



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2021 – 10:58 AM EST

PDB ID : 5V2C
Title : RE-REFINEMENT OF CRYSTAL STRUCTURE OF PHOTOSYSTEM II COMPLEX
Authors : Wang, J.; Wiwczar, J.M.; Brudvig, G.W.
Deposited on : 2017-03-03
Resolution : 1.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.17.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.17.1

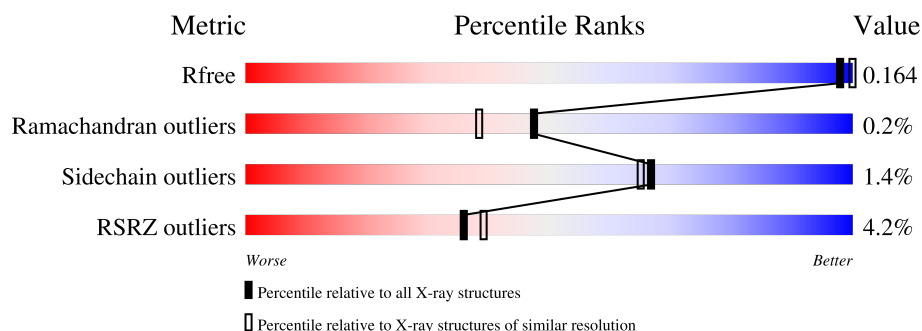
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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.



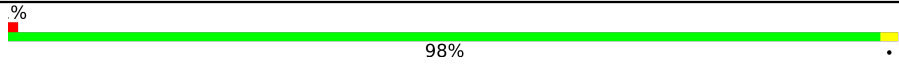
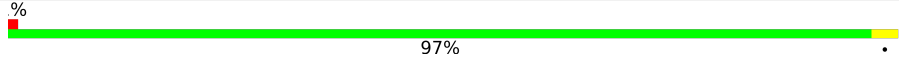
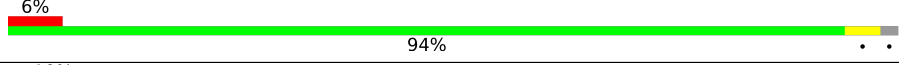
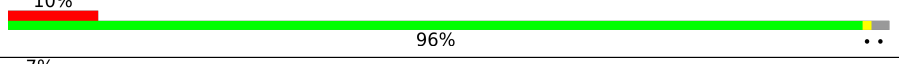
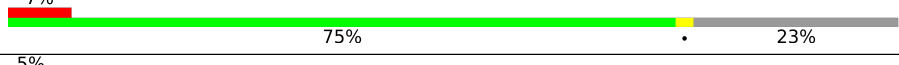
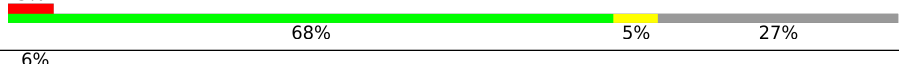
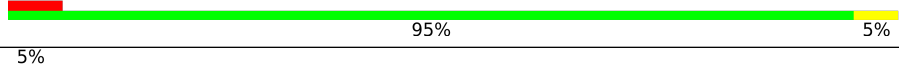
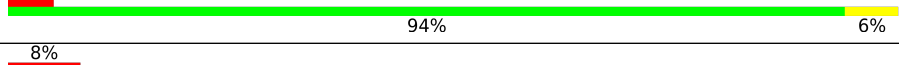
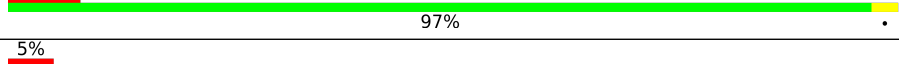
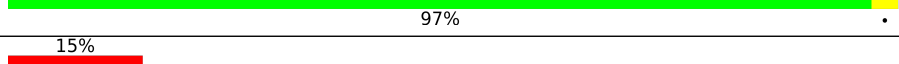
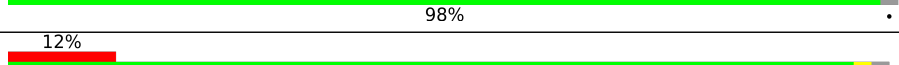
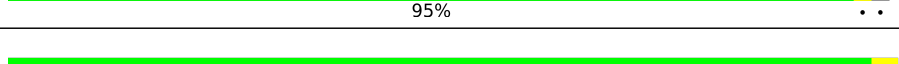
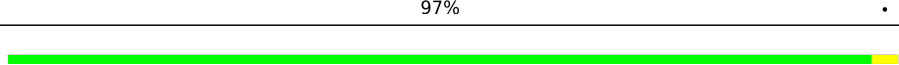
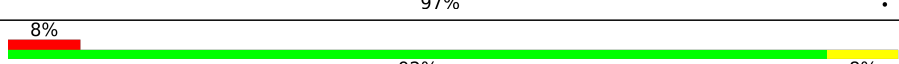
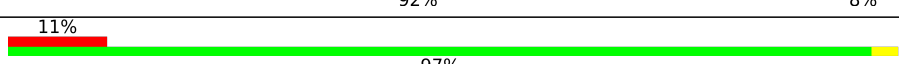
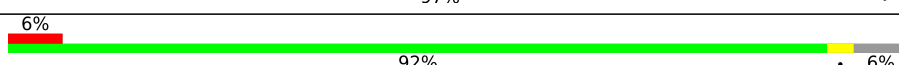
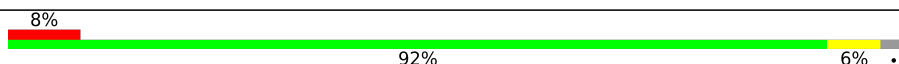
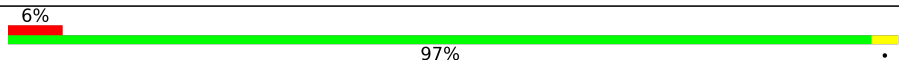
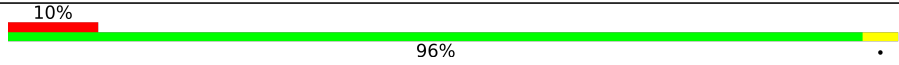

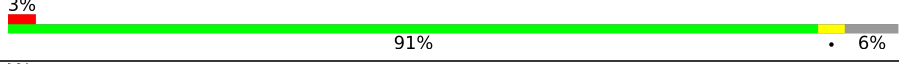
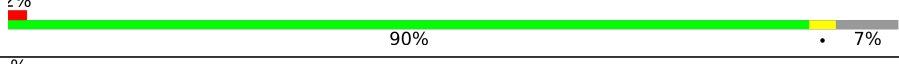
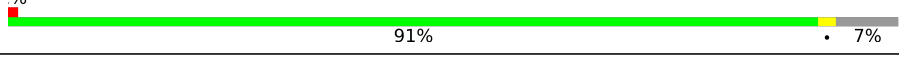
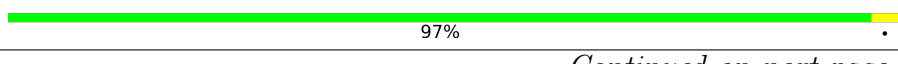

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	<div> <div>%</div> <div>95%</div> <div>..</div> </div>
1	a	344	<div> <div>%</div> <div>96%</div> <div>..</div> </div>
2	B	506	<div> <div>3%</div> <div>97%</div> <div>.</div> </div>
2	b	506	<div> <div>6%</div> <div>96%</div> <div>.</div> </div>
3	C	458	<div> <div>%</div> <div>97%</div> <div>..</div> </div>
3	c	458	<div> <div>3%</div> <div>97%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	342	
4	d	342	
5	E	83	
5	e	83	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	245	
13	o	245	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	

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Mol	Chain	Length	Quality of chain
16	v	137	
17	Y	30	
17	y	30	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	A	606	X	-	-	-
24	CLA	A	607	X	-	-	-
24	CLA	A	609	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	609	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	B	617	X	-	-	-
24	CLA	C	501	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	D	404	X	-	-	-
24	CLA	D	405	X	-	-	-
24	CLA	a	407	X	-	-	-
24	CLA	a	408	X	-	-	-
24	CLA	a	410	X	-	-	-
24	CLA	b	602	X	-	-	-
24	CLA	b	603	X	-	-	-
24	CLA	b	604	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	-
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24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	c	501	X	-	-	-
24	CLA	c	502	X	-	-	-
24	CLA	c	503	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	d	403	X	-	-	-
24	CLA	d	404	X	-	-	-
24	CLA	d	405	X	-	-	-
28	SQD	h	105	-	-	-	X
30	GOL	C	528	-	X	-	-
30	GOL	O	307	-	-	-	X
30	GOL	o	303	-	-	-	X
30	GOL	v	205	-	-	-	X
31	LMT	C	533	-	-	-	X
31	LMT	j	103	-	-	-	X
33	PG4	B	642	-	-	-	X
33	PG4	B	643	-	-	-	X
33	PG4	C	534	-	-	-	X
33	PG4	b	637	-	-	-	X
33	PG4	e	103	-	-	-	X
33	PG4	e	104	-	-	-	X
34	PGE	B	646	-	-	-	X
34	PGE	B	650	-	-	-	X
34	PGE	D	415	-	-	-	X
34	PGE	E	105	-	-	-	X
34	PGE	E	107	-	-	-	X
34	PGE	E	108	-	-	-	X
34	PGE	H	110	-	-	-	X
34	PGE	O	309	-	-	-	X
34	PGE	V	215	-	-	-	X
34	PGE	b	639	-	-	-	X
34	PGE	b	644	-	-	-	X
34	PGE	b	645	-	-	-	X
34	PGE	b	646	-	-	-	X
34	PGE	b	647	-	-	-	X
34	PGE	c	536	-	-	-	X
34	PGE	c	539	-	-	-	X
34	PGE	c	540	-	-	-	X
34	PGE	f	105	-	-	-	X
34	PGE	h	109	-	-	-	X
34	PGE	i	106	-	-	-	X
34	PGE	o	307	-	-	-	X
35	P6G	C	541	-	-	-	X
35	P6G	E	110	-	-	-	X
36	EDO	B	656	-	-	-	X
36	EDO	C	542	-	-	-	X
36	EDO	V	218	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	EDO	c	542	-	-	-	X
38	HTG	C	530	-	-	-	X
38	HTG	C	531	-	-	-	X
39	1PE	B	653	-	-	-	X
39	1PE	V	217	-	-	-	X

2 Entry composition

There are 46 unique types of molecules in this entry. The entry contains 57584 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	4	0
			2639	1730	434	460	15			
1	a	334	Total	C	N	O	S	0	4	0
			2639	1730	434	460	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	11	0
			4032	2646	671	702	13			
2	b	506	Total	C	N	O	S	0	10	0
			4037	2649	670	705	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	506	SER	-	expression tag	UNP D0VWR1
B	507	ASP	-	expression tag	UNP D0VWR1
b	506	SER	-	expression tag	UNP D0VWR1
b	507	ASP	-	expression tag	UNP D0VWR1

- 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	5	0
			3508	2297	585	613	13			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	c	458	Total	C	N	O	S	0	4	0
			3553	2324	592	624	13			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	16	GLU	-	expression tag	UNP D0VWR7
C	17	ALA	-	expression tag	UNP D0VWR7
C	18	ALA	-	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
c	16	GLU	-	expression tag	UNP D0VWR7
c	17	ALA	-	expression tag	UNP D0VWR7
c	18	ALA	-	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
			2731	1810	445	464	12			
4	d	342	Total	C	N	O	S	0	2	0
			2741	1815	448	466	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	3	0
			676	441	110	125				
5	e	81	Total	C	N	O		0	2	0
			668	436	107	125				

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	f	32	Total	C	N	O	S	0	0	0
			257	175	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	2	0
			525	351	86	86	2			
7	h	65	Total	C	N	O	S	0	1	0
			519	346	85	86	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	39	Total	C	N	O	S	0	2	0
			294	197	46	50	1			
9	j	39	Total	C	N	O	S	0	0	0
			281	187	43	50	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	2	GLU	MET	conflict	UNP Q7DGD4
j	2	GLU	MET	conflict	UNP Q7DGD4

- 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	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			
11	l	37	Total	C	N	O	S	0	2	0
			315	211	49	54	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	2	0
			286	190	42	53	1			
12	m	35	Total	C	N	O	S	0	2	0
			289	193	42	52	2			

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	245	Total	C	N	O	S	0	6	0
			1904	1192	317	391	4			
13	o	245	Total	C	N	O	S	0	5	0
			1902	1189	320	389	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	2	ALA	-	expression tag	UNP D0VWR2
O	3	ALA	-	expression tag	UNP D0VWR2
o	2	ALA	-	expression tag	UNP D0VWR2
o	3	ALA	-	expression tag	UNP D0VWR2

- 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	2	0
			271	190	36	42	3			
14	t	30	Total	C	N	O	S	0	2	0
			271	190	36	42	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O		0	2	0
			786	499	130	157				
15	u	97	Total	C	N	O		0	0	0
			774	491	129	154				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	2	0
			1077	683	181	209	4			
16	v	137	Total	C	N	O	S	0	1	0
			1072	680	180	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	29	Total	C	N	O	S	0	1	0
			219	145	37	34	3			
17	y	29	Total	C	N	O	S	0	1	0
			220	146	37	33	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	40	Total	C	N	O	S	0	1	0
			300	201	47	51	1			
18	x	40	Total	C	N	O	S	0	0	0
			295	196	47	51	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1	MET	-	initiating methionine	UNP D0VWR4

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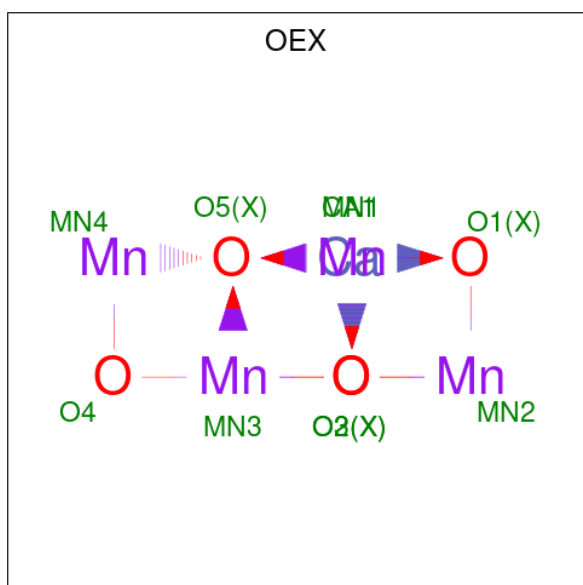
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Chain	Residue	Modelled	Actual	Comment	Reference
x	1	MET	-	initiating methionine	UNP D0VWR4

- 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 CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



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

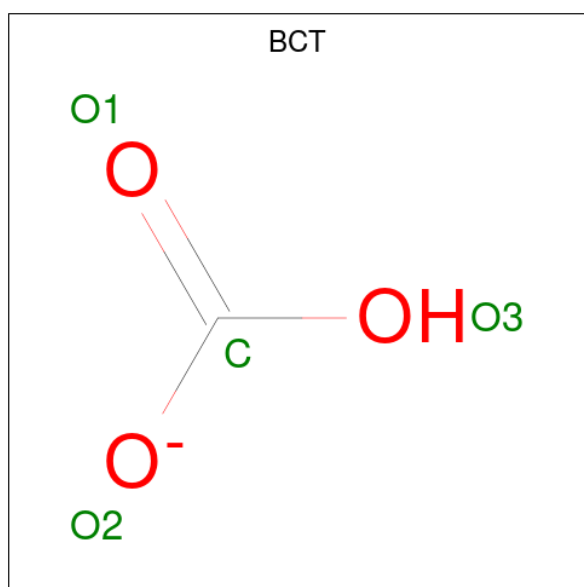
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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 (three-letter code: CL) (formula: Cl).

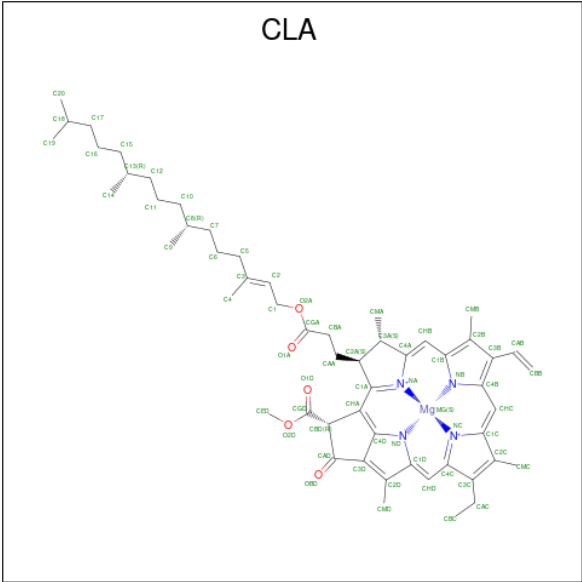
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		
22	V	1	Total	Cl	0	0
			1	1		
22	a	2	Total	Cl	0	0
			2	2		
22	v	1	Total	Cl	0	0
			1	1		

- Molecule 23 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	0
			4	1	3		
23	a	1	Total	C	O	0	0
			4	1	3		
23	m	1	Total	C	O	0	1
			8	2	6		

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
24	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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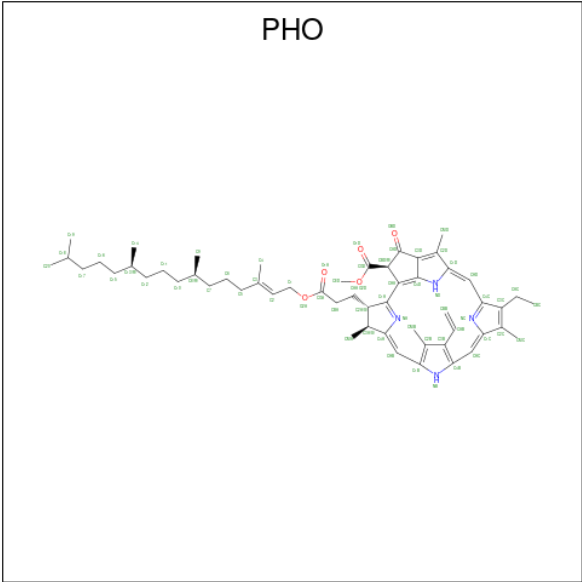
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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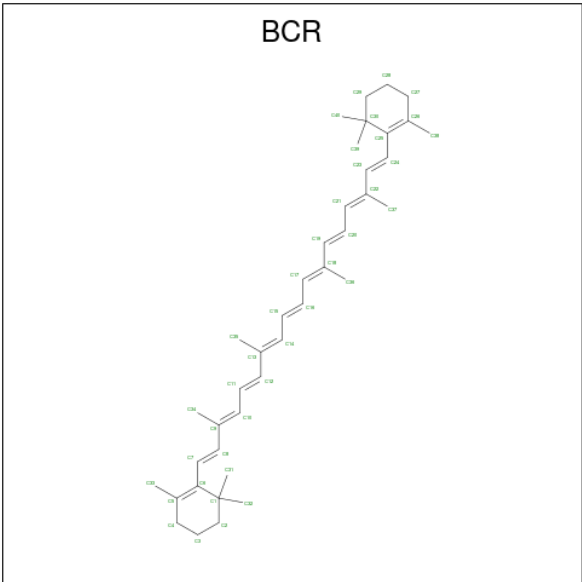
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	d	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	d	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	d	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



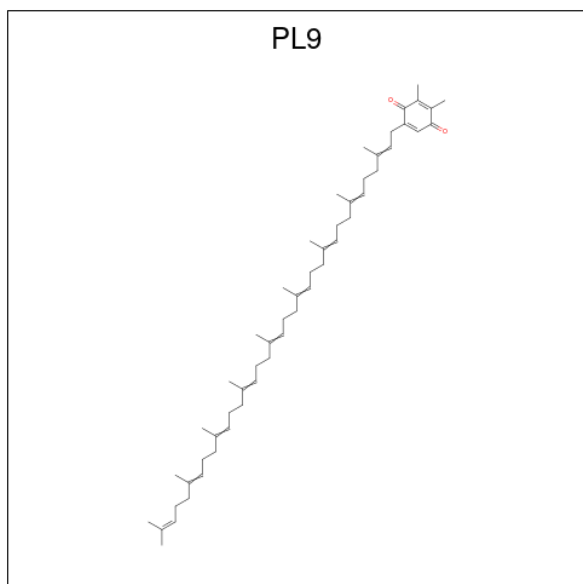
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	D	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



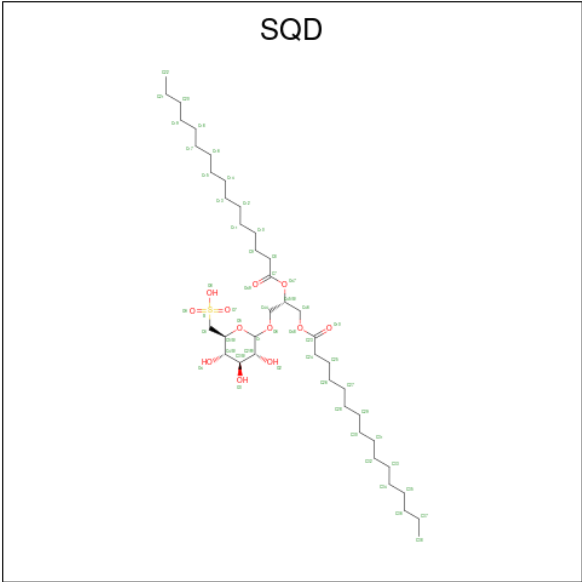
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total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

- Molecule 27 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 (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



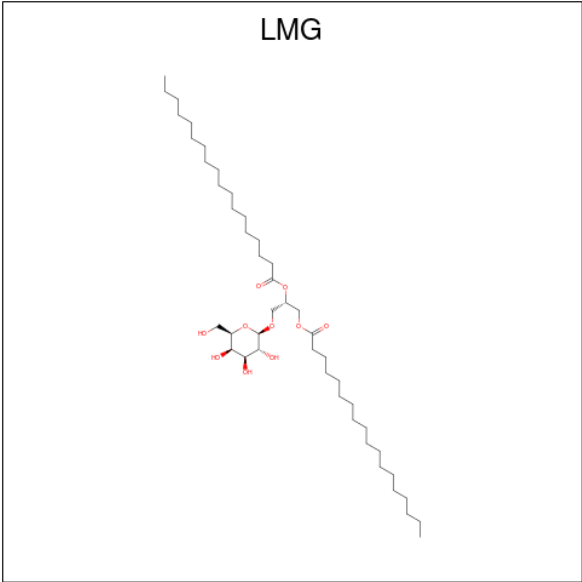
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			55	53	2		
27	D	1	Total	C	O	0	0
			55	53	2		
27	a	1	Total	C	O	0	0
			55	53	2		
27	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	F	1	Total	C	O	S	0	0
			54	41	12	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	b	1	Total	C	O	S	0	0
			54	41	12	1		
28	h	1	Total	C	O	S	0	0
			54	41	12	1		
28	l	1	Total	C	O	S	0	0
			54	41	12	1		
28	x	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			51	41	10		
29	B	1	Total	C	O	0	0
			51	41	10		
29	B	1	Total	C	O	0	0
			55	45	10		
29	C	1	Total	C	O	0	0
			51	41	10		
29	C	1	Total	C	O	0	0
			51	41	10		
29	C	1	Total	C	O	0	0
			55	45	10		
29	J	1	Total	C	O	0	0
			47	37	10		
29	a	1	Total	C	O	0	0
			51	41	10		
29	b	1	Total	C	O	0	0
			51	41	10		
29	c	1	Total	C	O	0	0
			51	41	10		
29	c	1	Total	C	O	0	0
			51	41	10		
29	d	1	Total	C	O	0	0
			55	45	10		
29	j	1	Total	C	O	0	0
			47	37	10		
29	z	1	Total	C	O	0	0
			55	45	10		

- Molecule 30 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	D	1	Total 6	C 3	O 3	0	0
30	D	1	Total 6	C 3	O 3	0	0
30	D	1	Total 6	C 3	O 3	0	0
30	F	1	Total 6	C 3	O 3	0	0
30	O	1	Total 6	C 3	O 3	0	0
30	O	1	Total 6	C 3	O 3	0	0
30	O	1	Total 6	C 3	O 3	0	0
30	O	1	Total 6	C 3	O 3	0	0
30	O	1	Total 6	C 3	O 3	0	0
30	T	1	Total 6	C 3	O 3	0	0
30	T	1	Total 6	C 3	O 3	0	0
30	U	1	Total 6	C 3	O 3	0	0
30	V	1	Total 6	C 3	O 3	0	0
30	V	1	Total 6	C 3	O 3	0	0
30	V	1	Total 6	C 3	O 3	0	0
30	V	1	Total 6	C 3	O 3	0	0
30	V	1	Total 6	C 3	O 3	0	0
30	a	1	Total 6	C 3	O 3	0	0
30	a	1	Total 6	C 3	O 3	0	0
30	b	1	Total 6	C 3	O 3	0	0
30	b	1	Total 6	C 3	O 3	0	0

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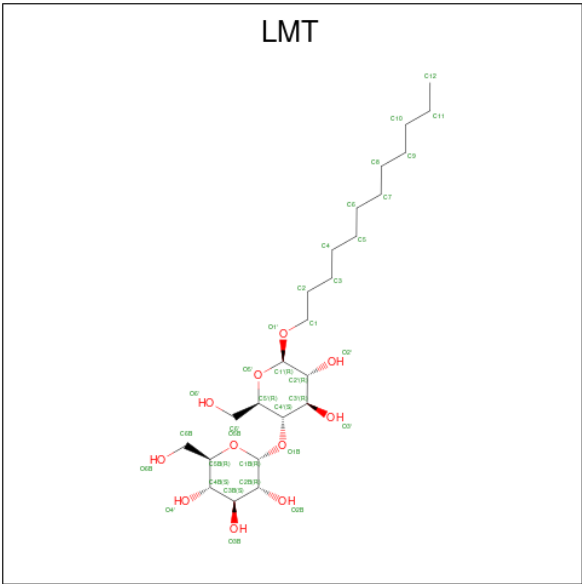
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	b	1	Total	C	O	0	0
			6	3	3		
30	b	1	Total	C	O	0	0
			6	3	3		
30	b	1	Total	C	O	0	0
			6	3	3		
30	b	1	Total	C	O	0	0
			6	3	3		
30	c	1	Total	C	O	0	0
			6	3	3		
30	c	1	Total	C	O	0	0
			6	3	3		
30	c	1	Total	C	O	0	0
			6	3	3		
30	c	1	Total	C	O	0	0
			6	3	3		
30	d	1	Total	C	O	0	0
			6	3	3		
30	d	1	Total	C	O	0	0
			6	3	3		
30	e	1	Total	C	O	0	0
			6	3	3		
30	f	1	Total	C	O	0	0
			6	3	3		
30	f	1	Total	C	O	0	0
			6	3	3		
30	m	1	Total	C	O	0	0
			6	3	3		
30	o	1	Total	C	O	0	0
			6	3	3		
30	o	1	Total	C	O	0	0
			6	3	3		
30	o	1	Total	C	O	0	0
			6	3	3		
30	t	1	Total	C	O	0	0
			6	3	3		
30	u	1	Total	C	O	0	0
			6	3	3		
30	u	1	Total	C	O	0	0
			6	3	3		
30	v	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	v	1	Total	C	O	0	0
			6	3	3		
30	v	1	Total	C	O	0	0
			6	3	3		
30	v	1	Total	C	O	0	0
			6	3	3		
30	v	1	Total	C	O	0	0
			6	3	3		
30	y	1	Total	C	O	0	0
			6	3	3		

- Molecule 31 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



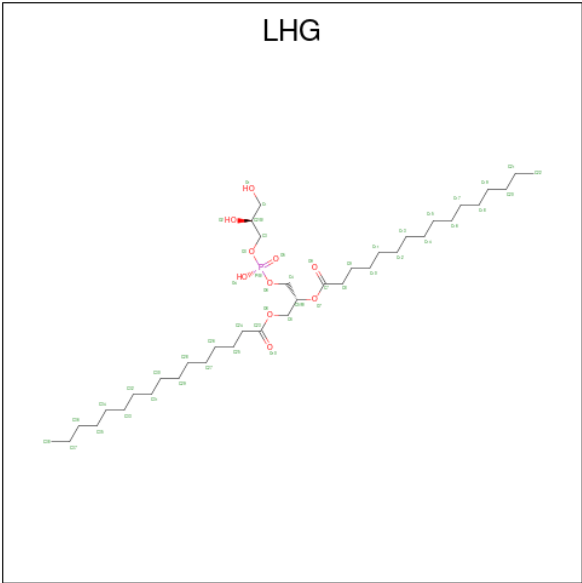
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	C	1	Total	C	O	0	0
			35	24	11		
31	F	1	Total	C	O	0	0
			35	24	11		
31	I	1	Total	C	O	0	0
			35	24	11		
31	J	1	Total	C	O	0	0
			35	24	11		

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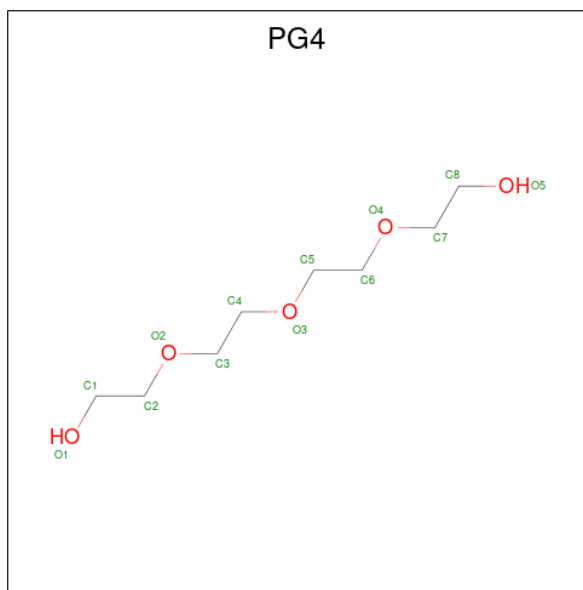
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	M	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total	C	O	0	0
			35	24	11		
31	Y	1	Total	C	O	0	0
			35	24	11		
31	a	1	Total	C	O	0	0
			35	24	11		
31	b	1	Total	C	O	0	0
			35	24	11		
31	c	1	Total	C	O	0	0
			35	24	11		
31	f	1	Total	C	O	0	0
			35	24	11		
31	j	1	Total	C	O	0	0
			35	24	11		
31	m	1	Total	C	O	0	0
			35	24	11		
31	m	1	Total	C	O	0	0
			35	24	11		
31	t	1	Total	C	O	0	0
			35	24	11		
31	u	1	Total	C	O	0	0
			35	24	11		

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	A	1	Total	C	O	P	0	0
			42	31	10	1		
32	B	1	Total	C	O	P	0	0
			49	38	10	1		
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	E	1	Total	C	O	P	0	0
			42	31	10	1		
32	a	1	Total	C	O	P	0	0
			41	30	10	1		
32	d	1	Total	C	O	P	0	0
			49	38	10	1		
32	d	1	Total	C	O	P	0	0
			49	38	10	1		
32	d	1	Total	C	O	P	0	0
			49	38	10	1		
32	e	1	Total	C	O	P	0	0
			42	31	10	1		
32	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 33 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	A	1	Total	C	O	0	0
			13	8	5		
33	B	1	Total	C	O	0	0
			13	8	5		
33	B	1	Total	C	O	0	0
			13	8	5		
33	B	1	Total	C	O	0	0
			13	8	5		
33	B	1	Total	C	O	0	0
			13	8	5		
33	B	1	Total	C	O	0	0
			13	8	5		
33	B	1	Total	C	O	0	0
			13	8	5		
33	B	1	Total	C	O	0	0
			13	8	5		
33	C	1	Total	C	O	0	0
			13	8	5		
33	C	1	Total	C	O	0	0
			13	8	5		
33	C	1	Total	C	O	0	0
			13	8	5		
33	C	1	Total	C	O	0	0
			13	8	5		
33	C	1	Total	C	O	0	0
			13	8	5		
33	D	1	Total	C	O	0	0
			13	8	5		
33	E	1	Total	C	O	0	0
			13	8	5		
33	E	1	Total	C	O	0	0
			13	8	5		
33	H	1	Total	C	O	0	0
			13	8	5		
33	H	1	Total	C	O	0	0
			13	8	5		
33	H	1	Total	C	O	0	0
			13	8	5		
33	H	1	Total	C	O	0	0
			13	8	5		
33	I	1	Total	C	O	0	0
			13	8	5		

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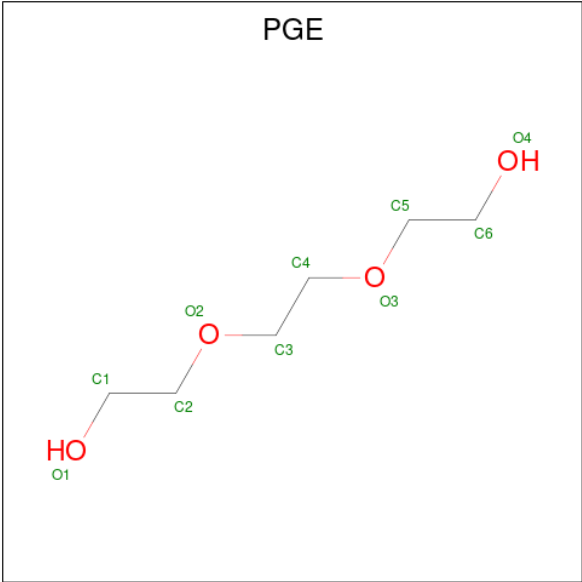
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	I	1	Total	C	O	0	0
			13	8	5		
33	I	1	Total	C	O	0	0
			13	8	5		
33	J	1	Total	C	O	0	0
			13	8	5		
33	J	1	Total	C	O	0	0
			13	8	5		
33	K	1	Total	C	O	0	0
			13	8	5		
33	U	1	Total	C	O	0	0
			13	8	5		
33	V	1	Total	C	O	0	0
			13	8	5		
33	V	1	Total	C	O	0	0
			13	8	5		
33	V	1	Total	C	O	0	0
			13	8	5		
33	V	1	Total	C	O	0	0
			13	8	5		
33	V	1	Total	C	O	0	0
			13	8	5		
33	X	1	Total	C	O	0	0
			13	8	5		
33	X	1	Total	C	O	0	0
			13	8	5		
33	X	1	Total	C	O	0	0
			13	8	5		
33	a	1	Total	C	O	0	0
			13	8	5		
33	a	1	Total	C	O	0	0
			13	8	5		
33	b	1	Total	C	O	0	0
			13	8	5		
33	b	1	Total	C	O	0	0
			13	8	5		
33	b	1	Total	C	O	0	0
			13	8	5		
33	b	1	Total	C	O	0	0
			13	8	5		
33	c	1	Total	C	O	0	0
			13	8	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	c	1	Total	C	O	0	0
			13	8	5		
33	c	1	Total	C	O	0	0
			13	8	5		
33	c	1	Total	C	O	0	0
			13	8	5		
33	d	1	Total	C	O	0	0
			13	8	5		
33	e	1	Total	C	O	0	0
			13	8	5		
33	e	1	Total	C	O	0	0
			13	8	5		
33	h	1	Total	C	O	0	0
			13	8	5		
33	i	1	Total	C	O	0	0
			13	8	5		
33	i	1	Total	C	O	0	0
			13	8	5		
33	i	1	Total	C	O	0	0
			13	8	5		
33	i	1	Total	C	O	0	0
			13	8	5		
33	j	1	Total	C	O	0	0
			13	8	5		
33	l	1	Total	C	O	0	0
			13	8	5		
33	x	1	Total	C	O	0	0
			13	8	5		

- Molecule 34 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	A	1	Total	C	O	0	0
			7	4	3		
34	A	1	Total	C	O	0	0
			10	6	4		
34	B	1	Total	C	O	0	0
			10	6	4		
34	B	1	Total	C	O	0	0
			10	6	4		
34	B	1	Total	C	O	0	0
			10	6	4		
34	B	1	Total	C	O	0	0
			10	6	4		
34	B	1	Total	C	O	0	0
			10	6	4		
34	B	1	Total	C	O	0	0
			10	6	4		
34	C	1	Total	C	O	0	0
			10	6	4		
34	C	1	Total	C	O	0	0
			10	6	4		
34	D	1	Total	C	O	0	0
			10	6	4		
34	E	1	Total	C	O	0	0
			10	6	4		
34	E	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	E	1	Total	C	O	0	0
			10	6	4		
34	E	1	Total	C	O	0	0
			10	6	4		
34	E	1	Total	C	O	0	0
			10	6	4		
34	E	1	Total	C	O	0	0
			10	6	4		
34	H	1	Total	C	O	0	0
			10	6	4		
34	H	1	Total	C	O	0	0
			10	6	4		
34	H	1	Total	C	O	0	0
			10	6	4		
34	H	1	Total	C	O	0	0
			10	6	4		
34	I	1	Total	C	O	0	0
			10	6	4		
34	J	1	Total	C	O	0	0
			10	6	4		
34	J	1	Total	C	O	0	0
			10	6	4		
34	J	1	Total	C	O	0	0
			10	6	4		
34	O	1	Total	C	O	0	0
			10	6	4		
34	O	1	Total	C	O	0	0
			10	6	4		
34	O	1	Total	C	O	0	0
			10	6	4		
34	T	1	Total	C	O	0	0
			7	4	3		
34	V	1	Total	C	O	0	0
			10	6	4		
34	V	1	Total	C	O	0	0
			10	6	4		
34	Y	1	Total	C	O	0	0
			10	6	4		
34	a	1	Total	C	O	0	0
			10	6	4		
34	a	1	Total	C	O	0	0
			10	6	4		

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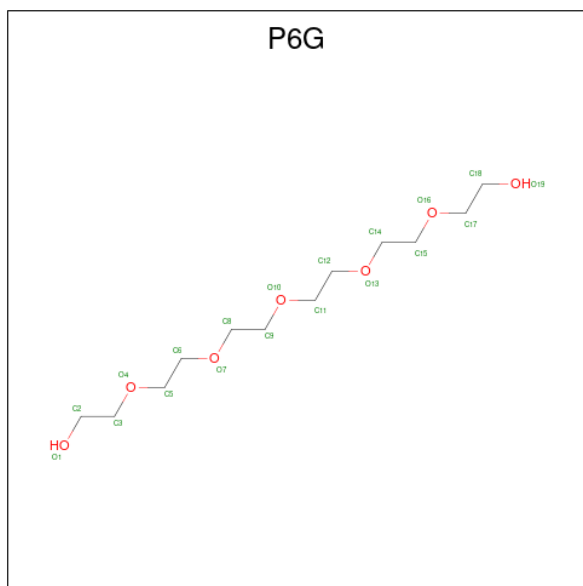
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	b	1	Total	C	O	0	0
			10	6	4		
34	b	1	Total	C	O	0	0
			10	6	4		
34	b	1	Total	C	O	0	0
			10	6	4		
34	b	1	Total	C	O	0	0
			10	6	4		
34	b	1	Total	C	O	0	0
			10	6	4		
34	b	1	Total	C	O	0	0
			10	6	4		
34	b	1	Total	C	O	0	0
			10	6	4		
34	b	1	Total	C	O	0	0
			10	6	4		
34	c	1	Total	C	O	0	0
			10	6	4		
34	c	1	Total	C	O	0	0
			10	6	4		
34	c	1	Total	C	O	0	0
			10	6	4		
34	c	1	Total	C	O	0	0
			10	6	4		
34	c	1	Total	C	O	0	0
			10	6	4		
34	f	1	Total	C	O	0	0
			10	6	4		
34	h	1	Total	C	O	0	0
			10	6	4		
34	h	1	Total	C	O	0	0
			10	6	4		
34	h	1	Total	C	O	0	0
			10	6	4		
34	h	1	Total	C	O	0	0
			10	6	4		
34	i	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	i	1	Total	C	O	0	0
			10	6	4		
34	j	1	Total	C	O	0	0
			10	6	4		
34	o	1	Total	C	O	0	0
			10	6	4		
34	o	1	Total	C	O	0	0
			10	6	4		
34	o	1	Total	C	O	0	0
			10	6	4		
34	t	1	Total	C	O	0	0
			10	6	4		
34	t	1	Total	C	O	0	0
			7	4	3		
34	x	1	Total	C	O	0	0
			10	6	4		

- Molecule 35 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	A	1	Total	C	O	0	0
			19	12	7		
35	A	1	Total	C	O	0	0
			19	12	7		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	B	1	Total	C	O	0	0
			19	12	7		
35	B	1	Total	C	O	0	0
			19	12	7		
35	C	1	Total	C	O	0	0
			19	12	7		
35	D	1	Total	C	O	0	0
			19	12	7		
35	D	1	Total	C	O	0	0
			19	12	7		
35	D	1	Total	C	O	0	0
			19	12	7		
35	E	1	Total	C	O	0	0
			19	12	7		
35	I	1	Total	C	O	0	0
			19	12	7		
35	T	1	Total	C	O	0	0
			19	12	7		
35	b	1	Total	C	O	0	0
			19	12	7		
35	b	1	Total	C	O	0	0
			19	12	7		
35	c	1	Total	C	O	0	0
			19	12	7		
35	d	1	Total	C	O	0	0
			19	12	7		
35	d	1	Total	C	O	0	0
			19	12	7		
35	j	1	Total	C	O	0	0
			19	12	7		

- Molecule 36 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	A	1	Total	C	O	0	0
			4	2	2		
36	B	1	Total	C	O	0	0
			4	2	2		
36	B	1	Total	C	O	0	0
			4	2	2		
36	B	1	Total	C	O	0	0
			4	2	2		
36	B	1	Total	C	O	0	0
			4	2	2		
36	C	1	Total	C	O	0	0
			4	2	2		
36	D	1	Total	C	O	0	0
			4	2	2		
36	E	1	Total	C	O	0	0
			4	2	2		
36	E	1	Total	C	O	0	0
			4	2	2		
36	H	1	Total	C	O	0	0
			4	2	2		
36	I	1	Total	C	O	0	0
			4	2	2		
36	J	1	Total	C	O	0	0
			4	2	2		
36	O	1	Total	C	O	0	0
			4	2	2		
36	V	1	Total	C	O	0	0
			4	2	2		

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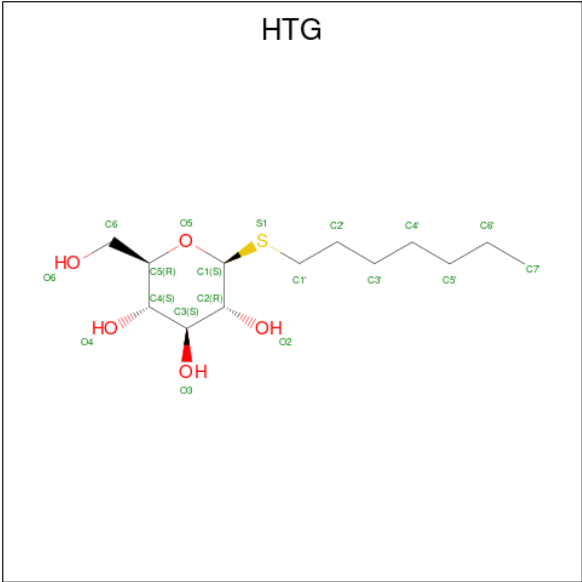
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	X	1	Total	C	O	0	0
			4	2	2		
36	a	1	Total	C	O	0	0
			4	2	2		
36	c	1	Total	C	O	0	0
			4	2	2		
36	d	1	Total	C	O	0	0
			4	2	2		
36	e	1	Total	C	O	0	0
			4	2	2		
36	i	1	Total	C	O	0	0
			4	2	2		
36	o	1	Total	C	O	0	0
			4	2	2		
36	o	1	Total	C	O	0	0
			4	2	2		

- Molecule 37 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	B	1	Total	Ca	0	0
			1	1		
37	O	1	Total	Ca	0	0
			1	1		
37	b	1	Total	Ca	0	0
			1	1		
37	c	1	Total	Ca	0	0
			1	1		
37	h	1	Total	Ca	0	0
			1	1		
37	o	1	Total	Ca	0	0
			1	1		

- Molecule 38 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: C₁₃H₂₆O₅S).



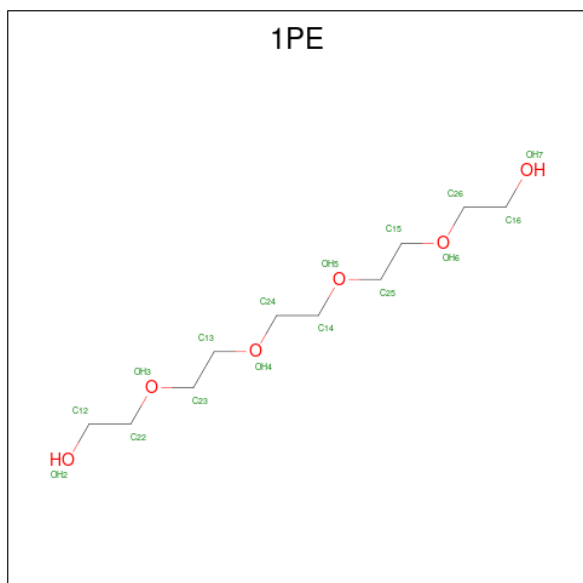
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	B	1	Total	C	O	S	0	0
			19	13	5	1		
38	B	1	Total	C	O	S	0	0
			19	13	5	1		
38	B	1	Total	C	O	S	0	0
			19	13	5	1		
38	B	1	Total	C	O	S	0	0
			19	13	5	1		
38	C	1	Total	C	O	S	0	0
			19	13	5	1		
38	C	1	Total	C	O	S	0	0
			19	13	5	1		
38	C	1	Total	C	O	S	0	0
			19	13	5	1		
38	C	1	Total	C	O	S	0	0
			19	13	5	1		
38	C	1	Total	C	O	S	0	0
			19	13	5	1		
38	H	1	Total	C	O	S	0	0
			19	13	5	1		
38	O	1	Total	C	O	S	0	0
			19	13	5	1		
38	V	1	Total	C	O	S	0	0
			19	13	5	1		
38	a	1	Total	C	O	S	0	0
			19	13	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	b	1	Total	C	O	S	0	0
			19	13	5	1		
38	b	1	Total	C	O	S	0	0
			19	13	5	1		
38	b	1	Total	C	O	S	0	0
			19	13	5	1		
38	b	1	Total	C	O	S	0	0
			19	13	5	1		
38	c	1	Total	C	O	S	0	0
			19	13	5	1		
38	c	1	Total	C	O	S	0	0
			19	13	5	1		
38	c	1	Total	C	O	S	0	0
			19	13	5	1		
38	h	1	Total	C	O	S	0	0
			19	13	5	1		
38	o	1	Total	C	O	S	0	0
			19	13	5	1		

- Molecule 39 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



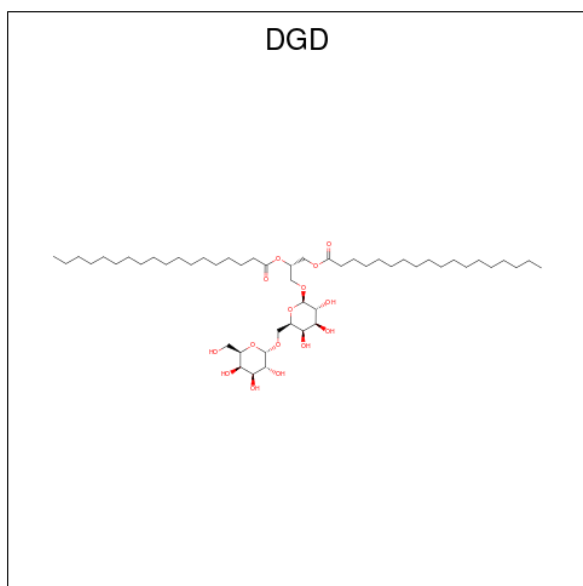
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
39	B	1	Total	C	O	0	0
			16	10	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
39	B	1	Total	C	O	0	0
			16	10	6		
39	L	1	Total	C	O	0	0
			16	10	6		
39	V	1	Total	C	O	0	0
			16	10	6		
39	e	1	Total	C	O	0	0
			16	10	6		
39	j	1	Total	C	O	0	0
			16	10	6		
39	x	1	Total	C	O	0	0
			16	10	6		

- Molecule 40 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
40	C	1	Total	C	O	0	0
			62	47	15		
40	C	1	Total	C	O	0	0
			56	41	15		
40	C	1	Total	C	O	0	0
			62	47	15		
40	D	1	Total	C	O	0	0
			66	51	15		
40	H	1	Total	C	O	0	0
			62	47	15		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
40	c	1	Total 62	C 47	O 15	0	0
40	c	1	Total 57	C 42	O 15	0	0
40	c	1	Total 62	C 47	O 15	0	0
40	d	1	Total 66	C 51	O 15	0	0
40	h	1	Total 62	C 47	O 15	0	0

- # HEM

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

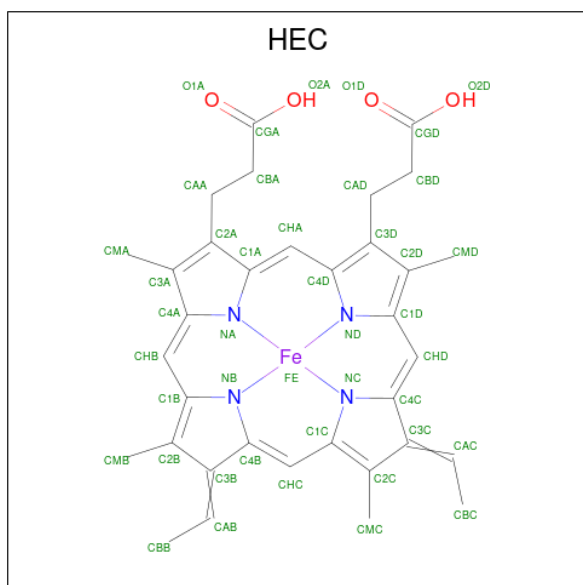
- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 42 | F | 1 | Total Mg
1 1 | 0 | 0 |
| 42 | J | 1 | Total Mg
1 1 | 0 | 0 |



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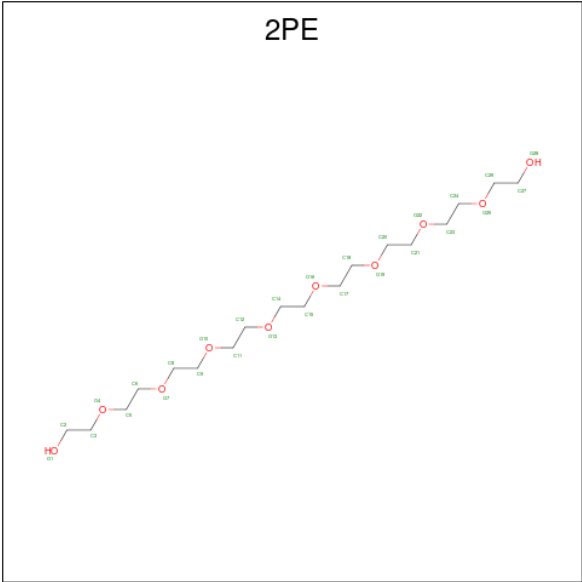
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	f	1	Total	Mg	0	0
			1	1		
42	j	1	Total	Mg	0	0
			1	1		

- Molecule 43 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



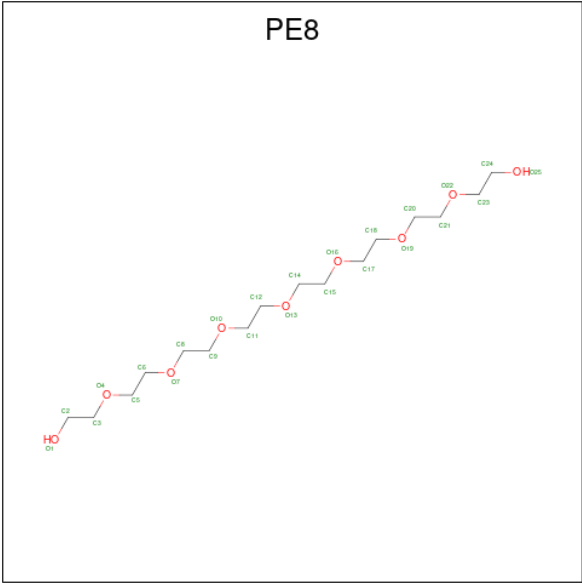
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
43	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
43	v	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 44 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: $C_{18}H_{38}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
44	V	1	Total	C	O	0	0
			28	18	10		

- Molecule 45 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (three-letter code: PE8) (formula: C₁₆H₃₄O₉).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
45	i	1	Total	C	O	0	0
			25	16	9		

- Molecule 46 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
46	A	191	Total O 191 191	0	0
46	B	413	Total O 413 413	0	0
46	C	320	Total O 320 320	0	0
46	D	169	Total O 170 170	0	1
46	E	57	Total O 57 57	0	0
46	F	17	Total O 17 17	0	0
46	H	63	Total O 63 63	0	0
46	I	16	Total O 16 16	0	0
46	J	17	Total O 17 17	0	0
46	K	15	Total O 15 15	0	0
46	L	23	Total O 23 23	0	0
46	M	33	Total O 33 33	0	0
46	O	254	Total O 254 254	0	0
46	T	27	Total O 27 27	0	0
46	U	112	Total O 112 112	0	0
46	V	149	Total O 149 149	0	0
46	Y	6	Total O 6 6	0	0
46	X	10	Total O 10 10	0	0
46	Z	4	Total O 4 4	0	0
46	a	177	Total O 177 177	0	0
46	b	421	Total O 421 421	0	0
46	c	329	Total O 329 329	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
46	d	188	Total 189	O 189	0	1
46	e	46	Total 46	O 46	0	0
46	f	15	Total 15	O 15	0	0
46	h	52	Total 52	O 52	0	0
46	i	22	Total 22	O 22	0	0
46	j	12	Total 12	O 12	0	0
46	k	9	Total 9	O 9	0	0
46	l	23	Total 23	O 23	0	0
46	m	24	Total 24	O 24	0	0
46	o	246	Total 246	O 246	0	0
46	t	17	Total 17	O 17	0	0
46	u	140	Total 140	O 140	0	0
46	v	154	Total 154	O 154	0	0
46	y	7	Total 7	O 7	0	0
46	x	8	Total 8	O 8	0	0
46	z	1	Total 1	O 1	0	0

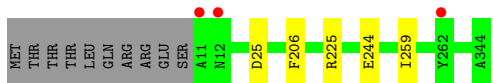
3 Residue-property plots

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

- Molecule 1: Photosystem II protein D1



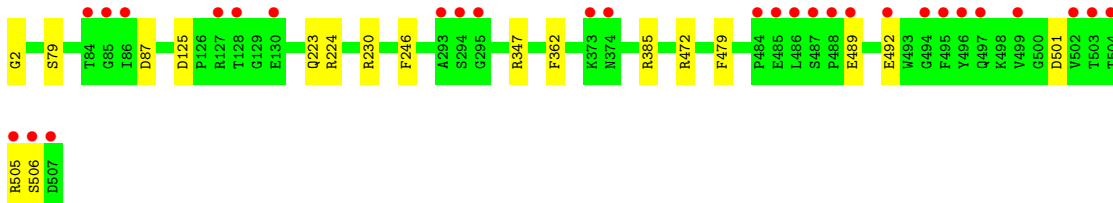
- Molecule 1: Photosystem II protein D1



- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein





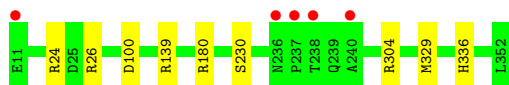
- Molecule 3: Photosystem II CP43 reaction center protein



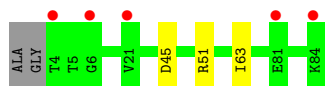
- Molecule 4: Photosystem II D2 protein



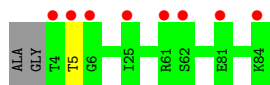
- Molecule 4: Photosystem II D2 protein



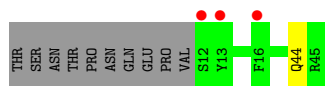
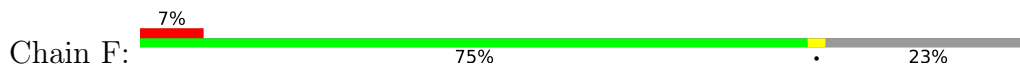
- Molecule 5: Cytochrome b559 subunit alpha



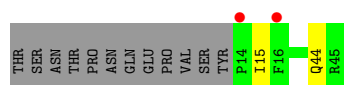
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit beta



- Molecule 6: Cytochrome b559 subunit beta



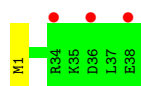
- Molecule 7: Photosystem II reaction center protein H



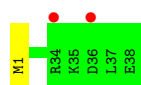
- Molecule 7: Photosystem II reaction center protein H



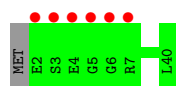
- Molecule 8: Photosystem II reaction center protein I



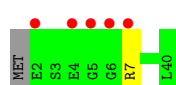
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K

Chain K:  97% .




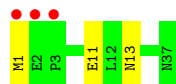
- Molecule 10: Photosystem II reaction center protein K

Chain k:  97% .



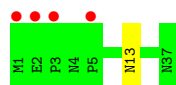
- Molecule 11: Photosystem II reaction center protein L

Chain L:  8% 92% 8% .




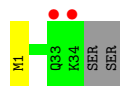
- Molecule 11: Photosystem II reaction center protein L

Chain l:  11% 97% .




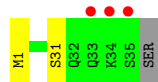
- Molecule 12: Photosystem II reaction center protein M

Chain M:  6% 92% 6% .



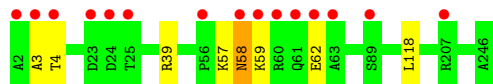
- Molecule 12: Photosystem II reaction center protein M

Chain m:  8% 92% 6% .

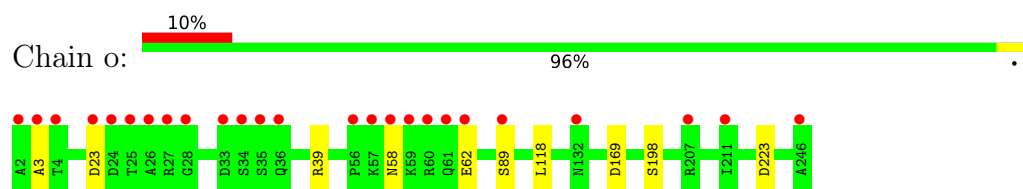


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

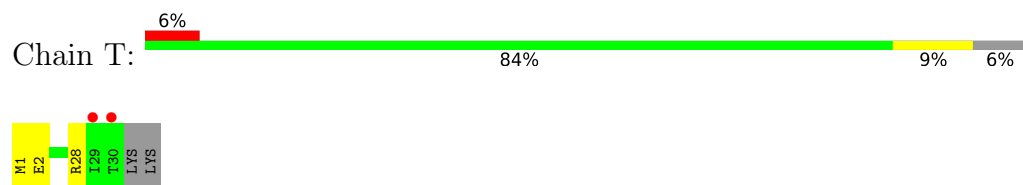
Chain O:  6% 97% .



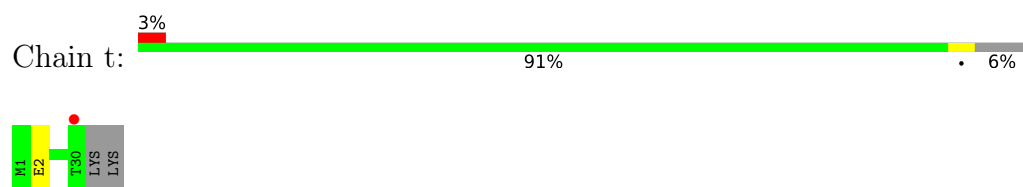
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



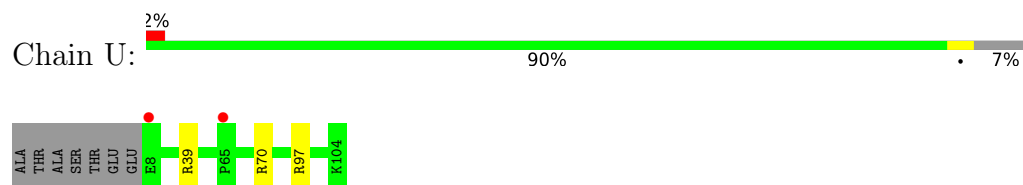
- Molecule 14: Photosystem II reaction center protein T



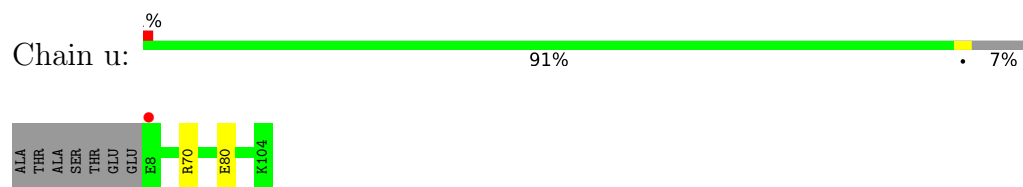
- Molecule 14: Photosystem II reaction center protein T



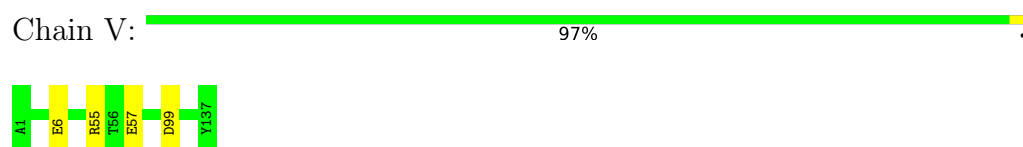
- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 16: Cytochrome c-550

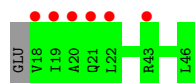


- Molecule 16: Cytochrome c-550

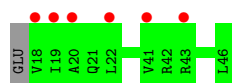




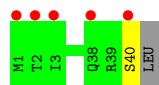
- Molecule 17: Photosystem II reaction center protein Ycf12



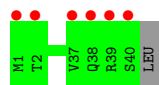
- Molecule 17: Photosystem II reaction center protein Ycf12



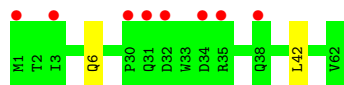
- Molecule 18: Photosystem II reaction center protein X



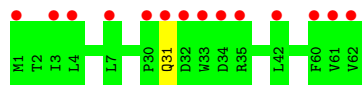
- Molecule 18: Photosystem II reaction center protein X



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	122.19Å 228.51Å 286.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	178.62 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (178.62-1.90) 99.9 (20.00-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.98 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.092 , 0.163 0.095 , 0.164	Depositor DCC
R_{free} test set	31202 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 81.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	57584	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BCT, DGD, 1PE, LMT, FE2, MHS, FME, MG, HTG, LHG, BCR, OEX, CLA, PG4, PL9, 2PE, PHO, EDO, P6G, PE8, LMG, CA, CL, HEC, SQD, GOL, PGE, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.99	2/2736 (0.1%)	0.88	4/3730 (0.1%)
1	a	0.93	0/2736	0.87	7/3730 (0.2%)
2	B	0.98	2/4205 (0.0%)	0.88	9/5727 (0.2%)
2	b	0.94	3/4207 (0.1%)	0.88	7/5731 (0.1%)
3	C	0.92	1/3636 (0.0%)	0.83	6/4950 (0.1%)
3	c	0.83	1/3679 (0.0%)	0.84	6/5008 (0.1%)
4	D	0.98	1/2816 (0.0%)	0.90	4/3836 (0.1%)
4	d	0.92	1/2829 (0.0%)	0.86	8/3852 (0.2%)
5	E	0.92	0/704	0.93	3/959 (0.3%)
5	e	0.86	0/693	0.83	0/944
6	F	0.84	0/284	0.71	0/387
6	f	0.74	0/265	0.74	0/360
7	H	1.01	2/544 (0.4%)	0.89	0/739
7	h	0.88	1/535 (0.2%)	0.75	0/728
8	I	0.90	0/311	0.81	0/419
8	i	0.86	0/311	0.83	0/419
9	J	0.87	0/306	0.74	0/413
9	j	0.75	0/287	0.77	0/388
10	K	0.80	0/303	0.75	0/416
10	k	0.75	0/303	0.77	0/416
11	L	1.00	1/319 (0.3%)	0.93	0/433
11	l	0.93	0/328	0.87	0/446
12	M	0.99	0/279	0.83	0/380
12	m	0.98	1/275 (0.4%)	0.88	0/375
13	O	0.90	0/1953	0.92	1/2649 (0.0%)
13	o	0.90	1/1948 (0.1%)	0.94	6/2641 (0.2%)
14	T	1.21	1/266 (0.4%)	1.06	1/362 (0.3%)
14	t	1.07	2/266 (0.8%)	0.91	0/362
15	U	0.85	0/803	0.92	2/1088 (0.2%)
15	u	0.98	1/785 (0.1%)	0.90	0/1064
16	V	0.95	3/1104 (0.3%)	0.89	3/1498 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.86	0/1096	0.84	4/1487 (0.3%)
17	Y	0.76	0/223	0.80	0/299
17	y	0.71	0/224	0.83	0/299
18	X	0.77	0/306	0.82	0/413
18	x	0.83	0/298	0.83	0/402
19	Z	0.74	0/490	0.79	0/669
19	z	0.73	0/490	0.70	0/669
All	All	0.92	24/43143 (0.1%)	0.87	71/58688 (0.1%)

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	66	GLY	C-O	7.92	1.36	1.23
7	H	66	GLY	C-OXT	7.84	1.38	1.23
14	t	2	GLU	CB-CG	-7.21	1.38	1.52
15	u	80	GLU	CD-OE2	-6.83	1.18	1.25
16	V	57	GLU	CG-CD	6.71	1.62	1.51

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	139	ARG	NE-CZ-NH1	14.27	127.43	120.30
4	D	139	ARG	NE-CZ-NH2	-9.74	115.43	120.30
2	B	357	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	a	225[A]	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	a	225[B]	ARG	NE-CZ-NH1	8.76	124.68	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	336/344 (98%)	332 (99%)	3 (1%)	1 (0%)	41	31
1	a	336/344 (98%)	330 (98%)	5 (2%)	1 (0%)	41	31
2	B	513/506 (101%)	508 (99%)	5 (1%)	0	100	100
2	b	514/506 (102%)	505 (98%)	9 (2%)	0	100	100
3	C	454/458 (99%)	444 (98%)	9 (2%)	1 (0%)	47	38
3	c	460/458 (100%)	446 (97%)	11 (2%)	3 (1%)	22	12
4	D	340/342 (99%)	331 (97%)	9 (3%)	0	100	100
4	d	341/342 (100%)	334 (98%)	7 (2%)	0	100	100
5	E	82/83 (99%)	82 (100%)	0	0	100	100
5	e	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	29 (97%)	0	1 (3%)	4	0
7	H	65/65 (100%)	58 (89%)	7 (11%)	0	100	100
7	h	64/65 (98%)	59 (92%)	4 (6%)	1 (2%)	9	2
8	I	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
8	i	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
9	J	39/40 (98%)	39 (100%)	0	0	100	100
9	j	37/40 (92%)	37 (100%)	0	0	100	100
10	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	37/37 (100%)	37 (100%)	0	0	100	100
12	M	34/36 (94%)	34 (100%)	0	0	100	100
12	m	34/36 (94%)	34 (100%)	0	0	100	100
13	O	249/245 (102%)	242 (97%)	3 (1%)	4 (2%)	9	2
13	o	248/245 (101%)	239 (96%)	8 (3%)	1 (0%)	34	24
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	29/32 (91%)	29 (100%)	0	0	100	100
15	U	97/104 (93%)	95 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	93 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	V	137/137 (100%)	132 (96%)	5 (4%)	0	100	100
16	v	136/137 (99%)	133 (98%)	3 (2%)	0	100	100
17	Y	28/30 (93%)	28 (100%)	0	0	100	100
17	y	28/30 (93%)	28 (100%)	0	0	100	100
18	X	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
18	x	38/41 (93%)	37 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
All	All	5280/5362 (98%)	5161 (98%)	106 (2%)	13 (0%)	47	38

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	58	ASN
13	O	59	LYS
3	C	416	SER
3	c	416[A]	SER
3	c	416[B]	SER

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	273/279 (98%)	271 (99%)	2 (1%)	84	84
1	a	273/279 (98%)	272 (100%)	1 (0%)	91	91
2	B	413/404 (102%)	407 (98%)	6 (2%)	65	62
2	b	414/404 (102%)	403 (97%)	11 (3%)	44	38
3	C	357/357 (100%)	354 (99%)	3 (1%)	81	82
3	c	361/357 (101%)	352 (98%)	9 (2%)	47	41
4	D	277/276 (100%)	275 (99%)	2 (1%)	84	84
4	d	278/276 (101%)	276 (99%)	2 (1%)	84	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	75/72 (104%)	75 (100%)	0	100	100
5	e	74/72 (103%)	73 (99%)	1 (1%)	67	65
6	F	28/38 (74%)	27 (96%)	1 (4%)	35	26
6	f	26/38 (68%)	25 (96%)	1 (4%)	33	24
7	H	56/54 (104%)	53 (95%)	3 (5%)	22	13
7	h	55/54 (102%)	52 (94%)	3 (6%)	21	12
8	I	34/34 (100%)	34 (100%)	0	100	100
8	i	34/34 (100%)	34 (100%)	0	100	100
9	J	29/28 (104%)	29 (100%)	0	100	100
9	j	27/28 (96%)	26 (96%)	1 (4%)	34	25
10	K	30/30 (100%)	29 (97%)	1 (3%)	38	29
10	k	30/30 (100%)	29 (97%)	1 (3%)	38	29
11	L	36/35 (103%)	34 (94%)	2 (6%)	21	11
11	l	37/35 (106%)	36 (97%)	1 (3%)	44	38
12	M	32/32 (100%)	32 (100%)	0	100	100
12	m	31/32 (97%)	31 (100%)	0	100	100
13	O	212/206 (103%)	208 (98%)	4 (2%)	57	53
13	o	211/206 (102%)	206 (98%)	5 (2%)	49	43
14	T	27/28 (96%)	27 (100%)	0	100	100
14	t	27/28 (96%)	27 (100%)	0	100	100
15	U	86/89 (97%)	85 (99%)	1 (1%)	71	70
15	u	84/89 (94%)	83 (99%)	1 (1%)	71	70
16	V	119/117 (102%)	119 (100%)	0	100	100
16	v	118/117 (101%)	118 (100%)	0	100	100
17	Y	23/23 (100%)	23 (100%)	0	100	100
17	y	23/23 (100%)	23 (100%)	0	100	100
18	X	34/34 (100%)	33 (97%)	1 (3%)	42	35
18	x	33/34 (97%)	33 (100%)	0	100	100
19	Z	52/52 (100%)	50 (96%)	2 (4%)	33	24
19	z	52/52 (100%)	51 (98%)	1 (2%)	57	53
All	All	4381/4376 (100%)	4315 (98%)	66 (2%)	67	62

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	k	10	LYS
13	o	23	ASP
19	z	31	GLN
15	U	70	ARG
13	O	118	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
3	c	201	ASN
13	o	124	ASN
3	c	373	ASN
4	d	332	GLN
13	o	147	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	FME	t	1[A]	-	8,9,10	0.91	0	7,9,11	0.99	0
4	MHS	D	336	4	7,11,12	0.82	0	6,14,16	2.64	4 (66%)
8	FME	i	1	8	8,9,10	0.49	0	7,9,11	1.45	1 (14%)
14	FME	T	1[B]	-	8,9,10	0.47	0	7,9,11	1.19	1 (14%)
14	FME	T	1[A]	-	8,9,10	0.60	0	7,9,11	1.29	2 (28%)
12	FME	m	1[B]	-	8,9,10	0.95	0	7,9,11	1.84	3 (42%)
14	FME	t	1[B]	-	8,9,10	0.66	0	7,9,11	1.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	FME	M	1	12	8,9,10	1.52	1 (12%)	7,9,11	1.55	1 (14%)
12	FME	m	1[A]	-	8,9,10	0.61	0	7,9,11	1.53	2 (28%)
4	MHS	d	336	4	7,11,12	1.17	0	6,14,16	1.96	1 (16%)
8	FME	I	1	8	8,9,10	0.75	0	7,9,11	1.09	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	t	1[A]	-	-	0/7/9/11	-
4	MHS	D	336	4	-	0/5/6/8	0/1/1/1
8	FME	i	1	8	-	0/7/9/11	-
14	FME	T	1[B]	-	-	2/7/9/11	-
14	FME	T	1[A]	-	-	0/7/9/11	-
12	FME	m	1[B]	-	-	3/7/9/11	-
14	FME	t	1[B]	-	-	2/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
12	FME	m	1[A]	-	-	1/7/9/11	-
4	MHS	d	336	4	-	0/5/6/8	0/1/1/1
8	FME	I	1	8	-	0/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	1	FME	CA-N	-3.01	1.42	1.46

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	336	MHS	CM-ND1-CG	5.06	131.17	124.44
4	d	336	MHS	CM-ND1-CG	4.39	130.28	124.44
12	M	1	FME	CG-CB-CA	2.91	121.03	112.95
12	m	1[B]	FME	CB-CG-SD	-2.90	97.90	113.48
8	i	1	FME	O-C-CA	-2.74	117.61	124.78

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	O-C-CA-CB
14	T	1[B]	FME	CB-CG-SD-CE
14	t	1[B]	FME	CB-CG-SD-CE
12	m	1[B]	FME	CB-CG-SD-CE
14	T	1[B]	FME	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 447 ligands modelled in this entry, 18 are monoatomic - leaving 429 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	$\# Z > 2$
29	LMG	C	526	-	55,55,55	1.05	2 (3%)	63,63,63	1.51	8 (12%)
38	HTG	b	632	-	19,19,19	0.97	1 (5%)	23,24,24	1.67	7 (30%)
34	PGE	t	105	-	6,6,9	0.67	0	5,5,8	0.49	0
38	HTG	C	522	-	19,19,19	1.09	1 (5%)	23,24,24	1.90	3 (13%)
34	PGE	T	104	-	6,6,9	1.04	0	5,5,8	0.54	0
31	LMT	m	102	-	36,36,36	0.98	1 (2%)	47,47,47	1.67	7 (14%)
30	GOL	D	402	-	5,5,5	0.78	0	5,5,5	1.28	1 (20%)
31	LMT	m	101	-	36,36,36	1.03	1 (2%)	47,47,47	1.09	5 (10%)
24	CLA	d	404	-	59,73,73	1.49	10 (16%)	67,113,113	2.34	19 (28%)
24	CLA	B	603	-	59,73,73	1.79	11 (18%)	67,113,113	2.08	15 (22%)
34	PGE	c	539	-	9,9,9	0.64	0	8,8,8	0.38	0
34	PGE	E	106	-	9,9,9	0.69	0	8,8,8	0.60	0
34	PGE	h	108	-	9,9,9	0.60	0	8,8,8	0.43	0
33	PG4	l	103	-	12,12,12	0.65	0	11,11,11	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	PG4	V	212	-	12,12,12	0.71	0	11,11,11	0.57	0
30	GOL	D	412	-	5,5,5	0.61	0	5,5,5	0.66	0
29	LMG	A	613	-	51,51,55	0.98	3 (5%)	59,59,63	1.02	3 (5%)
32	LHG	e	101	-	41,41,48	1.13	2 (4%)	44,47,54	1.18	4 (9%)
34	PGE	O	310	-	9,9,9	0.60	0	8,8,8	0.36	0
38	HTG	C	531	-	19,19,19	1.31	2 (10%)	23,24,24	1.01	2 (8%)
39	1PE	e	105	-	15,15,15	0.64	0	14,14,14	0.54	0
34	PGE	a	423	-	9,9,9	0.59	0	8,8,8	0.44	0
34	PGE	V	215	-	9,9,9	0.87	0	8,8,8	0.63	0
38	HTG	a	418	-	19,19,19	1.35	3 (15%)	23,24,24	1.84	8 (34%)
40	DGD	H	103	-	63,63,67	1.07	7 (11%)	77,77,81	1.22	11 (14%)
33	PG4	I	103	-	12,12,12	0.73	0	11,11,11	0.58	0
34	PGE	B	645	-	9,9,9	0.72	0	8,8,8	0.68	0
36	EDO	B	655	-	3,3,3	0.43	0	2,2,2	0.50	0
34	PGE	b	641	-	9,9,9	0.39	0	8,8,8	0.74	0
40	DGD	D	408	-	67,67,67	1.22	4 (5%)	81,81,81	1.61	10 (12%)
38	HTG	C	532	-	19,19,19	1.16	2 (10%)	23,24,24	1.79	5 (21%)
31	LMT	B	622	-	36,36,36	0.80	1 (2%)	47,47,47	1.45	7 (14%)
28	SQD	A	622	-	53,54,54	1.36	4 (7%)	62,65,65	1.52	9 (14%)
24	CLA	c	507	46	59,73,73	1.82	11 (18%)	67,113,113	2.14	18 (26%)
36	EDO	e	106	-	3,3,3	0.41	0	2,2,2	0.50	0
34	PGE	o	306	-	9,9,9	0.61	0	8,8,8	0.24	0
35	P6G	D	418	-	18,18,18	0.75	0	17,17,17	0.60	0
24	CLA	b	605	-	59,73,73	1.76	14 (23%)	67,113,113	2.78	21 (31%)
26	BCR	C	514	-	41,41,41	1.29	4 (9%)	56,56,56	1.85	13 (23%)
30	GOL	c	529	-	5,5,5	1.01	0	5,5,5	1.36	1 (20%)
39	1PE	V	217	-	15,15,15	0.94	0	14,14,14	1.01	1 (7%)
24	CLA	b	611	46	59,73,73	1.61	9 (15%)	67,113,113	2.40	23 (34%)
29	LMG	c	519	-	51,51,55	1.01	3 (5%)	59,59,63	1.39	8 (13%)
24	CLA	c	512	-	59,73,73	1.81	12 (20%)	67,113,113	2.30	21 (31%)
29	LMG	b	621	-	51,51,55	1.03	3 (5%)	59,59,63	1.66	7 (11%)
24	CLA	c	511	3	59,73,73	1.63	12 (20%)	67,113,113	2.09	20 (29%)
33	PG4	B	643	-	12,12,12	0.55	0	11,11,11	0.56	0
31	LMT	c	521	-	36,36,36	0.83	0	47,47,47	1.63	12 (25%)
30	GOL	u	201	-	5,5,5	0.72	0	5,5,5	1.10	0
26	BCR	C	515	-	41,41,41	0.98	1 (2%)	56,56,56	1.62	11 (19%)
32	LHG	a	419	-	40,40,48	1.21	3 (7%)	43,46,54	1.38	6 (13%)
35	P6G	j	106	-	18,18,18	0.80	0	17,17,17	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	PL9	A	611	-	55,55,55	1.35	7 (12%)	68,69,69	2.10	17 (25%)
38	HTG	c	522	-	19,19,19	0.72	0	23,24,24	1.44	3 (13%)
24	CLA	C	506	-	59,73,73	1.64	10 (16%)	67,113,113	2.27	17 (25%)
33	PG4	c	535	-	12,12,12	0.86	0	11,11,11	0.68	0
33	PG4	X	101	-	12,12,12	0.66	0	11,11,11	0.51	0
33	PG4	B	637	-	12,12,12	0.80	0	11,11,11	0.55	0
30	GOL	c	528	-	5,5,5	0.57	0	5,5,5	0.62	0
38	HTG	C	529	-	19,19,19	1.20	2 (10%)	23,24,24	2.27	4 (17%)
24	CLA	c	502	-	59,73,73	1.59	12 (20%)	67,113,113	2.38	17 (25%)
34	PGE	b	644	-	9,9,9	0.63	0	8,8,8	0.38	0
24	CLA	a	408	46	54,68,73	1.62	9 (16%)	61,107,113	2.37	18 (29%)
32	LHG	D	411	-	48,48,48	0.87	2 (4%)	51,54,54	0.84	3 (5%)
38	HTG	C	521	-	19,19,19	0.94	1 (5%)	23,24,24	1.05	1 (4%)
33	PG4	e	103	-	12,12,12	0.58	0	11,11,11	0.51	0
33	PG4	B	642	-	12,12,12	0.82	0	11,11,11	0.64	0
38	HTG	O	303	-	19,19,19	1.58	2 (10%)	23,24,24	1.07	2 (8%)
33	PG4	i	101	-	12,12,12	0.58	0	11,11,11	0.41	0
38	HTG	B	624	-	19,19,19	1.01	1 (5%)	23,24,24	1.90	5 (21%)
34	PGE	Y	102	-	9,9,9	0.79	0	8,8,8	0.62	0
26	BCR	b	618	-	41,41,41	1.14	3 (7%)	56,56,56	1.49	7 (12%)
34	PGE	A	620	-	6,6,9	0.64	0	5,5,8	0.90	0
26	BCR	A	610	-	41,41,41	1.23	5 (12%)	56,56,56	1.52	14 (25%)
31	LMT	Y	101	-	36,36,36	0.58	0	47,47,47	1.24	5 (10%)
35	P6G	B	651	-	18,18,18	0.52	0	17,17,17	0.67	0
36	EDO	B	656	-	3,3,3	1.06	0	2,2,2	0.21	0
33	PG4	c	532	-	12,12,12	0.90	0	11,11,11	0.81	0
24	CLA	b	602	46	59,73,73	1.81	10 (16%)	67,113,113	2.38	23 (34%)
30	GOL	a	415	-	5,5,5	1.09	0	5,5,5	1.12	1 (20%)
25	PHO	A	608	-	67,69,69	1.53	13 (19%)	85,99,99	1.79	17 (20%)
24	CLA	b	614	-	59,73,73	1.80	10 (16%)	67,113,113	2.16	16 (23%)
34	PGE	b	638	-	9,9,9	1.00	0	8,8,8	0.71	0
32	LHG	E	101	-	41,41,48	1.11	2 (4%)	44,47,54	1.14	3 (6%)
24	CLA	D	404	-	59,73,73	1.56	12 (20%)	67,113,113	2.24	20 (29%)
35	P6G	b	649	-	18,18,18	0.55	0	17,17,17	0.53	0
24	CLA	b	617	-	54,68,73	1.75	13 (24%)	61,107,113	2.62	22 (36%)
39	1PE	x	104	-	15,15,15	0.62	0	14,14,14	0.41	0
24	CLA	a	410	-	59,73,73	1.61	10 (16%)	67,113,113	2.31	22 (32%)
20	OEX	a	402	1,3,46	0,15,15	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	c	510	-	59,73,73	1.85	16 (27%)	67,113,113	2.10	15 (22%)
30	GOL	B	626	-	5,5,5	0.82	0	5,5,5	0.70	0
34	PGE	o	308	-	9,9,9	0.69	0	8,8,8	0.56	0
35	P6G	T	105	-	18,18,18	0.68	0	17,17,17	0.96	0
24	CLA	c	509	-	59,73,73	1.70	11 (18%)	67,113,113	2.15	16 (23%)
31	LMT	I	101	-	36,36,36	0.89	1 (2%)	47,47,47	1.52	9 (19%)
33	PG4	B	636	-	12,12,12	0.57	0	11,11,11	0.59	0
34	PGE	c	538	-	9,9,9	0.91	0	8,8,8	0.88	0
24	CLA	B	616	-	59,73,73	1.46	10 (16%)	67,113,113	2.08	14 (20%)
26	BCR	C	525	-	41,41,41	1.13	3 (7%)	56,56,56	1.68	11 (19%)
34	PGE	D	415	-	9,9,9	0.59	0	8,8,8	0.41	0
34	PGE	f	105	-	9,9,9	0.58	0	8,8,8	0.26	0
31	LMT	F	102	-	36,36,36	1.09	3 (8%)	47,47,47	1.26	5 (10%)
34	PGE	i	106	-	9,9,9	0.83	0	8,8,8	0.64	0
35	P6G	d	416	-	18,18,18	0.64	0	17,17,17	0.59	0
30	GOL	B	625	-	5,5,5	0.69	0	5,5,5	1.86	2 (40%)
32	LHG	A	618	-	41,41,48	1.22	2 (4%)	44,47,54	1.21	5 (11%)
31	LMT	f	101	-	36,36,36	0.94	1 (2%)	47,47,47	1.33	5 (10%)
30	GOL	v	206	-	5,5,5	0.31	0	5,5,5	0.52	0
33	PG4	X	102	-	12,12,12	0.85	0	11,11,11	0.79	0
33	PG4	B	638	-	12,12,12	0.81	0	11,11,11	0.76	0
38	HTG	B	623	-	19,19,19	1.00	1 (5%)	23,24,24	1.34	3 (13%)
29	LMG	B	621	-	51,51,55	1.09	4 (7%)	59,59,63	1.67	8 (13%)
25	PHO	a	409	-	67,69,69	1.65	11 (16%)	85,99,99	1.62	19 (22%)
34	PGE	j	105	-	9,9,9	0.64	0	8,8,8	0.59	0
30	GOL	t	101	-	5,5,5	1.24	0	5,5,5	1.10	1 (20%)
33	PG4	K	102	-	12,12,12	0.62	0	11,11,11	0.50	0
38	HTG	c	531	-	19,19,19	1.15	2 (10%)	23,24,24	1.87	7 (30%)
35	P6G	E	110	-	18,18,18	0.77	0	17,17,17	0.53	0
30	GOL	C	524	-	5,5,5	0.79	0	5,5,5	1.03	0
34	PGE	o	307	-	9,9,9	0.78	0	8,8,8	0.55	0
24	CLA	b	607	-	49,63,73	1.70	10 (20%)	55,101,113	2.24	20 (36%)
26	BCR	a	411	-	41,41,41	1.20	4 (9%)	56,56,56	1.34	6 (10%)
36	EDO	A	625	-	3,3,3	0.63	0	2,2,2	0.40	0
40	DGD	C	518	-	63,63,67	0.79	2 (3%)	77,77,81	1.10	6 (7%)
24	CLA	B	611	46	59,73,73	1.58	9 (15%)	67,113,113	2.48	24 (35%)
34	PGE	h	109	-	9,9,9	0.70	0	8,8,8	0.45	0
30	GOL	B	627	-	5,5,5	0.69	0	5,5,5	0.88	0
33	PG4	b	635	-	12,12,12	0.84	0	11,11,11	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	EDO	E	112	-	3,3,3	0.60	0	2,2,2	0.10	0
24	CLA	c	513	-	59,73,73	1.73	11 (18%)	67,113,113	2.24	17 (25%)
30	GOL	f	104	-	5,5,5	0.76	0	5,5,5	1.23	0
34	PGE	i	105	-	9,9,9	0.66	0	8,8,8	0.68	0
24	CLA	D	403	46	59,73,73	1.76	9 (15%)	67,113,113	2.10	14 (20%)
30	GOL	v	204	-	5,5,5	1.16	0	5,5,5	0.88	0
28	SQD	a	413	-	53,54,54	1.12	4 (7%)	62,65,65	2.14	12 (19%)
29	LMG	j	101	42	47,47,55	1.00	3 (6%)	55,55,63	1.04	3 (5%)
24	CLA	C	501	-	59,73,73	1.71	12 (20%)	67,113,113	2.62	17 (25%)
25	PHO	D	401	-	67,69,69	1.77	16 (23%)	85,99,99	1.72	16 (18%)
36	EDO	H	112	-	3,3,3	0.50	0	2,2,2	0.37	0
30	GOL	B	635	-	5,5,5	0.78	0	5,5,5	1.17	0
32	LHG	B	632	-	48,48,48	0.80	2 (4%)	51,54,54	1.30	7 (13%)
24	CLA	c	506	-	59,73,73	1.60	12 (20%)	67,113,113	2.09	19 (28%)
30	GOL	v	207	-	5,5,5	0.50	0	5,5,5	0.34	0
36	EDO	J	109	-	3,3,3	0.43	0	2,2,2	0.34	0
34	PGE	J	108	-	9,9,9	0.57	0	8,8,8	0.52	0
28	SQD	a	424	-	53,54,54	1.31	3 (5%)	62,65,65	2.01	14 (22%)
30	GOL	V	206	-	5,5,5	0.56	0	5,5,5	0.19	0
24	CLA	B	617	-	54,68,73	1.76	12 (22%)	61,107,113	2.38	21 (34%)
26	BCR	t	102	-	41,41,41	1.13	3 (7%)	56,56,56	1.98	18 (32%)
36	EDO	E	111	-	3,3,3	0.67	0	2,2,2	0.39	0
29	LMG	a	414	-	51,51,55	0.85	2 (3%)	59,59,63	1.26	5 (8%)
34	PGE	H	109	-	9,9,9	0.53	0	8,8,8	0.48	0
26	BCR	B	619	-	41,41,41	1.19	5 (12%)	56,56,56	1.45	8 (14%)
30	GOL	o	303	-	5,5,5	0.76	0	5,5,5	0.65	0
28	SQD	b	633	-	53,54,54	1.43	5 (9%)	62,65,65	1.99	16 (25%)
33	PG4	x	102	-	12,12,12	0.64	0	11,11,11	0.37	0
30	GOL	B	628	-	5,5,5	0.76	0	5,5,5	1.66	1 (20%)
39	1PE	j	107	-	15,15,15	0.63	0	14,14,14	0.63	0
34	PGE	B	647	-	9,9,9	0.70	0	8,8,8	0.67	0
30	GOL	c	525	-	5,5,5	0.46	0	5,5,5	1.43	1 (20%)
26	BCR	B	620	-	41,41,41	1.14	3 (7%)	56,56,56	1.37	7 (12%)
28	SQD	A	616	-	53,54,54	1.18	4 (7%)	62,65,65	1.56	10 (16%)
24	CLA	b	608	46	59,73,73	1.61	10 (16%)	67,113,113	1.79	12 (17%)
33	PG4	E	103	-	12,12,12	0.64	0	11,11,11	0.53	0
32	LHG	l	101	-	48,48,48	0.91	2 (4%)	51,54,54	1.18	3 (5%)
30	GOL	b	628	-	5,5,5	0.83	0	5,5,5	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	P6G	I	106	-	18,18,18	0.64	0	17,17,17	0.78	1 (5%)
34	PGE	E	109	-	9,9,9	0.84	0	8,8,8	0.58	0
31	LMT	C	533	-	36,36,36	0.68	1 (2%)	47,47,47	1.09	1 (2%)
26	BCR	B	618	-	41,41,41	0.98	0	56,56,56	1.54	10 (17%)
32	LHG	D	409	-	48,48,48	0.83	2 (4%)	51,54,54	1.48	5 (9%)
34	PGE	O	309	-	9,9,9	0.81	0	8,8,8	0.99	1 (12%)
34	PGE	t	104	-	9,9,9	0.83	0	8,8,8	0.70	0
26	BCR	d	406	-	41,41,41	1.48	4 (9%)	56,56,56	2.20	17 (30%)
24	CLA	B	606	-	59,73,73	1.72	11 (18%)	67,113,113	2.53	24 (35%)
38	HTG	b	631	-	19,19,19	1.32	2 (10%)	23,24,24	1.71	6 (26%)
27	PL9	d	407	-	55,55,55	1.27	8 (14%)	68,69,69	1.32	10 (14%)
24	CLA	D	405	-	59,73,73	1.59	8 (13%)	67,113,113	2.25	16 (23%)
33	PG4	J	105	-	12,12,12	0.69	0	11,11,11	0.37	0
30	GOL	f	103	42	5,5,5	0.67	0	5,5,5	0.89	0
24	CLA	B	610	-	59,73,73	1.46	7 (11%)	67,113,113	2.42	19 (28%)
36	EDO	o	311	-	3,3,3	0.48	0	2,2,2	0.28	0
24	CLA	B	614	-	59,73,73	1.61	10 (16%)	67,113,113	2.14	16 (23%)
33	PG4	i	104	-	12,12,12	0.51	0	11,11,11	0.41	0
30	GOL	T	101	-	5,5,5	0.94	0	5,5,5	0.86	0
33	PG4	B	640	-	12,12,12	0.67	0	11,11,11	0.43	0
30	GOL	T	103	-	5,5,5	0.73	0	5,5,5	0.70	0
36	EDO	O	311	-	3,3,3	0.67	0	2,2,2	0.29	0
31	LMT	M	101	-	36,36,36	0.96	3 (8%)	47,47,47	1.80	15 (31%)
38	HTG	b	623	-	19,19,19	1.21	2 (10%)	23,24,24	1.58	5 (21%)
30	GOL	m	103	-	5,5,5	0.28	0	5,5,5	0.57	0
31	LMT	t	103	-	36,36,36	0.85	0	47,47,47	1.40	8 (17%)
24	CLA	C	502	-	59,73,73	1.53	9 (15%)	67,113,113	2.29	18 (26%)
24	CLA	B	602	46	59,73,73	1.77	11 (18%)	67,113,113	2.87	25 (37%)
26	BCR	k	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.65	11 (19%)
40	DGD	c	517	-	58,58,67	1.00	4 (6%)	72,72,81	1.12	3 (4%)
41	HEM	E	113	6,5	27,50,50	1.08	1 (3%)	17,82,82	3.78	8 (47%)
31	LMT	J	103	-	36,36,36	0.93	1 (2%)	47,47,47	1.56	9 (19%)
35	P6G	d	415	-	18,18,18	0.69	0	17,17,17	0.96	1 (5%)
26	BCR	c	515	-	41,41,41	1.25	2 (4%)	56,56,56	1.65	12 (21%)
32	LHG	D	410	-	48,48,48	0.87	2 (4%)	51,54,54	0.98	1 (1%)
28	SQD	l	102	-	53,54,54	1.30	4 (7%)	62,65,65	1.86	14 (22%)
30	GOL	v	205	-	5,5,5	0.44	0	5,5,5	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	EDO	o	310	-	3,3,3	0.62	0	2,2,2	0.12	0
28	SQD	a	417	-	53,54,54	1.25	4 (7%)	62,65,65	1.26	5 (8%)
33	PG4	I	104	-	12,12,12	0.50	0	11,11,11	0.48	0
35	P6G	B	652	-	18,18,18	0.83	0	17,17,17	1.10	1 (5%)
34	PGE	h	107	-	9,9,9	0.77	0	8,8,8	0.69	0
38	HTG	V	204	-	19,19,19	0.97	1 (5%)	23,24,24	2.71	7 (30%)
35	P6G	A	624	-	18,18,18	0.59	0	17,17,17	0.55	0
32	LHG	d	410	-	48,48,48	0.80	2 (4%)	51,54,54	1.11	3 (5%)
24	CLA	C	505	-	59,73,73	1.81	12 (20%)	67,113,113	2.24	16 (23%)
30	GOL	O	302	-	5,5,5	1.49	1 (20%)	5,5,5	0.94	0
28	SQD	h	105	-	53,54,54	1.43	6 (11%)	62,65,65	1.53	9 (14%)
24	CLA	B	607	-	49,63,73	1.65	12 (24%)	55,101,113	2.59	17 (30%)
29	LMG	B	634	-	55,55,55	1.25	3 (5%)	63,63,63	1.42	12 (19%)
24	CLA	C	508	-	54,68,73	1.75	12 (22%)	61,107,113	2.51	17 (27%)
24	CLA	b	615	-	59,73,73	1.60	11 (18%)	67,113,113	2.04	20 (29%)
33	PG4	U	202	-	12,12,12	0.69	0	11,11,11	0.47	0
24	CLA	C	512	-	59,73,73	1.64	12 (20%)	67,113,113	2.07	21 (31%)
36	EDO	V	218	-	3,3,3	0.91	0	2,2,2	0.21	0
24	CLA	b	603	-	59,73,73	1.68	9 (15%)	67,113,113	2.14	18 (26%)
30	GOL	O	304	-	5,5,5	0.43	0	5,5,5	0.52	0
31	LMT	j	103	-	36,36,36	0.74	1 (2%)	47,47,47	1.43	4 (8%)
33	PG4	H	106	-	12,12,12	0.73	0	11,11,11	0.63	0
30	GOL	b	630	-	5,5,5	0.46	0	5,5,5	0.31	0
33	PG4	e	104	-	12,12,12	0.60	0	11,11,11	0.56	0
30	GOL	A	615	-	5,5,5	0.53	0	5,5,5	1.05	0
34	PGE	E	104	-	9,9,9	0.56	0	8,8,8	0.46	0
23	BCT	a	406	21	0,3,3	0.00	-	0,3,3	0.00	-
30	GOL	d	413	-	5,5,5	0.77	0	5,5,5	0.92	0
33	PG4	b	636	-	12,12,12	0.77	0	11,11,11	0.68	0
24	CLA	b	609	-	59,73,73	1.58	10 (16%)	67,113,113	2.23	19 (28%)
33	PG4	V	213	-	12,12,12	0.71	0	11,11,11	0.63	0
39	1PE	B	654	-	15,15,15	0.77	0	14,14,14	0.90	0
30	GOL	v	203	-	5,5,5	0.75	0	5,5,5	0.64	0
34	PGE	V	214	-	9,9,9	0.63	0	8,8,8	0.30	0
43	HEC	v	202	16	26,50,50	1.03	2 (7%)	18,82,82	1.94	7 (38%)
28	SQD	F	104	-	53,54,54	1.43	5 (9%)	62,65,65	2.09	17 (27%)
43	HEC	V	203	16	26,50,50	1.22	3 (11%)	18,82,82	1.78	5 (27%)
26	BCR	b	619	-	41,41,41	1.27	5 (12%)	56,56,56	1.78	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCT	m	104[B]	-	0,3,3	0.00	-	0,3,3	0.00	-
33	PG4	J	104	-	12,12,12	0.59	0	11,11,11	0.31	0
24	CLA	B	604	-	59,73,73	1.69	10 (16%)	67,113,113	2.33	17 (25%)
34	PGE	c	536	-	9,9,9	0.61	0	8,8,8	0.27	0
34	PGE	A	621	-	9,9,9	0.73	0	8,8,8	0.48	0
40	DGD	C	516	-	63,63,67	0.89	5 (7%)	77,77,81	1.29	10 (12%)
34	PGE	B	650	-	9,9,9	0.63	0	8,8,8	0.38	0
33	PG4	C	538	-	12,12,12	0.76	0	11,11,11	0.55	0
35	P6G	D	416	-	18,18,18	0.72	0	17,17,17	0.60	0
35	P6G	b	648	-	18,18,18	0.62	0	17,17,17	0.74	0
36	EDO	c	542	-	3,3,3	0.62	0	2,2,2	0.39	0
24	CLA	B	613	-	59,73,73	1.45	8 (13%)	67,113,113	1.80	12 (17%)
30	GOL	d	402	-	5,5,5	0.62	0	5,5,5	0.96	1 (20%)
24	CLA	C	507	46	59,73,73	1.72	11 (18%)	67,113,113	2.24	18 (26%)
40	DGD	c	516	-	63,63,67	0.90	3 (4%)	77,77,81	1.10	4 (5%)
31	LMT	u	203	-	36,36,36	1.28	4 (11%)	47,47,47	1.67	9 (19%)
30	GOL	a	416	-	5,5,5	0.62	0	5,5,5	0.79	0
24	CLA	A	606	-	59,73,73	1.71	9 (15%)	67,113,113	2.11	18 (26%)
33	PG4	C	535	-	12,12,12	0.95	0	11,11,11	0.83	0
33	PG4	I	102	-	12,12,12	0.61	0	11,11,11	0.42	0
33	PG4	C	534	-	12,12,12	0.72	0	11,11,11	0.41	0
28	SQD	x	101	-	53,54,54	1.26	4 (7%)	62,65,65	1.83	11 (17%)
34	PGE	b	639	-	9,9,9	0.62	0	8,8,8	0.44	0
26	BCR	c	527	-	41,41,41	1.04	2 (4%)	56,56,56	1.40	9 (16%)
33	PG4	V	209	-	12,12,12	0.85	0	11,11,11	1.01	1 (9%)
24	CLA	c	505	-	59,73,73	1.56	10 (16%)	67,113,113	2.32	17 (25%)
34	PGE	H	111	-	9,9,9	0.66	0	8,8,8	0.39	0
30	GOL	C	527	-	5,5,5	0.48	0	5,5,5	0.29	0
34	PGE	b	640	-	9,9,9	0.64	0	8,8,8	0.31	0
30	GOL	V	208	-	5,5,5	0.48	0	5,5,5	0.46	0
30	GOL	o	305	-	5,5,5	0.68	0	5,5,5	0.97	0
40	DGD	C	517	-	57,57,67	0.88	3 (5%)	71,71,81	1.09	2 (2%)
24	CLA	C	510	-	59,73,73	1.69	11 (18%)	67,113,113	2.19	19 (28%)
34	PGE	B	649	-	9,9,9	0.89	0	8,8,8	0.55	0
44	2PE	V	216	-	27,27,27	0.92	0	26,26,26	0.69	0
30	GOL	O	306	-	5,5,5	1.26	1 (20%)	5,5,5	1.12	1 (20%)
33	PG4	a	421	-	12,12,12	0.63	0	11,11,11	0.62	0
38	HTG	H	101	-	19,19,19	1.11	2 (10%)	23,24,24	1.56	5 (21%)
29	LMG	C	519	-	51,51,55	1.12	3 (5%)	59,59,63	1.52	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	HTG	C	530	-	19,19,19	1.05	1 (5%)	23,24,24	1.19	2 (8%)
34	PGE	x	103	-	9,9,9	0.60	0	8,8,8	0.58	0
34	PGE	c	540	-	9,9,9	0.67	0	8,8,8	0.46	0
33	PG4	H	105	-	12,12,12	0.74	0	11,11,11	0.48	0
24	CLA	C	503	-	59,73,73	1.75	11 (18%)	67,113,113	2.36	17 (25%)
26	BCR	b	620	-	41,41,41	1.00	2 (4%)	56,56,56	1.39	4 (7%)
34	PGE	I	105	-	9,9,9	0.96	0	8,8,8	0.75	0
24	CLA	b	613	-	59,73,73	1.75	13 (22%)	67,113,113	2.14	16 (23%)
30	GOL	A	614	-	5,5,5	1.17	0	5,5,5	0.88	0
34	PGE	B	644	-	9,9,9	0.57	0	8,8,8	0.44	0
34	PGE	E	105	-	9,9,9	0.73	0	8,8,8	0.47	0
38	HTG	c	530	-	19,19,19	1.69	3 (15%)	23,24,24	1.24	3 (13%)
30	GOL	b	629	-	5,5,5	0.67	0	5,5,5	1.11	0
33	PG4	D	414	-	12,12,12	0.66	0	11,11,11	0.51	0
33	PG4	a	420	-	12,12,12	0.57	0	11,11,11	0.38	0
30	GOL	b	625	-	5,5,5	0.52	0	5,5,5	1.54	1 (20%)
33	PG4	B	641	-	12,12,12	0.72	0	11,11,11	0.61	0
30	GOL	C	523	-	5,5,5	0.68	0	5,5,5	2.18	2 (40%)
30	GOL	U	201	-	5,5,5	0.53	0	5,5,5	1.10	0
24	CLA	B	615	-	49,63,73	1.78	8 (16%)	55,101,113	2.34	19 (34%)
40	DGD	c	518	-	63,63,67	0.91	3 (4%)	77,77,81	0.98	6 (7%)
30	GOL	e	102	-	5,5,5	0.69	0	5,5,5	0.81	0
29	LMG	C	520	-	51,51,55	1.26	3 (5%)	59,59,63	1.27	9 (15%)
27	PL9	D	407	-	55,55,55	1.43	8 (14%)	68,69,69	1.36	6 (8%)
24	CLA	C	513	-	59,73,73	1.66	10 (16%)	67,113,113	2.39	21 (31%)
34	PGE	o	309	-	9,9,9	0.84	0	8,8,8	0.71	0
36	EDO	X	104	-	3,3,3	0.95	0	2,2,2	0.48	0
27	PL9	a	412	-	55,55,55	1.35	2 (3%)	68,69,69	1.79	14 (20%)
29	LMG	d	412	-	55,55,55	1.05	3 (5%)	63,63,63	1.17	5 (7%)
34	PGE	a	422	-	9,9,9	0.67	0	8,8,8	0.73	0
40	DGD	h	104	-	63,63,67	1.12	5 (7%)	77,77,81	1.26	8 (10%)
30	GOL	V	201	-	5,5,5	1.03	0	5,5,5	0.49	0
38	HTG	B	631	-	19,19,19	1.10	3 (15%)	23,24,24	1.20	2 (8%)
33	PG4	c	533	-	12,12,12	0.59	0	11,11,11	0.48	0
34	PGE	b	642	-	9,9,9	0.66	0	8,8,8	0.20	0
40	DGD	d	408	-	67,67,67	1.32	4 (5%)	81,81,81	1.76	10 (12%)
29	LMG	J	101	42	47,47,55	0.74	2 (4%)	55,55,63	0.90	2 (3%)
24	CLA	c	501	-	59,73,73	1.51	8 (13%)	67,113,113	2.53	16 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	PGE	O	308	-	9,9,9	0.99	0	8,8,8	1.28	1 (12%)
31	LMT	M	102	-	36,36,36	0.90	0	47,47,47	1.57	2 (4%)
24	CLA	d	405	-	59,73,73	1.80	12 (20%)	67,113,113	2.18	18 (26%)
24	CLA	b	610	-	59,73,73	1.71	11 (18%)	67,113,113	2.31	18 (26%)
24	CLA	b	616	-	59,73,73	1.76	8 (13%)	67,113,113	2.27	17 (25%)
34	PGE	b	643	-	9,9,9	0.86	0	8,8,8	0.62	0
35	P6G	D	417	-	18,18,18	0.64	0	17,17,17	0.88	1 (5%)
31	LMT	a	401	-	36,36,36	0.83	1 (2%)	47,47,47	1.42	4 (8%)
31	LMT	b	622	-	36,36,36	0.84	1 (2%)	47,47,47	1.42	5 (10%)
34	PGE	c	537	-	9,9,9	0.54	0	8,8,8	0.35	0
34	PGE	H	108	-	9,9,9	0.60	0	8,8,8	0.60	0
38	HTG	o	301	-	19,19,19	2.03	2 (10%)	23,24,24	1.08	1 (4%)
24	CLA	B	605	-	59,73,73	1.63	10 (16%)	67,113,113	2.58	25 (37%)
33	PG4	b	634	-	12,12,12	0.81	0	11,11,11	0.68	0
30	GOL	u	202	-	5,5,5	0.81	0	5,5,5	0.39	0
30	GOL	c	526	-	5,5,5	0.39	0	5,5,5	0.84	0
30	GOL	V	207	-	5,5,5	0.76	0	5,5,5	0.81	0
38	HTG	c	523	-	19,19,19	0.92	2 (10%)	23,24,24	1.49	5 (21%)
41	HEM	e	107	6,5	27,50,50	0.84	1 (3%)	17,82,82	1.94	4 (23%)
26	BCR	H	102	-	41,41,41	1.07	3 (7%)	56,56,56	1.76	17 (30%)
36	EDO	C	542	-	3,3,3	0.51	0	2,2,2	0.37	0
34	PGE	J	106	-	9,9,9	0.63	0	8,8,8	0.34	0
20	OEX	A	601	1,3,46	0,15,15	0.00	-	-	-	-
35	P6G	A	623	-	18,18,18	0.69	0	17,17,17	0.56	0
33	PG4	B	639	-	12,12,12	0.90	0	11,11,11	0.73	0
30	GOL	y	101	-	5,5,5	0.66	0	5,5,5	0.69	0
24	CLA	C	509	-	59,73,73	1.47	8 (13%)	67,113,113	2.23	19 (28%)
38	HTG	B	630	-	19,19,19	1.09	2 (10%)	23,24,24	1.59	8 (34%)
33	PG4	V	210	-	12,12,12	0.91	0	11,11,11	0.78	0
36	EDO	a	425	-	3,3,3	0.61	0	2,2,2	0.06	0
30	GOL	b	627	-	5,5,5	1.23	1 (20%)	5,5,5	1.34	1 (20%)
29	LMG	c	520	-	51,51,55	1.18	3 (5%)	59,59,63	1.19	5 (8%)
45	PE8	i	107	-	24,24,24	0.69	0	23,23,23	0.69	0
32	LHG	d	411	-	48,48,48	1.00	3 (6%)	51,54,54	0.84	2 (3%)
24	CLA	C	504	46	54,68,73	1.81	13 (24%)	61,107,113	2.20	17 (27%)
34	PGE	C	540	-	9,9,9	0.60	0	8,8,8	0.33	0
26	BCR	T	102	-	41,41,41	1.05	4 (9%)	56,56,56	1.62	11 (19%)
34	PGE	J	107	-	9,9,9	0.68	0	8,8,8	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	B	608	46	59,73,73	1.57	8 (13%)	67,113,113	2.16	19 (28%)
30	GOL	C	528	-	5,5,5	0.67	0	5,5,5	3.00	3 (60%)
28	SQD	A	612	-	53,54,54	1.12	4 (7%)	62,65,65	2.16	14 (22%)
33	PG4	C	536	-	12,12,12	0.69	0	11,11,11	0.65	0
34	PGE	B	648	-	9,9,9	0.86	0	8,8,8	0.73	0
34	PGE	b	645	-	9,9,9	0.54	0	8,8,8	0.41	0
26	BCR	h	103	-	41,41,41	1.14	4 (9%)	56,56,56	1.76	16 (28%)
35	P6G	c	541	-	18,18,18	0.51	0	17,17,17	0.42	0
33	PG4	V	211	-	12,12,12	1.02	0	11,11,11	0.81	0
30	GOL	B	629	-	5,5,5	0.91	0	5,5,5	0.38	0
24	CLA	d	403	46	59,73,73	1.67	9 (15%)	67,113,113	1.93	16 (23%)
23	BCT	A	605	21	0,3,3	0.00	-	0,3,3	0.00	-
36	EDO	i	108	-	3,3,3	0.43	0	2,2,2	0.42	0
24	CLA	c	508	-	54,68,73	1.63	10 (18%)	61,107,113	2.54	19 (31%)
33	PG4	b	637	-	12,12,12	0.78	0	11,11,11	0.56	0
30	GOL	b	626	-	5,5,5	0.79	0	5,5,5	0.77	0
23	BCT	m	104[A]	-	0,3,3	0.00	-	0,3,3	0.00	-
39	1PE	L	101	-	15,15,15	0.68	0	14,14,14	0.67	0
25	PHO	d	401	-	67,69,69	1.60	11 (16%)	85,99,99	1.87	17 (20%)
26	BCR	D	406	-	41,41,41	1.43	5 (12%)	56,56,56	1.96	12 (21%)
34	PGE	B	646	-	9,9,9	0.54	0	8,8,8	0.48	0
30	GOL	B	633	-	5,5,5	1.24	1 (20%)	5,5,5	1.25	0
30	GOL	D	413	-	5,5,5	0.56	0	5,5,5	0.84	0
34	PGE	E	108	-	9,9,9	0.56	0	8,8,8	0.40	0
24	CLA	b	604	-	59,73,73	1.62	10 (16%)	67,113,113	2.25	20 (29%)
24	CLA	b	612	-	59,73,73	1.45	11 (18%)	67,113,113	2.32	19 (28%)
33	PG4	C	537	-	12,12,12	0.66	0	11,11,11	0.57	0
34	PGE	b	647	-	9,9,9	0.59	0	8,8,8	0.42	0
24	CLA	B	612	-	59,73,73	1.56	10 (16%)	67,113,113	2.44	17 (25%)
33	PG4	H	104	-	12,12,12	0.62	0	11,11,11	0.34	0
24	CLA	c	503	-	59,73,73	1.55	10 (16%)	67,113,113	1.94	17 (25%)
30	GOL	O	307	-	5,5,5	0.50	0	5,5,5	0.21	0
30	GOL	F	101	42	5,5,5	0.52	0	5,5,5	0.73	0
32	LHG	d	409	-	48,48,48	0.85	3 (6%)	51,54,54	1.37	6 (11%)
33	PG4	h	106	-	12,12,12	0.57	0	11,11,11	0.48	0
33	PG4	d	414	-	12,12,12	0.72	0	11,11,11	0.45	0
35	P6G	C	541	-	18,18,18	0.66	0	17,17,17	0.43	0
33	PG4	A	619	-	12,12,12	0.71	0	11,11,11	0.61	0
34	PGE	h	110	-	9,9,9	0.79	0	8,8,8	0.68	0
30	GOL	o	304	-	5,5,5	0.50	0	5,5,5	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	b	606	-	59,73,73	1.81	9 (15%)	67,113,113	2.47	24 (35%)
30	GOL	V	205	-	5,5,5	0.92	0	5,5,5	1.09	0
34	PGE	H	110	-	9,9,9	0.56	0	8,8,8	0.34	0
24	CLA	A	609	-	59,73,73	1.52	9 (15%)	67,113,113	2.40	20 (29%)
30	GOL	O	305	-	5,5,5	0.45	0	5,5,5	0.34	0
24	CLA	A	607	46	54,68,73	1.54	10 (18%)	61,107,113	2.27	16 (26%)
33	PG4	H	107	-	12,12,12	0.70	0	11,11,11	0.50	0
38	HTG	b	624	-	19,19,19	1.51	2 (10%)	23,24,24	1.32	2 (8%)
39	1PE	B	653	-	15,15,15	0.61	0	14,14,14	0.41	0
24	CLA	a	407	-	59,73,73	1.52	7 (11%)	67,113,113	2.12	19 (28%)
24	CLA	c	504	46	54,68,73	1.85	13 (24%)	61,107,113	2.29	18 (29%)
36	EDO	B	657	-	3,3,3	0.65	0	2,2,2	0.06	0
33	PG4	c	534	-	12,12,12	0.54	0	11,11,11	0.43	0
34	PGE	C	539	-	9,9,9	0.92	0	8,8,8	0.86	0
33	PG4	X	103	-	12,12,12	0.76	0	11,11,11	0.54	0
36	EDO	d	417	-	3,3,3	0.70	0	2,2,2	0.40	0
33	PG4	i	102	-	12,12,12	0.57	0	11,11,11	0.52	0
26	BCR	c	514	-	41,41,41	1.21	5 (12%)	56,56,56	1.70	14 (25%)
36	EDO	B	658	-	3,3,3	0.46	0	2,2,2	0.44	0
34	PGE	b	646	-	9,9,9	0.66	0	8,8,8	0.51	0
34	PGE	E	107	-	9,9,9	0.77	0	8,8,8	0.76	0
33	PG4	E	102	-	12,12,12	0.61	0	11,11,11	0.58	0
29	LMG	z	101	-	55,55,55	1.03	2 (3%)	63,63,63	1.18	5 (7%)
26	BCR	K	101	-	41,41,41	0.97	1 (2%)	56,56,56	1.49	11 (19%)
33	PG4	i	103	-	12,12,12	0.64	0	11,11,11	0.48	0
36	EDO	I	107	-	3,3,3	0.75	0	2,2,2	0.20	0
33	PG4	j	104	-	12,12,12	0.70	0	11,11,11	0.72	0
38	HTG	h	101	-	19,19,19	1.17	2 (10%)	23,24,24	1.75	5 (21%)
24	CLA	B	609	-	59,73,73	1.47	8 (13%)	67,113,113	2.12	15 (22%)
24	CLA	C	511	3	59,73,73	1.67	8 (13%)	67,113,113	2.01	18 (26%)
36	EDO	D	419	-	3,3,3	0.71	0	2,2,2	0.08	0
31	LMT	A	617	-	36,36,36	1.10	2 (5%)	47,47,47	1.58	9 (19%)

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
29	LMG	C	526	-	-	27/50/70/70	0/1/1/1
38	HTG	b	632	-	-	2/10/30/30	0/1/1/1
34	PGE	t	105	-	-	1/4/4/7	-
38	HTG	C	522	-	-	4/10/30/30	0/1/1/1
34	PGE	T	104	-	-	1/4/4/7	-
31	LMT	m	102	-	-	3/21/61/61	0/2/2/2
30	GOL	D	402	-	-	2/4/4/4	-
31	LMT	m	101	-	-	5/21/61/61	0/2/2/2
24	CLA	d	404	-	3/3/20/25	2/37/135/135	-
24	CLA	B	603	-	3/3/20/25	5/37/135/135	-
34	PGE	c	539	-	-	1/7/7/7	-
34	PGE	E	106	-	-	3/7/7/7	-
34	PGE	h	108	-	-	4/7/7/7	-
33	PG4	l	103	-	-	3/10/10/10	-
33	PG4	V	212	-	-	5/10/10/10	-
30	GOL	D	412	-	-	4/4/4/4	-
29	LMG	A	613	-	-	20/46/66/70	0/1/1/1
32	LHG	e	101	-	-	26/46/46/53	-
34	PGE	O	310	-	-	5/7/7/7	-
38	HTG	C	531	-	-	7/10/30/30	0/1/1/1
39	1PE	e	105	-	-	7/13/13/13	-
34	PGE	a	423	-	-	2/7/7/7	-
34	PGE	V	215	-	-	4/7/7/7	-
38	HTG	a	418	-	-	7/10/30/30	0/1/1/1
40	DGD	H	103	-	-	10/51/91/95	0/2/2/2
33	PG4	I	103	-	-	5/10/10/10	-
34	PGE	B	645	-	-	5/7/7/7	-
36	EDO	B	655	-	-	0/1/1/1	-
34	PGE	b	641	-	-	3/7/7/7	-
40	DGD	D	408	-	-	30/55/95/95	0/2/2/2
38	HTG	C	532	-	-	2/10/30/30	0/1/1/1
31	LMT	B	622	-	-	6/21/61/61	0/2/2/2
28	SQD	A	622	-	-	25/49/69/69	0/1/1/1
24	CLA	c	507	46	3/3/20/25	2/37/135/135	-
36	EDO	e	106	-	-	1/1/1/1	-
34	PGE	o	306	-	-	3/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	P6G	D	418	-	-	7/16/16/16	-
24	CLA	b	605	-	3/3/20/25	7/37/135/135	-
26	BCR	C	514	-	-	0/29/63/63	0/2/2/2
30	GOL	c	529	-	-	2/4/4/4	-
39	1PE	V	217	-	-	5/13/13/13	-
24	CLA	b	611	46	3/3/20/25	5/37/135/135	-
29	LMG	c	519	-	-	19/46/66/70	0/1/1/1
24	CLA	c	512	-	3/3/20/25	8/37/135/135	-
29	LMG	b	621	-	-	13/46/66/70	0/1/1/1
24	CLA	c	511	3	3/3/20/25	2/37/135/135	-
33	PG4	B	643	-	-	5/10/10/10	-
31	LMT	c	521	-	-	8/21/61/61	0/2/2/2
30	GOL	u	201	-	-	0/4/4/4	-
26	BCR	C	515	-	-	2/29/63/63	0/2/2/2
32	LHG	a	419	-	-	22/45/45/53	-
35	P6G	j	106	-	-	8/16/16/16	-
27	PL9	A	611	-	-	9/53/73/73	0/1/1/1
38	HTG	c	522	-	-	4/10/30/30	0/1/1/1
24	CLA	C	506	-	3/3/20/25	11/37/135/135	-
33	PG4	c	535	-	-	4/10/10/10	-
33	PG4	X	101	-	-	3/10/10/10	-
33	PG4	B	637	-	-	4/10/10/10	-
30	GOL	c	528	-	-	4/4/4/4	-
38	HTG	C	529	-	-	5/10/30/30	0/1/1/1
24	CLA	c	502	-	3/3/20/25	3/37/135/135	-
34	PGE	b	644	-	-	3/7/7/7	-
24	CLA	a	408	46	3/3/19/25	5/31/129/135	-
32	LHG	D	411	-	-	8/53/53/53	-
38	HTG	C	521	-	-	4/10/30/30	0/1/1/1
33	PG4	e	103	-	-	4/10/10/10	-
33	PG4	B	642	-	-	5/10/10/10	-
38	HTG	O	303	-	-	1/10/30/30	0/1/1/1
33	PG4	i	101	-	-	7/10/10/10	-
38	HTG	B	624	-	-	4/10/30/30	0/1/1/1
34	PGE	Y	102	-	-	4/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	b	618	-	-	1/29/63/63	0/2/2/2
34	PGE	A	620	-	-	2/4/4/7	-
26	BCR	A	610	-	-	2/29/63/63	0/2/2/2
31	LMT	Y	101	-	-	11/21/61/61	0/2/2/2
35	P6G	B	651	-	-	7/16/16/16	-
36	EDO	B	656	-	-	1/1/1/1	-
33	PG4	c	532	-	-	6/10/10/10	-
24	CLA	b	602	46	3/3/20/25	15/37/135/135	-
30	GOL	a	415	-	-	0/4/4/4	-
25	PHO	A	608	-	-	2/53/103/103	0/5/6/6
24	CLA	b	614	-	3/3/20/25	0/37/135/135	-
34	PGE	b	638	-	-	3/7/7/7	-
32	LHG	E	101	-	-	16/46/46/53	-
24	CLA	D	404	-	3/3/20/25	4/37/135/135	-
35	P6G	b	649	-	-	10/16/16/16	-
24	CLA	b	617	-	3/3/19/25	6/31/129/135	-
39	1PE	x	104	-	-	9/13/13/13	-
24	CLA	a	410	-	3/3/20/25	9/37/135/135	-
24	CLA	c	510	-	3/3/20/25	5/37/135/135	-
30	GOL	B	626	-	-	0/4/4/4	-
34	PGE	o	308	-	-	5/7/7/7	-
35	P6G	T	105	-	-	12/16/16/16	-
24	CLA	c	509	-	3/3/20/25	7/37/135/135	-
31	LMT	I	101	-	-	7/21/61/61	0/2/2/2
33	PG4	B	636	-	-	4/10/10/10	-
34	PGE	c	538	-	-	2/7/7/7	-
24	CLA	B	616	-	2/2/20/25	6/37/135/135	-
26	BCR	C	525	-	-	2/29/63/63	0/2/2/2
34	PGE	D	415	-	-	6/7/7/7	-
34	PGE	f	105	-	-	2/7/7/7	-
31	LMT	F	102	-	-	6/21/61/61	0/2/2/2
34	PGE	i	106	-	-	4/7/7/7	-
35	P6G	d	416	-	-	8/16/16/16	-
30	GOL	B	625	-	-	2/4/4/4	-
32	LHG	A	618	-	-	23/46/46/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	f	101	-	-	3/21/61/61	0/2/2/2
30	GOL	v	206	-	-	2/4/4/4	-
33	PG4	X	102	-	-	4/10/10/10	-
33	PG4	B	638	-	-	6/10/10/10	-
38	HTG	B	623	-	-	3/10/30/30	0/1/1/1
29	LMG	B	621	-	-	12/46/66/70	0/1/1/1
25	PHO	a	409	-	-	2/53/103/103	0/5/6/6
34	PGE	j	105	-	-	4/7/7/7	-
30	GOL	t	101	-	-	0/4/4/4	-
33	PG4	K	102	-	-	4/10/10/10	-
38	HTG	c	531	-	-	8/10/30/30	0/1/1/1
35	P6G	E	110	-	-	11/16/16/16	-
30	GOL	C	524	-	-	0/4/4/4	-
34	PGE	o	307	-	-	5/7/7/7	-
24	CLA	b	607	-	3/3/18/25	3/25/123/135	-
26	BCR	a	411	-	-	0/29/63/63	0/2/2/2
36	EDO	A	625	-	-	0/1/1/1	-
40	DGD	C	518	-	-	10/51/91/95	0/2/2/2
24	CLA	B	611	46	3/3/20/25	4/37/135/135	-
34	PGE	h	109	-	-	4/7/7/7	-
30	GOL	B	627	-	-	2/4/4/4	-
33	PG4	b	635	-	-	5/10/10/10	-
36	EDO	E	112	-	-	0/1/1/1	-
24	CLA	c	513	-	3/3/20/25	1/37/135/135	-
30	GOL	f	104	-	-	4/4/4/4	-
34	PGE	i	105	-	-	4/7/7/7	-
24	CLA	D	403	46	3/3/20/25	5/37/135/135	-
30	GOL	v	204	-	-	1/4/4/4	-
28	SQD	a	413	-	-	19/49/69/69	0/1/1/1
29	LMG	j	101	42	-	9/42/62/70	0/1/1/1
24	CLA	C	501	-	3/3/20/25	4/37/135/135	-
25	PHO	D	401	-	-	2/53/103/103	0/5/6/6
36	EDO	H	112	-	-	1/1/1/1	-
30	GOL	B	635	-	-	0/4/4/4	-
32	LHG	B	632	-	-	12/53/53/53	-
24	CLA	c	506	-	3/3/20/25	6/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	GOL	v	207	-	-	2/4/4/4	-
36	EDO	J	109	-	-	0/1/1/1	-
34	PGE	J	108	-	-	4/7/7/7	-
28	SQD	a	424	-	-	22/49/69/69	0/1/1/1
30	GOL	V	206	-	-	0/4/4/4	-
24	CLA	B	617	-	3/3/19/25	8/31/129/135	-
26	BCR	t	102	-	-	2/29/63/63	0/2/2/2
36	EDO	E	111	-	-	1/1/1/1	-
29	LMG	a	414	-	-	25/46/66/70	0/1/1/1
34	PGE	H	109	-	-	5/7/7/7	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
30	GOL	o	303	-	-	2/4/4/4	-
28	SQD	b	633	-	-	17/49/69/69	0/1/1/1
33	PG4	x	102	-	-	3/10/10/10	-
30	GOL	B	628	-	-	0/4/4/4	-
39	1PE	j	107	-	-	5/13/13/13	-
34	PGE	B	647	-	-	2/7/7/7	-
30	GOL	c	525	-	-	2/4/4/4	-
26	BCR	B	620	-	-	1/29/63/63	0/2/2/2
28	SQD	A	616	-	-	18/49/69/69	0/1/1/1
24	CLA	b	608	46	3/3/20/25	2/37/135/135	-
33	PG4	E	103	-	-	4/10/10/10	-
32	LHG	l	101	-	-	13/53/53/53	-
30	GOL	b	628	-	-	0/4/4/4	-
35	P6G	I	106	-	-	10/16/16/16	-
34	PGE	E	109	-	-	4/7/7/7	-
31	LMT	C	533	-	-	12/21/61/61	0/2/2/2
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
32	LHG	D	409	-	-	7/53/53/53	-
34	PGE	O	309	-	-	5/7/7/7	-
34	PGE	t	104	-	-	2/7/7/7	-
26	BCR	d	406	-	-	2/29/63/63	0/2/2/2
24	CLA	B	606	-	3/3/20/25	4/37/135/135	-
38	HTG	b	631	-	-	2/10/30/30	0/1/1/1
27	PL9	d	407	-	-	2/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	D	405	-	3/3/20/25	7/37/135/135	-
33	PG4	J	105	-	-	6/10/10/10	-
30	GOL	f	103	42	-	1/4/4/4	-
24	CLA	B	610	-	3/3/20/25	1/37/135/135	-
36	EDO	o	311	-	-	1/1/1/1	-
24	CLA	B	614	-	3/3/20/25	2/37/135/135	-
33	PG4	i	104	-	-	5/10/10/10	-
30	GOL	T	101	-	-	0/4/4/4	-
33	PG4	B	640	-	-	5/10/10/10	-
30	GOL	T	103	-	-	3/4/4/4	-
36	EDO	O	311	-	-	1/1/1/1	-
31	LMT	M	101	-	-	2/21/61/61	0/2/2/2
38	HTG	b	623	-	-	2/10/30/30	0/1/1/1
30	GOL	m	103	-	-	0/4/4/4	-
31	LMT	t	103	-	-	7/21/61/61	0/2/2/2
24	CLA	C	502	-	3/3/20/25	5/37/135/135	-
24	CLA	B	602	46	3/3/20/25	12/37/135/135	-
26	BCR	k	101	-	-	0/29/63/63	0/2/2/2
40	DGD	c	517	-	-	15/46/86/95	0/2/2/2
41	HEM	E	113	6,5	-	1/6/54/54	-
31	LMT	J	103	-	-	10/21/61/61	0/2/2/2
35	P6G	d	415	-	-	8/16/16/16	-
26	BCR	c	515	-	-	0/29/63/63	0/2/2/2
32	LHG	D	410	-	-	9/53/53/53	-
28	SQD	l	102	-	-	18/49/69/69	0/1/1/1
30	GOL	v	205	-	-	2/4/4/4	-
36	EDO	o	310	-	-	0/1/1/1	-
28	SQD	a	417	-	-	15/49/69/69	0/1/1/1
33	PG4	I	104	-	-	4/10/10/10	-
35	P6G	B	652	-	-	7/16/16/16	-
34	PGE	h	107	-	-	4/7/7/7	-
38	HTG	V	204	-	-	2/10/30/30	0/1/1/1
35	P6G	A	624	-	-	9/16/16/16	-
32	LHG	d	410	-	-	9/53/53/53	-
24	CLA	C	505	-	3/3/20/25	3/37/135/135	-
30	GOL	O	302	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	SQD	h	105	-	-	26/49/69/69	0/1/1/1
24	CLA	B	607	-	3/3/18/25	4/25/123/135	-
29	LMG	B	634	-	-	18/50/70/70	0/1/1/1
24	CLA	C	508	-	3/3/19/25	4/31/129/135	-
24	CLA	b	615	-	3/3/20/25	11/37/135/135	-
33	PG4	U	202	-	-	3/10/10/10	-
24	CLA	C	512	-	3/3/20/25	4/37/135/135	-
36	EDO	V	218	-	-	1/1/1/1	-
24	CLA	b	603	-	3/3/20/25	4/37/135/135	-
30	GOL	O	304	-	-	0/4/4/4	-
31	LMT	j	103	-	-	9/21/61/61	0/2/2/2
33	PG4	H	106	-	-	4/10/10/10	-
30	GOL	b	630	-	-	0/4/4/4	-
33	PG4	e	104	-	-	4/10/10/10	-
30	GOL	A	615	-	-	2/4/4/4	-
34	PGE	E	104	-	-	1/7/7/7	-
30	GOL	d	413	-	-	4/4/4/4	-
33	PG4	b	636	-	-	6/10/10/10	-
24	CLA	b	609	-	3/3/20/25	1/37/135/135	-
33	PG4	V	213	-	-	4/10/10/10	-
39	1PE	B	654	-	-	5/13/13/13	-
30	GOL	v	203	-	-	0/4/4/4	-
34	PGE	V	214	-	-	4/7/7/7	-
43	HEC	v	202	16	-	0/6/54/54	-
28	SQD	F	104	-	-	18/49/69/69	0/1/1/1
43	HEC	V	203	16	-	0/6/54/54	-
26	BCR	b	619	-	-	0/29/63/63	0/2/2/2
33	PG4	J	104	-	-	2/10/10/10	-
24	CLA	B	604	-	3/3/20/25	4/37/135/135	-
34	PGE	c	536	-	-	3/7/7/7	-
34	PGE	A	621	-	-	3/7/7/7	-
40	DGD	C	516	-	-	17/51/91/95	0/2/2/2
34	PGE	B	650	-	-	2/7/7/7	-
33	PG4	C	538	-	-	2/10/10/10	-
35	P6G	D	416	-	-	9/16/16/16	-
35	P6G	b	648	-	-	7/16/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	EDO	c	542	-	-	1/1/1/1	-
24	CLA	B	613	-	3/3/20/25	2/37/135/135	-
30	GOL	d	402	-	-	2/4/4/4	-
24	CLA	C	507	46	2/2/20/25	7/37/135/135	-
40	DGD	c	516	-	-	17/51/91/95	0/2/2/2
31	LMT	u	203	-	-	12/21/61/61	0/2/2/2
30	GOL	a	416	-	-	2/4/4/4	-
24	CLA	A	606	-	3/3/20/25	5/37/135/135	-
33	PG4	C	535	-	-	3/10/10/10	-
33	PG4	I	102	-	-	6/10/10/10	-
33	PG4	C	534	-	-	5/10/10/10	-
28	SQD	x	101	-	-	23/49/69/69	0/1/1/1
34	PGE	b	639	-	-	3/7/7/7	-
26	BCR	c	527	-	-	1/29/63/63	0/2/2/2
33	PG4	V	209	-	-	5/10/10/10	-
24	CLA	c	505	-	3/3/20/25	2/37/135/135	-
34	PGE	H	111	-	-	3/7/7/7	-
30	GOL	C	527	-	-	2/4/4/4	-
34	PGE	b	640	-	-	3/7/7/7	-
30	GOL	V	208	-	-	4/4/4/4	-
30	GOL	o	305	-	-	2/4/4/4	-
40	DGD	C	517	-	-	14/45/85/95	0/2/2/2
24	CLA	C	510	-	3/3/20/25	3/37/135/135	-
34	PGE	B	649	-	-	3/7/7/7	-
44	2PE	V	216	-	-	14/25/25/25	-
30	GOL	O	306	-	-	0/4/4/4	-
33	PG4	a	421	-	-	4/10/10/10	-
38	HTG	H	101	-	-	3/10/30/30	0/1/1/1
29	LMG	C	519	-	-	15/46/66/70	0/1/1/1
38	HTG	C	530	-	-	3/10/30/30	0/1/1/1
34	PGE	x	103	-	-	2/7/7/7	-
34	PGE	c	540	-	-	4/7/7/7	-
33	PG4	H	105	-	-	4/10/10/10	-
24	CLA	C	503	-	3/3/20/25	4/37/135/135	-
26	BCR	b	620	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	PGE	I	105	-	-	2/7/7/7	-
24	CLA	b	613	-	3/3/20/25	3/37/135/135	-
30	GOL	A	614	-	-	0/4/4/4	-
34	PGE	B	644	-	-	3/7/7/7	-
34	PGE	E	105	-	-	4/7/7/7	-
38	HTG	c	530	-	-	3/10/30/30	0/1/1/1
30	GOL	b	629	-	-	2/4/4/4	-
33	PG4	D	414	-	-	5/10/10/10	-
33	PG4	a	420	-	-	3/10/10/10	-
30	GOL	b	625	-	-	3/4/4/4	-
33	PG4	B	641	-	-	4/10/10/10	-
30	GOL	C	523	-	-	1/4/4/4	-
30	GOL	U	201	-	-	1/4/4/4	-
24	CLA	B	615	-	3/3/18/25	4/25/123/135	-
40	DGD	c	518	-	-	14/51/91/95	0/2/2/2
30	GOL	e	102	-	-	0/4/4/4	-
29	LMG	C	520	-	-	17/46/66/70	0/1/1/1
27	PL9	D	407	-	-	1/53/73/73	0/1/1/1
24	CLA	C	513	-	3/3/20/25	8/37/135/135	-
34	PGE	o	309	-	-	5/7/7/7	-
36	EDO	X	104	-	-	0/1/1/1	-
27	PL9	a	412	-	-	10/53/73/73	0/1/1/1
29	LMG	d	412	-	-	25/50/70/70	0/1/1/1
34	PGE	a	422	-	-	5/7/7/7	-
40	DGD	h	104	-	-	10/51/91/95	0/2/2/2
30	GOL	V	201	-	-	0/4/4/4	-
38	HTG	B	631	-	-	3/10/30/30	0/1/1/1
33	PG4	c	533	-	-	5/10/10/10	-
34	PGE	b	642	-	-	3/7/7/7	-
40	DGD	d	408	-	-	31/55/95/95	0/2/2/2
29	LMG	J	101	42	-	6/42/62/70	0/1/1/1
24	CLA	c	501	-	3/3/20/25	4/37/135/135	-
34	PGE	O	308	-	-	5/7/7/7	-
31	LMT	M	102	-	-	7/21/61/61	0/2/2/2
24	CLA	d	405	-	3/3/20/25	6/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	610	-	3/3/20/25	2/37/135/135	-
24	CLA	b	616	-	2/2/20/25	4/37/135/135	-
34	PGE	b	643	-	-	3/7/7/7	-
35	P6G	D	417	-	-	8/16/16/16	-
31	LMT	a	401	-	-	9/21/61/61	0/2/2/2
31	LMT	b	622	-	-	9/21/61/61	0/2/2/2
34	PGE	c	537	-	-	4/7/7/7	-
34	PGE	H	108	-	-	5/7/7/7	-
38	HTG	o	301	-	-	0/10/30/30	0/1/1/1
24	CLA	B	605	-	3/3/20/25	5/37/135/135	-
33	PG4	b	634	-	-	3/10/10/10	-
30	GOL	u	202	-	-	0/4/4/4	-
30	GOL	c	526	-	-	0/4/4/4	-
30	GOL	V	207	-	-	0/4/4/4	-
38	HTG	c	523	-	-	3/10/30/30	0/1/1/1
41	HEM	e	107	6,5	-	1/6/54/54	-
26	BCR	H	102	-	-	0/29/63/63	0/2/2/2
36	EDO	C	542	-	-	1/1/1/1	-
34	PGE	J	106	-	-	3/7/7/7	-
35	P6G	A	623	-	-	9/16/16/16	-
33	PG4	B	639	-	-	4/10/10/10	-
30	GOL	y	101	-	-	2/4/4/4	-
24	CLA	C	509	-	3/3/20/25	7/37/135/135	-
38	HTG	B	630	-	-	4/10/30/30	0/1/1/1
33	PG4	V	210	-	-	7/10/10/10	-
36	EDO	a	425	-	-	1/1/1/1	-
30	GOL	b	627	-	-	0/4/4/4	-
29	LMG	c	520	-	-	17/46/66/70	0/1/1/1
45	PE8	i	107	-	-	14/22/22/22	-
32	LHG	d	411	-	-	10/53/53/53	-
24	CLA	C	504	46	3/3/19/25	4/31/129/135	-
34	PGE	C	540	-	-	4/7/7/7	-
26	BCR	T	102	-	-	2/29/63/63	0/2/2/2
34	PGE	J	107	-	-	3/7/7/7	-
24	CLA	B	608	46	3/3/20/25	1/37/135/135	-
30	GOL	C	528	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	SQD	A	612	-	-	11/49/69/69	0/1/1/1
33	PG4	C	536	-	-	5/10/10/10	-
34	PGE	B	648	-	-	3/7/7/7	-
34	PGE	b	645	-	-	4/7/7/7	-
26	BCR	h	103	-	-	0/29/63/63	0/2/2/2
35	P6G	c	541	-	-	4/16/16/16	-
33	PG4	V	211	-	-	3/10/10/10	-
30	GOL	B	629	-	-	0/4/4/4	-
24	CLA	d	403	46	3/3/20/25	5/37/135/135	-
36	EDO	i	108	-	-	0/1/1/1	-
24	CLA	c	508	-	3/3/19/25	2/31/129/135	-
33	PG4	b	637	-	-	5/10/10/10	-
30	GOL	b	626	-	-	0/4/4/4	-
39	1PE	L	101	-	-	5/13/13/13	-
25	PHO	d	401	-	-	3/53/103/103	0/5/6/6
26	BCR	D	406	-	-	0/29/63/63	0/2/2/2
34	PGE	B	646	-	-	4/7/7/7	-
30	GOL	B	633	-	-	4/4/4/4	-
30	GOL	D	413	-	-	2/4/4/4	-
34	PGE	E	108	-	-	2/7/7/7	-
24	CLA	b	604	-	3/3/20/25	4/37/135/135	-
24	CLA	b	612	-	3/3/20/25	3/37/135/135	-
33	PG4	C	537	-	-	6/10/10/10	-
34	PGE	b	647	-	-	3/7/7/7	-
24	CLA	B	612	-	3/3/20/25	3/37/135/135	-
33	PG4	H	104	-	-	3/10/10/10	-
24	CLA	c	503	-	3/3/20/25	2/37/135/135	-
30	GOL	O	307	-	-	2/4/4/4	-
30	GOL	F	101	42	-	2/4/4/4	-
32	LHG	d	409	-	-	7/53/53/53	-
33	PG4	h	106	-	-	3/10/10/10	-
33	PG4	d	414	-	-	3/10/10/10	-
35	P6G	C	541	-	-	8/16/16/16	-
33	PG4	A	619	-	-	3/10/10/10	-
34	PGE	h	110	-	-	3/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	GOL	o	304	-	-	4/4/4/4	-
24	CLA	b	606	-	3/3/20/25	3/37/135/135	-
30	GOL	V	205	-	-	0/4/4/4	-
34	PGE	H	110	-	-	4/7/7/7	-
24	CLA	A	609	-	3/3/20/25	11/37/135/135	-
30	GOL	O	305	-	-	2/4/4/4	-
24	CLA	A	607	46	3/3/19/25	3/31/129/135	-
33	PG4	H	107	-	-	4/10/10/10	-
38	HTG	b	624	-	-	5/10/30/30	0/1/1/1
39	1PE	B	653	-	-	4/13/13/13	-
24	CLA	a	407	-	3/3/20/25	2/37/135/135	-
24	CLA	c	504	46	3/3/19/25	4/31/129/135	-
36	EDO	B	657	-	-	0/1/1/1	-
33	PG4	c	534	-	-	6/10/10/10	-
34	PGE	C	539	-	-	3/7/7/7	-
33	PG4	X	103	-	-	4/10/10/10	-
36	EDO	d	417	-	-	1/1/1/1	-
33	PG4	i	102	-	-	4/10/10/10	-
26	BCR	c	514	-	-	0/29/63/63	0/2/2/2
36	EDO	B	658	-	-	1/1/1/1	-
34	PGE	b	646	-	-	4/7/7/7	-
34	PGE	E	107	-	-	4/7/7/7	-
33	PG4	E	102	-	-	8/10/10/10	-
29	LMG	z	101	-	-	31/50/70/70	0/1/1/1
26	BCR	K	101	-	-	2/29/63/63	0/2/2/2
33	PG4	i	103	-	-	6/10/10/10	-
36	EDO	I	107	-	-	0/1/1/1	-
33	PG4	j	104	-	-	8/10/10/10	-
38	HTG	h	101	-	-	5/10/30/30	0/1/1/1
24	CLA	B	609	-	3/3/20/25	1/37/135/135	-
24	CLA	C	511	3	3/3/20/25	0/37/135/135	-
36	EDO	D	419	-	-	0/1/1/1	-
31	LMT	A	617	-	-	8/21/61/61	0/2/2/2

The worst 5 of 1097 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	403	CLA	OBD-CAD	8.12	1.33	1.22
38	o	301	HTG	C1'-S1	-7.89	1.71	1.81
27	a	412	PL9	C7-C3	7.55	1.59	1.51
24	b	614	CLA	OBD-CAD	7.07	1.32	1.22
24	C	505	CLA	OBD-CAD	6.86	1.31	1.22

The worst 5 of 2264 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	E	113	HEM	CAD-CBD-CGD	11.43	131.84	112.67
24	c	508	CLA	C4D-C3D-CAD	-11.16	102.24	108.47
24	c	502	CLA	C4D-C3D-CAD	-10.91	102.38	108.47
24	C	508	CLA	C4D-C3D-CAD	-10.27	102.74	108.47
24	A	609	CLA	C4D-C3D-CAD	-9.59	103.12	108.47

5 of 207 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	606	CLA	NA
24	A	606	CLA	ND
24	A	606	CLA	NC
24	A	607	CLA	NA
24	A	607	CLA	ND

5 of 2168 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	605	CLA	C1-C2-C3-C4
24	B	605	CLA	C2-C3-C5-C6
24	B	606	CLA	C1-C2-C3-C4
24	B	607	CLA	CHA-CBD-CGD-O1D
24	B	615	CLA	CHA-CBD-CGD-O1D

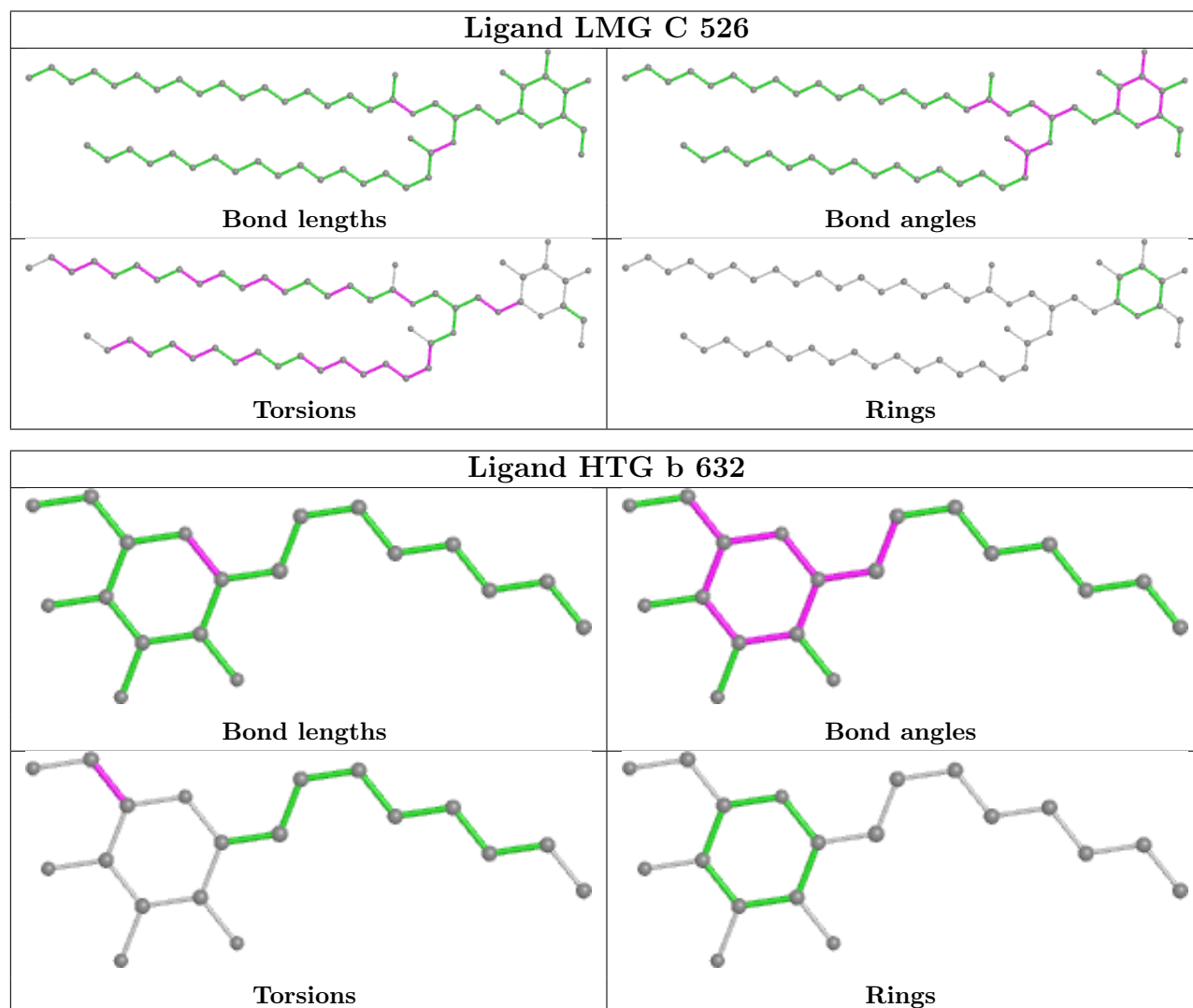
There are no ring outliers.

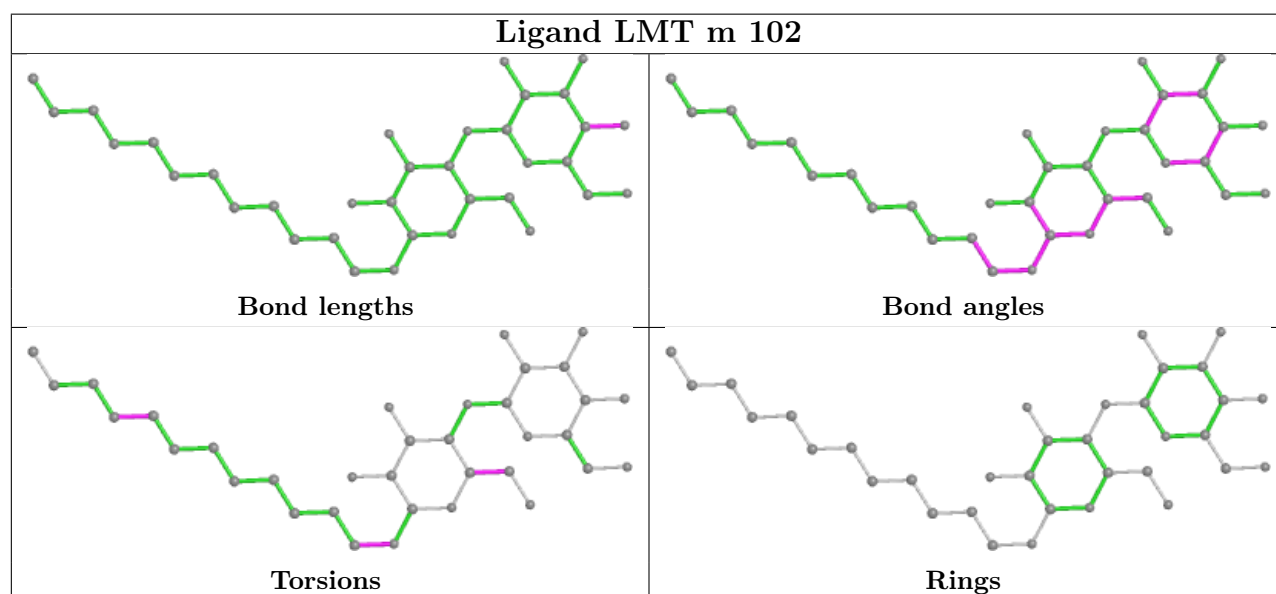
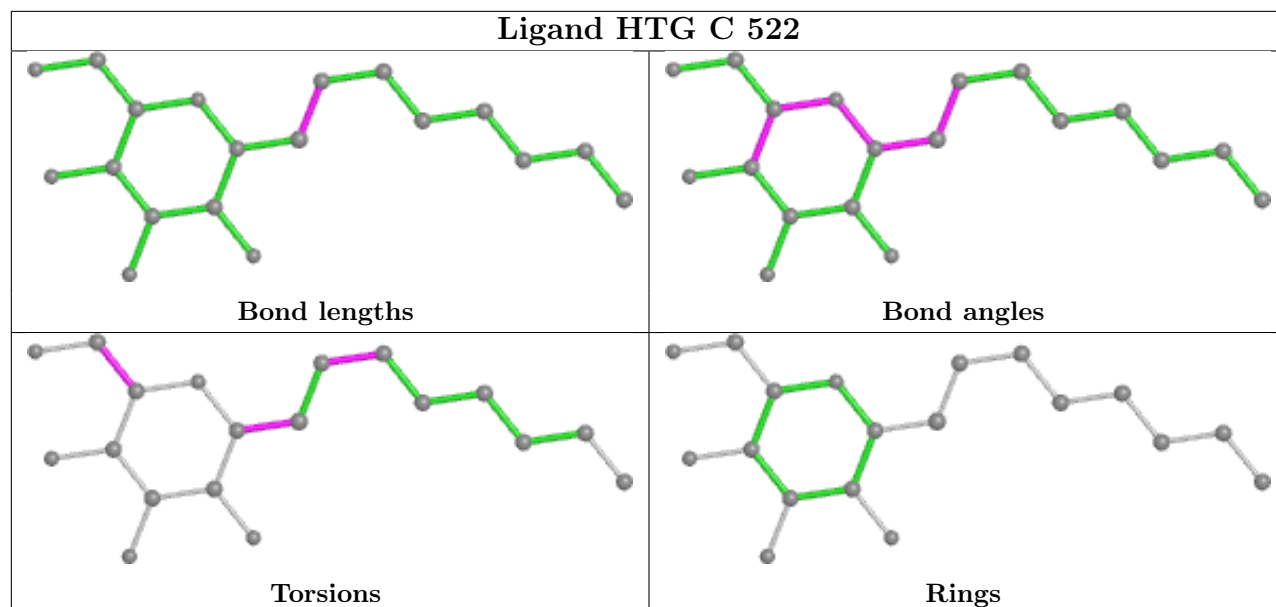
1 monomer is involved in 1 short contact:

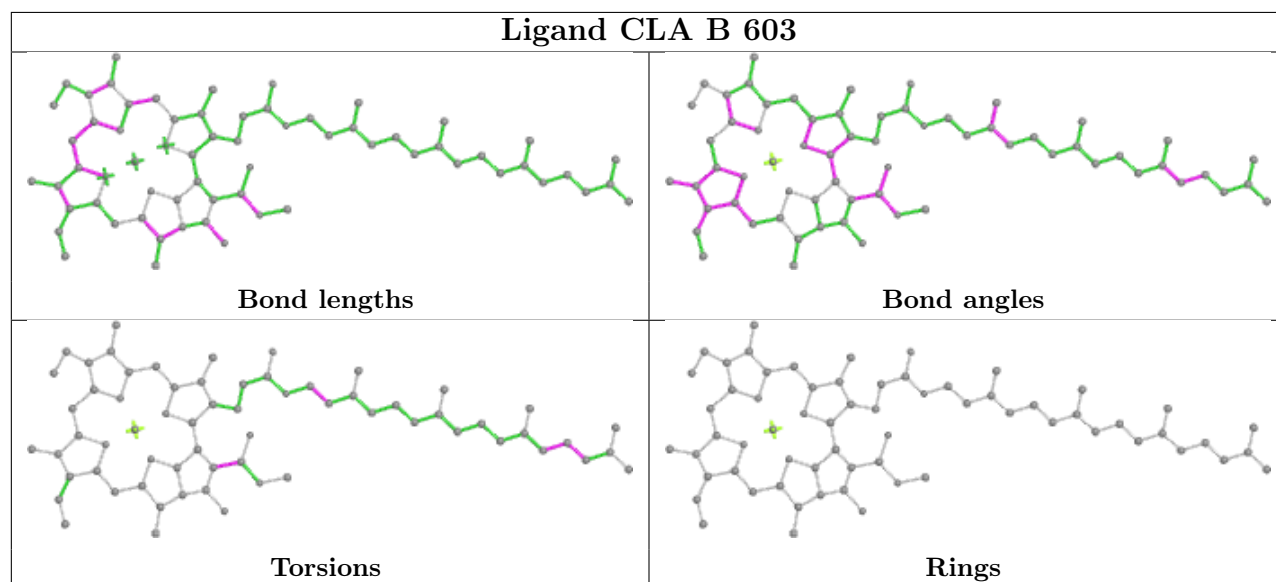
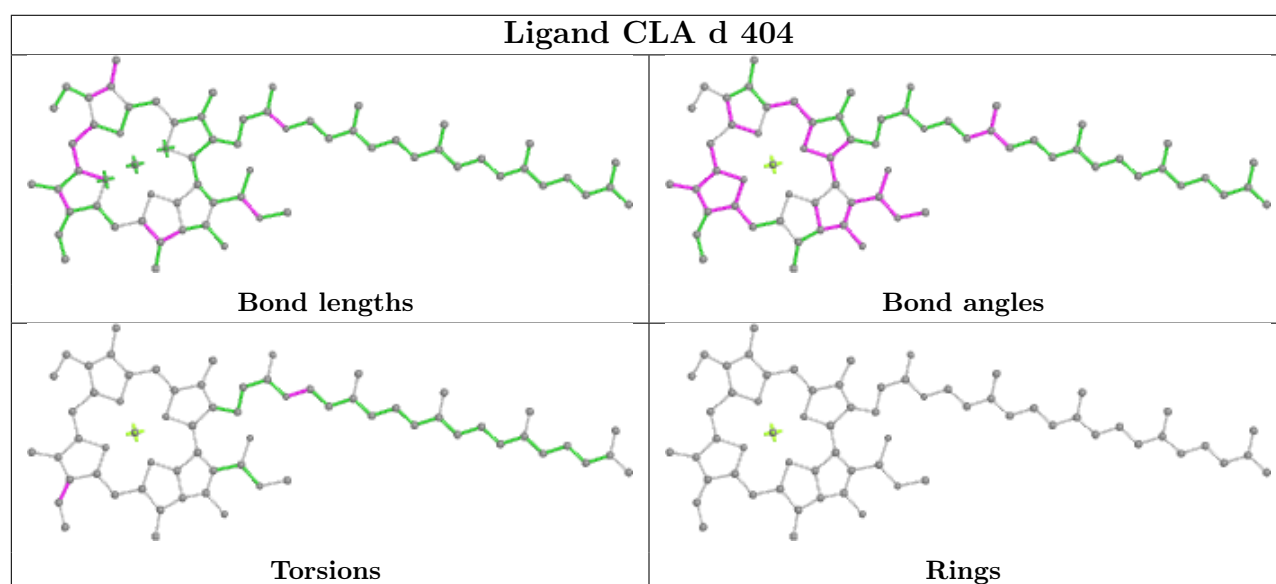
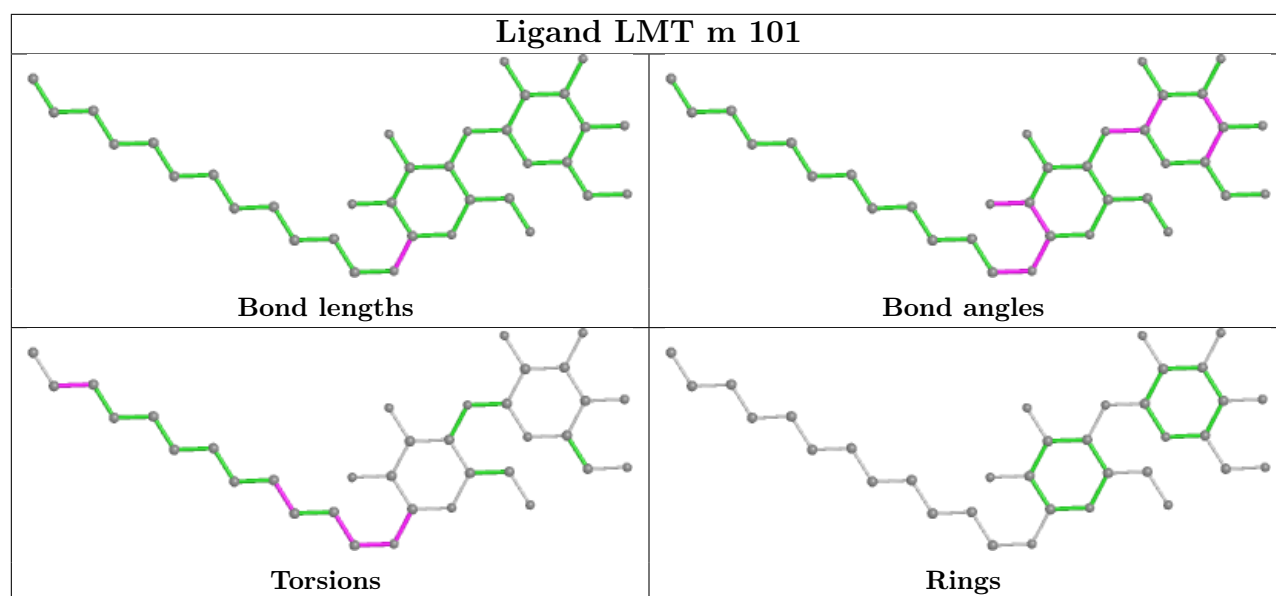
Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	d	408	DGD	0	1

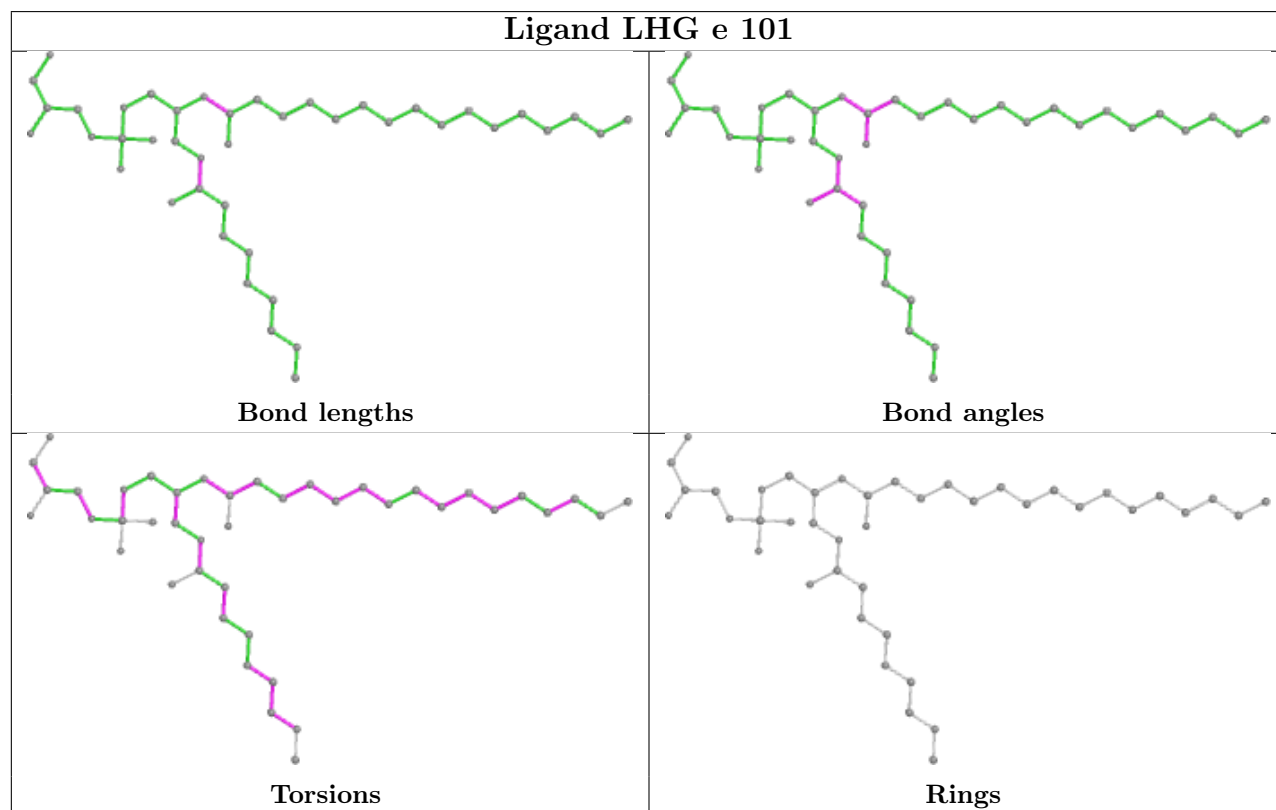
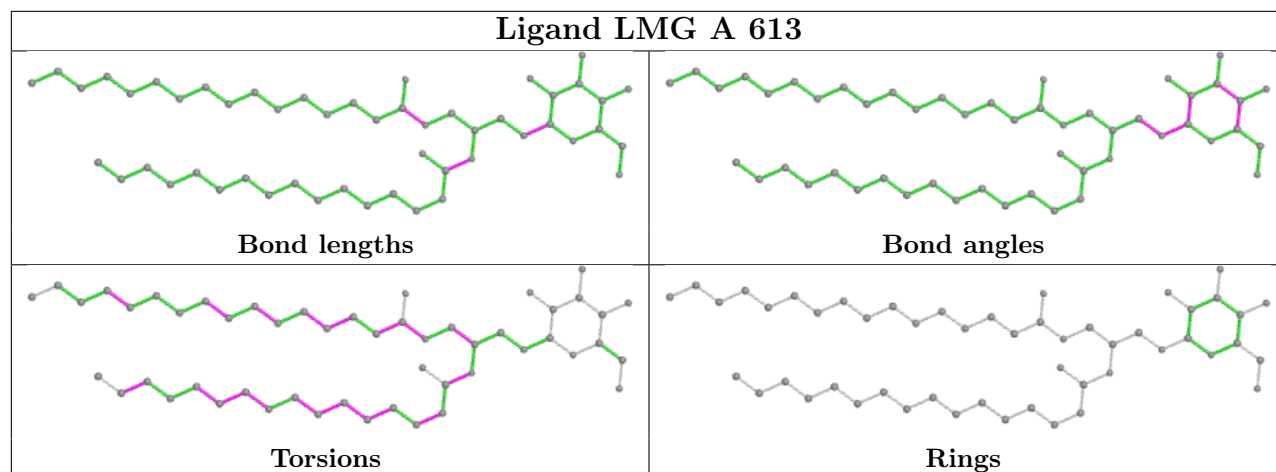
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

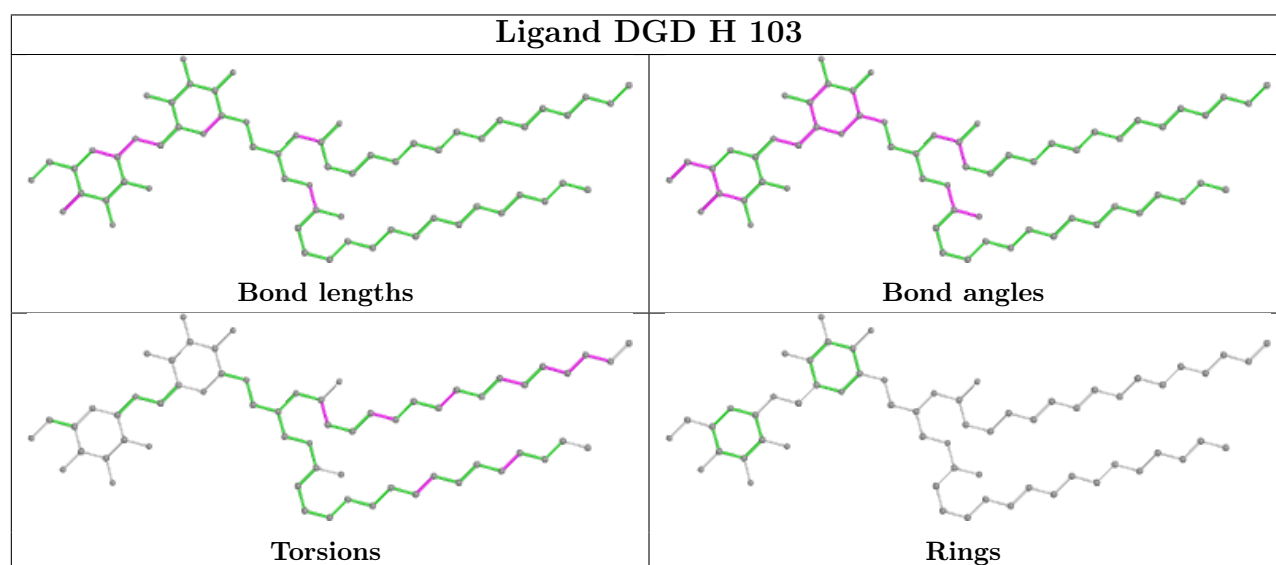
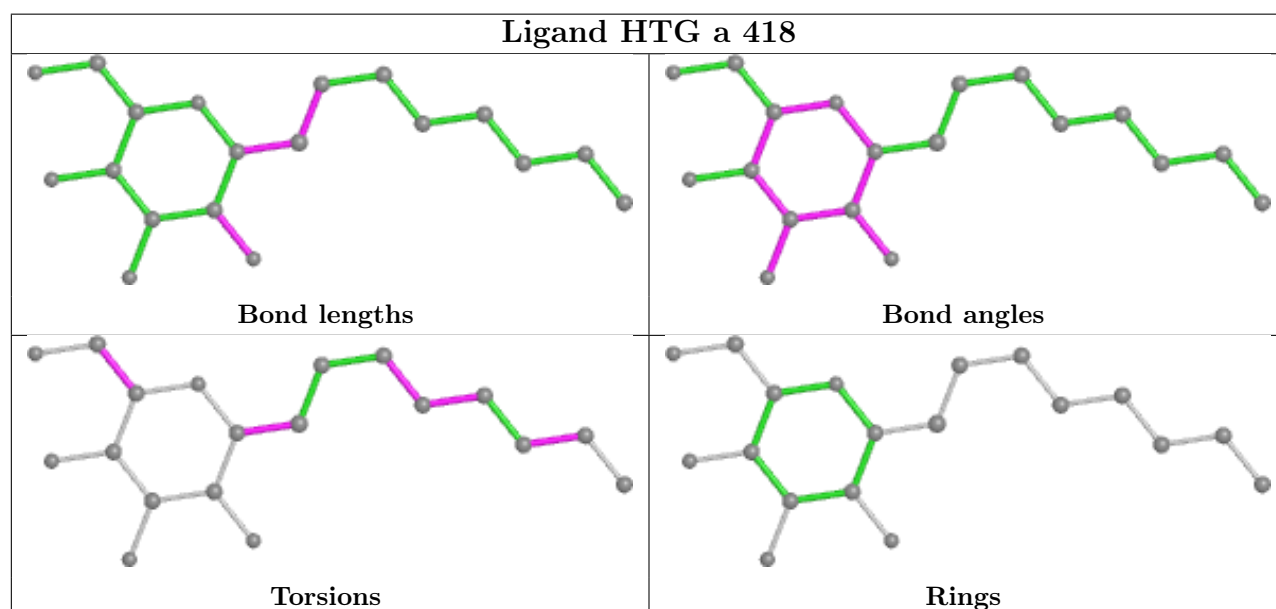
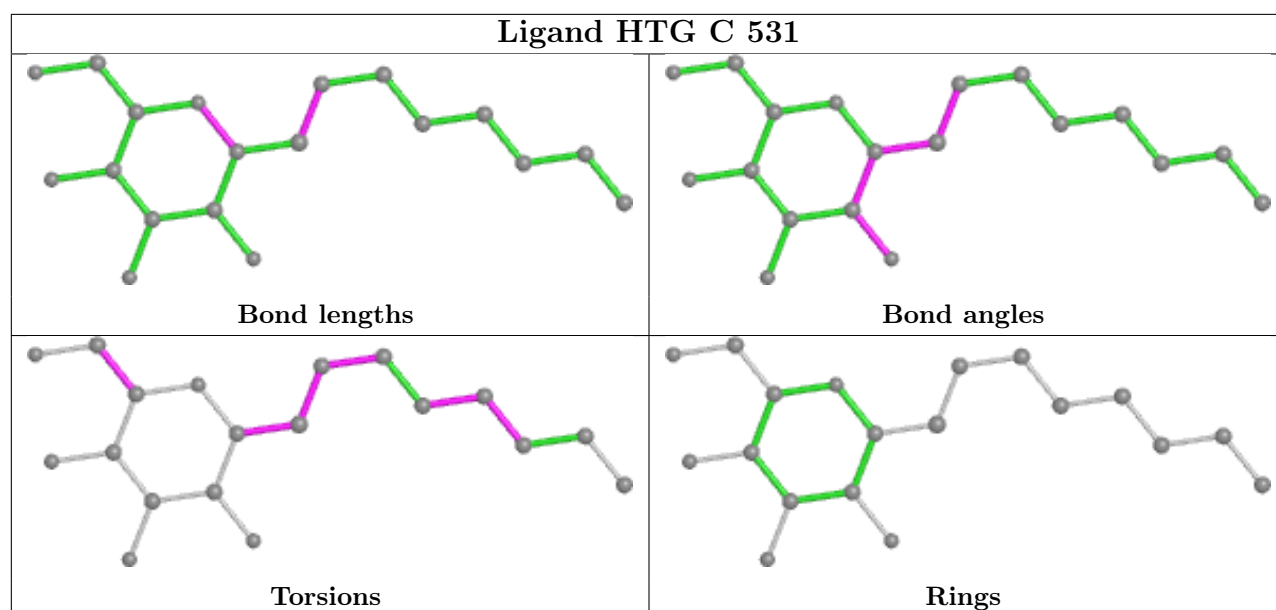
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

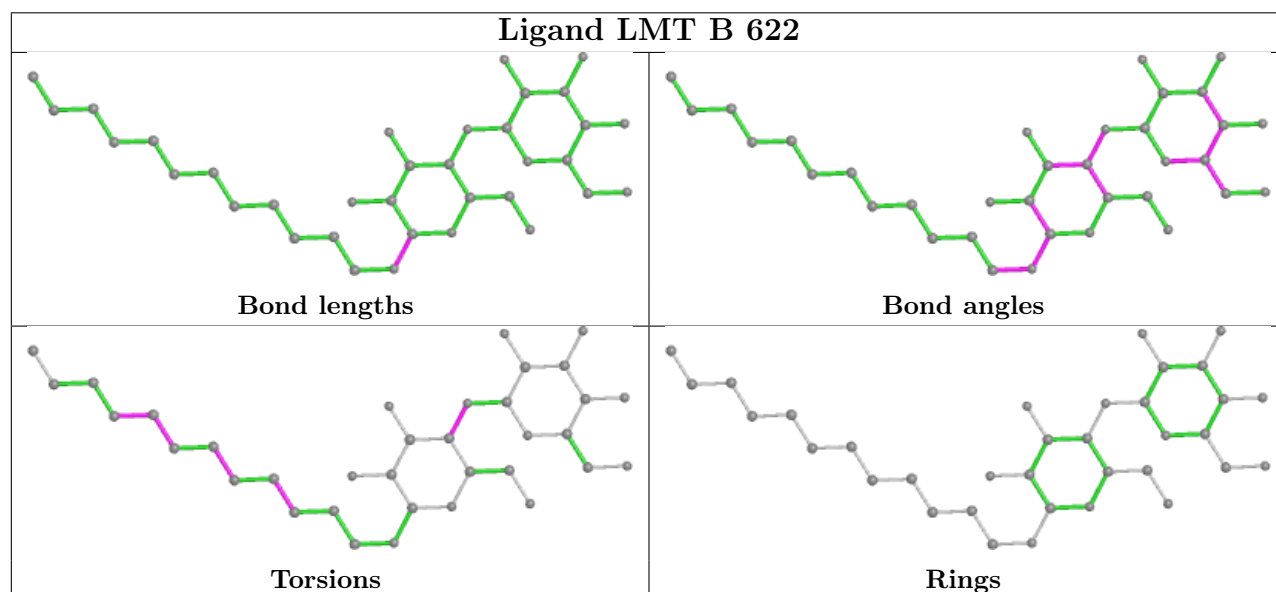
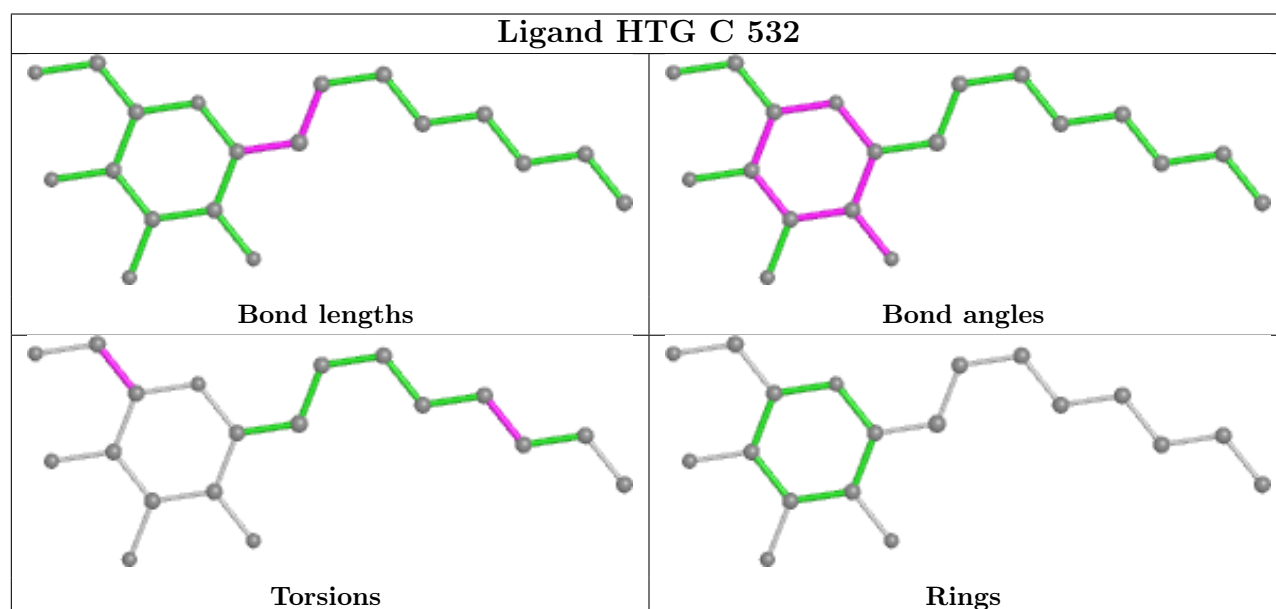
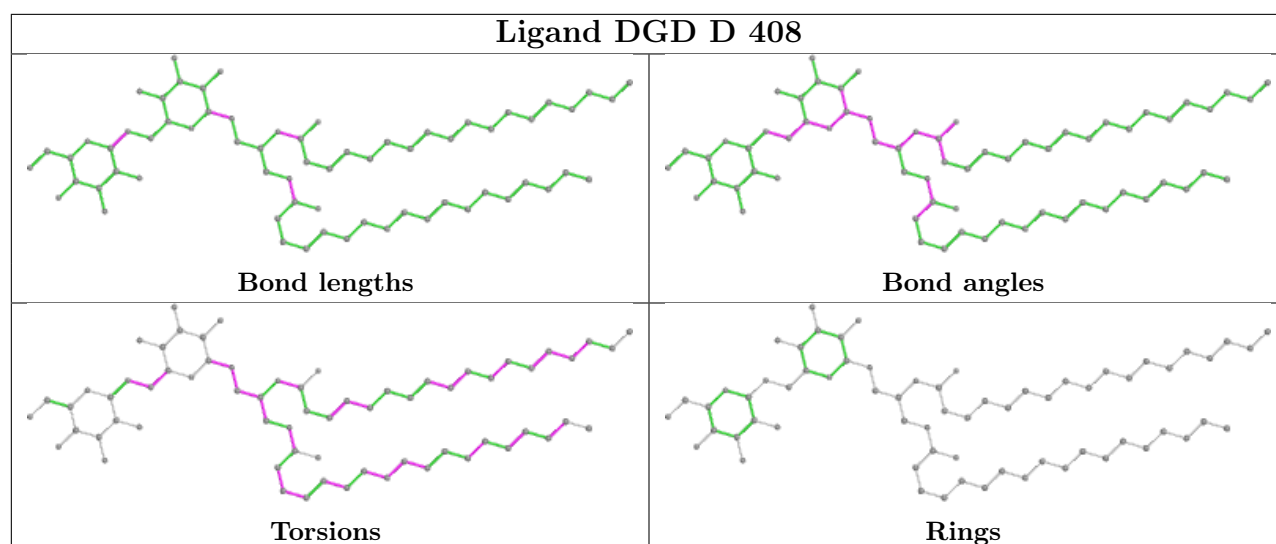


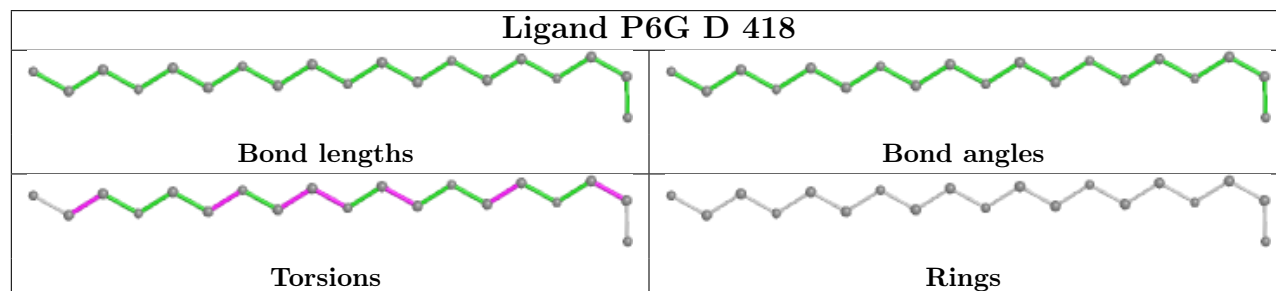
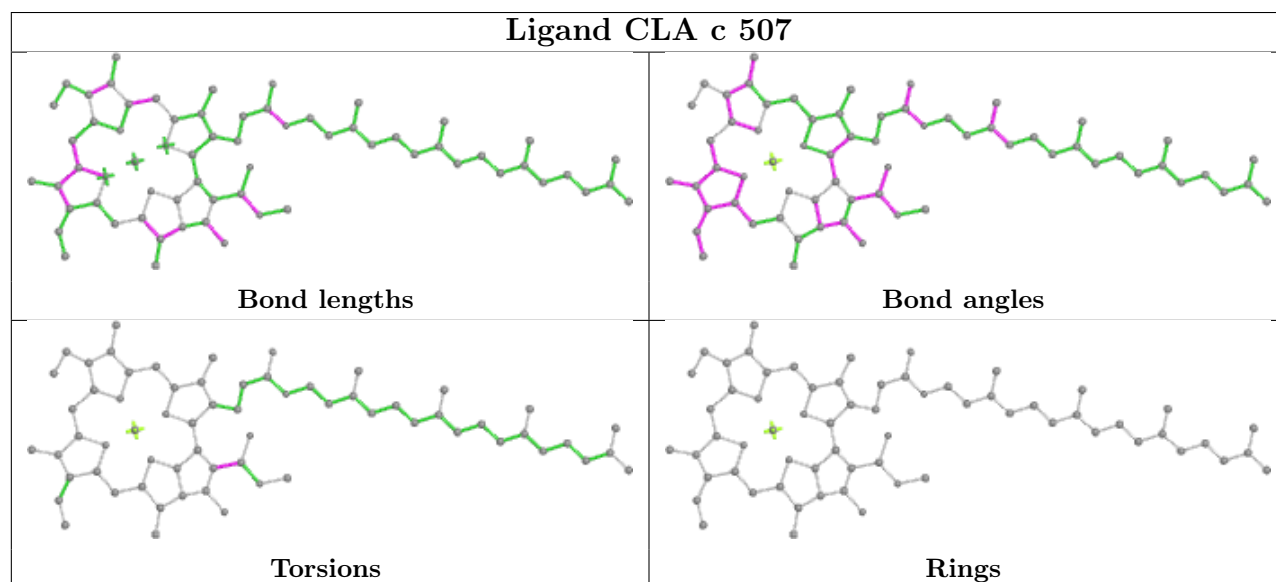
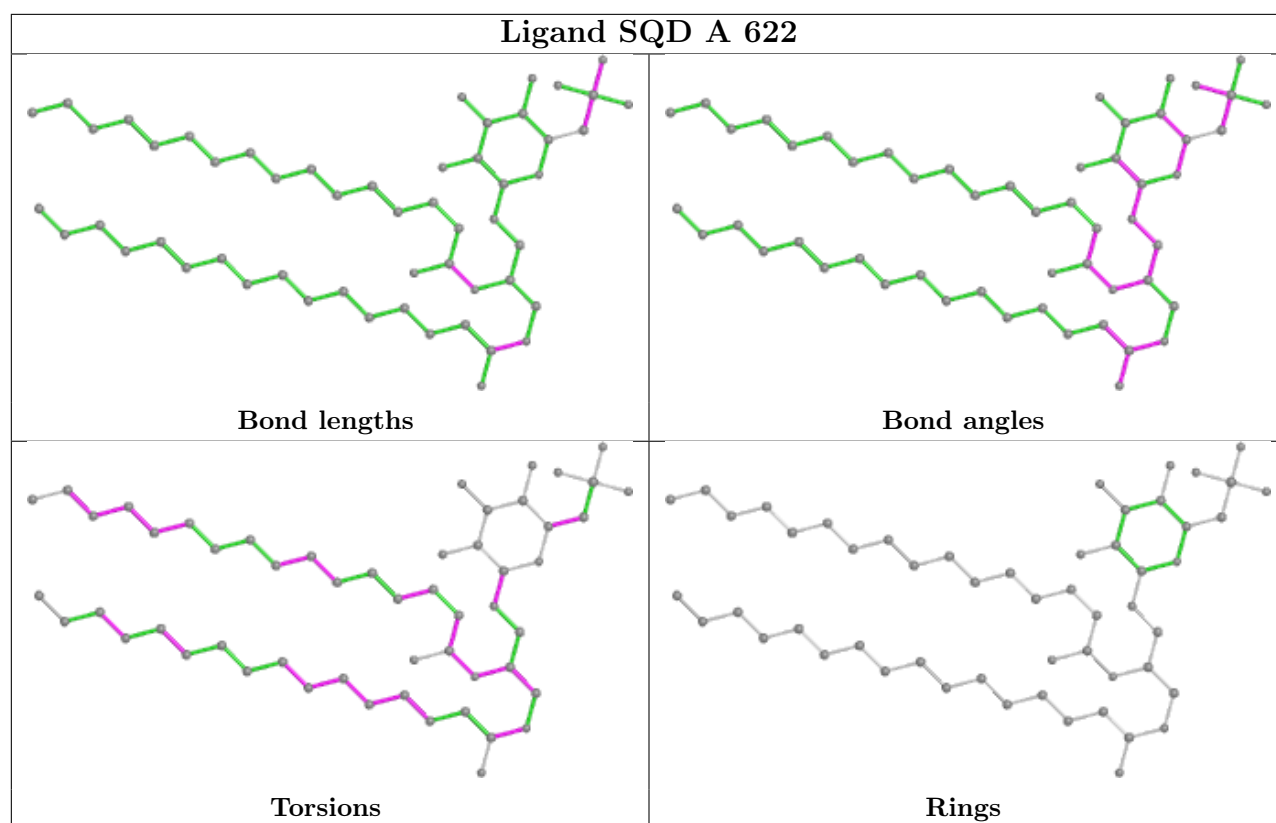


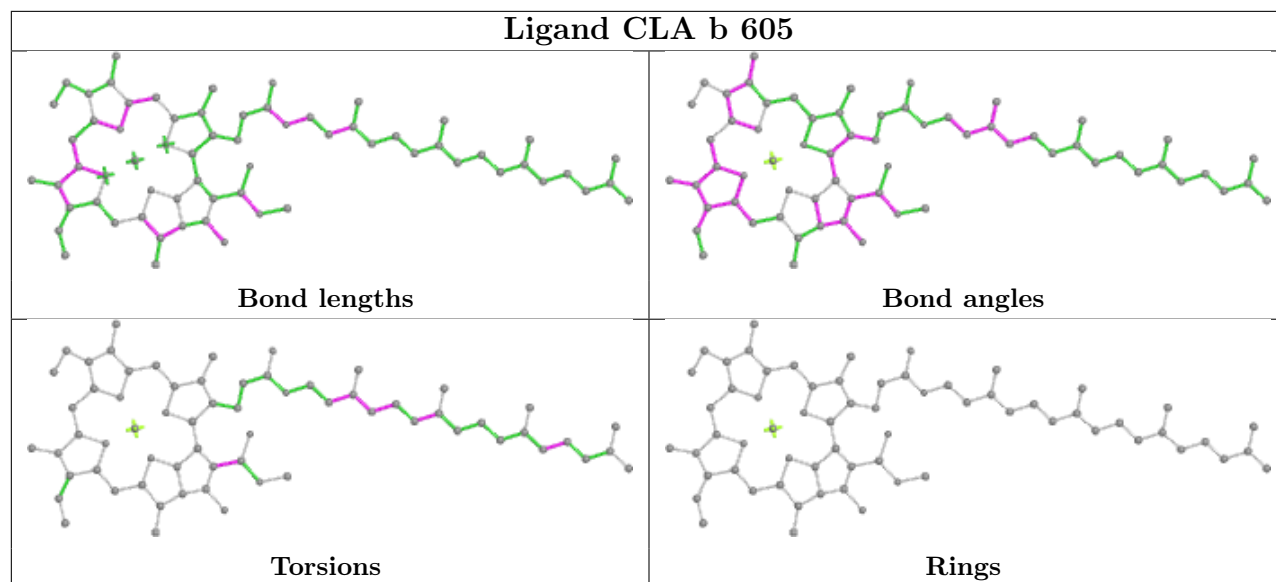
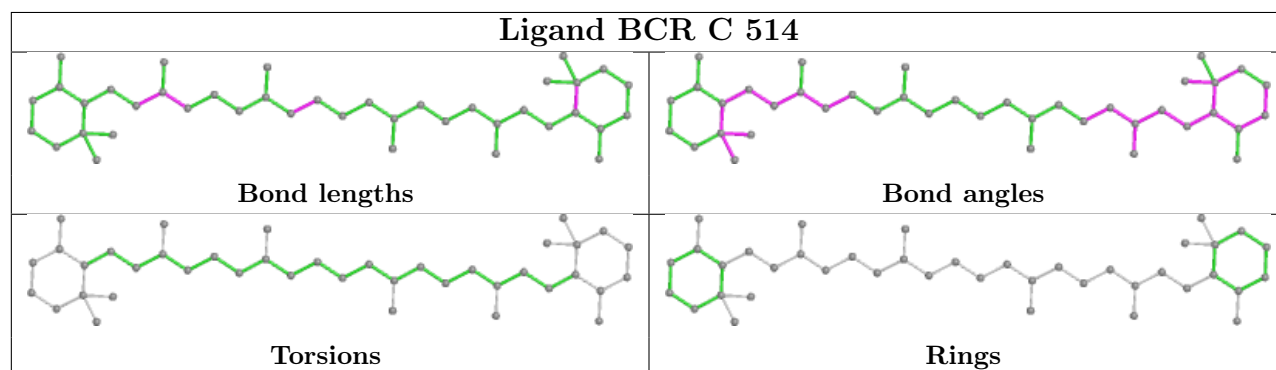
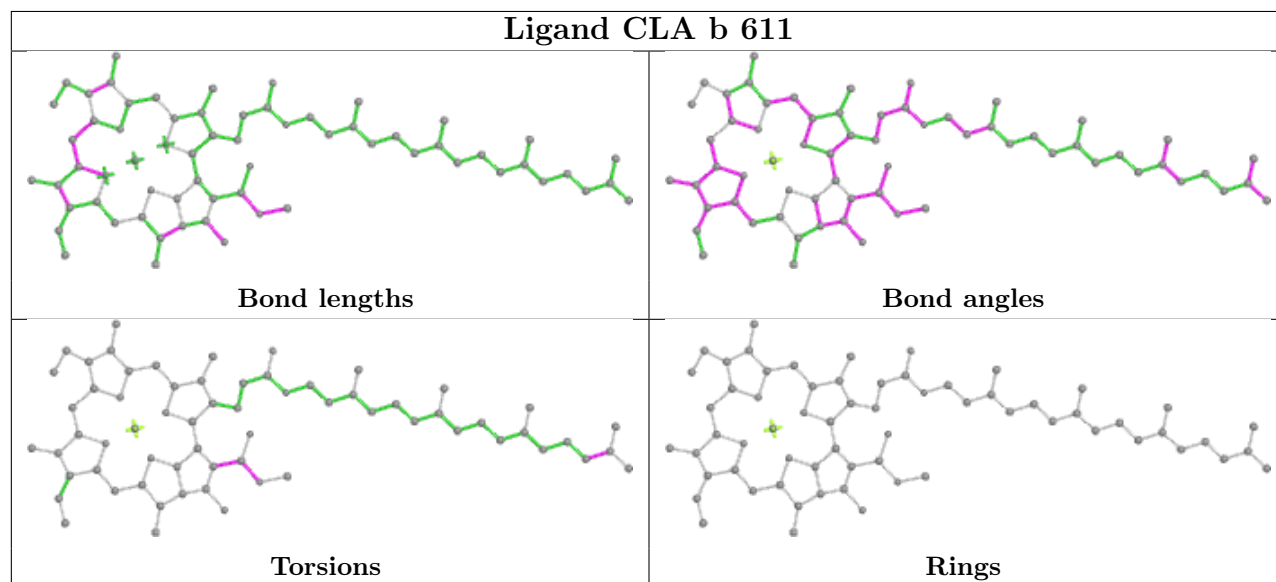


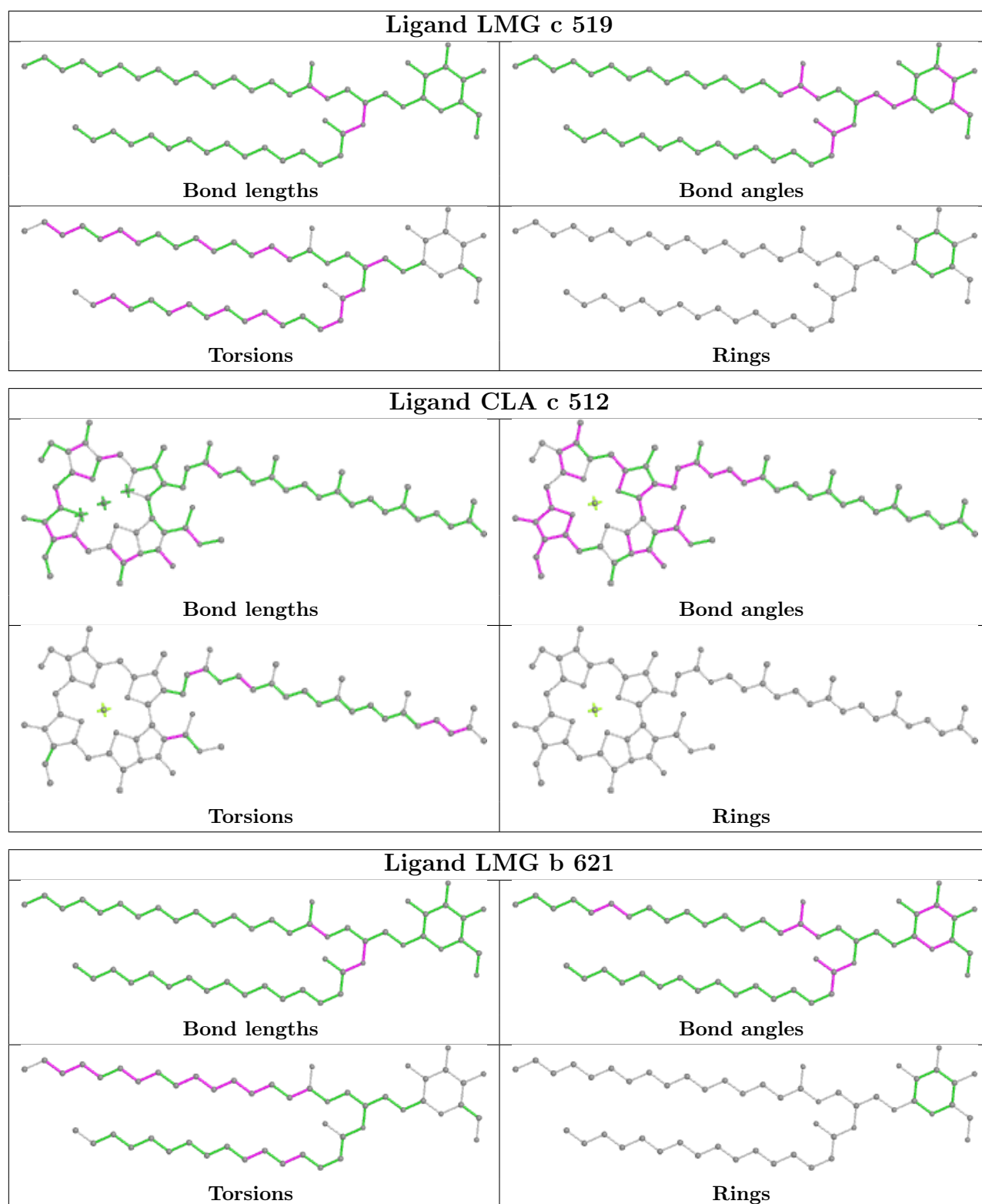




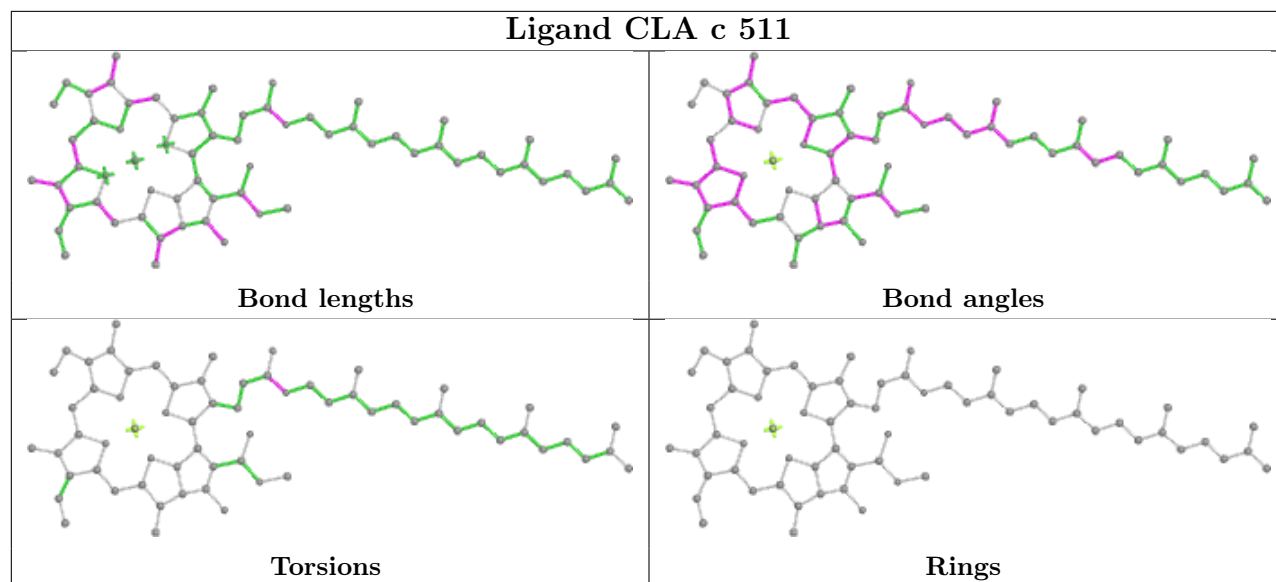




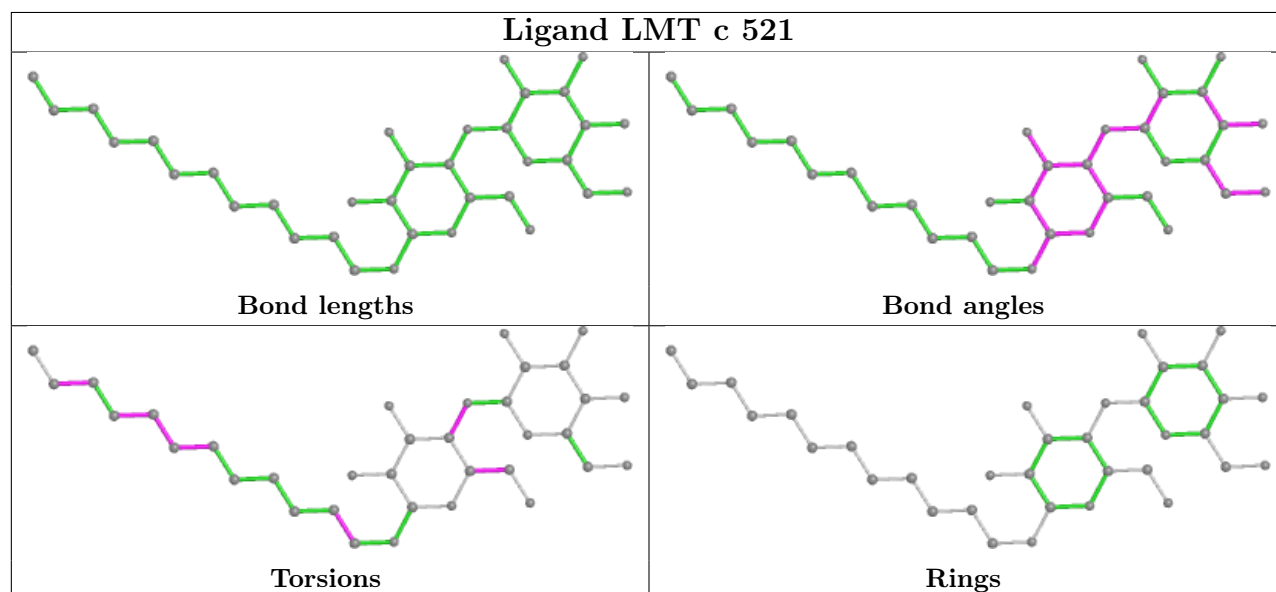
Ligand CLA b 605**Ligand BCR C 514****Ligand CLA b 611**



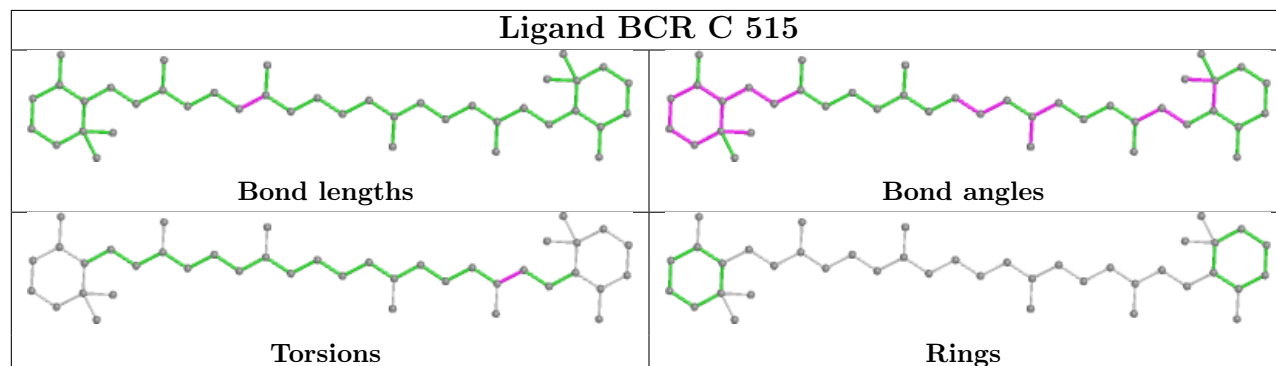
Ligand CLA c 511

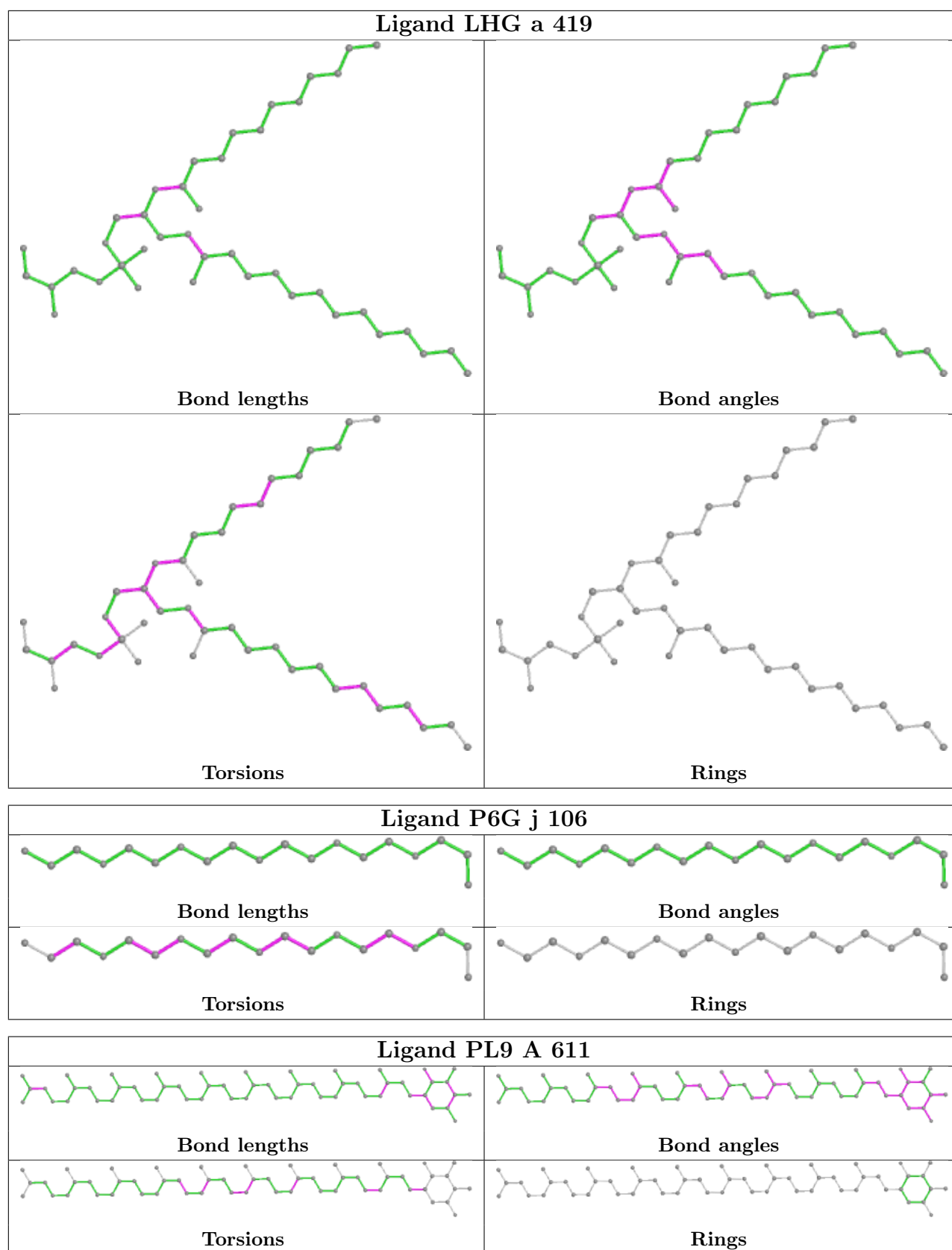


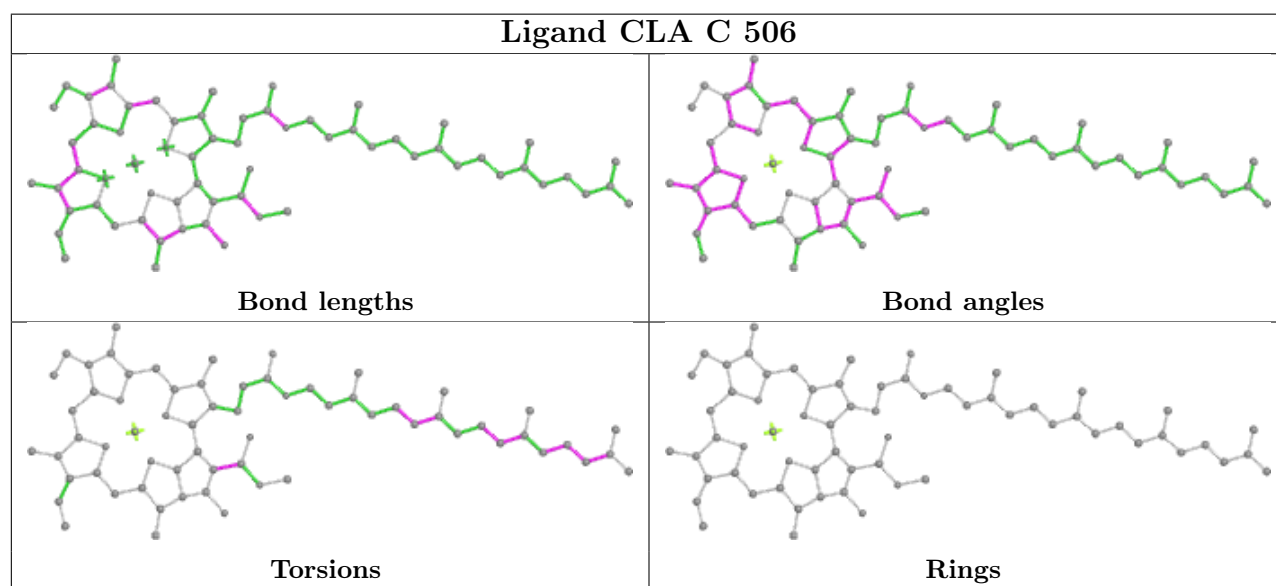
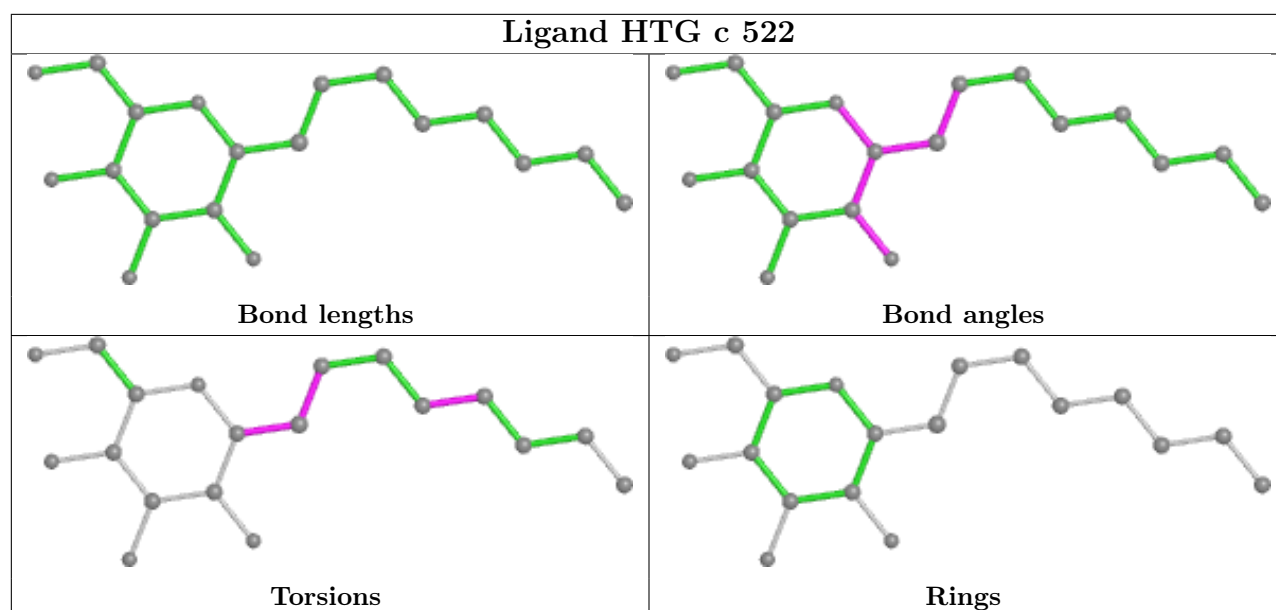
Ligand LMT c 521

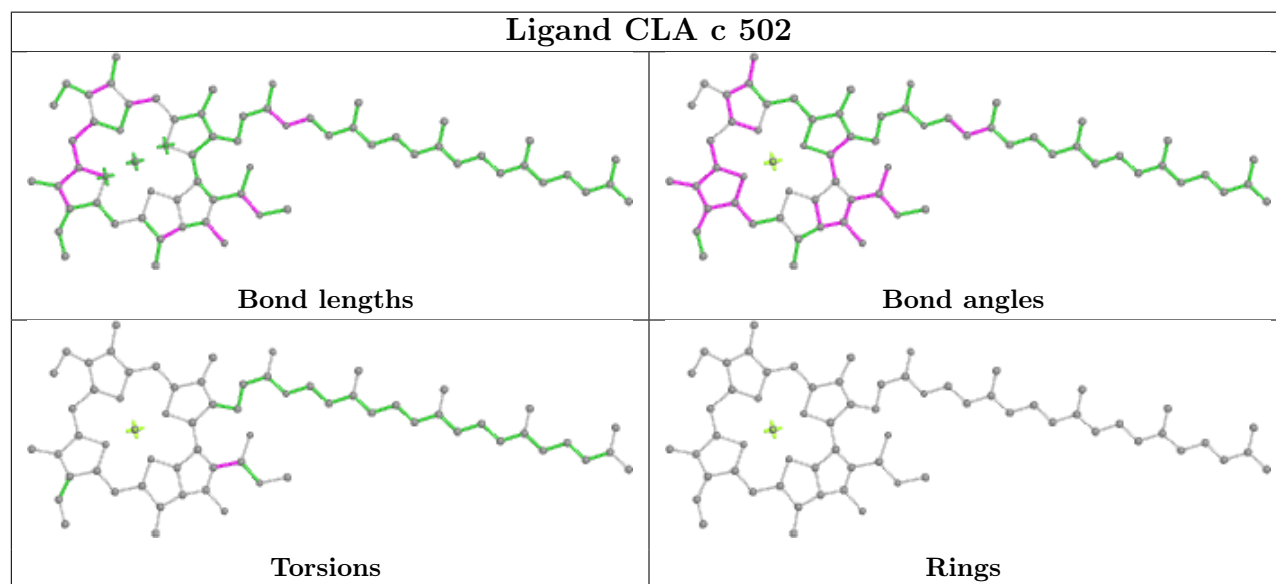
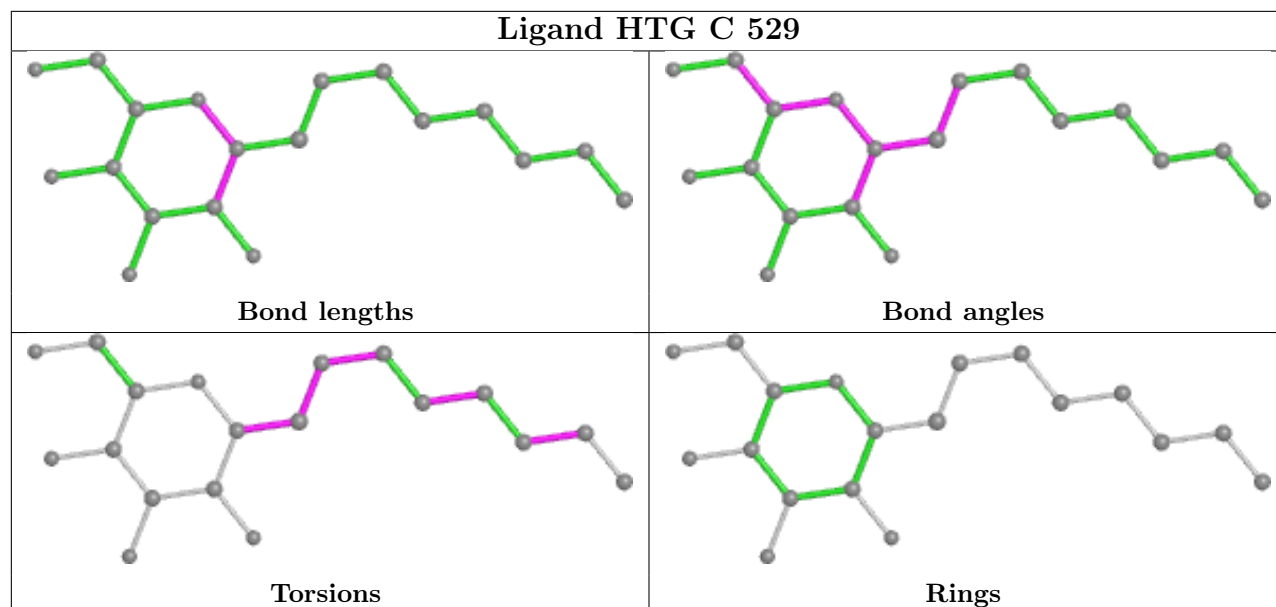


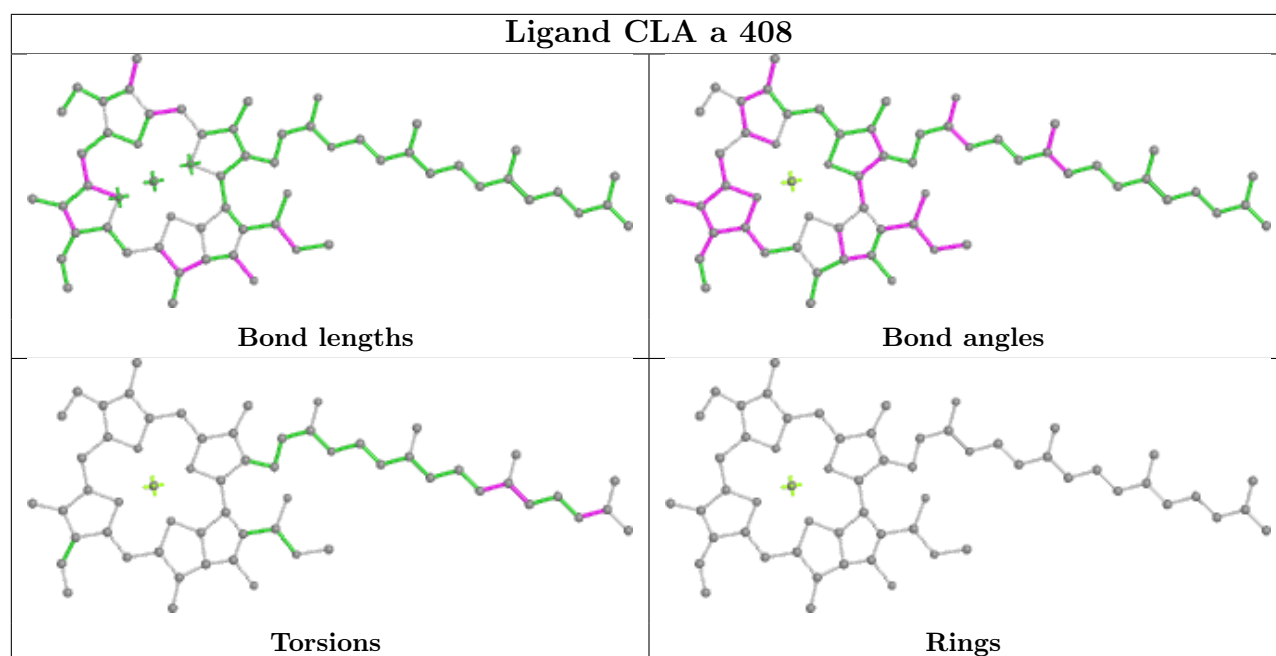
Ligand BCR C 515

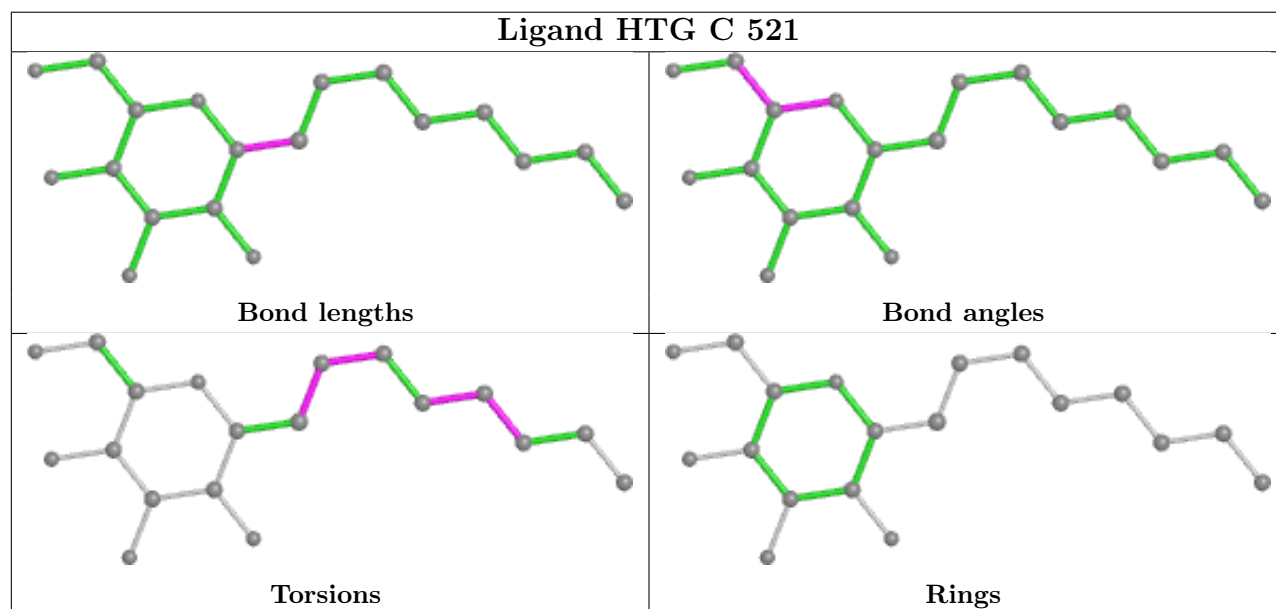
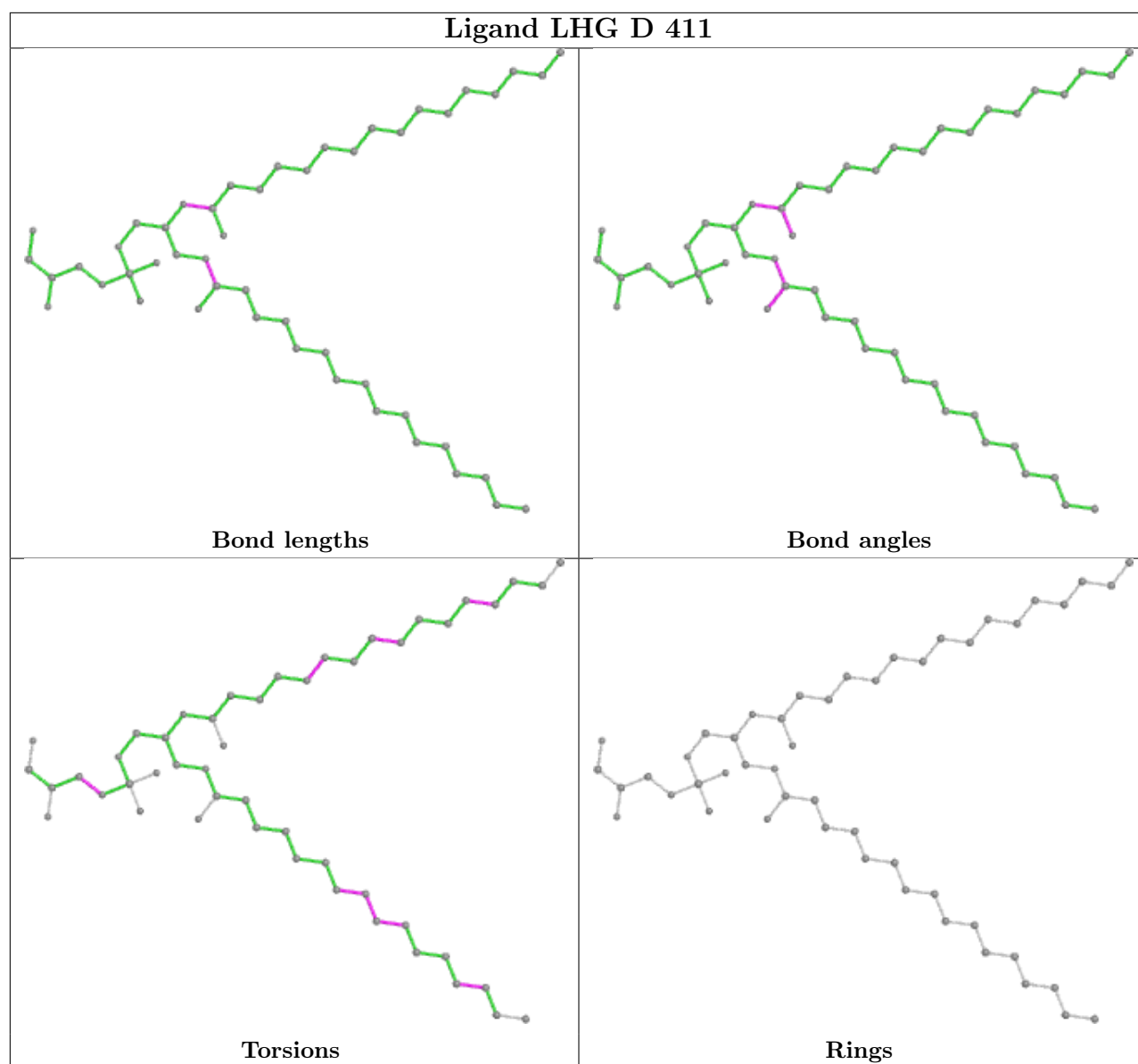


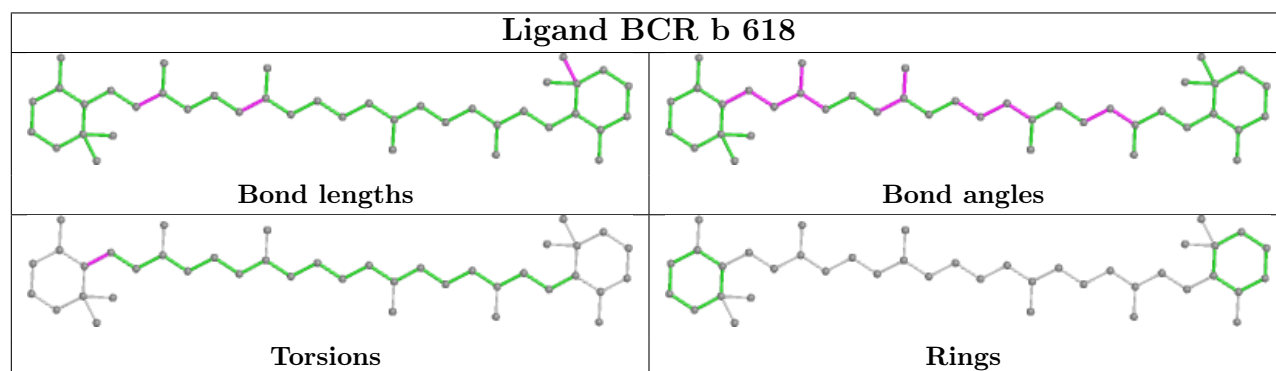
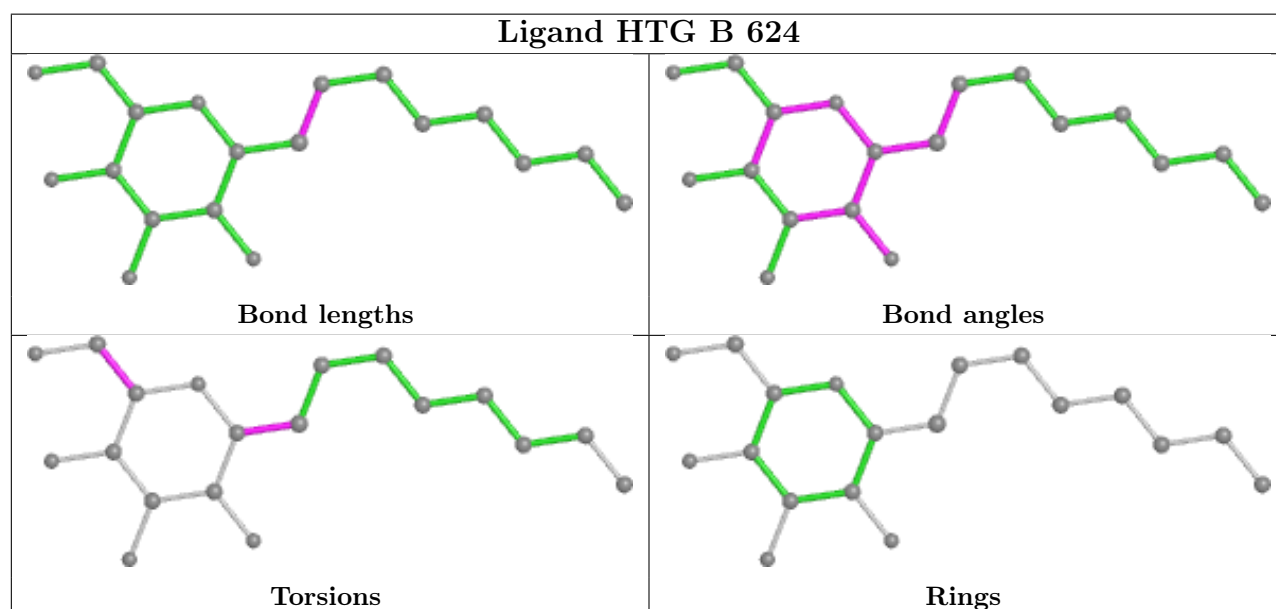
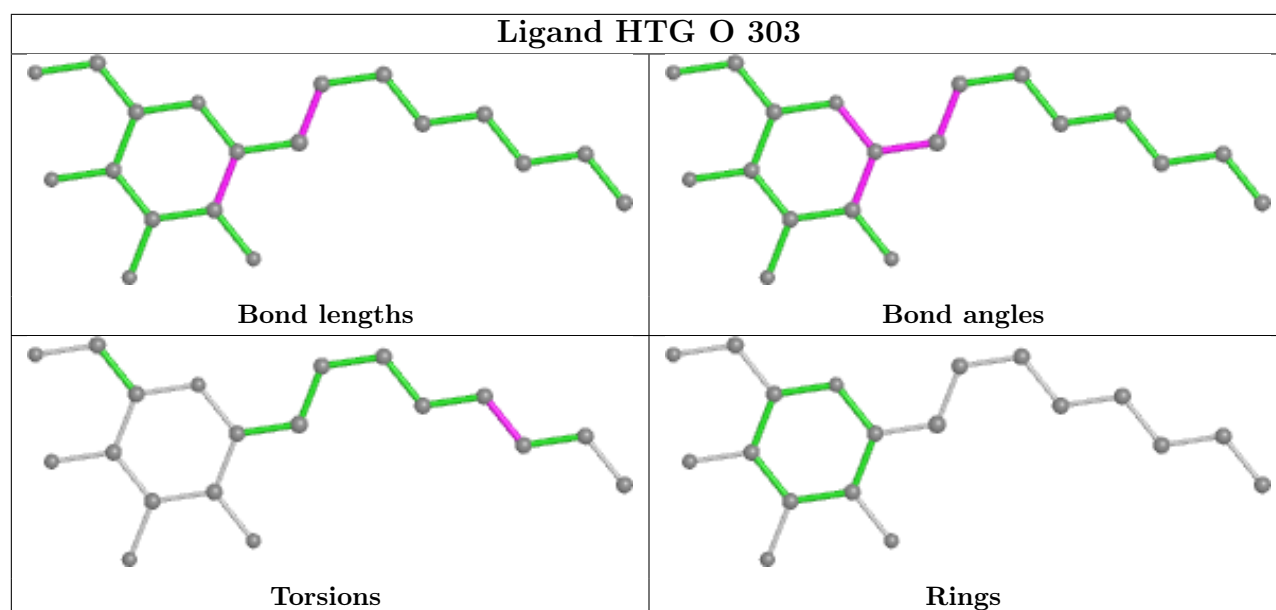


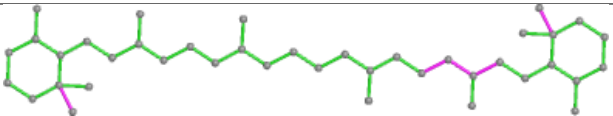
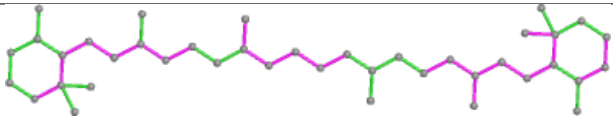
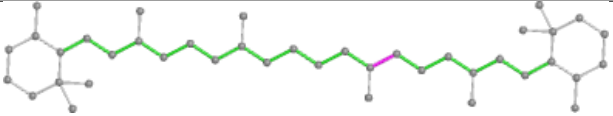
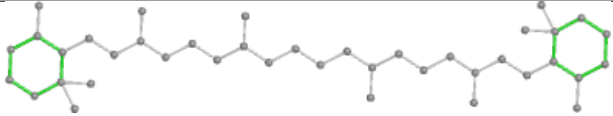


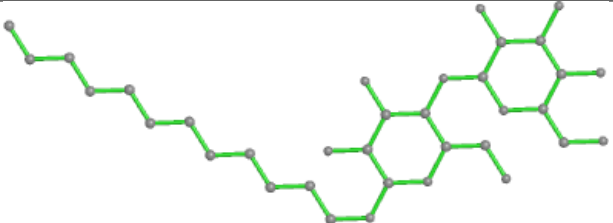
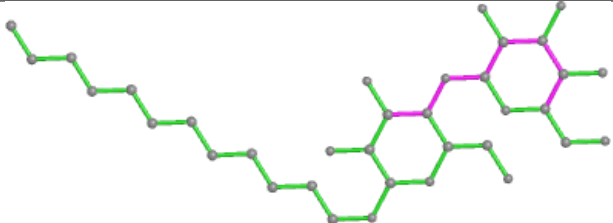
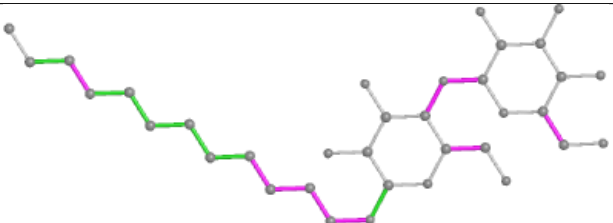
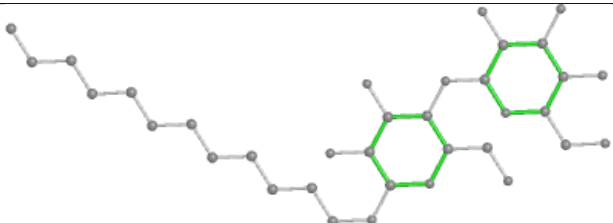


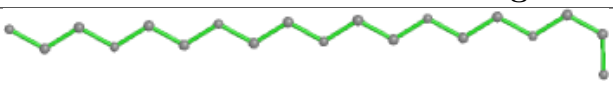
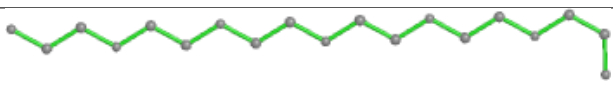
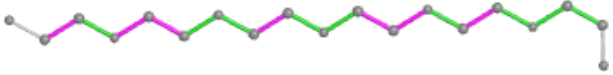
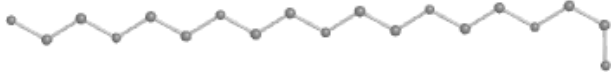




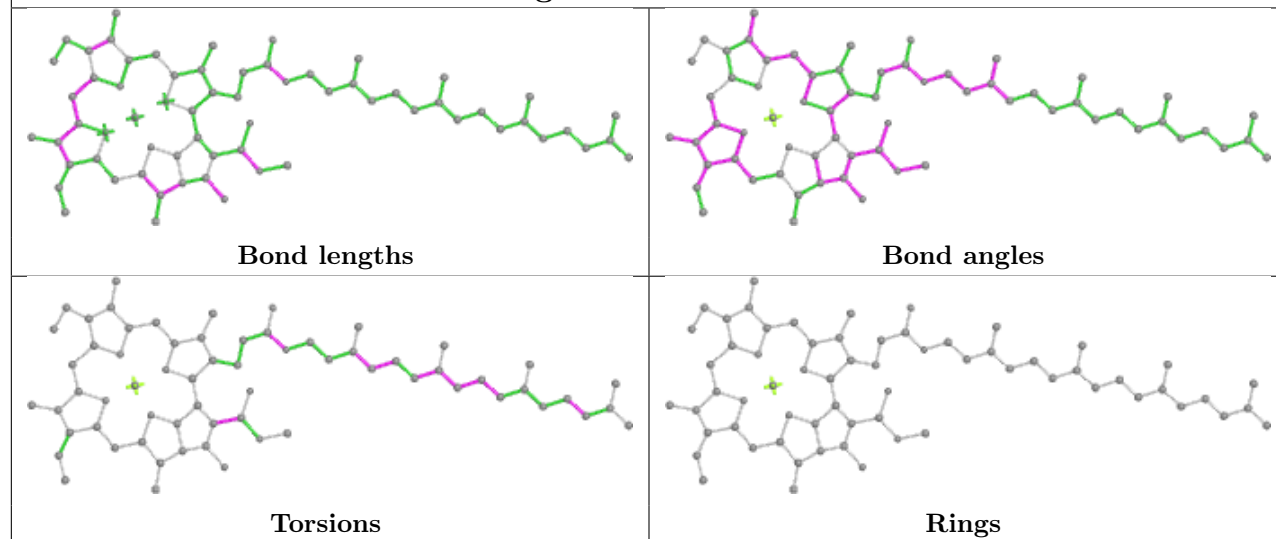


Ligand BCR A 610	
	Bond lengths
	Bond angles
	Torsions
	Rings

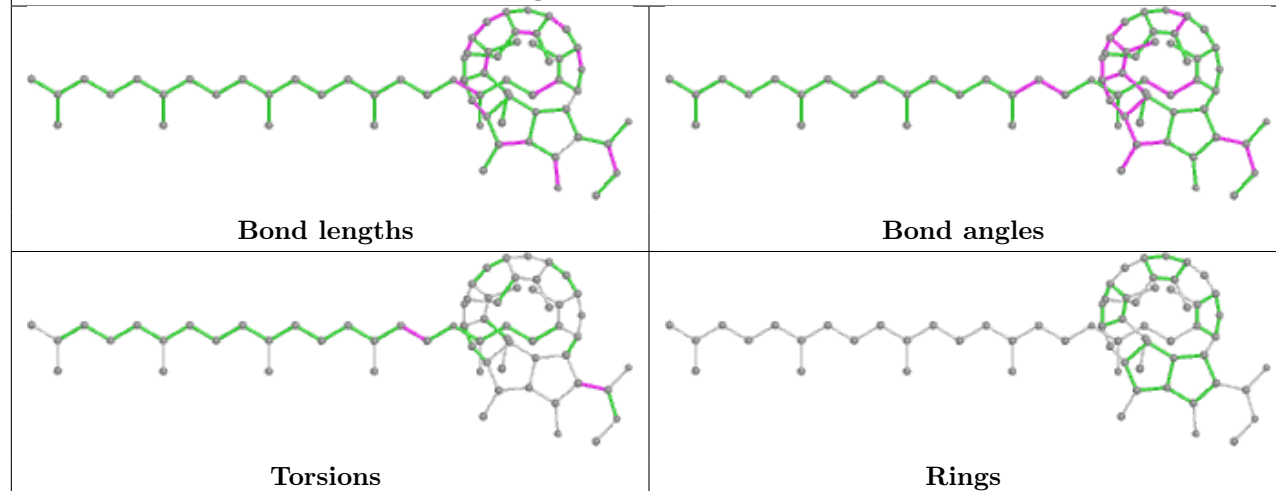
Ligand LMT Y 101	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand P6G B 651	
	Bond lengths
	Bond angles
	Torsions
	Rings

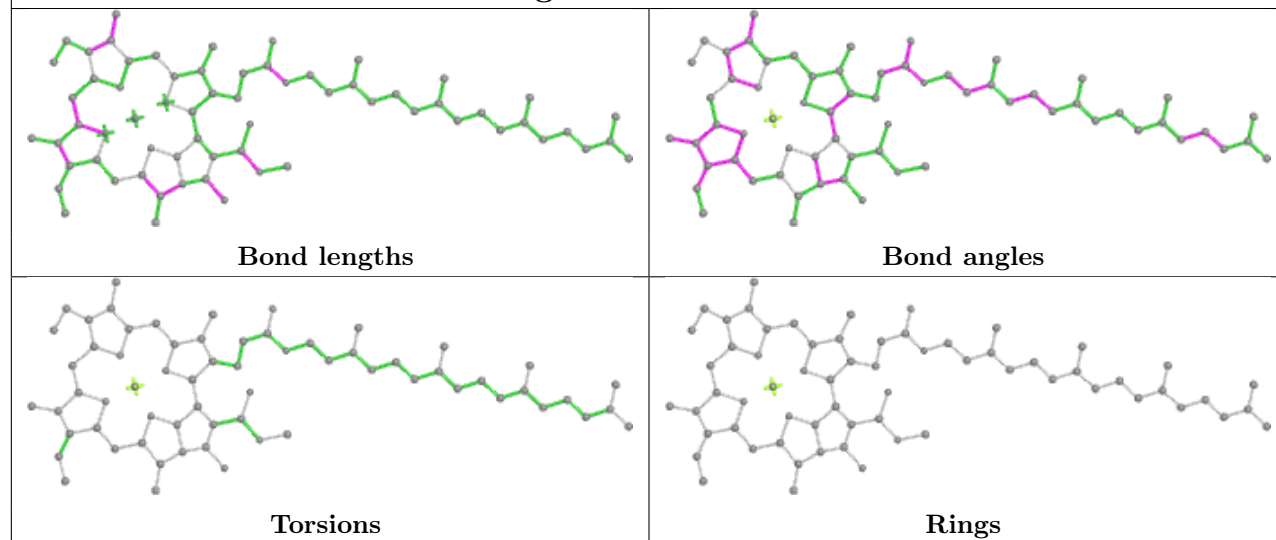
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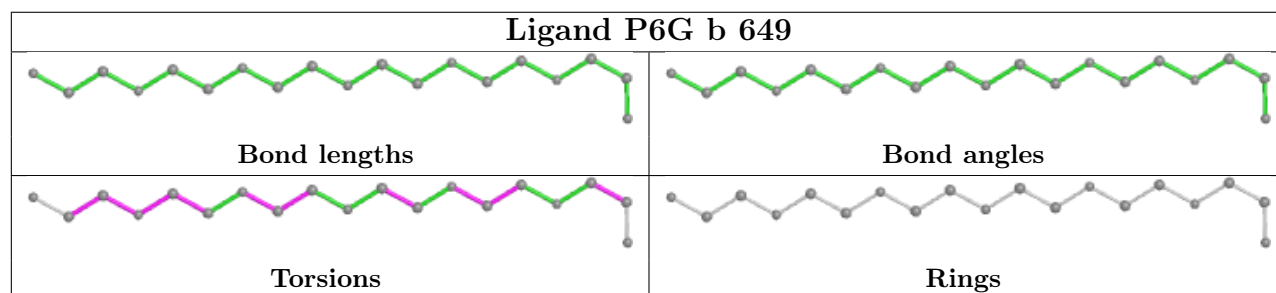
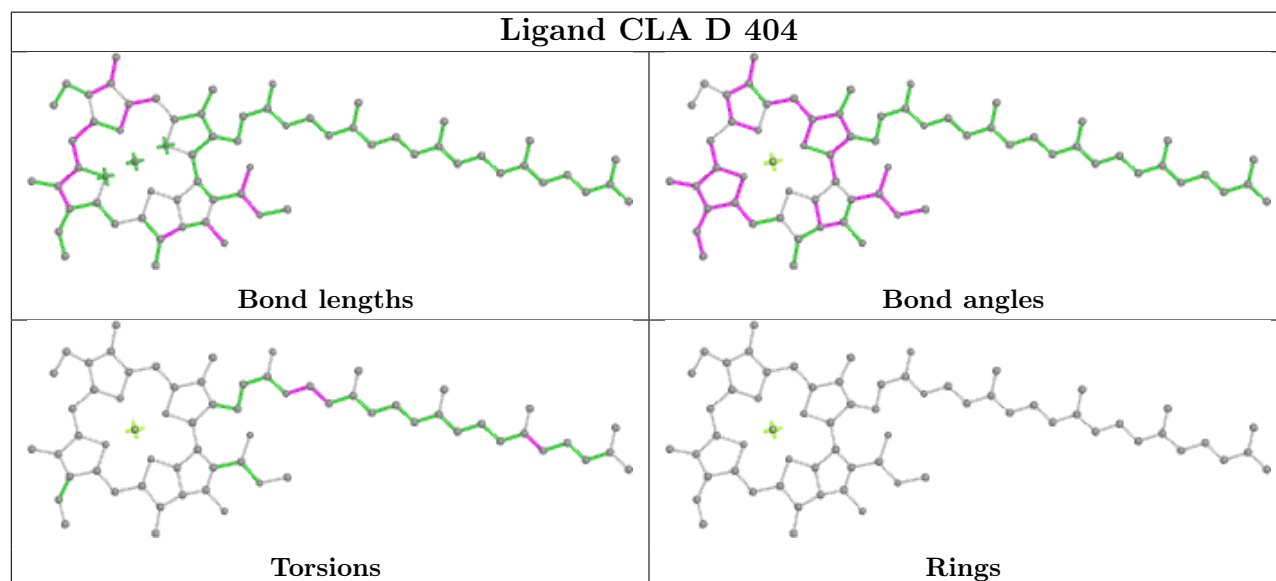
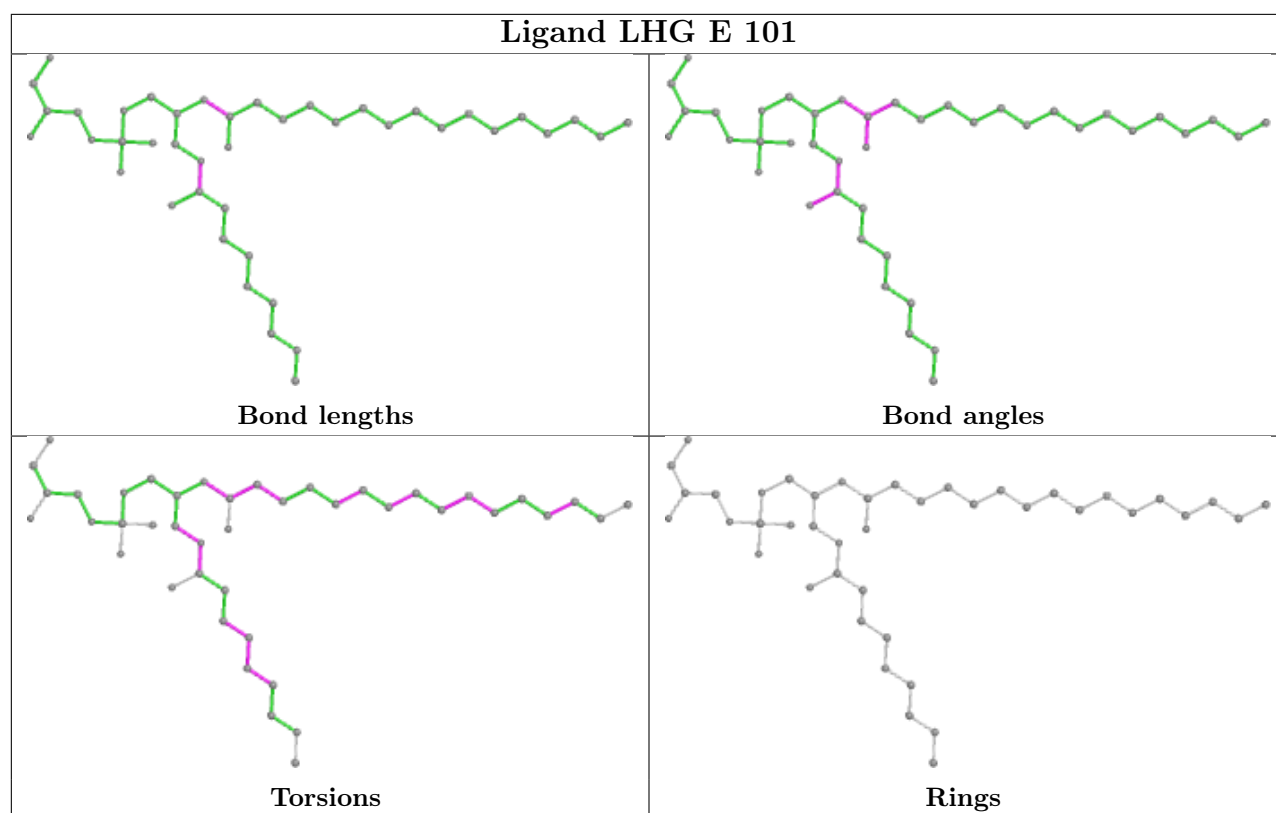


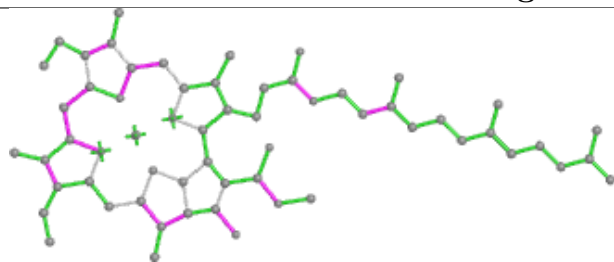
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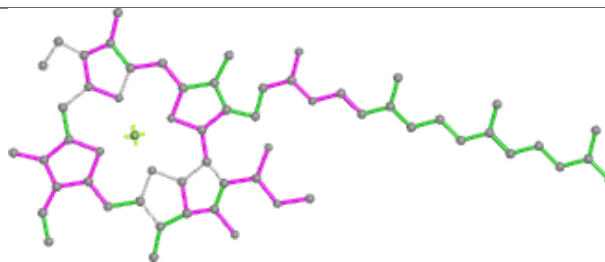
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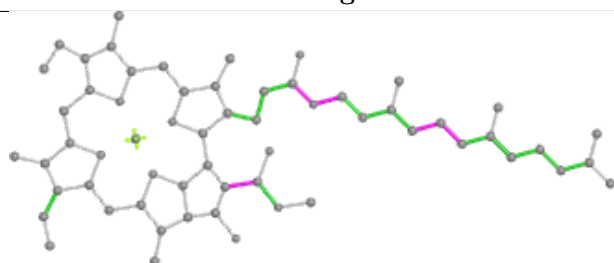


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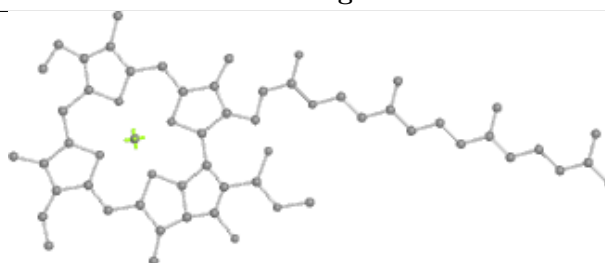
Bond lengths



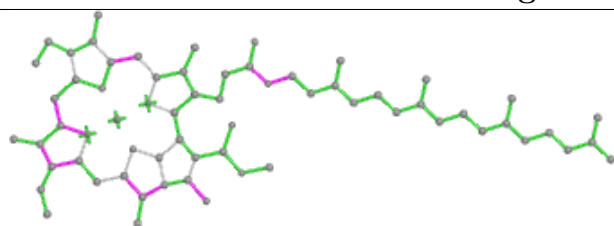
Bond angles



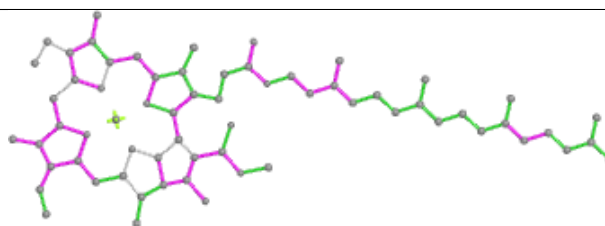
Torsions



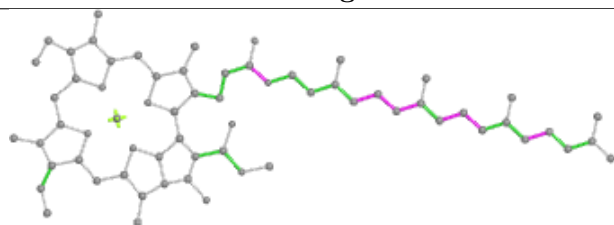
Rings

Ligand CLA a 410

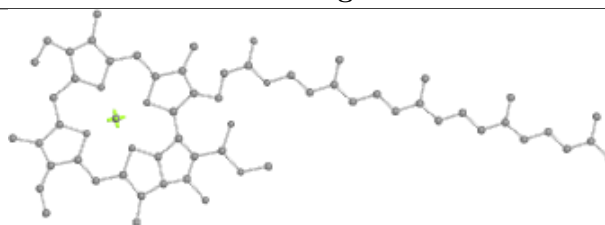
Bond lengths



Bond angles

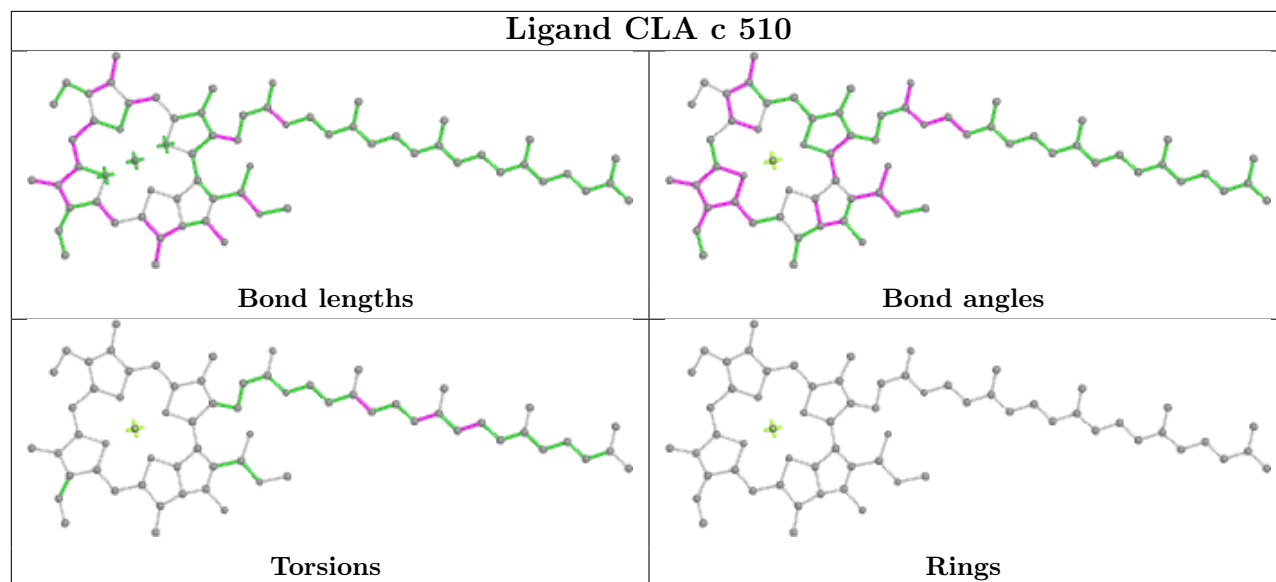


Torsions

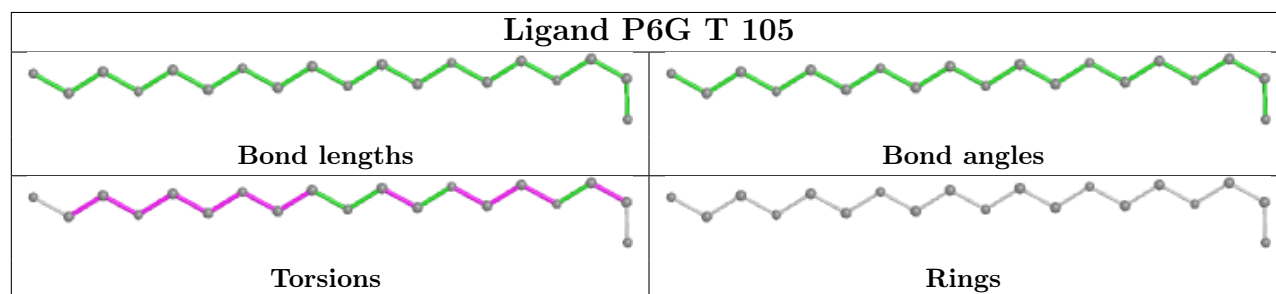


Rings

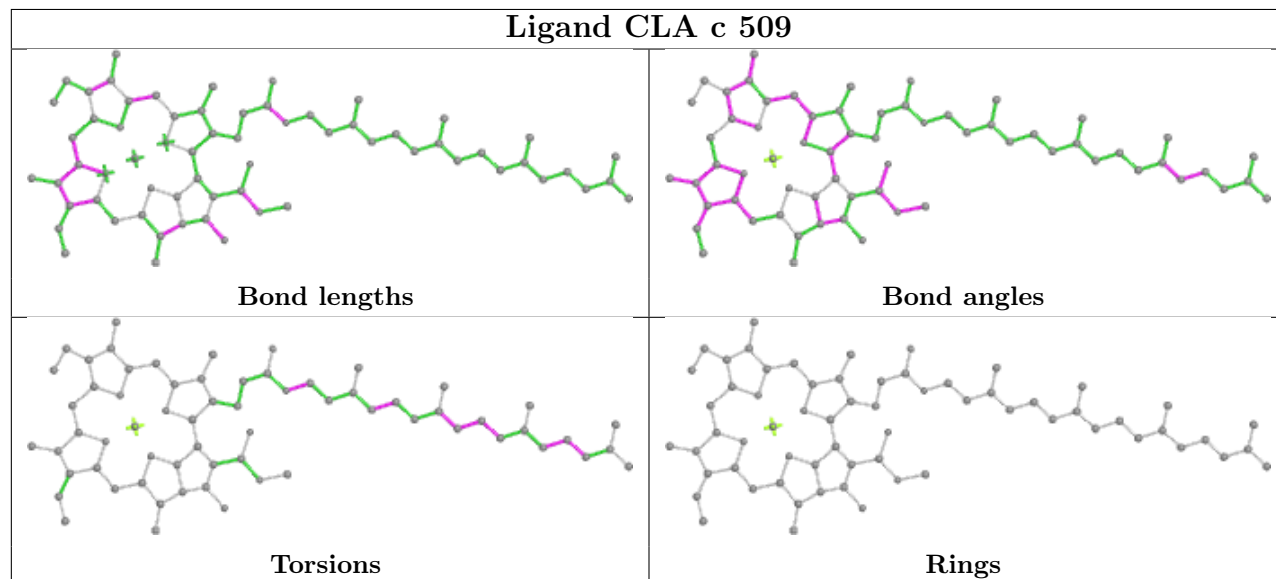
Ligand CLA c 510

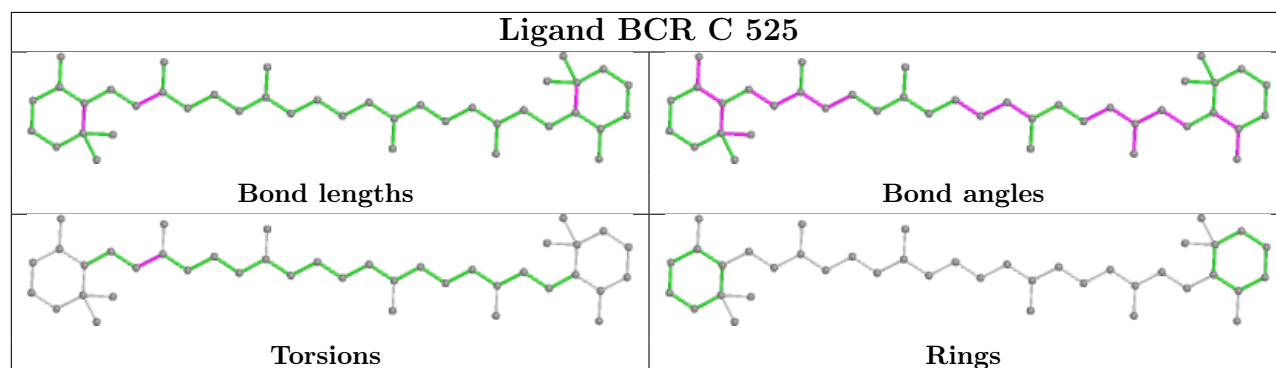
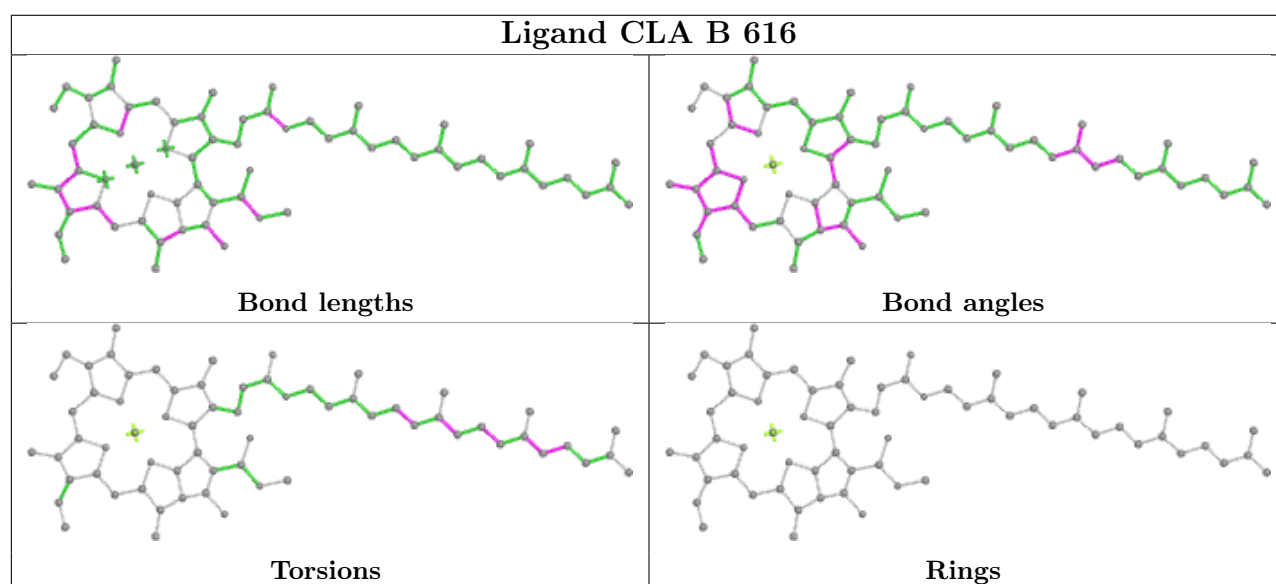
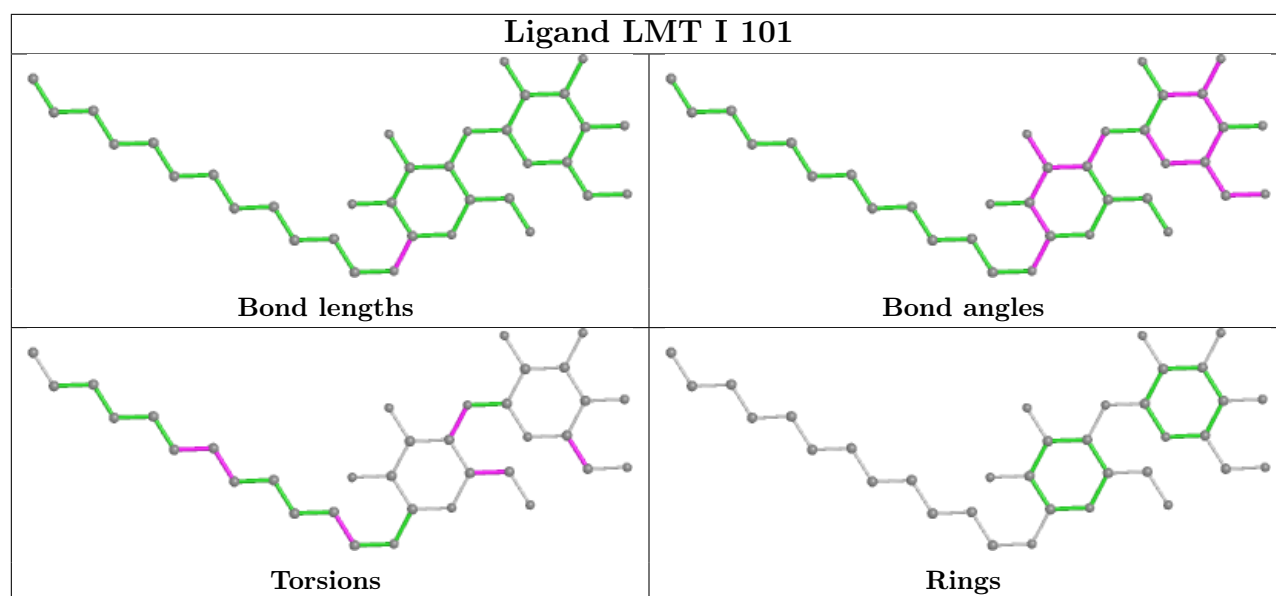


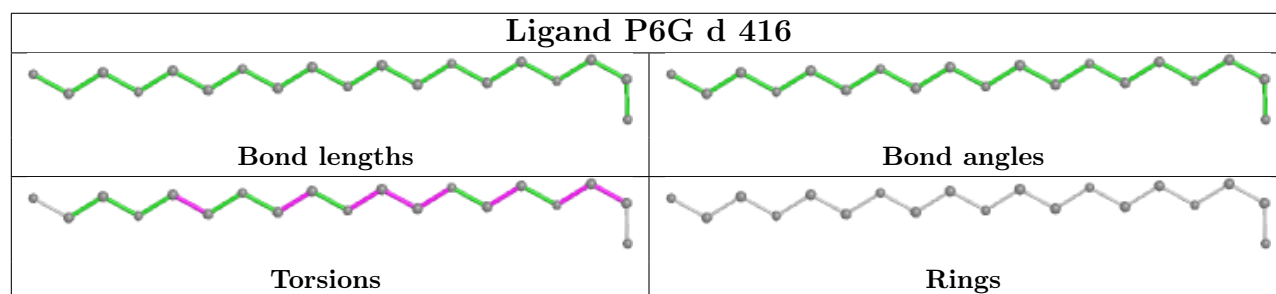
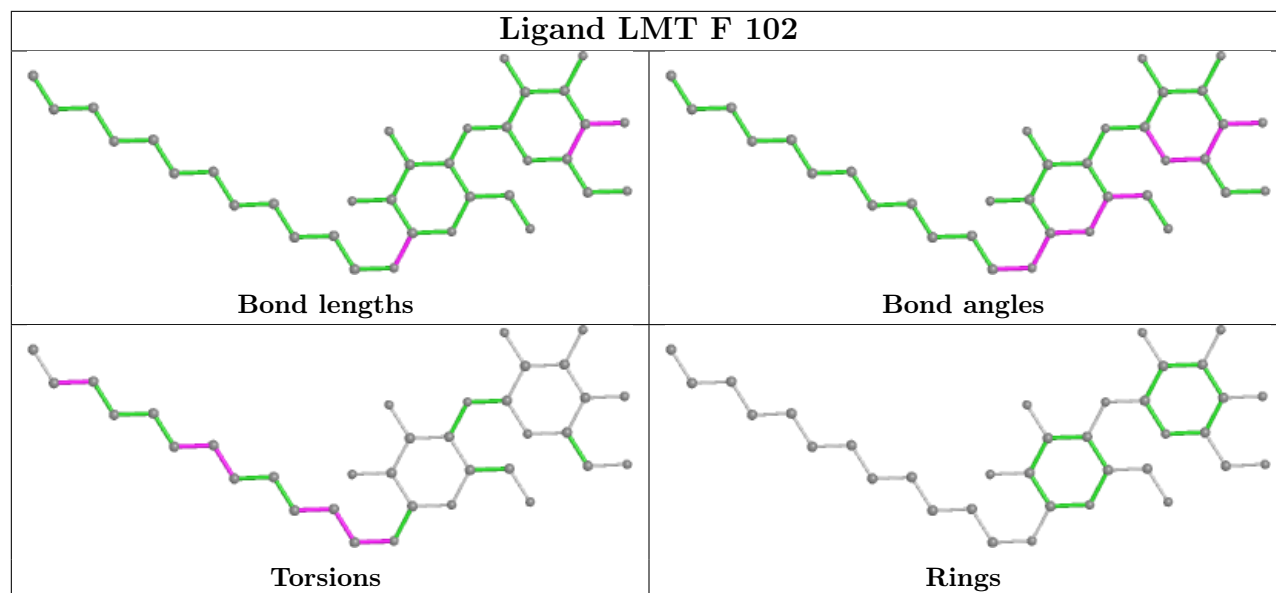
Ligand P6G T 105

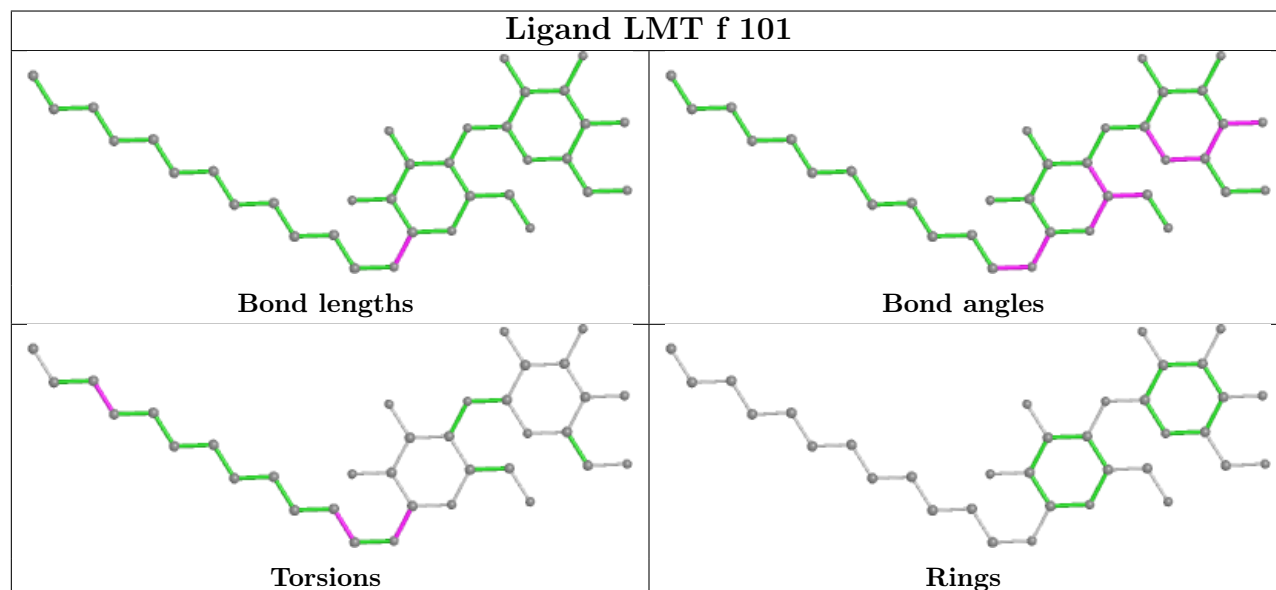
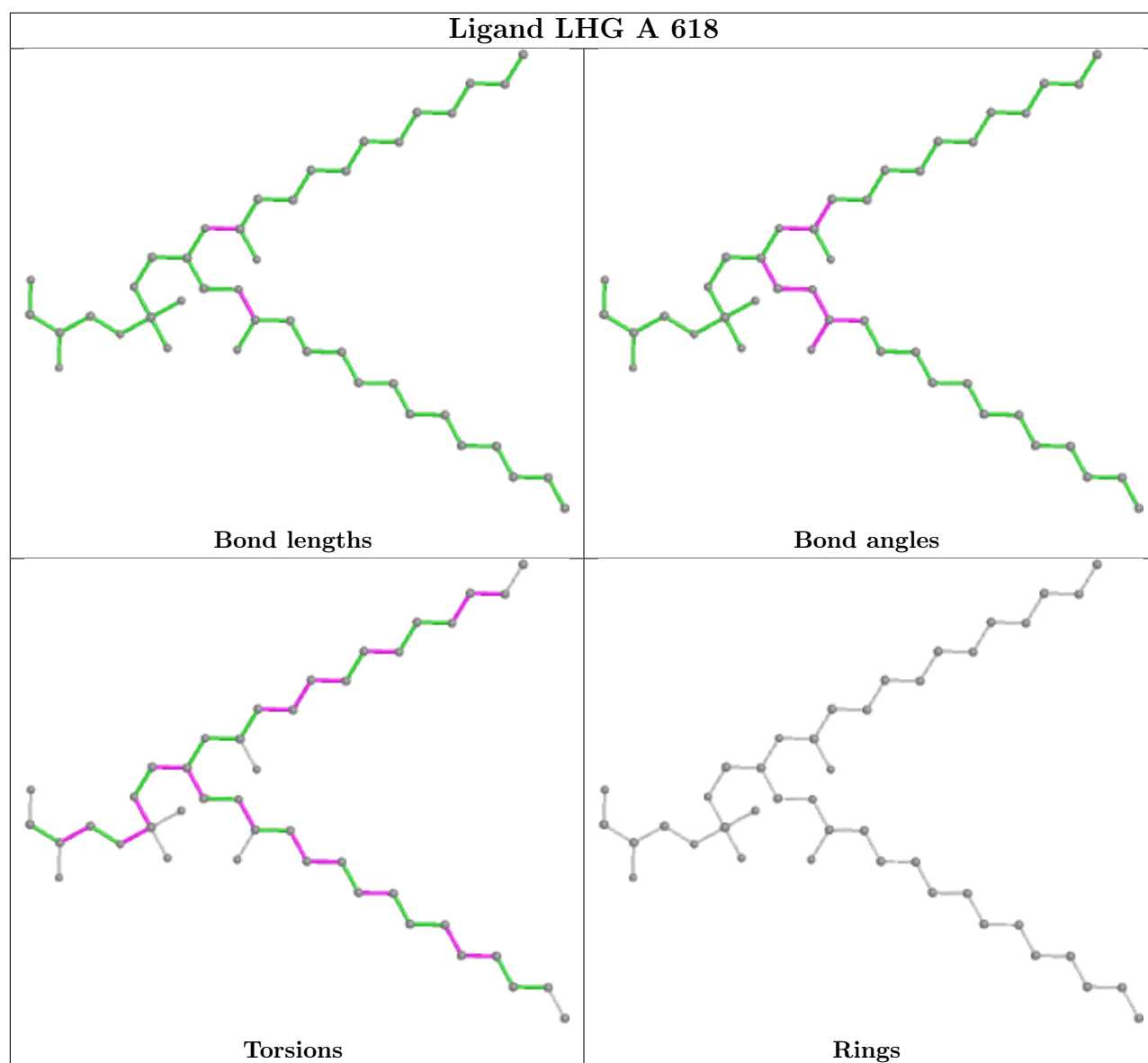


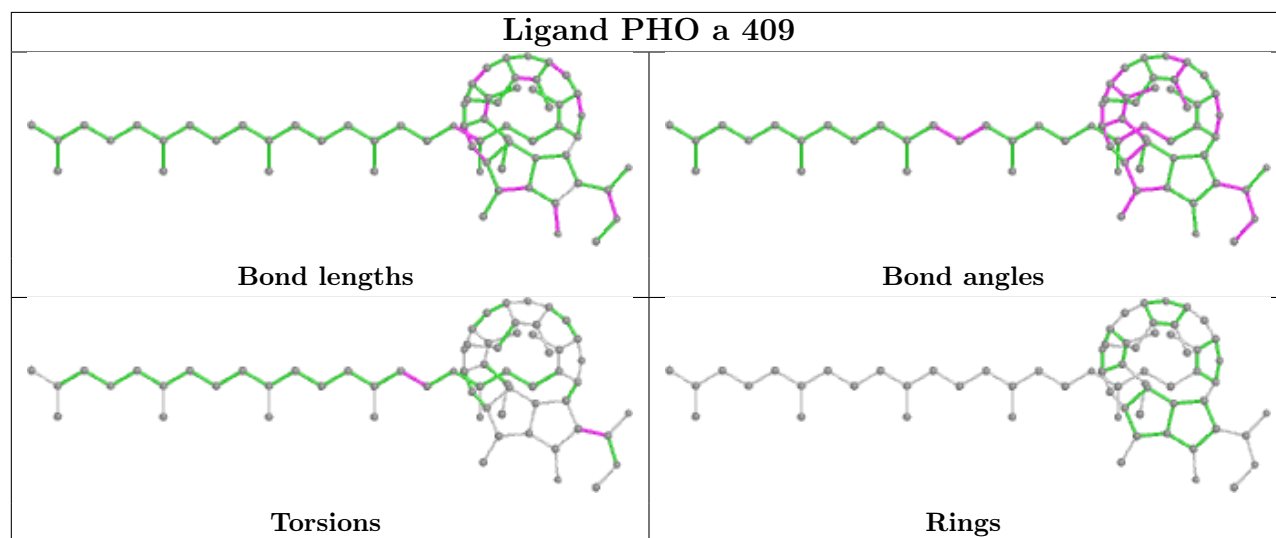
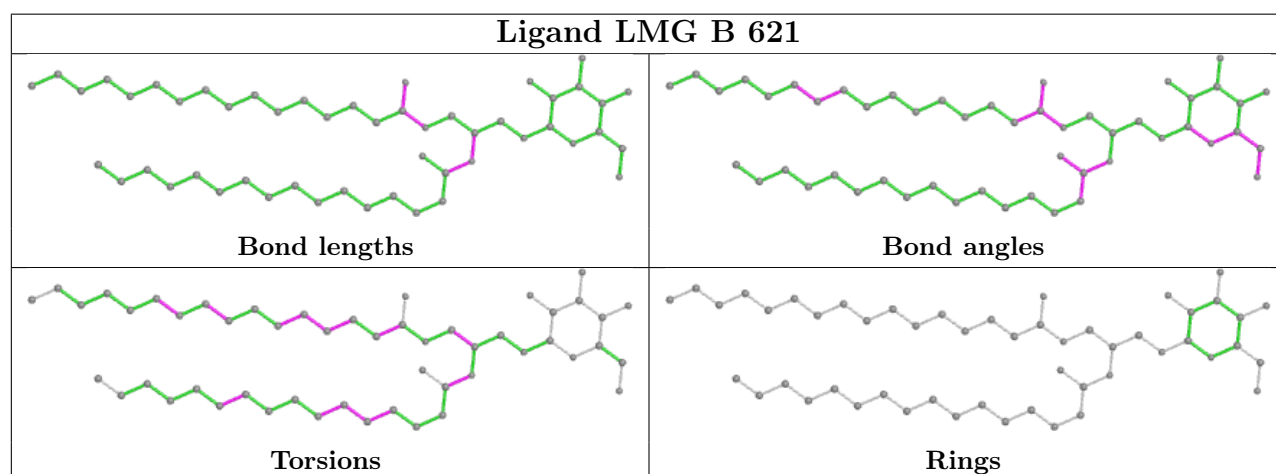
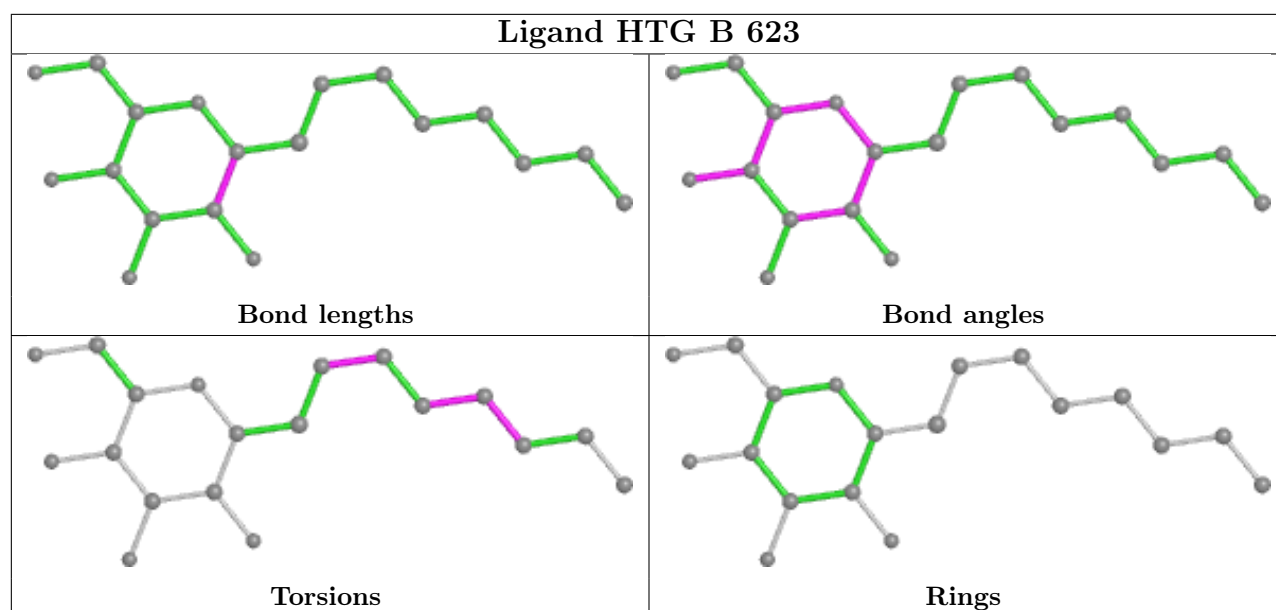
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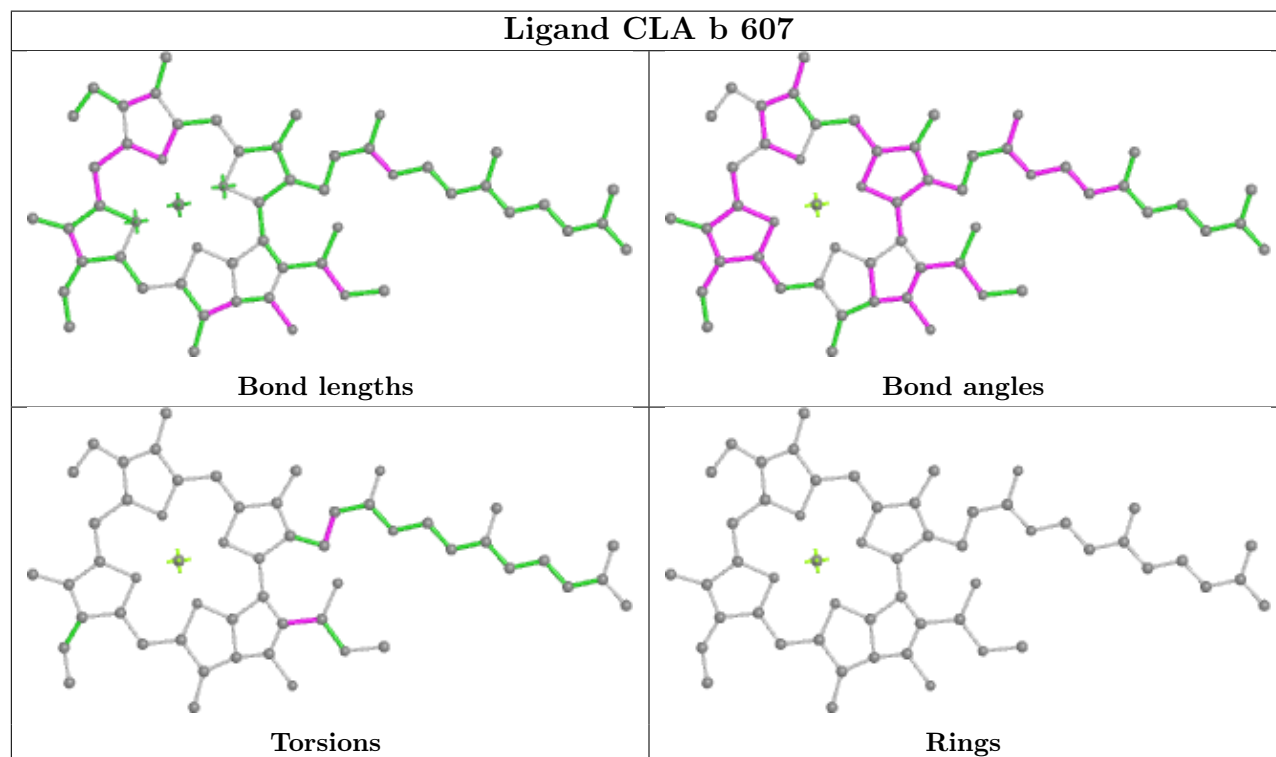
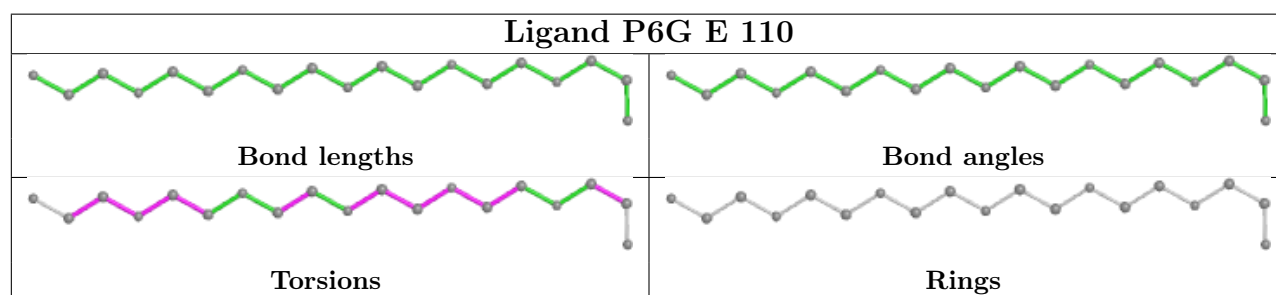
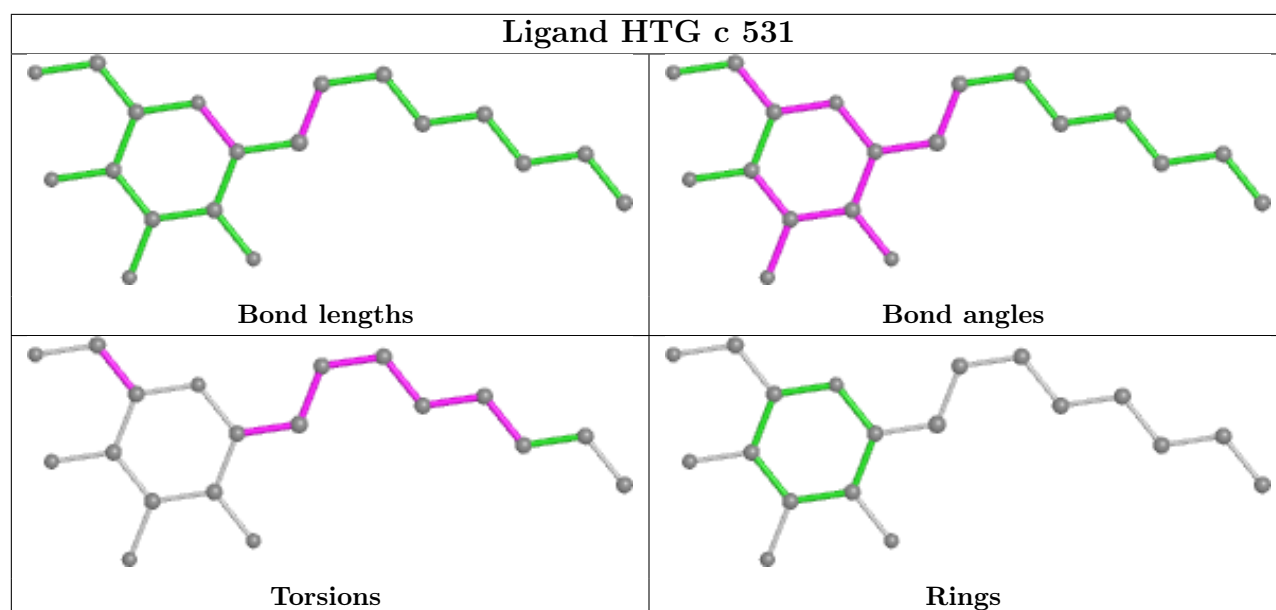


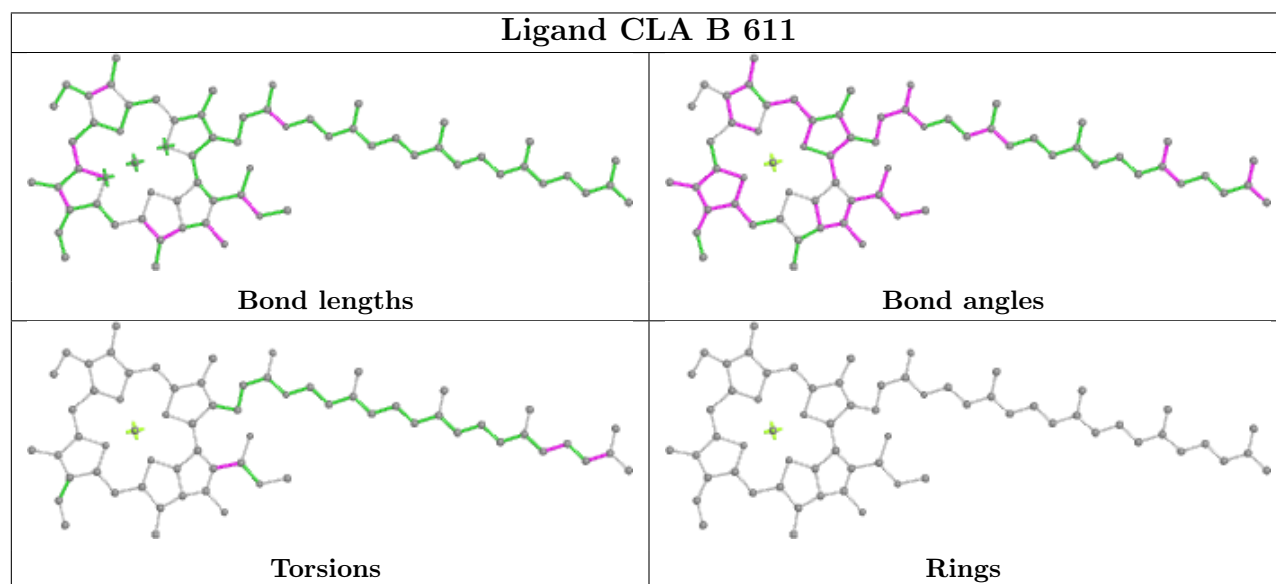
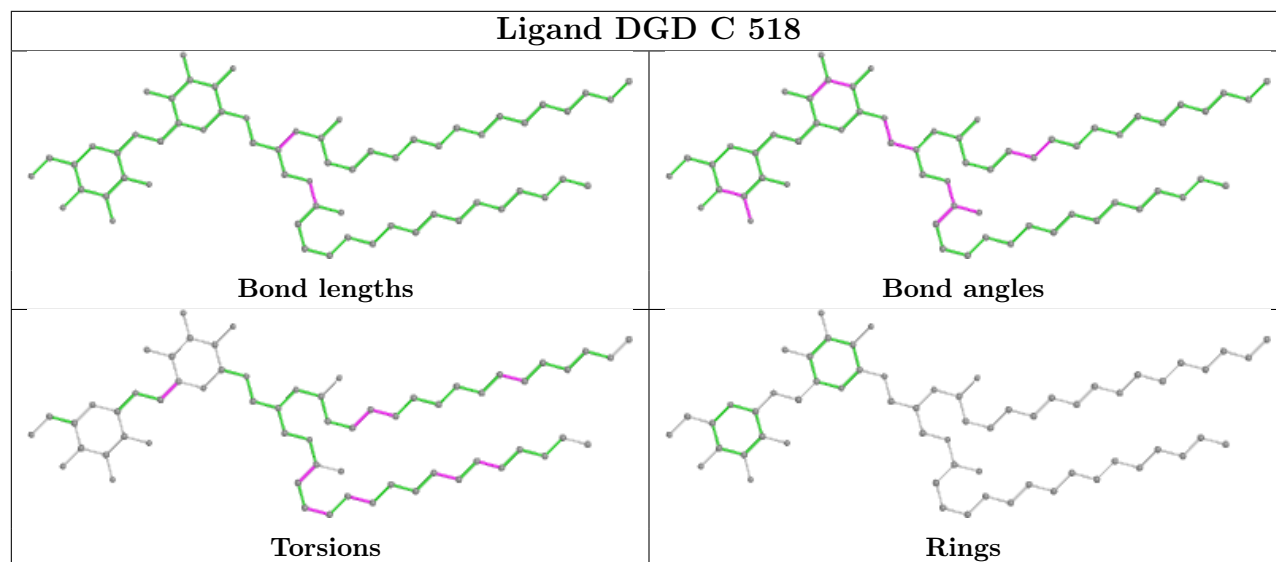
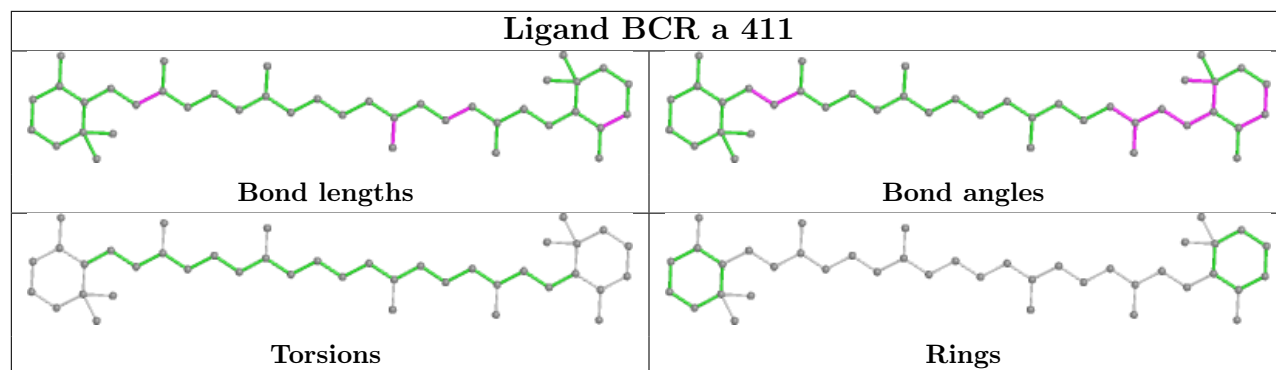


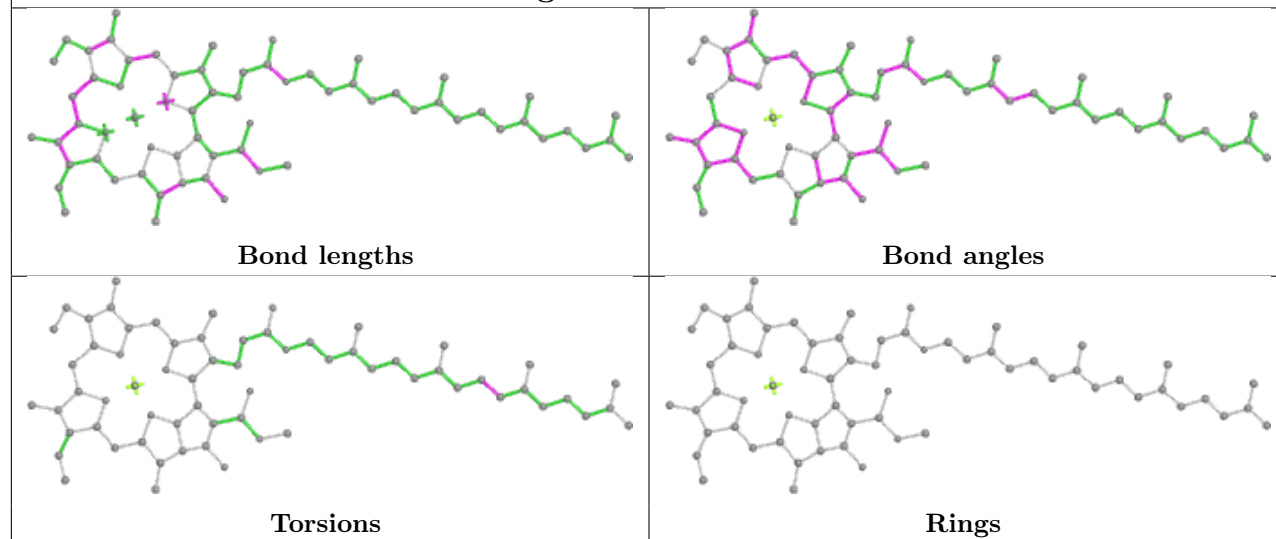
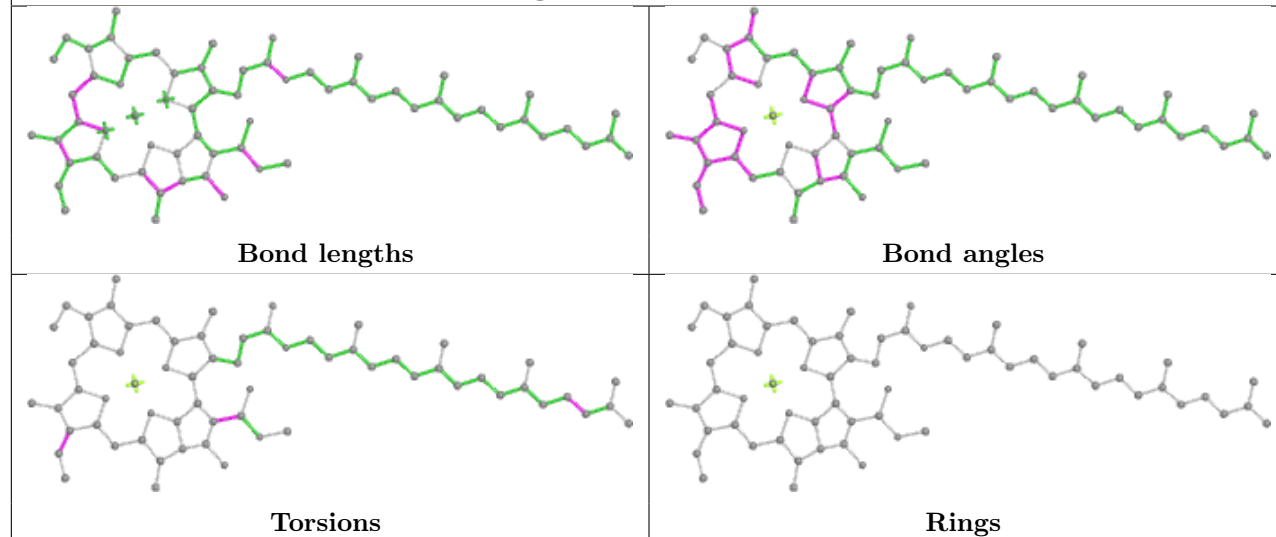


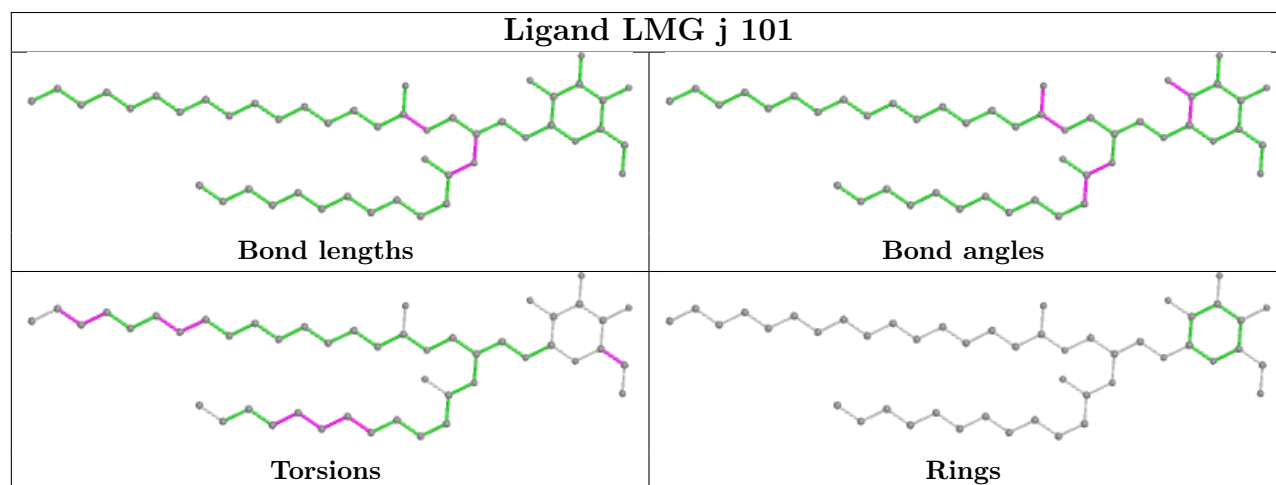
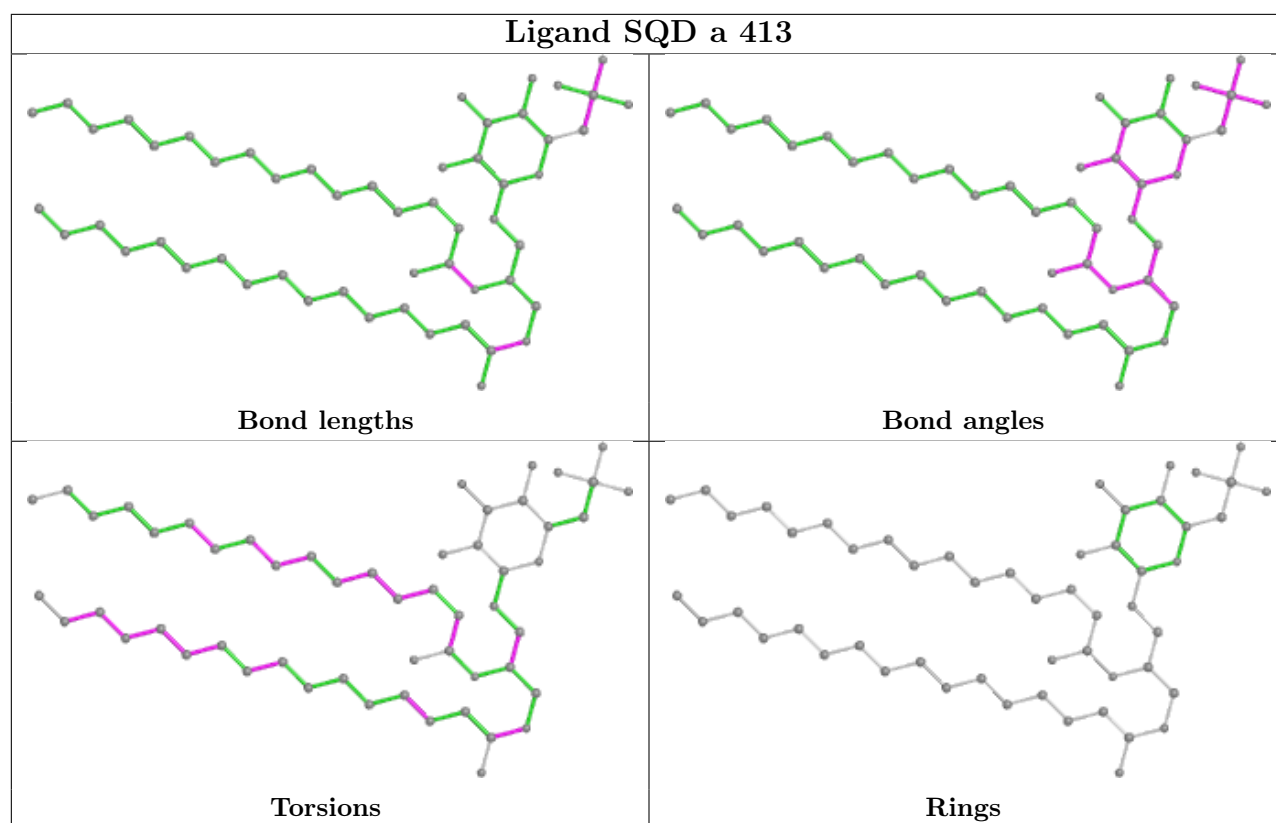


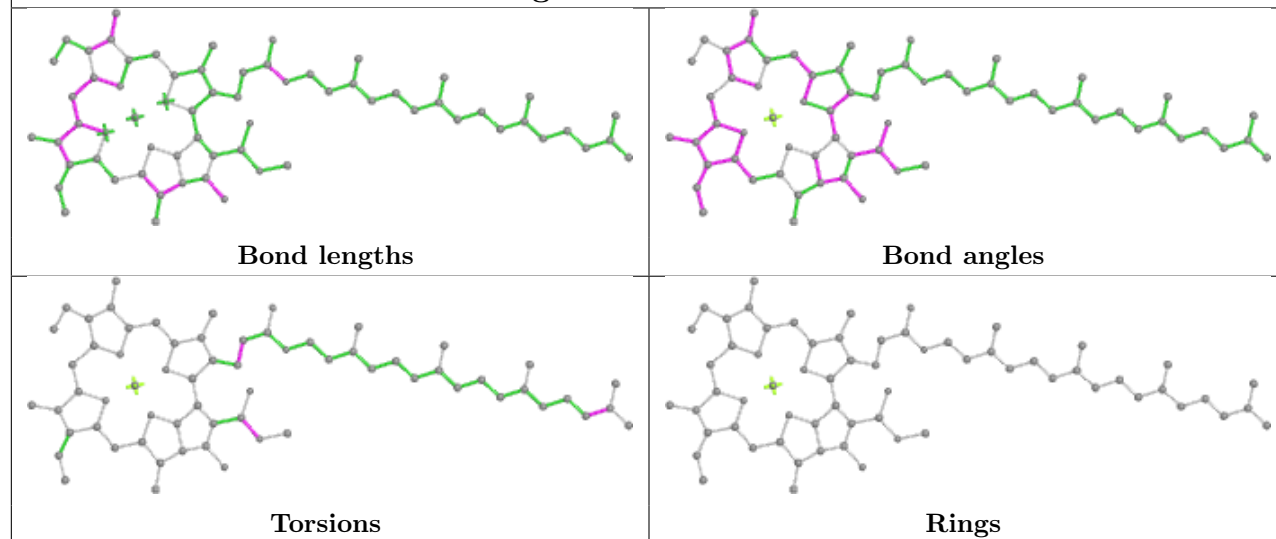
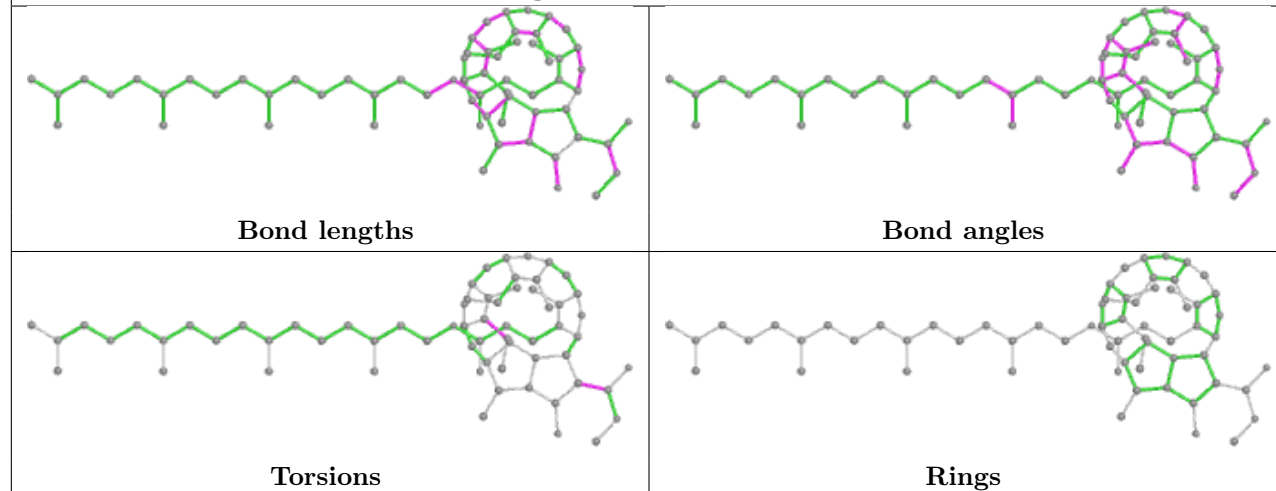


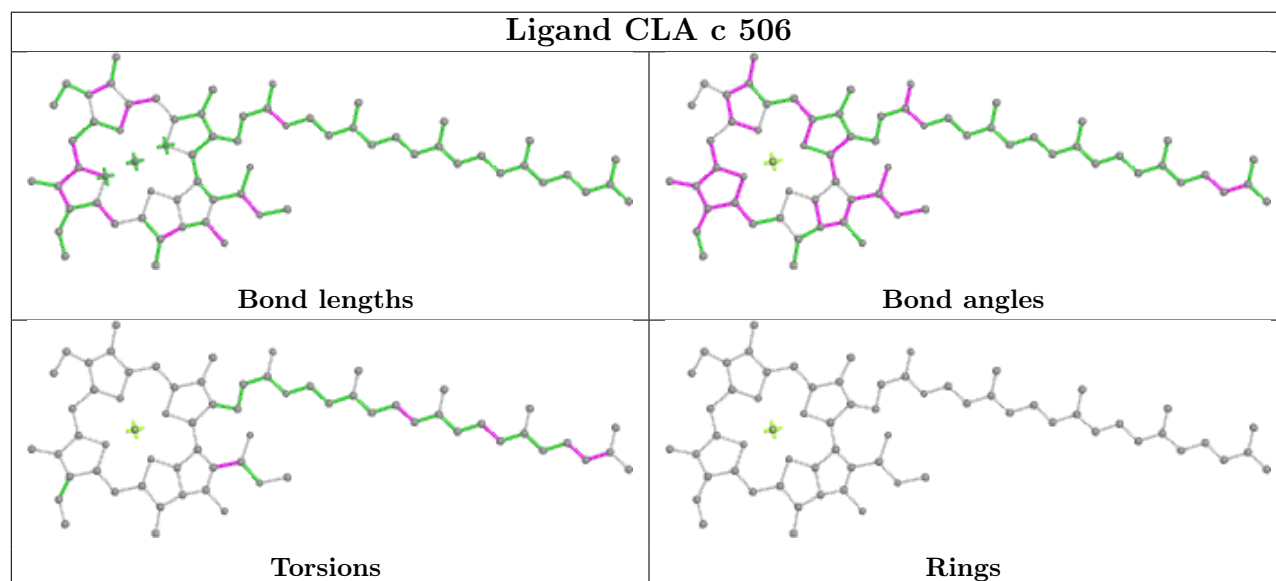
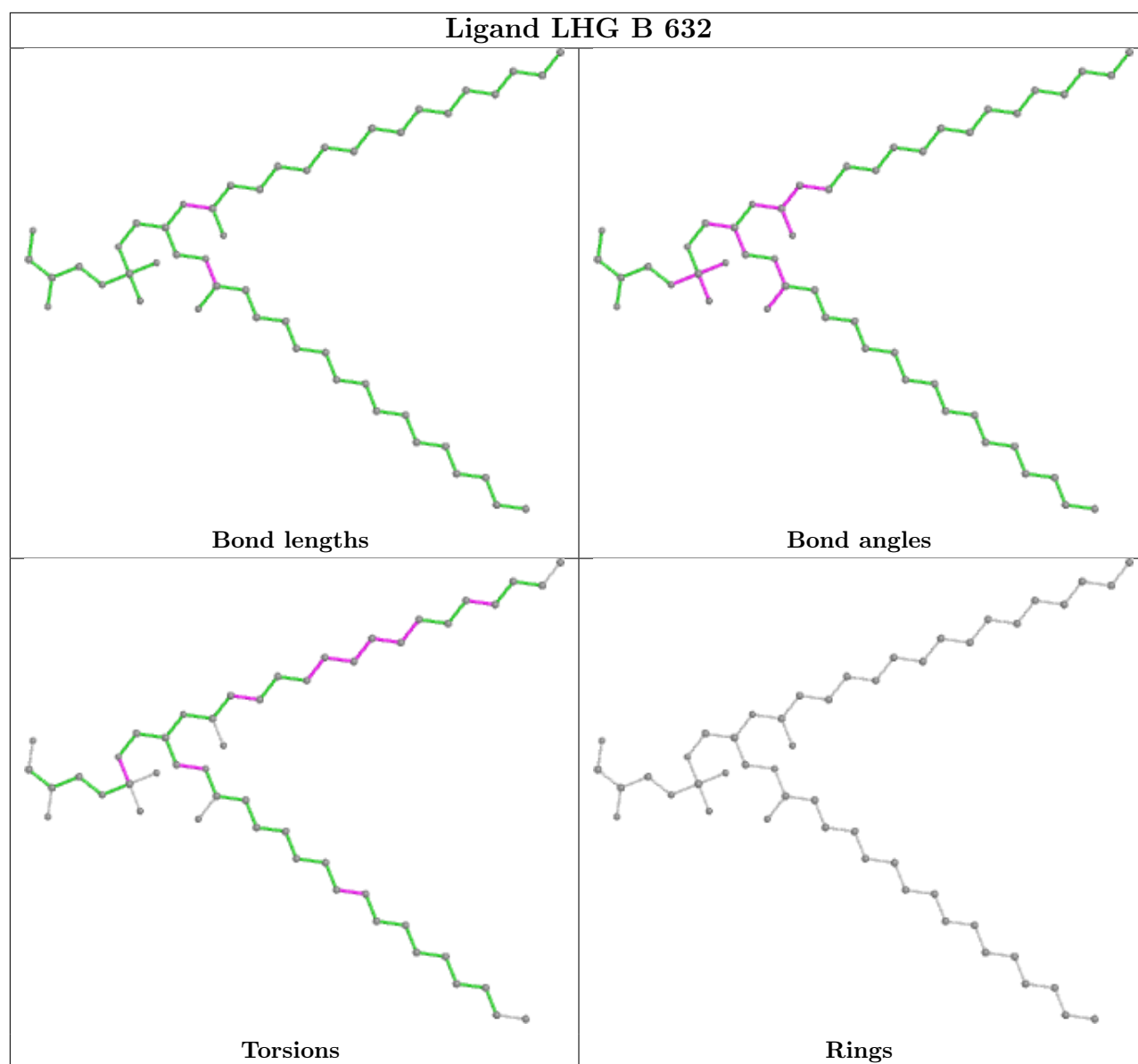


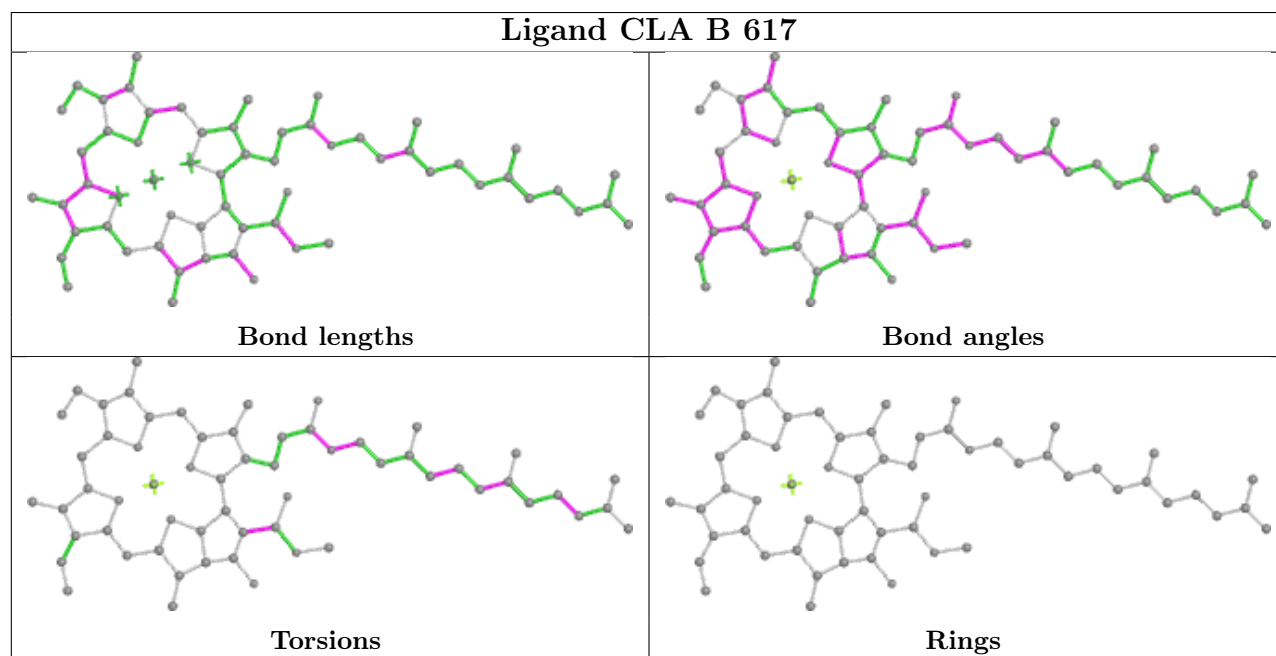
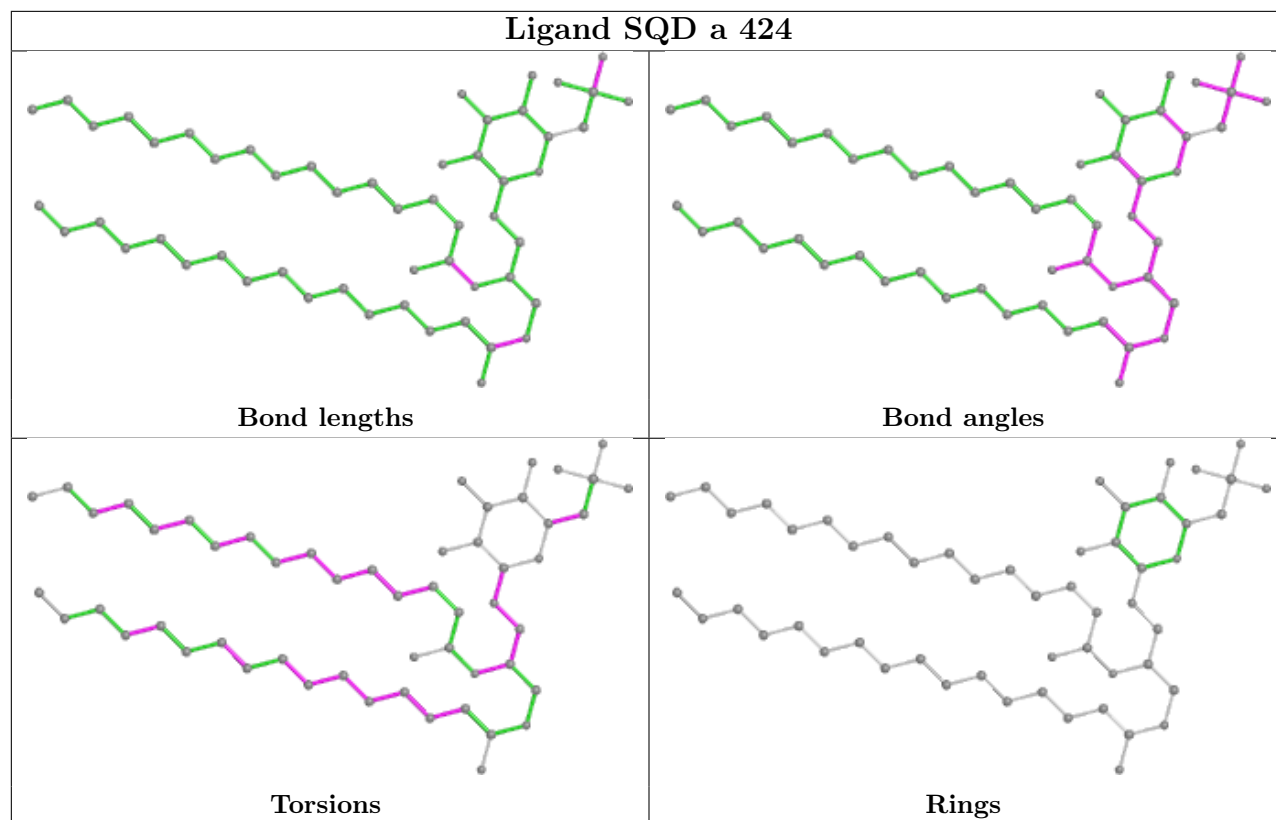


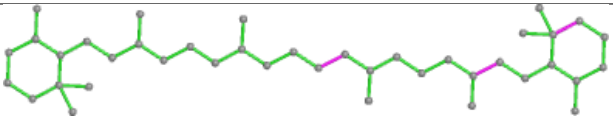
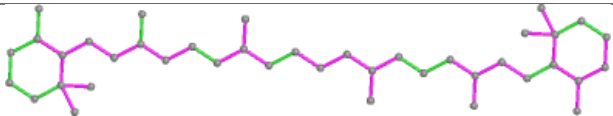
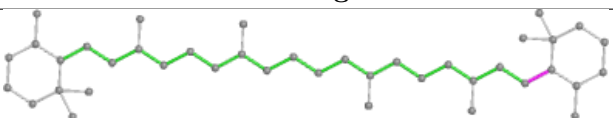
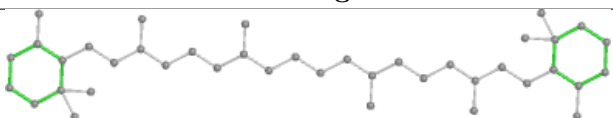
Ligand CLA c 513**Ligand CLA D 403**

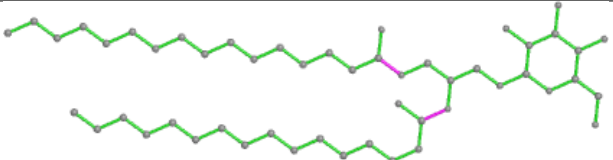
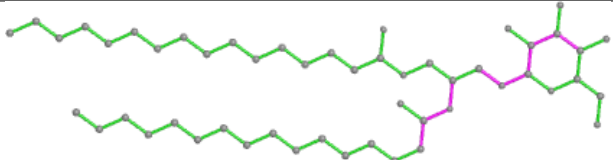
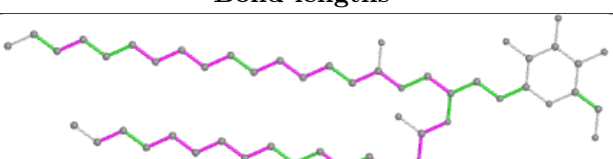
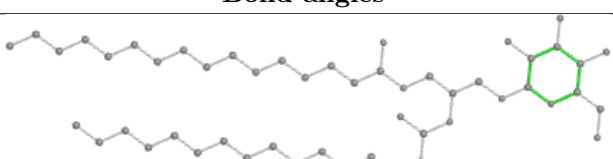


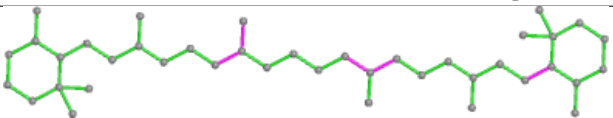
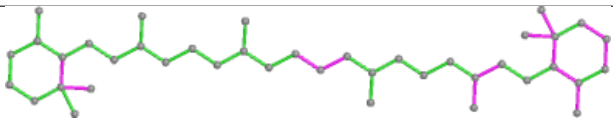
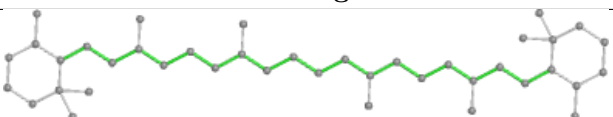
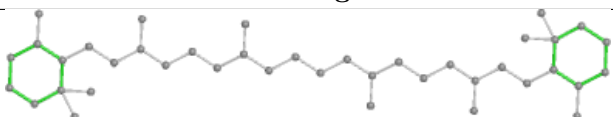
Ligand CLA C 501**Ligand PHO D 401**

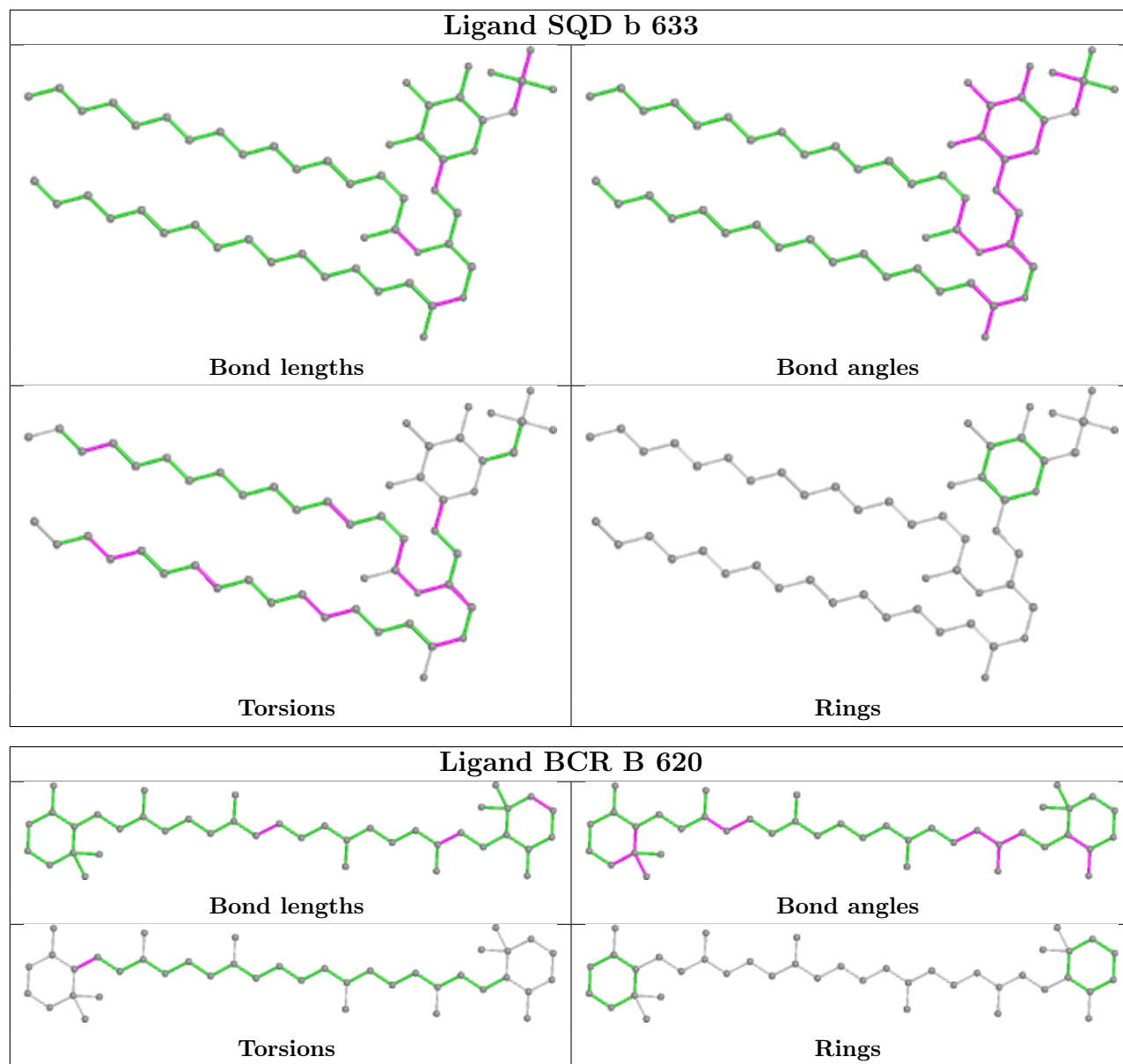


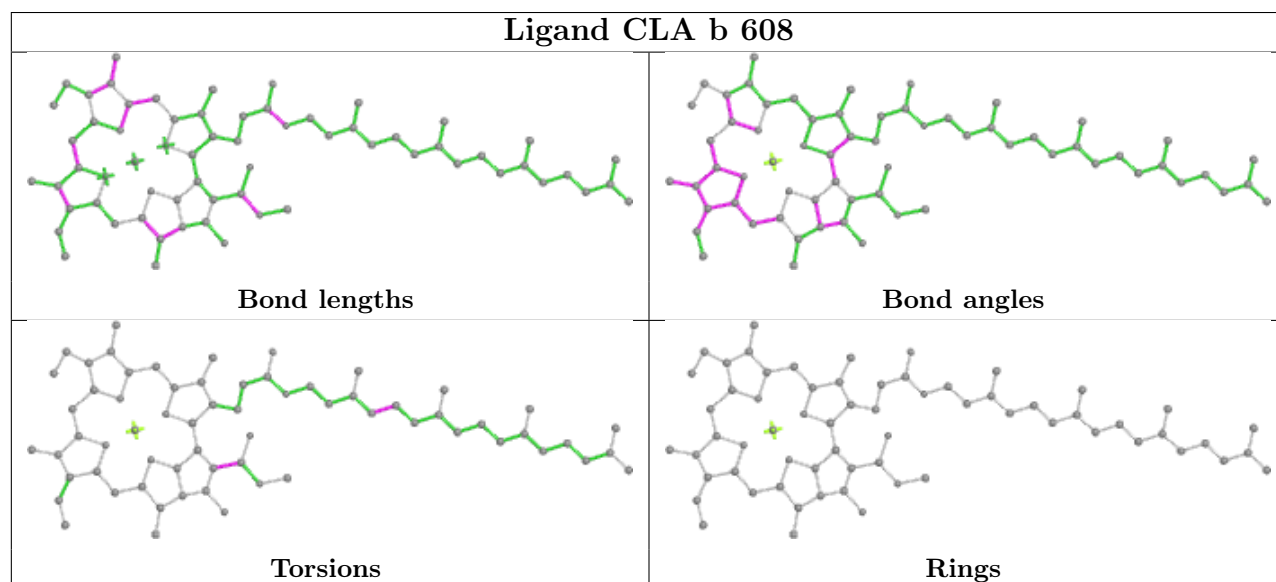
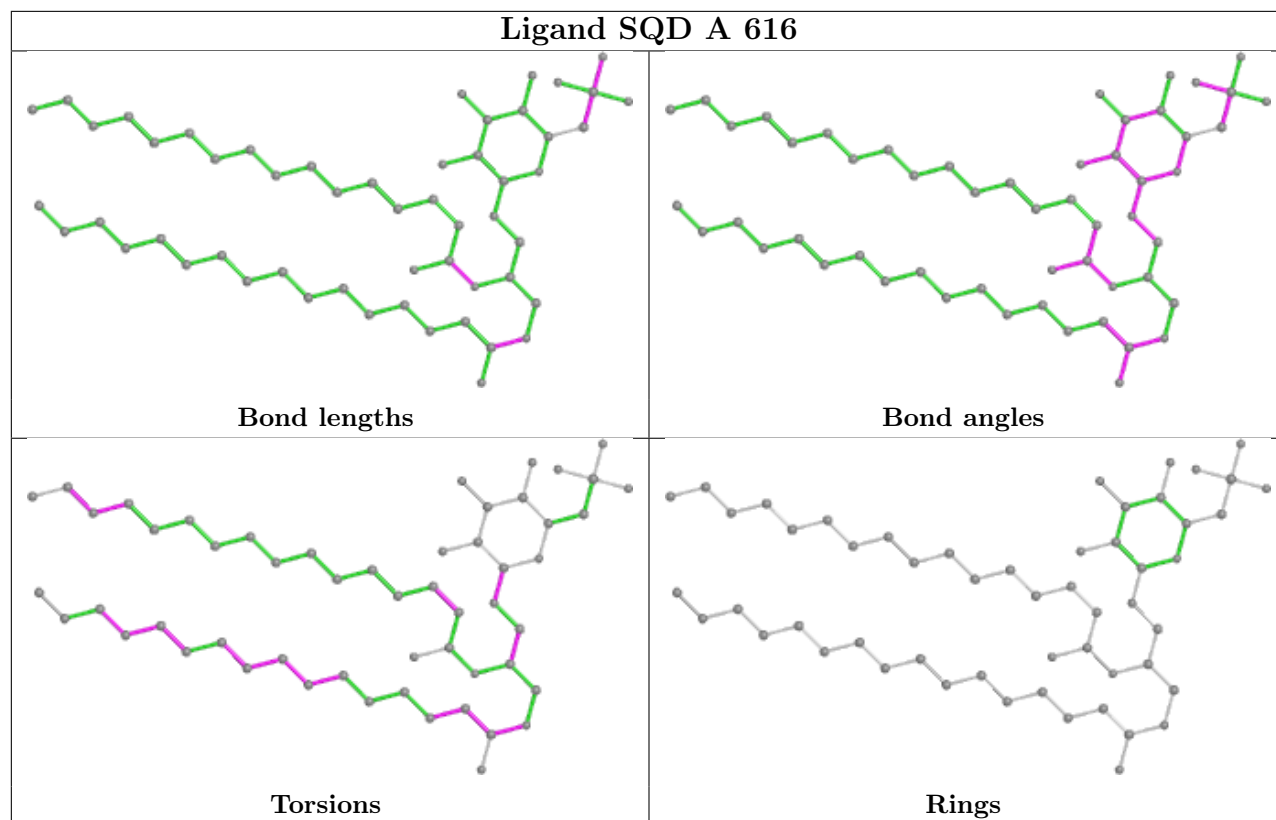


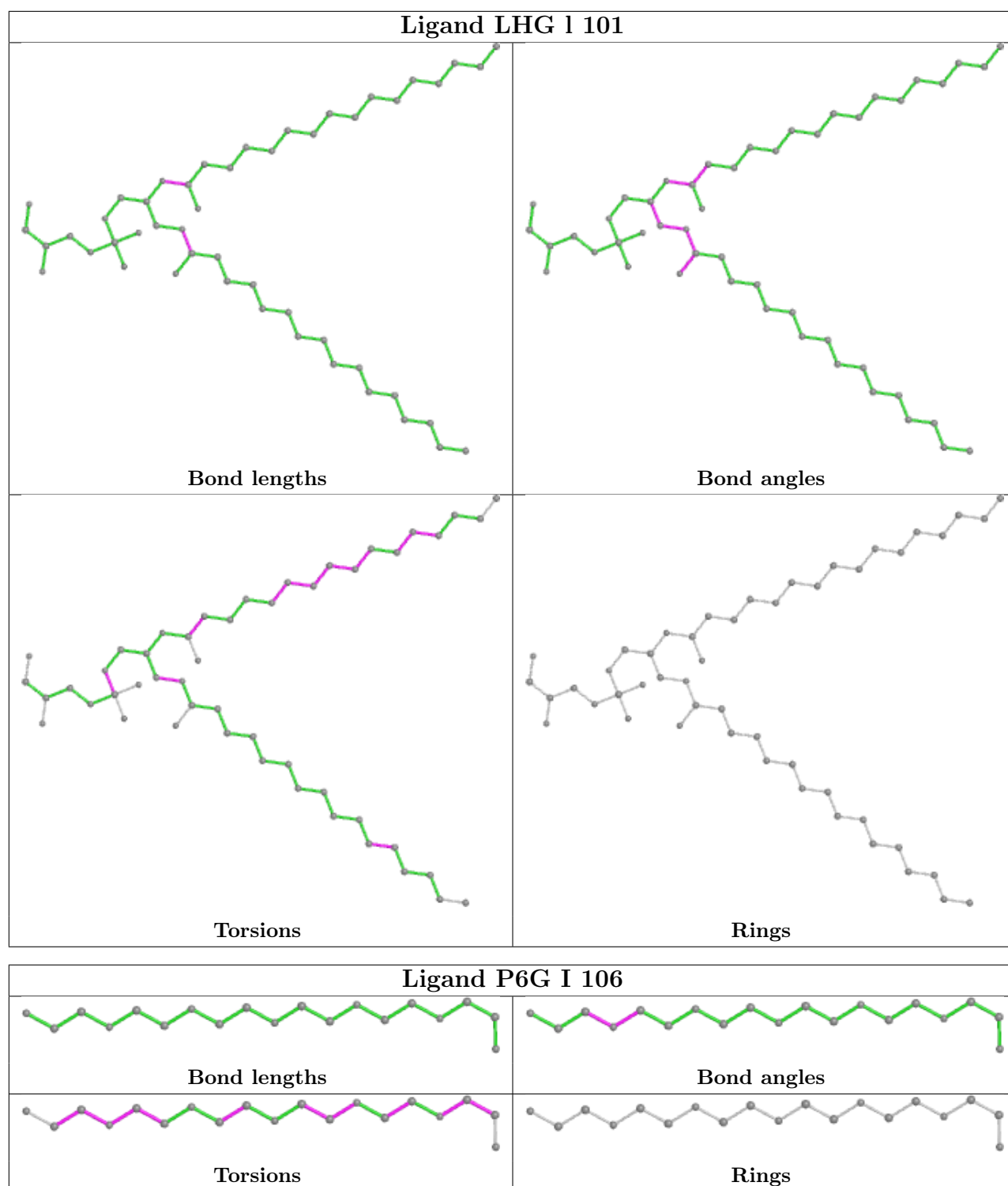
Ligand BCR t 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

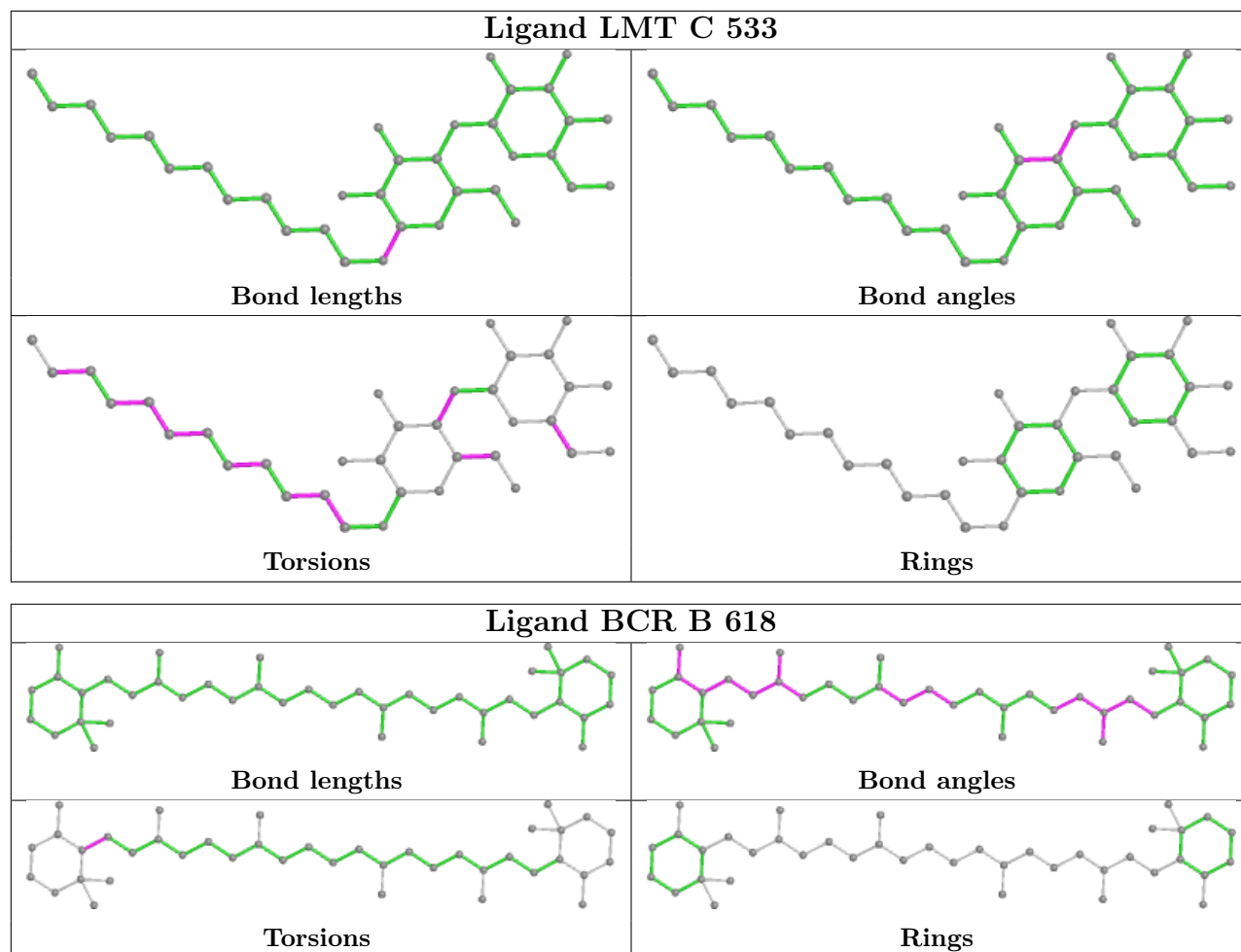
Ligand LMG a 414	
	
Bond lengths	Bond angles
	
Torsions	Rings

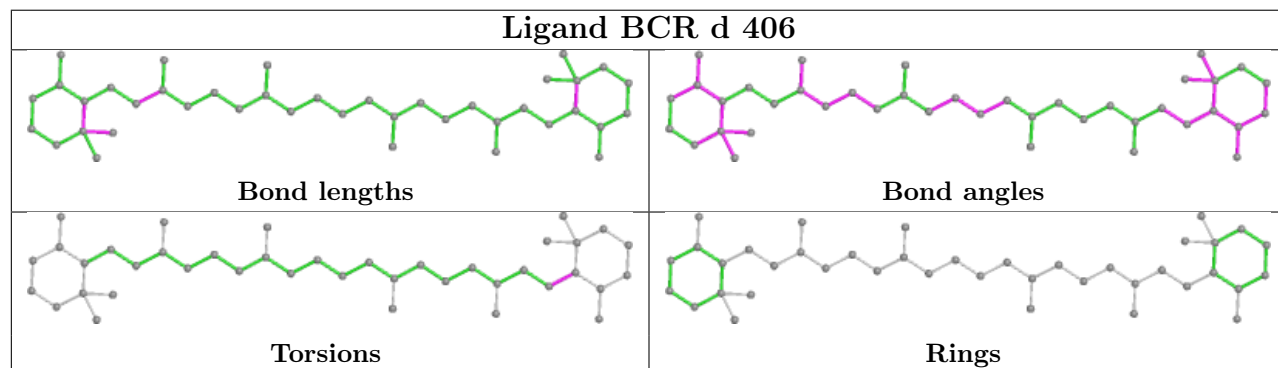
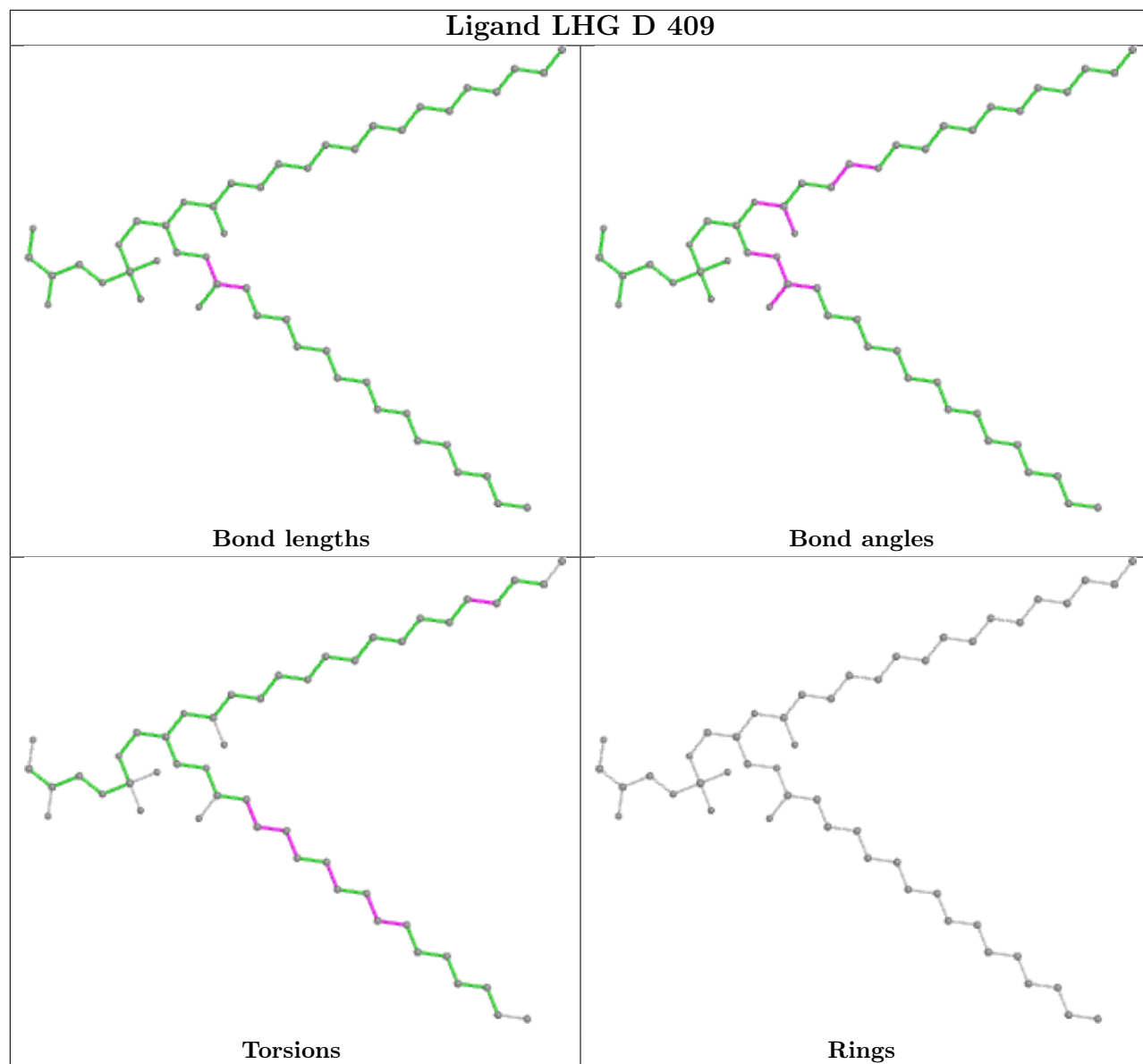
Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

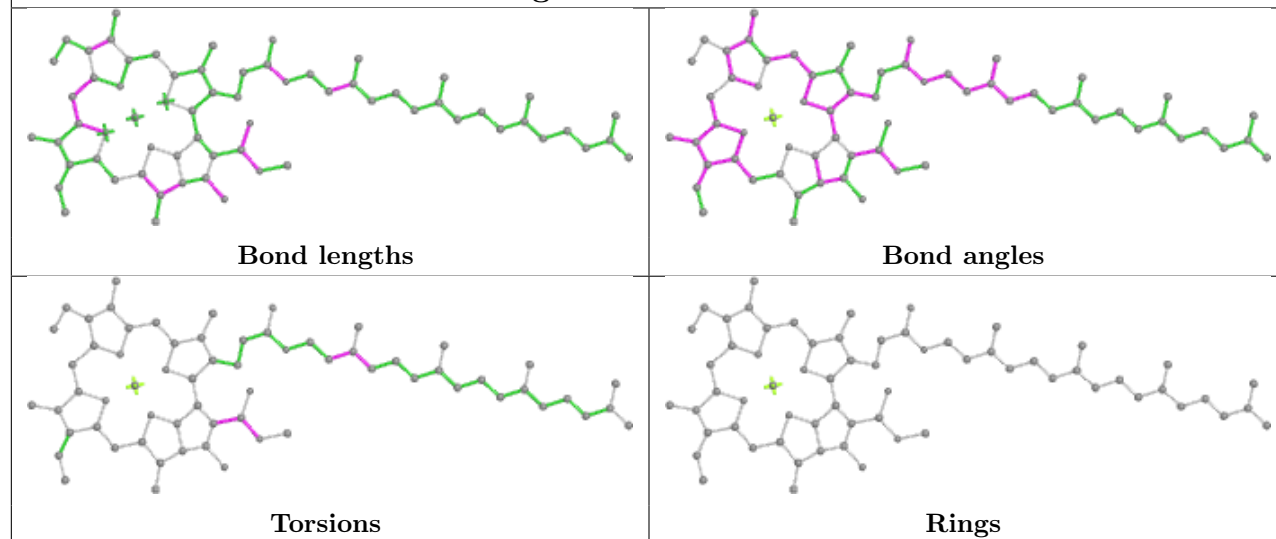
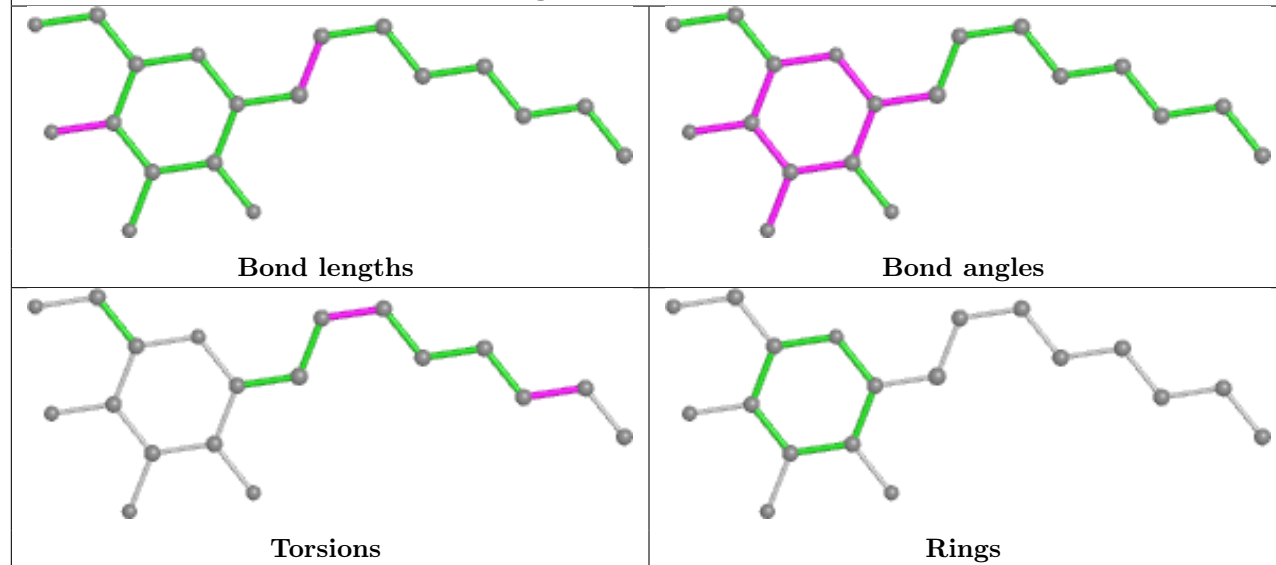
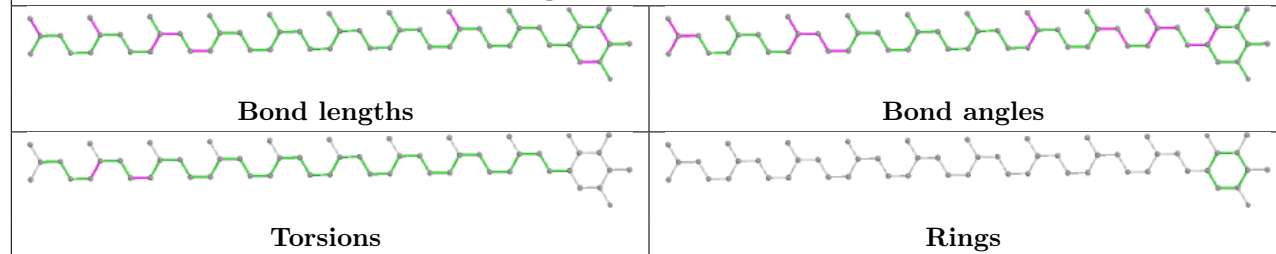


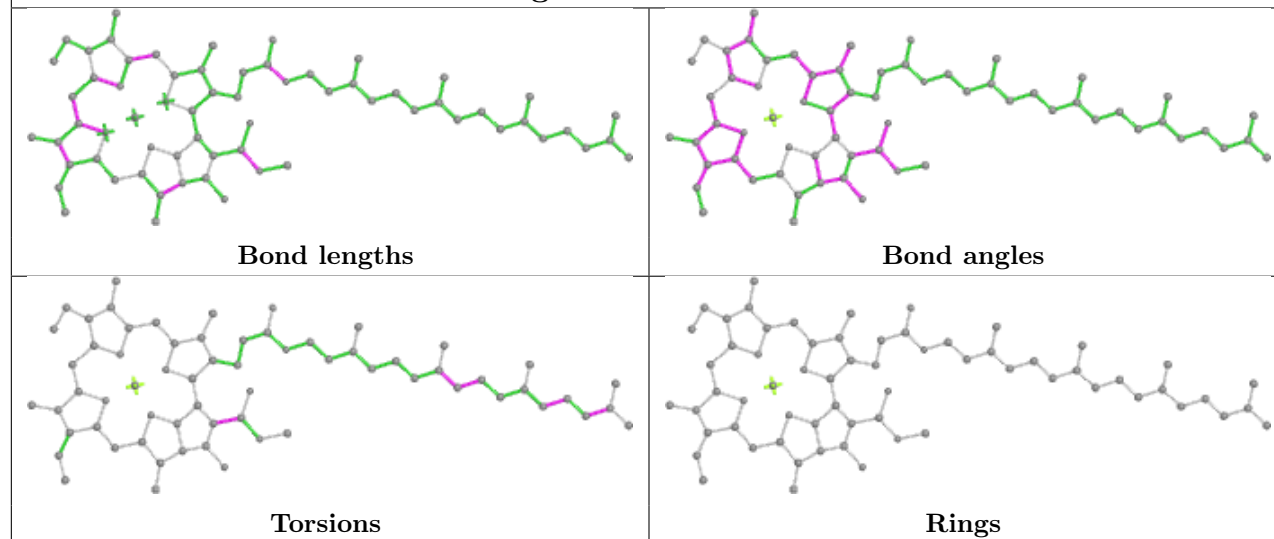
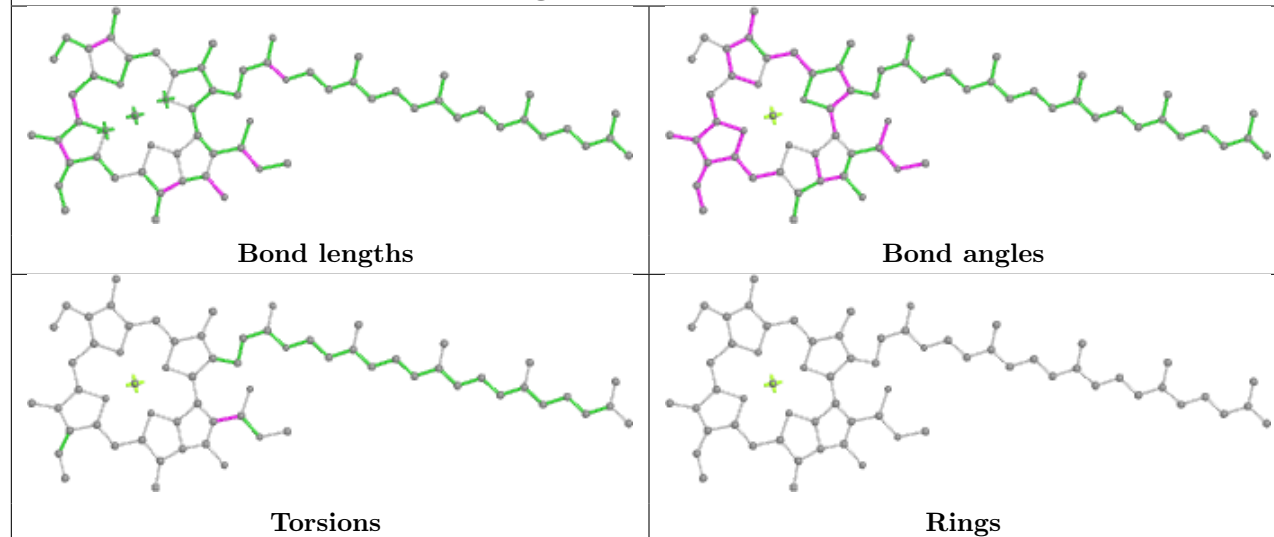
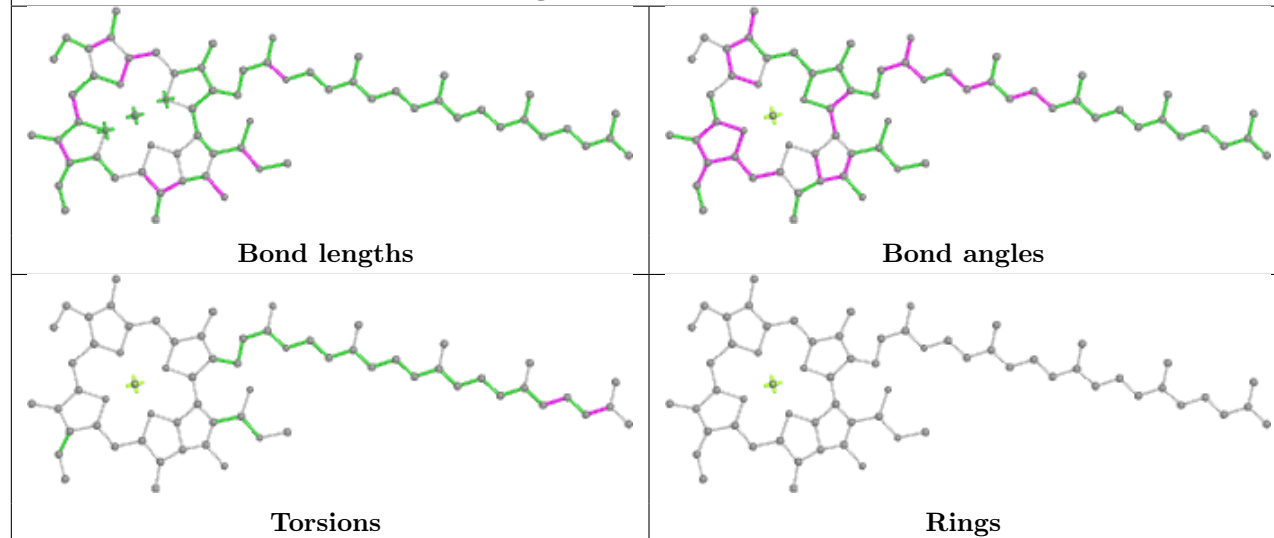


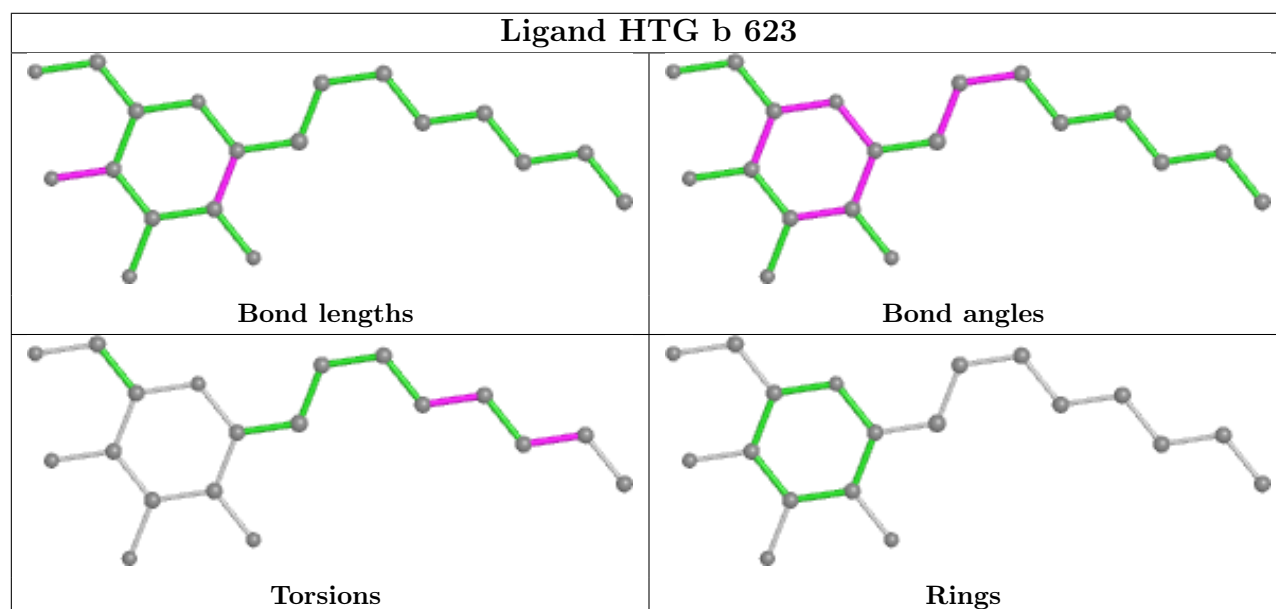
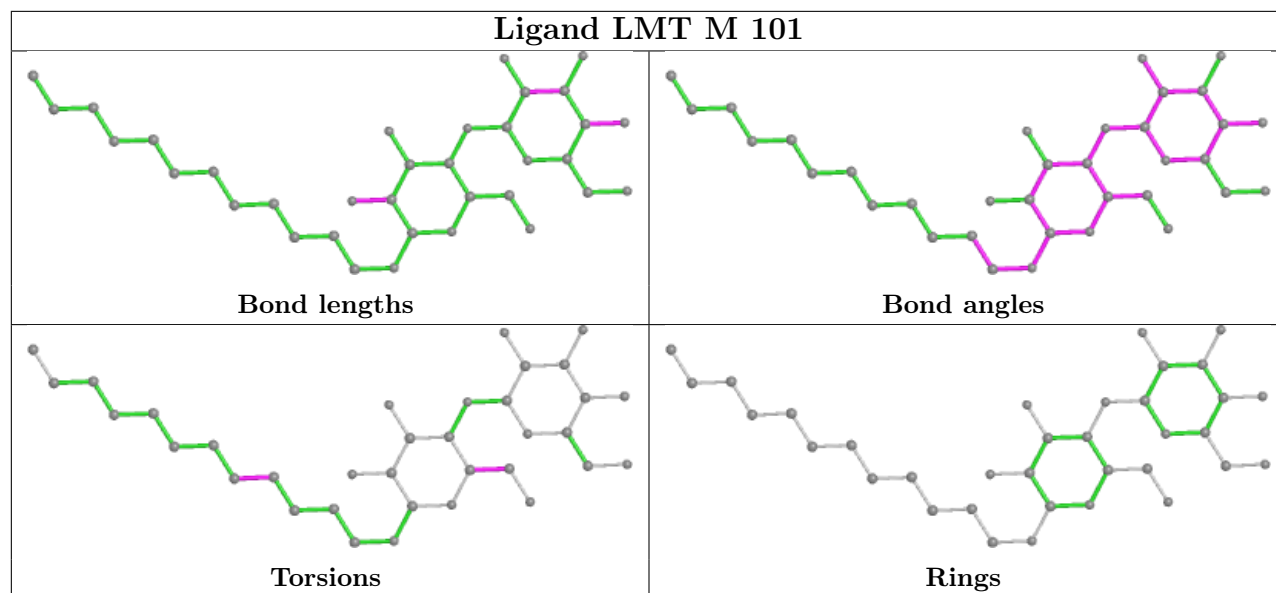


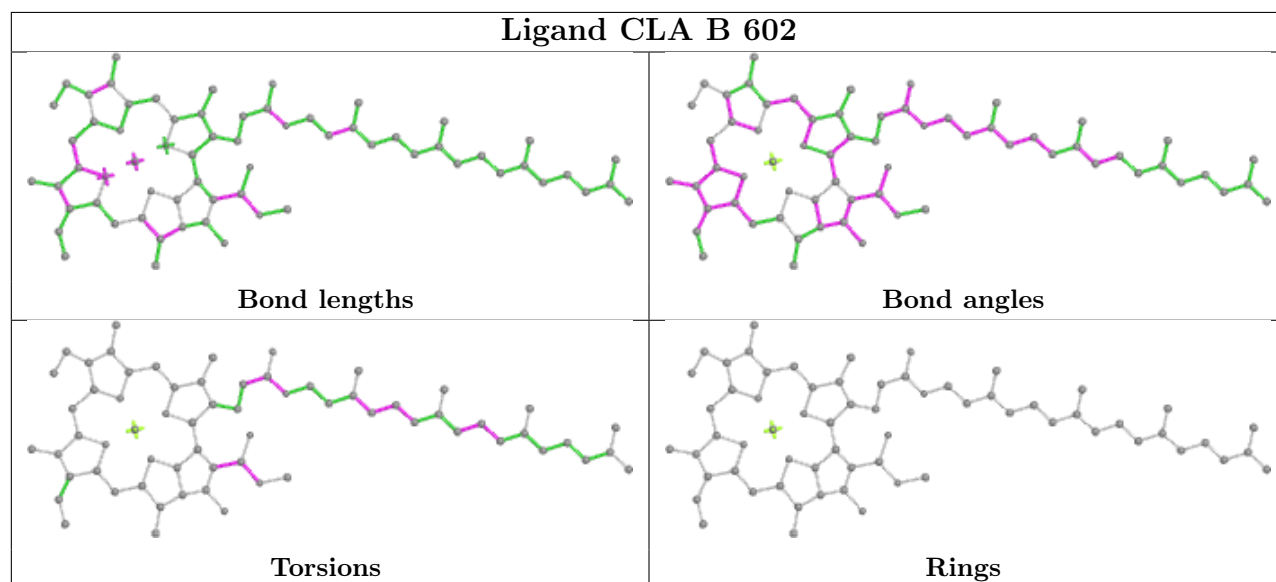
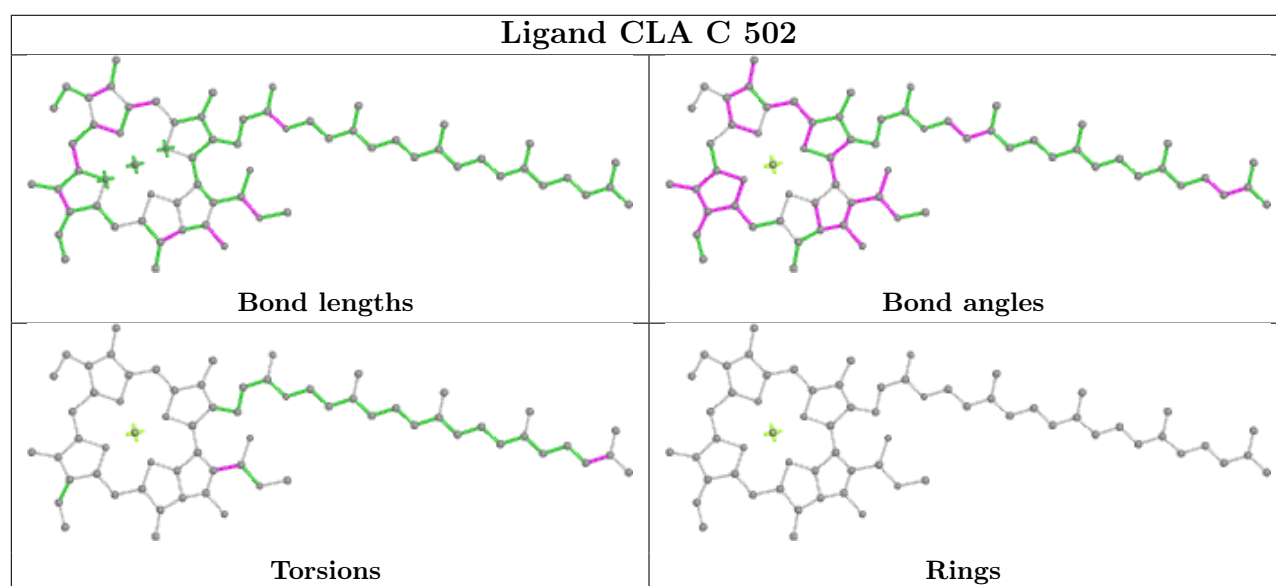
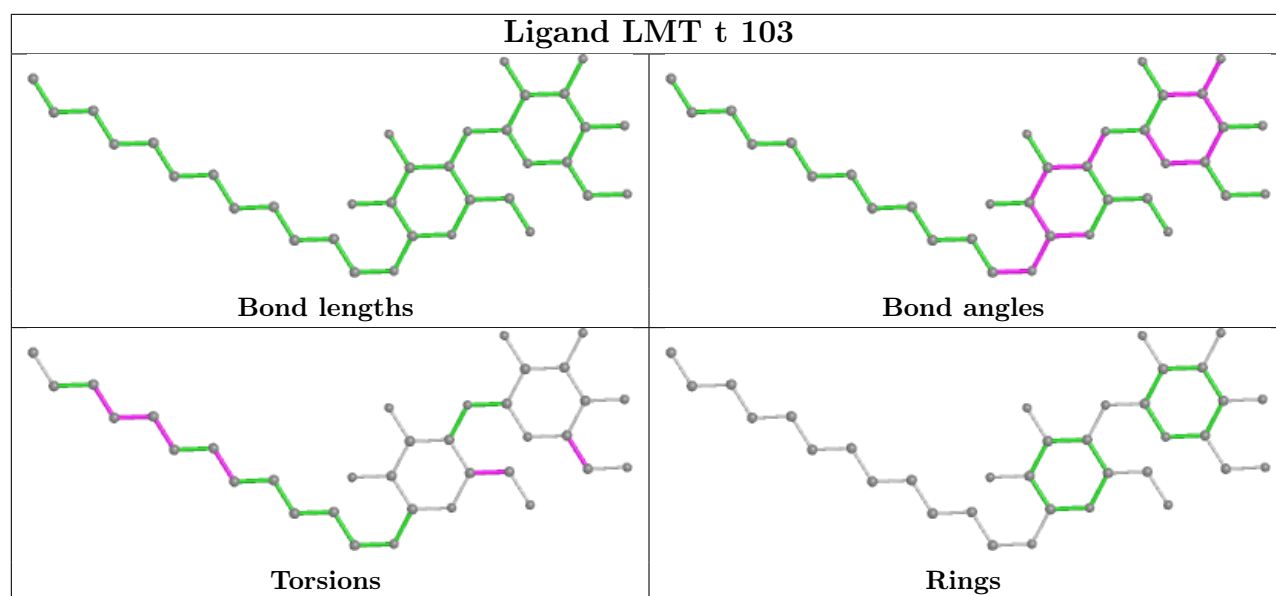


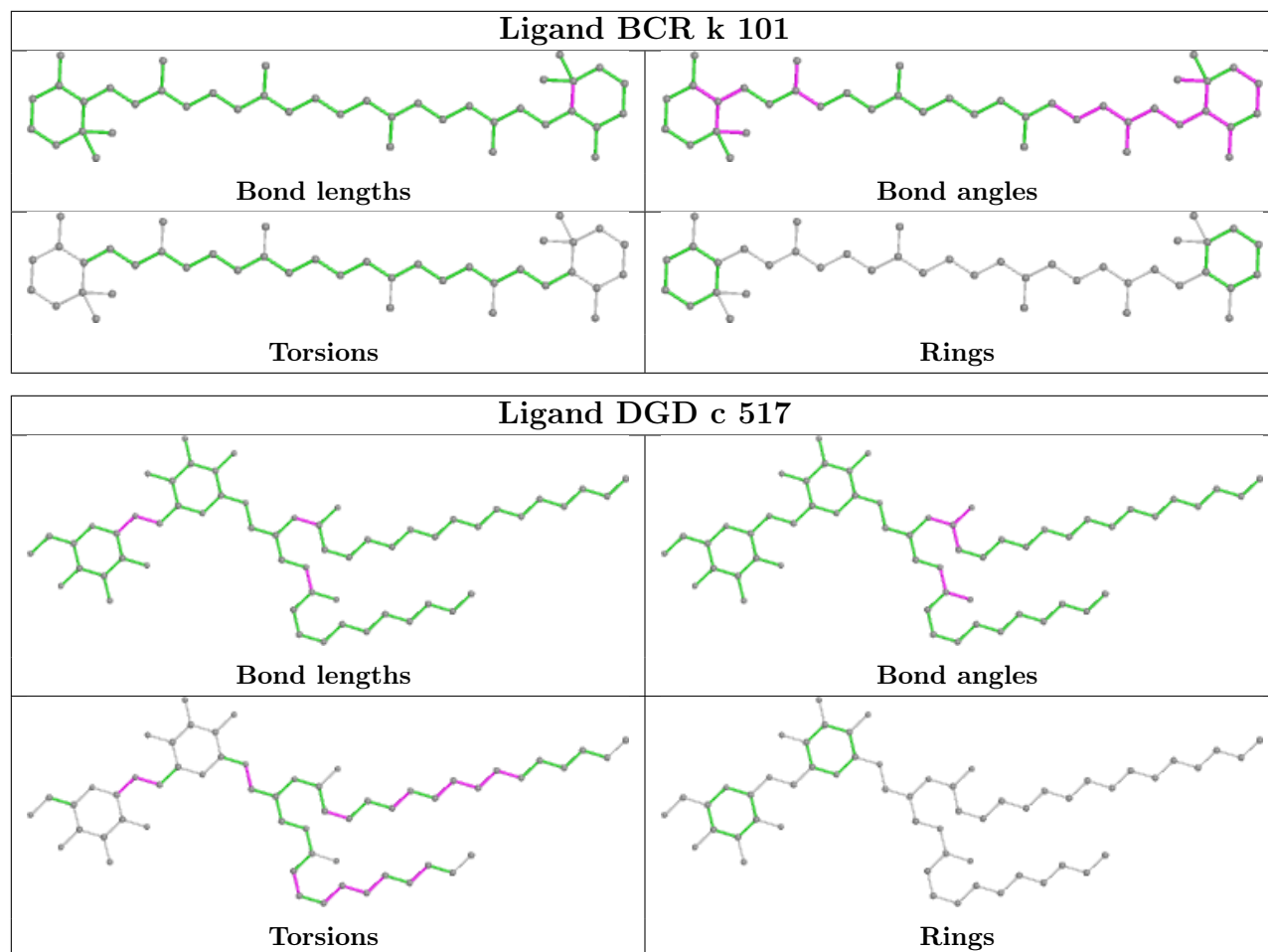


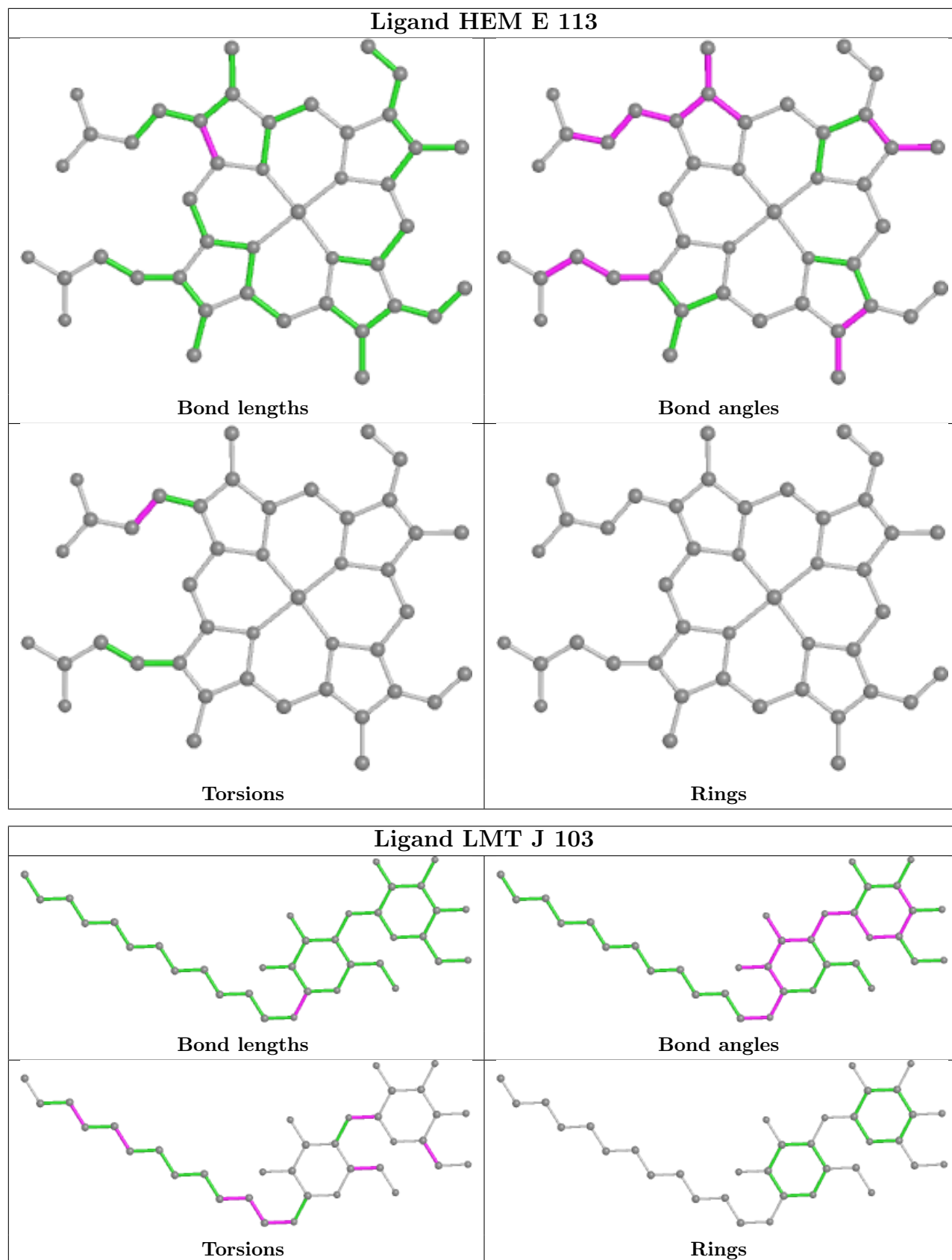
Ligand CLA B 606**Ligand HTG b 631****Ligand PL9 d 407**

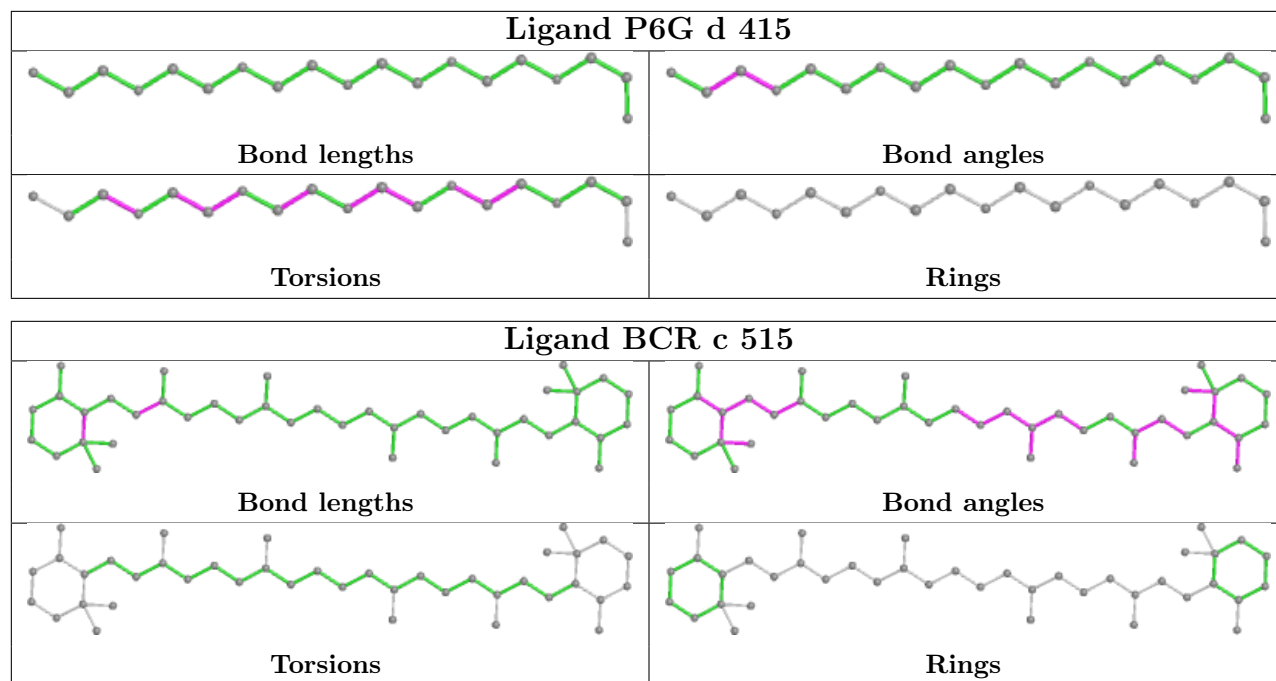
Ligand CLA D 405**Ligand CLA B 610****Ligand CLA B 614**

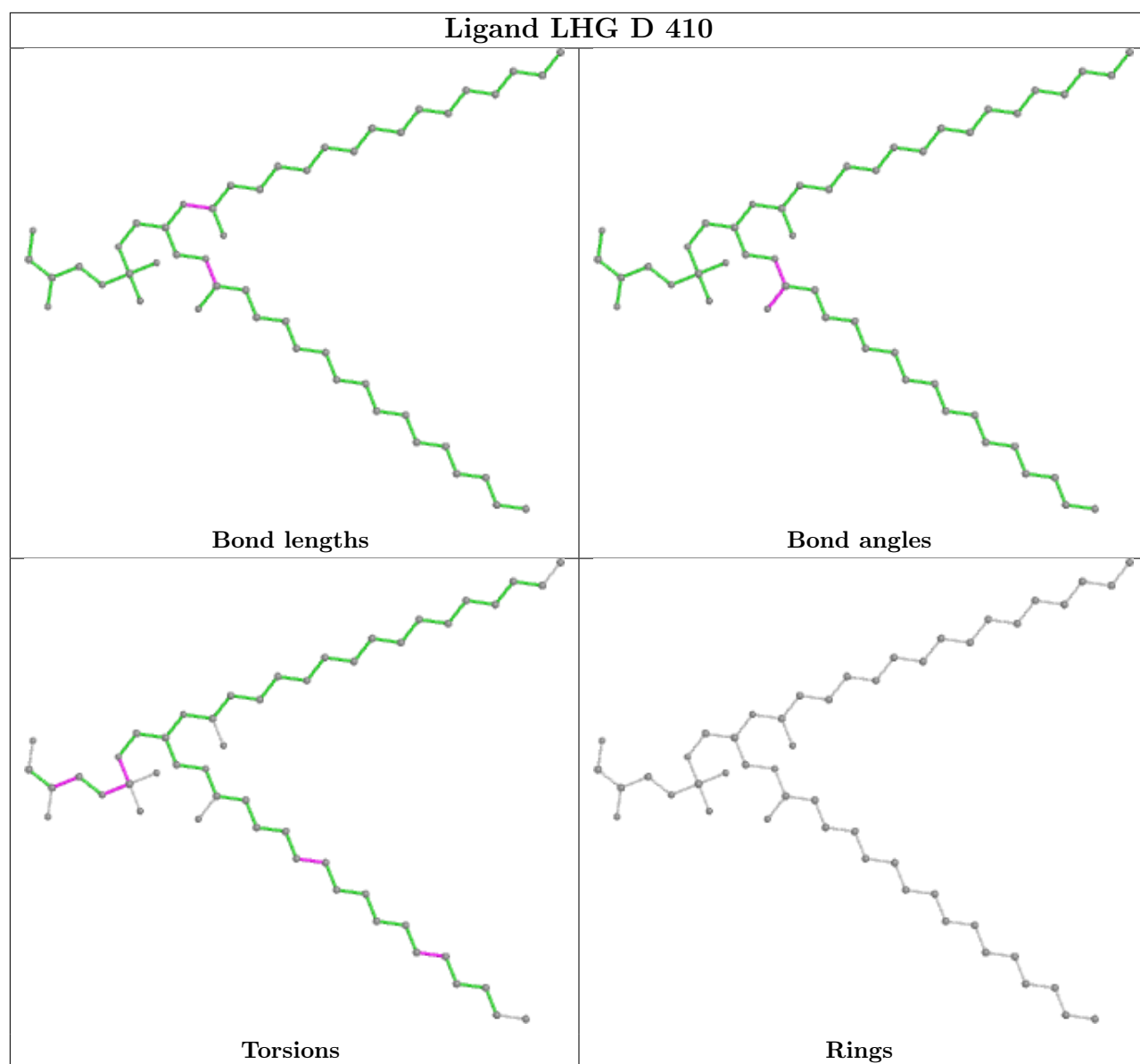


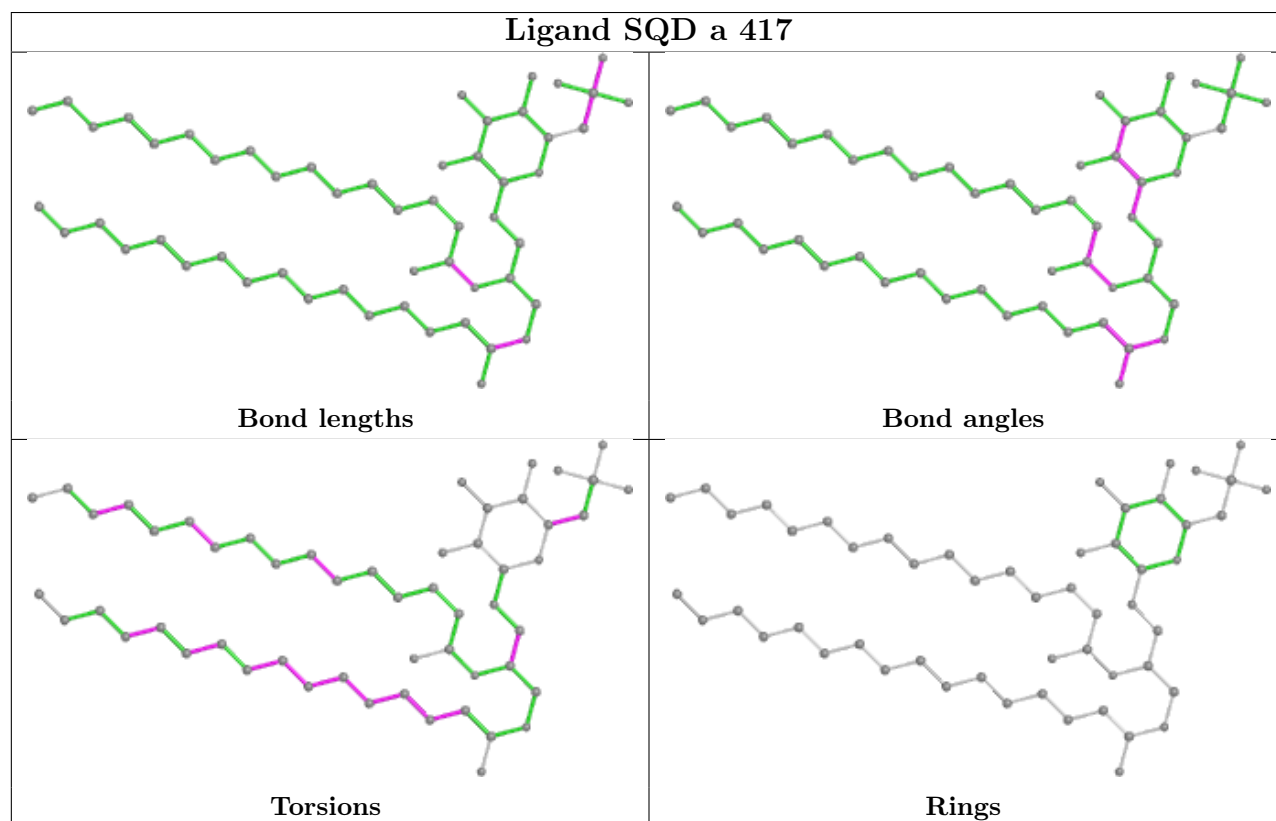
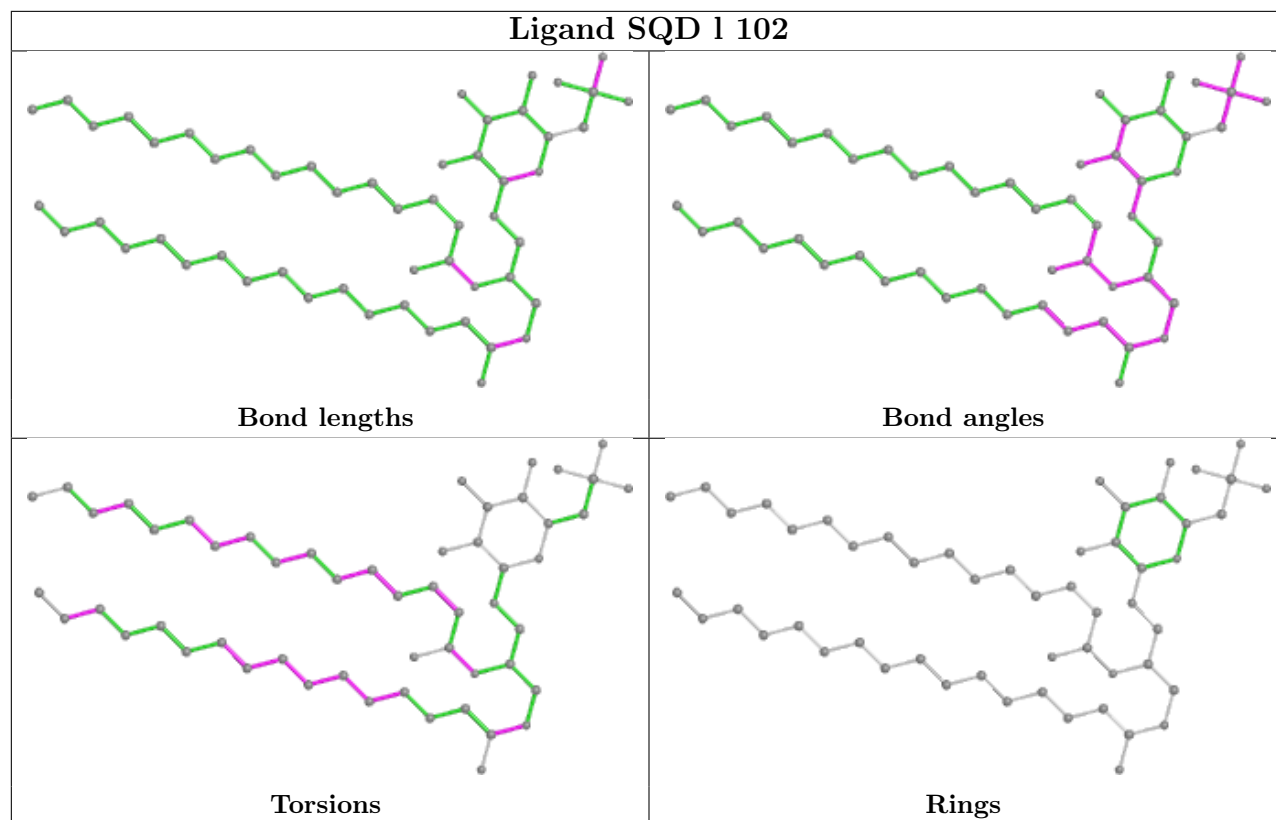


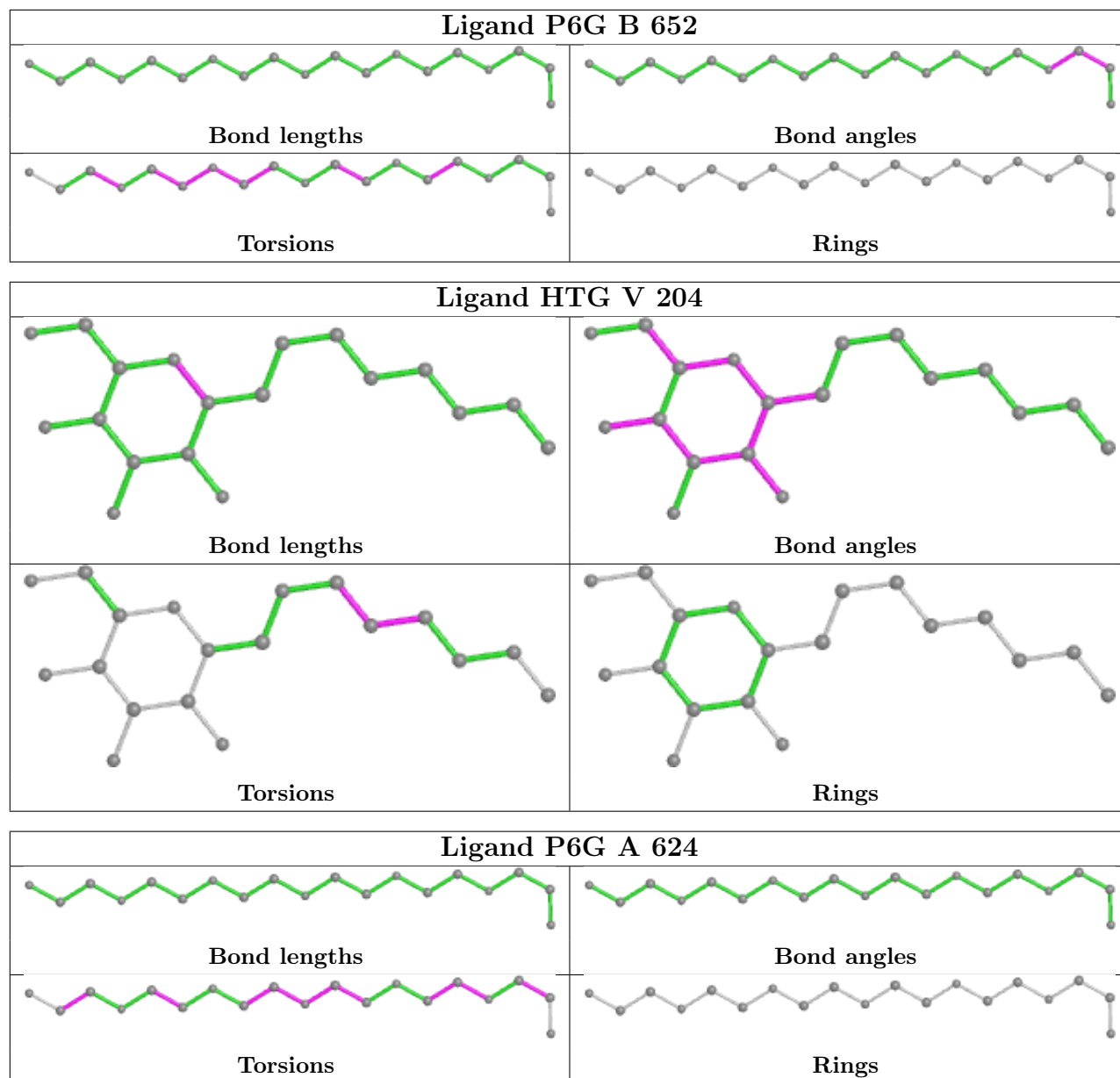


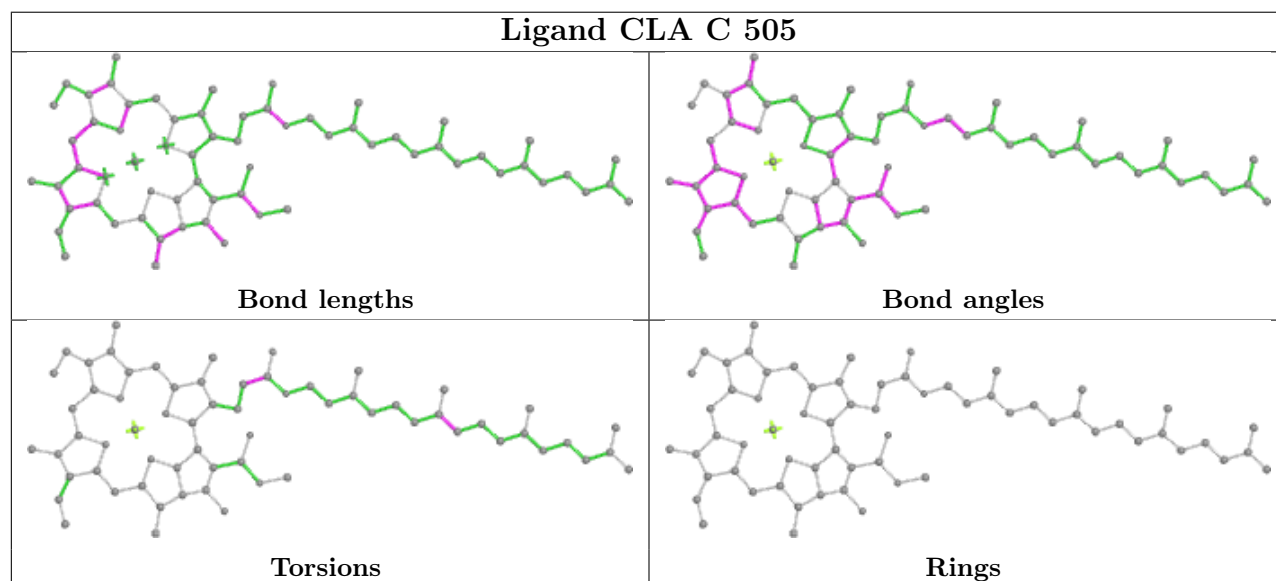
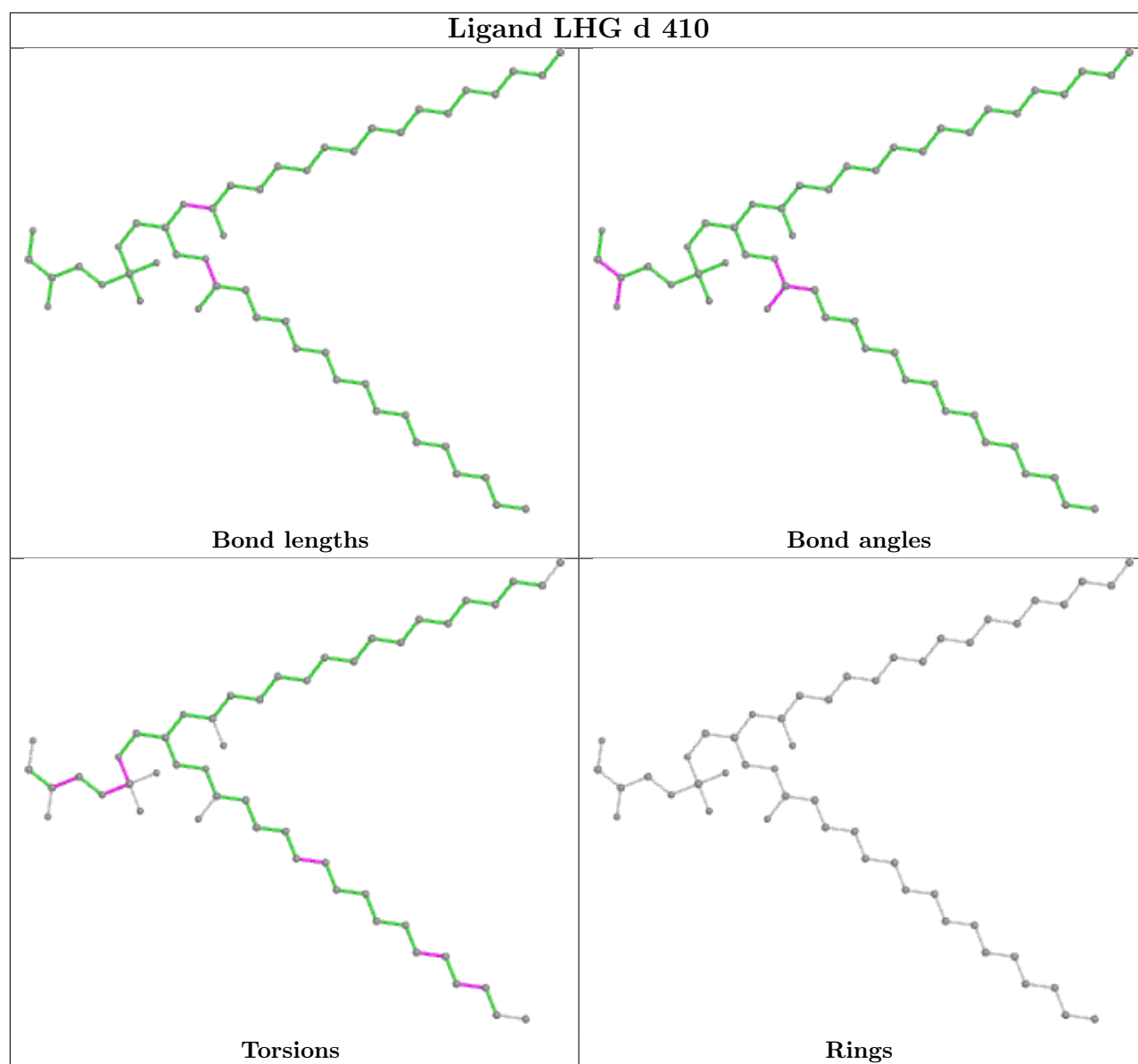


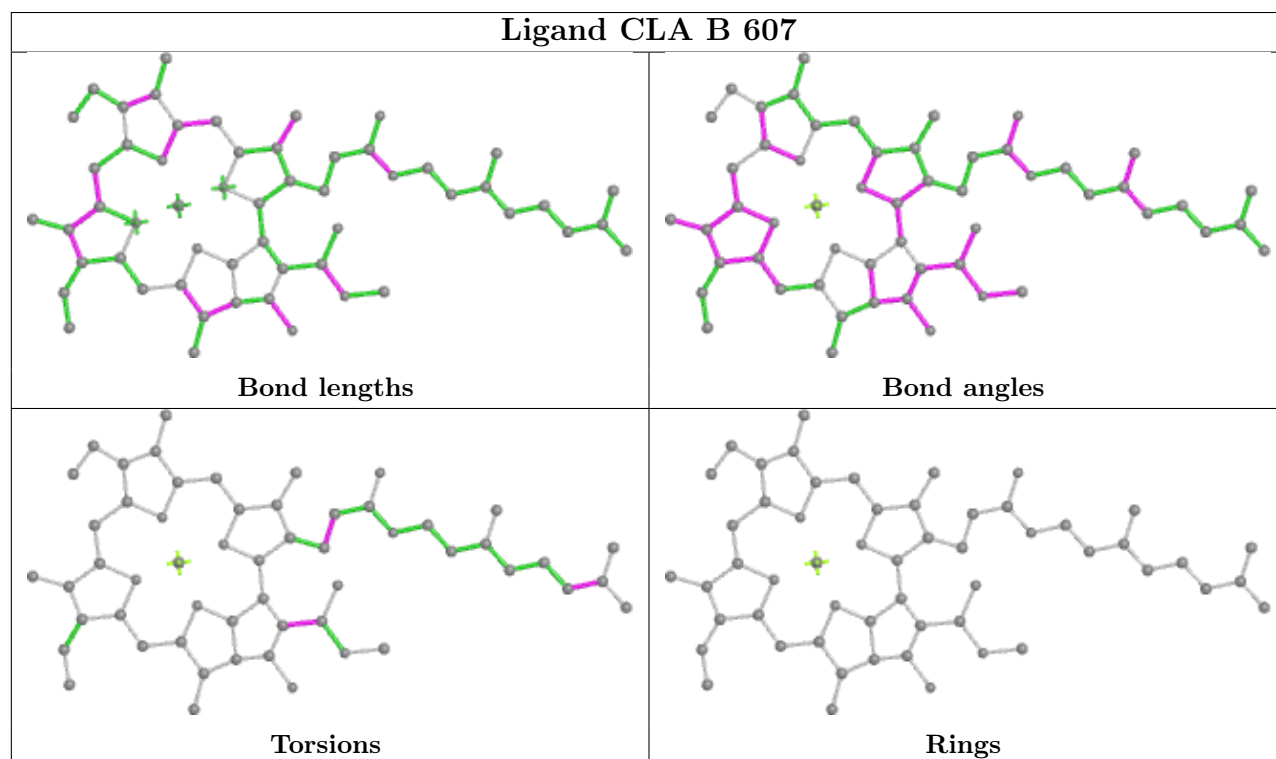
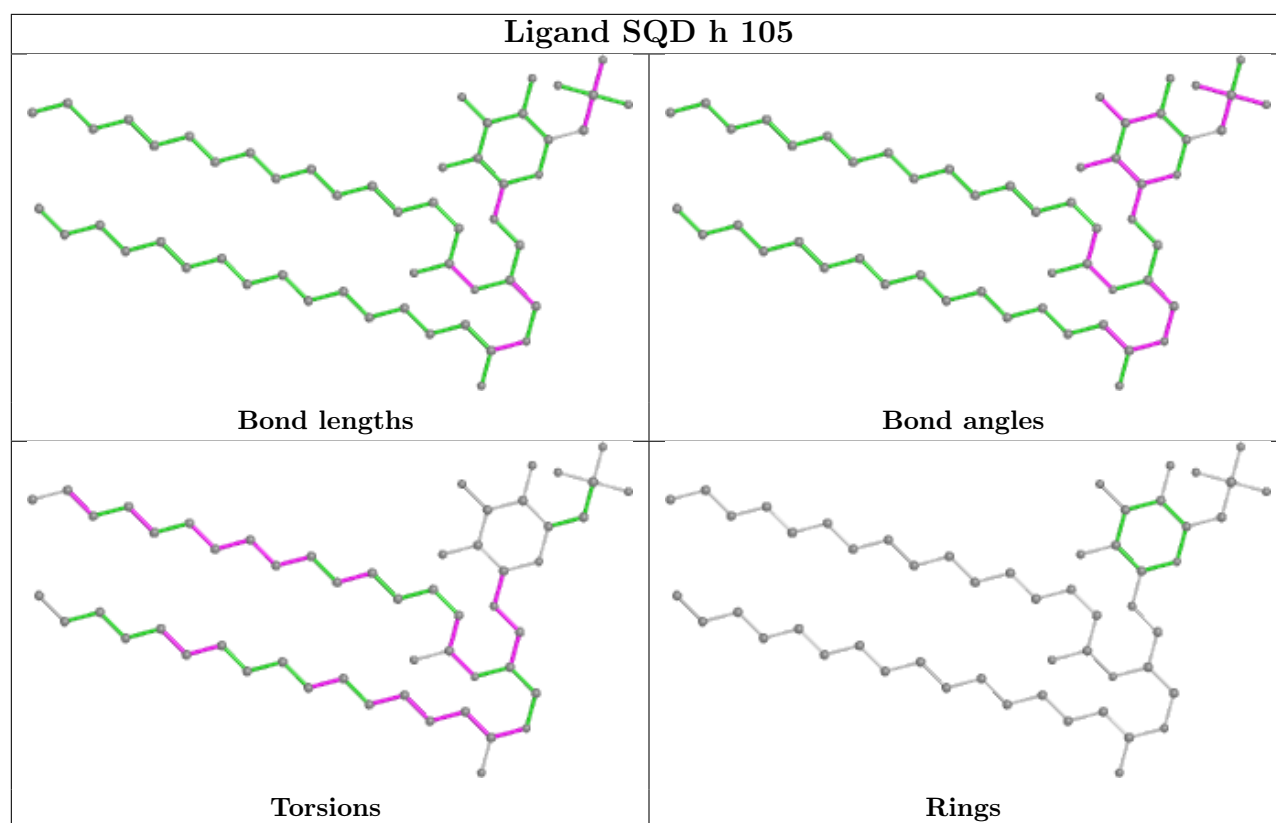


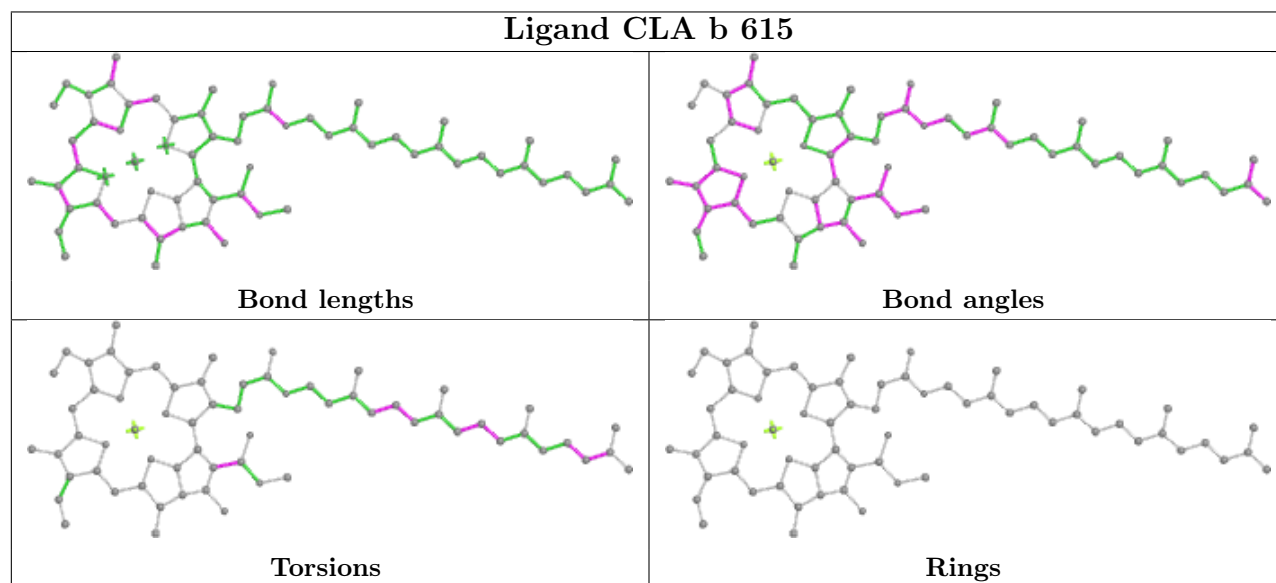
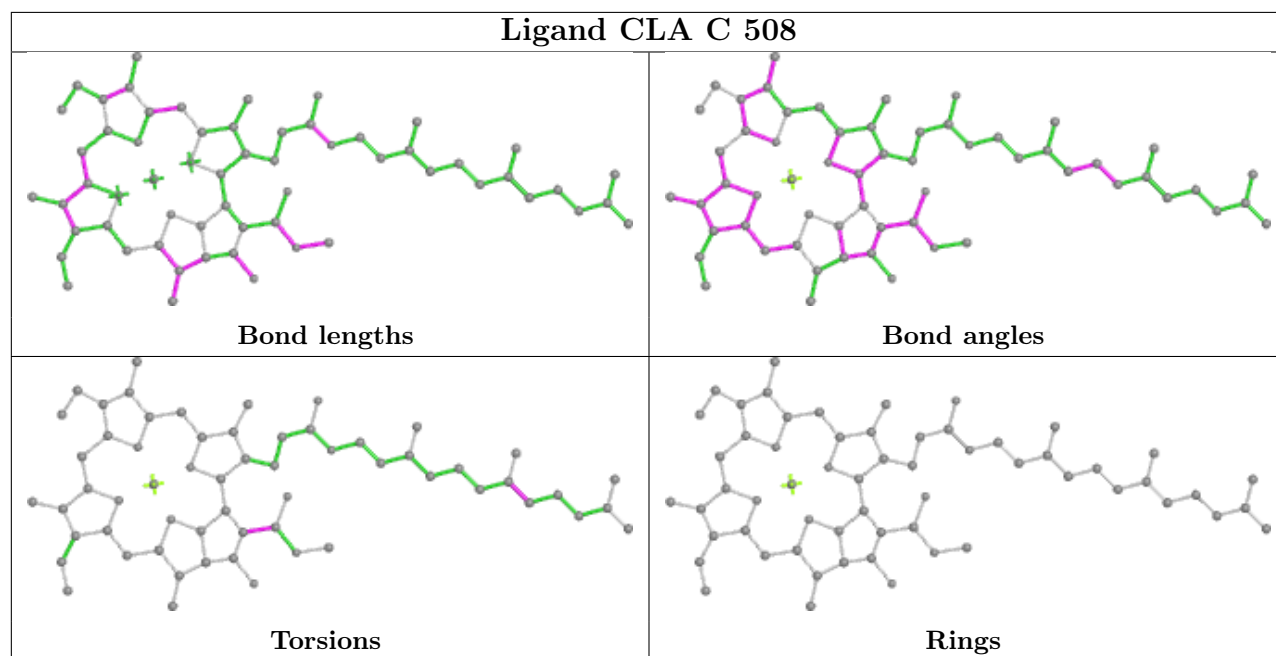
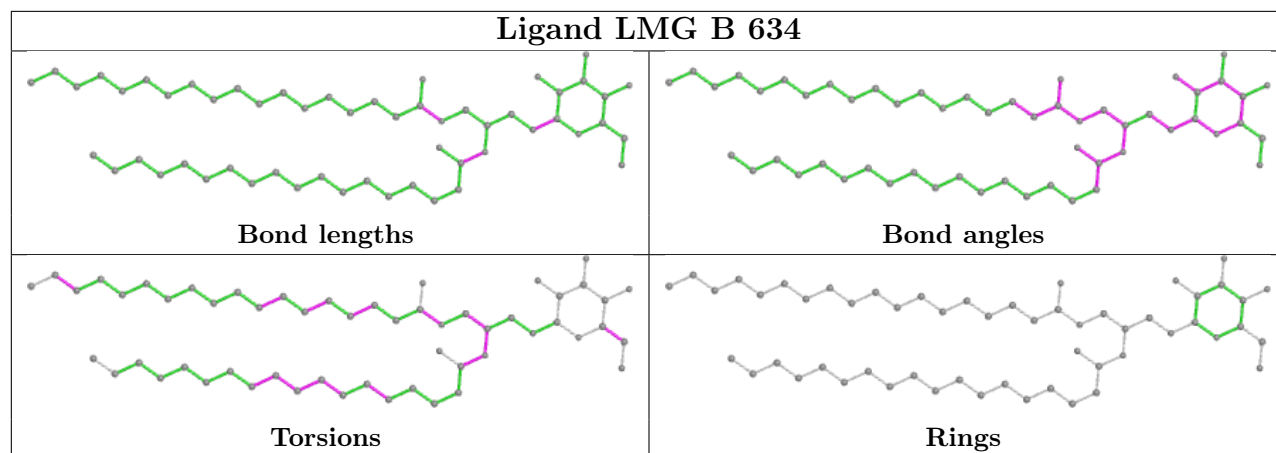




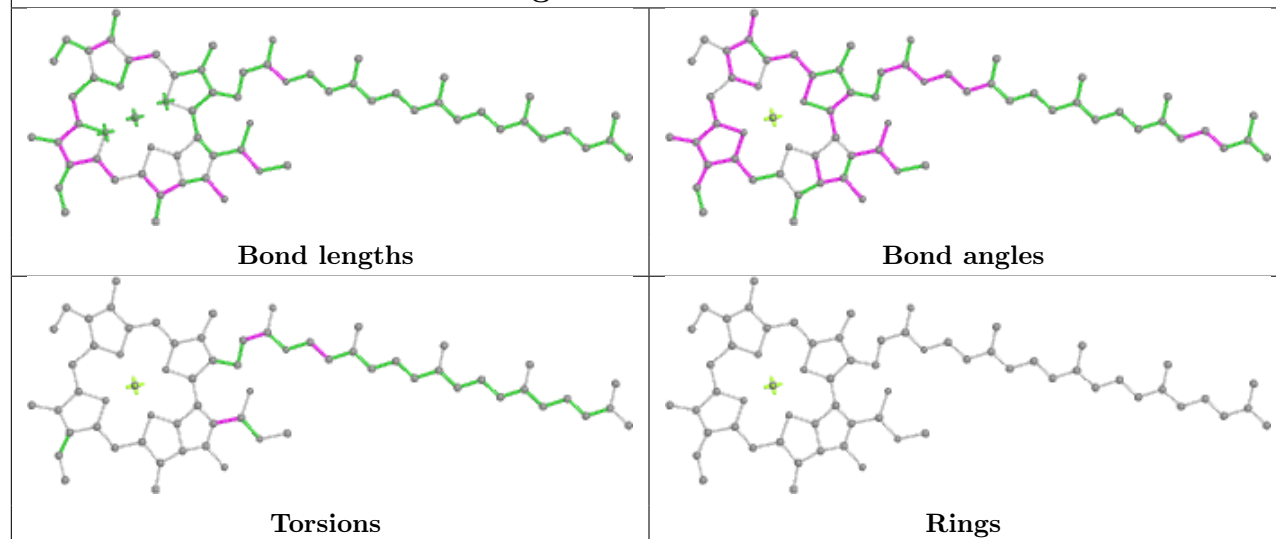




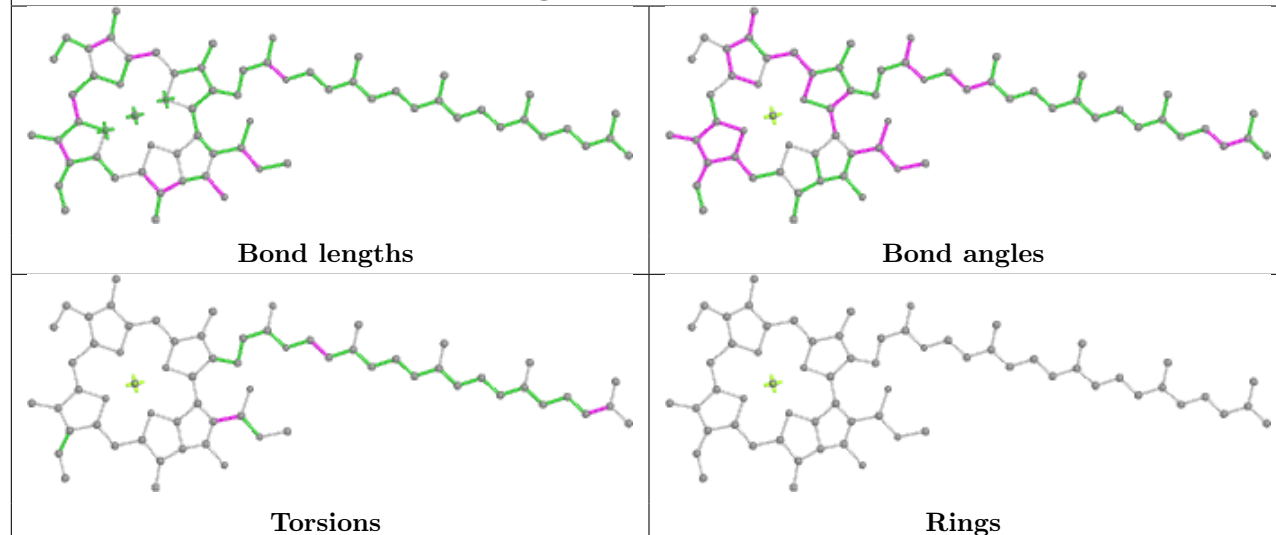




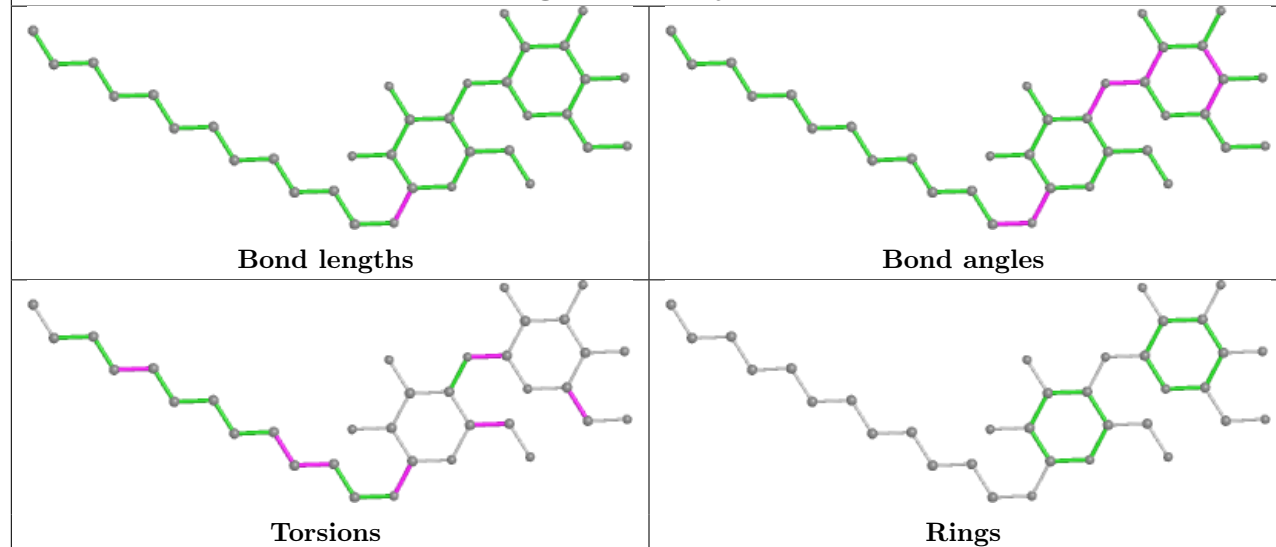
Ligand CLA C 512



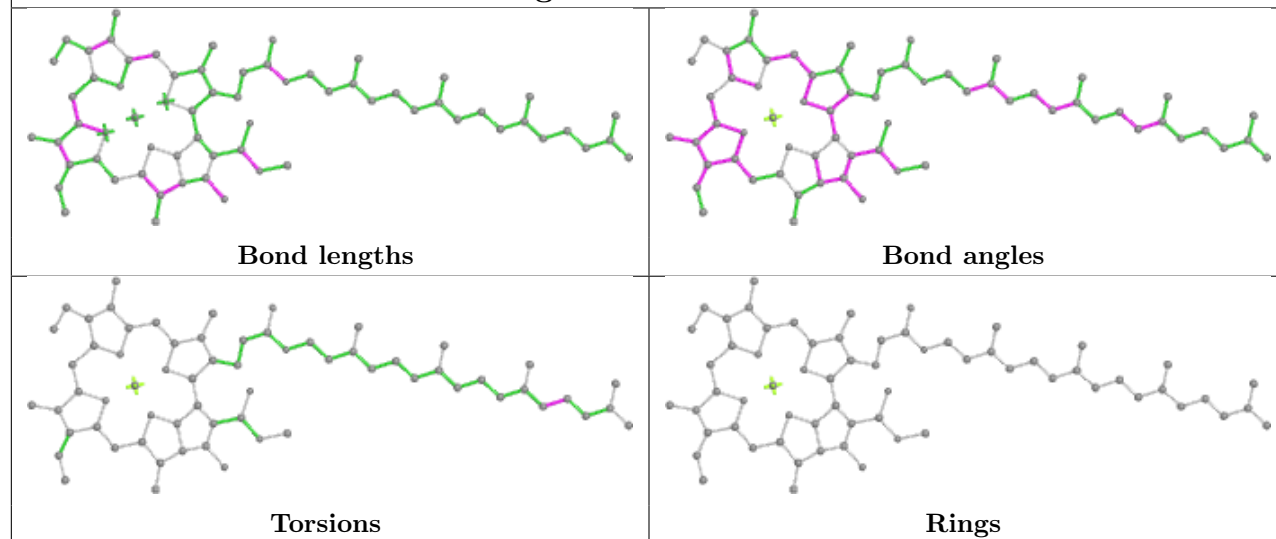
Ligand CLA b 603



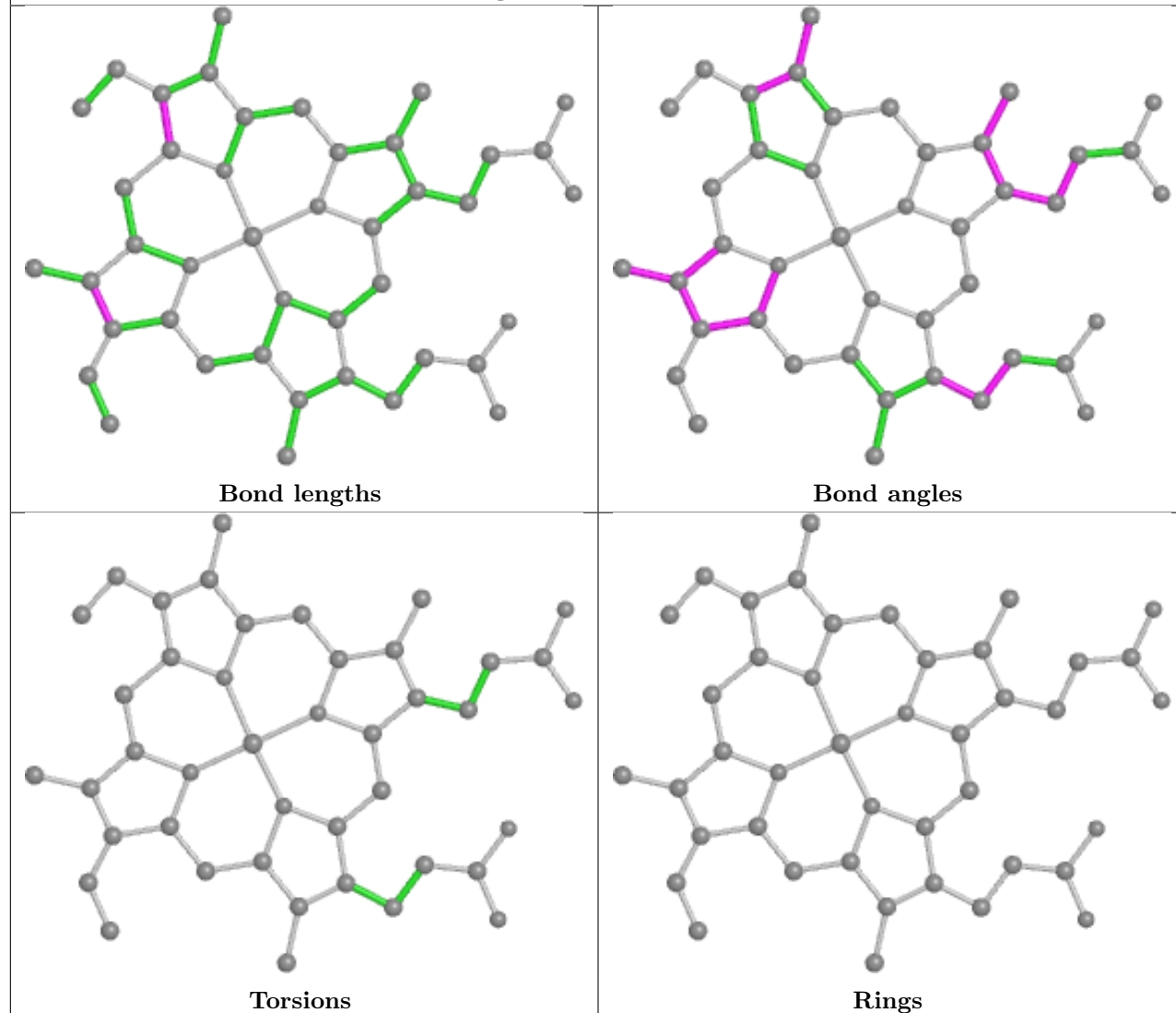
Ligand LMT j 103

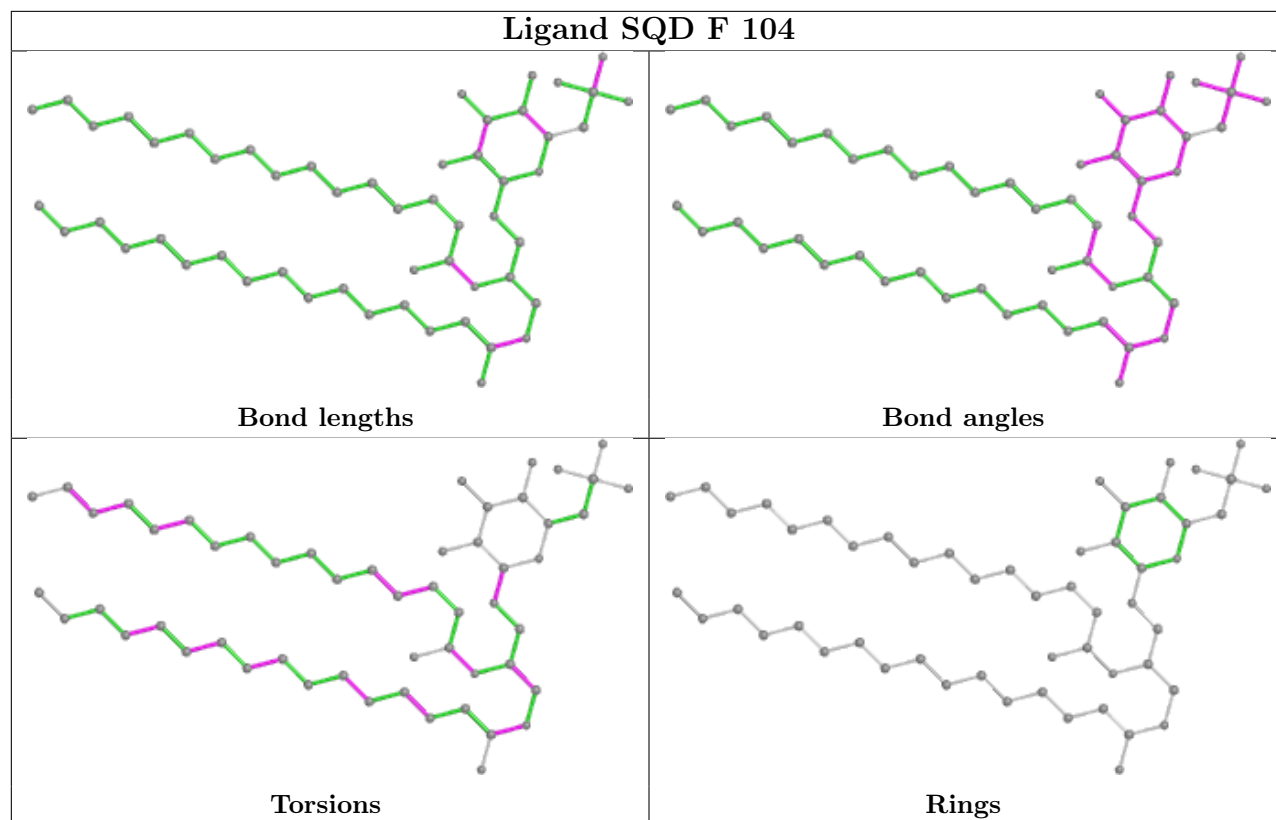


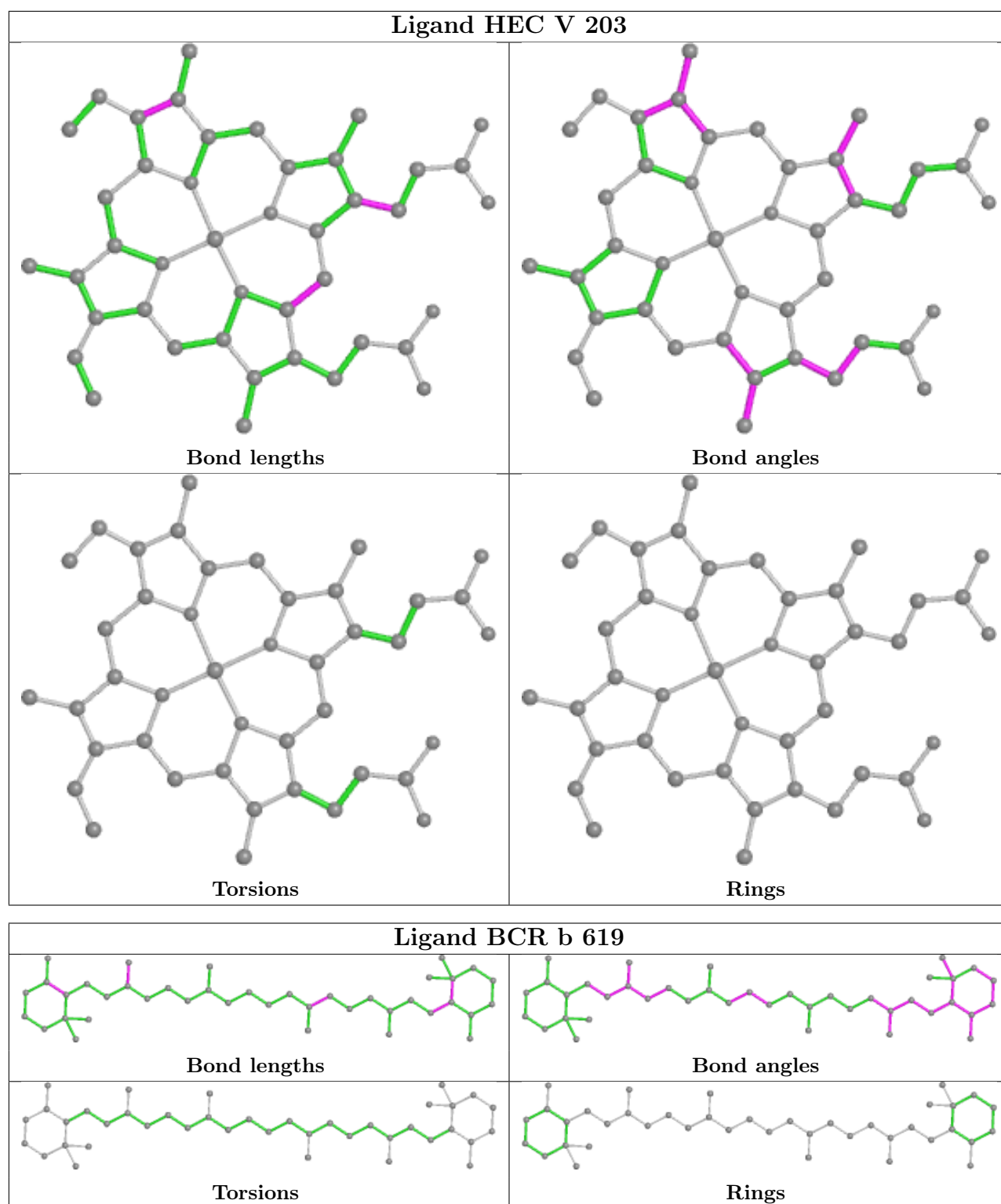
Ligand CLA b 609

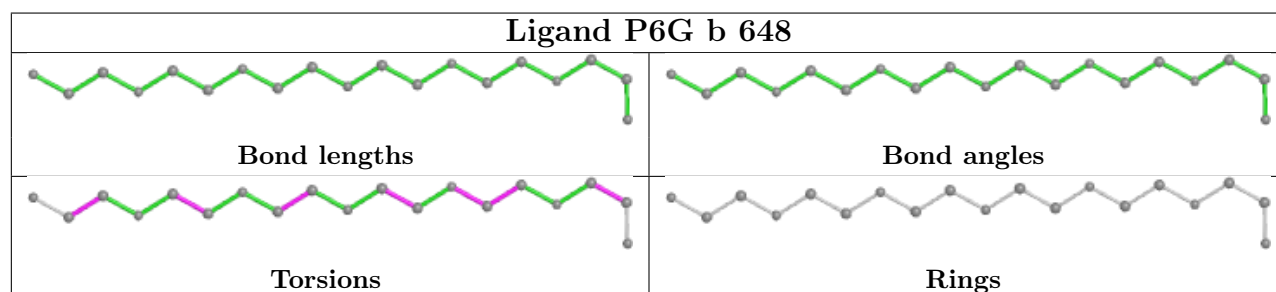
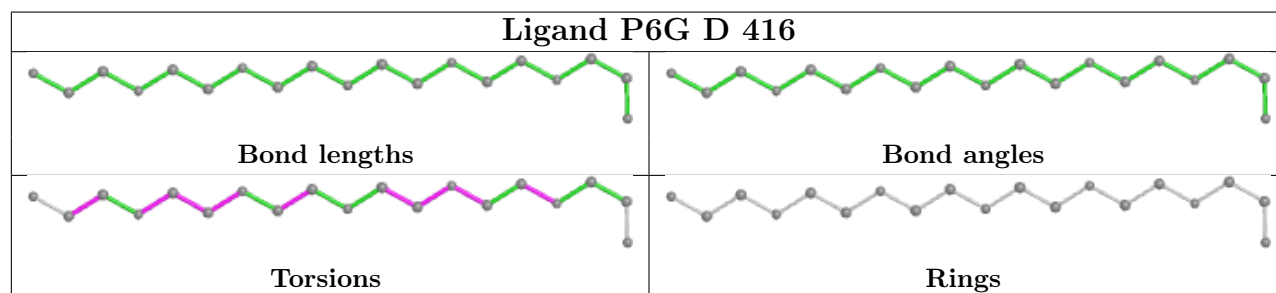
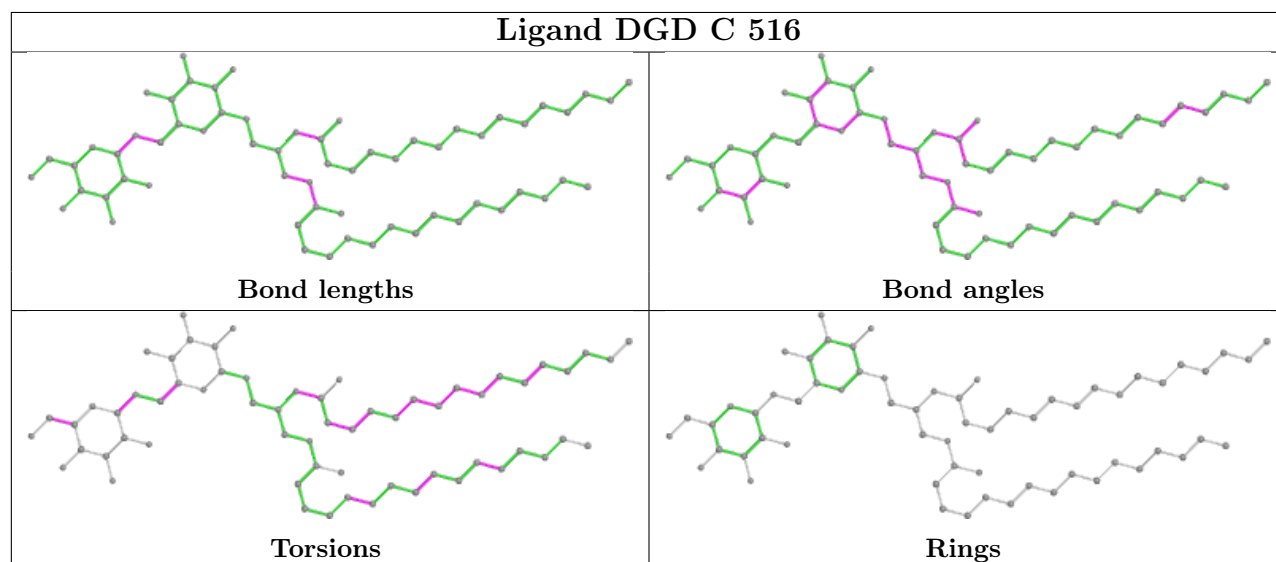
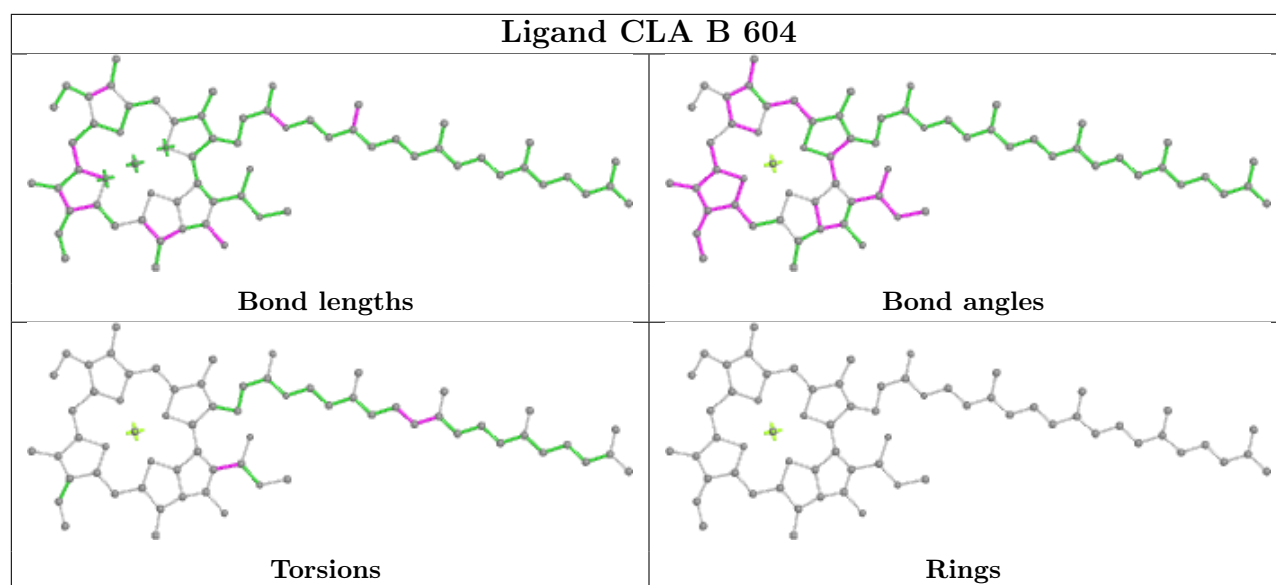


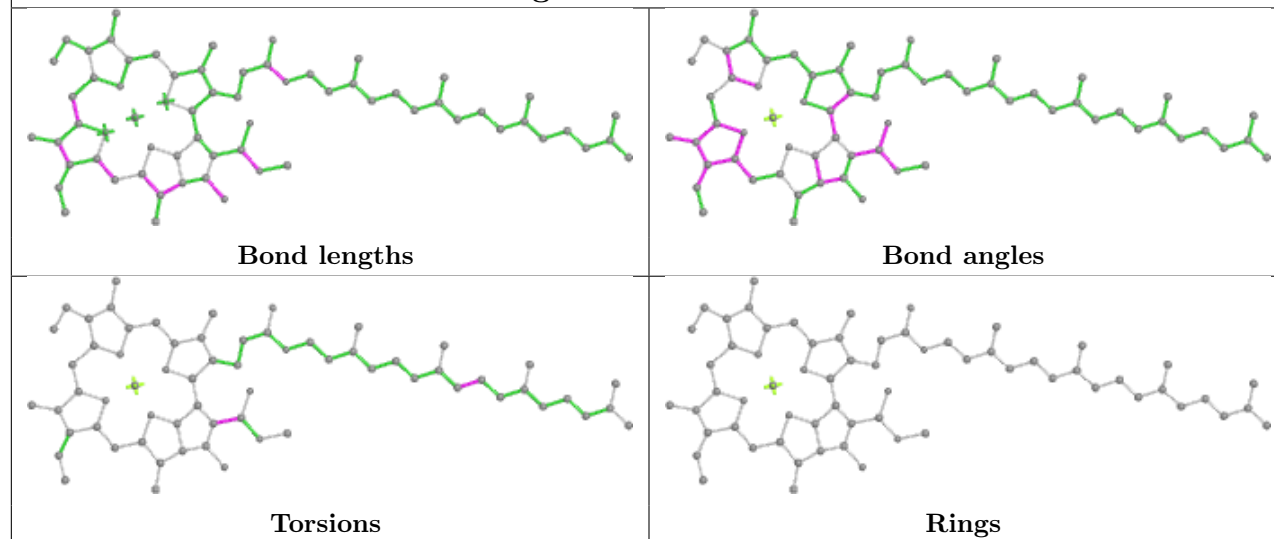
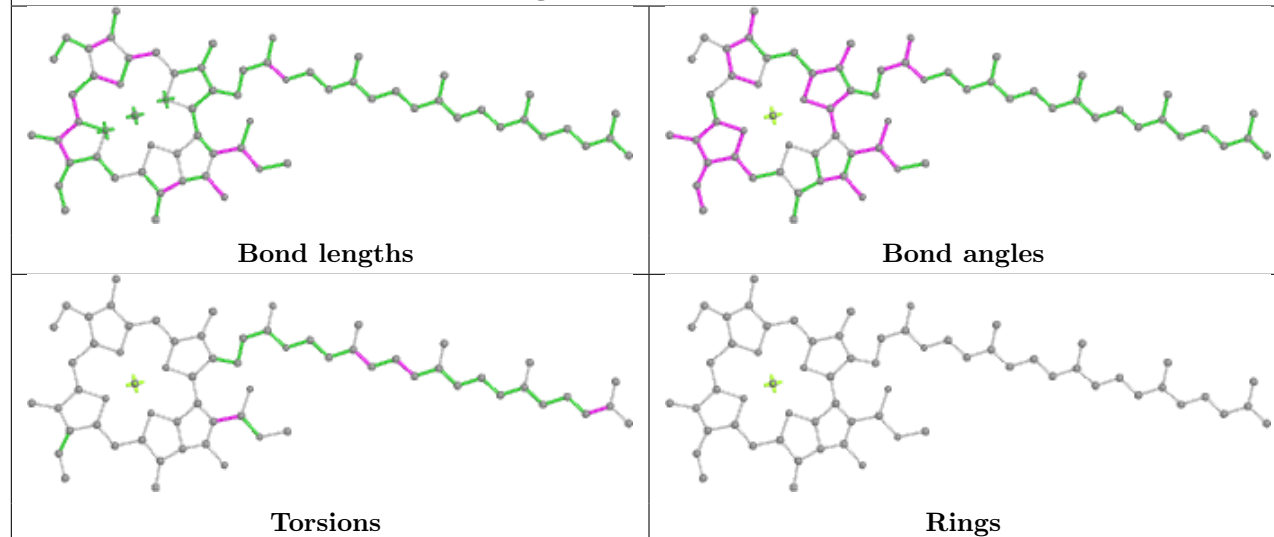
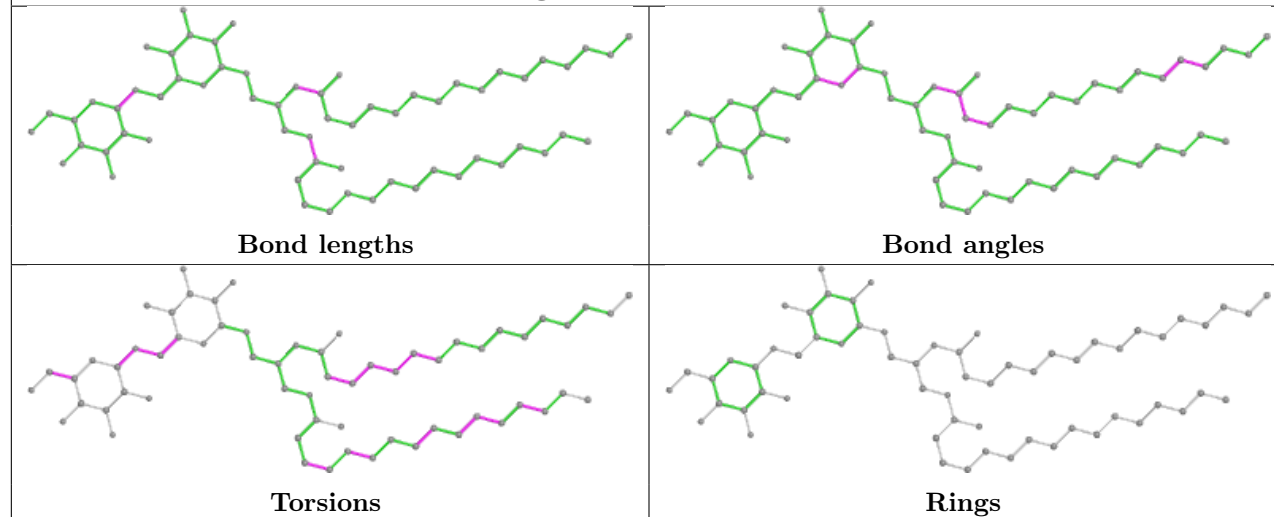
Ligand HEC v 202

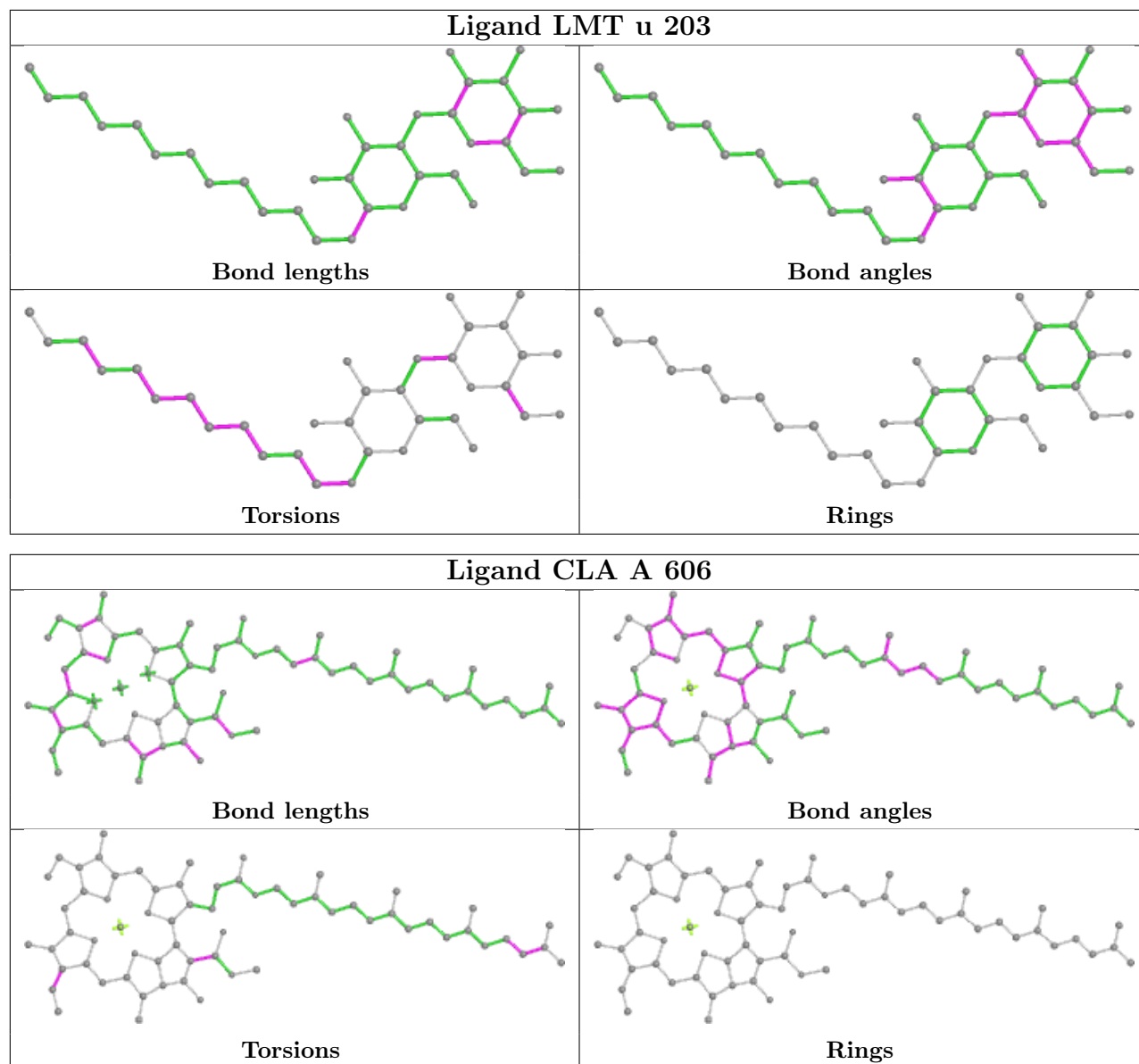


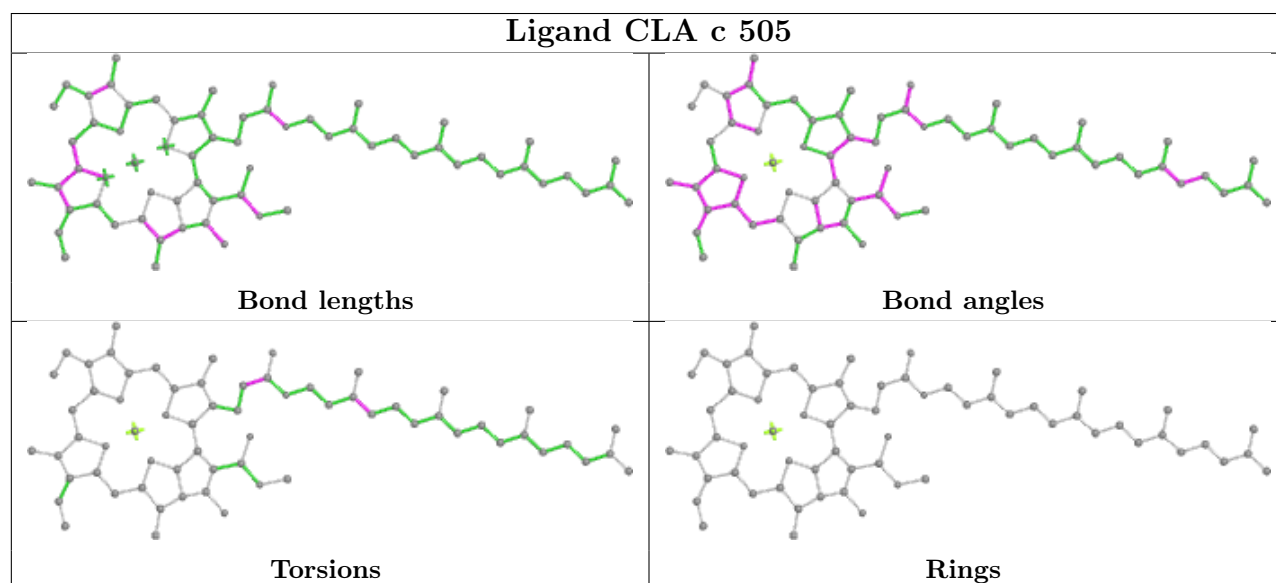
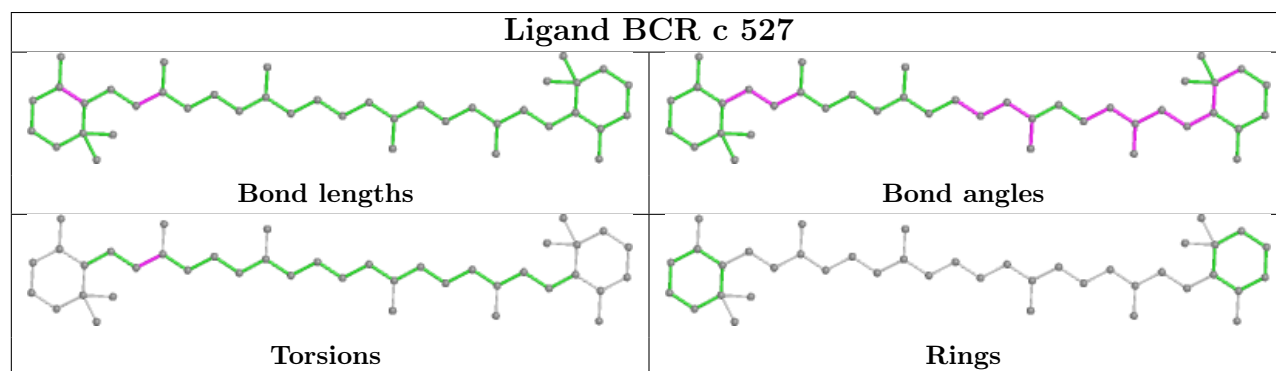
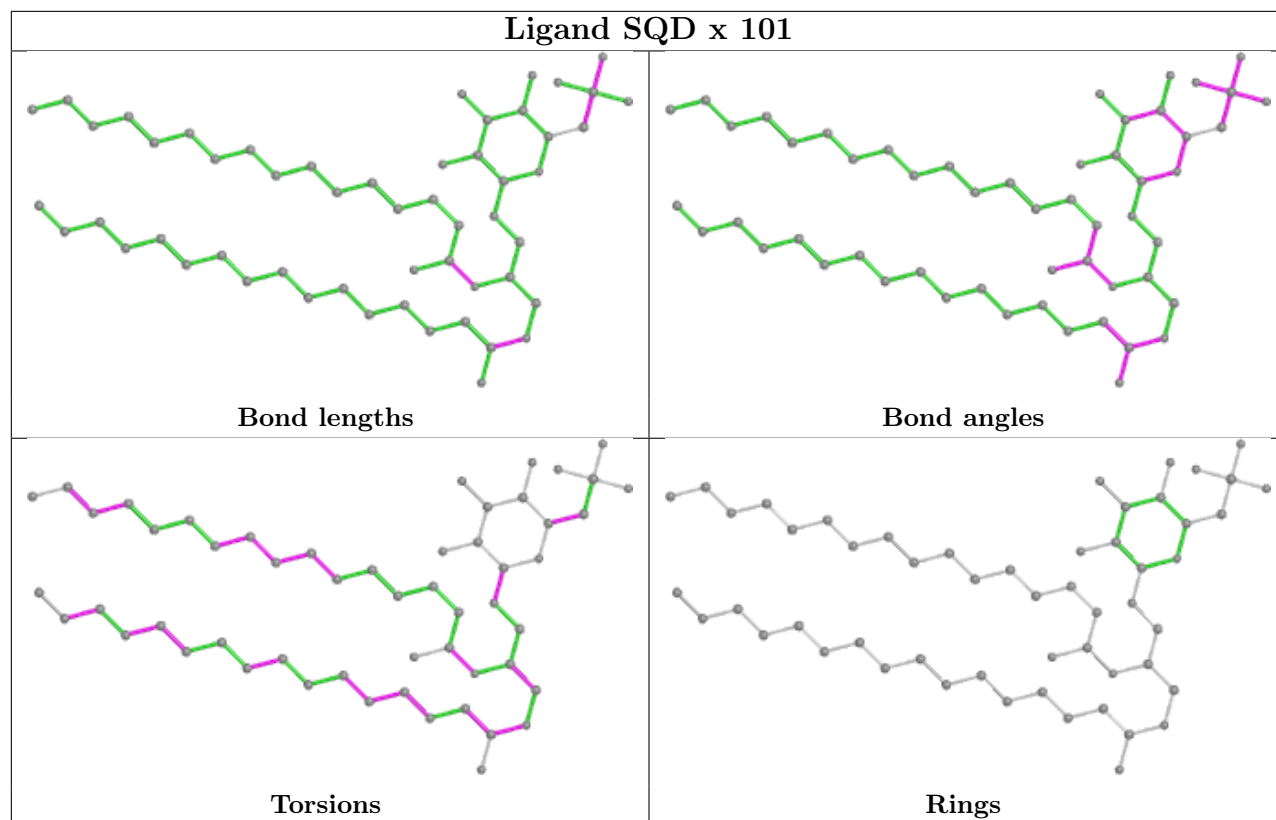


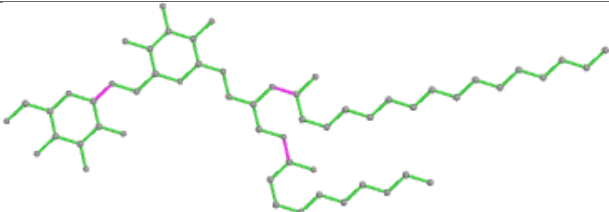
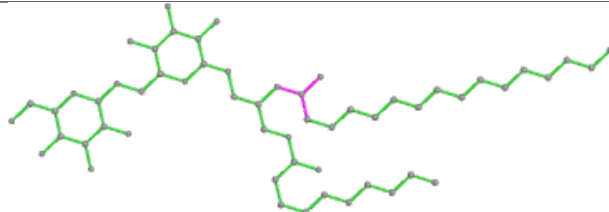
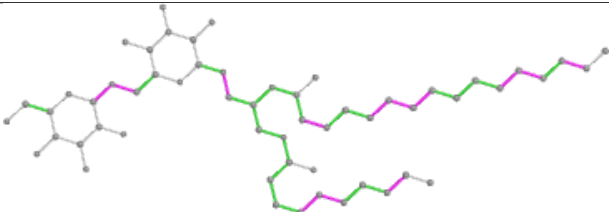
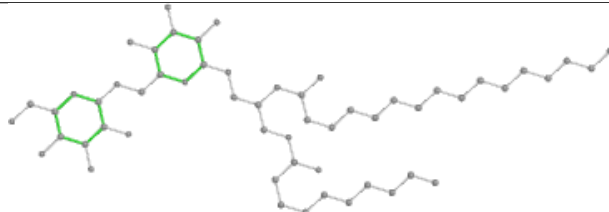


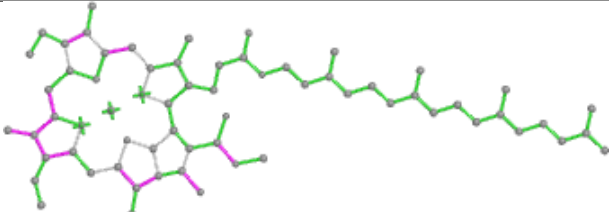
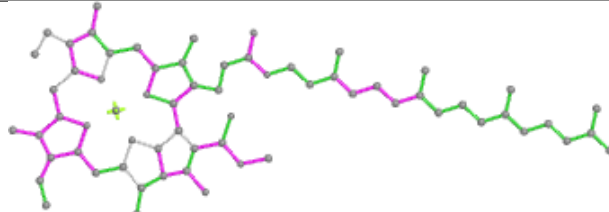
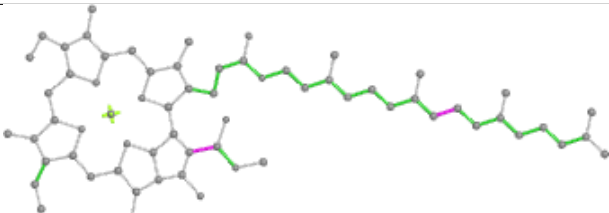
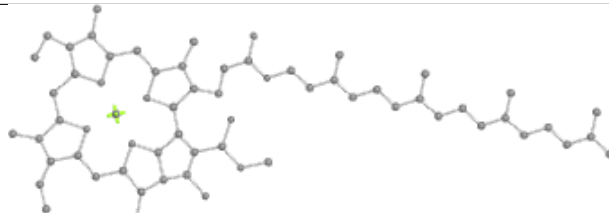






Ligand CLA B 613**Ligand CLA C 507****Ligand DGD c 516**

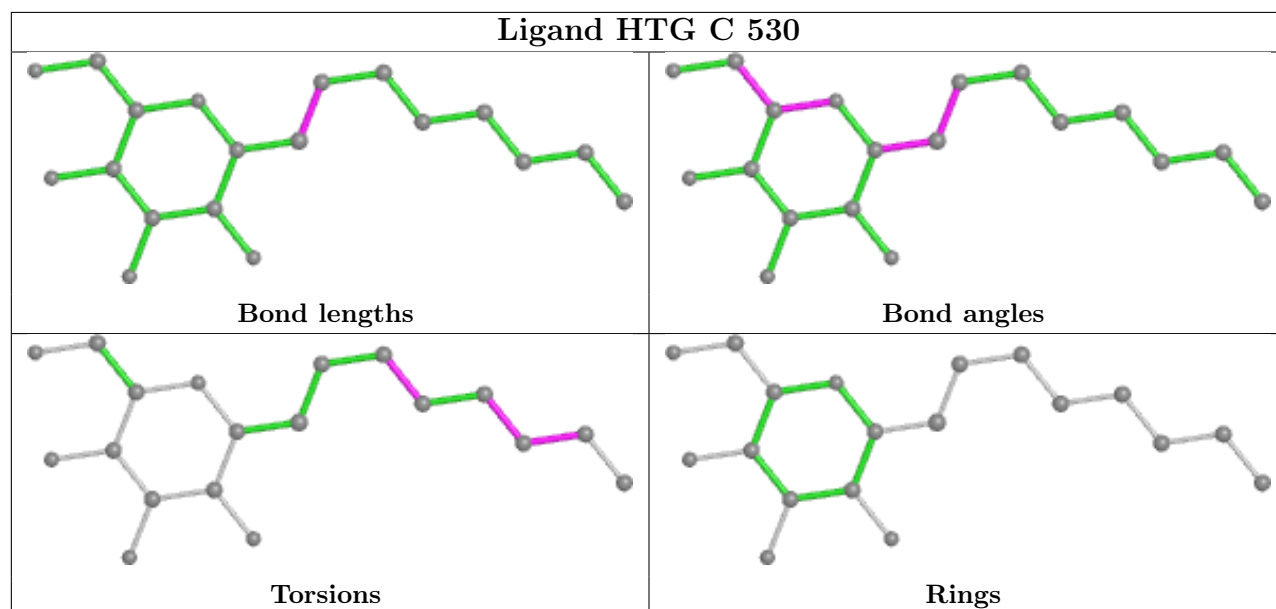
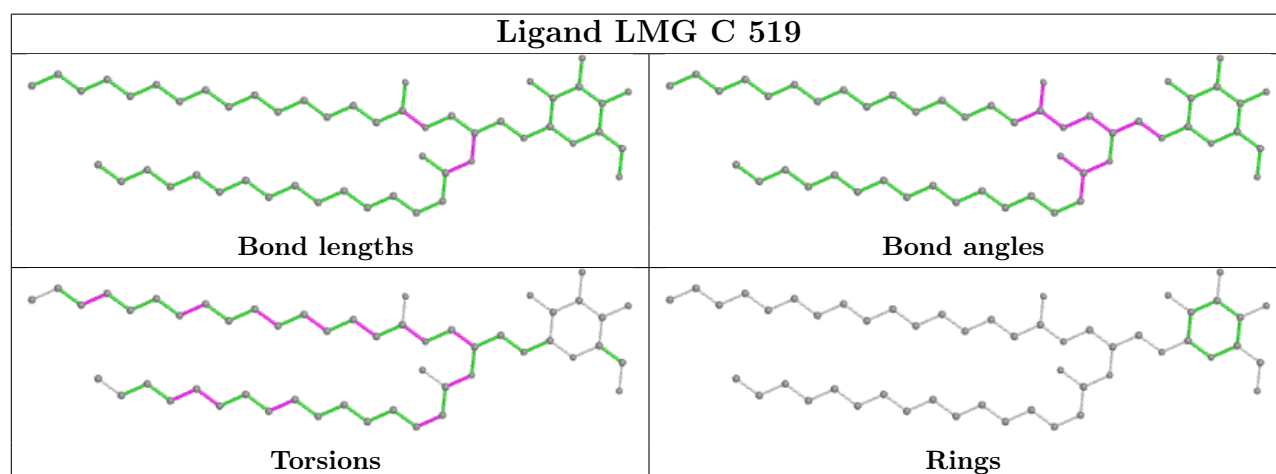
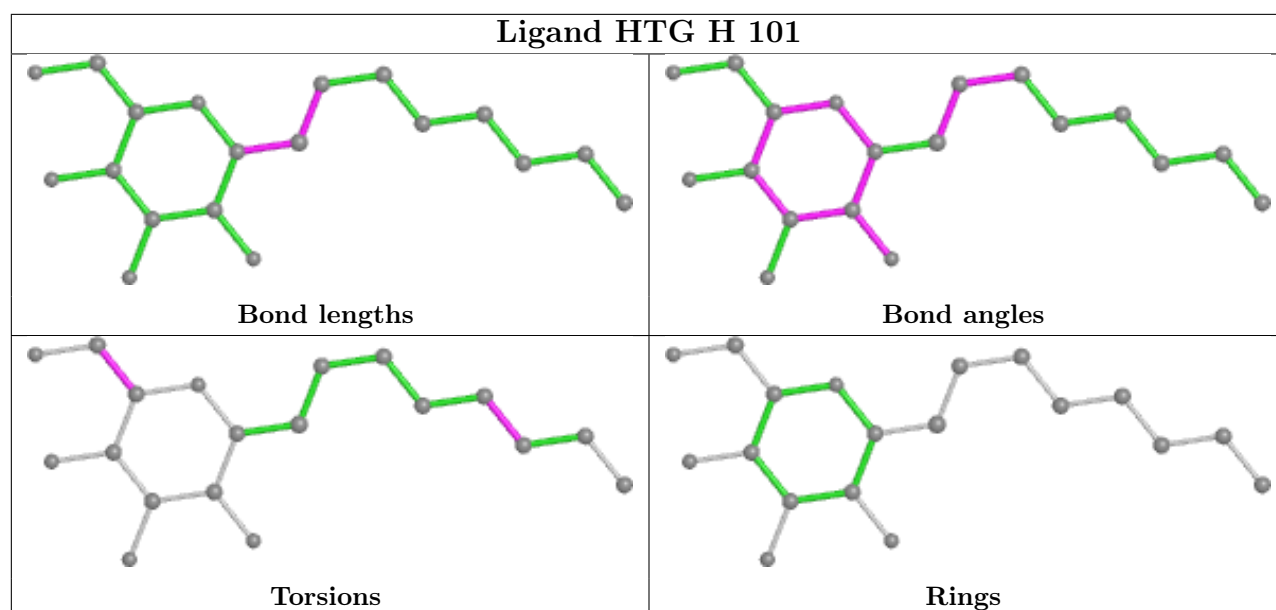


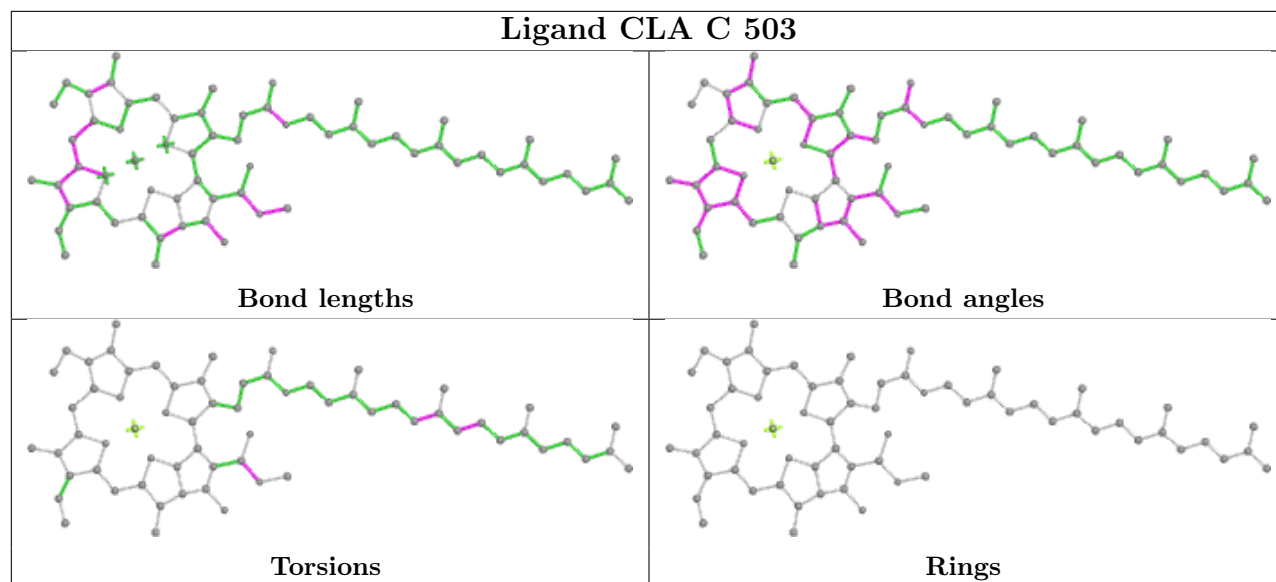
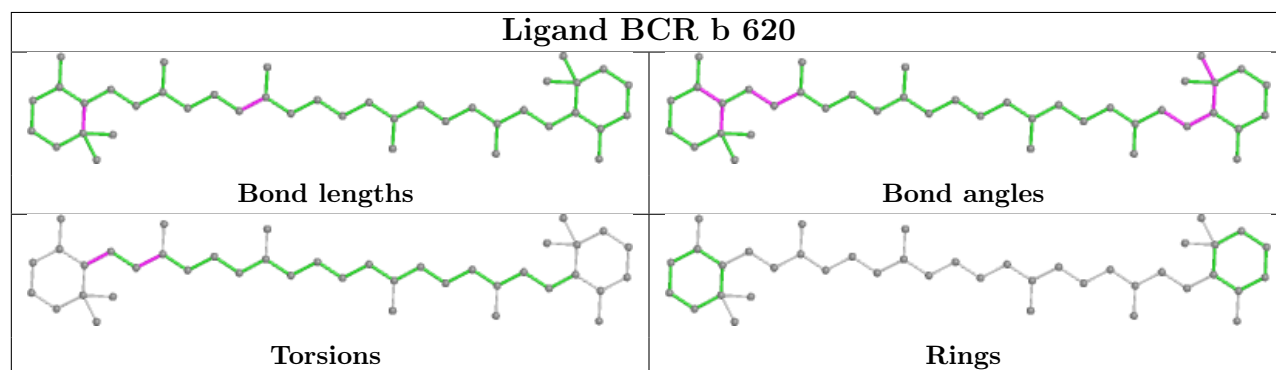
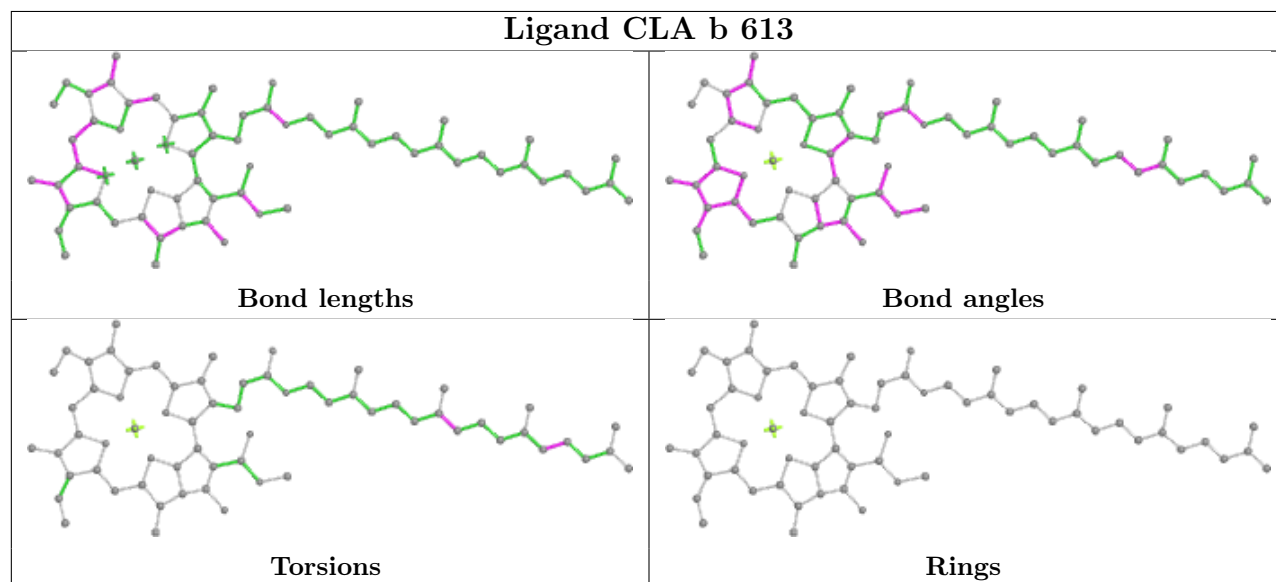


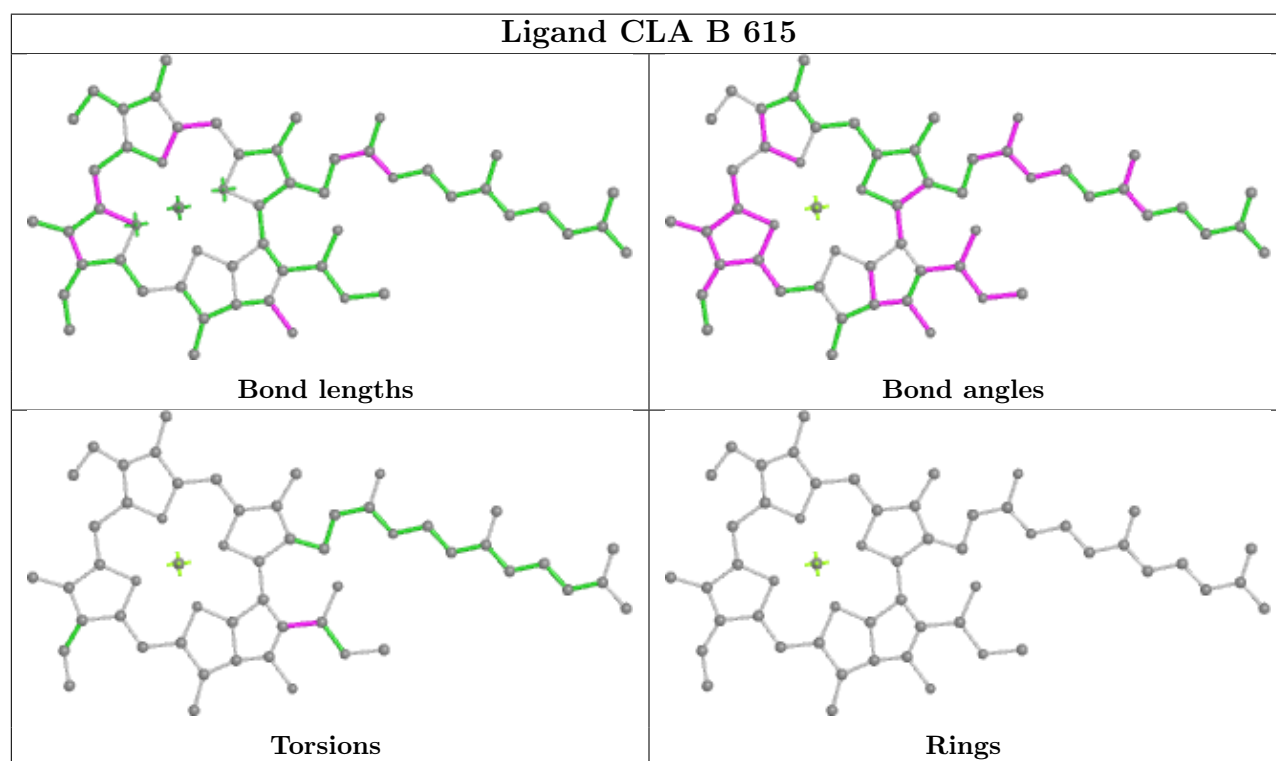
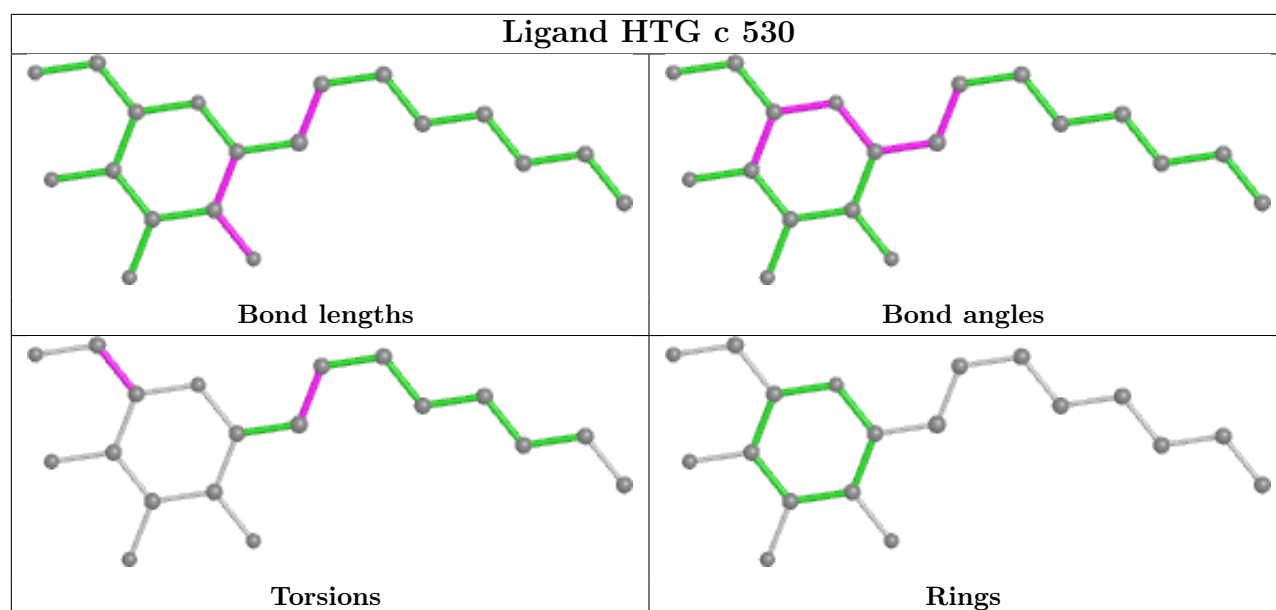
Ligand DGD C 517	
	
Bond lengths	Bond angles
	
Torsions	Rings

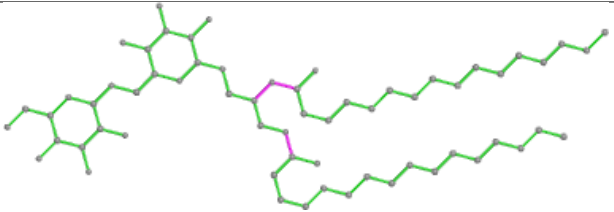
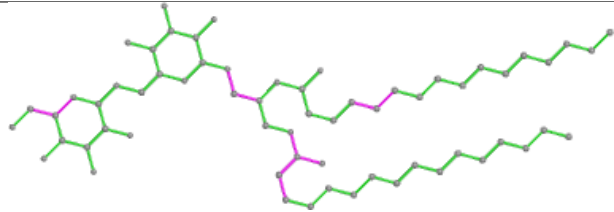
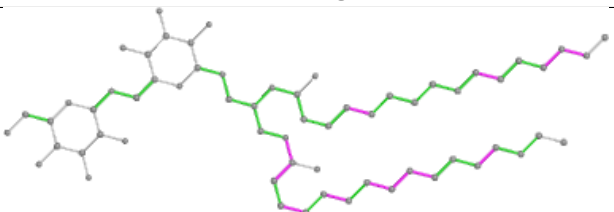
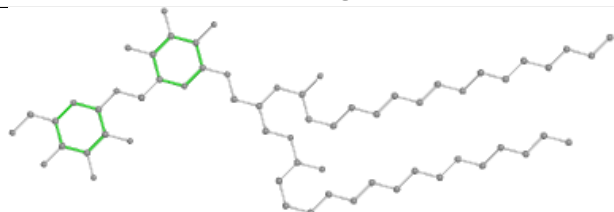
Ligand CLA C 510	
	
Bond lengths	Bond angles
	
Torsions	Rings

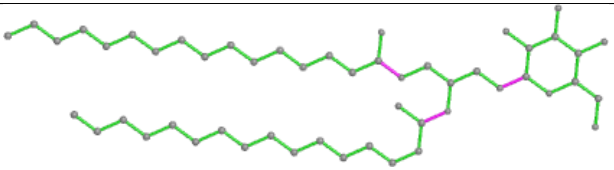
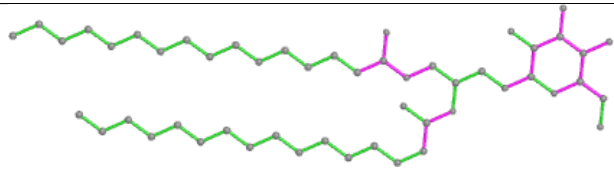
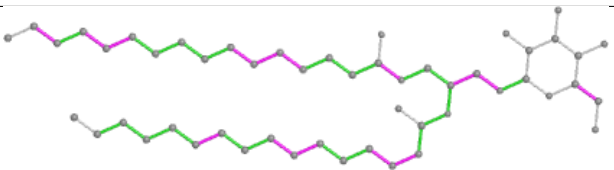
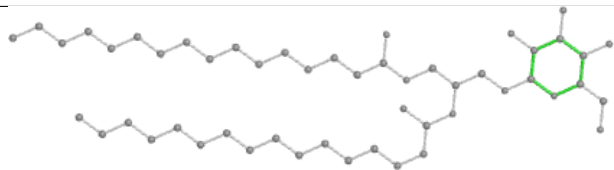
Ligand 2PE V 216	
	
Bond lengths	Bond angles
	
Torsions	Rings

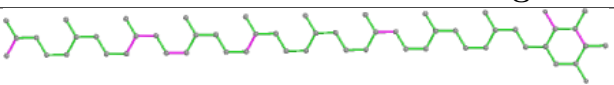
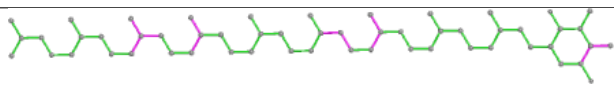
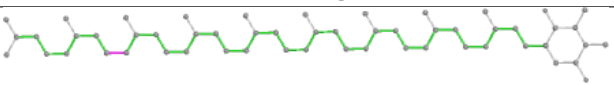
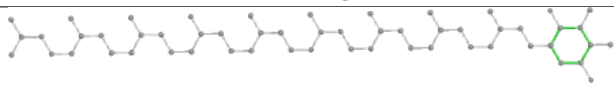


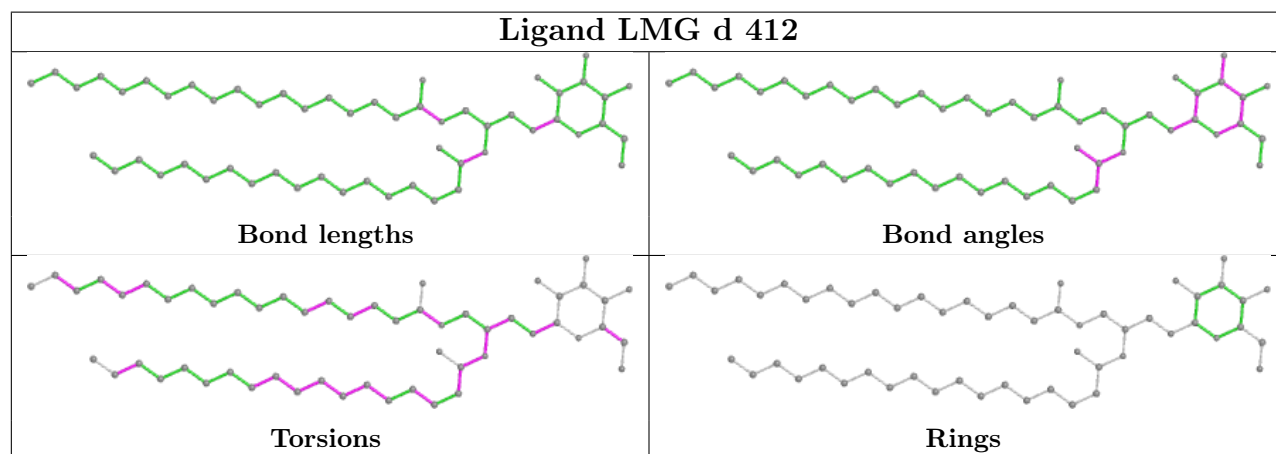
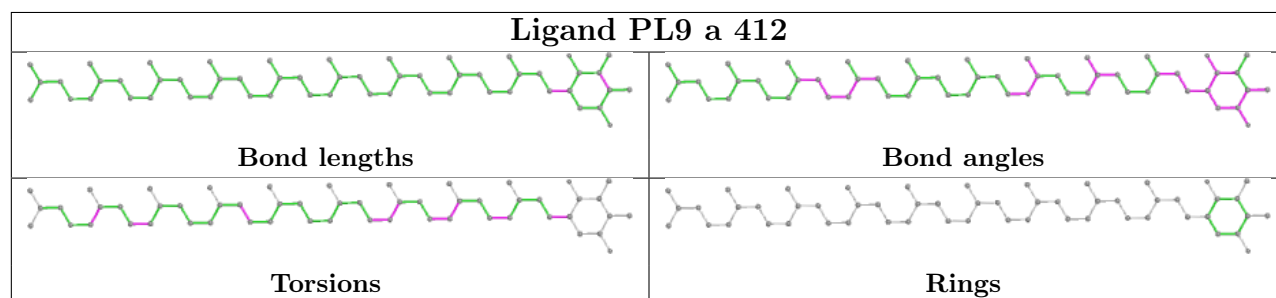
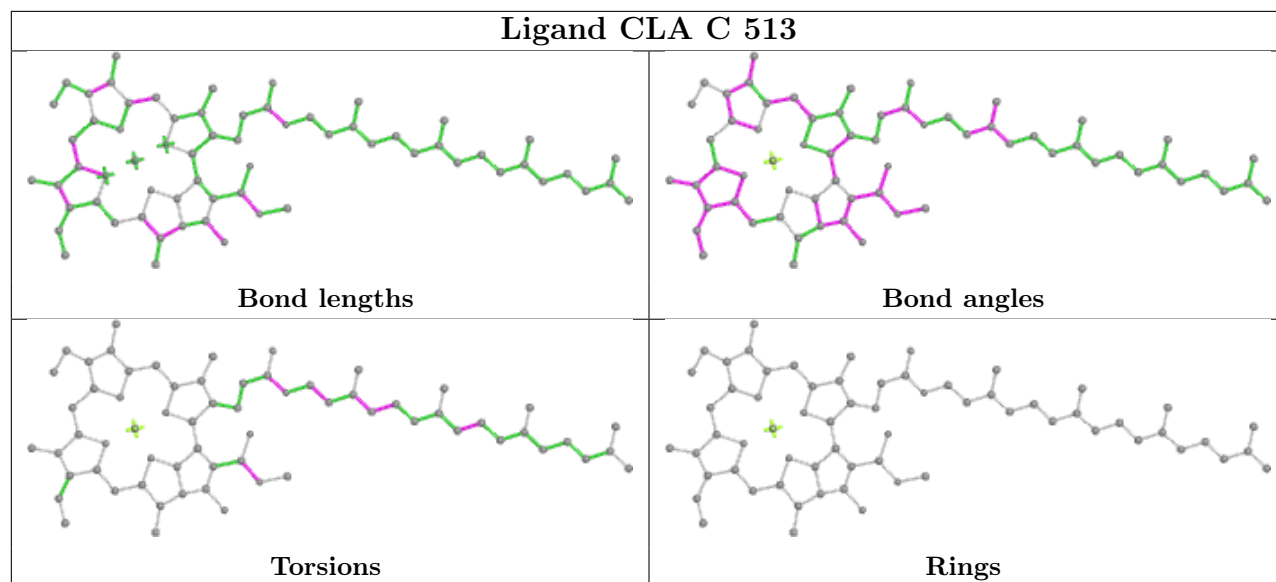
Ligand CLA C 503**Ligand BCR b 620****Ligand CLA b 613**

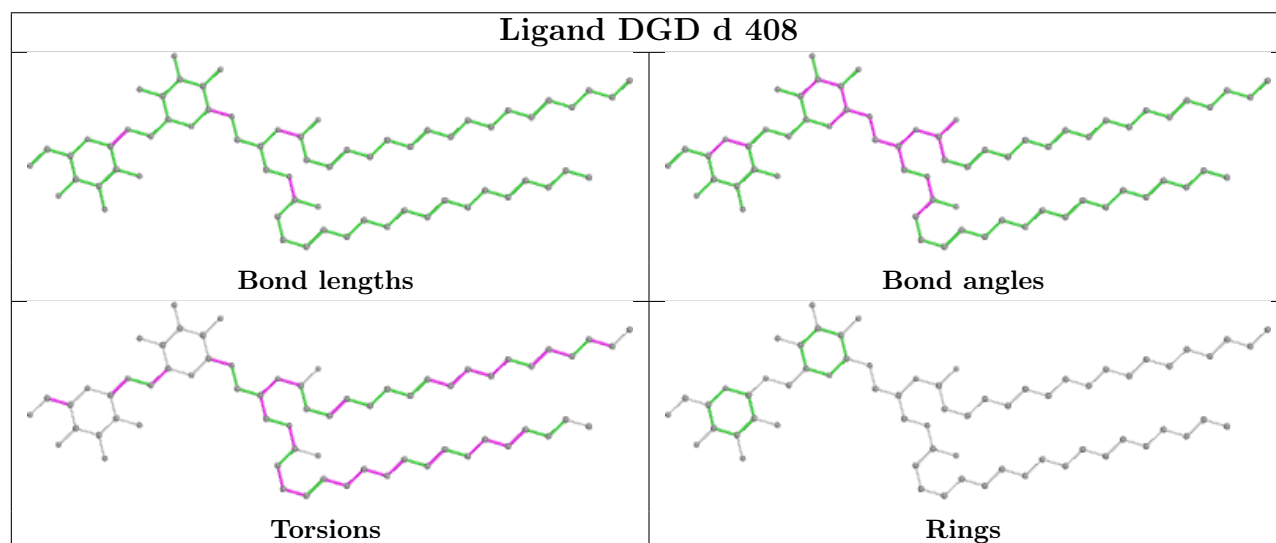
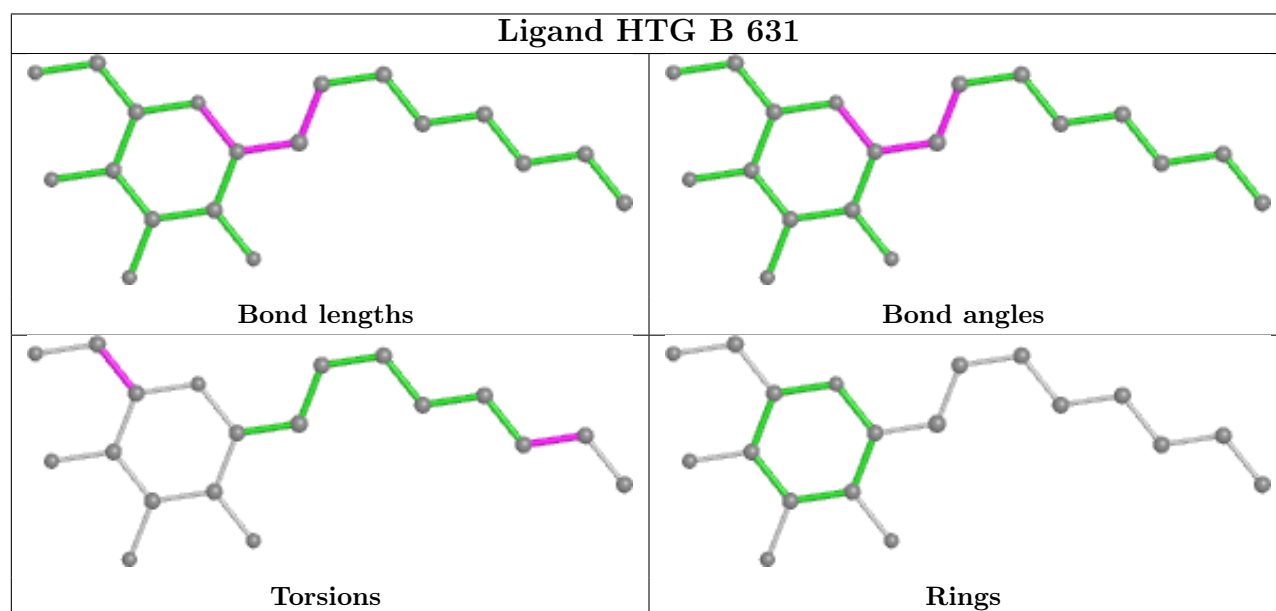
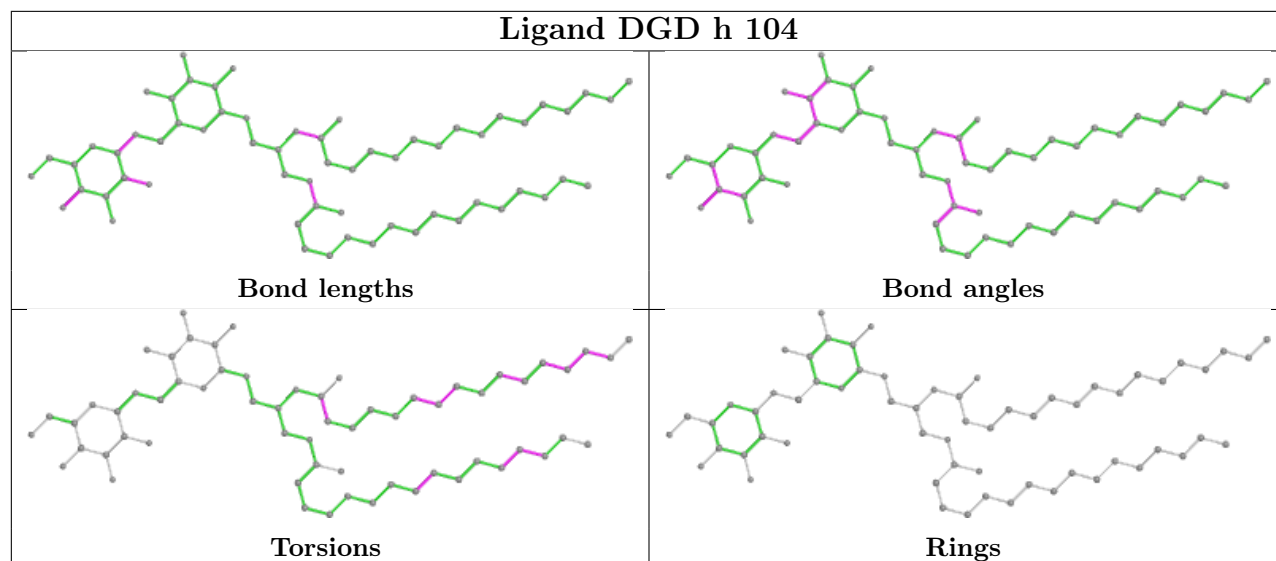


Ligand DGD c 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

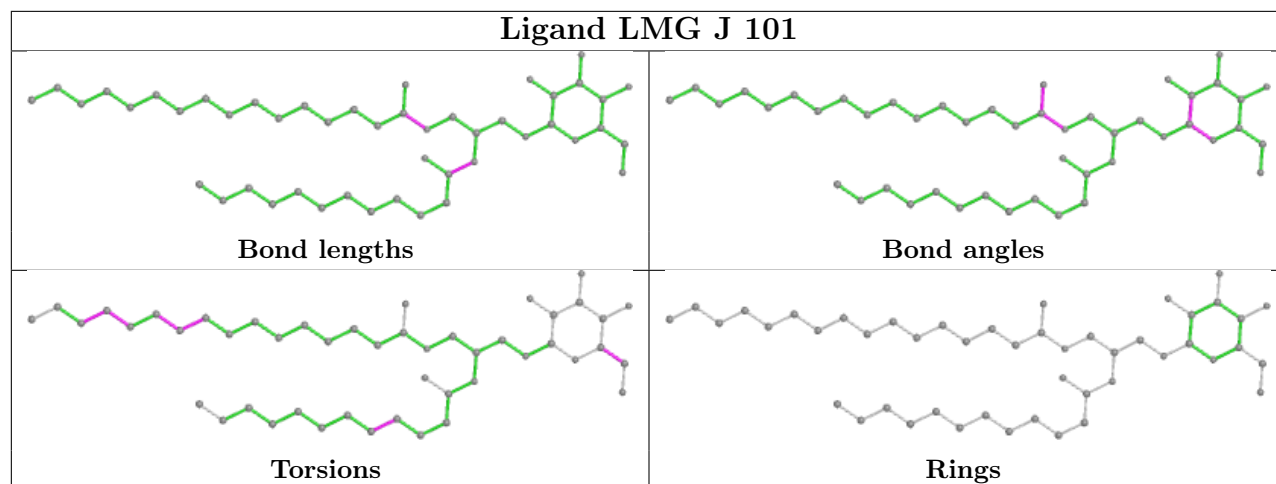
Ligand LMG C 520	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 D 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

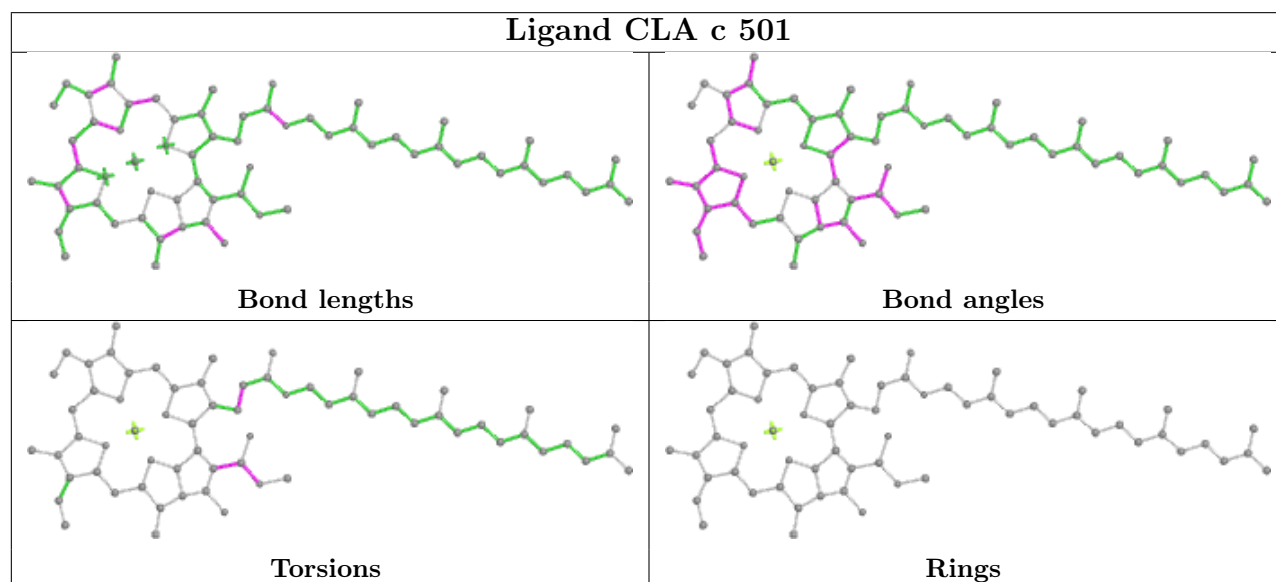




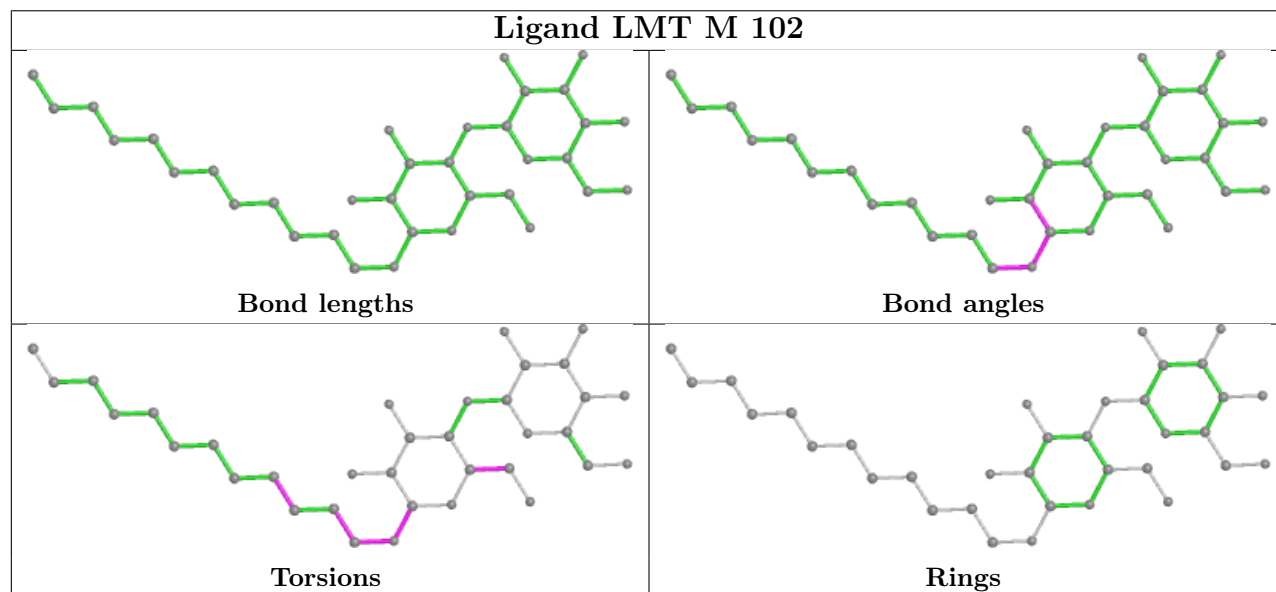
Ligand LMG J 101



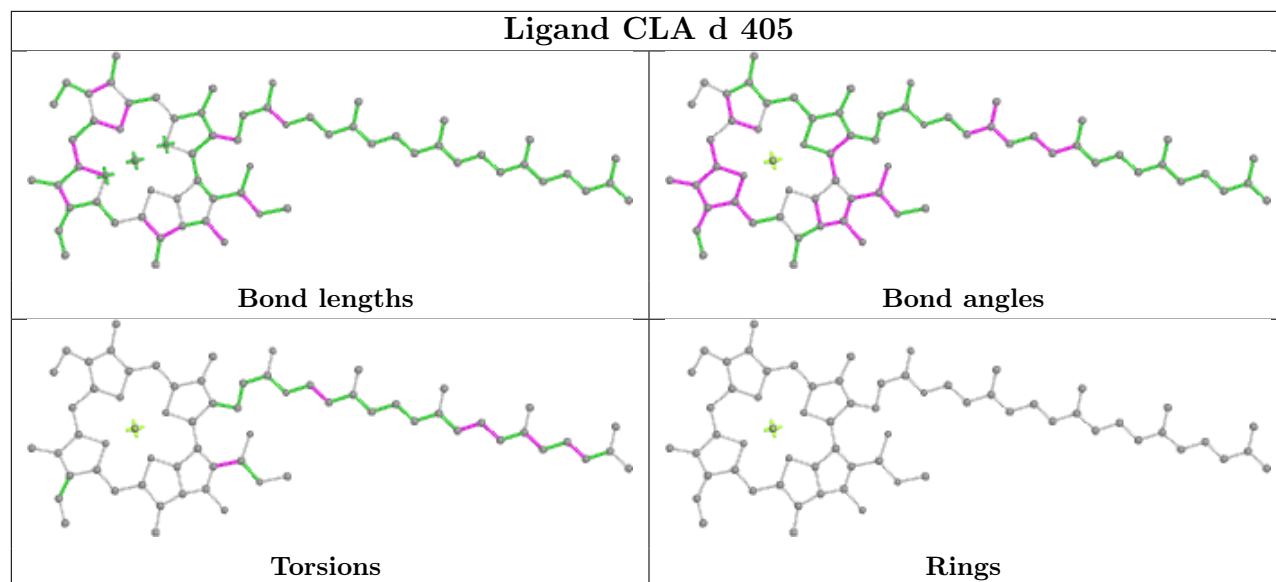
Ligand CLA c 501



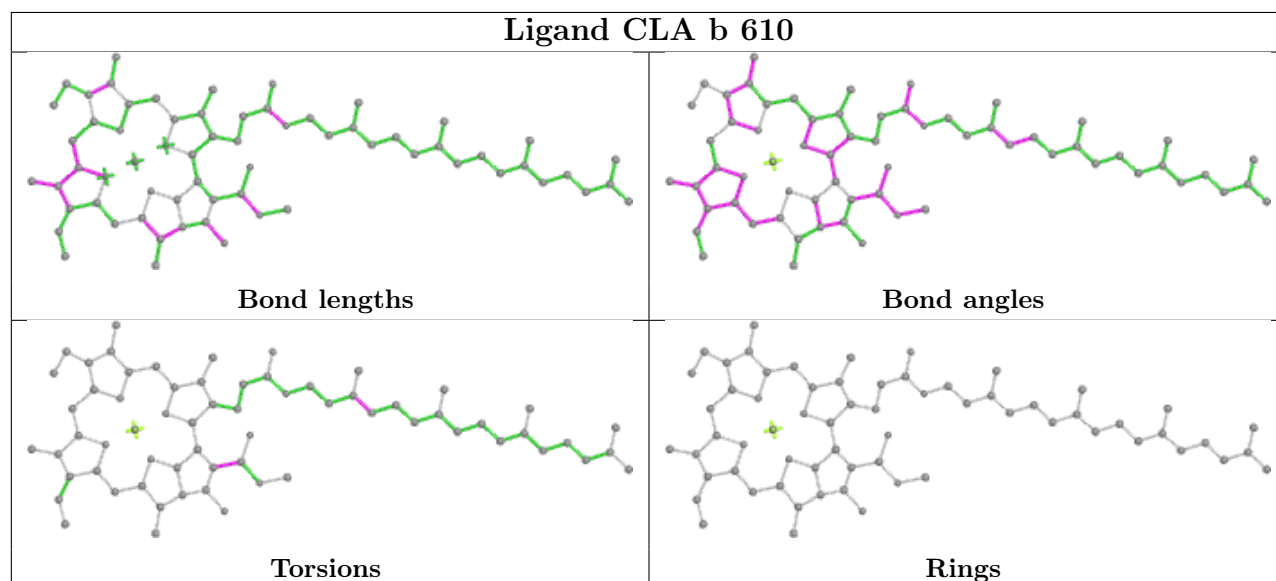
Ligand LMT M 102



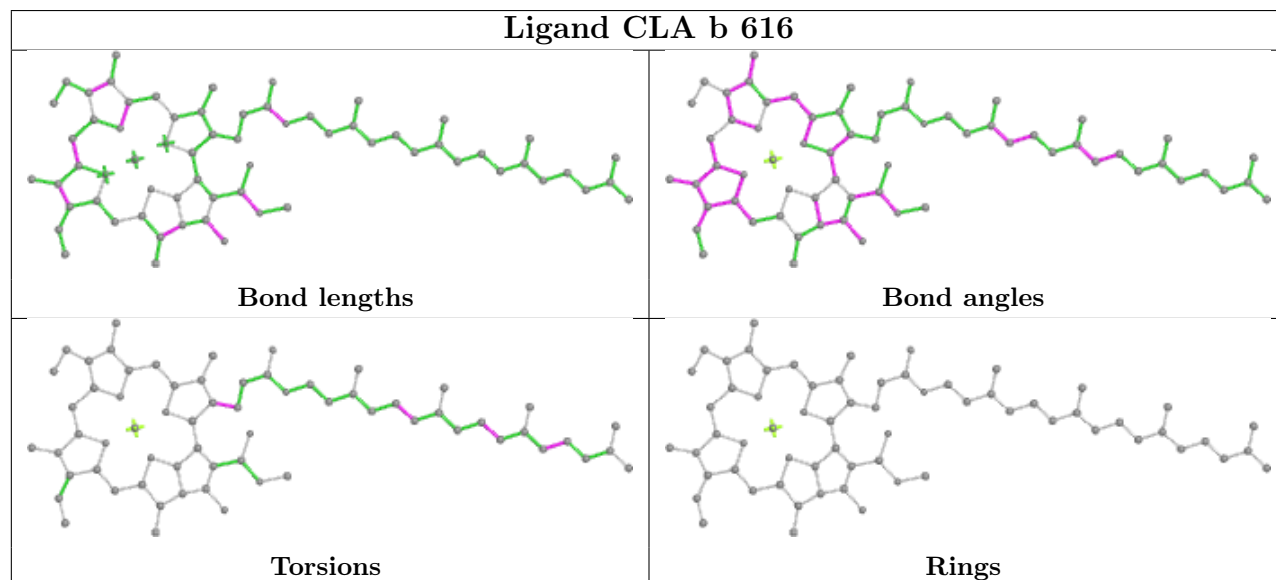
Ligand CLA d 405

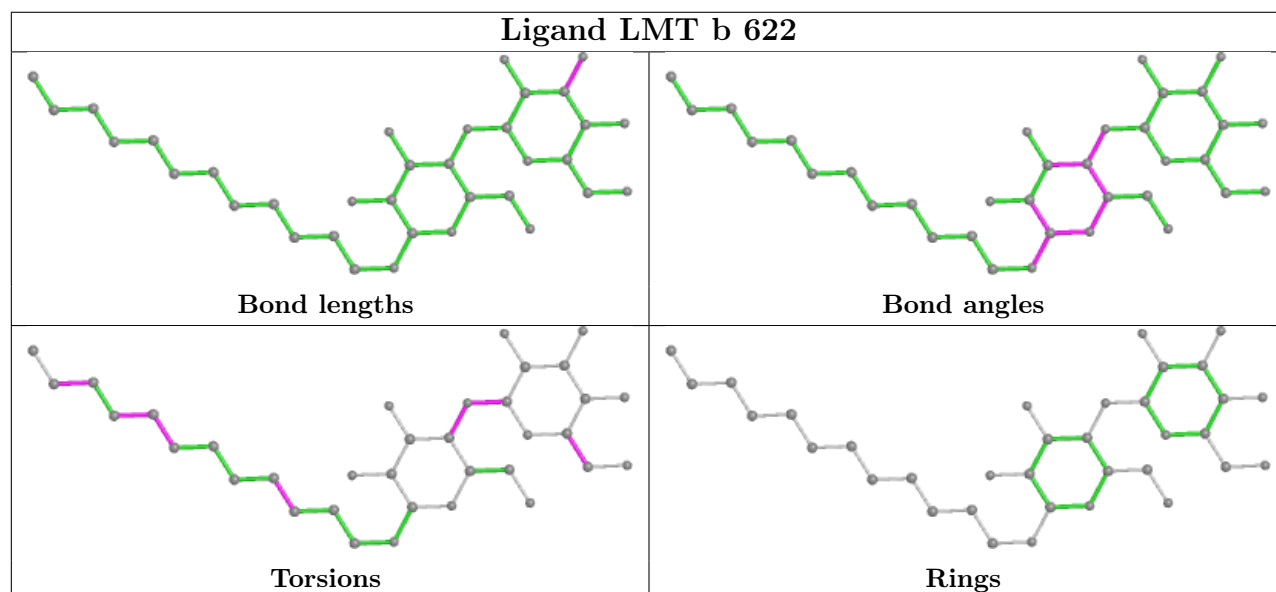
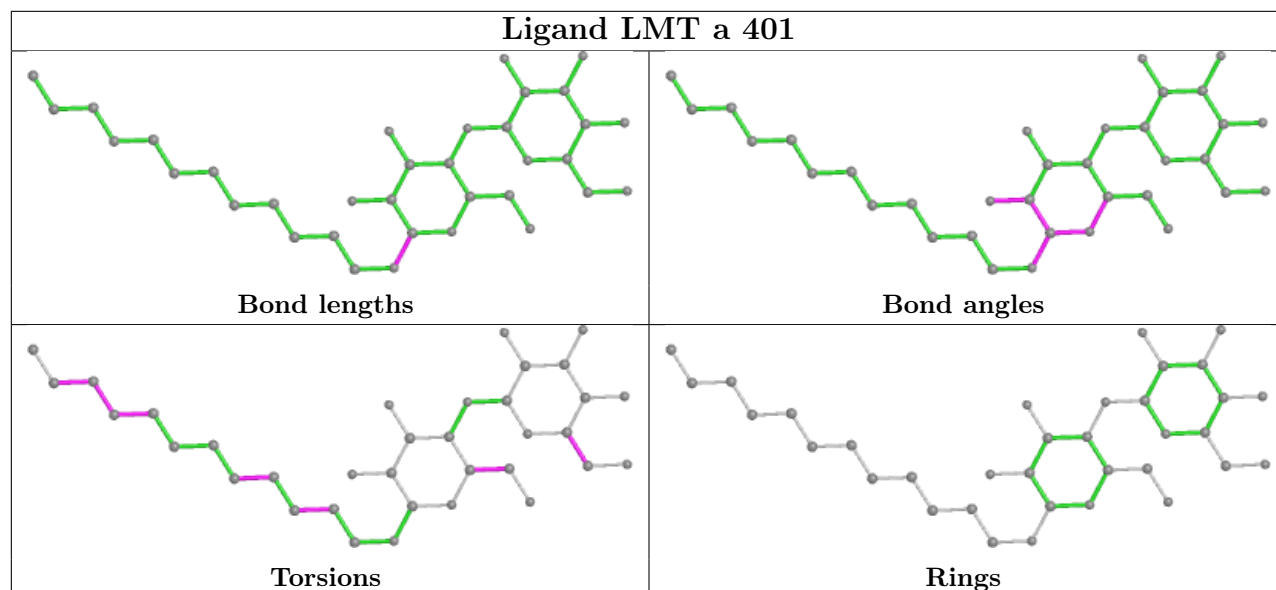
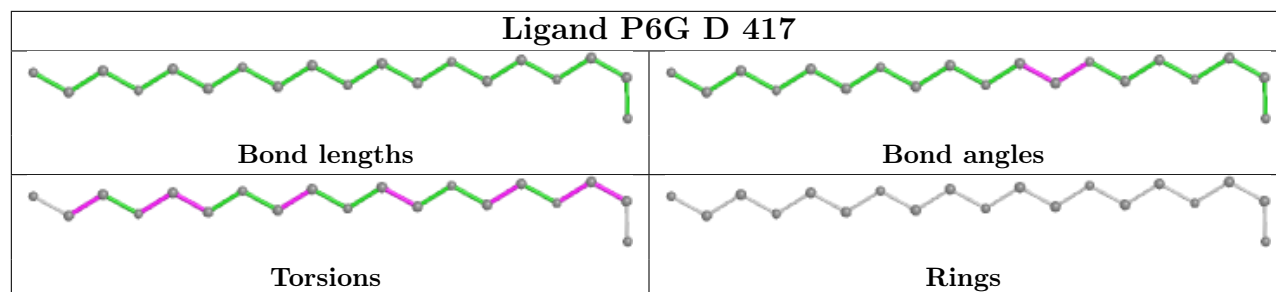


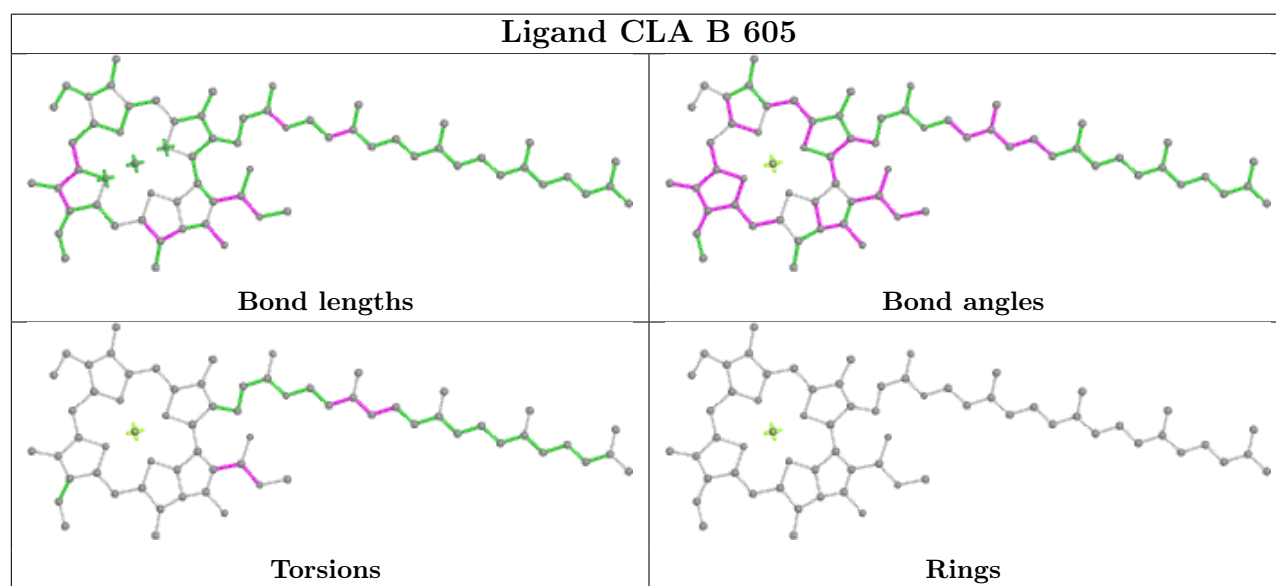
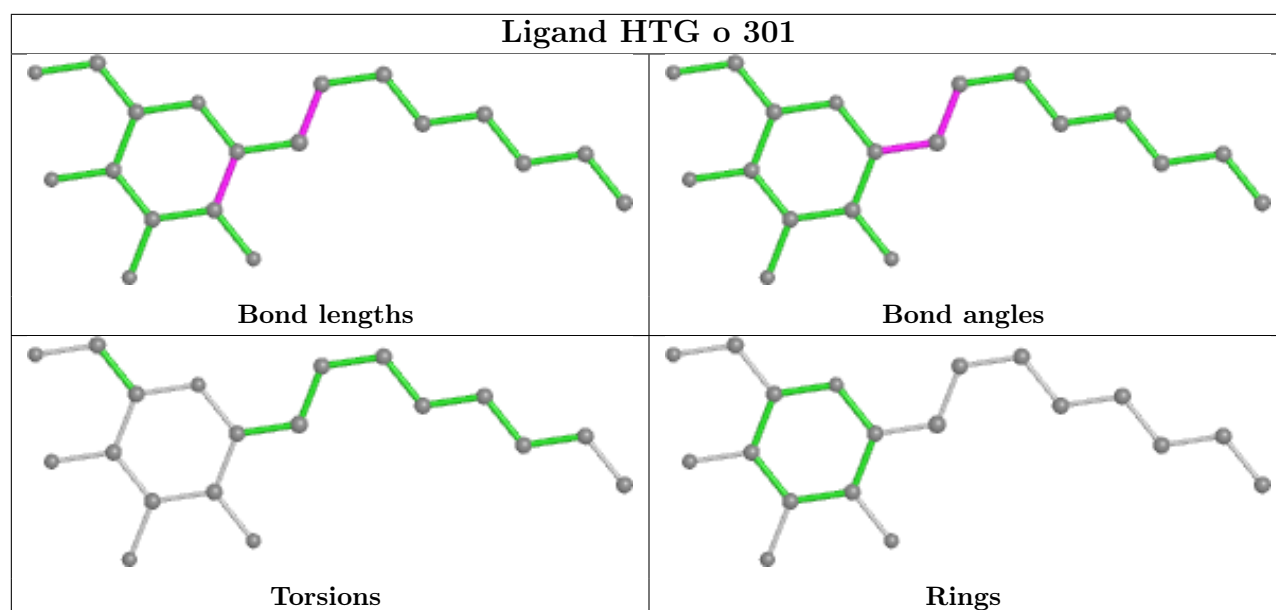
Ligand CLA b 610



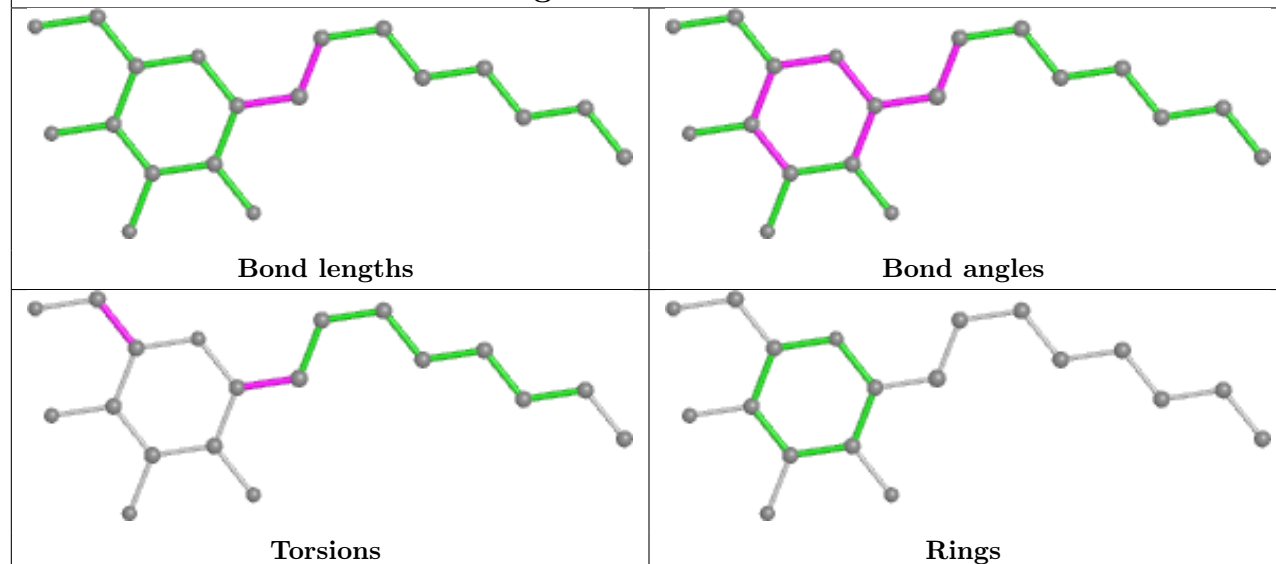
Ligand CLA b 616



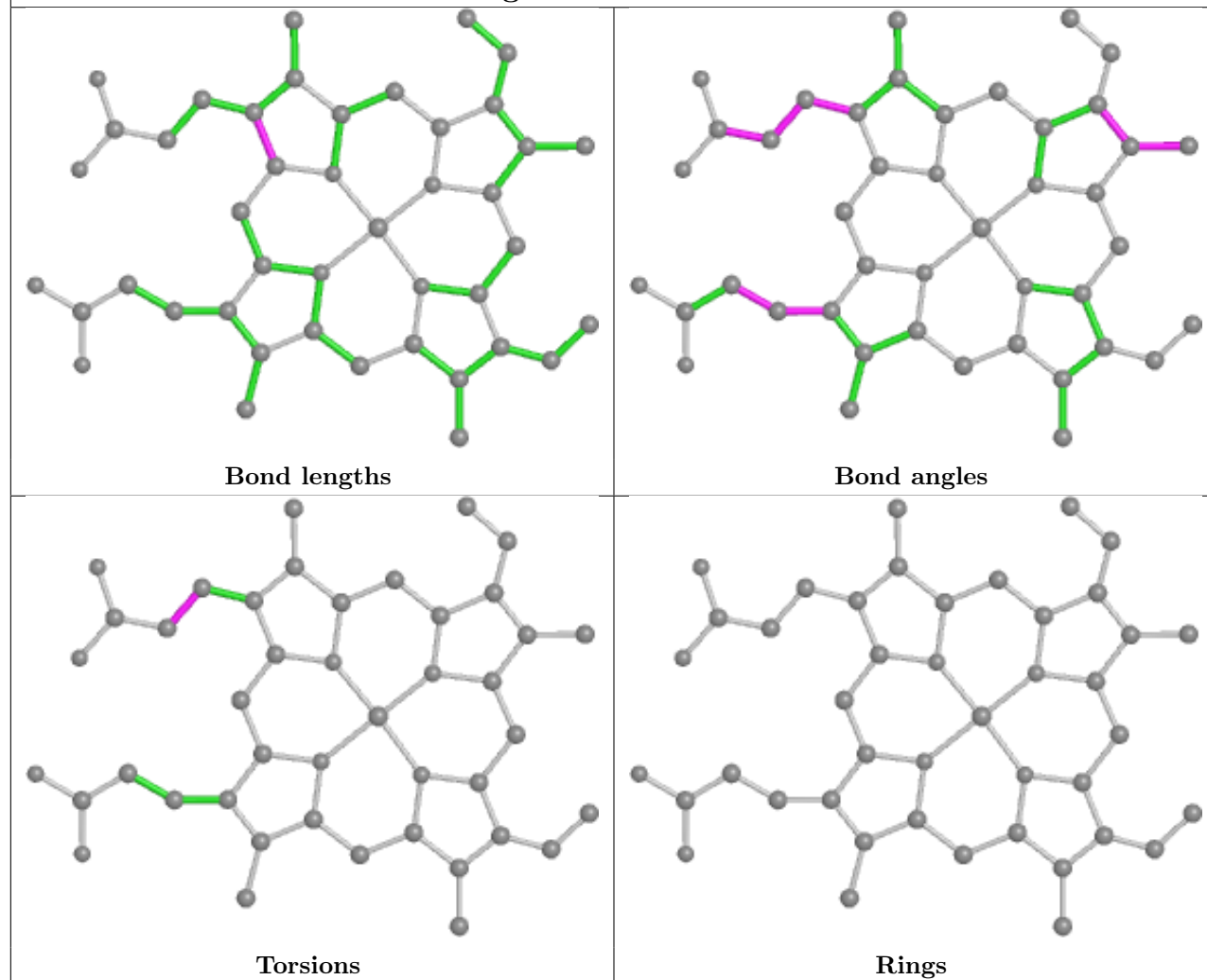


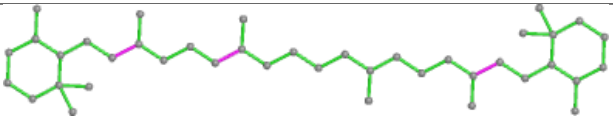
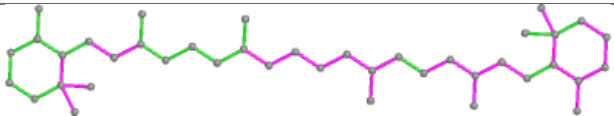
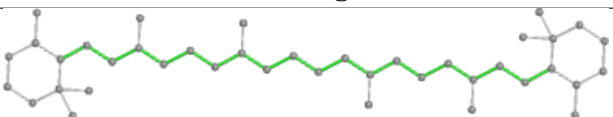
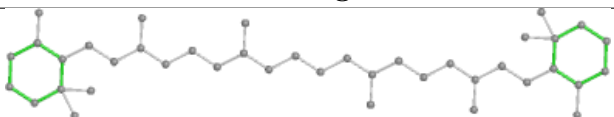


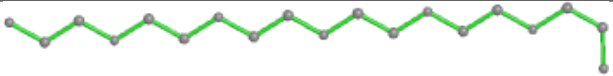
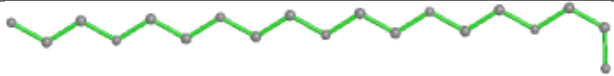
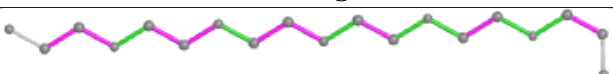
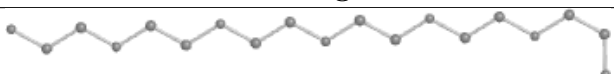
Ligand HTG c 523

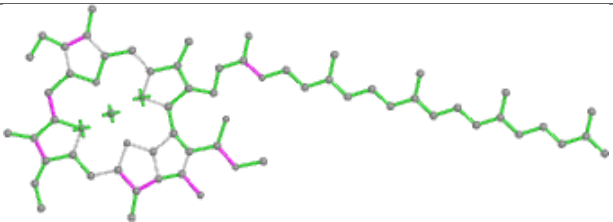
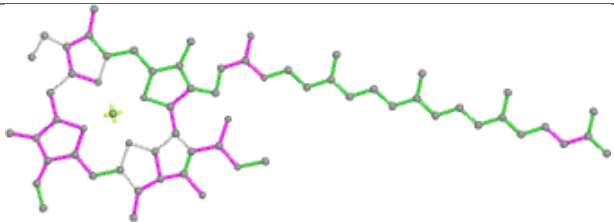
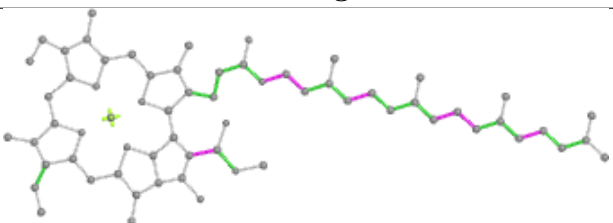
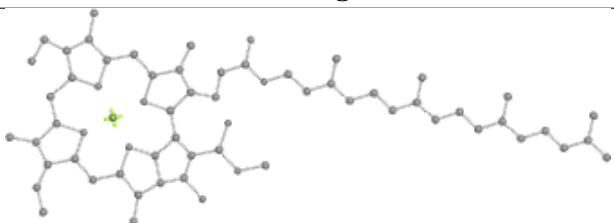


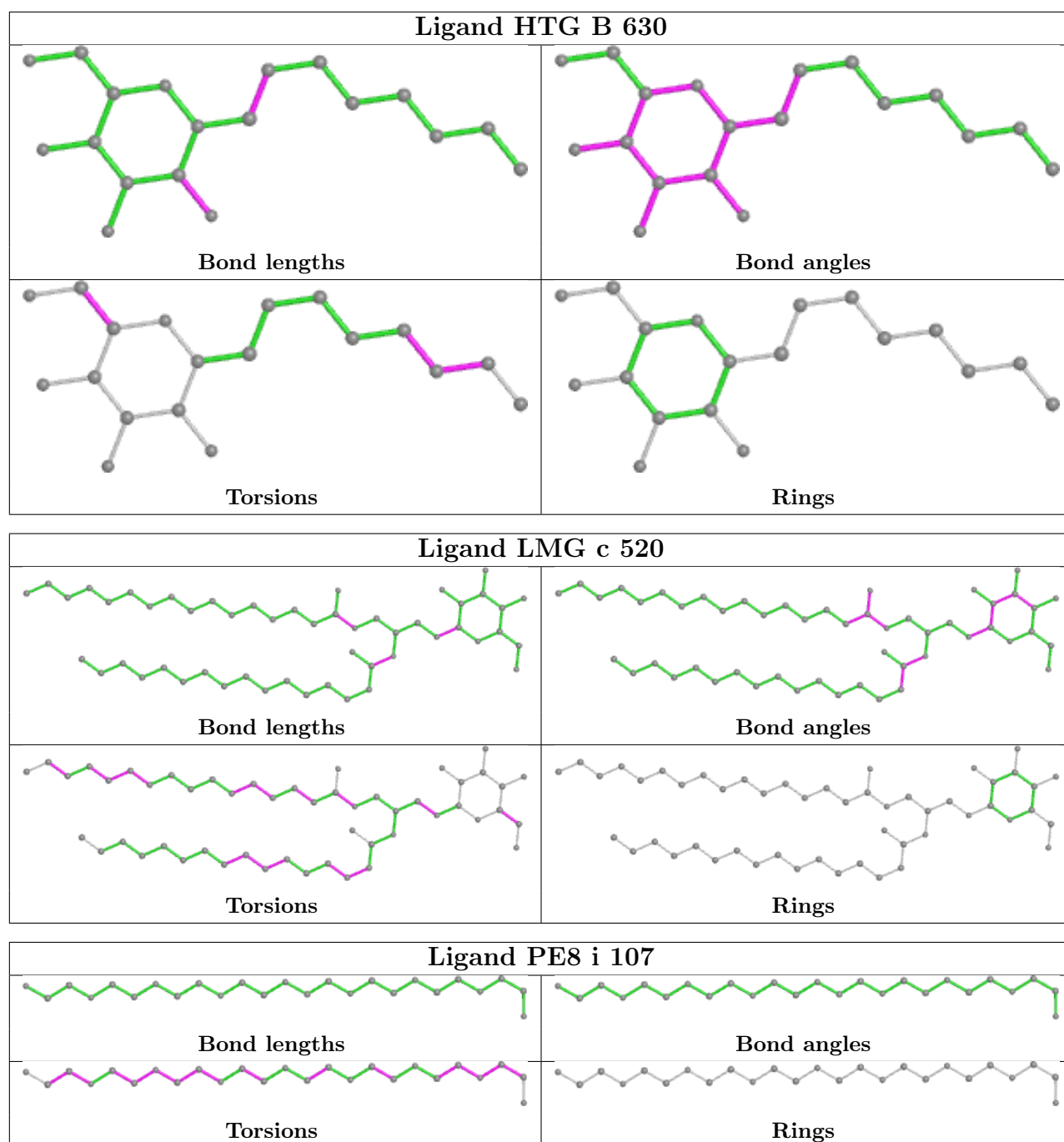
Ligand HEM e 107

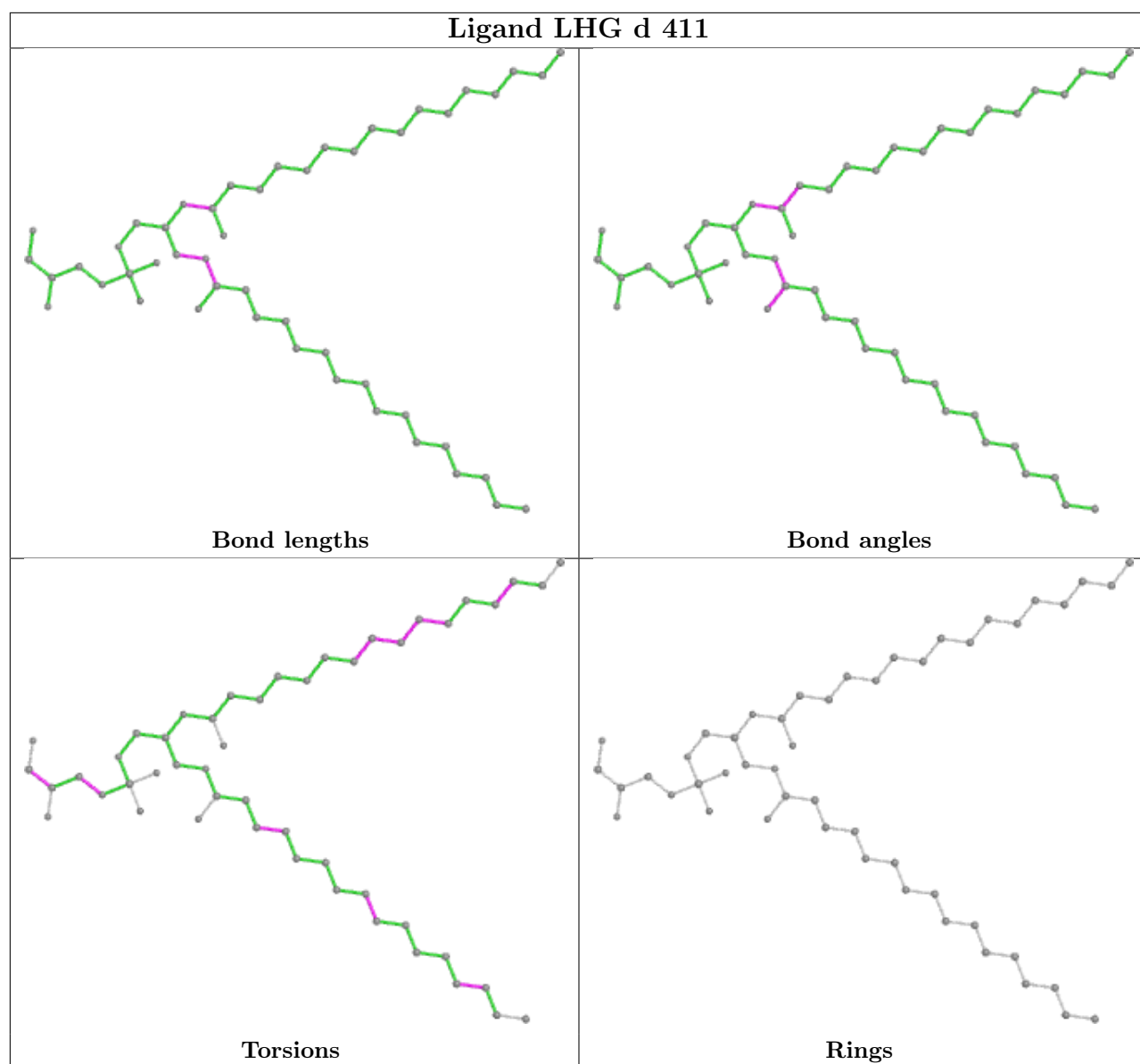


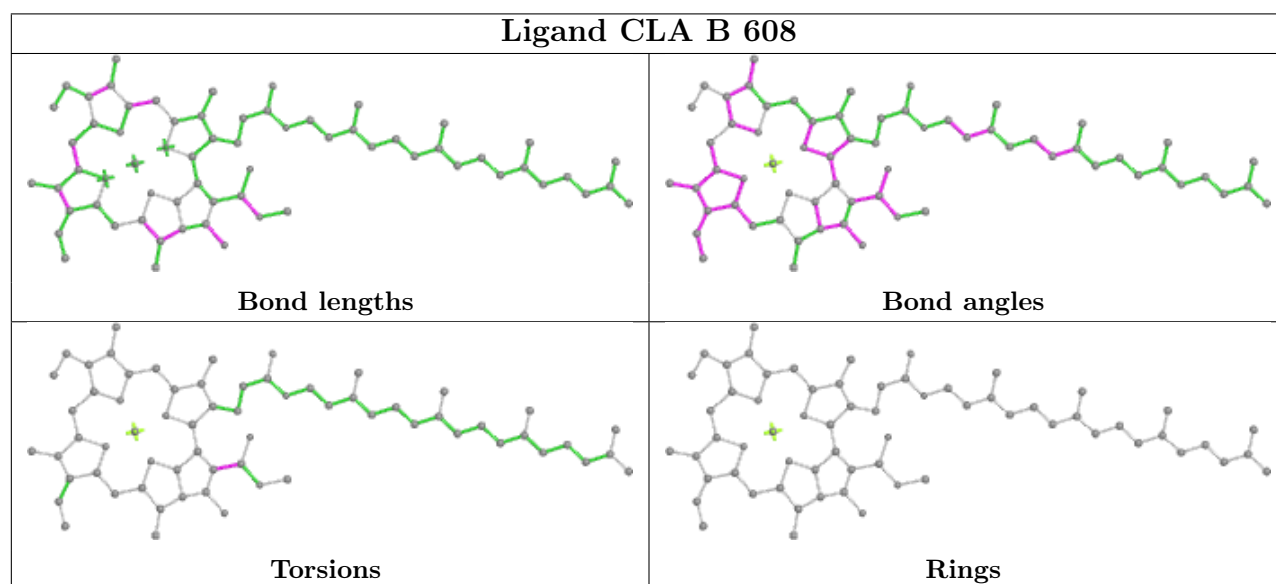
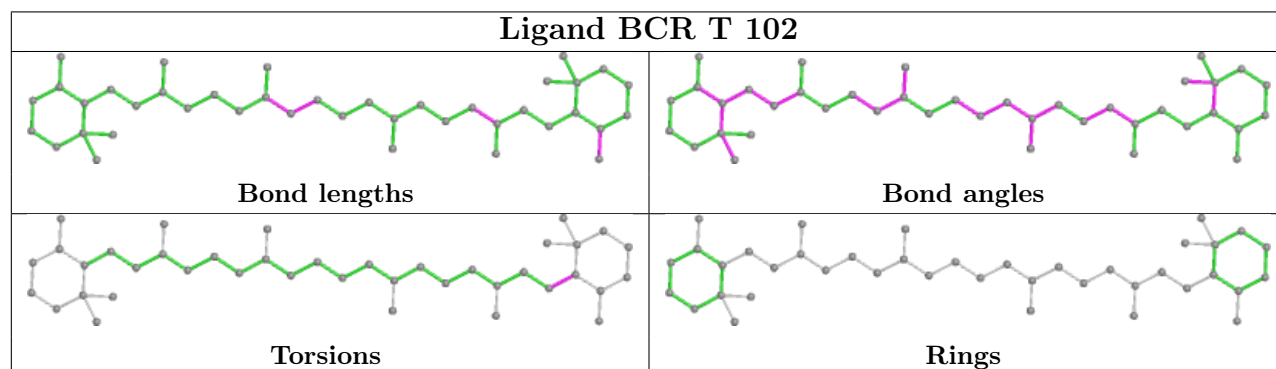
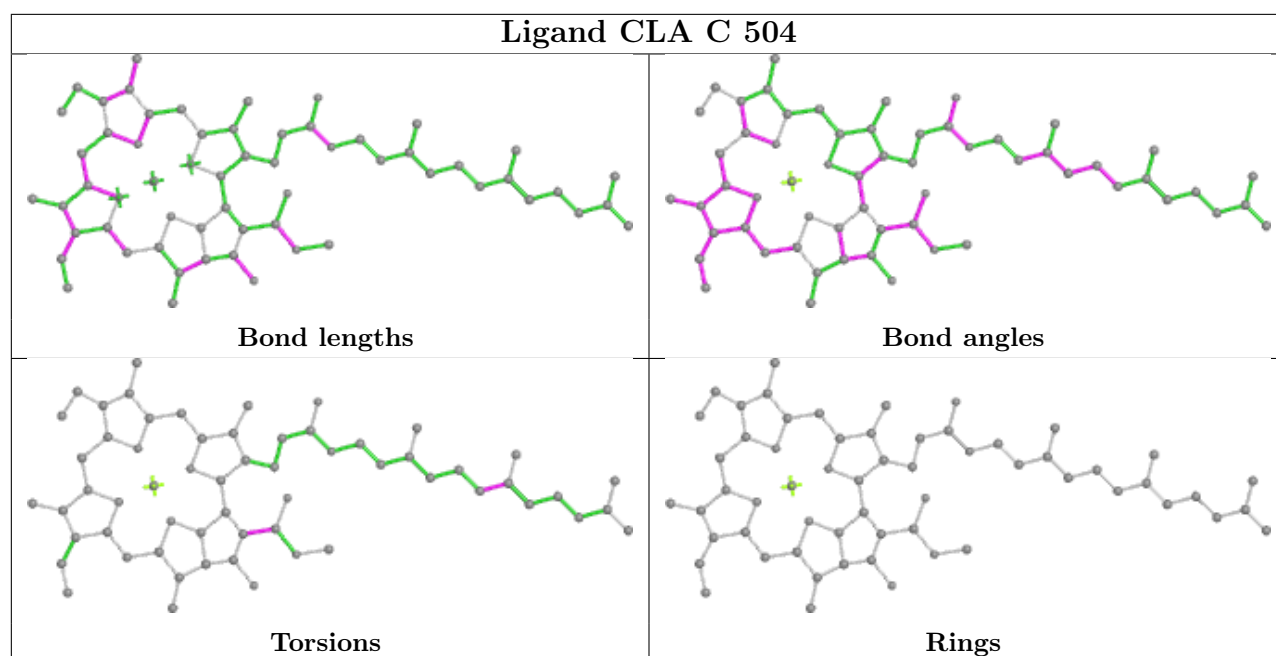
Ligand BCR H 102	
	Bond lengths
	Bond angles
	Torsions
	Rings

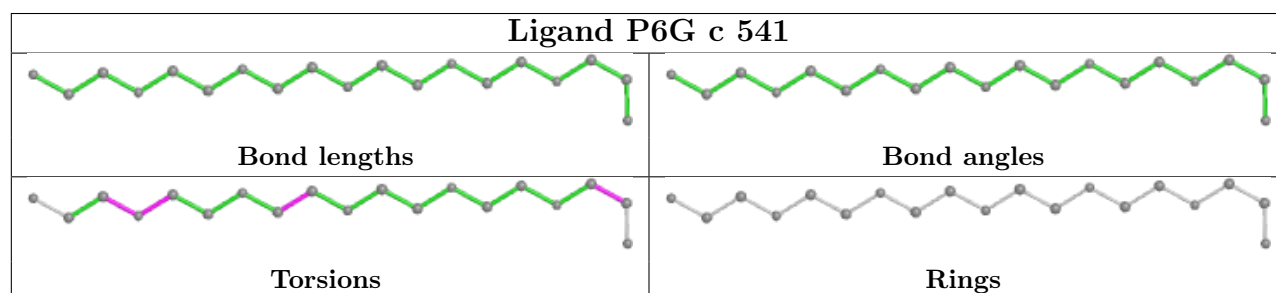
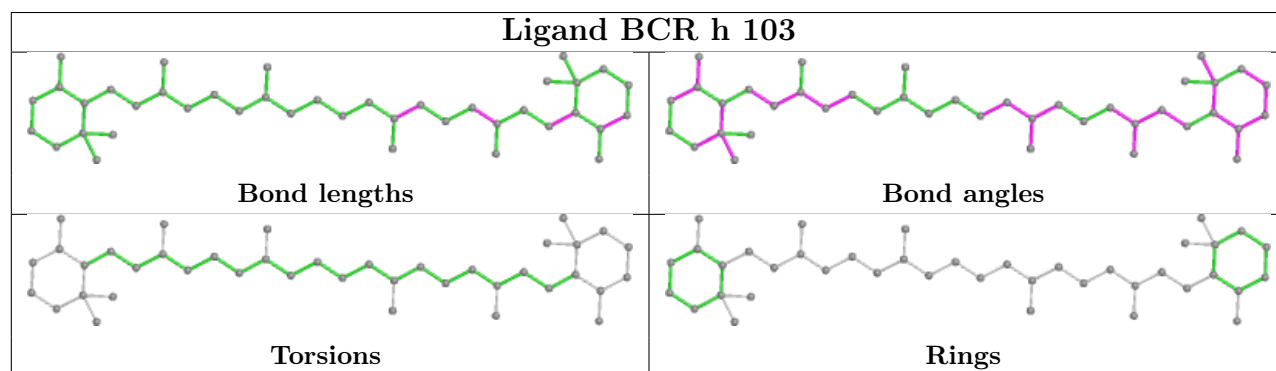
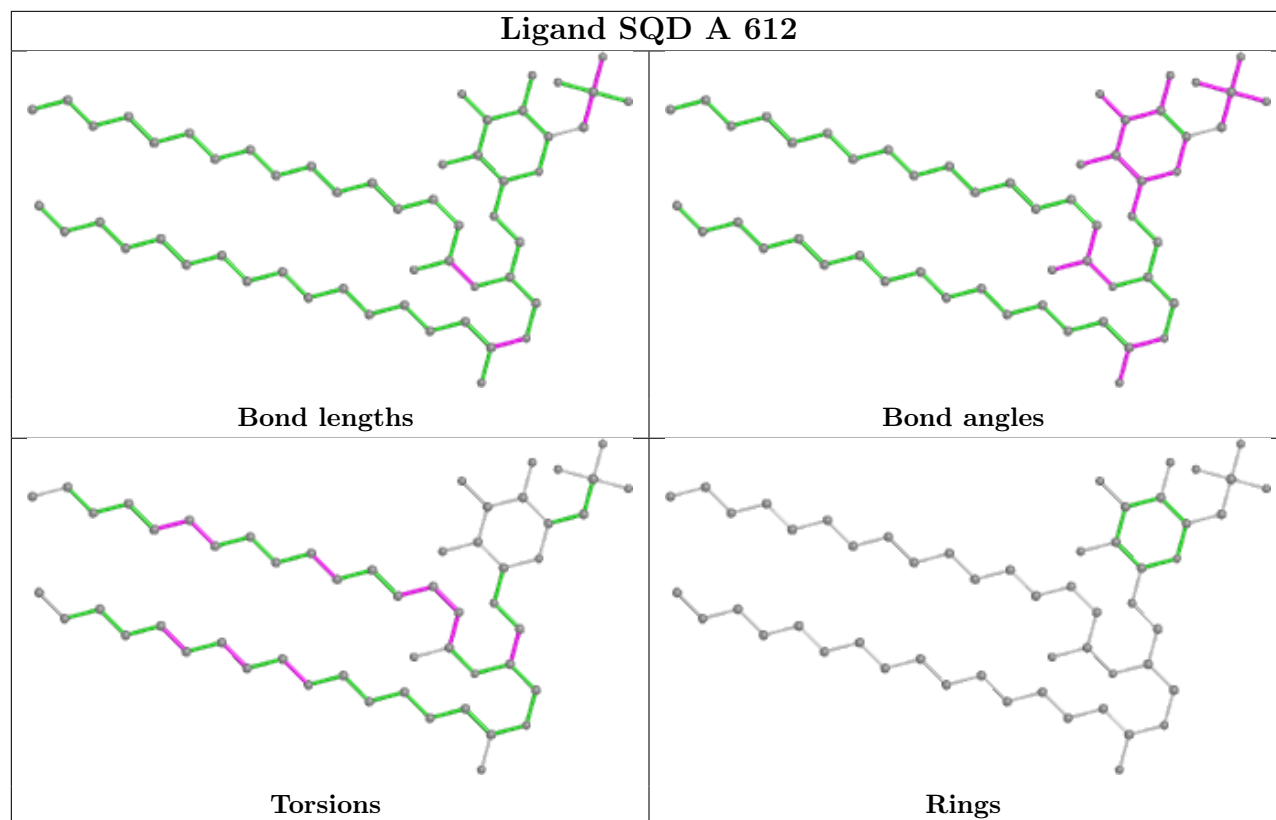
Ligand P6G A 623	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand CLA C 509	
	Bond lengths
	Bond angles
	Torsions
	Rings

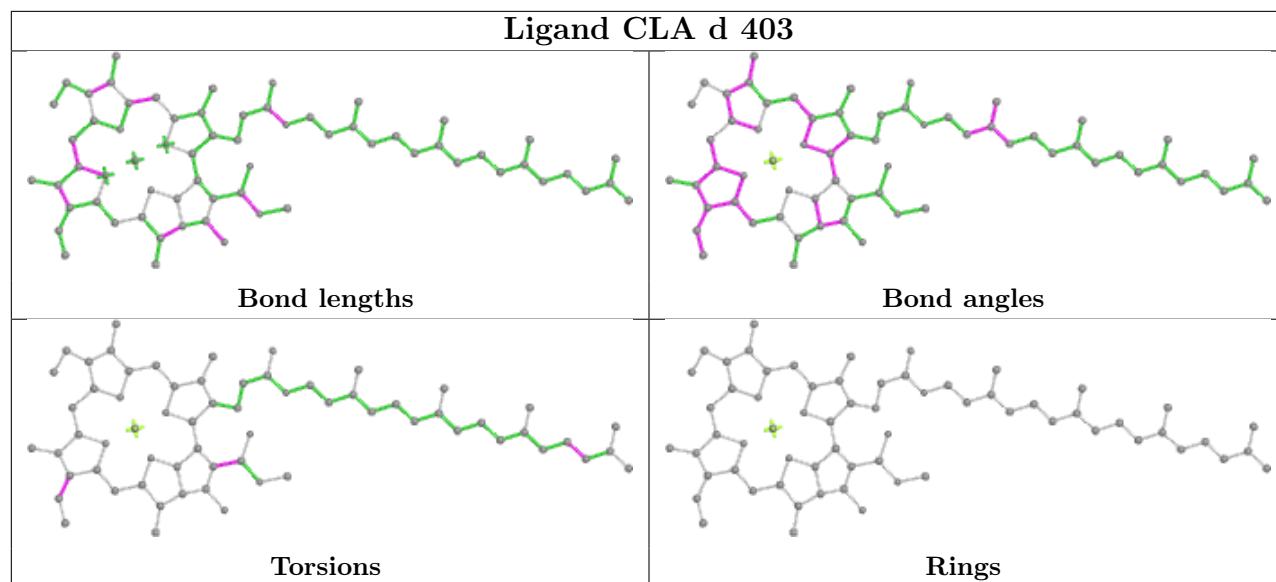




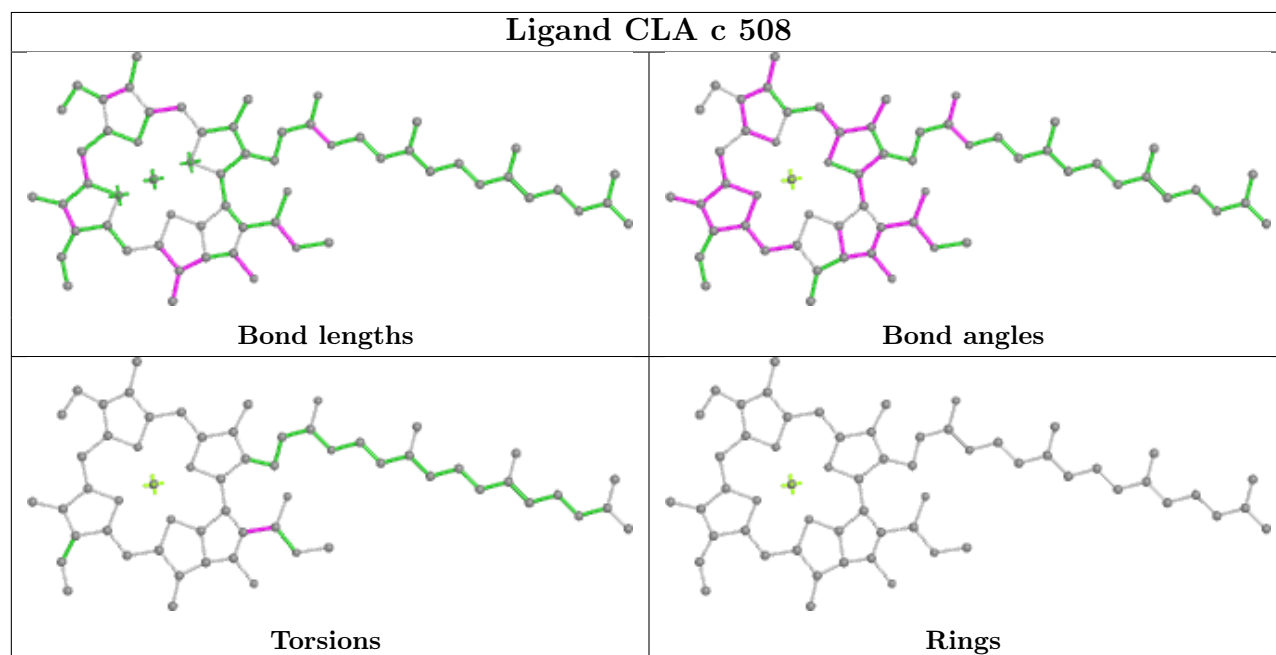




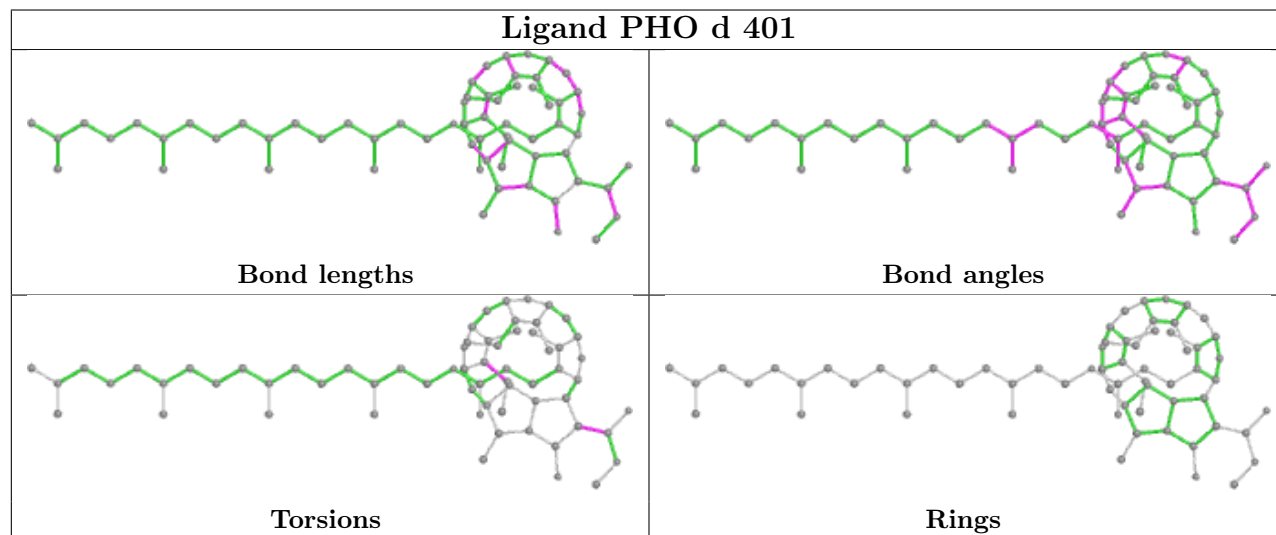
Ligand CLA d 403

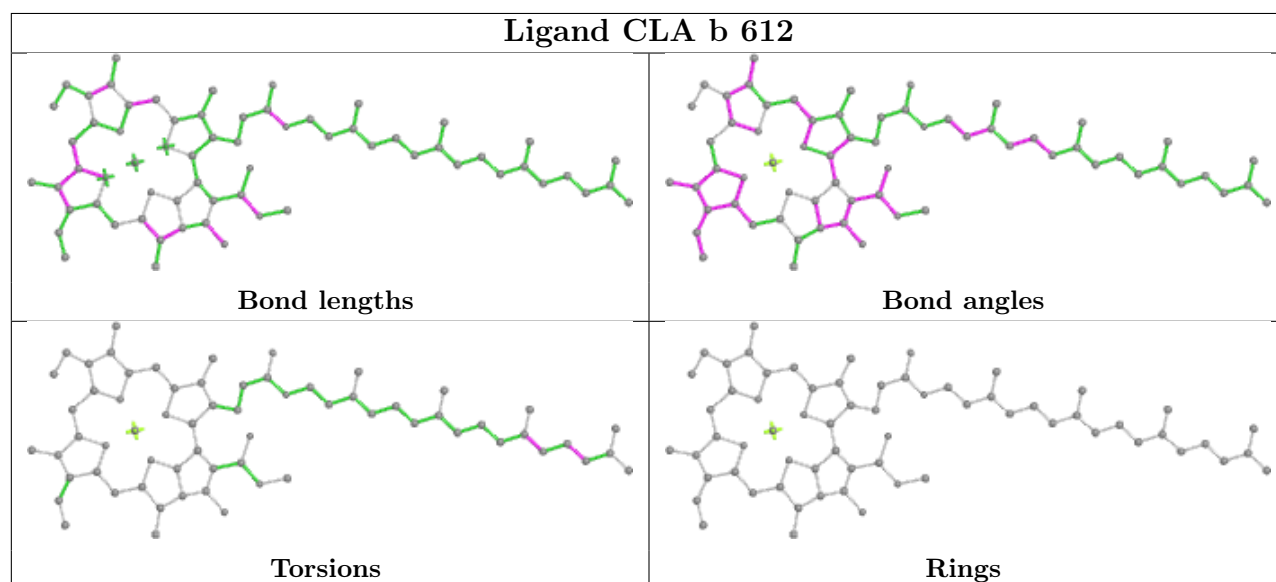
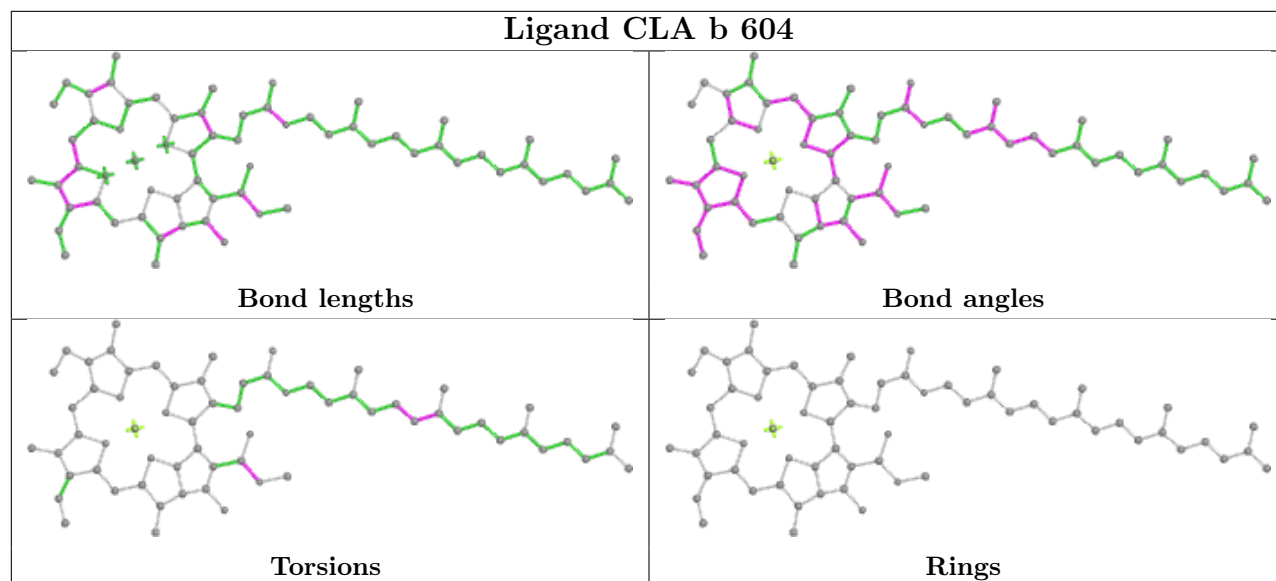
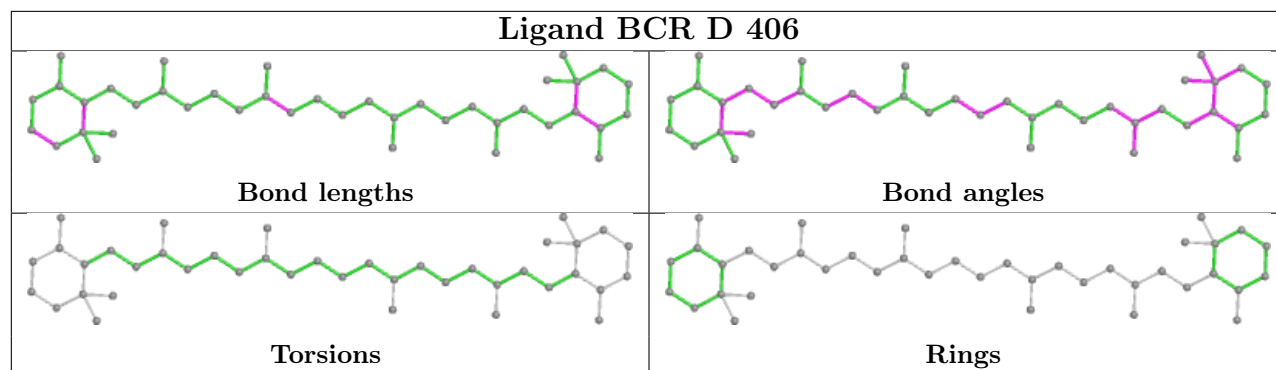


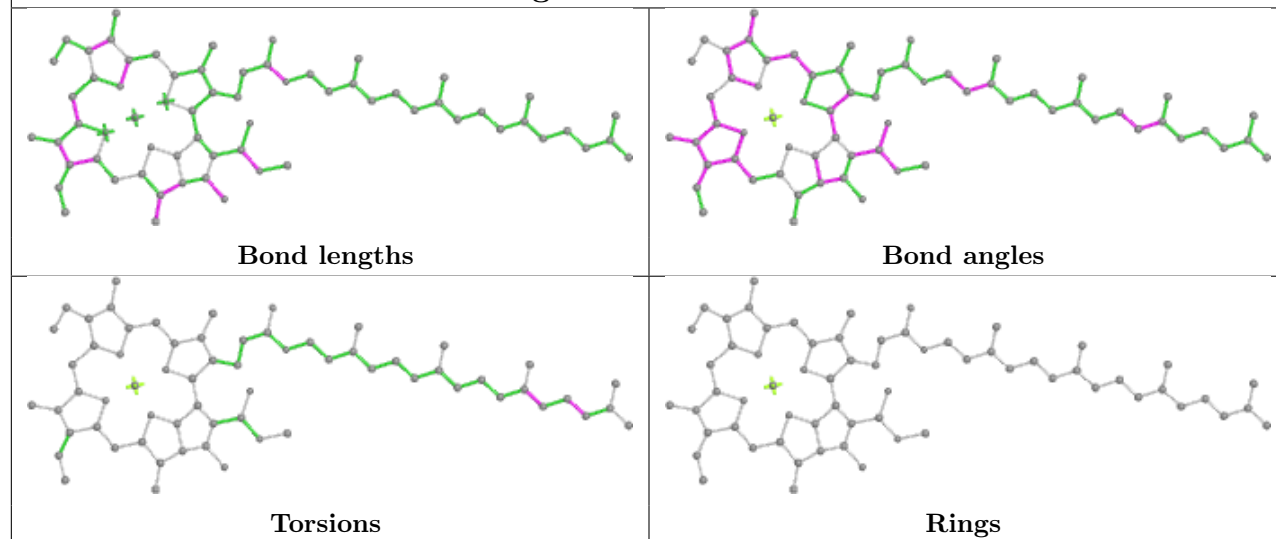
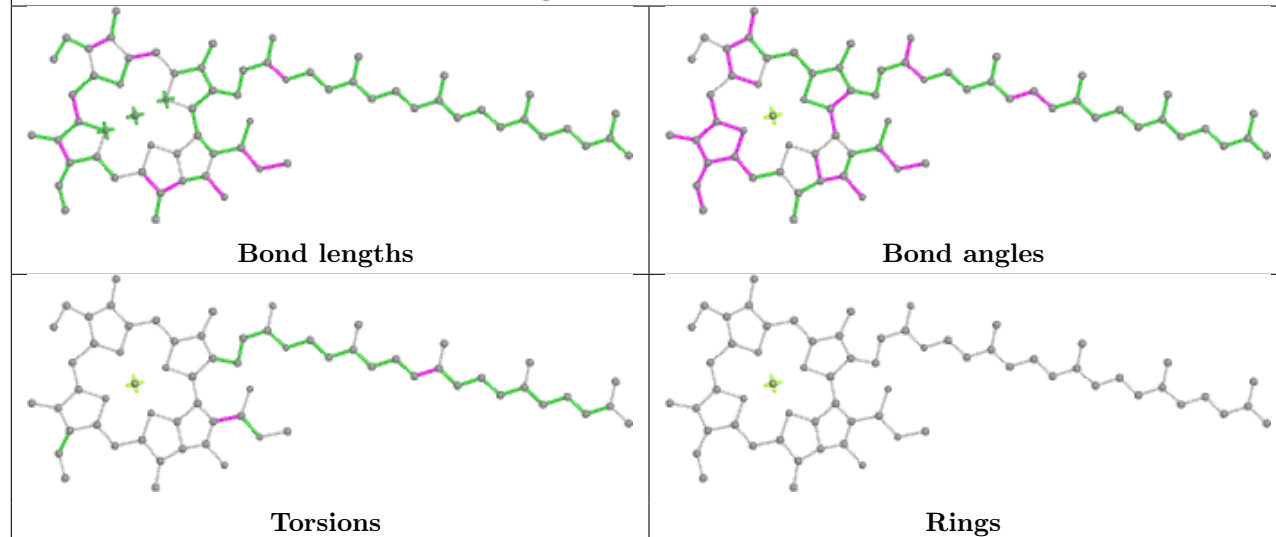
Ligand CLA c 508

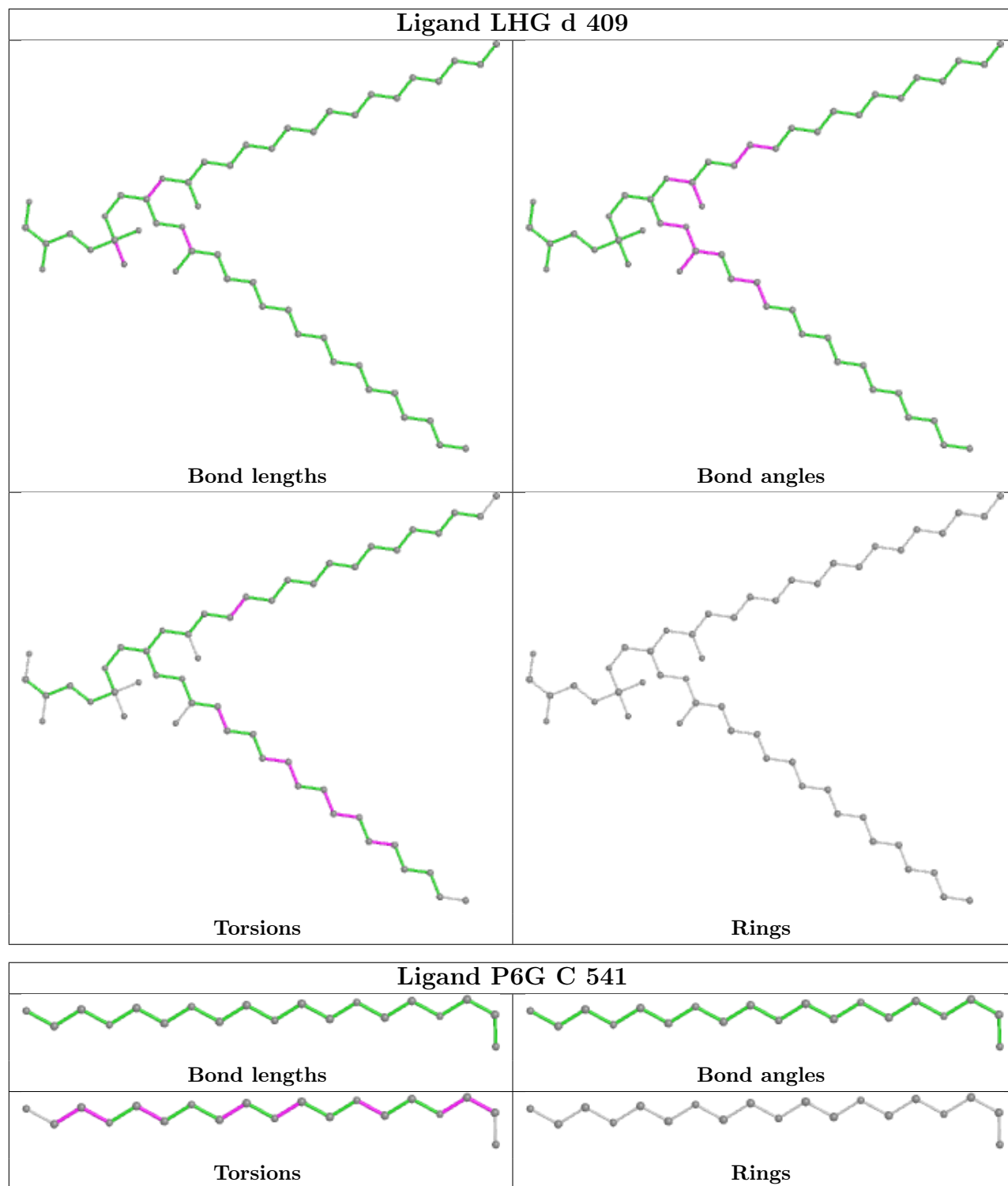


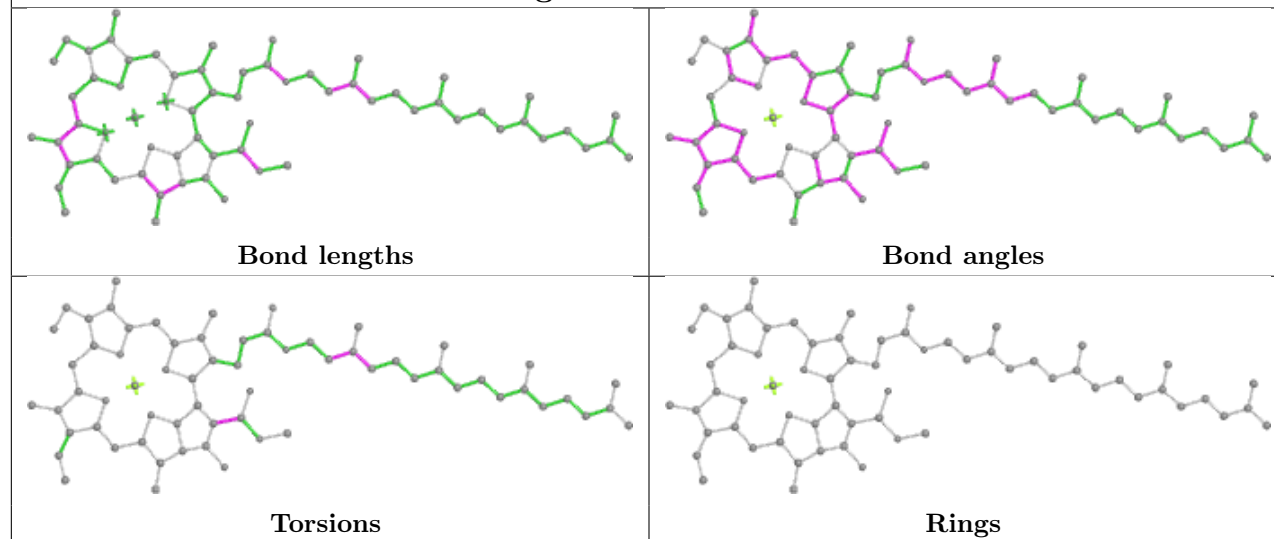
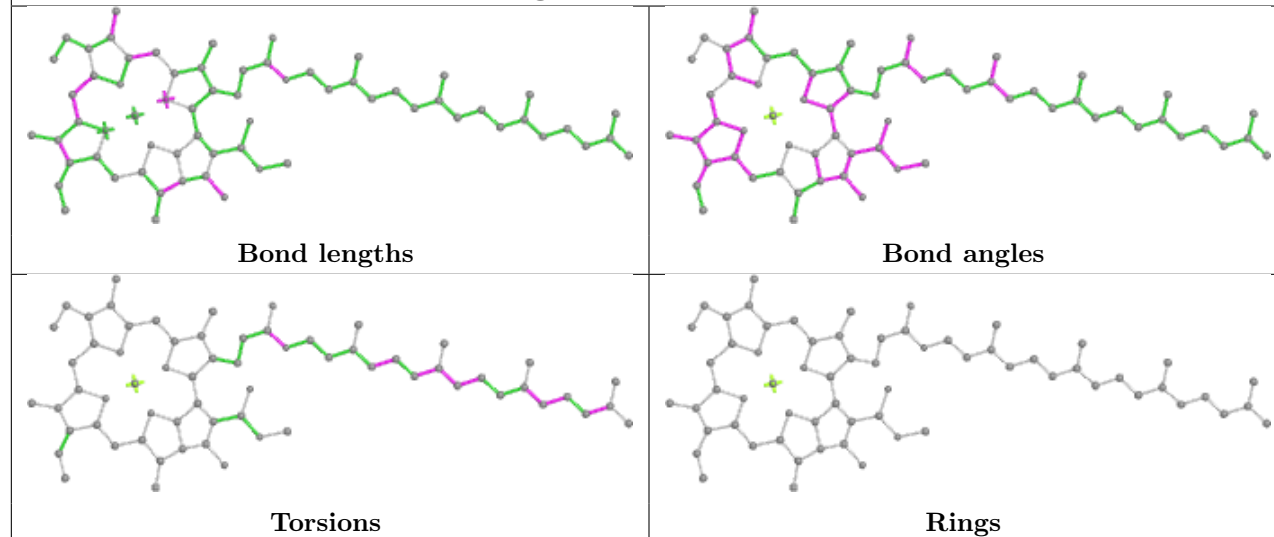
Ligand PHO d 401



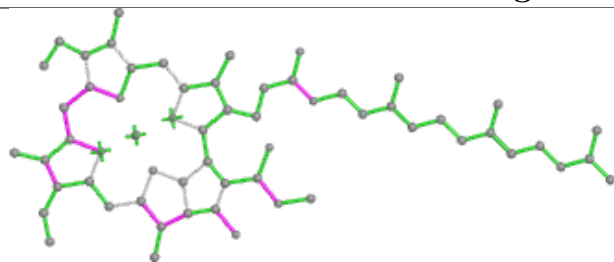


Ligand CLA B 612**Ligand CLA c 503**

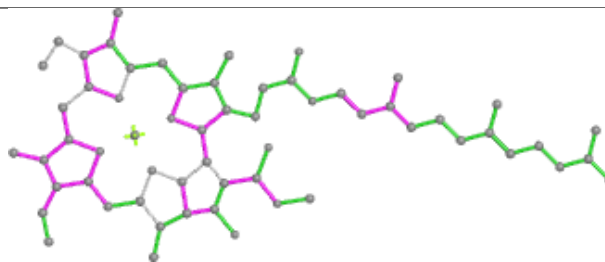


Ligand CLA b 606**Ligand CLA A 609**

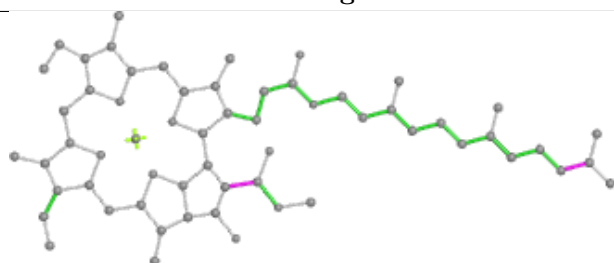
Ligand CLA A 607



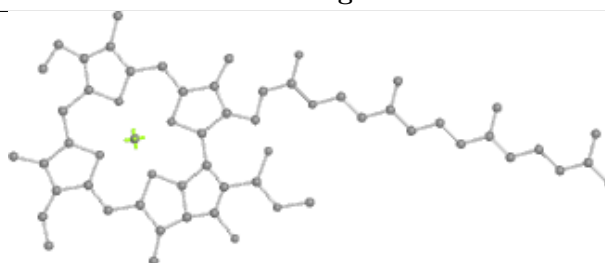
Bond lengths



Bond angles

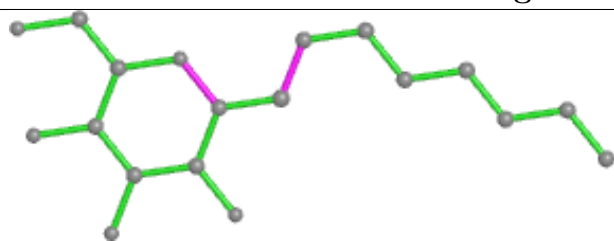


Torsions

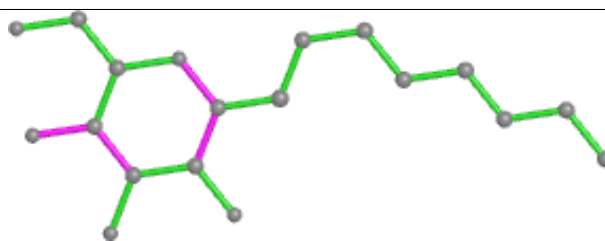


Rings

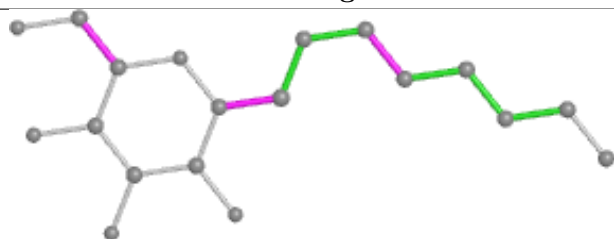
Ligand HTG b 624



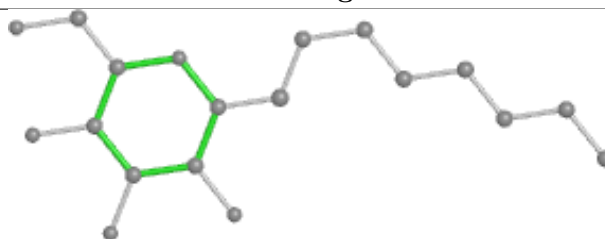
Bond lengths



Bond angles

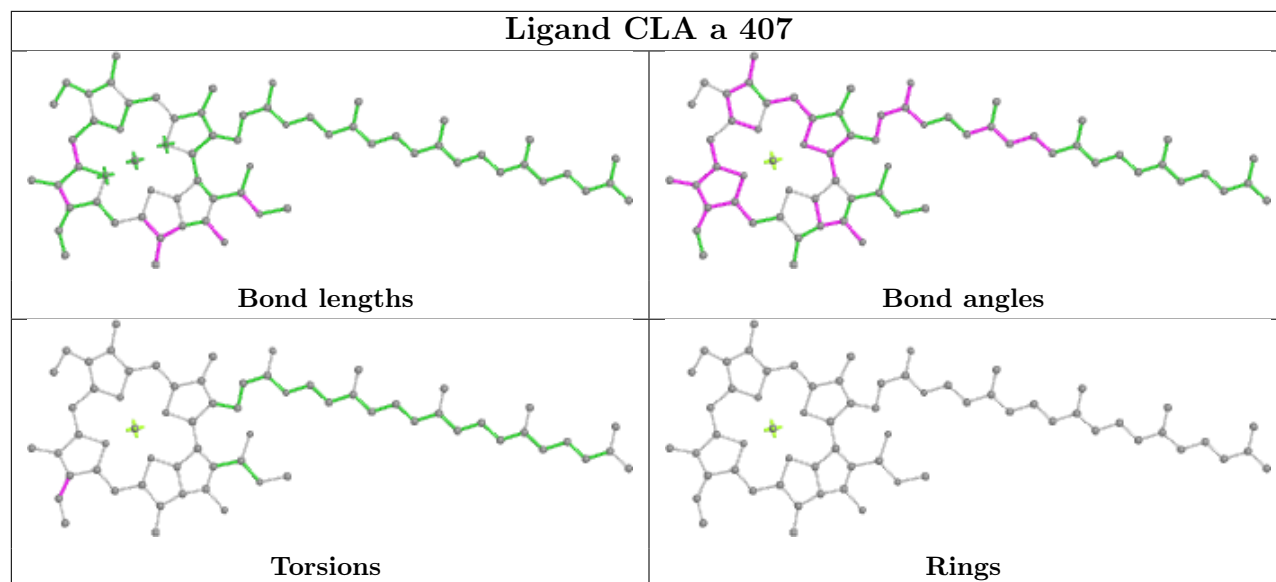


Torsions

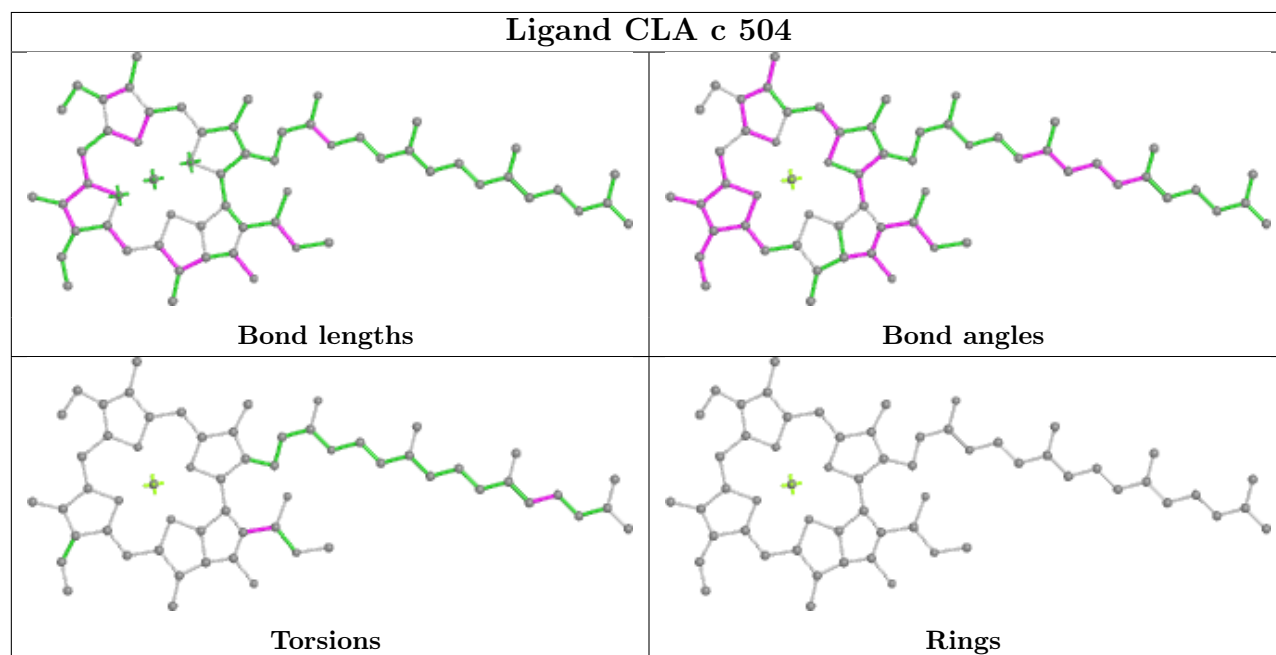


Rings

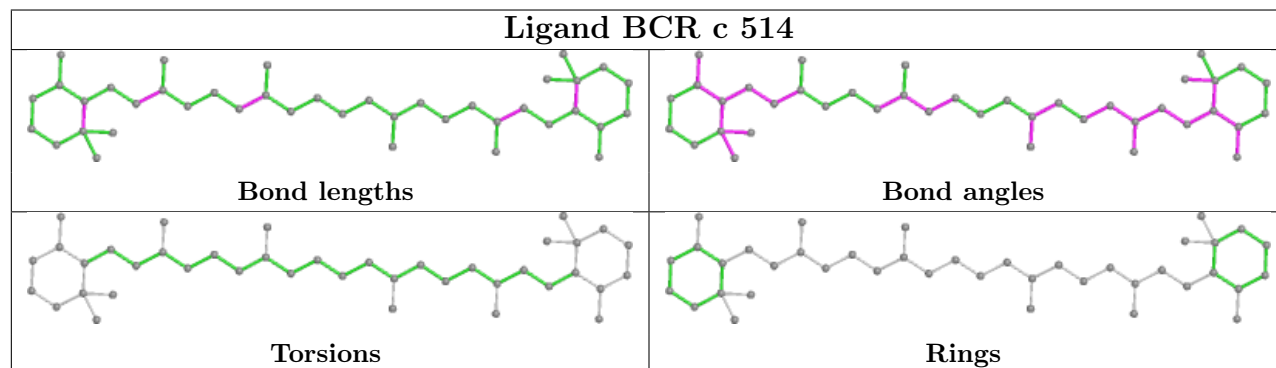
Ligand CLA a 407

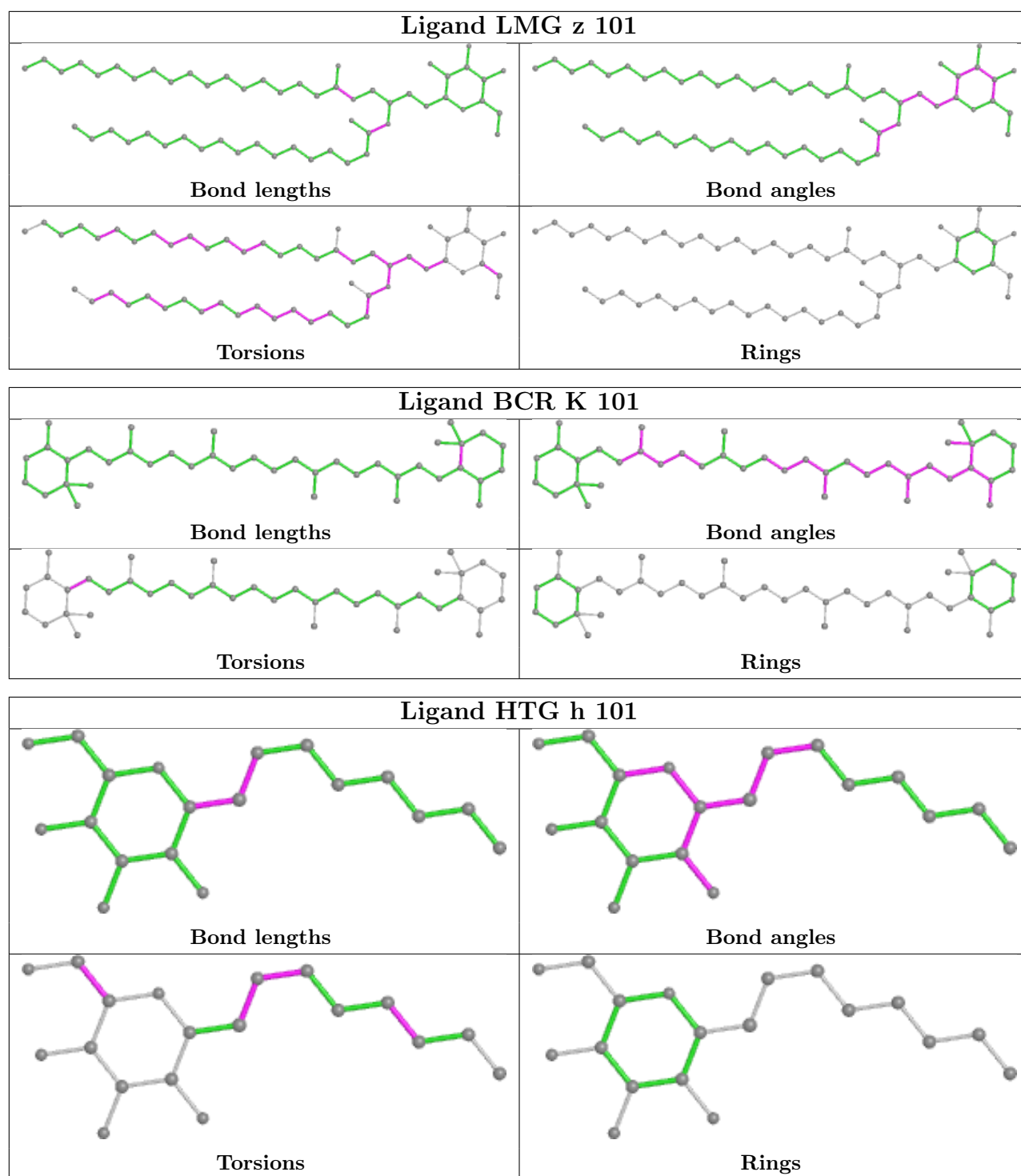


Ligand CLA c 504

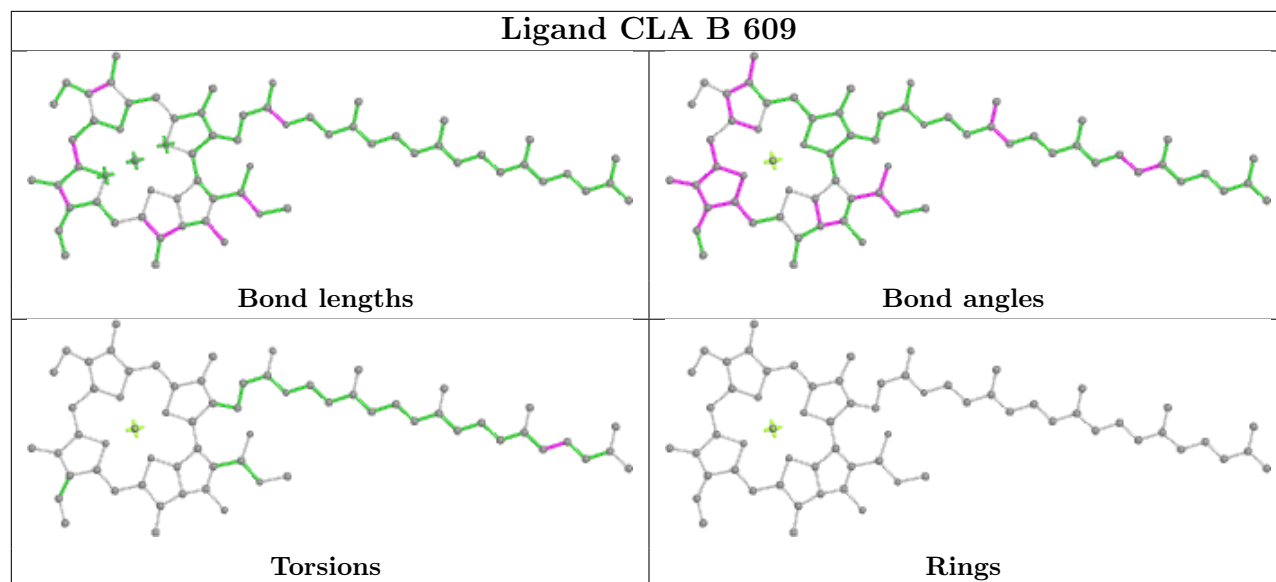


Ligand BCR c 514

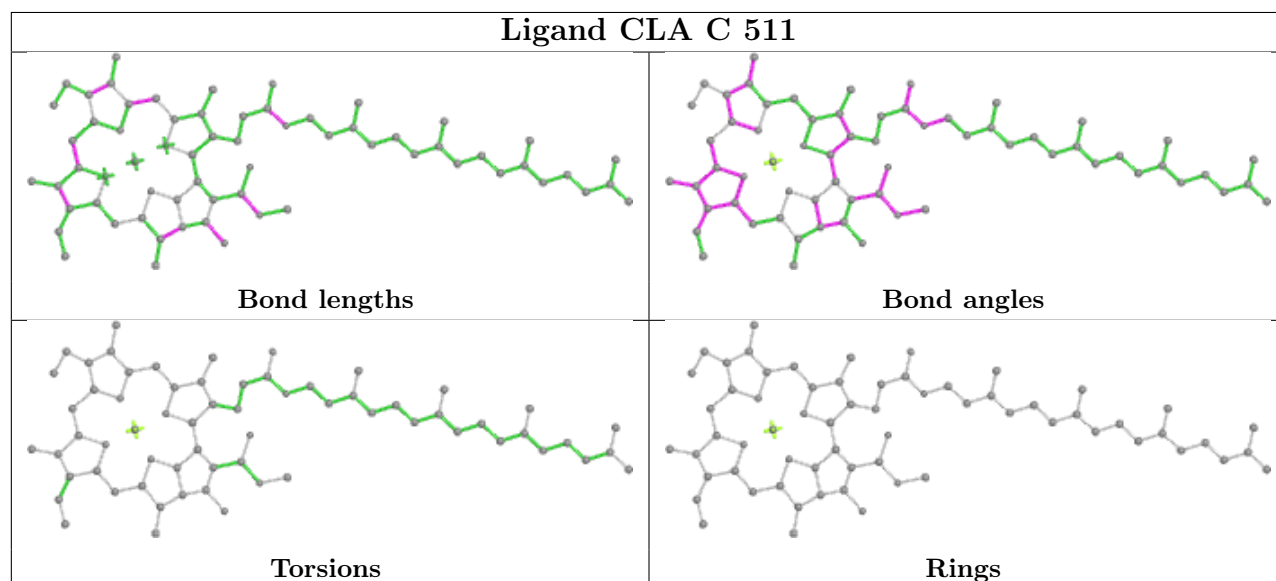




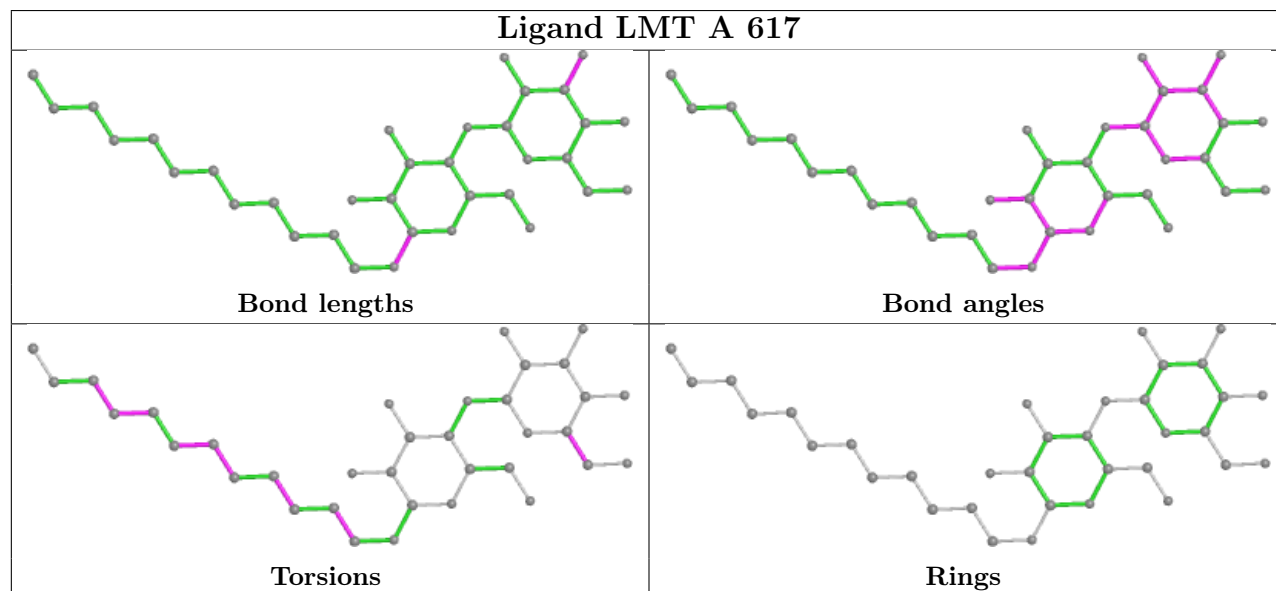
Ligand CLA B 609



Ligand CLA C 511



Ligand LMT A 617



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%)	-0.86	2 (0%) 89 90	16, 22, 46, 78	0
1	a	334/344 (97%)	-0.83	3 (0%) 84 85	17, 24, 52, 89	0
2	B	504/506 (99%)	-0.63	17 (3%) 45 48	17, 26, 57, 92	0
2	b	506/506 (100%)	-0.49	29 (5%) 23 26	19, 29, 71, 129	0
3	C	451/458 (98%)	-0.75	4 (0%) 84 85	19, 31, 46, 87	0
3	c	458/458 (100%)	-0.62	12 (2%) 56 58	24, 35, 51, 108	0
4	D	341/342 (99%)	-0.88	4 (1%) 79 81	16, 23, 40, 114	0
4	d	341/342 (99%)	-0.82	5 (1%) 73 76	18, 26, 44, 110	0
5	E	81/83 (97%)	-0.23	5 (6%) 20 23	26, 41, 66, 92	0
5	e	81/83 (97%)	0.25	8 (9%) 7 8	32, 46, 75, 118	0
6	F	34/44 (77%)	-0.37	3 (8%) 10 11	26, 33, 63, 82	0
6	f	32/44 (72%)	-0.22	2 (6%) 20 22	30, 38, 78, 117	0
7	H	65/65 (100%)	-0.43	4 (6%) 20 23	23, 33, 47, 123	0
7	h	65/65 (100%)	-0.22	3 (4%) 32 35	26, 38, 56, 116	0
8	I	37/38 (97%)	-0.35	3 (8%) 12 13	28, 35, 75, 91	0
8	i	37/38 (97%)	-0.38	2 (5%) 25 29	27, 34, 67, 89	0
9	J	39/40 (97%)	-0.30	6 (15%) 2 2	24, 36, 108, 130	0
9	j	39/40 (97%)	-0.26	5 (12%) 3 4	29, 43, 75, 89	0
10	K	37/37 (100%)	-0.54	0 100 100	31, 37, 56, 70	0
10	k	37/37 (100%)	-0.48	0 100 100	36, 44, 64, 75	0
11	L	37/37 (100%)	-0.45	3 (8%) 12 13	15, 21, 70, 92	0
11	l	37/37 (100%)	-0.33	4 (10%) 5 6	18, 22, 70, 95	0
12	M	33/36 (91%)	-0.59	2 (6%) 21 24	19, 22, 44, 88	0
12	m	34/36 (94%)	-0.49	3 (8%) 10 11	20, 24, 75, 98	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	245/245 (100%)	-0.11	15 (6%) 21 24	18, 33, 69, 128	0
13	o	245/245 (100%)	0.04	25 (10%) 6 8	21, 34, 84, 136	0
14	T	29/32 (90%)	-0.66	2 (6%) 16 19	18, 23, 47, 101	0
14	t	29/32 (90%)	-0.81	1 (3%) 45 48	19, 23, 44, 81	0
15	U	97/104 (93%)	-0.53	2 (2%) 63 66	21, 31, 58, 95	0
15	u	97/104 (93%)	-0.58	1 (1%) 82 84	24, 31, 47, 84	0
16	V	137/137 (100%)	-0.76	0 100 100	20, 29, 46, 66	0
16	v	137/137 (100%)	-0.49	4 (2%) 51 54	26, 38, 58, 73	0
17	Y	29/30 (96%)	1.34	6 (20%) 1 1	36, 49, 76, 109	0
17	y	29/30 (96%)	1.18	6 (20%) 1 1	46, 60, 81, 92	0
18	X	40/41 (97%)	0.24	5 (12%) 3 4	30, 40, 100, 118	0
18	x	40/41 (97%)	0.28	6 (15%) 2 2	36, 43, 112, 132	0
19	Z	62/62 (100%)	0.22	8 (12%) 3 3	37, 47, 86, 94	0
19	z	62/62 (100%)	0.82	14 (22%) 0 0	50, 62, 101, 117	0
All	All	5272/5362 (98%)	-0.52	224 (4%) 36 39	15, 30, 65, 136	0

The worst 5 of 224 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	2	ALA	13.7
7	h	66	GLY	13.4
13	o	3	ALA	13.1
13	O	2	ALA	12.7
17	Y	19	ILE	12.0

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
12	FME	m	1[A]	10/11	0.97	0.10	24,30,61,84	7
12	FME	m	1[B]	10/11	0.97	0.10	30,33,55,66	7
12	FME	M	1	10/11	0.98	0.07	27,32,64,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MHS	D	336	11/12	0.98	0.07	23,28,37,38	0
8	FME	I	1	10/11	0.98	0.05	26,32,40,44	0
14	FME	t	1[A]	10/11	0.98	0.07	20,24,39,42	7
14	FME	t	1[B]	10/11	0.98	0.07	20,24,31,36	7
14	FME	T	1[A]	10/11	0.99	0.07	21,25,47,47	7
14	FME	T	1[B]	10/11	0.99	0.07	21,25,32,35	7
4	MHS	d	336	11/12	0.99	0.05	27,32,44,44	0
8	FME	i	1	10/11	0.99	0.06	30,33,36,37	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(\AA^2)	Q<0.9
30	GOL	O	307	6/6	0.35	0.78	116,117,120,123	0
31	LMT	Y	101	35/35	0.38	0.39	61,118,170,188	0
31	LMT	j	103	35/35	0.40	0.44	68,114,162,168	0
39	1PE	B	653	16/16	0.41	0.61	103,121,137,148	0
34	PGE	f	105	10/10	0.43	0.55	91,98,114,127	0
38	HTG	C	529	19/19	0.46	0.27	70,102,136,144	0
28	SQD	h	105	54/54	0.51	0.45	76,100,195,214	0
31	LMT	C	533	35/35	0.52	0.56	72,121,170,191	0
34	PGE	i	106	10/10	0.52	0.52	78,95,100,103	0
34	PGE	c	536	10/10	0.54	0.58	87,105,124,125	0
30	GOL	v	205	6/6	0.54	0.70	102,122,135,152	0
33	PG4	e	103	13/13	0.54	0.40	72,107,125,136	0
34	PGE	E	107	10/10	0.54	0.59	73,106,142,143	0
34	PGE	E	108	10/10	0.54	0.41	52,65,68,73	10
34	PGE	b	646	10/10	0.56	0.46	70,102,120,121	0
33	PG4	C	534	13/13	0.56	0.54	81,103,119,119	0
35	P6G	D	418	19/19	0.59	0.39	68,99,126,131	0
34	PGE	J	106	10/10	0.61	0.39	85,121,129,138	0
34	PGE	o	307	10/10	0.62	0.55	90,112,130,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	PGE	D	415	10/10	0.63	0.60	86,105,110,122	0
36	EDO	E	111	4/4	0.63	0.24	66,83,90,97	0
38	HTG	H	101	19/19	0.65	0.24	50,94,122,122	0
34	PGE	h	110	10/10	0.65	0.26	71,99,111,117	0
34	PGE	c	540	10/10	0.66	0.42	82,92,110,113	0
33	PG4	X	103	13/13	0.66	0.38	78,99,111,115	0
39	1PE	j	107	16/16	0.66	0.29	74,106,155,159	0
38	HTG	h	101	19/19	0.67	0.28	62,86,123,141	0
33	PG4	B	636	13/13	0.67	0.35	71,98,116,121	0
33	PG4	c	533	13/13	0.67	0.38	77,90,105,109	0
40	DGD	D	408	66/66	0.67	0.29	56,88,142,175	0
34	PGE	J	107	10/10	0.68	0.26	87,137,168,170	0
34	PGE	E	105	10/10	0.68	0.60	90,96,116,118	0
34	PGE	B	650	10/10	0.68	0.51	88,109,126,128	0
38	HTG	c	530	19/19	0.68	0.31	66,104,128,145	0
38	HTG	c	531	19/19	0.69	0.31	59,99,122,124	0
34	PGE	b	644	10/10	0.69	0.47	83,100,113,125	0
30	GOL	y	101	6/6	0.69	0.30	82,90,98,101	0
39	1PE	V	217	16/16	0.69	0.55	63,93,120,133	0
35	P6G	C	541	19/19	0.69	0.49	79,103,127,142	0
33	PG4	J	104	13/13	0.69	0.36	74,82,107,108	0
30	GOL	o	303	6/6	0.70	0.47	79,96,110,126	0
36	EDO	V	218	4/4	0.70	0.46	87,88,88,96	0
33	PG4	J	105	13/13	0.70	0.37	75,88,110,115	0
38	HTG	C	530	19/19	0.70	0.48	98,124,143,150	0
34	PGE	E	106	10/10	0.70	0.35	85,95,111,116	0
34	PGE	b	647	10/10	0.70	0.59	77,97,109,109	0
33	PG4	b	637	13/13	0.71	0.52	74,97,124,130	0
33	PG4	K	102	13/13	0.71	0.25	56,70,102,109	0
33	PG4	C	536	13/13	0.71	0.24	66,72,93,103	0
34	PGE	B	646	10/10	0.71	0.45	83,95,114,119	0
33	PG4	b	634	13/13	0.71	0.29	78,90,111,123	0
31	LMT	J	103	35/35	0.72	0.27	47,78,115,134	0
33	PG4	B	640	13/13	0.72	0.21	66,86,95,99	0
31	LMT	u	203	35/35	0.72	0.39	42,77,115,137	0
38	HTG	C	532	19/19	0.72	0.32	57,85,128,156	0
34	PGE	h	108	10/10	0.73	0.31	70,75,101,105	0
29	LMG	d	412	55/55	0.73	0.25	47,77,119,137	0
38	HTG	C	531	19/19	0.73	0.44	72,109,139,142	0
33	PG4	H	106	13/13	0.74	0.31	38,53,67,74	13
33	PG4	B	643	13/13	0.74	0.45	75,92,114,118	0
38	HTG	B	624	19/19	0.74	0.28	47,103,125,143	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	PG4	E	103	13/13	0.74	0.24	59,76,89,105	0
35	P6G	I	106	19/19	0.74	0.26	56,81,119,121	0
36	EDO	A	625	4/4	0.75	0.16	70,71,80,80	0
33	PG4	e	104	13/13	0.75	0.50	78,94,120,120	0
34	PGE	H	111	10/10	0.75	0.36	82,100,121,127	0
34	PGE	c	539	10/10	0.75	0.48	80,90,104,104	0
33	PG4	B	642	13/13	0.76	0.47	66,86,115,120	0
38	HTG	a	418	19/19	0.76	0.28	53,84,123,124	0
36	EDO	c	542	4/4	0.76	0.68	88,91,102,107	0
36	EDO	o	311	4/4	0.76	0.35	81,83,83,86	0
33	PG4	j	104	13/13	0.76	0.24	78,97,113,116	0
33	PG4	C	538	13/13	0.76	0.34	65,93,115,123	0
34	PGE	b	639	10/10	0.76	0.44	79,97,111,119	0
36	EDO	D	419	4/4	0.76	0.33	66,70,78,97	0
39	1PE	x	104	16/16	0.76	0.35	85,105,130,136	0
34	PGE	H	110	10/10	0.76	0.53	91,103,116,118	0
44	2PE	V	216	28/28	0.76	0.36	44,91,110,123	0
28	SQD	A	622	54/54	0.77	0.27	63,85,136,187	0
34	PGE	H	109	10/10	0.77	0.38	84,95,102,105	0
38	HTG	b	624	19/19	0.77	0.23	54,91,117,133	0
34	PGE	O	309	10/10	0.77	0.48	62,86,111,111	0
34	PGE	V	215	10/10	0.77	0.50	66,90,103,111	0
36	EDO	B	657	4/4	0.77	0.34	93,95,100,102	0
34	PGE	I	105	10/10	0.78	0.20	60,83,95,99	0
33	PG4	V	212	13/13	0.78	0.29	82,96,120,123	0
36	EDO	X	104	4/4	0.78	0.25	73,80,83,88	0
35	P6G	c	541	19/19	0.78	0.32	43,61,68,72	19
33	PG4	c	535	13/13	0.78	0.35	69,89,109,115	0
34	PGE	b	645	10/10	0.78	0.44	106,110,126,134	0
38	HTG	b	632	19/19	0.78	0.20	49,79,119,135	0
33	PG4	B	637	13/13	0.78	0.18	68,82,106,106	0
33	PG4	E	102	13/13	0.79	0.35	62,81,106,120	0
33	PG4	X	102	13/13	0.79	0.27	77,95,113,114	0
34	PGE	h	109	10/10	0.79	0.49	84,97,111,113	0
36	EDO	B	656	4/4	0.79	0.43	78,87,100,107	0
30	GOL	e	102	6/6	0.79	0.36	79,91,112,117	0
36	EDO	C	542	4/4	0.79	0.48	77,84,88,96	0
38	HTG	B	631	19/19	0.79	0.21	46,90,129,147	0
40	DGD	d	408	66/66	0.79	0.35	57,89,155,184	0
35	P6G	E	110	19/19	0.79	0.46	49,95,111,122	0
33	PG4	V	211	13/13	0.80	0.38	54,89,114,120	0
28	SQD	a	424	54/54	0.80	0.26	63,83,134,198	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	LMT	m	101	35/35	0.80	0.20	45,62,75,92	0
31	LMT	t	103	35/35	0.80	0.22	32,75,110,117	0
35	P6G	b	649	19/19	0.80	0.26	71,103,125,128	0
33	PG4	B	638	13/13	0.80	0.34	66,84,114,130	0
34	PGE	B	649	10/10	0.81	0.24	66,82,101,105	0
34	PGE	Y	102	10/10	0.81	0.17	61,84,103,104	0
33	PG4	B	641	13/13	0.81	0.34	74,97,107,115	0
29	LMG	B	634	55/55	0.81	0.19	39,69,141,167	0
33	PG4	i	103	13/13	0.81	0.37	74,85,98,105	0
30	GOL	C	527	6/6	0.81	0.49	96,108,112,135	0
34	PGE	B	645	10/10	0.81	0.36	68,81,89,93	0
34	PGE	o	306	10/10	0.81	0.46	70,92,102,103	0
29	LMG	C	526	55/55	0.81	0.23	47,83,115,124	0
34	PGE	V	214	10/10	0.82	0.43	50,86,96,98	0
29	LMG	z	101	55/55	0.82	0.21	49,95,120,160	0
36	EDO	e	106	4/4	0.82	0.11	72,76,79,89	0
32	LHG	e	101	42/49	0.82	0.27	60,105,123,171	0
33	PG4	V	210	13/13	0.82	0.38	53,84,115,120	0
31	LMT	F	102	35/35	0.82	0.28	43,81,105,126	0
33	PG4	H	107	13/13	0.82	0.20	68,83,105,110	0
33	PG4	V	213	13/13	0.82	0.48	68,80,103,112	0
33	PG4	I	103	13/13	0.82	0.23	73,97,121,129	0
31	LMT	b	622	35/35	0.82	0.22	49,76,124,132	0
34	PGE	c	537	10/10	0.82	0.28	96,106,120,123	0
34	PGE	c	538	10/10	0.82	0.29	68,102,115,129	0
33	PG4	A	619	13/13	0.83	0.22	83,96,112,112	0
33	PG4	H	104	13/13	0.83	0.39	83,98,117,119	0
34	PGE	A	621	10/10	0.83	0.20	66,116,120,129	0
34	PGE	H	108	10/10	0.83	0.29	66,86,129,136	0
33	PG4	C	535	13/13	0.84	0.33	66,74,108,121	0
34	PGE	i	105	10/10	0.84	0.23	70,81,89,92	0
33	PG4	B	639	13/13	0.84	0.21	64,79,104,115	0
33	PG4	X	101	13/13	0.84	0.35	63,89,105,108	0
35	P6G	d	416	19/19	0.84	0.17	43,61,100,111	0
30	GOL	v	203	6/6	0.84	0.17	66,79,82,98	0
35	P6G	A	623	19/19	0.84	0.18	48,60,95,96	0
33	PG4	H	105	13/13	0.84	0.25	72,87,126,147	0
33	PG4	a	420	13/13	0.84	0.18	79,94,105,106	0
34	PGE	b	641	10/10	0.85	0.21	99,104,114,125	0
38	HTG	c	523	19/19	0.85	0.31	65,86,104,106	0
32	LHG	A	618	42/49	0.85	0.22	49,90,145,167	0
33	PG4	x	102	13/13	0.85	0.48	79,95,107,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
38	HTG	C	522	19/19	0.85	0.24	50,83,100,110	0
29	LMG	c	520	51/55	0.85	0.22	47,76,100,124	0
33	PG4	d	414	13/13	0.85	0.26	65,79,85,87	0
39	1PE	e	105	16/16	0.85	0.21	77,93,116,121	0
29	LMG	C	520	51/55	0.85	0.20	38,79,108,121	0
30	GOL	f	104	6/6	0.85	0.31	94,115,135,150	0
31	LMT	f	101	35/35	0.85	0.28	54,85,110,119	0
33	PG4	i	104	13/13	0.85	0.15	56,71,90,91	0
36	EDO	o	310	4/4	0.85	0.32	60,65,77,90	0
36	EDO	H	112	4/4	0.86	0.26	70,85,94,95	0
33	PG4	U	202	13/13	0.86	0.32	52,80,100,102	0
34	PGE	A	620	7/10	0.86	0.11	68,77,83,87	0
31	LMT	M	101	35/35	0.86	0.14	34,51,70,73	0
34	PGE	a	423	10/10	0.86	0.26	78,91,107,107	0
31	LMT	M	102	35/35	0.86	0.17	43,59,82,96	0
31	LMT	B	622	35/35	0.86	0.16	46,73,107,123	0
33	PG4	i	101	13/13	0.86	0.17	71,84,95,98	0
33	PG4	i	102	13/13	0.86	0.25	65,71,81,82	0
33	PG4	b	636	13/13	0.86	0.21	71,79,90,93	0
31	LMT	a	401	35/35	0.86	0.16	37,52,75,83	0
28	SQD	F	104	54/54	0.86	0.26	55,80,110,135	0
34	PGE	x	103	10/10	0.86	0.58	81,98,110,112	0
34	PGE	O	310	10/10	0.86	0.57	58,81,122,137	0
36	EDO	E	112	4/4	0.86	0.17	84,94,96,100	0
36	EDO	I	107	4/4	0.87	0.16	84,89,91,96	0
34	PGE	o	308	10/10	0.87	0.22	48,87,100,104	0
33	PG4	C	537	13/13	0.87	0.23	67,76,92,108	0
33	PG4	b	635	13/13	0.87	0.15	58,76,103,109	0
34	PGE	E	109	10/10	0.87	0.32	51,93,103,106	0
28	SQD	l	102	54/54	0.87	0.14	46,71,104,172	0
33	PG4	I	104	13/13	0.87	0.15	65,73,90,93	0
34	PGE	j	105	10/10	0.87	0.22	73,109,124,125	0
33	PG4	D	414	13/13	0.87	0.33	86,95,105,110	0
30	GOL	B	633	6/6	0.87	0.16	69,71,84,97	0
34	PGE	B	648	10/10	0.88	0.21	55,75,82,93	0
34	PGE	o	309	10/10	0.88	0.36	53,78,92,97	0
34	PGE	J	108	10/10	0.88	0.29	80,98,116,120	0
30	GOL	O	302	6/6	0.88	0.12	51,55,67,70	0
34	PGE	b	638	10/10	0.88	0.18	55,77,90,93	0
30	GOL	B	635	6/6	0.88	0.28	46,67,79,83	0
34	PGE	C	540	10/10	0.88	0.25	74,83,102,111	0
28	SQD	b	633	54/54	0.89	0.13	46,66,104,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	LHG	a	419	41/49	0.89	0.20	52,85,176,193	0
28	SQD	x	101	54/54	0.89	0.20	62,84,132,147	0
33	PG4	c	534	13/13	0.89	0.28	69,85,99,112	0
30	GOL	O	305	6/6	0.89	0.34	55,65,71,77	0
34	PGE	b	643	10/10	0.89	0.21	70,85,103,116	0
39	1PE	B	654	16/16	0.89	0.21	46,68,92,105	0
29	LMG	A	613	51/55	0.90	0.13	45,60,82,95	0
35	P6G	B	652	19/19	0.90	0.28	42,84,105,109	0
31	LMT	m	102	35/35	0.90	0.12	28,50,66,82	0
30	GOL	O	304	6/6	0.90	0.36	60,69,79,88	0
28	SQD	A	616	54/54	0.90	0.13	39,65,102,107	0
30	GOL	u	201	6/6	0.90	0.24	43,70,71,77	0
32	LHG	E	101	42/49	0.90	0.18	54,80,100,127	0
29	LMG	a	414	51/55	0.90	0.13	42,64,80,90	0
34	PGE	b	640	10/10	0.90	0.20	61,88,103,118	0
34	PGE	B	647	10/10	0.90	0.31	78,92,122,122	0
30	GOL	d	413	6/6	0.90	0.17	74,88,114,116	0
34	PGE	h	107	10/10	0.90	0.17	67,78,92,95	0
45	PE8	i	107	25/25	0.90	0.14	44,66,104,122	0
30	GOL	u	202	6/6	0.91	0.22	50,56,61,63	0
35	P6G	A	624	19/19	0.91	0.10	70,85,105,113	0
33	PG4	c	532	13/13	0.91	0.19	70,78,98,101	0
31	LMT	I	101	35/35	0.91	0.15	57,83,111,113	0
30	GOL	b	626	6/6	0.91	0.10	42,46,50,54	0
27	PL9	A	611	55/55	0.91	0.13	39,63,96,107	0
38	HTG	c	522	19/19	0.91	0.23	60,74,96,106	0
28	SQD	a	417	54/54	0.92	0.10	40,64,93,101	0
31	LMT	A	617	35/35	0.92	0.15	37,55,92,105	0
39	1PE	L	101	16/16	0.92	0.12	56,72,99,100	0
33	PG4	V	209	13/13	0.92	0.26	51,84,95,101	0
24	CLA	C	513	65/65	0.92	0.11	33,44,73,92	0
30	GOL	v	207	6/6	0.92	0.31	63,73,86,86	0
35	P6G	d	415	19/19	0.92	0.12	51,64,88,97	0
34	PGE	E	104	10/10	0.92	0.12	67,76,99,106	0
33	PG4	a	421	13/13	0.92	0.09	76,89,99,102	0
31	LMT	c	521	35/35	0.92	0.26	54,77,95,101	0
36	EDO	a	425	4/4	0.92	0.24	74,78,96,120	0
30	GOL	c	529	6/6	0.93	0.33	27,31,39,40	6
34	PGE	t	104	10/10	0.93	0.09	60,79,99,100	0
35	P6G	b	648	19/19	0.93	0.11	59,66,80,84	0
34	PGE	a	422	10/10	0.93	0.14	72,75,85,92	0
33	PG4	h	106	13/13	0.93	0.22	67,76,106,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
37	CA	h	102	1/1	0.93	0.12	97,97,97,97	0
38	HTG	b	631	19/19	0.93	0.11	41,48,77,98	0
30	GOL	A	615	6/6	0.93	0.11	34,54,62,66	0
38	HTG	B	630	19/19	0.93	0.11	38,50,78,82	0
27	PL9	a	412	55/55	0.93	0.12	46,69,101,108	0
30	GOL	T	103	6/6	0.93	0.14	62,79,91,111	0
24	CLA	b	602	65/65	0.93	0.13	28,47,99,111	0
30	GOL	B	626	6/6	0.94	0.12	34,41,49,61	0
30	GOL	m	103	6/6	0.94	0.15	47,69,88,116	0
29	LMG	c	519	51/55	0.94	0.12	34,67,104,112	0
24	CLA	c	513	65/65	0.94	0.10	37,51,89,99	0
34	PGE	B	644	10/10	0.94	0.09	58,71,117,137	0
35	P6G	j	106	19/19	0.94	0.09	50,74,98,112	0
34	PGE	O	308	10/10	0.94	0.29	31,62,83,96	0
30	GOL	U	201	6/6	0.94	0.24	40,67,78,98	0
26	BCR	C	514	40/40	0.94	0.10	31,41,50,57	0
30	GOL	D	412	6/6	0.94	0.13	55,80,95,102	0
33	PG4	I	102	13/13	0.94	0.19	62,73,97,112	0
26	BCR	c	514	40/40	0.94	0.12	39,51,58,60	0
26	BCR	d	406	40/40	0.94	0.08	28,36,70,82	0
34	PGE	t	105	7/10	0.95	0.12	58,79,84,87	0
36	EDO	B	658	4/4	0.95	0.25	82,84,89,110	0
24	CLA	c	512	65/65	0.95	0.09	30,44,74,79	0
30	GOL	v	206	6/6	0.95	0.09	50,54,66,75	0
38	HTG	V	204	19/19	0.95	0.27	36,52,89,102	0
24	CLA	B	602	65/65	0.95	0.10	27,39,92,115	0
35	P6G	B	651	19/19	0.95	0.07	49,63,77,81	0
30	GOL	C	523	6/6	0.95	0.17	35,46,56,62	0
24	CLA	b	617	60/65	0.95	0.10	26,31,82,92	0
36	EDO	J	109	4/4	0.95	0.10	78,79,85,96	0
30	GOL	C	528	6/6	0.95	0.27	24,27,36,38	6
26	BCR	D	406	40/40	0.95	0.07	23,28,60,65	0
34	PGE	C	539	10/10	0.95	0.23	56,73,94,96	0
35	P6G	T	105	19/19	0.95	0.10	42,59,85,88	0
34	PGE	b	642	10/10	0.95	0.09	51,65,87,92	0
36	EDO	i	108	4/4	0.95	0.21	70,71,76,87	0
30	GOL	o	305	6/6	0.95	0.08	51,56,61,62	0
30	GOL	t	101	6/6	0.95	0.15	44,49,56,62	0
33	PG4	l	103	13/13	0.95	0.09	48,64,71,74	0
30	GOL	a	416	6/6	0.95	0.12	39,57,72,77	0
30	GOL	D	413	6/6	0.95	0.21	58,67,76,84	0
34	PGE	T	104	7/10	0.95	0.10	76,77,96,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
38	HTG	C	521	19/19	0.95	0.14	53,65,84,85	0
36	EDO	B	655	4/4	0.95	0.31	45,50,57,88	0
30	GOL	c	528	6/6	0.95	0.22	78,79,88,89	0
26	BCR	H	102	40/40	0.96	0.08	23,33,52,55	0
24	CLA	C	512	65/65	0.96	0.08	31,39,74,85	0
29	LMG	C	519	51/55	0.96	0.10	29,59,104,117	0
30	GOL	O	306	6/6	0.96	0.13	39,45,55,97	0
26	BCR	C	525	40/40	0.96	0.10	26,33,39,41	0
26	BCR	k	101	40/40	0.96	0.08	34,40,51,54	0
24	CLA	c	506	65/65	0.96	0.08	26,37,83,95	0
38	HTG	B	623	19/19	0.96	0.09	28,40,74,88	0
30	GOL	V	207	6/6	0.96	0.13	44,49,52,55	0
30	GOL	B	627	6/6	0.96	0.08	35,44,48,48	0
30	GOL	F	101	6/6	0.96	0.11	43,48,50,54	0
40	DGD	h	104	62/66	0.96	0.08	25,35,49,55	0
30	GOL	b	629	6/6	0.96	0.14	36,42,45,50	0
35	P6G	D	417	19/19	0.96	0.09	35,56,89,111	0
24	CLA	a	410	65/65	0.97	0.09	20,25,98,113	0
30	GOL	A	614	6/6	0.97	0.09	33,37,38,44	0
36	EDO	d	417	4/4	0.97	0.09	46,49,52,58	0
30	GOL	f	103	6/6	0.97	0.11	50,53,56,56	0
24	CLA	d	405	65/65	0.97	0.08	25,33,91,101	0
30	GOL	B	625	6/6	0.97	0.07	32,36,38,50	0
28	SQD	A	612	54/54	0.97	0.07	31,55,78,87	0
37	CA	b	601	1/1	0.97	0.19	72,72,72,72	0
30	GOL	o	304	6/6	0.97	0.08	45,53,55,62	0
26	BCR	B	619	40/40	0.97	0.07	20,26,50,62	0
30	GOL	B	629	6/6	0.97	0.09	31,39,60,64	0
24	CLA	C	506	65/65	0.97	0.08	28,39,97,106	0
26	BCR	C	515	40/40	0.97	0.09	28,33,52,59	0
24	CLA	C	510	65/65	0.97	0.07	22,29,41,48	0
24	CLA	c	503	65/65	0.97	0.07	26,35,42,52	0
35	P6G	D	416	19/19	0.97	0.06	38,60,84,87	0
24	CLA	c	504	60/65	0.97	0.06	25,31,67,75	0
30	GOL	D	402	6/6	0.97	0.12	31,37,43,44	0
26	BCR	K	101	40/40	0.97	0.08	27,36,45,47	0
26	BCR	T	102	40/40	0.97	0.07	20,29,45,60	0
38	HTG	O	303	19/19	0.97	0.07	27,31,50,65	0
26	BCR	a	411	40/40	0.97	0.06	20,25,31,32	0
26	BCR	b	619	40/40	0.97	0.07	21,28,47,57	0
38	HTG	b	623	19/19	0.97	0.09	26,42,77,81	0
29	LMG	B	621	51/55	0.97	0.07	27,39,54,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
26	BCR	b	620	40/40	0.97	0.07	24,32,45,48	0
22	CL	V	202	1/1	0.97	0.05	68,68,68,68	0
26	BCR	c	515	40/40	0.97	0.08	26,35,47,55	0
30	GOL	T	101	6/6	0.97	0.12	52,52,56,59	0
26	BCR	c	527	40/40	0.97	0.09	34,42,53,59	0
29	LMG	J	101	47/55	0.97	0.07	23,29,74,83	0
30	GOL	V	201	6/6	0.97	0.06	28,30,35,39	0
38	HTG	o	301	19/19	0.97	0.08	25,32,41,63	0
24	CLA	c	511	65/65	0.97	0.08	28,36,47,52	0
30	GOL	V	208	6/6	0.97	0.07	65,70,82,83	0
30	GOL	a	415	6/6	0.97	0.07	29,39,45,45	0
29	LMG	b	621	51/55	0.97	0.08	28,39,53,103	0
26	BCR	h	103	40/40	0.97	0.06	25,35,50,53	0
30	GOL	b	627	6/6	0.97	0.07	40,47,52,54	0
24	CLA	B	617	60/65	0.97	0.07	21,27,90,107	0
30	GOL	b	630	6/6	0.97	0.08	30,39,52,53	0
40	DGD	H	103	62/66	0.97	0.08	21,31,45,54	0
40	DGD	c	516	62/66	0.97	0.08	23,35,77,86	0
40	DGD	c	517	57/66	0.97	0.07	27,34,75,108	0
26	BCR	t	102	40/40	0.97	0.07	21,29,48,53	0
36	EDO	O	311	4/4	0.97	0.22	42,54,57,72	0
41	HEM	e	107	43/43	0.97	0.10	40,47,74,103	0
29	LMG	j	101	47/55	0.97	0.09	26,35,80,91	0
30	GOL	d	402	6/6	0.97	0.08	35,39,45,48	0
23	BCT	A	605	4/4	0.98	0.06	27,31,35,52	0
32	LHG	d	410	49/49	0.98	0.08	21,27,42,51	0
32	LHG	d	411	49/49	0.98	0.09	26,31,79,84	0
24	CLA	C	501	65/65	0.98	0.06	25,30,48,57	0
24	CLA	C	502	65/65	0.98	0.06	21,27,37,54	0
24	CLA	C	503	65/65	0.98	0.06	26,30,38,43	0
24	CLA	C	504	60/65	0.98	0.06	20,26,70,81	0
24	CLA	C	505	65/65	0.98	0.06	23,29,47,52	0
26	BCR	b	618	40/40	0.98	0.07	19,26,33,37	0
23	BCT	a	406	4/4	0.98	0.05	27,28,31,49	0
24	CLA	C	507	65/65	0.98	0.06	27,33,48,64	0
24	CLA	C	508	60/65	0.98	0.07	23,29,51,61	0
24	CLA	C	509	65/65	0.98	0.09	27,33,50,57	0
30	GOL	V	205	6/6	0.98	0.09	26,34,37,43	0
30	GOL	V	206	6/6	0.98	0.17	33,35,42,42	0
23	BCT	m	104[A]	4/4	0.98	0.11	18,34,38,38	4
24	CLA	C	511	65/65	0.98	0.08	26,33,40,45	0
23	BCT	m	104[B]	4/4	0.98	0.11	7,13,18,19	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CLA	A	607	60/65	0.98	0.06	17,20,66,78	0
30	GOL	b	625	6/6	0.98	0.07	34,39,44,54	0
24	CLA	D	404	65/65	0.98	0.06	13,18,35,40	0
24	CLA	D	405	65/65	0.98	0.06	22,29,91,98	0
30	GOL	b	628	6/6	0.98	0.06	32,34,35,44	0
27	PL9	D	407	55/55	0.98	0.07	17,22,33,48	0
24	CLA	a	407	65/65	0.98	0.07	17,20,27,41	0
30	GOL	c	525	6/6	0.98	0.20	47,49,64,80	0
30	GOL	c	526	6/6	0.98	0.07	24,28,29,32	0
37	CA	B	601	1/1	0.98	0.21	82,82,82,82	0
37	CA	O	301	1/1	0.98	0.08	53,53,53,53	0
27	PL9	d	407	55/55	0.98	0.07	19,24,31,39	0
24	CLA	a	408	60/65	0.98	0.07	18,25,73,85	0
37	CA	o	302	1/1	0.98	0.08	55,55,55,55	0
24	CLA	A	609	65/65	0.98	0.07	19,24,109,130	0
22	CL	v	201	1/1	0.98	0.07	72,72,72,72	0
24	CLA	b	603	65/65	0.98	0.07	21,28,39,43	0
28	SQD	a	413	54/54	0.98	0.07	33,54,92,96	0
24	CLA	b	605	65/65	0.98	0.06	17,23,53,59	0
24	CLA	b	606	65/65	0.98	0.06	20,25,33,39	0
24	CLA	b	607	55/65	0.98	0.07	22,27,36,49	0
24	CLA	b	608	65/65	0.98	0.06	17,22,31,37	0
24	CLA	b	610	65/65	0.98	0.07	23,30,35,44	0
24	CLA	b	611	65/65	0.98	0.05	23,28,38,44	0
24	CLA	b	613	65/65	0.98	0.07	20,25,32,41	0
24	CLA	b	614	65/65	0.98	0.06	19,23,48,54	0
24	CLA	b	615	65/65	0.98	0.06	18,26,94,117	0
24	CLA	b	616	65/65	0.98	0.05	22,29,47,56	0
24	CLA	B	603	65/65	0.98	0.06	21,26,33,38	0
24	CLA	c	501	65/65	0.98	0.06	27,35,49,53	0
24	CLA	B	605	65/65	0.98	0.06	17,21,55,58	0
24	CLA	B	606	65/65	0.98	0.07	18,22,34,38	0
24	CLA	c	505	65/65	0.98	0.06	25,29,44,50	0
24	CLA	B	607	55/65	0.98	0.06	19,25,33,49	0
24	CLA	c	507	65/65	0.98	0.07	28,34,50,59	0
24	CLA	c	508	60/65	0.98	0.06	23,29,52,62	0
24	CLA	c	510	65/65	0.98	0.06	26,32,41,48	0
24	CLA	B	608	65/65	0.98	0.06	16,20,32,38	0
24	CLA	B	610	65/65	0.98	0.07	22,27,33,37	0
24	CLA	B	611	65/65	0.98	0.06	20,24,38,51	0
24	CLA	B	613	65/65	0.98	0.06	17,23,30,39	0
25	PHO	A	608	64/64	0.98	0.06	17,19,26,26	0

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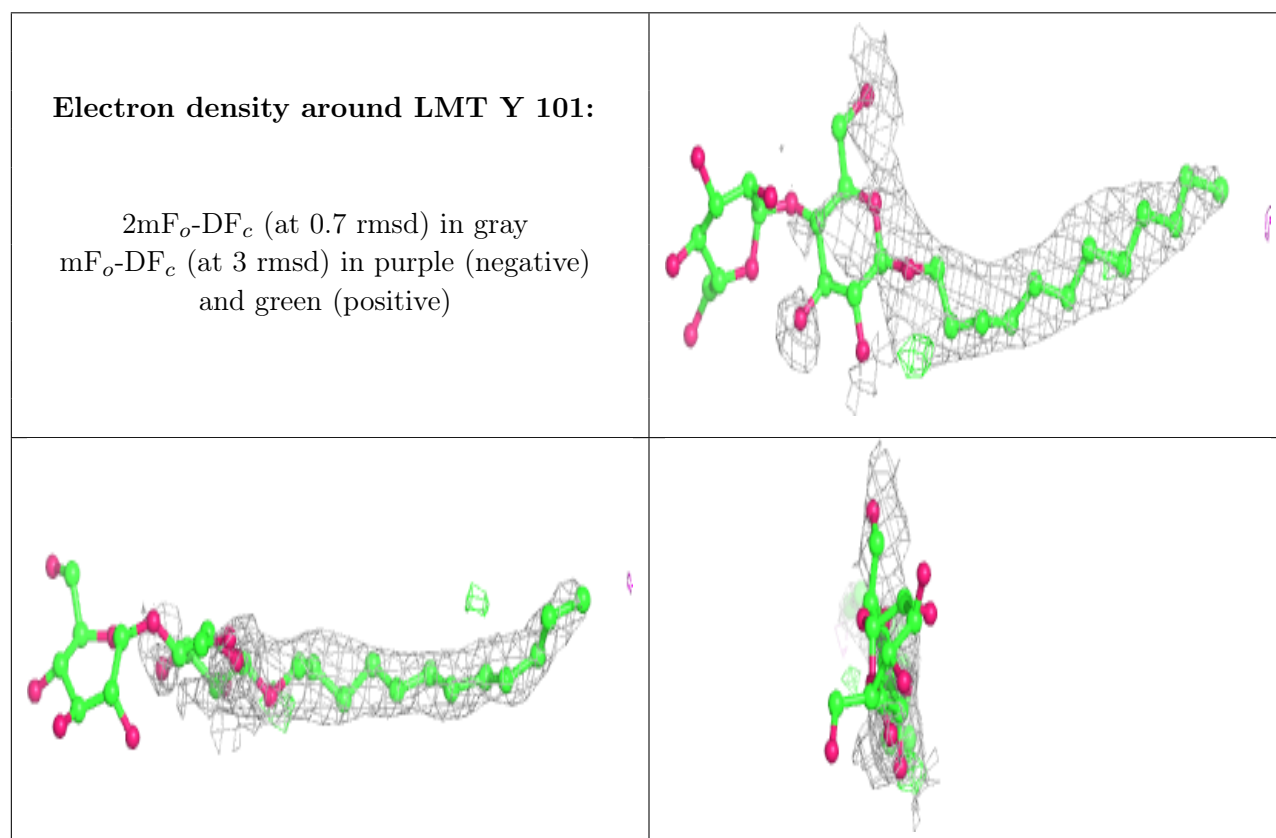
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	PHO	D	401	64/64	0.98	0.06	17,23,31,41	0
25	PHO	a	409	64/64	0.98	0.07	17,21,26,32	0
25	PHO	d	401	64/64	0.98	0.07	20,25,31,41	0
40	DGD	C	516	62/66	0.98	0.07	20,31,90,104	0
40	DGD	C	517	56/66	0.98	0.07	21,31,74,88	0
40	DGD	C	518	62/66	0.98	0.07	20,30,71,80	0
26	BCR	A	610	40/40	0.98	0.07	20,25,32,35	0
26	BCR	B	618	40/40	0.98	0.07	21,25,33,34	0
24	CLA	B	614	65/65	0.98	0.06	17,21,48,64	0
26	BCR	B	620	40/40	0.98	0.06	22,31,46,50	0
40	DGD	c	518	62/66	0.98	0.06	25,36,65,81	0
24	CLA	B	615	55/65	0.98	0.06	17,23,55,82	0
32	LHG	B	632	49/49	0.98	0.08	20,30,52,61	0
41	HEM	E	113	43/43	0.98	0.07	35,42,61,68	0
32	LHG	D	409	49/49	0.98	0.07	25,35,45,55	0
42	MG	F	103	1/1	0.98	0.09	32,32,32,32	0
43	HEC	v	202	43/43	0.98	0.08	26,31,34,38	0
32	LHG	D	411	49/49	0.98	0.08	23,31,81,89	0
24	CLA	B	616	65/65	0.98	0.06	21,27,48,56	0
30	GOL	v	204	6/6	0.99	0.06	30,36,41,50	0
24	CLA	B	612	65/65	0.99	0.05	16,21,35,39	0
32	LHG	l	101	49/49	0.99	0.07	23,30,49,62	0
24	CLA	c	502	65/65	0.99	0.07	24,30,41,50	0
24	CLA	b	604	65/65	0.99	0.05	22,28,38,45	0
24	CLA	d	403	65/65	0.99	0.05	17,20,29,38	0
24	CLA	d	404	65/65	0.99	0.07	17,21,37,43	0
24	CLA	b	612	65/65	0.99	0.06	18,24,37,42	0
30	GOL	B	628	6/6	0.99	0.07	34,40,48,49	0
24	CLA	B	609	65/65	0.99	0.06	19,24,33,40	0
24	CLA	A	606	65/65	0.99	0.08	14,18,27,44	0
24	CLA	D	403	65/65	0.99	0.06	14,18,28,44	0
32	LHG	D	410	49/49	0.99	0.08	21,27,41,48	0
24	CLA	B	604	65/65	0.99	0.05	19,23,34,41	0
30	GOL	C	524	6/6	0.99	0.07	21,22,24,26	0
42	MG	J	102	1/1	0.99	0.04	27,27,27,27	0
42	MG	f	102	1/1	0.99	0.07	45,45,45,45	0
42	MG	j	102	1/1	0.99	0.05	35,35,35,35	0
43	HEC	V	203	43/43	0.99	0.06	20,24,27,29	0
24	CLA	c	509	65/65	0.99	0.07	25,33,52,53	0
32	LHG	d	409	49/49	0.99	0.08	27,37,48,52	0
24	CLA	b	609	65/65	0.99	0.05	22,27,37,44	0
37	CA	c	524	1/1	1.00	0.08	45,45,45,45	0

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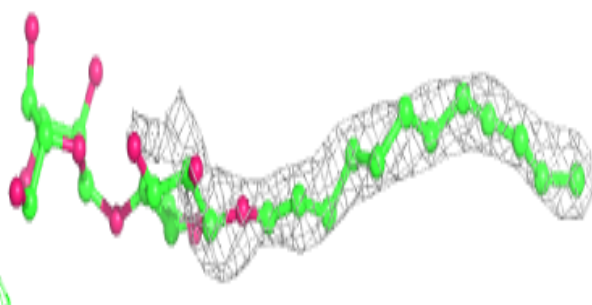
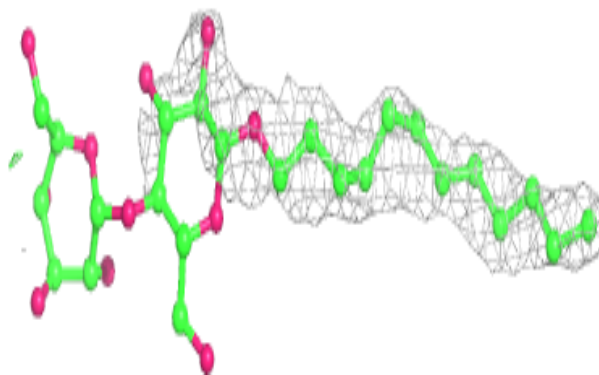
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	OEX	a	402	10/10	1.00	0.02	23,24,26,27	0
21	FE2	A	602	1/1	1.00	0.02	25,25,25,25	0
21	FE2	a	403	1/1	1.00	0.02	25,25,25,25	0
22	CL	A	603	1/1	1.00	0.01	23,23,23,23	0
22	CL	A	604	1/1	1.00	0.04	21,21,21,21	0
20	OEX	A	601	10/10	1.00	0.02	20,21,24,26	0
22	CL	a	404	1/1	1.00	0.02	28,28,28,28	0
22	CL	a	405	1/1	1.00	0.02	25,25,25,25	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.

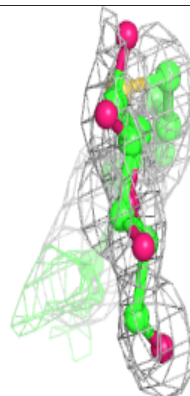
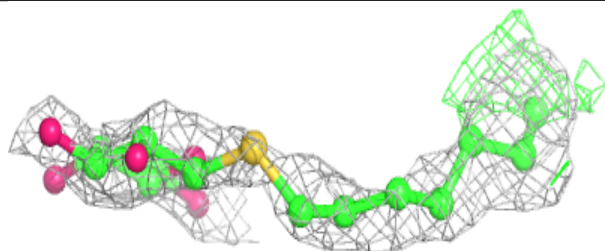
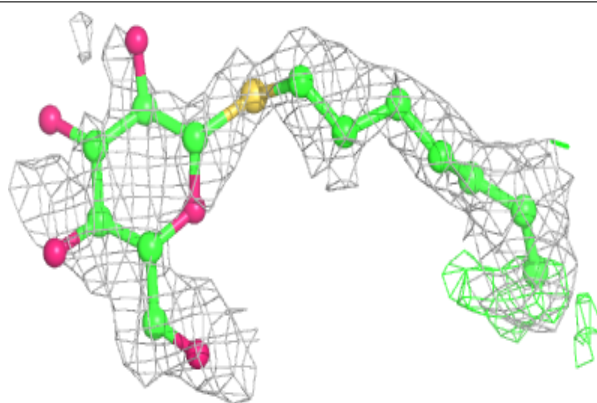


Electron density around LMT j 103:

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

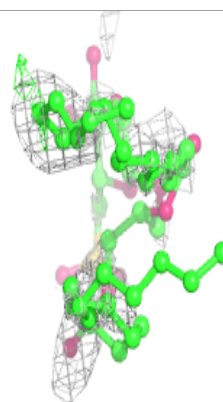
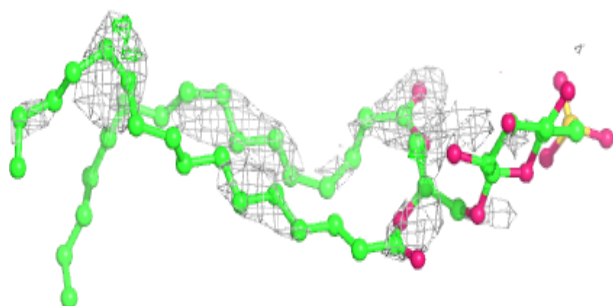
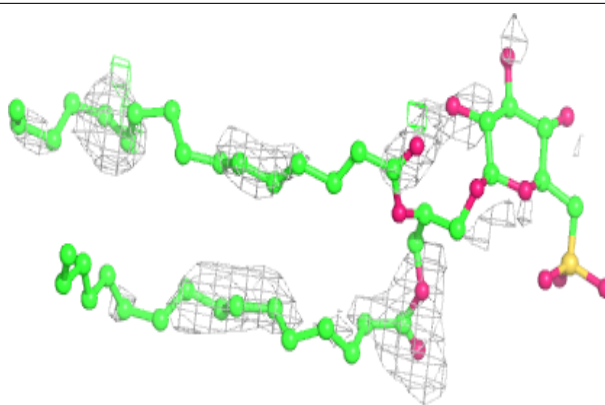
**Electron density around HTG C 529:**

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

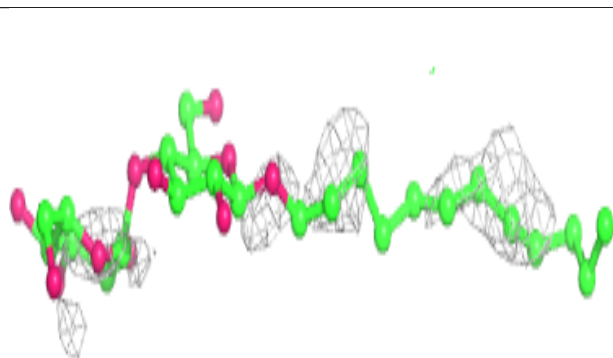
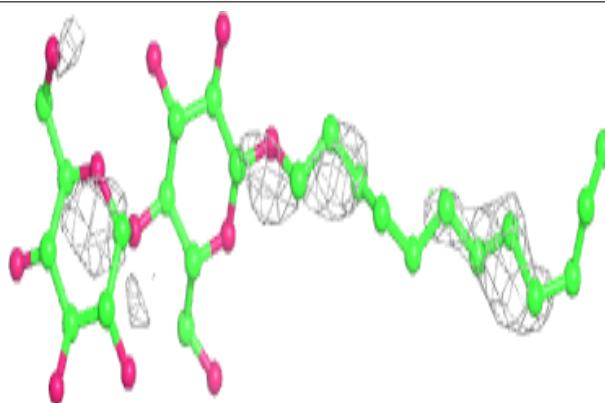


Electron density around SQD h 105:

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

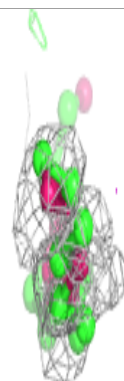
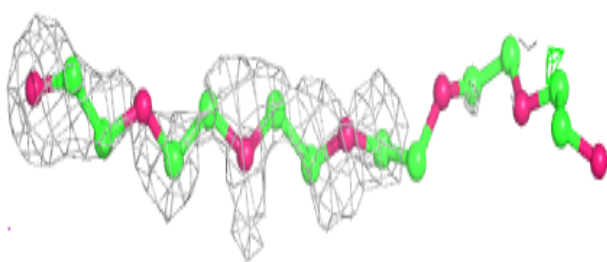
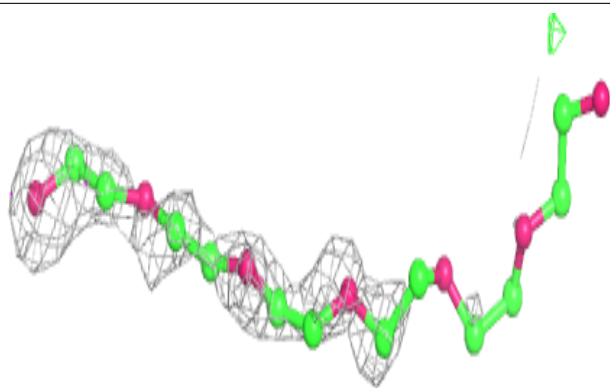
**Electron density around LMT C 533:**

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

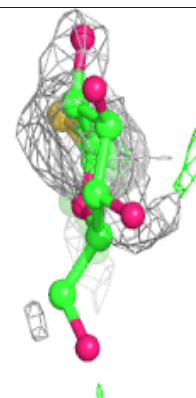
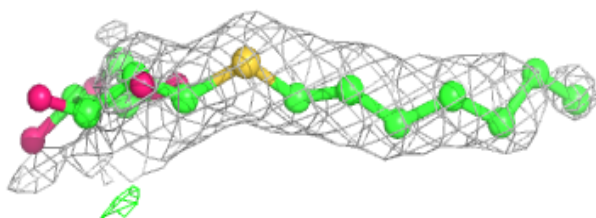
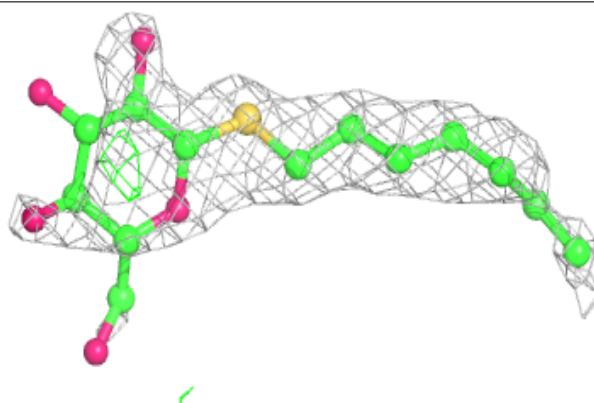


Electron density around P6G D 418:

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

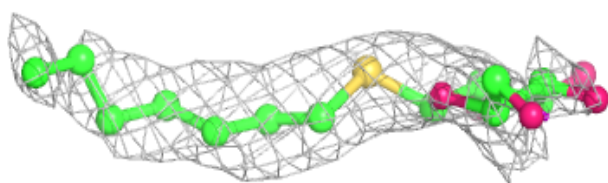
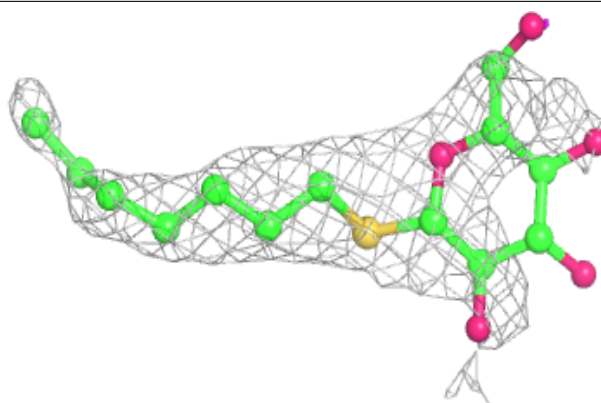
**Electron density around HTG H 101:**

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

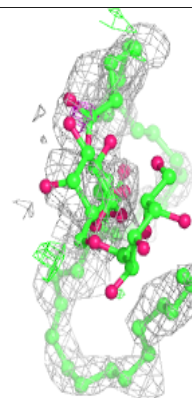
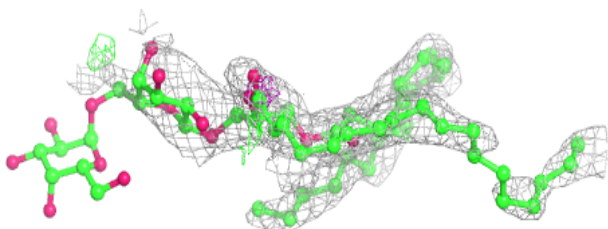
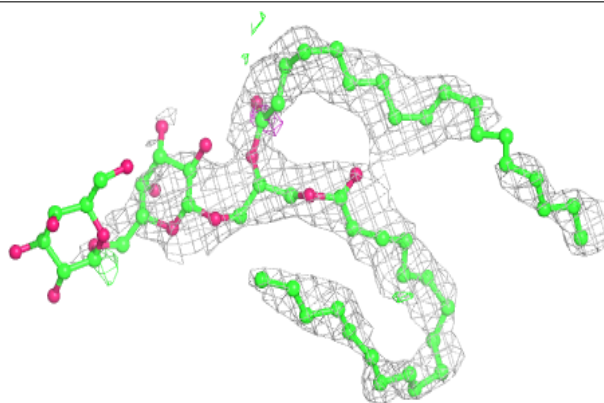


Electron density around HTG h 101:

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

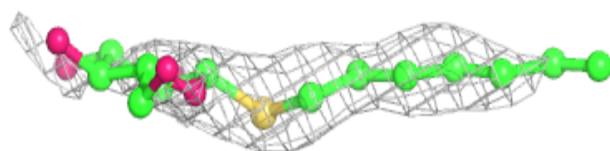
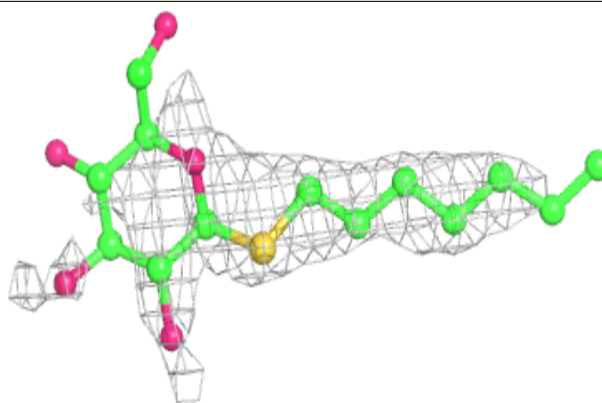
**Electron density around DGD D 408:**

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

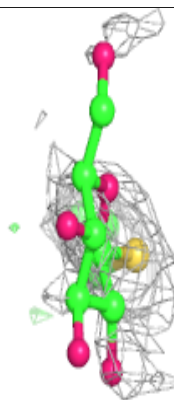
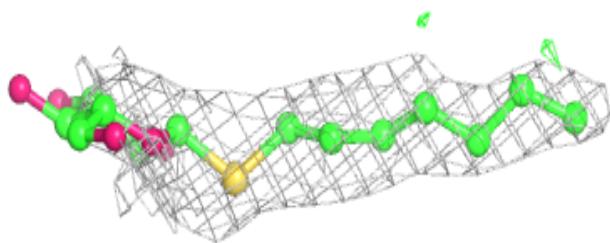
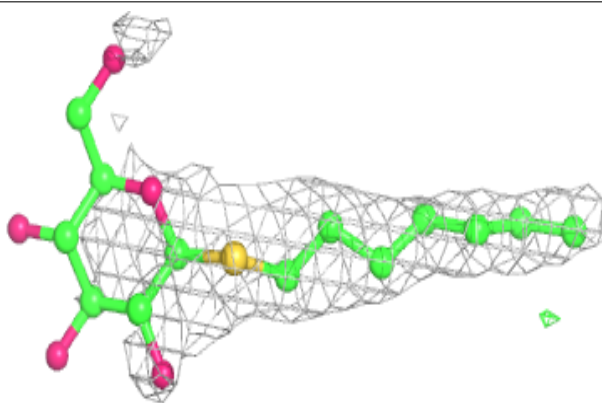


Electron density around HTG c 530:

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

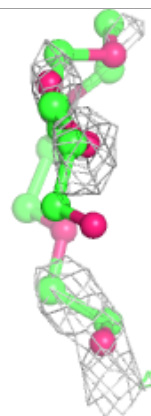
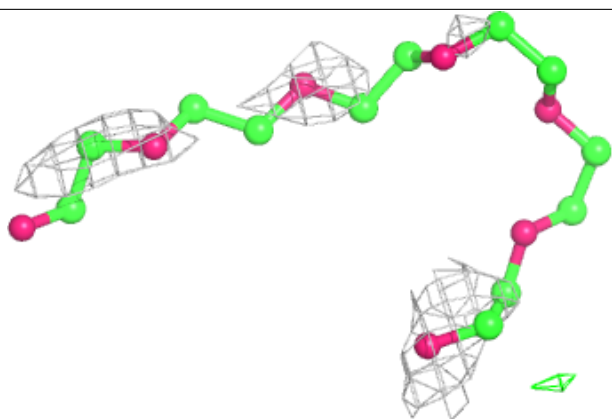
**Electron density around HTG c 531:**

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

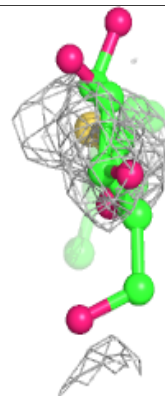
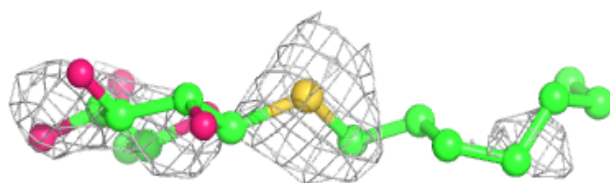
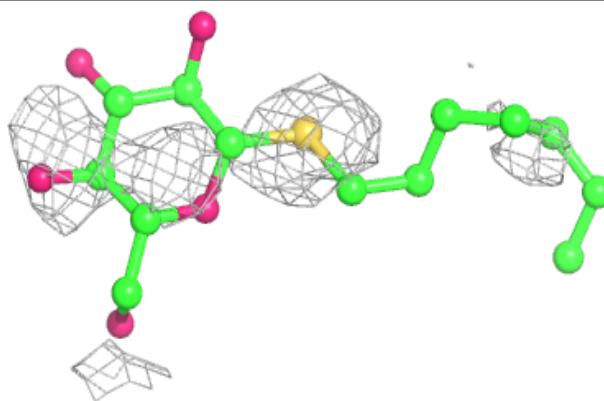


Electron density around P6G C 541:

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

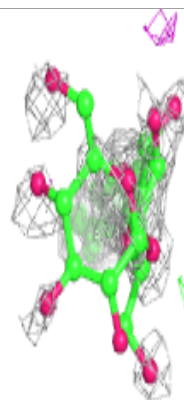
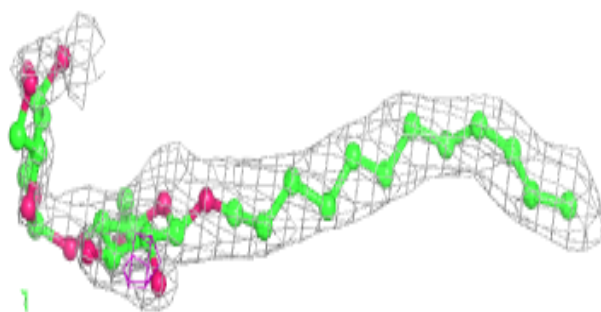
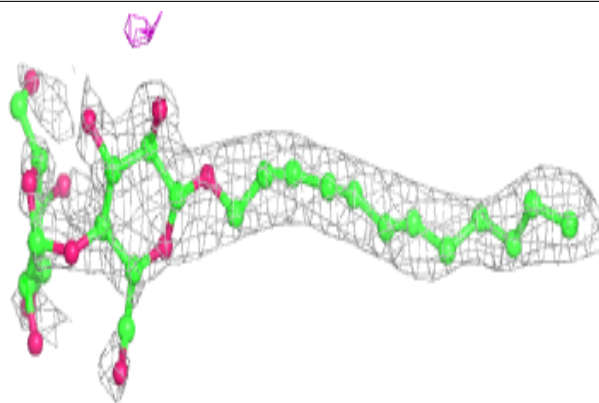
**Electron density around HTG C 530:**

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

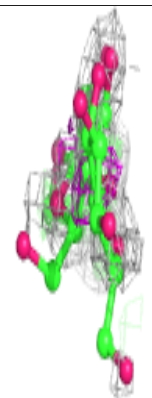
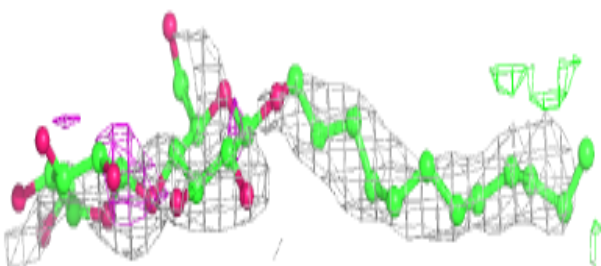
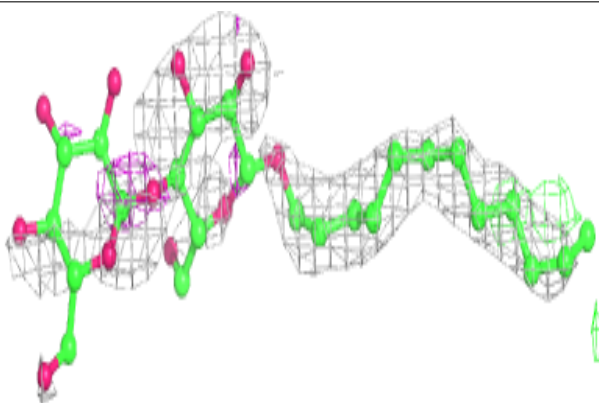


Electron density around LMT J 103:

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

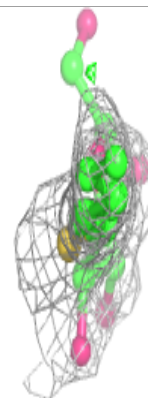
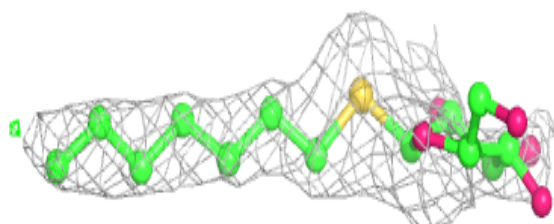
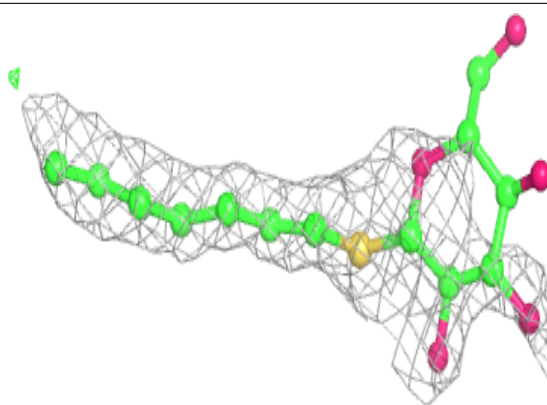
**Electron density around LMT u 203:**

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

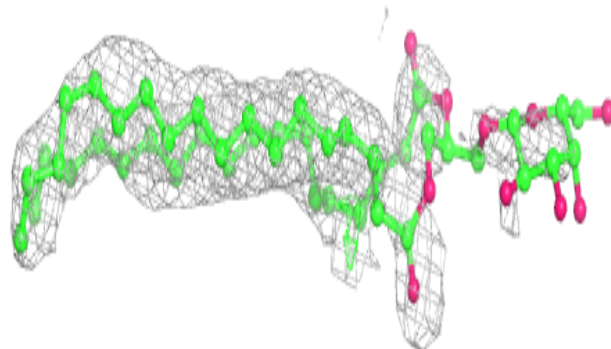
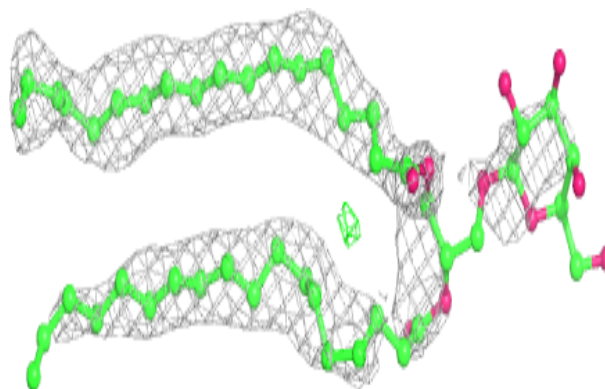


Electron density around HTG C 532:

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

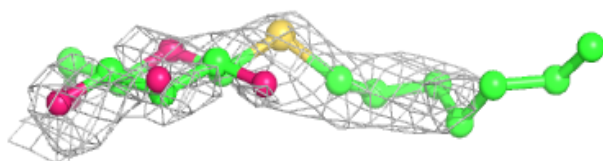
**Electron density around LMG d 412:**

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

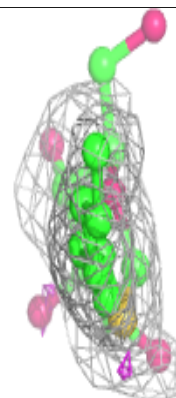
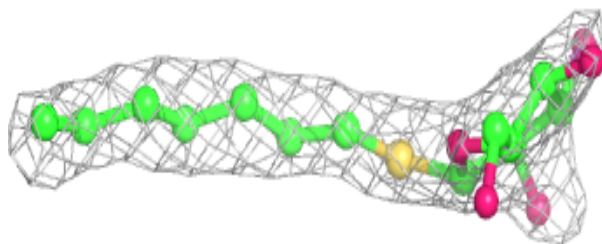
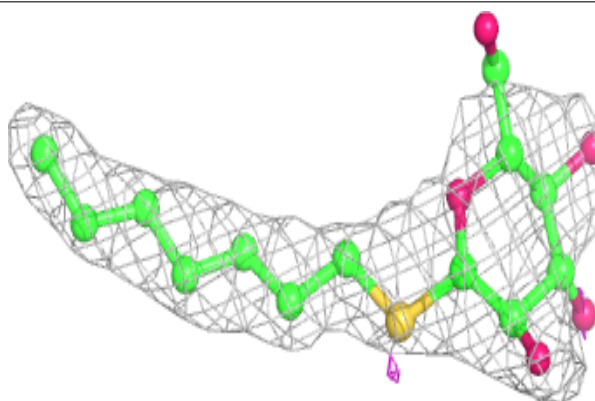


Electron density around HTG C 531:

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

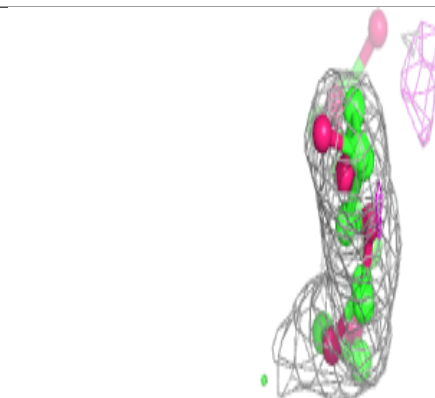
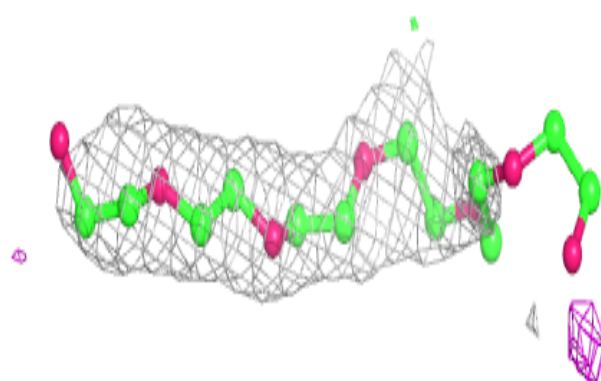
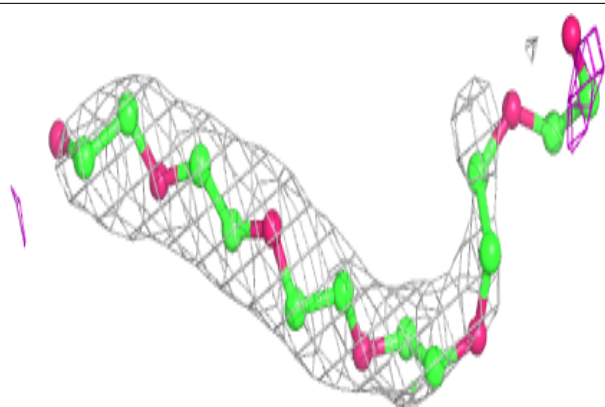
**Electron density around HTG B 624:**

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

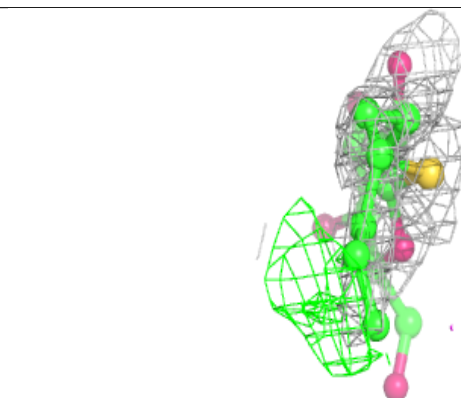
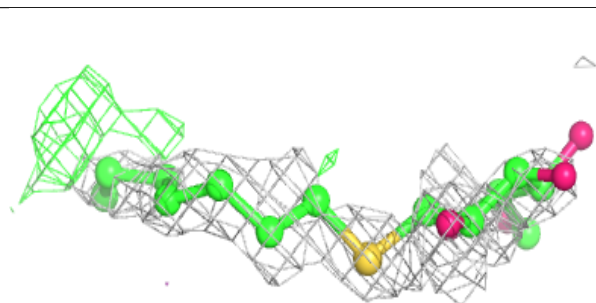
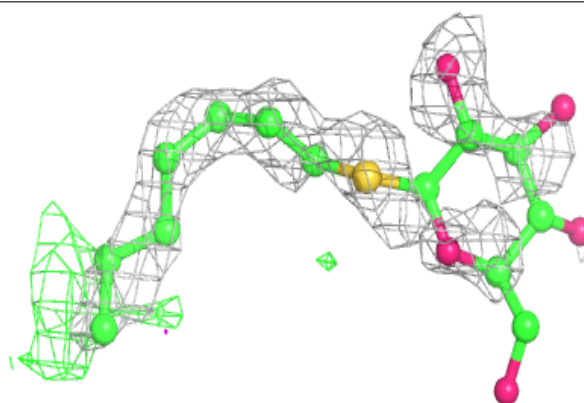


Electron density around P6G I 106:

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

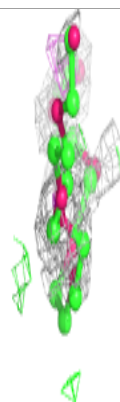
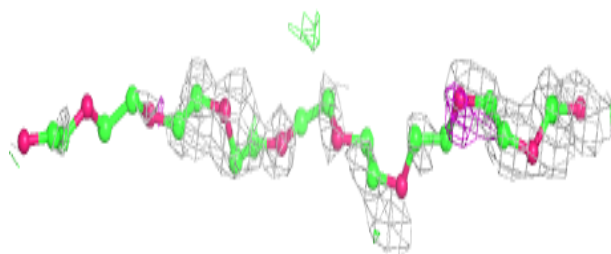
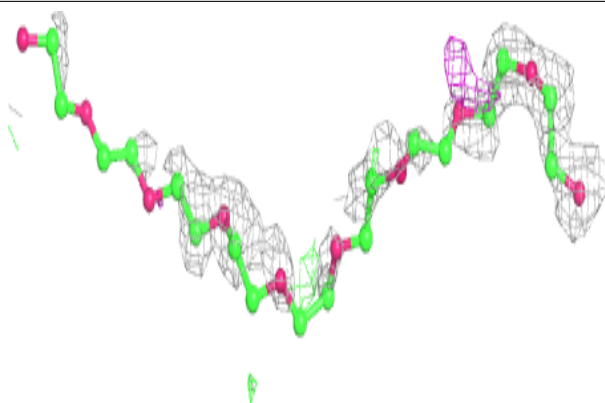
**Electron density around HTG a 418:**

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



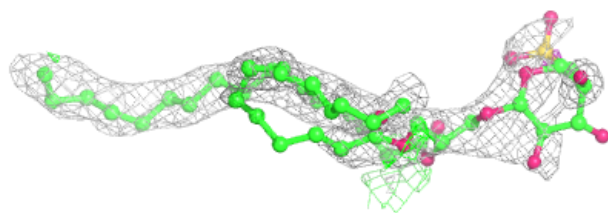
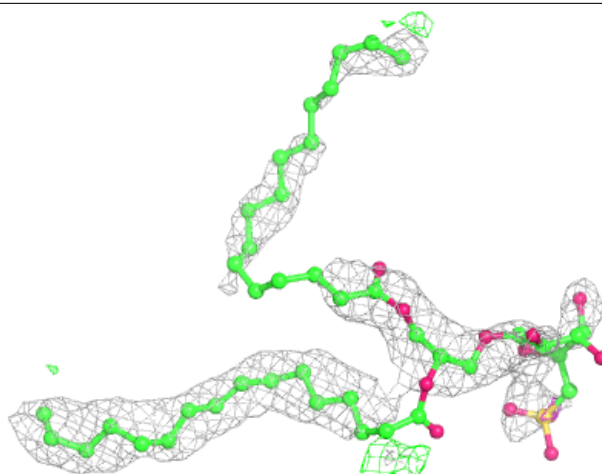
Electron density around 2PE V 216:

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



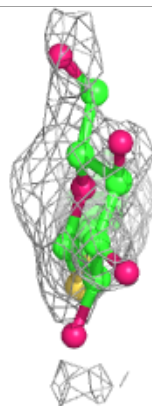
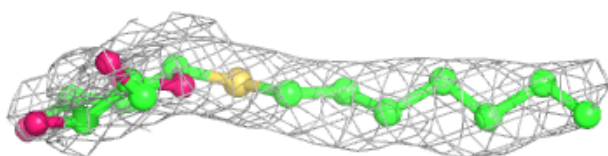
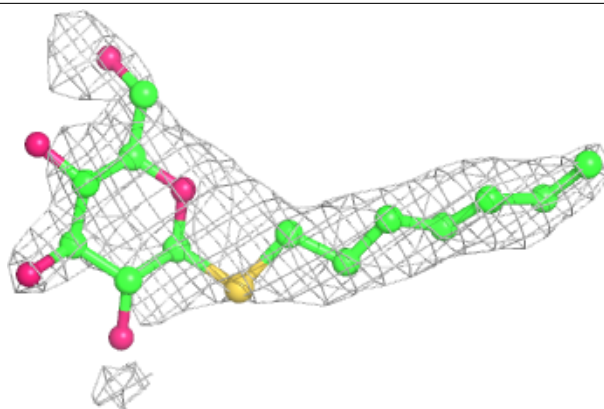
Electron density around SQD A 622:

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

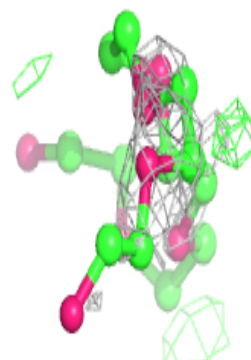
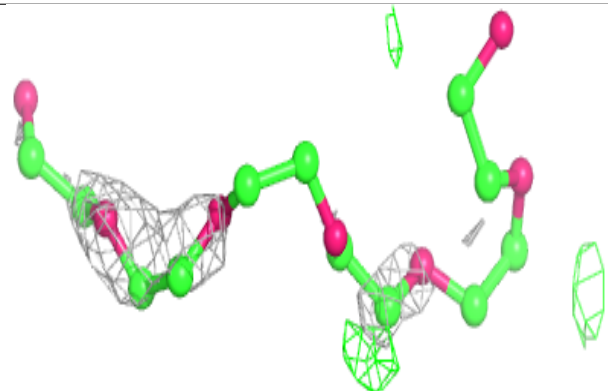
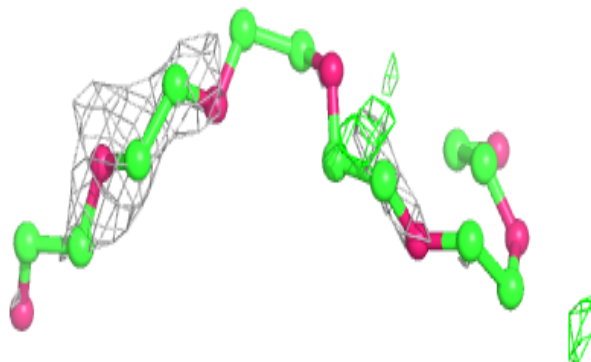


Electron density around HTG b 624:

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

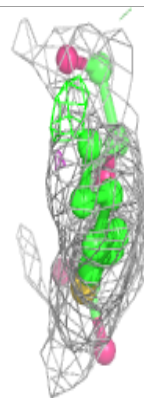
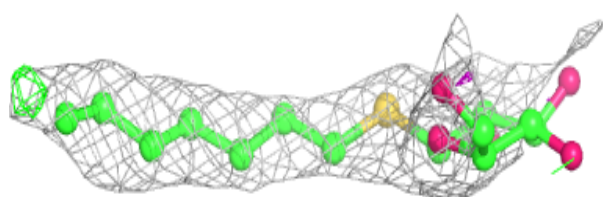
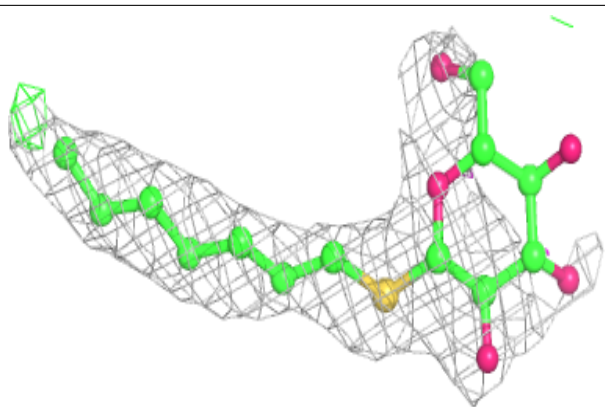
**Electron density around P6G c 541:**

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

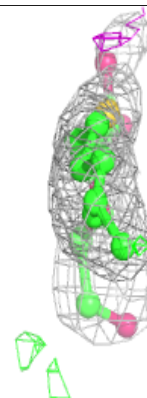
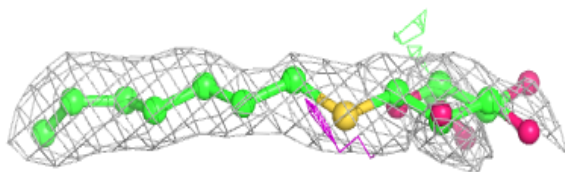
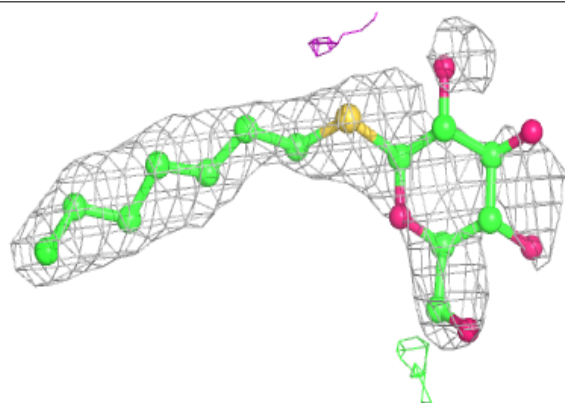


Electron density around HTG b 632:

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

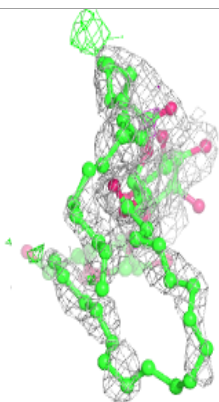
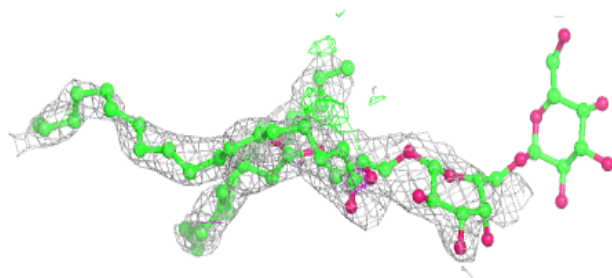
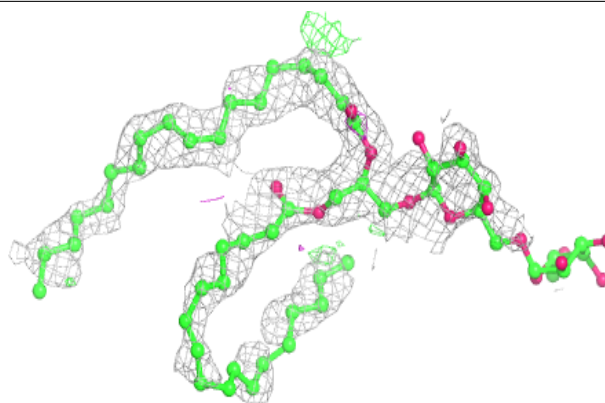
**Electron density around HTG B 631:**

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

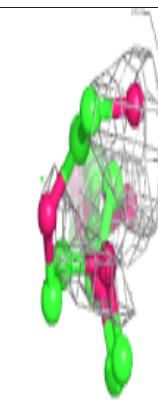
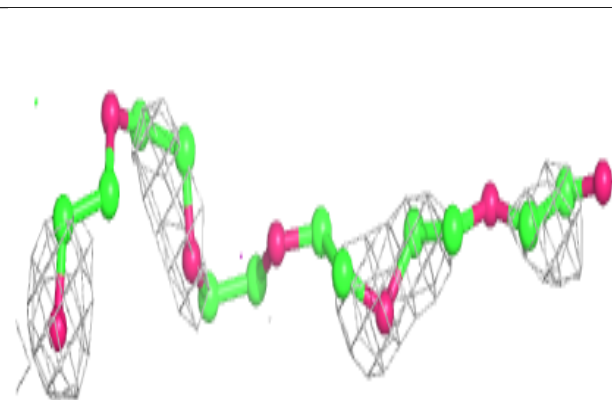
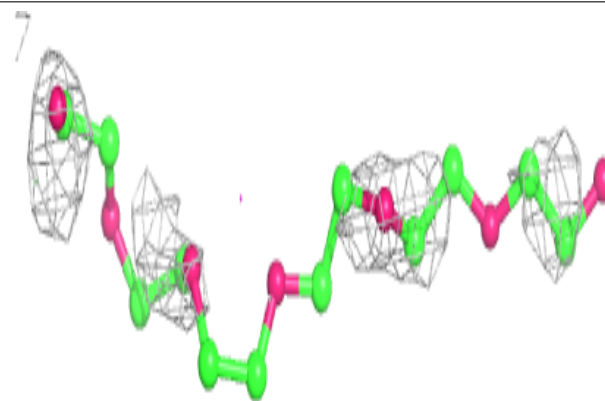


Electron density around DGD d 408:

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

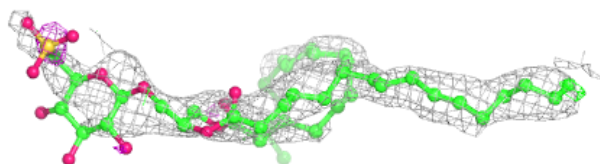
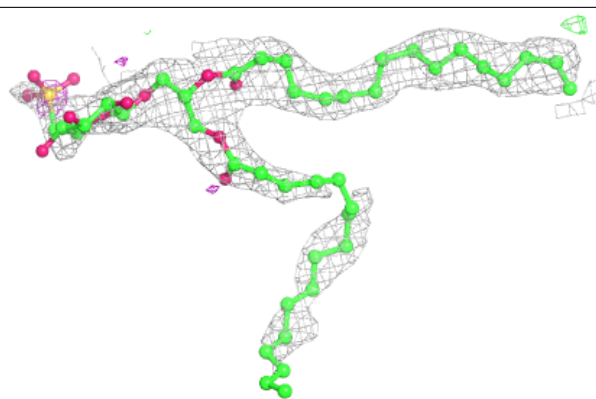
**Electron density around P6G E 110:**

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

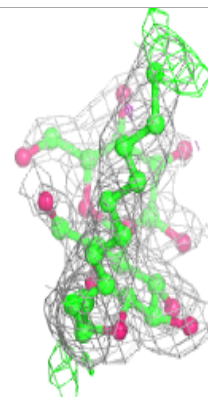
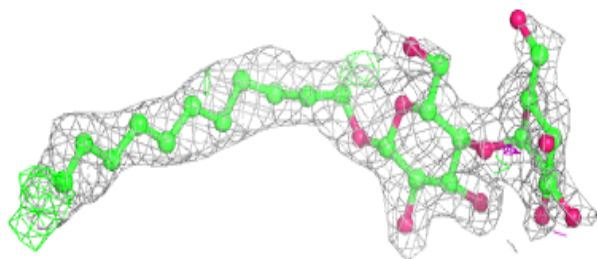
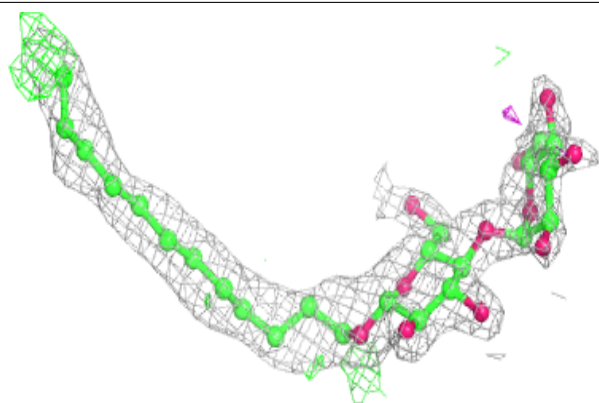


Electron density around SQD a 424:

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

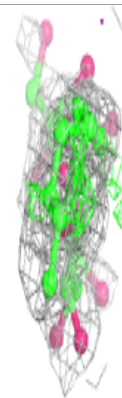
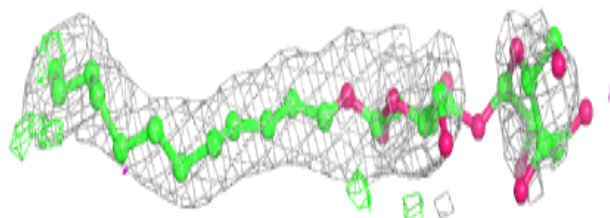
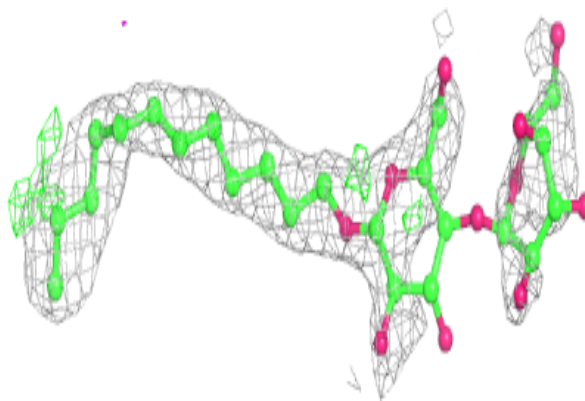
**Electron density around LMT m 101:**

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

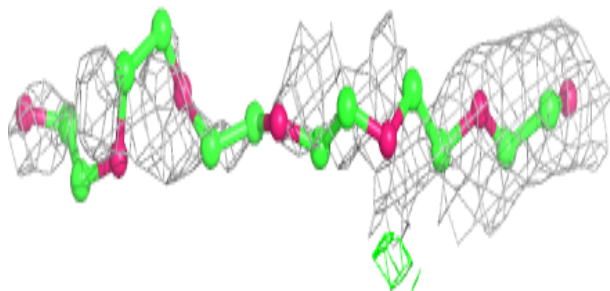
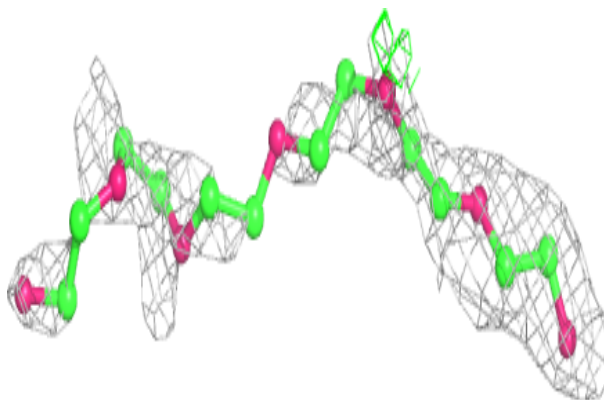


Electron density around LMT t 103:

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

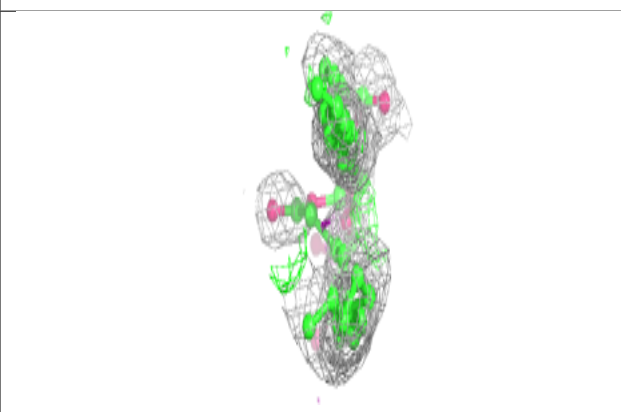
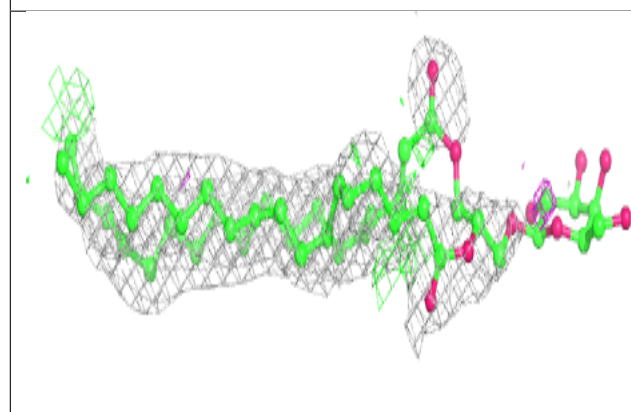
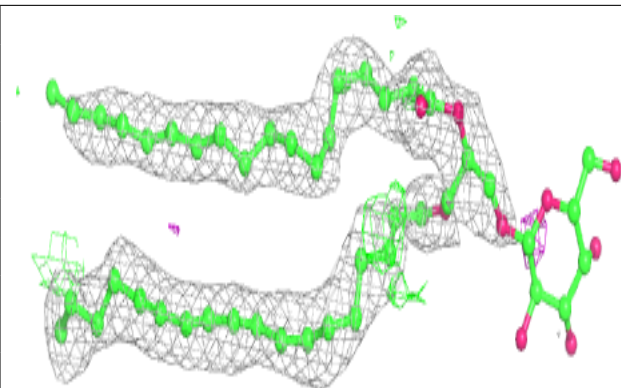
**Electron density around P6G b 649:**

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

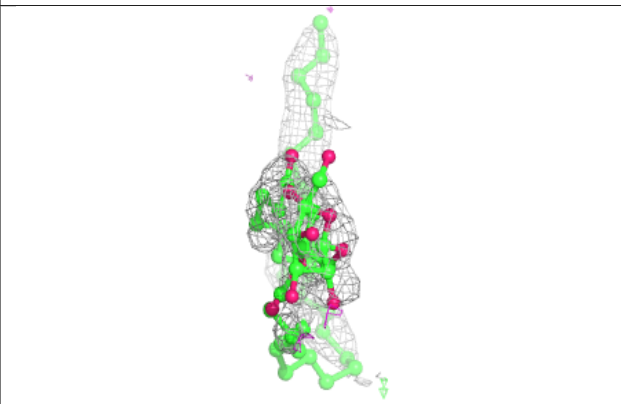
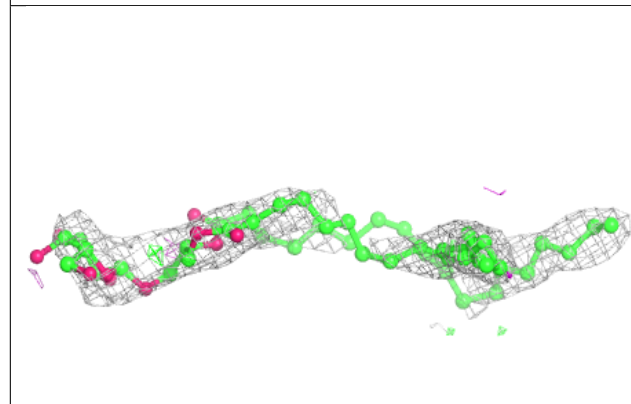
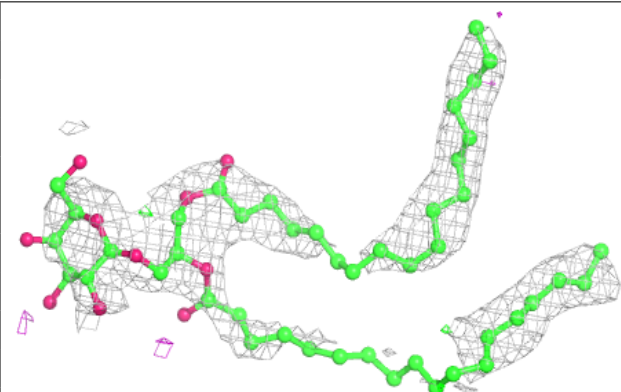


Electron density around LMG B 634:

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

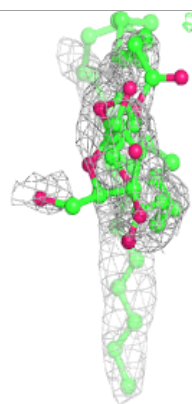
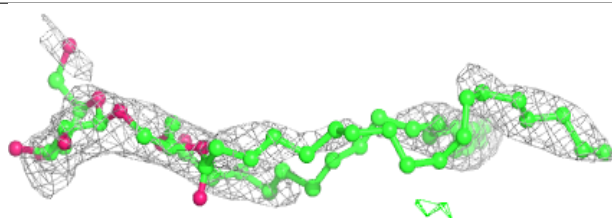
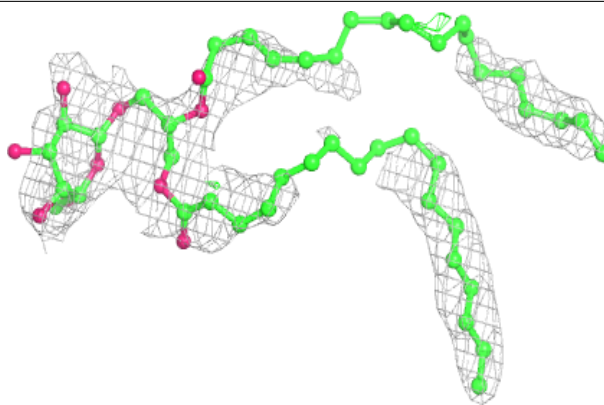
**Electron density around LMG C 526:**

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

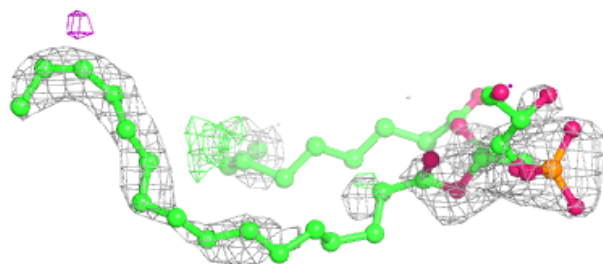
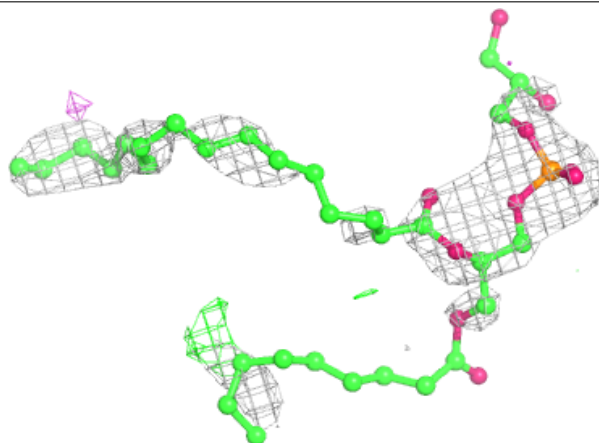


Electron density around LMG z 101:

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

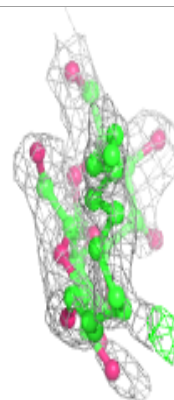
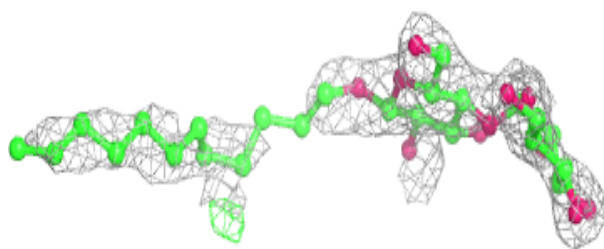
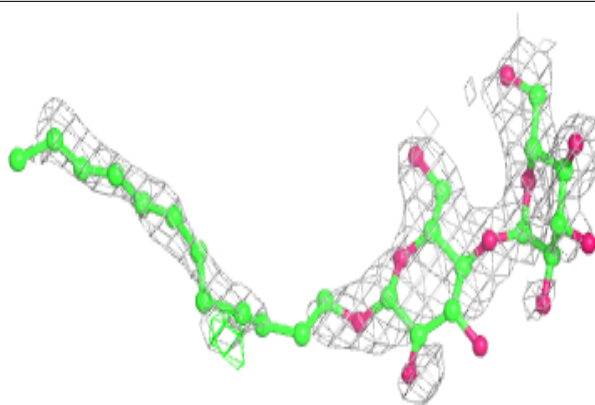
**Electron density around LHG e 101:**

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

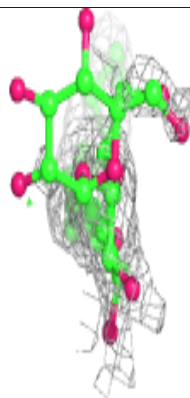
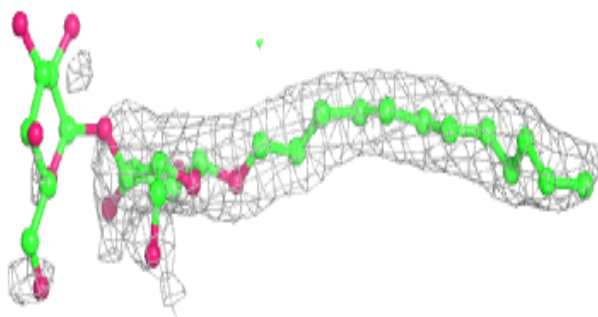
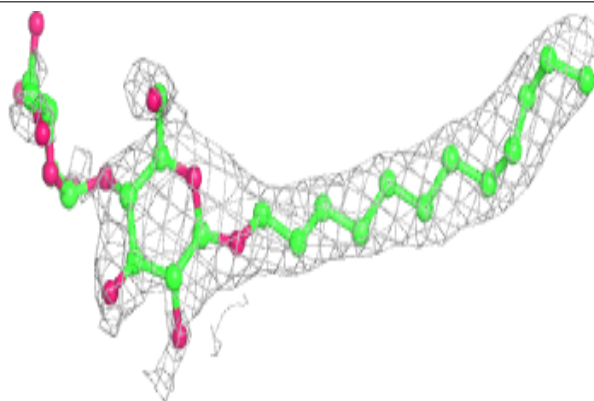


Electron density around LMT F 102:

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

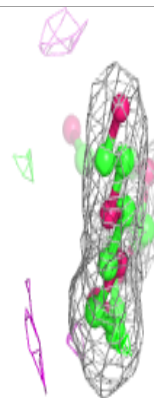
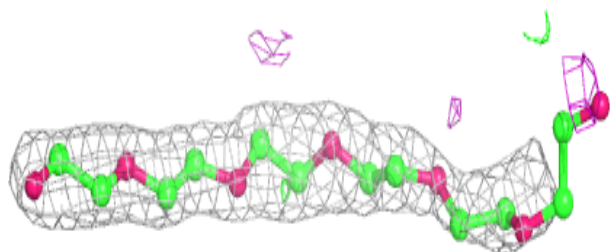
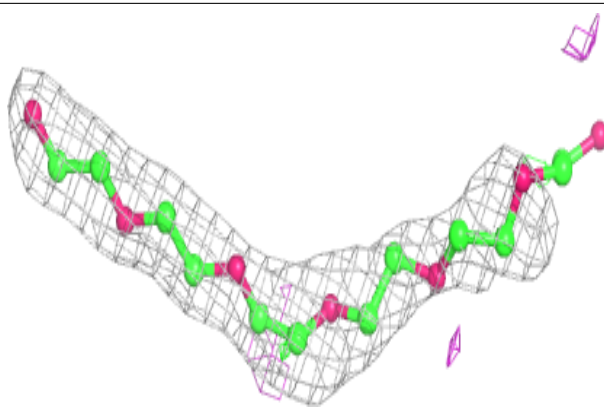
**Electron density around LMT b 622:**

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

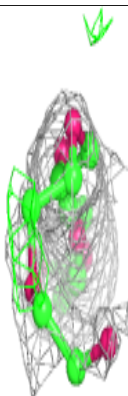
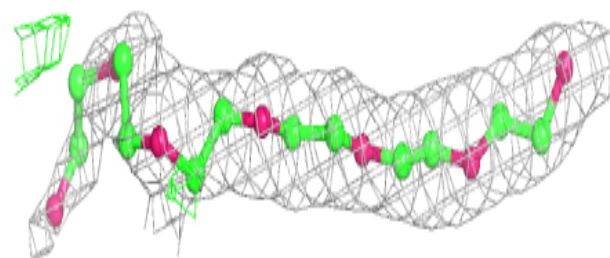
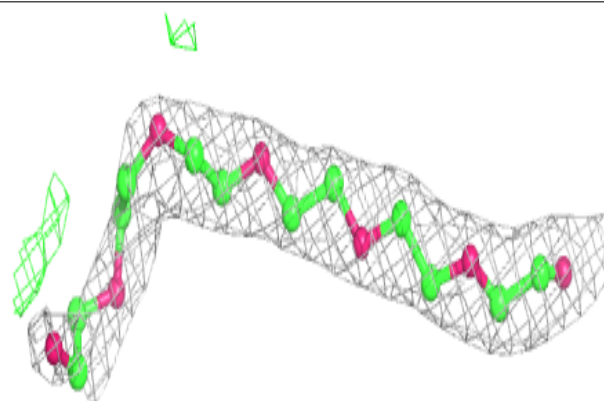


Electron density around P6G d 416:

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

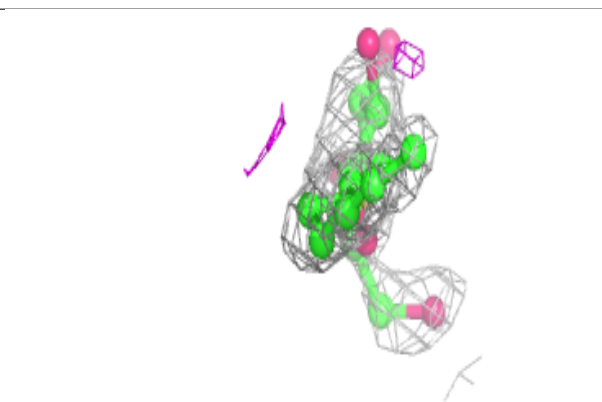
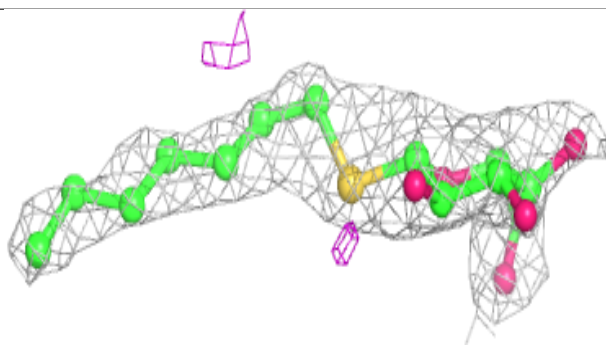
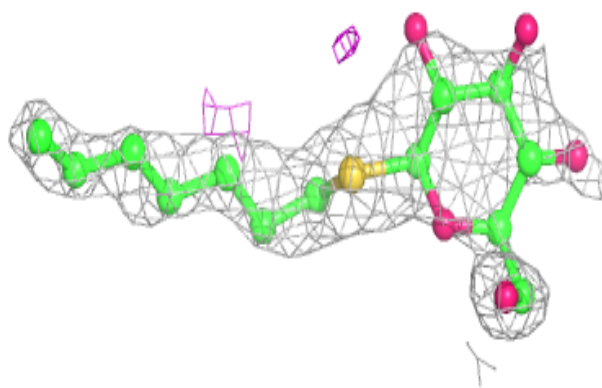
**Electron density around P6G A 623:**

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

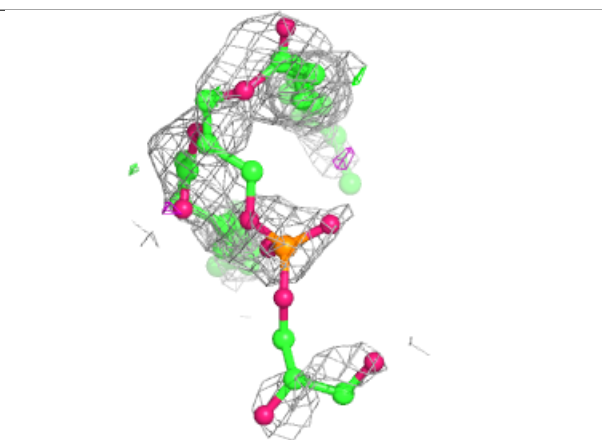
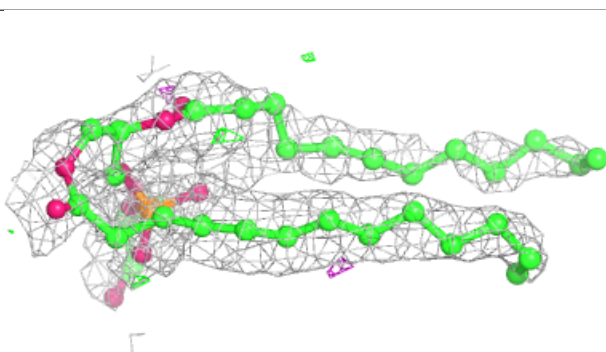
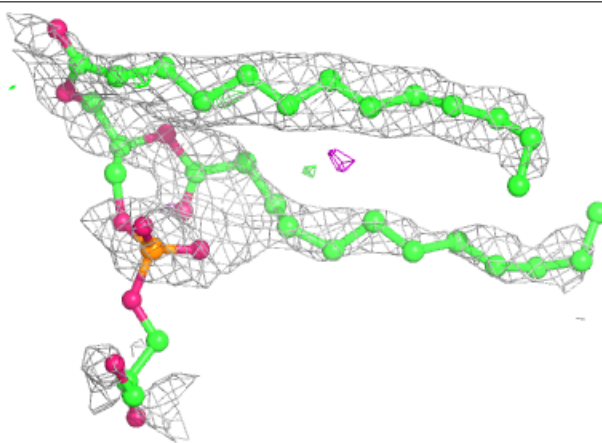


Electron density around HTG c 523:

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

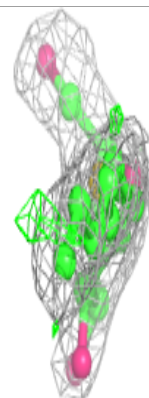
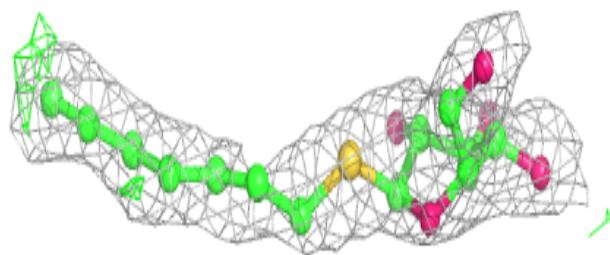
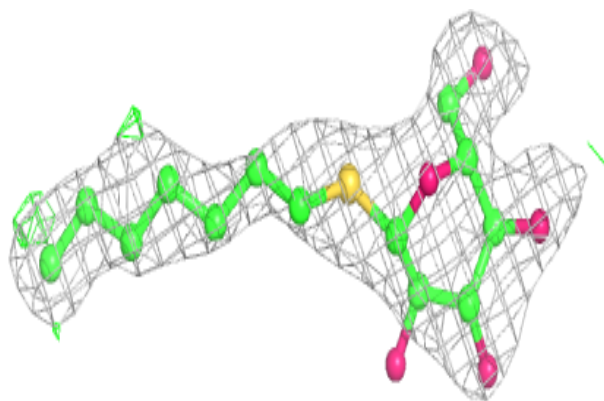
**Electron density around LHG A 618:**

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

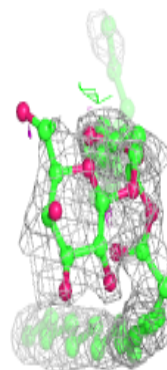
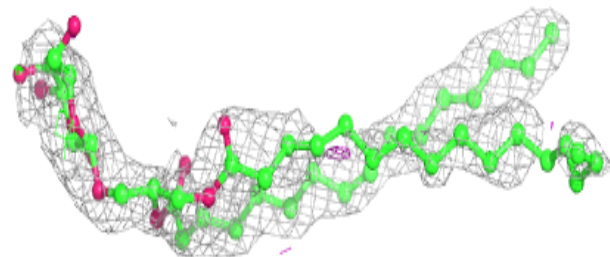
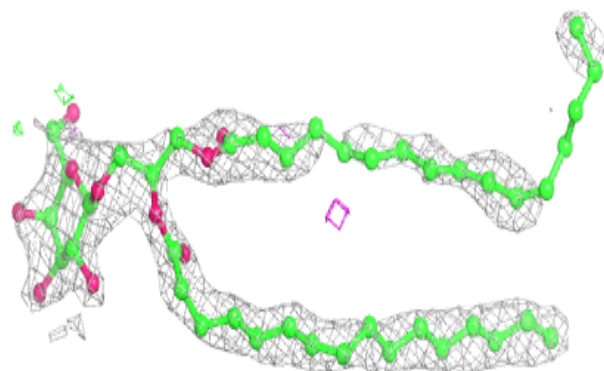


Electron density around HTG C 522:

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

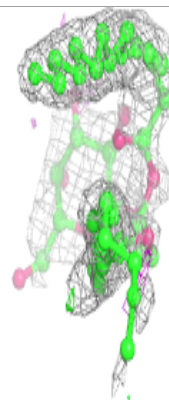
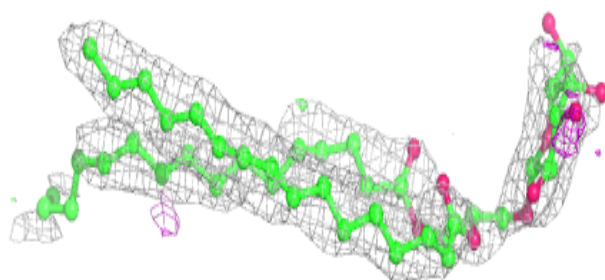
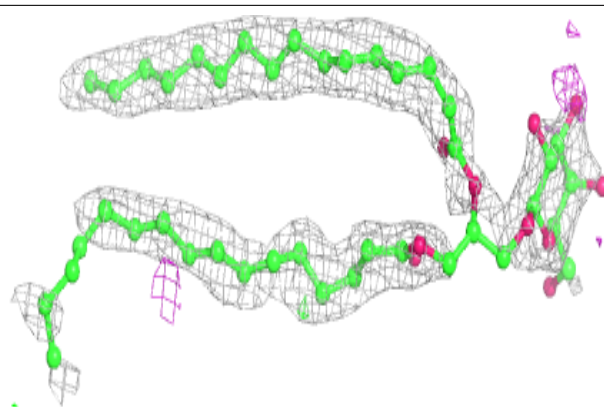
**Electron density around LMG c 520:**

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

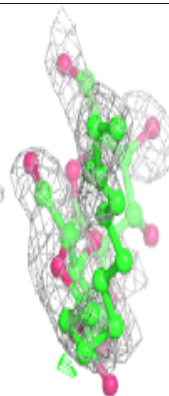
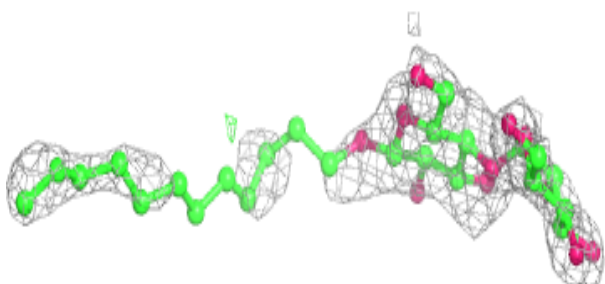
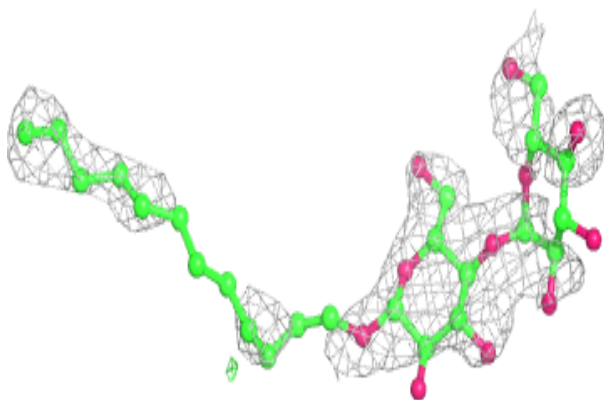


Electron density around LMG C 520:

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

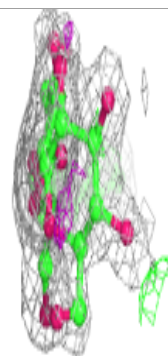
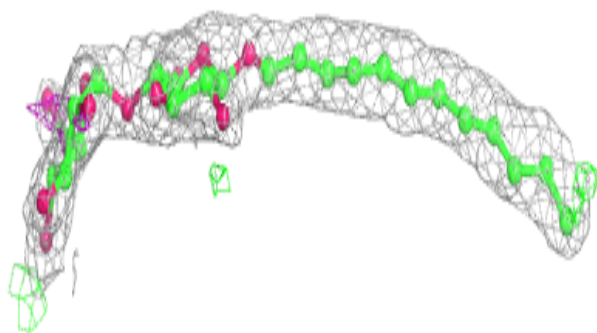
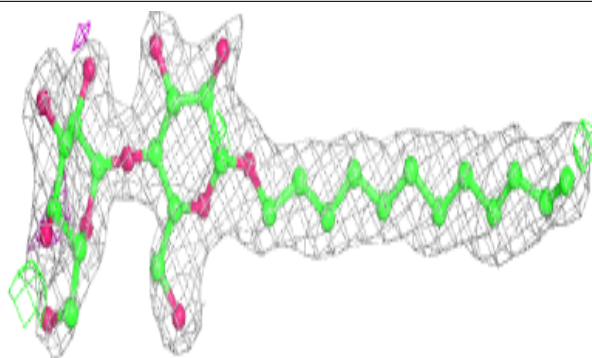
**Electron density around LMT f 101:**

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

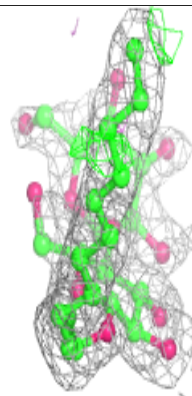
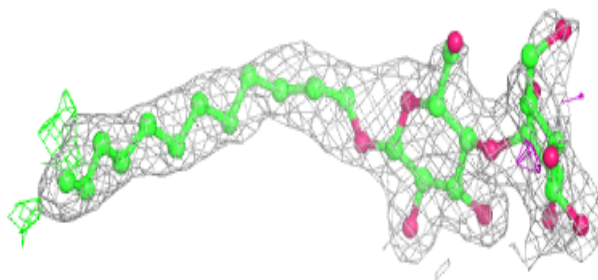
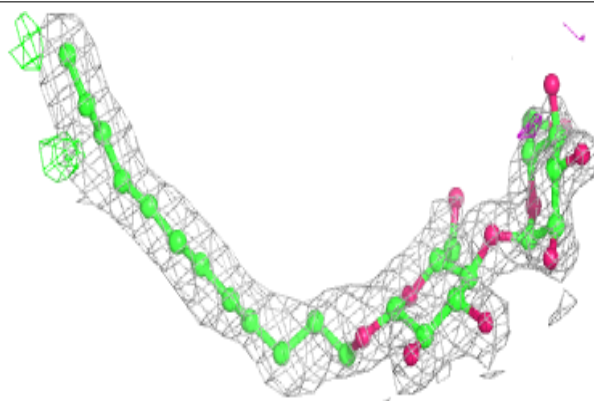


Electron density around LMT M 101:

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

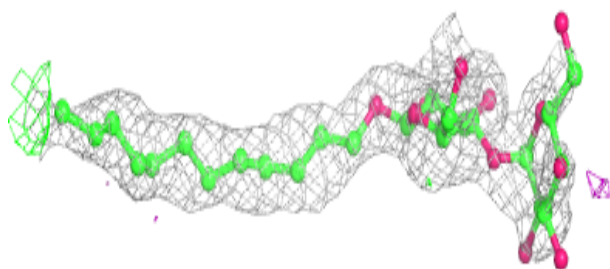
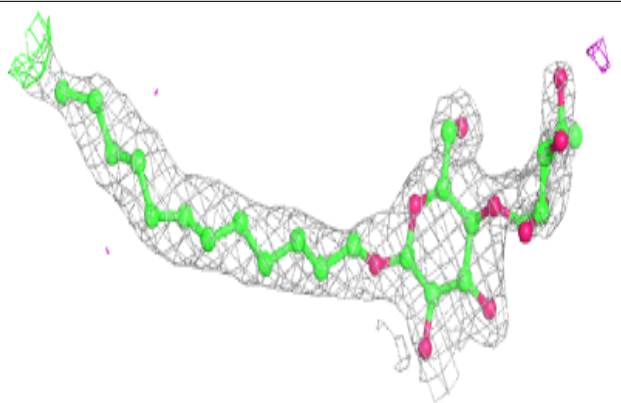
**Electron density around LMT M 102:**

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

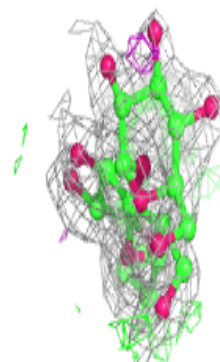
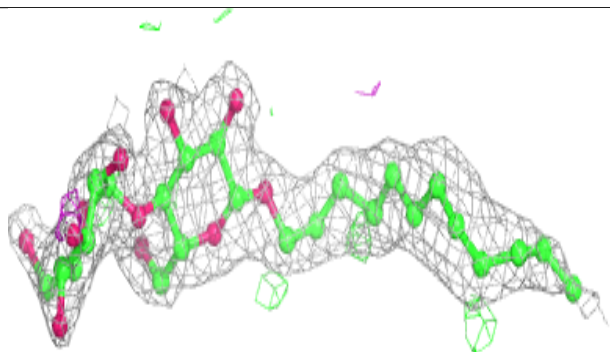
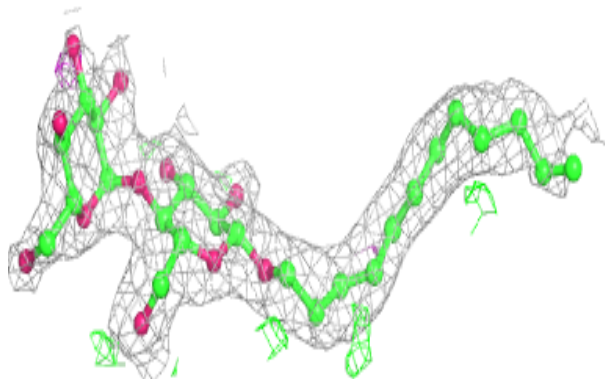


Electron density around LMT B 622:

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

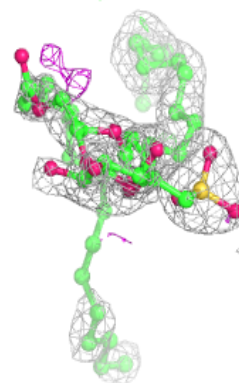
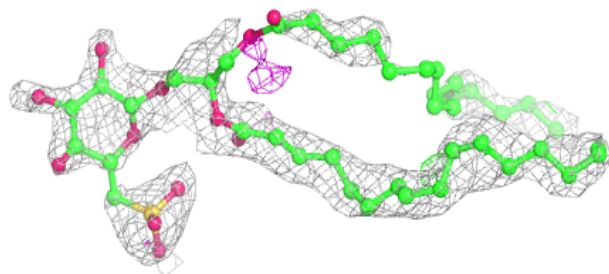
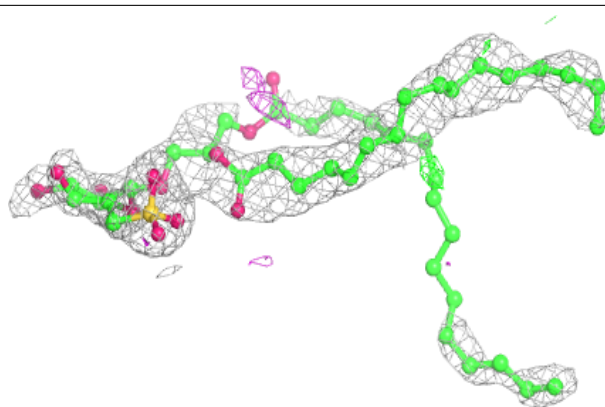
**Electron density around LMT a 401:**

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

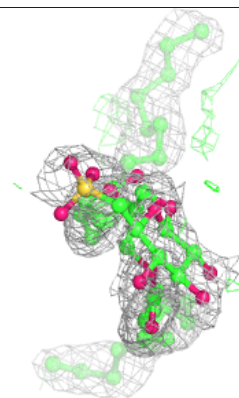
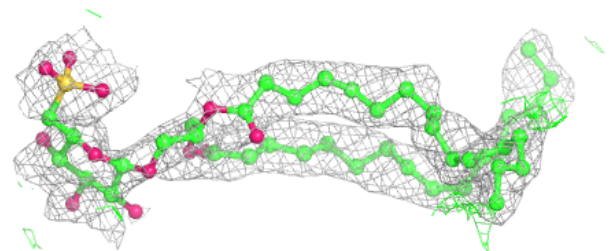
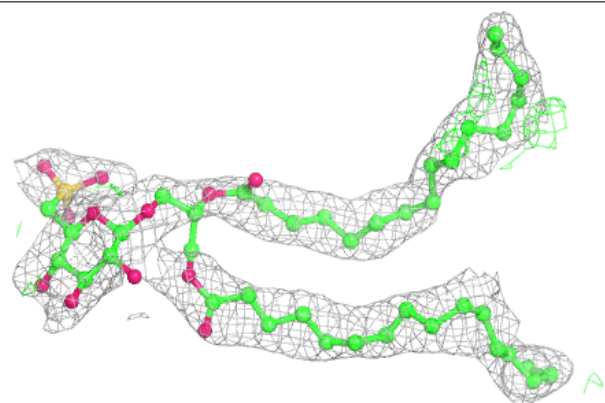


Electron density around SQD F 104:

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

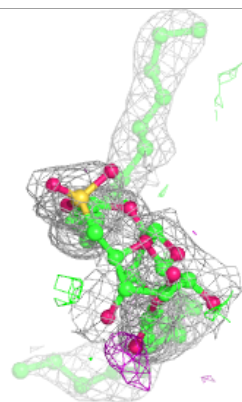
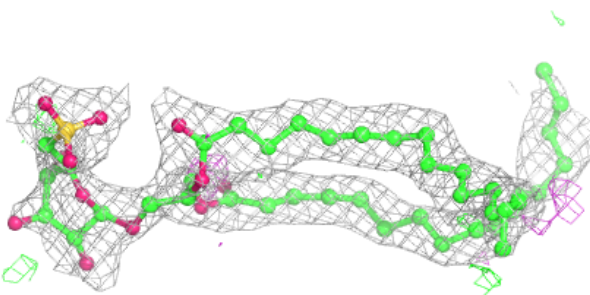
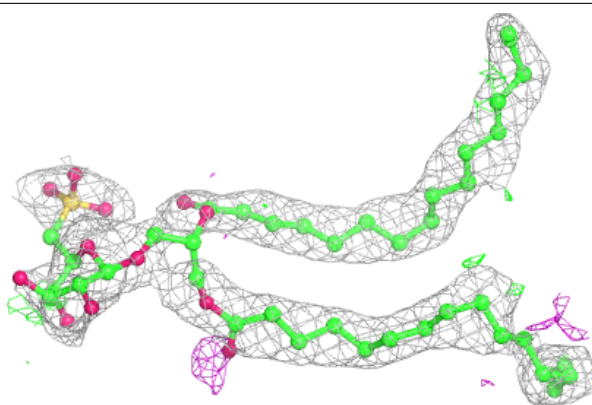
**Electron density around SQD I 102:**

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

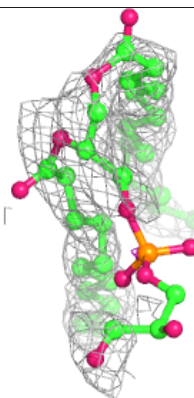
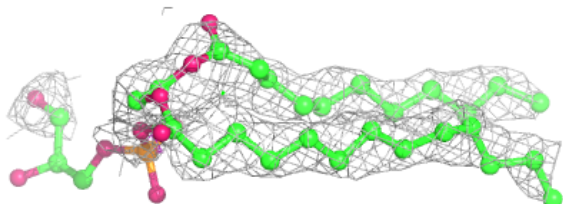
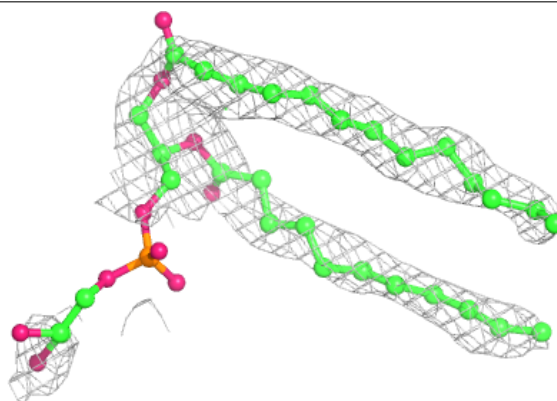


Electron density around SQD b 633:

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

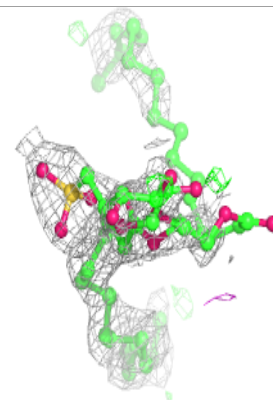
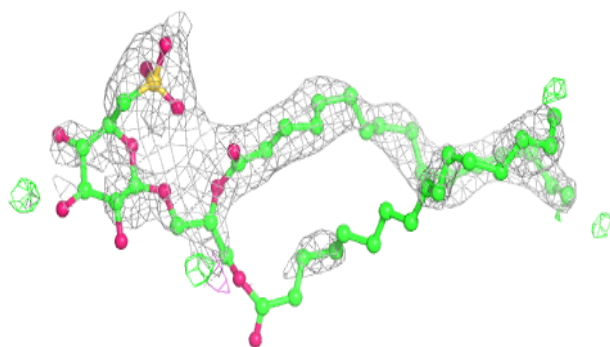
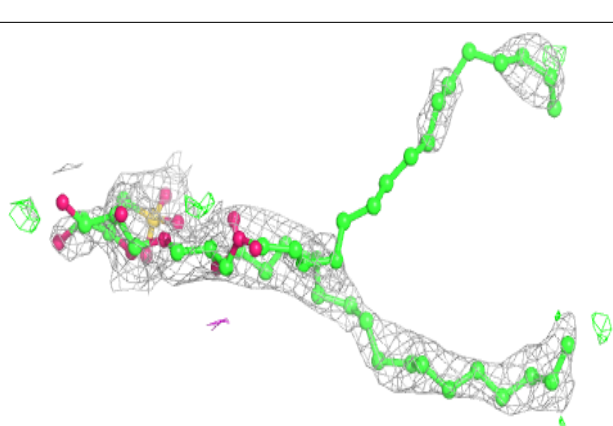
**Electron density around LHG a 419:**

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

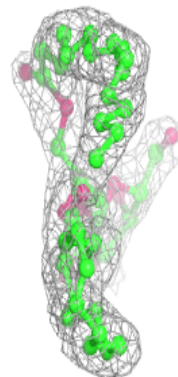
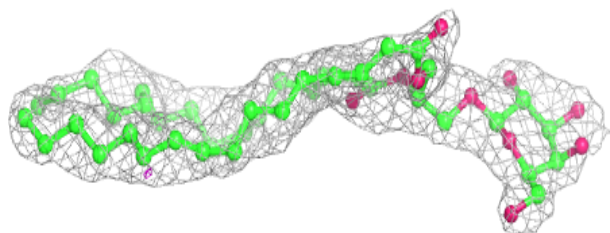
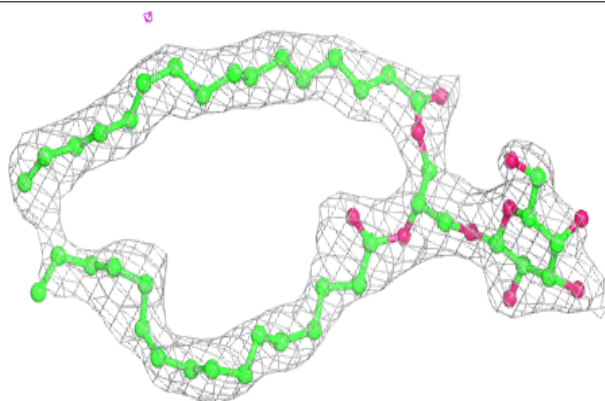


Electron density around SQD x 101:

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

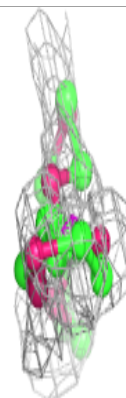
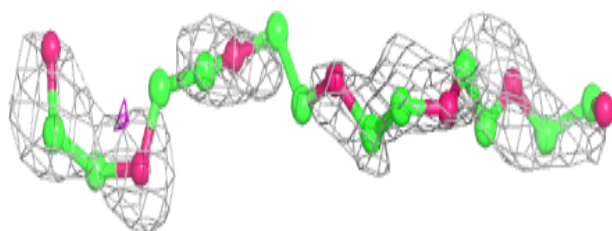
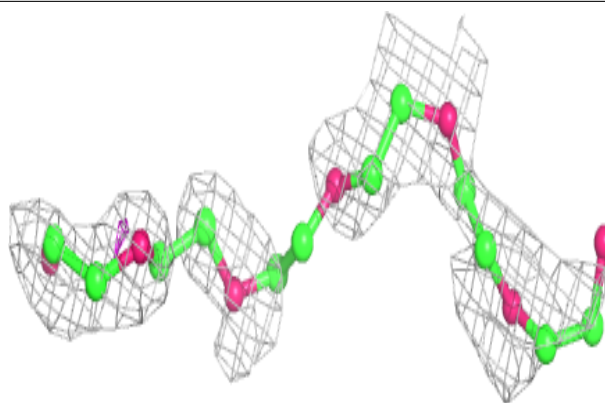
**Electron density around LMG A 613:**

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

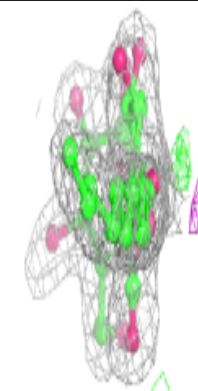
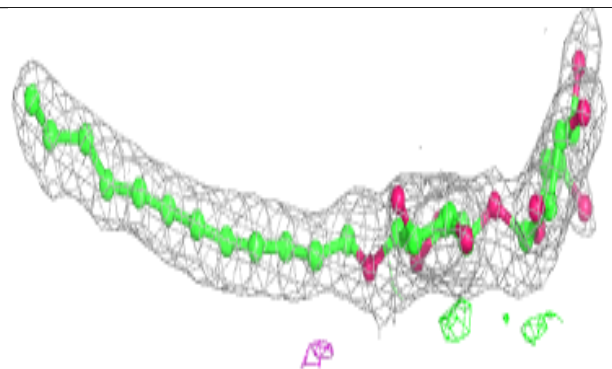
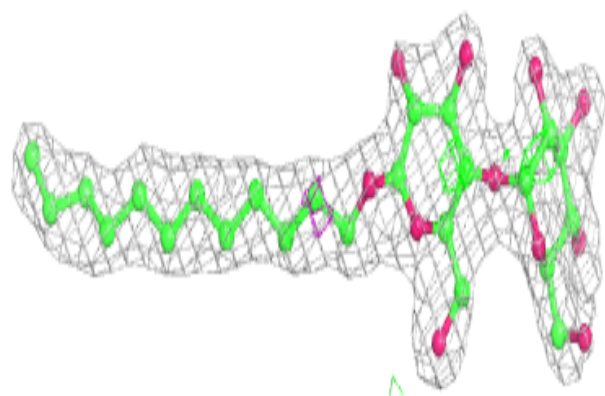


Electron density around P6G B 652:

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

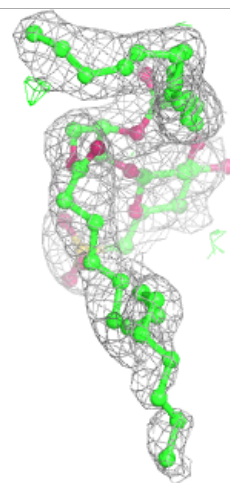
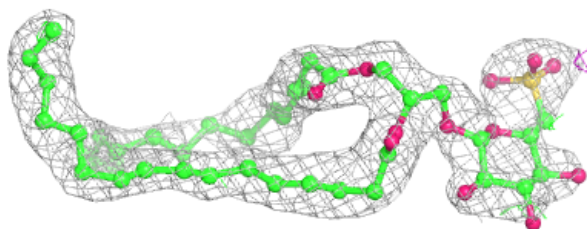
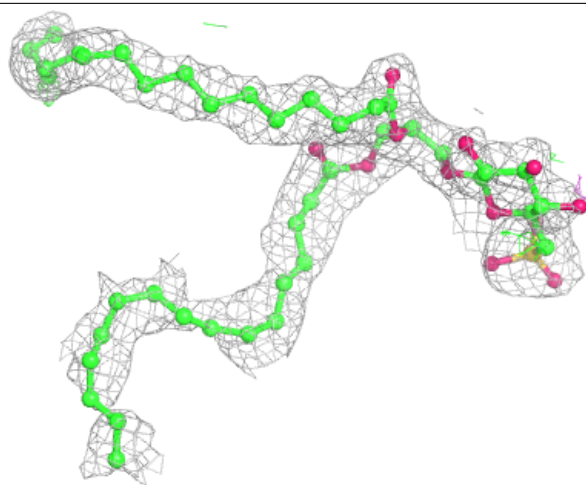
**Electron density around LMT m 102:**

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



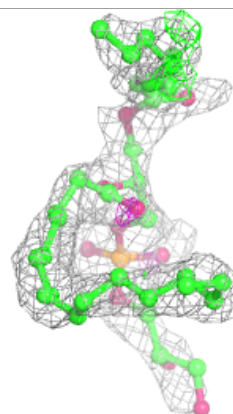
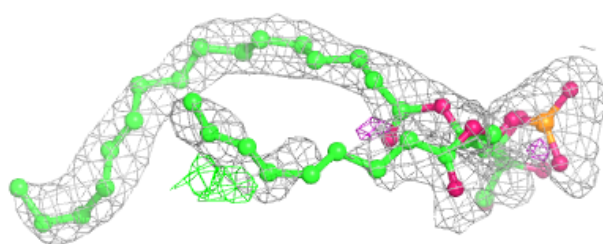
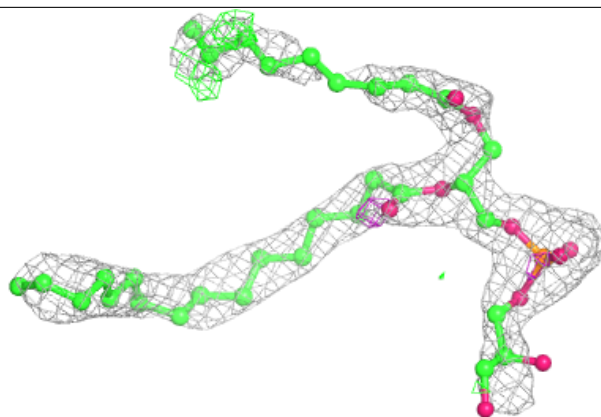
Electron density around SQD A 616:

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

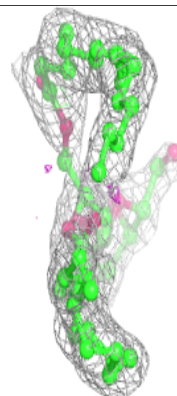
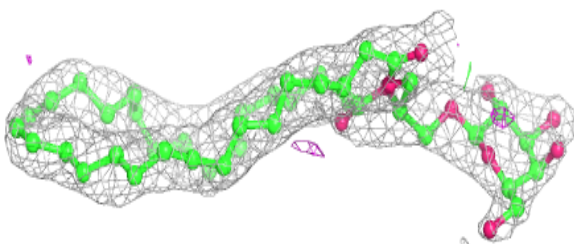
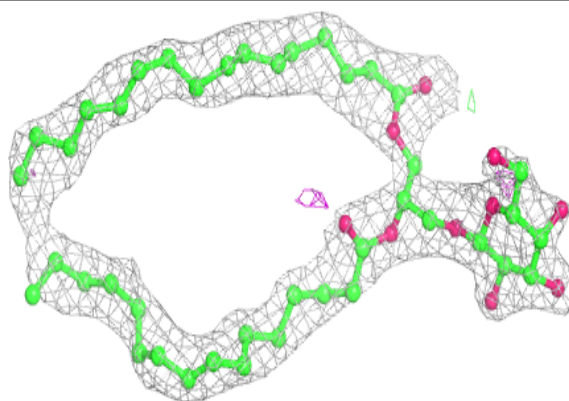


Electron density around LHG E 101:

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

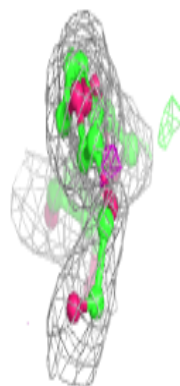
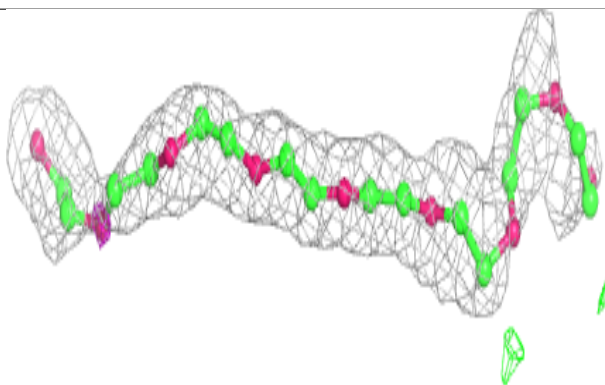
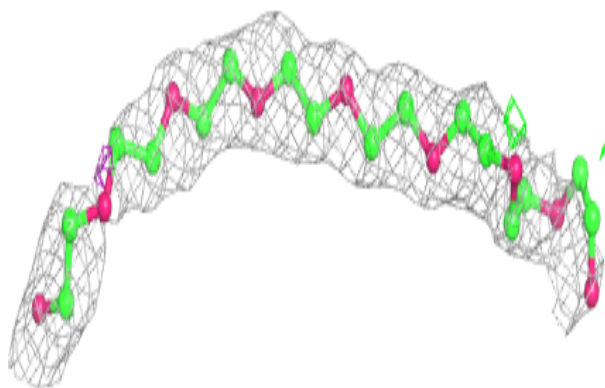
**Electron density around LMG a 414:**

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

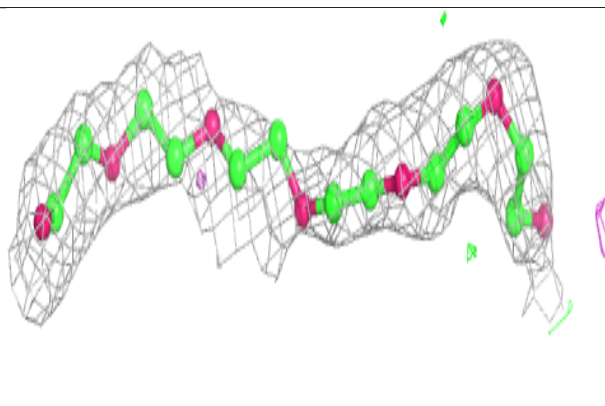
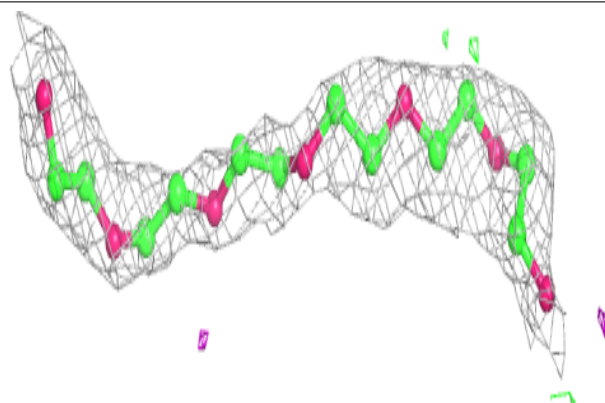


Electron density around PE8 i 107:

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

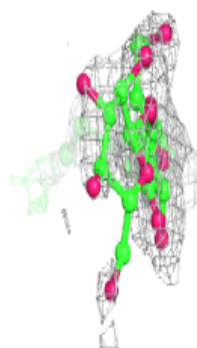
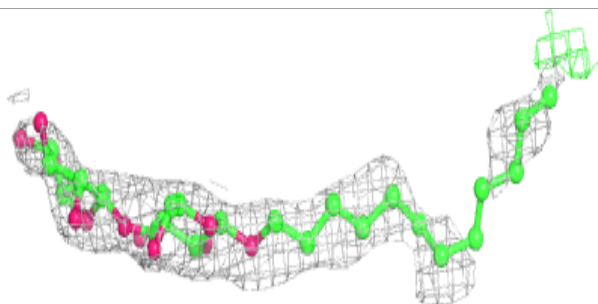
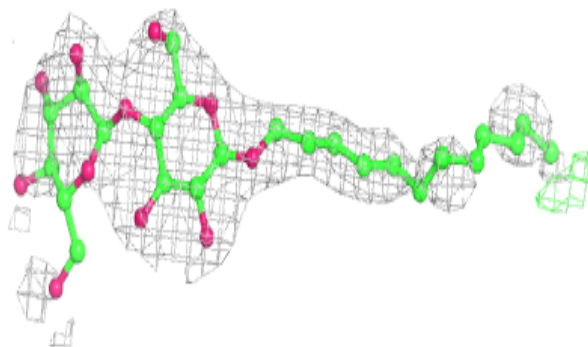
**Electron density around P6G A 624:**

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

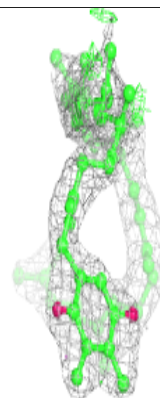
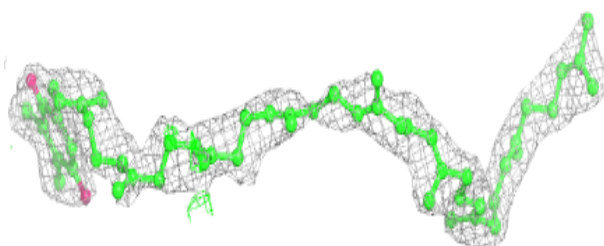
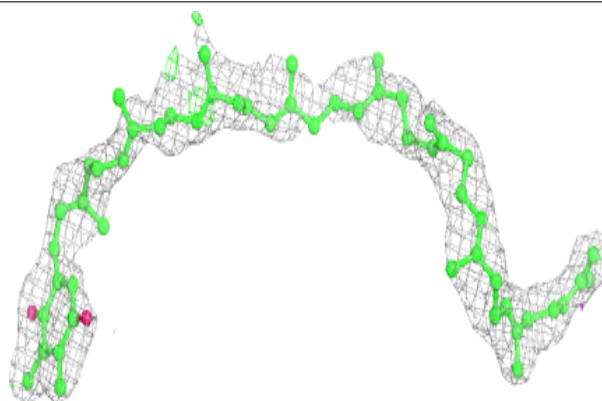


Electron density around LMT I 101:

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

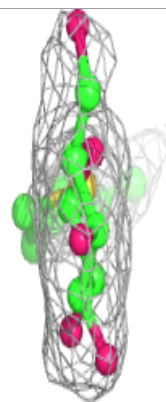
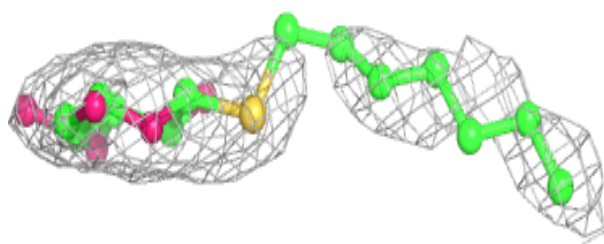
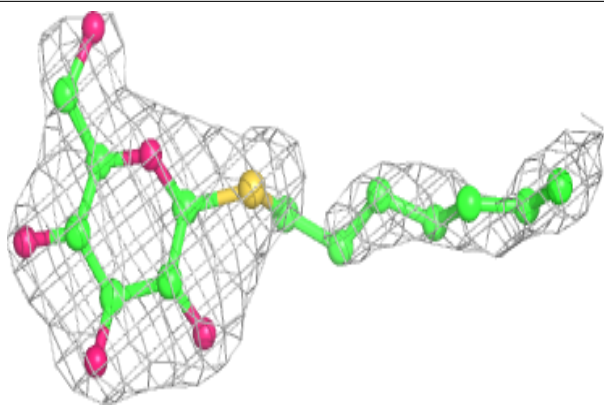
**Electron density around PL9 A 611:**

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

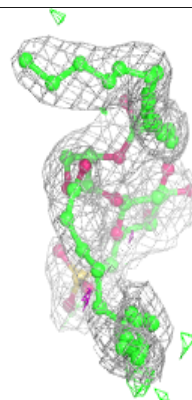
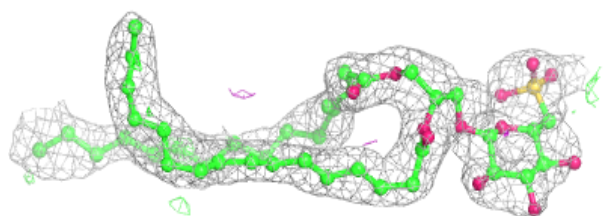
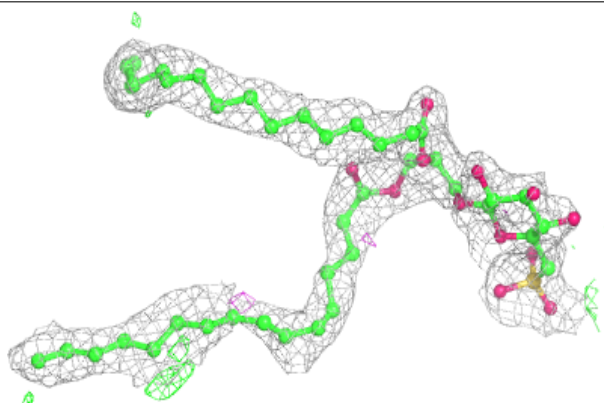


Electron density around HTG c 522:

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

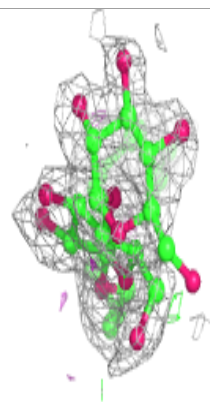
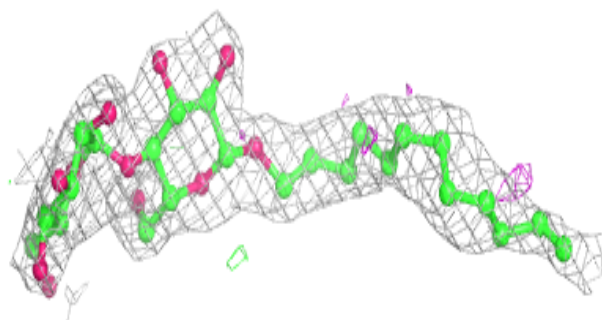
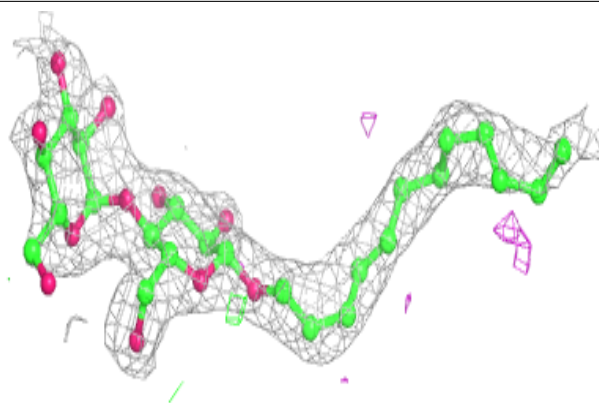
**Electron density around SQD a 417:**

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

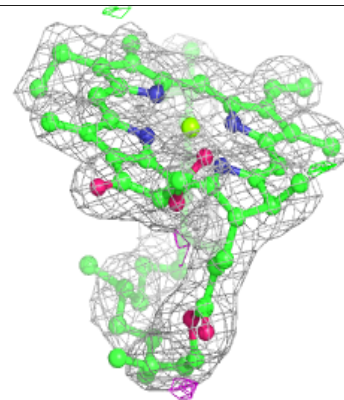
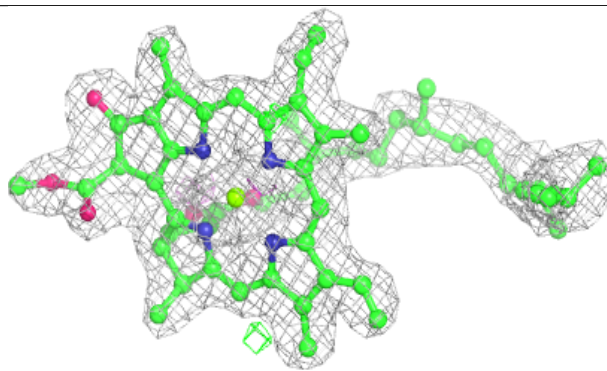
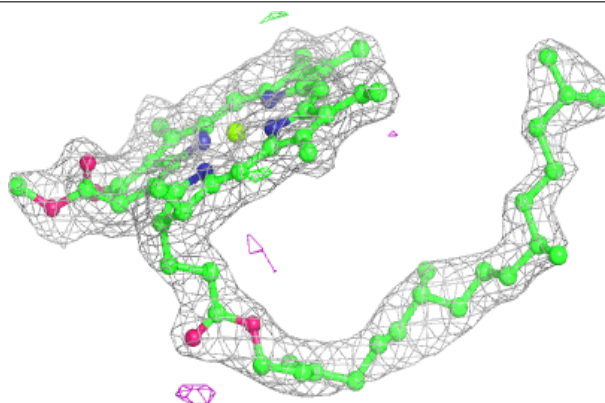


Electron density around LMT A 617:

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

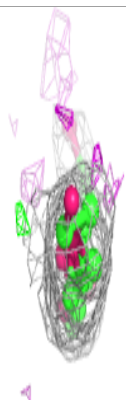
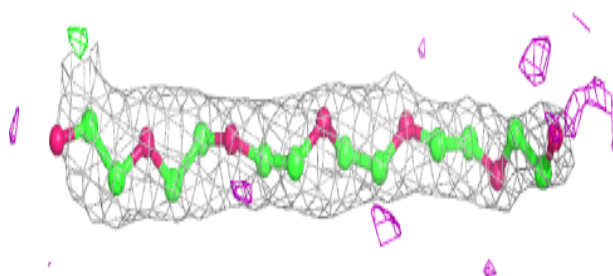
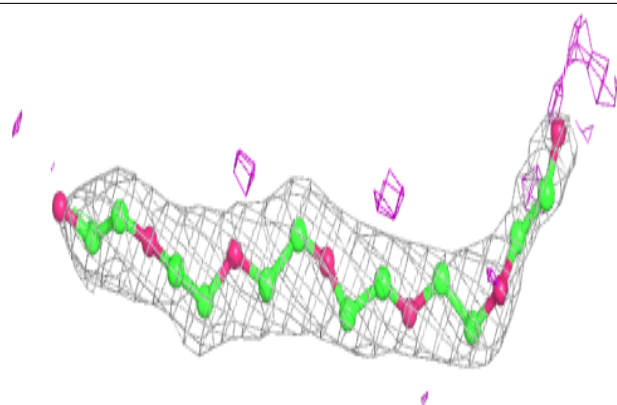
**Electron density around CLA C 513:**

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

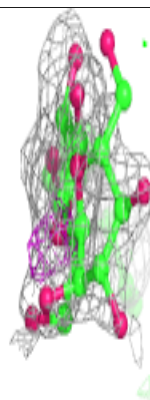
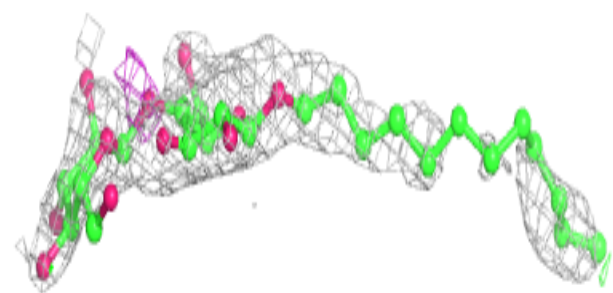
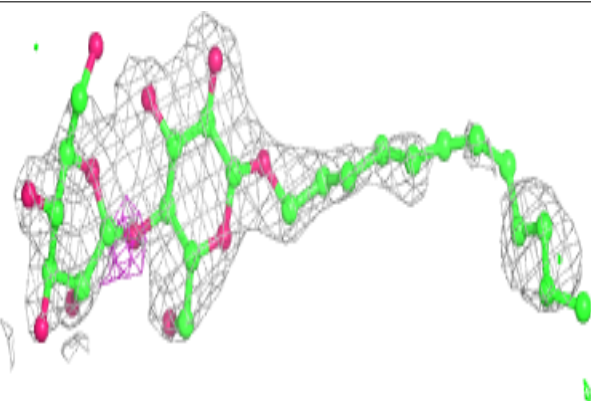


Electron density around P6G d 415:

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

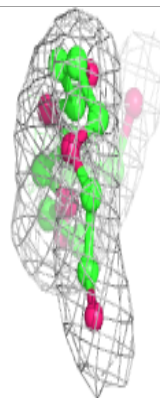
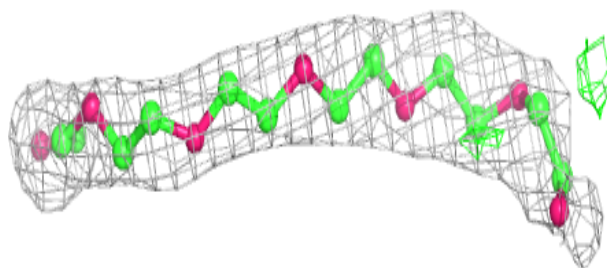
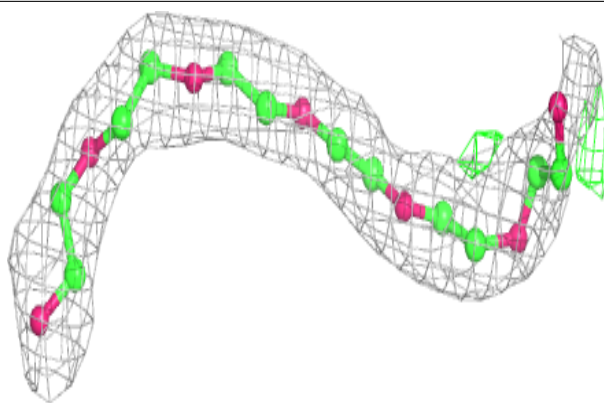
**Electron density around LMT c 521:**

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

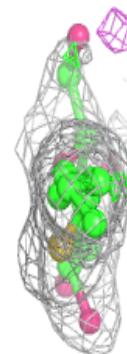
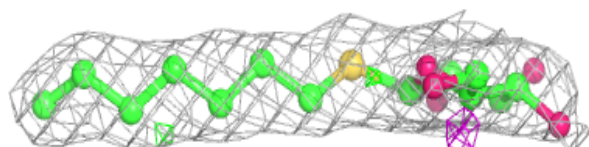
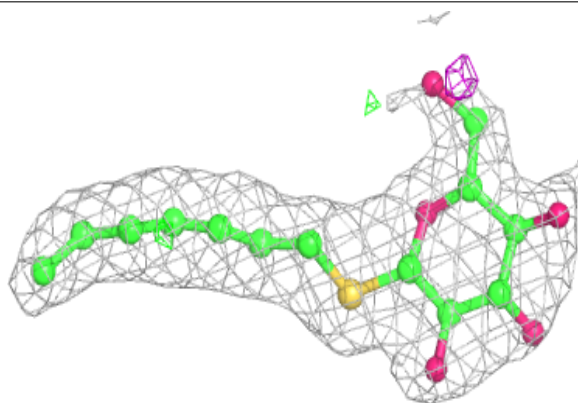


Electron density around P6G b 648:

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

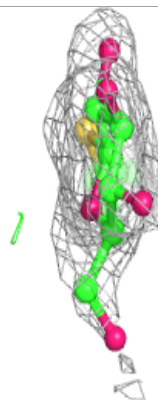
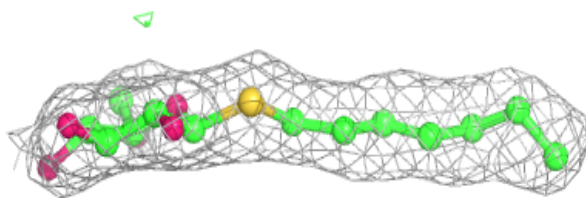
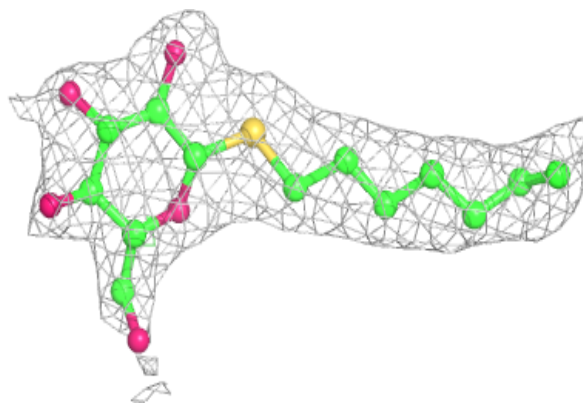
**Electron density around HTG b 631:**

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

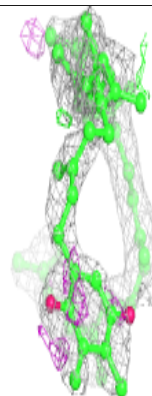
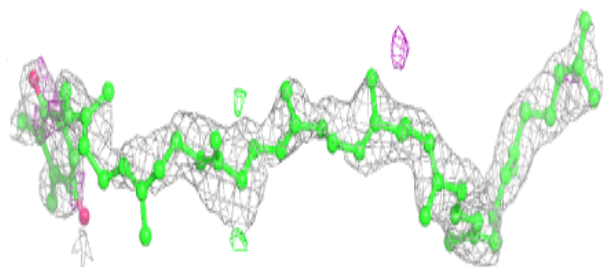
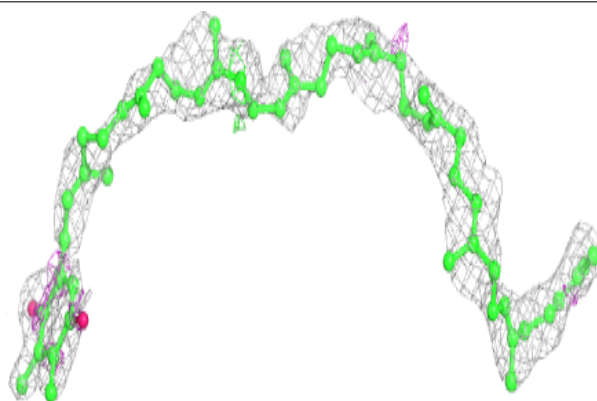


Electron density around HTG B 630:

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

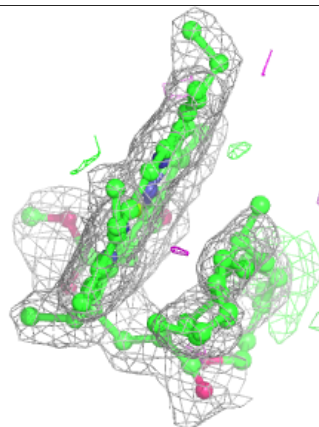
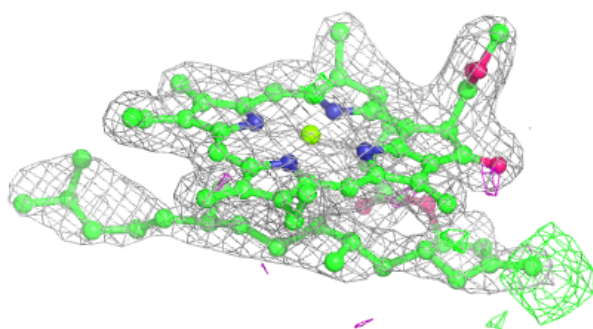
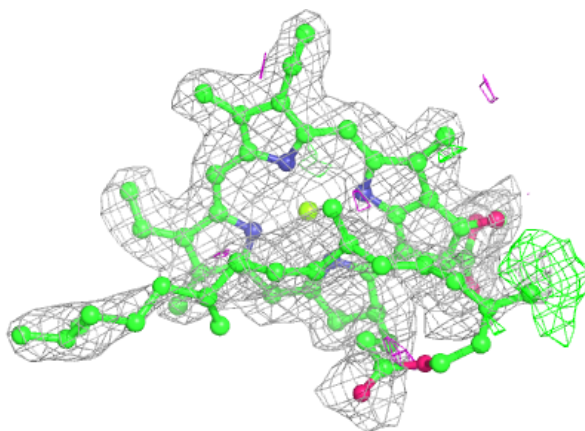
**Electron density around PL9 a 412:**

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



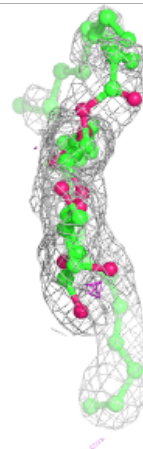
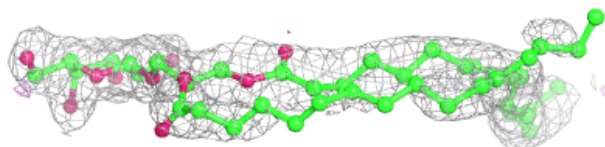
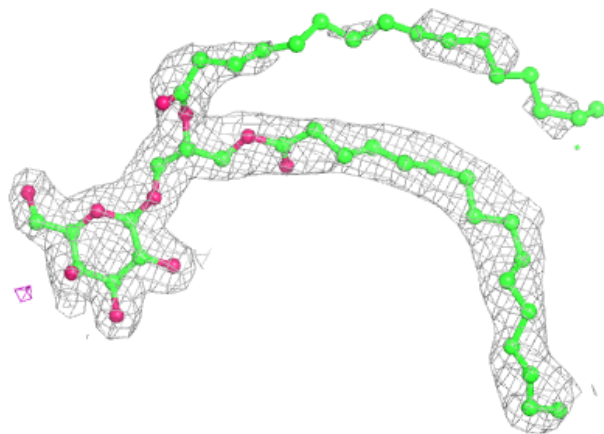
Electron density around CLA b 602:

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

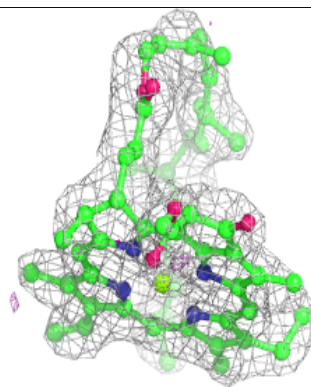
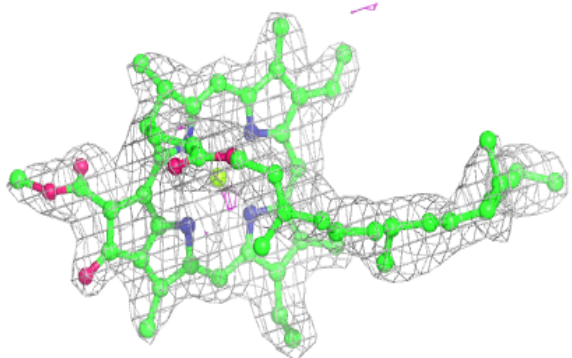
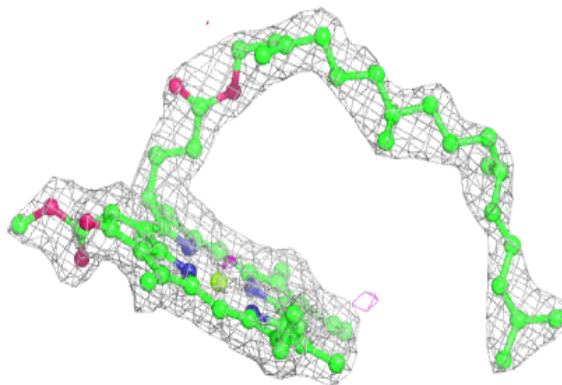


Electron density around LMG c 519:

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

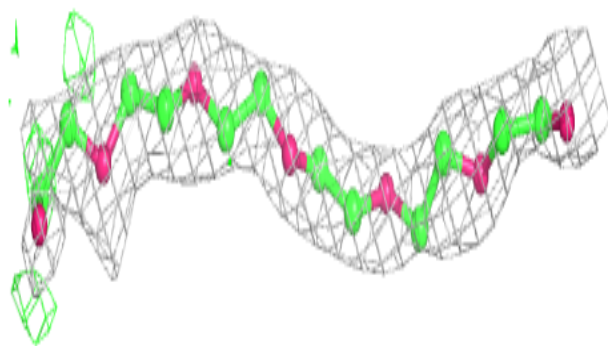
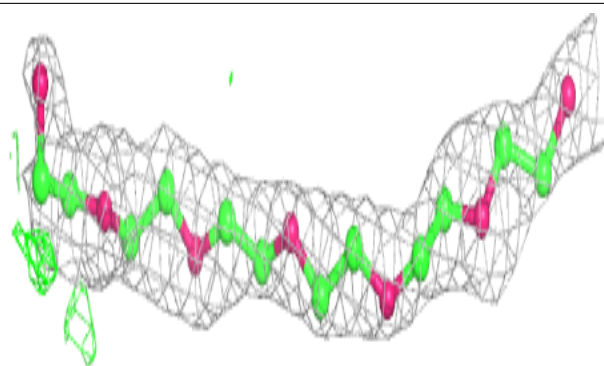
**Electron density around CLA c 513:**

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

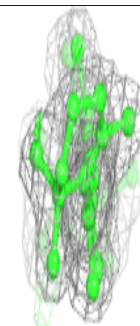
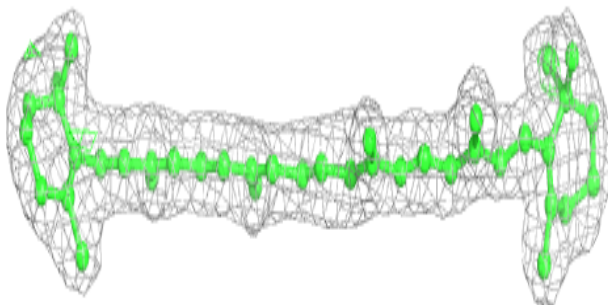
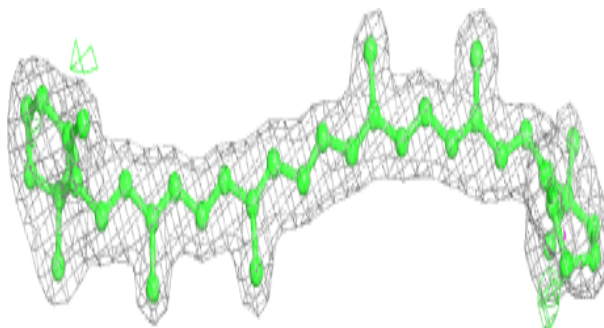


Electron density around P6G j 106:

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

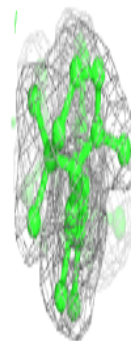
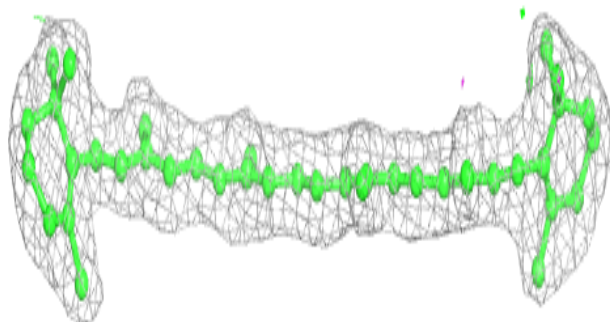
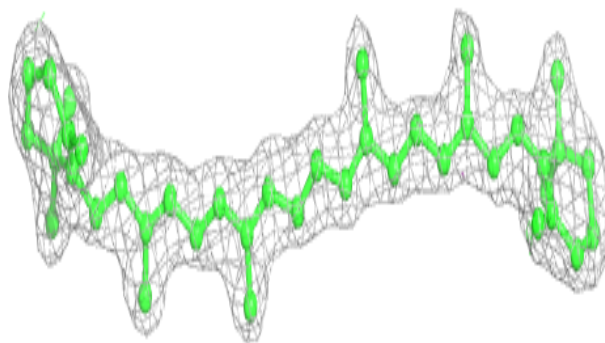
**Electron density around BCR C 514:**

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

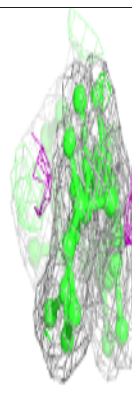
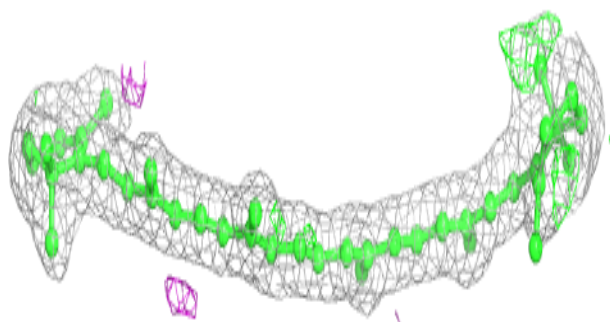
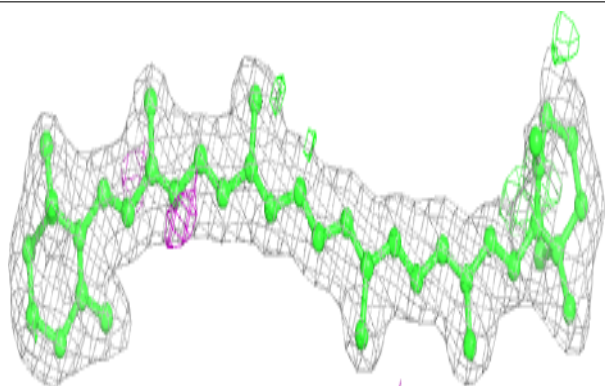


Electron density around BCR c 514:

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

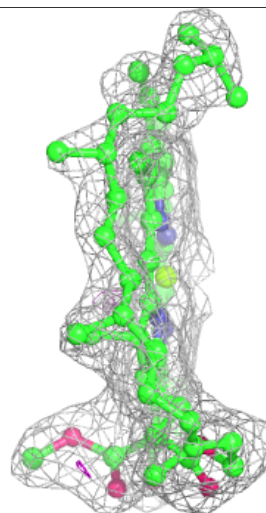
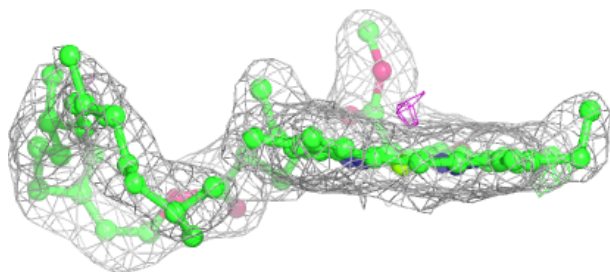
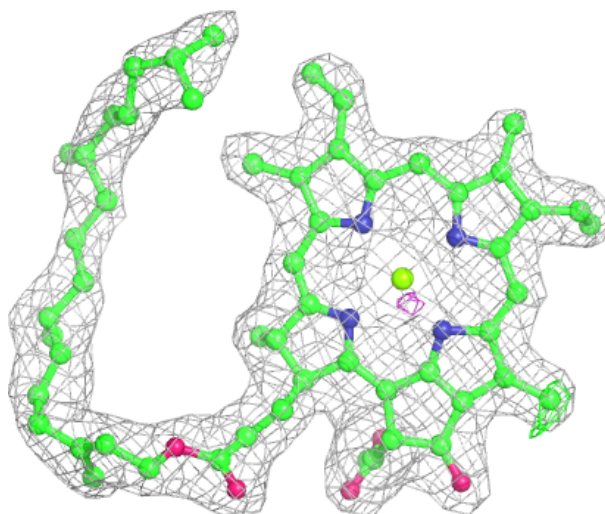
**Electron density around BCR d 406:**

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



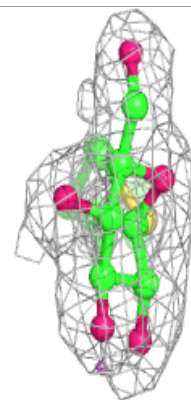
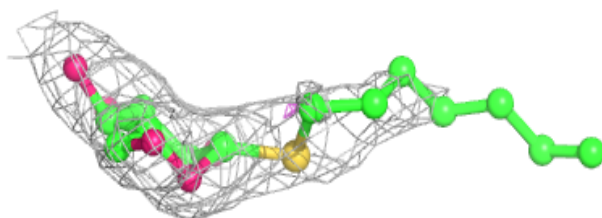
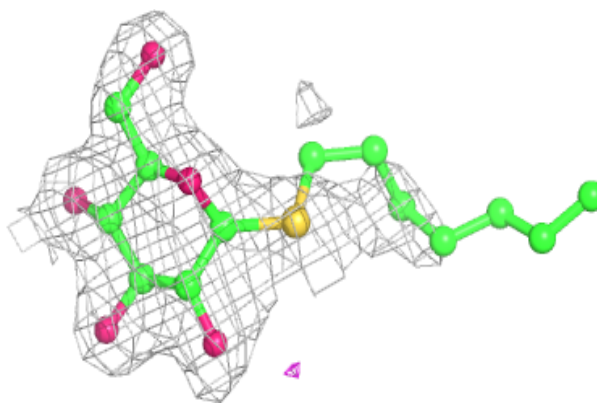
Electron density around CLA c 512:

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

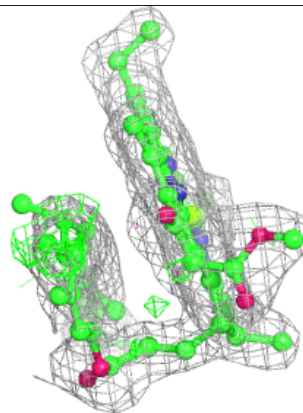
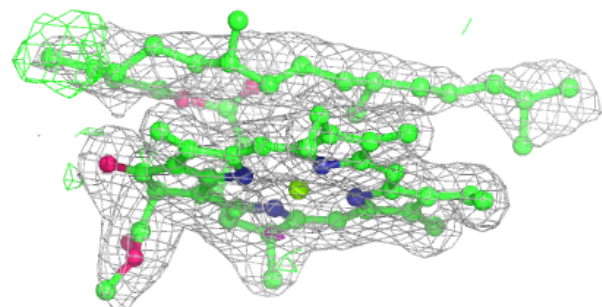
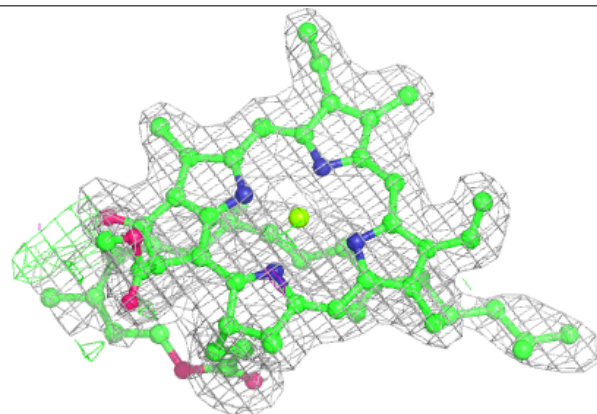


Electron density around HTG V 204:

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

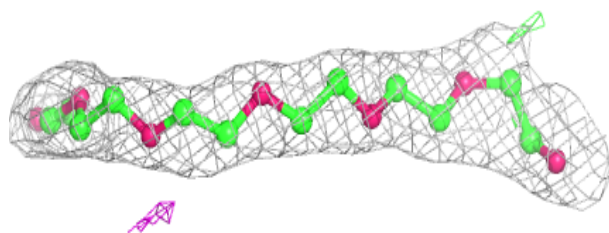
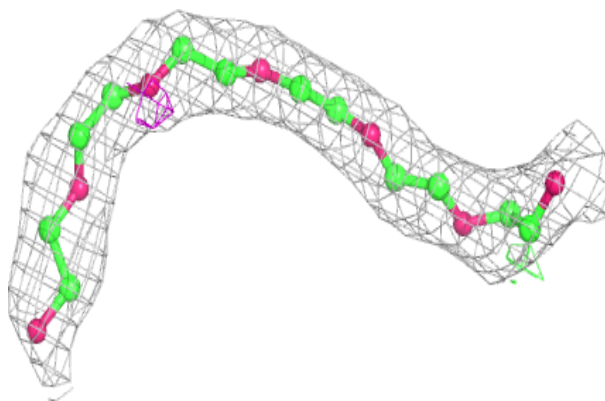
**Electron density around CLA B 602:**

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



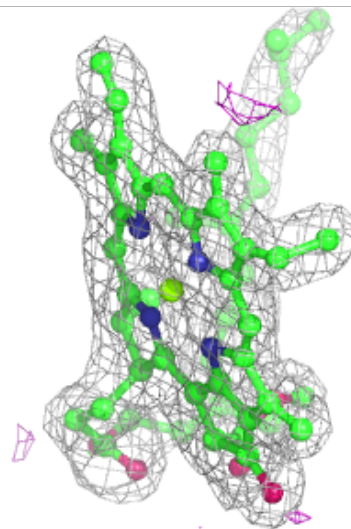
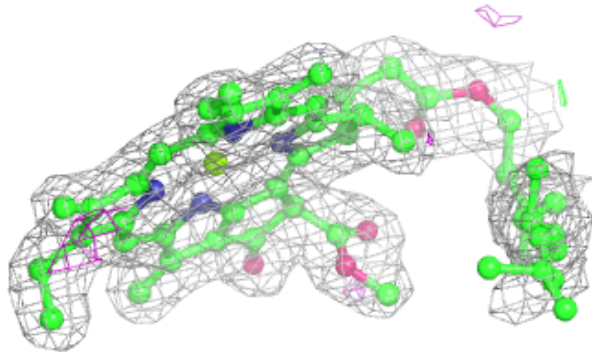
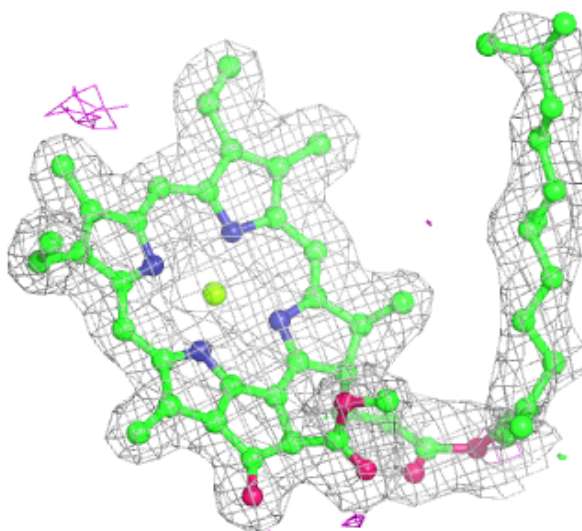
Electron density around P6G B 651:

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



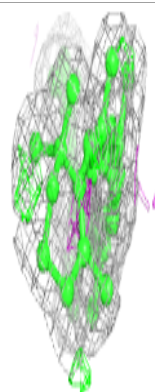
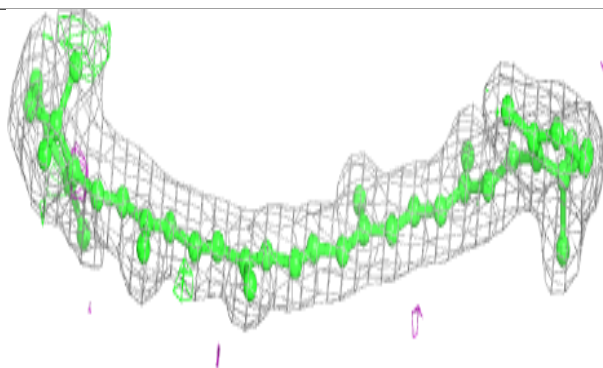
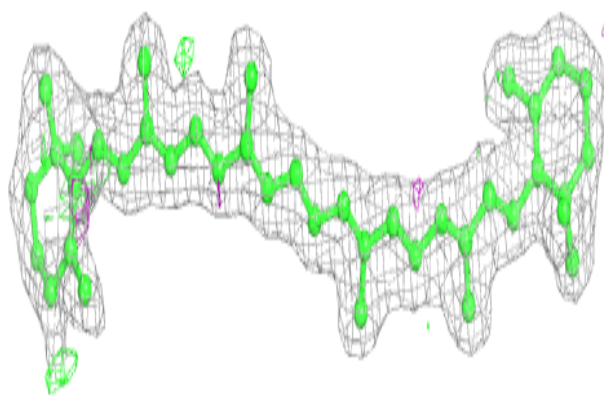
Electron density around CLA b 617:

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

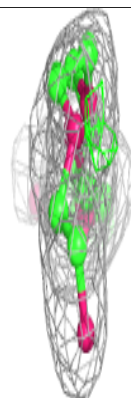
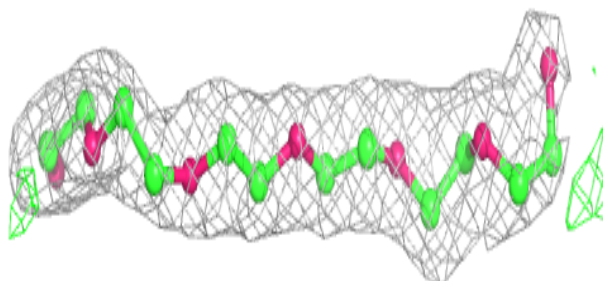
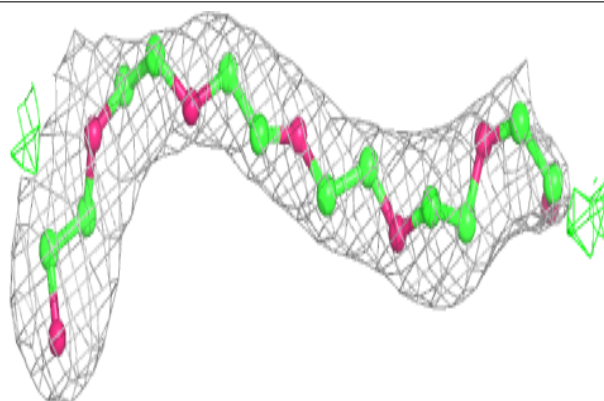


Electron density around BCR D 406:

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

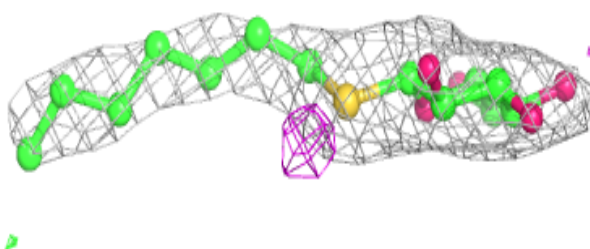
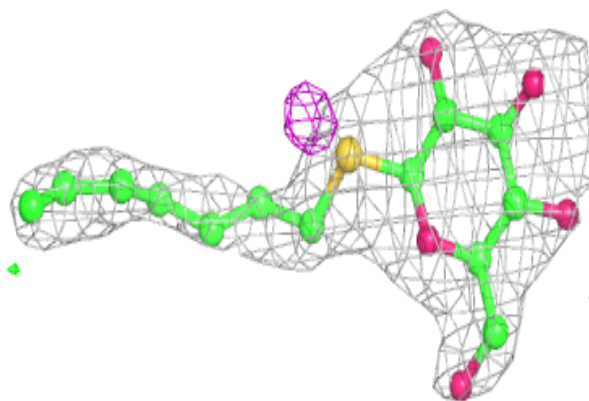
**Electron density around P6G T 105:**

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

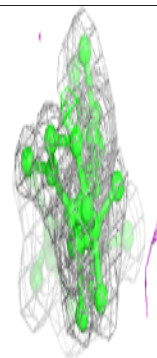
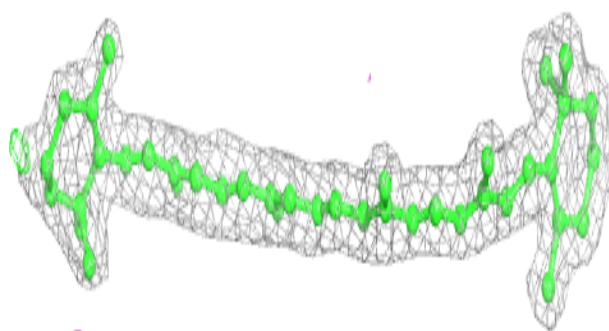
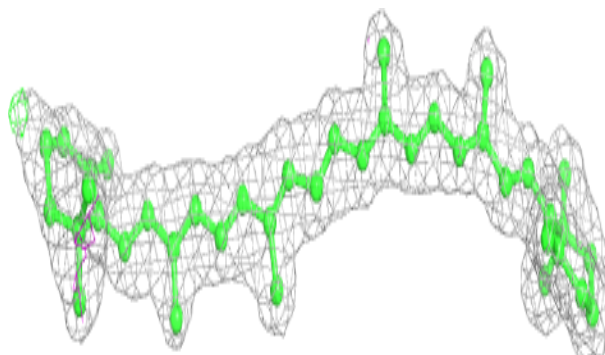


Electron density around HTG C 521:

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

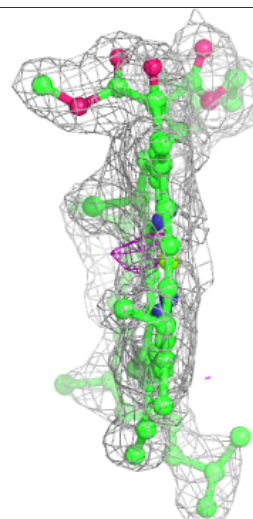
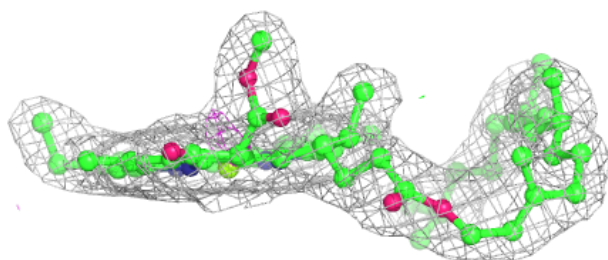
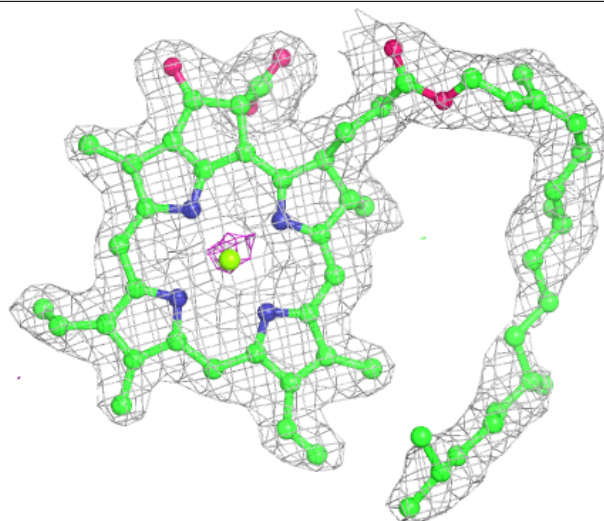
**Electron density around BCR H 102:**

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



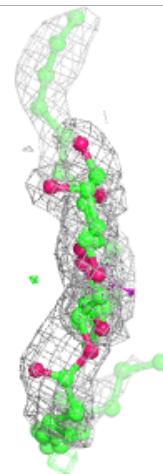
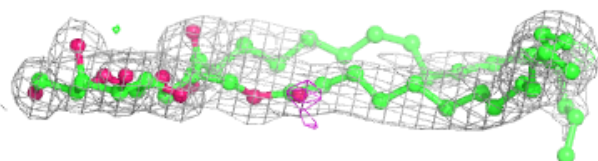
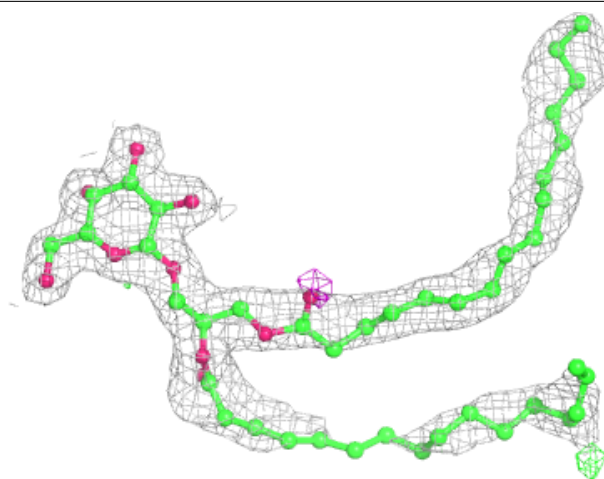
Electron density around CLA C 512:

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



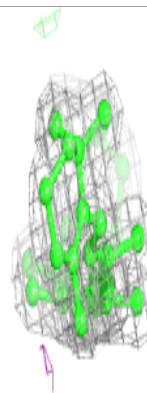
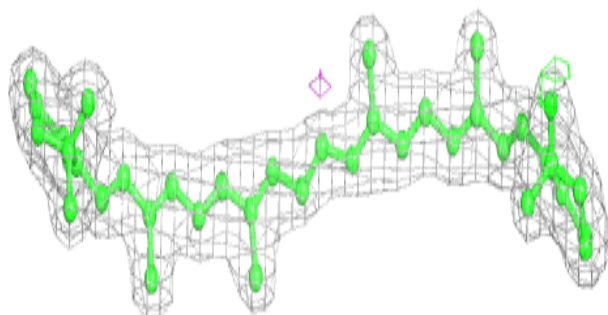
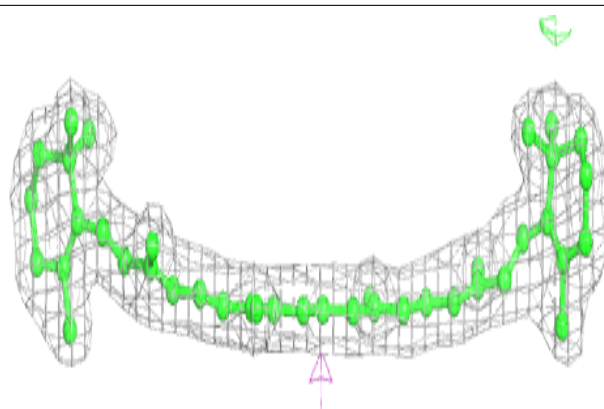
Electron density around LMG C 519:

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

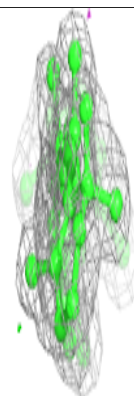
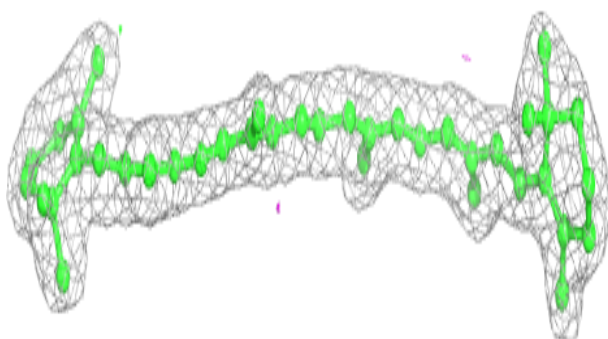
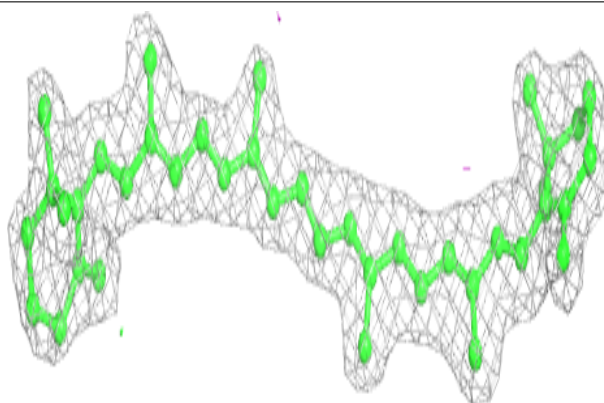


Electron density around BCR C 525:

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

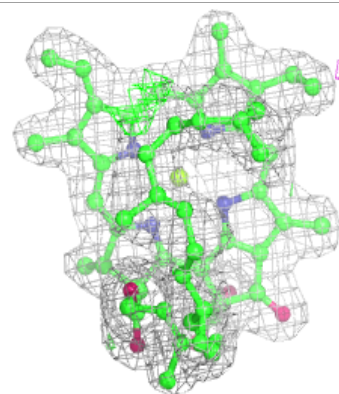
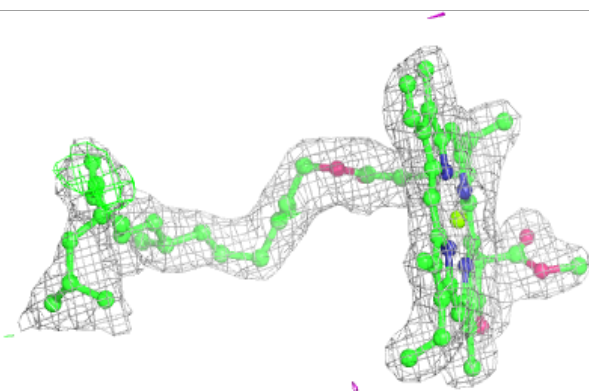
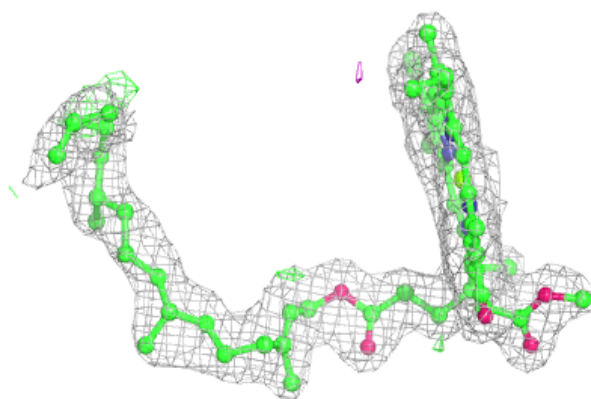
**Electron density around BCR k 101:**

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

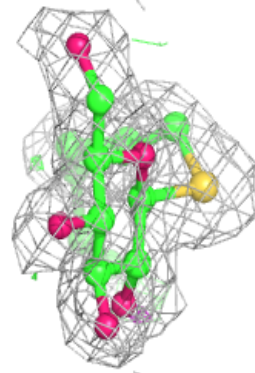
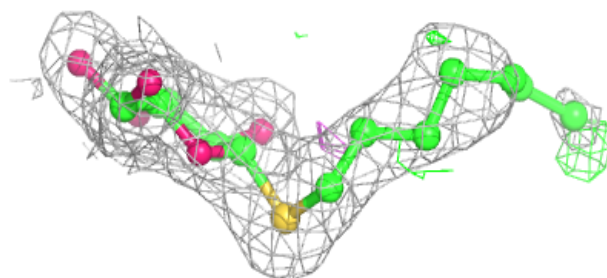
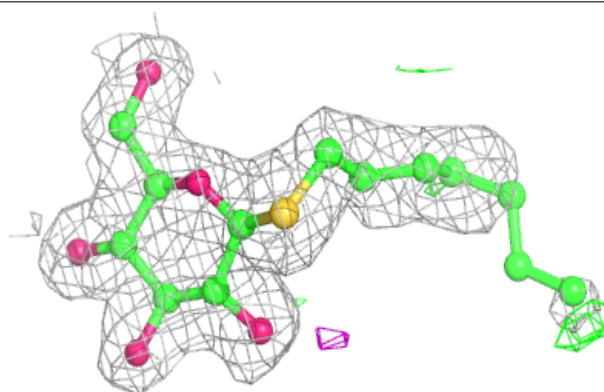


Electron density around CLA c 506:

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

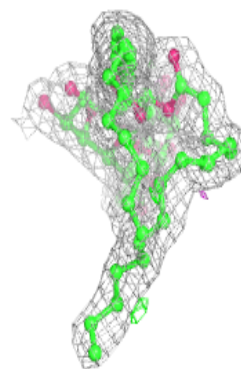
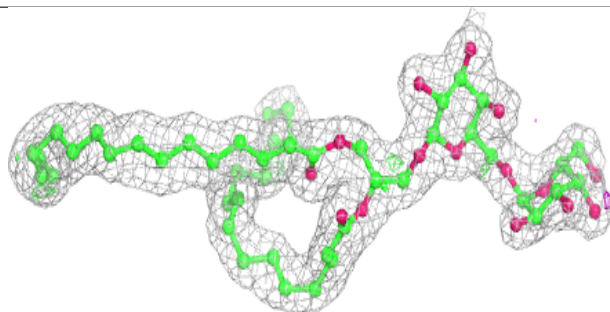
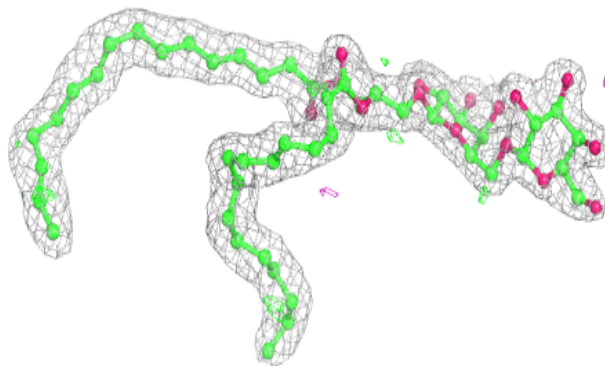
**Electron density around HTG B 623:**

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

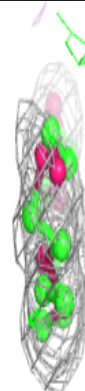
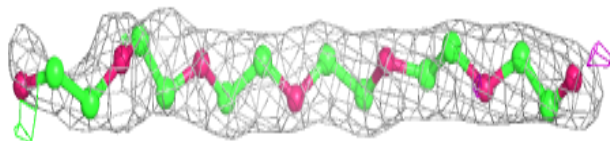
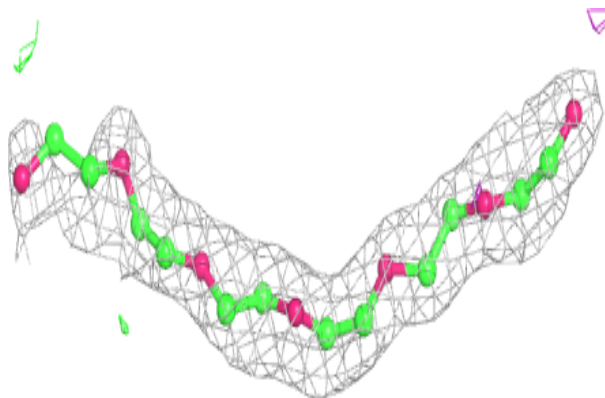


Electron density around DGD h 104:

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

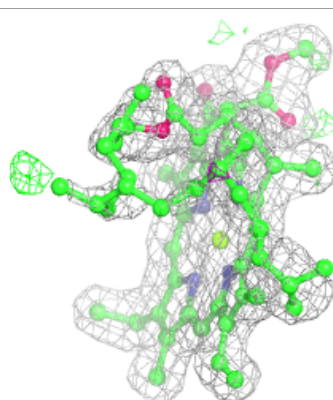
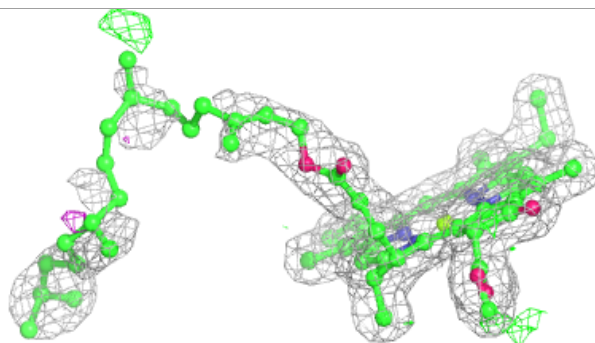
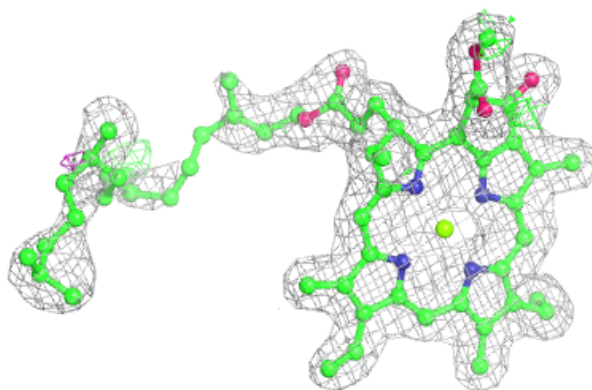
**Electron density around P6G D 417:**

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

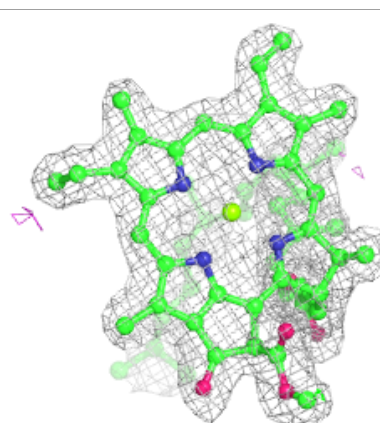
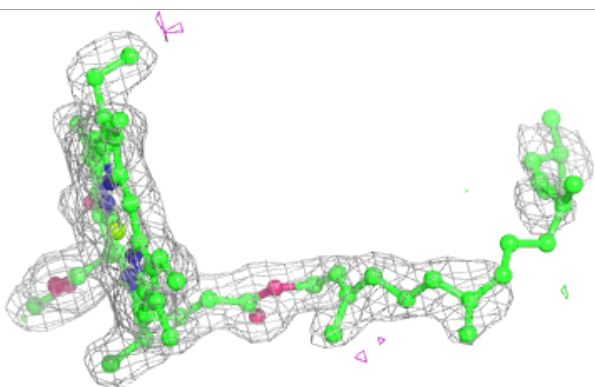
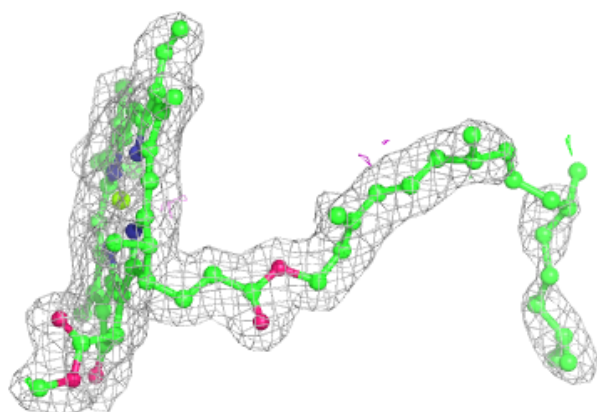


Electron density around CLA a 410:

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

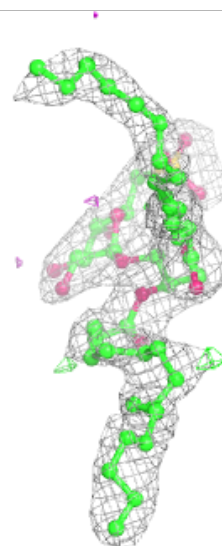
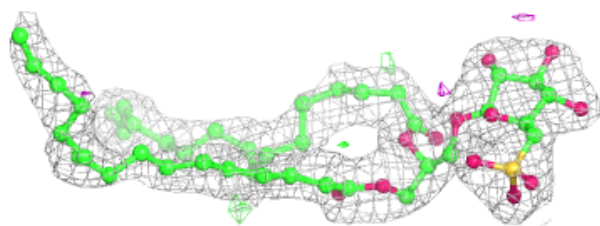
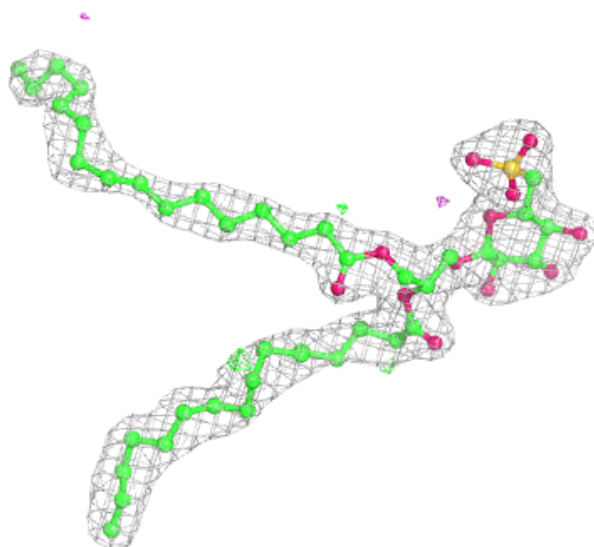
**Electron density around CLA d 405:**

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



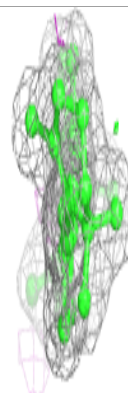
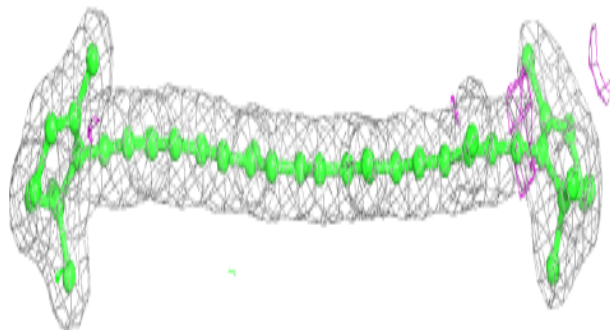
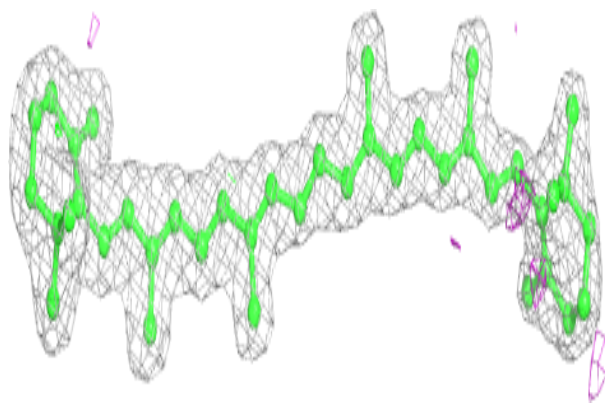
Electron density around SQD A 612:

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

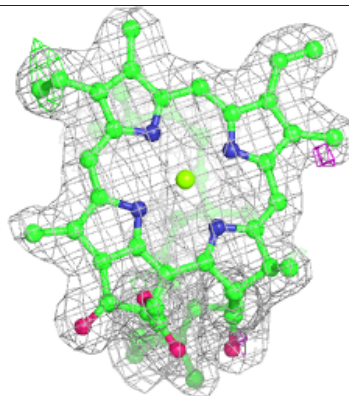
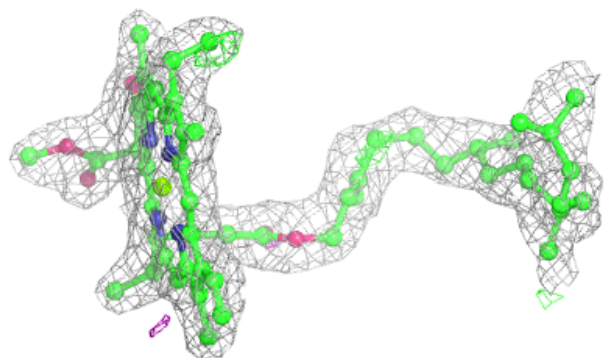
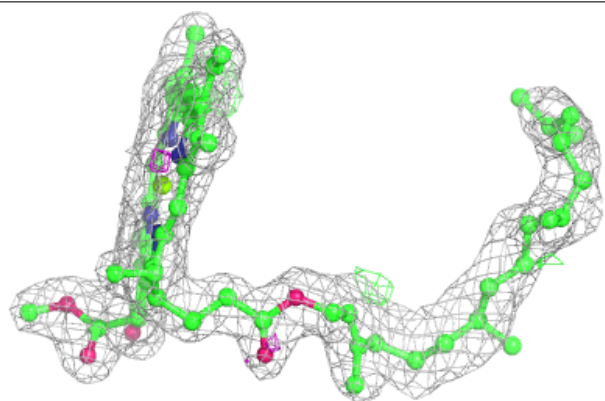


Electron density around BCR B 619:

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

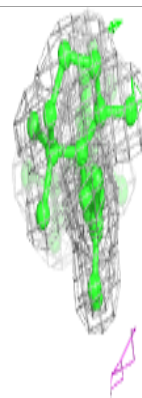
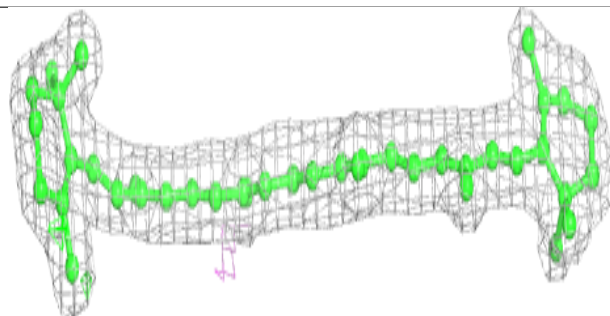
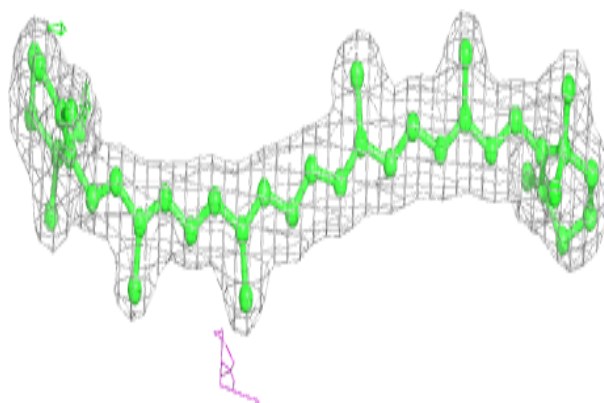
**Electron density around CLA C 506:**

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



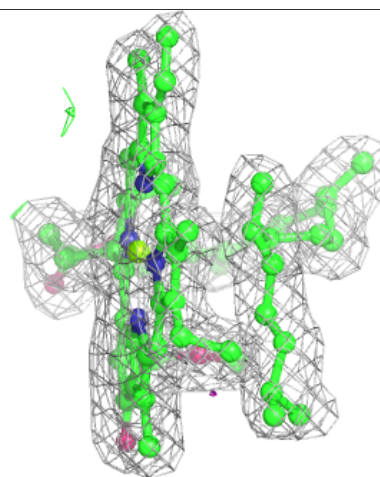
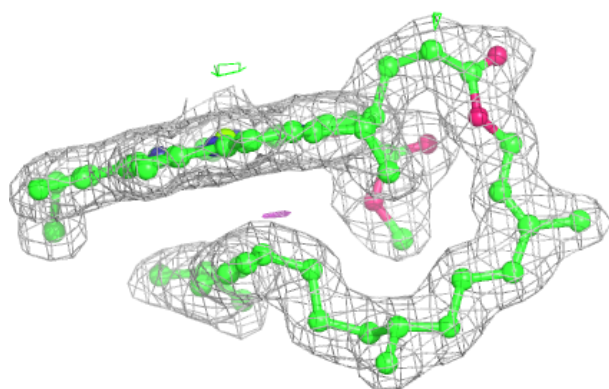
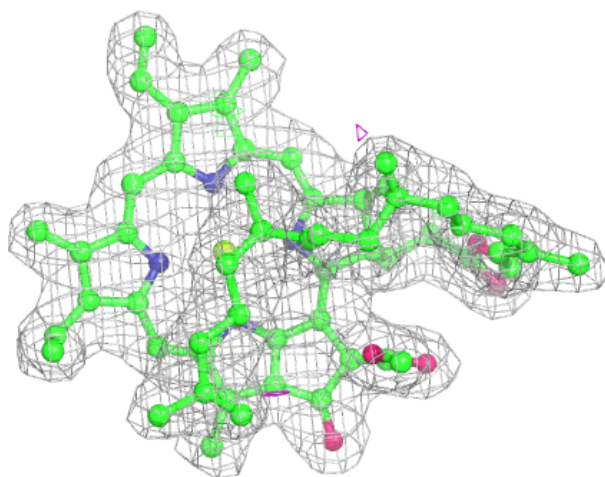
Electron density around BCR C 515:

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



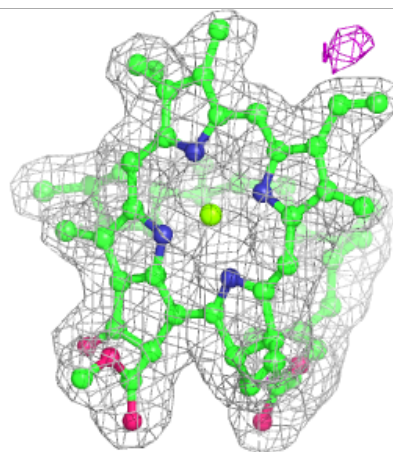
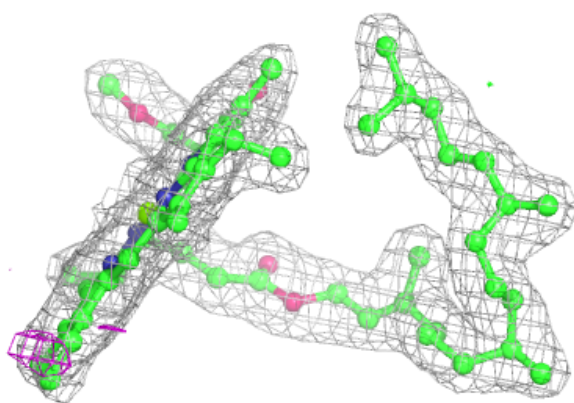
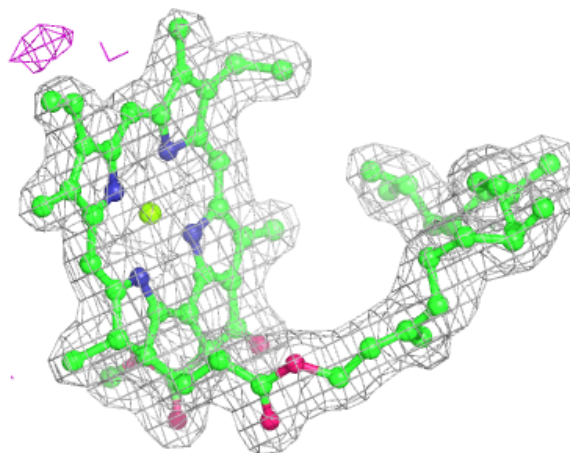
Electron density around CLA C 510:

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



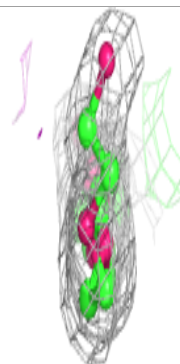
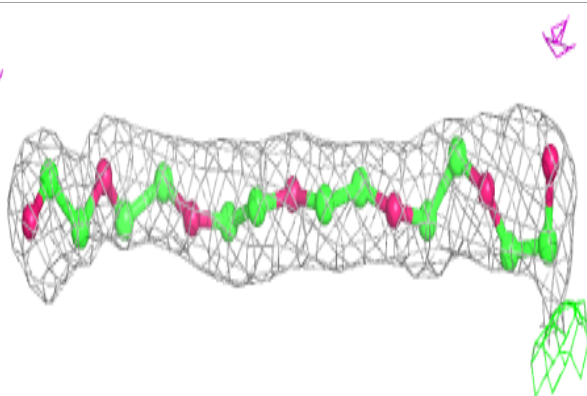
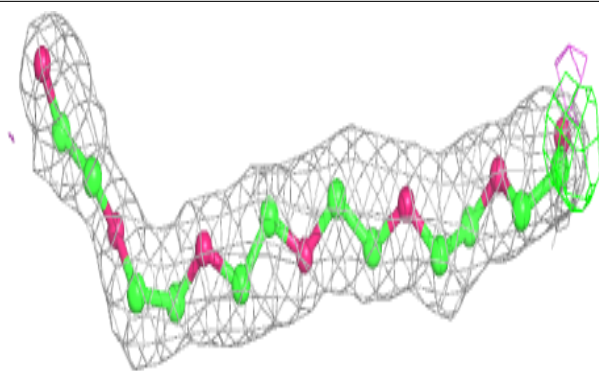
Electron density around CLA c 503:

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

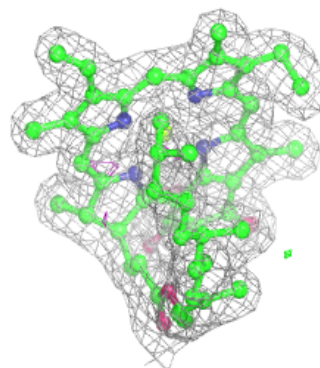
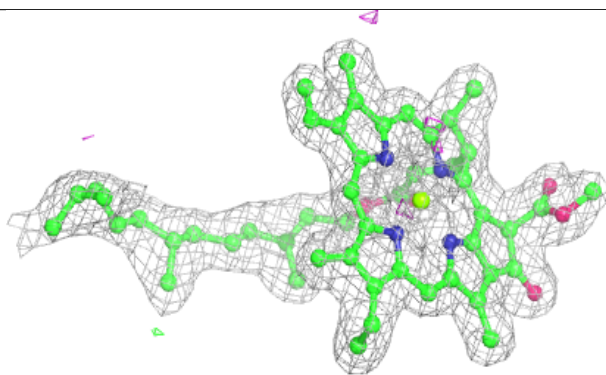
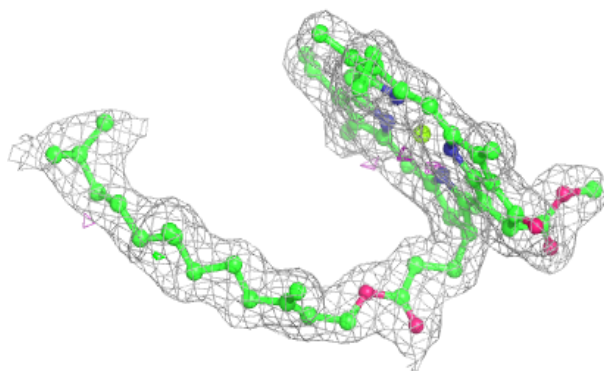


Electron density around P6G D 416:

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

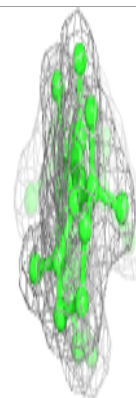
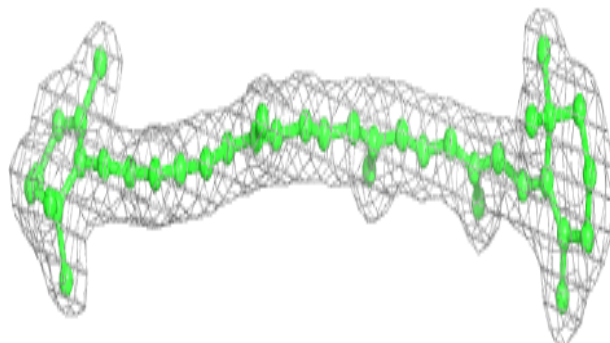
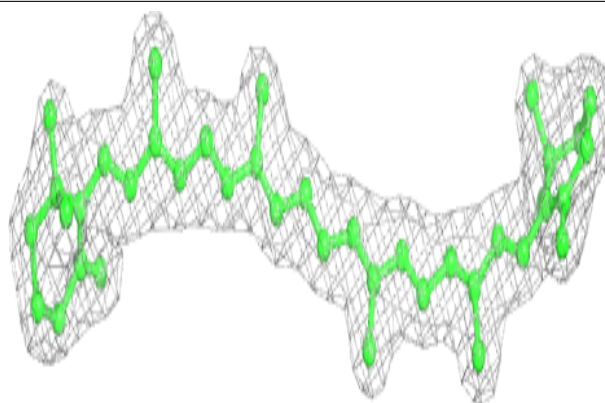
**Electron density around CLA c 504:**

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

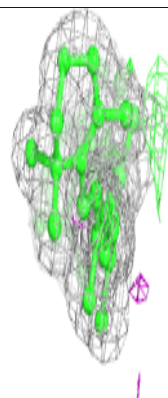
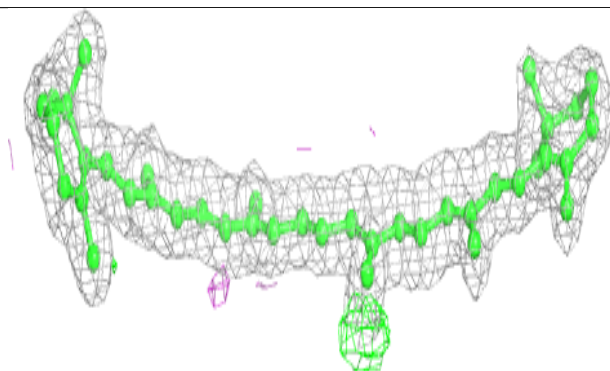
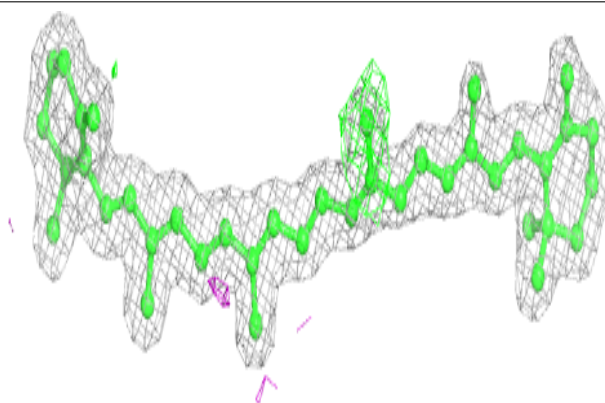


Electron density around BCR K 101:

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

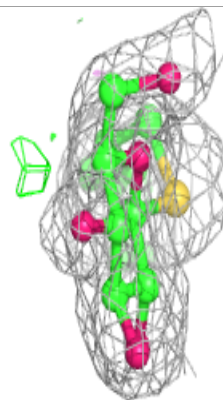
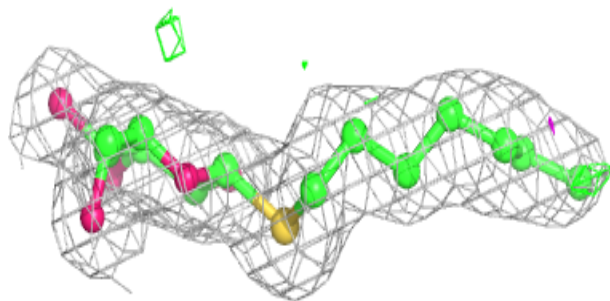
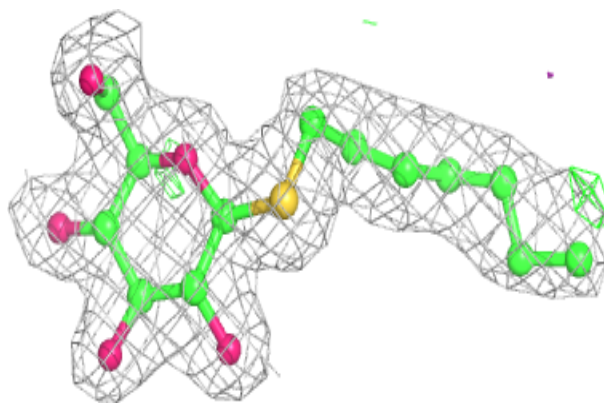
**Electron density around BCR T 102:**

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

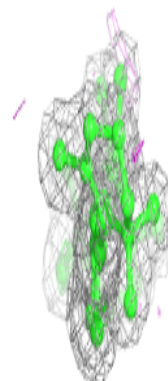
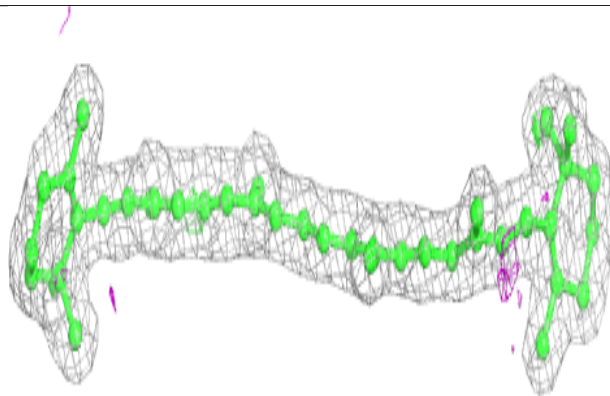
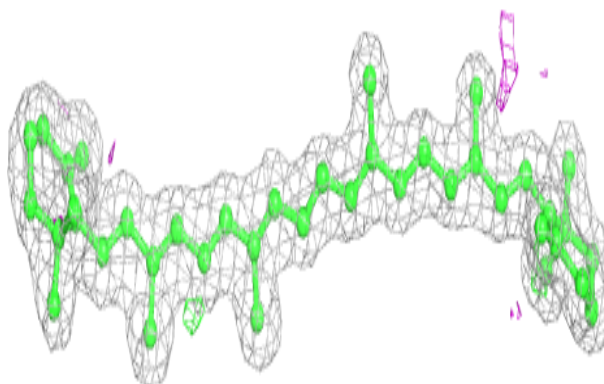


Electron density around HTG O 303:

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

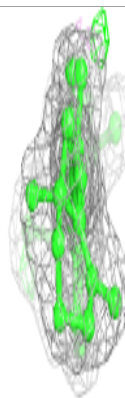
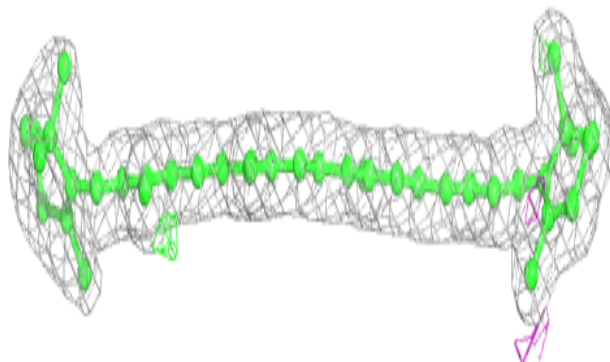
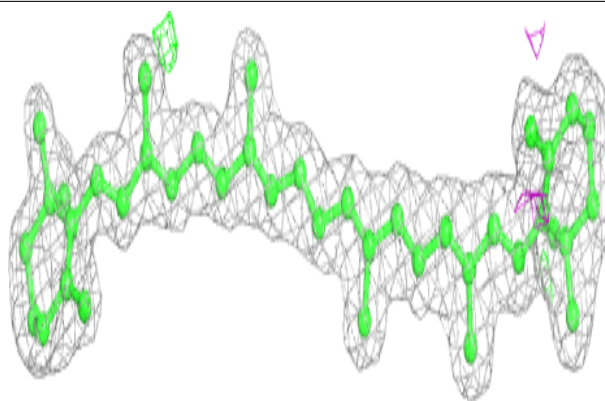
**Electron density around BCR a 411:**

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

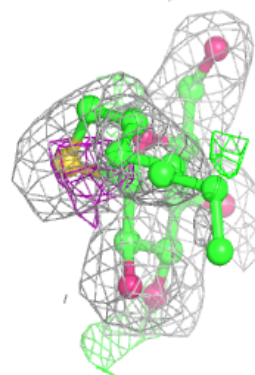
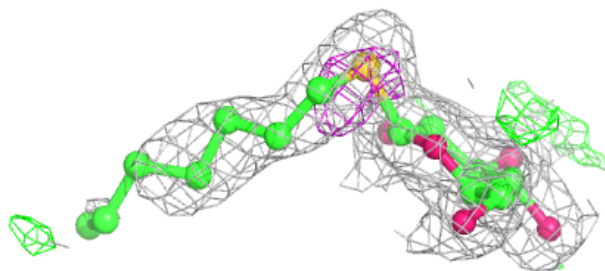
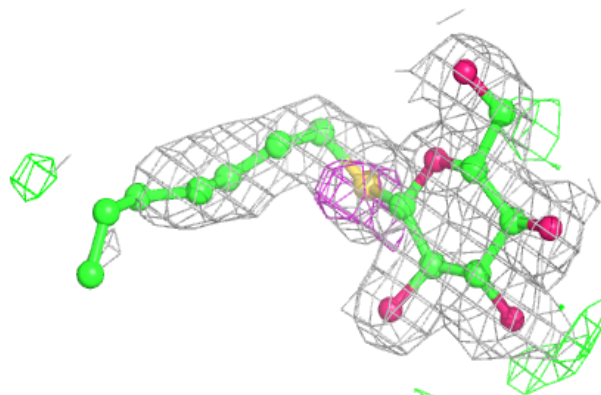


Electron density around BCR b 619:

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

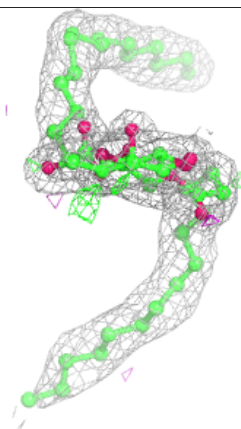
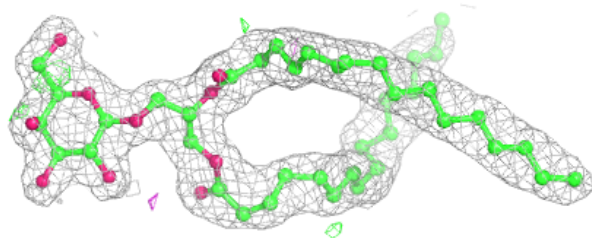
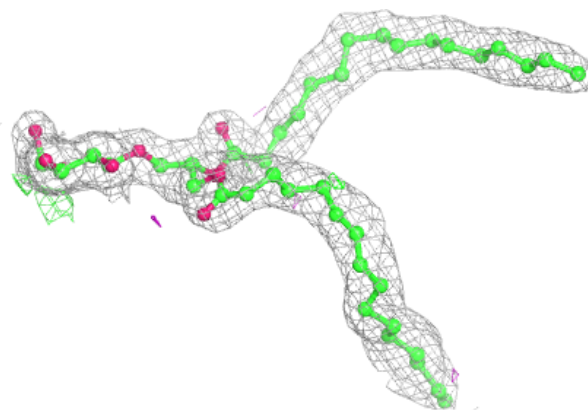
**Electron density around HTG b 623:**

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

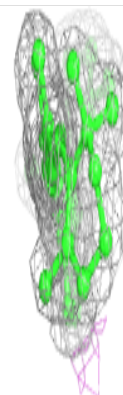
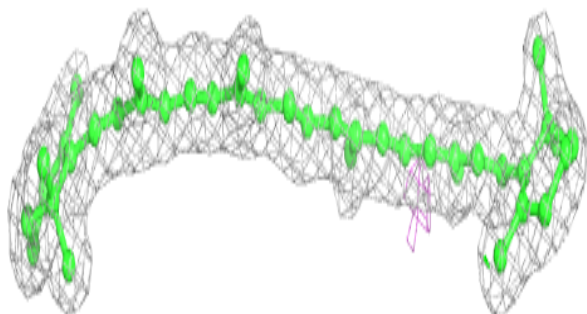
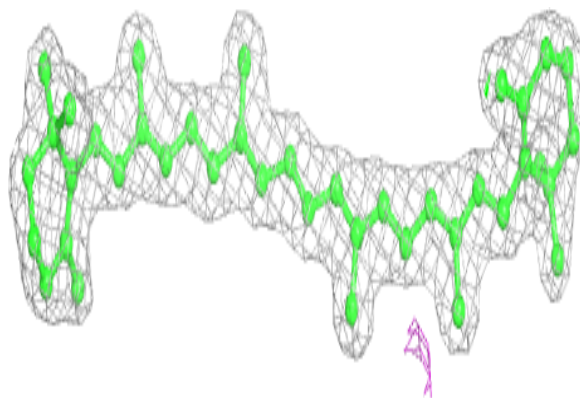


Electron density around LMG B 621:

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

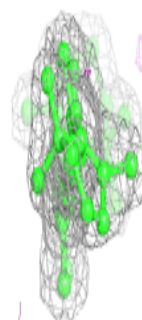
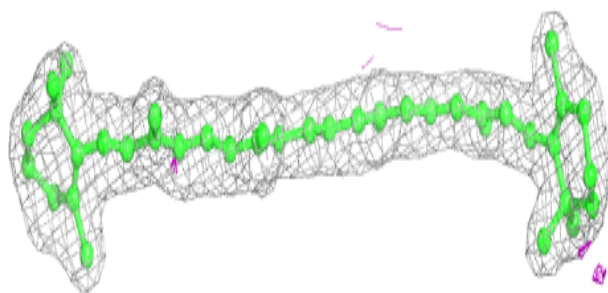
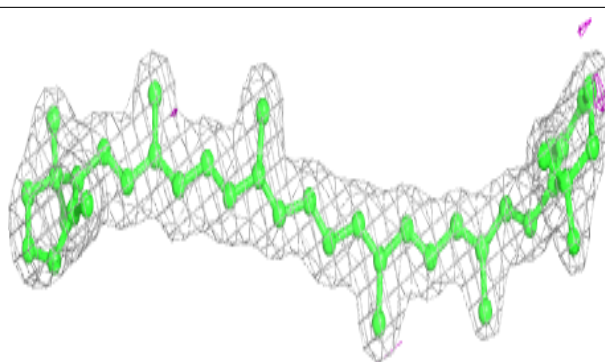
**Electron density around BCR b 620:**

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

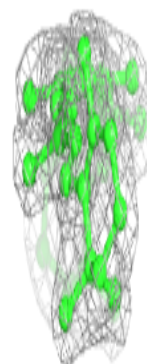
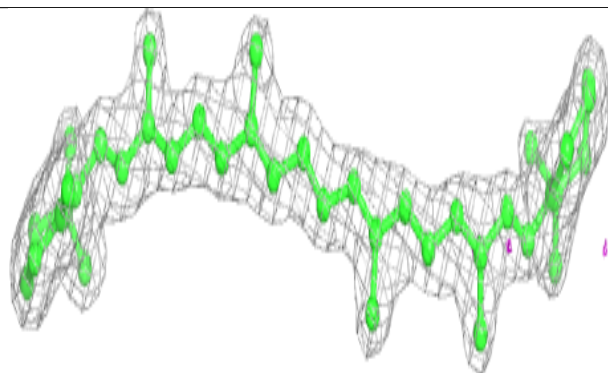
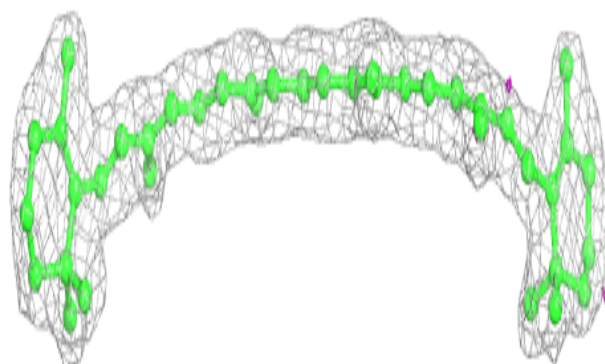


Electron density around BCR c 515:

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

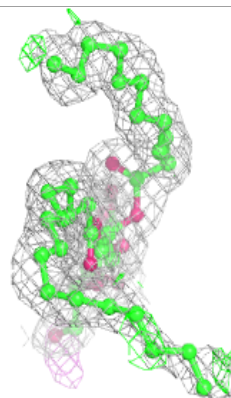
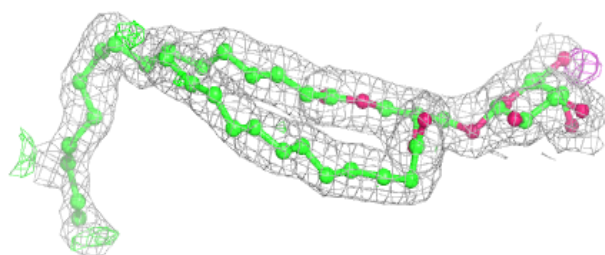
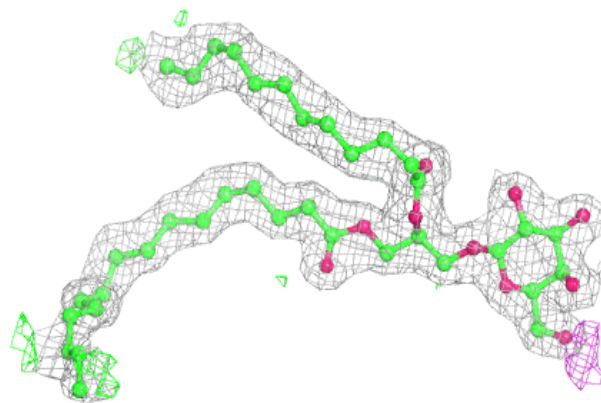
**Electron density around BCR c 527:**

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

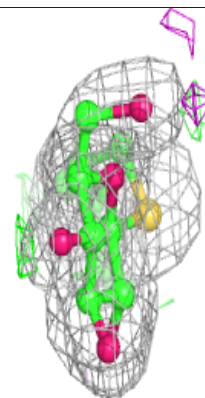
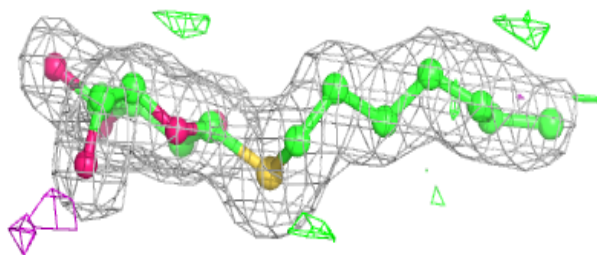
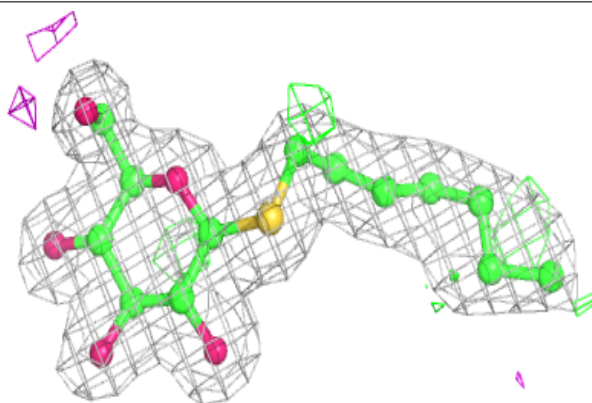


Electron density around LMG J 101:

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

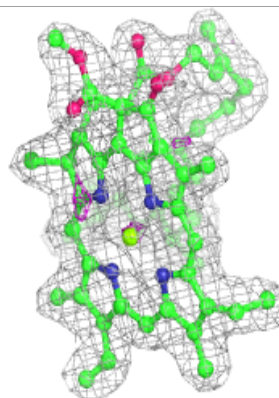
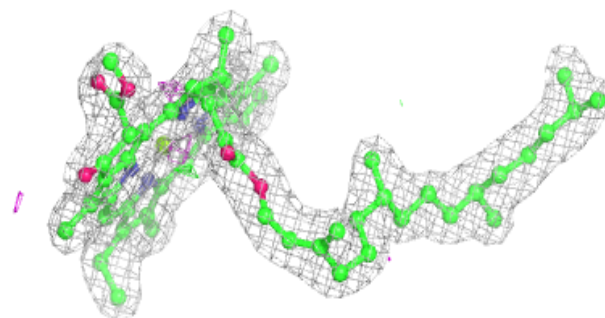
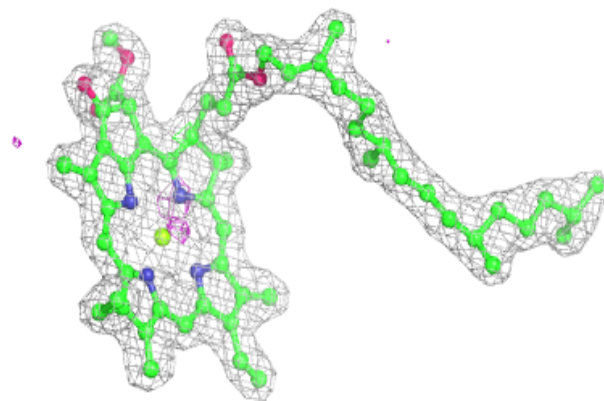
**Electron density around HTG o 301:**

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

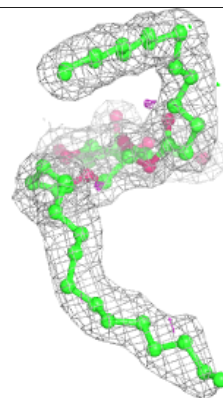
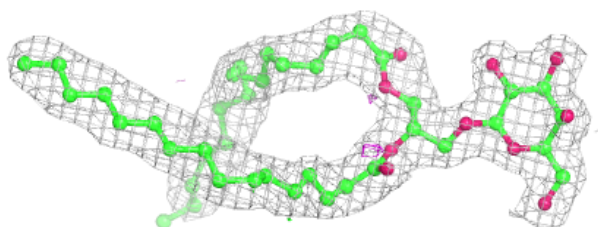
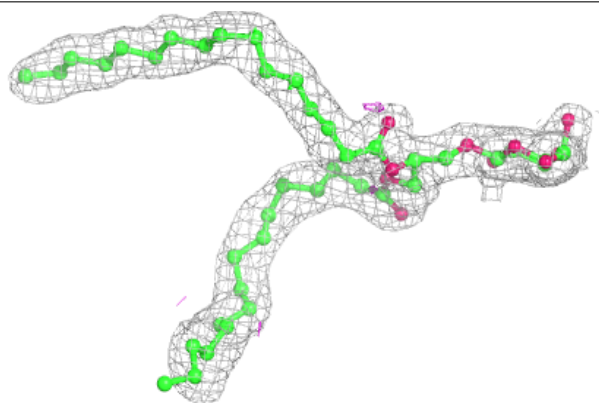


Electron density around CLA c 511:

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

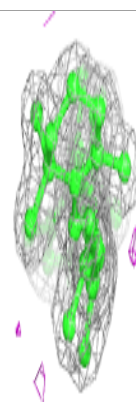
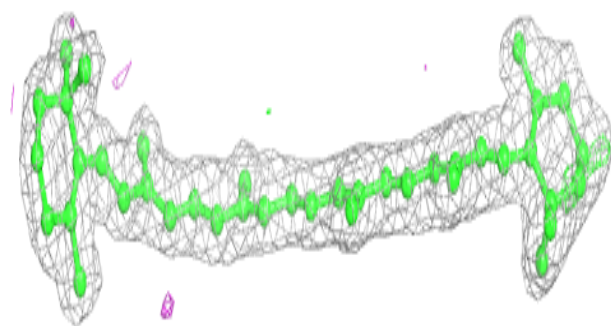
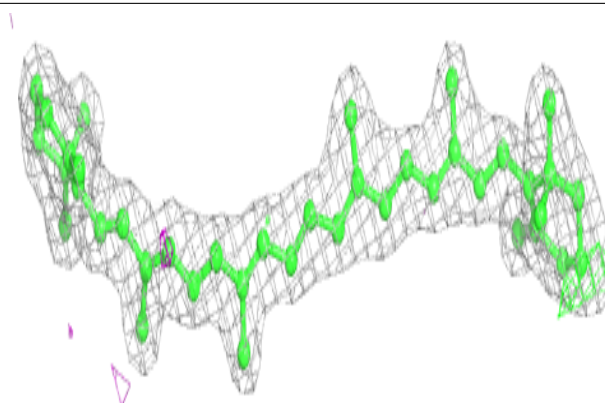
**Electron density around LMG b 621:**

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



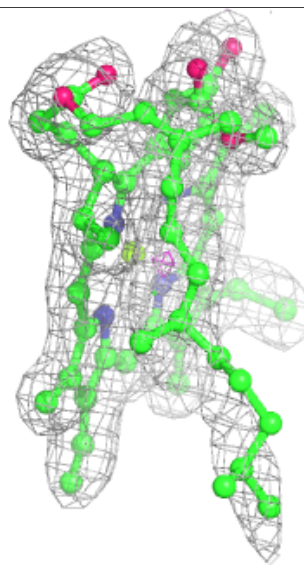
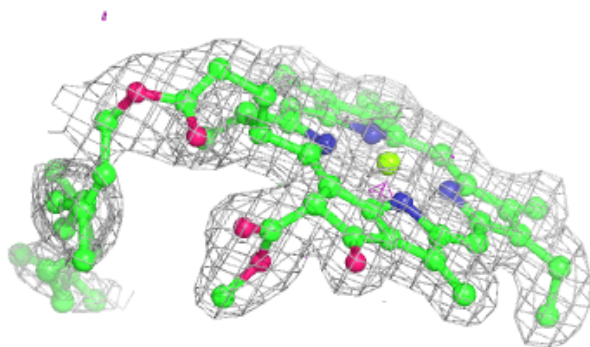
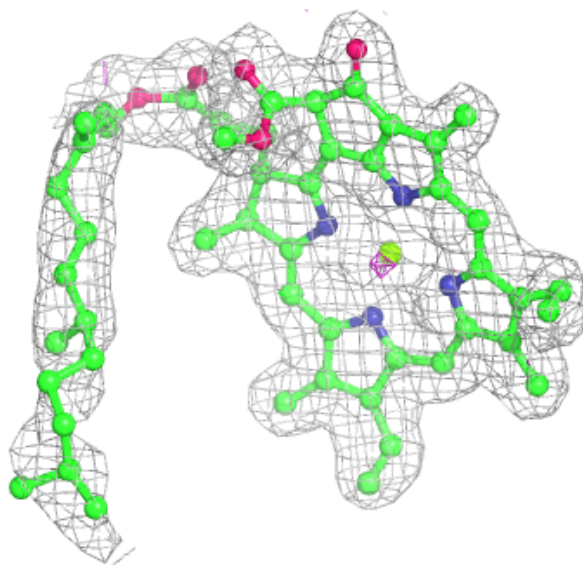
Electron density around BCR h 103:

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



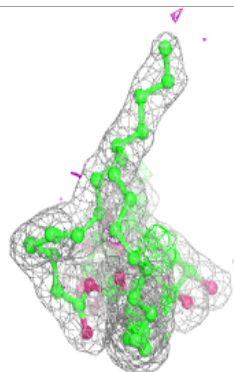
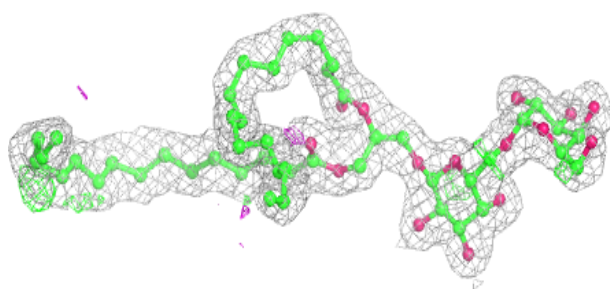
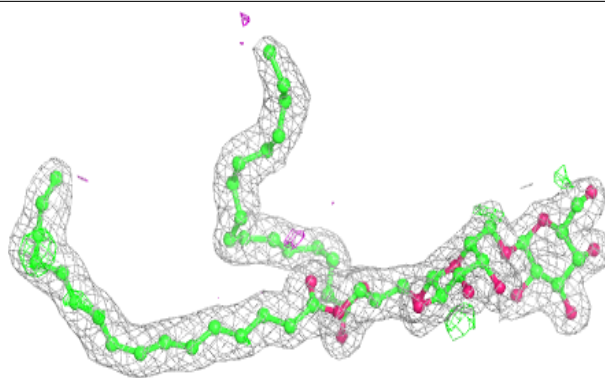
Electron density around CLA B 617:

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

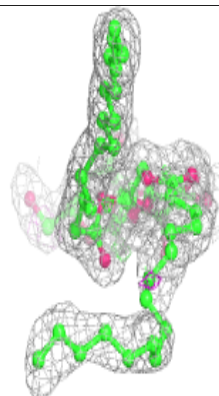
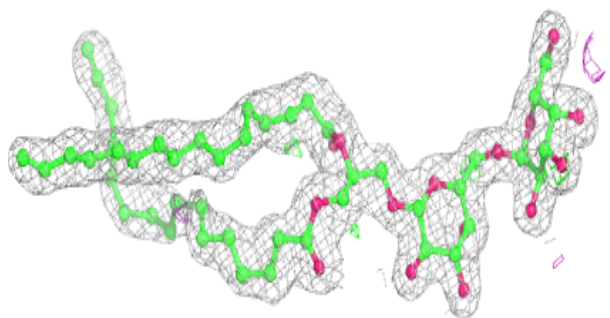
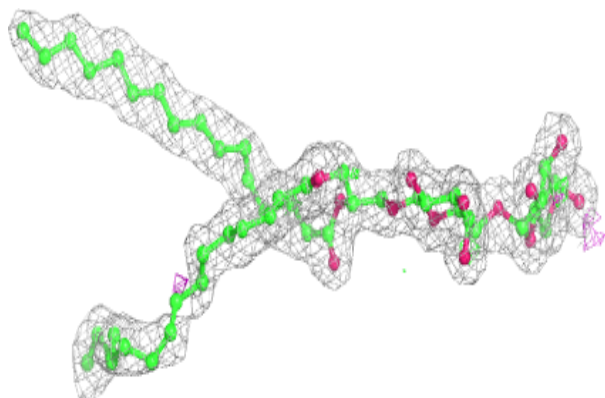


Electron density around DGD H 103:

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

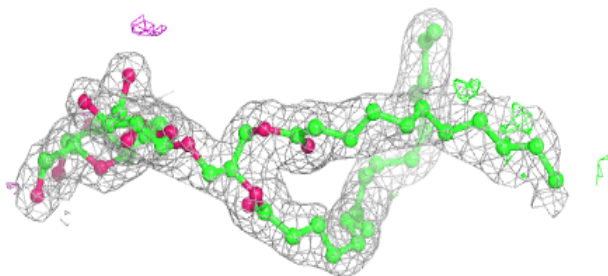
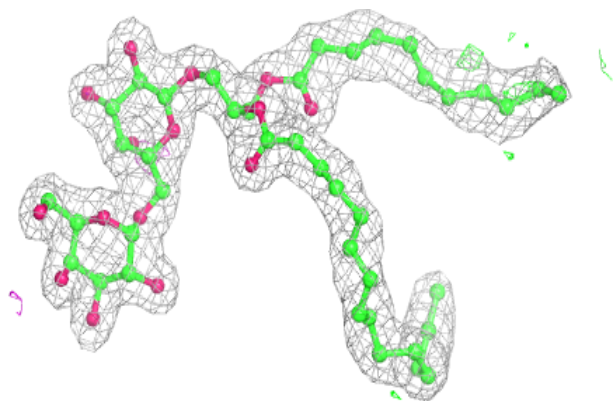
**Electron density around DGD c 516:**

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

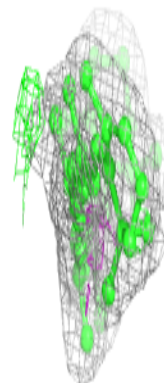
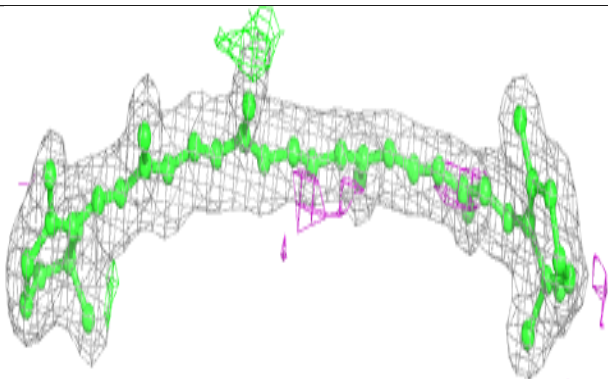
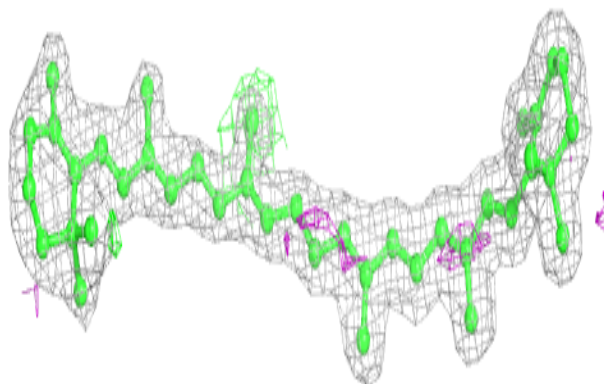


Electron density around DGD c 517:

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

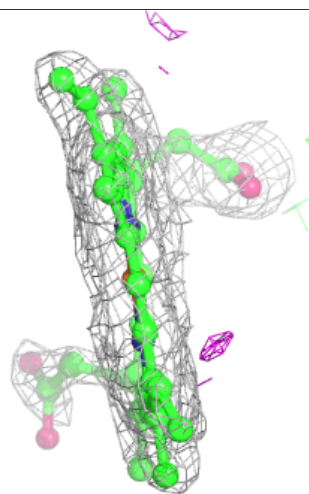
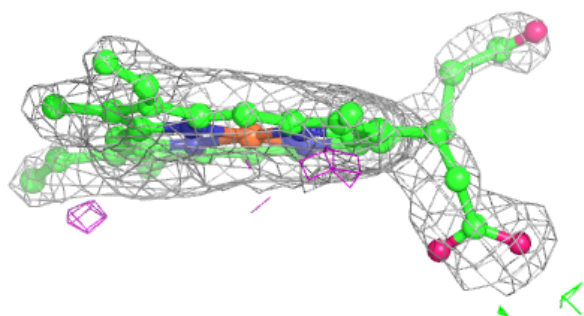
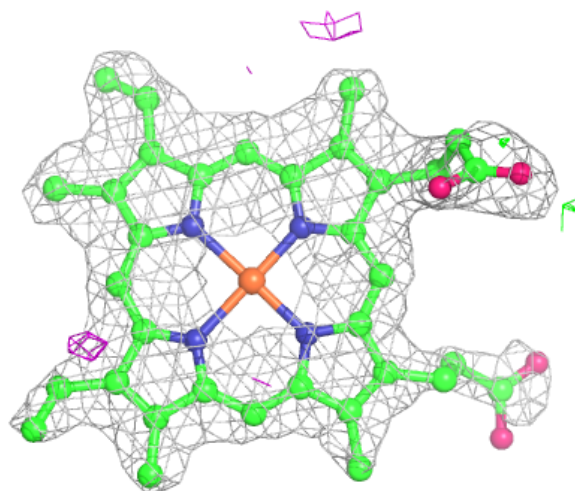
**Electron density around BCR t 102:**

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



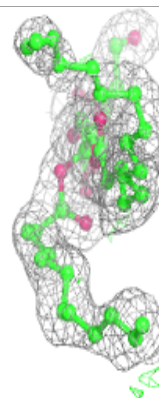
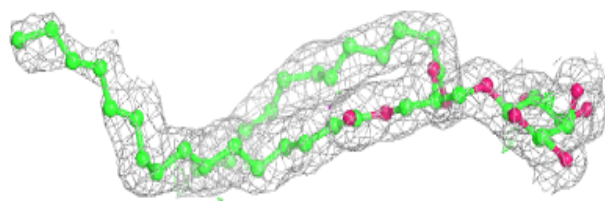
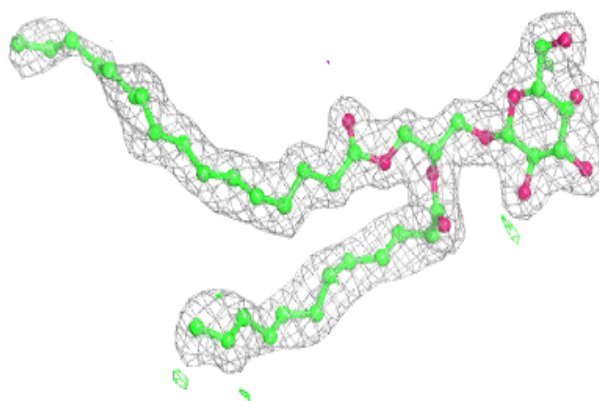
Electron density around HEM e 107:

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

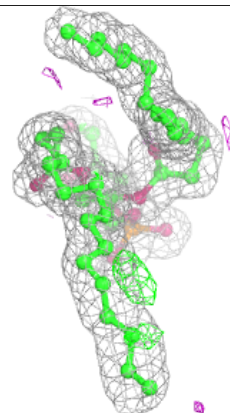
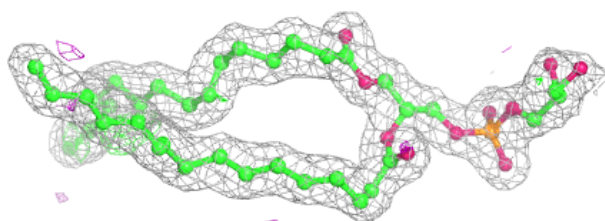
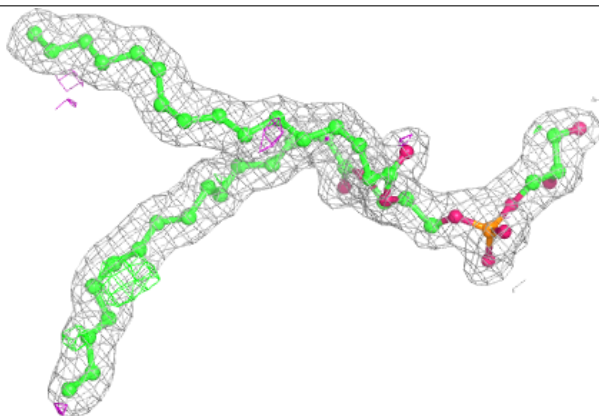


Electron density around LMG j 101:

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

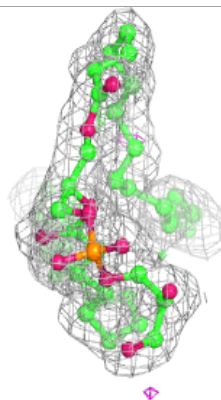
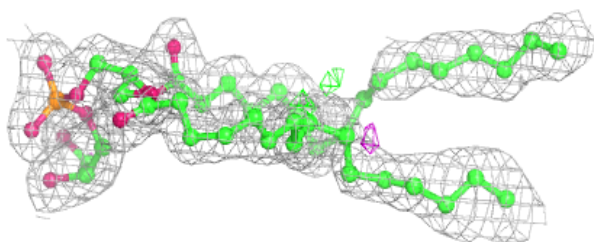
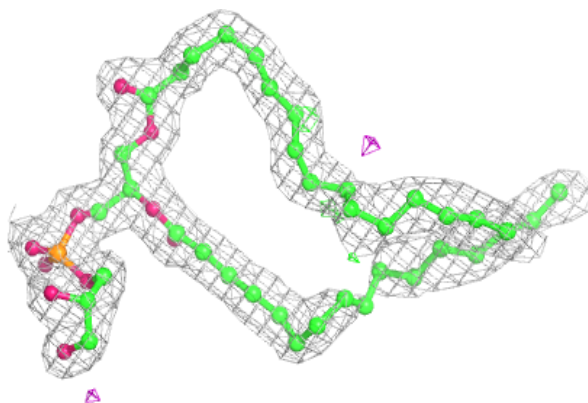
**Electron density around LHG d 410:**

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

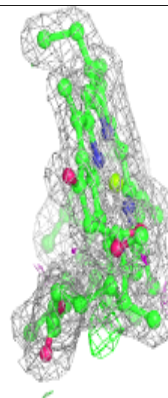
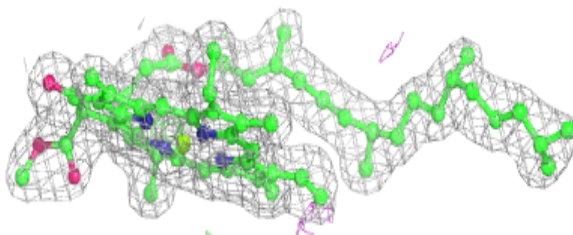
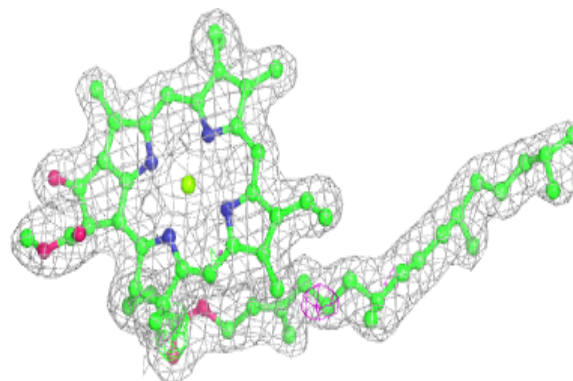


Electron density around LHG d 411:

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

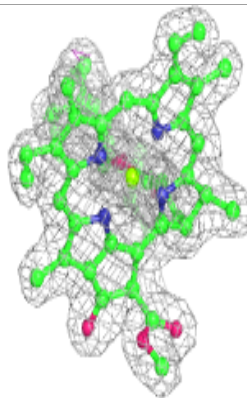
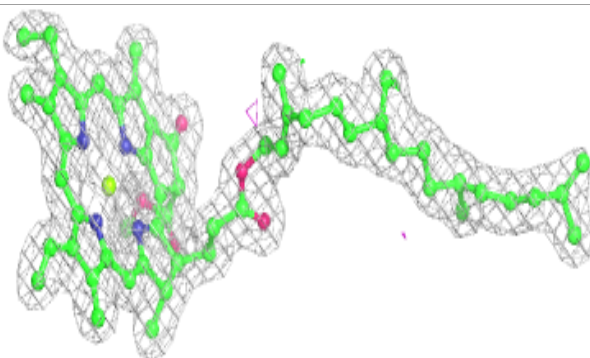
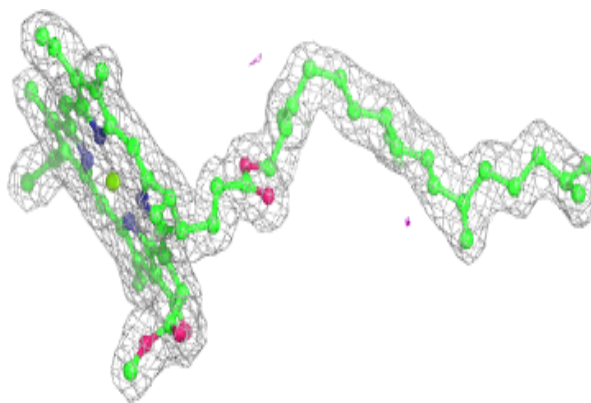
**Electron density around CLA C 501:**

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



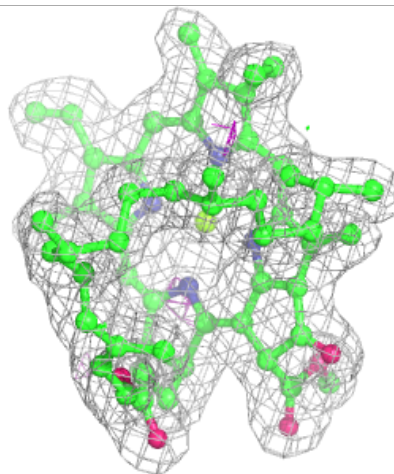
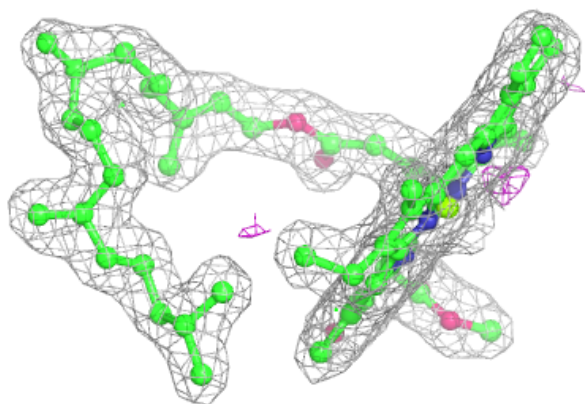
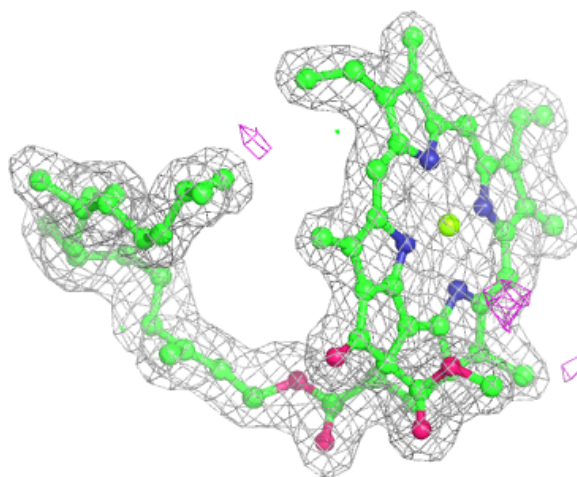
Electron density around CLA C 502:

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



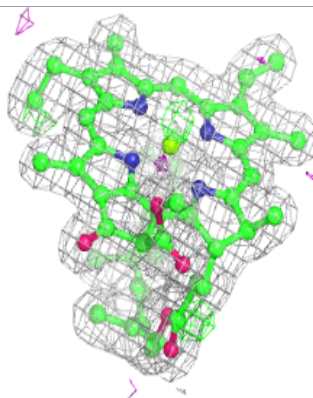
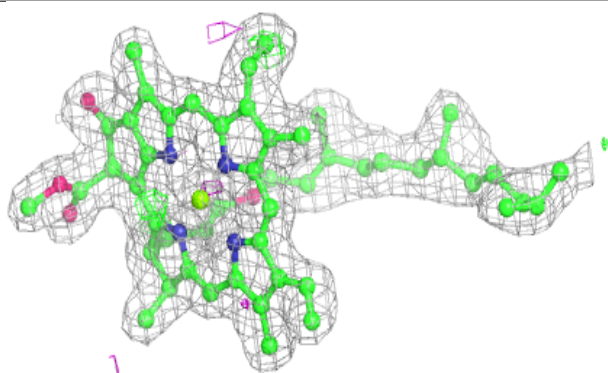
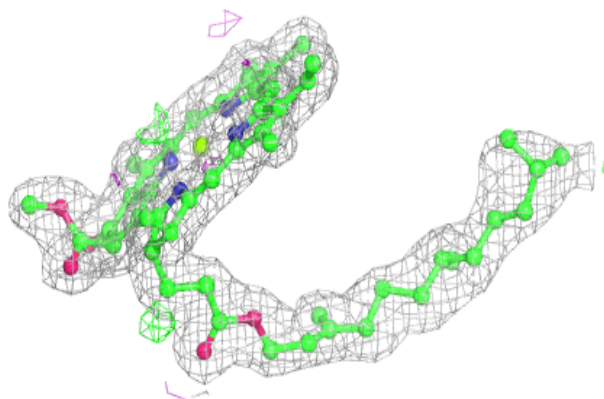
Electron density around CLA C 503:

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

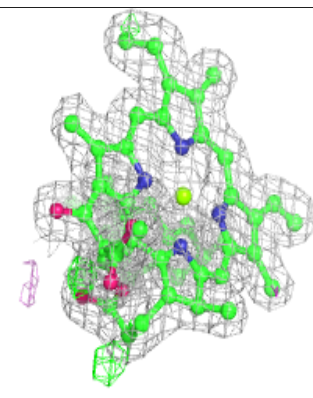
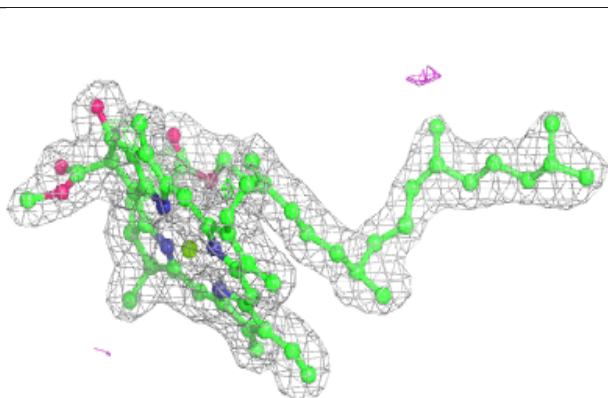
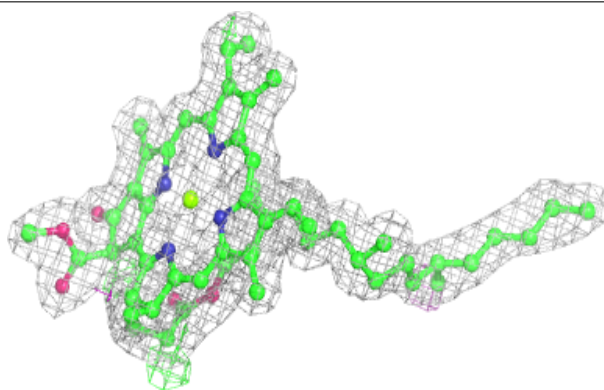


Electron density around CLA C 504:

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

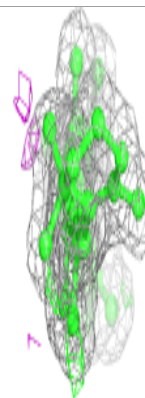
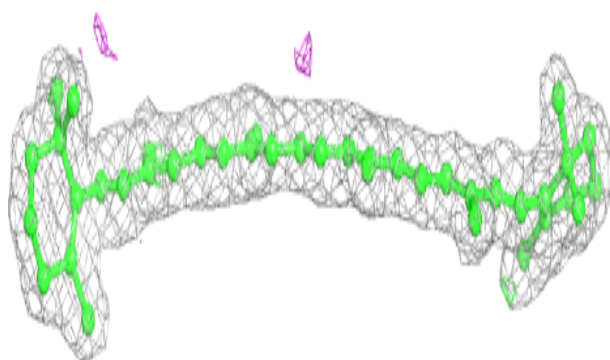
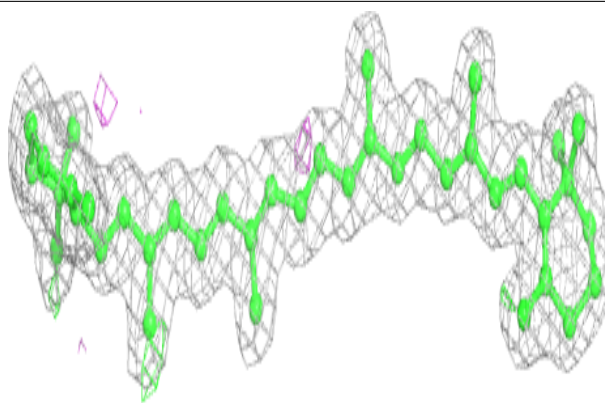
**Electron density around CLA C 505:**

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



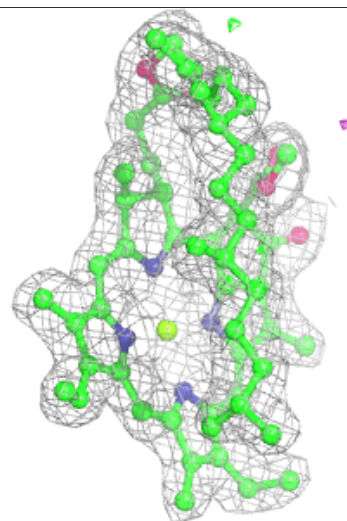
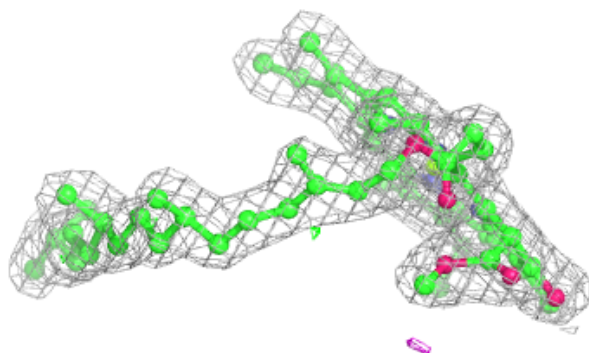
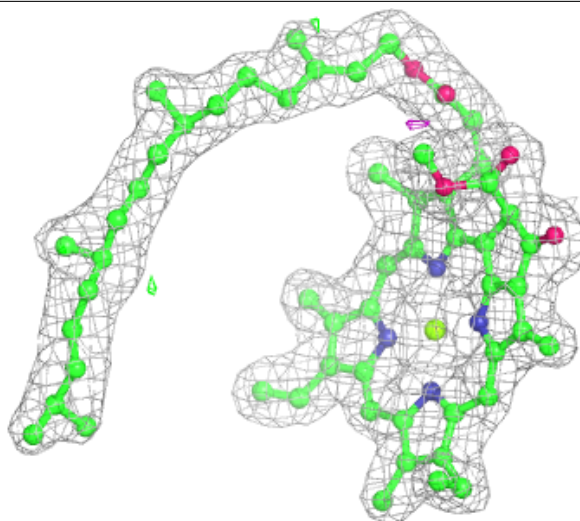
Electron density around BCR b 618:

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



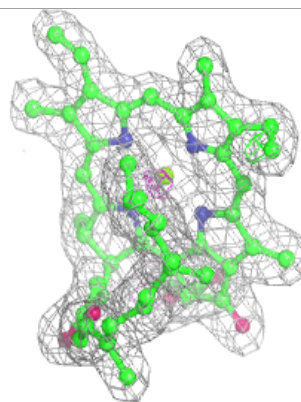
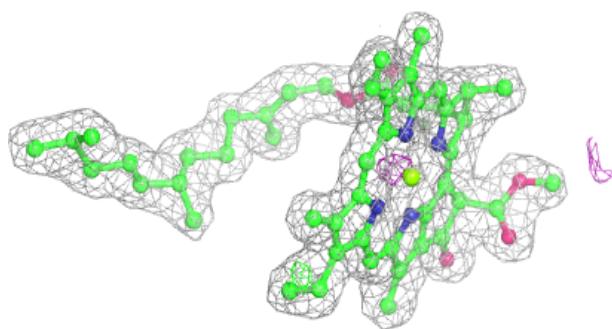
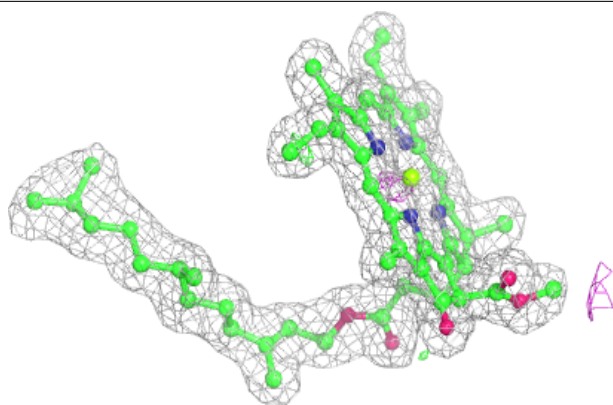
Electron density around CLA C 507:

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



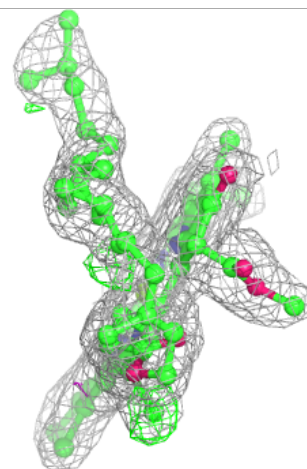
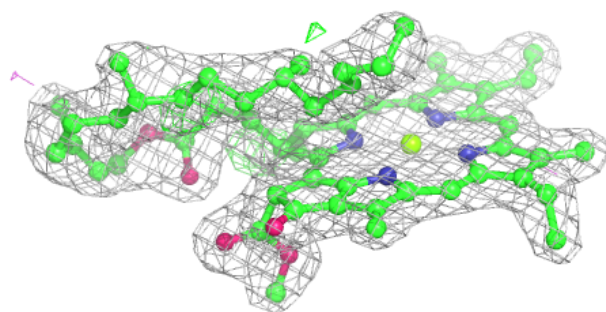
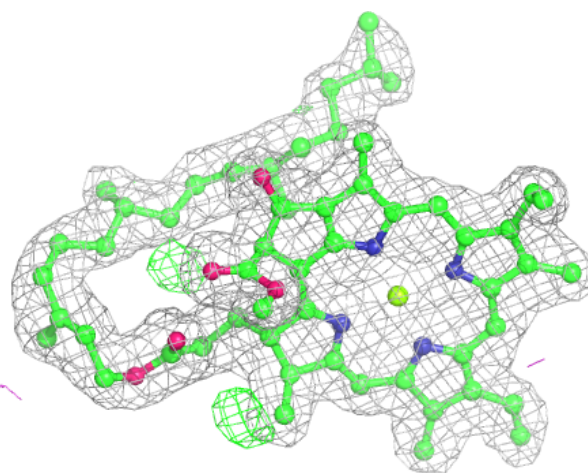
Electron density around CLA C 508:

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



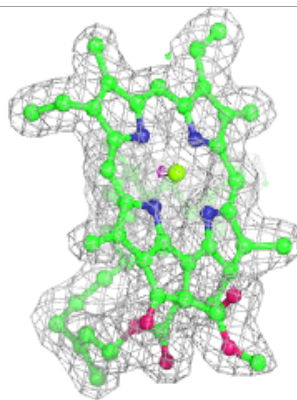
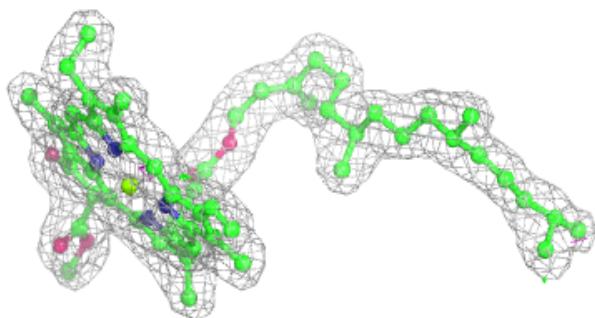
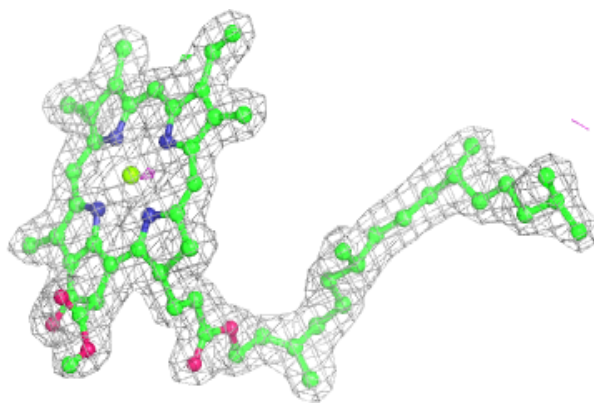
Electron density around CLA C 509:

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

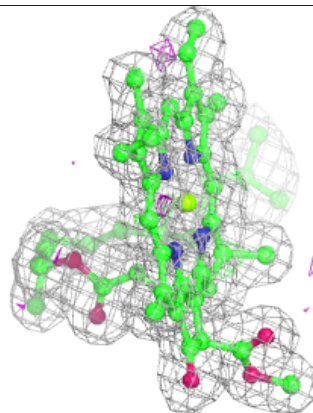
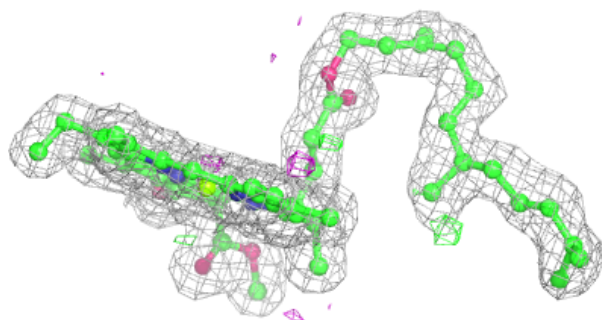
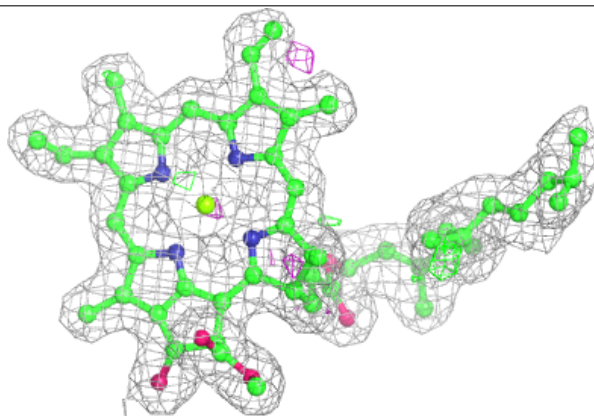


Electron density around CLA C 511:

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

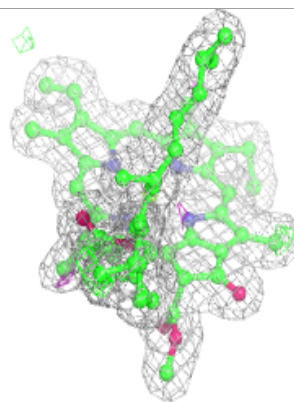
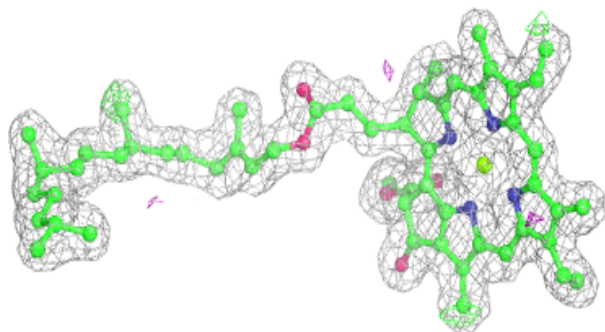
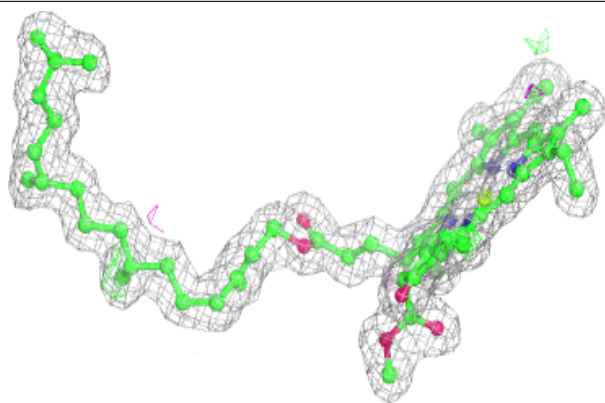
**Electron density around CLA A 607:**

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

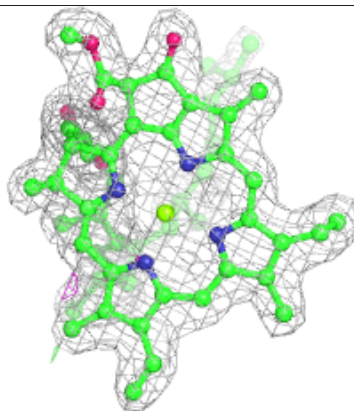
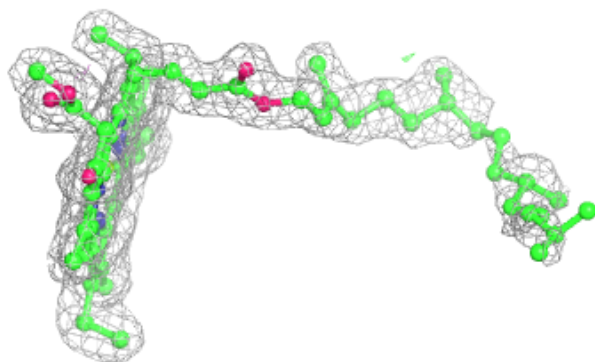
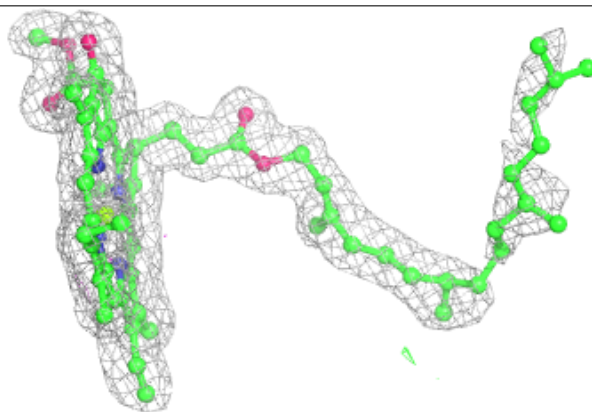


Electron density around CLA D 404:

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

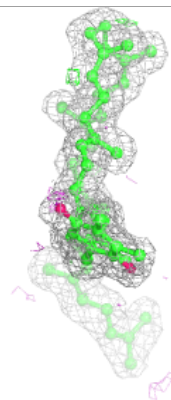
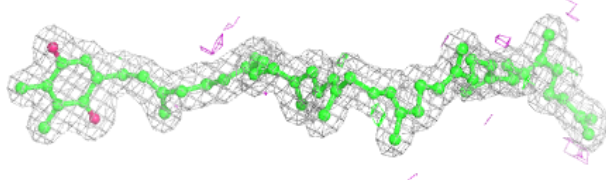
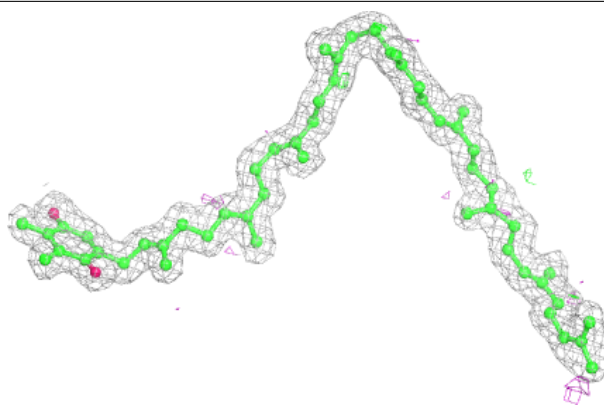
**Electron density around CLA D 405:**

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

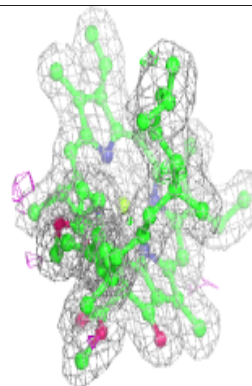
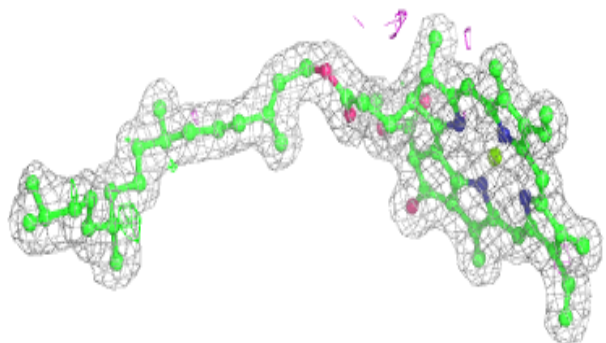
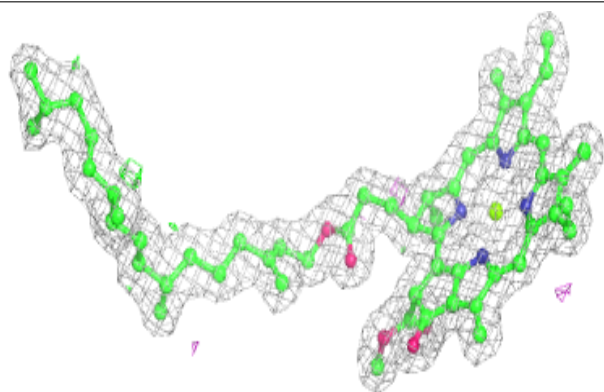


Electron density around PL9 D 407:

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

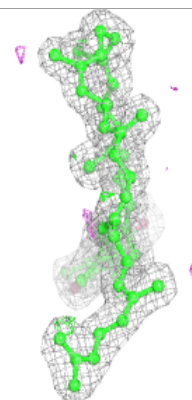
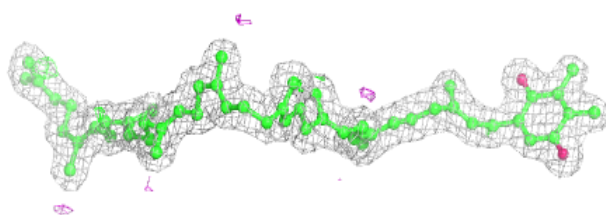
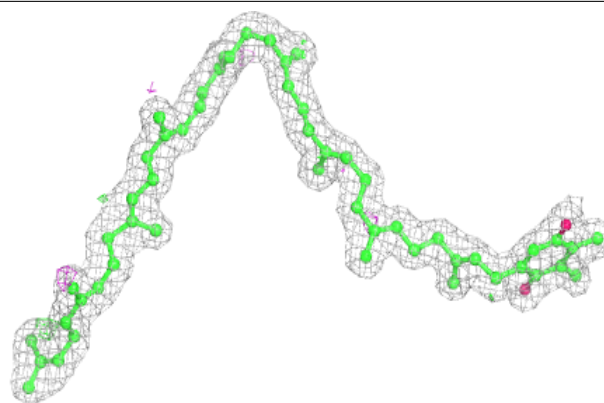
**Electron density around CLA a 407:**

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

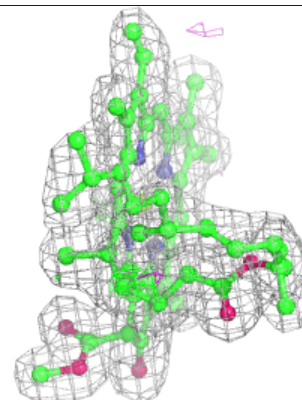
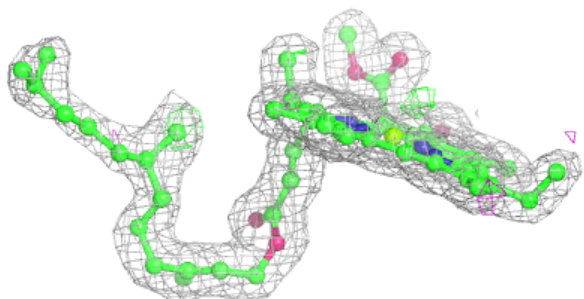
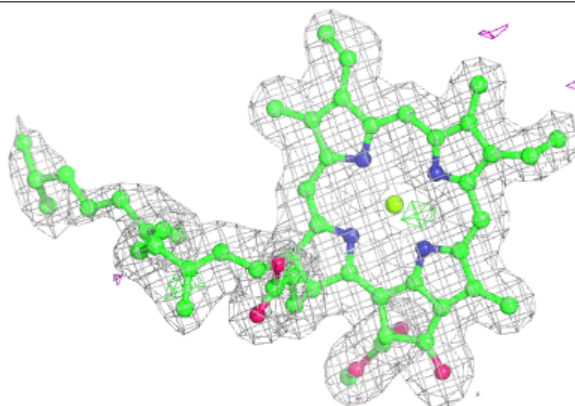


Electron density around PL9 d 407:

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

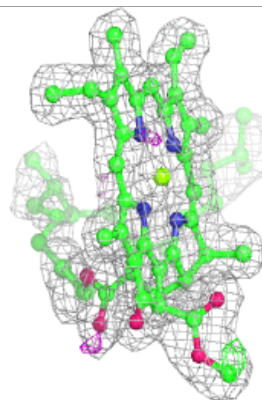
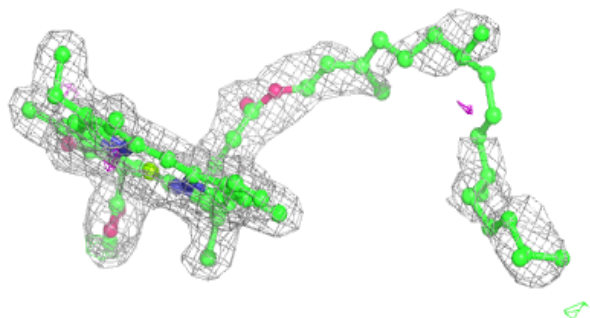
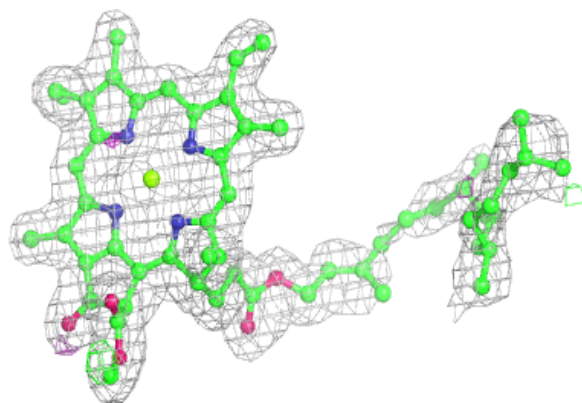
**Electron density around CLA a 408:**

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

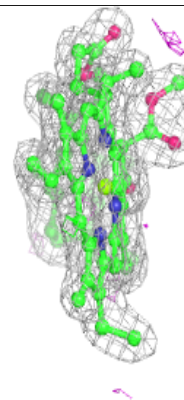
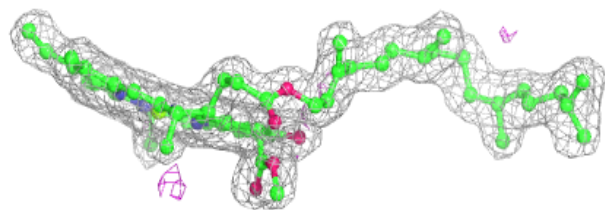
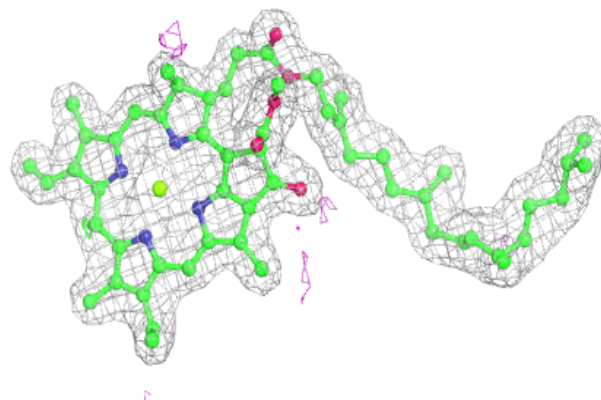


Electron density around CLA A 609:

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

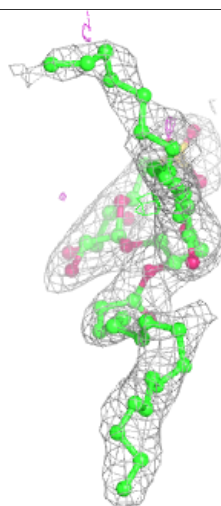
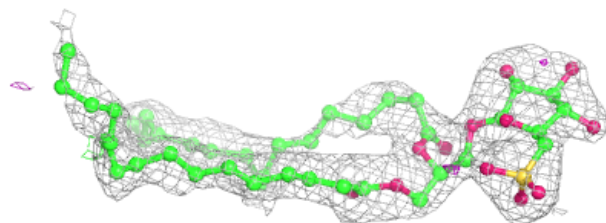
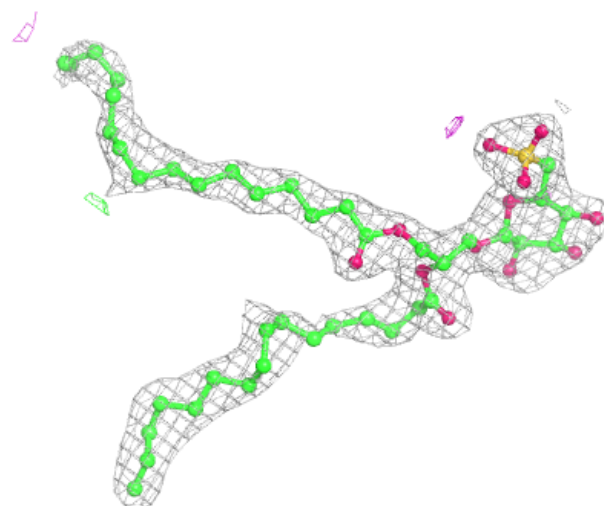
**Electron density around CLA b 603:**

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



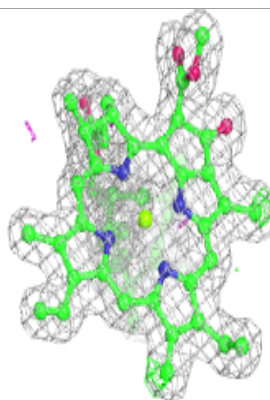
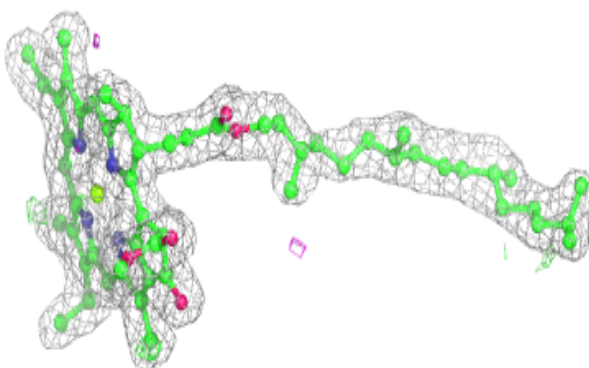
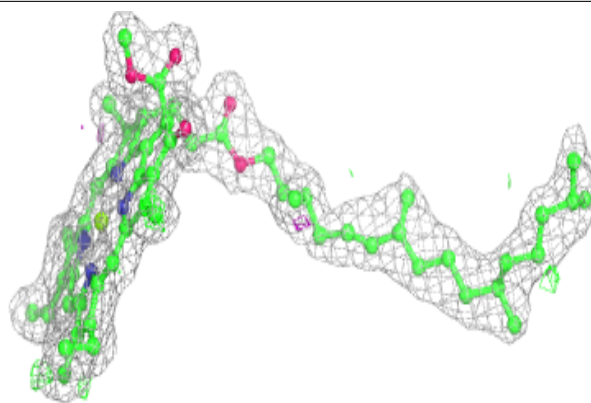
Electron density around SQD a 413:

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

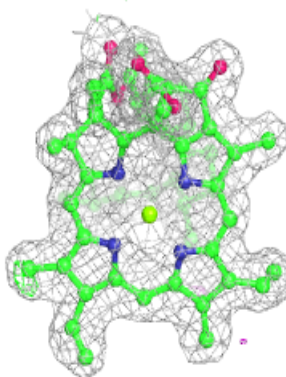
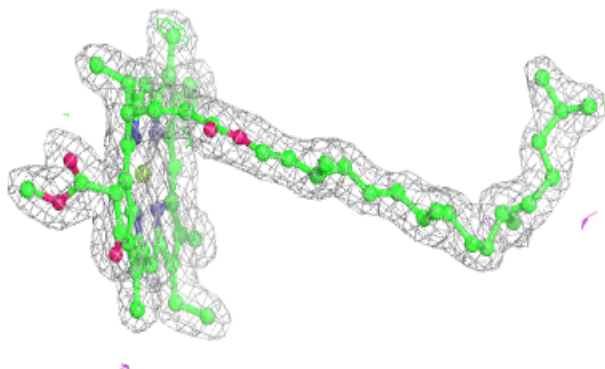
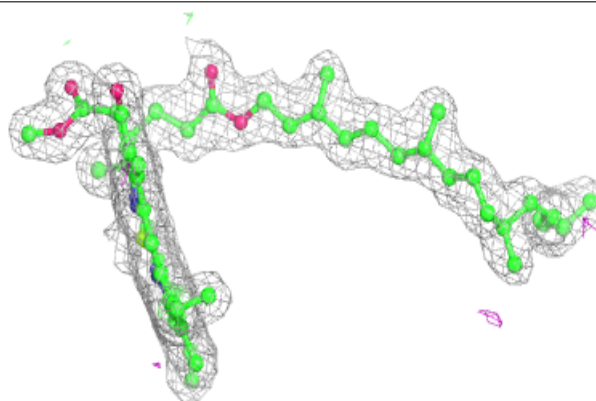


Electron density around CLA b 605:

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

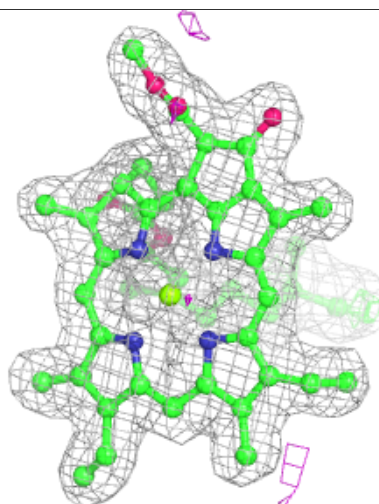
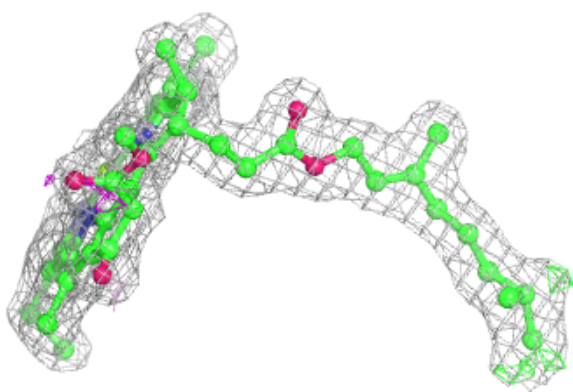
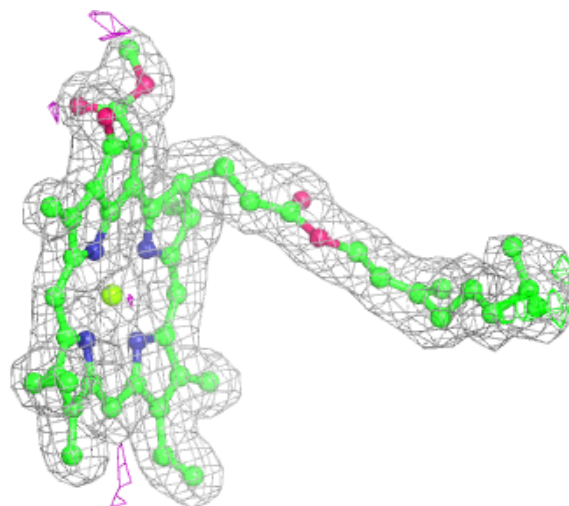
**Electron density around CLA b 606:**

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



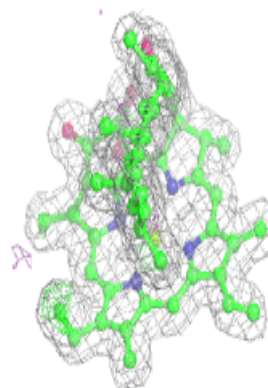
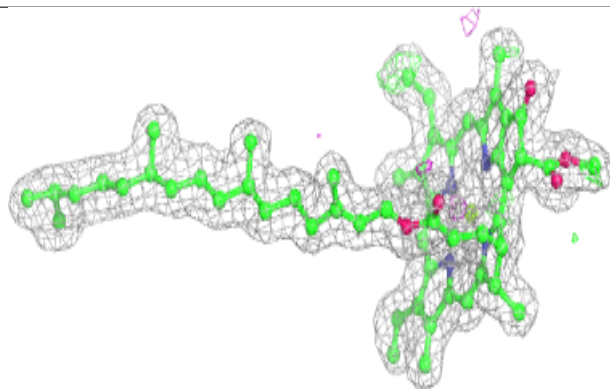
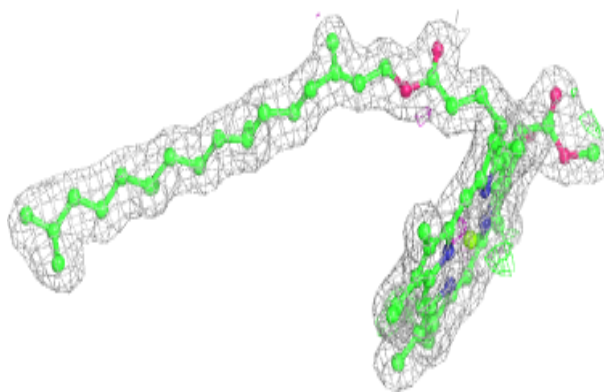
Electron density around CLA b 607:

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

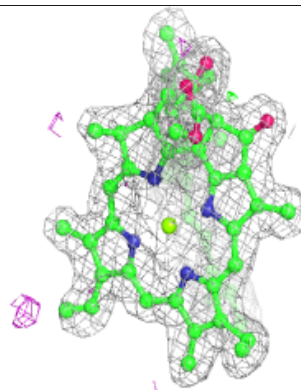
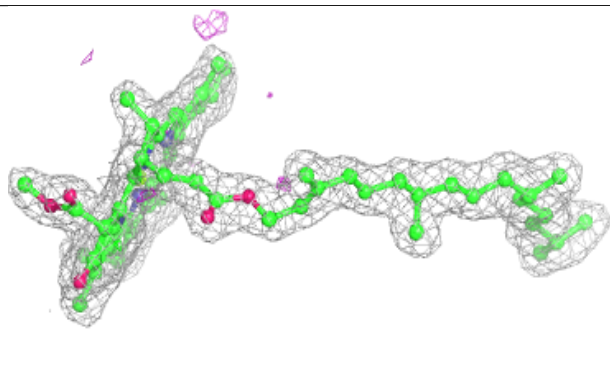
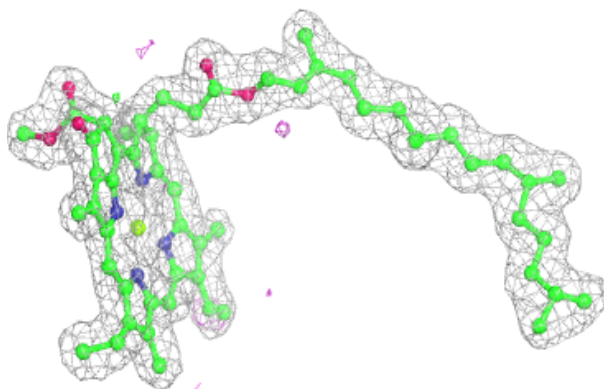


Electron density around CLA b 608:

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

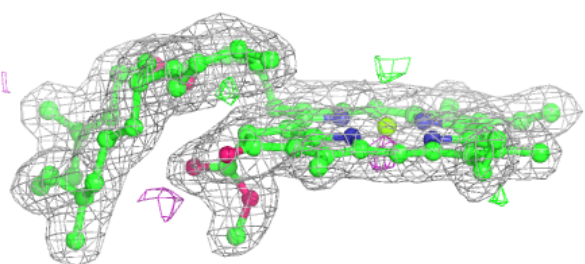
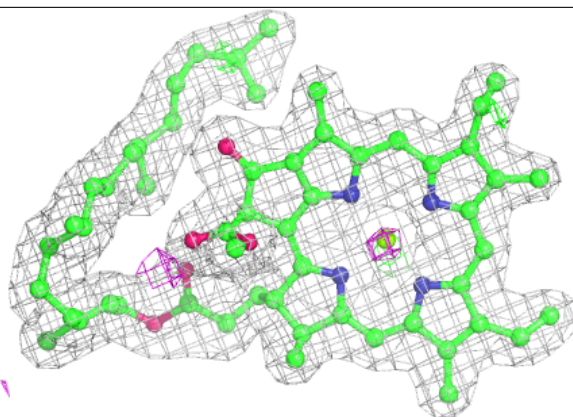
**Electron density around CLA b 610:**

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

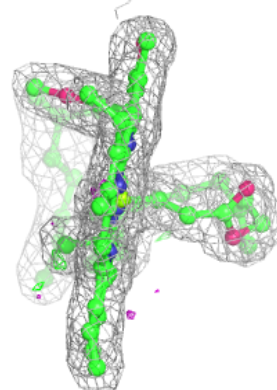
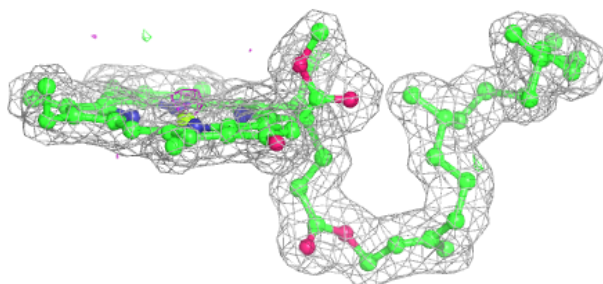
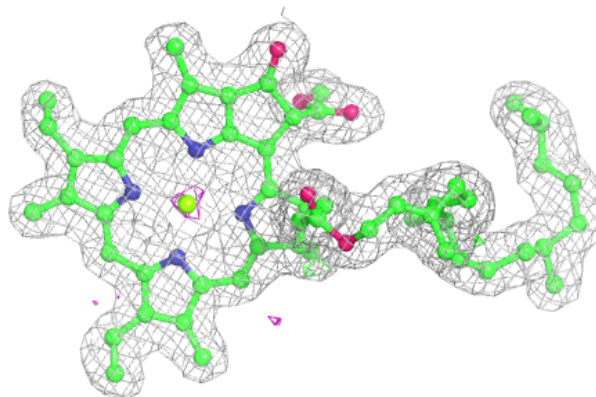


Electron density around CLA b 611:

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

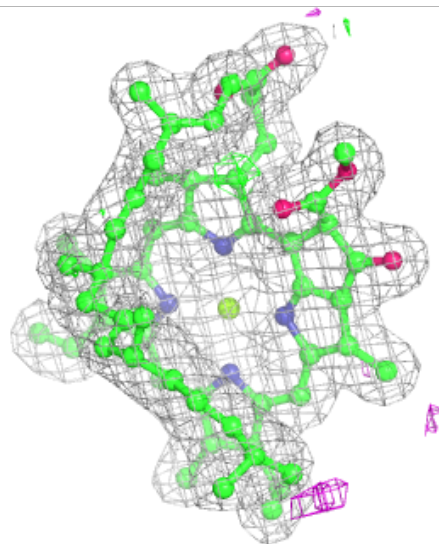
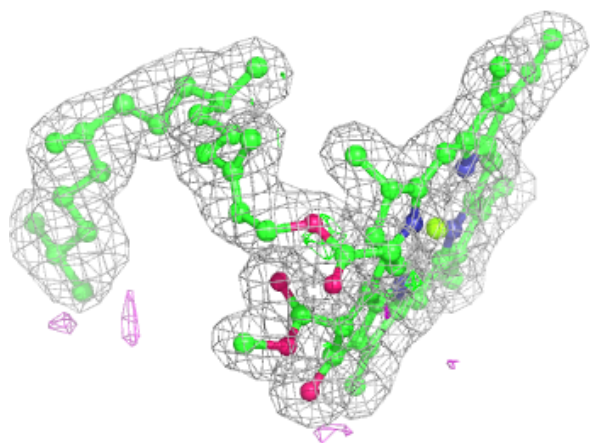
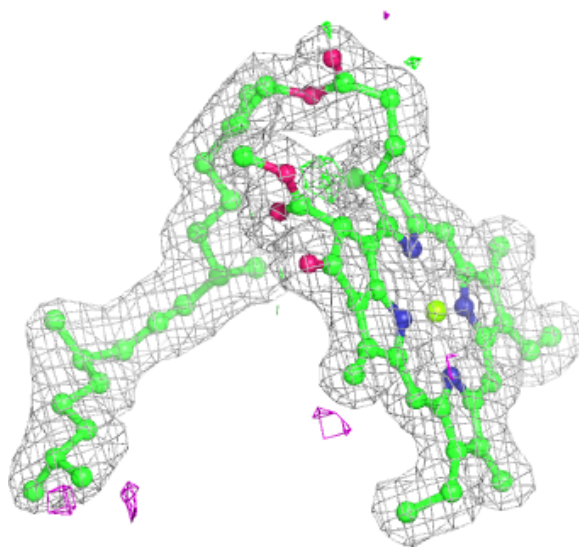
**Electron density around CLA b 613:**

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



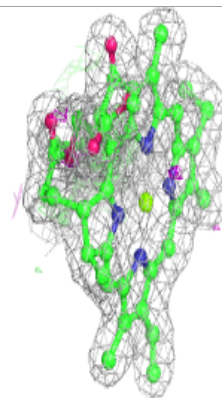
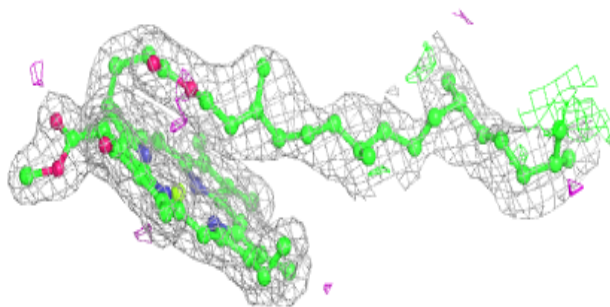
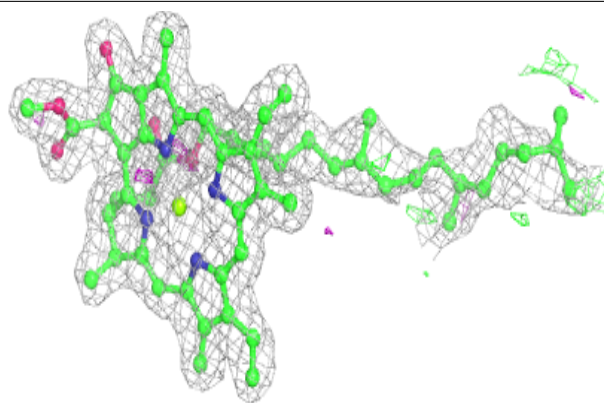
Electron density around CLA b 614:

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



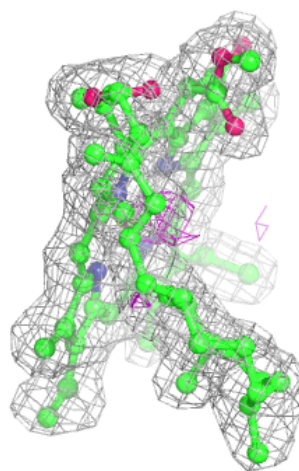
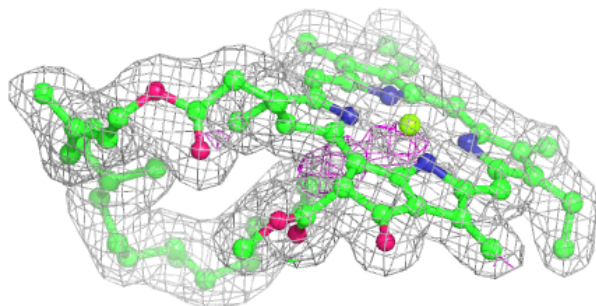
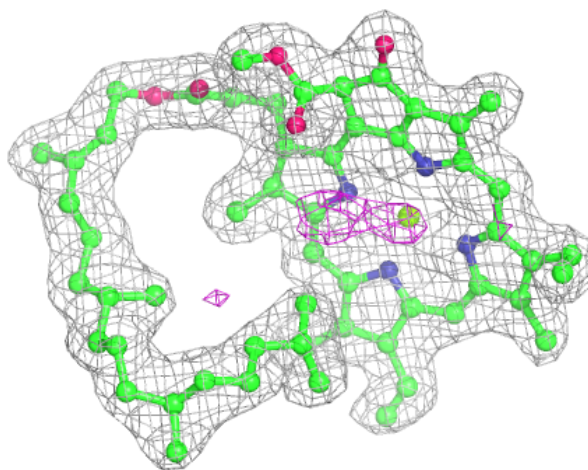
Electron density around CLA b 615:

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



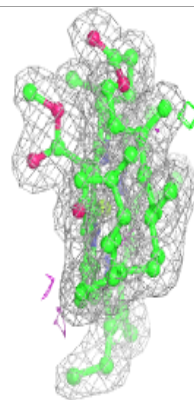
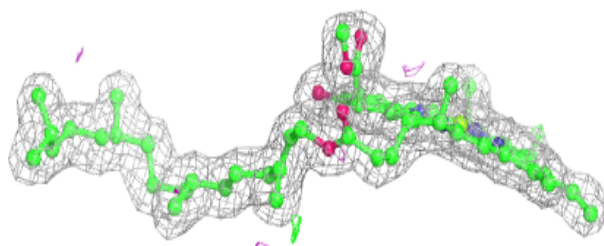
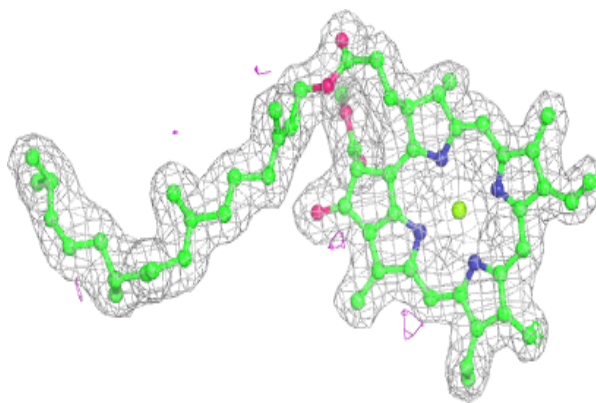
Electron density around CLA b 616:

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

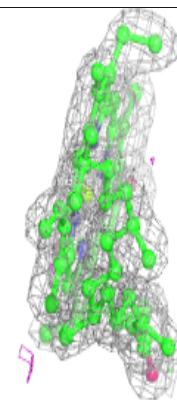
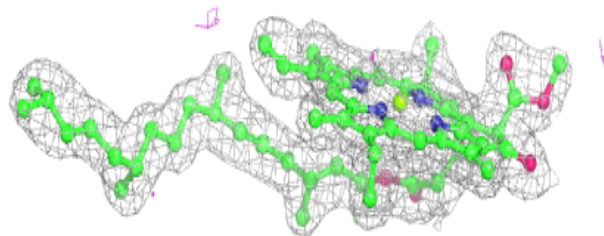
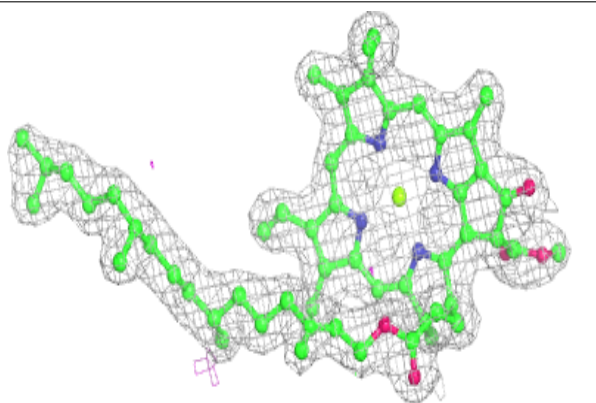


Electron density around CLA B 603:

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

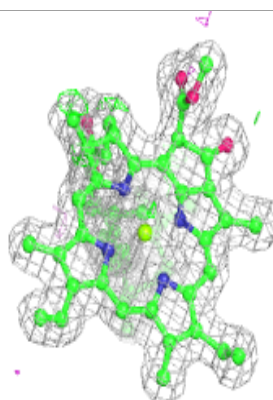
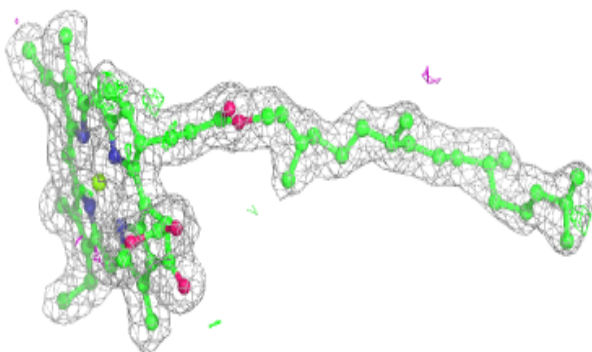
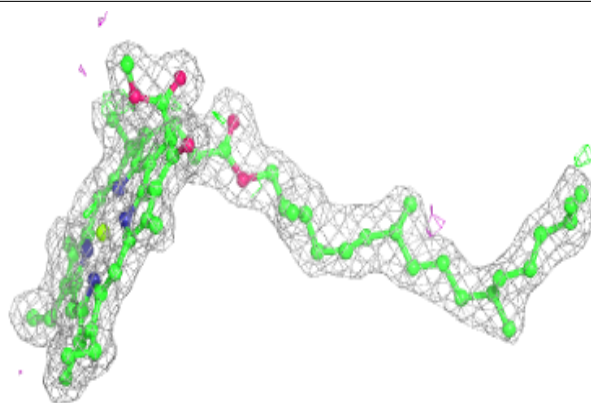
**Electron density around CLA c 501:**

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

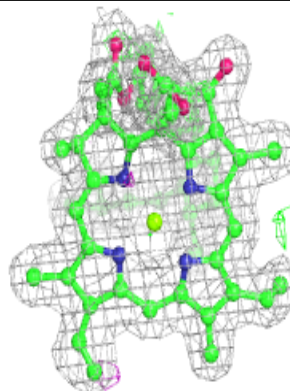
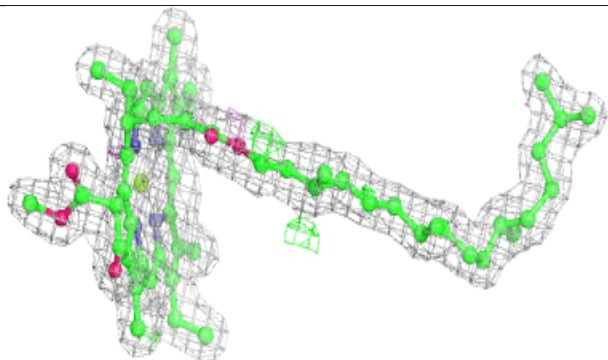
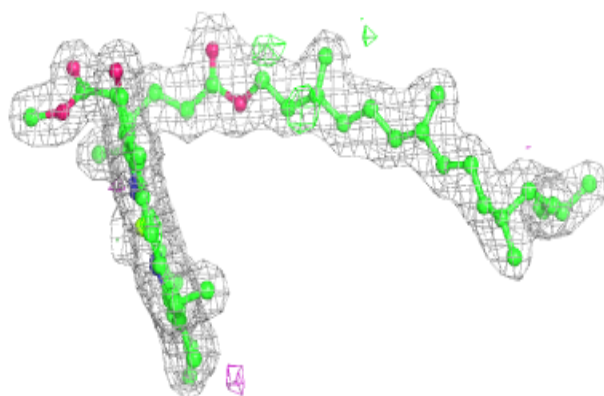


Electron density around CLA B 605:

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

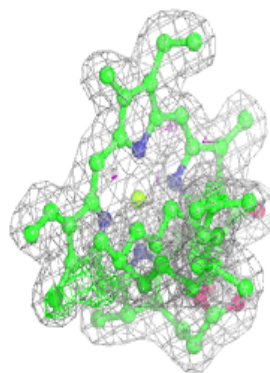
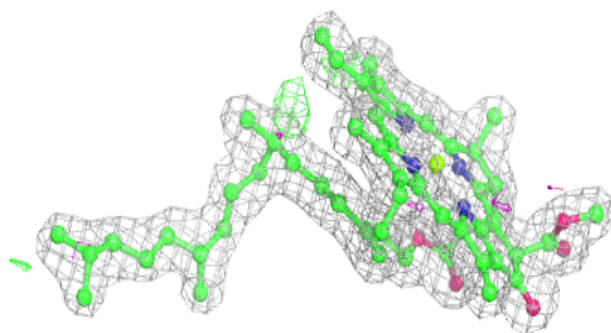
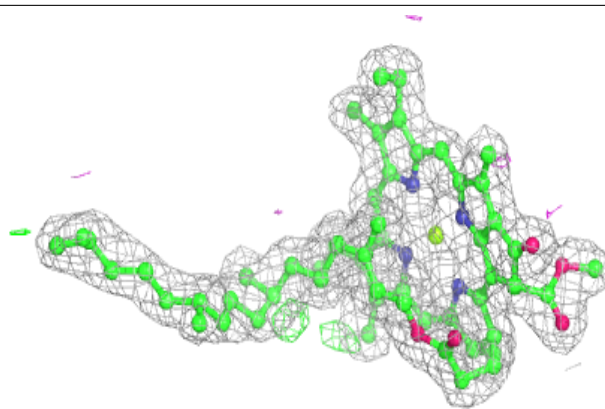
**Electron density around CLA B 606:**

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



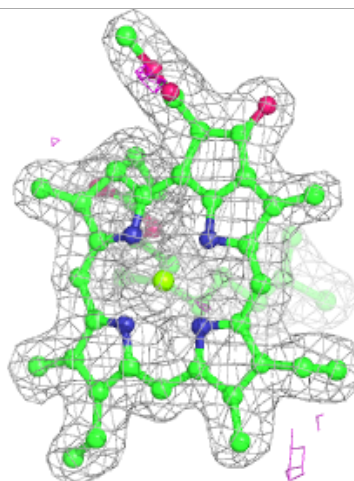
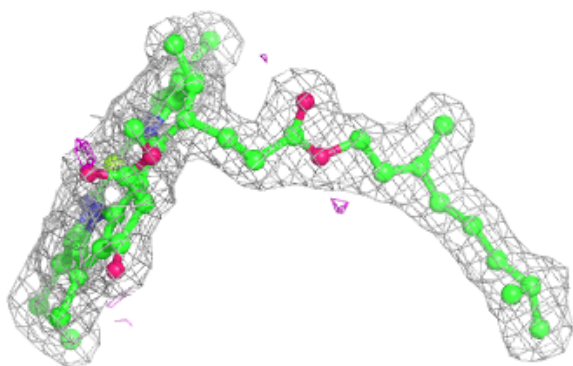
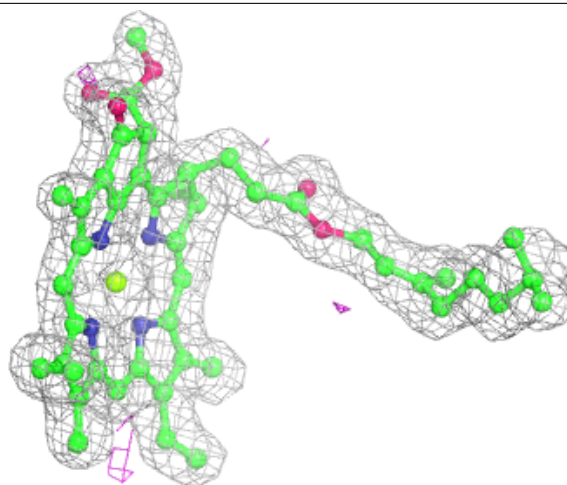
Electron density around CLA c 505:

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



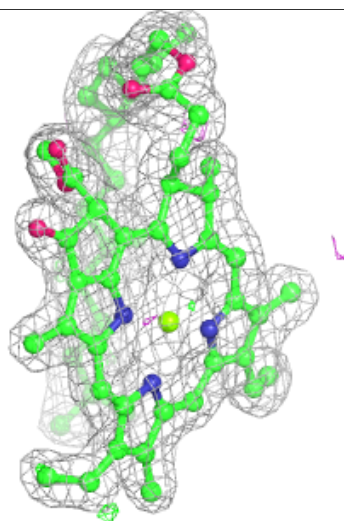
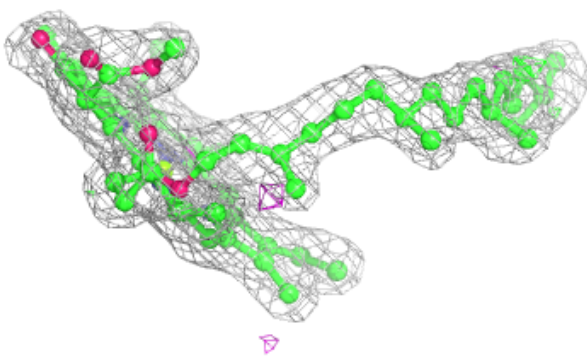
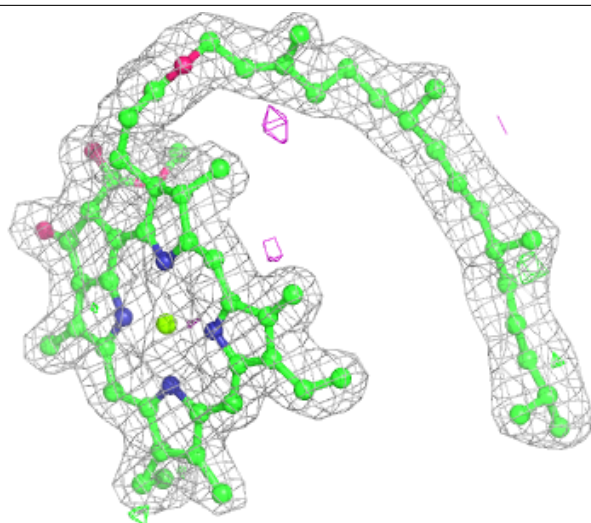
Electron density around CLA B 607:

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



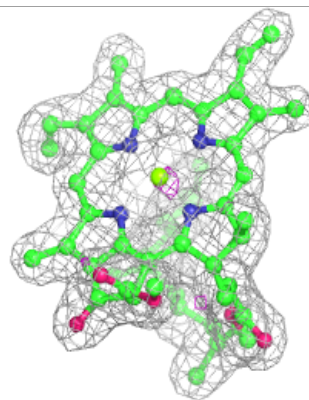
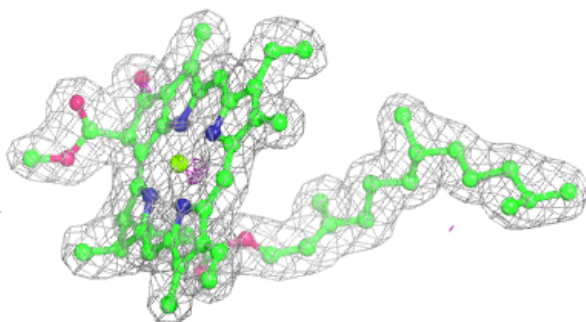
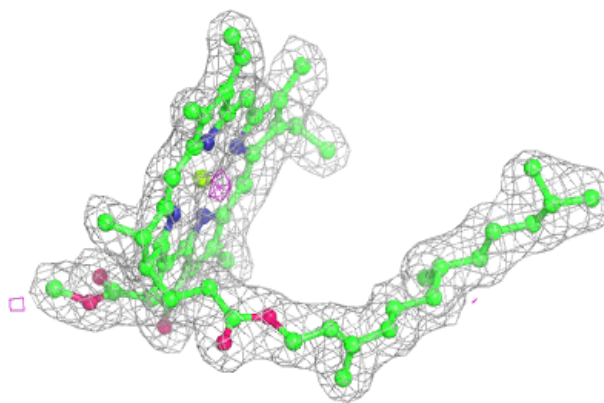
Electron density around CLA c 507:

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



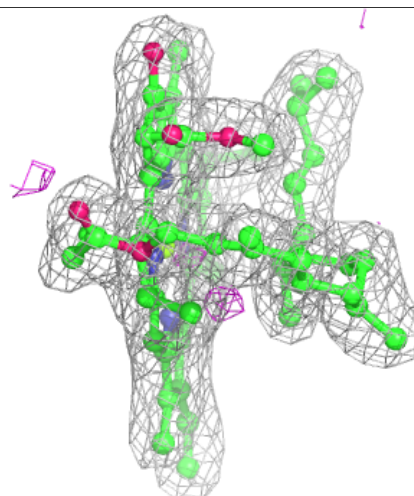
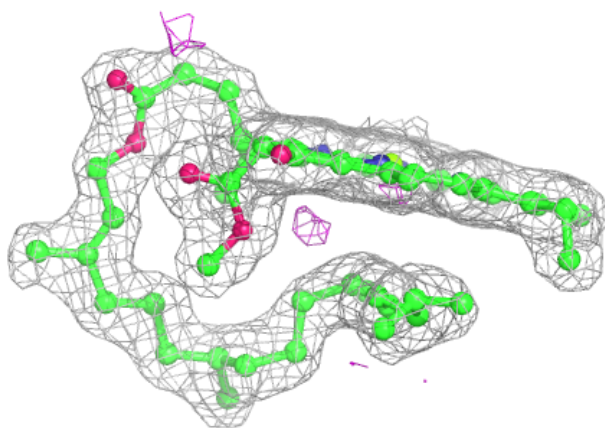
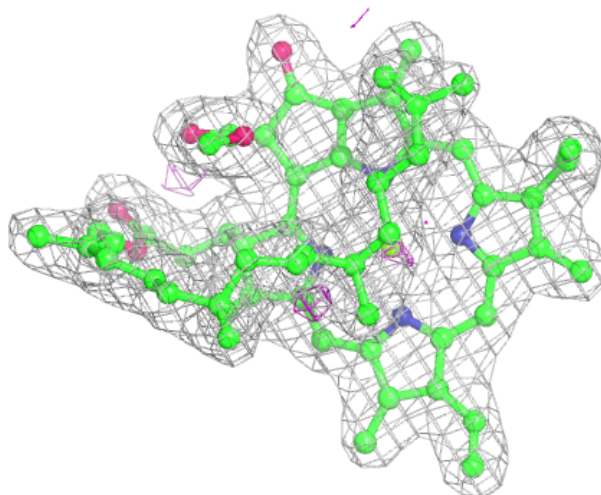
Electron density around CLA c 508:

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



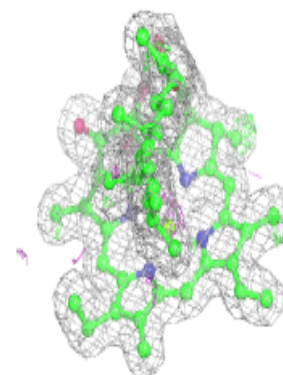
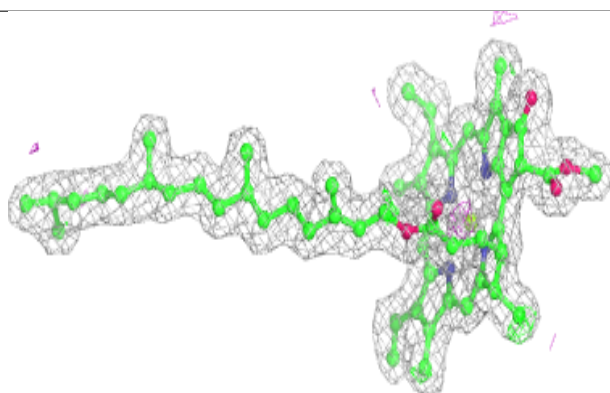
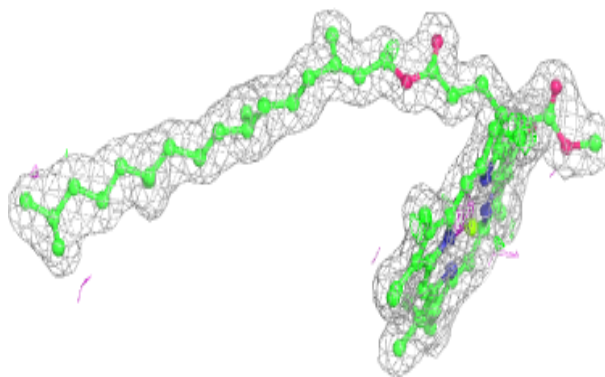
Electron density around CLA c 510:

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

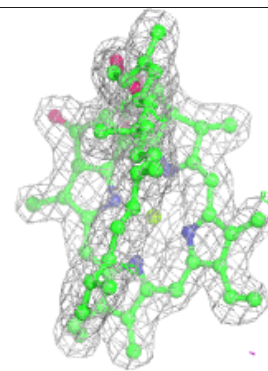
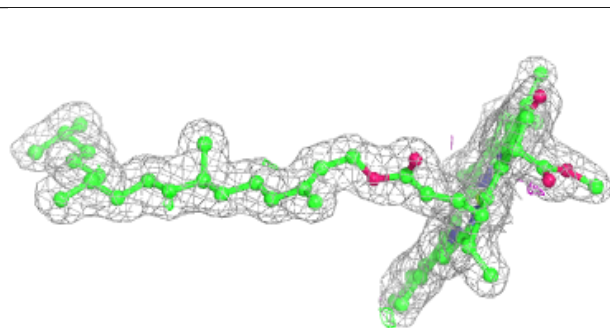
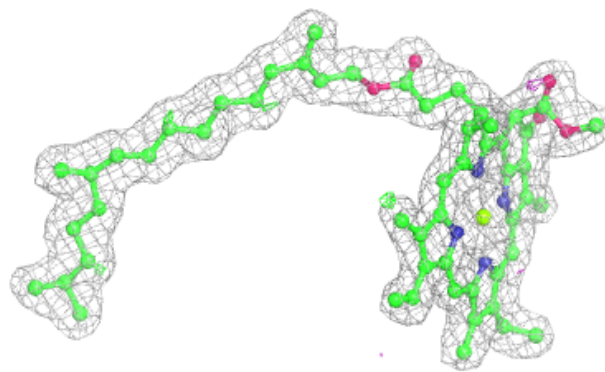


Electron density around CLA B 608:

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

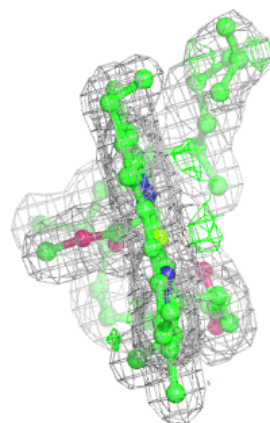
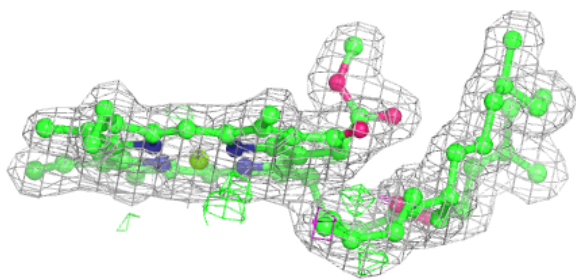
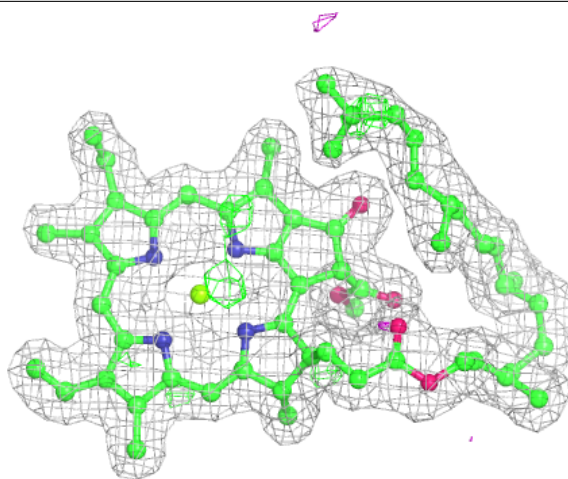
**Electron density around CLA B 610:**

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



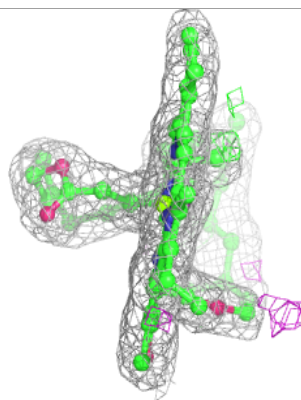
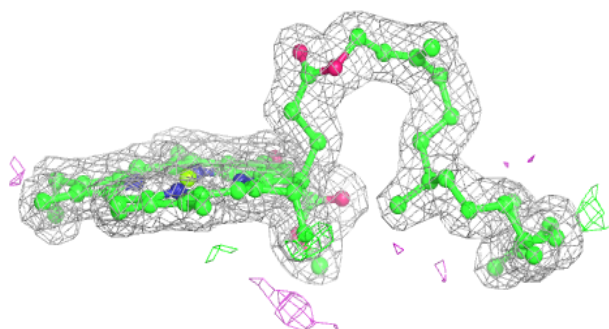
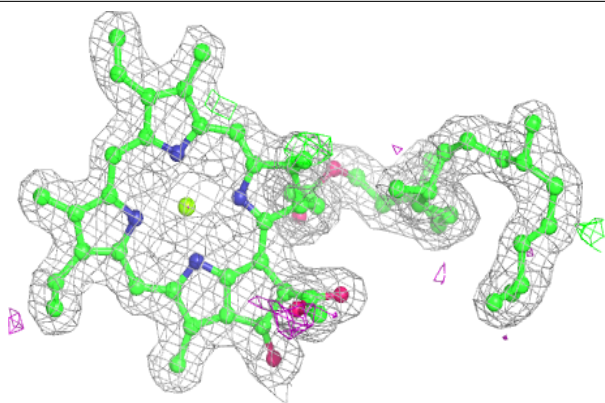
Electron density around CLA B 611:

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



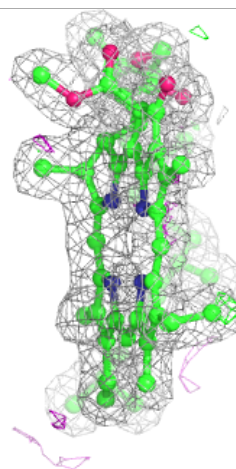
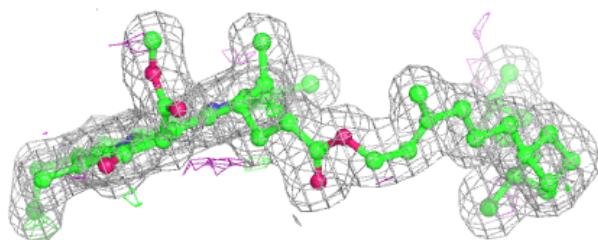
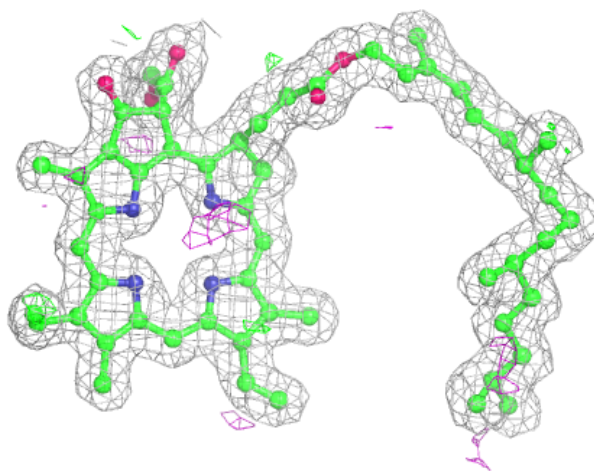
Electron density around CLA B 613:

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



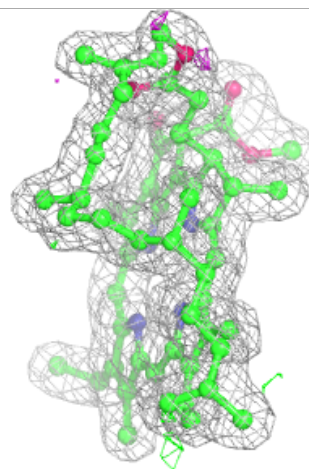
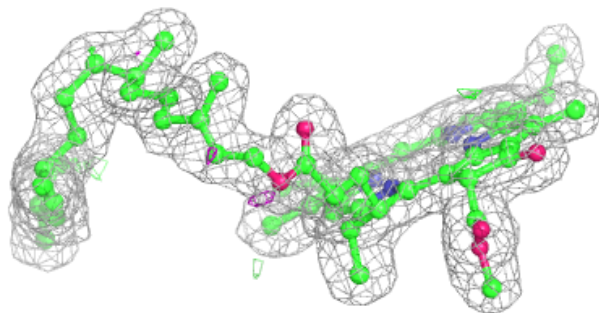
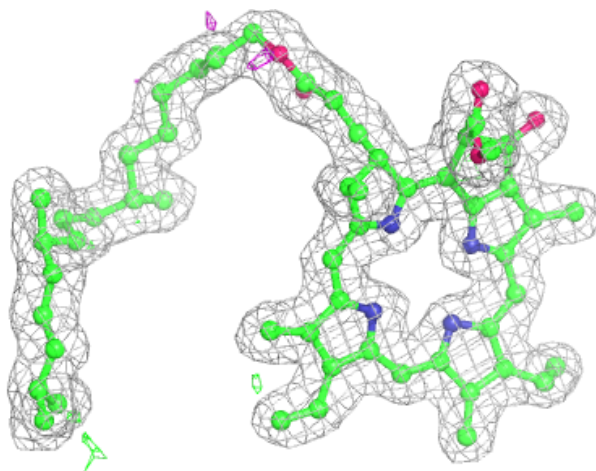
Electron density around PHO A 608:

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



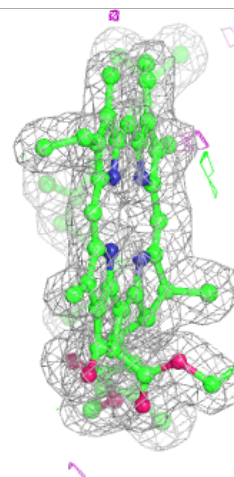
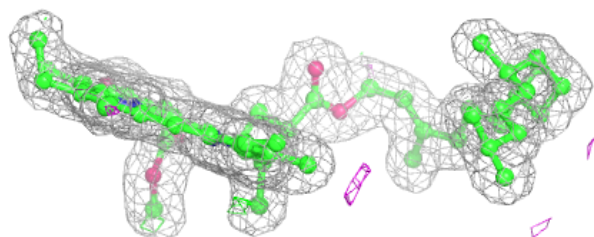
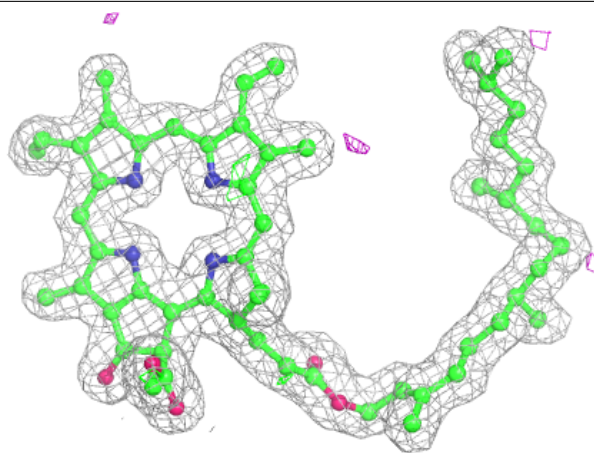
Electron density around PHO D 401:

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



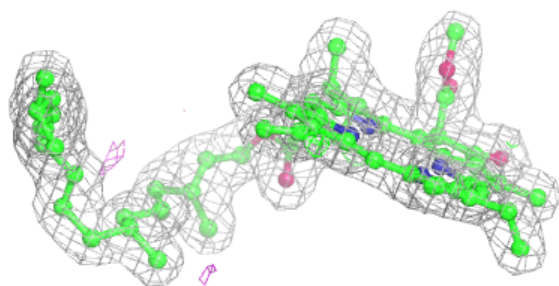
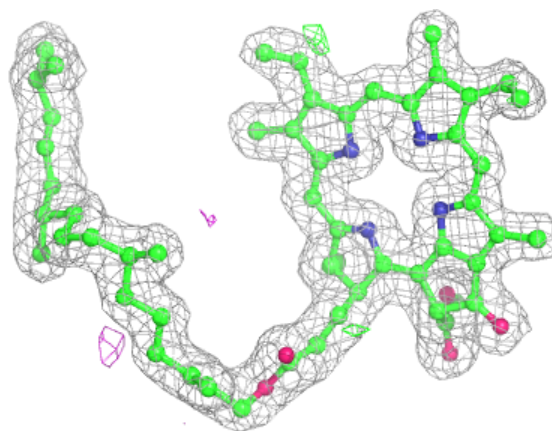
Electron density around PHO a 409:

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

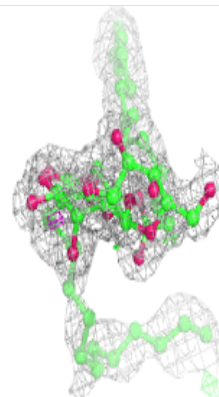
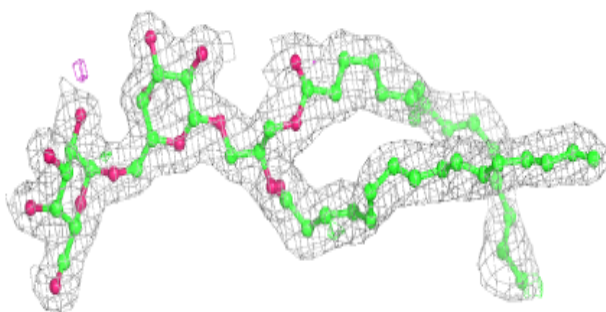
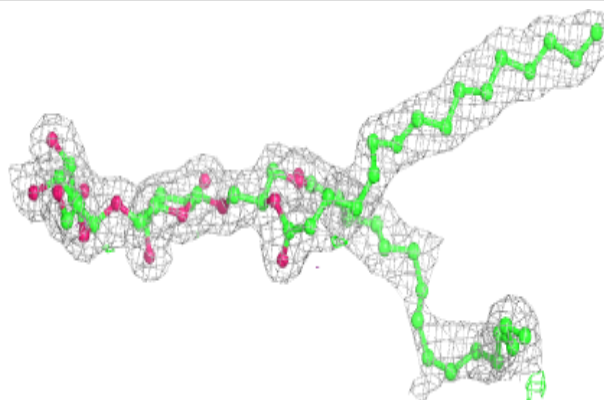


Electron density around PHO d 401:

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

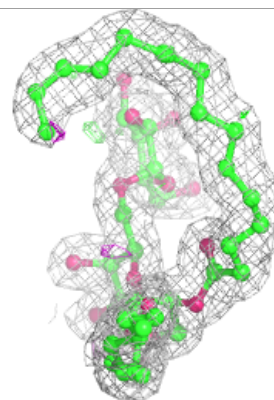
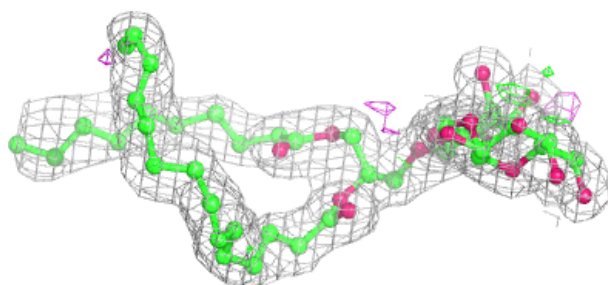
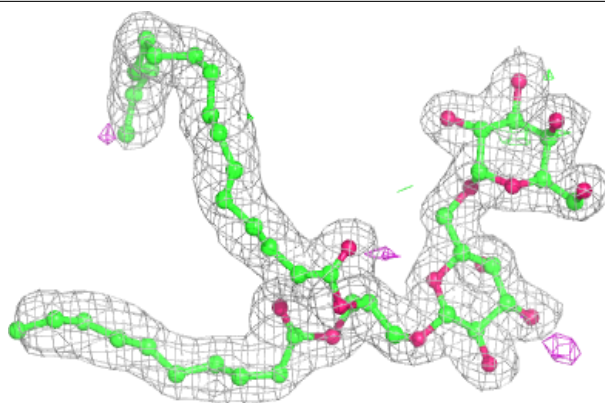
**Electron density around DGD C 516:**

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

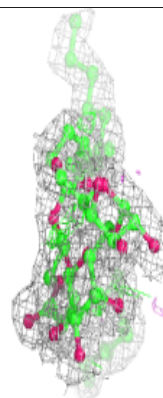
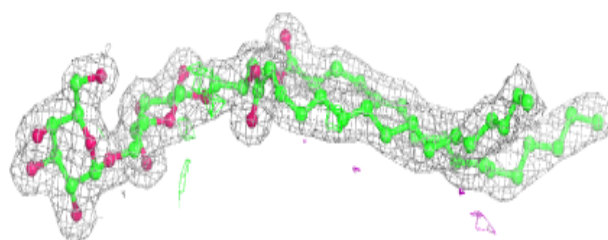
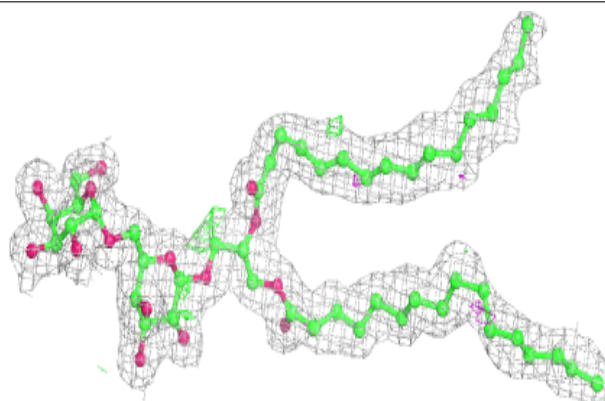


Electron density around DGD C 517:

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

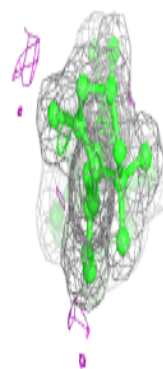
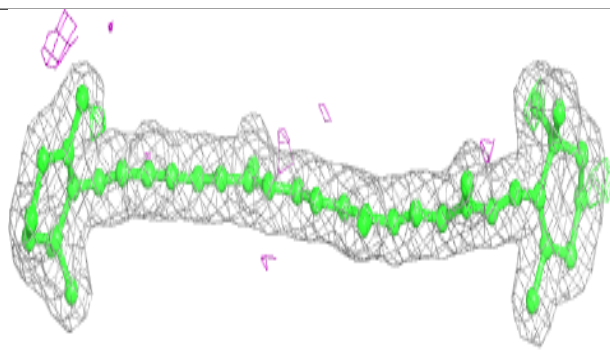
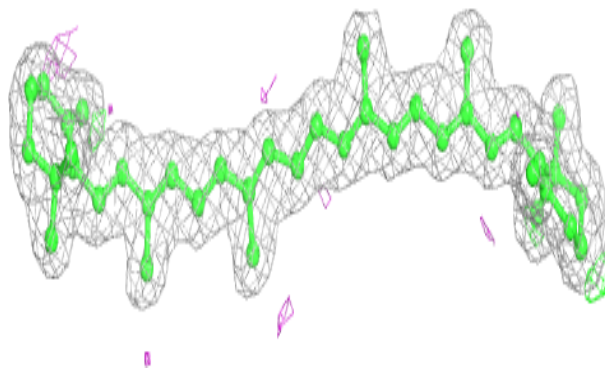
**Electron density around DGD C 518:**

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

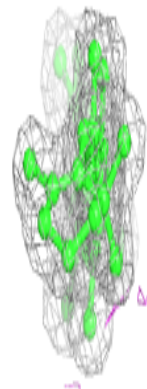
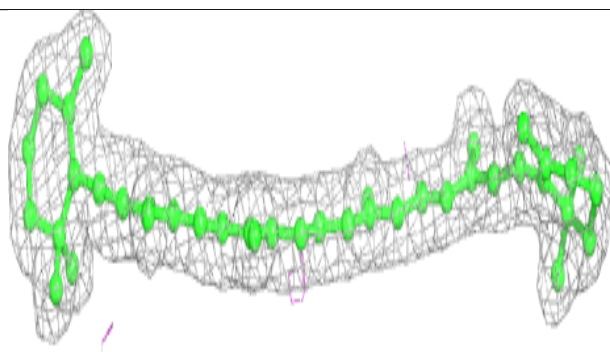
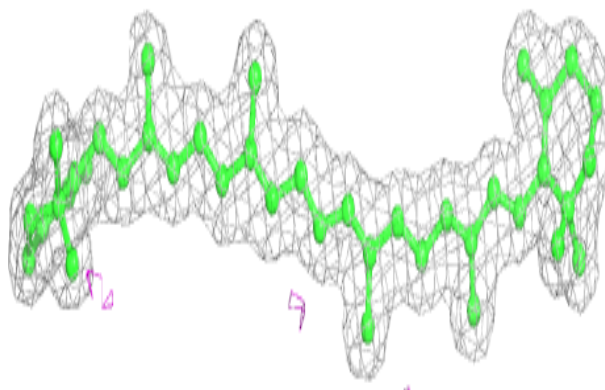


Electron density around BCR A 610:

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

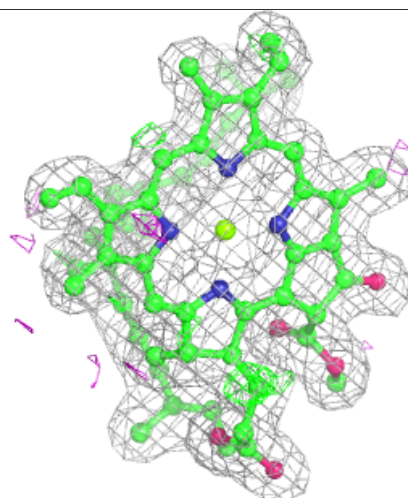
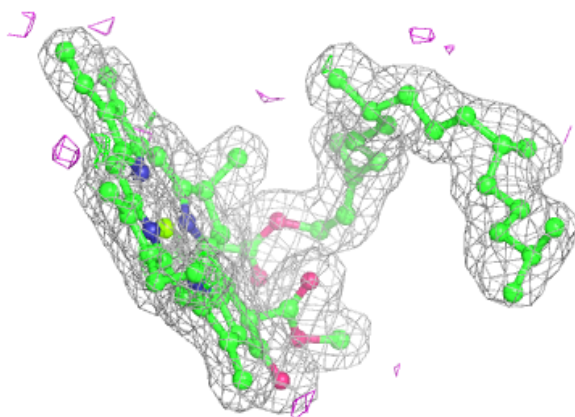
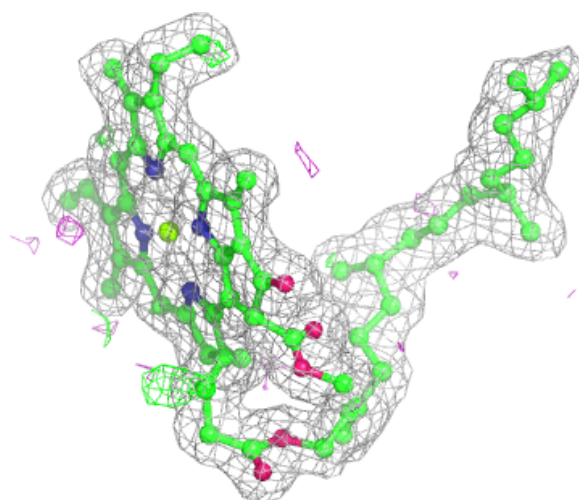
**Electron density around BCR B 618:**

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



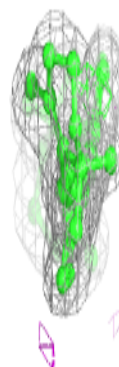
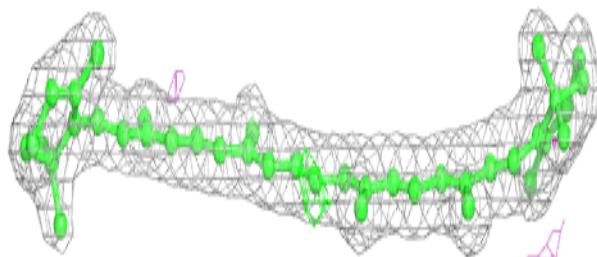
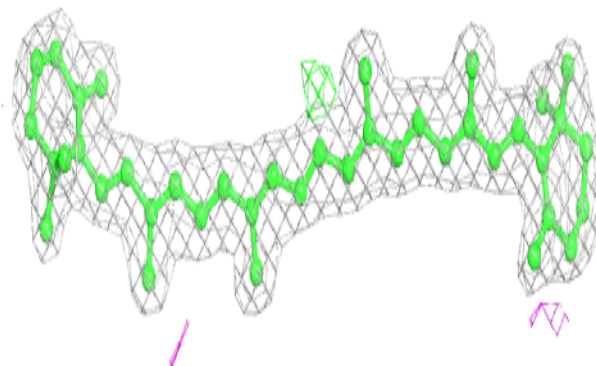
Electron density around CLA B 614:

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

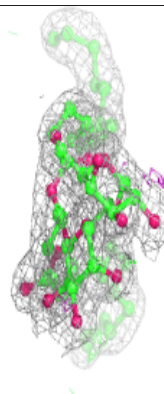
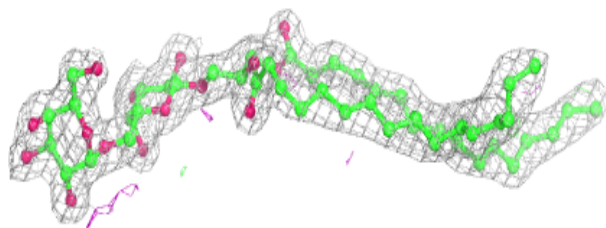
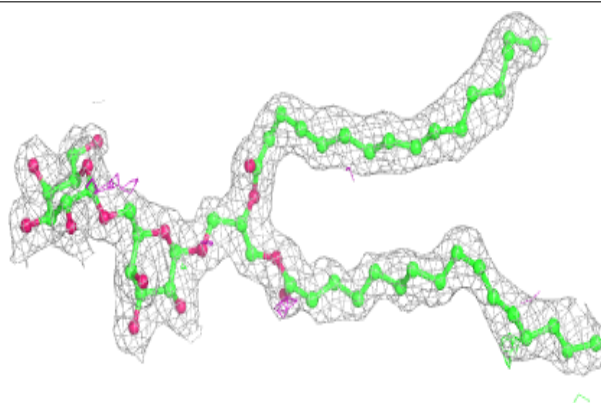


Electron density around BCR B 620:

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

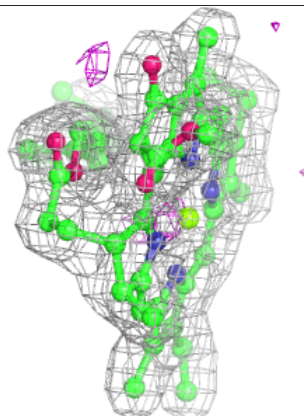
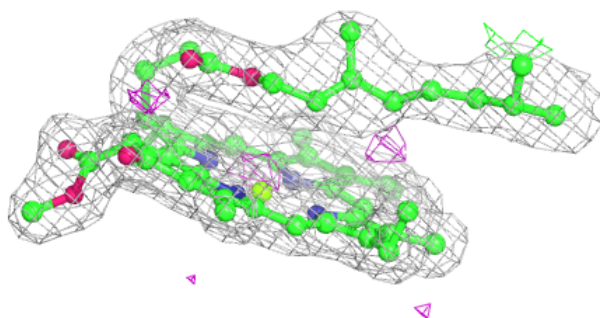
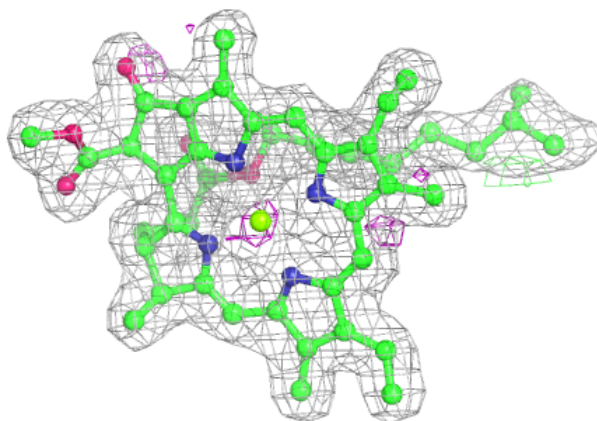
**Electron density around DGD c 518:**

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



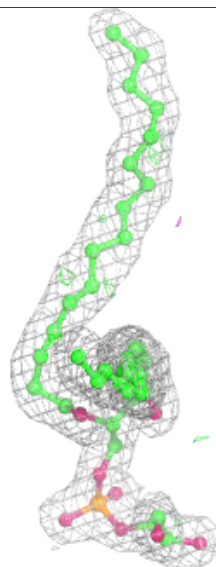
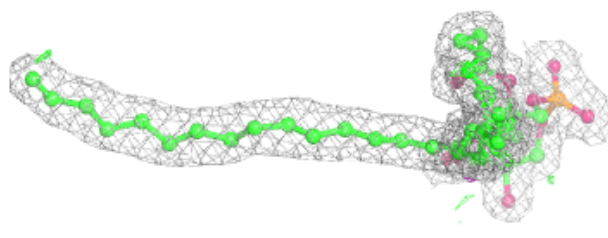
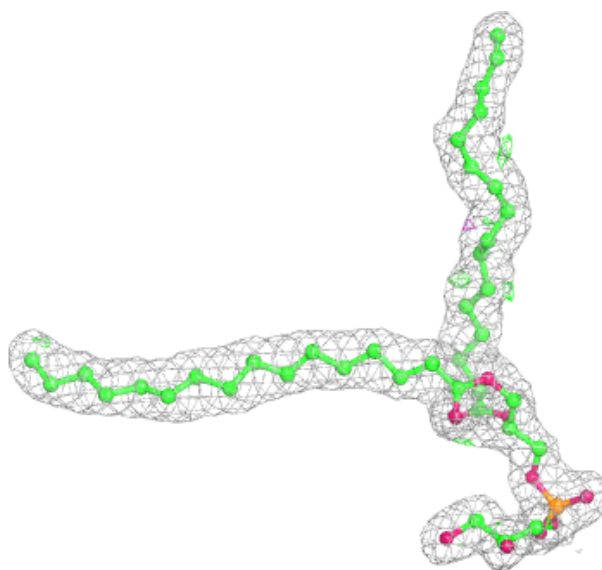
Electron density around CLA B 615:

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



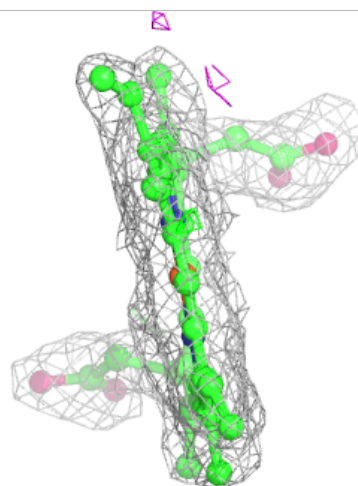
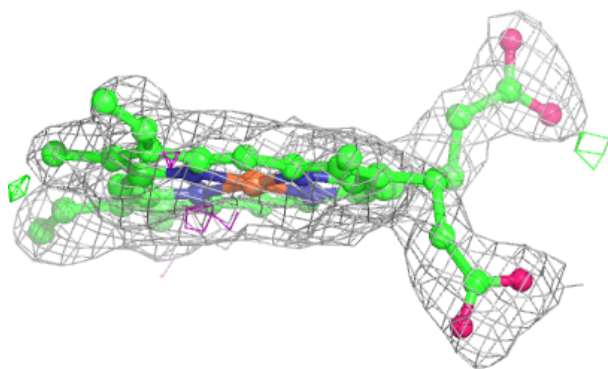
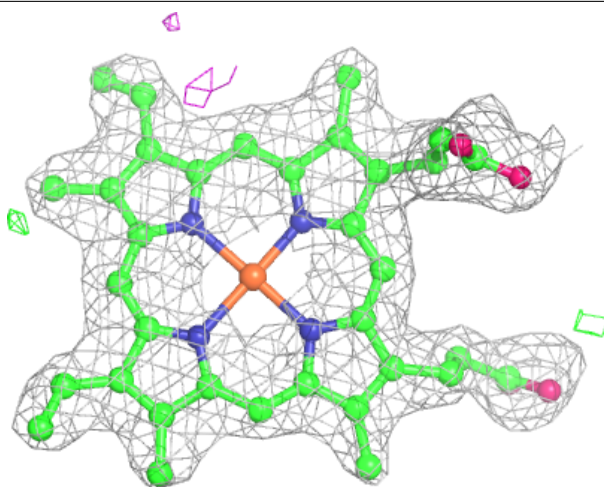
Electron density around LHG B 632:

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



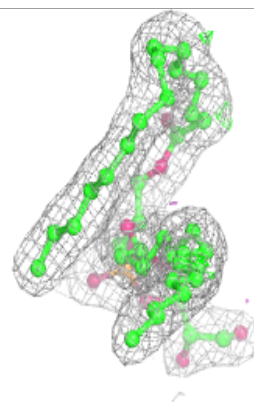
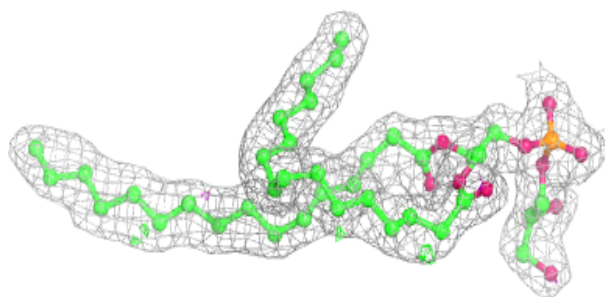
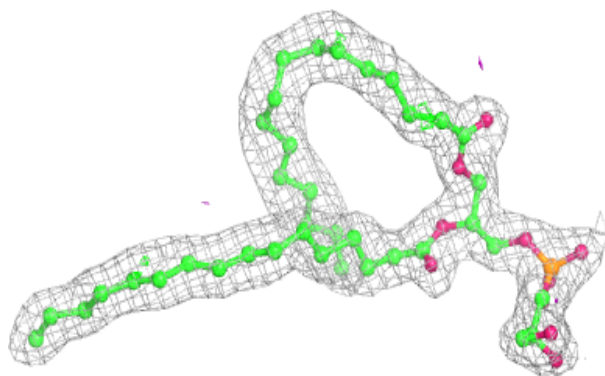
Electron density around HEM E 113:

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



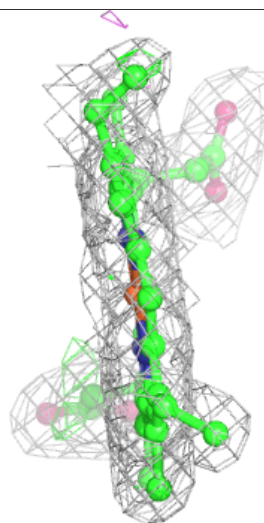
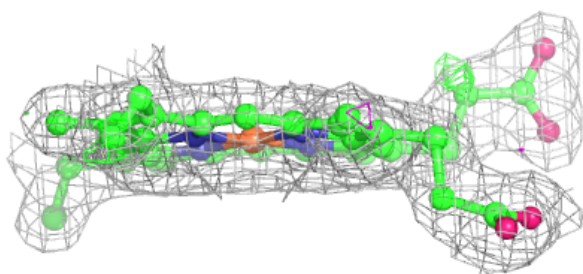
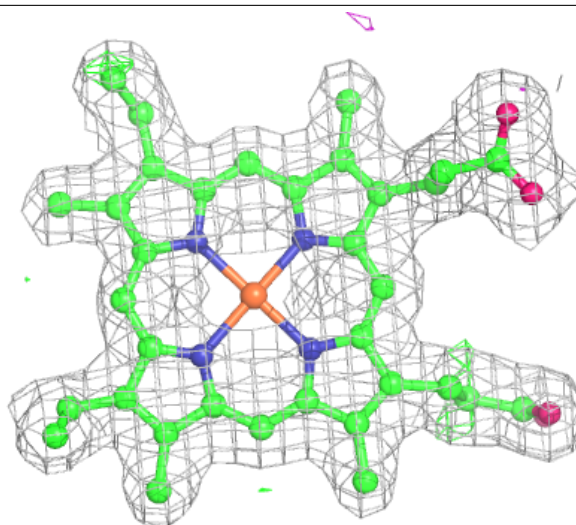
Electron density around LHG D 409:

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



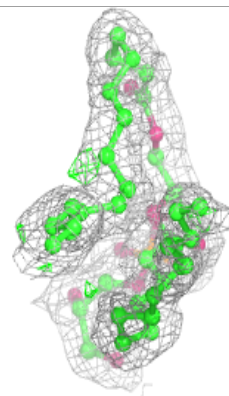
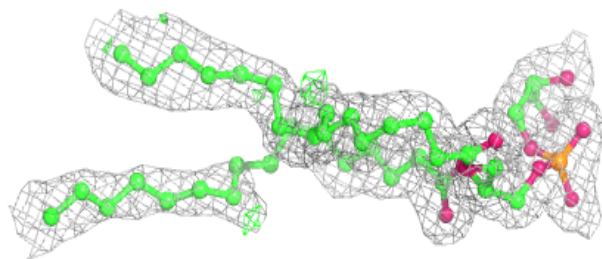
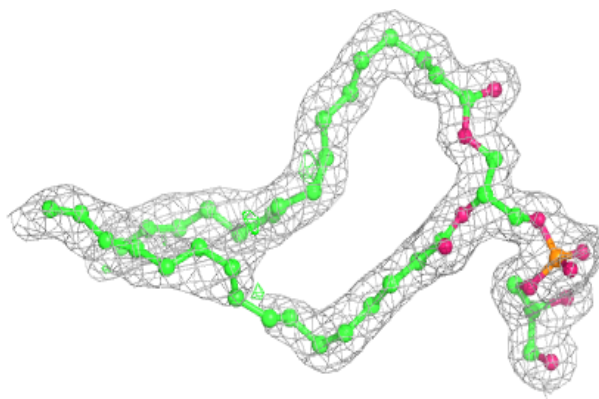
Electron density around HEC v 202:

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



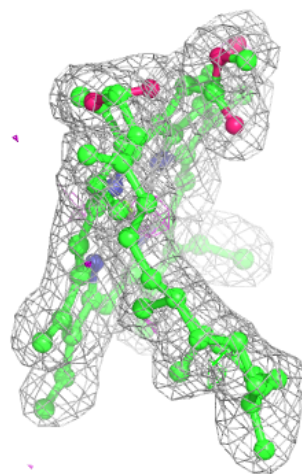
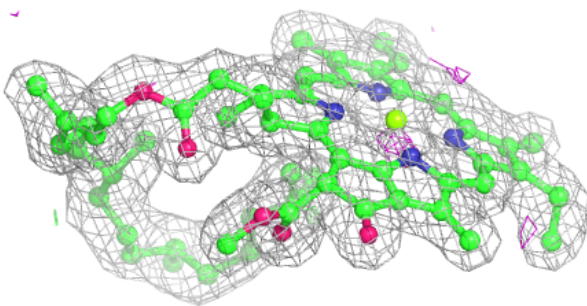
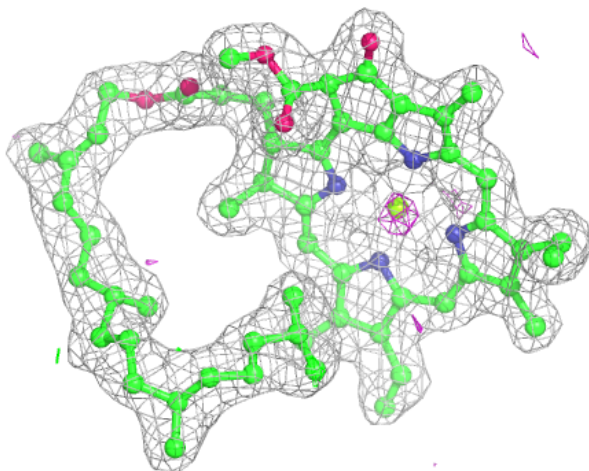
Electron density around LHG D 411:

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



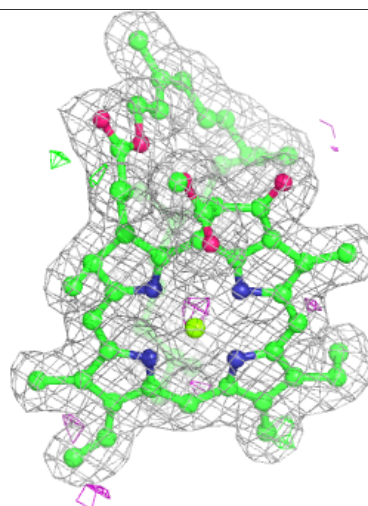
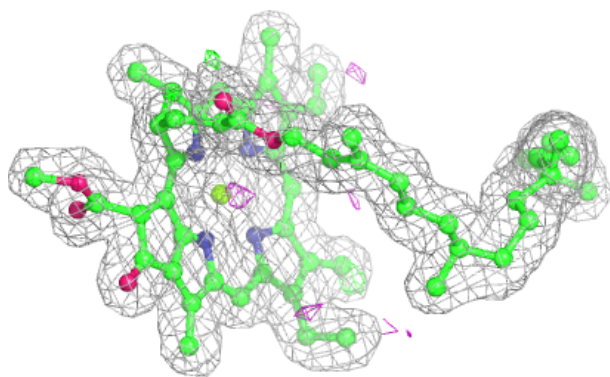
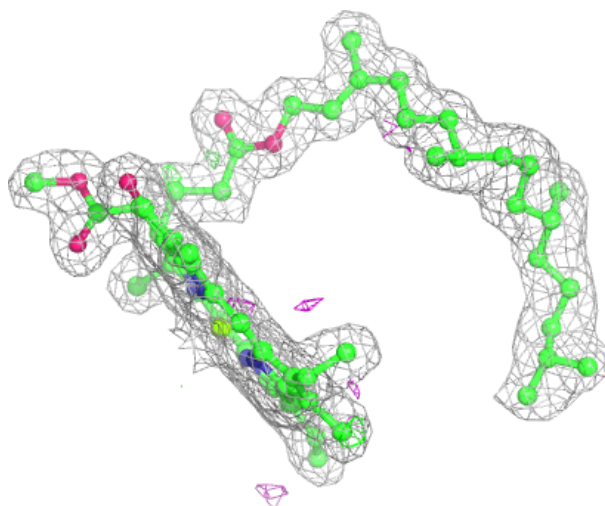
Electron density around CLA B 616:

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



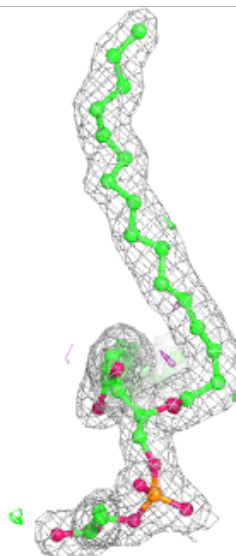
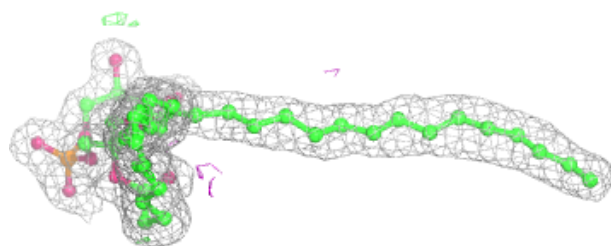
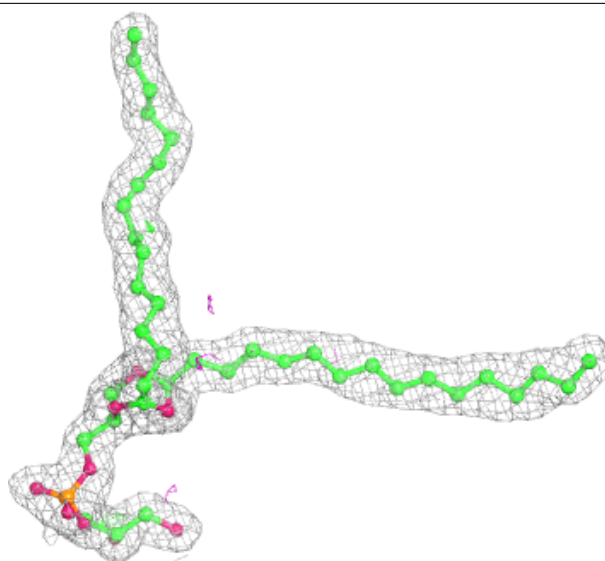
Electron density around CLA B 612:

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



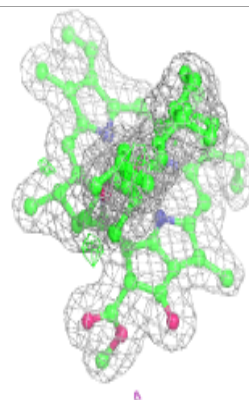
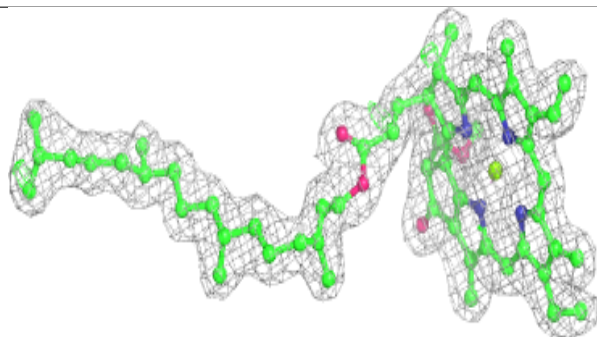
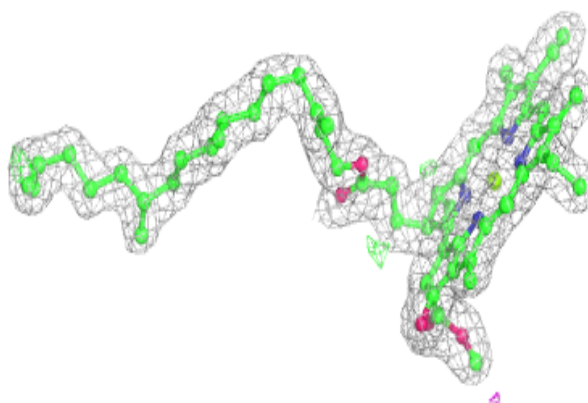
Electron density around LHG 1 101:

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

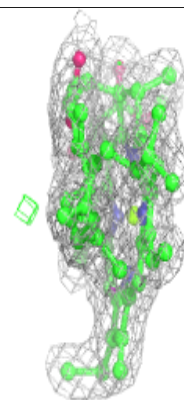
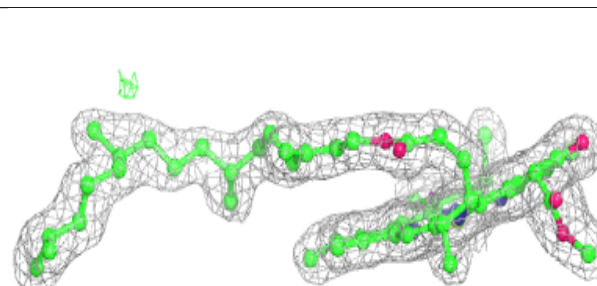
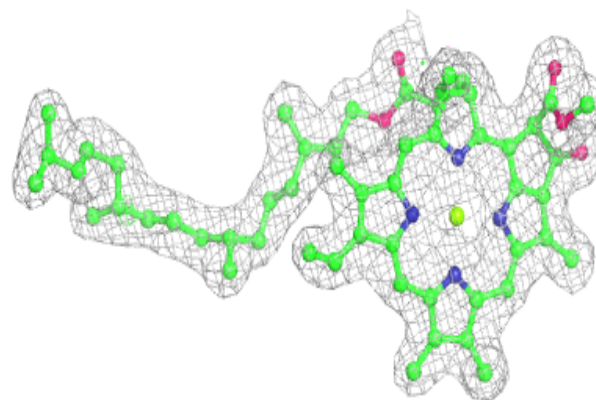


Electron density around CLA c 502:

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

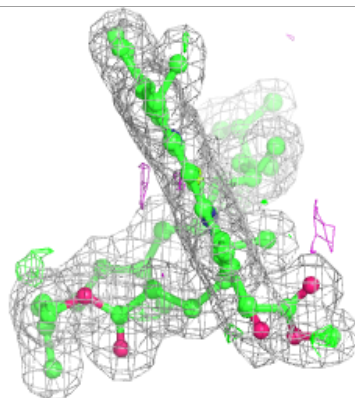
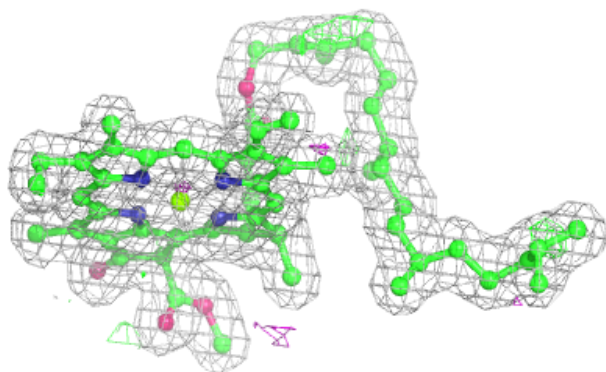
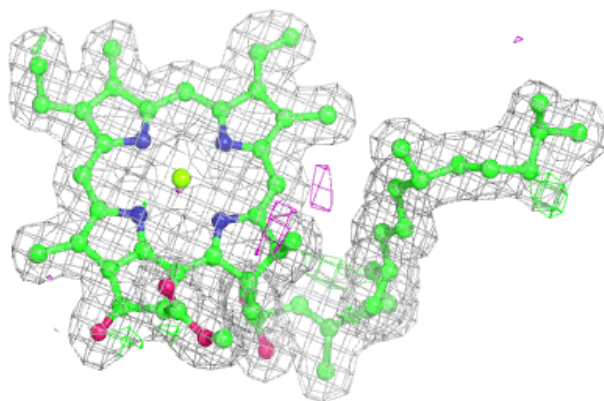
**Electron density around CLA b 604:**

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

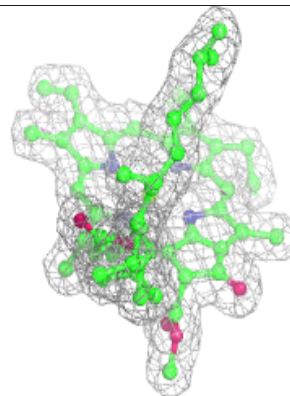
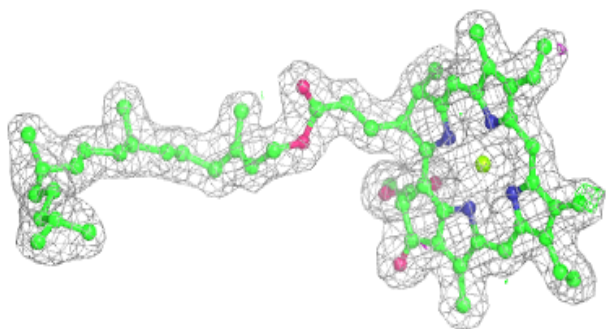
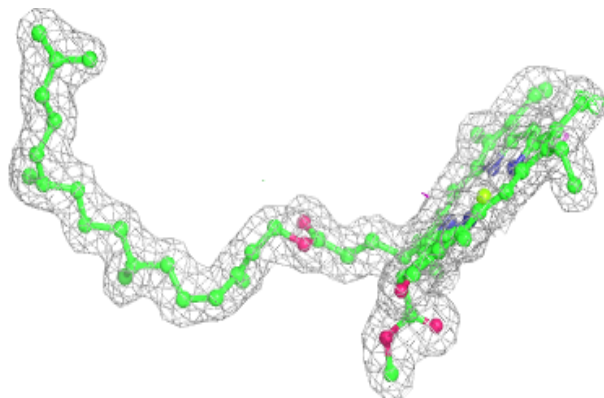


Electron density around CLA d 403:

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

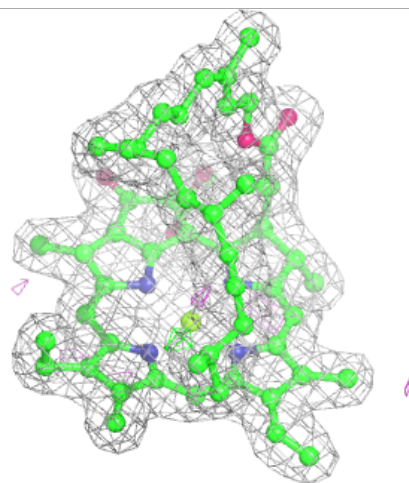
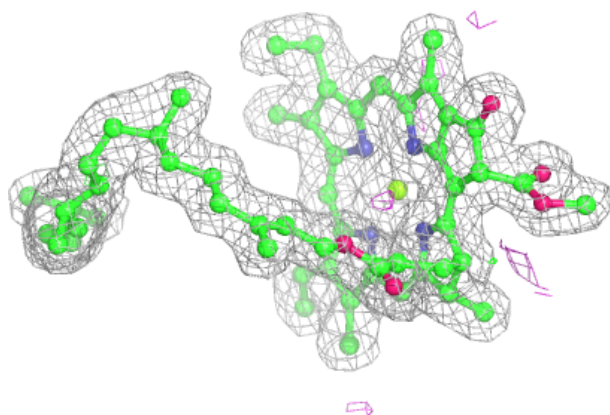
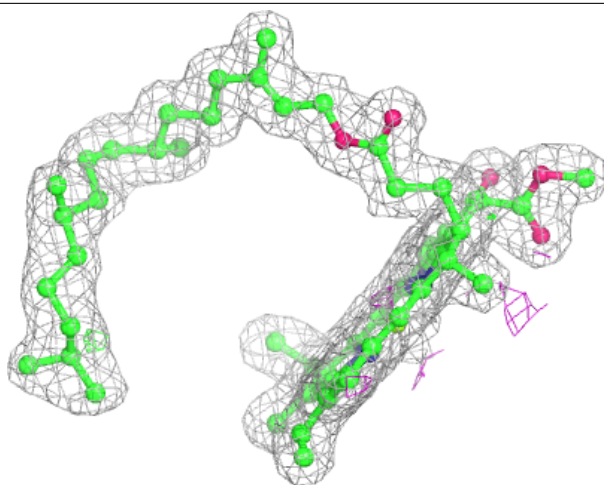
**Electron density around CLA d 404:**

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



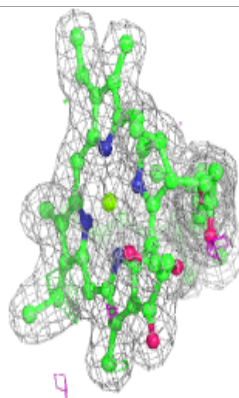
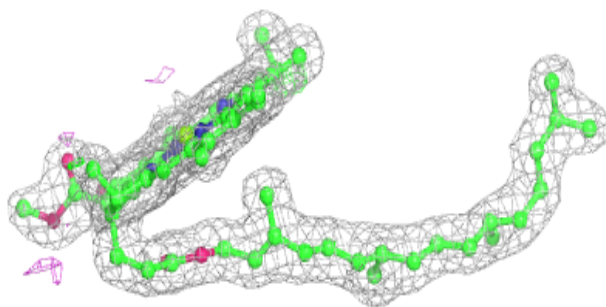
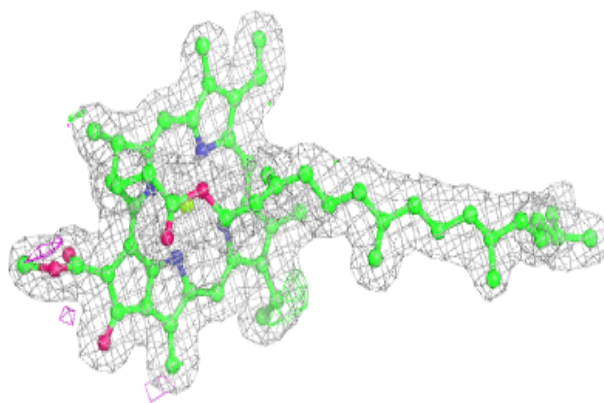
Electron density around CLA b 612:

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

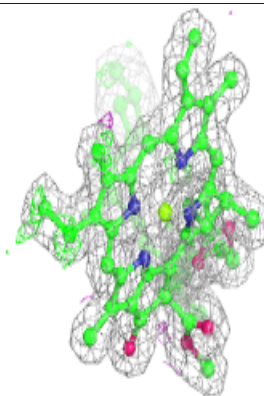
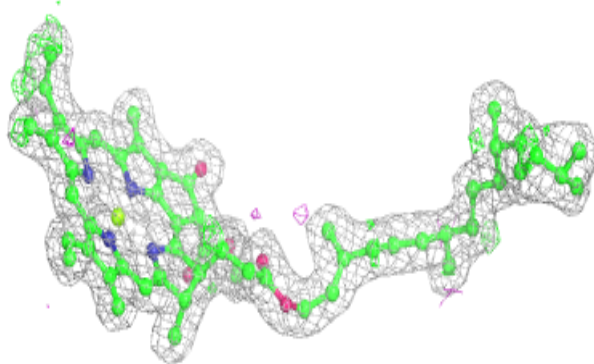
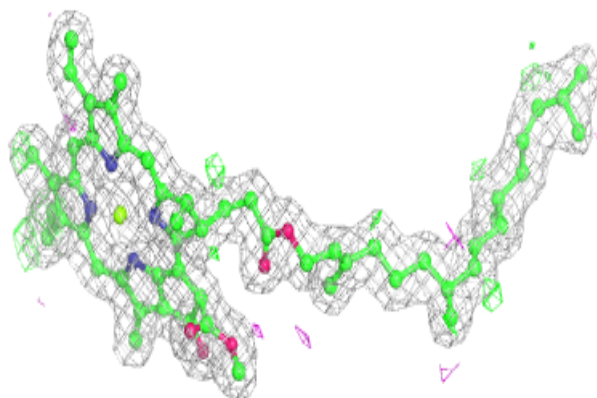


Electron density around CLA B 609:

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

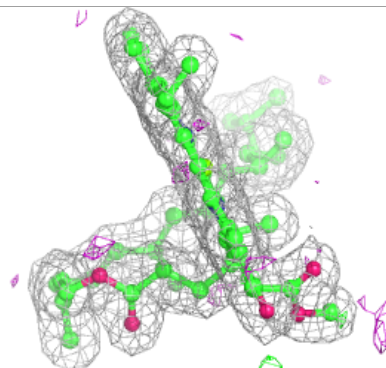
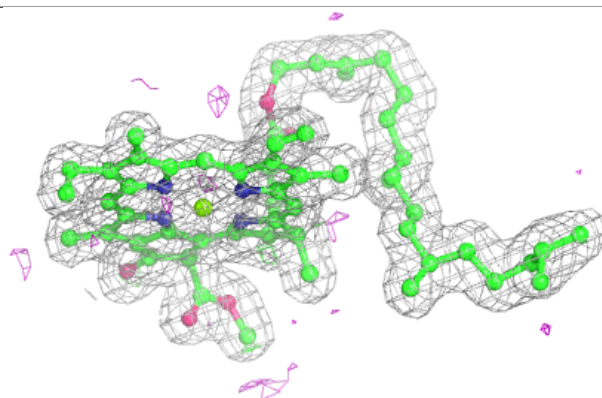
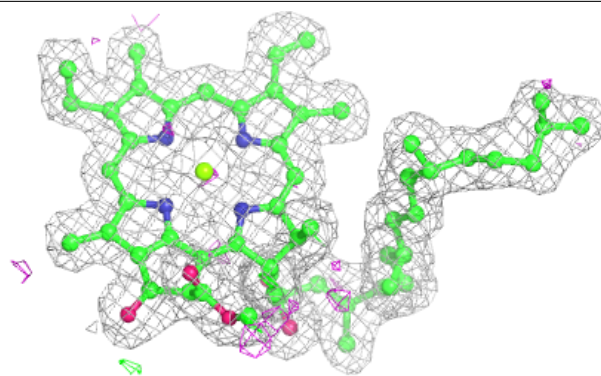
**Electron density around CLA A 606:**

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

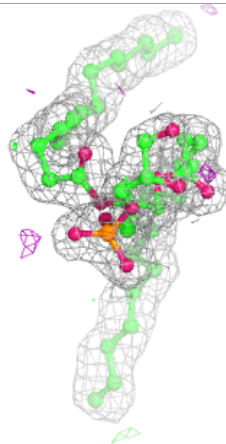
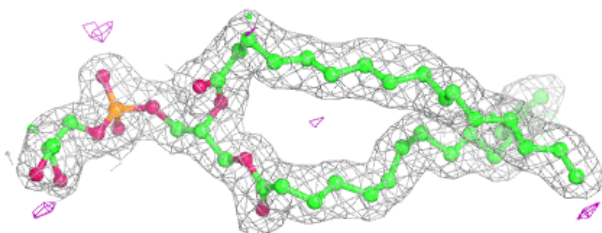
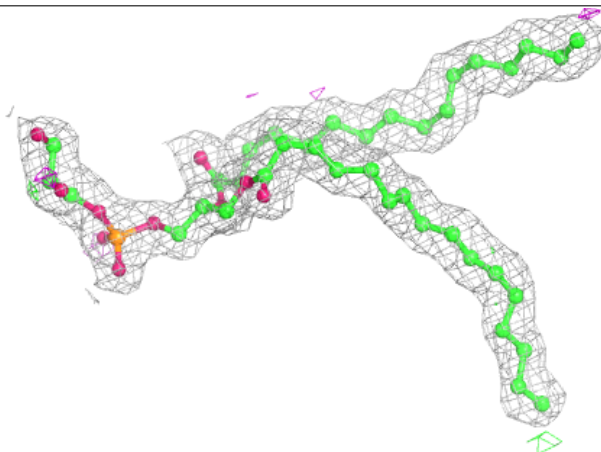


Electron density around CLA D 403:

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

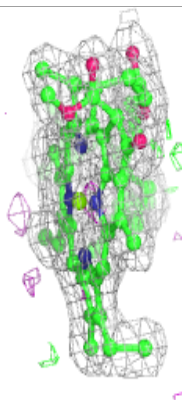
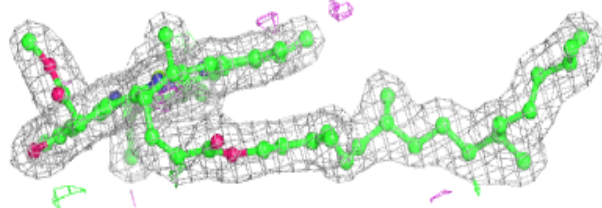
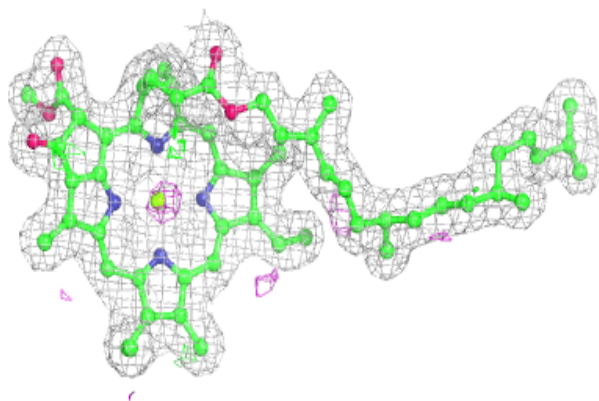
**Electron density around LHG D 410:**

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



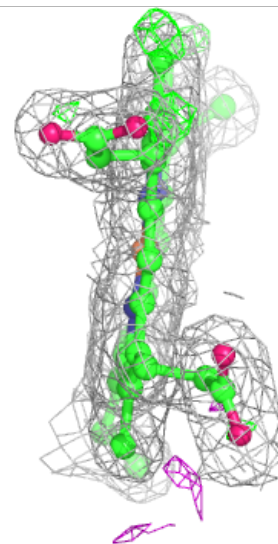
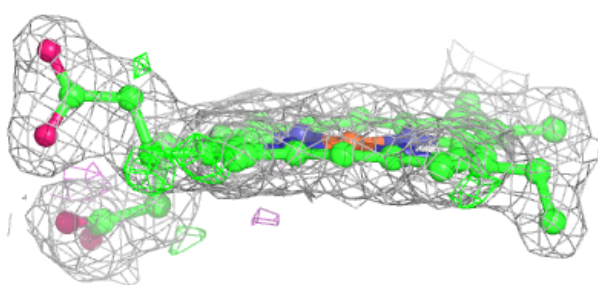
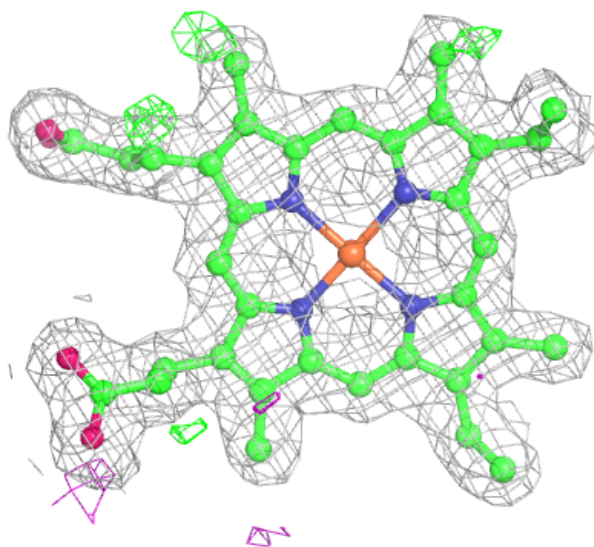
Electron density around CLA B 604:

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



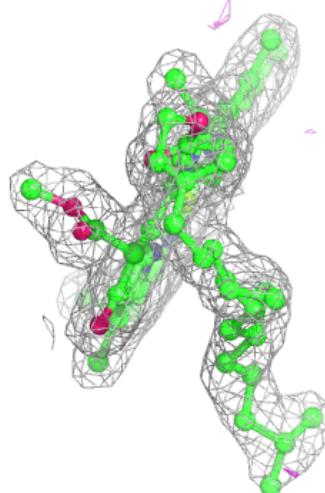
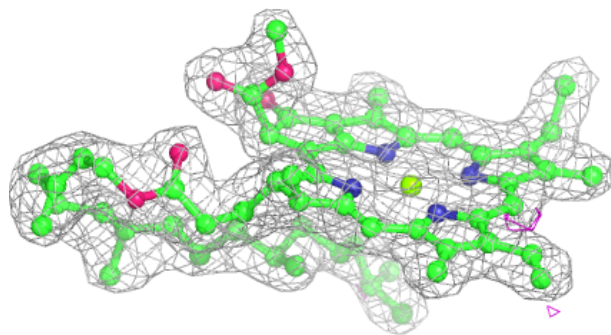
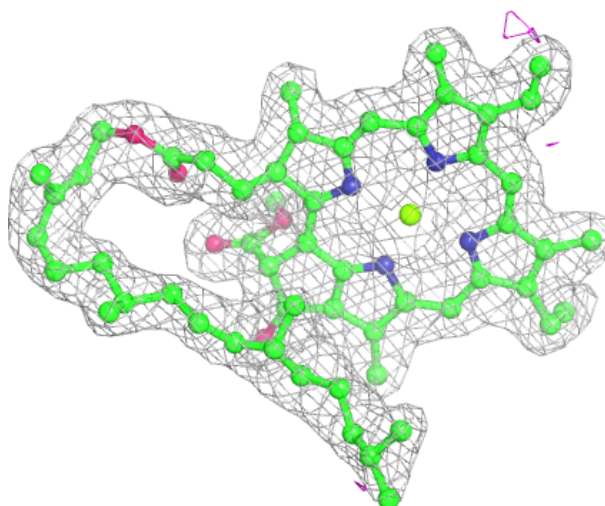
Electron density around HEC V 203:

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



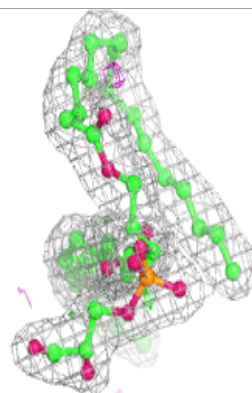
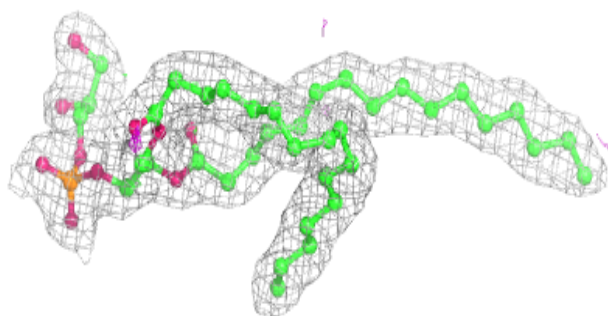
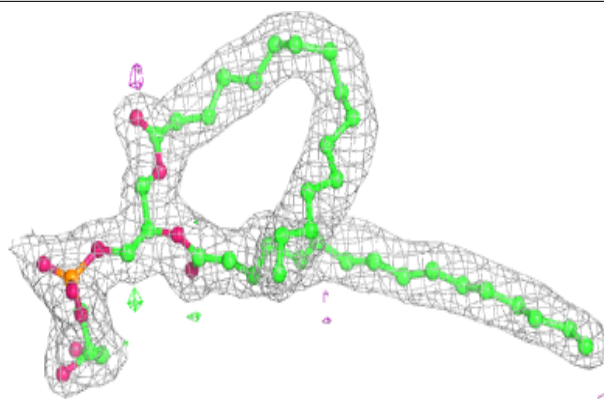
Electron density around CLA c 509:

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

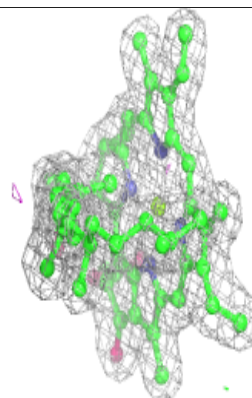
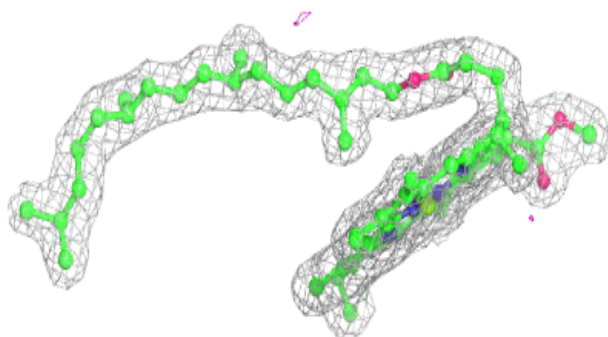
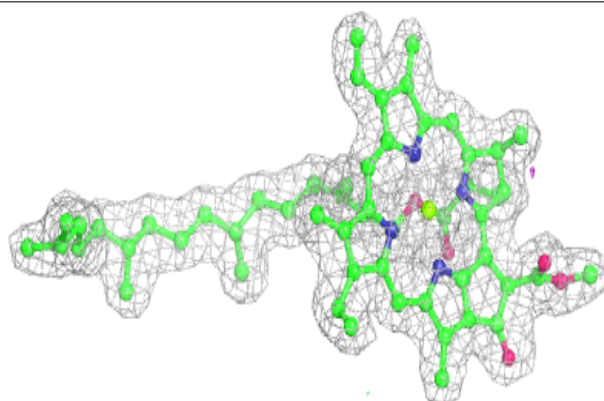


Electron density around LHG d 409:

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

**Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.