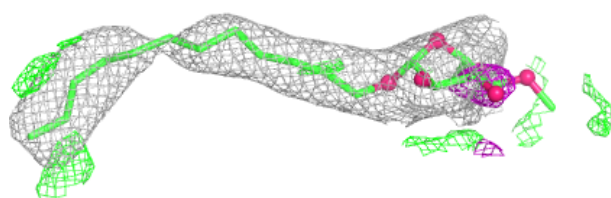
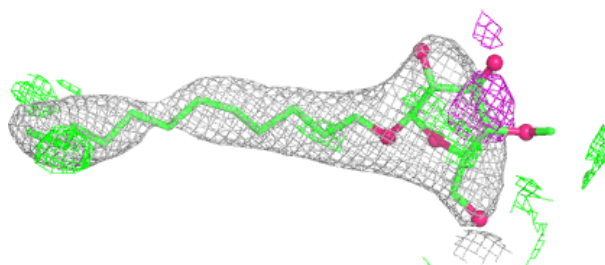
**Electron density around HTG b 623:**

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

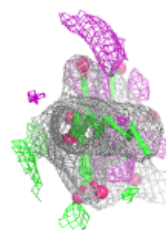
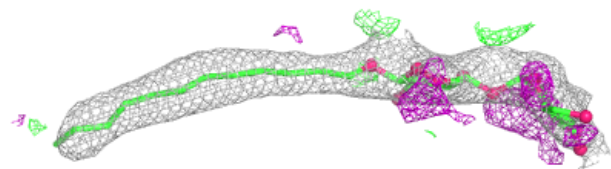
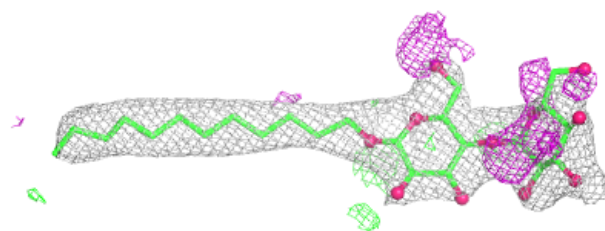


Electron density around LMT B 631:

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

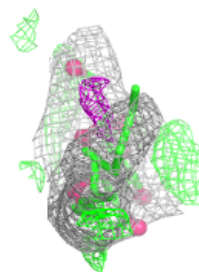
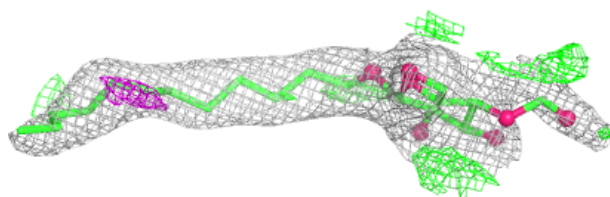
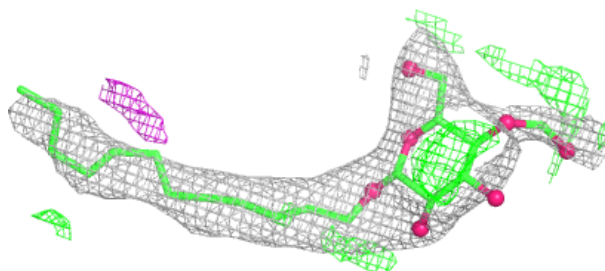
**Electron density around LMT m 103:**

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

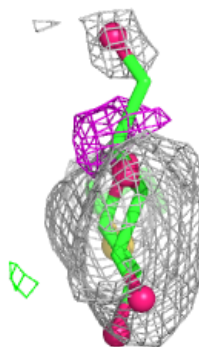
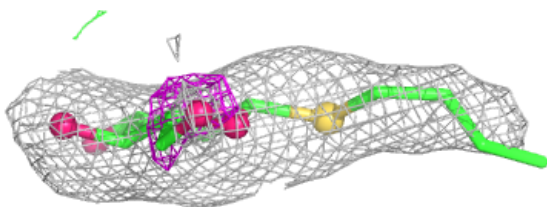
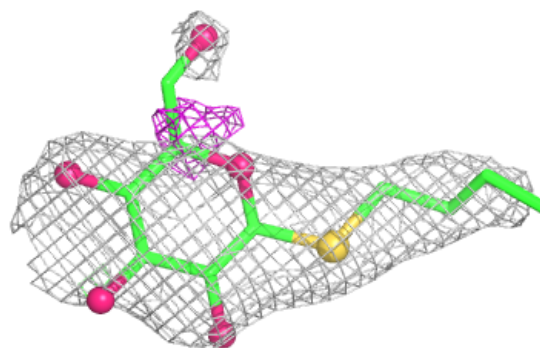


Electron density around LMT t 101:

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

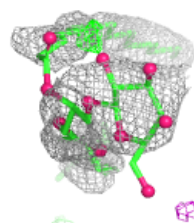
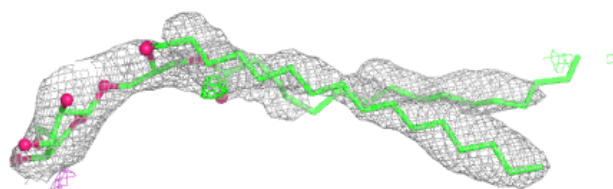
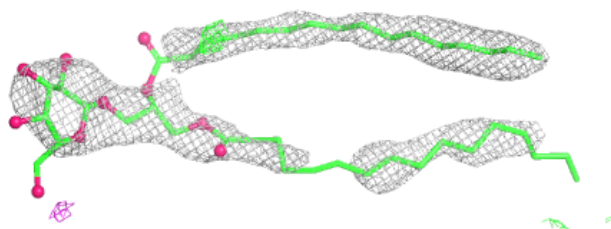
**Electron density around HTG d 409:**

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

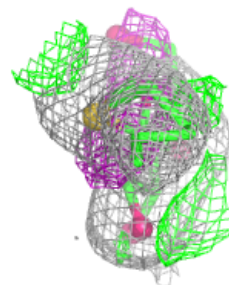
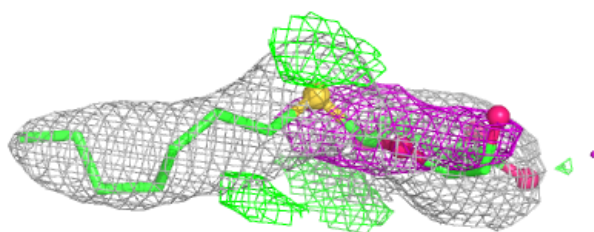
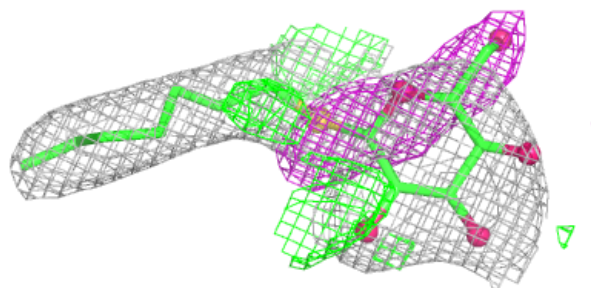


Electron density around LMG c 521:

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

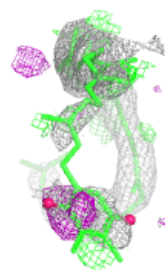
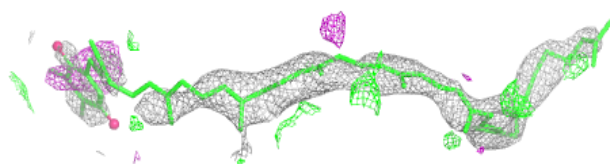
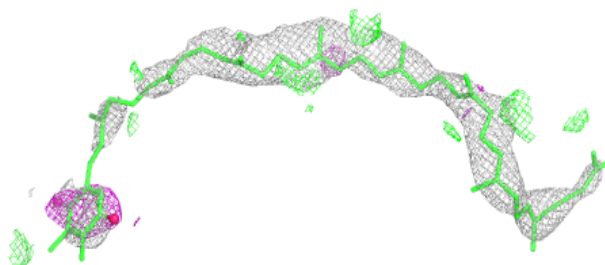
**Electron density around HTG B 622:**

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

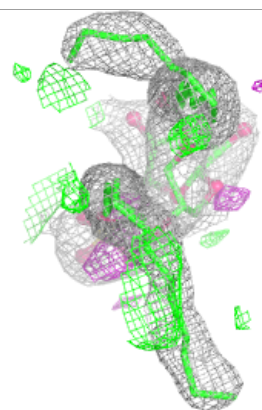
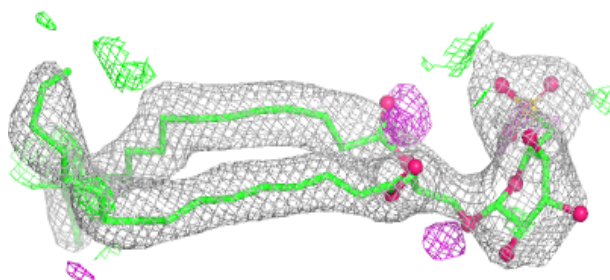
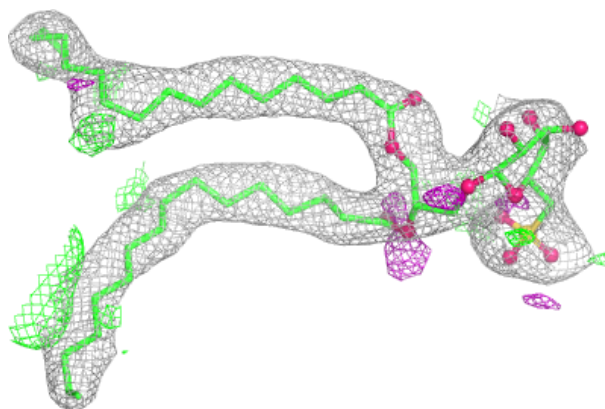


Electron density around PL9 a 415:

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

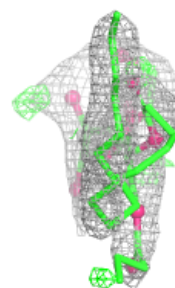
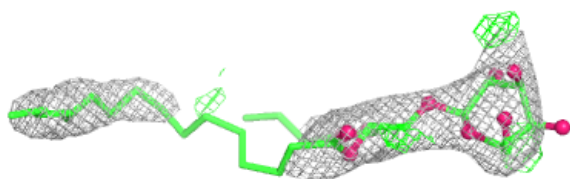
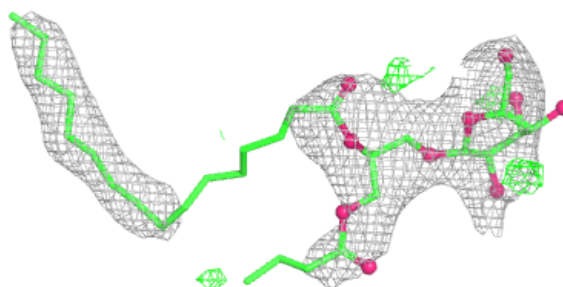
**Electron density around SQD B 620:**

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

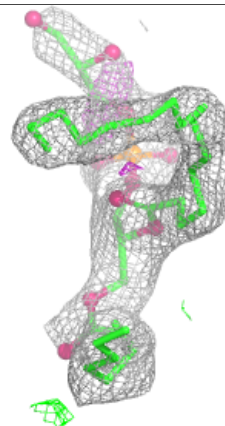
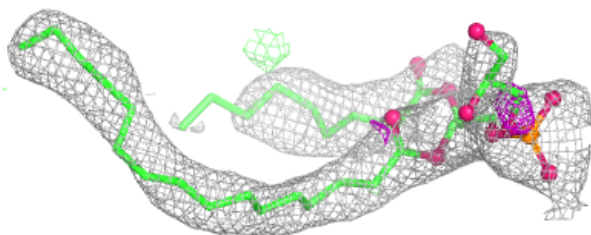
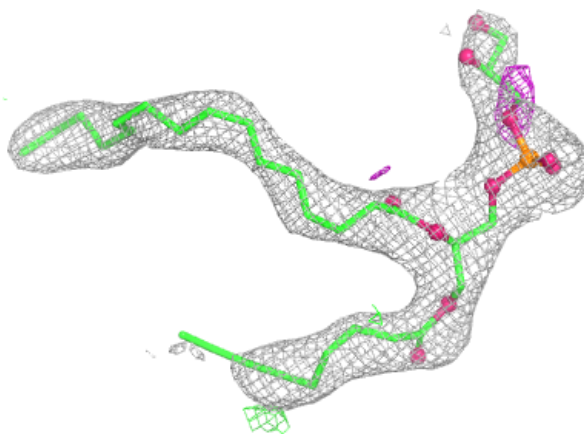


Electron density around LMG z 101:

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

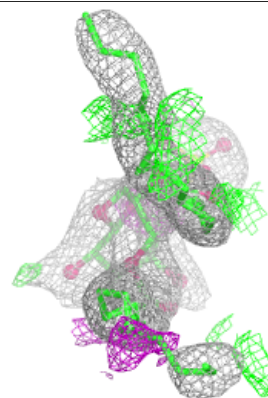
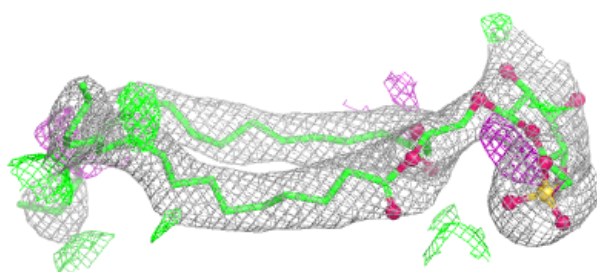
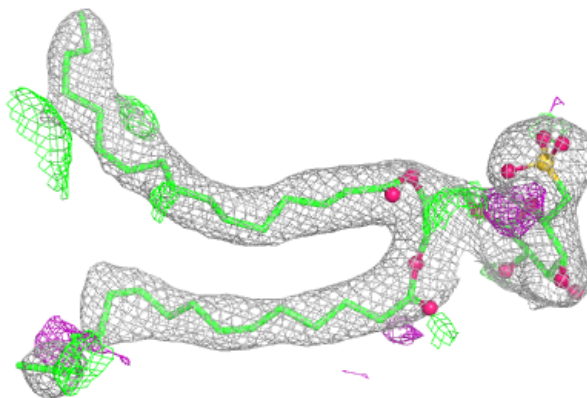
**Electron density around LHG E 101:**

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

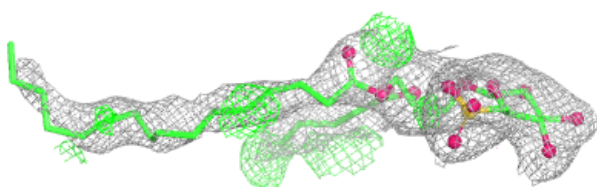
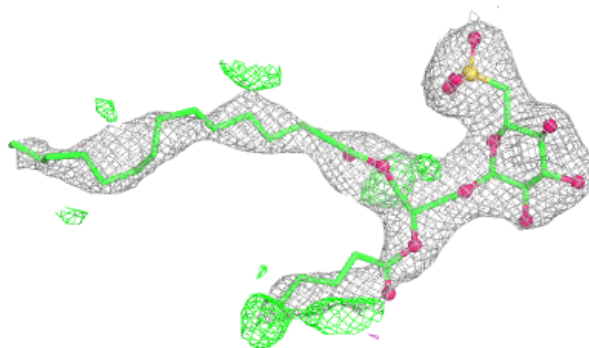


Electron density around SQD b 620:

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

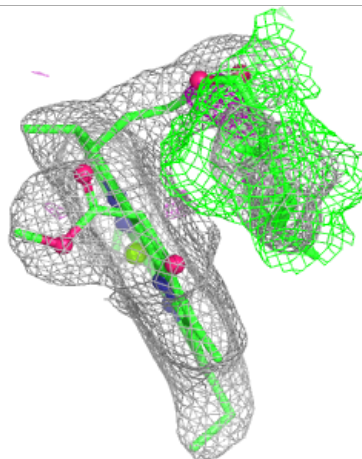
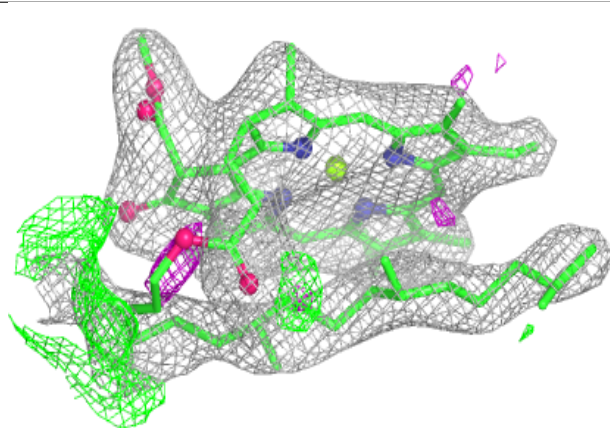
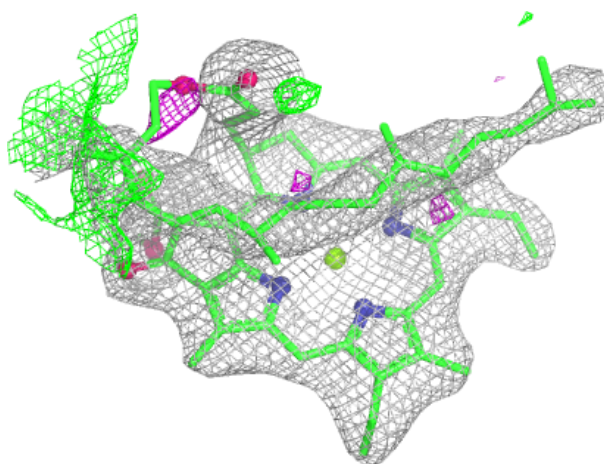
**Electron density around SQD F 103:**

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



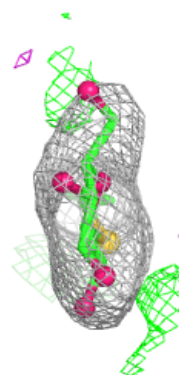
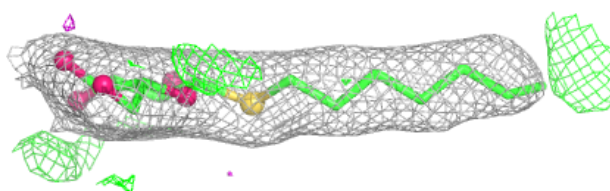
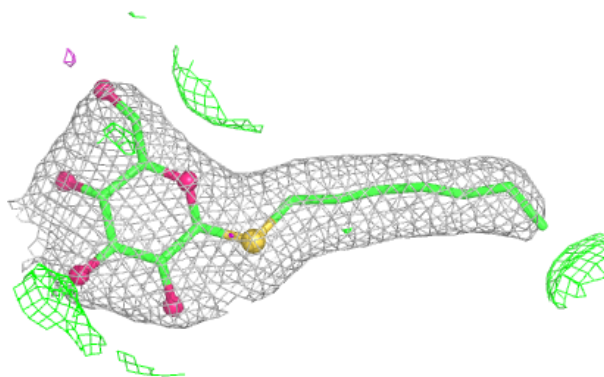
Electron density around CLA b 601:

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

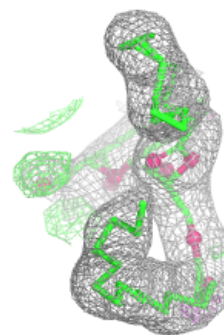
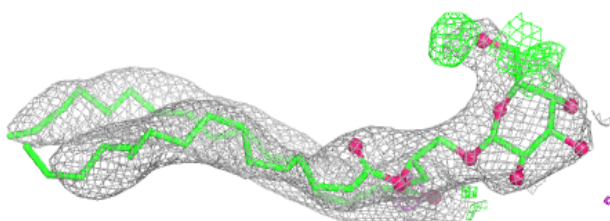
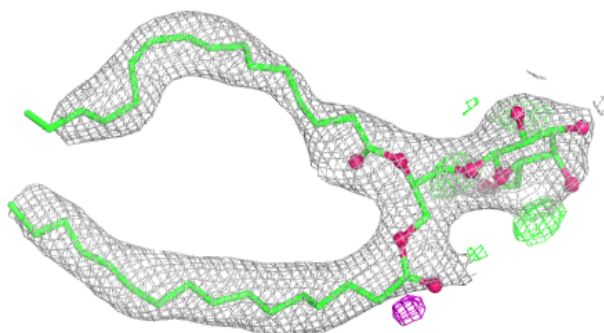


Electron density around HTG B 625:

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

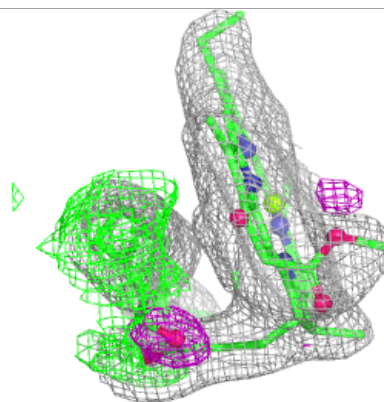
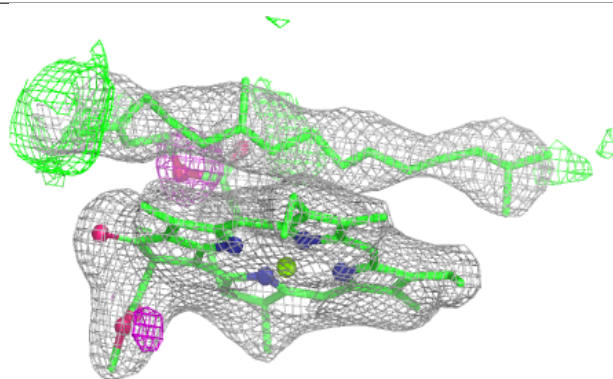
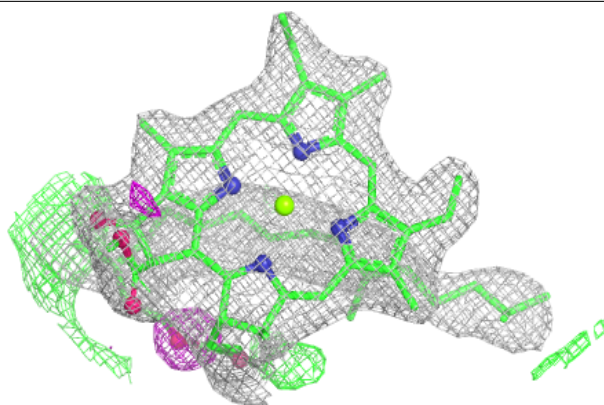
**Electron density around LMG A 419:**

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

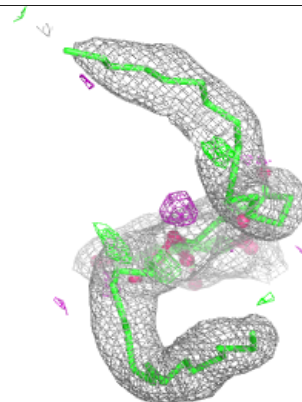
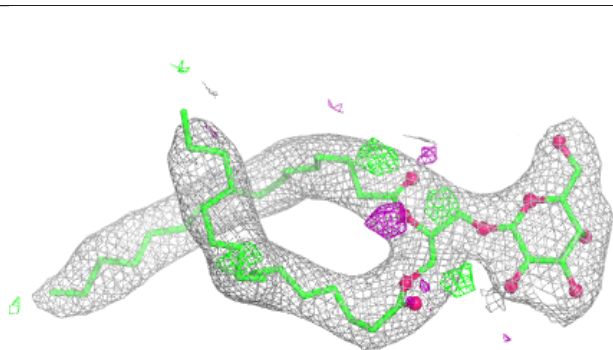
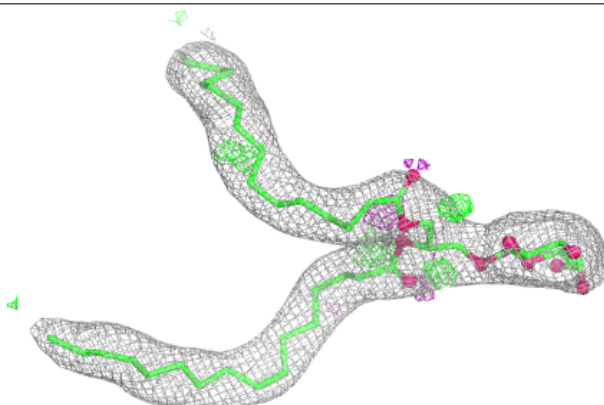


Electron density around CLA B 601:

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

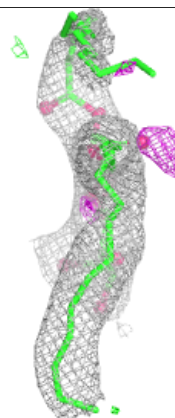
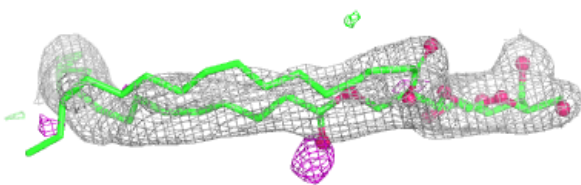
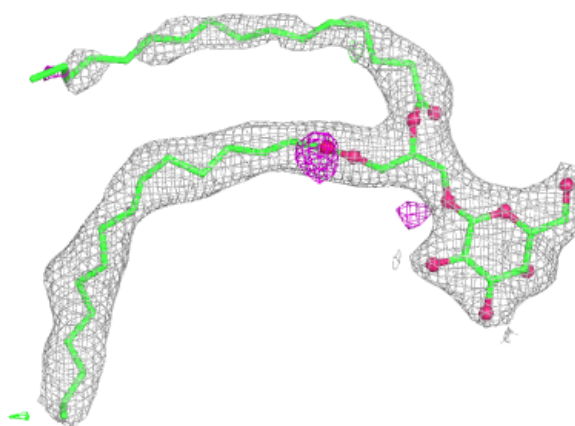
**Electron density around LMG B 621:**

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

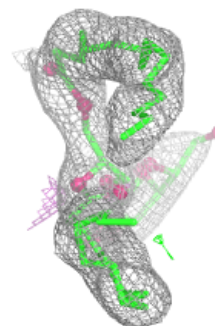
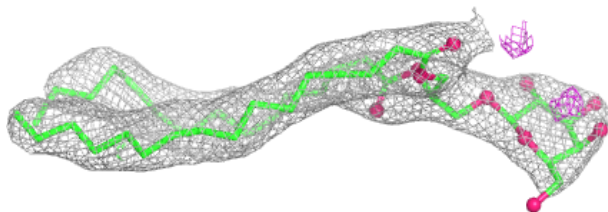
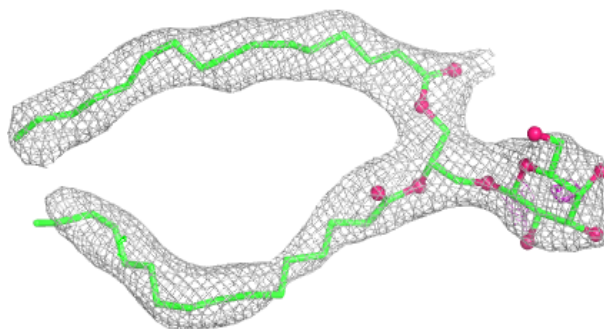


Electron density around LMG C 518:

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

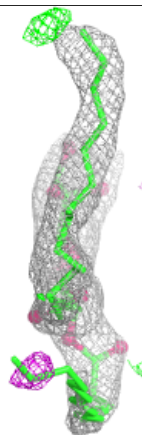
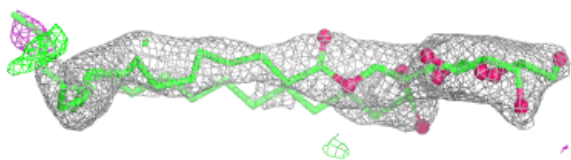
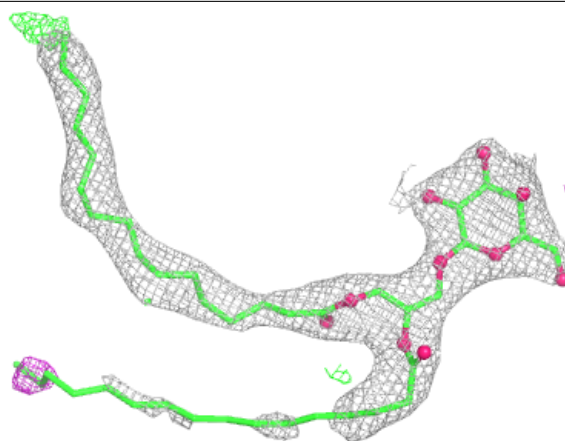
**Electron density around LMG a 418:**

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

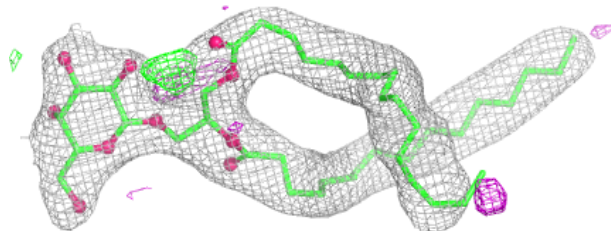
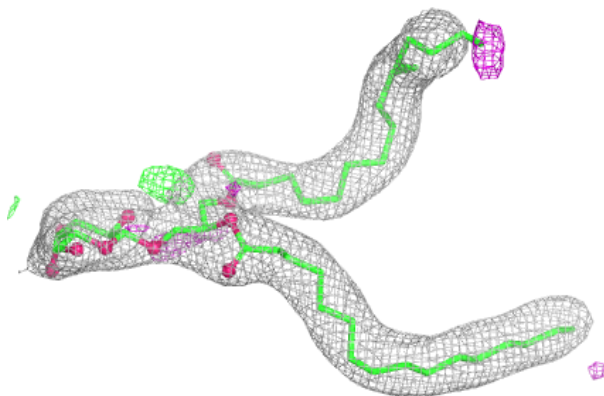


Electron density around LMG c 520:

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

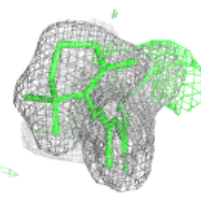
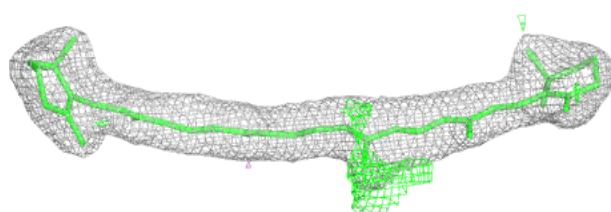
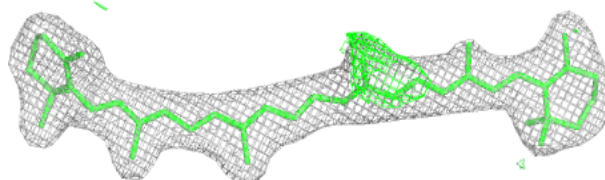
**Electron density around LMG m 101:**

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

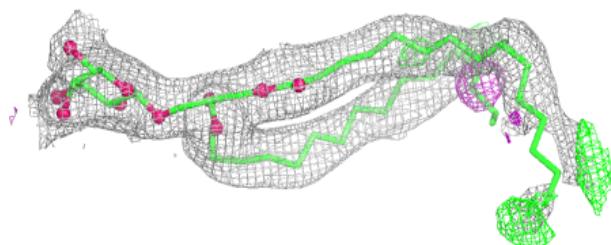
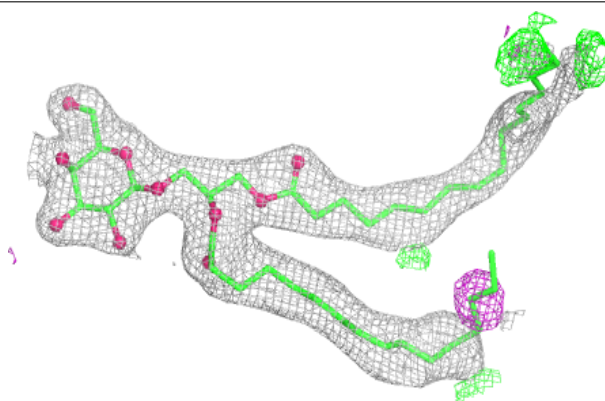


Electron density around BCR T 102:

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

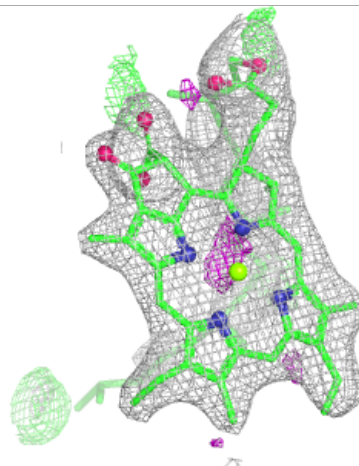
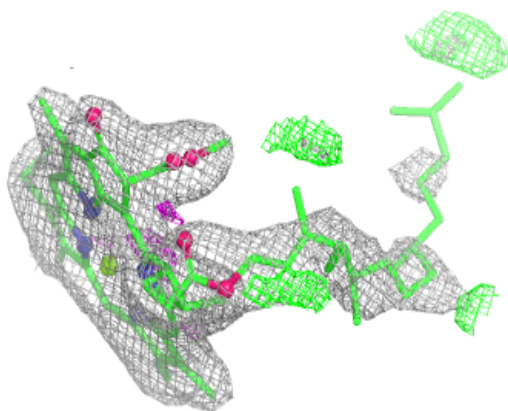
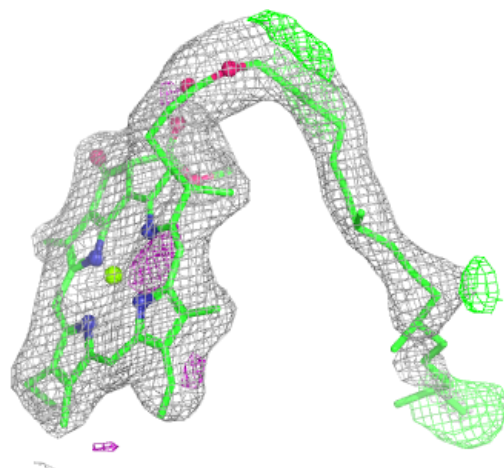
**Electron density around LMG D 411:**

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



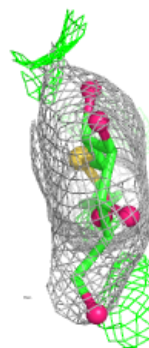
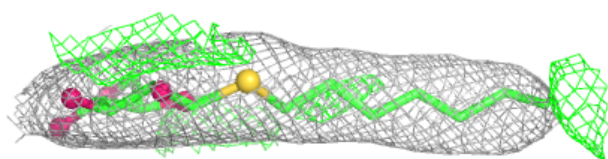
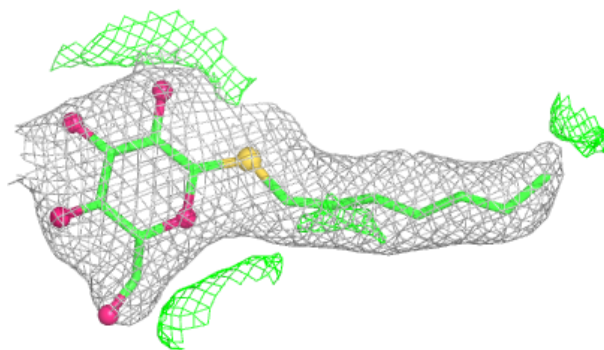
Electron density around CLA b 616:

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

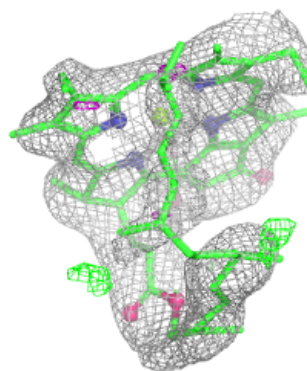
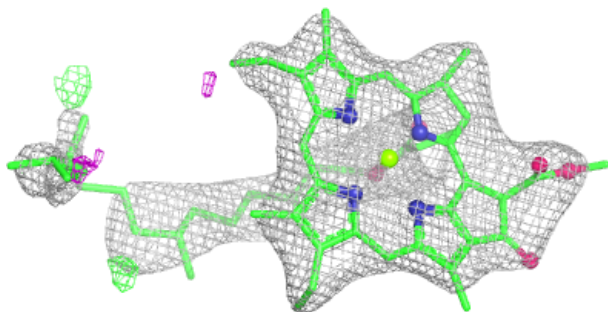
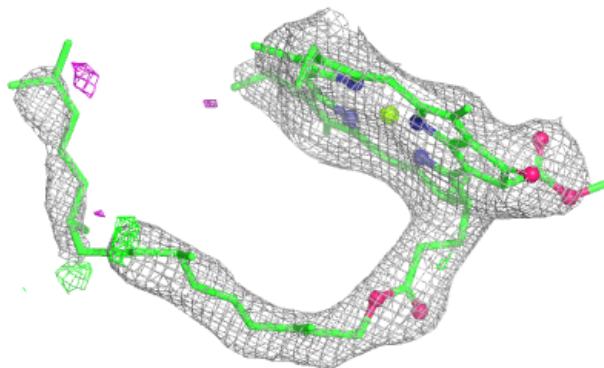


Electron density around HTG b 625:

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

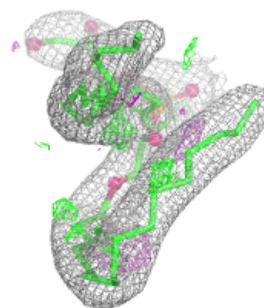
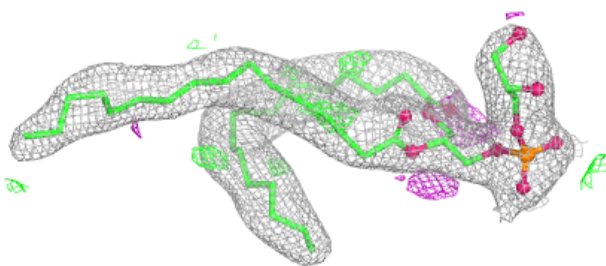
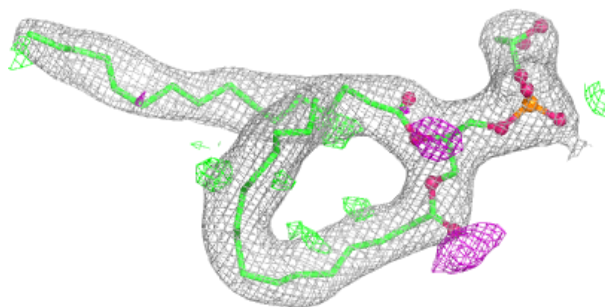
**Electron density around CLA c 514:**

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

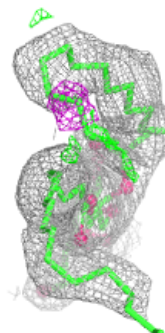
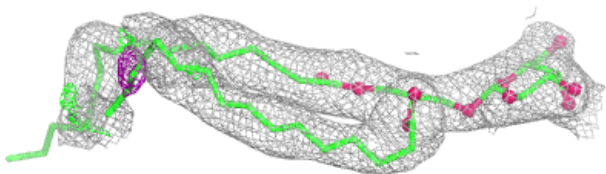
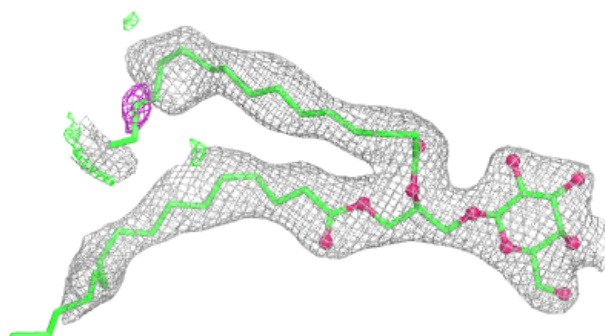


Electron density around LHG A 420:

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

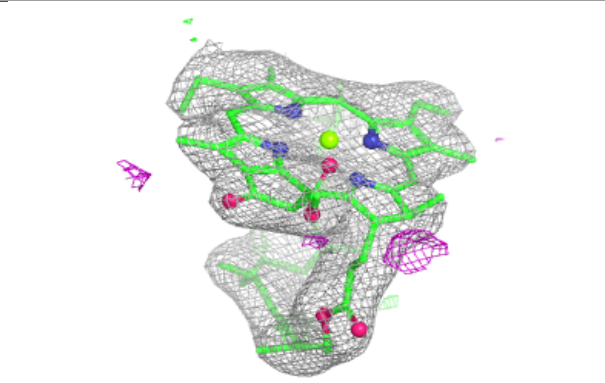
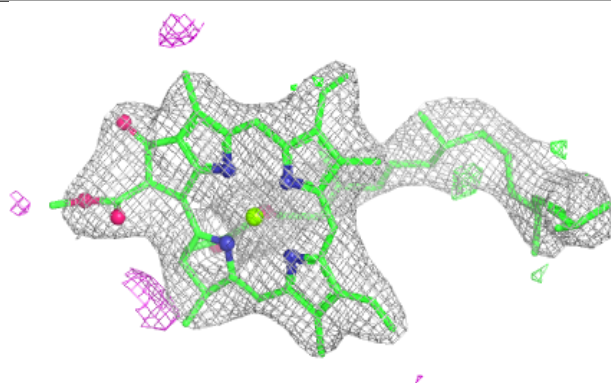
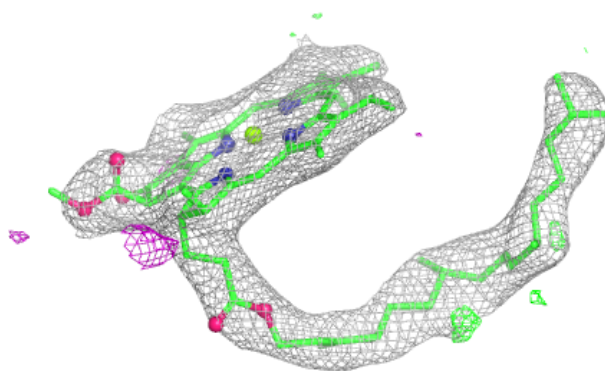
**Electron density around LMG d 410:**

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

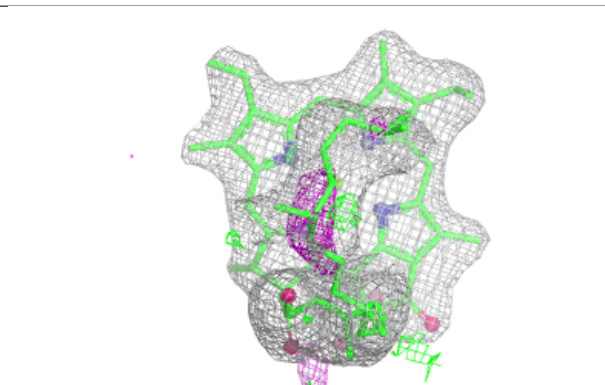
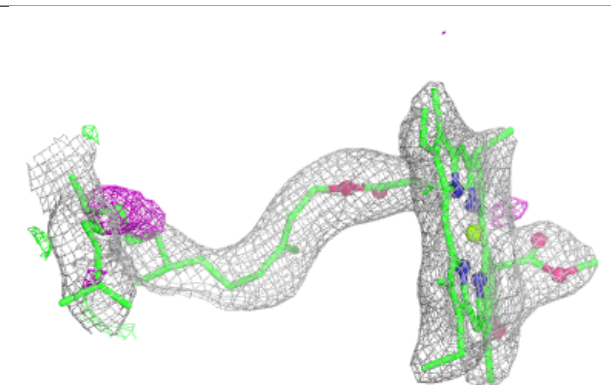
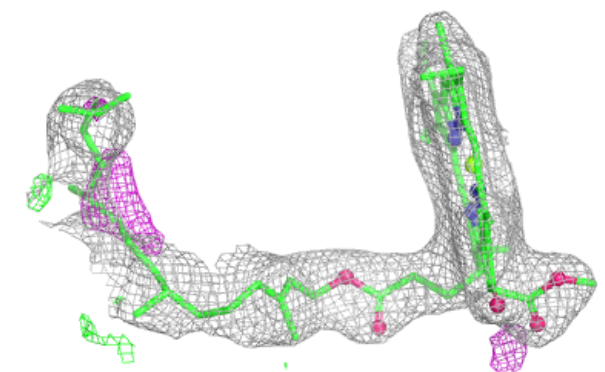


Electron density around CLA C 513:

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

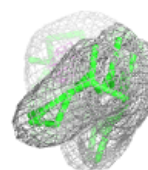
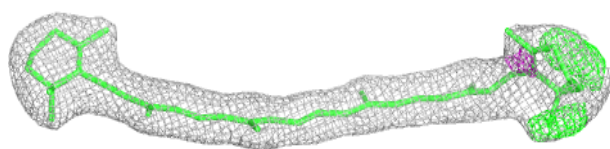
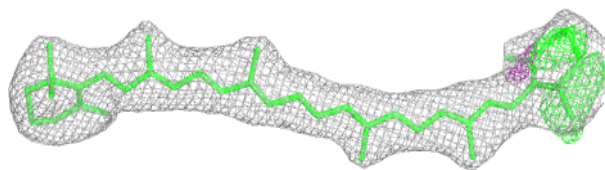
**Electron density around CLA C 506:**

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

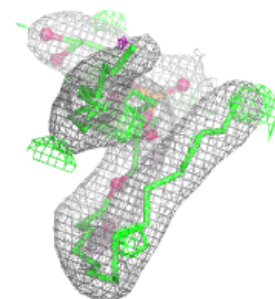
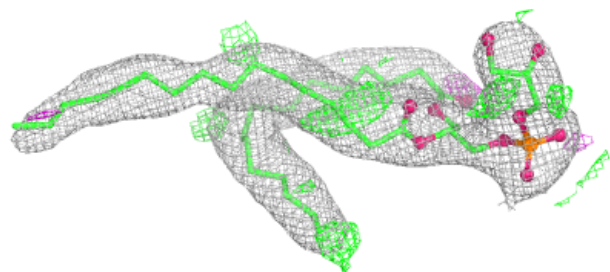
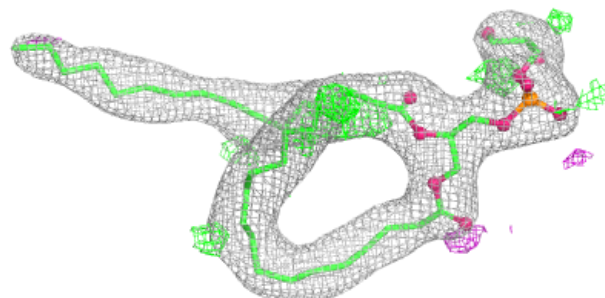


Electron density around BCR d 403:

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

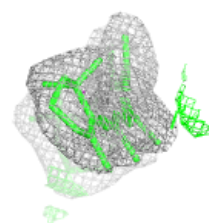
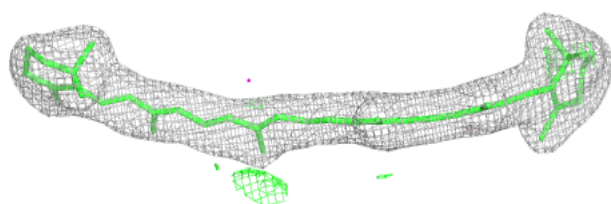
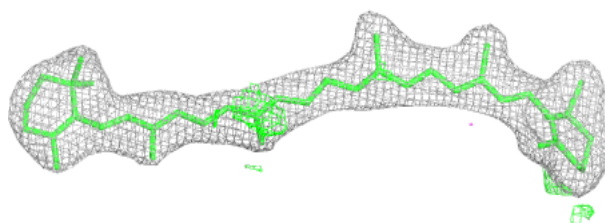
**Electron density around LHG d 411:**

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

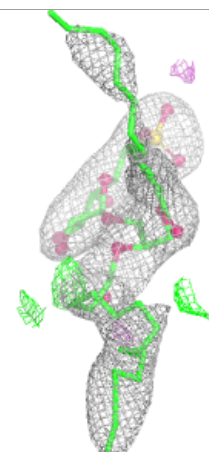
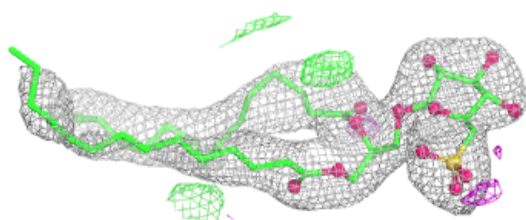
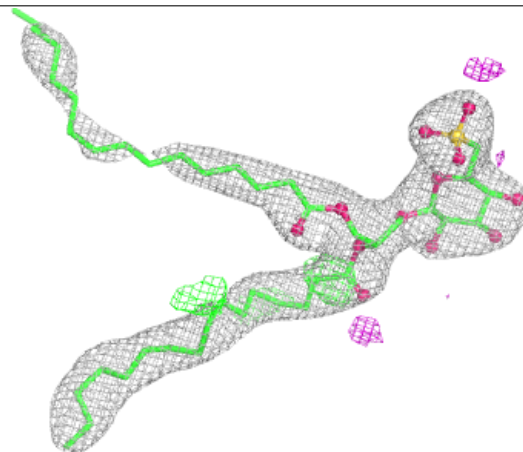


Electron density around BCR t 102:

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

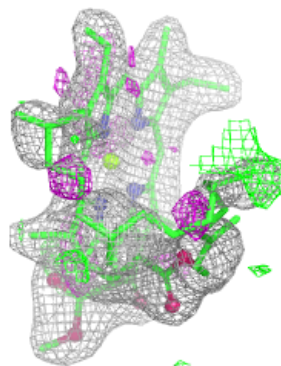
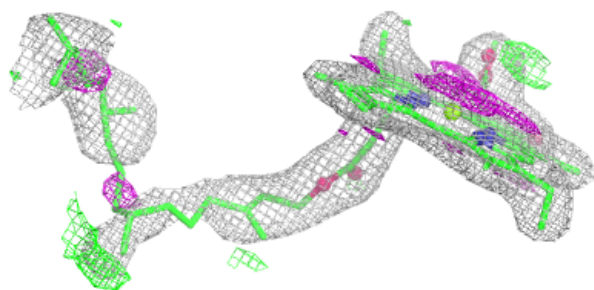
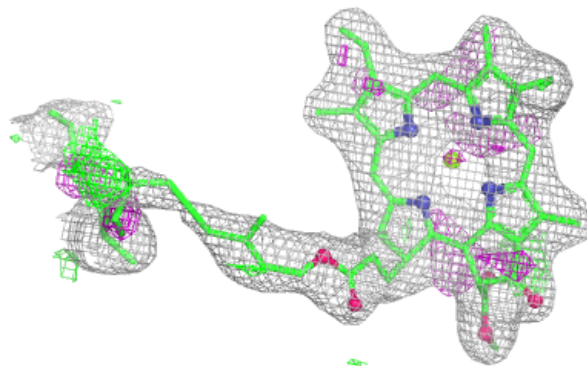
**Electron density around SQD A 410:**

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

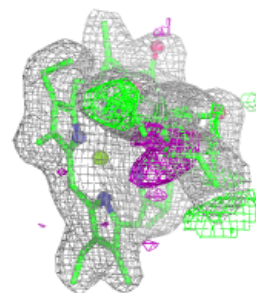
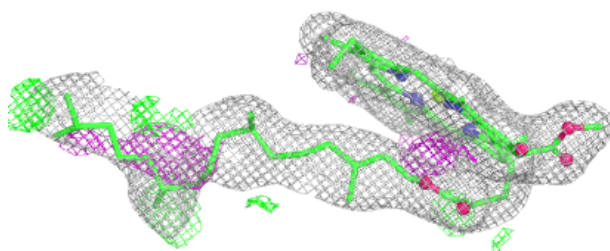
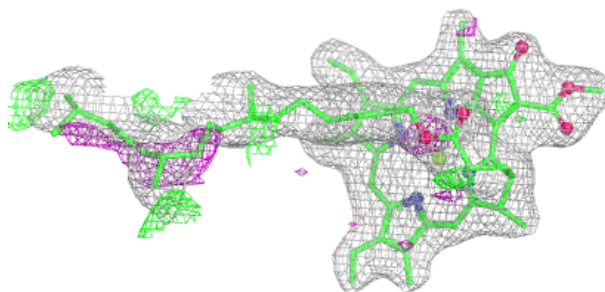


Electron density around CLA A 408:

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

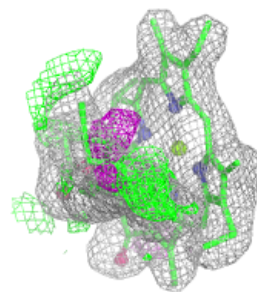
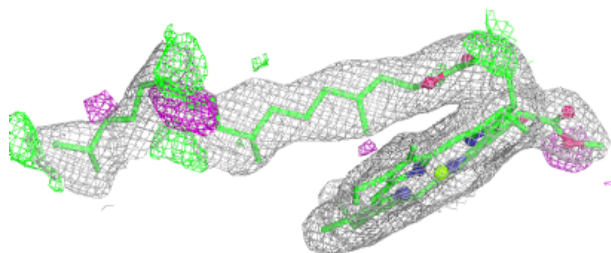
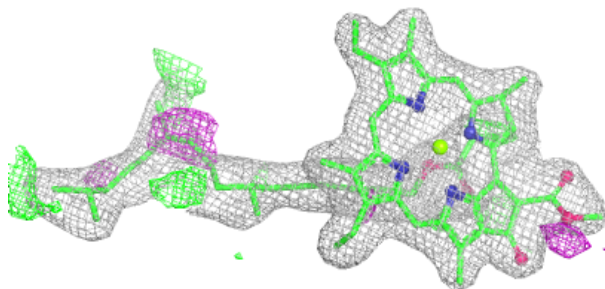
**Electron density around CLA B 614:**

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



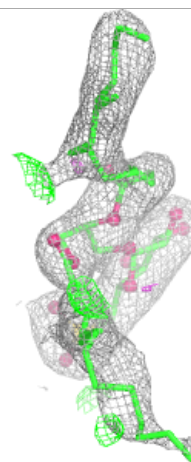
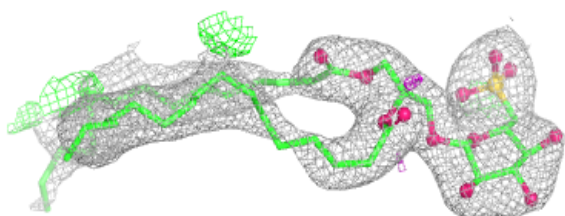
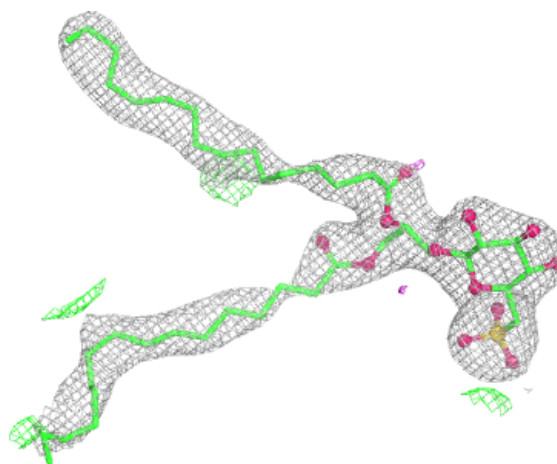
Electron density around CLA b 614:

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



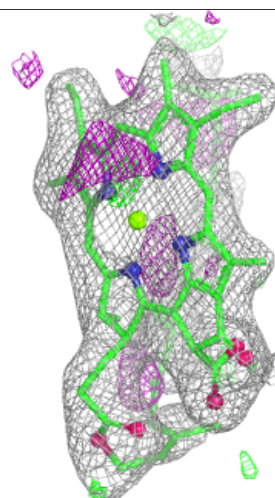
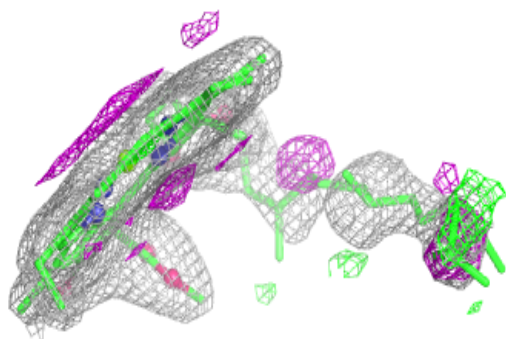
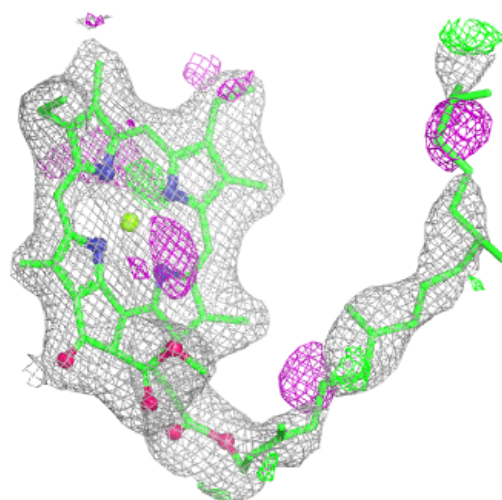
Electron density around SQD a 411:

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



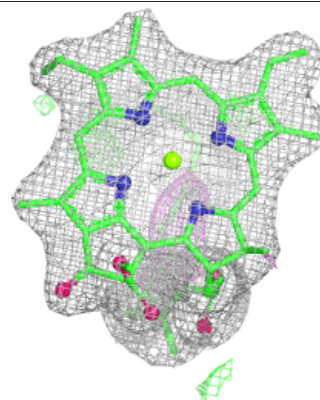
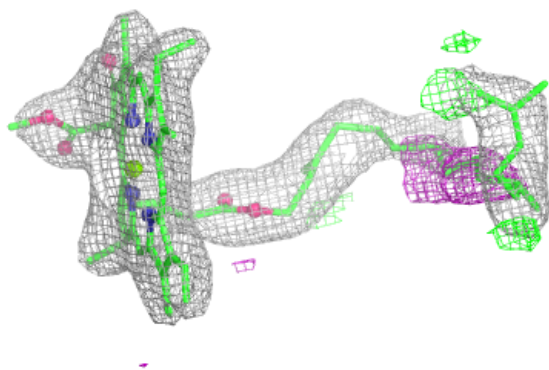
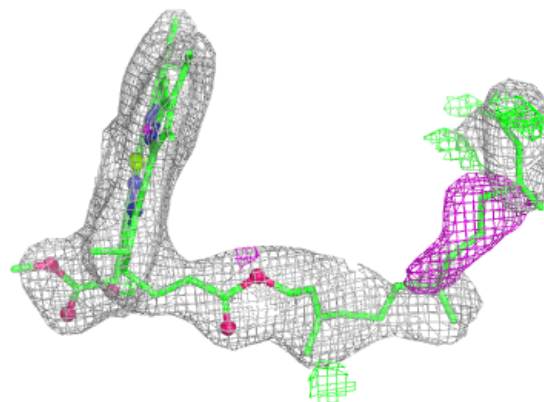
Electron density around CLA B 616:

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



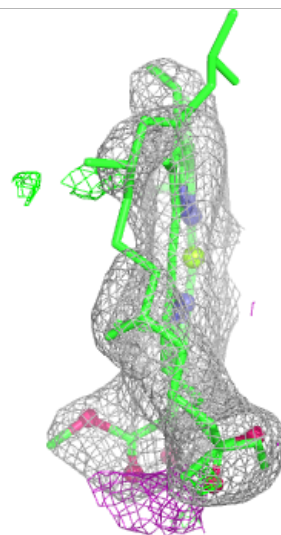
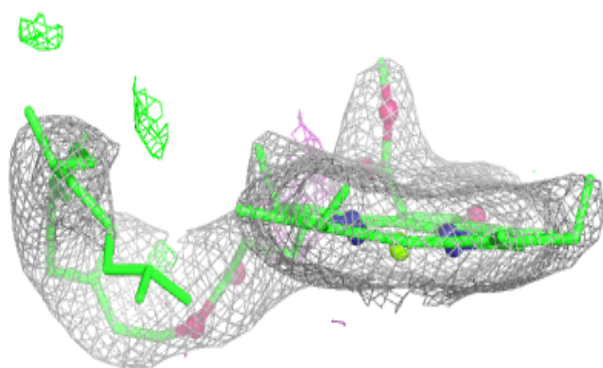
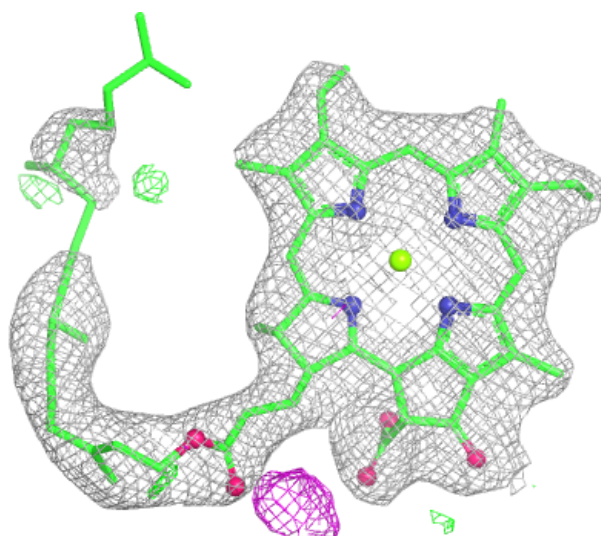
Electron density around CLA c 507:

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



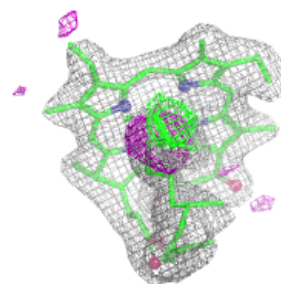
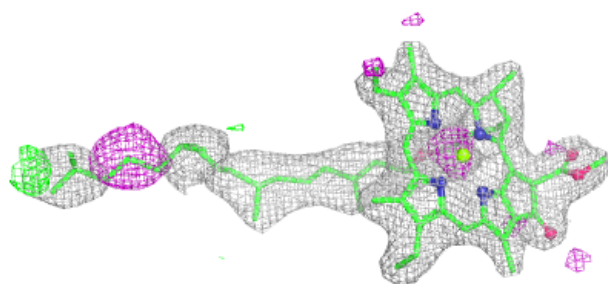
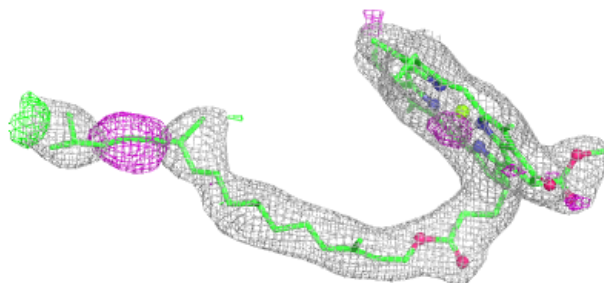
Electron density around CLA c 513:

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

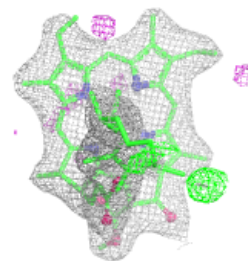
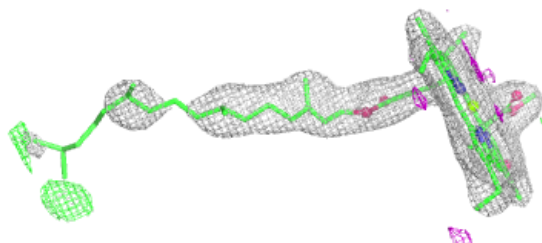
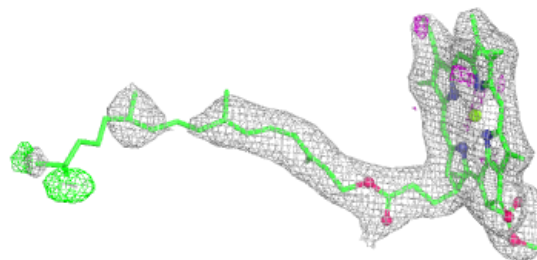


Electron density around CLA C 504:

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

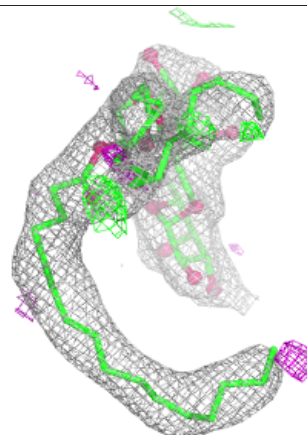
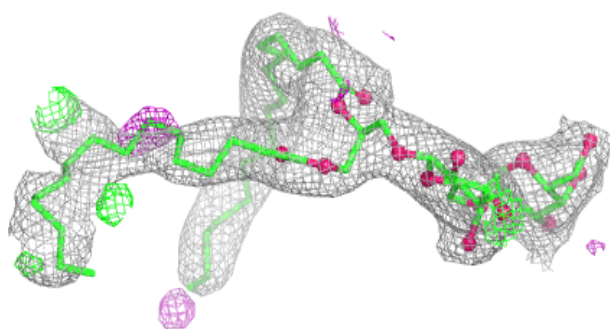
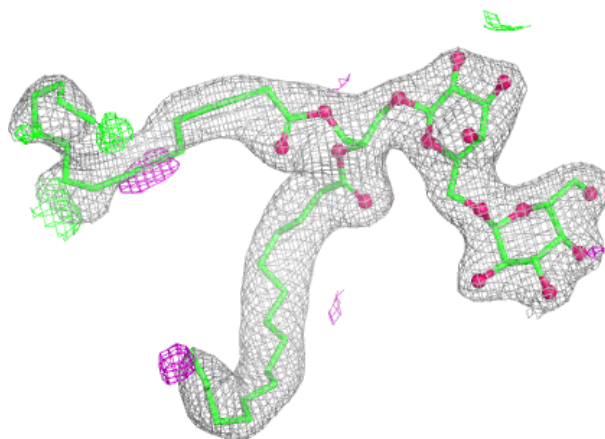
**Electron density around CLA d 402:**

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

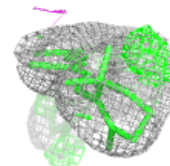
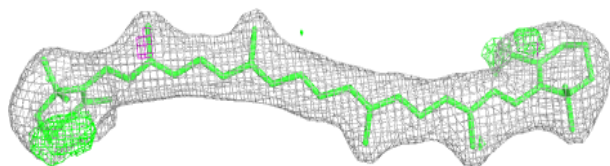
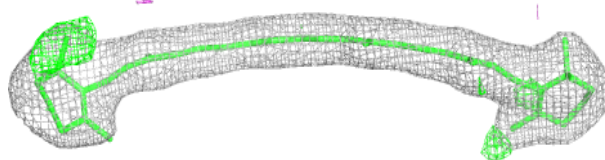


Electron density around DGD C 516:

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

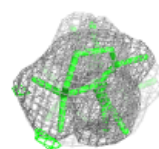
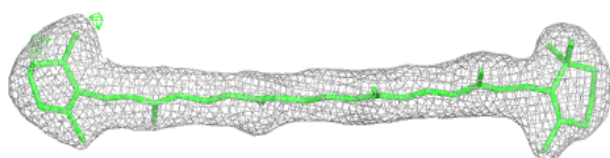
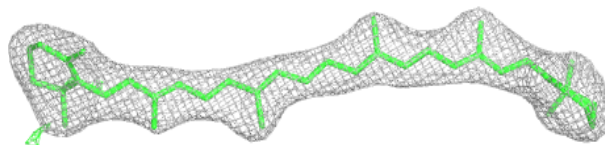
**Electron density around BCR D 404:**

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

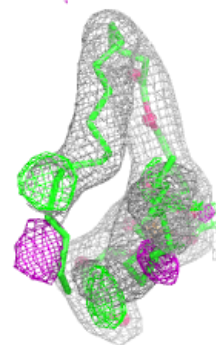
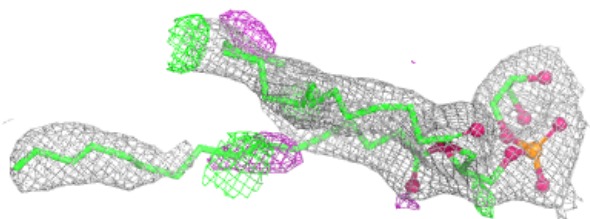
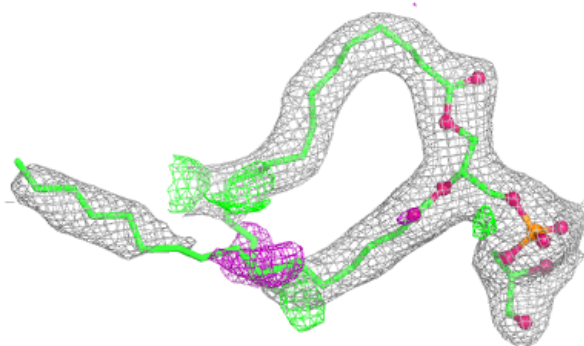


Electron density around BCR K 101:

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

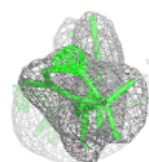
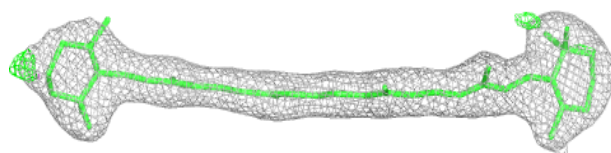
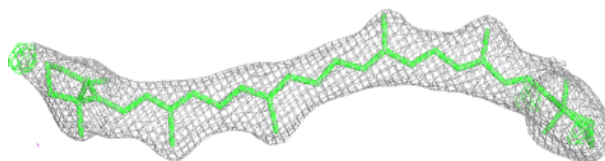
**Electron density around LHG D 407:**

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

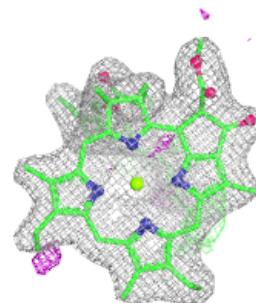
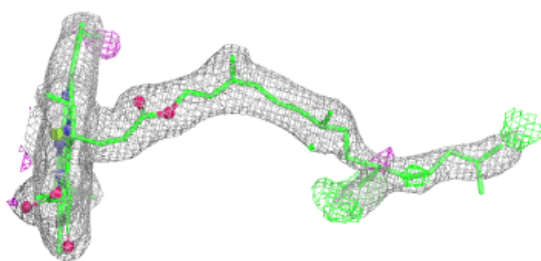
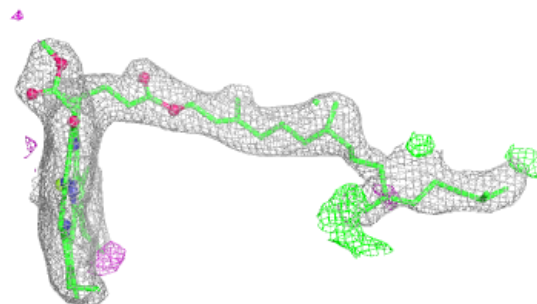


Electron density around BCR h 101:

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

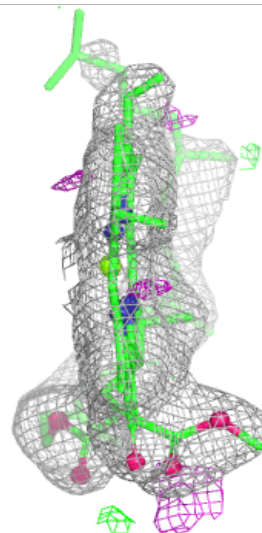
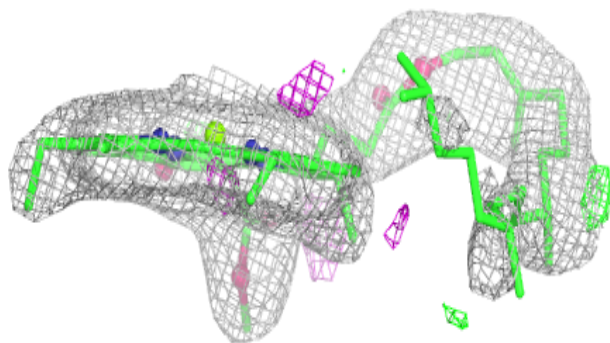
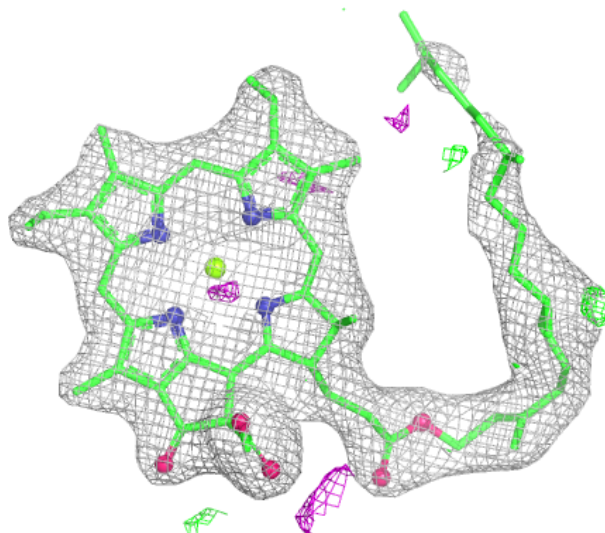
**Electron density around CLA b 606:**

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



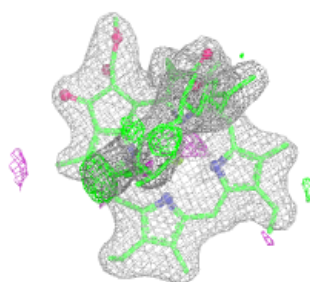
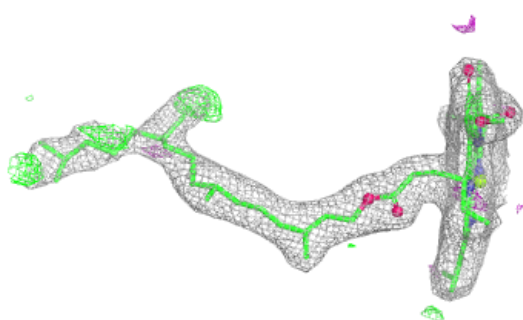
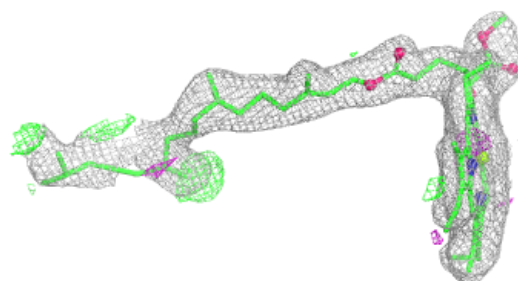
Electron density around CLA C 512:

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

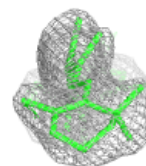
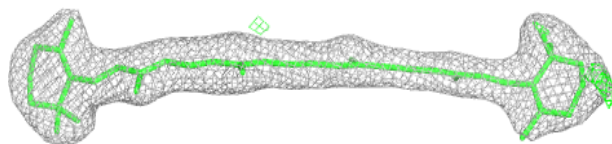
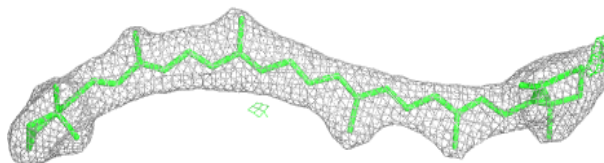


Electron density around CLA B 606:

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

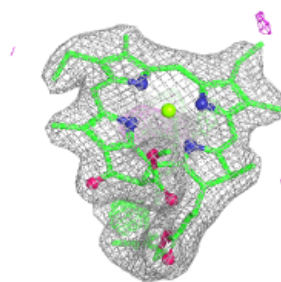
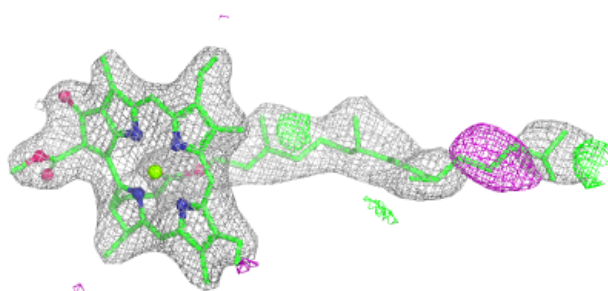
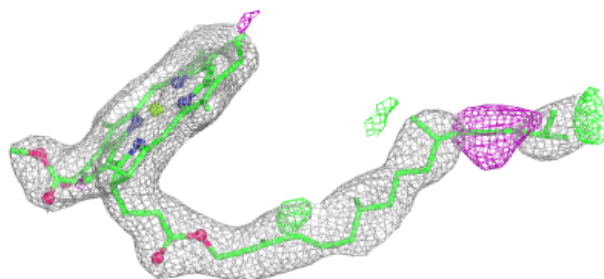
**Electron density around BCR H 101:**

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

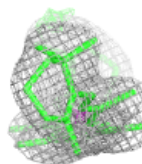
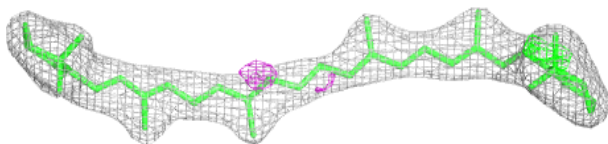
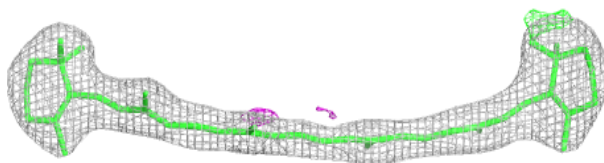


Electron density around CLA c 505:

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

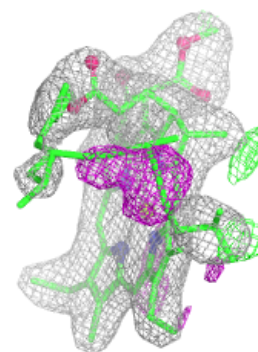
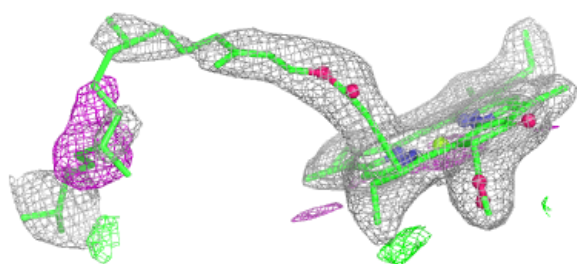
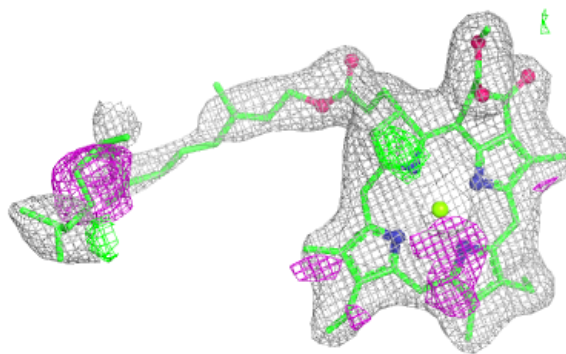
**Electron density around BCR K 103:**

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

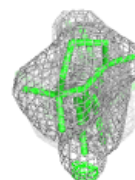
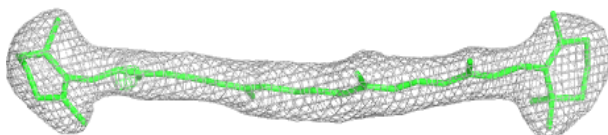
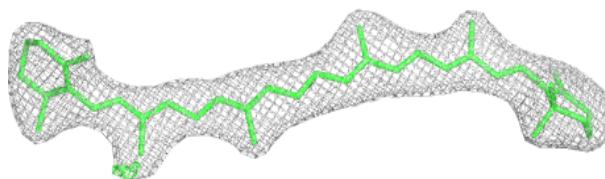


Electron density around CLA a 409:

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

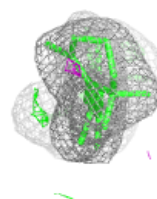
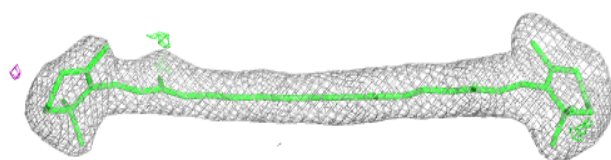
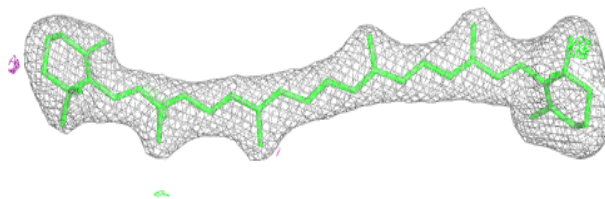
**Electron density around BCR Y 101:**

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

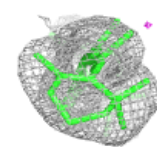
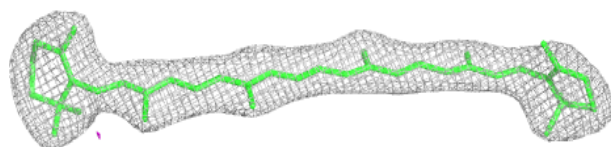
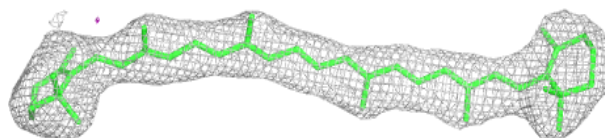


Electron density around BCR b 618:

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

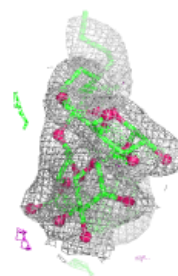
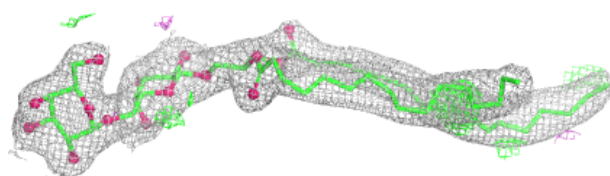
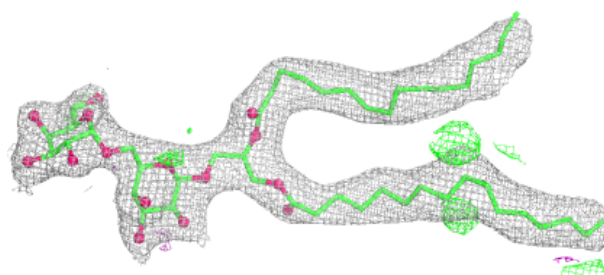
**Electron density around BCR c 515:**

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

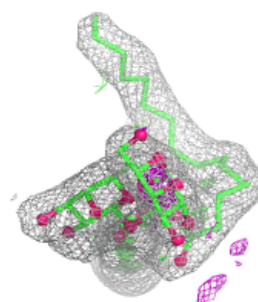
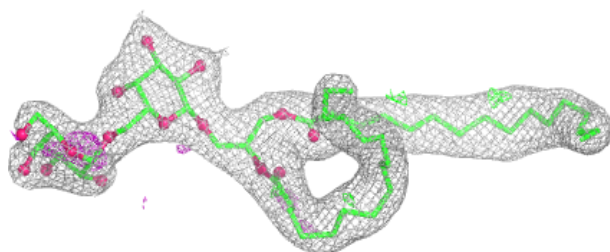
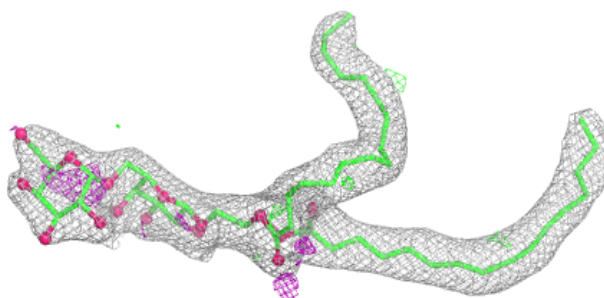


Electron density around DGD C 517:

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

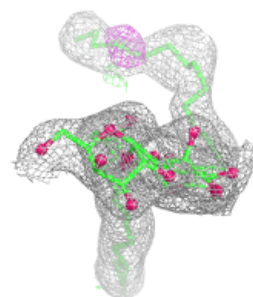
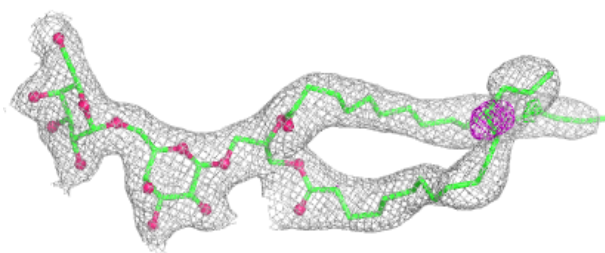
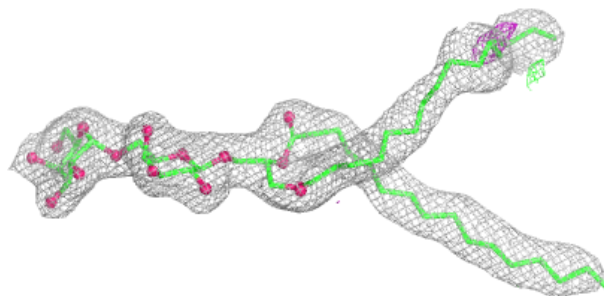
**Electron density around DGD H 102:**

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

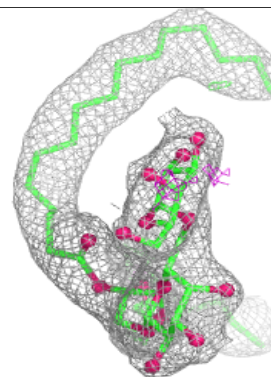
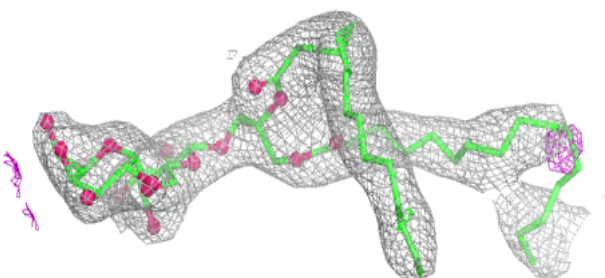
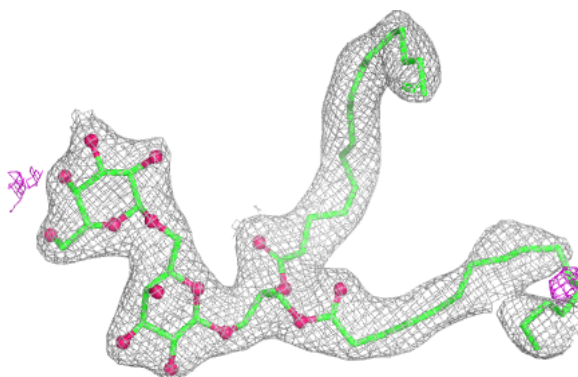


Electron density around DGD c 517:

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

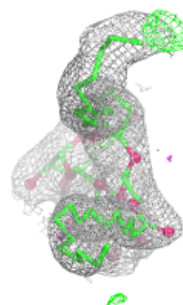
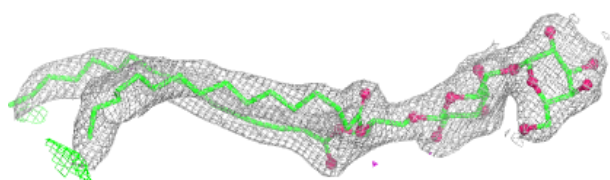
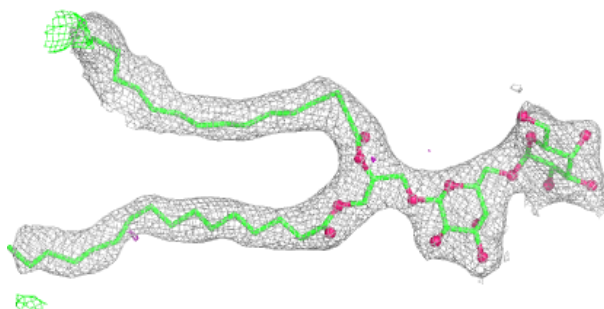
**Electron density around DGD c 518:**

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

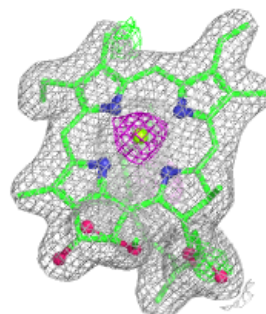
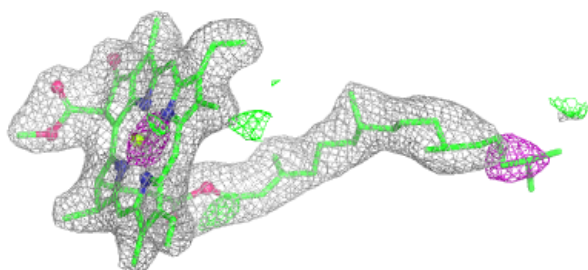
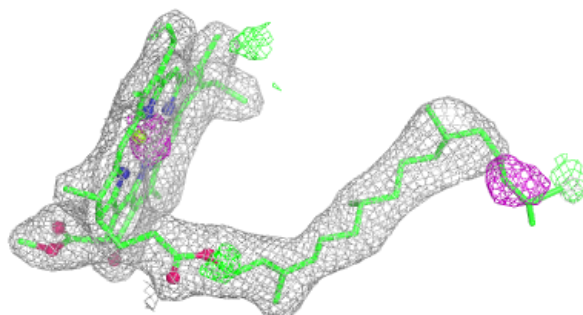


Electron density around DGD c 519:

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

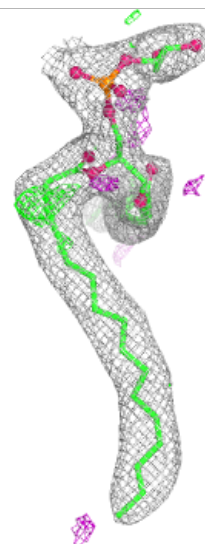
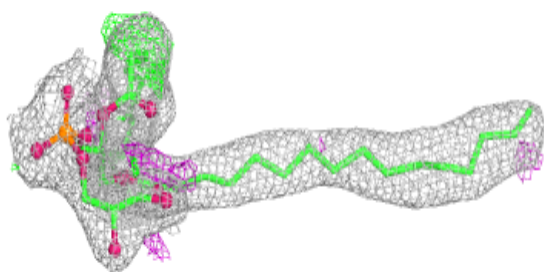
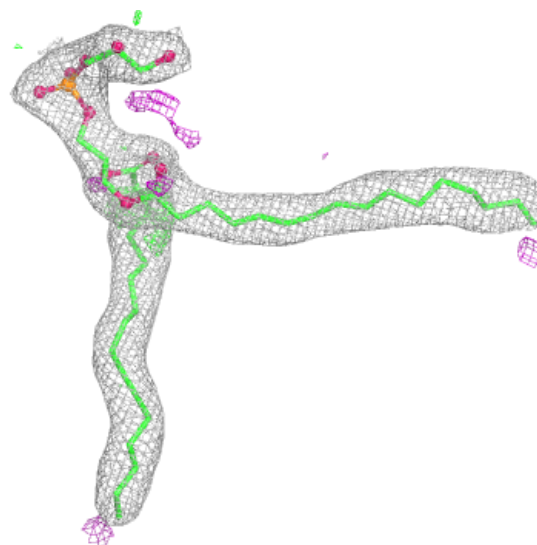
**Electron density around CLA C 508:**

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



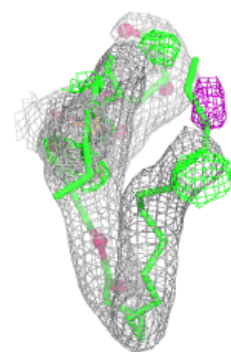
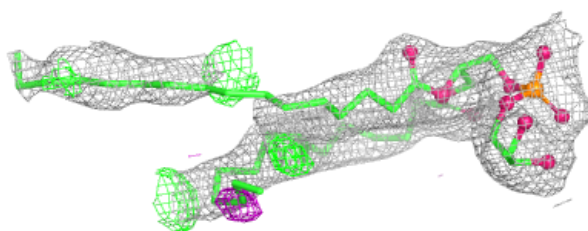
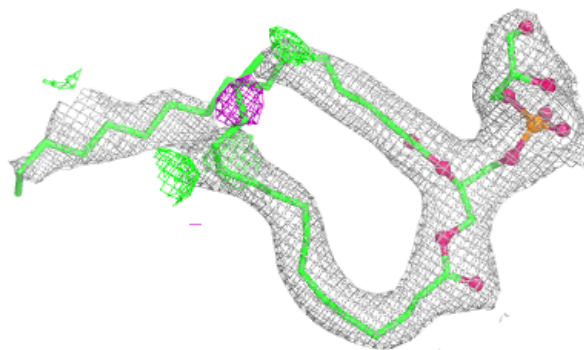
Electron density around LHG b 630:

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

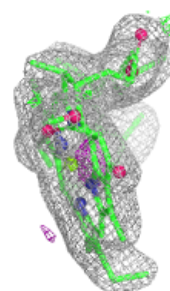
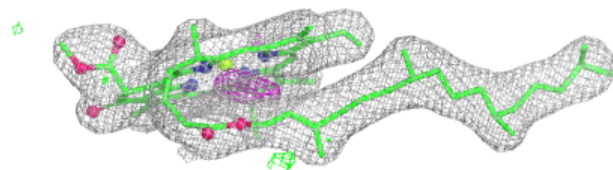
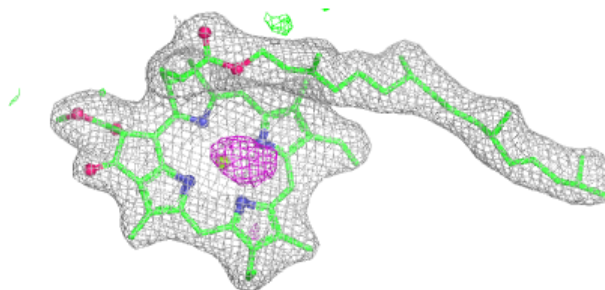


Electron density around LHG d 406:

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

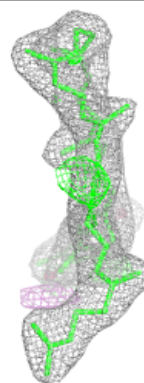
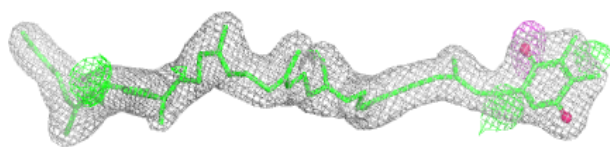
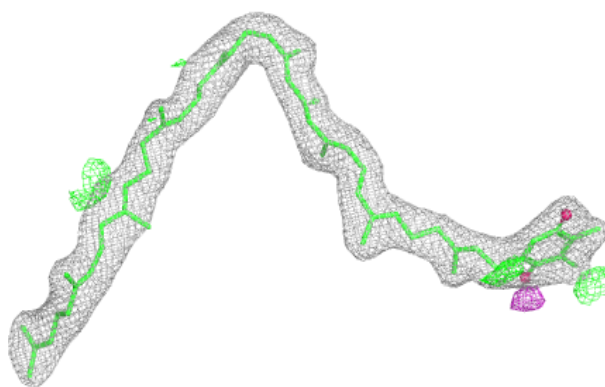
**Electron density around CLA C 501:**

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

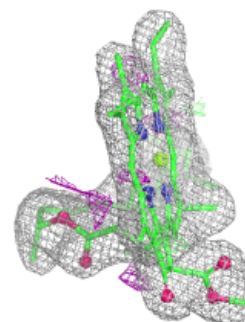
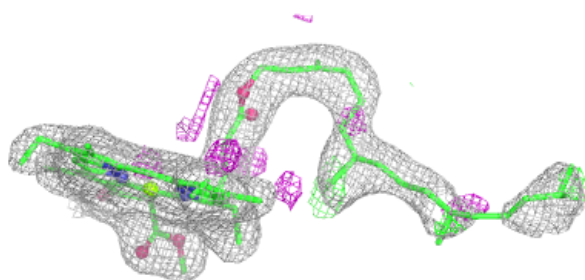
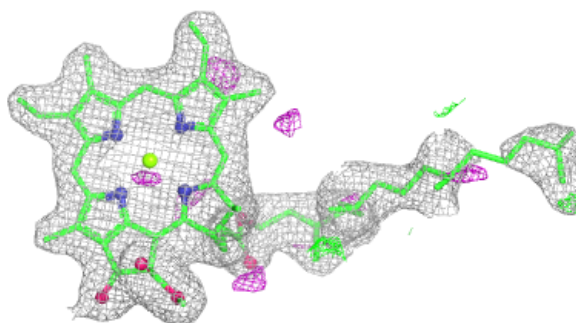


Electron density around PL9 D 405:

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

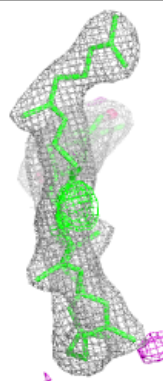
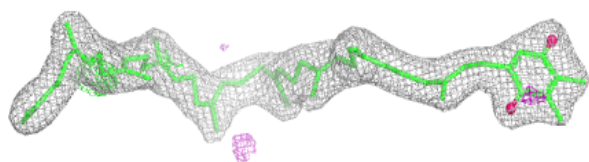
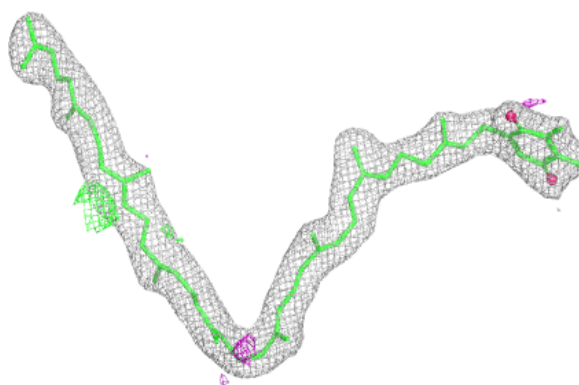
**Electron density around CLA A 406:**

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

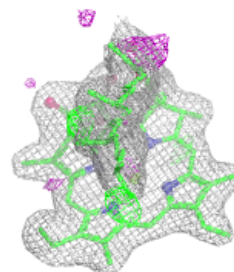
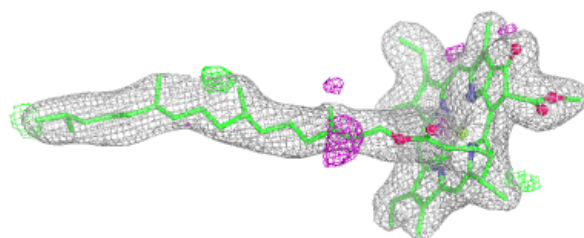
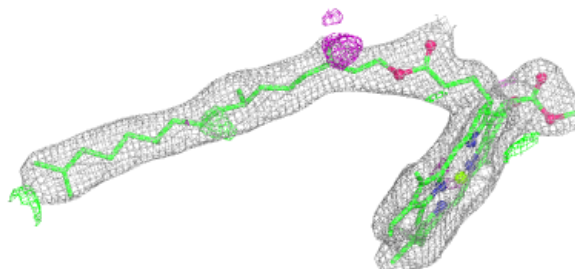


Electron density around PL9 d 404:

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

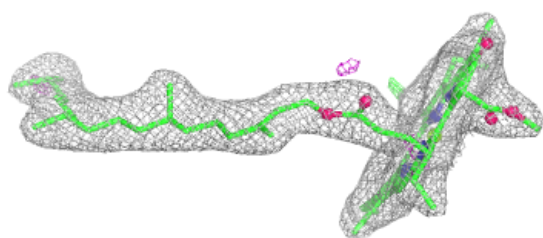
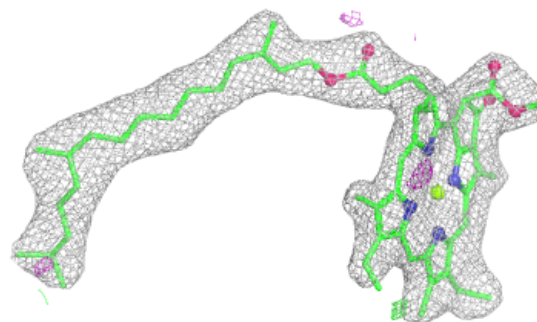
**Electron density around CLA b 607:**

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

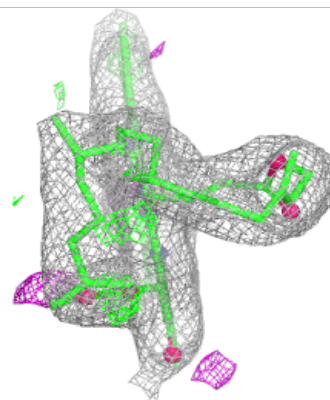
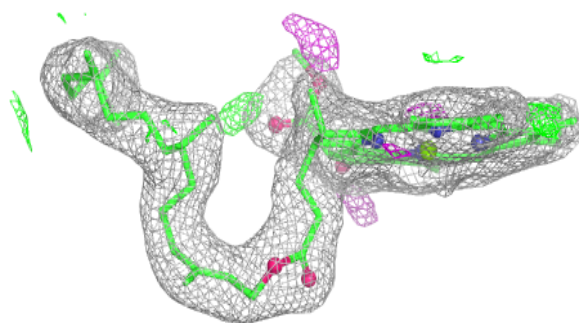
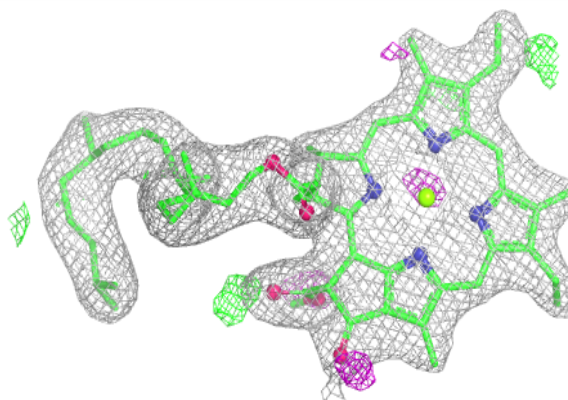


Electron density around CLA b 609:

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

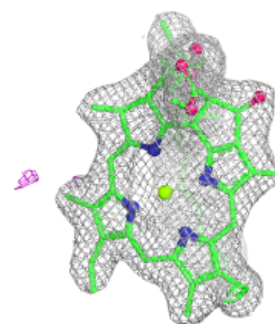
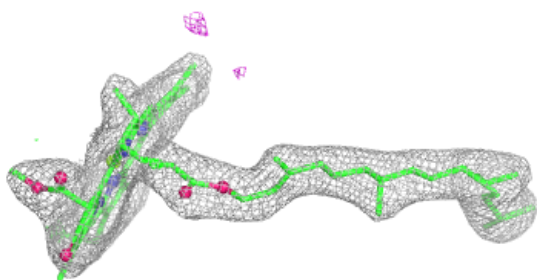
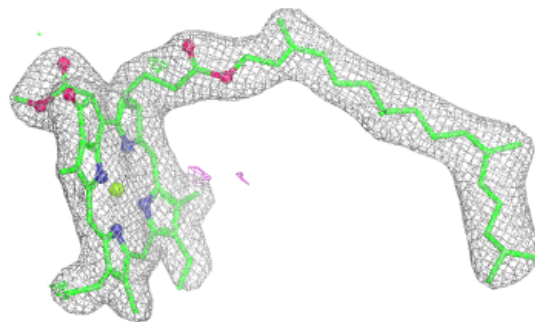
**Electron density around CLA b 612:**

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

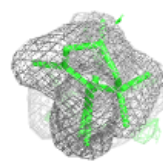
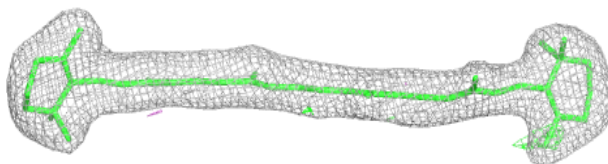
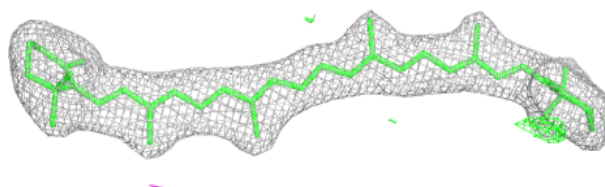


Electron density around CLA B 609:

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

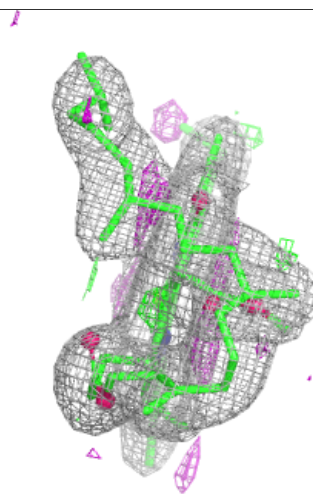
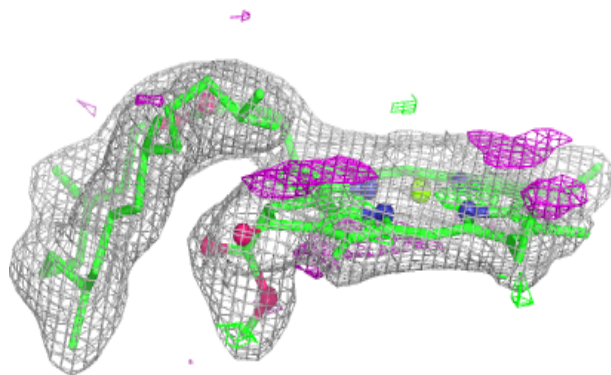
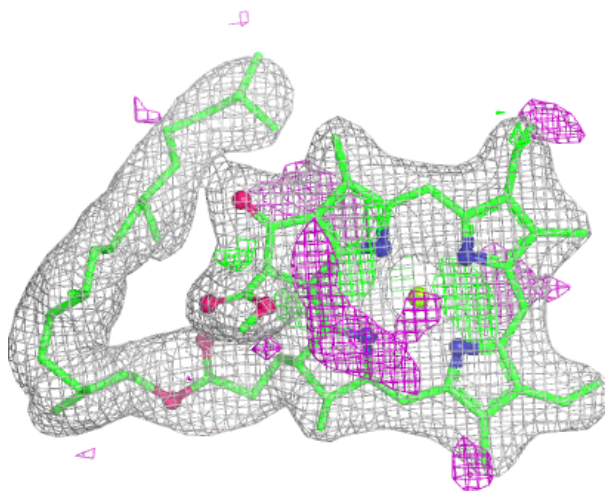
**Electron density around BCR a 410:**

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



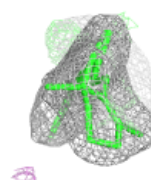
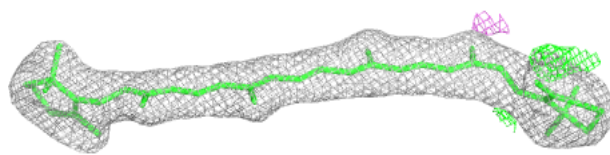
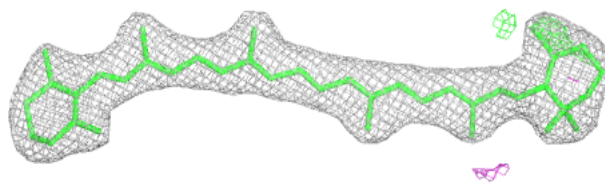
Electron density around CLA B 610:

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



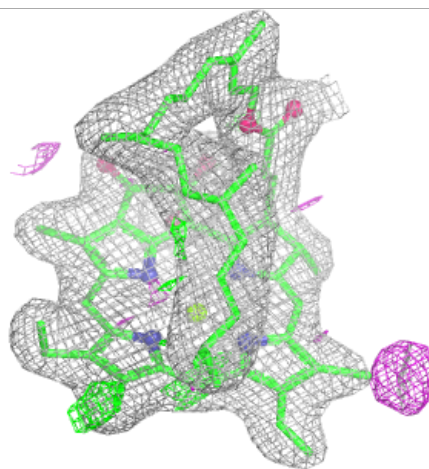
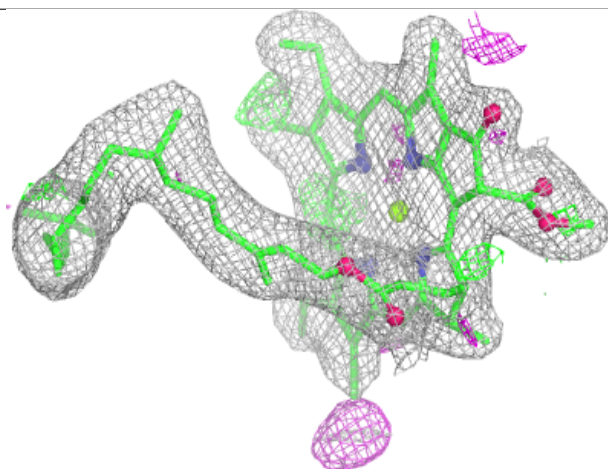
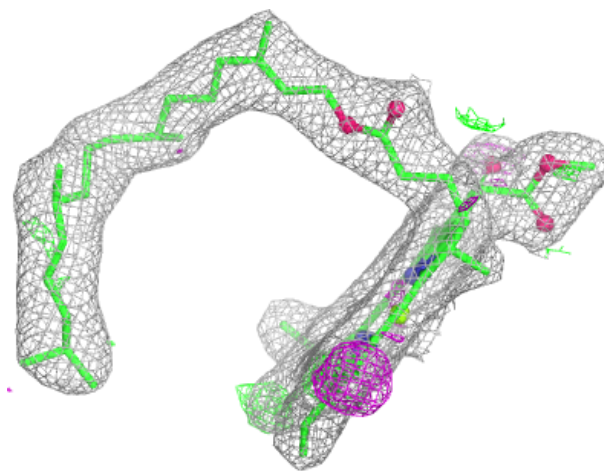
Electron density around BCR b 619:

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



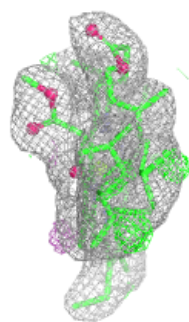
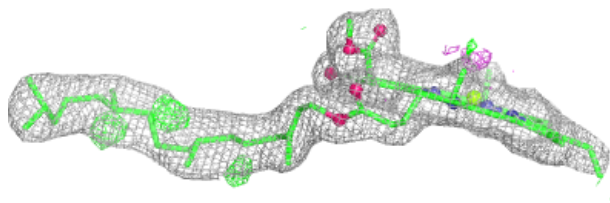
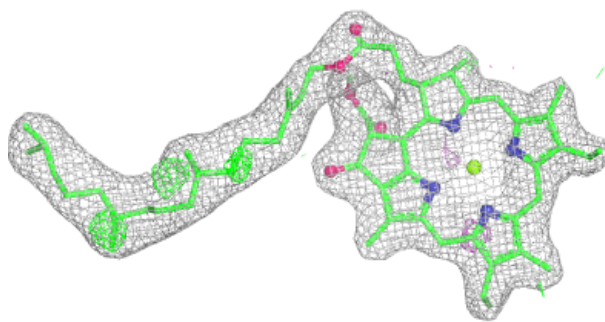
Electron density around CLA B 611:

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



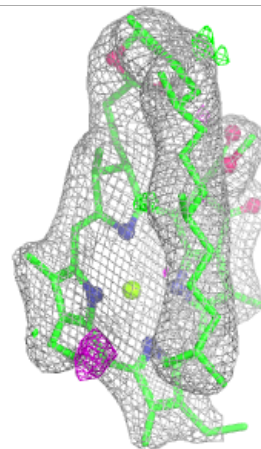
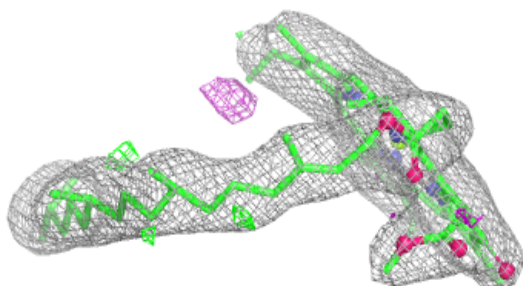
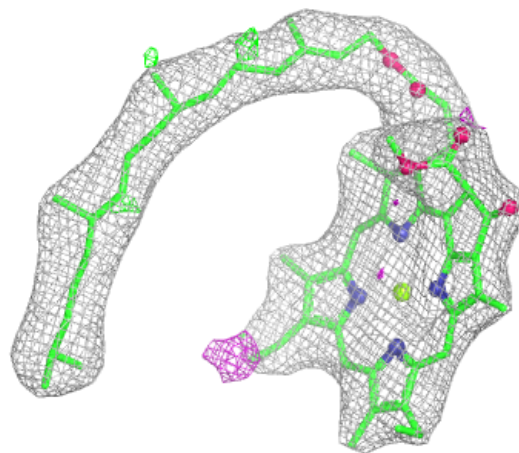
Electron density around CLA B 602:

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



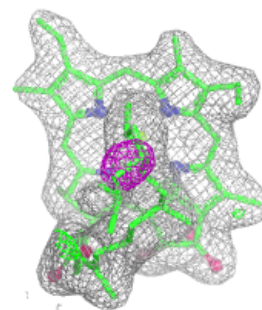
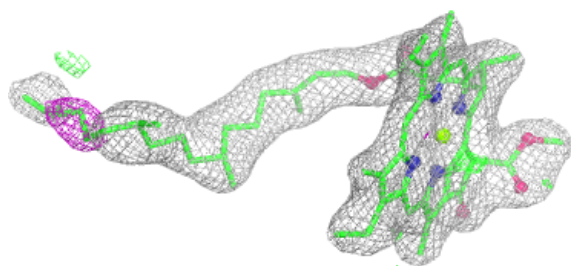
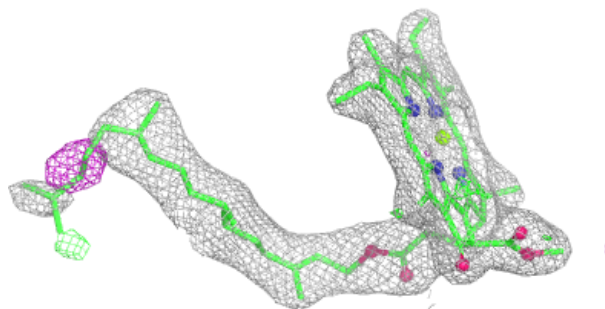
Electron density around CLA c 508:

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

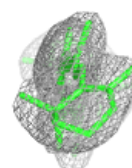
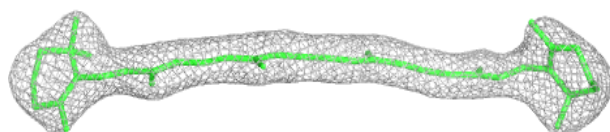
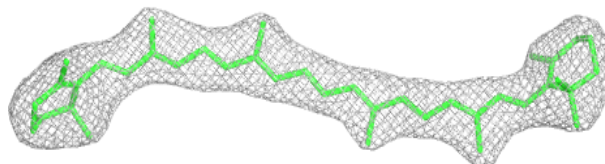


Electron density around CLA c 509:

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

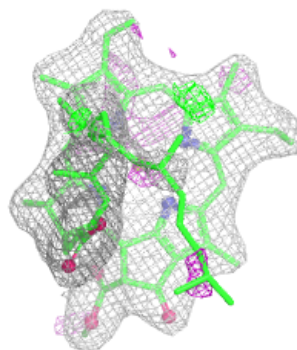
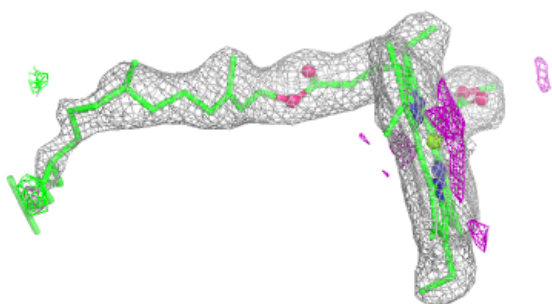
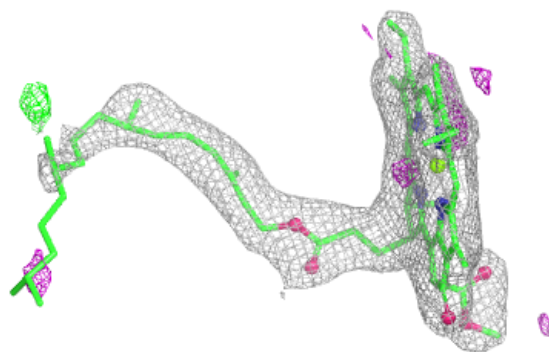
**Electron density around BCR y 101:**

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

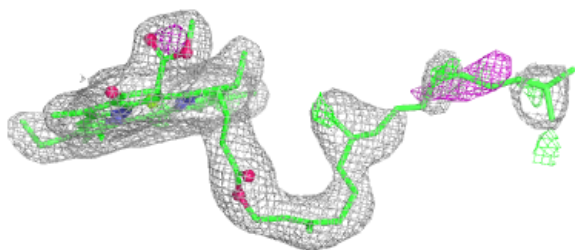
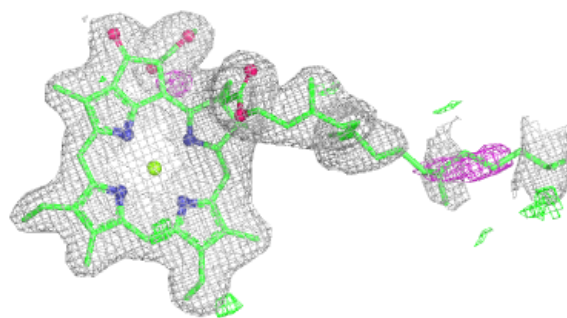


Electron density around CLA D 403:

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

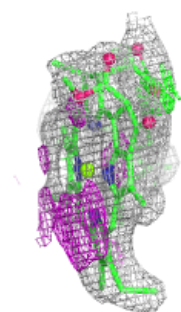
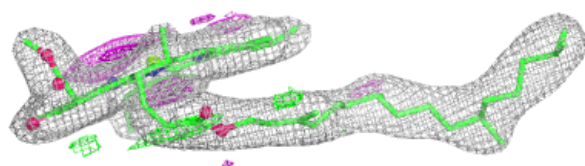
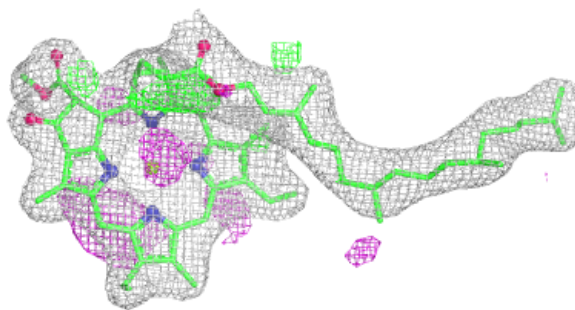
**Electron density around CLA a 407:**

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

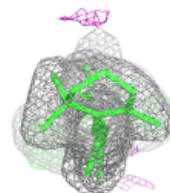
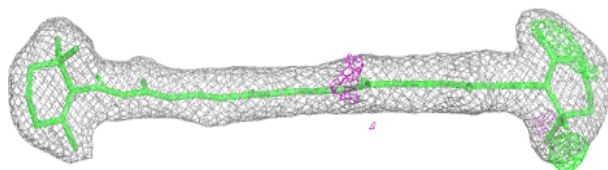
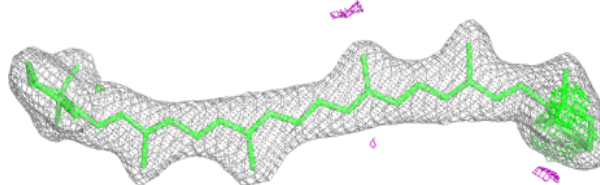


Electron density around CLA B 603:

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

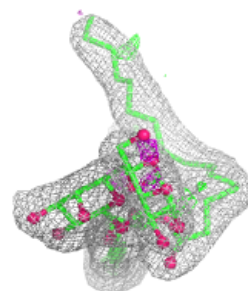
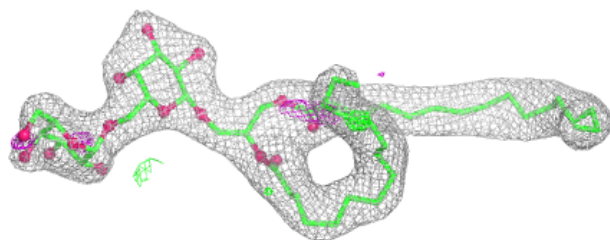
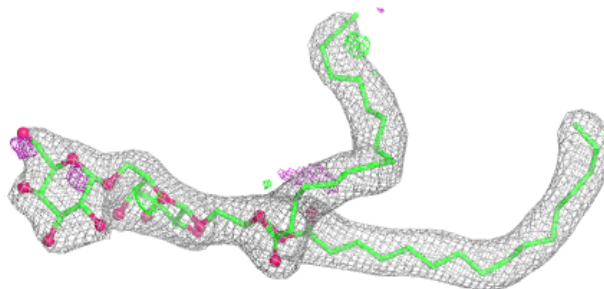
**Electron density around BCR A 409:**

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

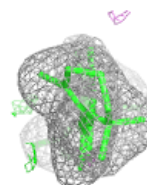
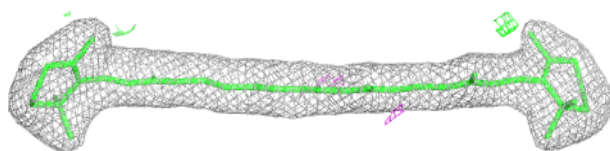
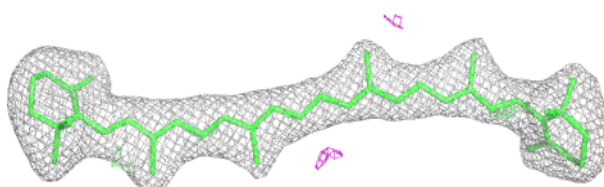


Electron density around DGD h 102:

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

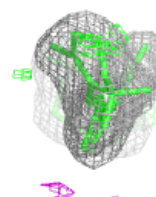
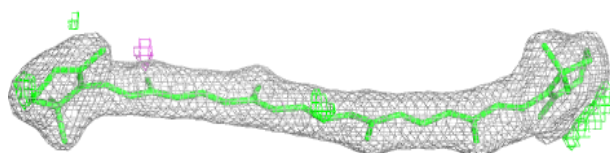
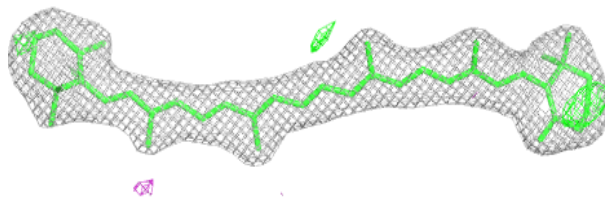
**Electron density around BCR B 618:**

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

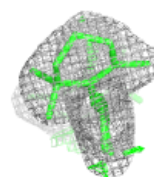
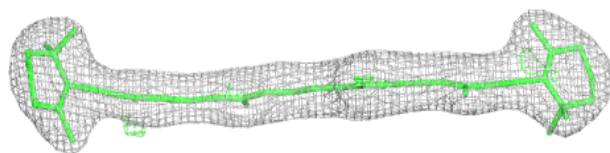
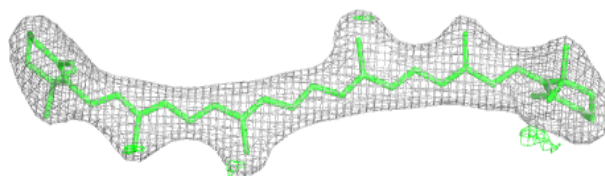


Electron density around BCR B 619:

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

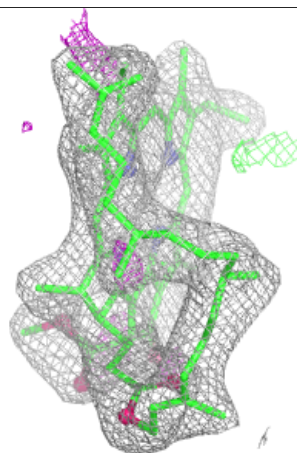
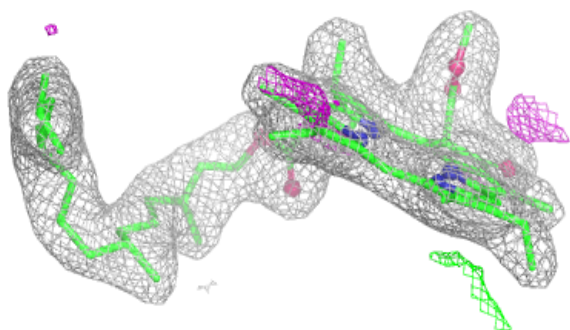
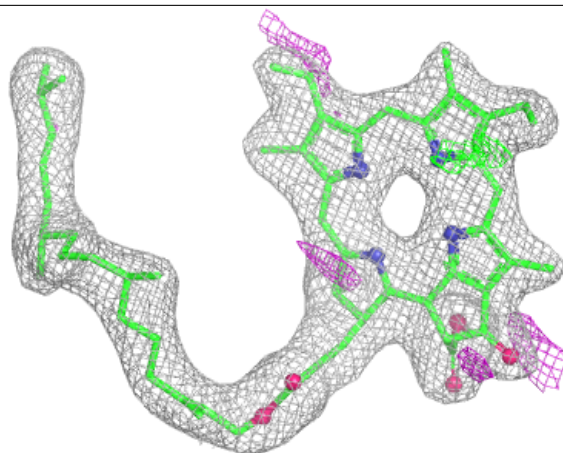
**Electron density around BCR C 514:**

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



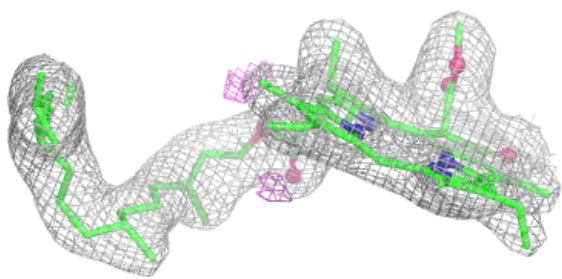
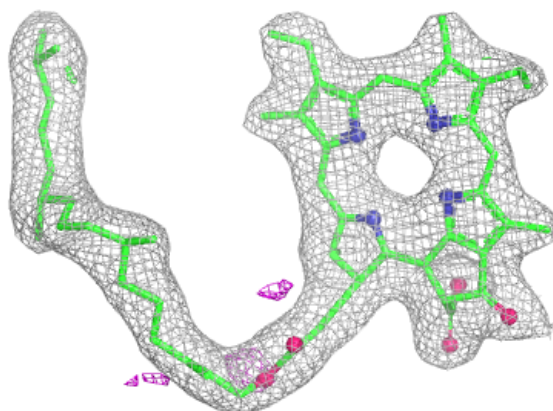
Electron density around PHO A 416:

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



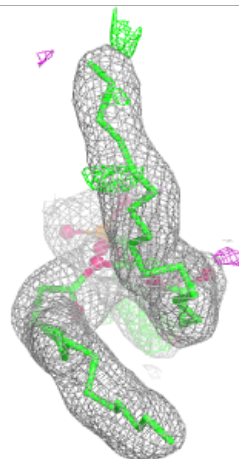
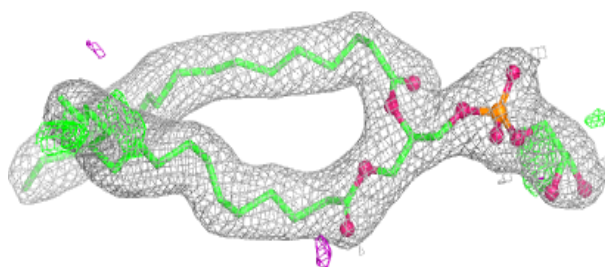
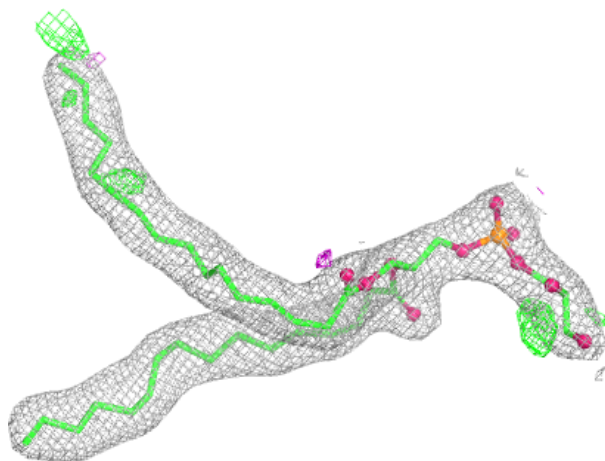
Electron density around PHO a 417:

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



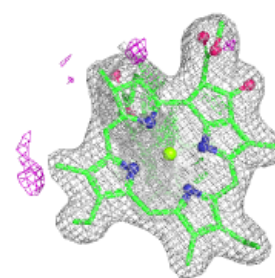
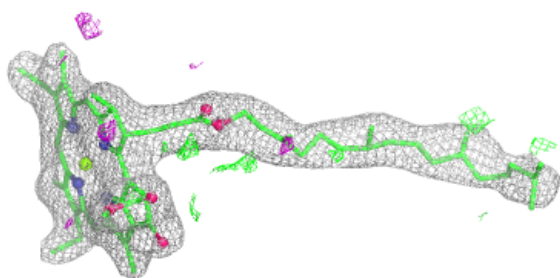
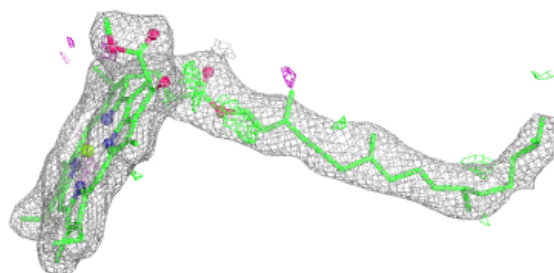
Electron density around LHG d 405:

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

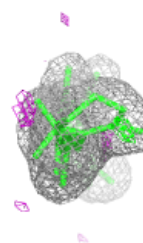
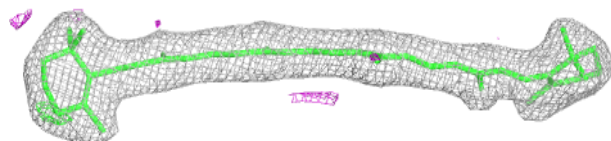
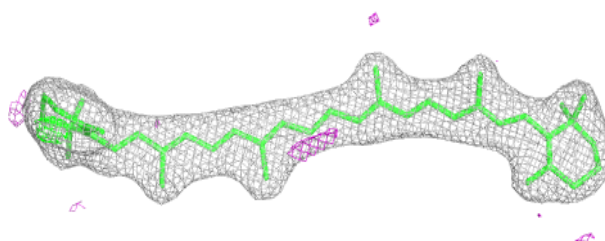


Electron density around CLA b 604:

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

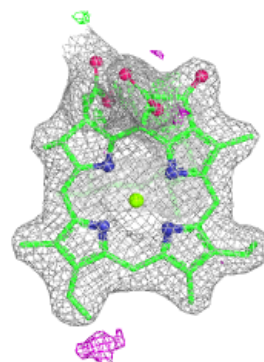
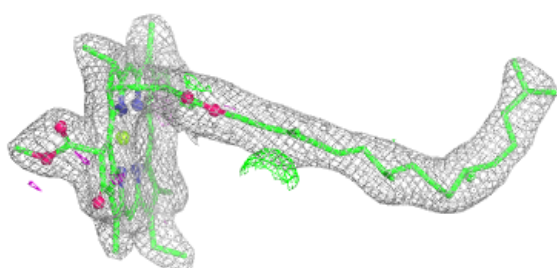
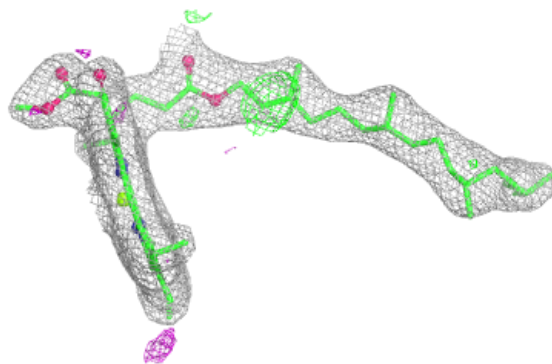
**Electron density around BCR B 617:**

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

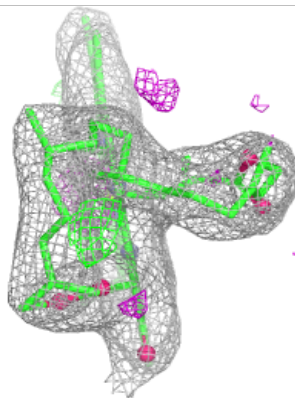
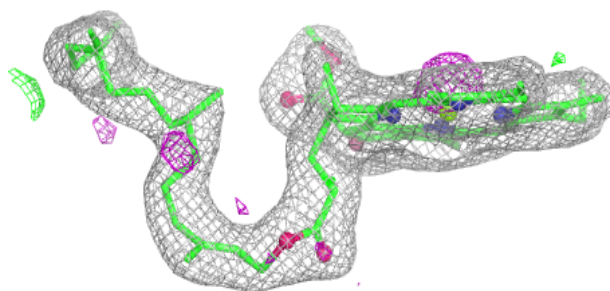
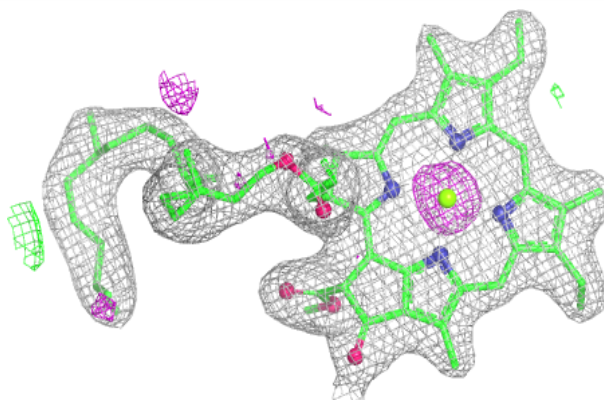


Electron density around CLA b 605:

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

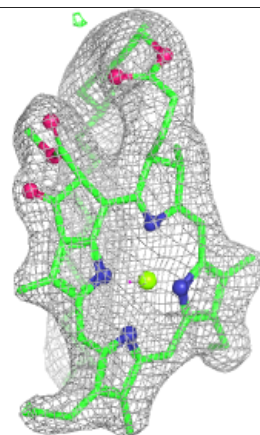
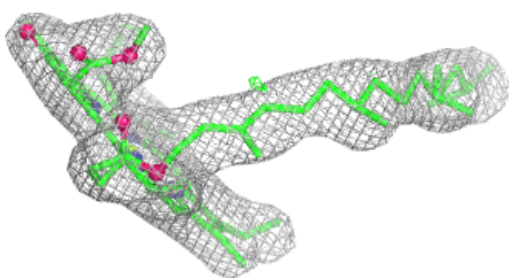
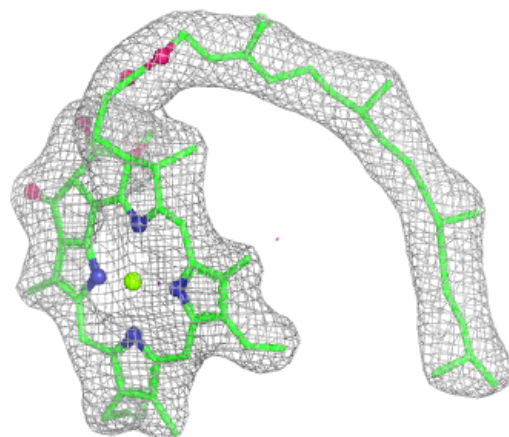
**Electron density around CLA B 612:**

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



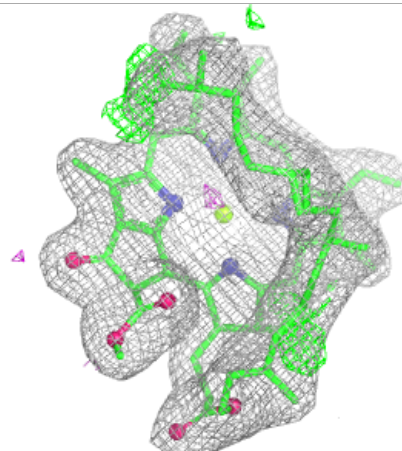
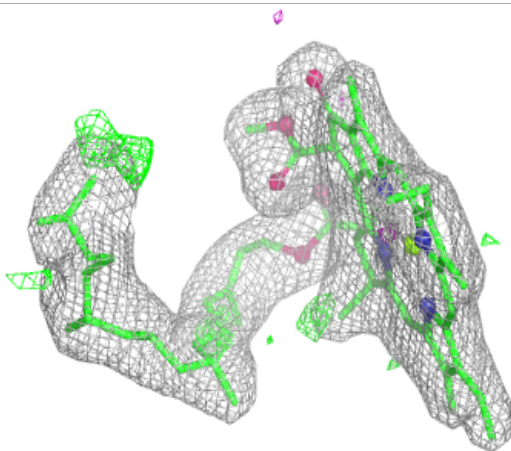
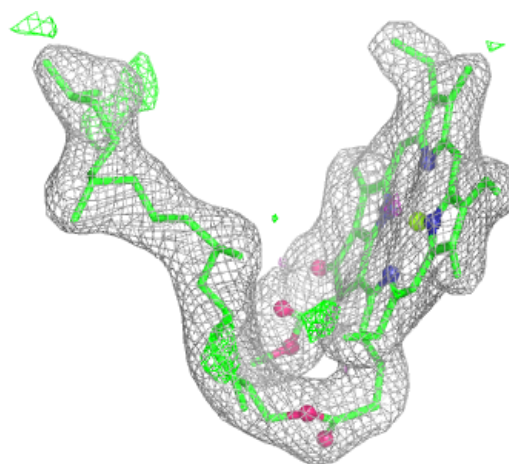
Electron density around CLA C 507:

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



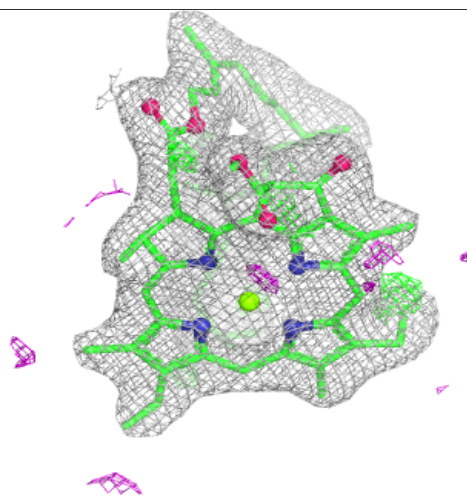
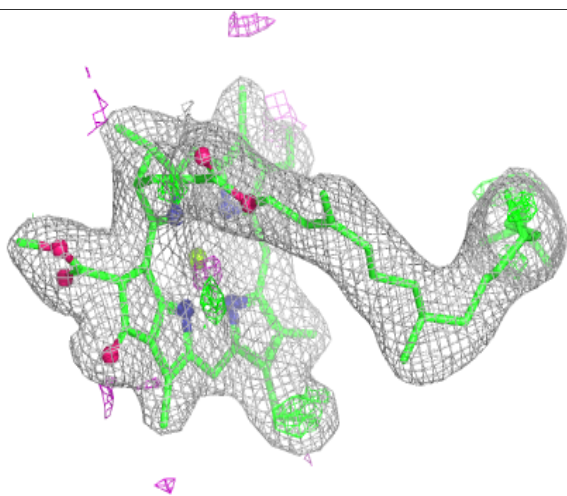
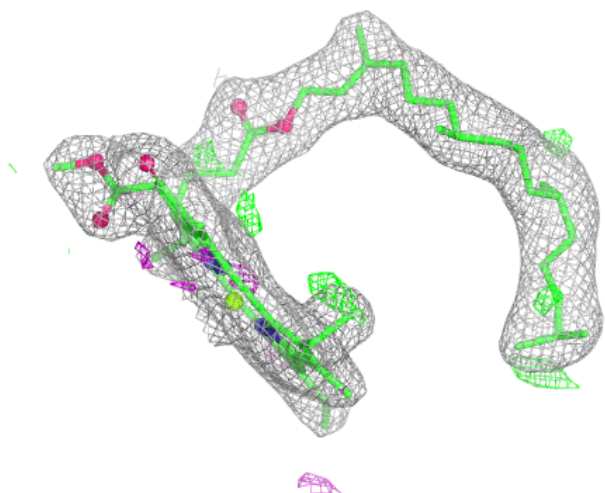
Electron density around CLA B 613:

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



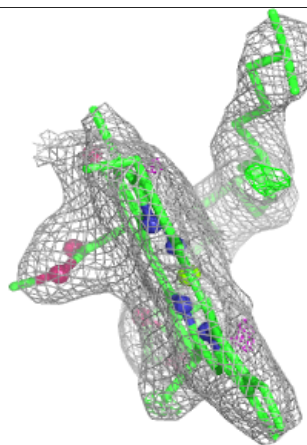
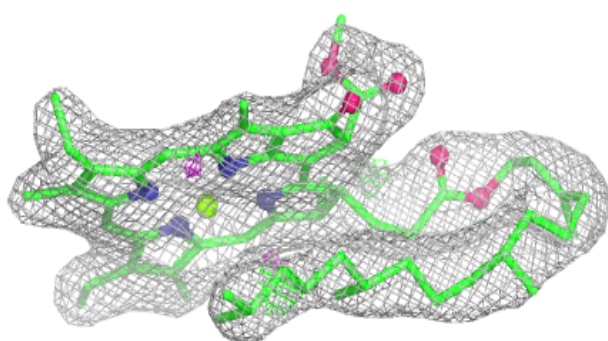
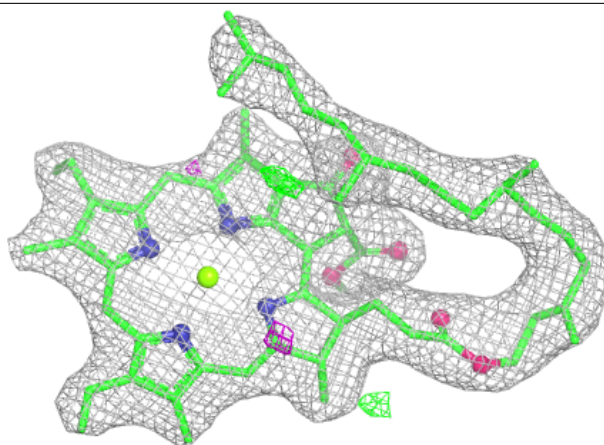
Electron density around CLA b 611:

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



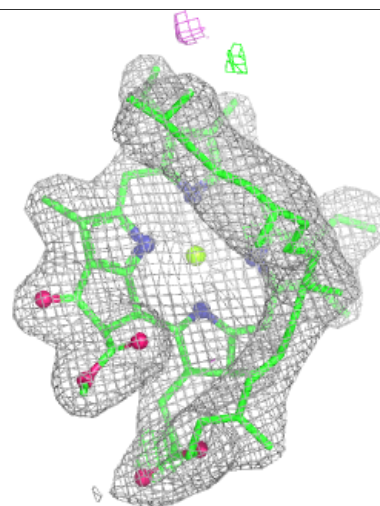
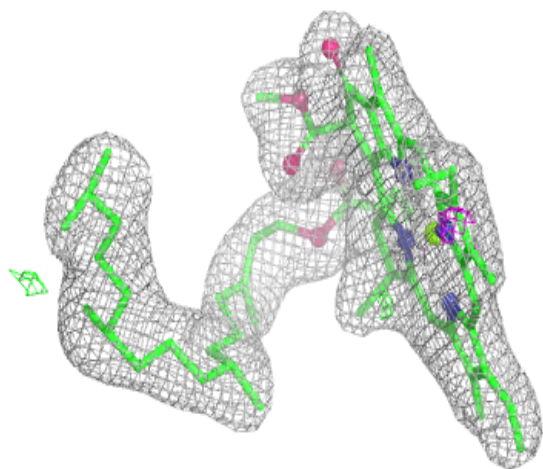
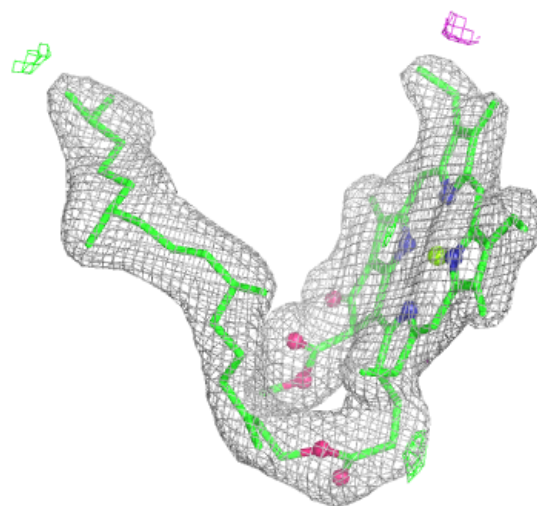
Electron density around CLA C 509:

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



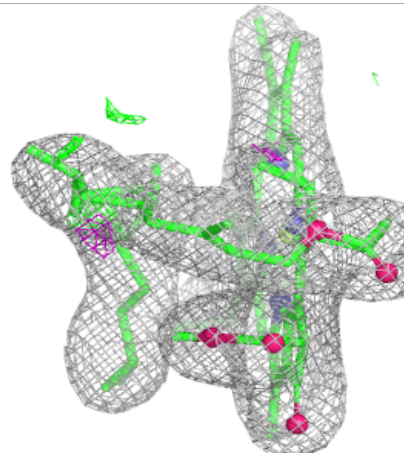
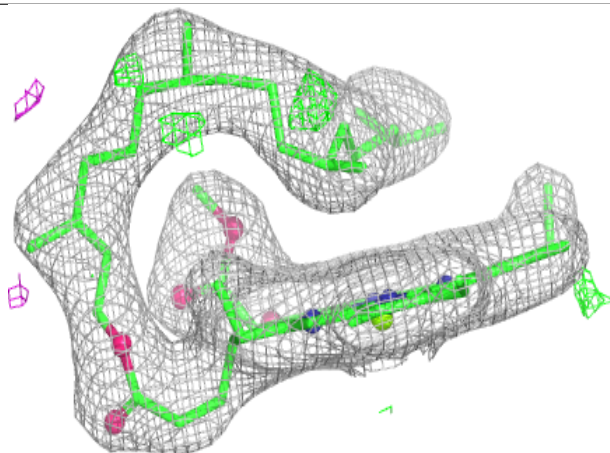
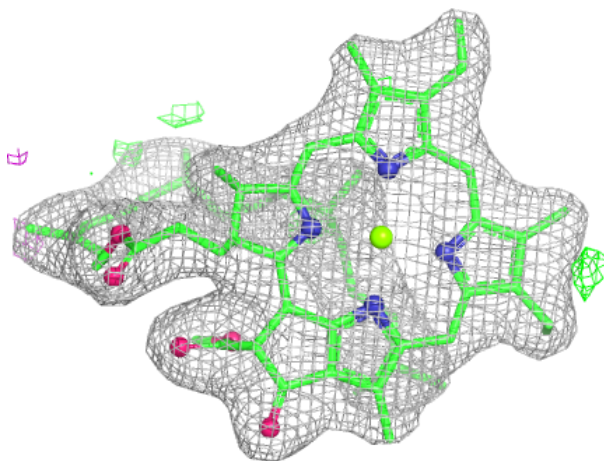
Electron density around CLA b 613:

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



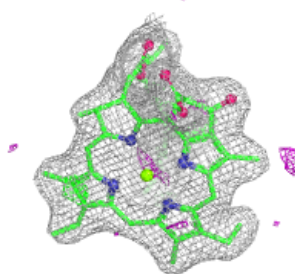
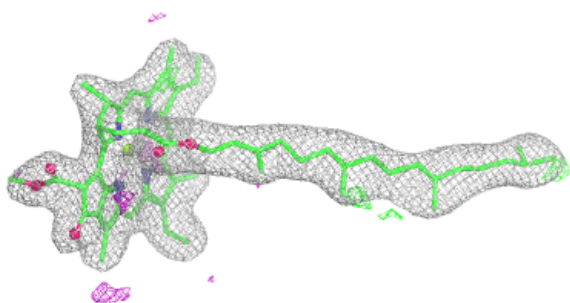
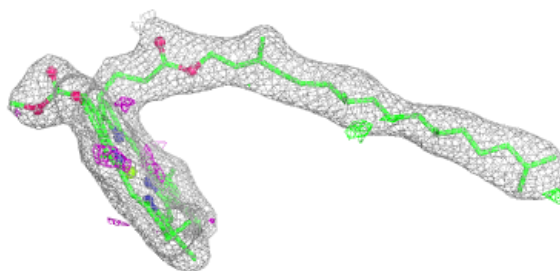
Electron density around CLA C 510:

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

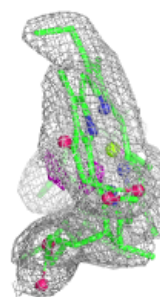
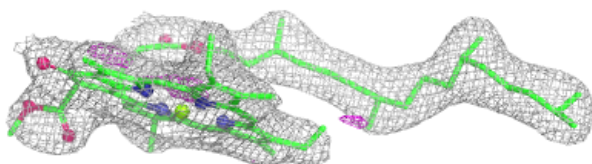
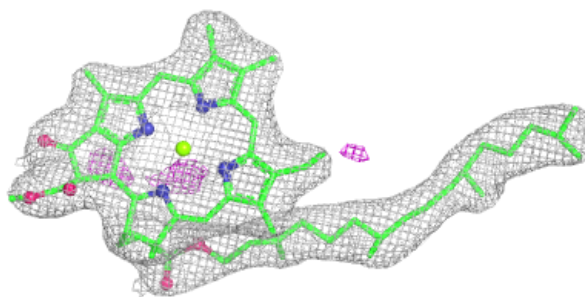


Electron density around CLA B 607:

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

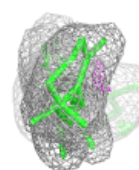
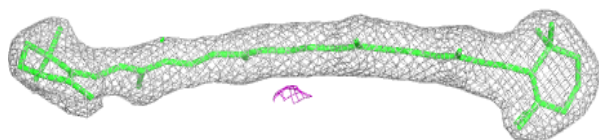
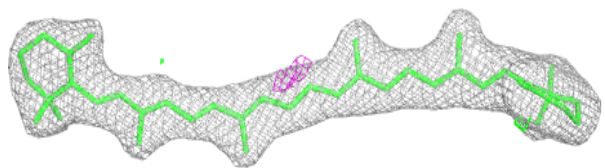
**Electron density around CLA c 502:**

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

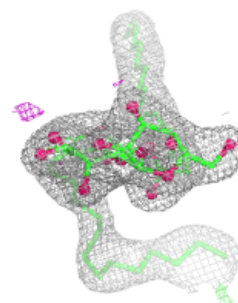
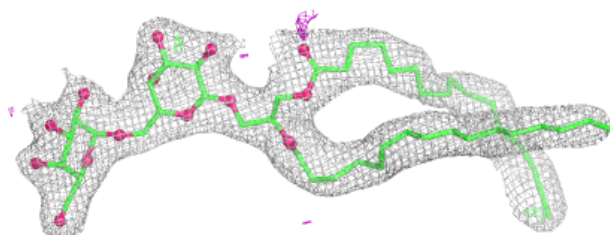
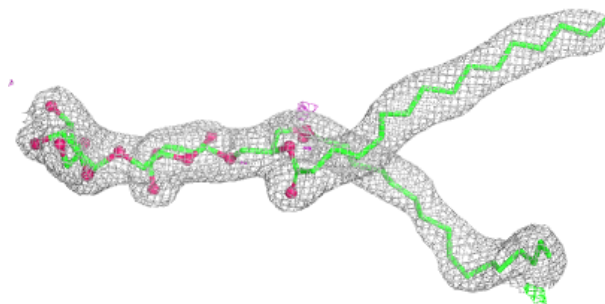


Electron density around BCR b 617:

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

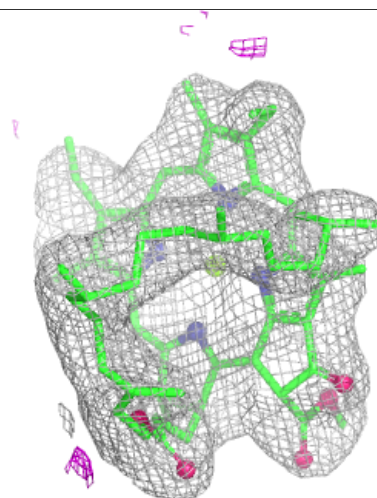
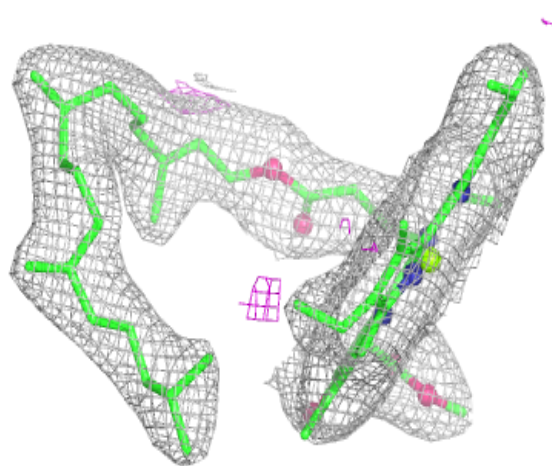
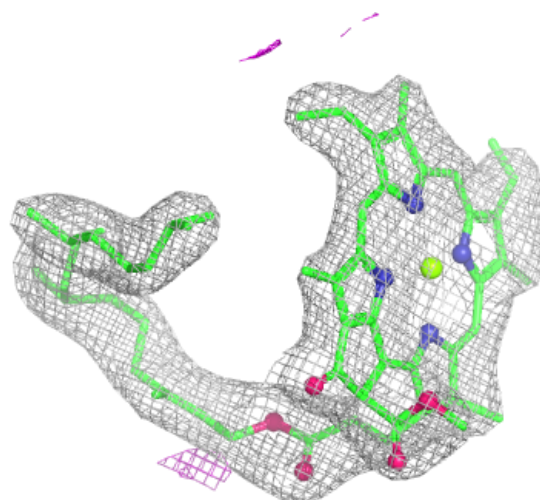
**Electron density around DGD C 515:**

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



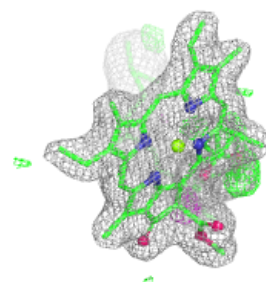
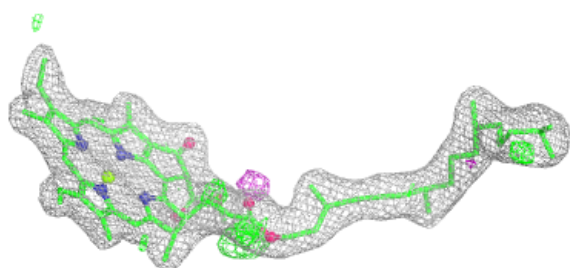
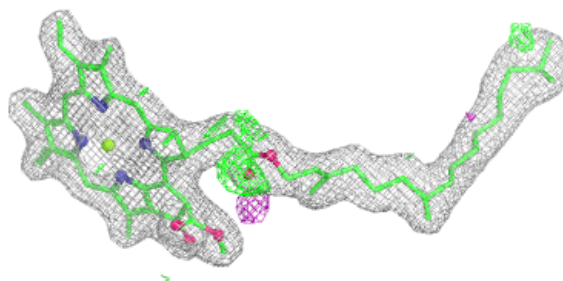
Electron density around CLA c 504:

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

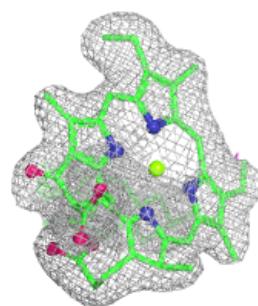
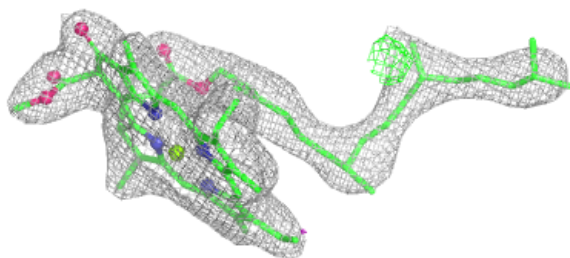
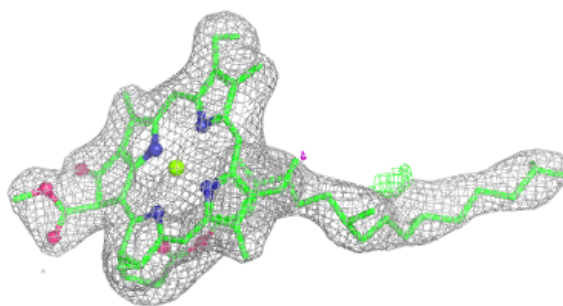


Electron density around CLA A 404:

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

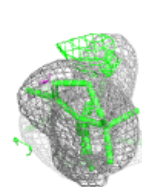
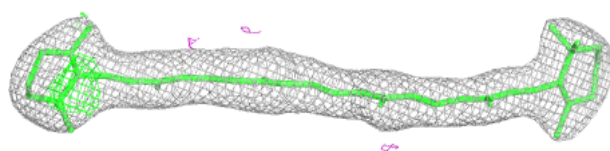
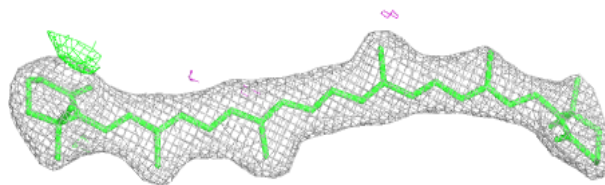
**Electron density around CLA c 506:**

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

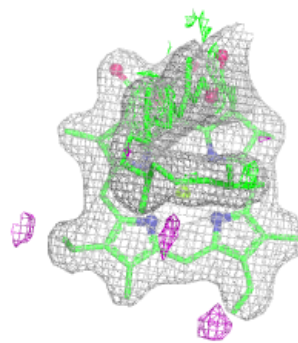
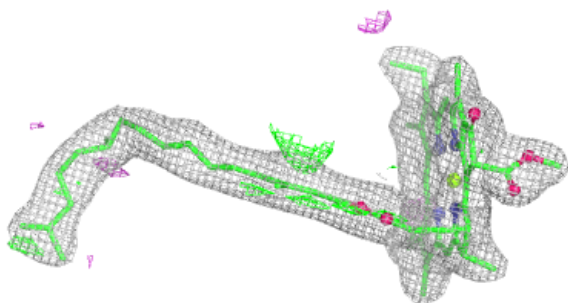
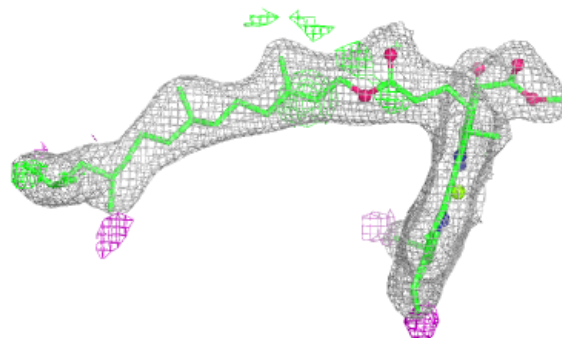


Electron density around BCR c 516:

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

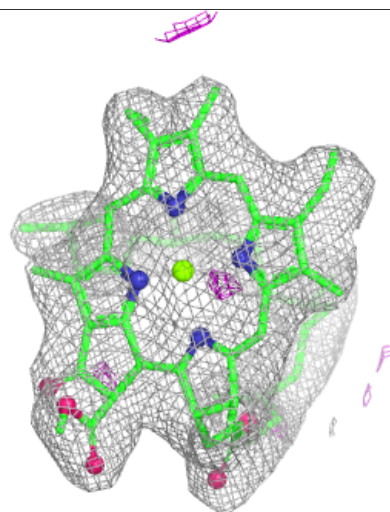
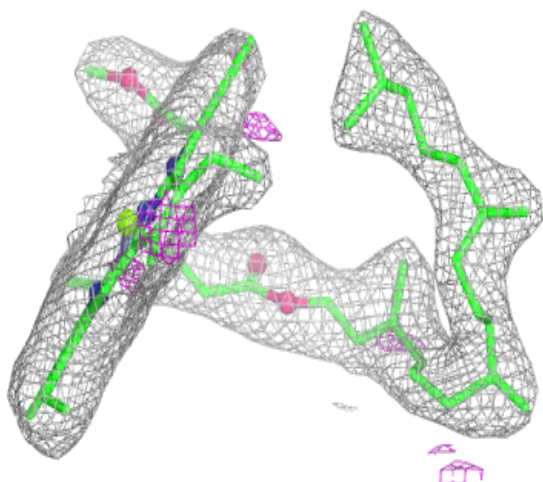
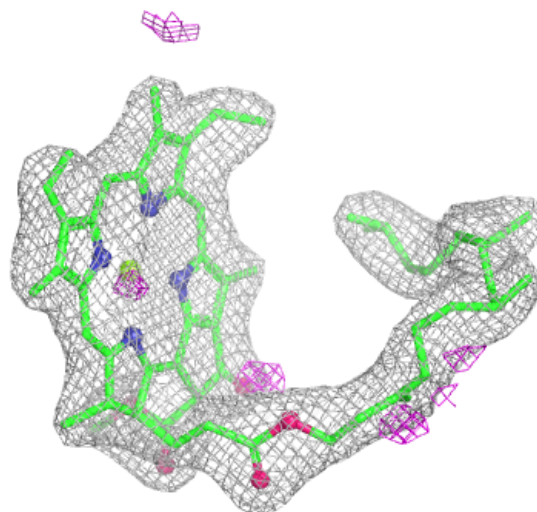
**Electron density around CLA B 605:**

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



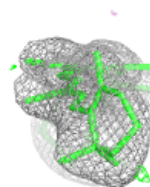
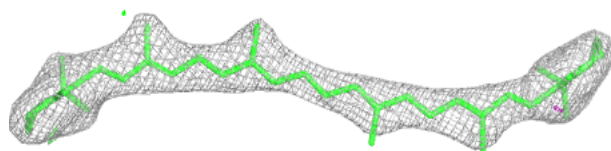
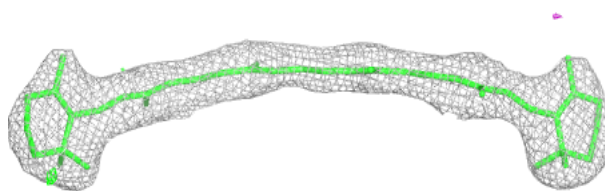
Electron density around CLA C 503:

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

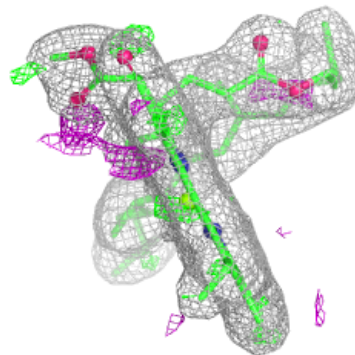
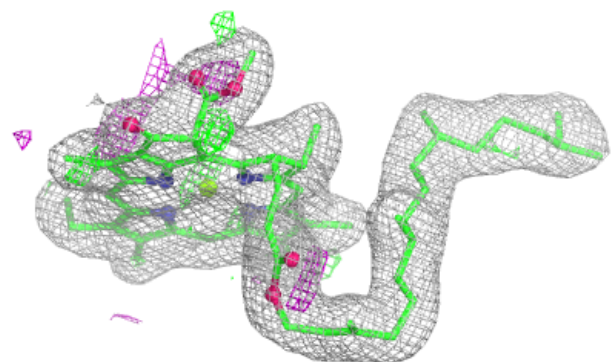
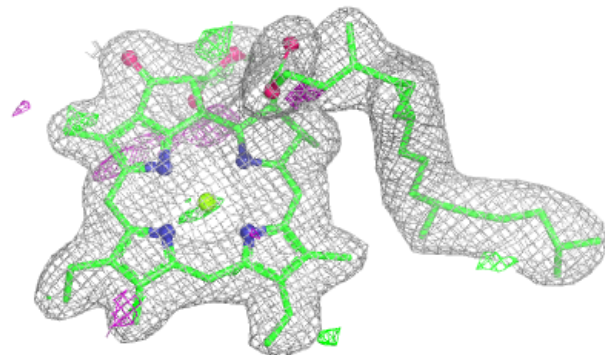


Electron density around BCR k 101:

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

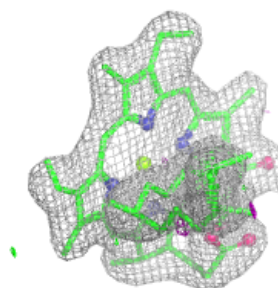
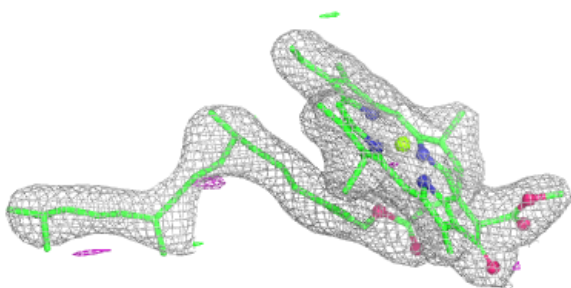
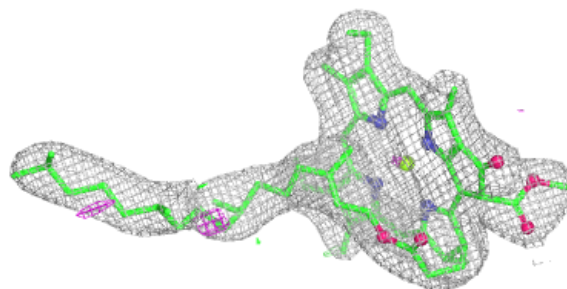
**Electron density around CLA A 405:**

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



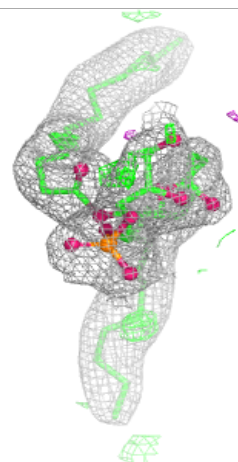
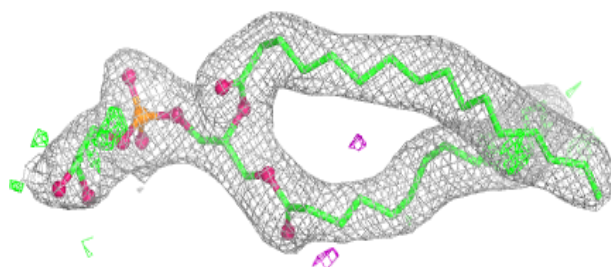
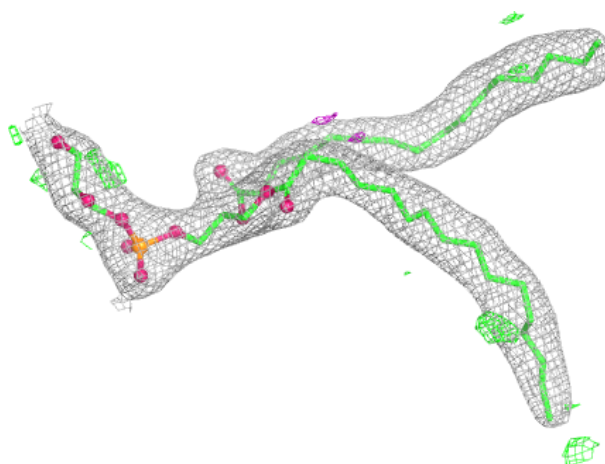
Electron density around CLA C 505:

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



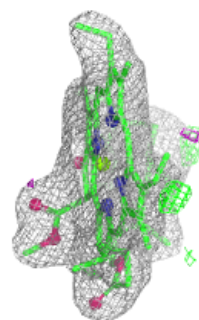
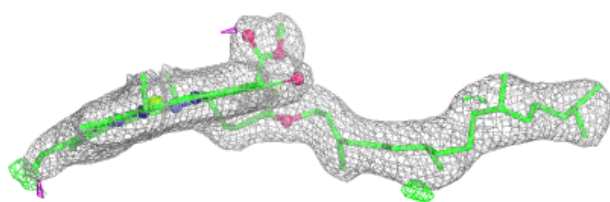
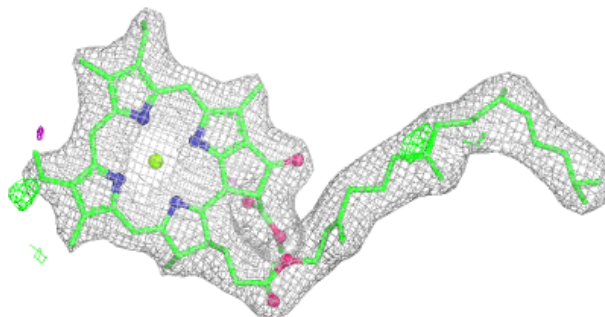
Electron density around LHG D 406:

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

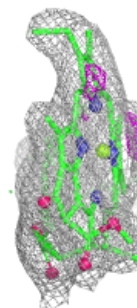
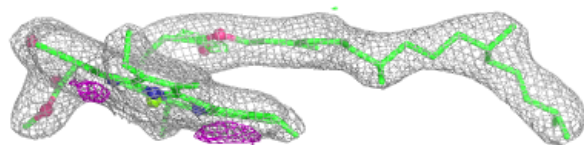
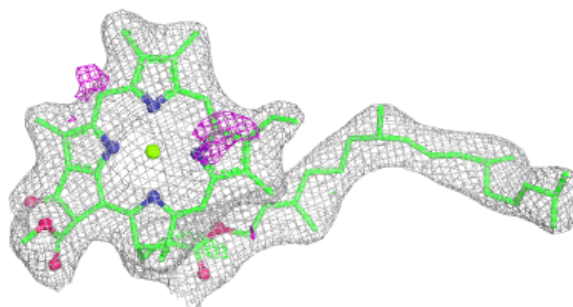


Electron density around CLA b 602:

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

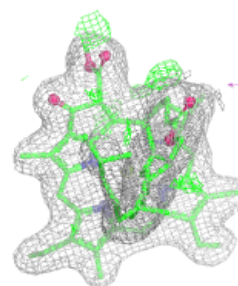
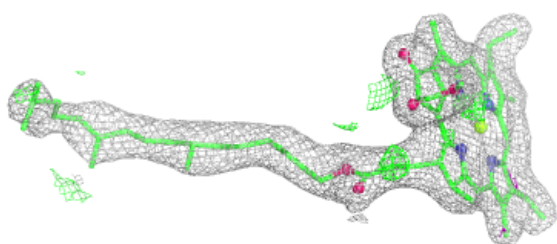
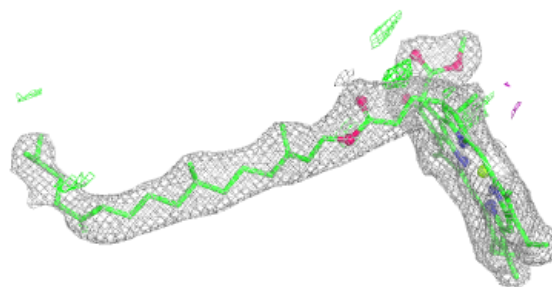
**Electron density around CLA b 603:**

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

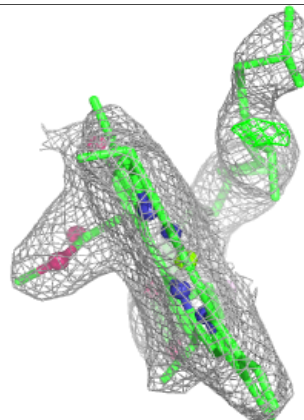
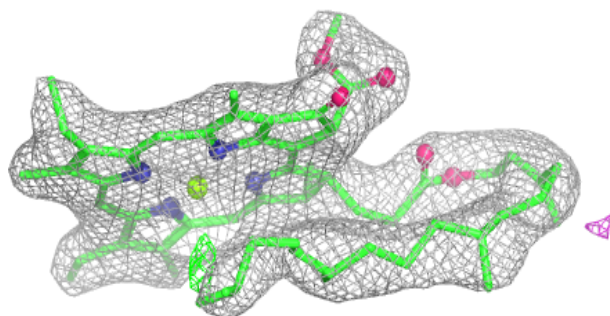
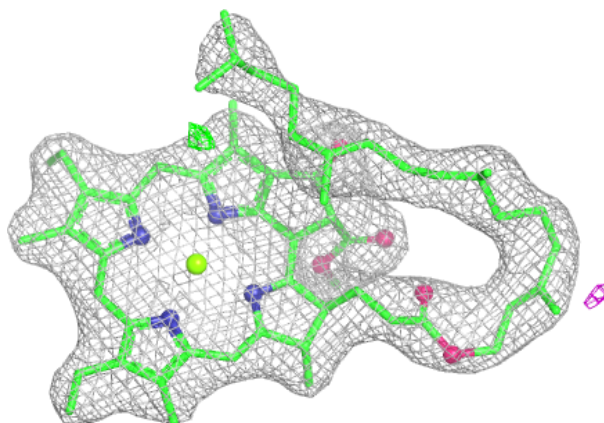


Electron density around CLA B 604:

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

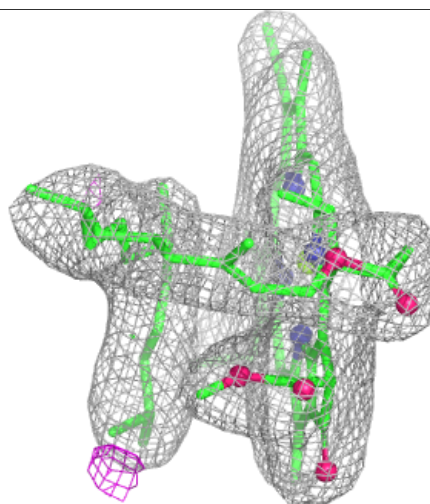
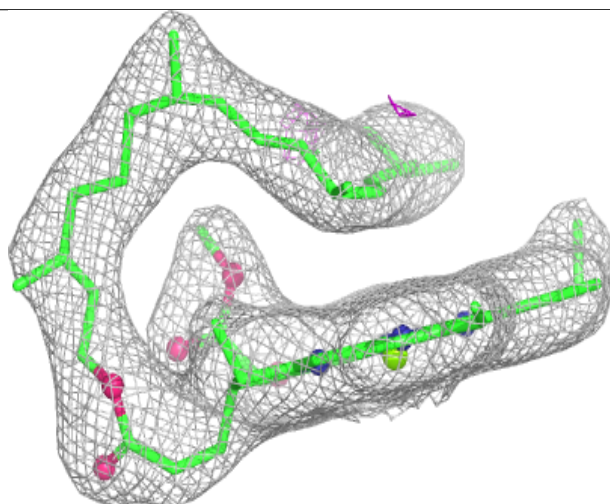
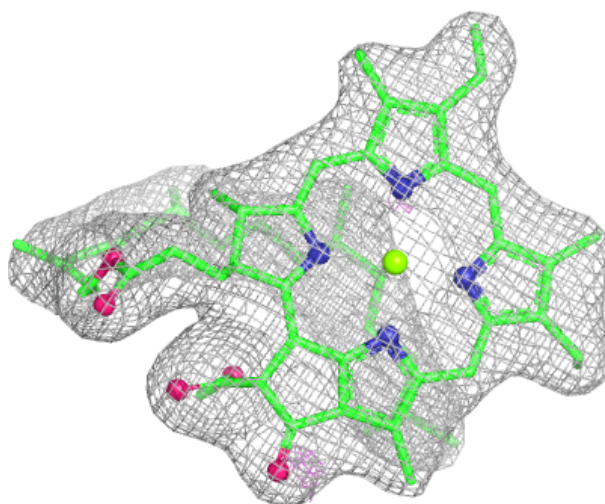
**Electron density around CLA c 510:**

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



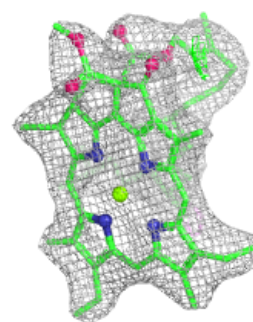
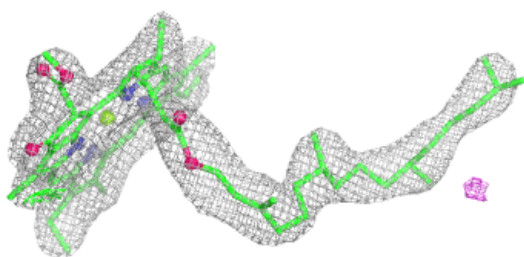
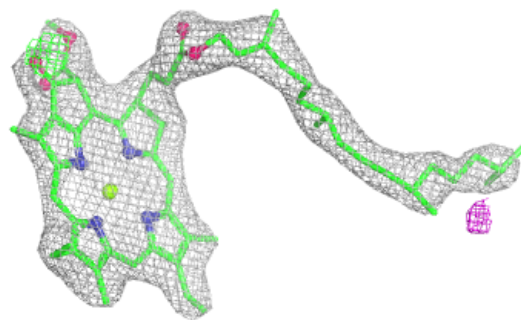
Electron density around CLA c 511:

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

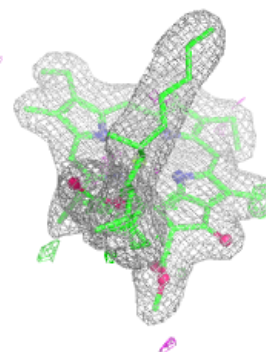
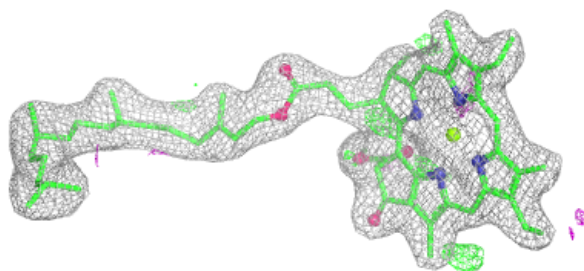
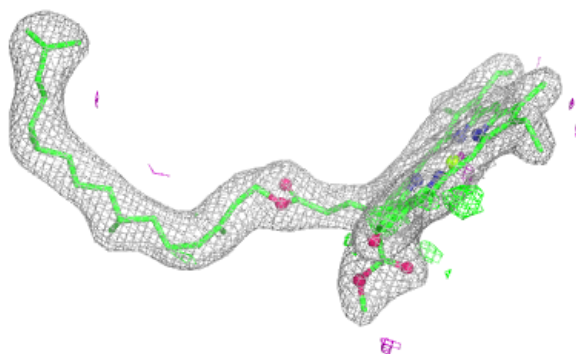


Electron density around CLA c 512:

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

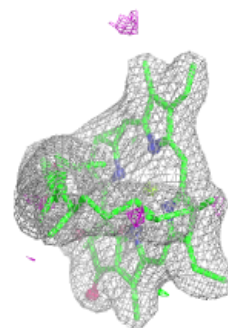
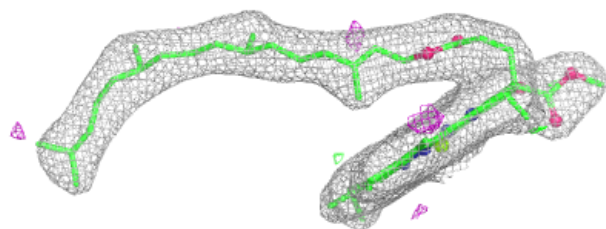
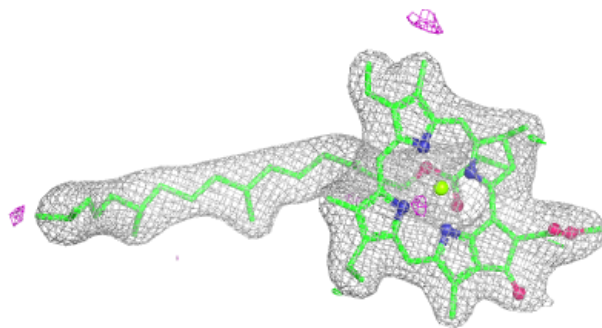
**Electron density around CLA D 402:**

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

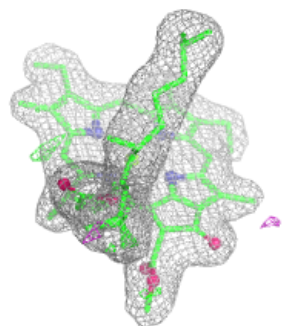
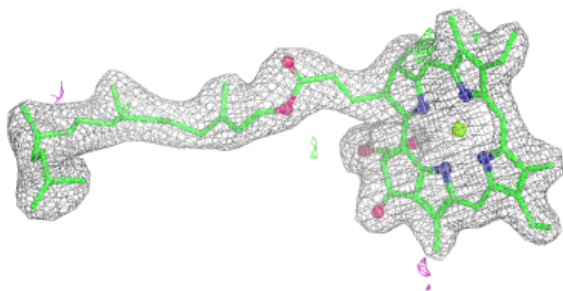
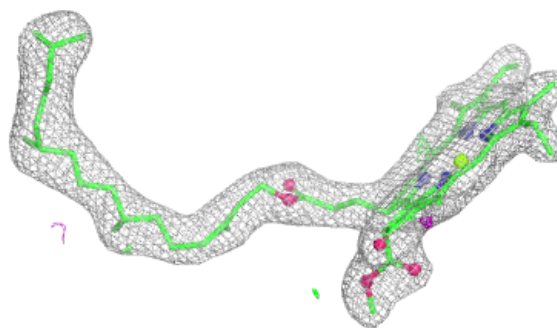


Electron density around CLA B 608:

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

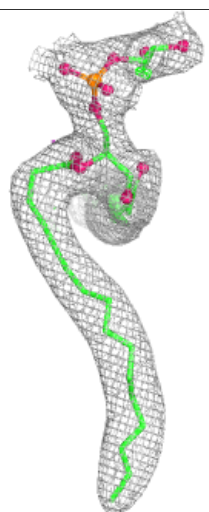
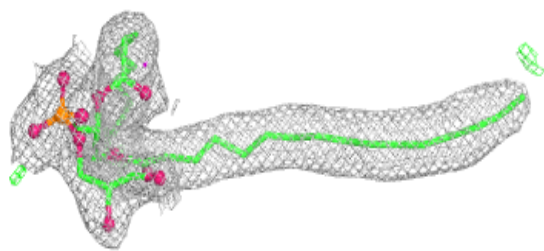
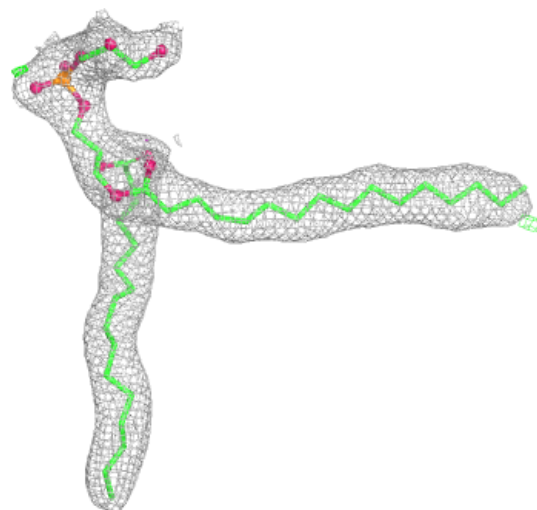
**Electron density around CLA d 401:**

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



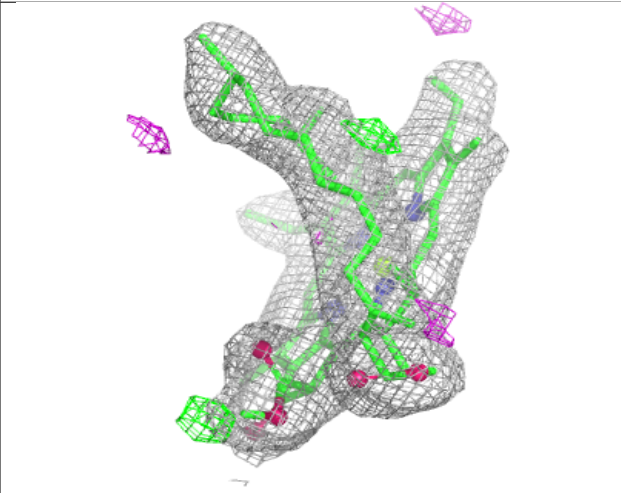
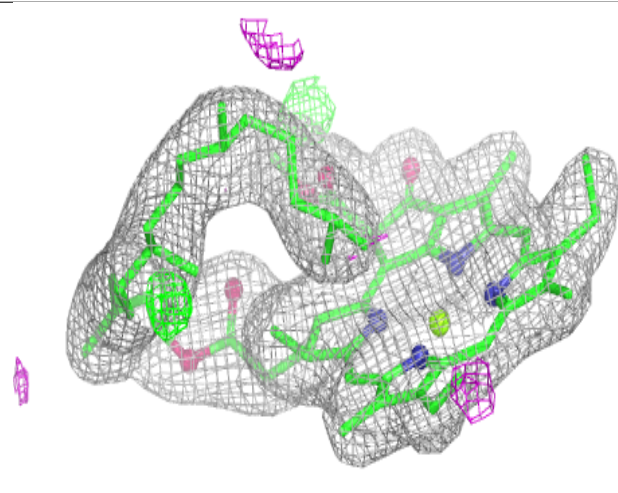
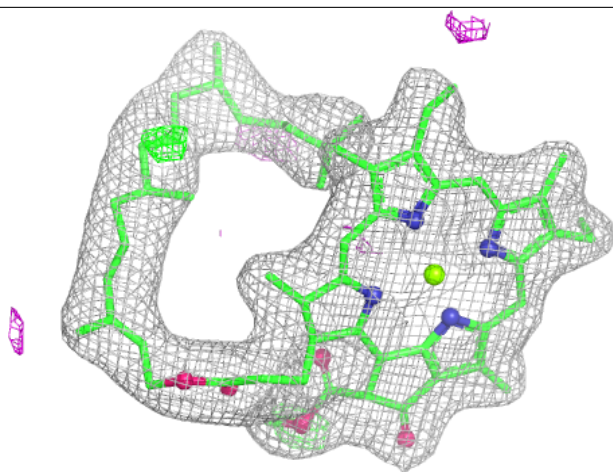
Electron density around LHG L 101:

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



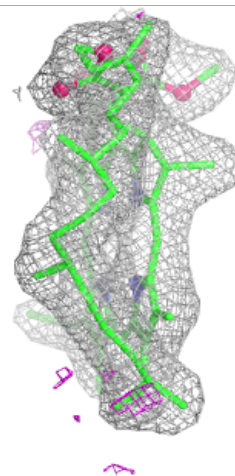
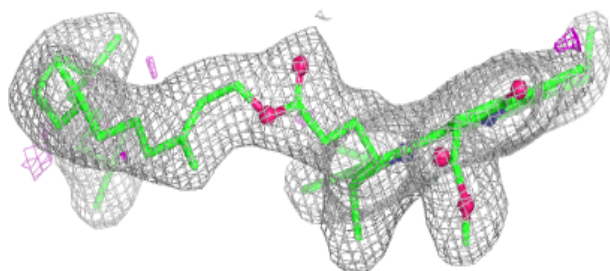
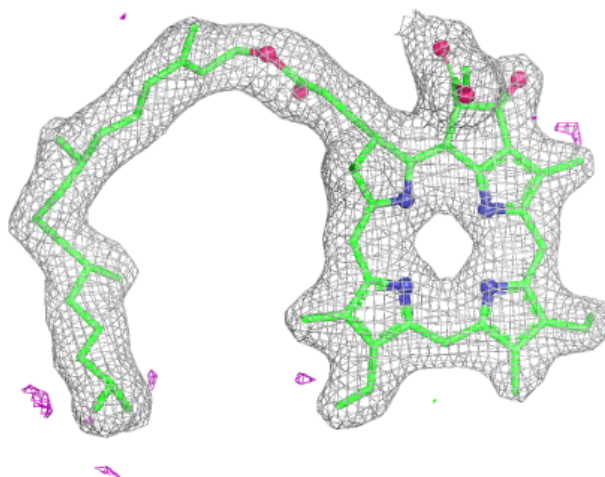
Electron density around CLA b 615:

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



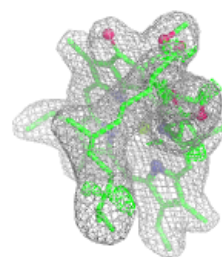
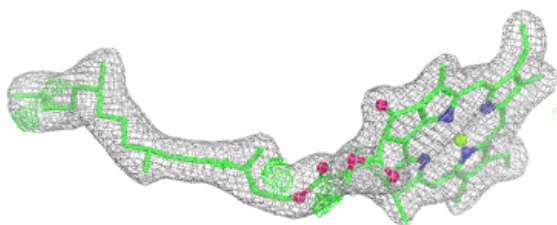
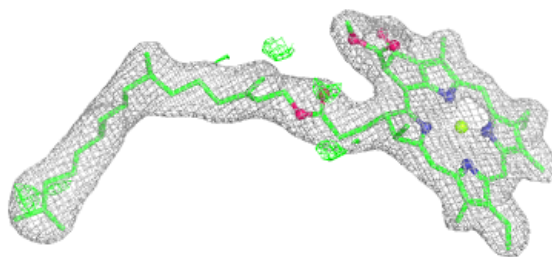
Electron density around PHO A 407:

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



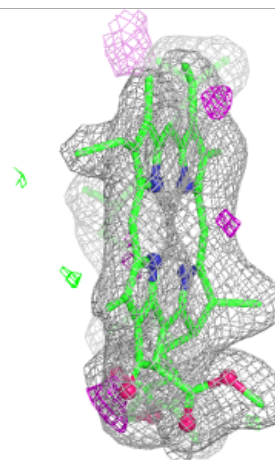
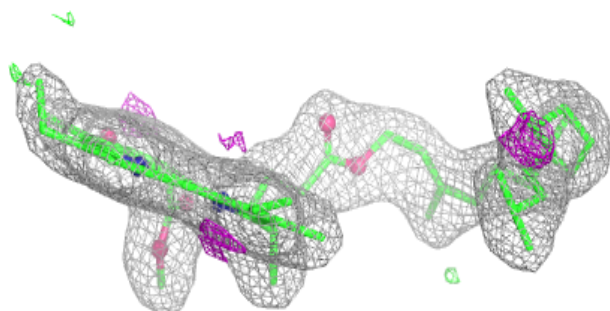
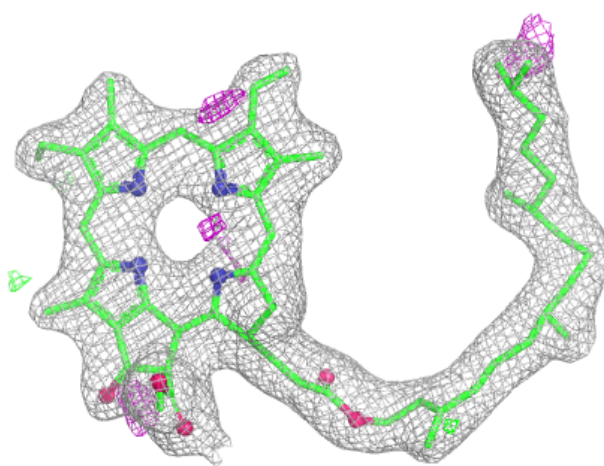
Electron density around CLA a 405:

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



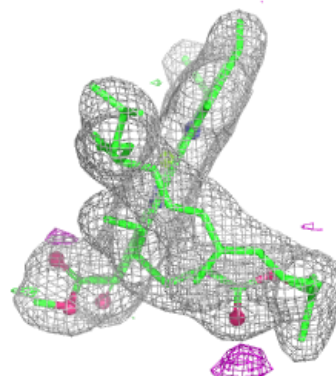
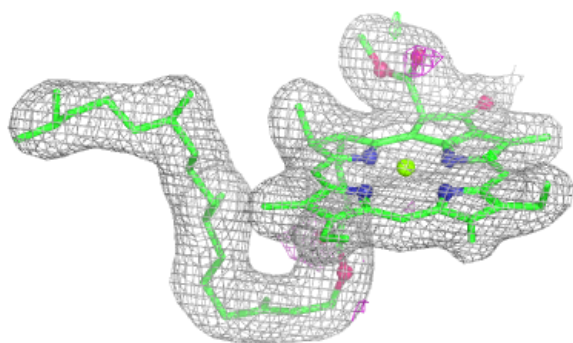
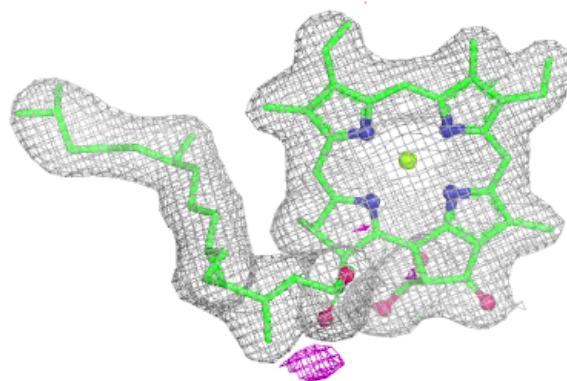
Electron density around PHO a 408:

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

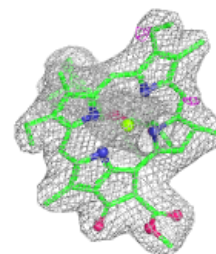
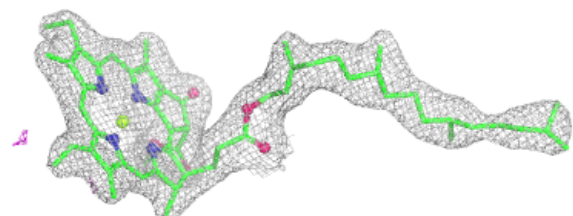
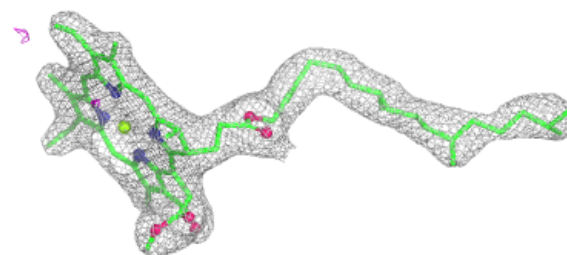


Electron density around CLA a 406:

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

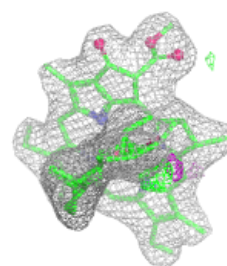
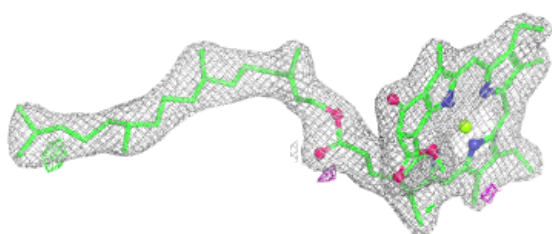
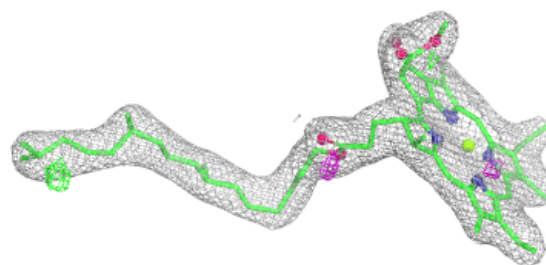
**Electron density around CLA c 503:**

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

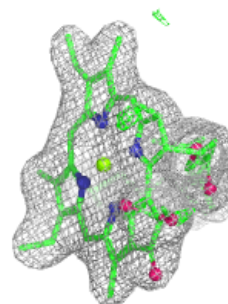
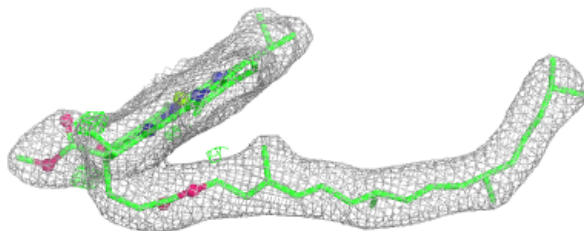
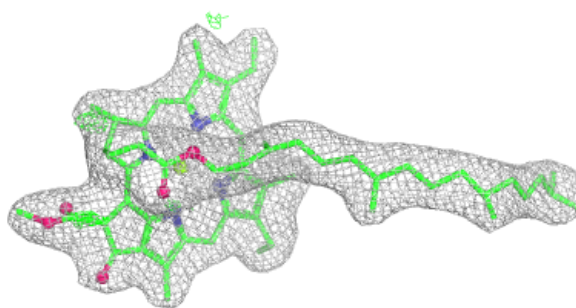


Electron density around CLA C 502:

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

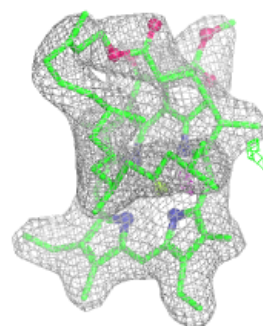
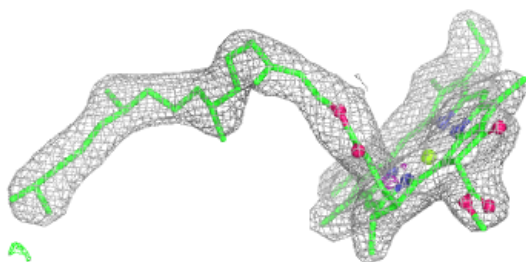
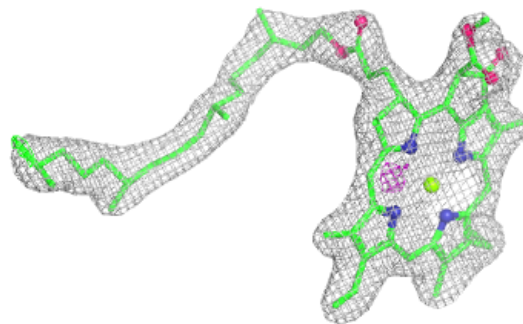
**Electron density around CLA b 608:**

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

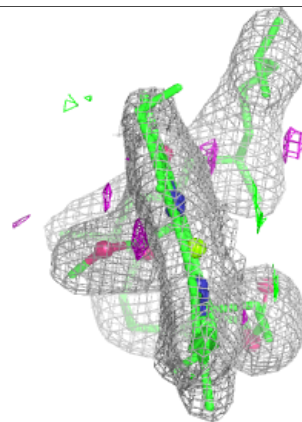
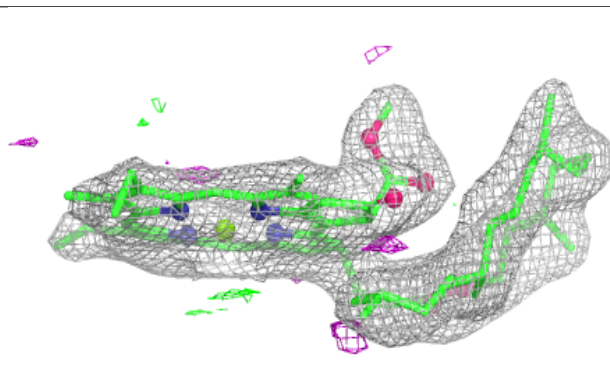
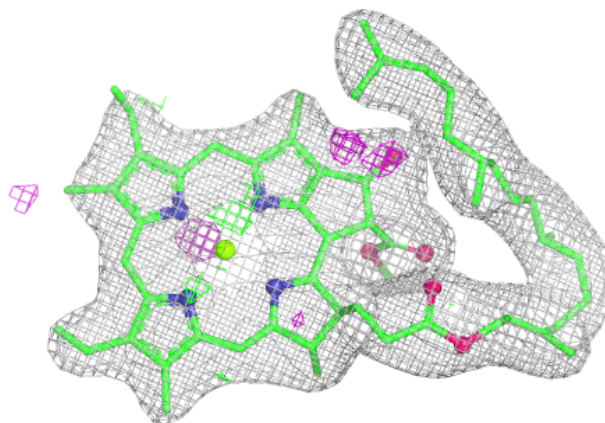


Electron density around CLA C 511:

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

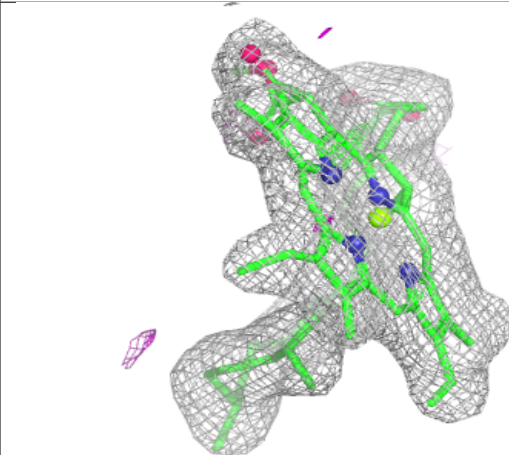
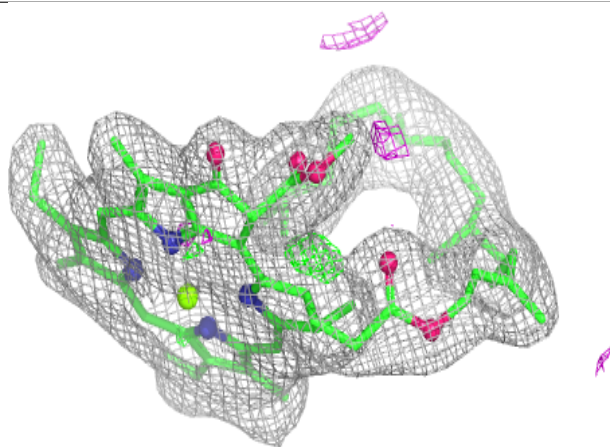
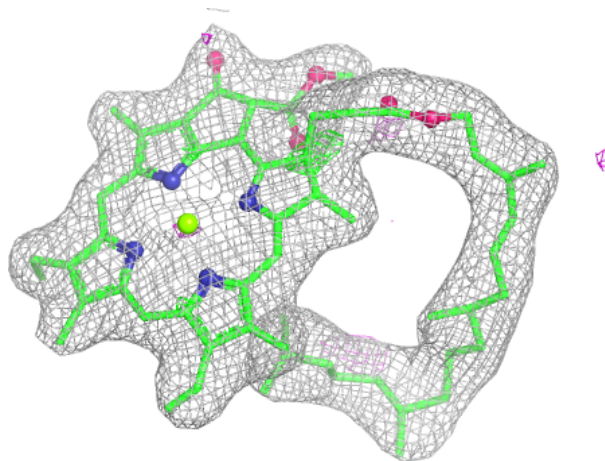
**Electron density around CLA b 610:**

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



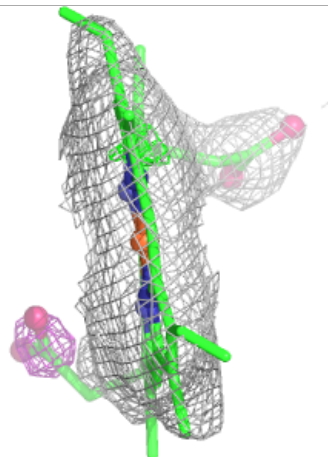
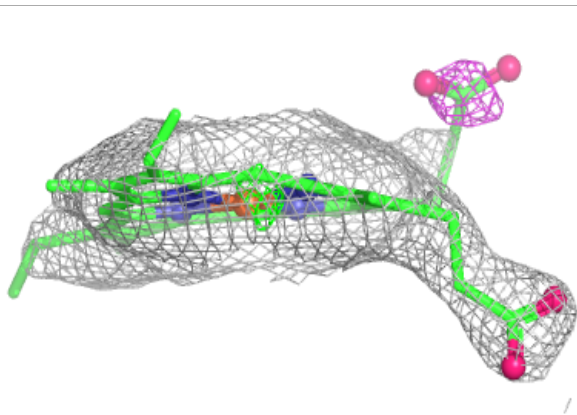
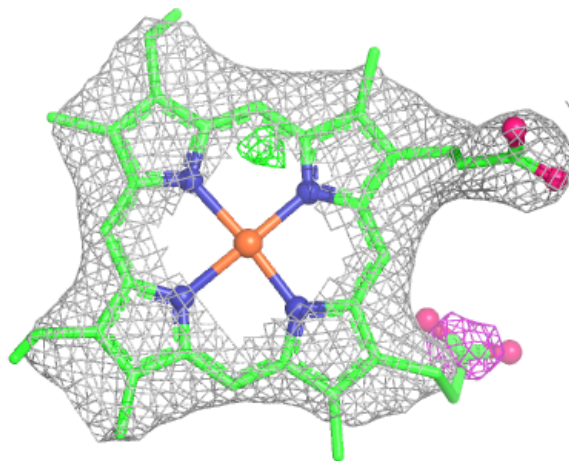
Electron density around CLA B 615:

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



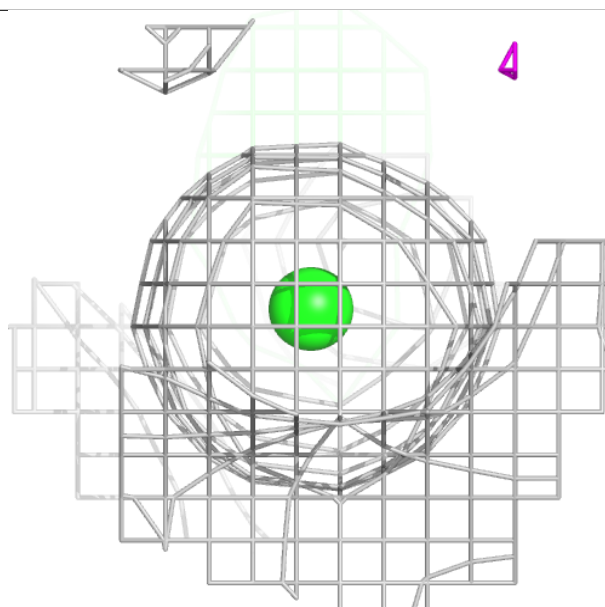
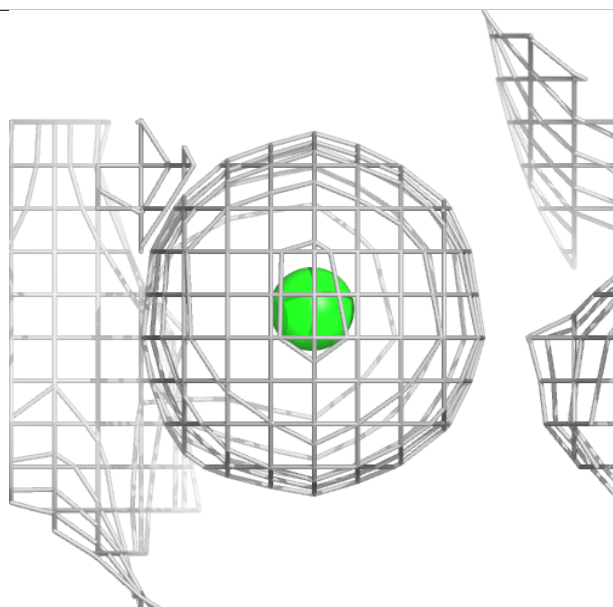
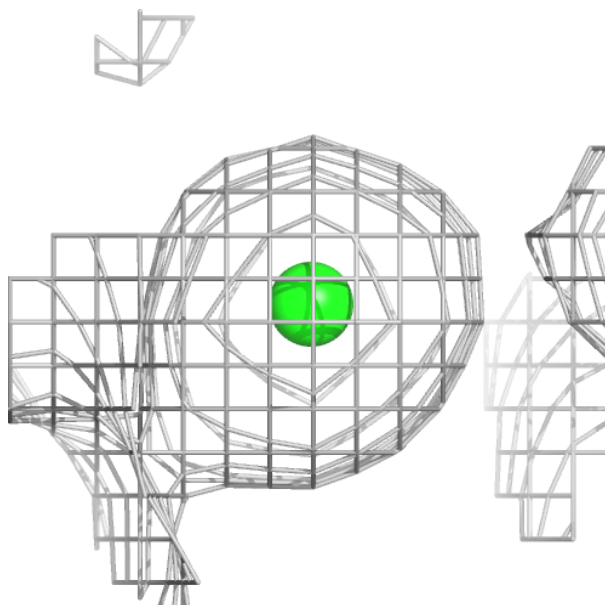
Electron density around HEM f 101:

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



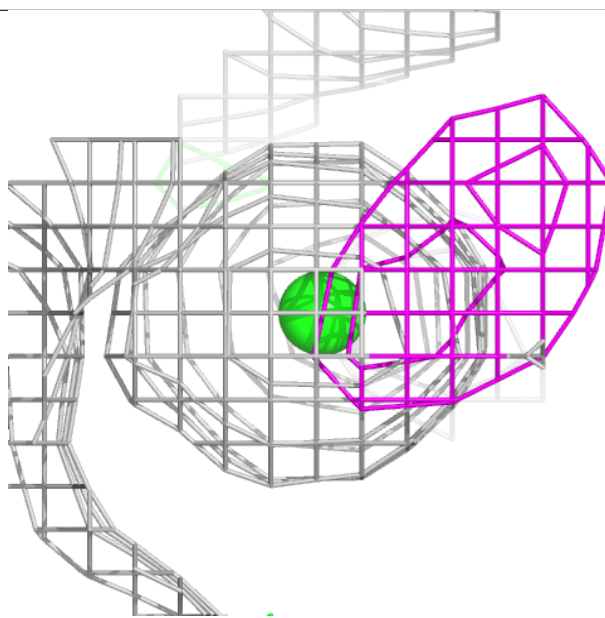
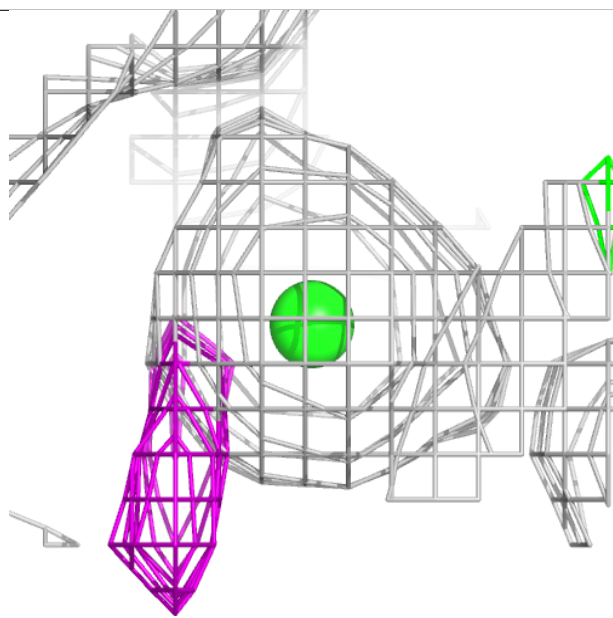
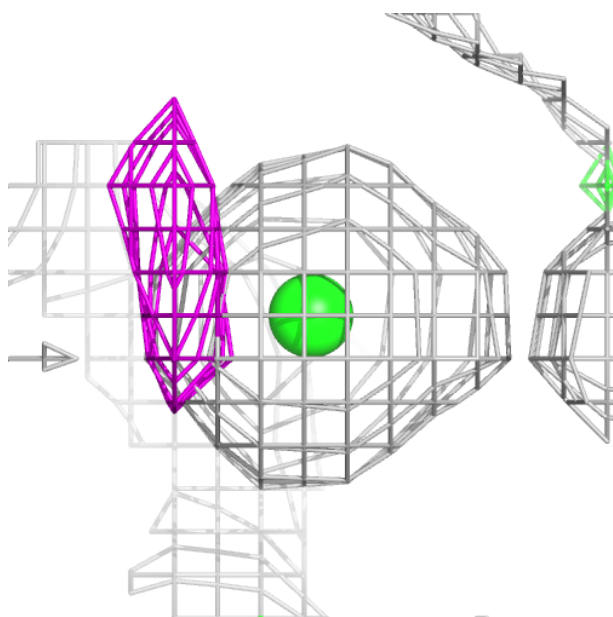
Electron density around CL A 403:

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



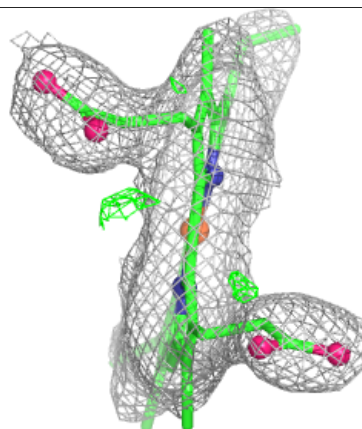
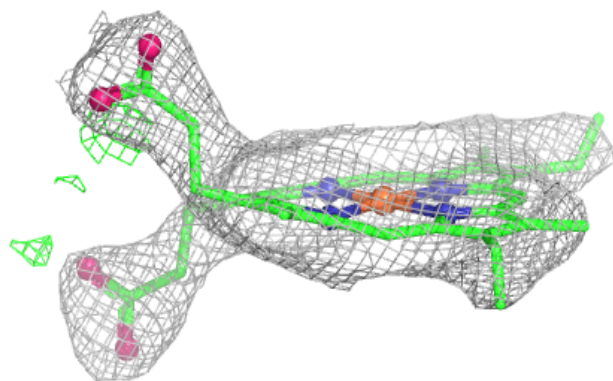
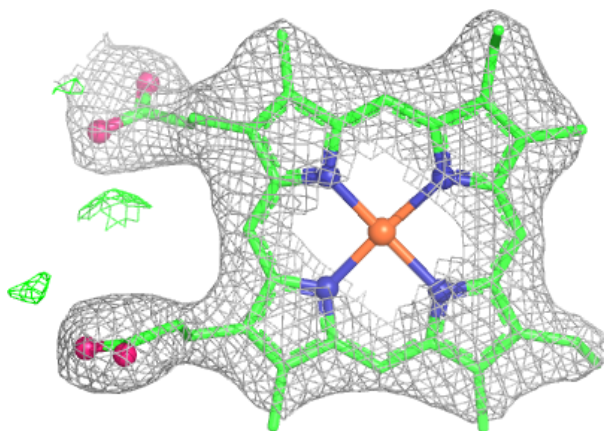
Electron density around CL a 403:

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



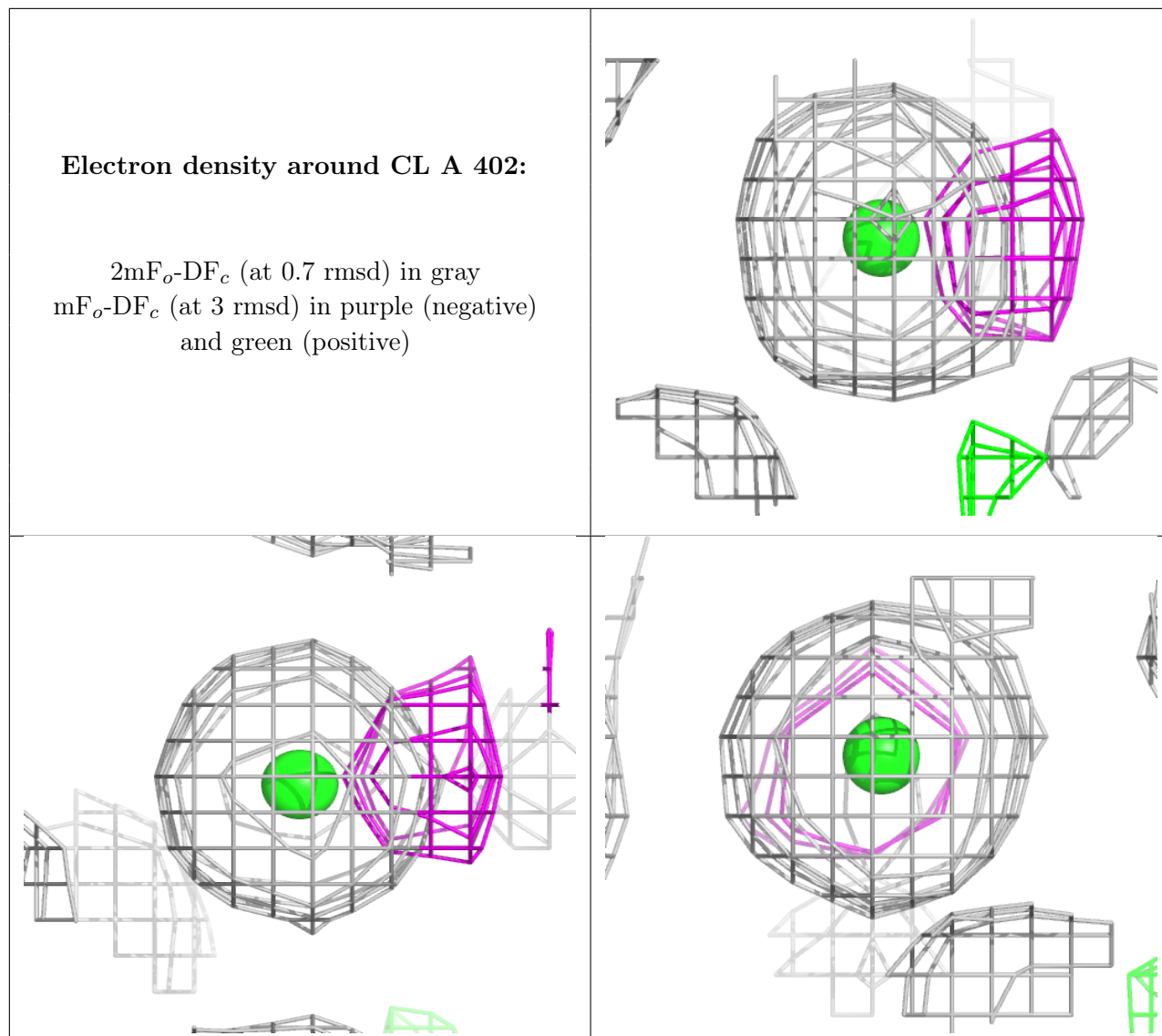
Electron density around HEM F 102:

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



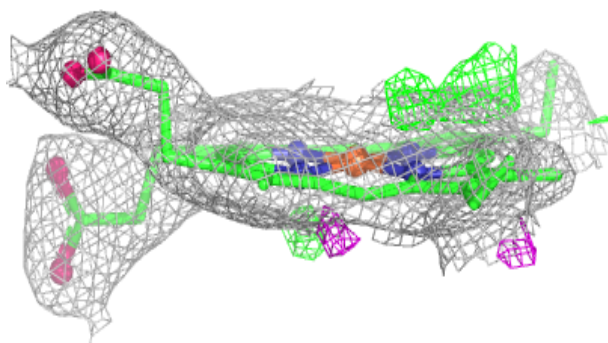
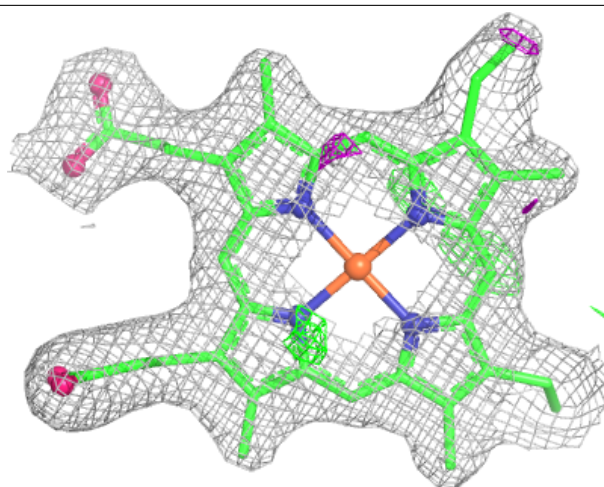
Electron density around CL A 402:

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



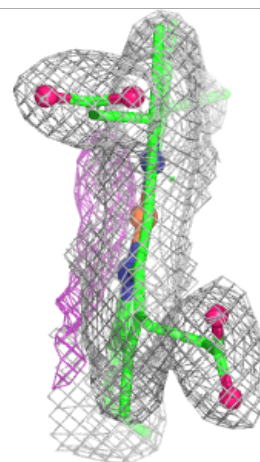
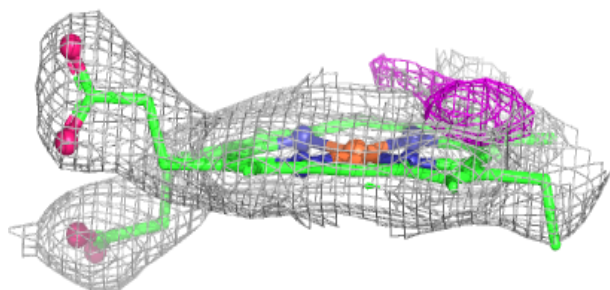
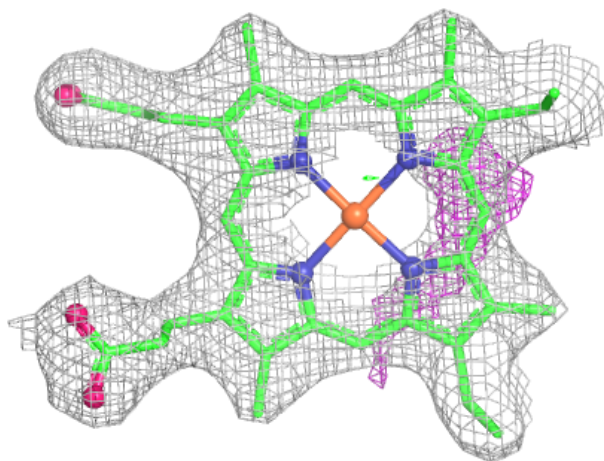
Electron density around HEC V 201:

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



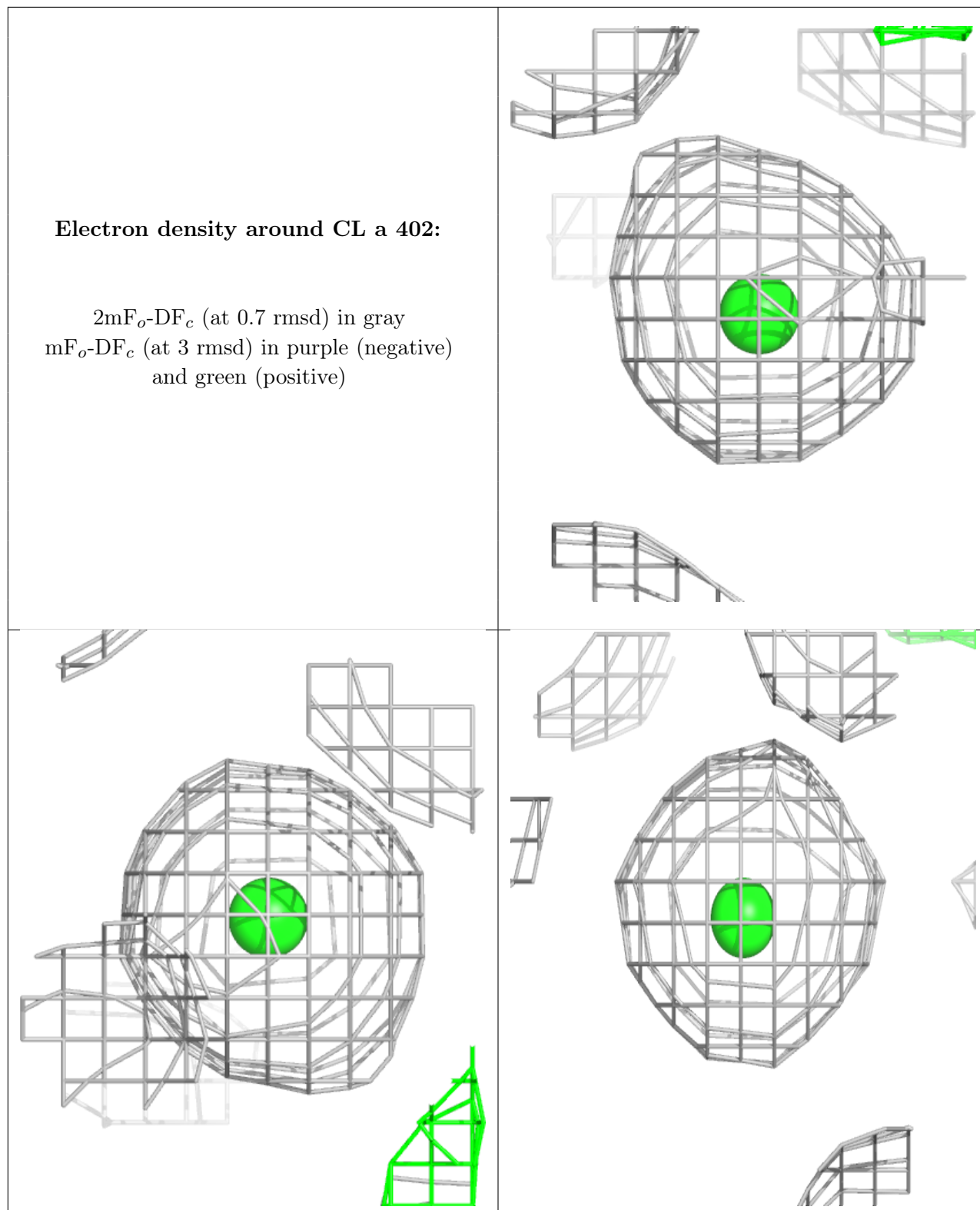
Electron density around HEC v 201:

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



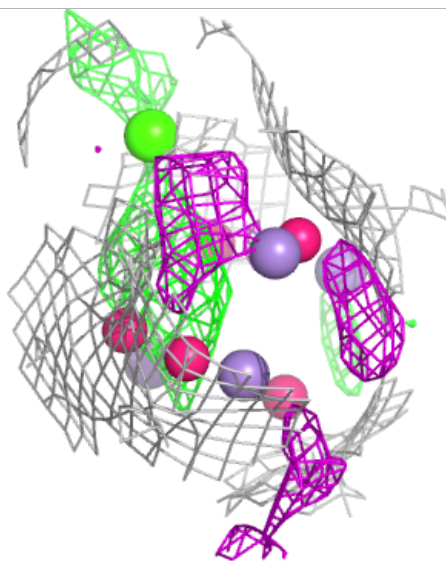
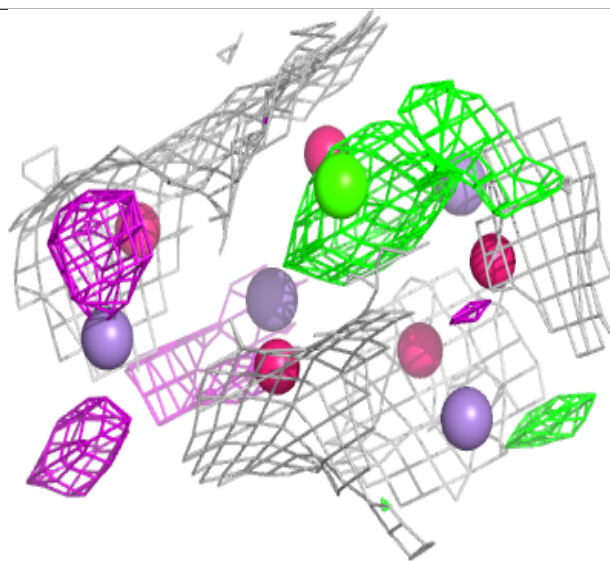
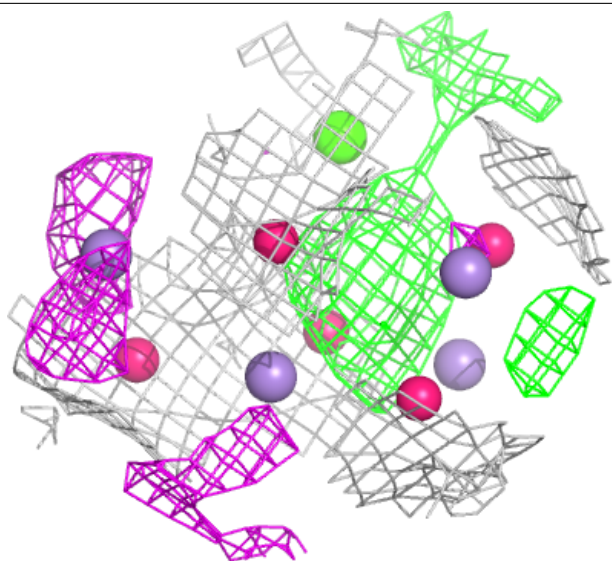
Electron density around CL a 402:

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



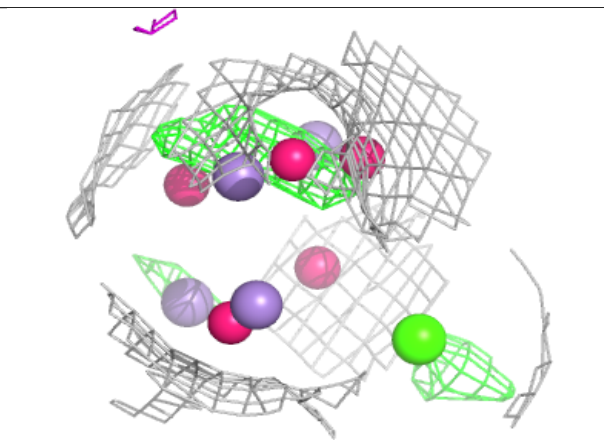
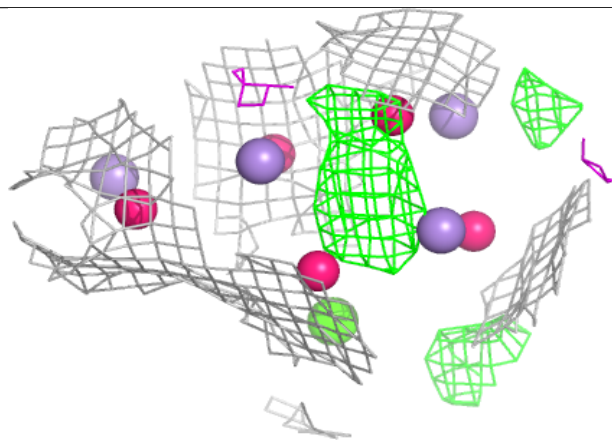
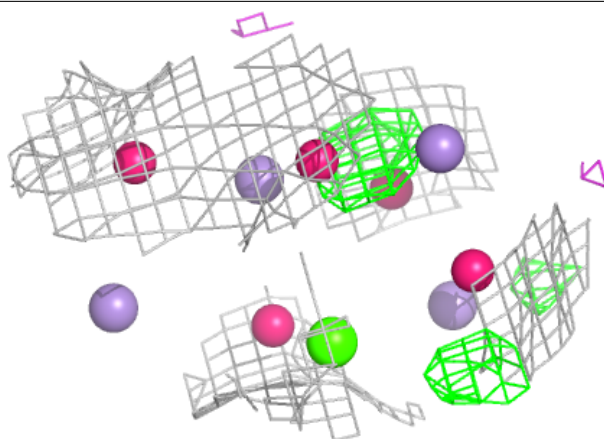
Electron density around OEX A 413:

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



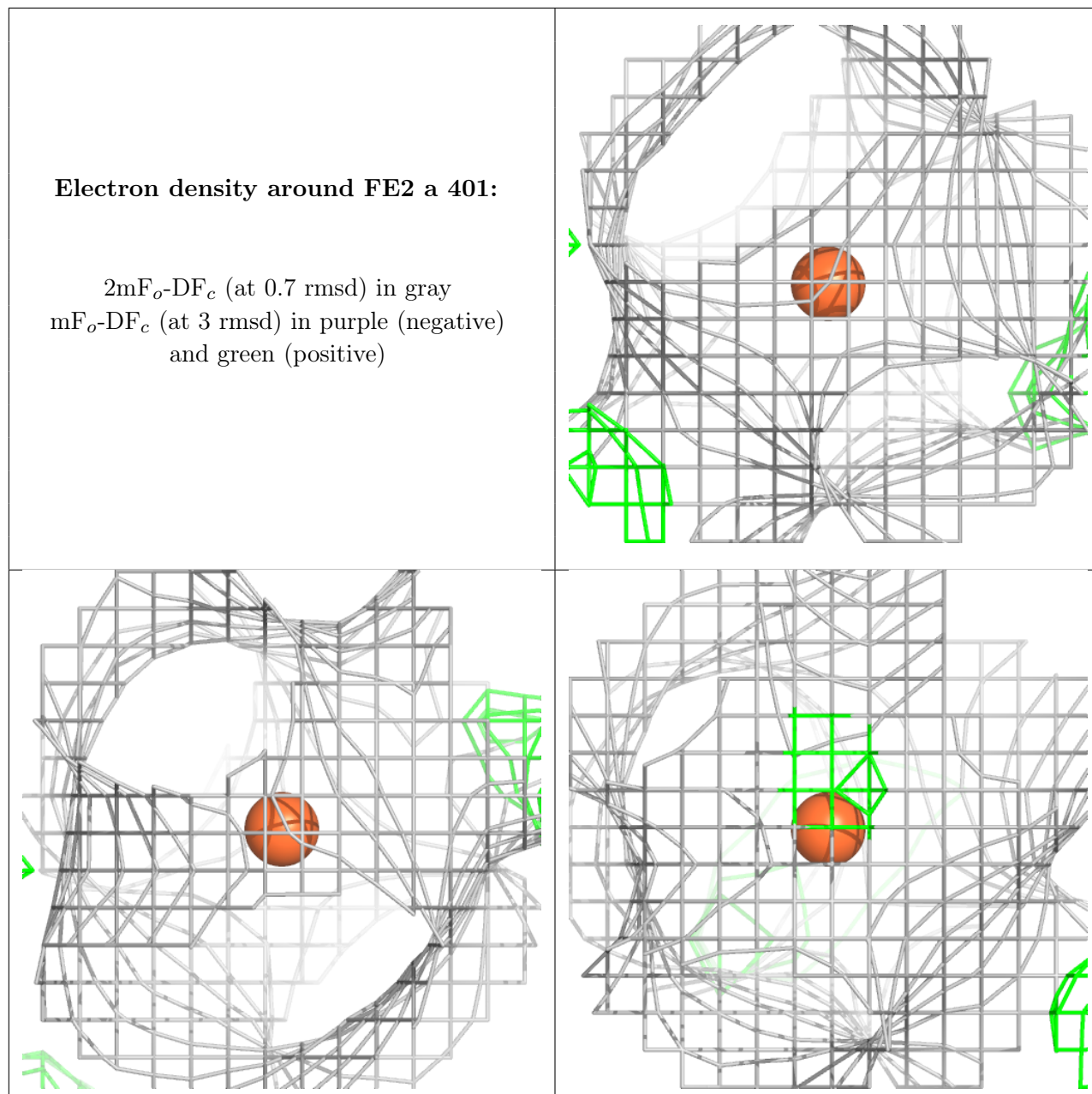
Electron density around OEX a 414:

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



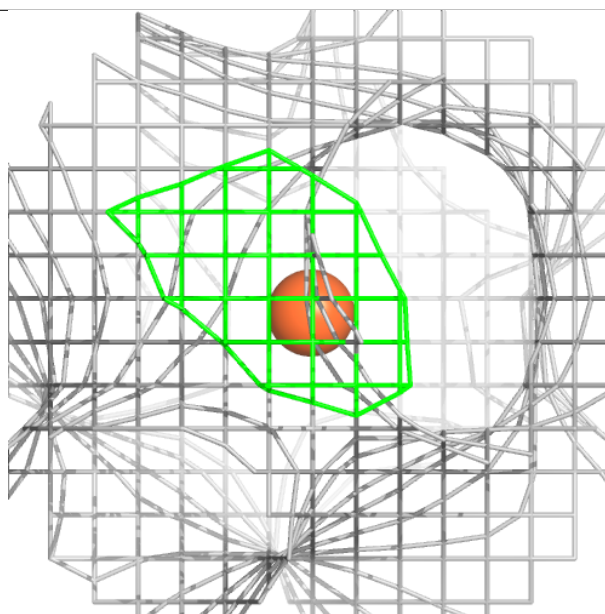
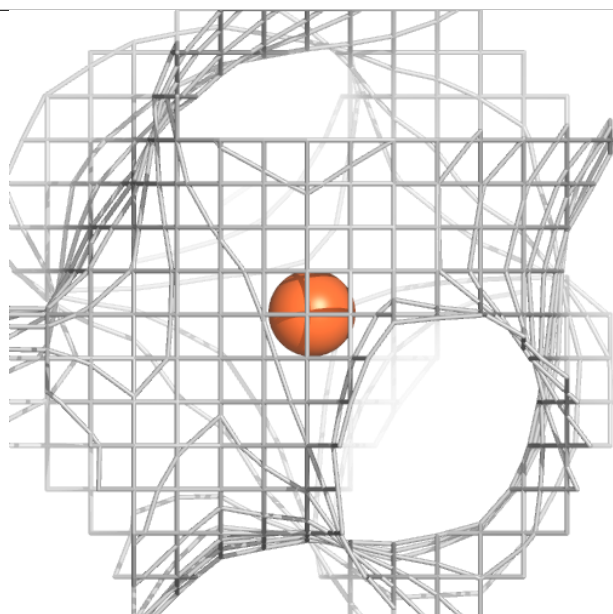
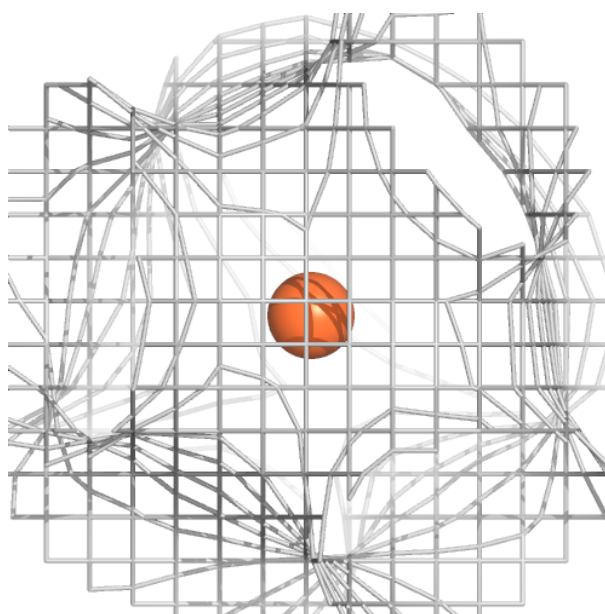
Electron density around FE2 a 401:

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



Electron density around FE2 A 401:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.