



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2026 – 08:01 AM EDT

PDB ID : 5V2C / pdb_00005v2c
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

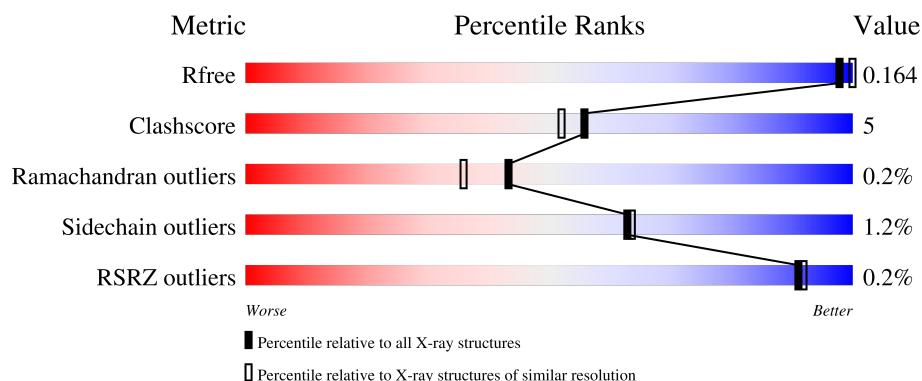
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



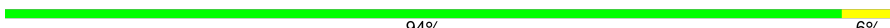
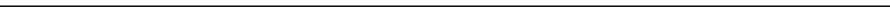
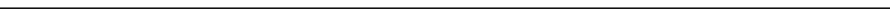
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	91% 6% .
1	a	344	90% 7% .
2	B	506	93% 7%
2	b	506	92% 7%
3	C	458	91% 7% .

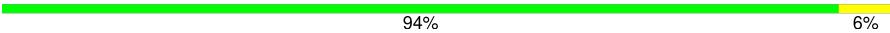
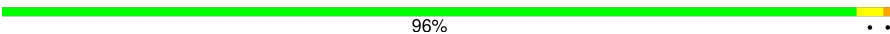
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	c	458	 91% 8%
4	D	342	 93% 7%
4	d	342	 94% 6%
5	E	83	 86% 12% •
5	e	83	 89% 8% •
6	F	44	 68% 9% 23%
6	f	44	 57% 16% 27%
7	H	65	 2% 92% 5% •
7	h	65	 3% 91% 8% •
8	I	38	 95% 5%
8	i	38	 95% • •
9	J	40	 85% 10% • •
9	j	40	 88% 8% • •
10	K	37	 92% 8%
10	k	37	 86% 14%
11	L	37	 86% 11% •
11	l	37	 89% 8% •
12	M	36	 75% 17% • 6%
12	m	36	 83% 14% •
13	O	245	 90% 9% •
13	o	245	 90% 9%
14	T	32	 88% 6% 6%
14	t	32	 91% • 6%
15	U	104	 90% • 7%
15	u	104	 87% 6% • 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	V	137	
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
22	CL	v	201	-	-	X	-
23	BCT	A	605	-	X	-	-
23	BCT	a	406	-	X	-	-
30	GOL	C	523	-	-	X	-
30	GOL	C	528	-	X	X	-
30	GOL	c	529	-	-	X	-
43	HEC	V	203	X	-	-	-
43	HEC	v	202	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			

Continued on next page...

Continued from previous page...

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			

Continued on next page...

Continued from previous page...

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

Continued on next page...

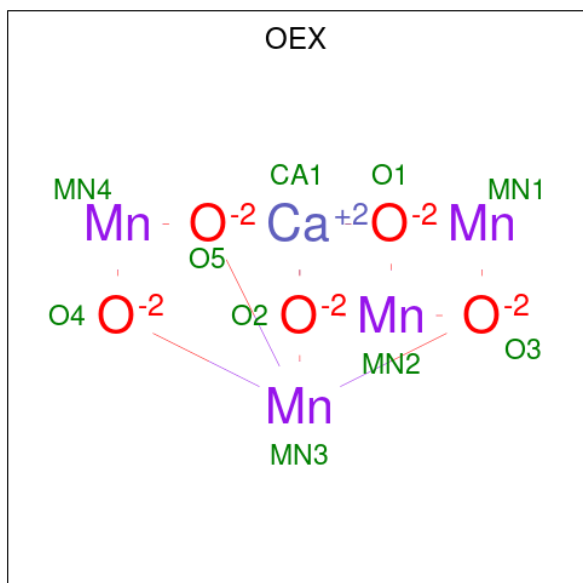
Continued from previous page...

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 (CCD ID: 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		

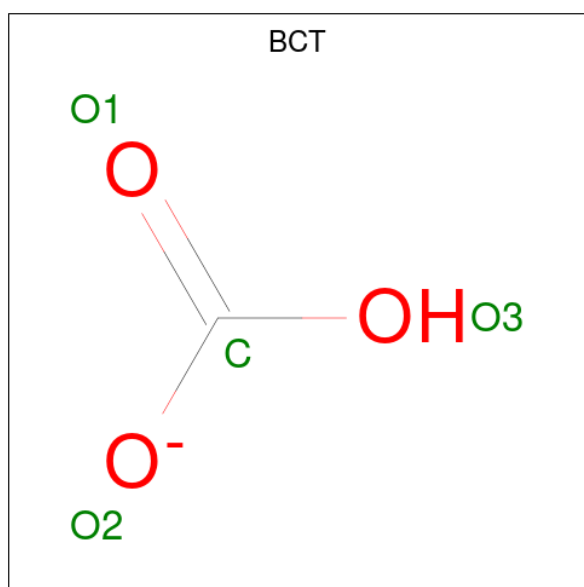
- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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 (CCD ID: 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 (CCD ID: BCT) (formula: CHO_3).



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 (CCD ID: CLA) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$).



Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

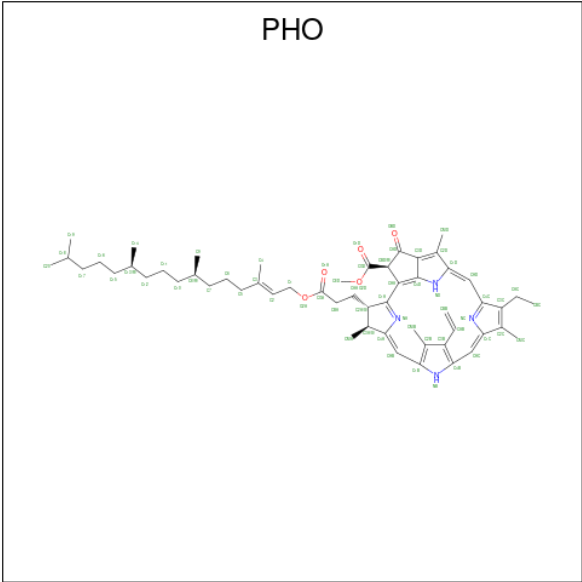
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

Continued on next page...

Continued from previous page...

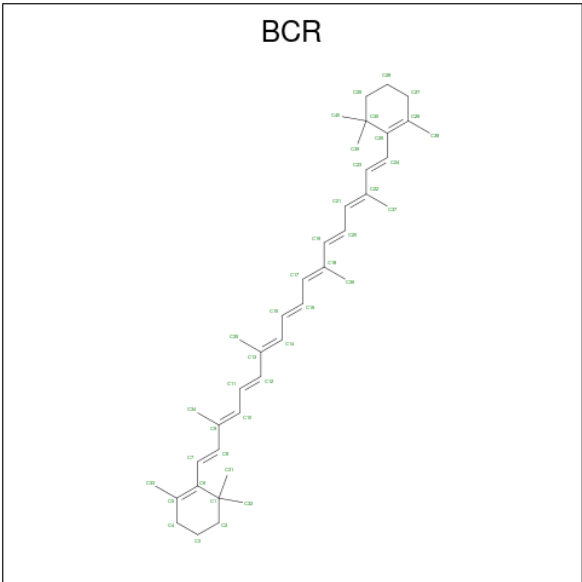
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 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 (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



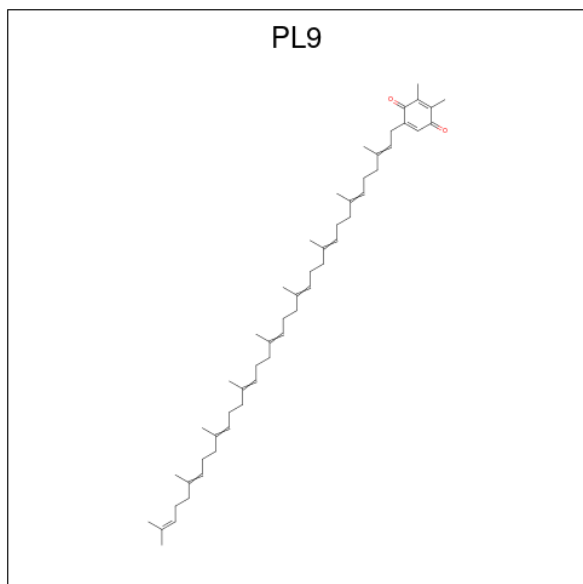
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	D	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	d	1	Total	C	N	O	0	0
			64	55	4	5		

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



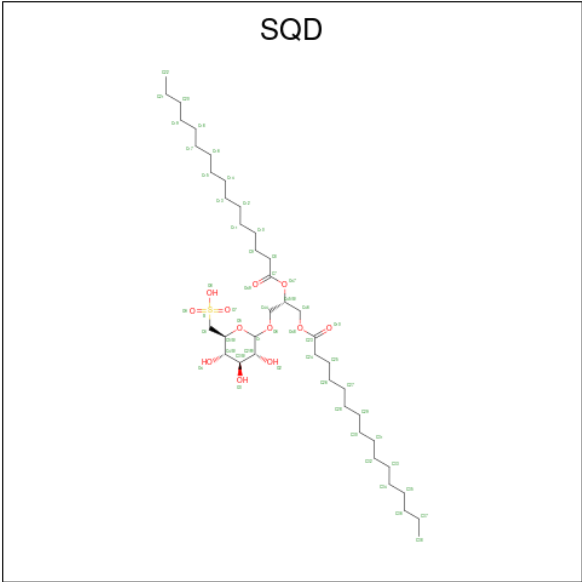
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total 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 (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



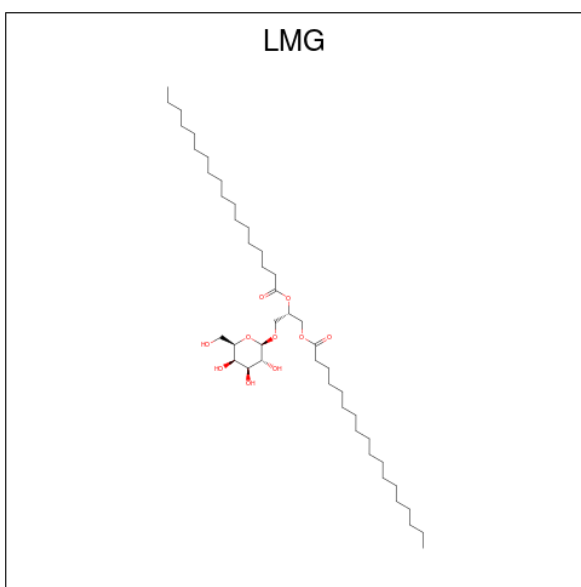
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			55	53	2		
27	D	1	Total	C	O	0	0
			55	53	2		
27	a	1	Total	C	O	0	0
			55	53	2		
27	d	1	Total	C	O	0	0
			55	53	2		

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



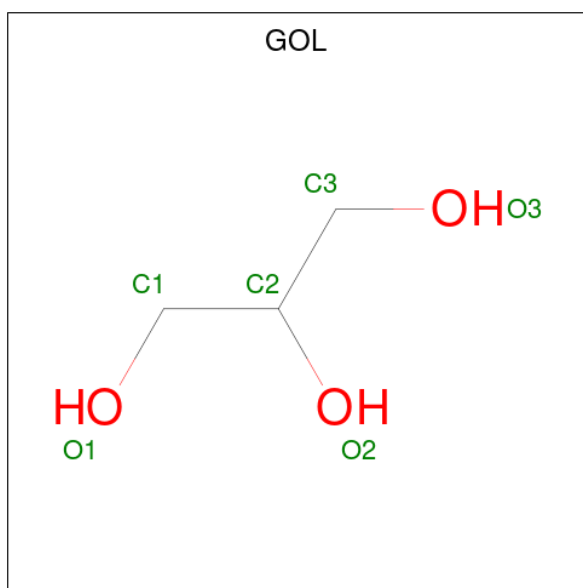
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	F	1	Total	C	O	S	0	0
			54	41	12	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	a	1	Total	C	O	S	0	0
			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 (CCD ID: 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 (CCD ID: 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		
30	C	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

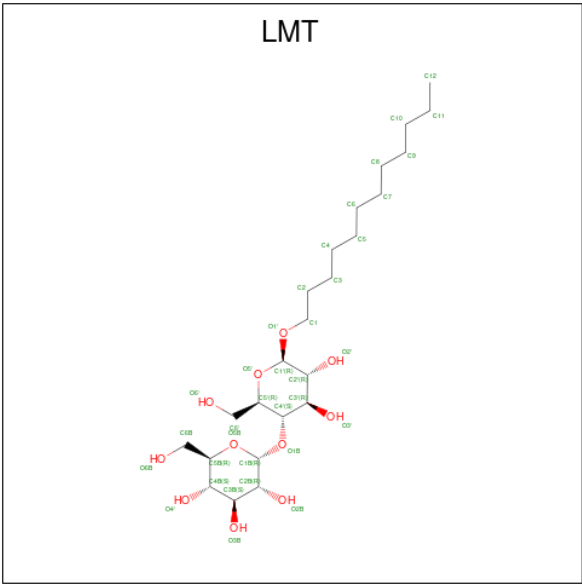
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	b	1	Total	C	O	0	0
			6	3	3		
30	b	1	Total	C	O	0	0
			6	3	3		
30	b	1	Total	C	O	0	0
			6	3	3		
30	b	1	Total	C	O	0	0
			6	3	3		
30	c	1	Total	C	O	0	0
			6	3	3		
30	c	1	Total	C	O	0	0
			6	3	3		
30	c	1	Total	C	O	0	0
			6	3	3		
30	c	1	Total	C	O	0	0
			6	3	3		
30	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		

Continued on next page...

Continued from previous page...

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-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



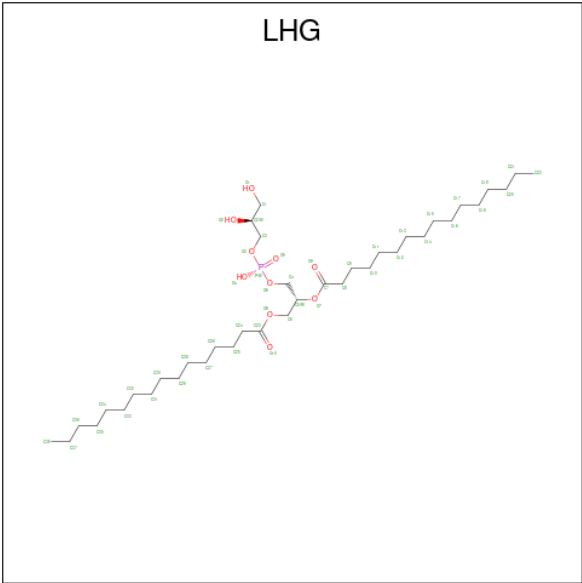
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	C	1	Total	C	O	0	0
			35	24	11		
31	F	1	Total	C	O	0	0
			35	24	11		
31	I	1	Total	C	O	0	0
			35	24	11		
31	J	1	Total	C	O	0	0
			35	24	11		

Continued on next page...

Continued from previous page...

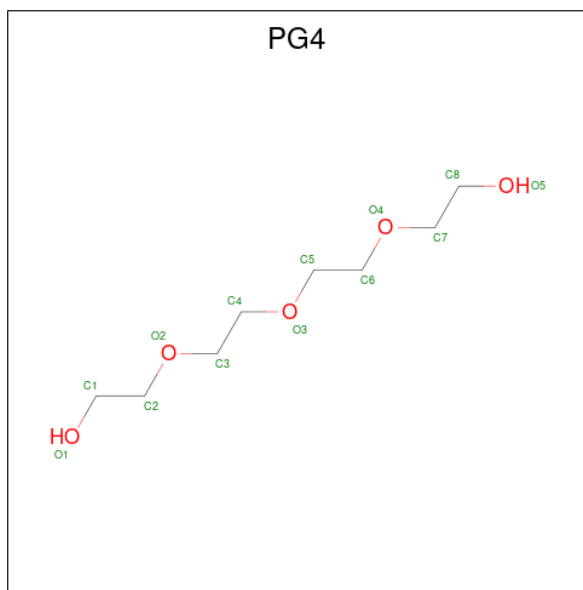
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	M	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total	C	O	0	0
			35	24	11		
31	Y	1	Total	C	O	0	0
			35	24	11		
31	a	1	Total	C	O	0	0
			35	24	11		
31	b	1	Total	C	O	0	0
			35	24	11		
31	c	1	Total	C	O	0	0
			35	24	11		
31	f	1	Total	C	O	0	0
			35	24	11		
31	j	1	Total	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 (CCD ID: 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 (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



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	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		

Continued on next page...

Continued from previous page...

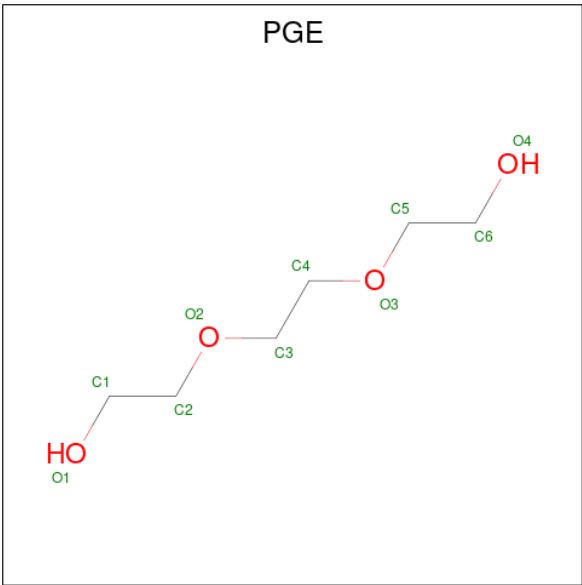
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	I	1	Total	C	O	0	0
			13	8	5		
33	I	1	Total	C	O	0	0
			13	8	5		
33	J	1	Total	C	O	0	0
			13	8	5		
33	J	1	Total	C	O	0	0
			13	8	5		
33	K	1	Total	C	O	0	0
			13	8	5		
33	U	1	Total	C	O	0	0
			13	8	5		
33	V	1	Total	C	O	0	0
			13	8	5		
33	V	1	Total	C	O	0	0
			13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

Continued on next page...

Continued from previous page...

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 (CCD ID: 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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

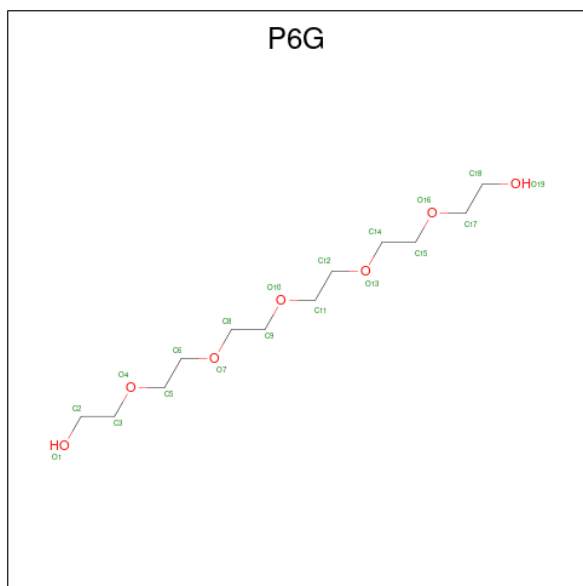
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	b	1	Total	C	O	0	0
			10	6	4		
34	b	1	Total	C	O	0	0
			10	6	4		
34	b	1	Total	C	O	0	0
			10	6	4		
34	b	1	Total	C	O	0	0
			10	6	4		
34	b	1	Total	C	O	0	0
			10	6	4		
34	b	1	Total	C	O	0	0
			10	6	4		
34	b	1	Total	C	O	0	0
			10	6	4		
34	b	1	Total	C	O	0	0
			10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

Continued on next page...

Continued from previous page...

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 (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



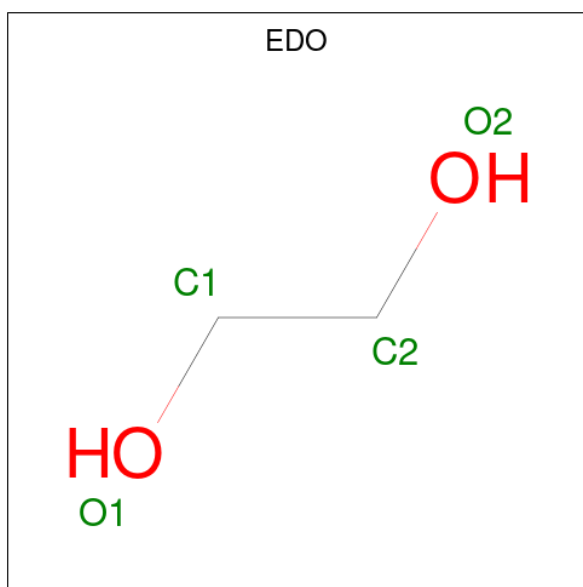
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	A	1	Total	C	O	0	0
			19	12	7		
35	A	1	Total	C	O	0	0
			19	12	7		

Continued on next page...

Continued from previous page...

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 (CCD ID: 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		

Continued on next page...

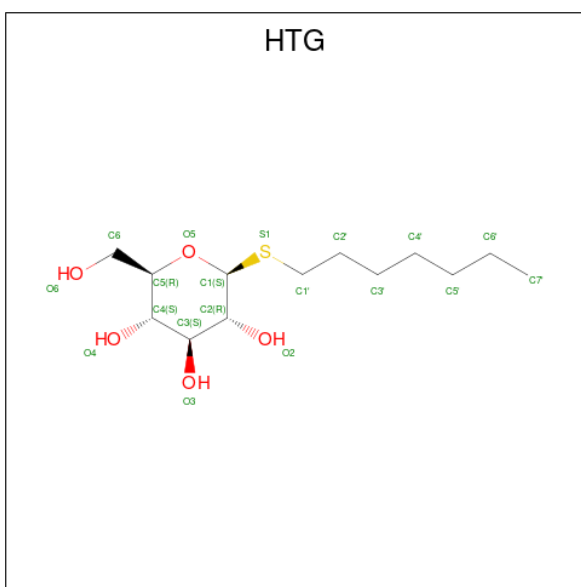
Continued from previous page...

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

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

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

- Molecule 38 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C₁₃H₂₆O₅S).



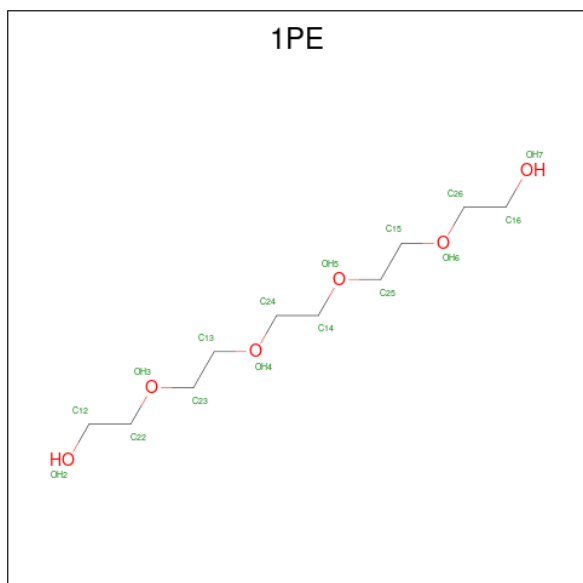
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	B	1	Total 19	C 13	O 5	S 1	0	0
38	B	1	Total 19	C 13	O 5	S 1	0	0
38	B	1	Total 19	C 13	O 5	S 1	0	0
38	B	1	Total 19	C 13	O 5	S 1	0	0
38	C	1	Total 19	C 13	O 5	S 1	0	0
38	C	1	Total 19	C 13	O 5	S 1	0	0
38	C	1	Total 19	C 13	O 5	S 1	0	0
38	C	1	Total 19	C 13	O 5	S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

Continued on next page...

Continued from previous page...

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 (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



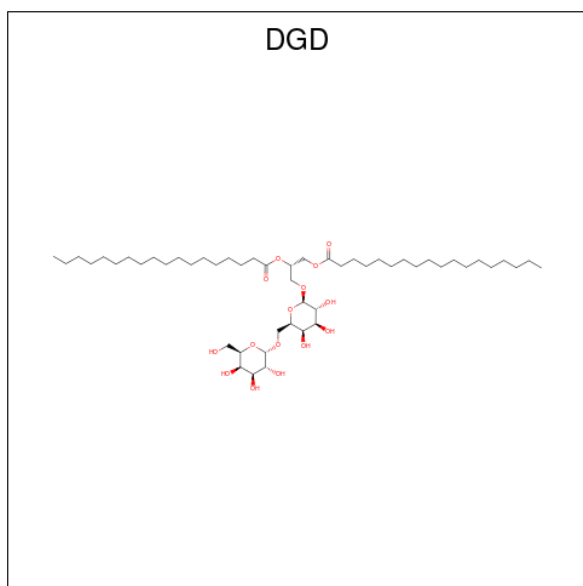
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
39	B	1	Total	C	O	0	0
			16	10	6		

Continued on next page...

Continued from previous page...

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) (CCD ID: 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		

Continued on next page...

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

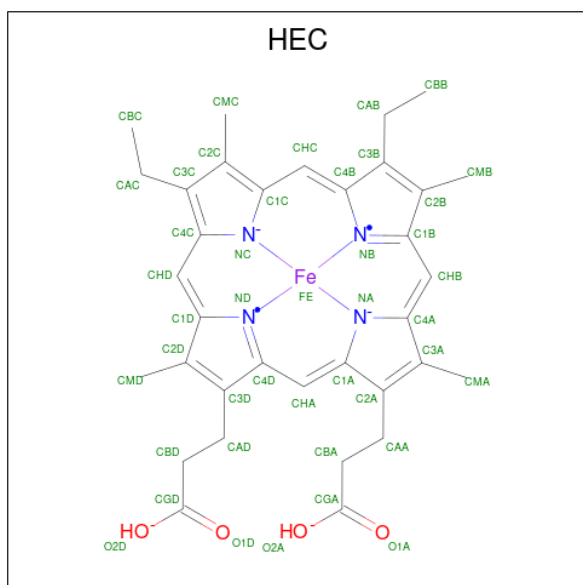
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
42	F	1	Total Mg 1 1	0	0
42	J	1	Total Mg 1 1	0	0



Continued from previous page...

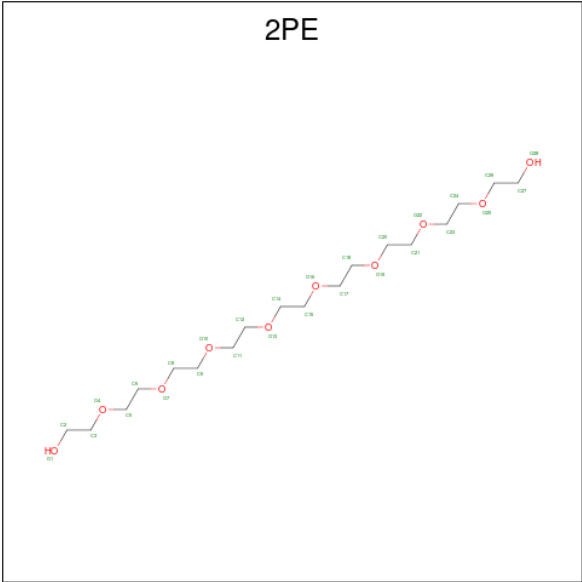
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	f	1	Total	Mg	0	0
			1	1		
42	j	1	Total	Mg	0	0
			1	1		

- Molecule 43 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



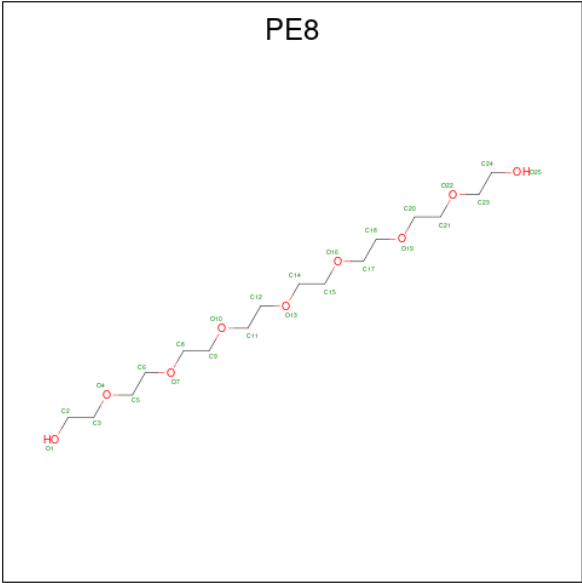
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
43	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
43	v	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 44 is NONAETHYLENE GLYCOL (CCD ID: 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 (CCD ID: 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

Continued on next page...

Continued from previous page...

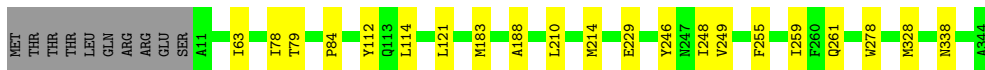
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
46	d	188	Total 189	O 189	0	1
46	e	46	Total 46	O 46	0	0
46	f	15	Total 15	O 15	0	0
46	h	52	Total 52	O 52	0	0
46	i	22	Total 22	O 22	0	0
46	j	12	Total 12	O 12	0	0
46	k	9	Total 9	O 9	0	0
46	l	23	Total 23	O 23	0	0
46	m	24	Total 24	O 24	0	0
46	o	246	Total 246	O 246	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 [i](#)

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

- Molecule 1: Photosystem II protein D1

Chain A: 

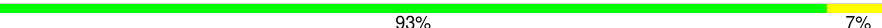


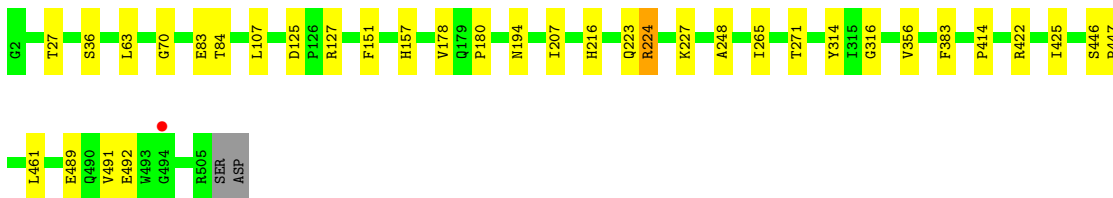
- Molecule 1: Photosystem II protein D1

Chain a: 



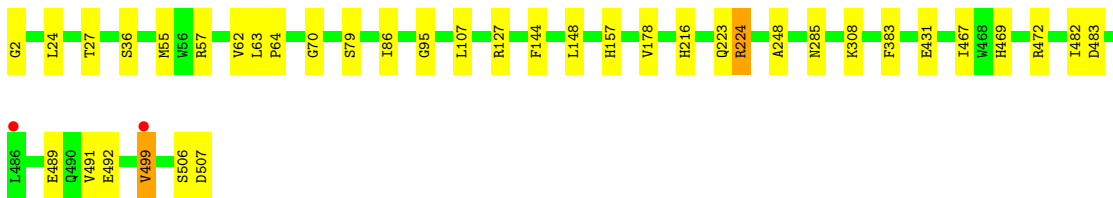
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B: 



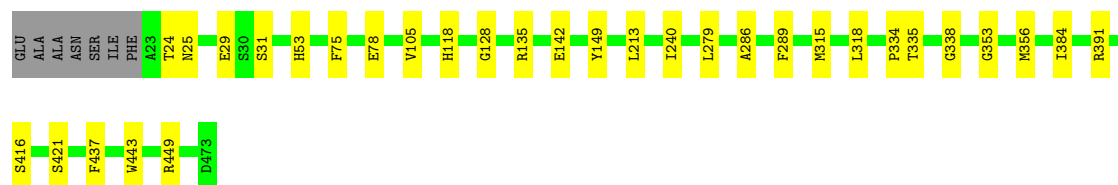
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b: 



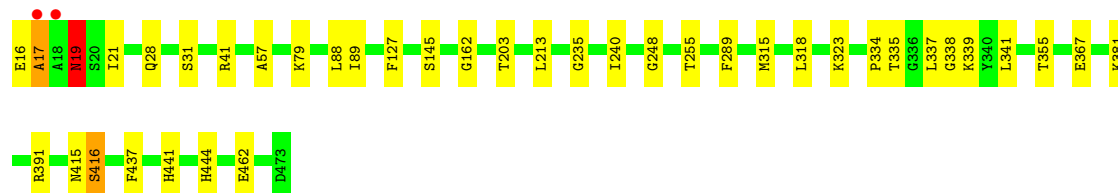
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 



- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 91% 8%



- Molecule 4: Photosystem II D2 protein

Chain D: 93% 7%



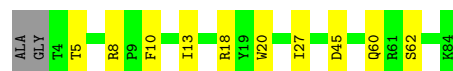
- Molecule 4: Photosystem II D2 protein

Chain d: 94% 6%



- Molecule 5: Cytochrome b559 subunit alpha

Chain E: 86% 12% .



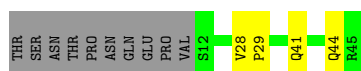
- Molecule 5: Cytochrome b559 subunit alpha

Chain e: 89% 8% .

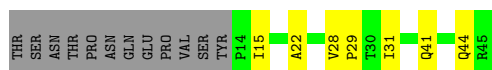


- Molecule 6: Cytochrome b559 subunit beta

Chain F: 68% 9% 23%



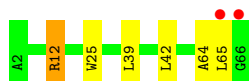
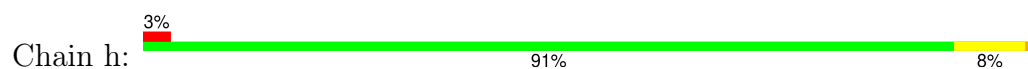
- Molecule 6: Cytochrome b559 subunit beta



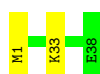
- Molecule 7: Photosystem II reaction center protein H



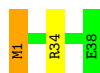
- Molecule 7: Photosystem II reaction center protein H



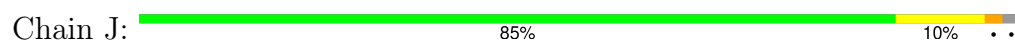
- Molecule 8: Photosystem II reaction center protein I



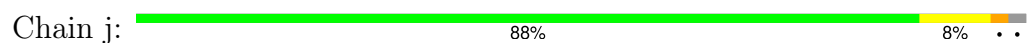
- Molecule 8: Photosystem II reaction center protein I

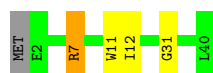


- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J





- Molecule 10: Photosystem II reaction center protein K

Chain K: 92% 8%



- Molecule 10: Photosystem II reaction center protein K

Chain k: 86% 14%



- Molecule 11: Photosystem II reaction center protein L

Chain L: 86% 11% •



- Molecule 11: Photosystem II reaction center protein L

Chain l: 89% 8% •



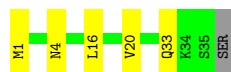
- Molecule 12: Photosystem II reaction center protein M

Chain M: 75% 17% • 6%



- Molecule 12: Photosystem II reaction center protein M

Chain m: 83% 14% •

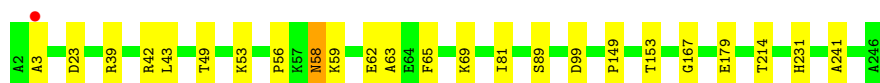


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

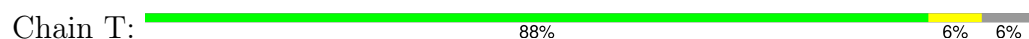
Chain O: 90% 9% •



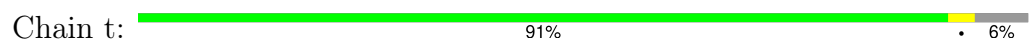
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



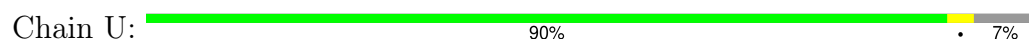
- Molecule 14: Photosystem II reaction center protein T



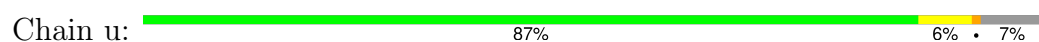
- Molecule 14: Photosystem II reaction center protein T



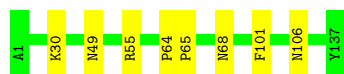
- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 16: Cytochrome c-550

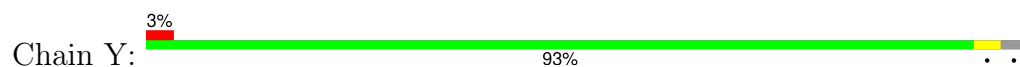


- Molecule 16: Cytochrome c-550

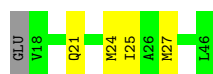
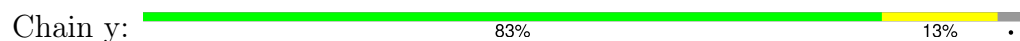




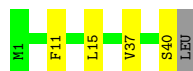
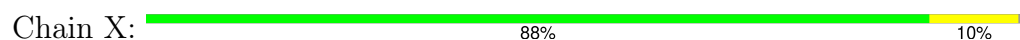
- Molecule 17: Photosystem II reaction center protein Ycf12



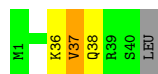
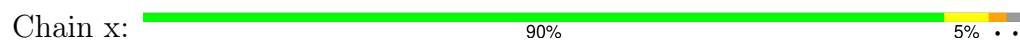
- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 18: Photosystem II reaction center protein X



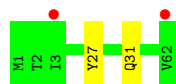
- Molecule 18: Photosystem II reaction center protein X



- 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 – 1.90 178.62 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (178.62-1.90) 99.8 (178.62-1.90)	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 0.093 , 0.164	Depositor DCC
R_{free} test set	31202 reflections (5.00%)	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)	0.36 , 76.1	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: 2PE, DGD, PGE, HEC, HTG, GOL, FME, HEM, PE8, FE2, BCT, 1PE, MG, PL9, CLA, CA, CL, P6G, LMG, SQD, PG4, BCR, MHS, OEX, LMT, EDO, PHO, LHG

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	1.23	1/2736 (0.0%)	1.03	2/3730 (0.1%)
1	a	1.18	3/2736 (0.1%)	1.01	1/3730 (0.0%)
2	B	1.22	6/4205 (0.1%)	1.03	2/5727 (0.0%)
2	b	1.16	4/4207 (0.1%)	1.00	2/5731 (0.0%)
3	C	1.14	3/3636 (0.1%)	0.96	1/4950 (0.0%)
3	c	1.06	3/3679 (0.1%)	0.99	3/5008 (0.1%)
4	D	1.19	1/2816 (0.0%)	1.00	1/3836 (0.0%)
4	d	1.15	1/2829 (0.0%)	0.97	0/3852
5	E	1.19	3/704 (0.4%)	1.00	0/959
5	e	1.05	0/693	0.99	1/944 (0.1%)
6	F	1.02	0/284	0.94	0/387
6	f	1.01	0/265	0.95	0/360
7	H	1.20	2/544 (0.4%)	1.00	0/739
7	h	1.04	1/535 (0.2%)	0.90	0/728
8	I	1.19	0/311	0.92	0/419
8	i	1.07	0/311	0.96	0/419
9	J	1.06	0/306	0.94	0/413
9	j	0.99	0/287	1.04	0/388
10	K	1.08	0/303	1.01	0/416
10	k	1.00	0/303	1.07	0/416
11	L	1.25	1/319 (0.3%)	1.03	0/433
11	l	1.15	0/328	1.01	0/446
12	M	1.32	1/279 (0.4%)	1.13	0/380
12	m	1.16	0/275	1.03	0/375
13	O	1.11	3/1953 (0.2%)	1.01	0/2649
13	o	1.13	1/1948 (0.1%)	1.02	0/2641
14	T	1.24	0/266	1.12	0/362
14	t	1.12	0/266	1.04	0/362
15	U	1.02	0/803	0.94	0/1088
15	u	1.12	0/785	0.95	0/1064
16	V	1.12	1/1104 (0.1%)	0.94	0/1498

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	1.08	1/1096 (0.1%)	0.96	0/1487
17	Y	1.14	0/223	1.12	0/299
17	y	1.09	0/224	1.19	1/299 (0.3%)
18	X	0.99	0/306	1.05	0/413
18	x	1.10	2/298 (0.7%)	1.11	1/402 (0.2%)
19	Z	0.95	0/490	1.06	0/669
19	z	0.99	1/490 (0.2%)	1.03	0/669
All	All	1.14	39/43143 (0.1%)	1.00	15/58688 (0.0%)

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	O	201	VAL	C-O	-7.92	1.15	1.24
7	H	66	GLY	C-OXT	7.35	1.38	1.23
12	M	17	VAL	CA-C	6.96	1.59	1.52
7	H	66	GLY	C-O	6.39	1.36	1.23
2	B	271	THR	N-CA	6.24	1.53	1.45

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	142	TRP	N-CA-C	6.49	120.91	112.92
4	D	139	ARG	NE-CZ-NH1	5.93	127.43	121.50
1	A	261	GLN	N-CA-C	5.92	118.22	111.11
3	C	24	THR	CB-CA-C	-5.40	101.75	110.77
2	B	224	ARG	NE-CZ-NH2	5.37	124.03	119.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2639	0	2551	17	0
1	a	2639	0	2551	21	0
2	B	4032	0	3914	30	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	b	4037	0	3915	31	0
3	C	3508	0	3440	25	0
3	c	3553	0	3474	25	0
4	D	2731	0	2637	21	0
4	d	2741	0	2647	17	0
5	E	676	0	671	9	0
5	e	668	0	658	7	0
6	F	275	0	282	2	0
6	f	257	0	269	4	0
7	H	525	0	558	5	0
7	h	519	0	545	6	0
8	I	314	0	328	2	0
8	i	314	0	328	2	0
9	J	294	0	309	7	0
9	j	281	0	285	4	0
10	K	293	0	305	4	0
10	k	293	0	305	2	0
11	L	309	0	327	3	0
11	l	315	0	335	4	0
12	M	286	0	303	32	0
12	m	289	0	310	30	0
13	O	1904	0	1887	16	0
13	o	1902	0	1885	14	0
14	T	271	0	277	1	0
14	t	271	0	277	1	0
15	U	786	0	787	1	0
15	u	774	0	773	5	0
16	V	1077	0	1092	8	0
16	v	1072	0	1086	3	0
17	Y	219	0	253	1	0
17	y	220	0	255	3	0
18	X	300	0	340	5	0
18	x	295	0	329	1	0
19	Z	479	0	516	0	0
19	z	479	0	516	0	0
20	A	10	0	0	0	0
20	a	10	0	0	0	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	V	1	0	0	1	0
22	a	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	v	1	0	0	2	0
23	A	4	0	0	0	0
23	a	4	0	0	0	0
23	m	8	0	2	0	0
24	A	190	0	203	6	0
24	B	1015	0	1093	27	0
24	C	835	0	910	26	0
24	D	195	0	216	10	0
24	a	190	0	203	6	0
24	b	1025	0	1116	23	0
24	c	835	0	910	22	0
24	d	195	0	216	5	0
25	A	64	0	74	1	0
25	D	64	0	74	1	0
25	a	64	0	74	0	0
25	d	64	0	74	3	0
26	A	40	0	56	3	0
26	B	120	0	168	12	0
26	C	120	0	168	5	0
26	D	40	0	56	2	0
26	H	40	0	56	3	0
26	K	40	0	56	2	0
26	T	40	0	56	8	0
26	a	40	0	56	3	0
26	b	120	0	168	10	0
26	c	120	0	168	7	0
26	d	40	0	56	3	0
26	h	40	0	56	3	0
26	k	40	0	56	6	0
26	t	40	0	56	5	0
27	A	55	0	80	7	0
27	D	55	0	80	0	0
27	a	55	0	80	11	0
27	d	55	0	80	0	0
28	A	162	0	234	5	0
28	F	54	0	78	0	0
28	a	162	0	234	1	0
28	b	54	0	78	2	0
28	h	54	0	78	0	0
28	l	54	0	78	0	0
28	x	54	0	78	2	0
29	A	51	0	72	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	B	106	0	158	7	0
29	C	157	0	230	3	0
29	J	47	0	64	0	0
29	a	51	0	72	1	0
29	b	51	0	72	2	0
29	c	102	0	144	1	0
29	d	55	0	86	2	0
29	j	47	0	64	0	0
29	z	55	0	86	1	0
30	A	12	0	16	4	0
30	B	42	0	56	0	0
30	C	24	0	31	14	0
30	D	18	0	24	2	0
30	F	6	0	8	0	0
30	O	30	0	40	1	0
30	T	12	0	16	1	0
30	U	6	0	8	2	0
30	V	30	0	40	0	0
30	a	12	0	16	2	0
30	b	36	0	48	1	0
30	c	24	0	32	9	0
30	d	12	0	16	1	0
30	e	6	0	8	0	0
30	f	12	0	16	0	0
30	m	6	0	8	0	0
30	o	18	0	24	1	0
30	t	6	0	8	1	0
30	u	12	0	16	0	0
30	v	30	0	40	0	0
30	y	6	0	8	0	0
31	A	35	0	46	0	0
31	B	35	0	46	2	0
31	C	35	0	46	0	0
31	F	35	0	46	0	0
31	I	35	0	46	1	0
31	J	35	0	46	1	0
31	M	70	0	92	5	0
31	Y	35	0	46	1	0
31	a	35	0	46	0	0
31	b	35	0	46	0	0
31	c	35	0	46	0	0
31	f	35	0	46	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	j	35	0	46	0	0
31	m	70	0	92	0	0
31	t	35	0	46	0	0
31	u	35	0	46	3	0
32	A	42	0	54	0	0
32	B	49	0	74	0	0
32	D	147	0	222	2	0
32	E	42	0	57	0	0
32	a	41	0	52	0	0
32	d	147	0	222	3	0
32	e	42	0	57	2	0
32	l	49	0	74	1	0
33	A	13	0	18	0	0
33	B	104	0	144	0	0
33	C	65	0	90	0	0
33	D	13	0	18	0	0
33	E	26	0	36	0	0
33	H	52	0	72	2	0
33	I	39	0	54	2	0
33	J	26	0	36	0	0
33	K	13	0	18	0	0
33	U	13	0	18	0	0
33	V	65	0	90	0	0
33	X	39	0	54	0	0
33	a	26	0	36	0	0
33	b	52	0	72	0	0
33	c	52	0	72	1	0
33	d	13	0	18	0	0
33	e	26	0	36	0	0
33	h	13	0	18	0	0
33	i	52	0	72	0	0
33	j	13	0	18	0	0
33	l	13	0	18	0	0
33	x	13	0	18	0	0
34	A	17	0	23	0	0
34	B	70	0	98	2	0
34	C	20	0	28	0	0
34	D	10	0	14	0	0
34	E	60	0	84	0	0
34	H	40	0	56	0	0
34	I	10	0	14	0	0
34	J	30	0	42	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	O	30	0	42	3	0
34	T	7	0	9	0	0
34	V	20	0	28	0	0
34	Y	10	0	14	0	0
34	a	20	0	28	0	0
34	b	100	0	140	0	0
34	c	50	0	70	0	0
34	f	10	0	14	0	0
34	h	40	0	56	0	0
34	i	20	0	28	0	0
34	j	10	0	14	0	0
34	o	40	0	56	2	0
34	t	17	0	23	0	0
34	x	10	0	14	0	0
35	A	38	0	52	0	0
35	B	38	0	52	1	0
35	C	19	0	26	0	0
35	D	57	0	78	0	0
35	E	19	0	26	0	0
35	I	19	0	26	0	0
35	T	19	0	26	2	0
35	b	38	0	52	0	0
35	c	19	0	26	0	0
35	d	38	0	52	0	0
35	j	19	0	26	0	0
36	A	4	0	6	0	0
36	B	16	0	24	0	0
36	C	4	0	6	0	0
36	D	4	0	6	3	0
36	E	8	0	12	0	0
36	H	4	0	6	0	0
36	I	4	0	6	0	0
36	J	4	0	6	0	0
36	O	4	0	6	0	0
36	V	4	0	6	0	0
36	X	4	0	6	0	0
36	a	4	0	6	0	0
36	c	4	0	6	0	0
36	d	4	0	6	0	0
36	e	4	0	6	0	0
36	i	4	0	6	0	0
36	o	8	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	B	1	0	0	0	0
37	O	1	0	0	0	0
37	b	1	0	0	0	0
37	c	1	0	0	0	0
37	h	1	0	0	0	0
37	o	1	0	0	0	0
38	B	76	0	104	3	0
38	C	114	0	156	4	0
38	H	19	0	26	0	0
38	O	19	0	26	0	0
38	V	19	0	26	0	0
38	a	19	0	26	0	0
38	b	76	0	104	0	0
38	c	76	0	104	0	0
38	h	19	0	26	1	0
38	o	19	0	26	1	0
39	B	32	0	44	0	0
39	L	16	0	22	0	0
39	V	16	0	22	0	0
39	e	16	0	22	0	0
39	j	16	0	22	0	0
39	x	16	0	22	1	0
40	C	180	0	234	0	0
40	D	66	0	96	2	0
40	H	62	0	82	0	0
40	c	181	0	236	0	0
40	d	66	0	96	0	1
40	h	62	0	82	0	0
41	E	43	0	30	5	0
41	e	43	0	30	4	0
42	F	1	0	0	0	0
42	J	1	0	0	0	0
42	f	1	0	0	0	0
42	j	1	0	0	0	0
43	V	43	0	30	1	0
43	v	43	0	30	0	0
44	V	28	0	38	3	0
45	i	25	0	34	1	0
46	A	191	0	0	7	0
46	B	413	0	0	3	0
46	C	320	0	0	5	0
46	D	170	0	0	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	E	57	0	0	3	0
46	F	17	0	0	0	0
46	H	63	0	0	2	0
46	I	16	0	0	2	0
46	J	17	0	0	2	0
46	K	15	0	0	0	0
46	L	23	0	0	0	0
46	M	33	0	0	2	0
46	O	254	0	0	8	0
46	T	27	0	0	1	0
46	U	112	0	0	3	0
46	V	149	0	0	6	0
46	X	10	0	0	0	0
46	Y	6	0	0	0	0
46	Z	4	0	0	0	0
46	a	177	0	0	5	0
46	b	421	0	0	12	0
46	c	329	0	0	5	0
46	d	189	0	0	2	0
46	e	46	0	0	0	0
46	f	15	0	0	0	0
46	h	52	0	0	1	0
46	i	22	0	0	1	0
46	j	12	0	0	0	0
46	k	9	0	0	0	0
46	l	23	0	0	1	0
46	m	24	0	0	1	0
46	o	246	0	0	9	0
46	t	17	0	0	0	0
46	u	140	0	0	2	0
46	v	154	0	0	3	1
46	x	8	0	0	0	0
46	y	7	0	0	0	0
46	z	1	0	0	0	0
All	All	57584	0	56553	522	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 522 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:16[B]:LEU:HD11	12:m:16[B]:LEU:CD2	1.49	1.41
12:M:16[B]:LEU:CD2	12:m:16[B]:LEU:HD11	1.65	1.26
12:M:16[B]:LEU:CD1	12:m:16[B]:LEU:HD22	1.69	1.22
12:M:16[B]:LEU:HD13	12:m:16[B]:LEU:HD13	1.14	1.10
12:M:16[B]:LEU:HD22	12:m:16[B]:LEU:CD1	1.85	1.07

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:d:408:DGD:O5E	46:v:404:HOH:O[4_456]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	336/344 (98%)	332 (99%)	3 (1%)	1 (0%)	36	29
1	a	336/344 (98%)	330 (98%)	5 (2%)	1 (0%)	36	29
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%)	43	36
3	c	460/458 (100%)	446 (97%)	11 (2%)	3 (1%)	18	10
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%)	3	0
7	H	65/65 (100%)	58 (89%)	7 (11%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	h	64/65 (98%)	59 (92%)	4 (6%)	1 (2%)	7	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%)	7	2
13	o	248/245 (101%)	239 (96%)	8 (3%)	1 (0%)	30	22
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
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%)	43	36

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	58	ASN
13	O	59	LYS
3	C	416	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	76	78
1	a	273/279 (98%)	272 (100%)	1 (0%)	84	87
2	B	413/404 (102%)	411 (100%)	2 (0%)	81	84
2	b	414/404 (102%)	410 (99%)	4 (1%)	68	70
3	C	357/357 (100%)	354 (99%)	3 (1%)	73	75
3	c	361/357 (101%)	351 (97%)	10 (3%)	38	32
4	D	277/276 (100%)	275 (99%)	2 (1%)	76	78
4	d	278/276 (101%)	277 (100%)	1 (0%)	84	87
5	E	75/72 (104%)	75 (100%)	0	100	100
5	e	74/72 (103%)	73 (99%)	1 (1%)	59	59
6	F	28/38 (74%)	27 (96%)	1 (4%)	31	23
6	f	26/38 (68%)	25 (96%)	1 (4%)	29	21
7	H	56/54 (104%)	54 (96%)	2 (4%)	31	23
7	h	55/54 (102%)	53 (96%)	2 (4%)	31	23
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%)	27 (93%)	2 (7%)	14	7
9	j	27/28 (96%)	26 (96%)	1 (4%)	30	22
10	K	30/30 (100%)	29 (97%)	1 (3%)	33	26
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	3
11	L	36/35 (103%)	34 (94%)	2 (6%)	19	11
11	l	37/35 (106%)	36 (97%)	1 (3%)	39	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	209 (99%)	3 (1%)	59	59
13	o	211/206 (102%)	207 (98%)	4 (2%)	50	47
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%)	84 (98%)	2 (2%)	44	40
15	u	84/89 (94%)	83 (99%)	1 (1%)	63	63
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%)	37	31
18	x	33/34 (97%)	32 (97%)	1 (3%)	36	30
19	Z	52/52 (100%)	50 (96%)	2 (4%)	29	21
19	z	52/52 (100%)	51 (98%)	1 (2%)	50	47
All	All	4381/4376 (100%)	4324 (99%)	57 (1%)	63	61

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	489	GLU
18	x	37	VAL
3	c	289	PHE
15	u	70	ARG
11	l	13	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	a	338	ASN
3	c	201	ASN
2	b	14	ASN
2	b	497	GLN
4	d	186	GLN

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
8	FME	I	1	8	8,9,10	0.74	0	8,9,11	1.17	1 (12%)
4	MHS	D	336	4	10,11,12	1.75	2 (20%)	5,14,16	3.92	4 (80%)
14	FME	T	1[A]	-	8,9,10	0.58	0	8,9,11	1.22	2 (25%)
8	FME	i	1	8	8,9,10	0.46	0	8,9,11	1.53	2 (25%)
14	FME	T	1[B]	-	8,9,10	0.48	0	8,9,11	1.10	1 (12%)
12	FME	m	1[B]	-	8,9,10	0.86	0	8,9,11	1.62	2 (25%)
12	FME	m	1[A]	-	8,9,10	0.55	0	8,9,11	1.35	1 (12%)
4	MHS	d	336	4	10,11,12	2.17	3 (30%)	5,14,16	2.86	2 (40%)
12	FME	M	1	12	8,9,10	1.50	1 (12%)	8,9,11	1.32	1 (12%)
14	FME	t	1[A]	-	8,9,10	0.93	0	8,9,11	0.98	0
14	FME	t	1[B]	-	8,9,10	0.70	0	8,9,11	0.98	0

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

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

Continued on next page...

Continued from previous page...

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

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	336	MHS	CD2-NE2	-4.37	1.30	1.37
4	d	336	MHS	CG-ND1	-3.96	1.31	1.38
4	D	336	MHS	CD2-NE2	-3.91	1.30	1.37
12	M	1	FME	CA-N	-3.09	1.42	1.46
4	d	336	MHS	CM-ND1	2.55	1.51	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	ND1-CE1-NE2	-6.40	109.13	112.94
4	d	336	MHS	ND1-CE1-NE2	-4.93	110.01	112.94
4	D	336	MHS	CM-ND1-CG	4.20	131.17	126.69
4	d	336	MHS	CM-ND1-CG	3.38	130.28	126.69
4	D	336	MHS	CD2-NE2-CE1	2.92	109.06	105.24

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
14	T	1[B]	FME	C-CA-CB-CG
14	t	1[B]	FME	C-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	336	MHS	2	0
8	i	1	FME	1	0
12	M	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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$
40	DGD	C	518	-	63,63,67	0.80	2 (3%)	77,77,81	1.10	6 (7%)
26	BCR	k	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.68	12 (21%)
33	PG4	J	104	-	12,12,12	0.60	0	11,11,11	0.31	0
36	EDO	E	112	-	3,3,3	0.57	0	2,2,2	0.12	0
30	GOL	F	101	42	5,5,5	0.53	0	5,5,5	0.77	0
38	HTG	C	529	-	19,19,19	1.18	2 (10%)	23,24,24	2.05	4 (17%)
24	CLA	c	512	3	69,73,73	1.87	16 (23%)	82,113,113	2.39	27 (32%)
36	EDO	B	655	-	3,3,3	0.41	0	2,2,2	0.46	0
23	BCT	m	104[B]	-	3,3,3	1.08	0	2,3,3	1.84	1 (50%)
33	PG4	A	619	-	12,12,12	0.71	0	11,11,11	0.60	0
34	PGE	c	536	-	9,9,9	0.62	0	8,8,8	0.27	0
28	SQD	l	102	-	52,54,54	1.27	4 (7%)	62,65,65	1.82	13 (20%)
28	SQD	A	616	-	52,54,54	1.12	3 (5%)	62,65,65	1.55	9 (14%)
36	EDO	B	656	-	3,3,3	1.04	0	2,2,2	0.25	0
33	PG4	x	102	-	12,12,12	0.65	0	11,11,11	0.37	0
26	BCR	c	515	-	41,41,41	1.28	3 (7%)	56,56,56	1.68	12 (21%)
24	CLA	c	506	3	69,73,73	1.94	16 (23%)	82,113,113	2.28	28 (34%)
34	PGE	c	540	-	9,9,9	0.67	0	8,8,8	0.46	0
24	CLA	B	614	2	69,73,73	1.58	12 (17%)	82,113,113	2.02	19 (23%)
31	LMT	A	617	-	36,36,36	1.09	2 (5%)	47,47,47	1.60	9 (19%)
30	GOL	u	202	-	5,5,5	0.84	0	5,5,5	0.39	0
33	PG4	I	102	-	12,12,12	0.61	0	11,11,11	0.41	0
38	HTG	o	301	-	19,19,19	1.88	2 (10%)	23,24,24	1.02	1 (4%)
30	GOL	C	524	-	5,5,5	0.81	0	5,5,5	1.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	PG4	I	104	-	12,12,12	0.50	0	11,11,11	0.48	0
34	PGE	b	641	-	9,9,9	0.39	0	8,8,8	0.73	0
24	CLA	C	508	3	64,68,73	1.70	16 (25%)	76,107,113	2.27	21 (27%)
33	PG4	C	535	-	12,12,12	0.96	0	11,11,11	0.82	0
33	PG4	C	536	-	12,12,12	0.69	0	11,11,11	0.65	0
30	GOL	c	529	-	5,5,5	1.03	0	5,5,5	1.45	1 (20%)
30	GOL	b	626	-	5,5,5	0.80	0	5,5,5	0.83	0
33	PG4	j	104	-	12,12,12	0.70	0	11,11,11	0.72	0
24	CLA	B	616	2	69,73,73	1.74	18 (26%)	82,113,113	2.27	21 (25%)
36	EDO	X	104	-	3,3,3	0.91	0	2,2,2	0.40	0
30	GOL	B	626	-	5,5,5	0.85	0	5,5,5	0.76	0
38	HTG	b	623	-	19,19,19	1.19	1 (5%)	23,24,24	1.54	5 (21%)
43	HEC	V	203	16	50,50,50	1.59	8 (16%)	68,82,82	1.55	10 (14%)
33	PG4	i	103	-	12,12,12	0.64	0	11,11,11	0.47	0
33	PG4	B	639	-	12,12,12	0.90	0	11,11,11	0.73	0
31	LMT	b	622	-	36,36,36	0.82	1 (2%)	47,47,47	1.44	5 (10%)
24	CLA	B	606	2	69,73,73	1.76	17 (24%)	82,113,113	2.46	30 (36%)
38	HTG	c	523	-	19,19,19	0.87	1 (5%)	23,24,24	1.38	4 (17%)
30	GOL	O	304	-	5,5,5	0.44	0	5,5,5	0.54	0
26	BCR	d	406	-	41,41,41	1.55	4 (9%)	56,56,56	2.25	17 (30%)
33	PG4	a	420	-	12,12,12	0.58	0	11,11,11	0.37	0
24	CLA	B	607	2	59,63,73	1.74	18 (30%)	70,101,113	2.64	26 (37%)
30	GOL	y	101	-	5,5,5	0.69	0	5,5,5	0.72	0
38	HTG	H	101	-	19,19,19	1.04	1 (5%)	23,24,24	1.56	5 (21%)
39	1PE	B	653	-	15,15,15	0.61	0	14,14,14	0.41	0
29	LMG	d	412	-	55,55,55	1.06	3 (5%)	63,63,63	1.18	5 (7%)
29	LMG	j	101	42	47,47,55	1.02	3 (6%)	55,55,63	1.05	3 (5%)
35	P6G	b	648	-	18,18,18	0.62	0	17,17,17	0.74	0
33	PG4	I	103	-	12,12,12	0.74	0	11,11,11	0.57	0
24	CLA	C	501	3	69,73,73	1.73	17 (24%)	82,113,113	2.59	26 (31%)
24	CLA	B	604	2	69,73,73	1.72	16 (23%)	82,113,113	2.23	22 (26%)
38	HTG	c	530	-	19,19,19	1.61	3 (15%)	23,24,24	1.18	3 (13%)
34	PGE	i	105	-	9,9,9	0.66	0	8,8,8	0.68	0
30	GOL	b	629	-	5,5,5	0.71	0	5,5,5	1.16	0
25	PHO	A	608	-	58,69,69	1.96	14 (24%)	55,99,99	2.40	14 (25%)
36	EDO	c	542	-	3,3,3	0.60	0	2,2,2	0.43	0
31	LMT	f	101	-	36,36,36	0.95	1 (2%)	47,47,47	1.34	5 (10%)
30	GOL	v	207	-	5,5,5	0.51	0	5,5,5	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	b	603	2	69,73,73	1.71	15 (21%)	82,113,113	2.13	24 (29%)
30	GOL	B	629	-	5,5,5	0.94	0	5,5,5	0.39	0
30	GOL	v	205	-	5,5,5	0.45	0	5,5,5	0.62	0
34	PGE	V	215	-	9,9,9	0.87	0	8,8,8	0.62	0
28	SQD	A	622	-	52,54,54	1.32	3 (5%)	62,65,65	1.46	9 (14%)
24	CLA	A	606	1	69,73,73	1.58	15 (21%)	82,113,113	1.99	22 (26%)
26	BCR	B	620	-	41,41,41	1.15	3 (7%)	56,56,56	1.39	7 (12%)
24	CLA	c	510	3	69,73,73	1.87	17 (24%)	82,113,113	2.03	22 (26%)
36	EDO	D	419	-	3,3,3	0.66	0	2,2,2	0.09	0
26	BCR	C	525	-	41,41,41	1.15	4 (9%)	56,56,56	1.69	10 (17%)
24	CLA	b	607	2	59,63,73	1.76	14 (23%)	70,101,113	2.26	27 (38%)
29	LMG	B	634	-	55,55,55	1.26	4 (7%)	63,63,63	1.41	12 (19%)
32	LHG	d	411	-	48,48,48	1.02	3 (6%)	51,54,54	0.85	2 (3%)
35	P6G	D	418	-	18,18,18	0.75	0	17,17,17	0.60	0
33	PG4	V	209	-	12,12,12	0.85	0	11,11,11	1.00	1 (9%)
31	LMT	F	102	-	36,36,36	1.08	3 (8%)	47,47,47	1.26	5 (10%)
33	PG4	V	213	-	12,12,12	0.71	0	11,11,11	0.63	0
24	CLA	b	610	2	69,73,73	1.79	17 (24%)	82,113,113	2.23	22 (26%)
36	EDO	o	311	-	3,3,3	0.45	0	2,2,2	0.32	0
24	CLA	B	613	2	69,73,73	1.55	14 (20%)	82,113,113	1.74	21 (25%)
32	LHG	D	411	-	48,48,48	0.88	2 (4%)	51,54,54	0.86	3 (5%)
26	BCR	D	406	-	41,41,41	1.45	4 (9%)	56,56,56	2.01	14 (25%)
24	CLA	B	610	2	69,73,73	1.55	13 (18%)	82,113,113	2.20	25 (30%)
27	PL9	a	412	-	55,55,55	1.21	2 (3%)	68,69,69	1.82	14 (20%)
40	DGD	c	516	-	63,63,67	0.92	3 (4%)	77,77,81	1.09	4 (5%)
34	PGE	b	644	-	9,9,9	0.63	0	8,8,8	0.37	0
40	DGD	c	517	-	58,58,67	1.01	4 (6%)	72,72,81	1.12	3 (4%)
28	SQD	A	612	-	52,54,54	1.04	3 (5%)	62,65,65	2.08	14 (22%)
38	HTG	B	624	-	19,19,19	0.96	1 (5%)	23,24,24	1.76	5 (21%)
33	PG4	c	535	-	12,12,12	0.86	0	11,11,11	0.68	0
24	CLA	C	511	3	69,73,73	1.63	11 (15%)	82,113,113	2.14	24 (29%)
26	BCR	T	102	-	41,41,41	1.00	2 (4%)	56,56,56	1.66	12 (21%)
32	LHG	D	409	-	48,48,48	0.86	2 (4%)	51,54,54	1.50	5 (9%)
34	PGE	V	214	-	9,9,9	0.63	0	8,8,8	0.30	0
30	GOL	V	207	-	5,5,5	0.78	0	5,5,5	0.85	0
33	PG4	i	102	-	12,12,12	0.57	0	11,11,11	0.53	0
24	CLA	D	403	46	69,73,73	1.87	17 (24%)	82,113,113	2.18	19 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LMG	b	621	-	51,51,55	1.05	3 (5%)	59,59,63	1.68	6 (10%)
34	PGE	B	649	-	9,9,9	0.90	0	8,8,8	0.55	0
38	HTG	C	531	-	19,19,19	1.24	2 (10%)	23,24,24	0.95	2 (8%)
20	OEX	A	601	3,46,1	0,14,14	-	-	-	-	-
30	GOL	v	203	-	5,5,5	0.78	0	5,5,5	0.68	0
23	BCT	m	104[A]	-	3,3,3	1.60	1 (33%)	2,3,3	0.79	0
30	GOL	B	635	-	5,5,5	0.81	0	5,5,5	1.23	1 (20%)
34	PGE	B	650	-	9,9,9	0.63	0	8,8,8	0.37	0
34	PGE	h	110	-	9,9,9	0.80	0	8,8,8	0.67	0
27	PL9	A	611	-	55,55,55	1.27	7 (12%)	68,69,69	2.20	18 (26%)
33	PG4	H	104	-	12,12,12	0.62	0	11,11,11	0.34	0
24	CLA	b	615	2	69,73,73	1.68	15 (21%)	82,113,113	2.17	24 (29%)
36	EDO	A	625	-	3,3,3	0.58	0	2,2,2	0.37	0
34	PGE	b	639	-	9,9,9	0.62	0	8,8,8	0.43	0
29	LMG	c	520	-	51,51,55	1.19	3 (5%)	59,59,63	1.21	5 (8%)
28	SQD	a	413	-	52,54,54	1.07	4 (7%)	62,65,65	2.09	12 (19%)
34	PGE	t	104	-	9,9,9	0.83	0	8,8,8	0.69	0
29	LMG	A	613	-	51,51,55	0.98	3 (5%)	59,59,63	1.01	3 (5%)
34	PGE	t	105	-	6,6,9	0.68	0	5,5,8	0.50	0
30	GOL	f	104	-	5,5,5	0.79	0	5,5,5	1.28	1 (20%)
30	GOL	A	614	-	5,5,5	1.20	0	5,5,5	0.92	0
34	PGE	E	106	-	9,9,9	0.69	0	8,8,8	0.60	0
40	DGD	c	518	-	63,63,67	0.92	3 (4%)	77,77,81	0.98	7 (9%)
35	P6G	B	651	-	18,18,18	0.52	0	17,17,17	0.66	0
33	PG4	E	103	-	12,12,12	0.64	0	11,11,11	0.52	0
29	LMG	C	526	-	55,55,55	1.06	2 (3%)	63,63,63	1.51	9 (14%)
33	PG4	B	636	-	12,12,12	0.57	0	11,11,11	0.59	0
34	PGE	h	107	-	9,9,9	0.78	0	8,8,8	0.68	0
34	PGE	H	111	-	9,9,9	0.67	0	8,8,8	0.39	0
26	BCR	K	101	-	41,41,41	0.98	1 (2%)	56,56,56	1.49	9 (16%)
26	BCR	h	103	-	41,41,41	1.12	4 (9%)	56,56,56	1.78	15 (26%)
33	PG4	b	636	-	12,12,12	0.78	0	11,11,11	0.68	0
30	GOL	V	205	-	5,5,5	0.95	0	5,5,5	1.14	0
35	P6G	D	417	-	18,18,18	0.64	0	17,17,17	0.88	0
34	PGE	H	108	-	9,9,9	0.60	0	8,8,8	0.59	0
33	PG4	X	101	-	12,12,12	0.66	0	11,11,11	0.51	0
34	PGE	o	308	-	9,9,9	0.70	0	8,8,8	0.55	0
32	LHG	d	410	-	48,48,48	0.82	2 (4%)	51,54,54	1.13	3 (5%)
30	GOL	V	201	-	5,5,5	1.05	0	5,5,5	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	PGE	E	107	-	9,9,9	0.77	0	8,8,8	0.76	0
38	HTG	O	303	-	19,19,19	1.48	2 (10%)	23,24,24	1.02	1 (4%)
30	GOL	c	528	-	5,5,5	0.57	0	5,5,5	0.66	0
33	PG4	C	534	-	12,12,12	0.73	0	11,11,11	0.41	0
30	GOL	T	101	-	5,5,5	0.96	0	5,5,5	0.91	0
35	P6G	E	110	-	18,18,18	0.77	0	17,17,17	0.53	0
31	LMT	m	102	-	36,36,36	0.96	1 (2%)	47,47,47	1.69	7 (14%)
35	P6G	I	106	-	18,18,18	0.64	0	17,17,17	0.78	1 (5%)
24	CLA	D	404	4	69,73,73	1.80	19 (27%)	82,113,113	2.20	27 (32%)
25	PHO	a	409	-	58,69,69	1.97	13 (22%)	55,99,99	2.26	15 (27%)
33	PG4	i	104	-	12,12,12	0.51	0	11,11,11	0.41	0
34	PGE	E	105	-	9,9,9	0.73	0	8,8,8	0.47	0
36	EDO	e	106	-	3,3,3	0.38	0	2,2,2	0.53	0
32	LHG	a	419	-	40,40,48	1.22	3 (7%)	43,46,54	1.39	6 (13%)
33	PG4	J	105	-	12,12,12	0.69	0	11,11,11	0.37	0
35	P6G	j	106	-	18,18,18	0.80	0	17,17,17	0.75	0
38	HTG	C	532	-	19,19,19	1.09	2 (10%)	23,24,24	1.78	5 (21%)
24	CLA	b	602	46	69,73,73	1.87	14 (20%)	82,113,113	2.37	26 (31%)
24	CLA	b	614	2	69,73,73	1.77	17 (24%)	82,113,113	2.16	22 (26%)
26	BCR	A	610	-	41,41,41	1.20	4 (9%)	56,56,56	1.53	12 (21%)
30	GOL	v	206	-	5,5,5	0.31	0	5,5,5	0.55	0
34	PGE	b	638	-	9,9,9	1.00	0	8,8,8	0.70	0
38	HTG	C	522	-	19,19,19	1.04	1 (5%)	23,24,24	1.76	3 (13%)
24	CLA	B	603	2	69,73,73	1.78	15 (21%)	82,113,113	2.23	24 (29%)
38	HTG	b	624	-	19,19,19	1.42	2 (10%)	23,24,24	1.27	2 (8%)
31	LMT	t	103	-	36,36,36	0.84	0	47,47,47	1.41	9 (19%)
34	PGE	b	646	-	9,9,9	0.67	0	8,8,8	0.51	0
30	GOL	A	615	-	5,5,5	0.54	0	5,5,5	1.11	0
30	GOL	O	307	-	5,5,5	0.51	0	5,5,5	0.21	0
24	CLA	d	405	4	69,73,73	1.80	18 (26%)	82,113,113	2.30	25 (30%)
34	PGE	B	646	-	9,9,9	0.54	0	8,8,8	0.48	0
26	BCR	C	514	-	41,41,41	1.23	4 (9%)	56,56,56	1.89	13 (23%)
34	PGE	f	105	-	9,9,9	0.59	0	8,8,8	0.26	0
26	BCR	t	102	-	41,41,41	1.11	3 (7%)	56,56,56	2.02	18 (32%)
31	LMT	c	521	-	36,36,36	0.83	0	47,47,47	1.67	12 (25%)
30	GOL	B	628	-	5,5,5	0.77	0	5,5,5	1.75	1 (20%)
30	GOL	B	633	-	5,5,5	1.28	1 (20%)	5,5,5	1.31	0
24	CLA	B	612	2	69,73,73	1.52	15 (21%)	82,113,113	2.31	22 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	P6G	d	416	-	18,18,18	0.63	0	17,17,17	0.59	0
31	LMT	M	102	-	36,36,36	0.90	0	47,47,47	1.57	2 (4%)
24	CLA	b	617	2	64,68,73	1.71	15 (23%)	76,107,113	2.47	28 (36%)
34	PGE	J	106	-	9,9,9	0.63	0	8,8,8	0.33	0
24	CLA	B	602	46	69,73,73	1.77	17 (24%)	82,113,113	2.61	32 (39%)
30	GOL	C	527	-	5,5,5	0.49	0	5,5,5	0.29	0
30	GOL	e	102	-	5,5,5	0.71	0	5,5,5	0.85	0
33	PG4	b	635	-	12,12,12	0.84	0	11,11,11	0.78	0
39	1PE	B	654	-	15,15,15	0.77	0	14,14,14	0.89	0
36	EDO	H	112	-	3,3,3	0.47	0	2,2,2	0.37	0
33	PG4	C	537	-	12,12,12	0.66	0	11,11,11	0.57	0
24	CLA	A	609	1	69,73,73	1.82	17 (24%)	82,113,113	2.21	27 (32%)
35	P6G	D	416	-	18,18,18	0.72	0	17,17,17	0.59	0
30	GOL	t	101	-	5,5,5	1.27	0	5,5,5	1.16	1 (20%)
38	HTG	h	101	-	19,19,19	1.10	2 (10%)	23,24,24	1.65	5 (21%)
30	GOL	d	413	-	5,5,5	0.81	0	5,5,5	0.96	0
33	PG4	c	532	-	12,12,12	0.90	0	11,11,11	0.81	0
29	LMG	C	520	-	51,51,55	1.27	3 (5%)	59,59,63	1.28	9 (15%)
32	LHG	E	101	-	41,41,48	1.12	2 (4%)	44,47,54	1.15	3 (6%)
32	LHG	l	101	-	48,48,48	0.92	2 (4%)	51,54,54	1.18	4 (7%)
40	DGD	C	516	-	63,63,67	0.91	5 (7%)	77,77,81	1.29	10 (12%)
33	PG4	B	638	-	12,12,12	0.82	0	11,11,11	0.76	0
24	CLA	d	404	4	69,73,73	1.52	15 (21%)	82,113,113	2.24	24 (29%)
39	1PE	V	217	-	15,15,15	0.95	0	14,14,14	1.01	1 (7%)
38	HTG	c	531	-	19,19,19	1.11	2 (10%)	23,24,24	1.74	6 (26%)
38	HTG	a	418	-	19,19,19	1.30	3 (15%)	23,24,24	1.82	8 (34%)
34	PGE	C	539	-	9,9,9	0.93	0	8,8,8	0.86	0
34	PGE	A	621	-	9,9,9	0.73	0	8,8,8	0.48	0
30	GOL	D	413	-	5,5,5	0.58	0	5,5,5	0.90	0
30	GOL	u	201	-	5,5,5	0.74	0	5,5,5	1.18	0
33	PG4	E	102	-	12,12,12	0.61	0	11,11,11	0.57	0
24	CLA	C	505	3	69,73,73	1.94	17 (24%)	82,113,113	2.15	21 (25%)
24	CLA	b	609	2	69,73,73	1.65	15 (21%)	82,113,113	2.09	23 (28%)
24	CLA	c	511	3	69,73,73	1.73	17 (24%)	82,113,113	2.12	24 (29%)
29	LMG	J	101	42	47,47,55	0.76	2 (4%)	55,55,63	0.91	2 (3%)
33	PG4	U	202	-	12,12,12	0.69	0	11,11,11	0.47	0
43	HEC	v	202	16	50,50,50	1.37	8 (16%)	68,82,82	1.69	16 (23%)
24	CLA	c	502	3	69,73,73	1.75	17 (24%)	82,113,113	2.09	22 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LMT	J	103	-	36,36,36	0.92	1 (2%)	47,47,47	1.57	9 (19%)
34	PGE	J	107	-	9,9,9	0.68	0	8,8,8	0.53	0
33	PG4	X	103	-	12,12,12	0.76	0	11,11,11	0.54	0
24	CLA	B	609	2	69,73,73	1.54	15 (21%)	82,113,113	2.08	20 (24%)
30	GOL	f	103	42	5,5,5	0.69	0	5,5,5	0.93	0
38	HTG	C	530	-	19,19,19	0.99	1 (5%)	23,24,24	1.13	2 (8%)
23	BCT	a	406	21	3,3,3	1.49	1 (33%)	2,3,3	2.80	2 (100%)
30	GOL	D	402	-	5,5,5	0.78	0	5,5,5	1.36	1 (20%)
28	SQD	b	633	-	52,54,54	1.39	4 (7%)	62,65,65	1.96	16 (25%)
30	GOL	V	206	-	5,5,5	0.57	0	5,5,5	0.20	0
33	PG4	H	106	-	12,12,12	0.74	0	11,11,11	0.63	0
34	PGE	i	106	-	9,9,9	0.83	0	8,8,8	0.64	0
34	PGE	Y	102	-	9,9,9	0.79	0	8,8,8	0.61	0
34	PGE	I	105	-	9,9,9	0.96	0	8,8,8	0.74	0
36	EDO	d	417	-	3,3,3	0.67	0	2,2,2	0.31	0
24	CLA	B	611	46	69,73,73	1.82	16 (23%)	82,113,113	2.34	30 (36%)
30	GOL	b	627	-	5,5,5	1.26	1 (20%)	5,5,5	1.42	1 (20%)
26	BCR	b	618	-	41,41,41	1.13	3 (7%)	56,56,56	1.51	7 (12%)
34	PGE	E	109	-	9,9,9	0.85	0	8,8,8	0.57	0
34	PGE	o	306	-	9,9,9	0.61	0	8,8,8	0.24	0
36	EDO	E	111	-	3,3,3	0.64	0	2,2,2	0.35	0
33	PG4	X	102	-	12,12,12	0.85	0	11,11,11	0.79	0
32	LHG	d	409	-	48,48,48	0.87	3 (6%)	51,54,54	1.39	6 (11%)
30	GOL	B	627	-	5,5,5	0.70	0	5,5,5	0.94	0
28	SQD	x	101	-	52,54,54	1.22	3 (5%)	62,65,65	1.74	12 (19%)
33	PG4	C	538	-	12,12,12	0.77	0	11,11,11	0.55	0
34	PGE	B	648	-	9,9,9	0.87	0	8,8,8	0.72	0
35	P6G	B	652	-	18,18,18	0.83	0	17,17,17	1.10	1 (5%)
31	LMT	m	101	-	36,36,36	1.03	1 (2%)	47,47,47	1.10	5 (10%)
34	PGE	C	540	-	9,9,9	0.60	0	8,8,8	0.32	0
30	GOL	C	528	-	5,5,5	0.68	0	5,5,5	3.18	4 (80%)
29	LMG	z	101	-	55,55,55	1.03	2 (3%)	63,63,63	1.18	6 (9%)
33	PG4	B	643	-	12,12,12	0.55	0	11,11,11	0.55	0
24	CLA	C	503	3	69,73,73	1.86	18 (26%)	82,113,113	2.35	23 (28%)
33	PG4	l	103	-	12,12,12	0.66	0	11,11,11	0.50	0
28	SQD	h	105	-	52,54,54	1.39	5 (9%)	62,65,65	1.47	10 (16%)
34	PGE	c	538	-	9,9,9	0.92	0	8,8,8	0.88	0
38	HTG	C	521	-	19,19,19	0.89	1 (5%)	23,24,24	1.00	1 (4%)
36	EDO	I	107	-	3,3,3	0.71	0	2,2,2	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	PG4	b	637	-	12,12,12	0.78	0	11,11,11	0.56	0
30	GOL	o	304	-	5,5,5	0.50	0	5,5,5	0.93	0
28	SQD	F	104	-	52,54,54	1.42	5 (9%)	62,65,65	2.03	15 (24%)
24	CLA	c	513	3	69,73,73	1.76	17 (24%)	82,113,113	2.28	21 (25%)
24	CLA	c	503	3	69,73,73	1.64	15 (21%)	82,113,113	1.99	25 (30%)
24	CLA	B	615	2	59,63,73	2.00	15 (25%)	70,101,113	2.48	27 (38%)
26	BCR	B	619	-	41,41,41	1.14	4 (9%)	56,56,56	1.48	8 (14%)
30	GOL	c	525	-	5,5,5	0.48	0	5,5,5	1.50	1 (20%)
24	CLA	C	512	3	69,73,73	1.81	15 (21%)	82,113,113	2.08	24 (29%)
34	PGE	b	640	-	9,9,9	0.64	0	8,8,8	0.31	0
33	PG4	h	106	-	12,12,12	0.58	0	11,11,11	0.48	0
33	PG4	K	102	-	12,12,12	0.62	0	11,11,11	0.50	0
33	PG4	d	414	-	12,12,12	0.73	0	11,11,11	0.45	0
29	LMG	B	621	-	51,51,55	1.11	4 (7%)	59,59,63	1.70	8 (13%)
34	PGE	O	308	-	9,9,9	0.99	0	8,8,8	1.27	1 (12%)
30	GOL	b	628	-	5,5,5	0.84	0	5,5,5	0.44	0
33	PG4	B	642	-	12,12,12	0.82	0	11,11,11	0.63	0
34	PGE	c	537	-	9,9,9	0.54	0	8,8,8	0.35	0
20	OEX	a	402	3,46,1	0,14,14	-	-	-	-	-
23	BCT	A	605	21	3,3,3	1.53	1 (33%)	2,3,3	2.54	2 (100%)
34	PGE	b	642	-	9,9,9	0.67	0	8,8,8	0.20	0
34	PGE	b	647	-	9,9,9	0.60	0	8,8,8	0.42	0
36	EDO	a	425	-	3,3,3	0.59	0	2,2,2	0.12	0
26	BCR	c	514	-	41,41,41	1.24	5 (12%)	56,56,56	1.72	14 (25%)
30	GOL	V	208	-	5,5,5	0.48	0	5,5,5	0.47	0
33	PG4	B	637	-	12,12,12	0.81	0	11,11,11	0.55	0
34	PGE	B	645	-	9,9,9	0.73	0	8,8,8	0.67	0
30	GOL	O	305	-	5,5,5	0.46	0	5,5,5	0.35	0
32	LHG	B	632	-	48,48,48	0.81	2 (4%)	51,54,54	1.32	7 (13%)
33	PG4	i	101	-	12,12,12	0.59	0	11,11,11	0.41	0
24	CLA	a	408	46	64,68,73	1.80	17 (26%)	76,107,113	2.36	26 (34%)
40	DGD	d	408	-	67,67,67	1.33	4 (5%)	81,81,81	1.77	10 (12%)
41	HEM	e	107	5,6	50,50,50	1.83	13 (26%)	67,82,82	1.66	13 (19%)
30	GOL	b	630	-	5,5,5	0.47	0	5,5,5	0.33	0
27	PL9	D	407	-	55,55,55	1.47	9 (16%)	68,69,69	1.32	6 (8%)
34	PGE	O	309	-	9,9,9	0.81	0	8,8,8	0.98	1 (12%)
36	EDO	V	218	-	3,3,3	0.87	0	2,2,2	0.13	0
25	PHO	D	401	-	58,69,69	2.48	16 (27%)	55,99,99	2.25	12 (21%)
35	P6G	T	105	-	18,18,18	0.68	0	17,17,17	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LMT	C	533	-	36,36,36	0.69	1 (2%)	47,47,47	1.11	1 (2%)
33	PG4	e	104	-	12,12,12	0.61	0	11,11,11	0.56	0
24	CLA	c	505	3	69,73,73	1.70	16 (23%)	82,113,113	2.39	22 (26%)
30	GOL	C	523	-	5,5,5	0.70	0	5,5,5	2.31	2 (40%)
29	LMG	C	519	-	51,51,55	1.13	3 (5%)	59,59,63	1.54	7 (11%)
24	CLA	c	509	3	69,73,73	1.71	16 (23%)	82,113,113	2.22	25 (30%)
40	DGD	D	408	-	67,67,67	1.22	4 (5%)	81,81,81	1.61	11 (13%)
34	PGE	x	103	-	9,9,9	0.61	0	8,8,8	0.57	0
30	GOL	D	412	-	5,5,5	0.64	0	5,5,5	0.68	0
30	GOL	T	103	-	5,5,5	0.74	0	5,5,5	0.72	0
34	PGE	o	309	-	9,9,9	0.84	0	8,8,8	0.71	0
24	CLA	D	405	4	69,73,73	1.74	13 (18%)	82,113,113	2.12	24 (29%)
24	CLA	a	407	1	69,73,73	1.69	19 (27%)	82,113,113	2.09	25 (30%)
24	CLA	d	403	46	69,73,73	1.70	14 (20%)	82,113,113	2.01	23 (28%)
29	LMG	c	519	-	51,51,55	1.02	3 (5%)	59,59,63	1.39	8 (13%)
34	PGE	b	643	-	9,9,9	0.86	0	8,8,8	0.61	0
35	P6G	b	649	-	18,18,18	0.55	0	17,17,17	0.52	0
24	CLA	C	502	3	69,73,73	1.64	16 (23%)	82,113,113	2.12	20 (24%)
32	LHG	e	101	-	41,41,48	1.13	2 (4%)	44,47,54	1.19	4 (9%)
39	1PE	j	107	-	15,15,15	0.63	0	14,14,14	0.62	0
36	EDO	o	310	-	3,3,3	0.59	0	2,2,2	0.06	0
30	GOL	O	306	-	5,5,5	1.29	1 (20%)	5,5,5	1.20	1 (20%)
24	CLA	c	507	46	69,73,73	1.86	17 (24%)	82,113,113	2.19	24 (29%)
31	LMT	j	103	-	36,36,36	0.75	1 (2%)	47,47,47	1.45	6 (12%)
31	LMT	u	203	-	36,36,36	1.27	2 (5%)	47,47,47	1.70	9 (19%)
24	CLA	B	608	46	69,73,73	1.58	14 (20%)	82,113,113	2.16	22 (26%)
29	LMG	a	414	-	51,51,55	0.86	2 (3%)	59,59,63	1.25	5 (8%)
30	GOL	o	305	-	5,5,5	0.69	0	5,5,5	1.03	0
24	CLA	b	605	2	69,73,73	1.81	17 (24%)	82,113,113	2.61	25 (30%)
24	CLA	C	509	3	69,73,73	1.61	16 (23%)	82,113,113	2.28	25 (30%)
24	CLA	b	611	46	69,73,73	1.66	16 (23%)	82,113,113	2.30	30 (36%)
24	CLA	A	607	46	64,68,73	1.84	16 (25%)	76,107,113	2.34	24 (31%)
36	EDO	J	109	-	3,3,3	0.40	0	2,2,2	0.39	0
45	PE8	i	107	-	24,24,24	0.69	0	23,23,23	0.69	0
34	PGE	B	644	-	9,9,9	0.57	0	8,8,8	0.45	0
33	PG4	e	103	-	12,12,12	0.58	0	11,11,11	0.50	0
40	DGD	H	103	-	63,63,67	1.08	7 (11%)	77,77,81	1.21	12 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	GOL	B	625	-	5,5,5	0.69	0	5,5,5	1.99	2 (40%)
28	SQD	a	417	-	52,54,54	1.17	3 (5%)	62,65,65	1.26	5 (8%)
26	BCR	B	618	-	41,41,41	0.95	0	56,56,56	1.55	9 (16%)
33	PG4	V	212	-	12,12,12	0.72	0	11,11,11	0.56	0
24	CLA	c	504	46	64,68,73	1.99	19 (29%)	76,107,113	2.47	25 (32%)
26	BCR	c	527	-	41,41,41	1.02	2 (4%)	56,56,56	1.40	9 (16%)
24	CLA	C	507	46	69,73,73	1.83	17 (24%)	82,113,113	2.34	25 (30%)
33	PG4	H	107	-	12,12,12	0.70	0	11,11,11	0.50	0
34	PGE	J	108	-	9,9,9	0.58	0	8,8,8	0.51	0
24	CLA	C	510	3	69,73,73	1.72	16 (23%)	82,113,113	2.12	25 (30%)
24	CLA	b	606	2	69,73,73	1.89	19 (27%)	82,113,113	2.47	30 (36%)
34	PGE	b	645	-	9,9,9	0.54	0	8,8,8	0.41	0
26	BCR	H	102	-	41,41,41	1.07	4 (9%)	56,56,56	1.78	18 (32%)
33	PG4	c	533	-	12,12,12	0.59	0	11,11,11	0.47	0
30	GOL	a	416	-	5,5,5	0.64	0	5,5,5	0.84	0
38	HTG	c	522	-	19,19,19	0.69	0	23,24,24	1.35	4 (17%)
31	LMT	B	622	-	36,36,36	0.80	1 (2%)	47,47,47	1.46	7 (14%)
26	BCR	a	411	-	41,41,41	1.21	5 (12%)	56,56,56	1.33	7 (12%)
27	PL9	d	407	-	55,55,55	1.31	9 (16%)	68,69,69	1.28	9 (13%)
36	EDO	C	542	-	3,3,3	0.48	0	2,2,2	0.39	0
24	CLA	C	504	46	64,68,73	1.70	14 (21%)	76,107,113	2.15	25 (32%)
30	GOL	a	415	-	5,5,5	1.10	0	5,5,5	1.18	1 (20%)
33	PG4	B	641	-	12,12,12	0.72	0	11,11,11	0.61	0
26	BCR	C	515	-	41,41,41	0.98	2 (4%)	56,56,56	1.65	12 (21%)
44	2PE	V	216	-	27,27,27	0.92	0	26,26,26	0.68	0
34	PGE	a	422	-	9,9,9	0.67	0	8,8,8	0.72	0
30	GOL	m	103	-	5,5,5	0.28	0	5,5,5	0.60	0
34	PGE	H	109	-	9,9,9	0.53	0	8,8,8	0.48	0
24	CLA	b	612	2	69,73,73	1.60	15 (21%)	82,113,113	2.27	25 (30%)
32	LHG	A	618	-	41,41,48	1.22	2 (4%)	44,47,54	1.23	5 (11%)
30	GOL	U	201	-	5,5,5	0.54	0	5,5,5	1.15	0
30	GOL	d	402	-	5,5,5	0.64	0	5,5,5	1.04	1 (20%)
33	PG4	b	634	-	12,12,12	0.82	0	11,11,11	0.67	0
26	BCR	b	620	-	41,41,41	0.98	2 (4%)	56,56,56	1.41	5 (8%)
30	GOL	v	204	-	5,5,5	1.18	0	5,5,5	0.91	0
35	P6G	C	541	-	18,18,18	0.66	0	17,17,17	0.43	0
41	HEM	E	113	5,6	50,50,50	1.90	13 (26%)	67,82,82	2.17	20 (29%)
38	HTG	B	623	-	19,19,19	1.00	1 (5%)	23,24,24	1.34	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	b	604	2	69,73,73	1.66	17 (24%)	82,113,113	2.25	27 (32%)
30	GOL	O	302	-	5,5,5	1.52	1 (20%)	5,5,5	0.99	0
24	CLA	a	410	1	69,73,73	1.74	13 (18%)	82,113,113	2.15	26 (31%)
26	BCR	b	619	-	41,41,41	1.26	5 (12%)	56,56,56	1.78	14 (25%)
38	HTG	V	204	-	19,19,19	0.94	1 (5%)	23,24,24	2.59	7 (30%)
38	HTG	b	632	-	19,19,19	0.94	1 (5%)	23,24,24	1.61	7 (30%)
35	P6G	A	623	-	18,18,18	0.69	0	17,17,17	0.56	0
38	HTG	B	631	-	19,19,19	1.05	2 (10%)	23,24,24	1.09	2 (8%)
33	PG4	B	640	-	12,12,12	0.67	0	11,11,11	0.43	0
33	PG4	H	105	-	12,12,12	0.74	0	11,11,11	0.48	0
24	CLA	B	605	2	69,73,73	1.76	18 (26%)	82,113,113	2.51	32 (39%)
34	PGE	H	110	-	9,9,9	0.56	0	8,8,8	0.33	0
34	PGE	A	620	-	6,6,9	0.65	0	5,5,8	0.90	0
31	LMT	M	101	-	36,36,36	0.94	2 (5%)	47,47,47	1.82	15 (31%)
24	CLA	b	613	2	69,73,73	1.77	19 (27%)	82,113,113	2.07	22 (26%)
24	CLA	C	513	3	69,73,73	1.62	14 (20%)	82,113,113	2.16	24 (29%)
31	LMT	I	101	-	36,36,36	0.89	1 (2%)	47,47,47	1.54	9 (19%)
34	PGE	h	109	-	9,9,9	0.71	0	8,8,8	0.45	0
34	PGE	E	108	-	9,9,9	0.56	0	8,8,8	0.39	0
34	PGE	a	423	-	9,9,9	0.60	0	8,8,8	0.44	0
31	LMT	Y	101	-	36,36,36	0.58	0	47,47,47	1.26	5 (10%)
34	PGE	c	539	-	9,9,9	0.65	0	8,8,8	0.38	0
24	CLA	B	617	2	64,68,73	1.80	18 (28%)	76,107,113	2.34	26 (34%)
35	P6G	c	541	-	18,18,18	0.51	0	17,17,17	0.41	0
39	1PE	L	101	-	15,15,15	0.68	0	14,14,14	0.66	0
34	PGE	O	310	-	9,9,9	0.61	0	8,8,8	0.36	0
34	PGE	o	307	-	9,9,9	0.78	0	8,8,8	0.55	0
33	PG4	V	210	-	12,12,12	0.91	0	11,11,11	0.78	0
36	EDO	B	658	-	3,3,3	0.45	0	2,2,2	0.47	0
33	PG4	D	414	-	12,12,12	0.67	0	11,11,11	0.51	0
39	1PE	x	104	-	15,15,15	0.62	0	14,14,14	0.41	0
34	PGE	h	108	-	9,9,9	0.60	0	8,8,8	0.42	0
34	PGE	D	415	-	9,9,9	0.60	0	8,8,8	0.41	0
33	PG4	a	421	-	12,12,12	0.63	0	11,11,11	0.61	0
24	CLA	c	508	3	64,68,73	1.72	15 (23%)	76,107,113	2.19	21 (27%)
33	PG4	V	211	-	12,12,12	1.03	0	11,11,11	0.80	0
30	GOL	b	625	-	5,5,5	0.53	0	5,5,5	1.63	2 (40%)
25	PHO	d	401	-	58,69,69	2.47	14 (24%)	55,99,99	2.60	17 (30%)
28	SQD	a	424	-	52,54,54	1.28	3 (5%)	62,65,65	1.91	14 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	PGE	E	104	-	9,9,9	0.57	0	8,8,8	0.45	0
24	CLA	b	616	2	69,73,73	1.65	11 (15%)	82,113,113	2.29	23 (28%)
35	P6G	d	415	-	18,18,18	0.70	0	17,17,17	0.96	1 (5%)
38	HTG	B	630	-	19,19,19	1.03	2 (10%)	23,24,24	1.52	7 (30%)
34	PGE	B	647	-	9,9,9	0.71	0	8,8,8	0.67	0
24	CLA	c	501	3	69,73,73	1.56	12 (17%)	82,113,113	2.45	24 (29%)
31	LMT	a	401	-	36,36,36	0.84	1 (2%)	47,47,47	1.44	4 (8%)
34	PGE	j	105	-	9,9,9	0.65	0	8,8,8	0.59	0
30	GOL	c	526	-	5,5,5	0.41	0	5,5,5	0.89	0
33	PG4	c	534	-	12,12,12	0.54	0	11,11,11	0.43	0
40	DGD	C	517	-	57,57,67	0.89	3 (5%)	71,71,81	1.10	2 (2%)
24	CLA	C	506	3	69,73,73	1.73	15 (21%)	82,113,113	2.14	22 (26%)
30	GOL	o	303	-	5,5,5	0.79	0	5,5,5	0.67	0
34	PGE	T	104	-	6,6,9	1.04	0	5,5,8	0.53	0
24	CLA	b	608	46	69,73,73	1.54	14 (20%)	82,113,113	1.81	20 (24%)
36	EDO	i	108	-	3,3,3	0.40	0	2,2,2	0.45	0
32	LHG	D	410	-	48,48,48	0.90	3 (6%)	51,54,54	0.99	1 (1%)
36	EDO	O	311	-	3,3,3	0.63	0	2,2,2	0.28	0
35	P6G	A	624	-	18,18,18	0.59	0	17,17,17	0.55	0
39	1PE	e	105	-	15,15,15	0.64	0	14,14,14	0.53	0
36	EDO	B	657	-	3,3,3	0.61	0	2,2,2	0.03	0
38	HTG	b	631	-	19,19,19	1.26	2 (10%)	23,24,24	1.64	6 (26%)
40	DGD	h	104	-	63,63,67	1.13	4 (6%)	77,77,81	1.25	8 (10%)

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
40	DGD	C	518	-	-	10/51/91/95	0/2/2/2
26	BCR	k	101	-	-	0/29/63/63	0/2/2/2
33	PG4	J	104	-	-	3/10/10/10	-
36	EDO	E	112	-	-	0/1/1/1	-
30	GOL	F	101	42	-	2/4/4/4	-
38	HTG	C	529	-	-	3/10/30/30	0/1/1/1
24	CLA	c	512	3	-	7/39/115/115	-
36	EDO	B	655	-	-	0/1/1/1	-
33	PG4	A	619	-	-	3/10/10/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	PGE	c	536	-	-	3/7/7/7	-
28	SQD	l	102	-	-	19/49/69/69	0/1/1/1
28	SQD	A	616	-	-	17/49/69/69	0/1/1/1
36	EDO	B	656	-	-	1/1/1/1	-
33	PG4	x	102	-	-	3/10/10/10	-
26	BCR	c	515	-	-	0/29/63/63	0/2/2/2
24	CLA	c	506	3	-	7/39/115/115	-
34	PGE	c	540	-	-	4/7/7/7	-
24	CLA	B	614	2	-	2/39/115/115	-
31	LMT	A	617	-	-	8/21/61/61	0/2/2/2
30	GOL	u	202	-	-	0/4/4/4	-
33	PG4	I	102	-	-	6/10/10/10	-
38	HTG	o	301	-	-	0/10/30/30	0/1/1/1
30	GOL	C	524	-	-	0/4/4/4	-
33	PG4	I	104	-	-	4/10/10/10	-
34	PGE	b	641	-	-	3/7/7/7	-
24	CLA	C	508	3	-	2/33/109/115	-
33	PG4	C	535	-	-	3/10/10/10	-
33	PG4	C	536	-	-	5/10/10/10	-
30	GOL	c	529	-	-	2/4/4/4	-
30	GOL	b	626	-	-	0/4/4/4	-
33	PG4	j	104	-	-	8/10/10/10	-
24	CLA	B	616	2	-	6/39/115/115	-
36	EDO	X	104	-	-	0/1/1/1	-
30	GOL	B	626	-	-	0/4/4/4	-
38	HTG	b	623	-	-	2/10/30/30	0/1/1/1
43	HEC	V	203	16	1/1/3/7	6/14/54/54	-
33	PG4	i	103	-	-	6/10/10/10	-
33	PG4	B	639	-	-	4/10/10/10	-
31	LMT	b	622	-	-	9/21/61/61	0/2/2/2
24	CLA	B	606	2	-	5/39/115/115	-
38	HTG	c	523	-	-	1/10/30/30	0/1/1/1
30	GOL	O	304	-	-	0/4/4/4	-
26	BCR	d	406	-	-	2/29/63/63	0/2/2/2
33	PG4	a	420	-	-	3/10/10/10	-
24	CLA	B	607	2	-	2/27/103/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	GOL	y	101	-	-	2/4/4/4	-
38	HTG	H	101	-	-	3/10/30/30	0/1/1/1
39	1PE	B	653	-	-	4/13/13/13	-
29	LMG	d	412	-	-	24/50/70/70	0/1/1/1
29	LMG	j	101	42	-	9/42/62/70	0/1/1/1
35	P6G	b	648	-	-	6/16/16/16	-
33	PG4	I	103	-	-	5/10/10/10	-
24	CLA	C	501	3	-	4/39/115/115	-
24	CLA	B	604	2	-	1/39/115/115	-
38	HTG	c	530	-	-	3/10/30/30	0/1/1/1
34	PGE	i	105	-	-	4/7/7/7	-
30	GOL	b	629	-	-	2/4/4/4	-
25	PHO	A	608	-	-	2/37/103/103	0/5/6/6
36	EDO	c	542	-	-	1/1/1/1	-
31	LMT	f	101	-	-	2/21/61/61	0/2/2/2
30	GOL	v	207	-	-	2/4/4/4	-
24	CLA	b	603	2	-	2/39/115/115	-
30	GOL	B	629	-	-	0/4/4/4	-
30	GOL	v	205	-	-	2/4/4/4	-
34	PGE	V	215	-	-	4/7/7/7	-
28	SQD	A	622	-	-	24/49/69/69	0/1/1/1
24	CLA	A	606	1	-	5/39/115/115	-
26	BCR	B	620	-	-	1/29/63/63	0/2/2/2
24	CLA	c	510	3	-	4/39/115/115	-
36	EDO	D	419	-	-	0/1/1/1	-
26	BCR	C	525	-	-	2/29/63/63	0/2/2/2
24	CLA	b	607	2	-	1/27/103/115	-
29	LMG	B	634	-	-	18/50/70/70	0/1/1/1
32	LHG	d	411	-	-	10/53/53/53	-
35	P6G	D	418	-	-	7/16/16/16	-
33	PG4	V	209	-	-	5/10/10/10	-
31	LMT	F	102	-	-	6/21/61/61	0/2/2/2
33	PG4	V	213	-	-	4/10/10/10	-
24	CLA	b	610	2	-	0/39/115/115	-
36	EDO	o	311	-	-	1/1/1/1	-
24	CLA	B	613	2	-	2/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LHG	D	411	-	-	8/53/53/53	-
26	BCR	D	406	-	-	0/29/63/63	0/2/2/2
24	CLA	B	610	2	-	1/39/115/115	-
27	PL9	a	412	-	-	10/53/73/73	0/1/1/1
40	DGD	c	516	-	-	16/51/91/95	0/2/2/2
34	PGE	b	644	-	-	3/7/7/7	-
40	DGD	c	517	-	-	15/46/86/95	0/2/2/2
28	SQD	A	612	-	-	11/49/69/69	0/1/1/1
38	HTG	B	624	-	-	3/10/30/30	0/1/1/1
33	PG4	c	535	-	-	3/10/10/10	-
24	CLA	C	511	3	-	0/39/115/115	-
26	BCR	T	102	-	-	1/29/63/63	0/2/2/2
32	LHG	D	409	-	-	7/53/53/53	-
34	PGE	V	214	-	-	4/7/7/7	-
30	GOL	V	207	-	-	0/4/4/4	-
33	PG4	i	102	-	-	4/10/10/10	-
24	CLA	D	403	46	-	3/39/115/115	-
29	LMG	b	621	-	-	13/46/66/70	0/1/1/1
34	PGE	B	649	-	-	3/7/7/7	-
38	HTG	C	531	-	-	7/10/30/30	0/1/1/1
30	GOL	v	203	-	-	0/4/4/4	-
30	GOL	B	635	-	-	0/4/4/4	-
34	PGE	B	650	-	-	2/7/7/7	-
34	PGE	h	110	-	-	3/7/7/7	-
27	PL9	A	611	-	-	10/53/73/73	0/1/1/1
33	PG4	H	104	-	-	3/10/10/10	-
24	CLA	b	615	2	-	9/39/115/115	-
36	EDO	A	625	-	-	0/1/1/1	-
34	PGE	b	639	-	-	3/7/7/7	-
29	LMG	c	520	-	-	17/46/66/70	0/1/1/1
28	SQD	a	413	-	-	19/49/69/69	0/1/1/1
34	PGE	t	104	-	-	2/7/7/7	-
29	LMG	A	613	-	-	19/46/66/70	0/1/1/1
34	PGE	t	105	-	-	1/4/4/7	-
30	GOL	f	104	-	-	4/4/4/4	-
30	GOL	A	614	-	-	0/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	PGE	E	106	-	-	3/7/7/7	-
40	DGD	c	518	-	-	15/51/91/95	0/2/2/2
35	P6G	B	651	-	-	5/16/16/16	-
33	PG4	E	103	-	-	4/10/10/10	-
29	LMG	C	526	-	-	27/50/70/70	0/1/1/1
33	PG4	B	636	-	-	3/10/10/10	-
34	PGE	h	107	-	-	4/7/7/7	-
34	PGE	H	111	-	-	3/7/7/7	-
26	BCR	K	101	-	-	2/29/63/63	0/2/2/2
26	BCR	h	103	-	-	0/29/63/63	0/2/2/2
33	PG4	b	636	-	-	6/10/10/10	-
30	GOL	V	205	-	-	0/4/4/4	-
35	P6G	D	417	-	-	8/16/16/16	-
34	PGE	H	108	-	-	5/7/7/7	-
33	PG4	X	101	-	-	3/10/10/10	-
34	PGE	o	308	-	-	5/7/7/7	-
32	LHG	d	410	-	-	8/53/53/53	-
30	GOL	V	201	-	-	0/4/4/4	-
34	PGE	E	107	-	-	5/7/7/7	-
38	HTG	O	303	-	-	1/10/30/30	0/1/1/1
30	GOL	c	528	-	-	3/4/4/4	-
33	PG4	C	534	-	-	5/10/10/10	-
30	GOL	T	101	-	-	0/4/4/4	-
35	P6G	E	110	-	-	11/16/16/16	-
31	LMT	m	102	-	-	3/21/61/61	0/2/2/2
35	P6G	I	106	-	-	10/16/16/16	-
24	CLA	D	404	4	-	3/39/115/115	-
25	PHO	a	409	-	-	1/37/103/103	0/5/6/6
33	PG4	i	104	-	-	5/10/10/10	-
34	PGE	E	105	-	-	4/7/7/7	-
36	EDO	e	106	-	-	1/1/1/1	-
32	LHG	a	419	-	-	21/45/45/53	-
33	PG4	J	105	-	-	6/10/10/10	-
35	P6G	j	106	-	-	7/16/16/16	-
38	HTG	C	532	-	-	2/10/30/30	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	602	46	-	14/39/115/115	-
24	CLA	b	614	2	-	0/39/115/115	-
26	BCR	A	610	-	-	2/29/63/63	0/2/2/2
30	GOL	v	206	-	-	2/4/4/4	-
34	PGE	b	638	-	-	3/7/7/7	-
38	HTG	C	522	-	-	3/10/30/30	0/1/1/1
24	CLA	B	603	2	-	2/39/115/115	-
38	HTG	b	624	-	-	4/10/30/30	0/1/1/1
31	LMT	t	103	-	-	7/21/61/61	0/2/2/2
34	PGE	b	646	-	-	4/7/7/7	-
30	GOL	A	615	-	-	1/4/4/4	-
30	GOL	O	307	-	-	2/4/4/4	-
24	CLA	d	405	4	-	4/39/115/115	-
34	PGE	B	646	-	-	4/7/7/7	-
26	BCR	C	514	-	-	0/29/63/63	0/2/2/2
34	PGE	f	105	-	-	2/7/7/7	-
26	BCR	t	102	-	-	1/29/63/63	0/2/2/2
31	LMT	c	521	-	-	9/21/61/61	0/2/2/2
30	GOL	B	628	-	-	0/4/4/4	-
30	GOL	B	633	-	-	4/4/4/4	-
24	CLA	B	612	2	-	3/39/115/115	-
35	P6G	d	416	-	-	8/16/16/16	-
31	LMT	M	102	-	-	7/21/61/61	0/2/2/2
24	CLA	b	617	2	-	5/33/109/115	-
34	PGE	J	106	-	-	3/7/7/7	-
24	CLA	B	602	46	-	12/39/115/115	-
30	GOL	C	527	-	-	2/4/4/4	-
30	GOL	e	102	-	-	0/4/4/4	-
33	PG4	b	635	-	-	5/10/10/10	-
39	1PE	B	654	-	-	4/13/13/13	-
36	EDO	H	112	-	-	1/1/1/1	-
33	PG4	C	537	-	-	6/10/10/10	-
24	CLA	A	609	1	-	10/39/115/115	-
35	P6G	D	416	-	-	9/16/16/16	-
30	GOL	t	101	-	-	0/4/4/4	-
38	HTG	h	101	-	-	4/10/30/30	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	GOL	d	413	-	-	4/4/4/4	-
33	PG4	c	532	-	-	6/10/10/10	-
29	LMG	C	520	-	-	17/46/66/70	0/1/1/1
32	LHG	E	101	-	-	16/46/46/53	-
32	LHG	l	101	-	-	12/53/53/53	-
40	DGD	C	516	-	-	17/51/91/95	0/2/2/2
33	PG4	B	638	-	-	6/10/10/10	-
24	CLA	d	404	4	-	1/39/115/115	-
39	1PE	V	217	-	-	4/13/13/13	-
38	HTG	c	531	-	-	8/10/30/30	0/1/1/1
38	HTG	a	418	-	-	7/10/30/30	0/1/1/1
34	PGE	C	539	-	-	3/7/7/7	-
34	PGE	A	621	-	-	3/7/7/7	-
30	GOL	D	413	-	-	2/4/4/4	-
30	GOL	u	201	-	-	0/4/4/4	-
33	PG4	E	102	-	-	8/10/10/10	-
24	CLA	C	505	3	-	2/39/115/115	-
24	CLA	b	609	2	-	1/39/115/115	-
24	CLA	c	511	3	-	2/39/115/115	-
29	LMG	J	101	42	-	6/42/62/70	0/1/1/1
33	PG4	U	202	-	-	3/10/10/10	-
43	HEC	v	202	16	1/1/3/7	4/14/54/54	-
24	CLA	c	502	3	-	2/39/115/115	-
31	LMT	J	103	-	-	10/21/61/61	0/2/2/2
34	PGE	J	107	-	-	3/7/7/7	-
33	PG4	X	103	-	-	4/10/10/10	-
24	CLA	B	609	2	-	1/39/115/115	-
30	GOL	f	103	42	-	1/4/4/4	-
38	HTG	C	530	-	-	3/10/30/30	0/1/1/1
30	GOL	D	402	-	-	2/4/4/4	-
28	SQD	b	633	-	-	18/49/69/69	0/1/1/1
30	GOL	V	206	-	-	0/4/4/4	-
33	PG4	H	106	-	-	4/10/10/10	-
34	PGE	i	106	-	-	4/7/7/7	-
34	PGE	Y	102	-	-	4/7/7/7	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	PGE	I	105	-	-	2/7/7/7	-
36	EDO	d	417	-	-	1/1/1/1	-
24	CLA	B	611	46	-	3/39/115/115	-
30	GOL	b	627	-	-	0/4/4/4	-
26	BCR	b	618	-	-	1/29/63/63	0/2/2/2
34	PGE	E	109	-	-	4/7/7/7	-
34	PGE	o	306	-	-	3/7/7/7	-
36	EDO	E	111	-	-	1/1/1/1	-
33	PG4	X	102	-	-	4/10/10/10	-
32	LHG	d	409	-	-	7/53/53/53	-
30	GOL	B	627	-	-	2/4/4/4	-
28	SQD	x	101	-	-	23/49/69/69	0/1/1/1
33	PG4	C	538	-	-	2/10/10/10	-
34	PGE	B	648	-	-	3/7/7/7	-
35	P6G	B	652	-	-	7/16/16/16	-
31	LMT	m	101	-	-	5/21/61/61	0/2/2/2
34	PGE	C	540	-	-	4/7/7/7	-
30	GOL	C	528	-	-	4/4/4/4	-
29	LMG	z	101	-	-	31/50/70/70	0/1/1/1
33	PG4	B	643	-	-	5/10/10/10	-
24	CLA	C	503	3	-	4/39/115/115	-
33	PG4	l	103	-	-	2/10/10/10	-
28	SQD	h	105	-	-	26/49/69/69	0/1/1/1
34	PGE	c	538	-	-	2/7/7/7	-
38	HTG	C	521	-	-	4/10/30/30	0/1/1/1
36	EDO	I	107	-	-	0/1/1/1	-
33	PG4	b	637	-	-	5/10/10/10	-
30	GOL	o	304	-	-	4/4/4/4	-
28	SQD	F	104	-	-	18/49/69/69	0/1/1/1
24	CLA	c	513	3	-	1/39/115/115	-
24	CLA	c	503	3	-	1/39/115/115	-
24	CLA	B	615	2	-	2/27/103/115	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
30	GOL	c	525	-	-	2/4/4/4	-
24	CLA	C	512	3	-	2/39/115/115	-
34	PGE	b	640	-	-	3/7/7/7	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	PG4	h	106	-	-	3/10/10/10	-
33	PG4	K	102	-	-	4/10/10/10	-
33	PG4	d	414	-	-	2/10/10/10	-
29	LMG	B	621	-	-	11/46/66/70	0/1/1/1
34	PGE	O	308	-	-	5/7/7/7	-
30	GOL	b	628	-	-	0/4/4/4	-
33	PG4	B	642	-	-	5/10/10/10	-
34	PGE	c	537	-	-	4/7/7/7	-
34	PGE	b	642	-	-	3/7/7/7	-
34	PGE	b	647	-	-	3/7/7/7	-
36	EDO	a	425	-	-	1/1/1/1	-
26	BCR	c	514	-	-	0/29/63/63	0/2/2/2
30	GOL	V	208	-	-	3/4/4/4	-
33	PG4	B	637	-	-	4/10/10/10	-
34	PGE	B	645	-	-	5/7/7/7	-
30	GOL	O	305	-	-	2/4/4/4	-
32	LHG	B	632	-	-	12/53/53/53	-
33	PG4	i	101	-	-	7/10/10/10	-
24	CLA	a	408	46	-	4/33/109/115	-
40	DGD	d	408	-	-	32/55/95/95	0/2/2/2
41	HEM	e	107	5,6	-	5/14/54/54	-
30	GOL	b	630	-	-	0/4/4/4	-
27	PL9	D	407	-	-	1/53/73/73	0/1/1/1
34	PGE	O	309	-	-	5/7/7/7	-
36	EDO	V	218	-	-	1/1/1/1	-
25	PHO	D	401	-	-	1/37/103/103	0/5/6/6
35	P6G	T	105	-	-	12/16/16/16	-
31	LMT	C	533	-	-	12/21/61/61	0/2/2/2
33	PG4	e	104	-	-	4/10/10/10	-
24	CLA	c	505	3	-	0/39/115/115	-
30	GOL	C	523	-	-	1/4/4/4	-
29	LMG	C	519	-	-	15/46/66/70	0/1/1/1
24	CLA	c	509	3	-	9/39/115/115	-
40	DGD	D	408	-	-	30/55/95/95	0/2/2/2
34	PGE	x	103	-	-	2/7/7/7	-
30	GOL	D	412	-	-	3/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	GOL	T	103	-	-	2/4/4/4	-
34	PGE	o	309	-	-	5/7/7/7	-
24	CLA	D	405	4	-	7/39/115/115	-
24	CLA	a	407	1	-	2/39/115/115	-
24	CLA	d	403	46	-	4/39/115/115	-
29	LMG	c	519	-	-	19/46/66/70	0/1/1/1
34	PGE	b	643	-	-	3/7/7/7	-
35	P6G	b	649	-	-	10/16/16/16	-
24	CLA	C	502	3	-	4/39/115/115	-
32	LHG	e	101	-	-	24/46/46/53	-
39	1PE	j	107	-	-	5/13/13/13	-
36	EDO	o	310	-	-	0/1/1/1	-
30	GOL	O	306	-	-	0/4/4/4	-
24	CLA	c	507	46	-	2/39/115/115	-
31	LMT	j	103	-	-	10/21/61/61	0/2/2/2
31	LMT	u	203	-	-	12/21/61/61	0/2/2/2
24	CLA	B	608	46	-	0/39/115/115	-
29	LMG	a	414	-	-	24/46/66/70	0/1/1/1
30	GOL	o	305	-	-	2/4/4/4	-
24	CLA	b	605	2	-	6/39/115/115	-
24	CLA	C	509	3	-	7/39/115/115	-
24	CLA	b	611	46	-	6/39/115/115	-
24	CLA	A	607	46	-	2/33/109/115	-
36	EDO	J	109	-	-	0/1/1/1	-
45	PE8	i	107	-	-	13/22/22/22	-
34	PGE	B	644	-	-	3/7/7/7	-
33	PG4	e	103	-	-	4/10/10/10	-
40	DGD	H	103	-	-	10/51/91/95	0/2/2/2
30	GOL	B	625	-	-	2/4/4/4	-
28	SQD	a	417	-	-	16/49/69/69	0/1/1/1
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
33	PG4	V	212	-	-	5/10/10/10	-
24	CLA	c	504	46	-	3/33/109/115	-
26	BCR	c	527	-	-	1/29/63/63	0/2/2/2
24	CLA	C	507	46	-	7/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	PG4	H	107	-	-	4/10/10/10	-
34	PGE	J	108	-	-	4/7/7/7	-
24	CLA	C	510	3	-	1/39/115/115	-
24	CLA	b	606	2	-	3/39/115/115	-
34	PGE	b	645	-	-	4/7/7/7	-
26	BCR	H	102	-	-	0/29/63/63	0/2/2/2
33	PG4	c	533	-	-	5/10/10/10	-
30	GOL	a	416	-	-	2/4/4/4	-
38	HTG	c	522	-	-	4/10/30/30	0/1/1/1
31	LMT	B	622	-	-	6/21/61/61	0/2/2/2
26	BCR	a	411	-	-	0/29/63/63	0/2/2/2
27	PL9	d	407	-	-	1/53/73/73	0/1/1/1
36	EDO	C	542	-	-	1/1/1/1	-
24	CLA	C	504	46	-	3/33/109/115	-
30	GOL	a	415	-	-	0/4/4/4	-
33	PG4	B	641	-	-	4/10/10/10	-
26	BCR	C	515	-	-	2/29/63/63	0/2/2/2
44	2PE	V	216	-	-	14/25/25/25	-
34	PGE	a	422	-	-	5/7/7/7	-
30	GOL	m	103	-	-	0/4/4/4	-
34	PGE	H	109	-	-	6/7/7/7	-
24	CLA	b	612	2	-	3/39/115/115	-
32	LHG	A	618	-	-	23/46/46/53	-
30	GOL	U	201	-	-	1/4/4/4	-
30	GOL	d	402	-	-	2/4/4/4	-
33	PG4	b	634	-	-	3/10/10/10	-
26	BCR	b	620	-	-	4/29/63/63	0/2/2/2
30	GOL	v	204	-	-	2/4/4/4	-
35	P6G	C	541	-	-	8/16/16/16	-
41	HEM	E	113	5,6	-	2/14/54/54	-
38	HTG	B	623	-	-	3/10/30/30	0/1/1/1
24	CLA	b	604	2	-	3/39/115/115	-
30	GOL	O	302	-	-	2/4/4/4	-
24	CLA	a	410	1	-	11/39/115/115	-
26	BCR	b	619	-	-	0/29/63/63	0/2/2/2
38	HTG	V	204	-	-	2/10/30/30	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	HTG	b	632	-	-	2/10/30/30	0/1/1/1
35	P6G	A	623	-	-	9/16/16/16	-
38	HTG	B	631	-	-	3/10/30/30	0/1/1/1
33	PG4	B	640	-	-	5/10/10/10	-
33	PG4	H	105	-	-	4/10/10/10	-
24	CLA	B	605	2	-	4/39/115/115	-
34	PGE	H	110	-	-	4/7/7/7	-
34	PGE	A	620	-	-	2/4/4/7	-
31	LMT	M	101	-	-	2/21/61/61	0/2/2/2
24	CLA	b	613	2	-	3/39/115/115	-
24	CLA	C	513	3	-	7/39/115/115	-
31	LMT	I	101	-	-	7/21/61/61	0/2/2/2
34	PGE	h	109	-	-	4/7/7/7	-
34	PGE	E	108	-	-	2/7/7/7	-
34	PGE	a	423	-	-	3/7/7/7	-
31	LMT	Y	101	-	-	12/21/61/61	0/2/2/2
34	PGE	c	539	-	-	1/7/7/7	-
24	CLA	B	617	2	-	8/33/109/115	-
35	P6G	c	541	-	-	5/16/16/16	-
39	1PE	L	101	-	-	5/13/13/13	-
34	PGE	O	310	-	-	5/7/7/7	-
34	PGE	o	307	-	-	5/7/7/7	-
33	PG4	V	210	-	-	8/10/10/10	-
36	EDO	B	658	-	-	1/1/1/1	-
33	PG4	D	414	-	-	5/10/10/10	-
39	1PE	x	104	-	-	9/13/13/13	-
34	PGE	h	108	-	-	4/7/7/7	-
34	PGE	D	415	-	-	6/7/7/7	-
33	PG4	a	421	-	-	3/10/10/10	-
24	CLA	c	508	3	-	0/33/109/115	-
33	PG4	V	211	-	-	3/10/10/10	-
30	GOL	b	625	-	-	3/4/4/4	-
25	PHO	d	401	-	-	2/37/103/103	0/5/6/6
28	SQD	a	424	-	-	22/49/69/69	0/1/1/1
34	PGE	E	104	-	-	1/7/7/7	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	616	2	-	4/39/115/115	-
35	P6G	d	415	-	-	8/16/16/16	-
38	HTG	B	630	-	-	4/10/30/30	0/1/1/1
34	PGE	B	647	-	-	3/7/7/7	-
24	CLA	c	501	3	-	2/39/115/115	-
31	LMT	a	401	-	-	9/21/61/61	0/2/2/2
34	PGE	j	105	-	-	4/7/7/7	-
30	GOL	c	526	-	-	0/4/4/4	-
33	PG4	c	534	-	-	6/10/10/10	-
40	DGD	C	517	-	-	14/45/85/95	0/2/2/2
24	CLA	C	506	3	-	10/39/115/115	-
30	GOL	o	303	-	-	2/4/4/4	-
34	PGE	T	104	-	-	1/4/4/7	-
24	CLA	b	608	46	-	1/39/115/115	-
36	EDO	i	108	-	-	0/1/1/1	-
32	LHG	D	410	-	-	8/53/53/53	-
36	EDO	O	311	-	-	1/1/1/1	-
35	P6G	A	624	-	-	9/16/16/16	-
39	1PE	e	105	-	-	7/13/13/13	-
36	EDO	B	657	-	-	0/1/1/1	-
38	HTG	b	631	-	-	2/10/30/30	0/1/1/1
40	DGD	h	104	-	-	10/51/91/95	0/2/2/2

The worst 5 of 1512 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	401	PHO	C1B-C2B	9.15	1.49	1.39
25	d	401	PHO	C1D-C2D	8.98	1.49	1.39
25	D	401	PHO	C1D-C2D	8.83	1.49	1.39
38	o	301	HTG	C1'-S1	-7.16	1.71	1.81
25	D	401	PHO	C3B-C2B	7.09	1.50	1.40

The worst 5 of 2716 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	401	PHO	C3B-C4B-NB	10.42	114.26	107.46
28	a	413	SQD	O6-C1-C2	9.34	122.46	108.27
40	d	408	DGD	O3G-C1D-C2D	9.10	122.09	108.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	608	PHO	C3B-C4B-NB	8.95	113.30	107.46
28	F	104	SQD	O6-C1-C2	8.89	121.78	108.27

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
43	V	203	HEC	NA
43	v	202	HEC	NA

5 of 2104 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	605	CLA	C1-C2-C3-C4
24	B	615	CLA	CAD-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O2D
24	C	507	CLA	CHA-CBD-CGD-O1D
24	C	507	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

156 monomers are involved in 318 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	k	101	BCR	6	0
38	C	529	HTG	1	0
24	c	512	CLA	2	0
28	A	616	SQD	1	0
26	c	515	BCR	4	0
24	c	506	CLA	3	0
24	B	614	CLA	1	0
38	o	301	HTG	1	0
33	I	104	PG4	2	0
24	C	508	CLA	1	0
30	c	529	GOL	7	0
24	B	616	CLA	1	0
43	V	203	HEC	1	0
24	B	606	CLA	2	0
26	d	406	BCR	3	0
24	B	607	CLA	3	0
29	d	412	LMG	2	0
24	C	501	CLA	1	0
24	B	604	CLA	2	0
30	b	629	GOL	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	608	PHO	1	0
28	A	622	SQD	2	0
24	A	606	CLA	4	0
26	B	620	BCR	4	0
24	c	510	CLA	3	0
36	D	419	EDO	3	0
26	C	525	BCR	1	0
24	b	607	CLA	1	0
29	B	634	LMG	6	0
32	d	411	LHG	1	0
24	b	610	CLA	4	0
32	D	411	LHG	1	0
26	D	406	BCR	2	0
24	B	610	CLA	4	0
27	a	412	PL9	11	0
28	A	612	SQD	2	0
24	C	511	CLA	1	0
26	T	102	BCR	8	0
32	D	409	LHG	1	0
24	D	403	CLA	3	0
29	b	621	LMG	2	0
38	C	531	HTG	1	0
27	A	611	PL9	7	0
24	b	615	CLA	3	0
29	A	613	LMG	3	0
30	A	614	GOL	1	0
29	C	526	LMG	3	0
26	K	101	BCR	2	0
26	h	103	BCR	3	0
34	o	308	PGE	2	0
32	d	410	LHG	1	0
24	D	404	CLA	2	0
38	C	532	HTG	1	0
24	b	602	CLA	2	0
24	b	614	CLA	1	0
26	A	610	BCR	3	0
30	A	615	GOL	3	0
24	d	405	CLA	1	0
34	B	646	PGE	2	0
26	C	514	BCR	1	0
26	t	102	BCR	5	0
31	M	102	LMT	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	b	617	CLA	1	0
24	B	602	CLA	11	0
24	A	609	CLA	1	0
30	t	101	GOL	1	0
38	h	101	HTG	1	0
30	d	413	GOL	1	0
32	l	101	LHG	1	0
24	d	404	CLA	2	0
24	C	505	CLA	2	0
24	b	609	CLA	1	0
24	c	502	CLA	2	0
31	J	103	LMT	1	0
30	D	402	GOL	1	0
28	b	633	SQD	2	0
33	H	106	PG4	2	0
24	B	611	CLA	1	0
26	b	618	BCR	1	0
32	d	409	LHG	1	0
28	x	101	SQD	2	0
35	B	652	P6G	1	0
30	C	528	GOL	10	0
29	z	101	LMG	1	0
24	C	503	CLA	1	0
38	C	521	HTG	1	0
24	c	503	CLA	2	0
24	B	615	CLA	2	0
26	B	619	BCR	4	0
30	c	525	GOL	2	0
24	C	512	CLA	3	0
29	B	621	LMG	1	0
34	O	308	PGE	3	0
26	c	514	BCR	1	0
30	O	305	GOL	1	0
24	a	408	CLA	1	0
40	d	408	DGD	0	1
41	e	107	HEM	4	0
25	D	401	PHO	1	0
35	T	105	P6G	2	0
24	c	505	CLA	6	0
30	C	523	GOL	4	0
24	c	509	CLA	1	0
40	D	408	DGD	2	0

Continued on next page...

Continued from previous page...

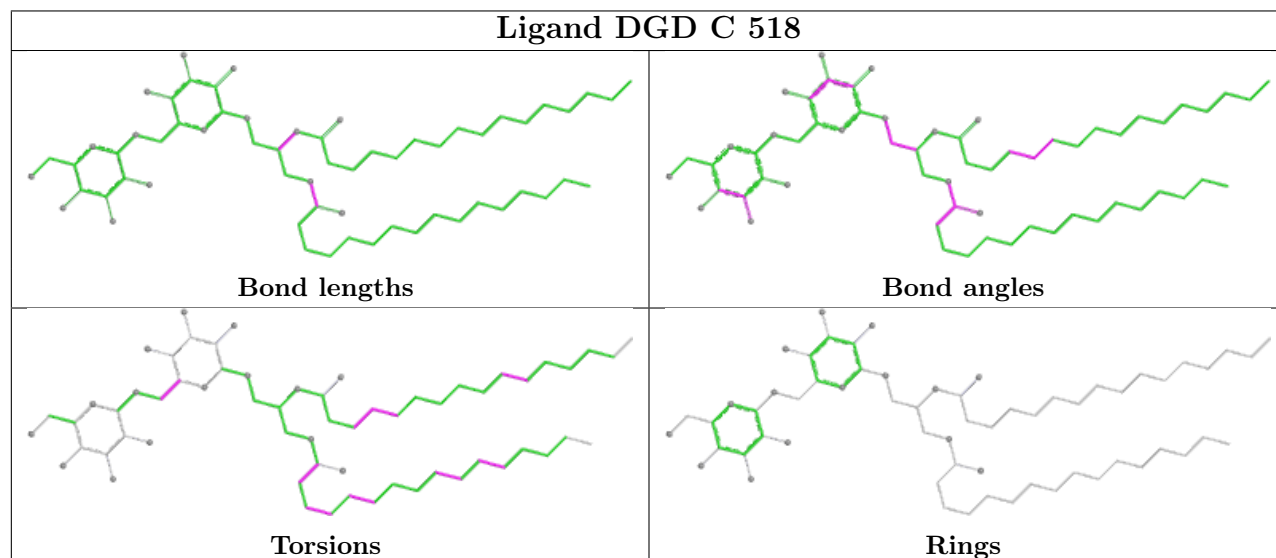
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	D	412	GOL	1	0
30	T	103	GOL	1	0
24	D	405	CLA	5	0
24	a	407	CLA	4	0
24	d	403	CLA	2	0
29	c	519	LMG	1	0
24	C	502	CLA	3	0
32	e	101	LHG	2	0
24	c	507	CLA	1	0
31	u	203	LMT	3	0
24	B	608	CLA	1	0
29	a	414	LMG	1	0
30	o	305	GOL	1	0
24	C	509	CLA	4	0
24	b	611	CLA	3	0
24	A	607	CLA	1	0
45	i	107	PE8	1	0
26	B	618	BCR	4	0
24	c	504	CLA	3	0
26	c	527	BCR	2	0
24	C	507	CLA	2	0
24	C	510	CLA	3	0
24	b	606	CLA	1	0
26	H	102	BCR	3	0
33	c	533	PG4	1	0
30	a	416	GOL	1	0
31	B	622	LMT	2	0
26	a	411	BCR	3	0
24	C	504	CLA	2	0
30	a	415	GOL	1	0
26	C	515	BCR	3	0
44	V	216	2PE	3	0
24	b	612	CLA	2	0
30	U	201	GOL	2	0
26	b	620	BCR	5	0
41	E	113	HEM	5	0
38	B	623	HTG	3	0
24	b	604	CLA	2	0
24	a	410	CLA	1	0
26	b	619	BCR	4	0
31	M	101	LMT	3	0
24	C	513	CLA	1	0

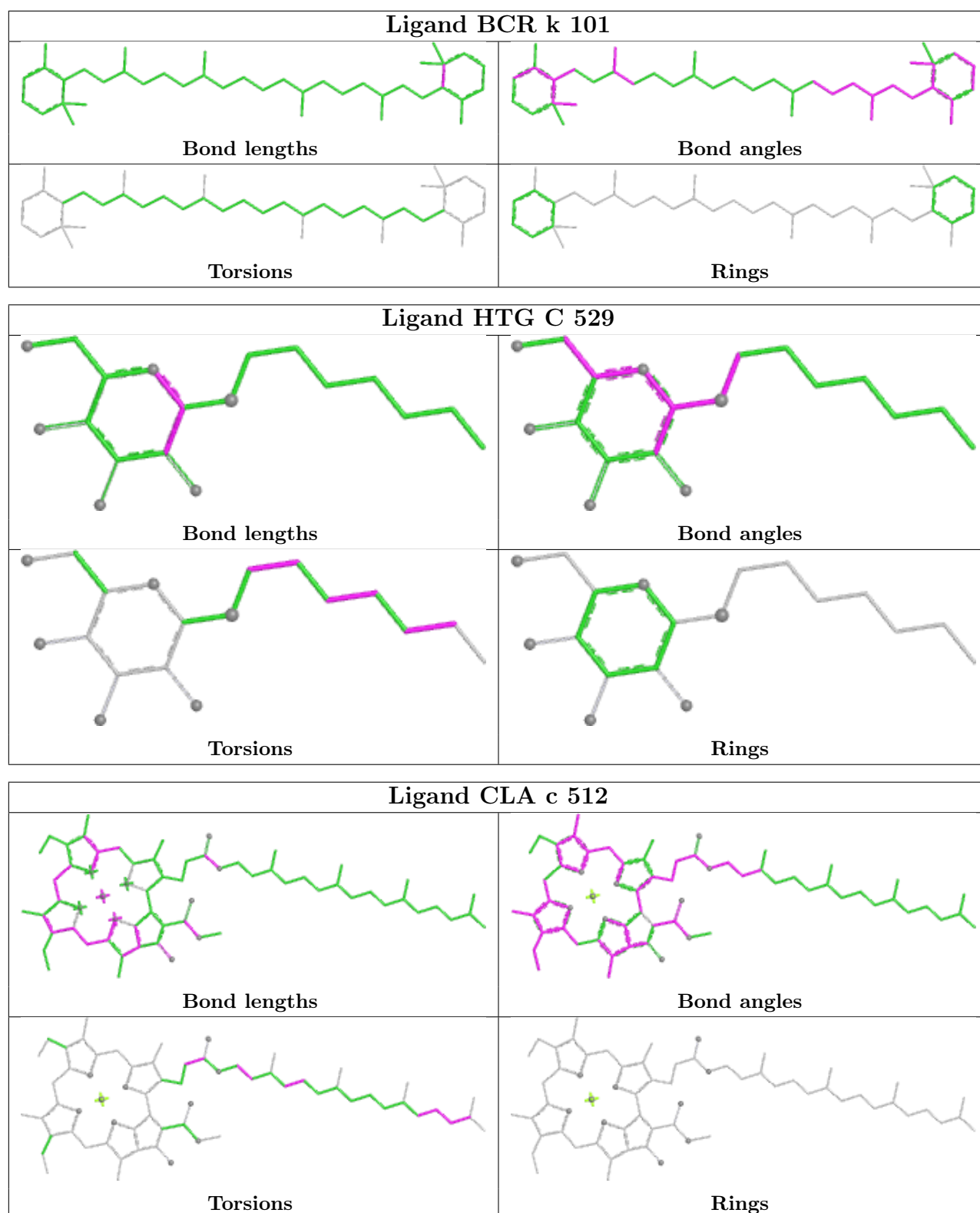
Continued on next page...

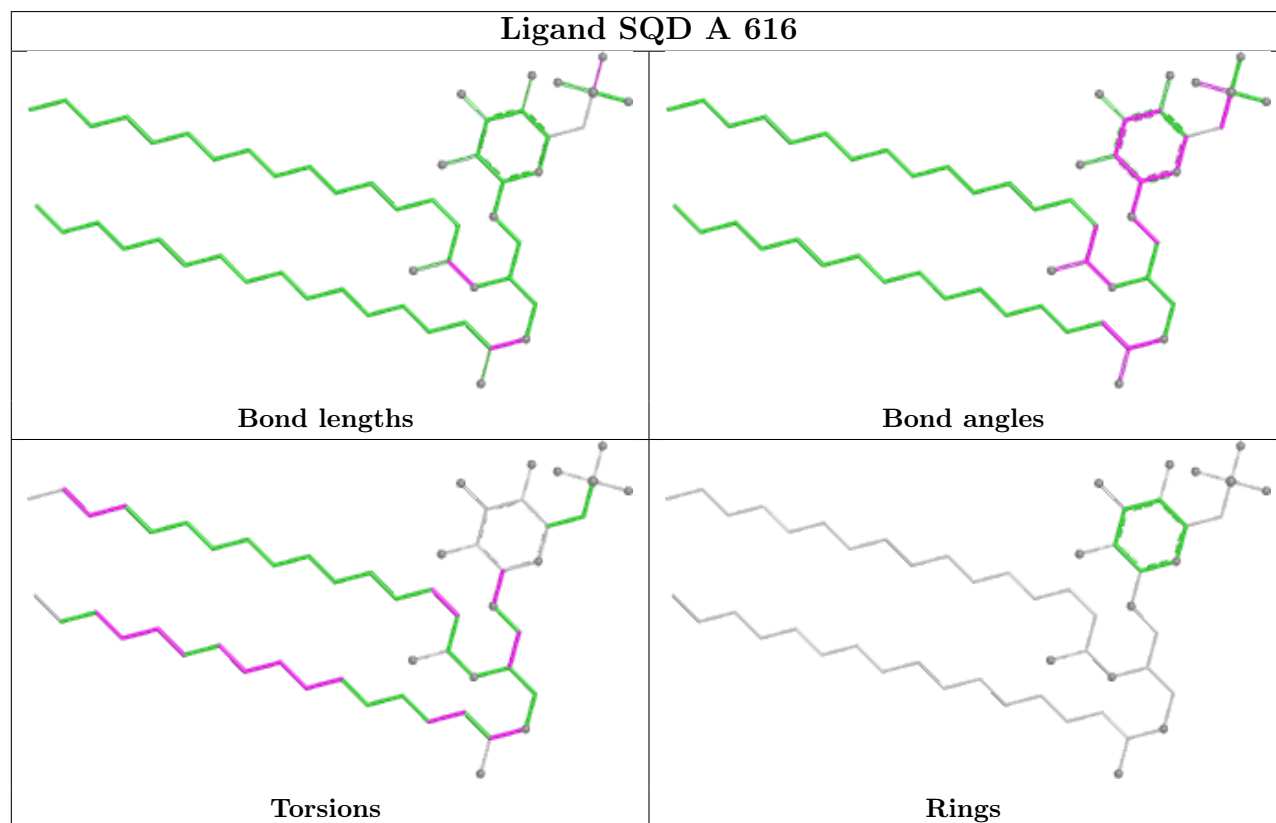
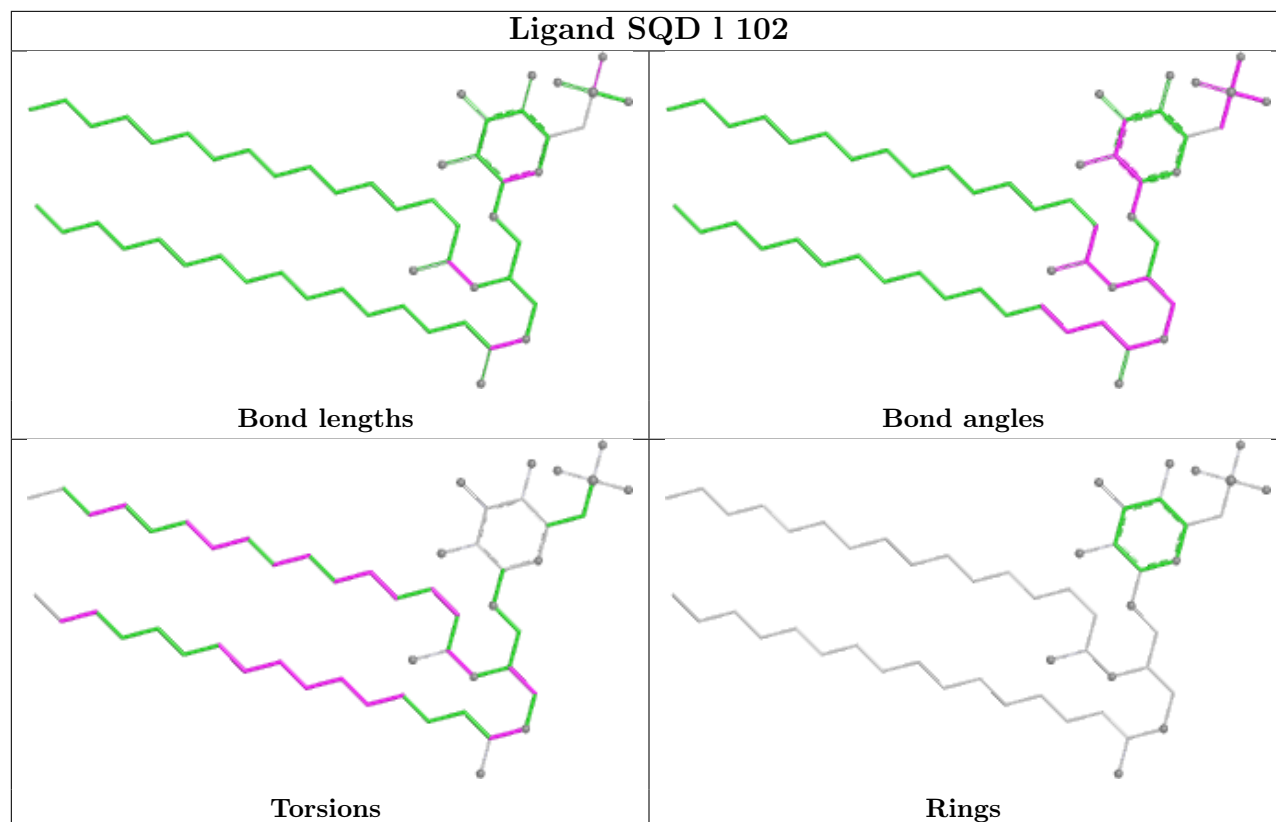
Continued from previous page...

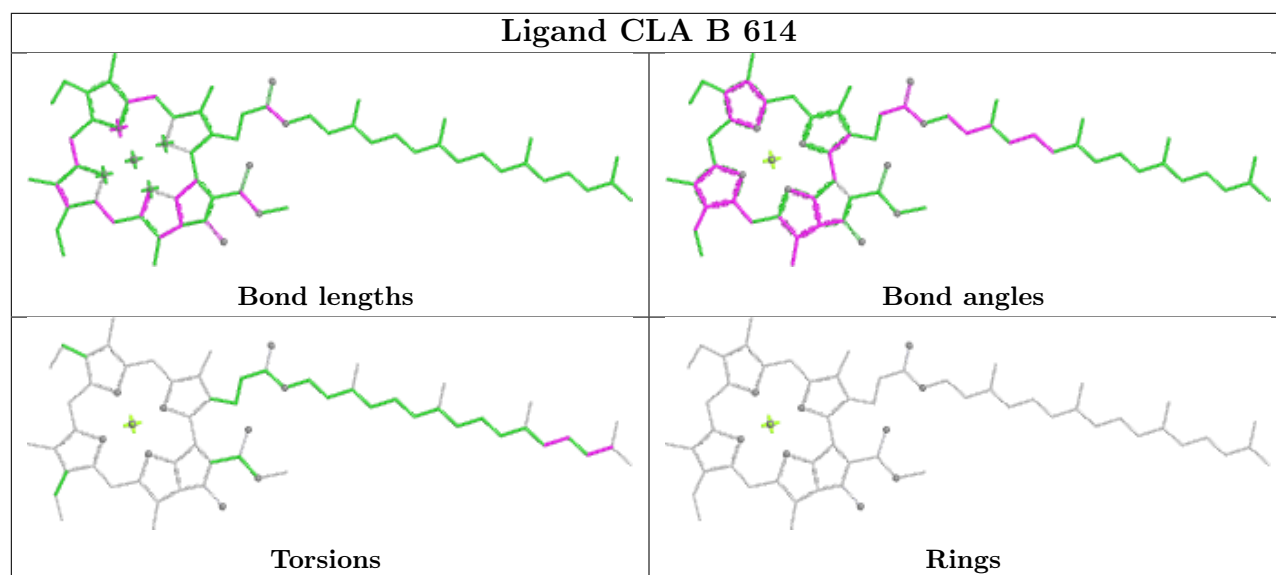
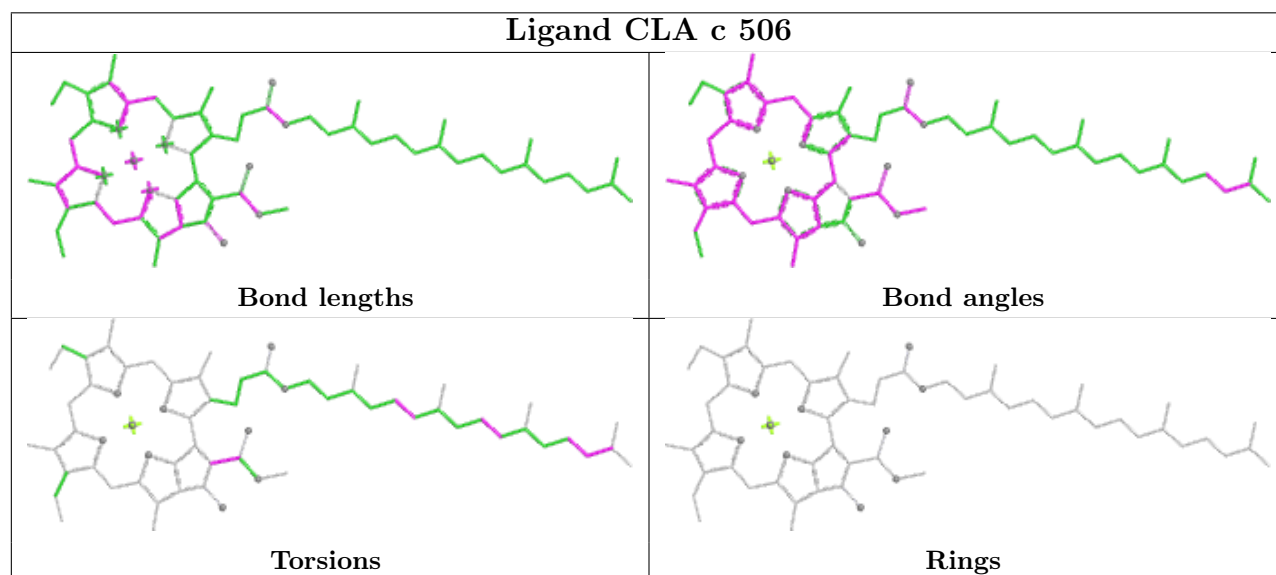
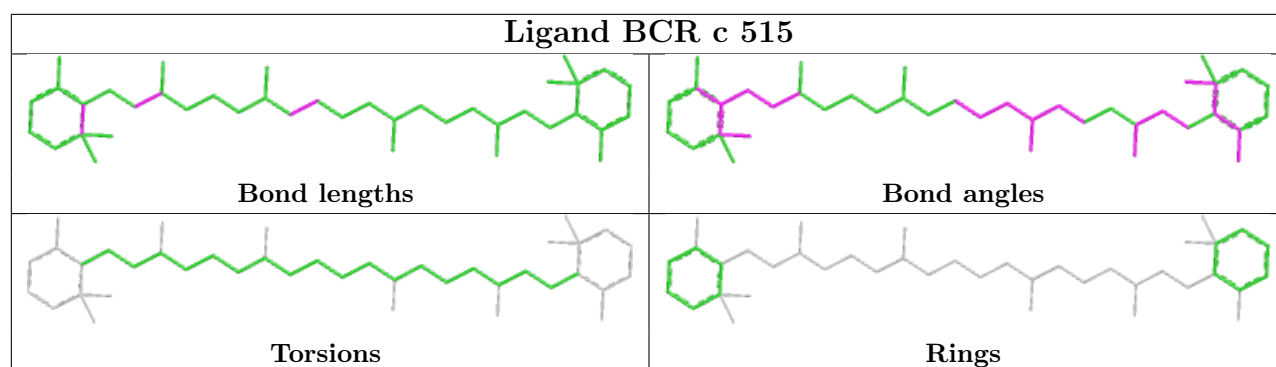
Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	I	101	LMT	1	0
31	Y	101	LMT	1	0
39	x	104	1PE	1	0
24	c	508	CLA	1	0
25	d	401	PHO	3	0
28	a	424	SQD	1	0
24	b	616	CLA	1	0
24	c	501	CLA	2	0
24	C	506	CLA	5	0
24	b	608	CLA	2	0

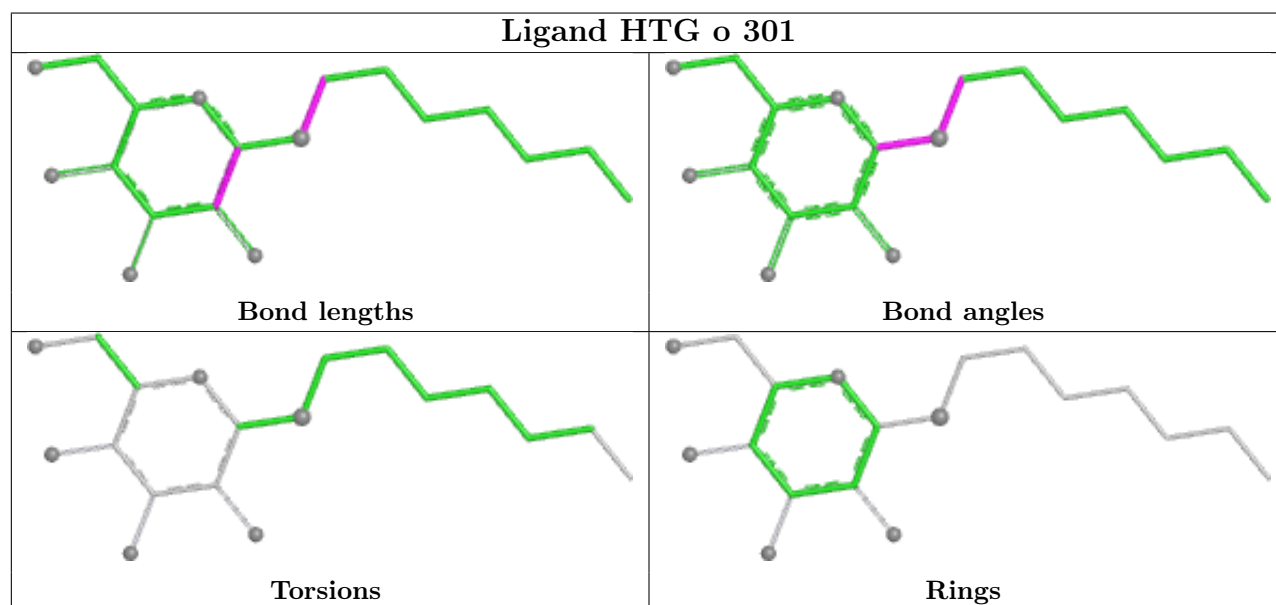
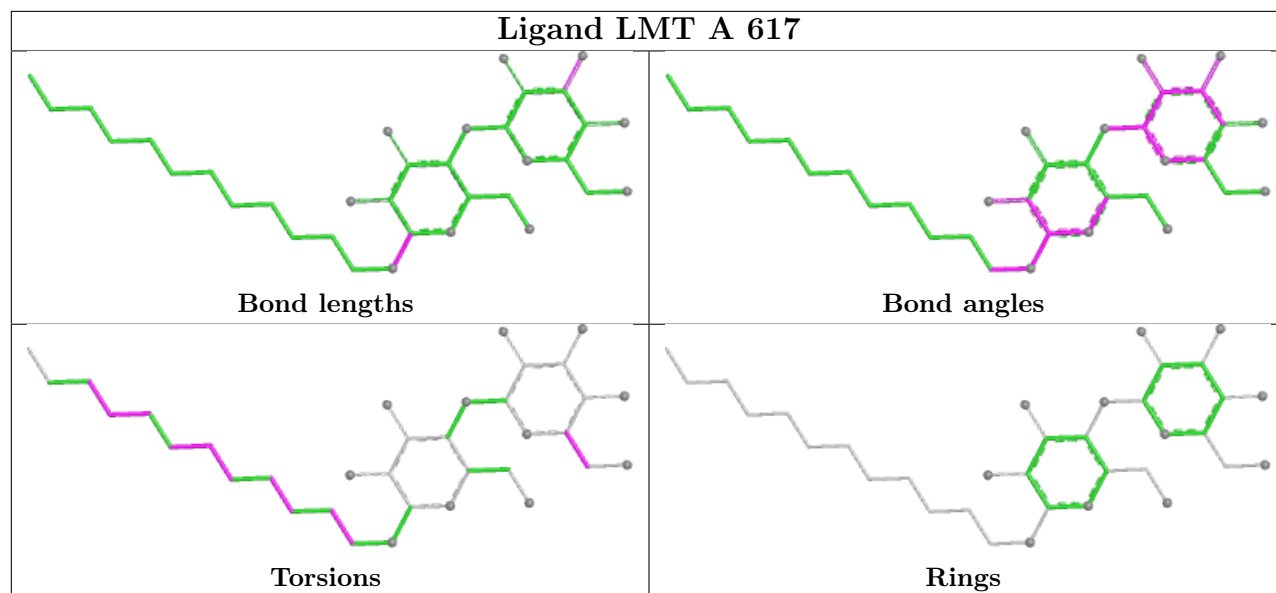
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

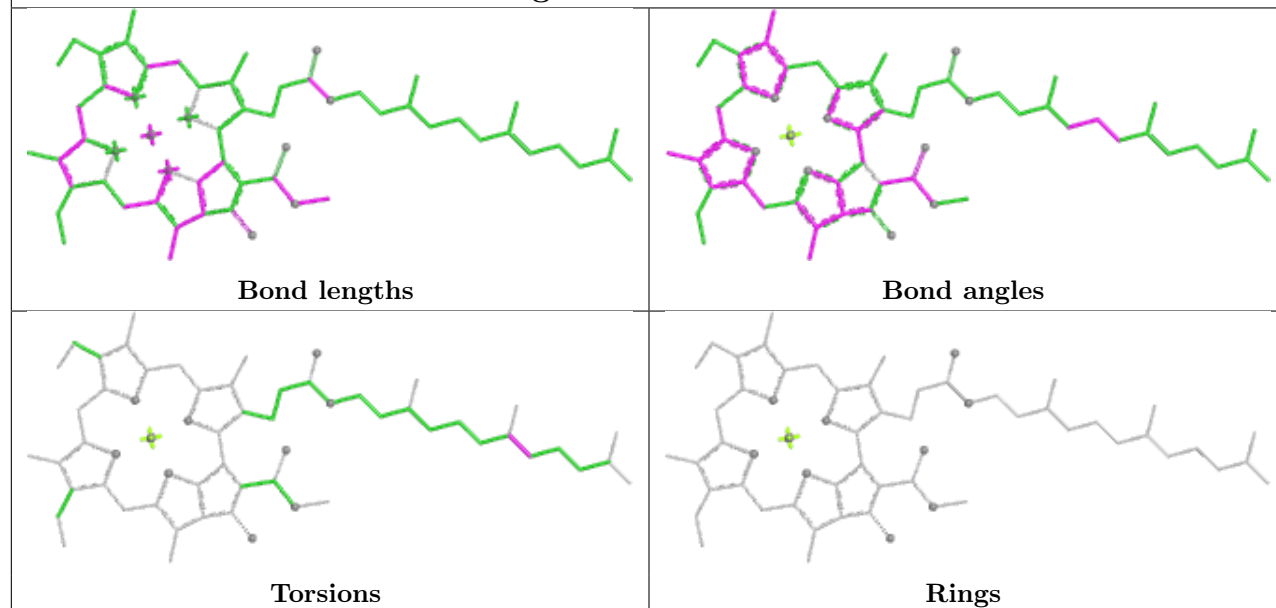
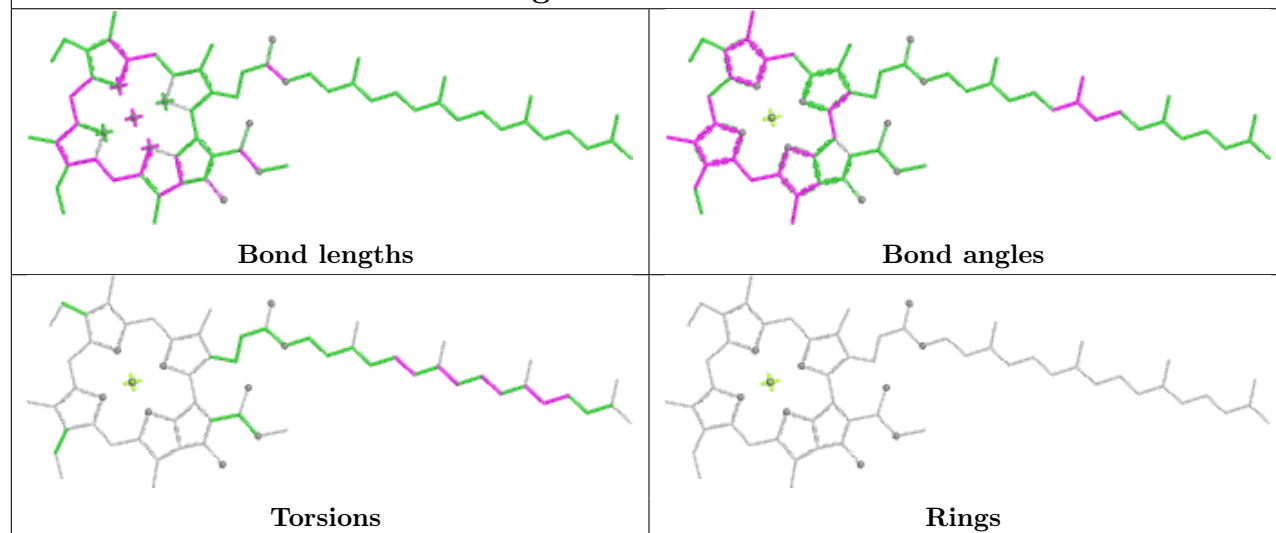


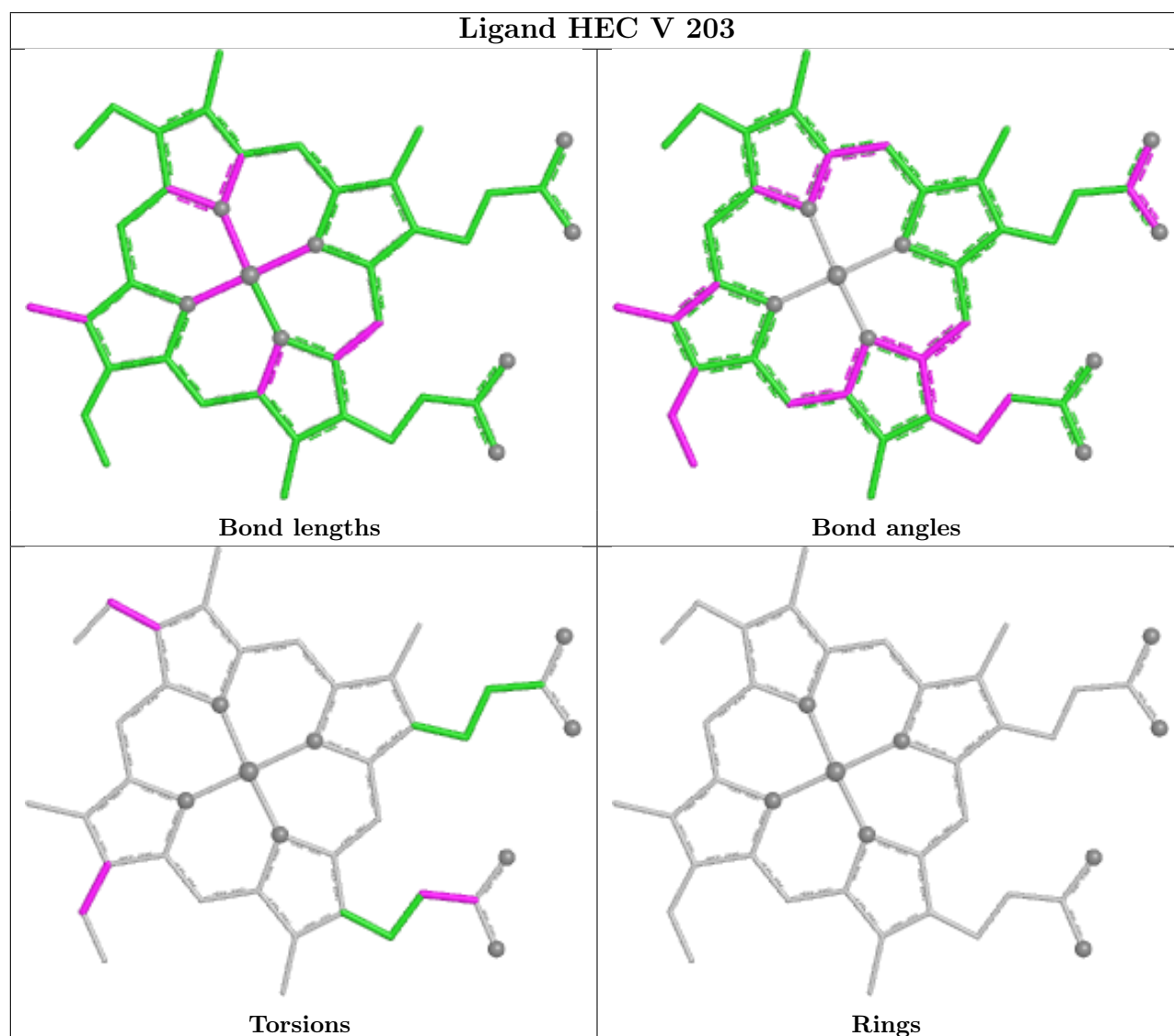
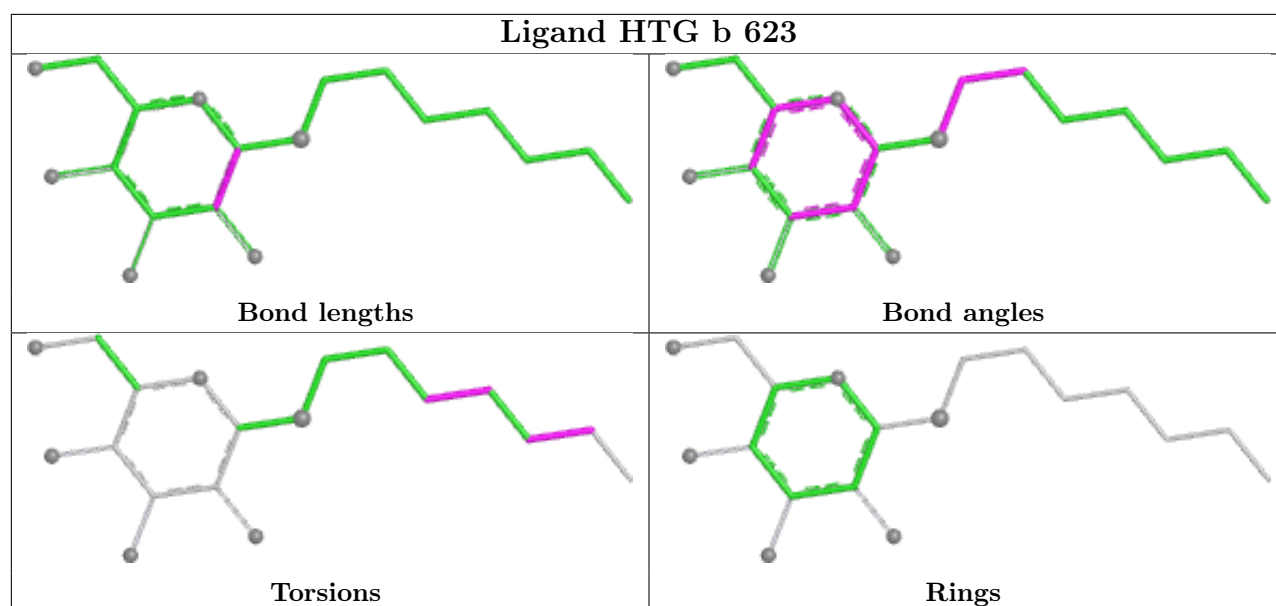


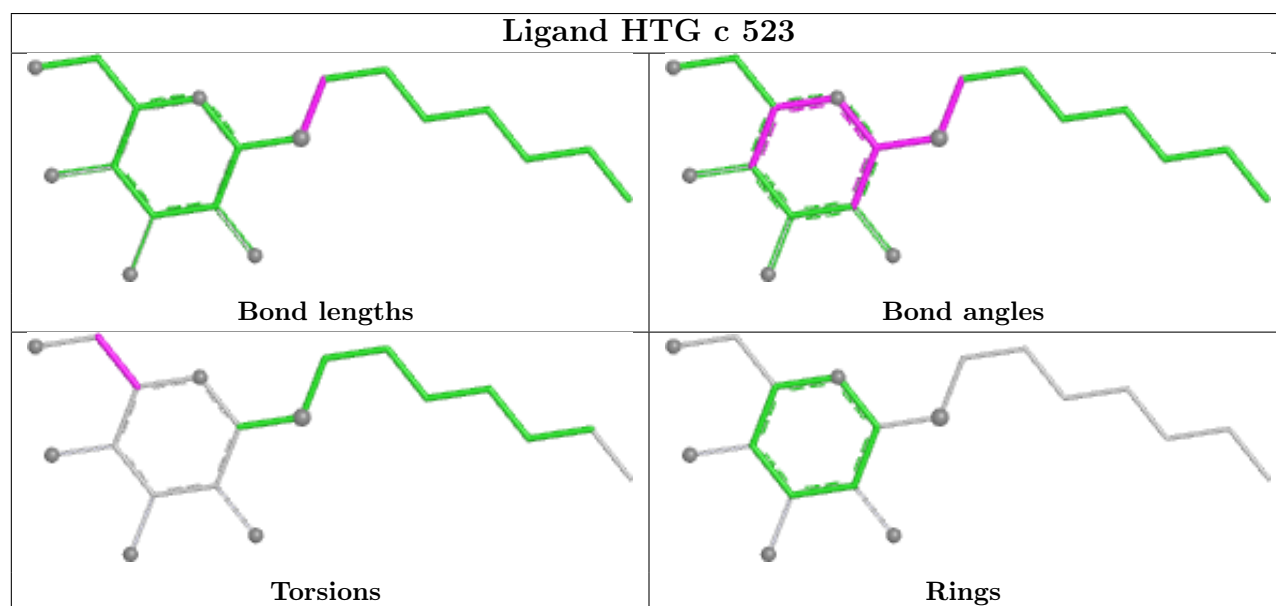
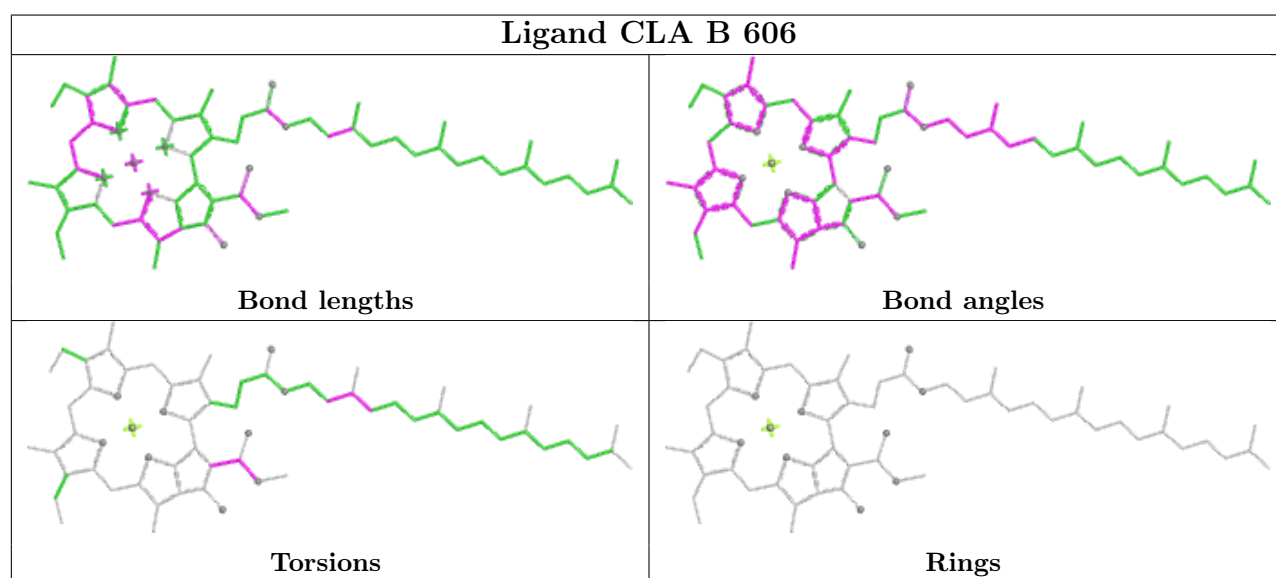
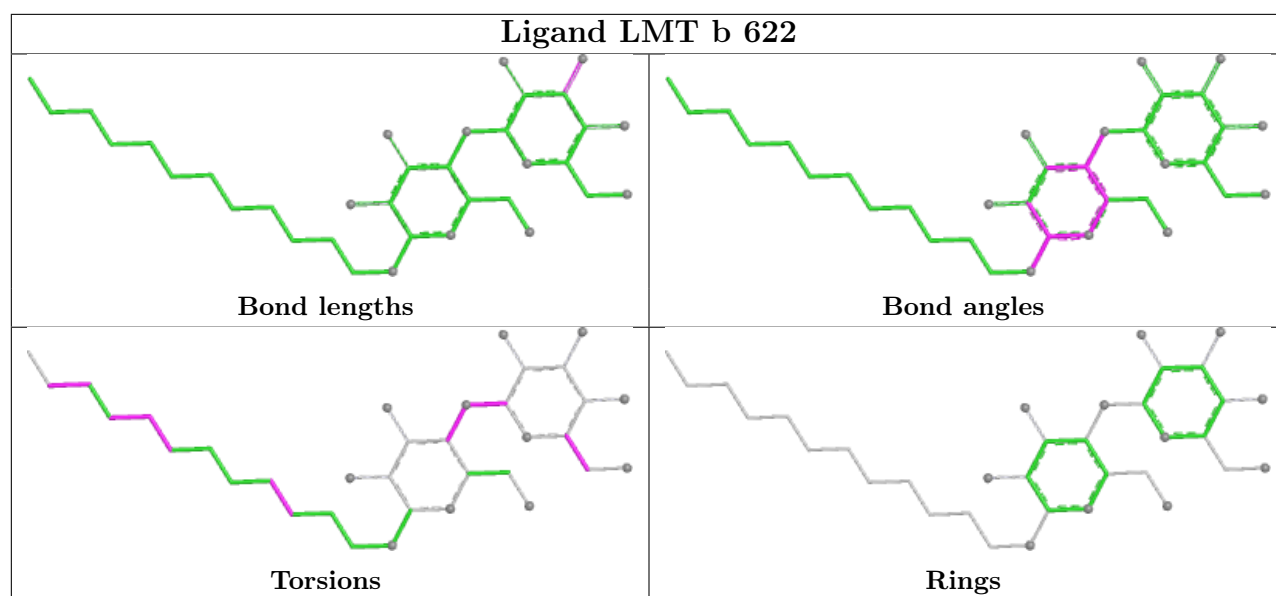


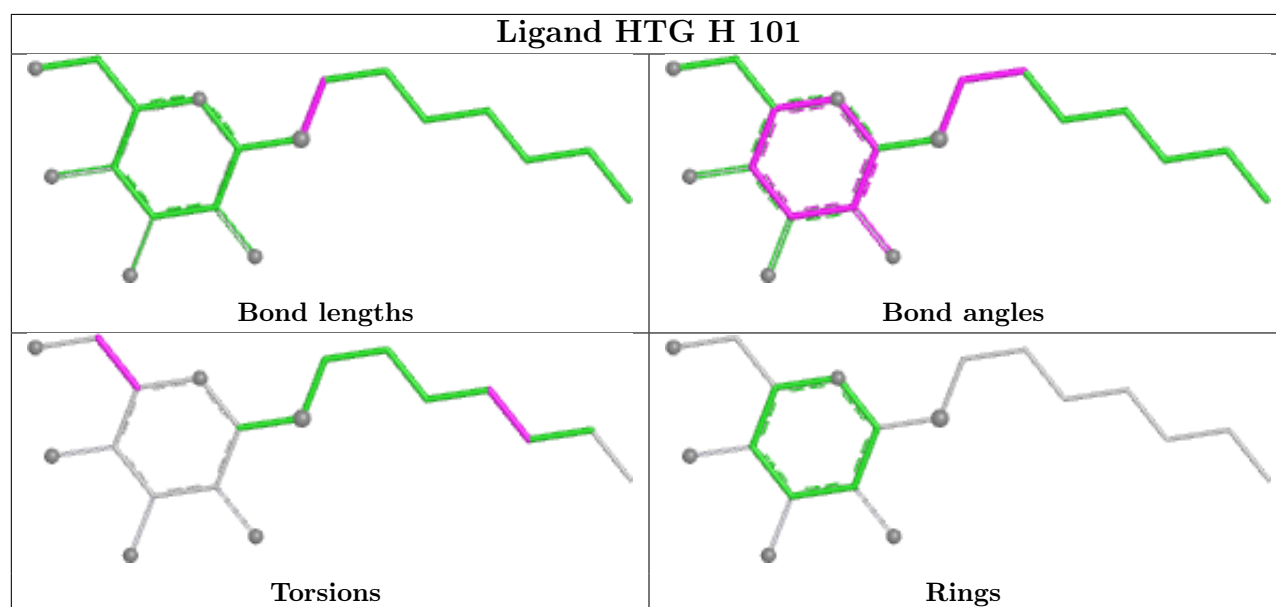
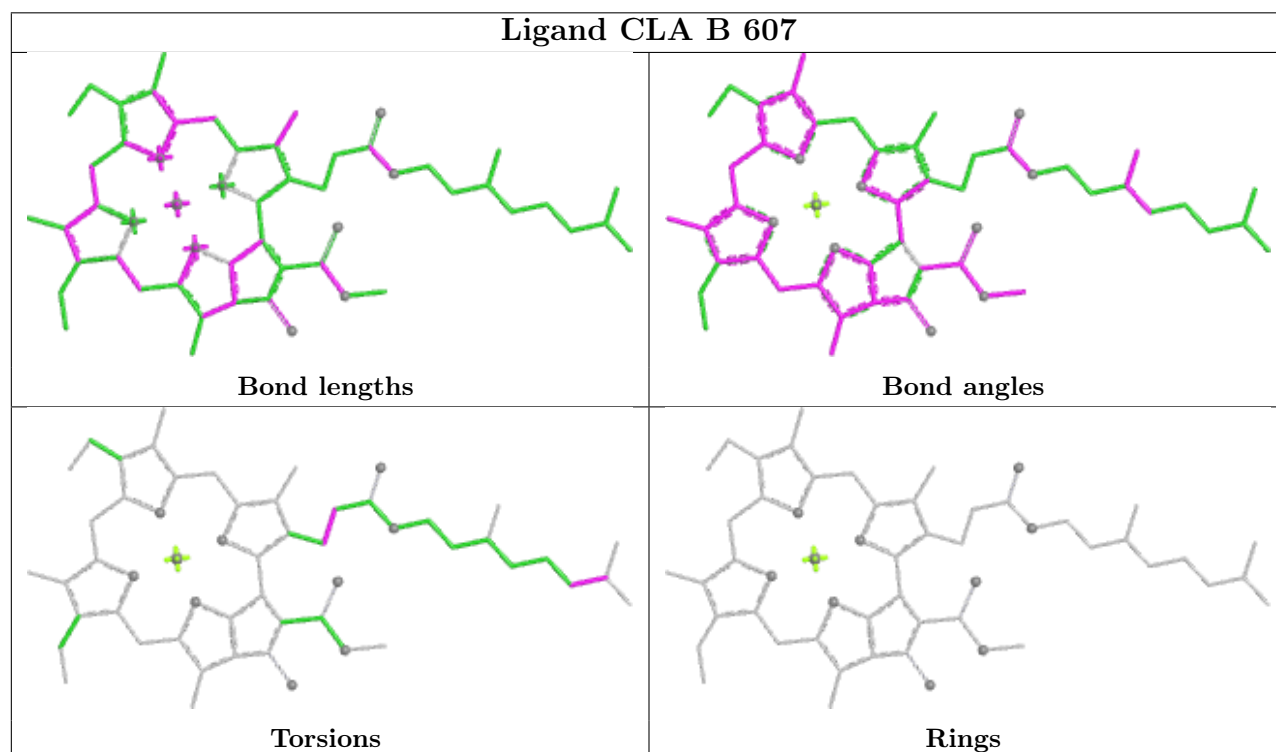
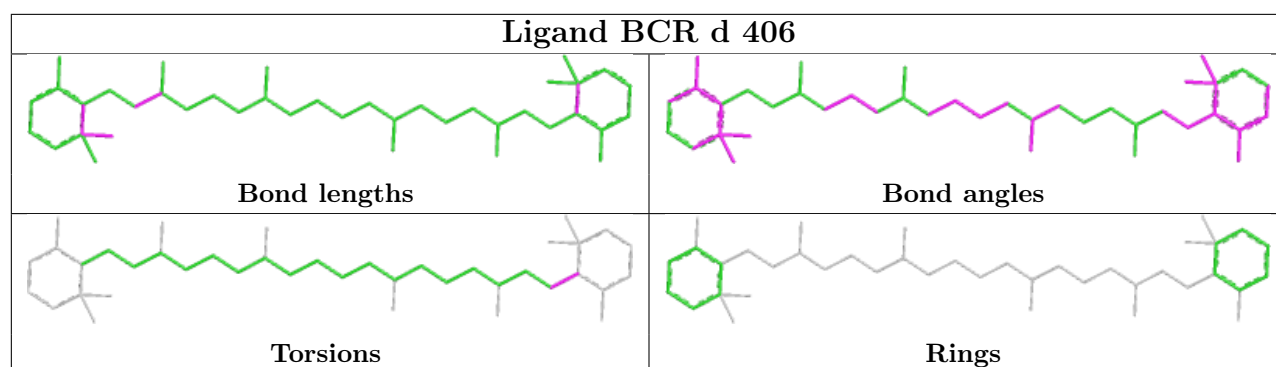


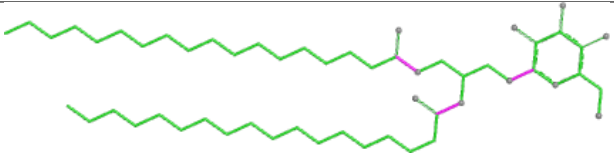
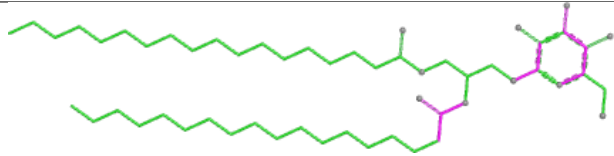
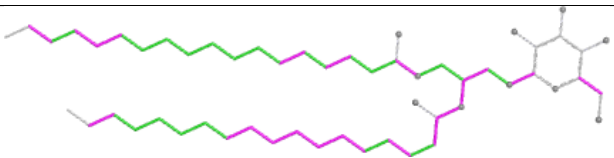
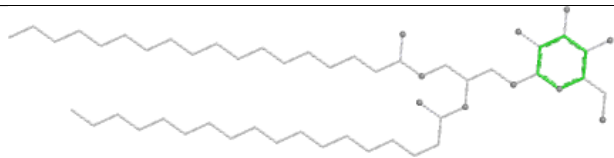
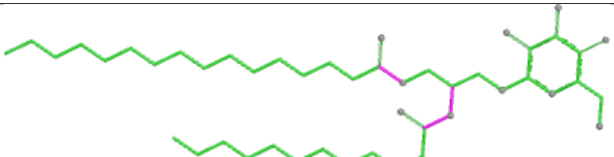
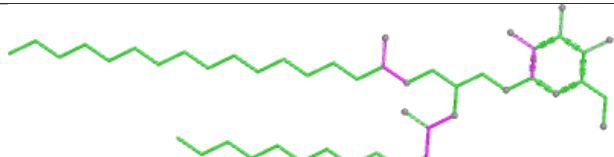
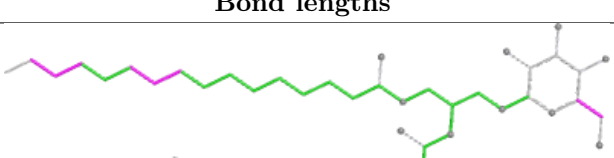
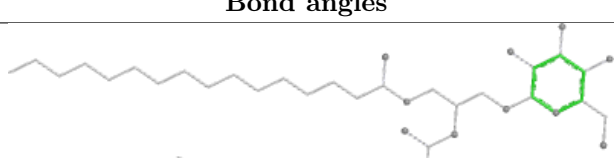
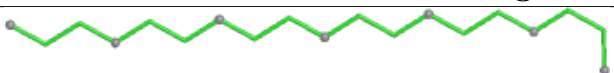
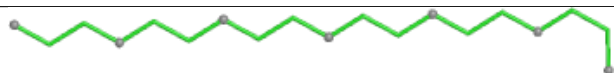
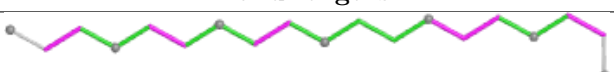
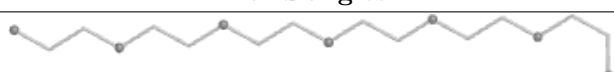


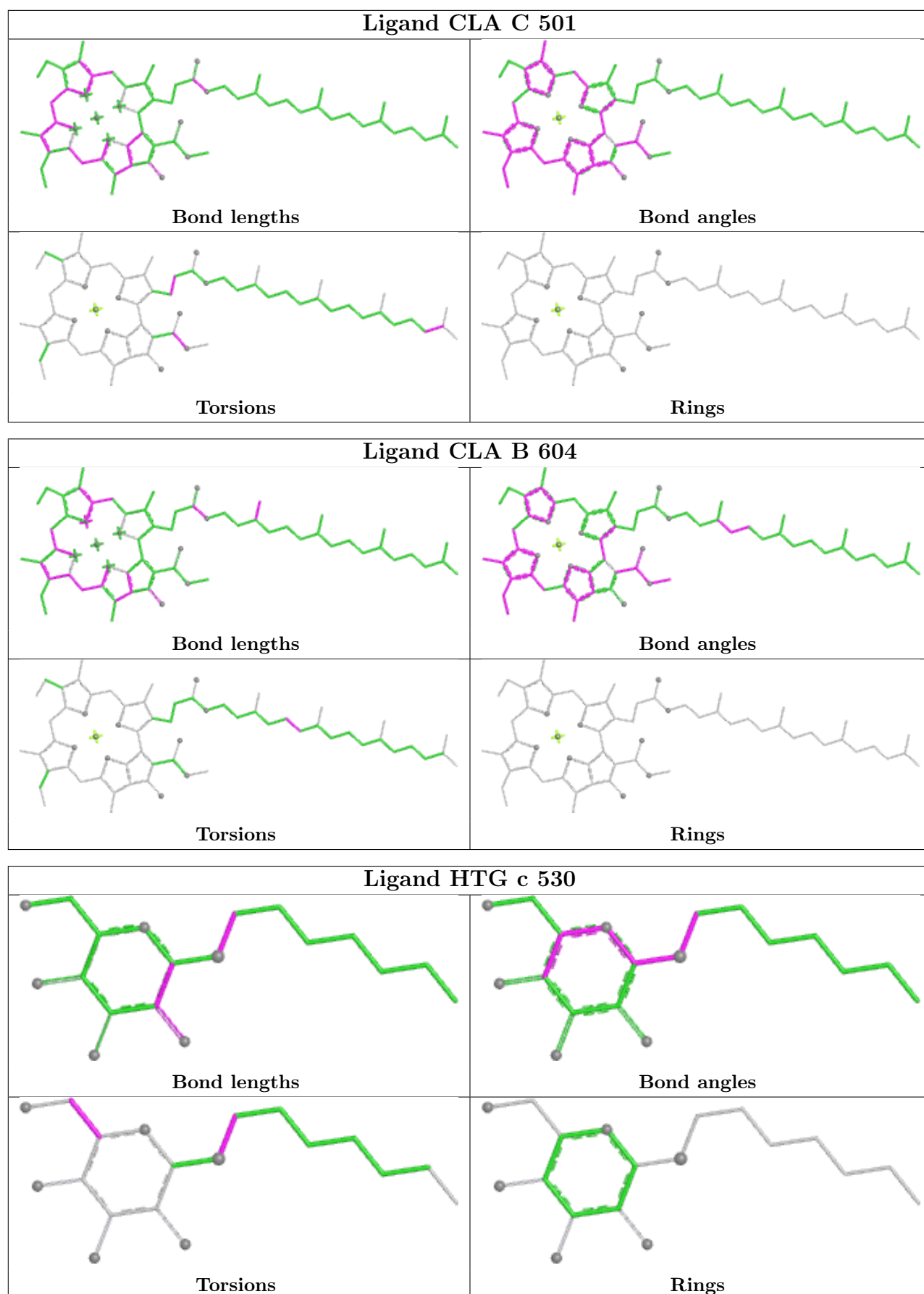
Ligand CLA C 508**Ligand CLA B 616**

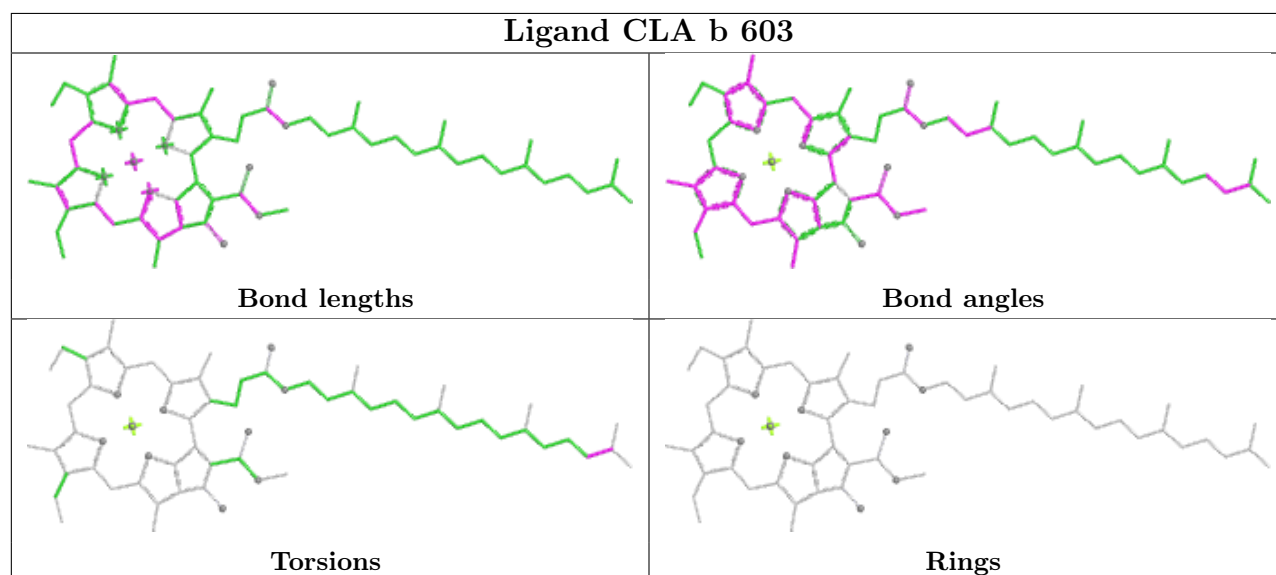
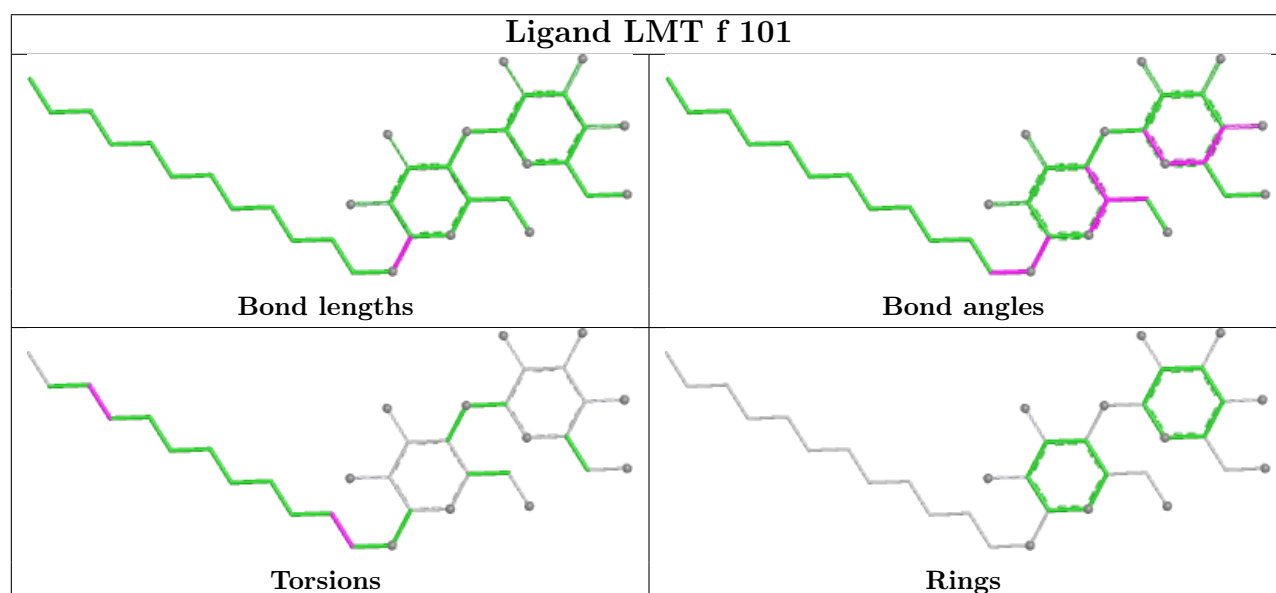
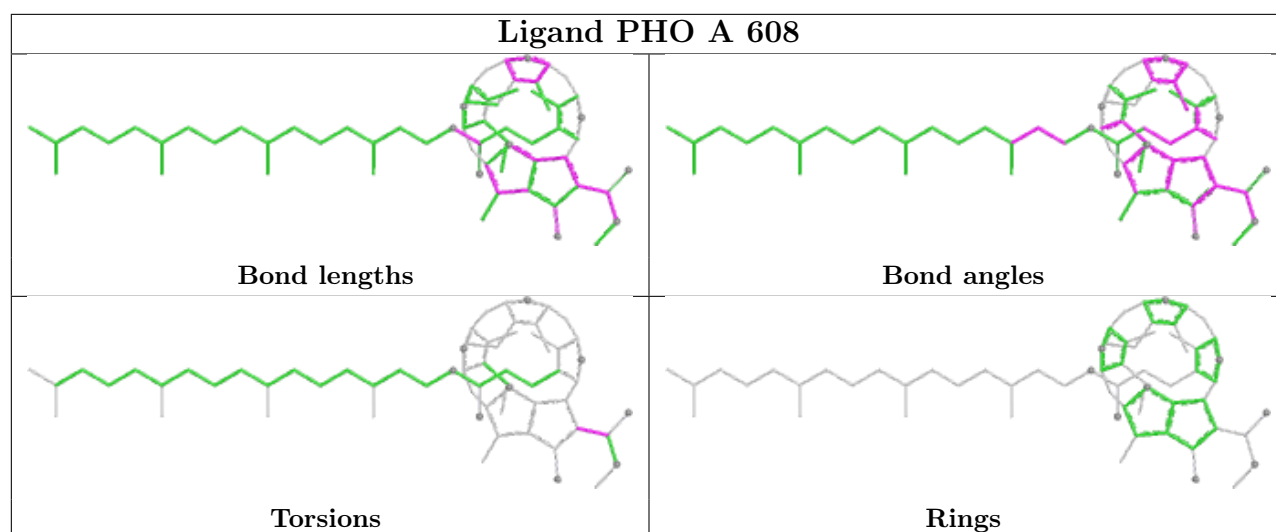


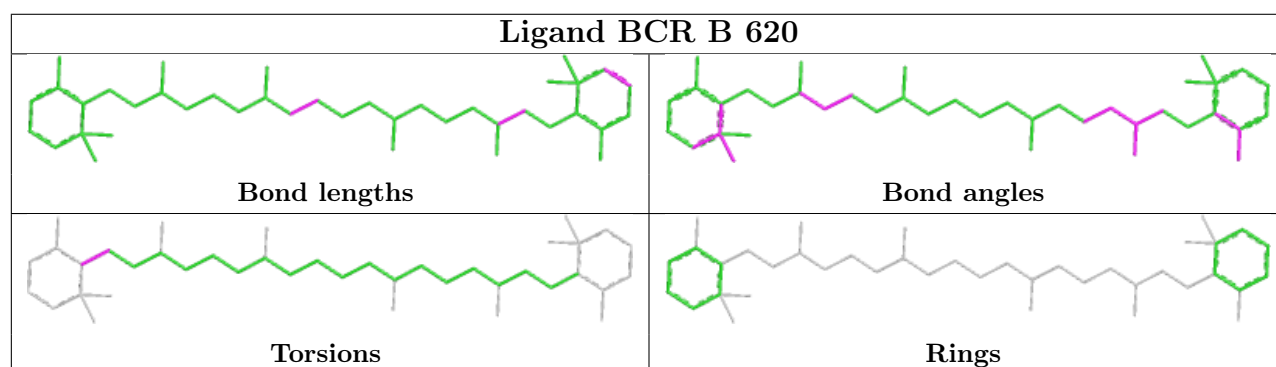
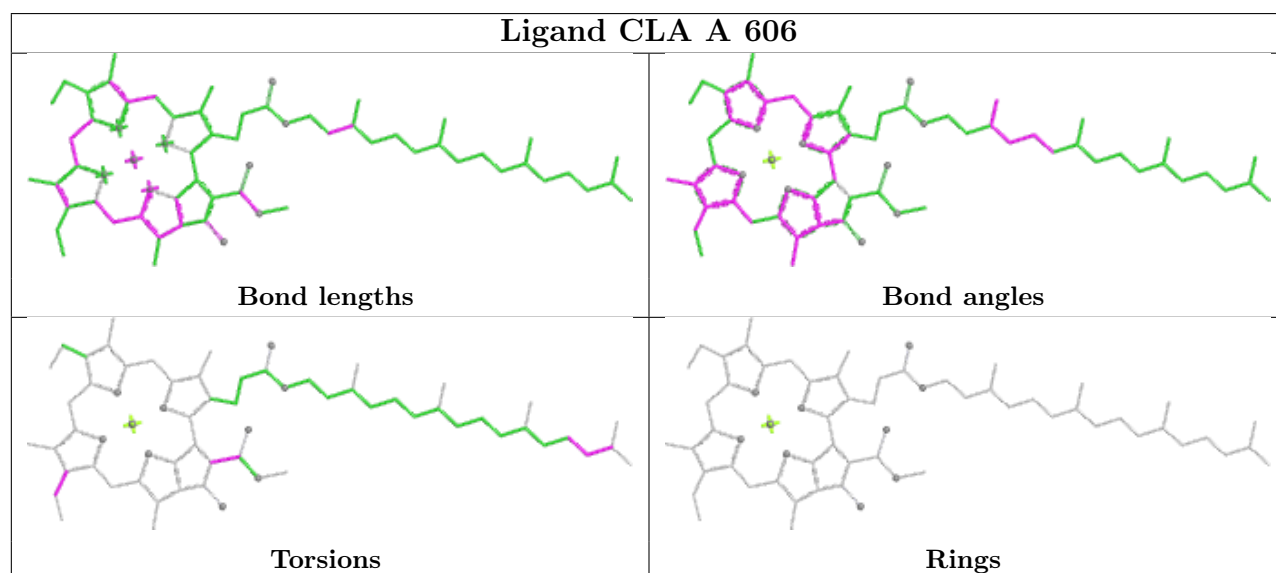
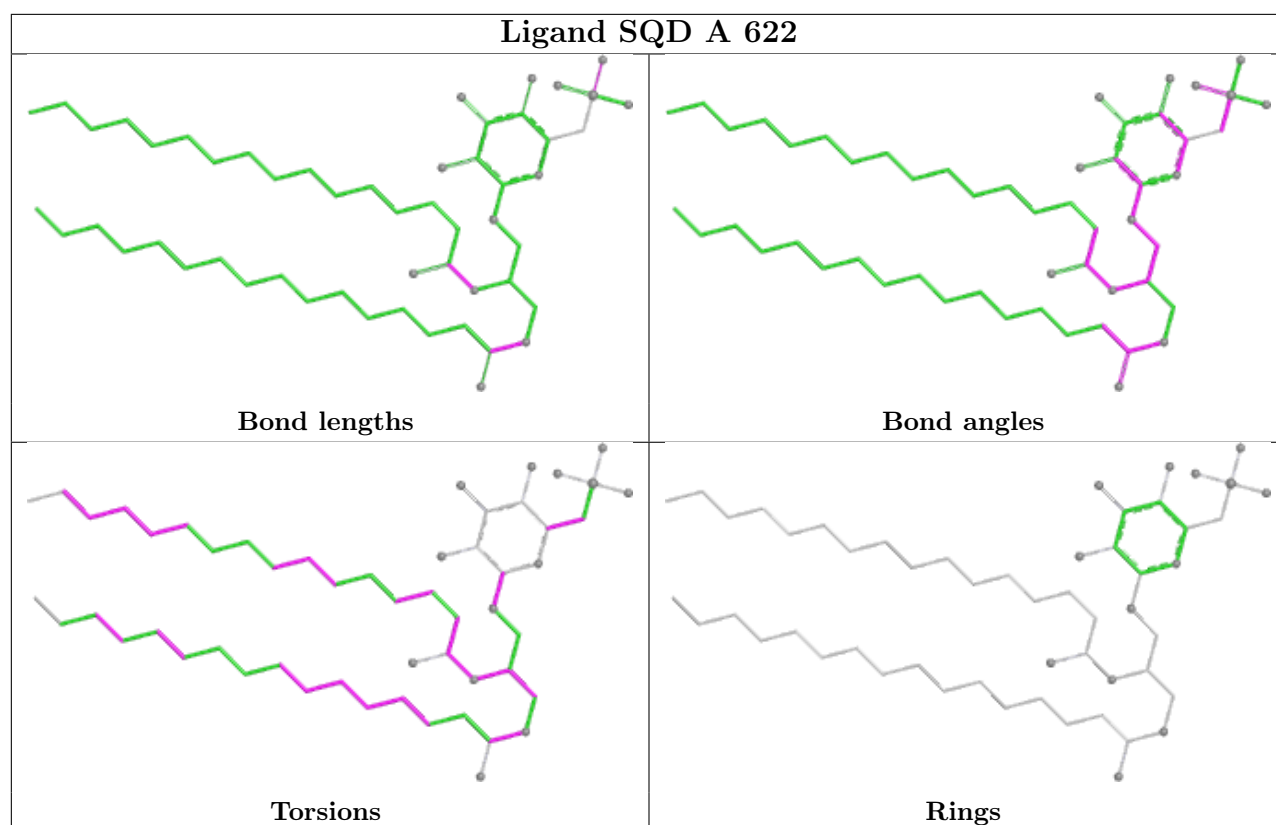




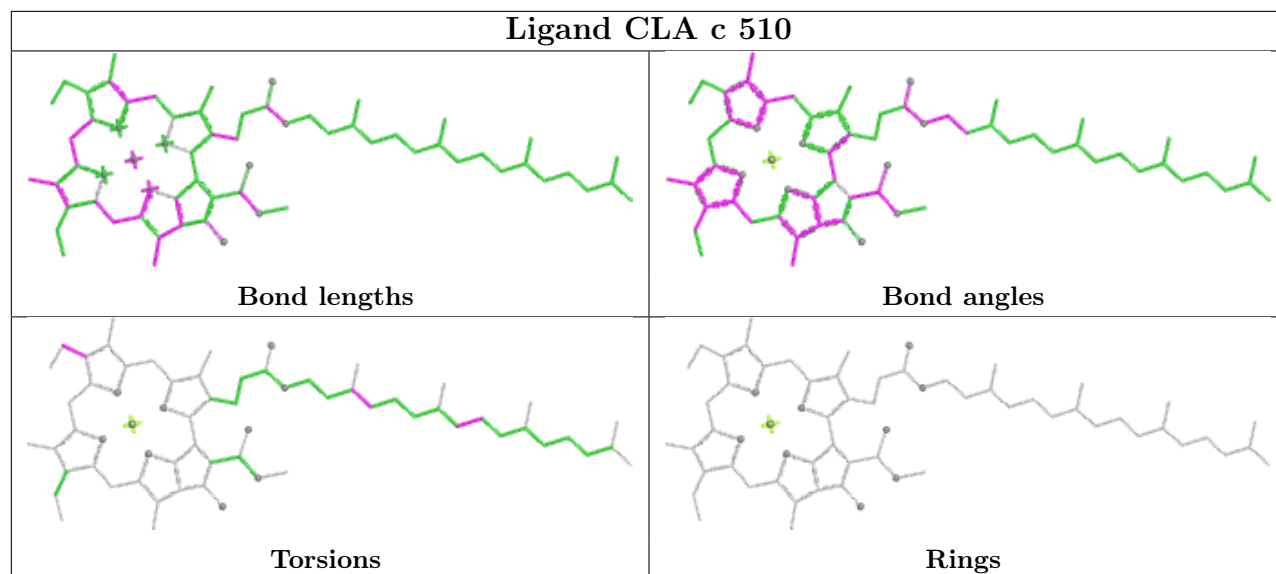
Ligand LMG d 412	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG j 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand P6G b 648	
 Bond lengths	 Bond angles
 Torsions	 Rings



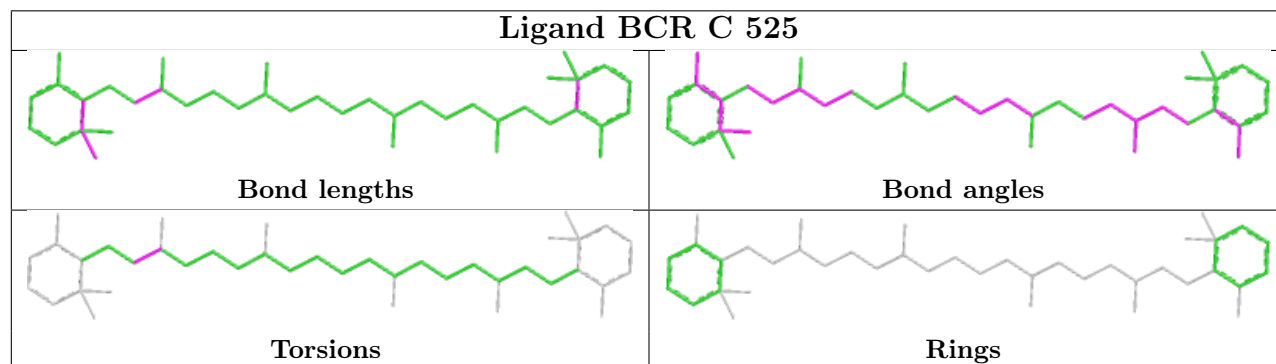




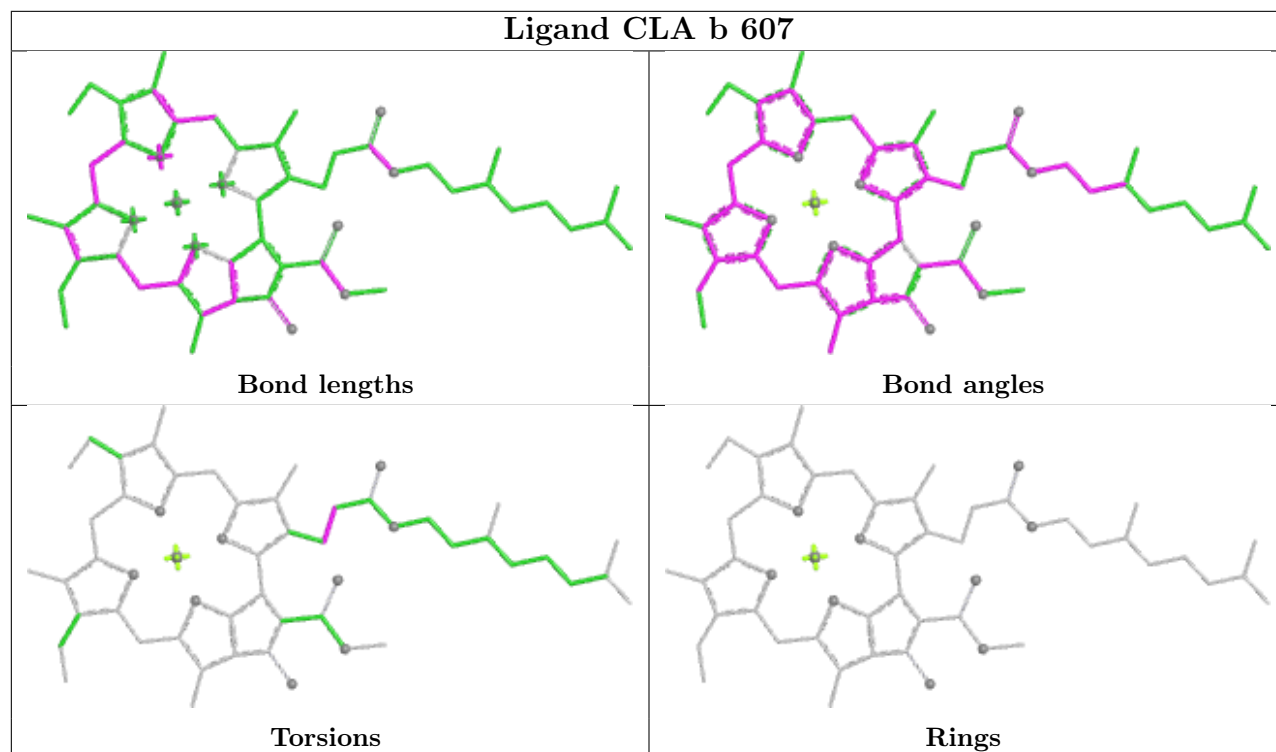
Ligand CLA c 510

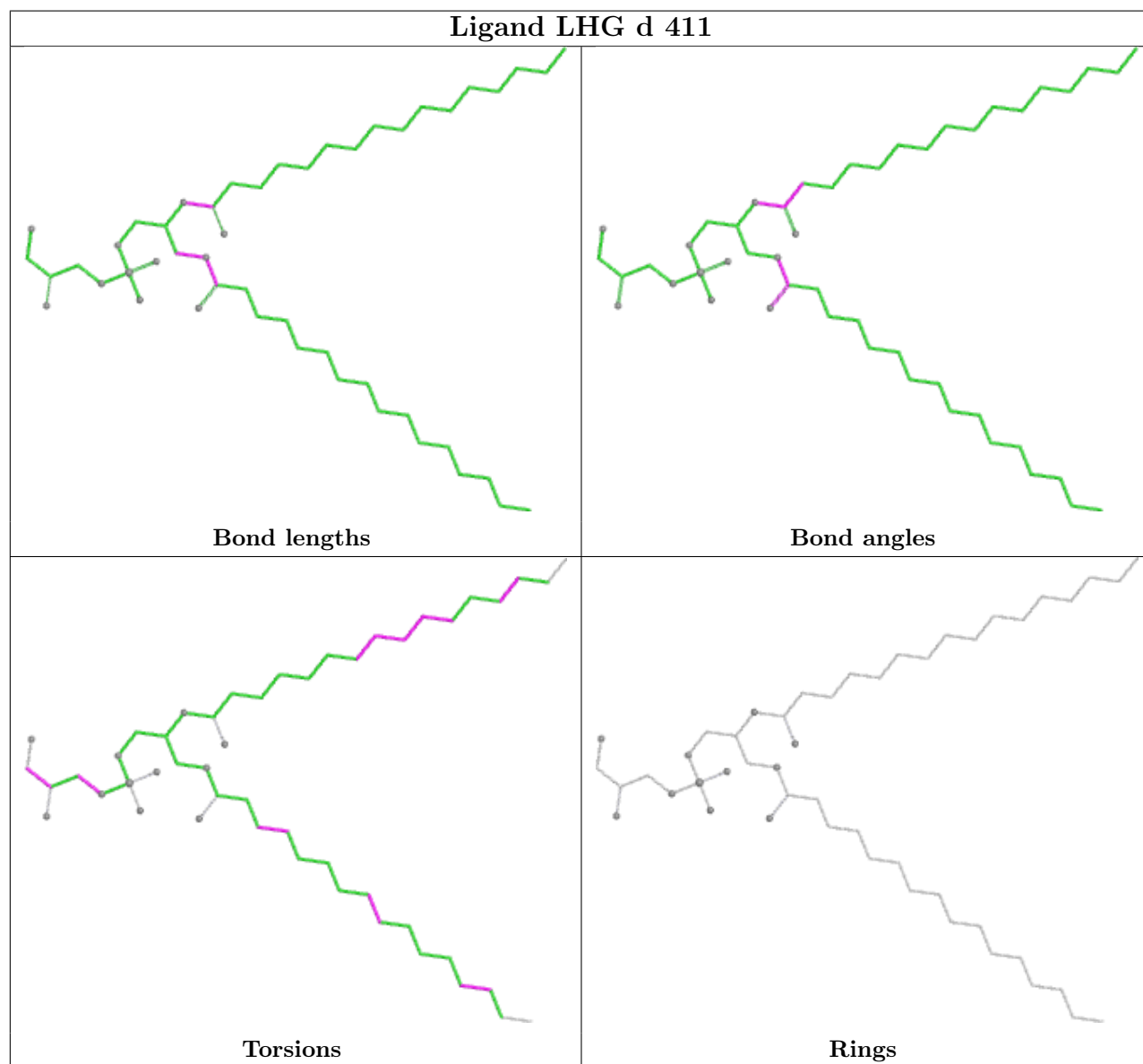
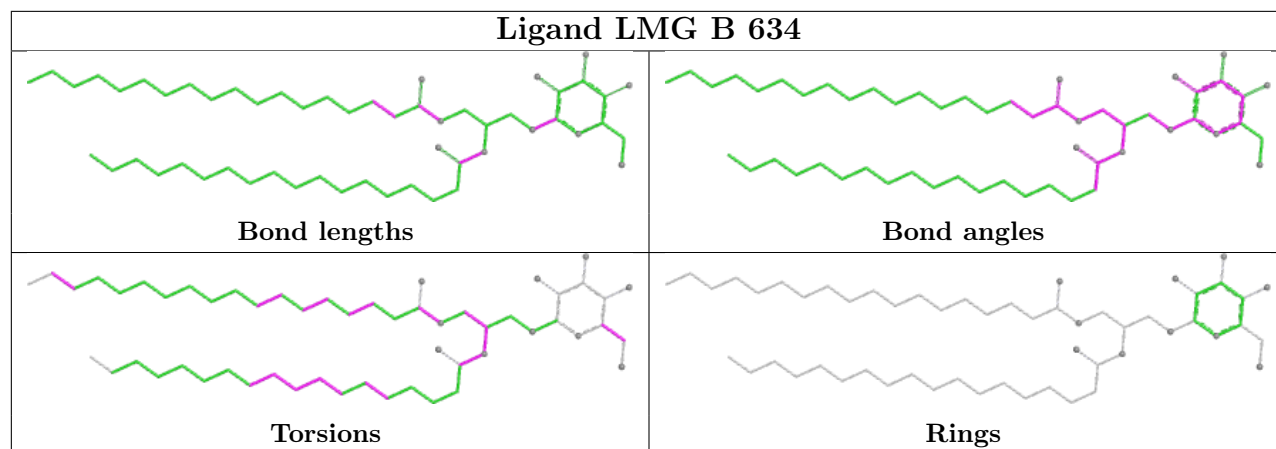


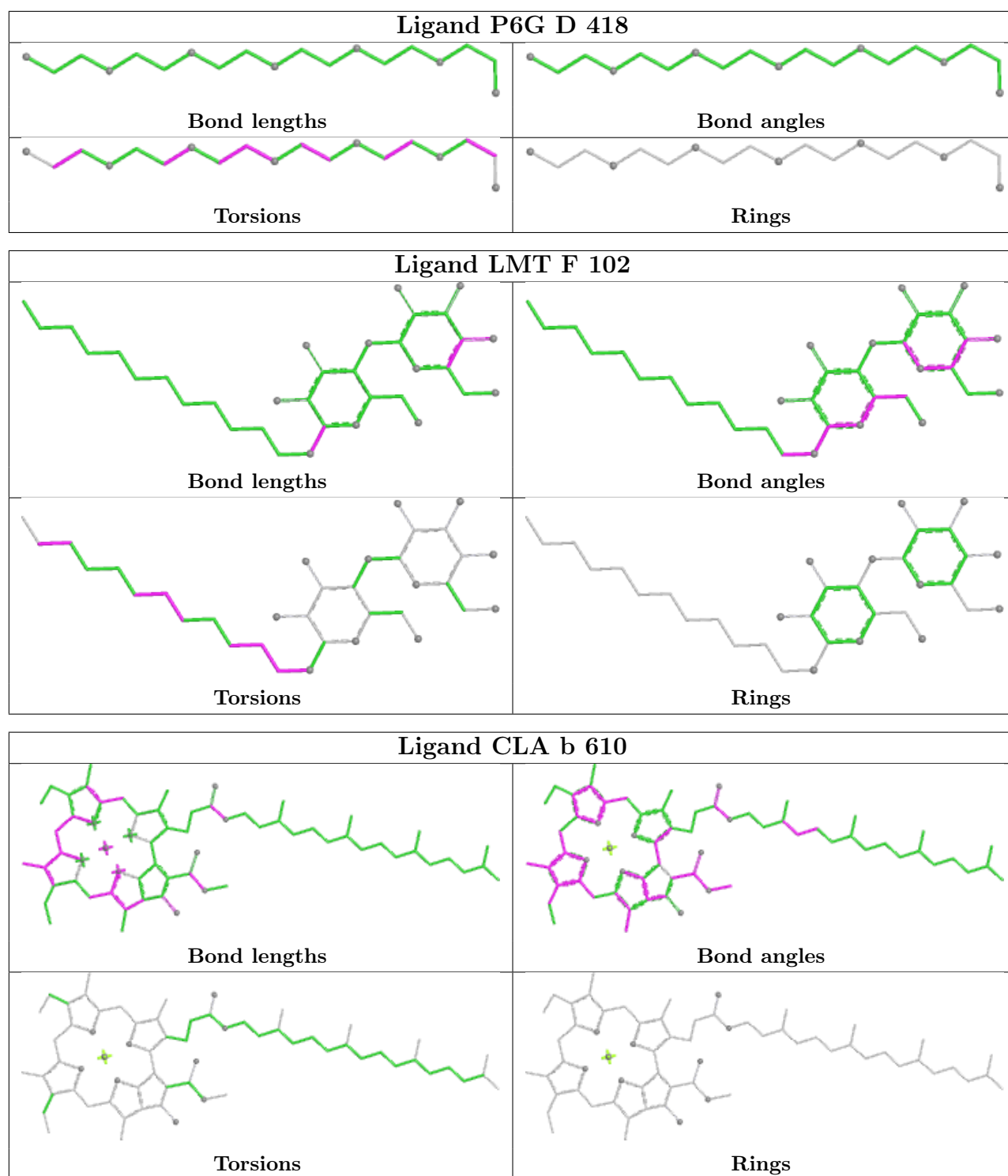
Ligand BCR C 525

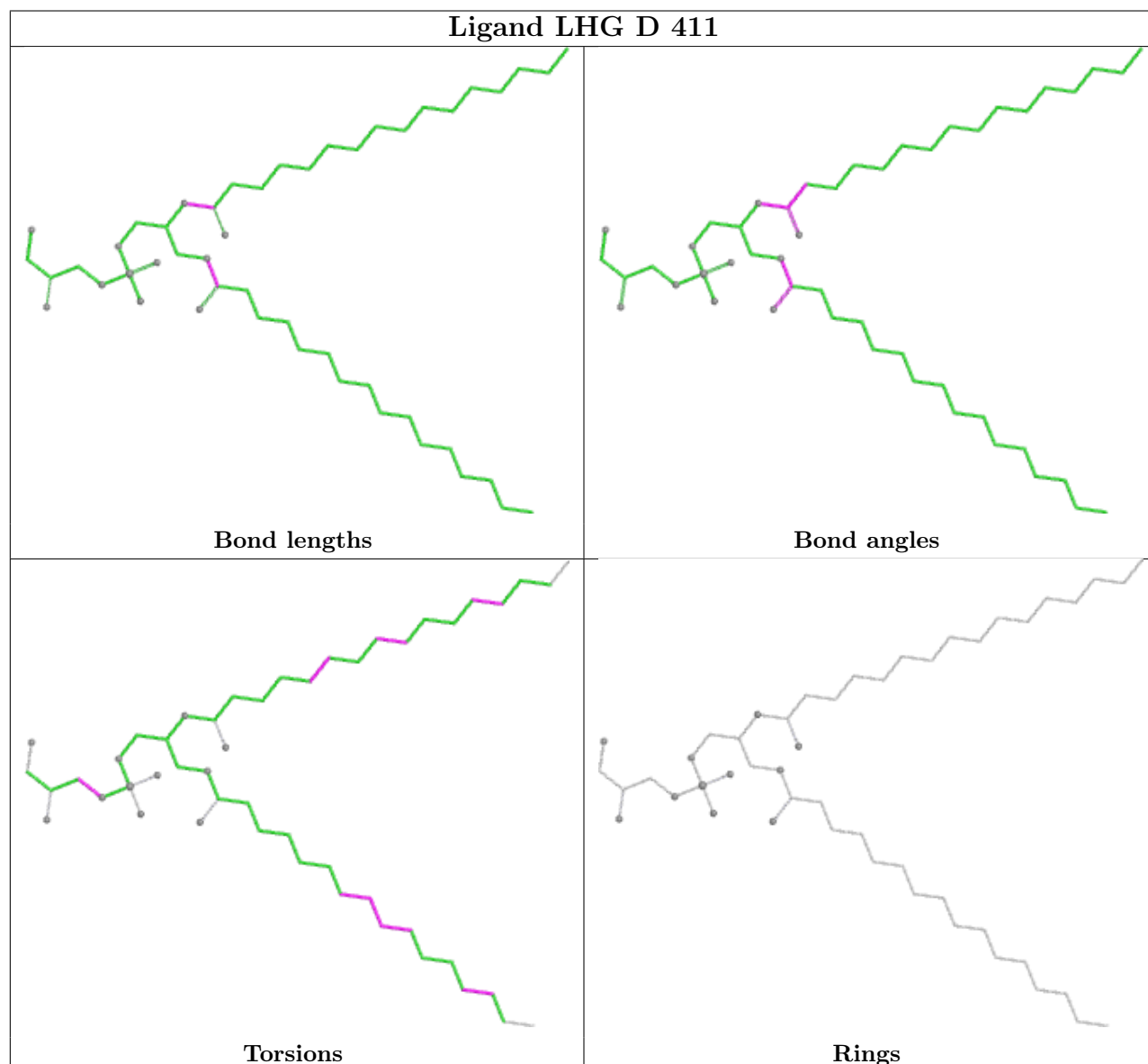
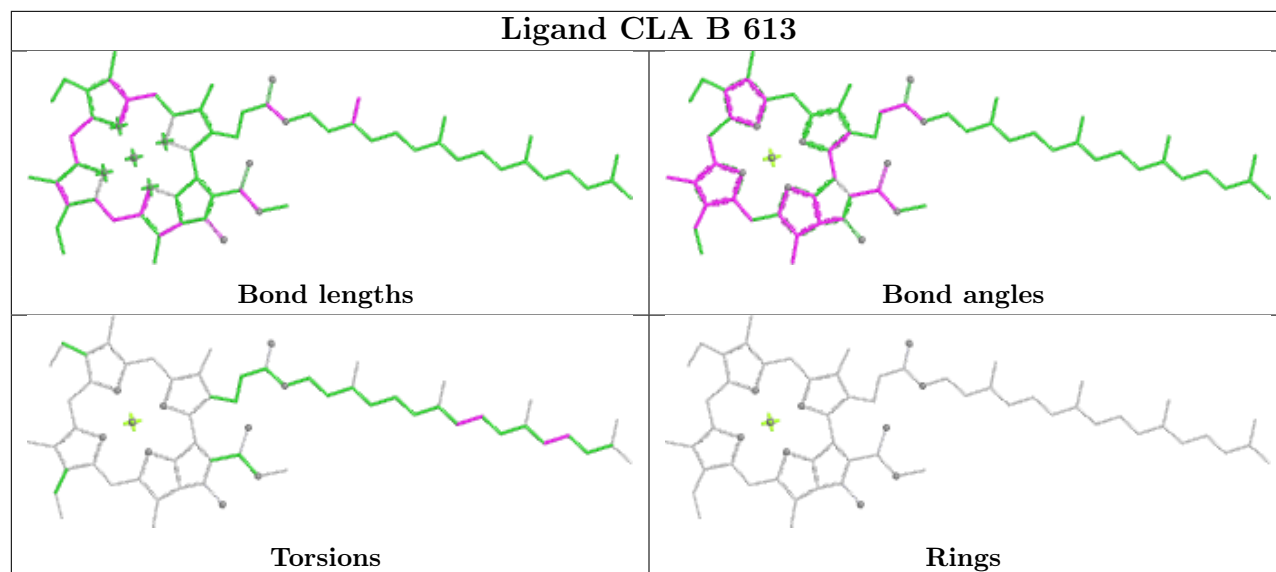


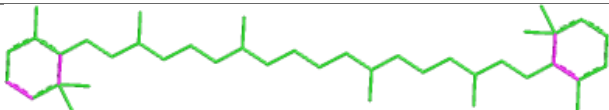
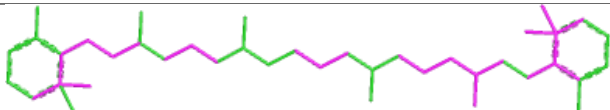
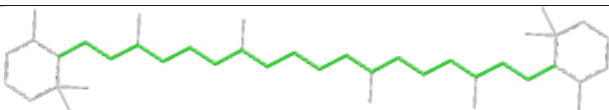
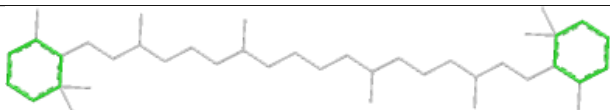
Ligand CLA b 607

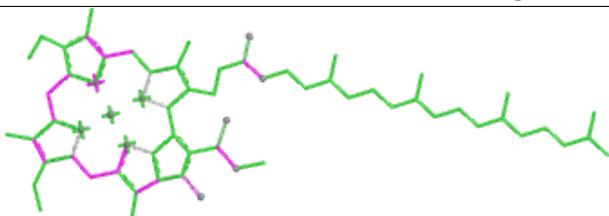
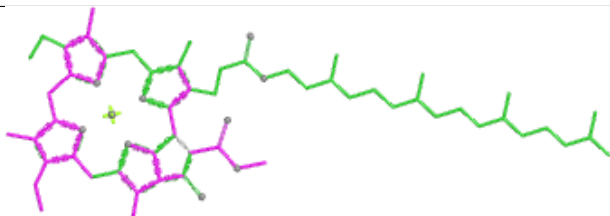
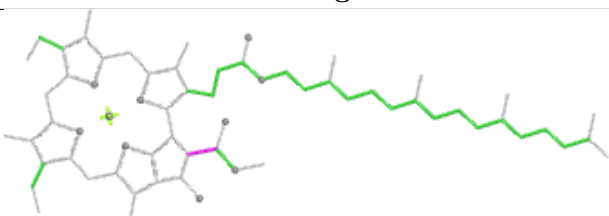
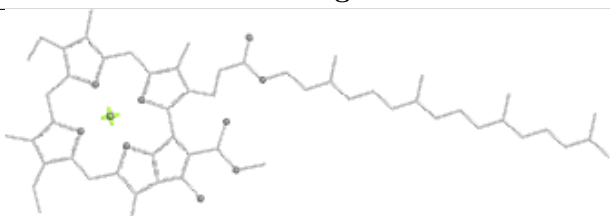


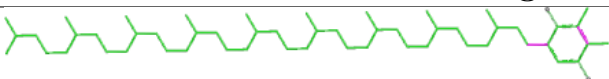
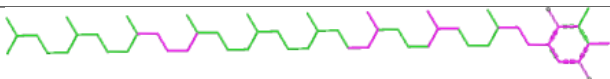
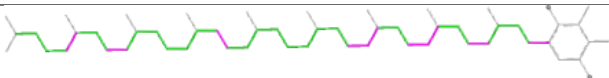
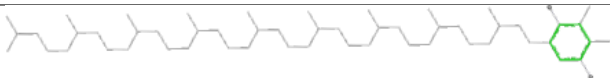


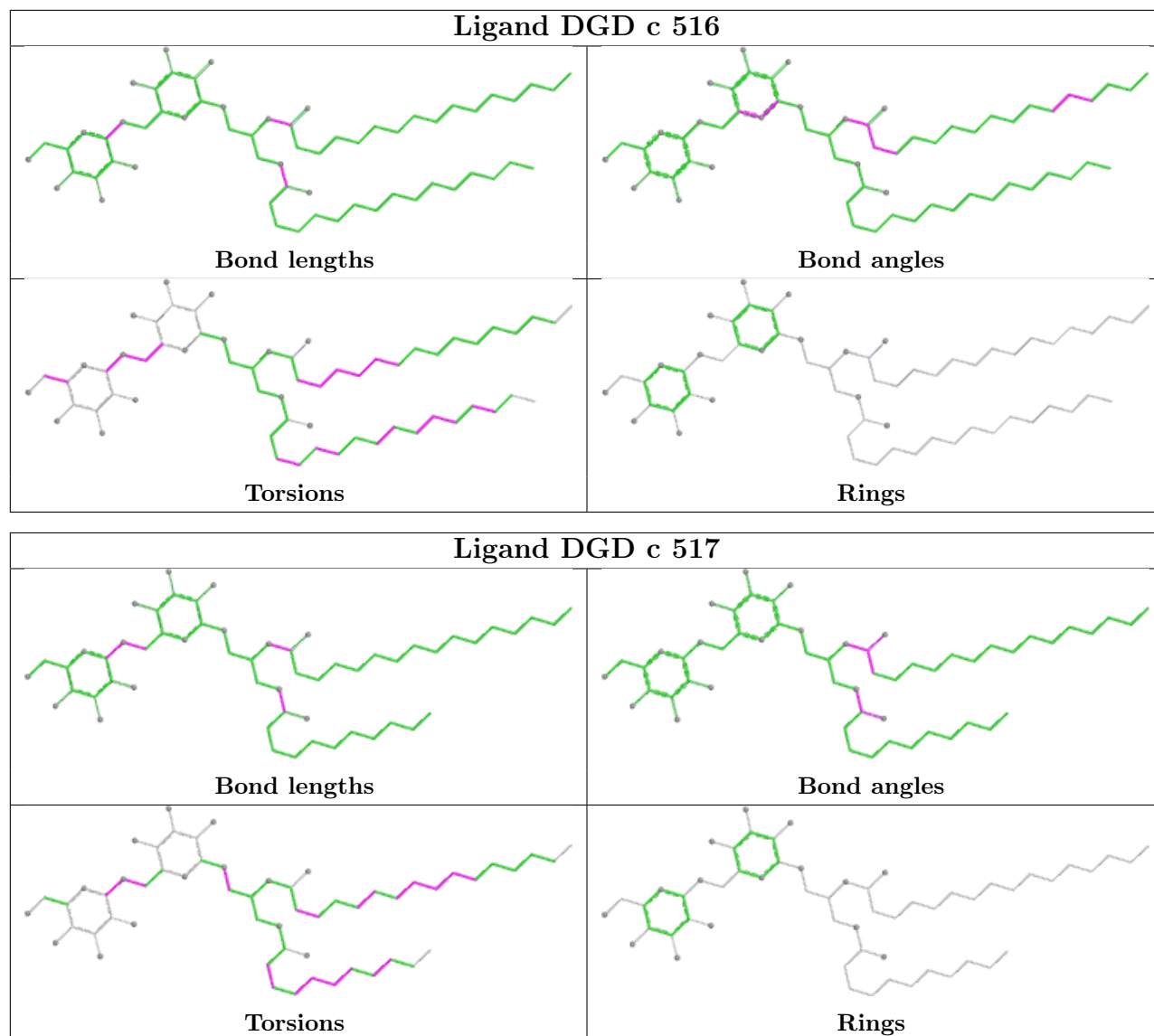


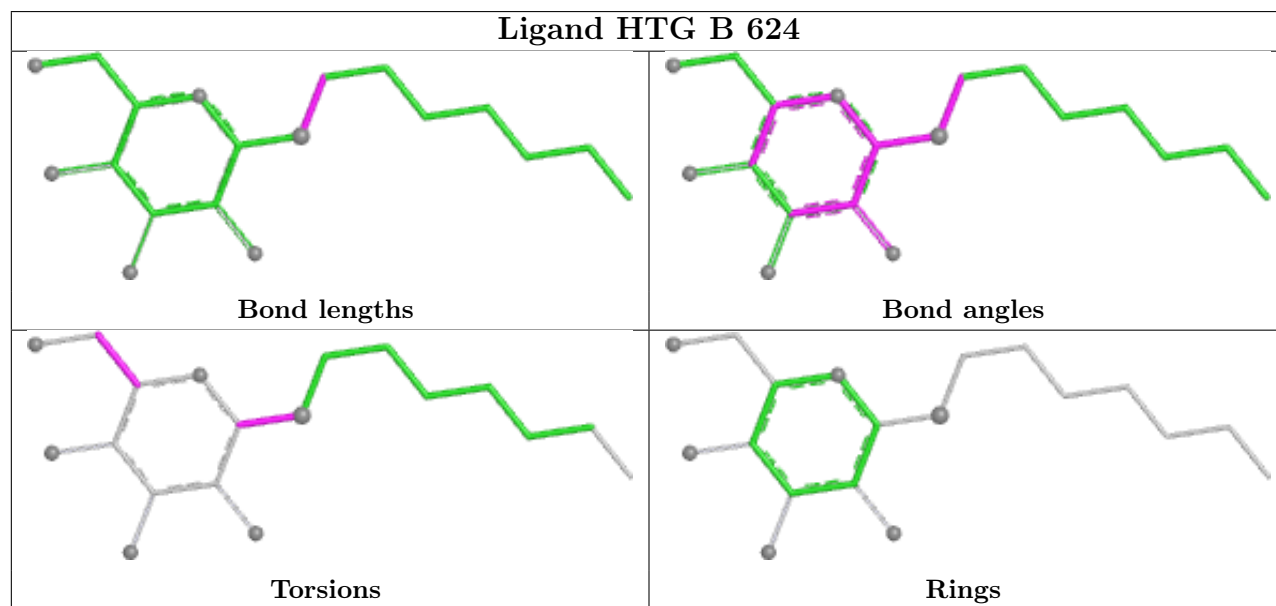
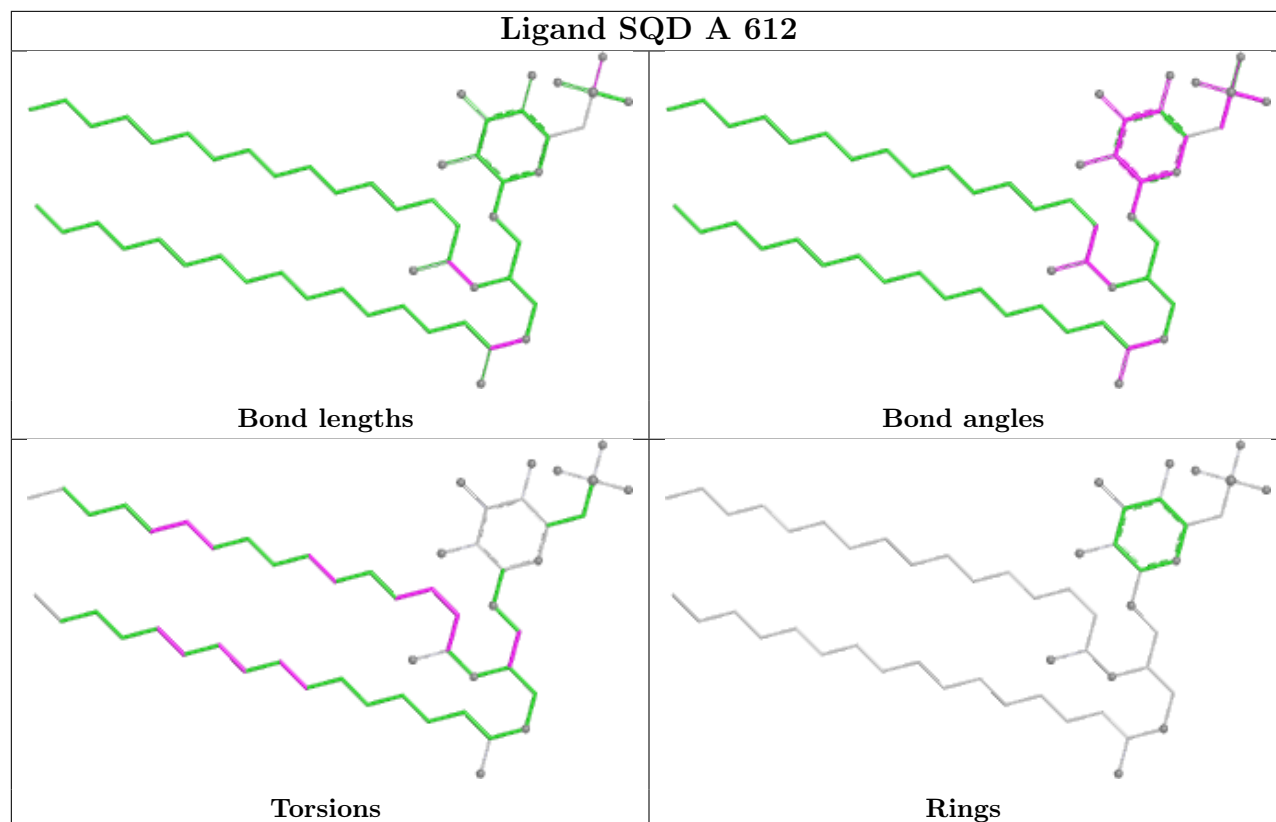


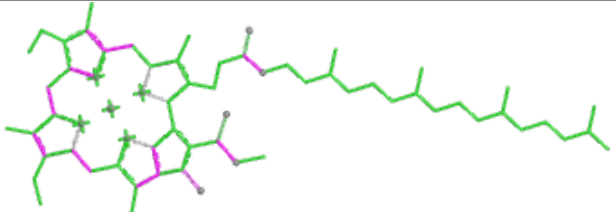
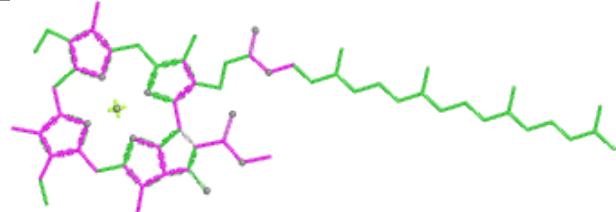
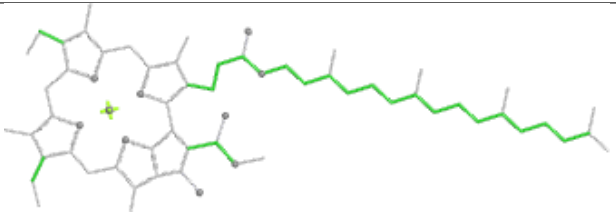
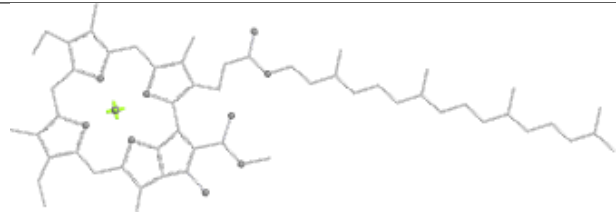
Ligand BCR D 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

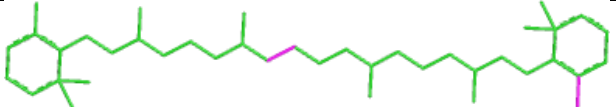
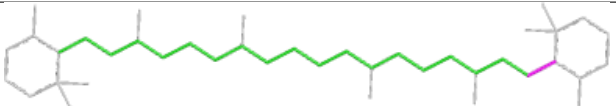
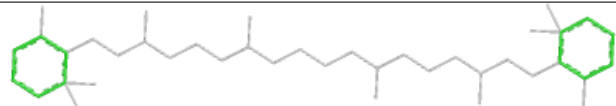
Ligand CLA B 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

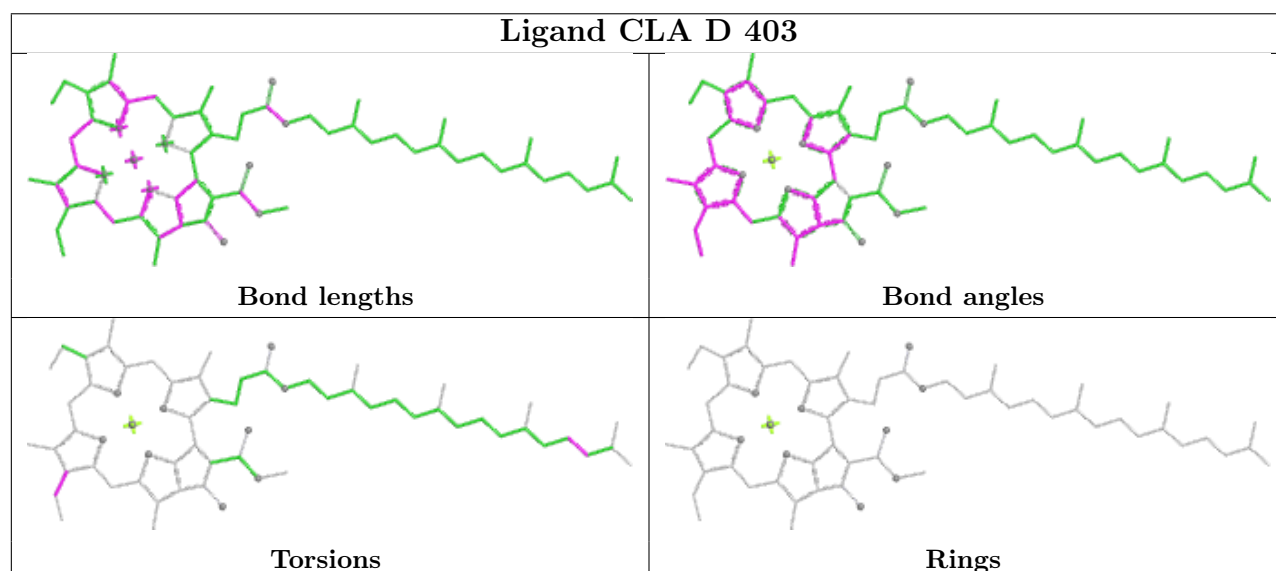
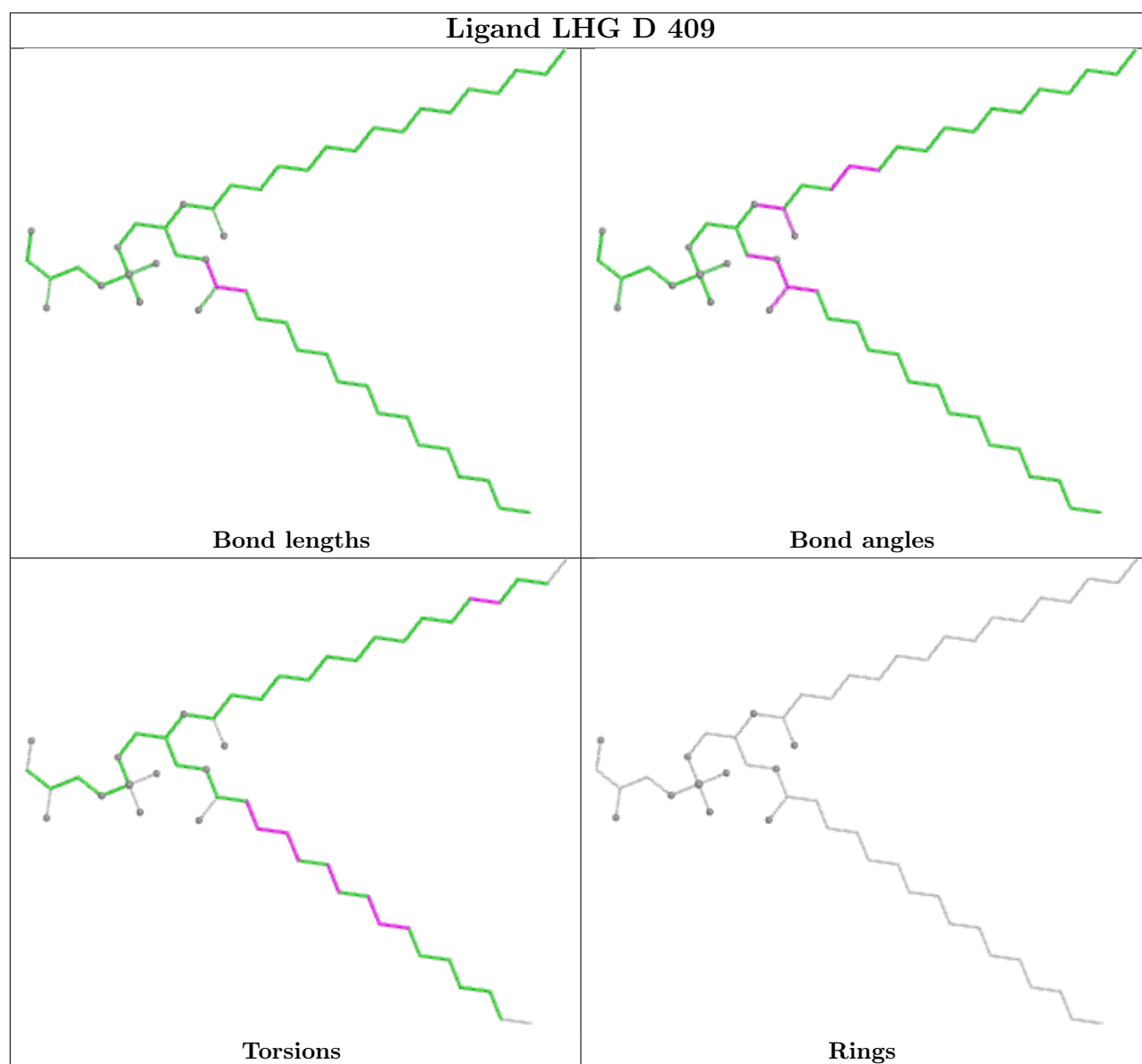
Ligand PL9 a 412	
	
Bond lengths	Bond angles
	
Torsions	Rings

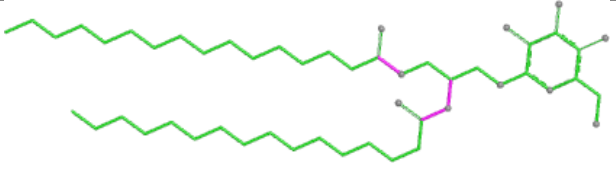
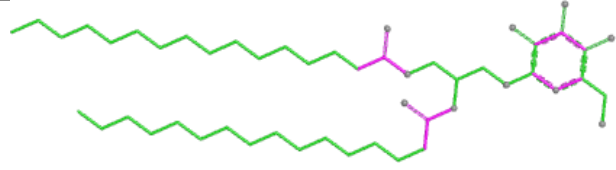
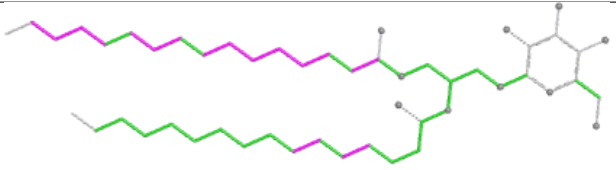
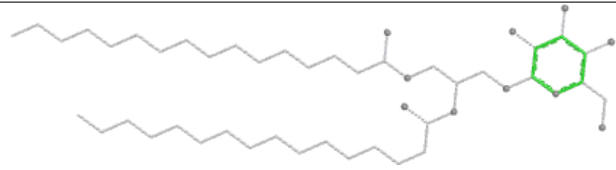


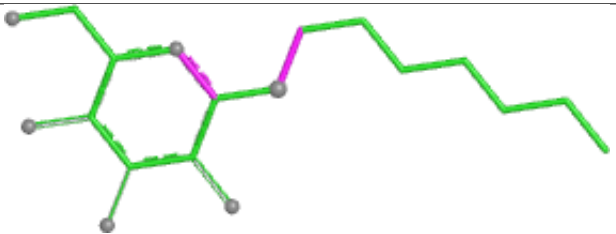
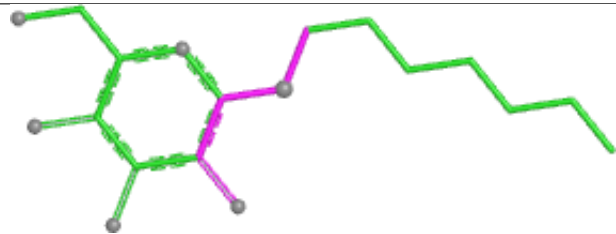
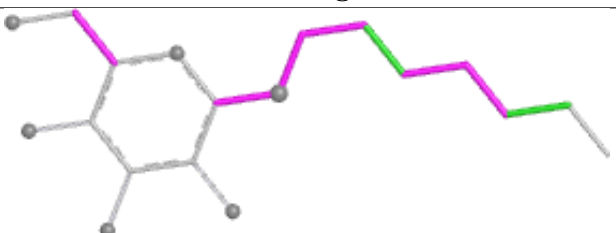
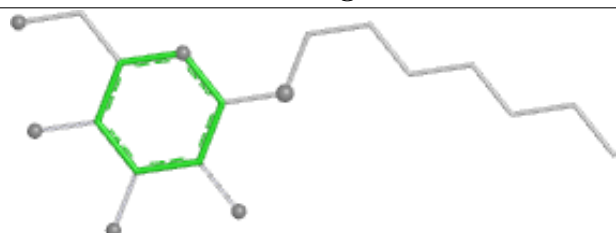


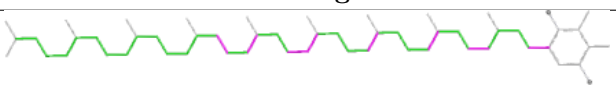
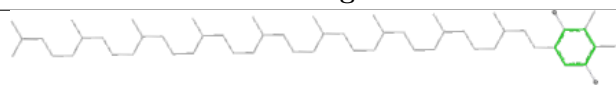
Ligand CLA C 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

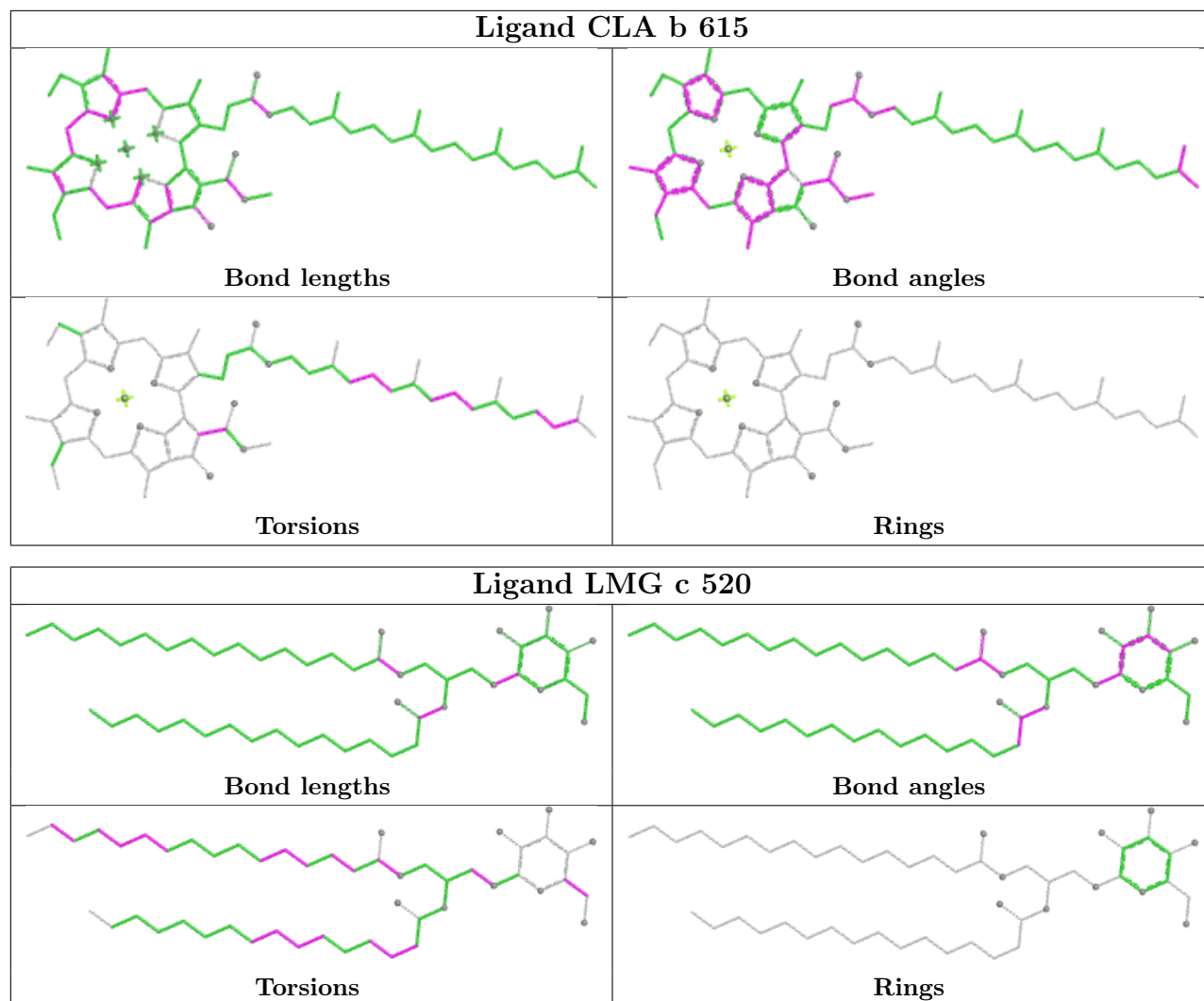
Ligand BCR T 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

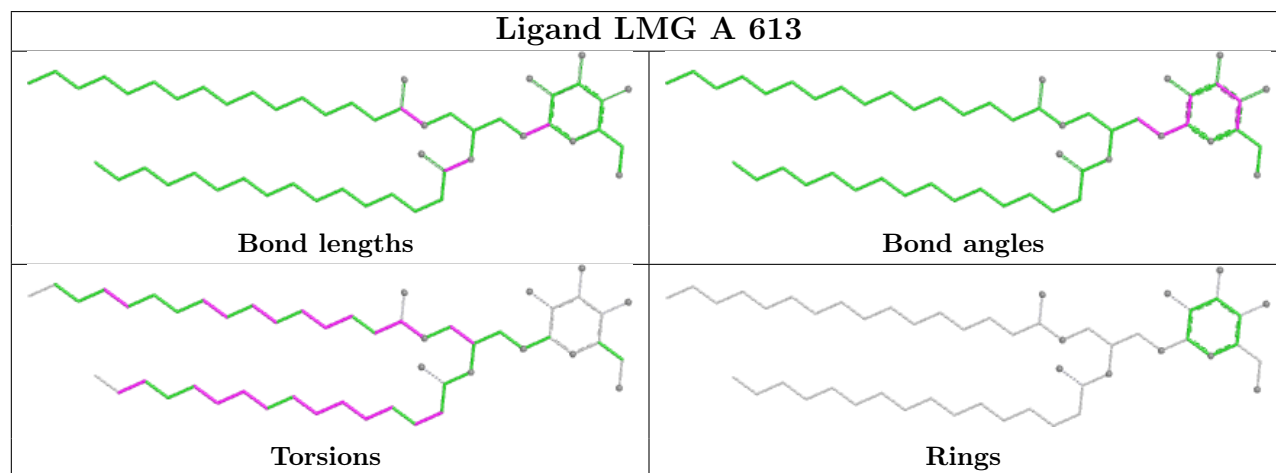
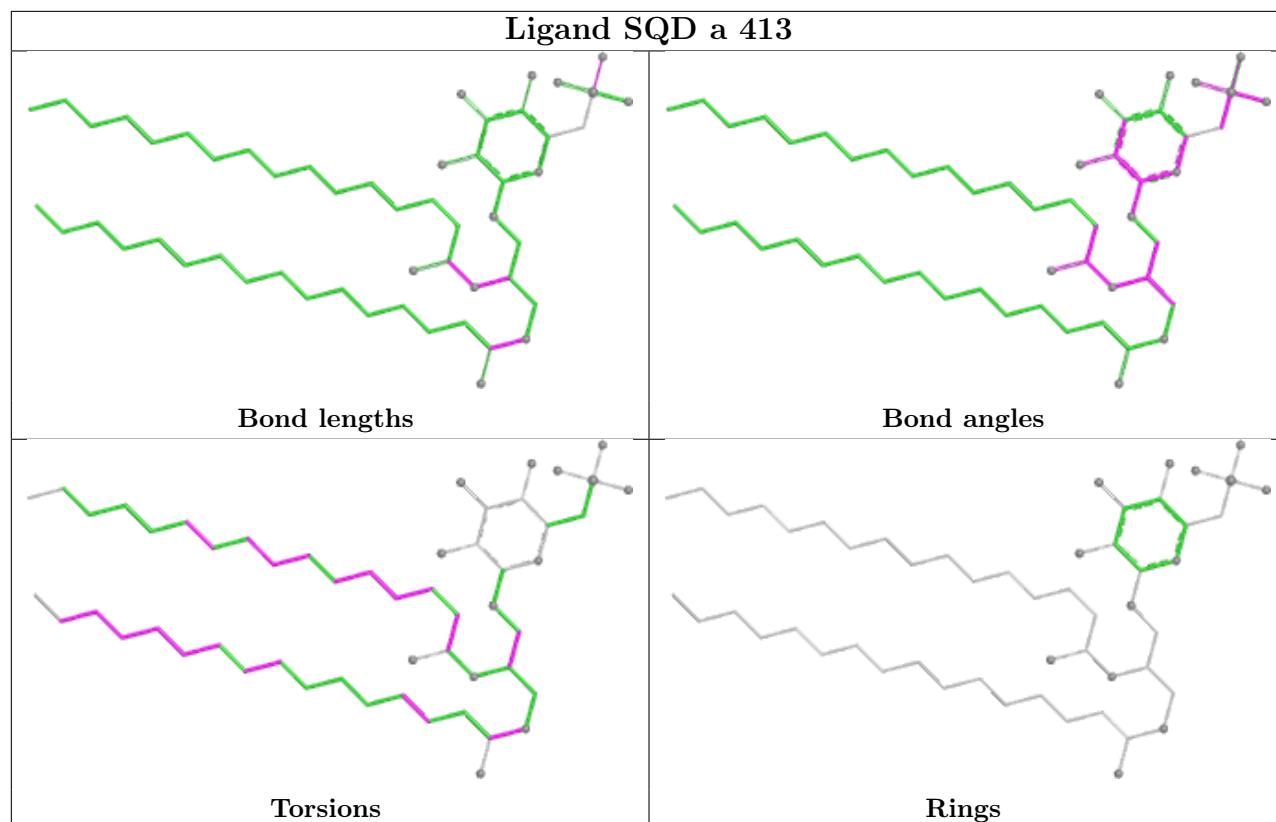


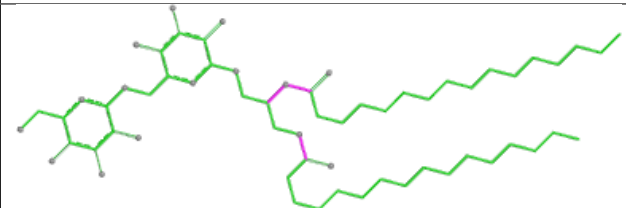
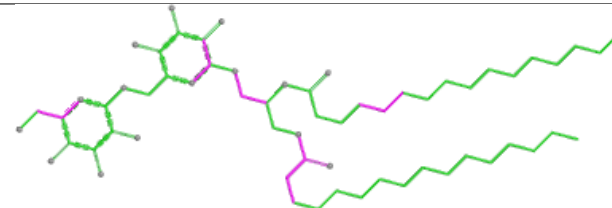
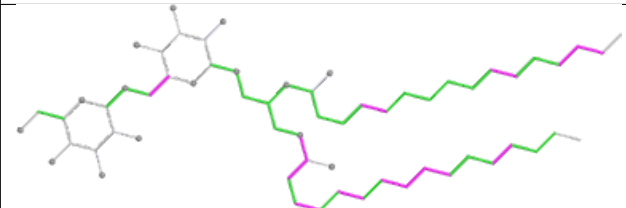
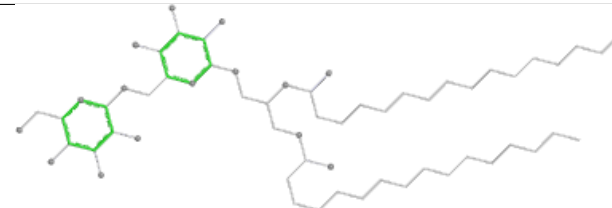
Ligand LMG b 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

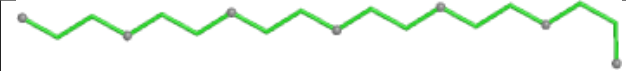
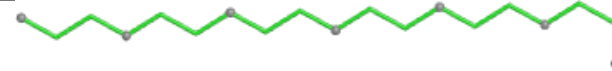
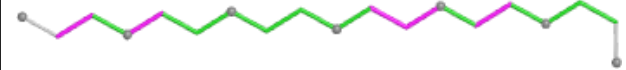
Ligand HTG C 531	
	
Bond lengths	Bond angles
	
Torsions	Rings

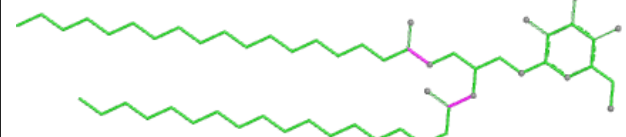
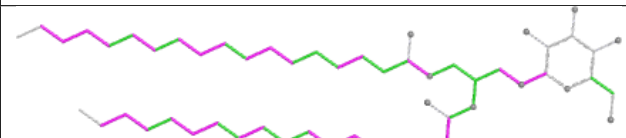
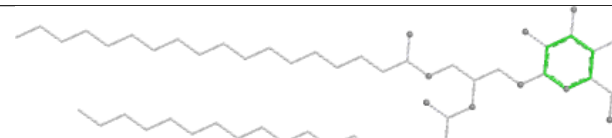
Ligand PL9 A 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

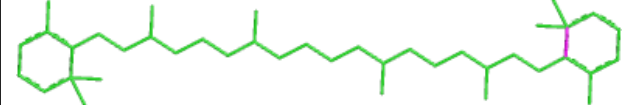
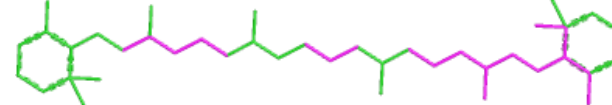
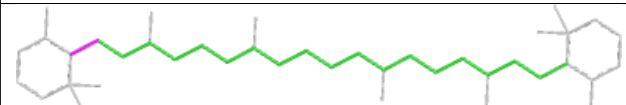
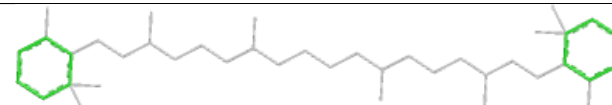


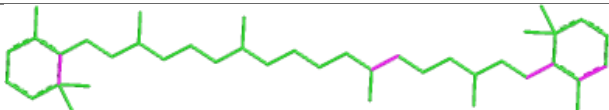
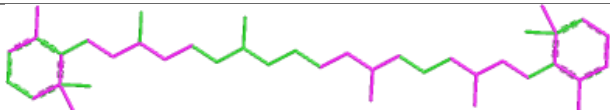
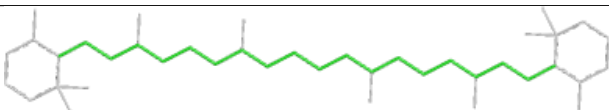
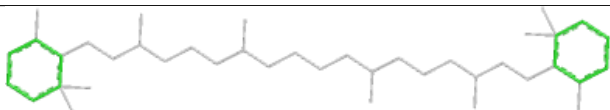


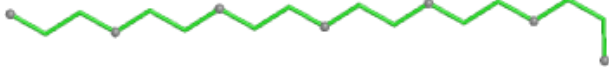
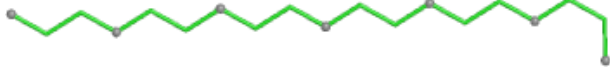
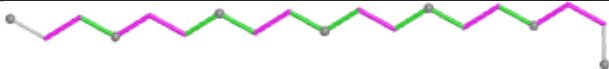
Ligand DGD c 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand P6G B 651	
	
Bond lengths	Bond angles
	
Torsions	Rings

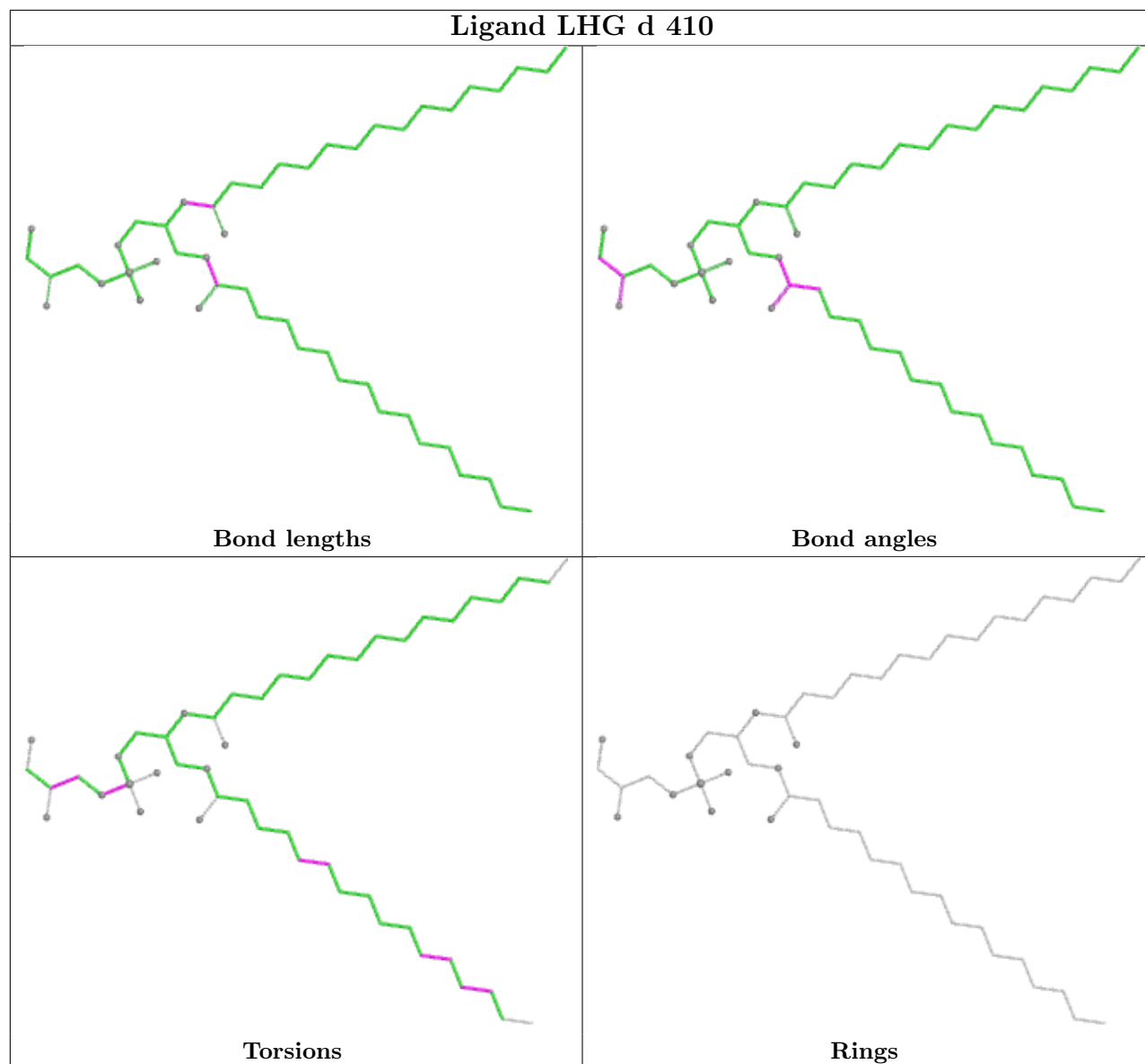
Ligand LMG C 526	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR K 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

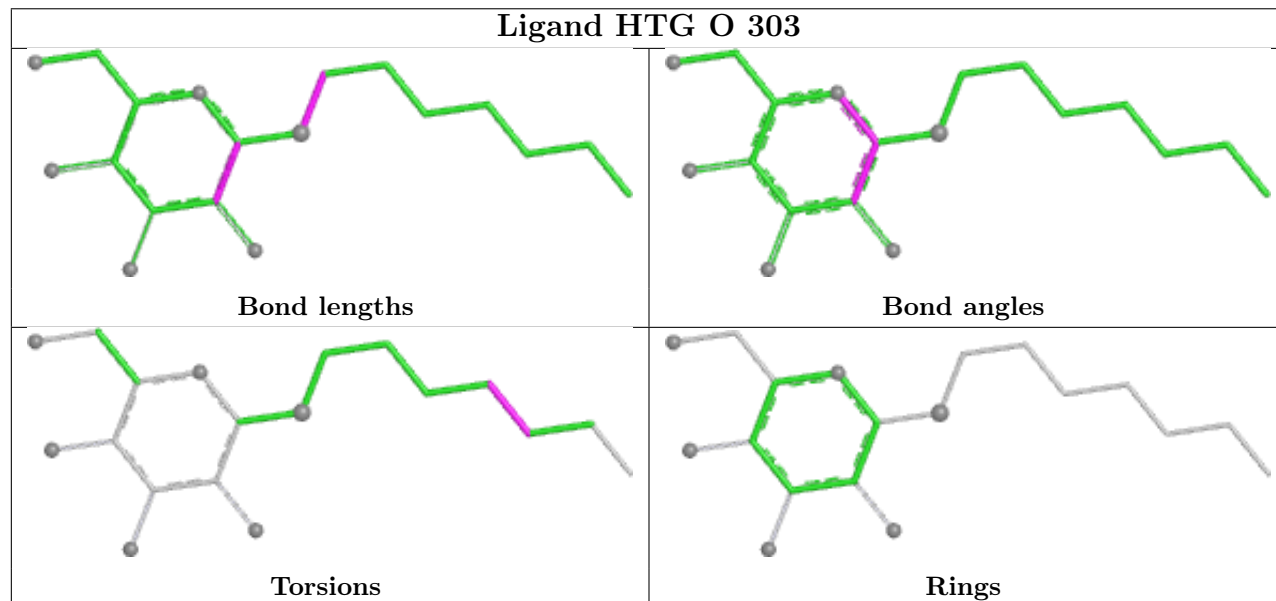
Ligand BCR h 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

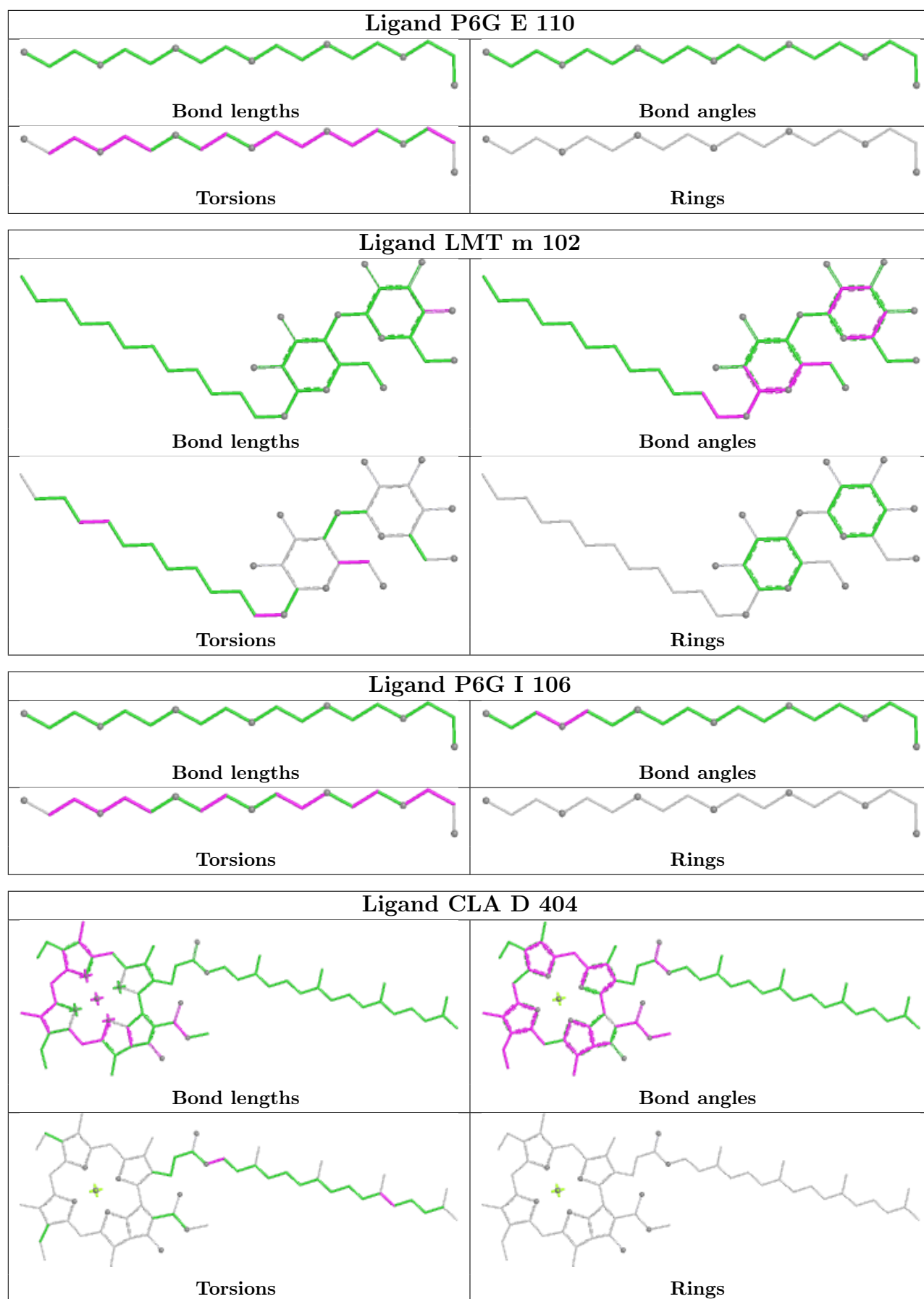
Ligand P6G D 417	
	
Bond lengths	Bond angles
	
Torsions	Rings

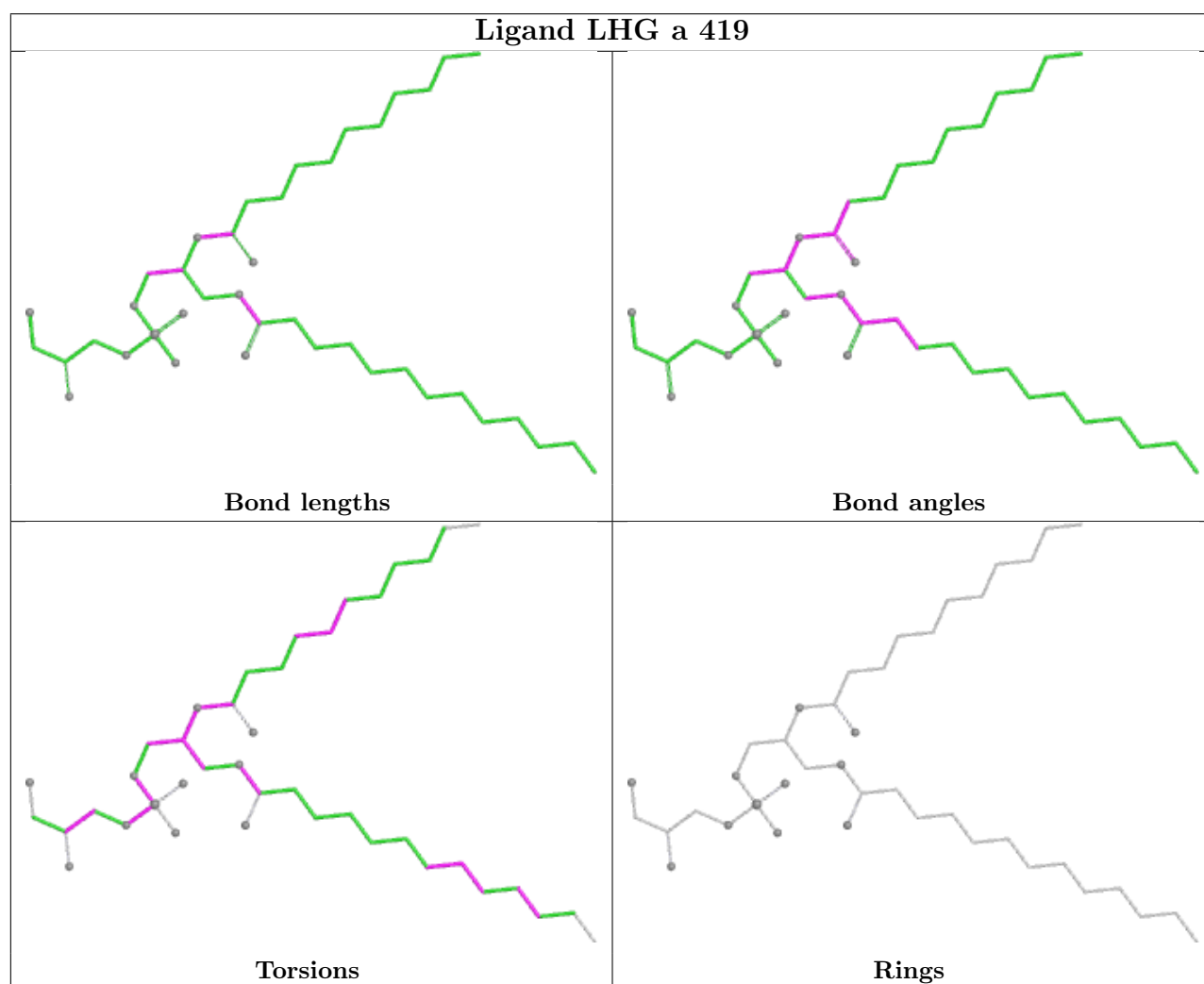
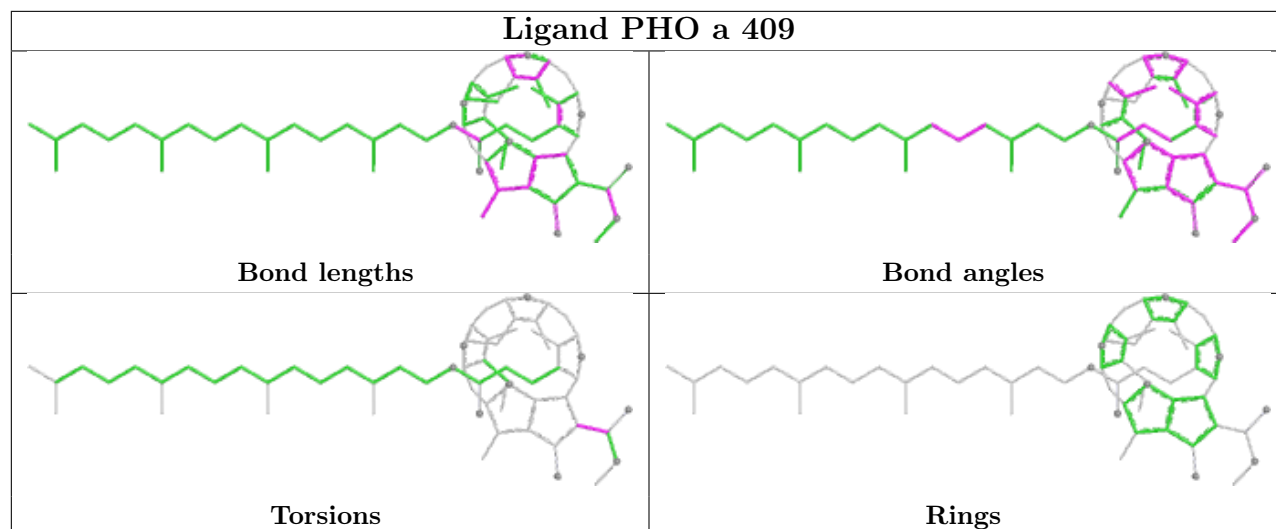
Ligand LHG d 410

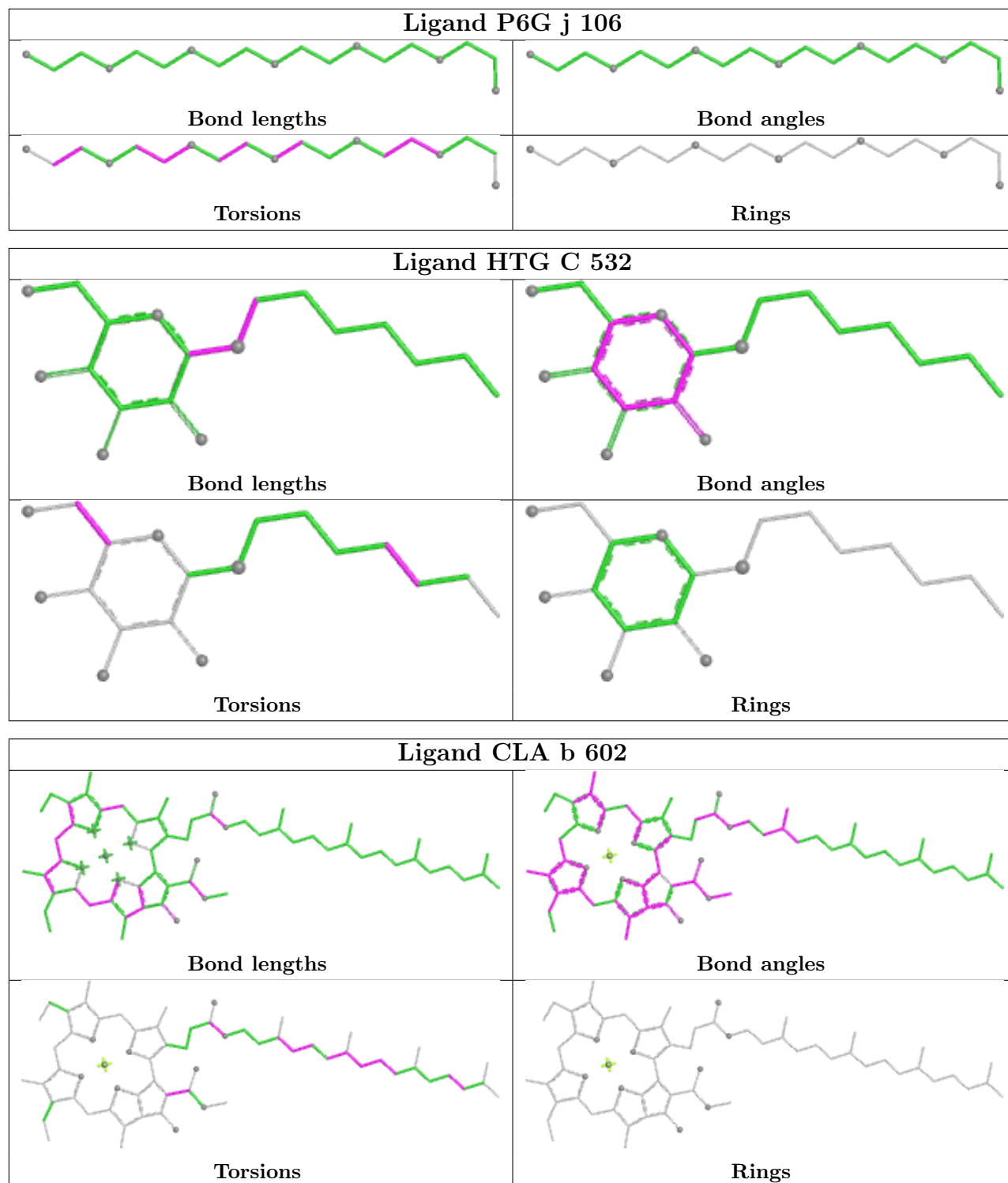


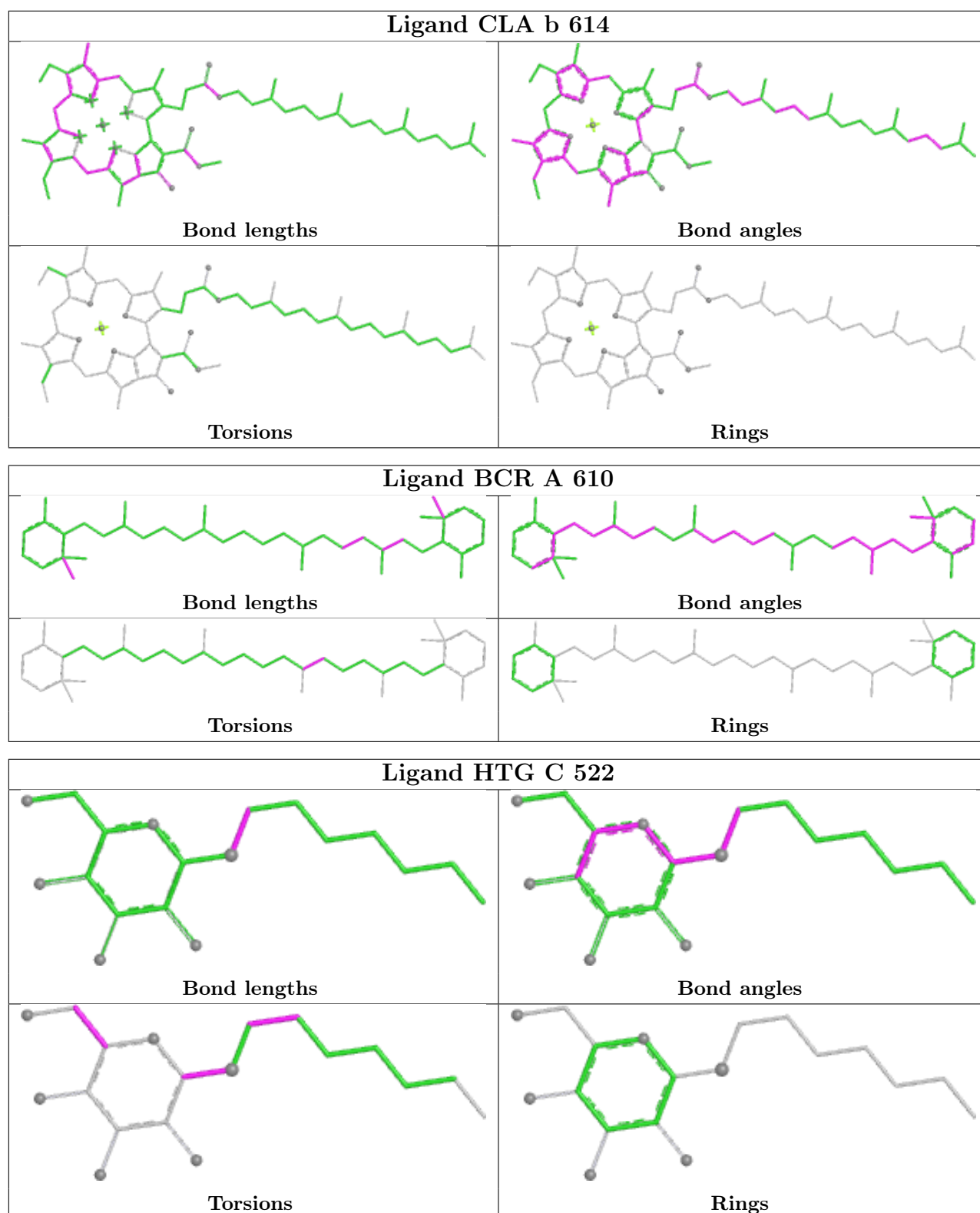
Ligand HTG O 303

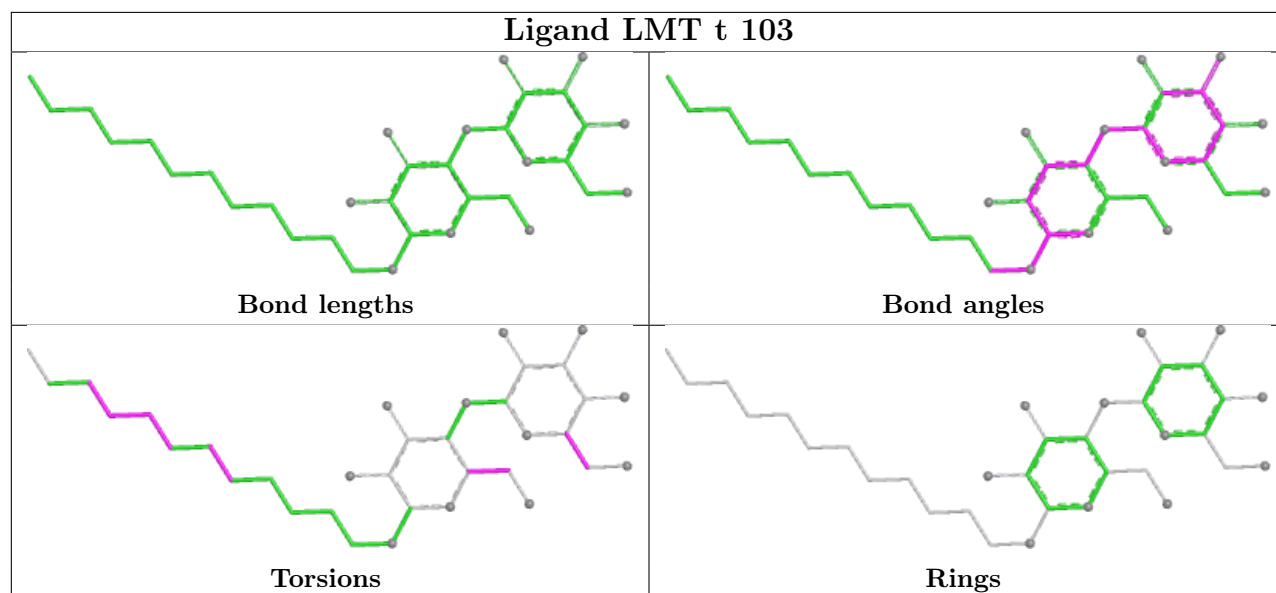
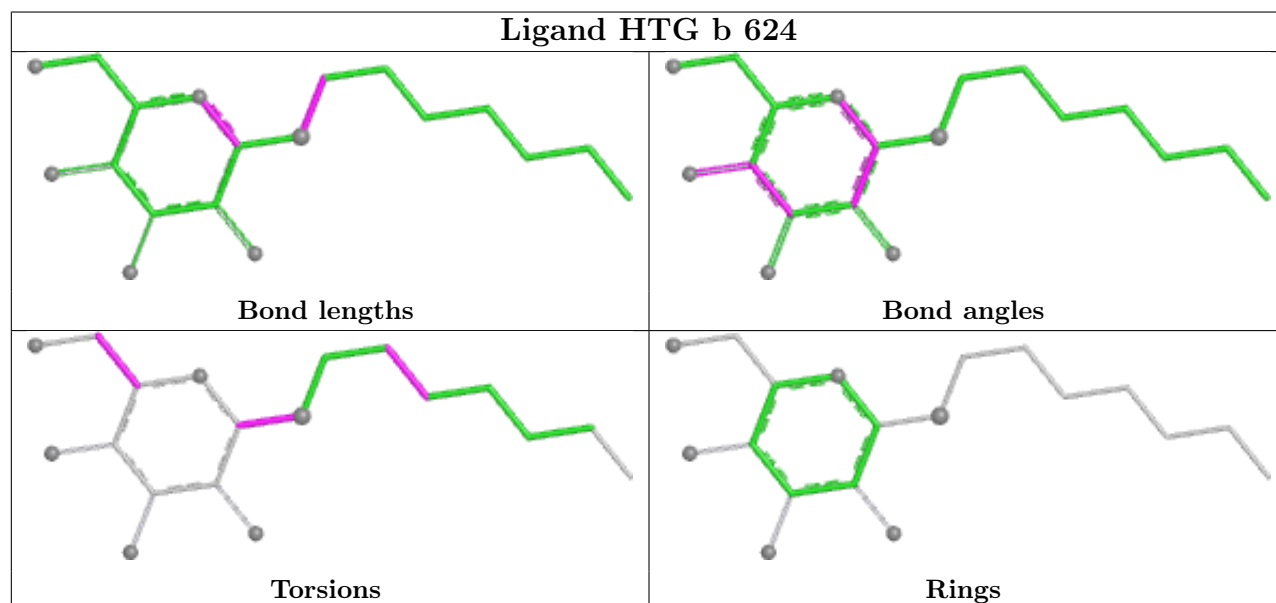
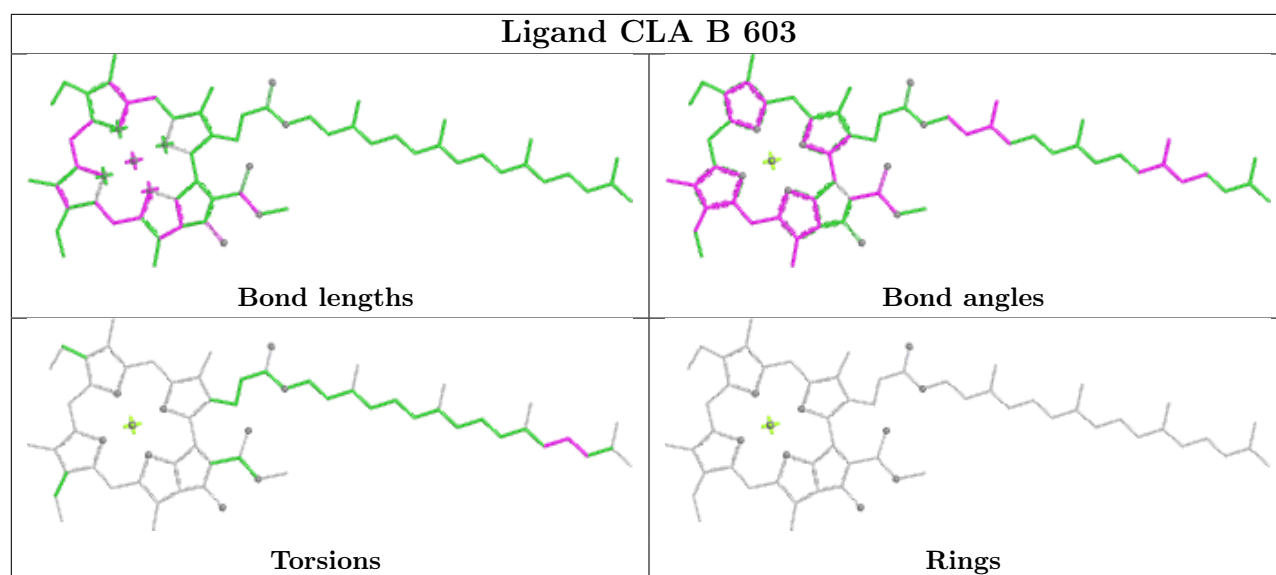


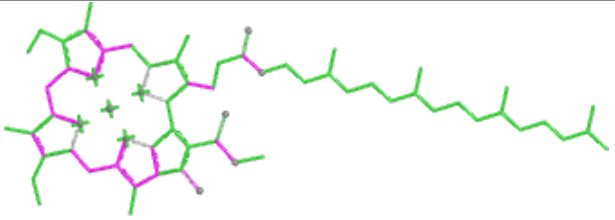
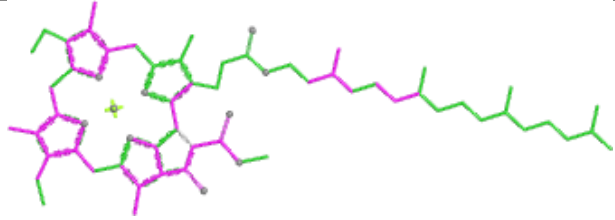
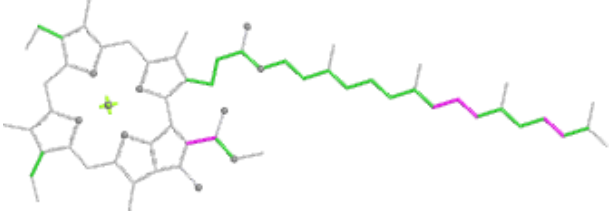
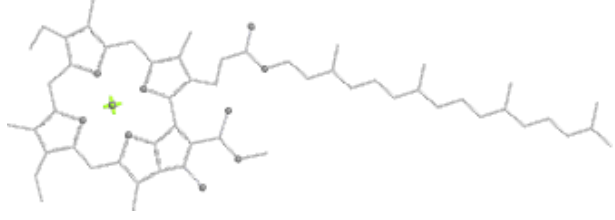
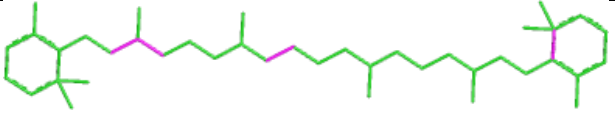
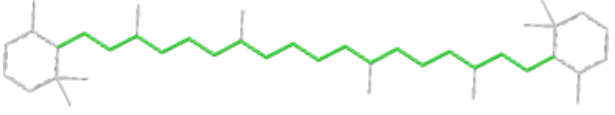
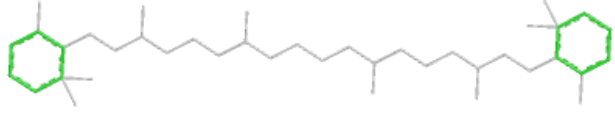
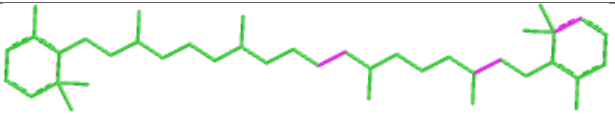
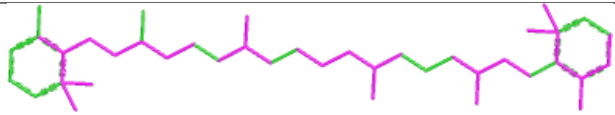
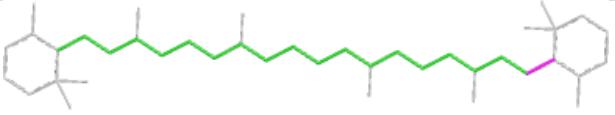
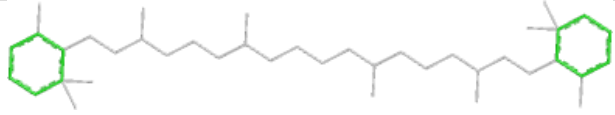


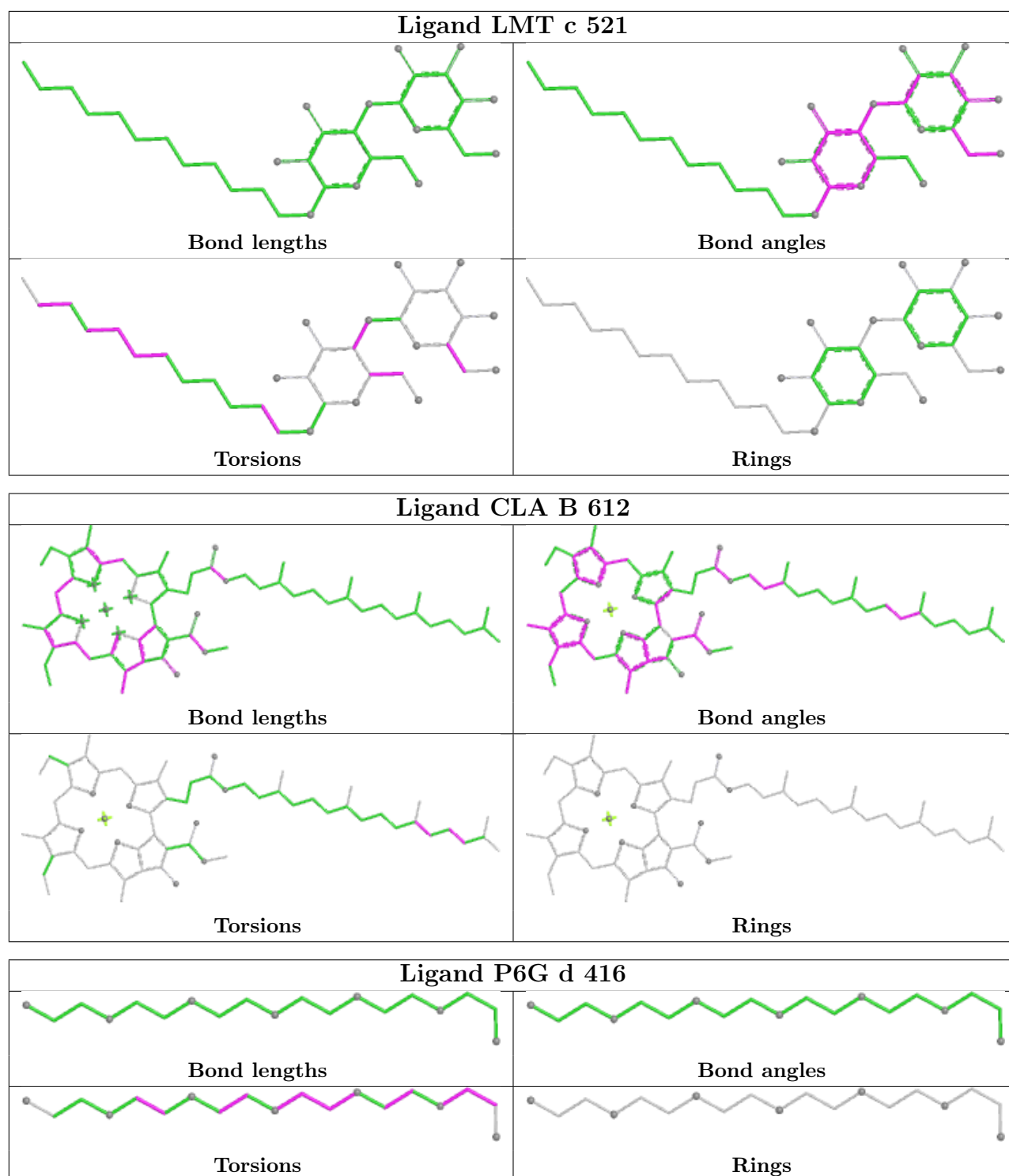


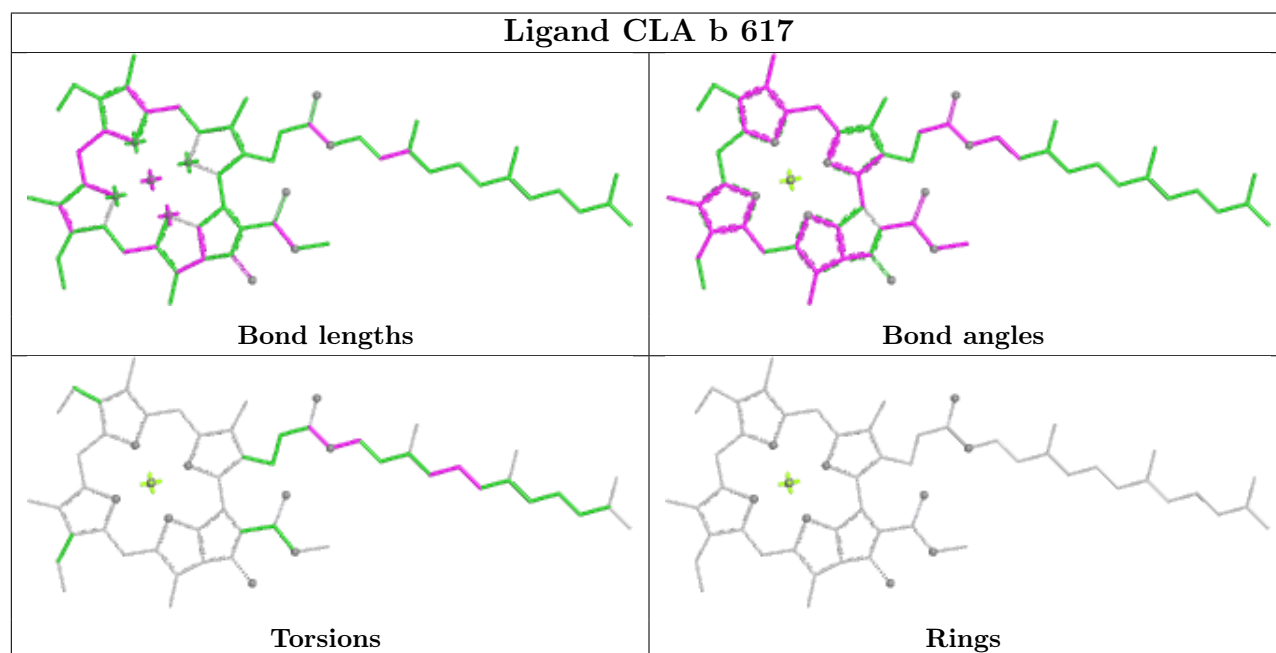
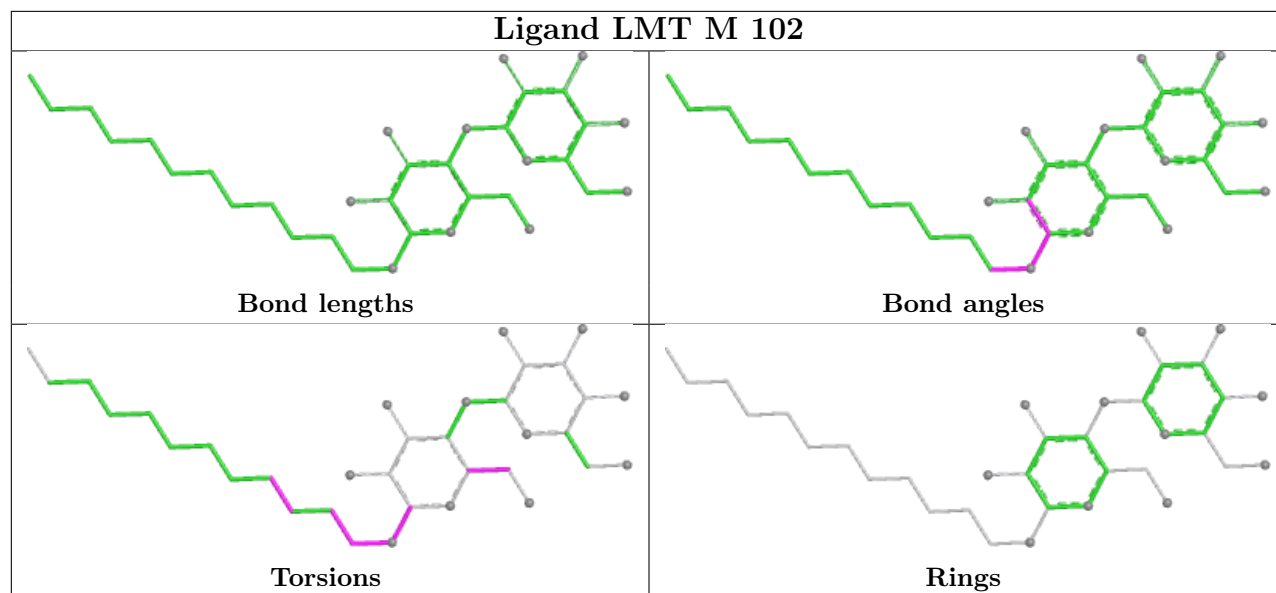


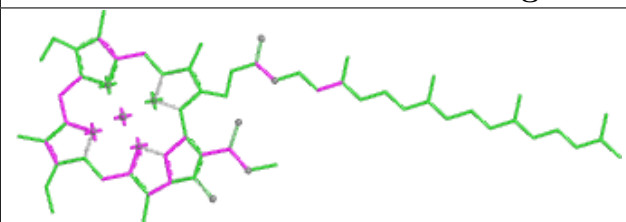
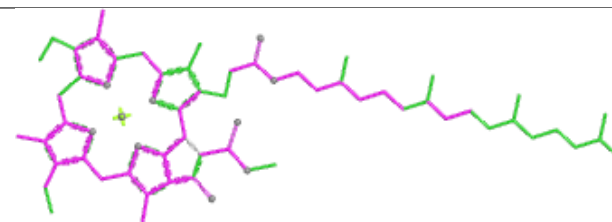
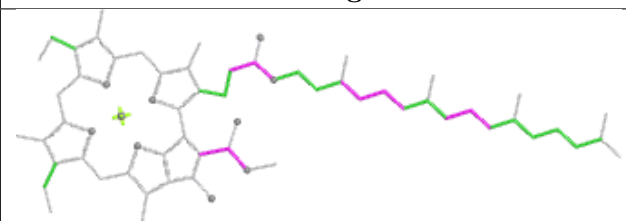
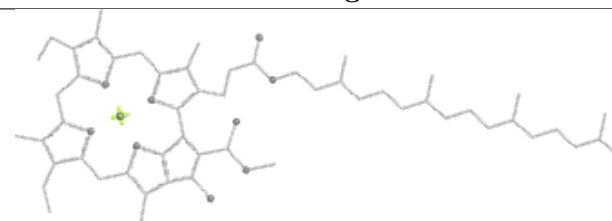
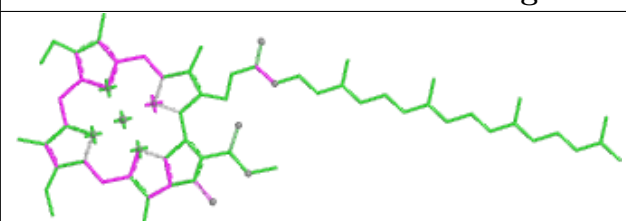
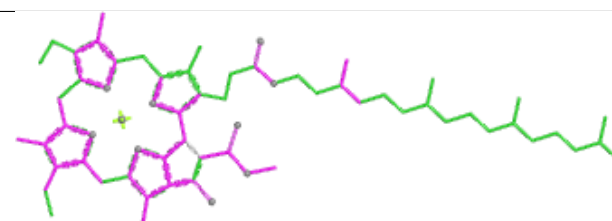
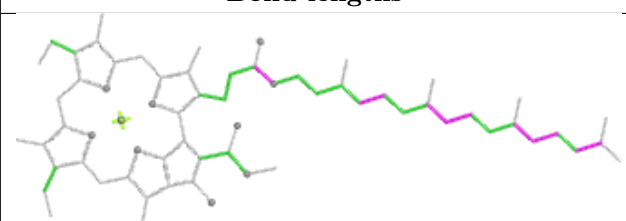
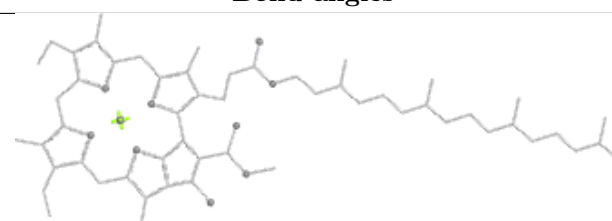
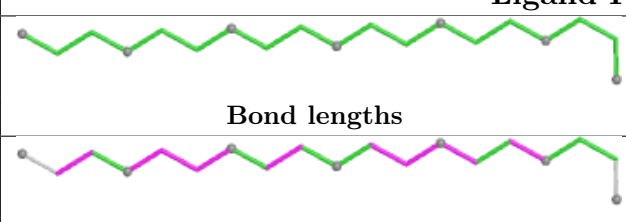
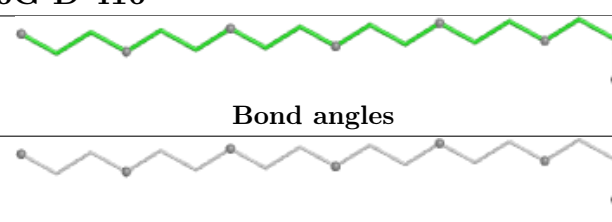
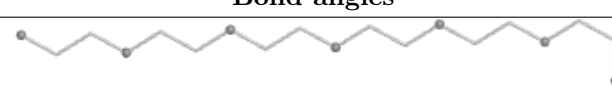


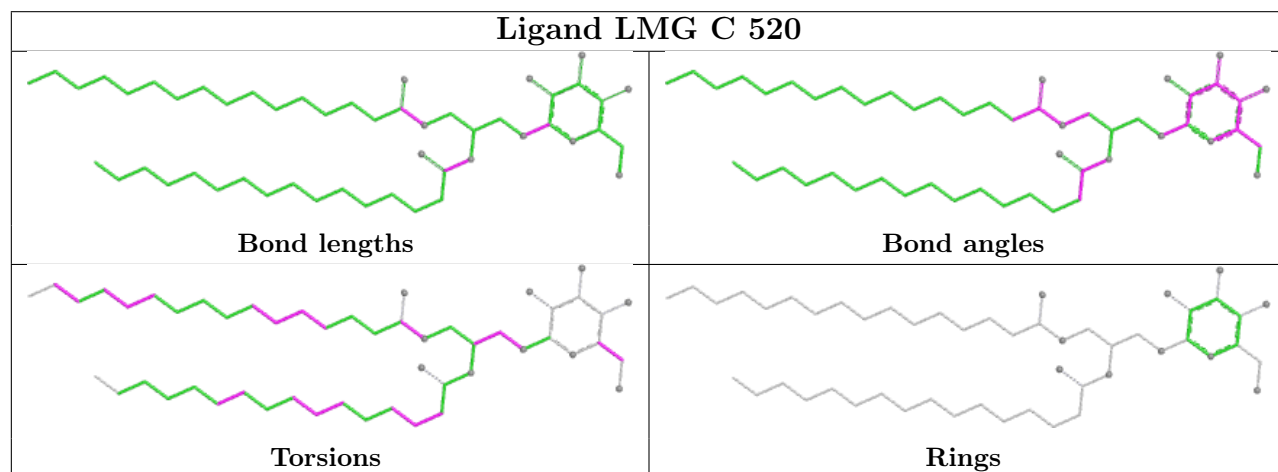
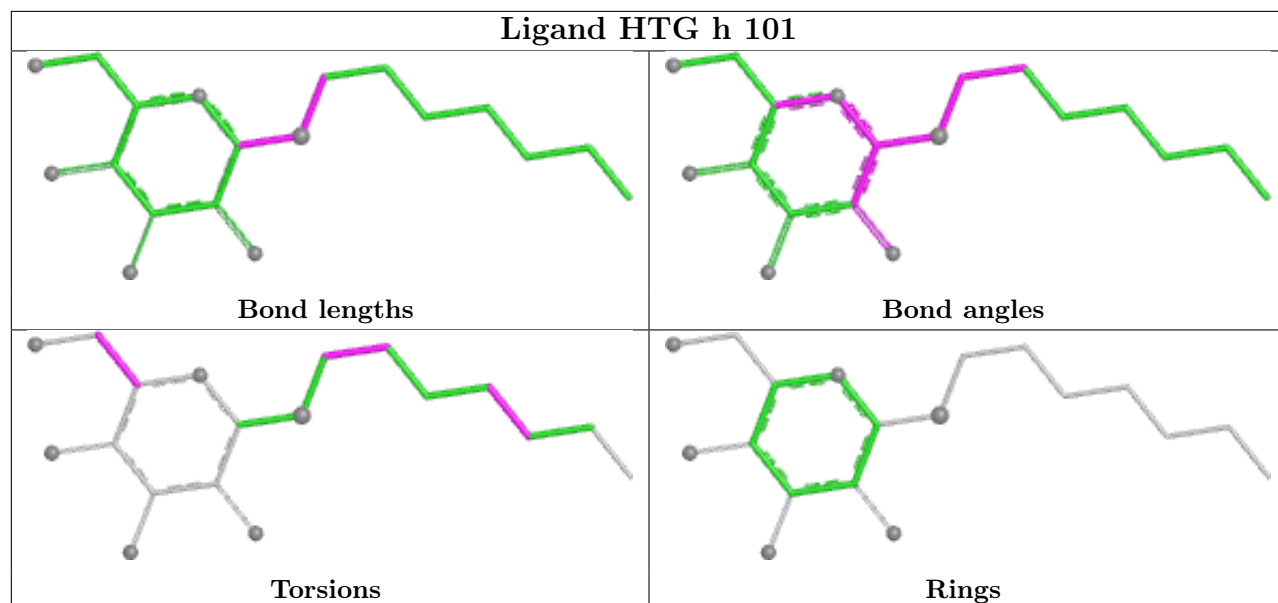


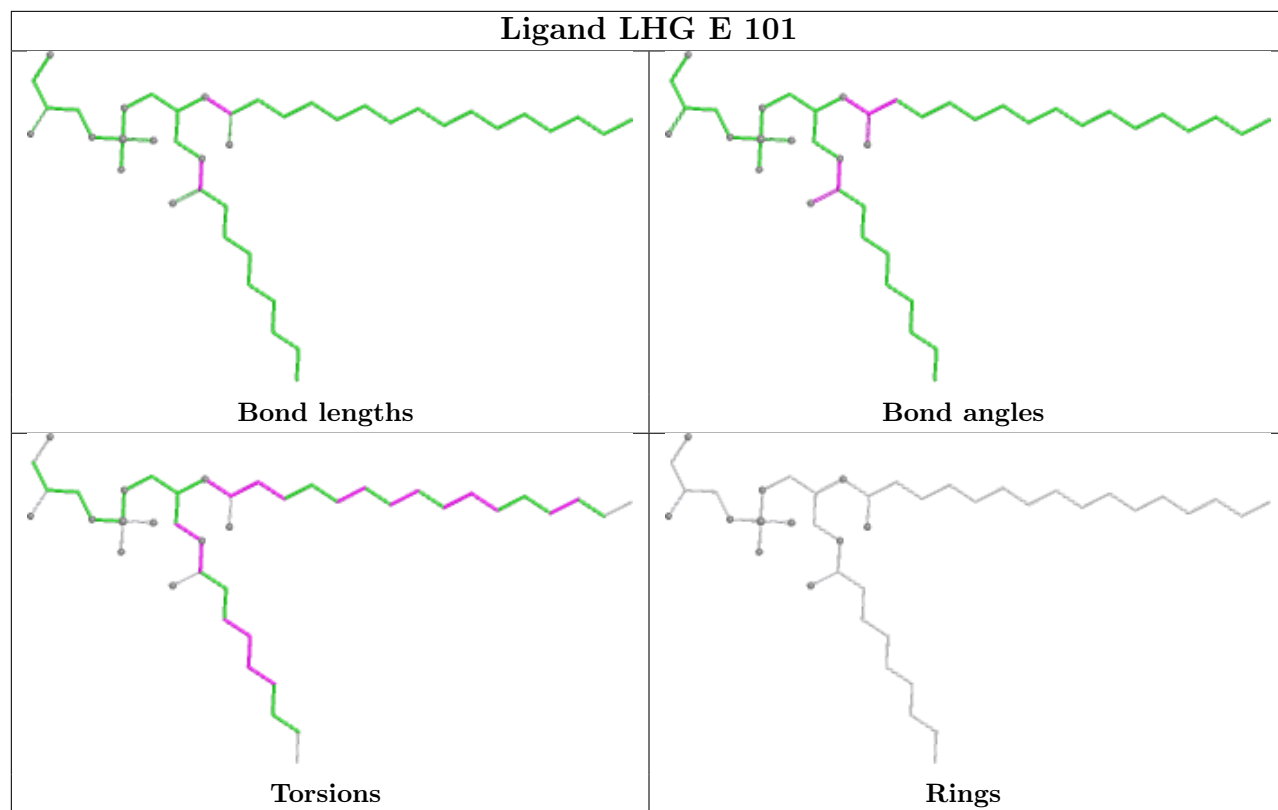
Ligand CLA d 405	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR C 514	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR t 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

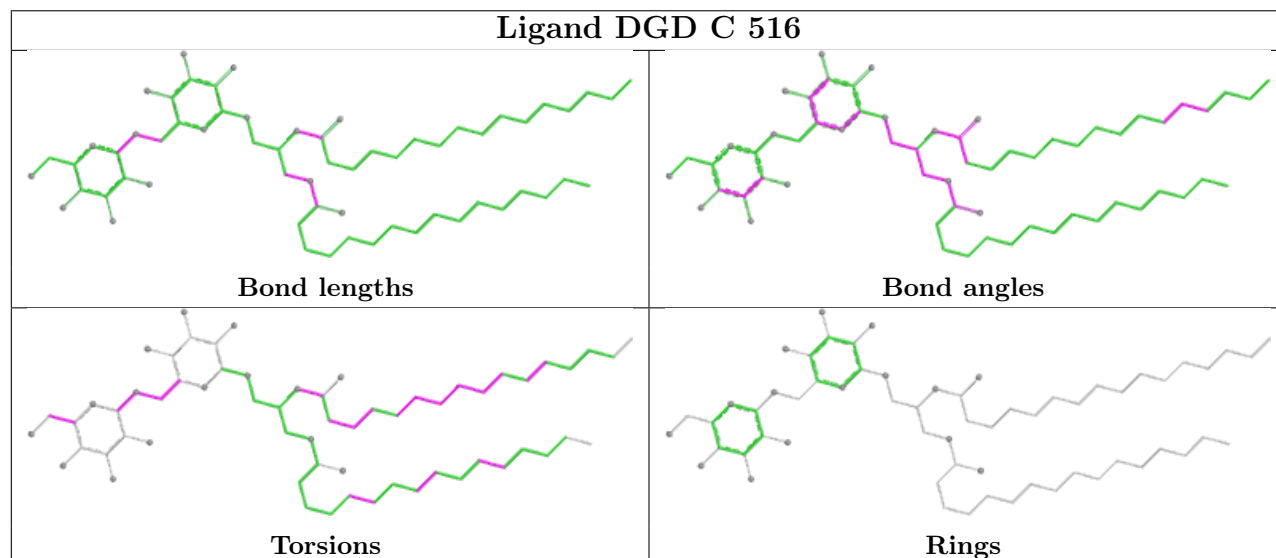
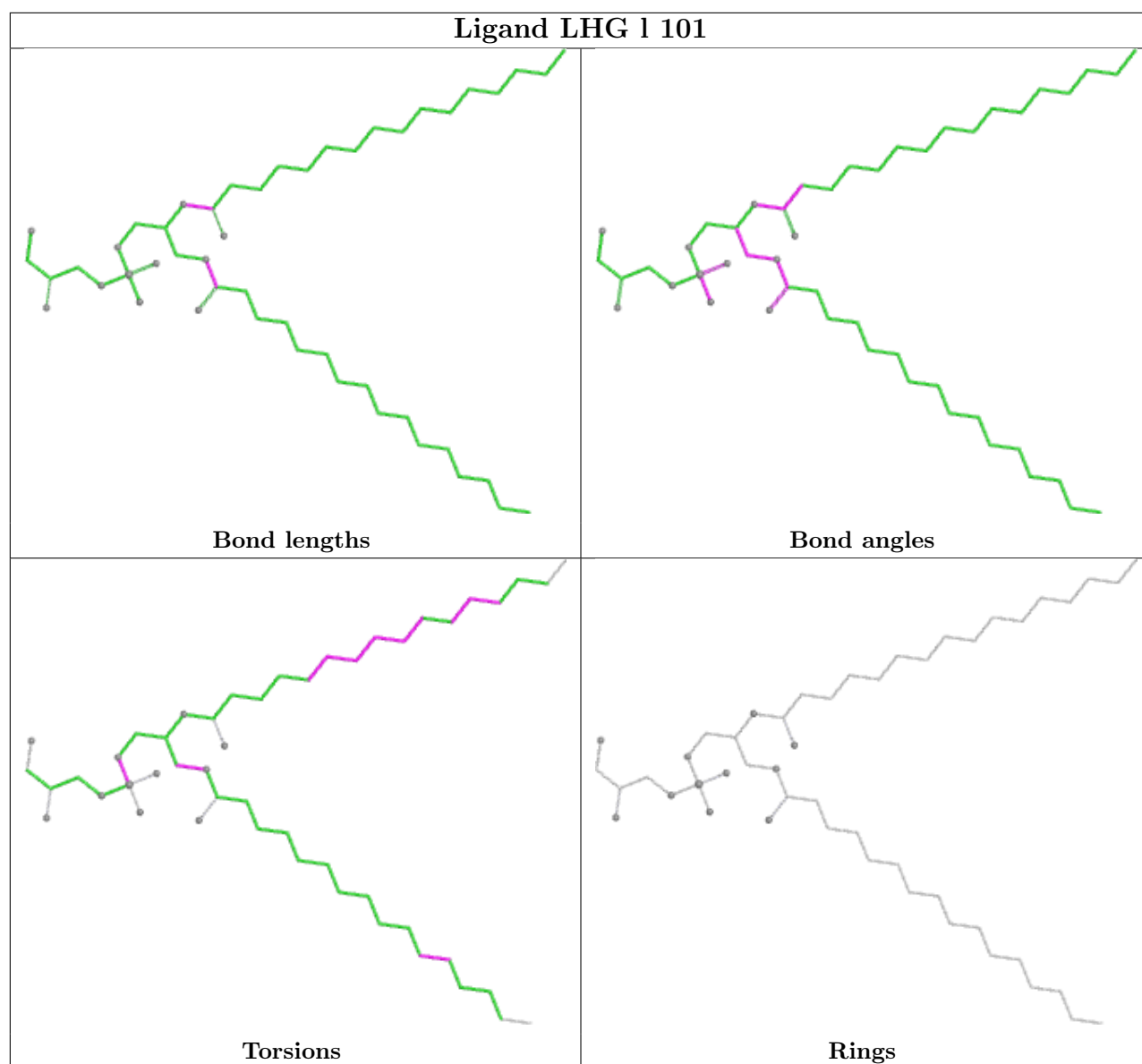


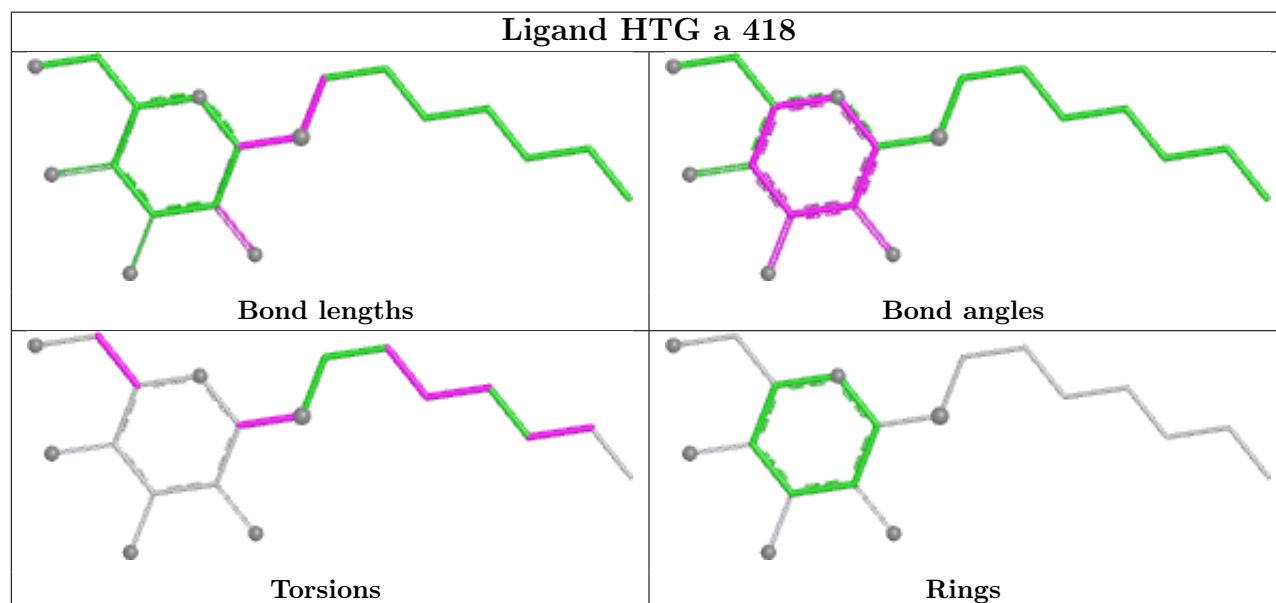
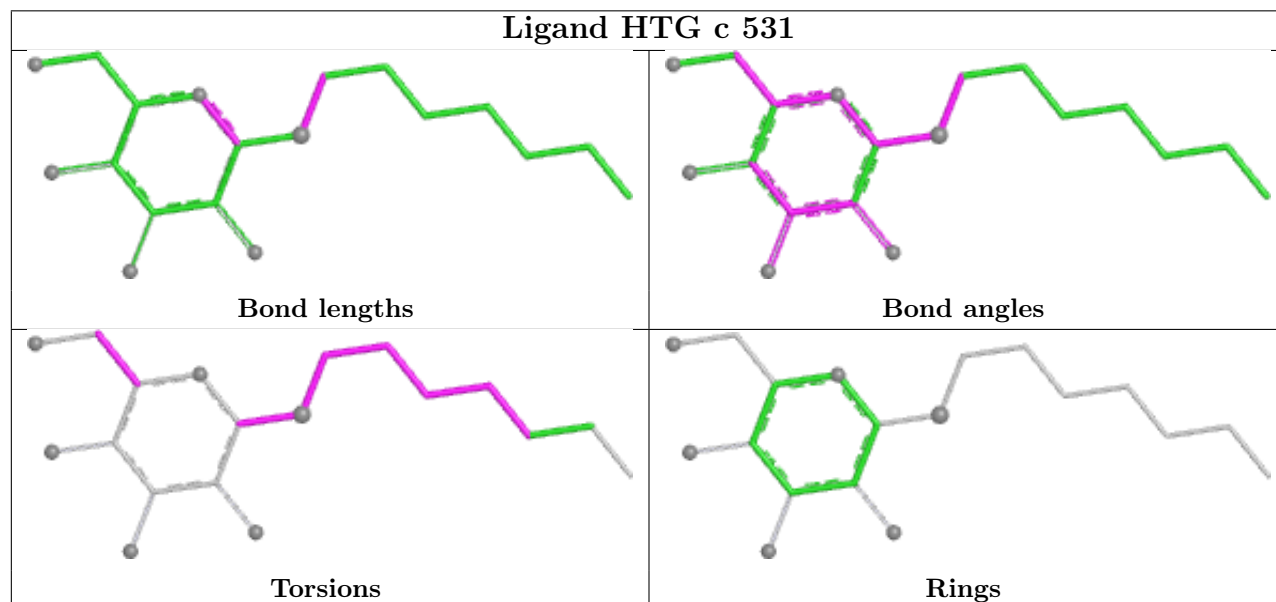
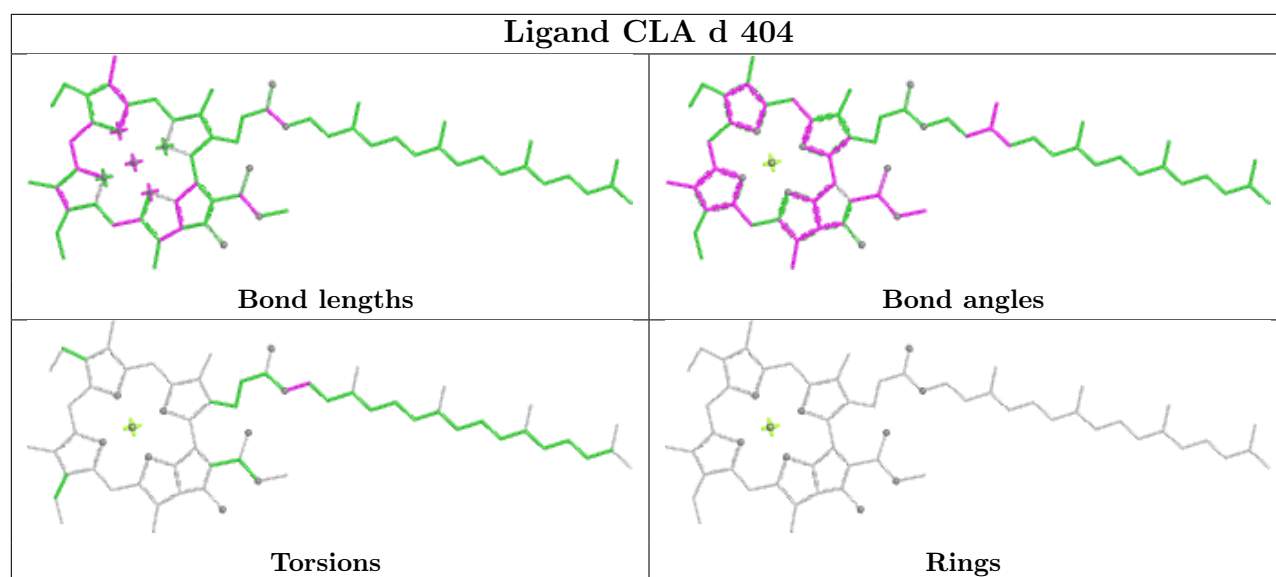


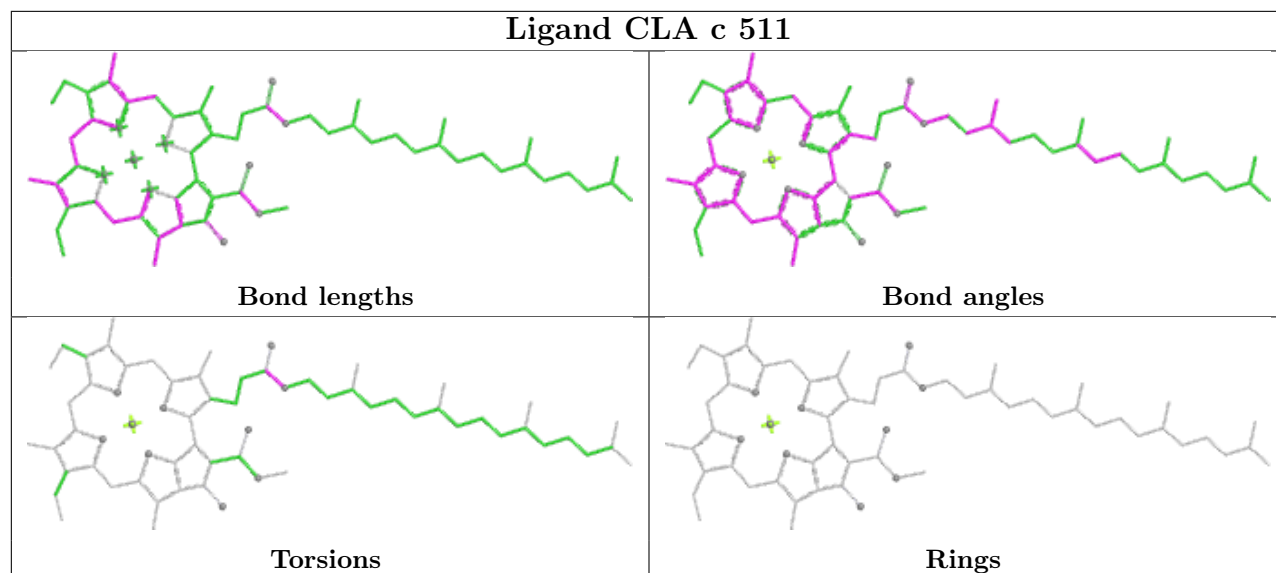
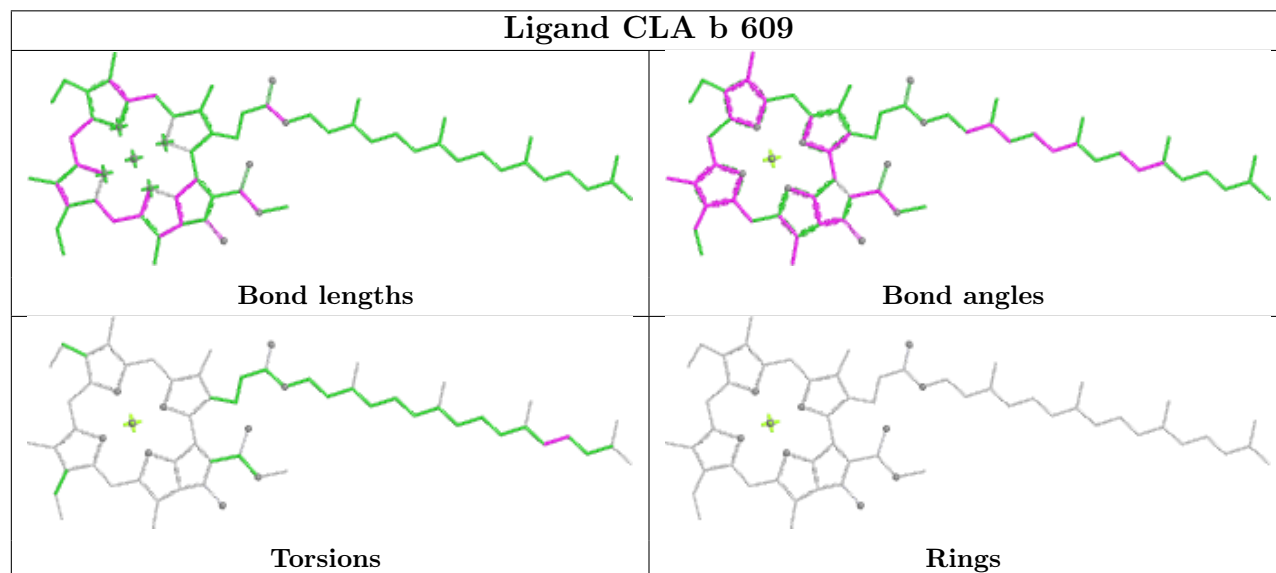
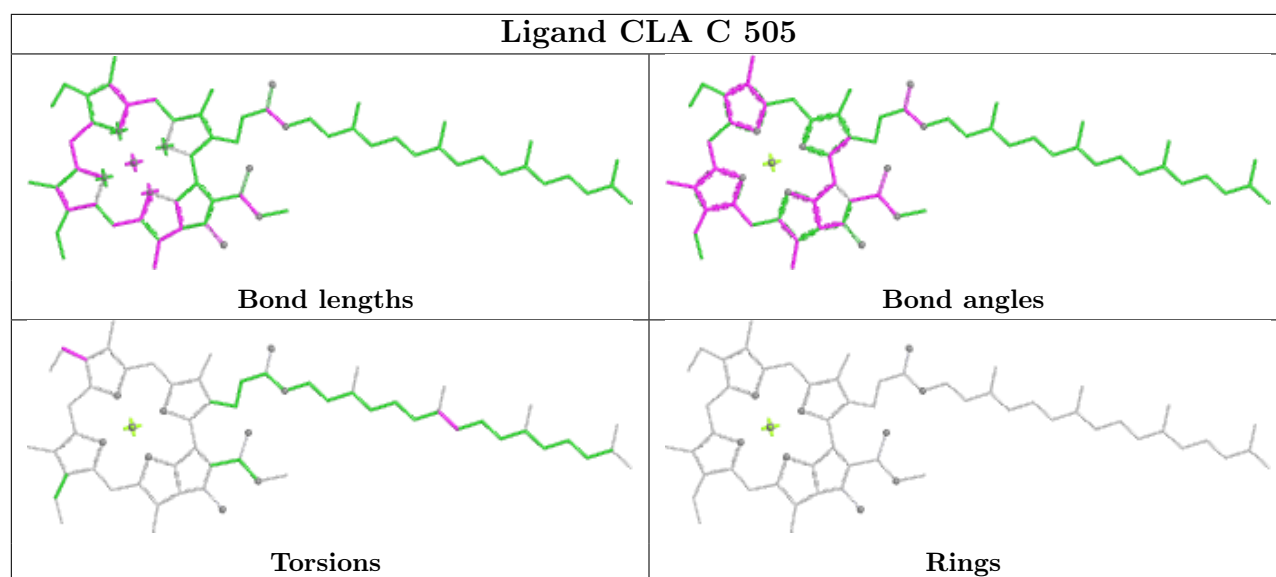
Ligand CLA B 602	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CLA A 609	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand P6G D 416	
	
Bond lengths	Bond angles
	
Torsions	Rings



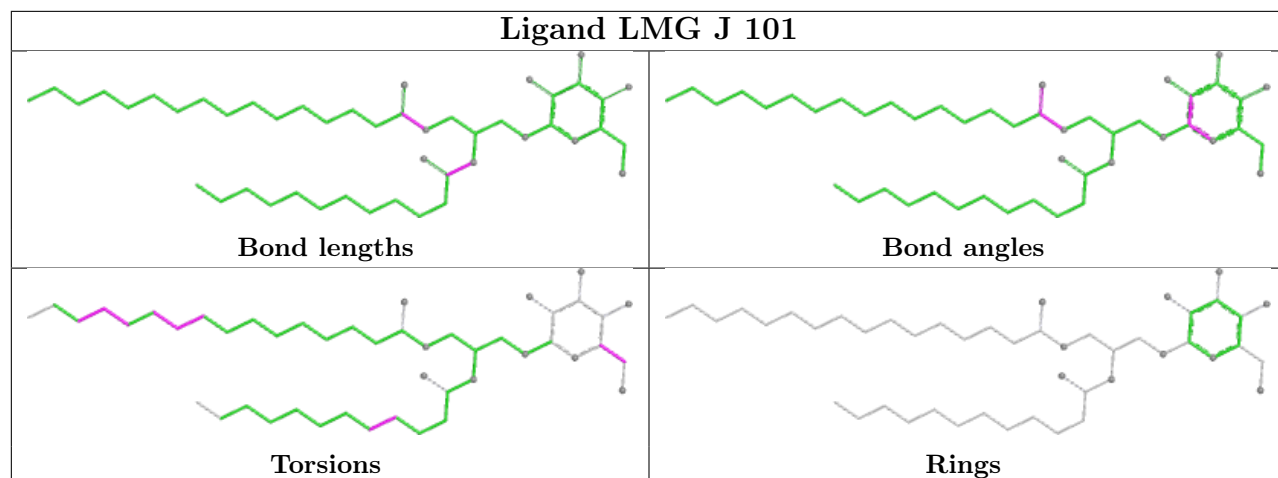




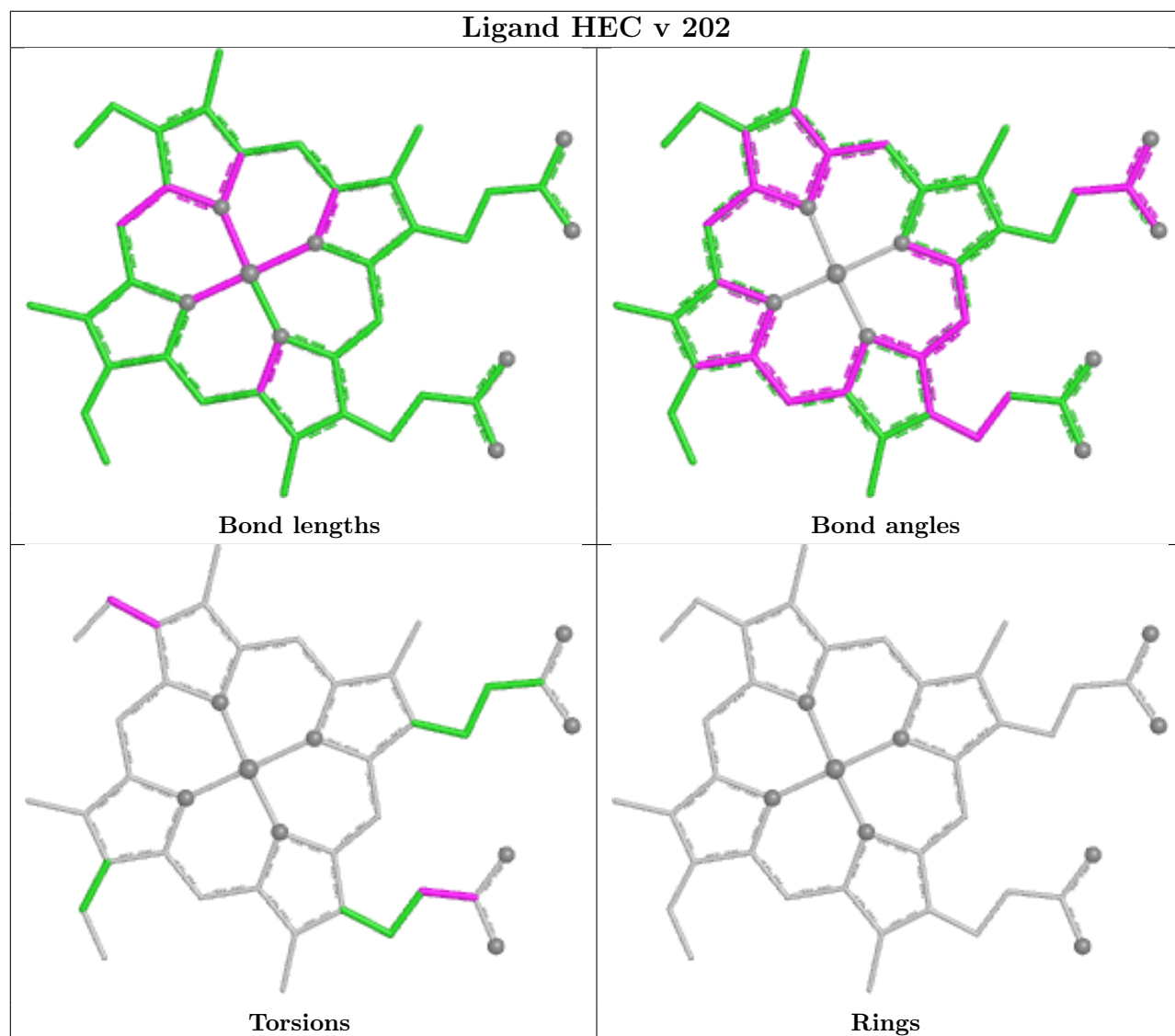




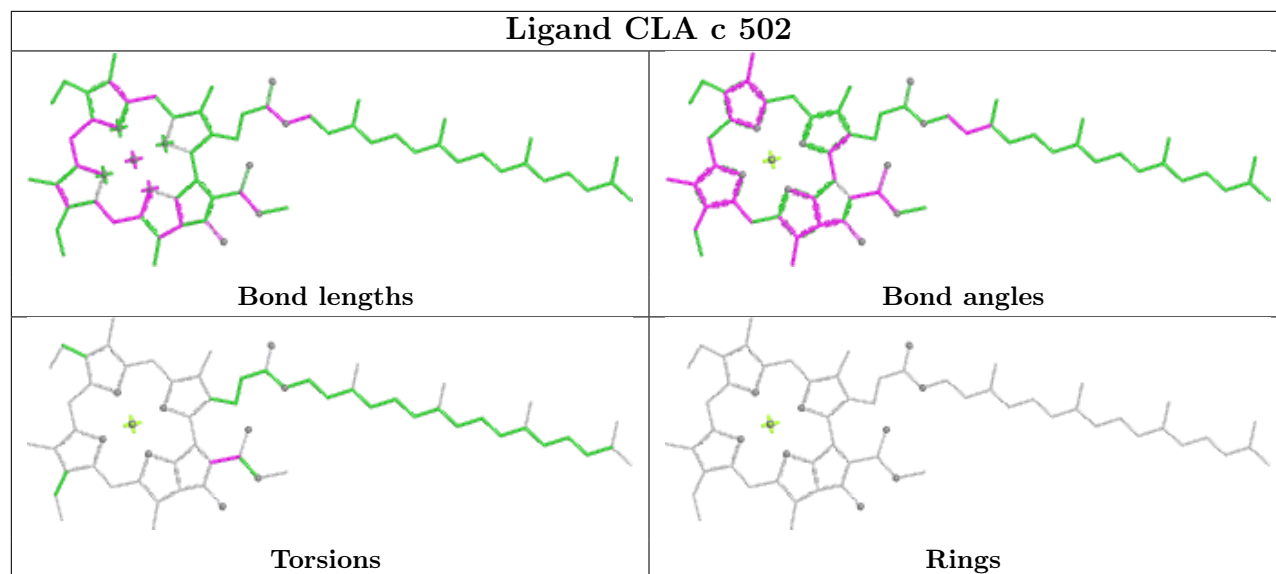
Ligand LMG J 101



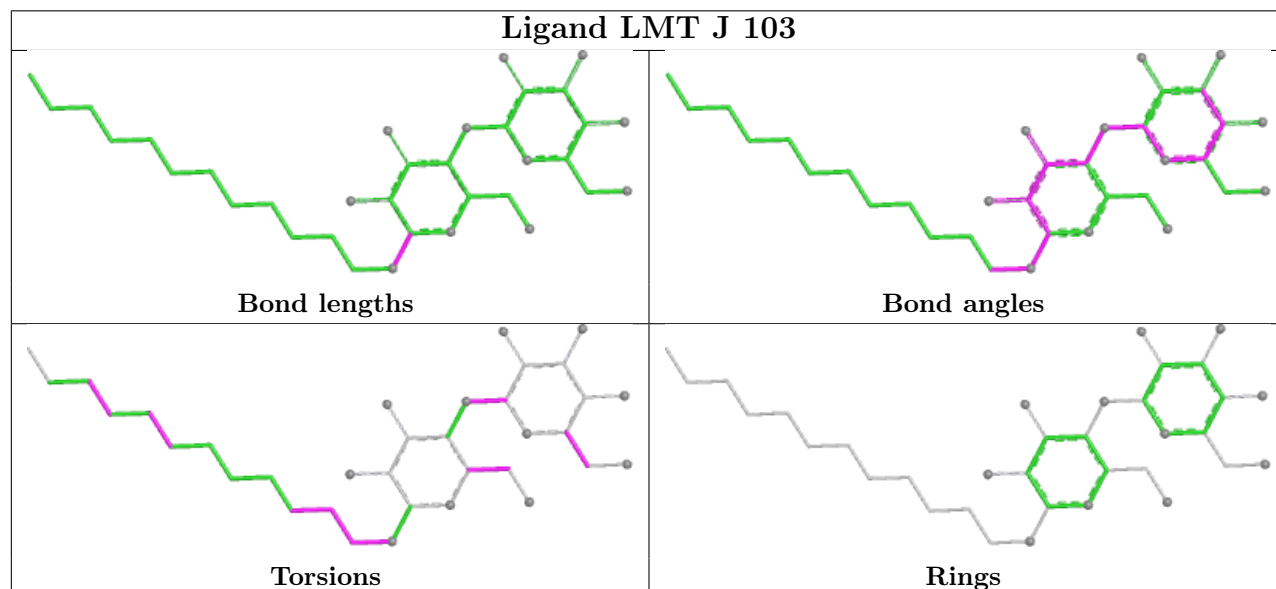
Ligand HEC v 202



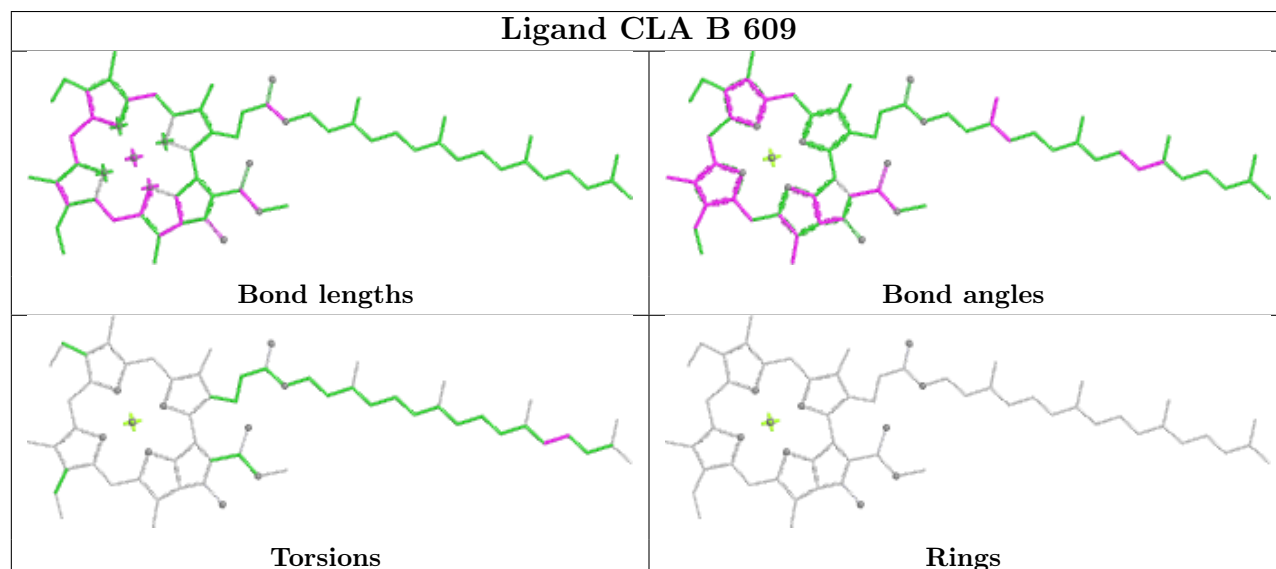
Ligand CLA c 502

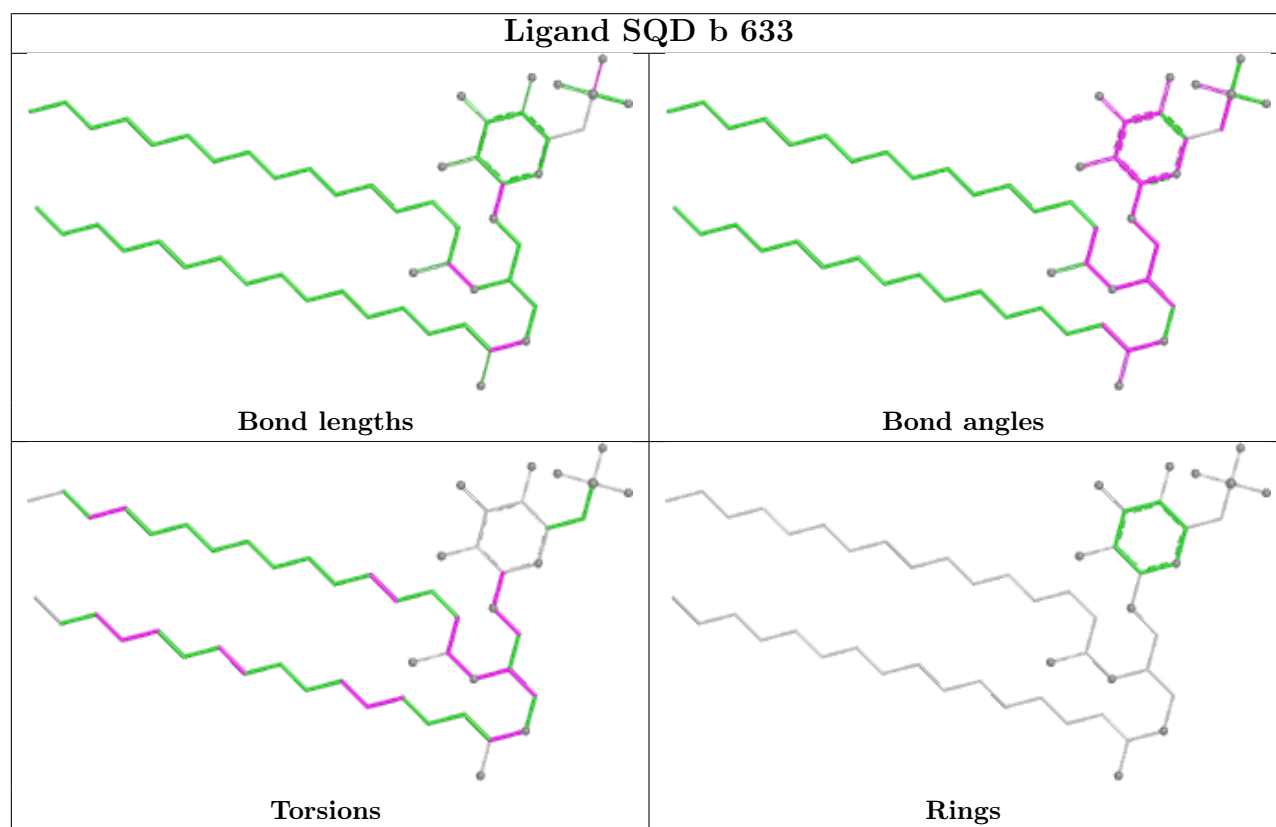
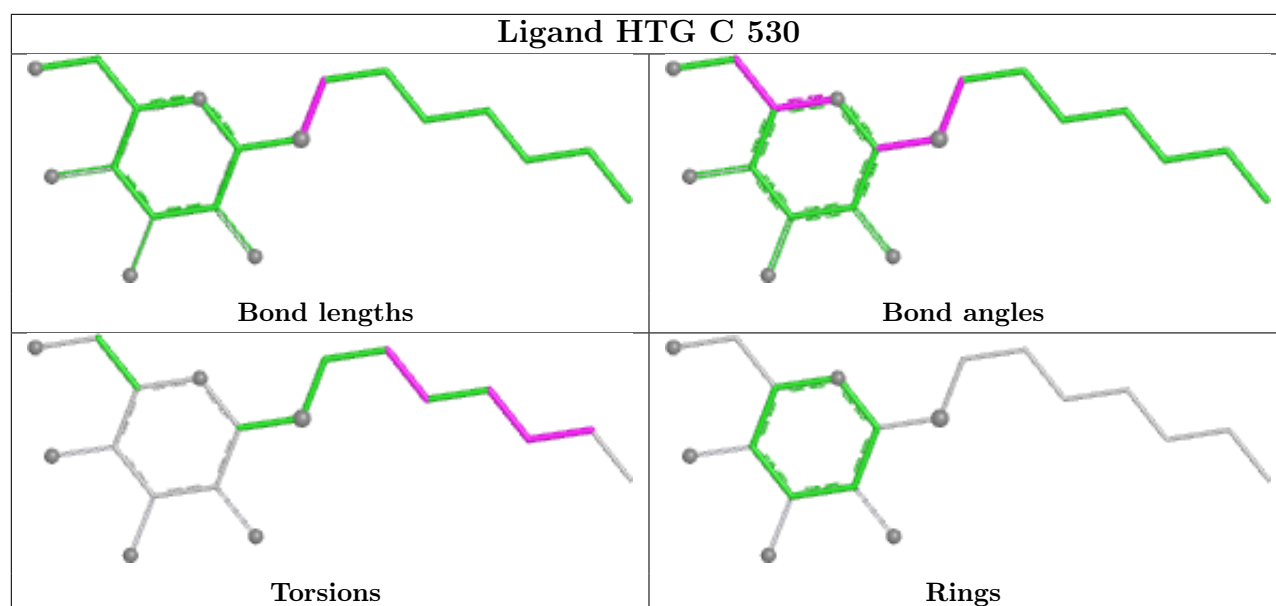


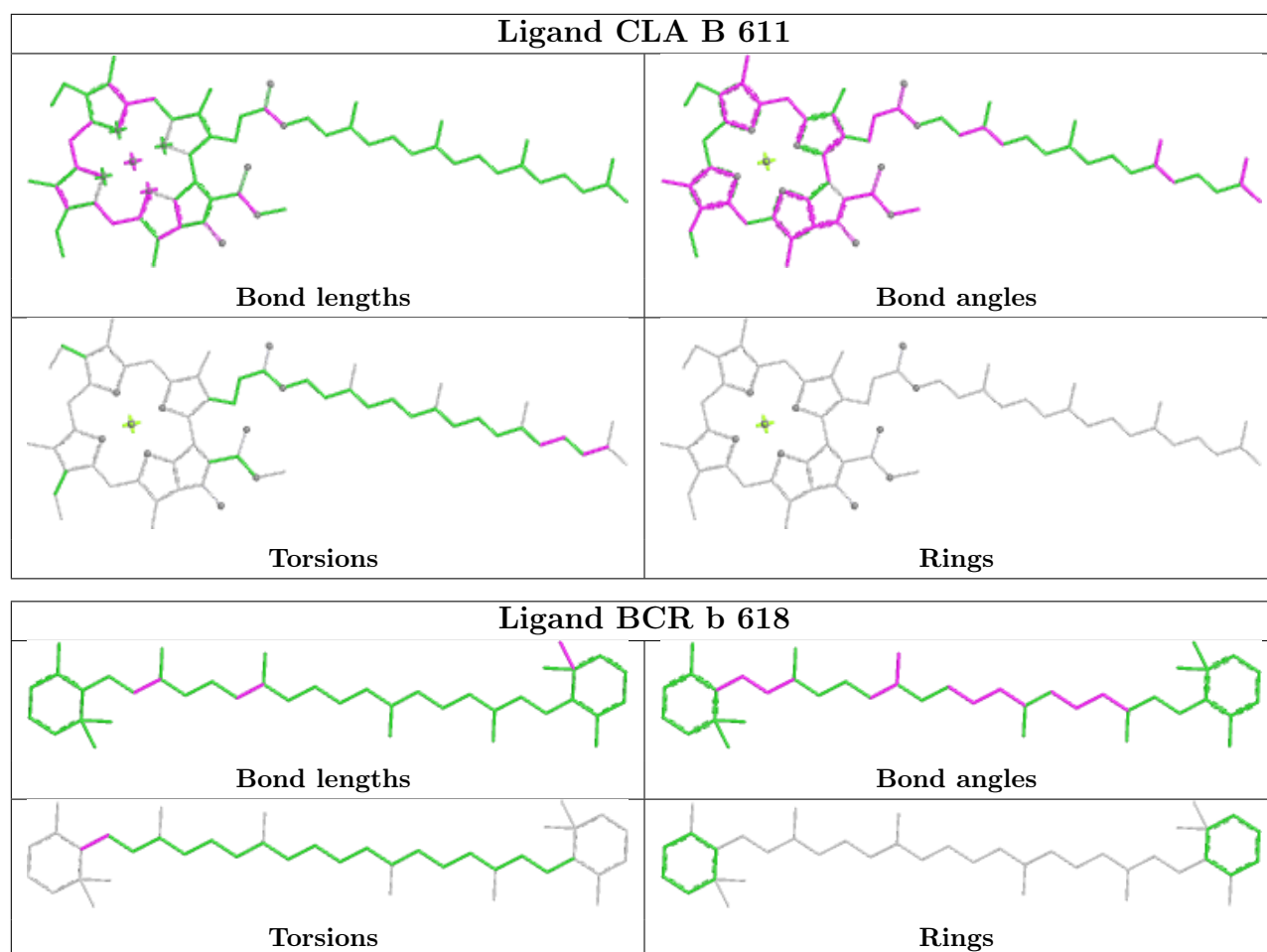
Ligand LMT J 103

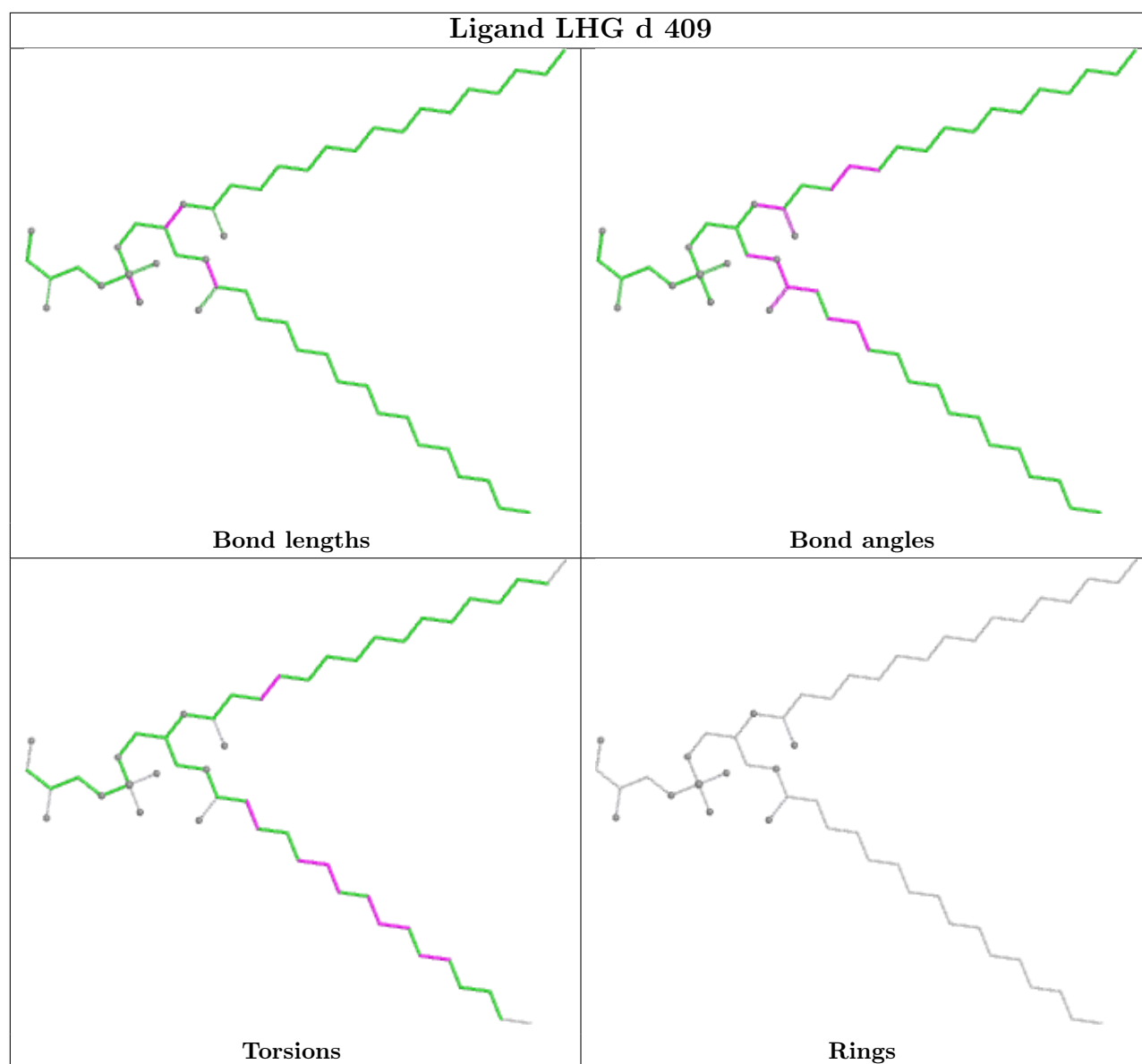


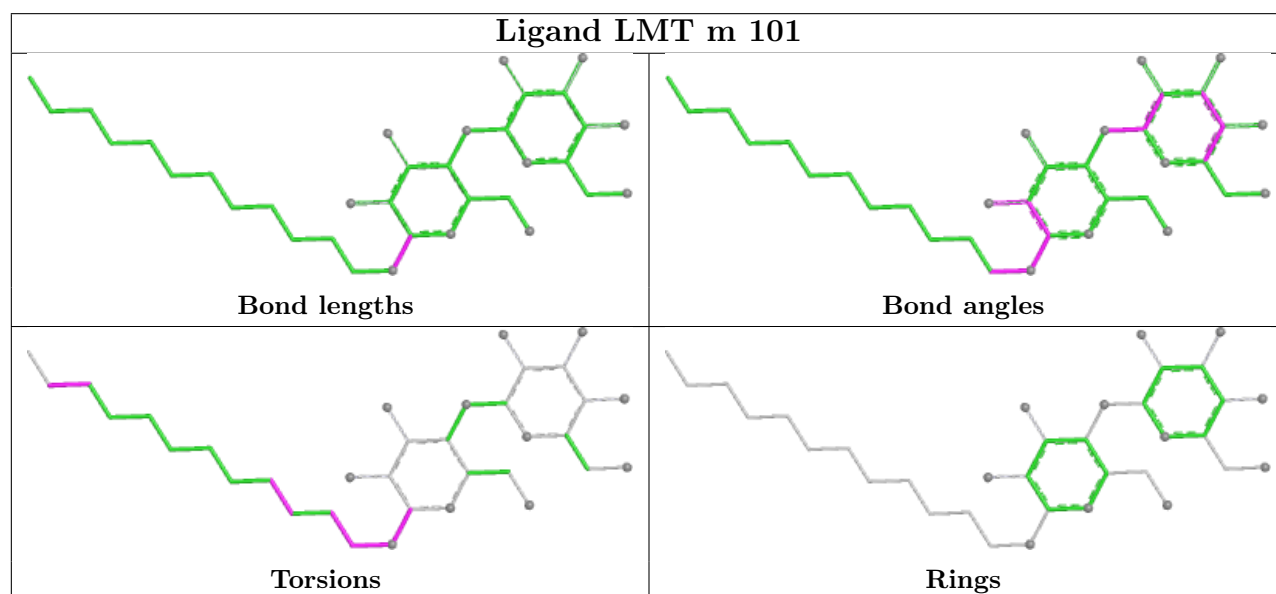
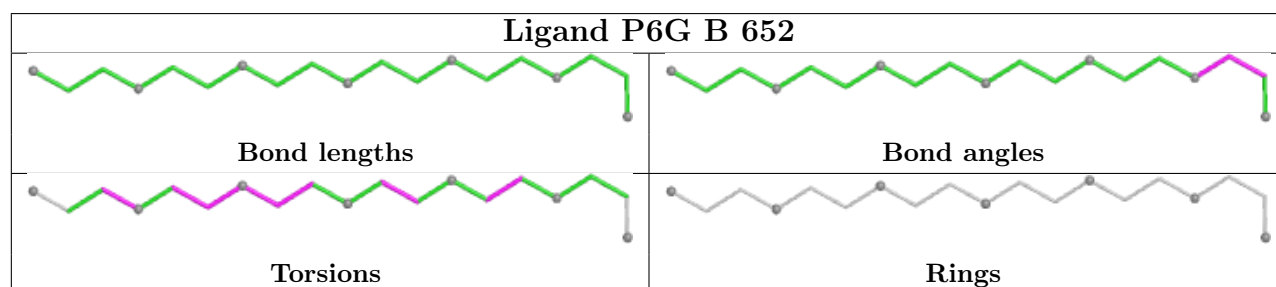
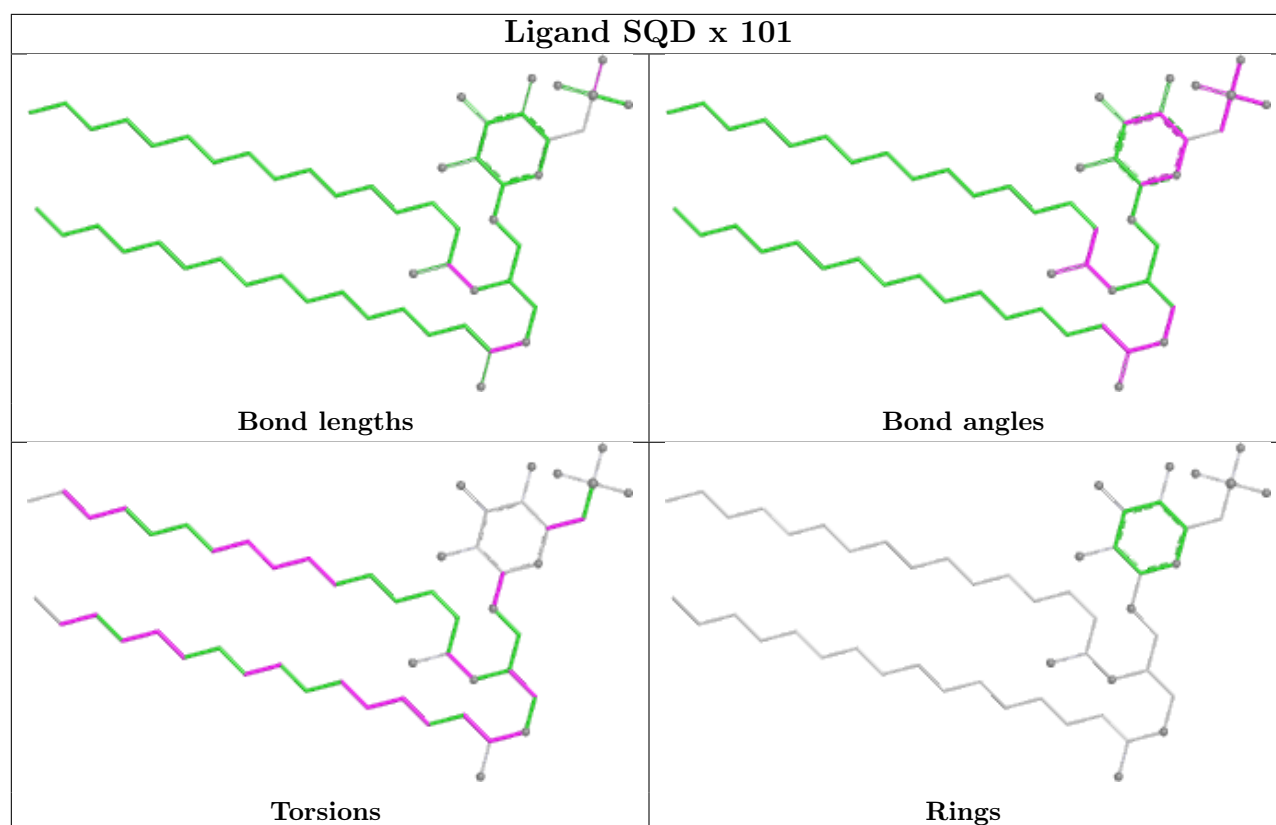
Ligand CLA B 609

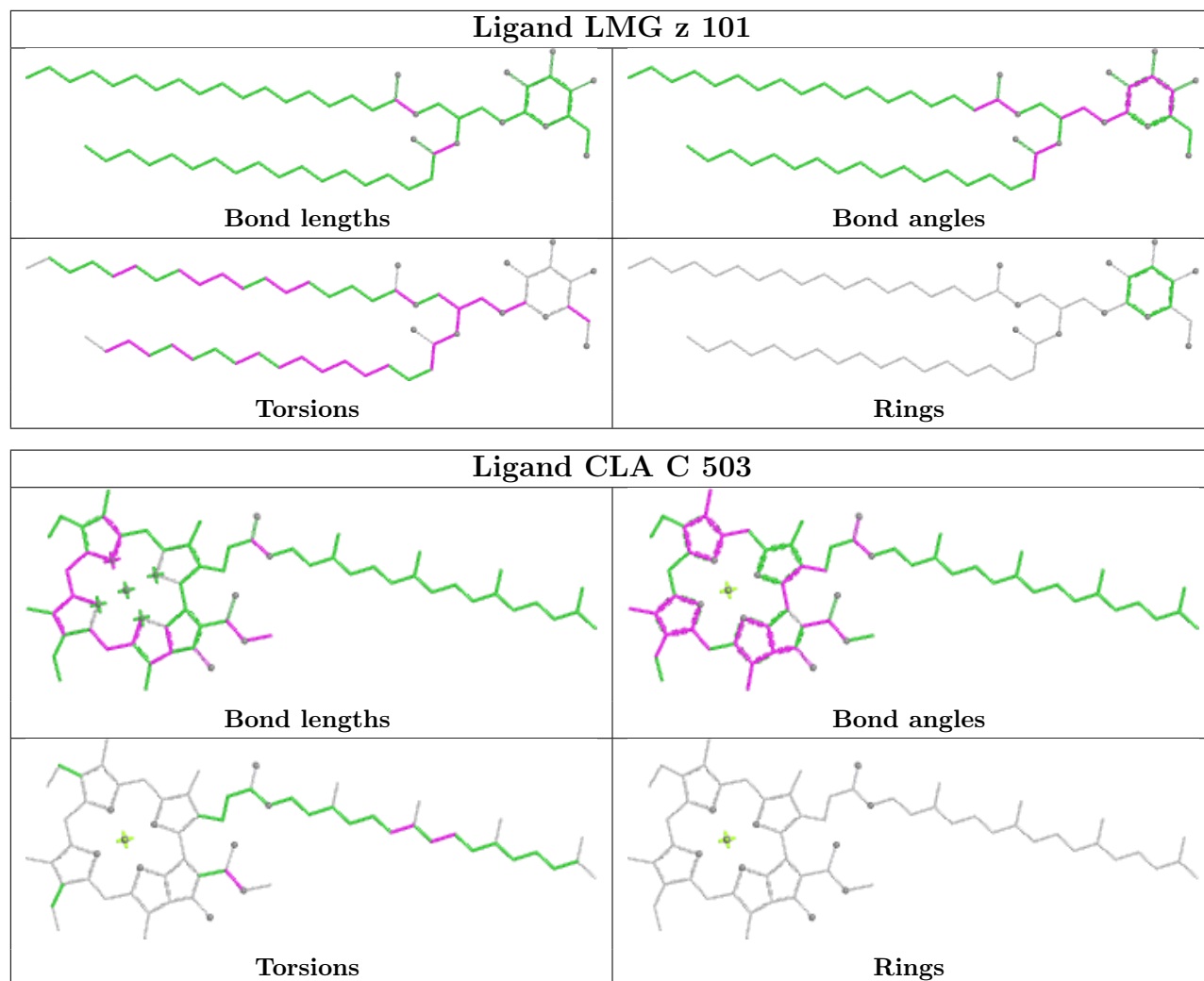


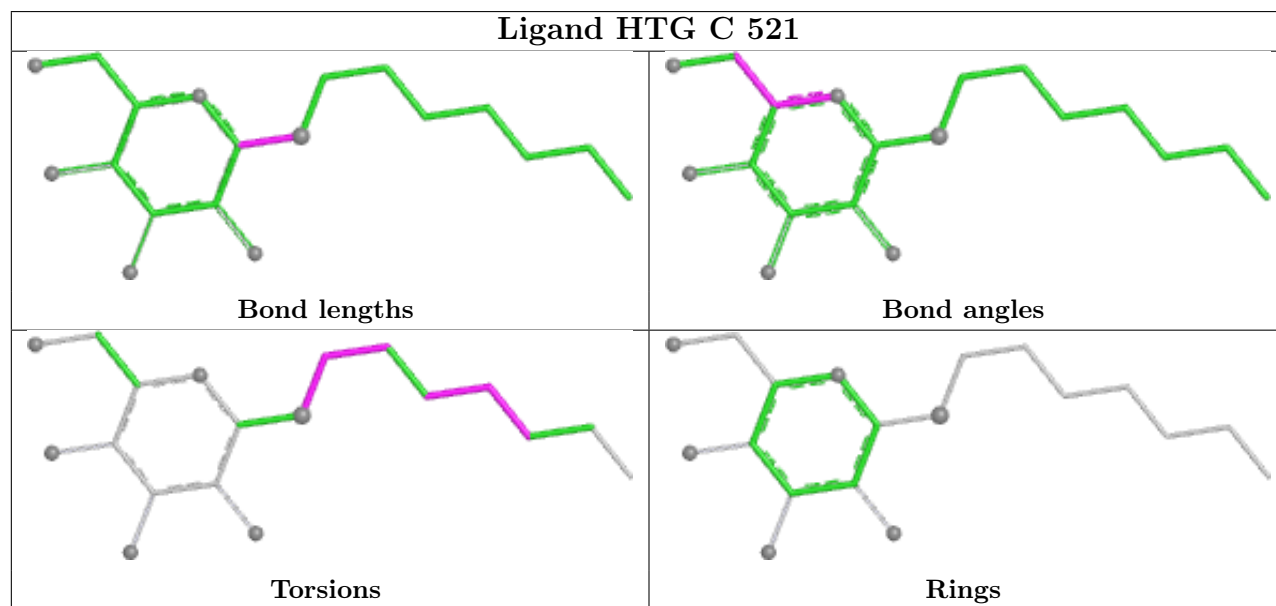
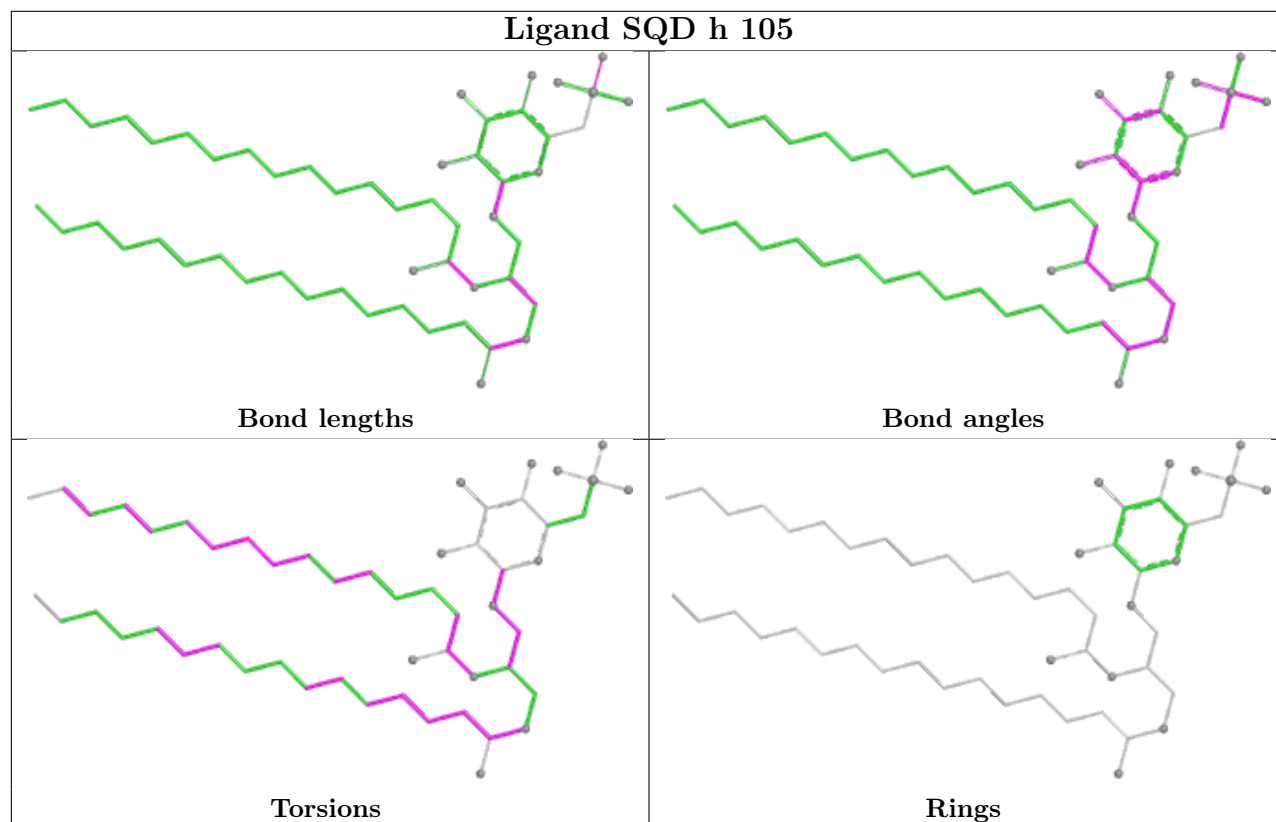


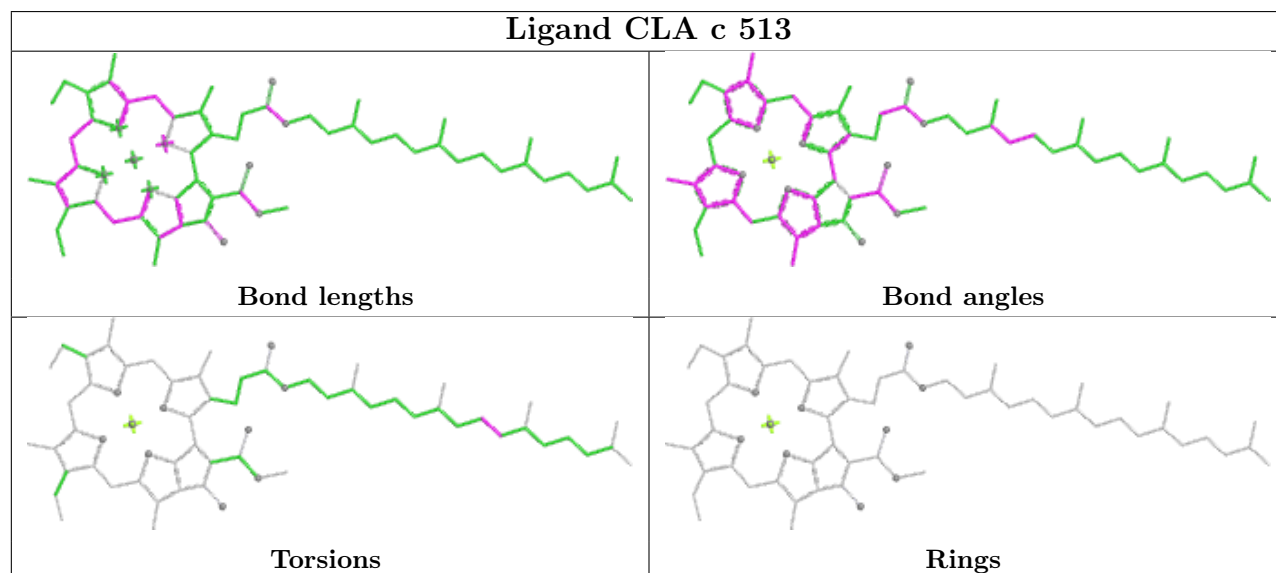
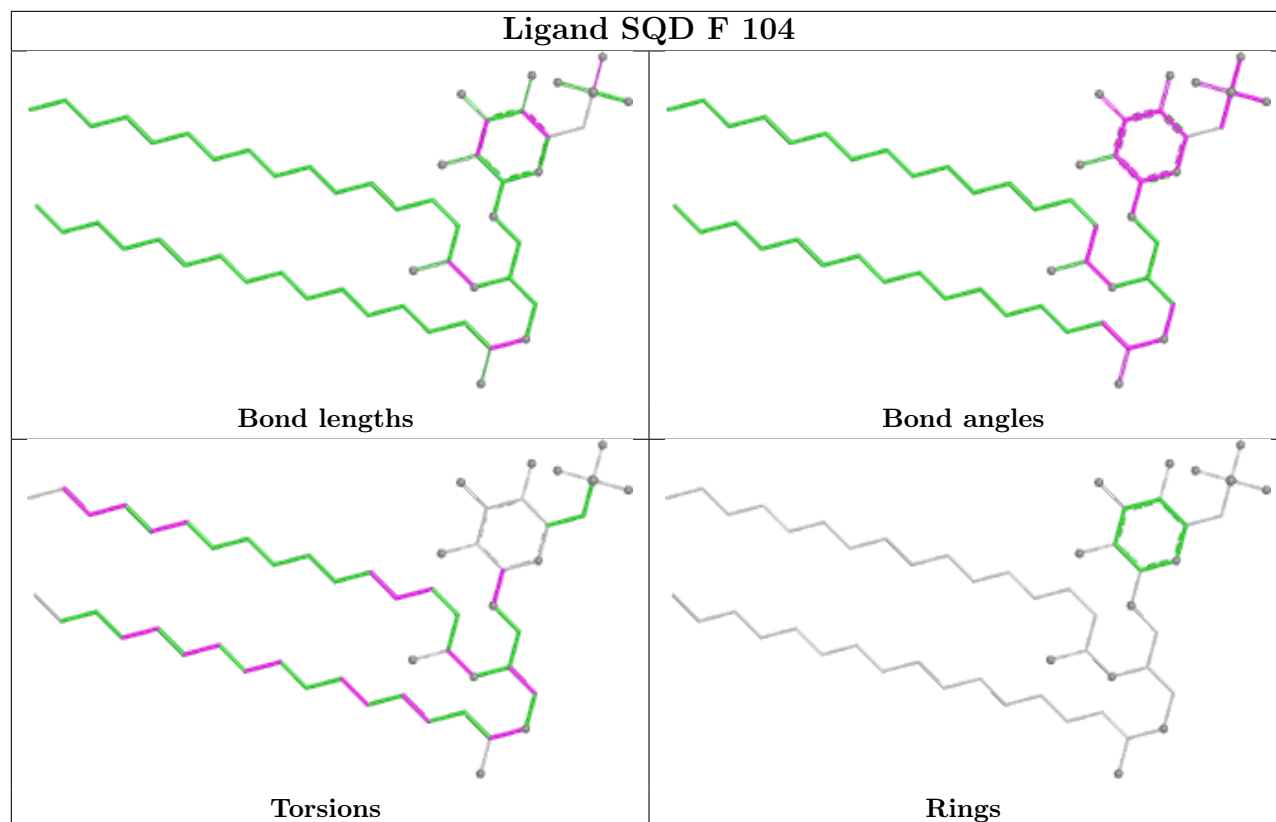


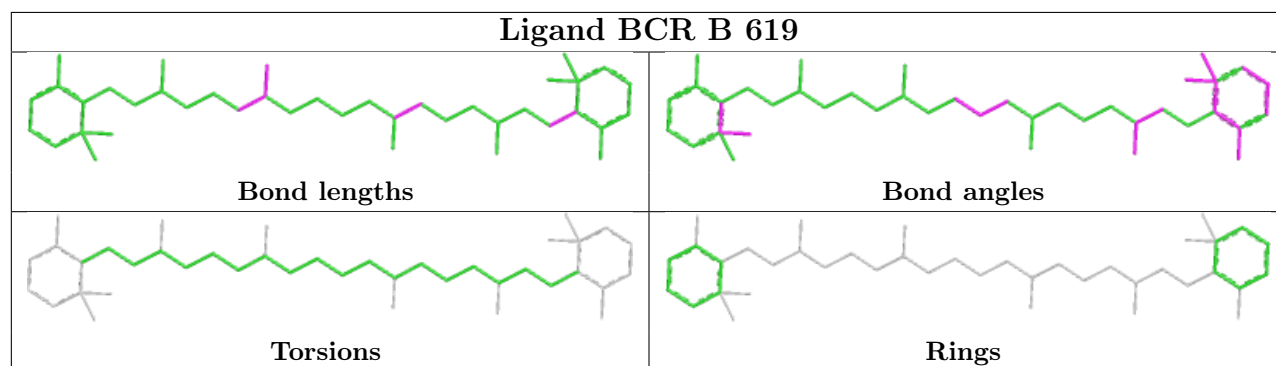
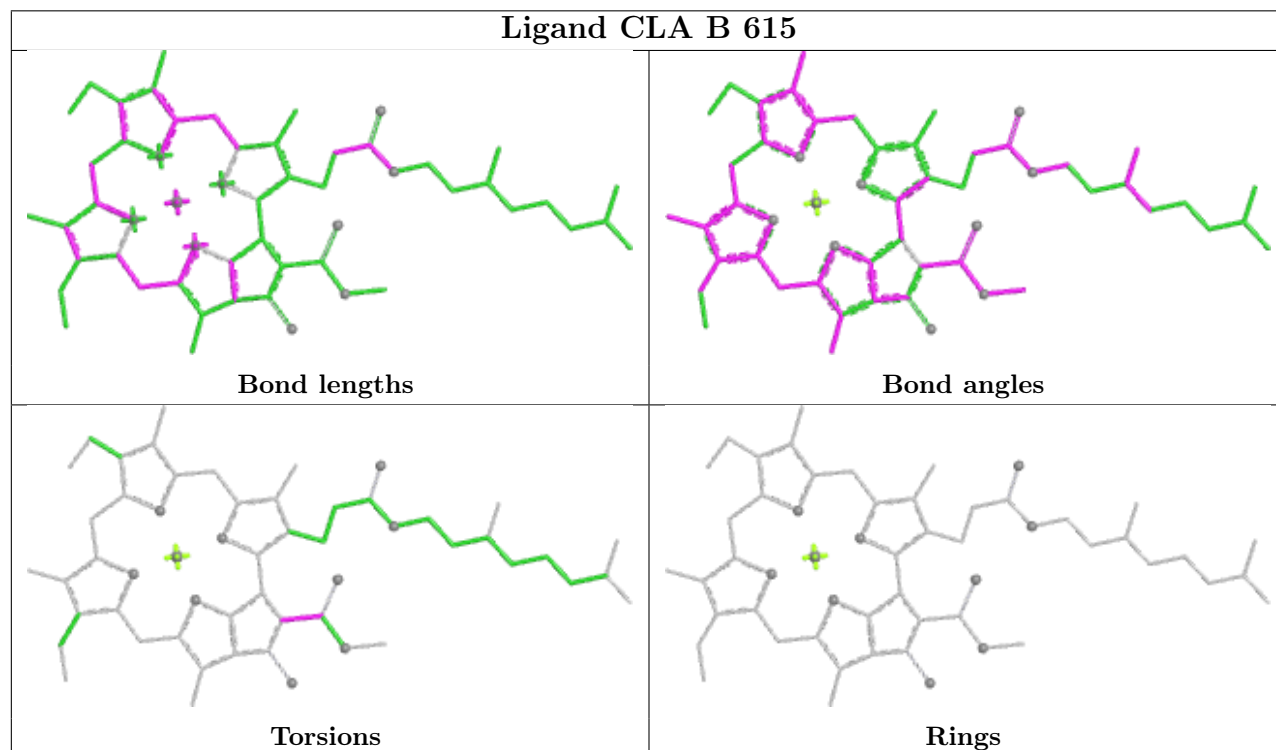
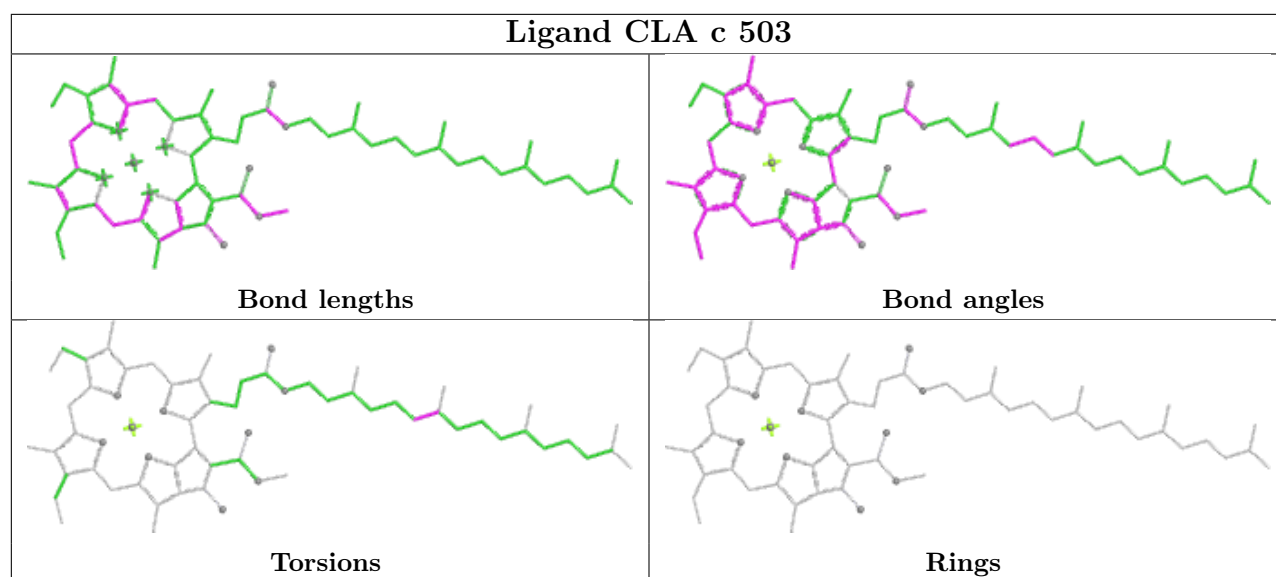


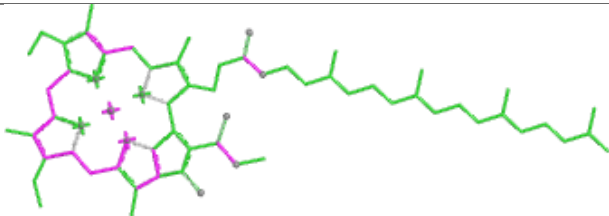
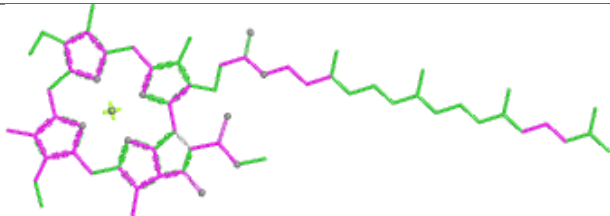
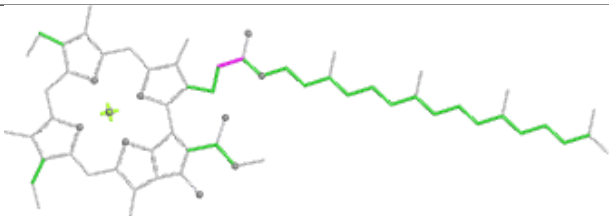
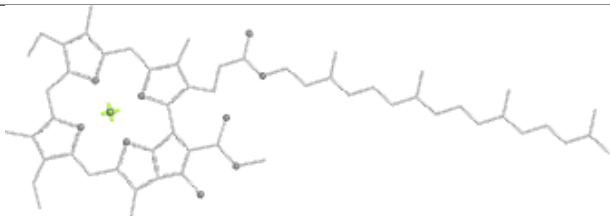


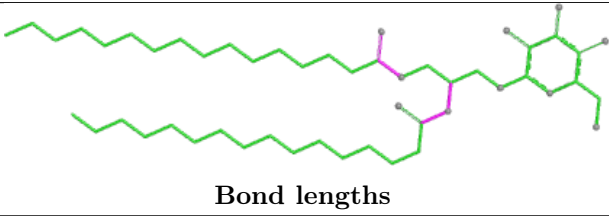
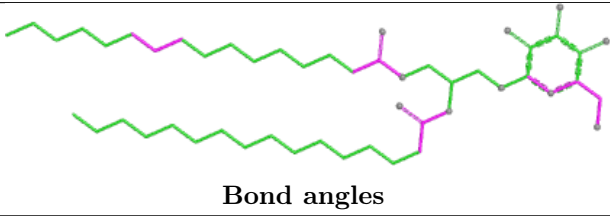
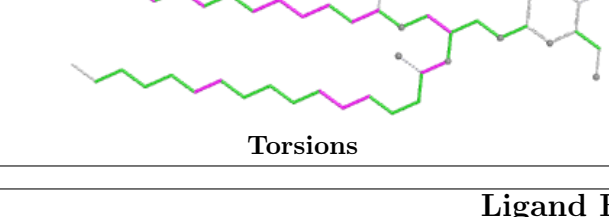
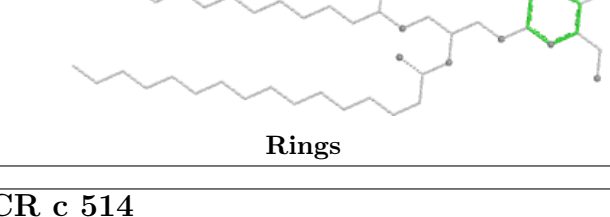


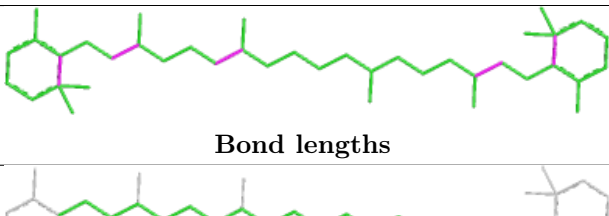
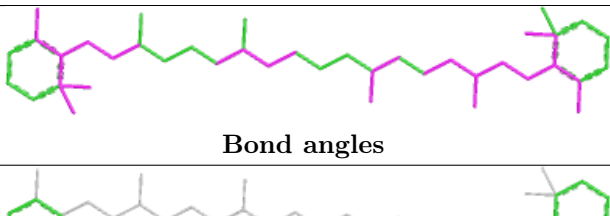


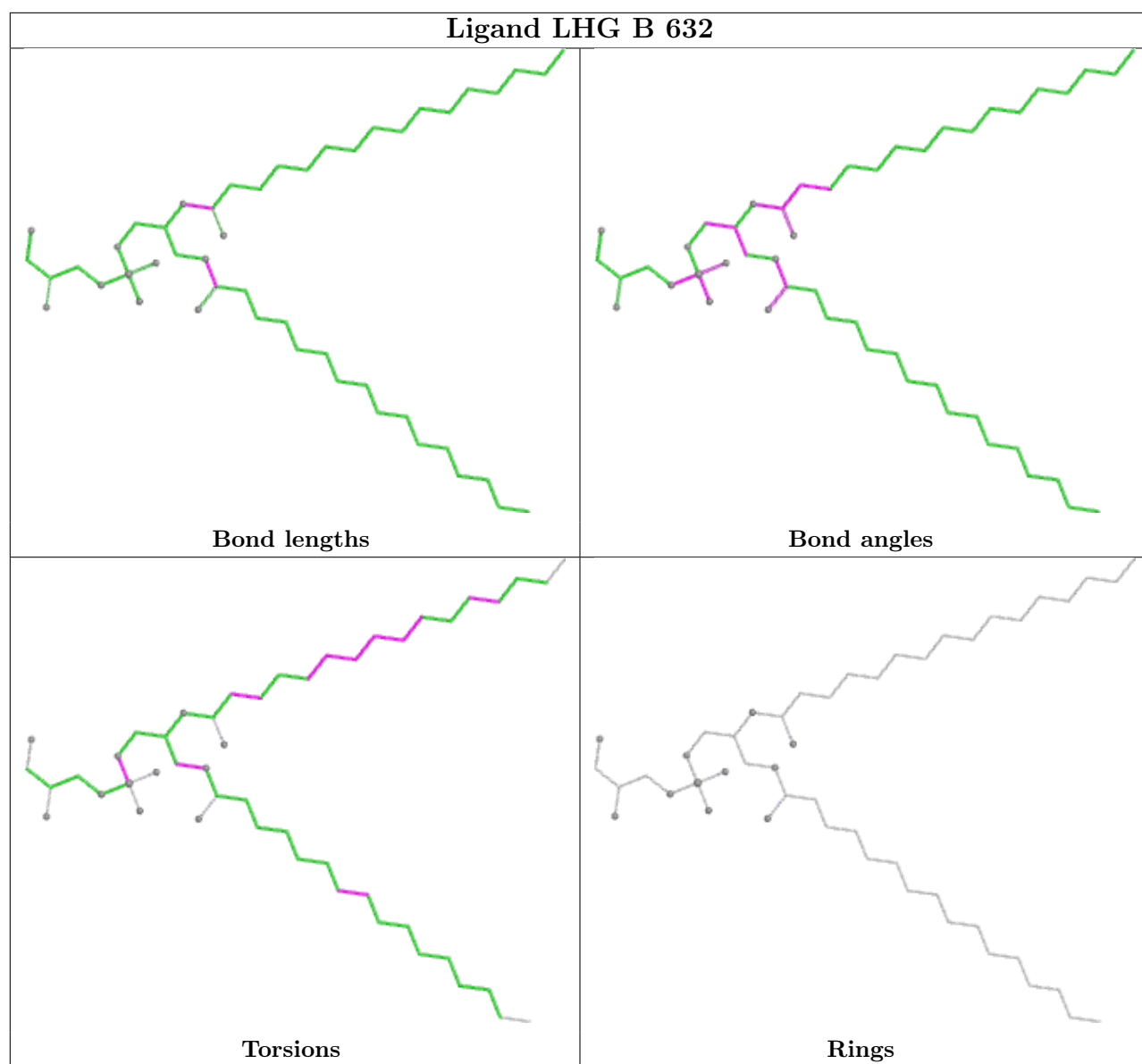


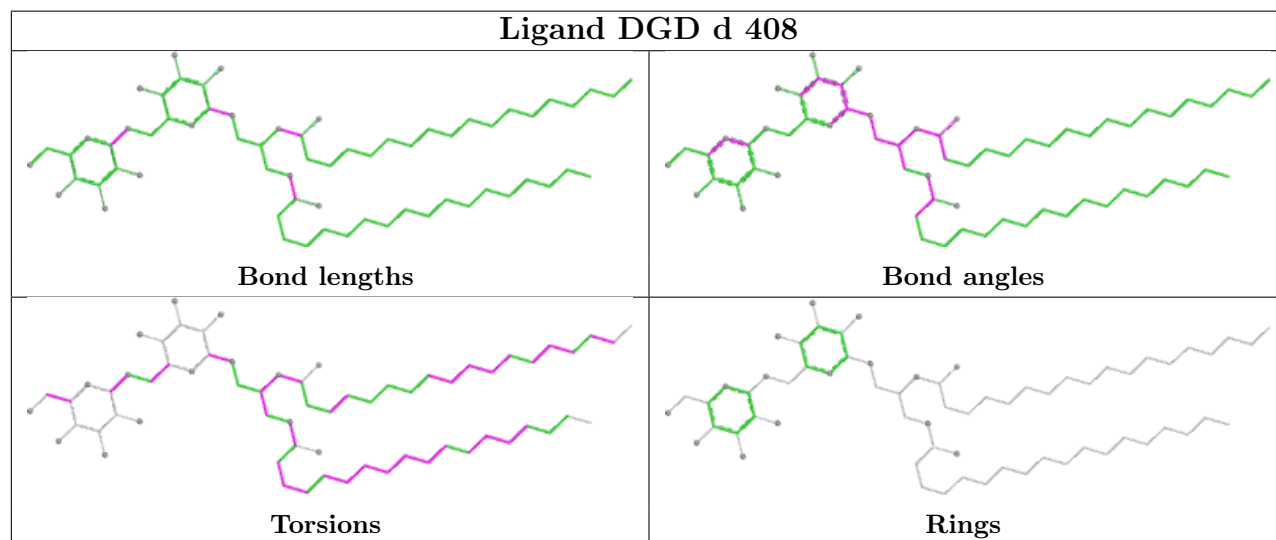
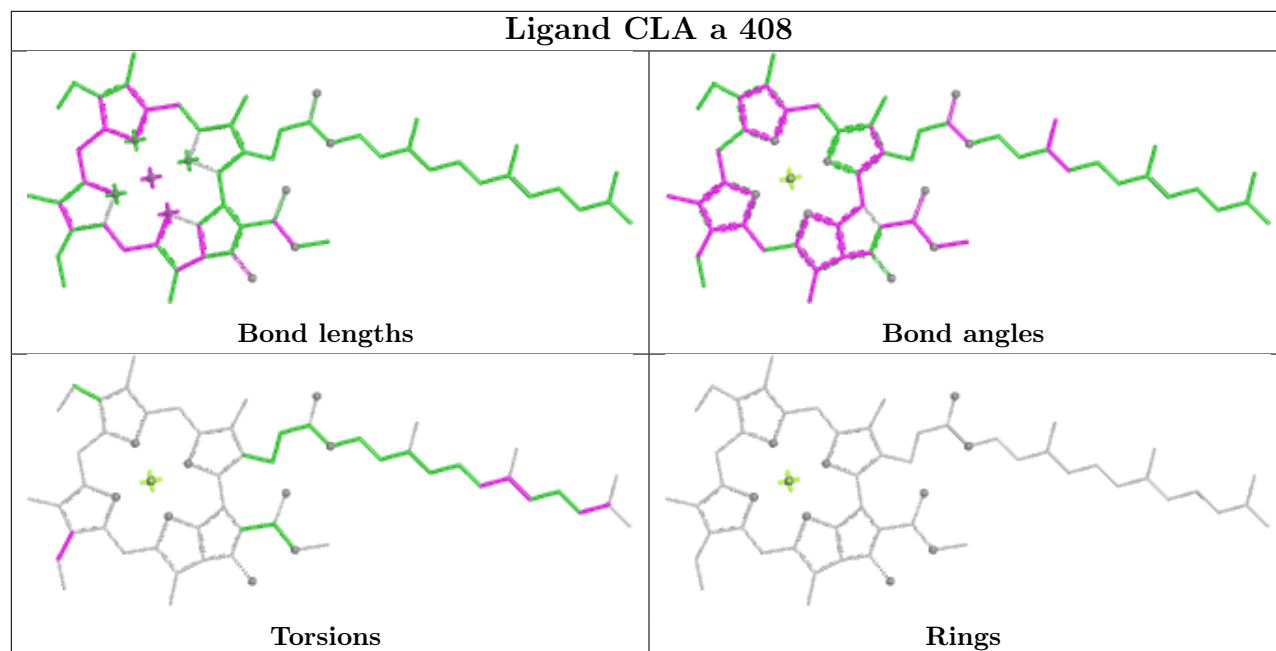


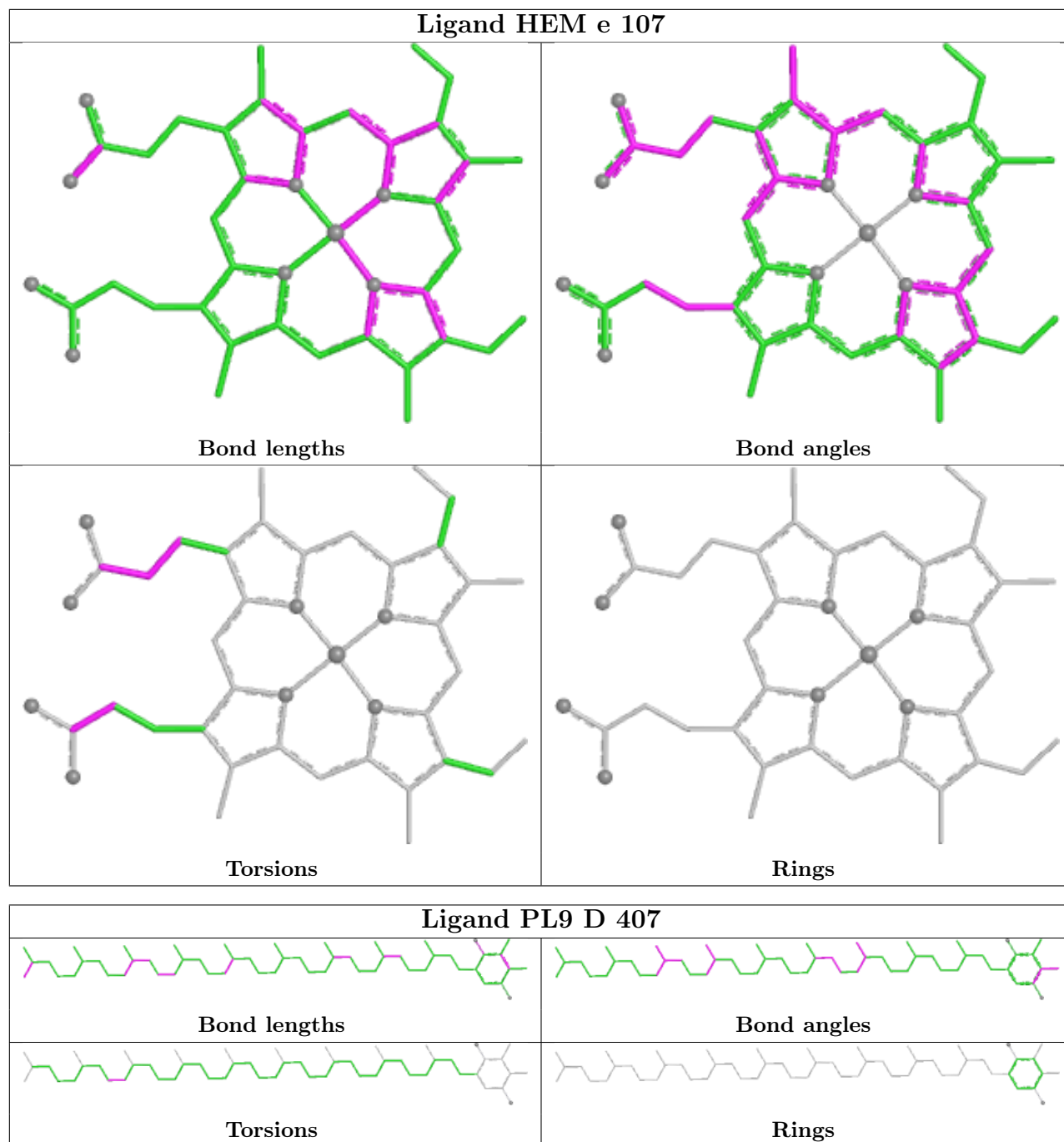
Ligand CLA C 512	
	
Bond lengths	Bond angles
	
Torsions	Rings

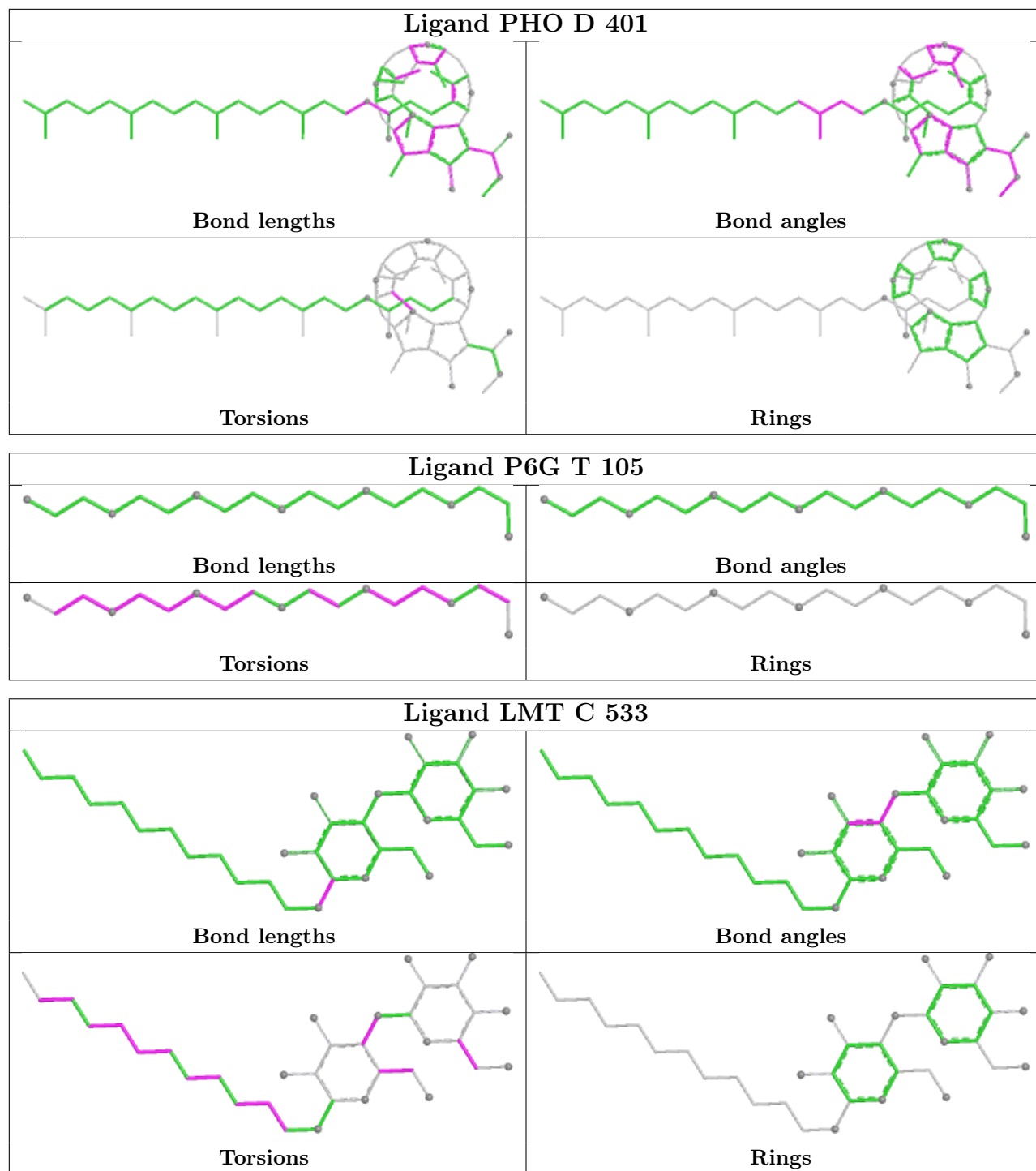
Ligand LMG B 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

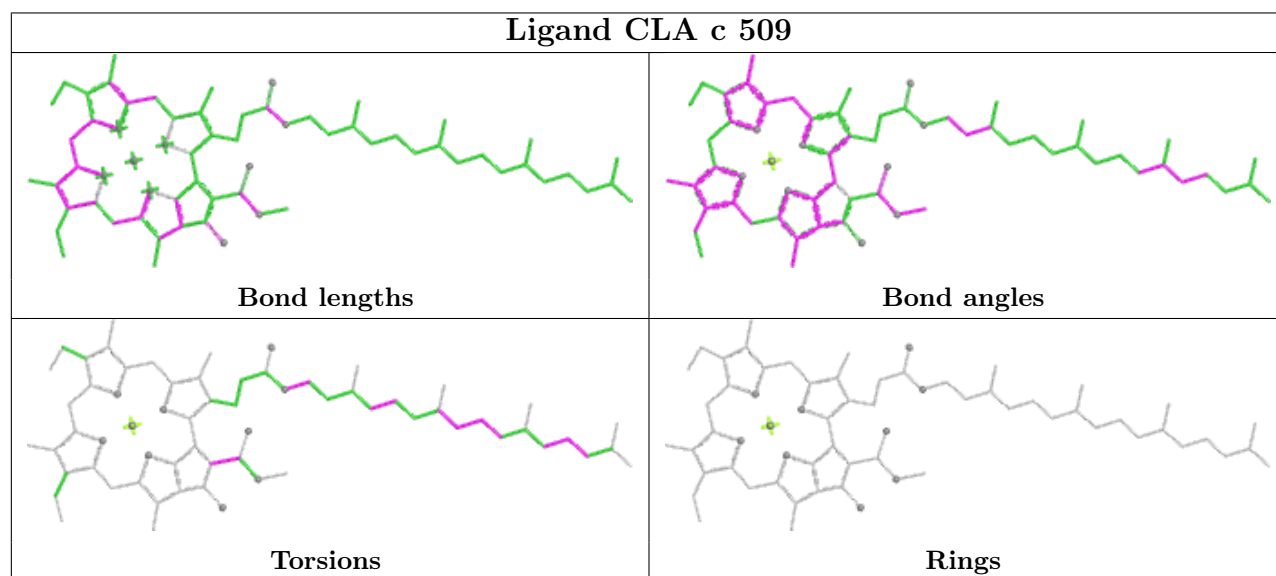
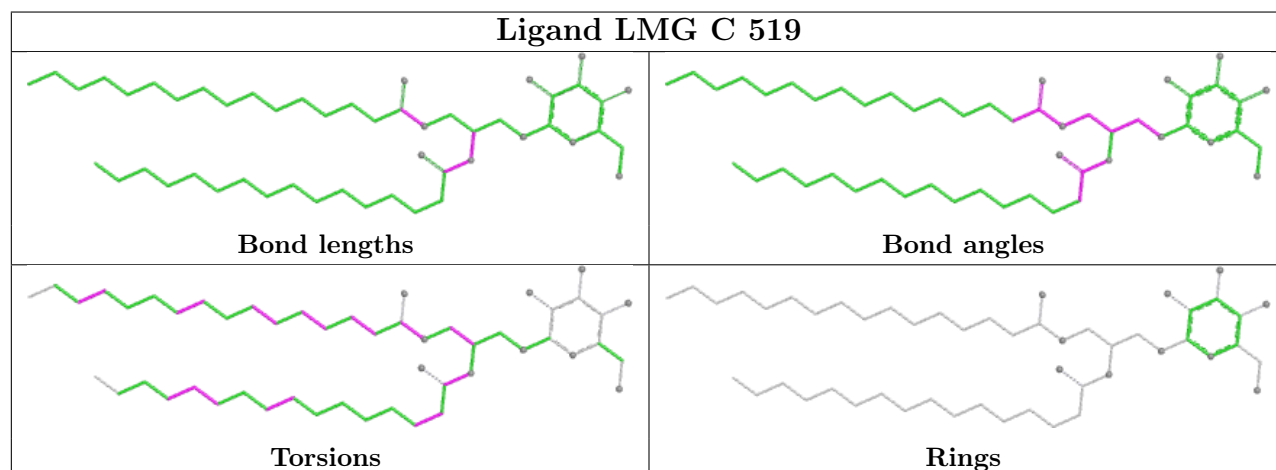
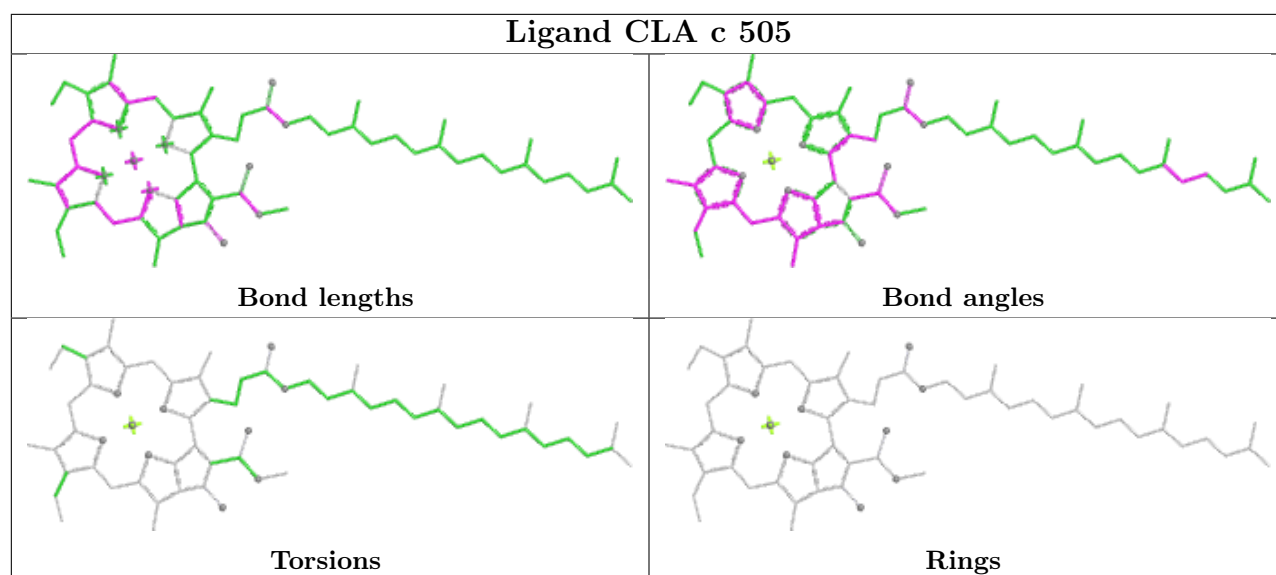
Ligand BCR c 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

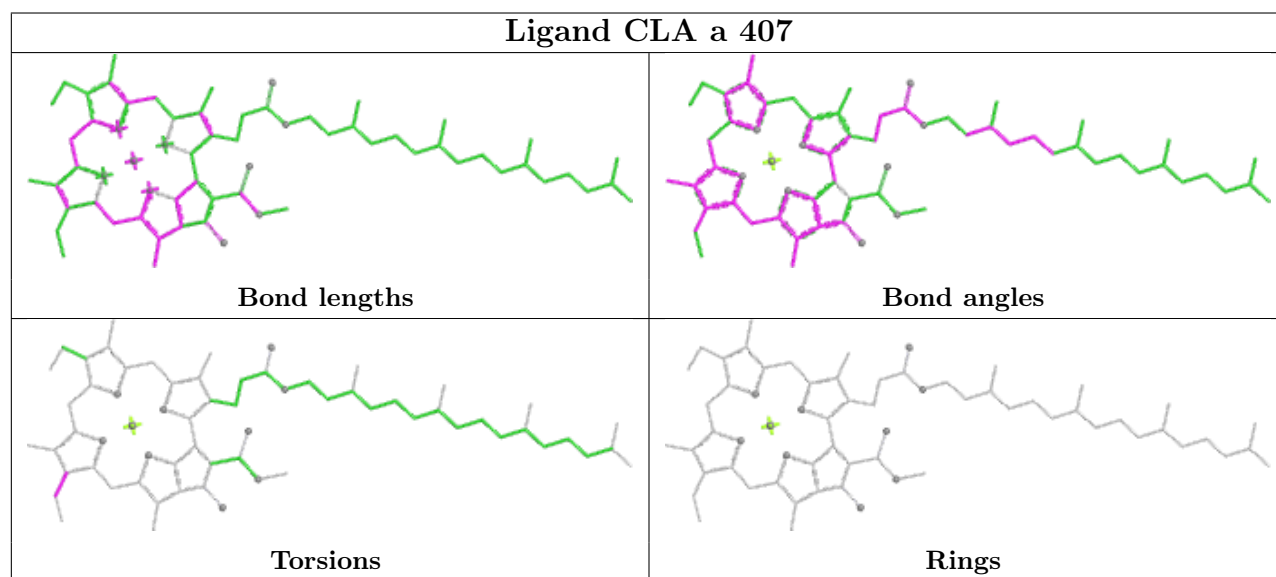
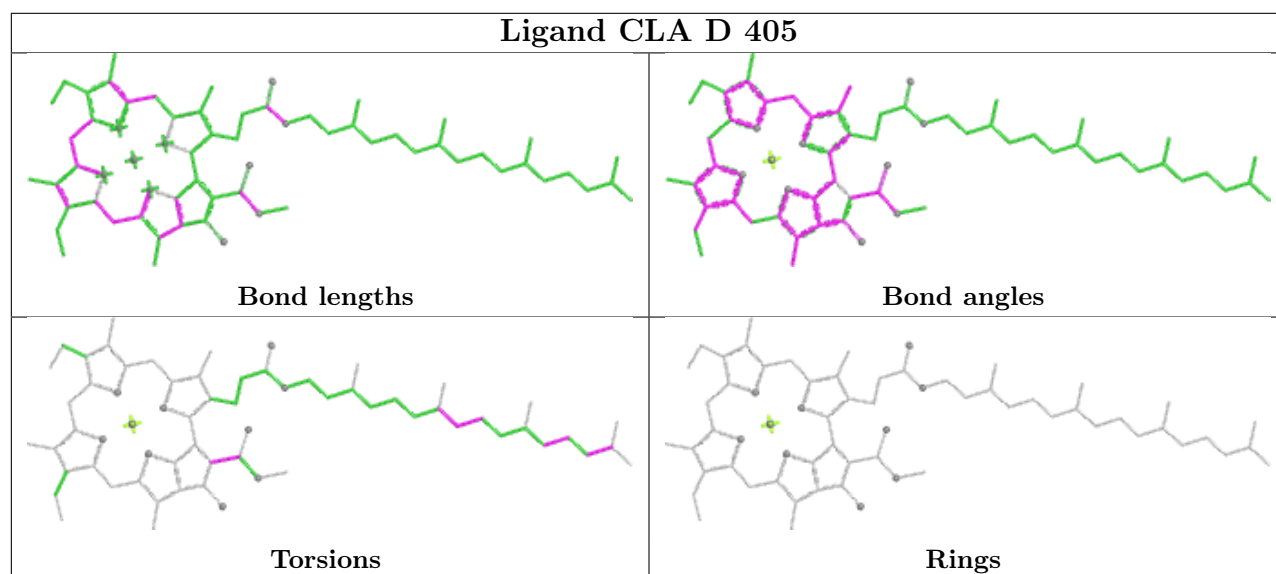
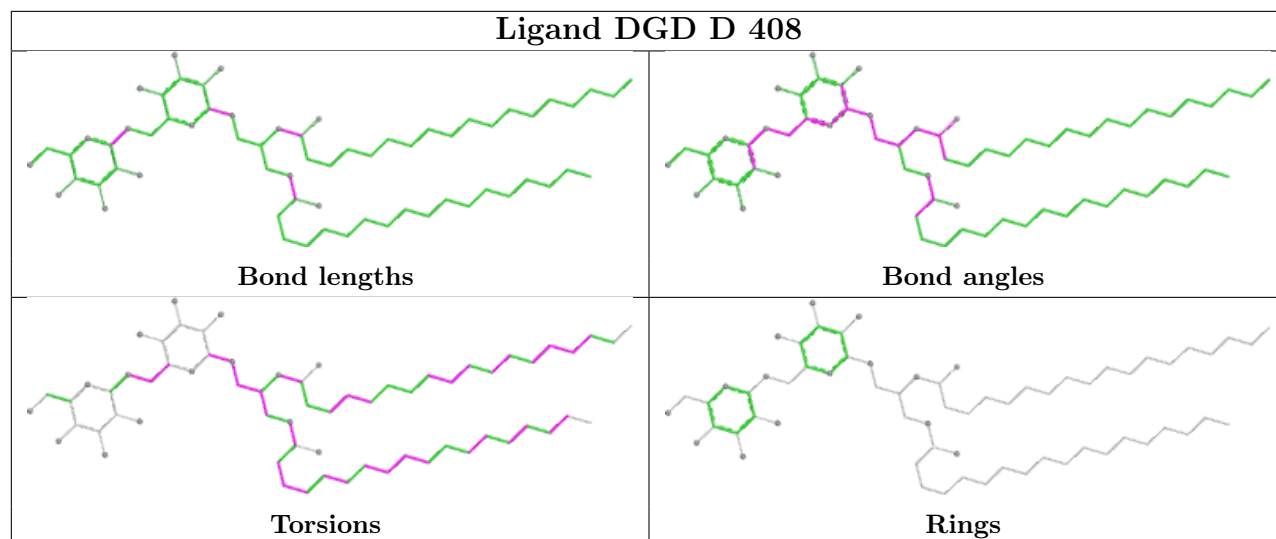


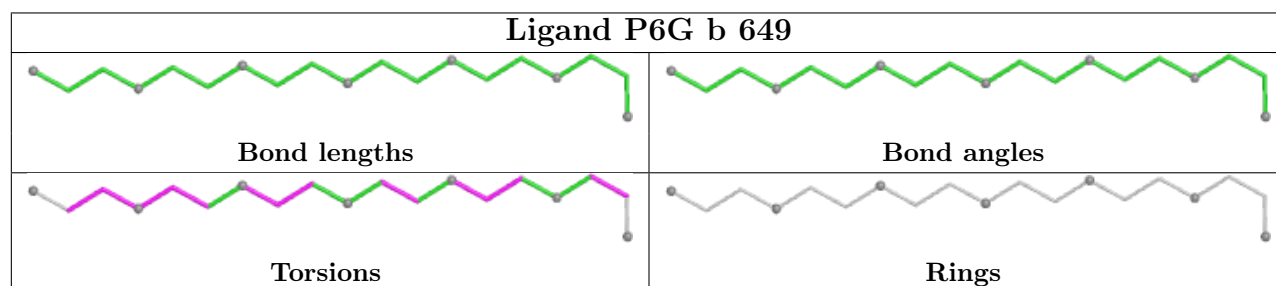
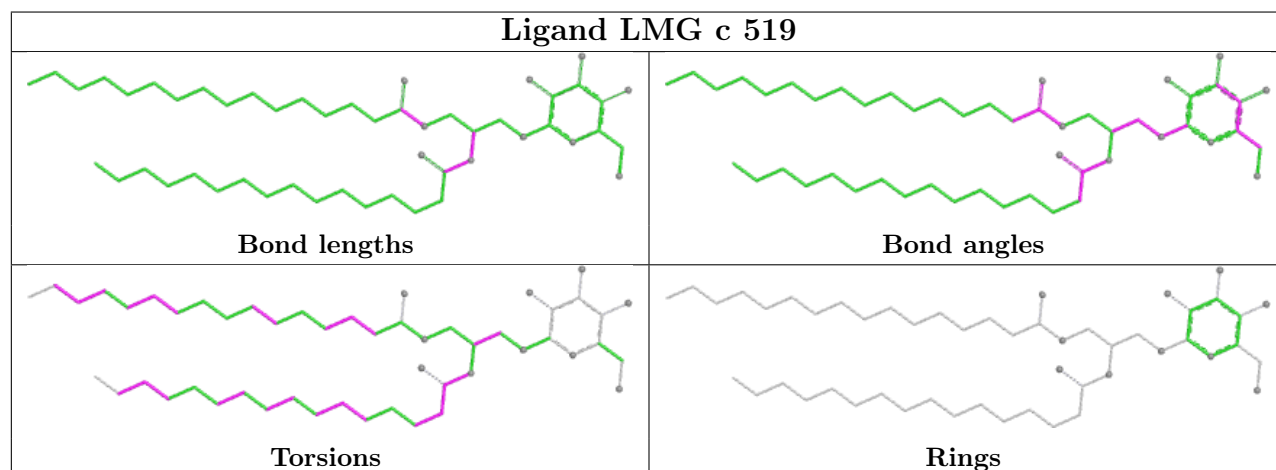
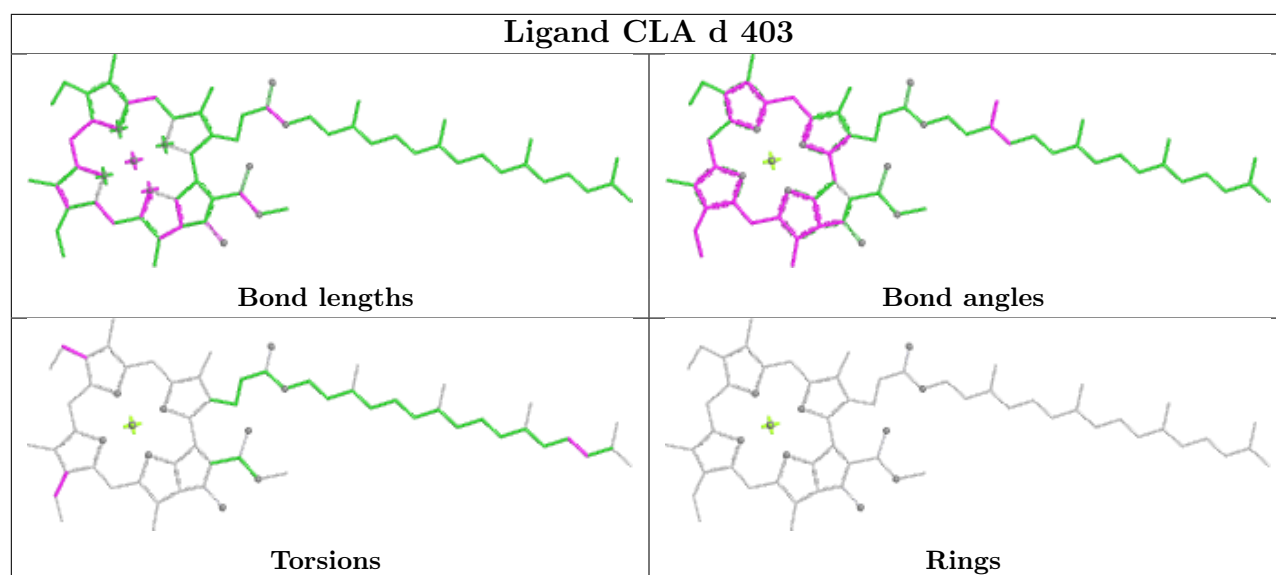


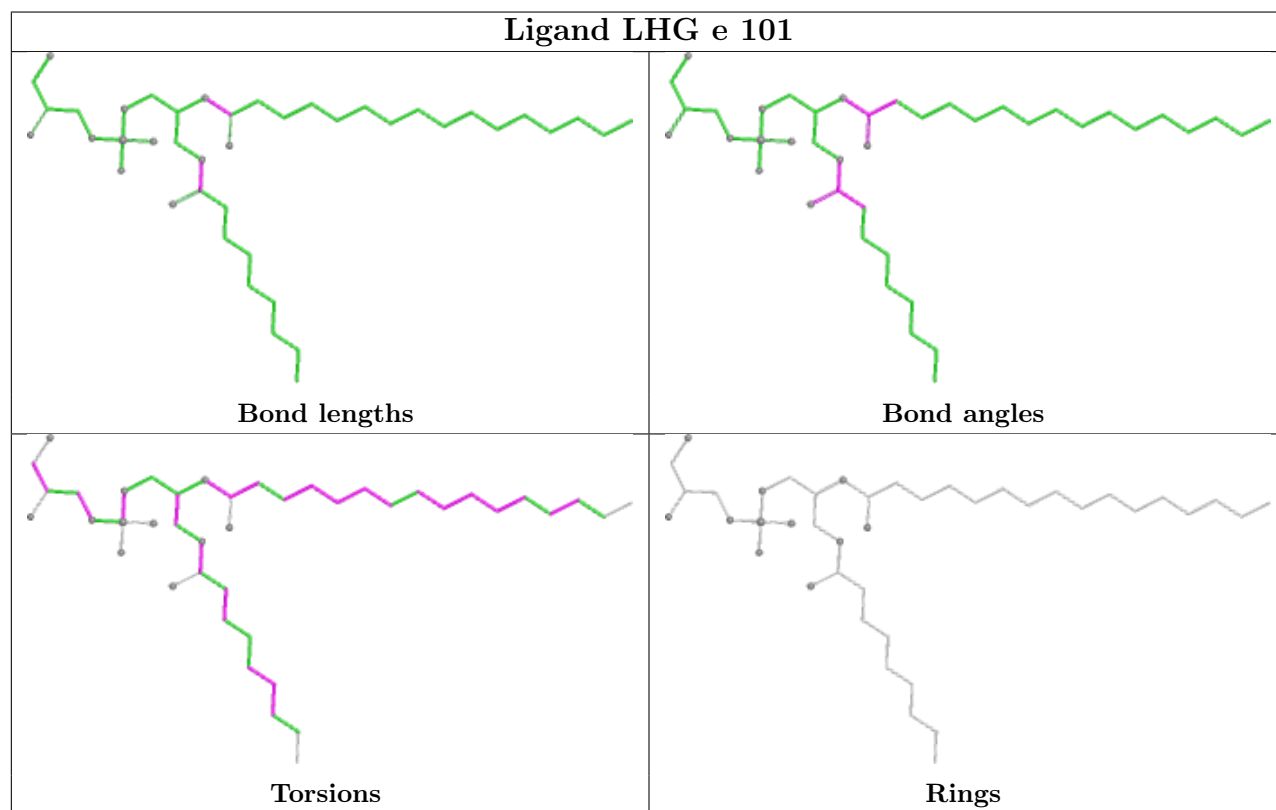
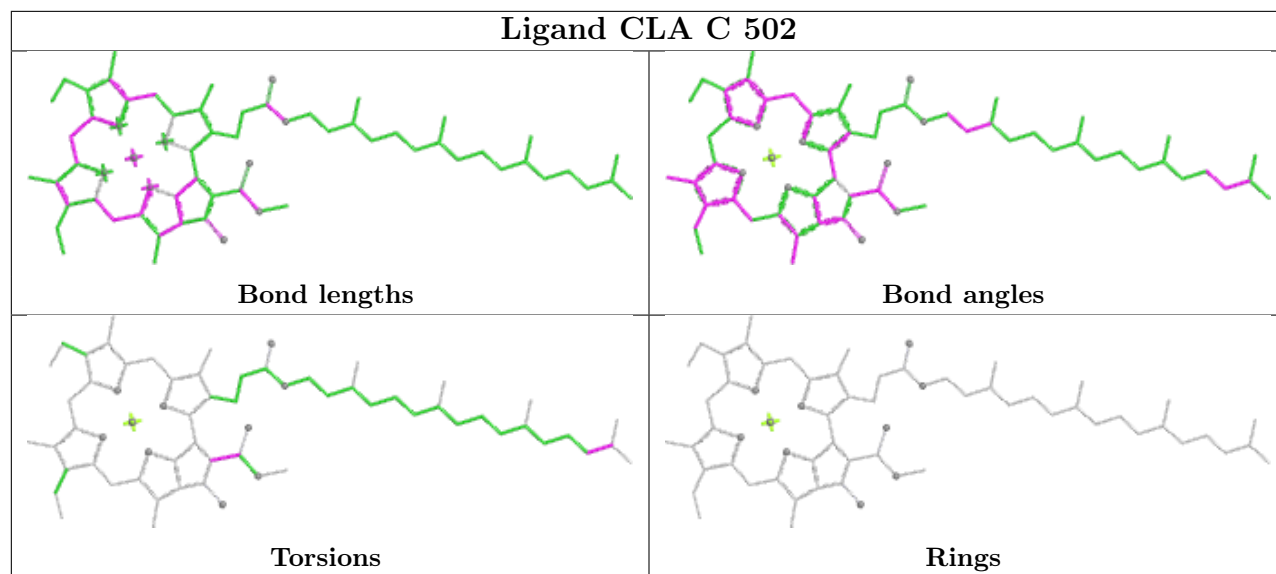


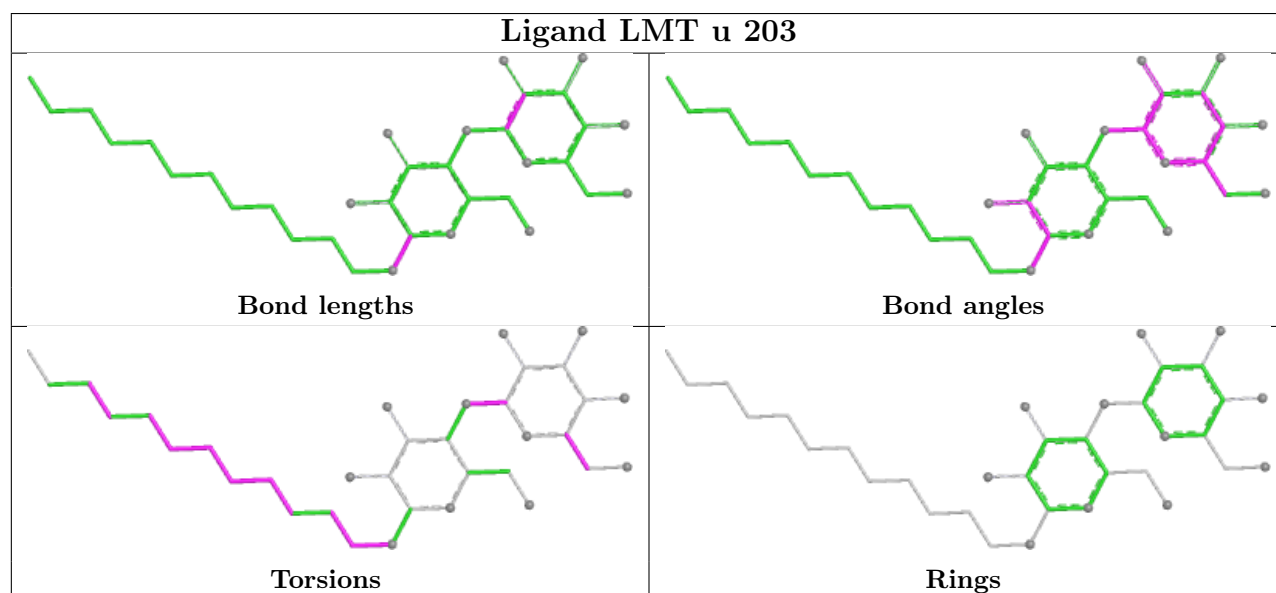
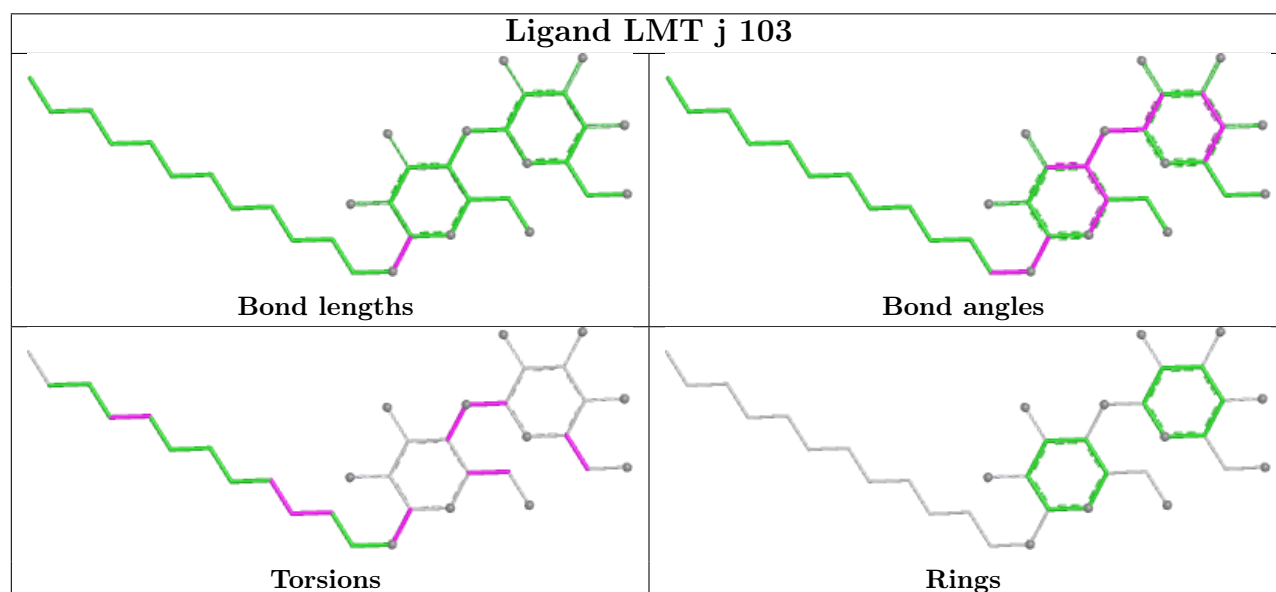
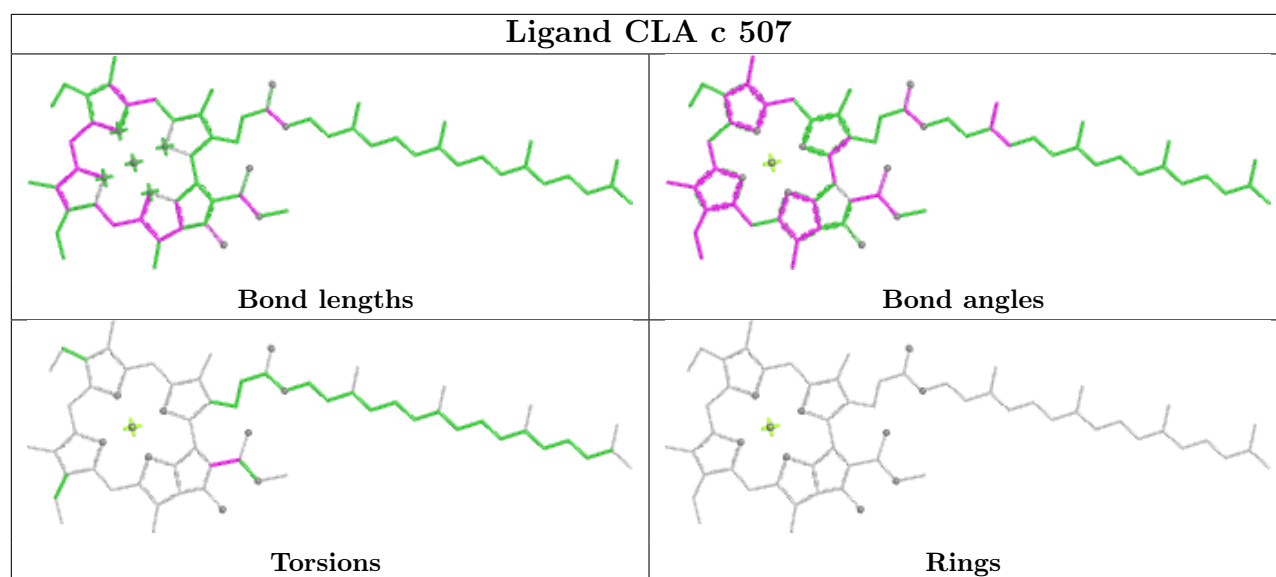


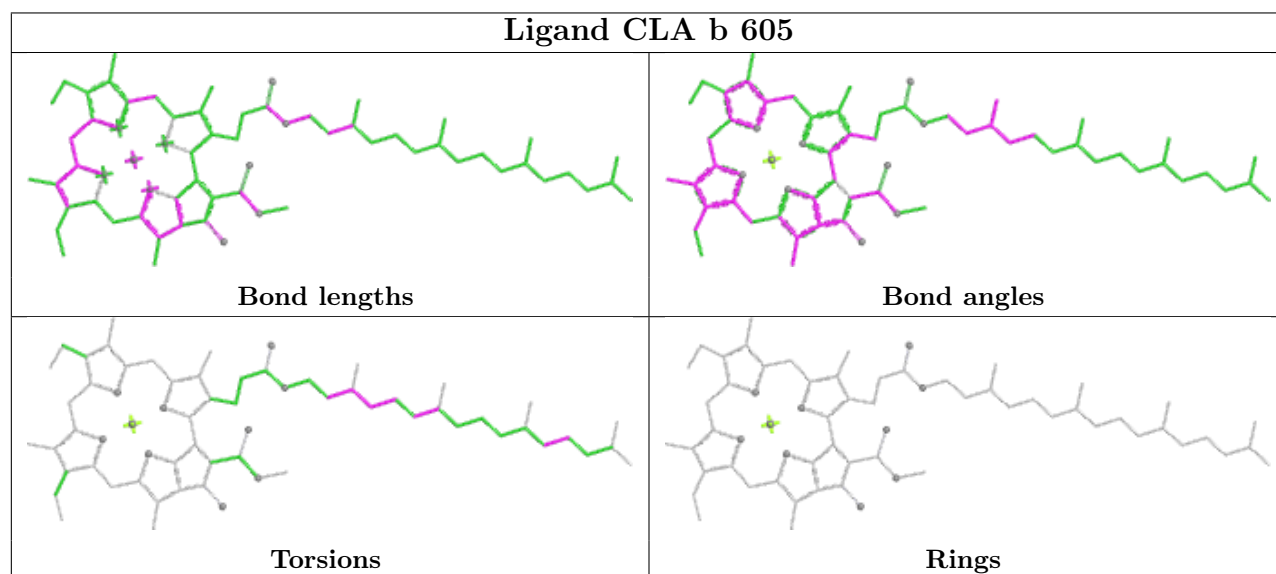
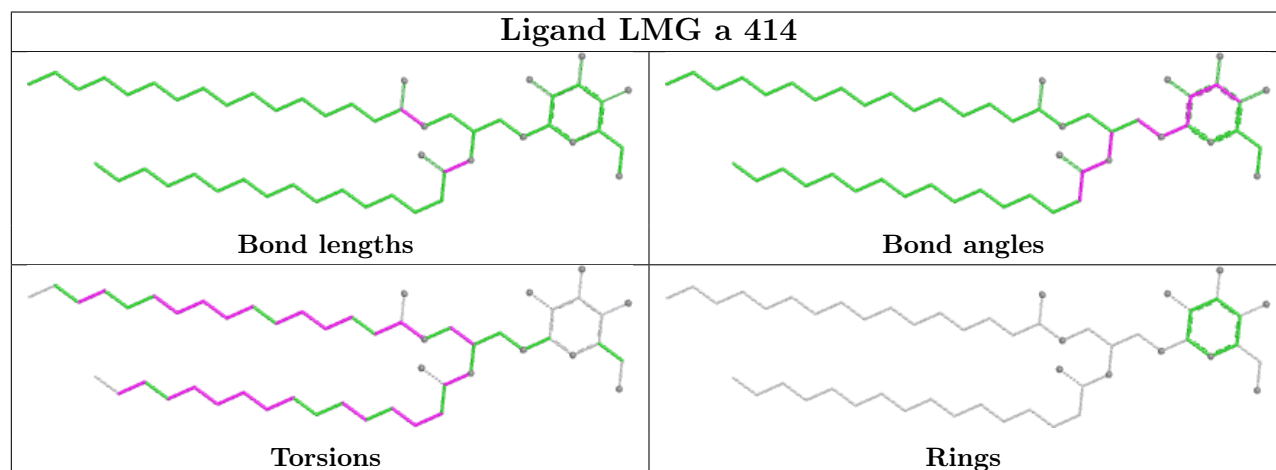
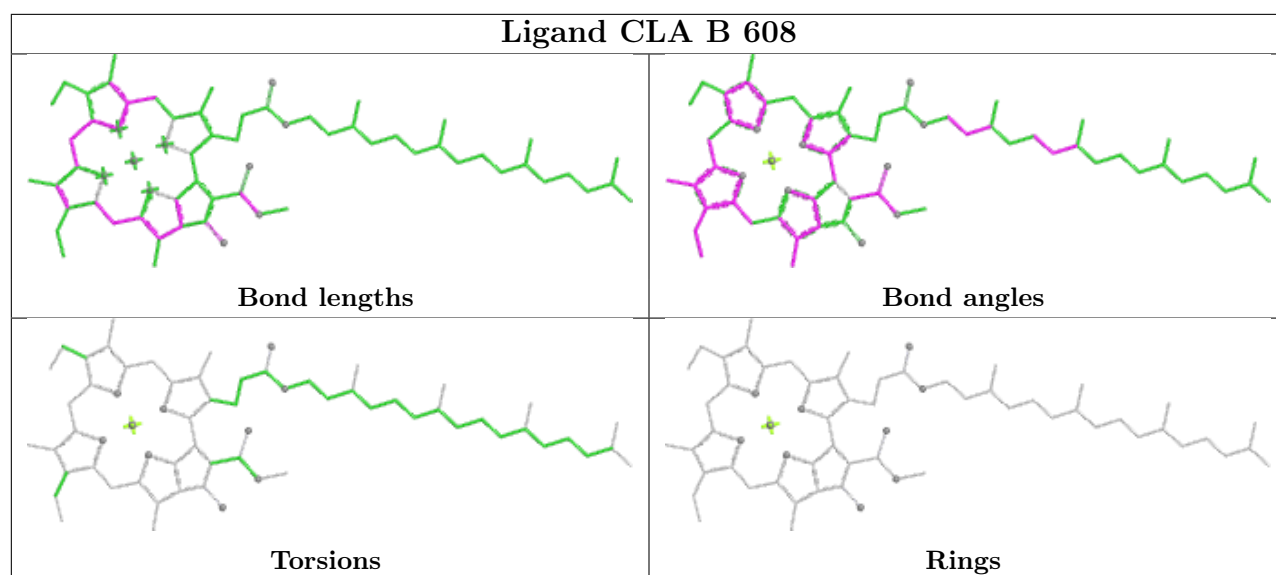


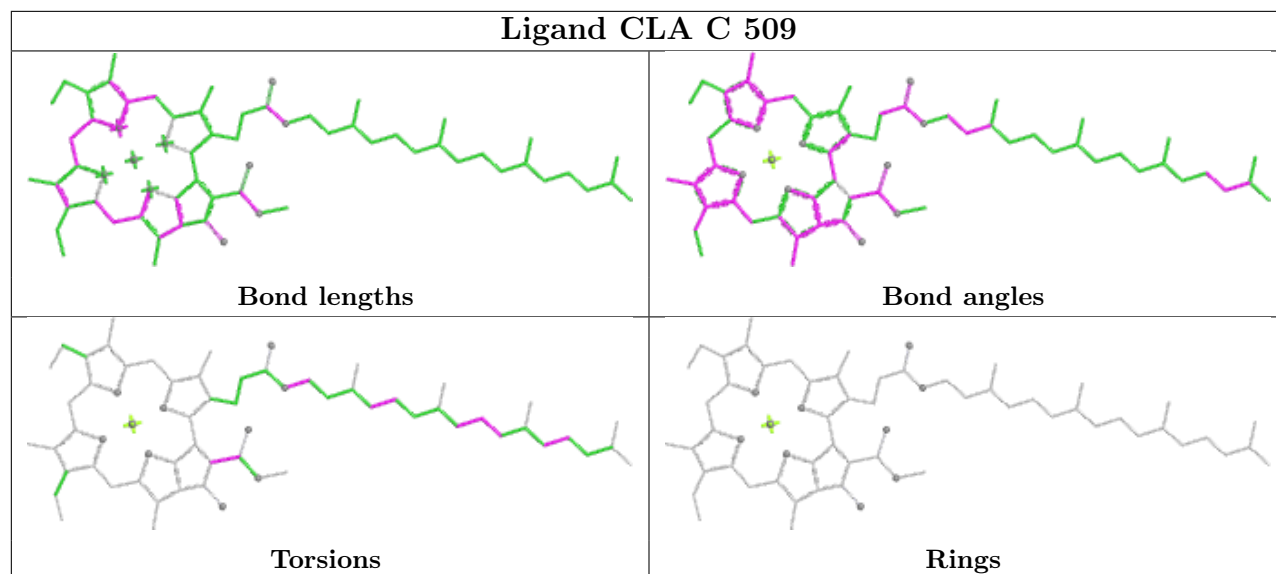
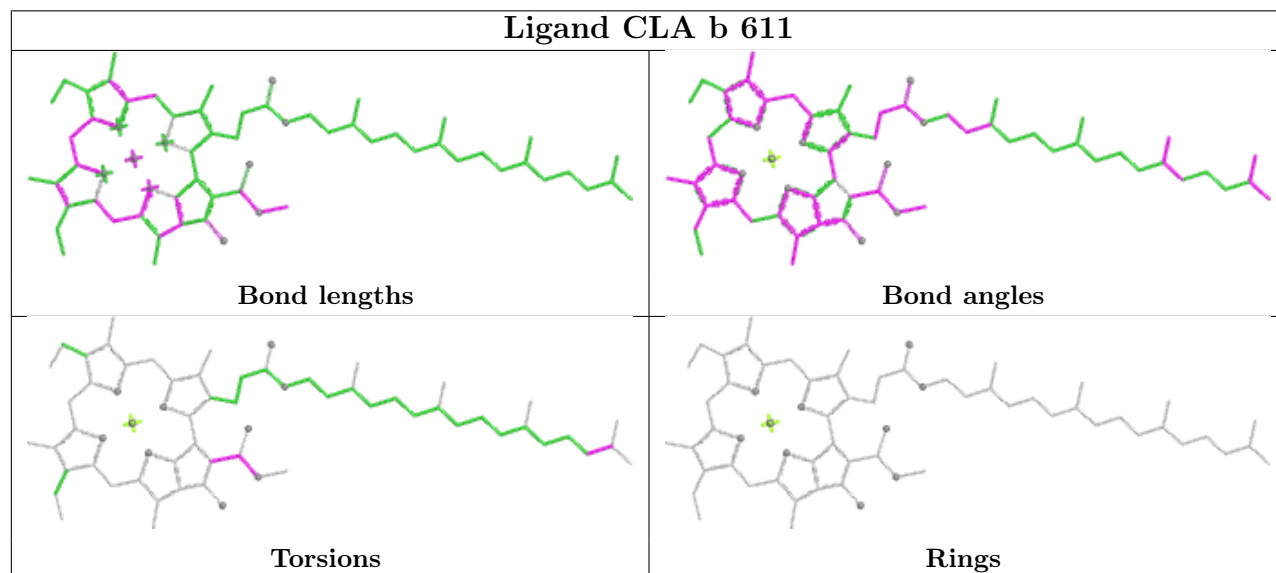




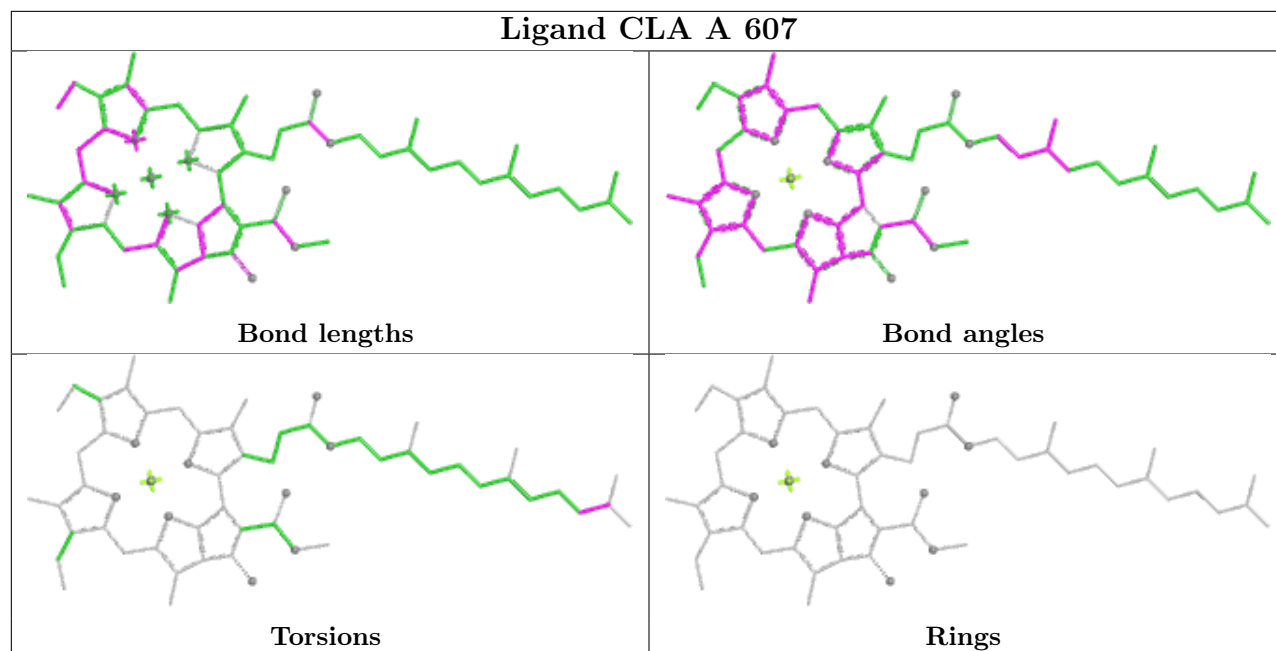




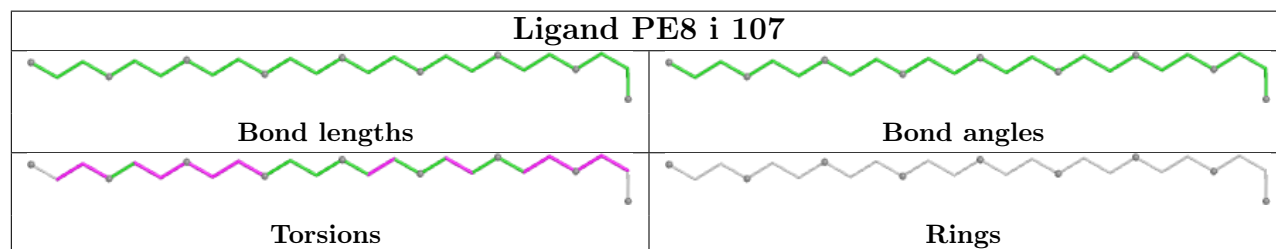


Ligand CLA C 509**Ligand CLA b 611**

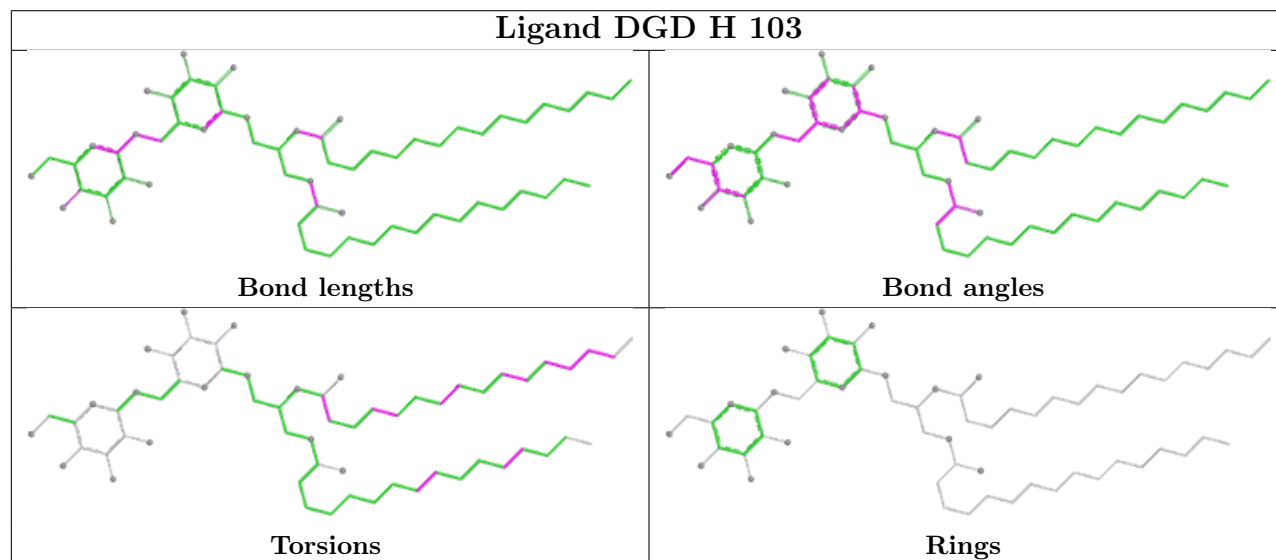
Ligand CLA A 607

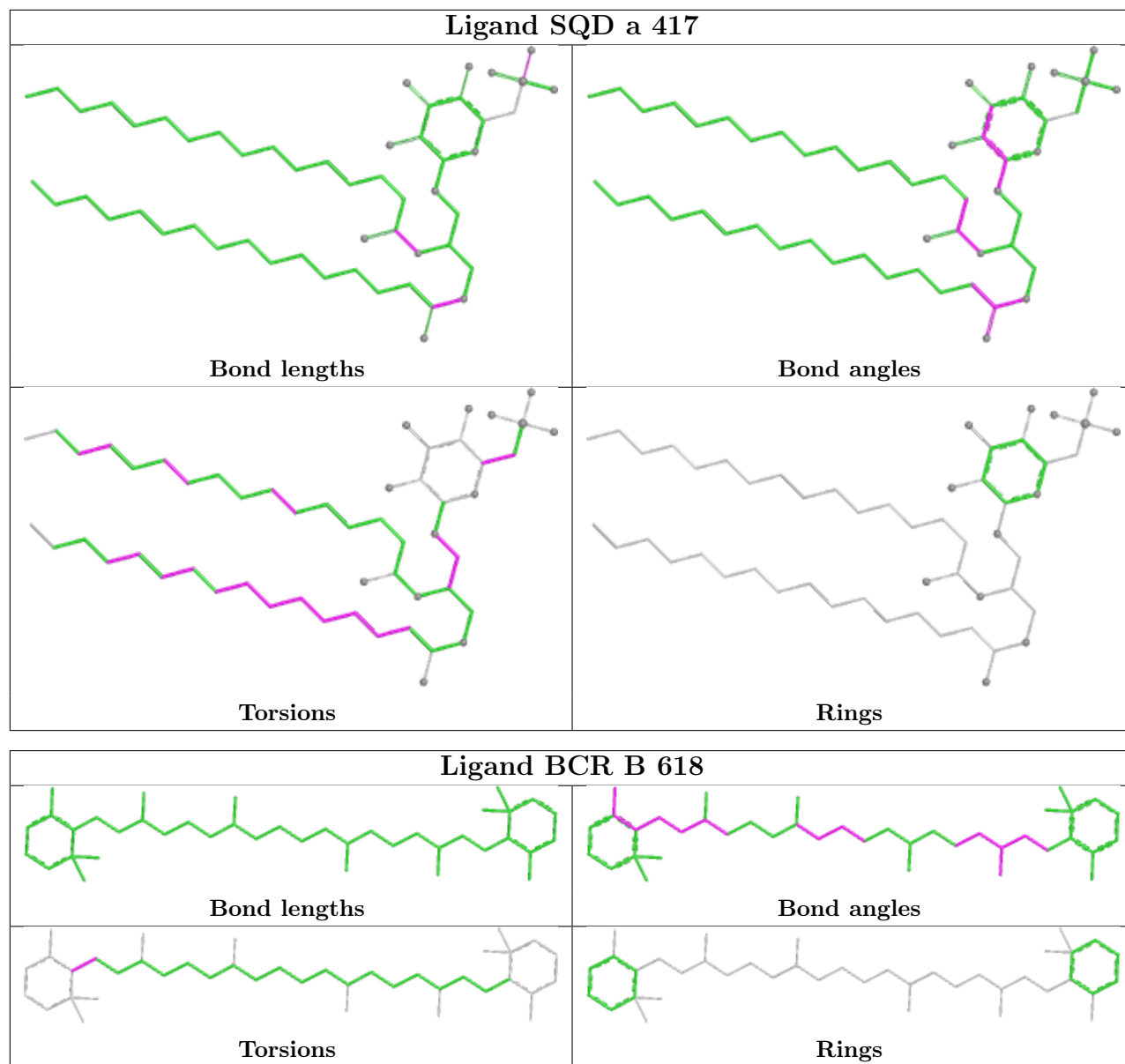


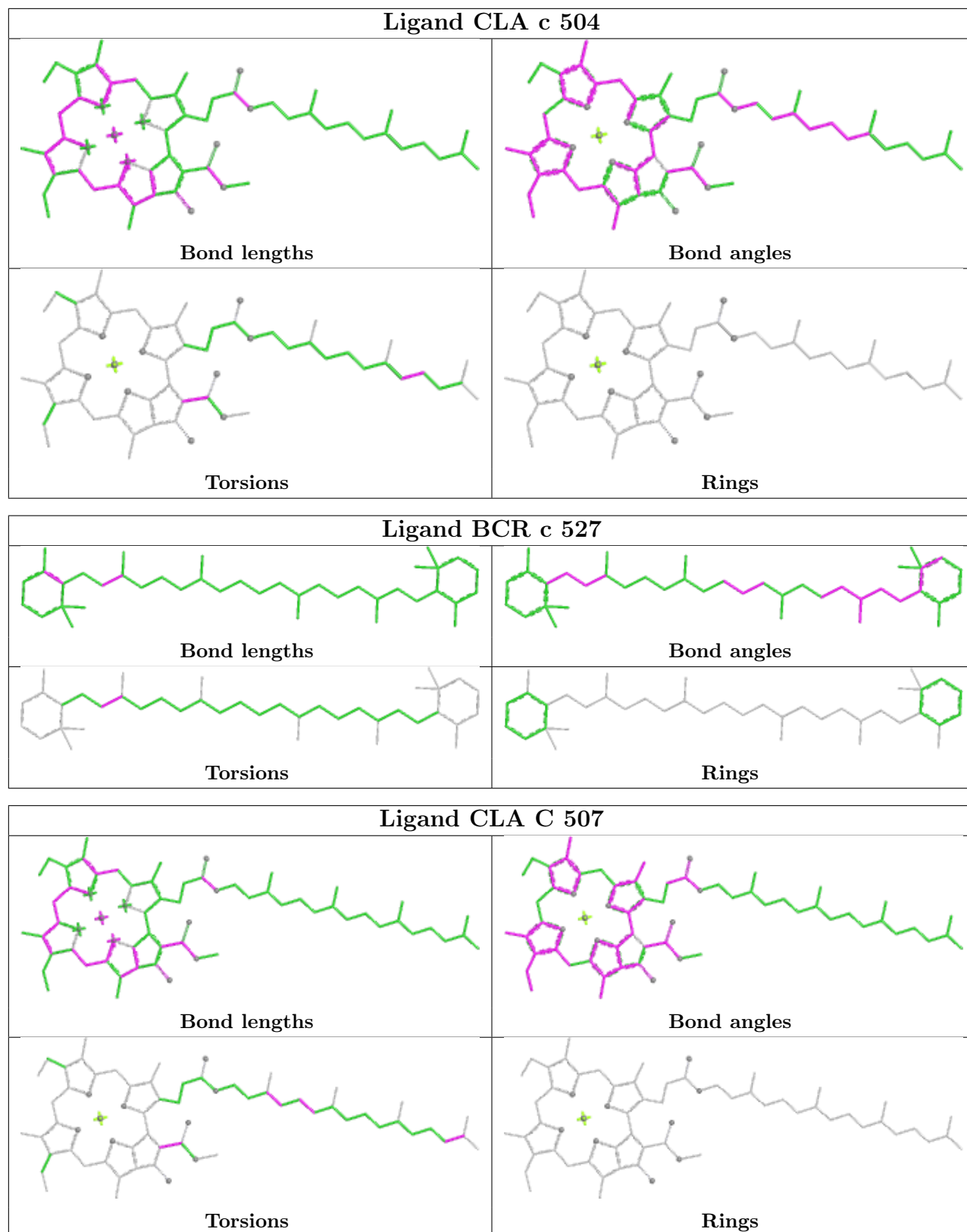
Ligand PE8 i 107

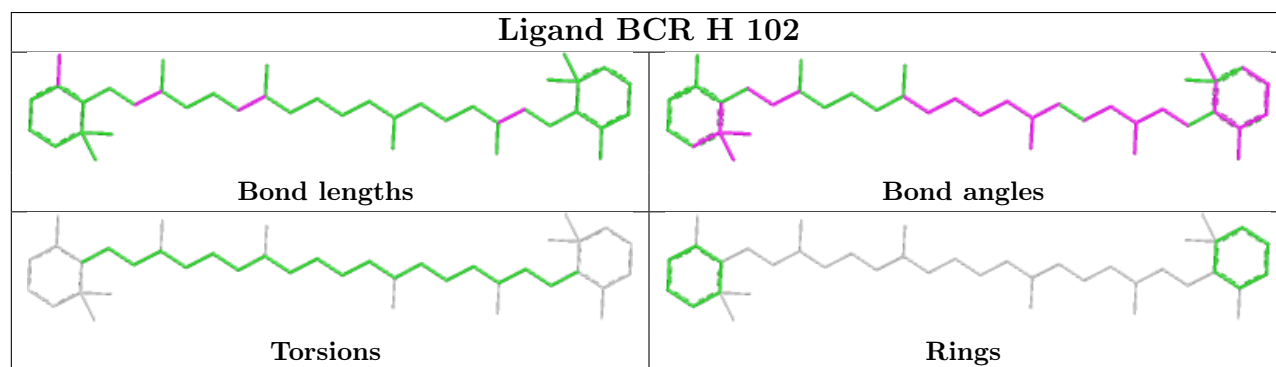
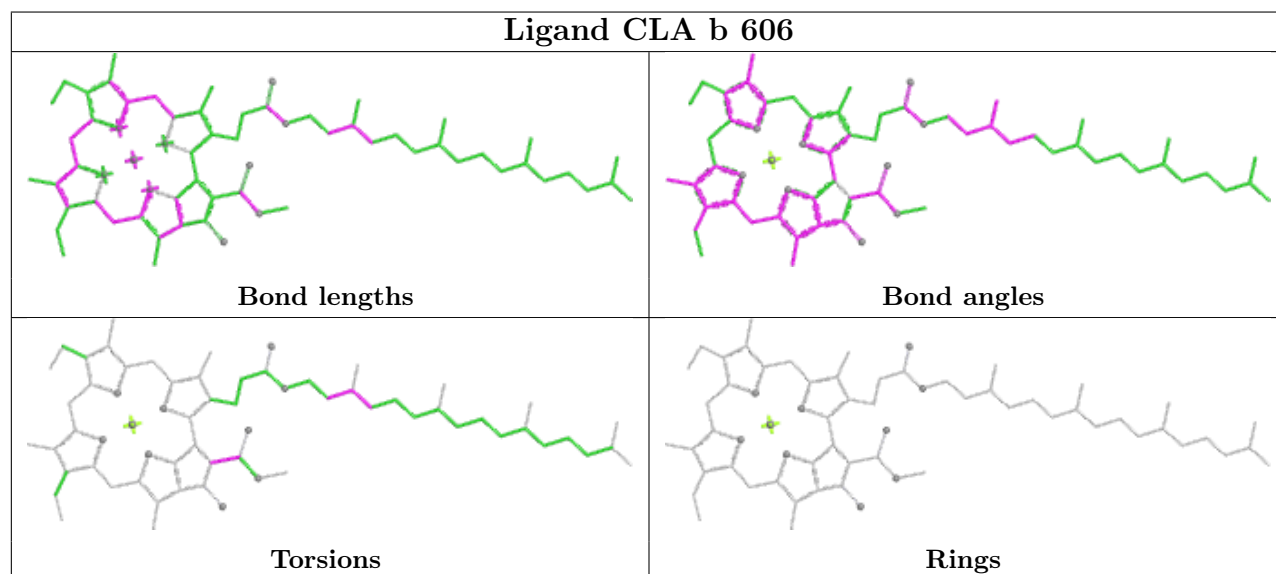
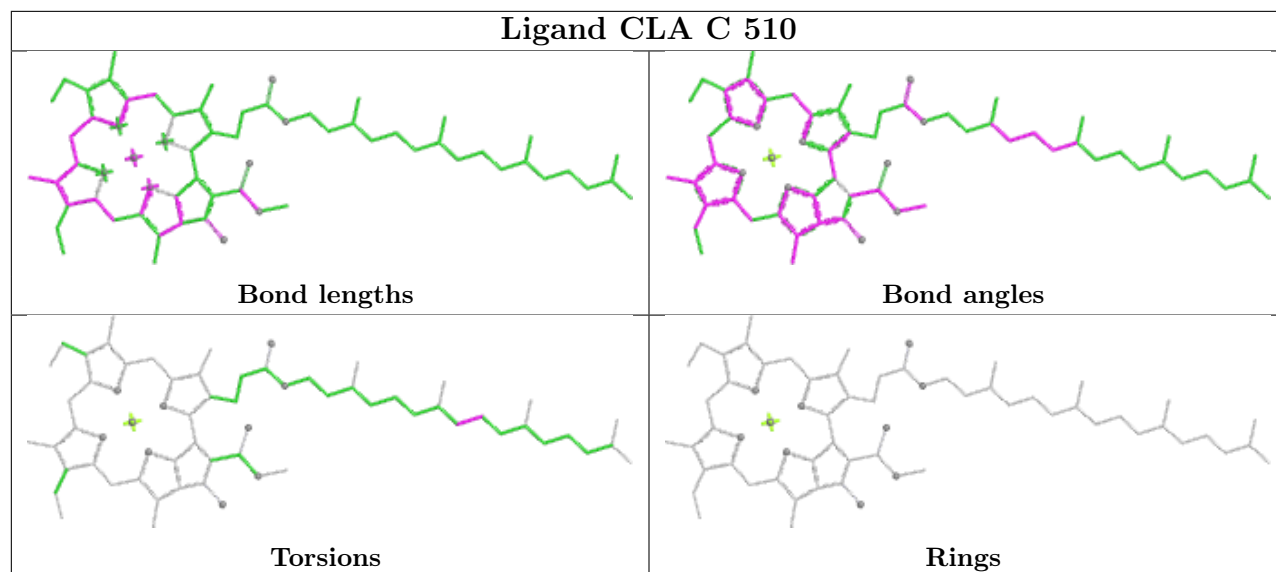


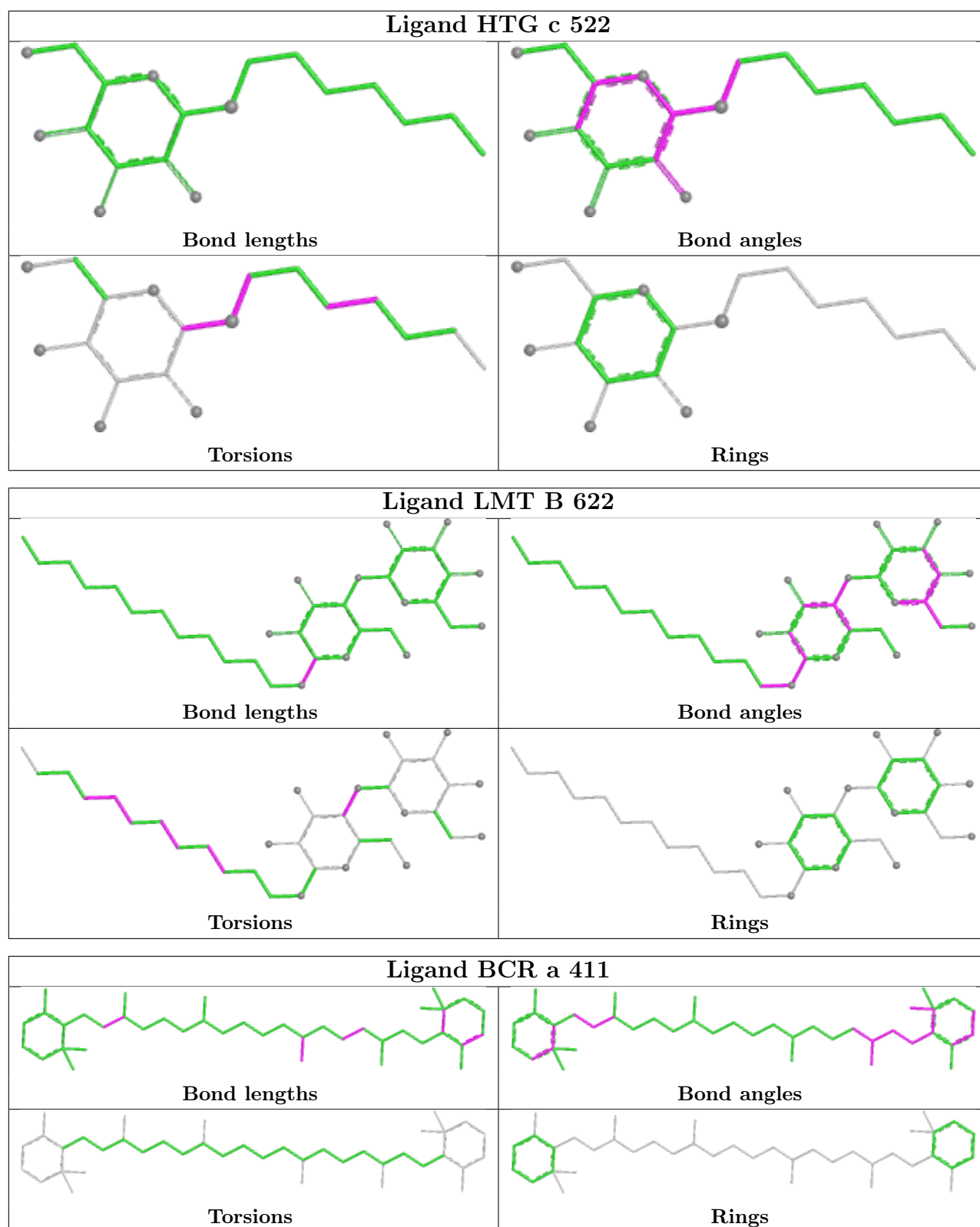
Ligand DGD H 103

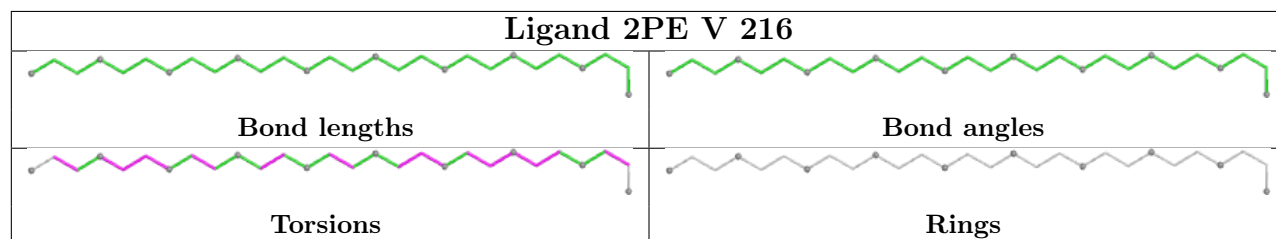
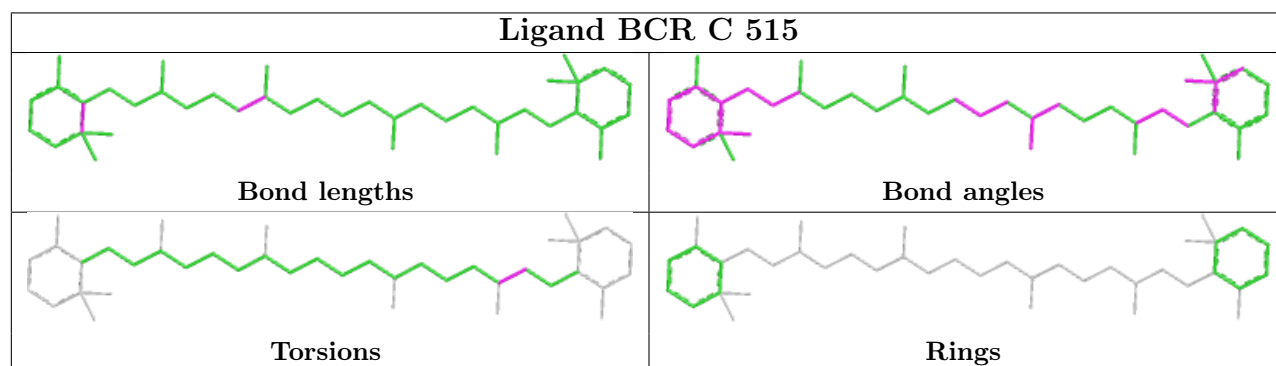
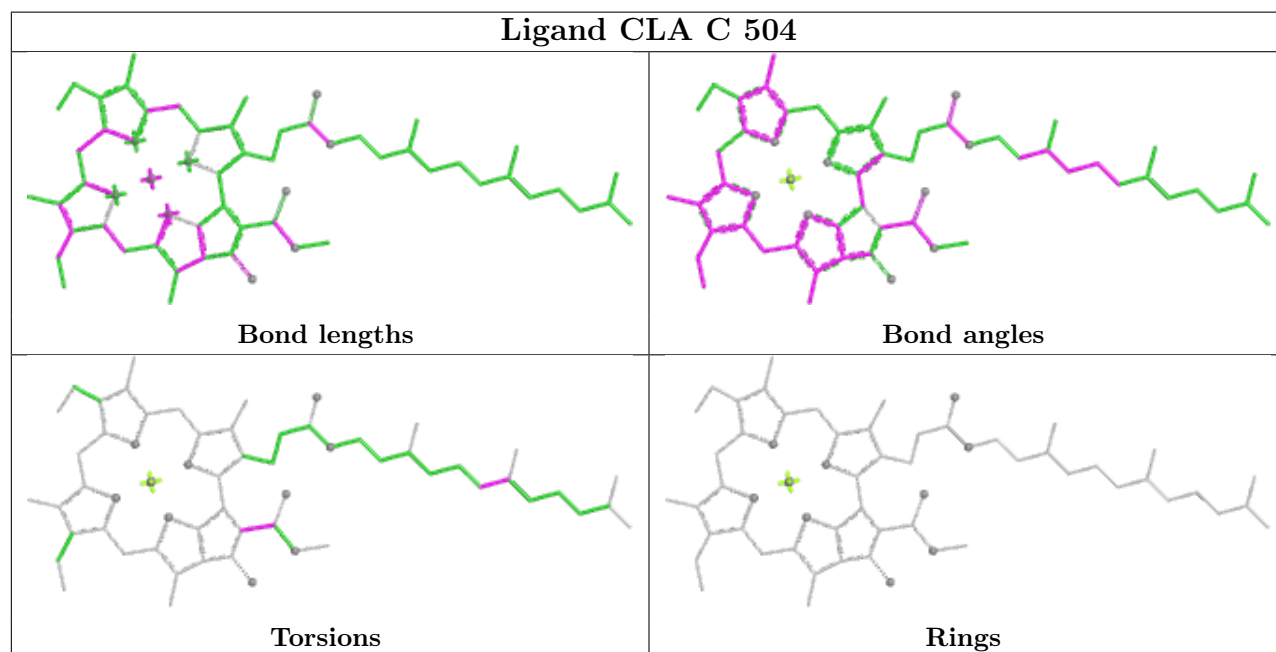
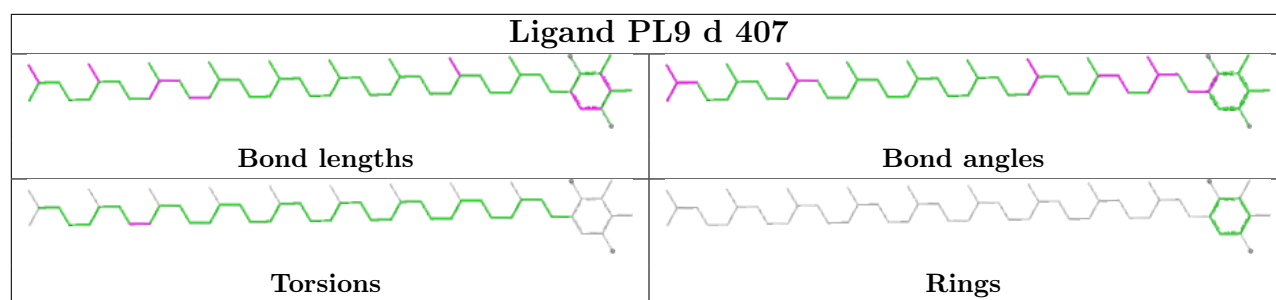


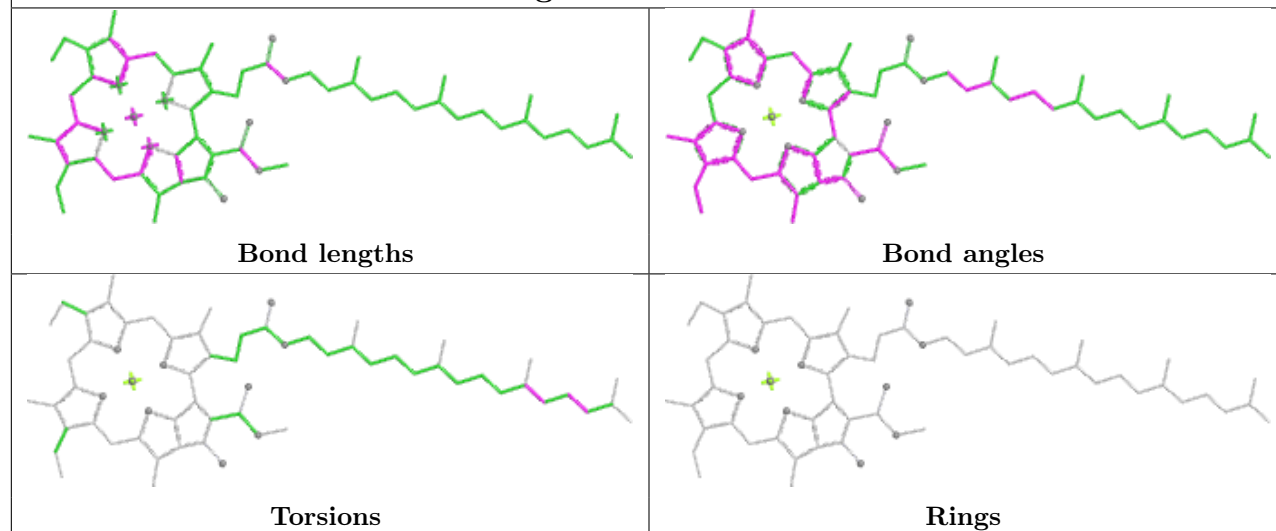
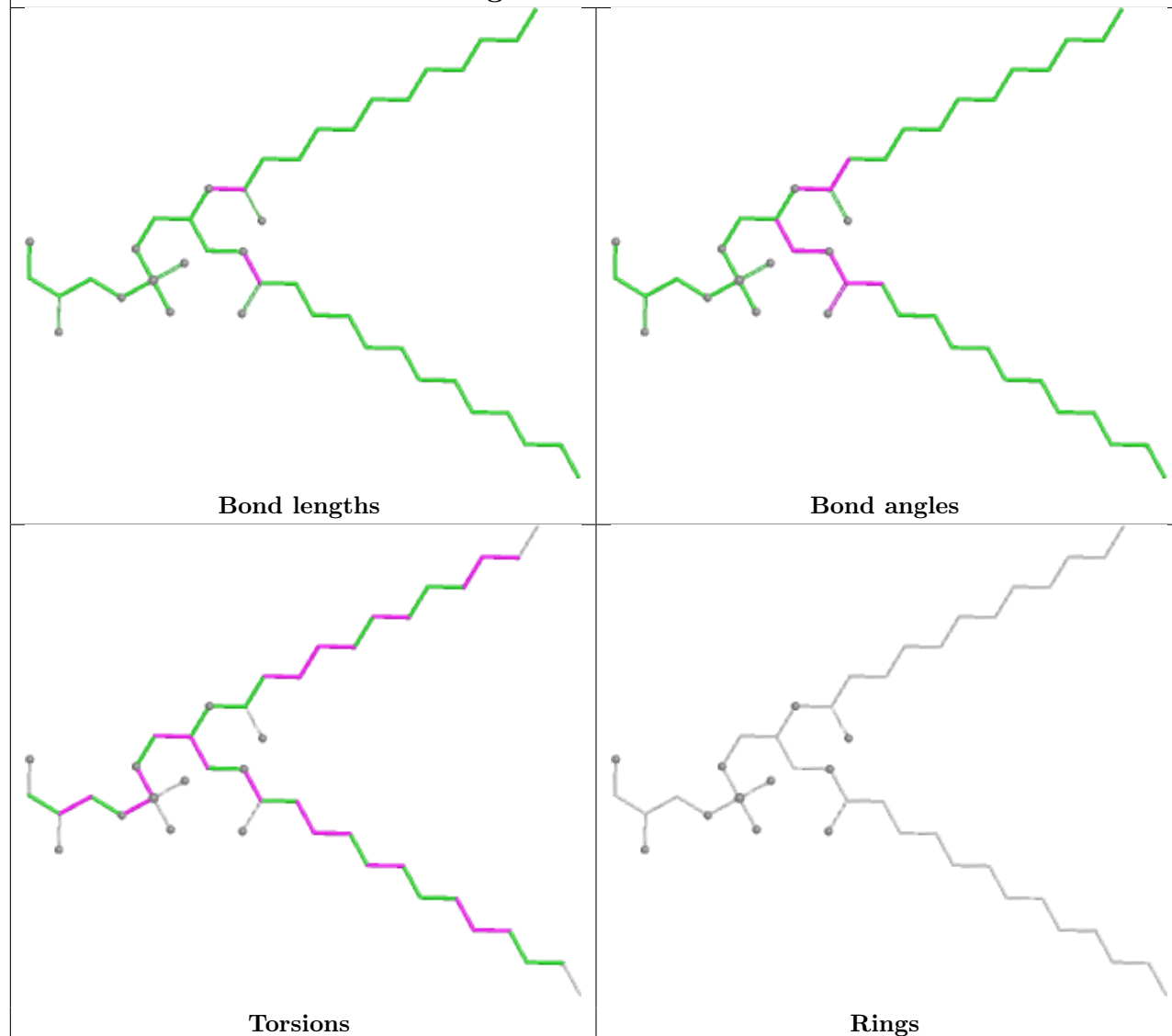


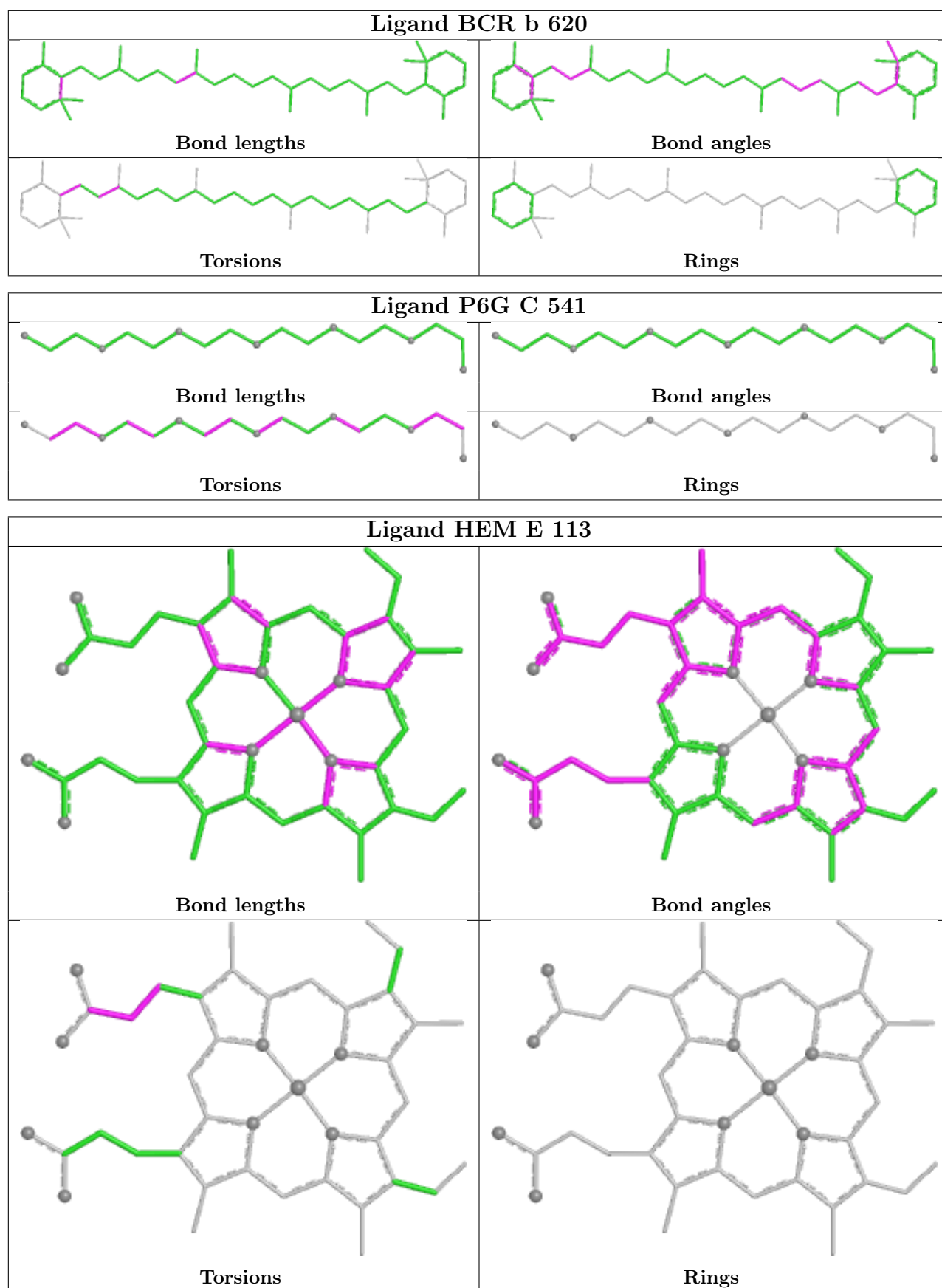


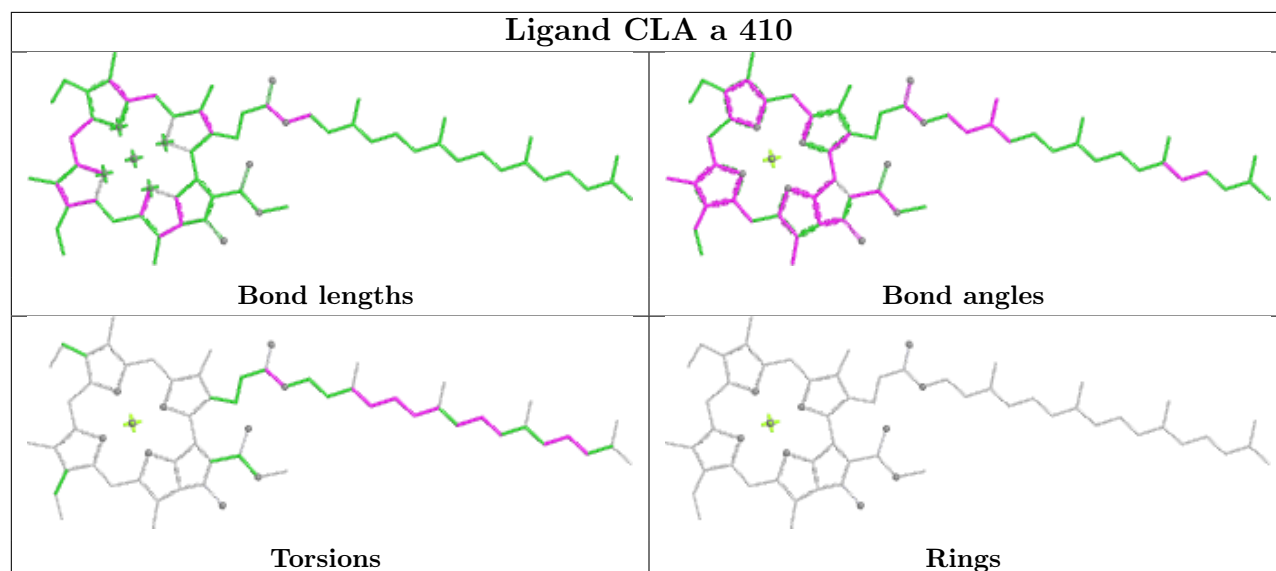
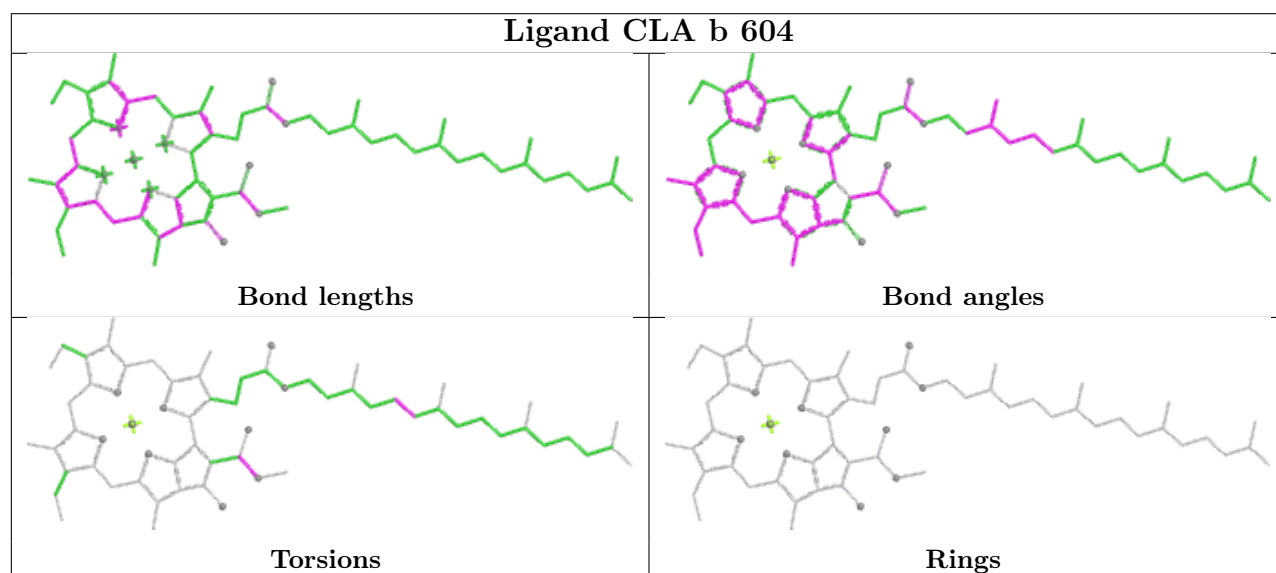
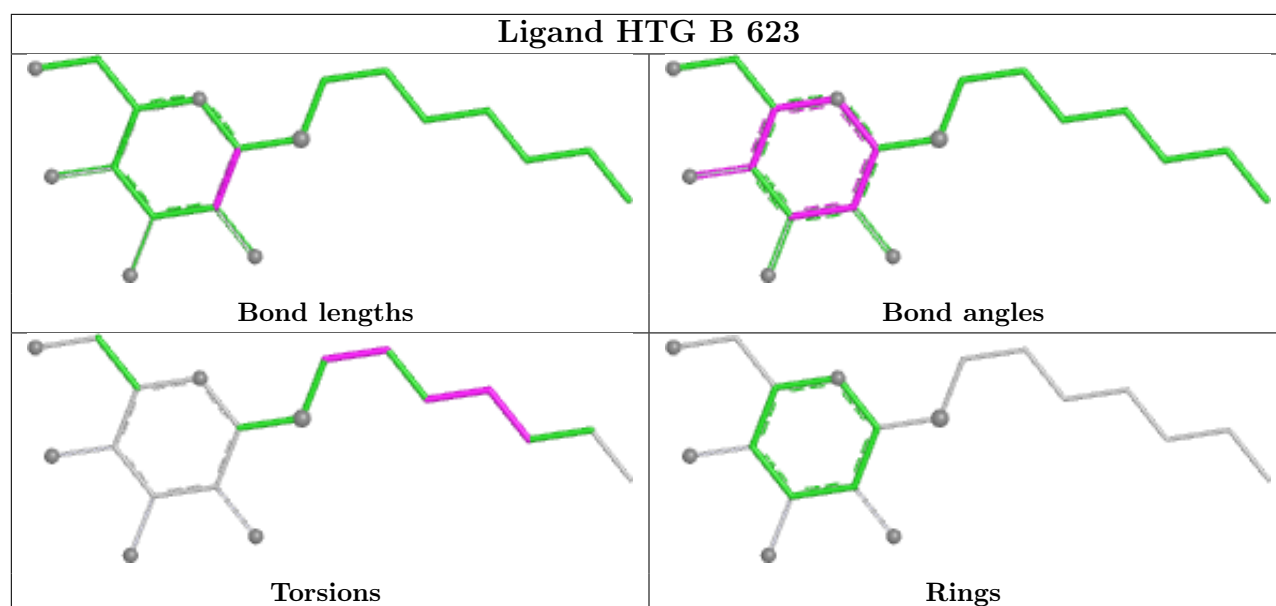




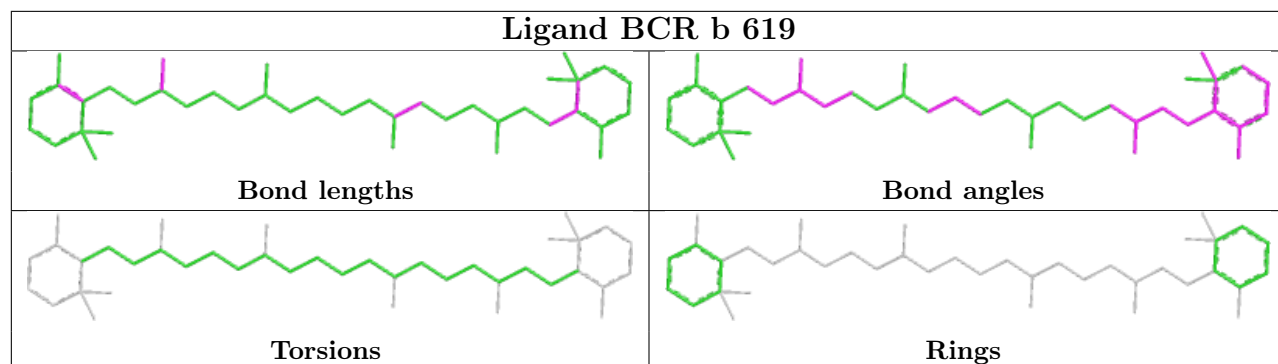


Ligand CLA b 612**Ligand LHG A 618**

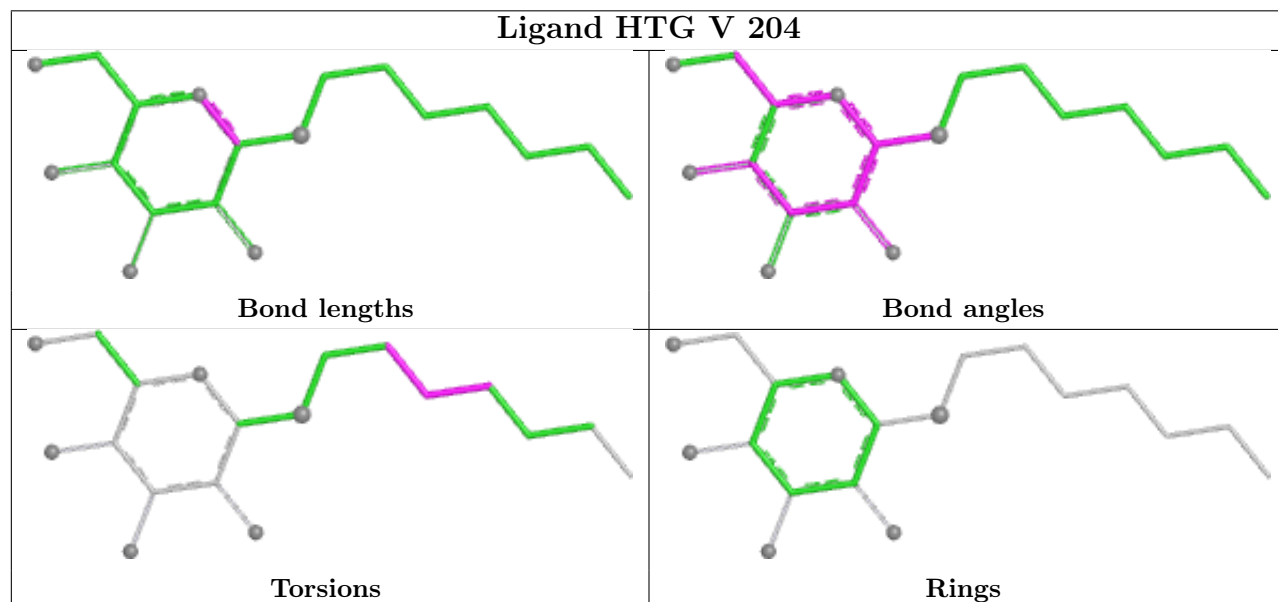




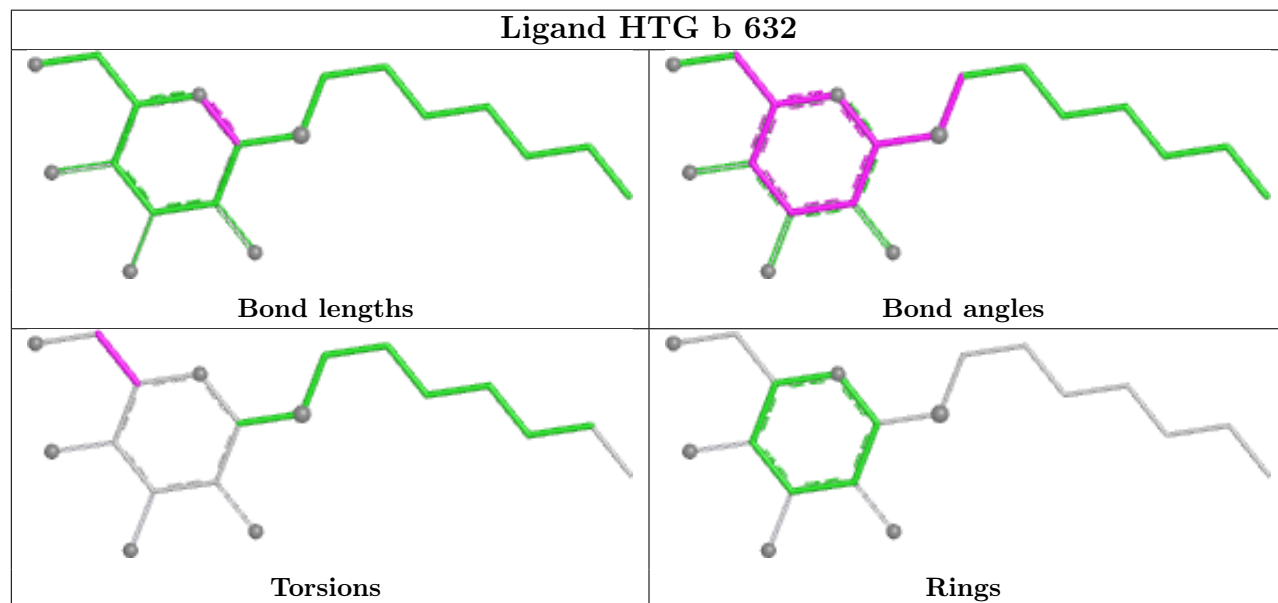
Ligand BCR b 619

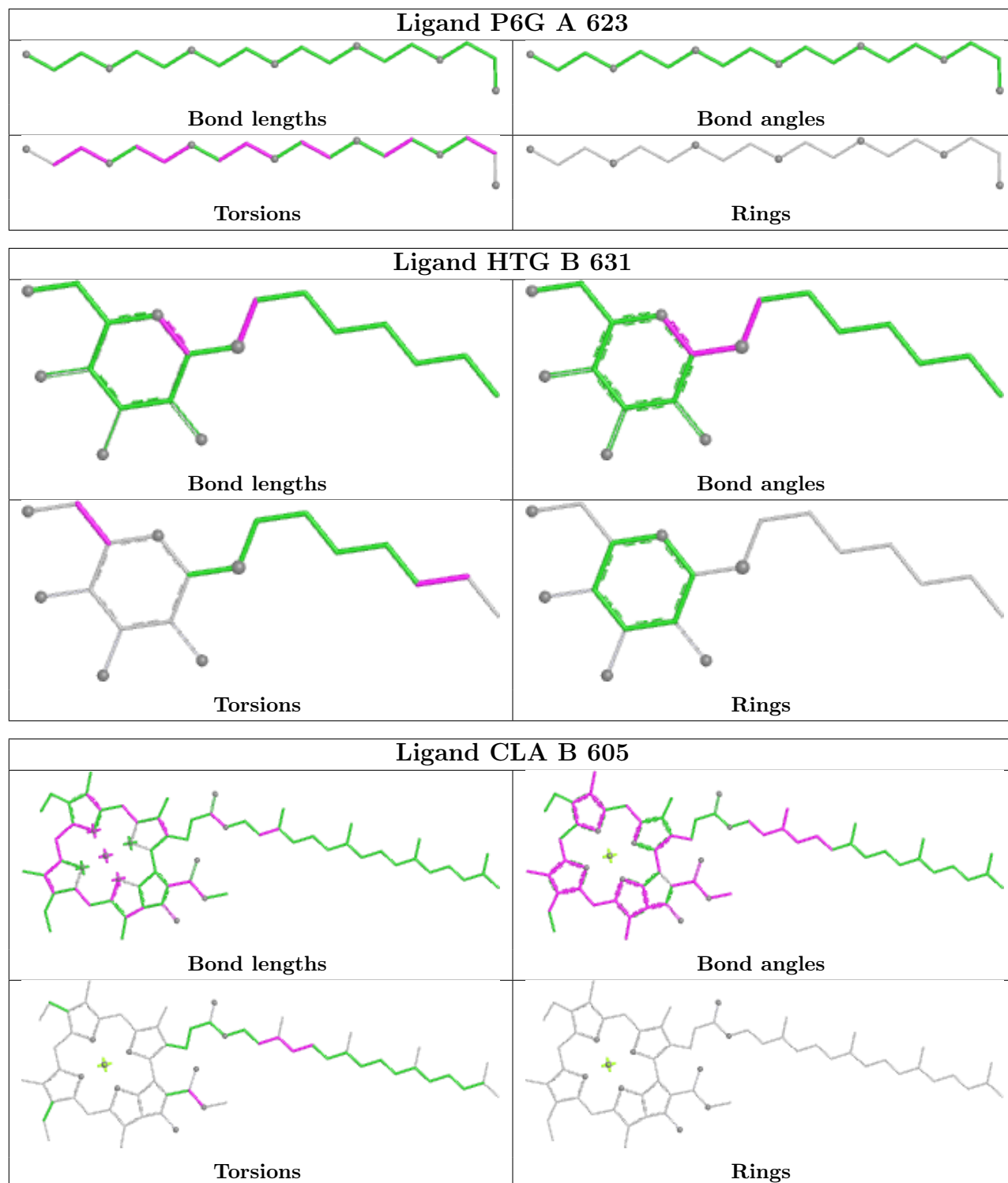


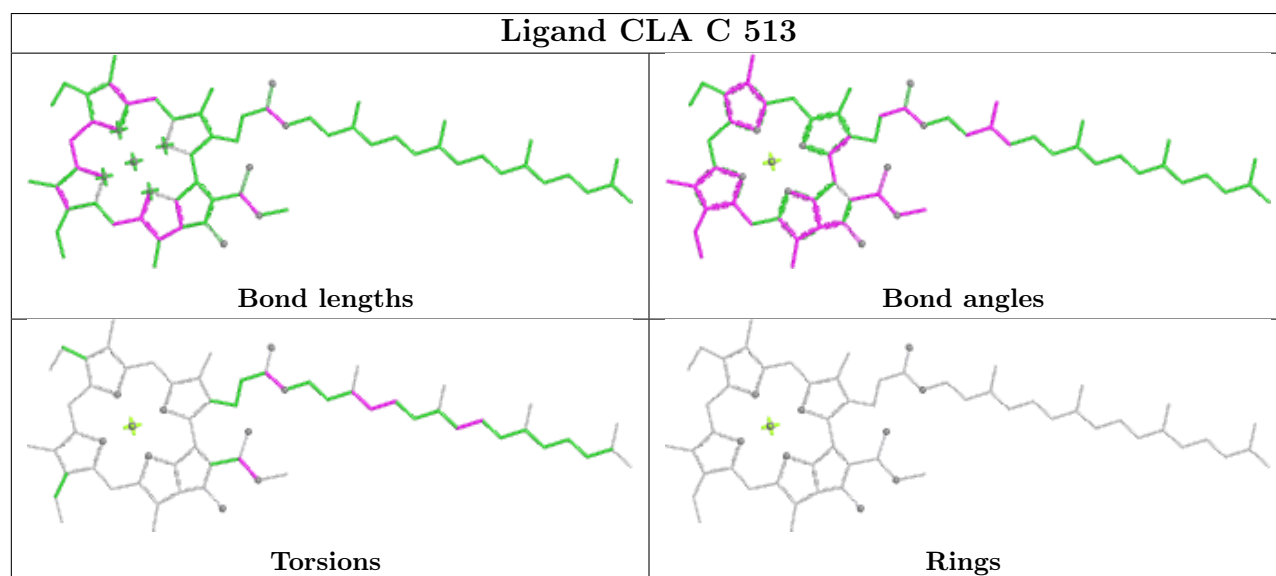
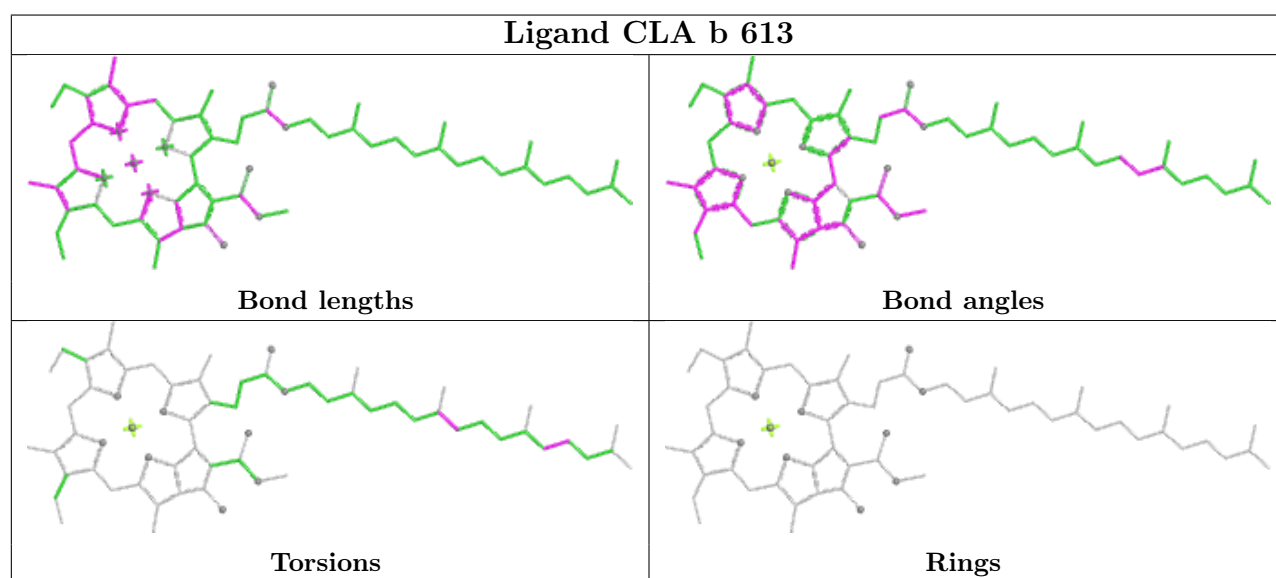
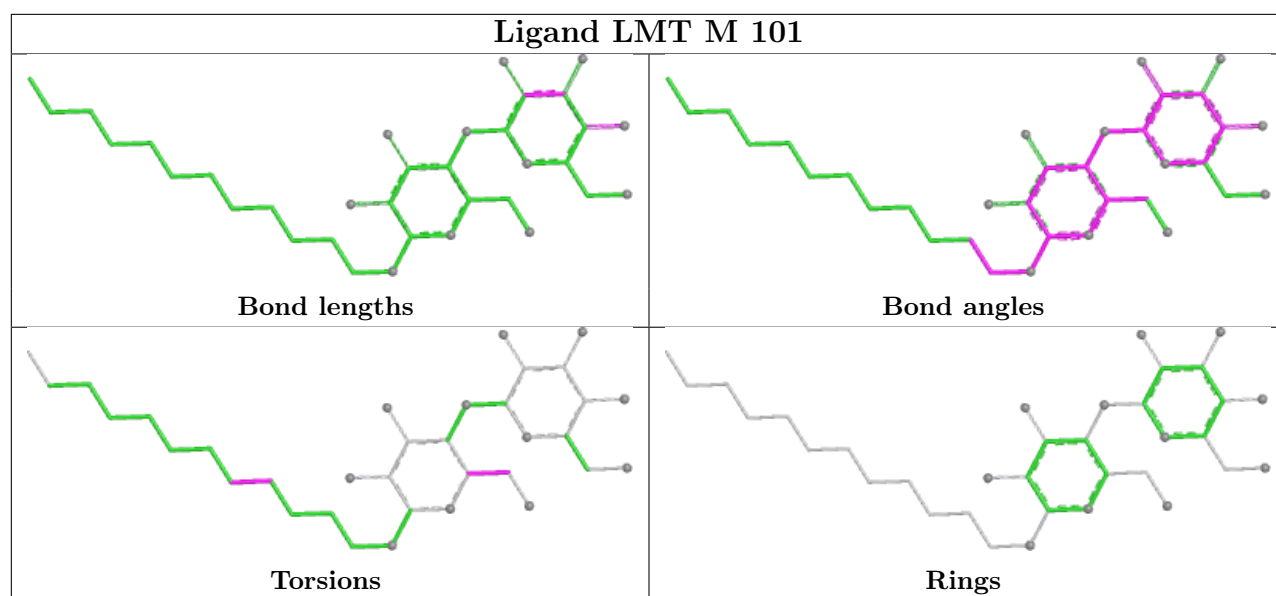
Ligand HTG V 204

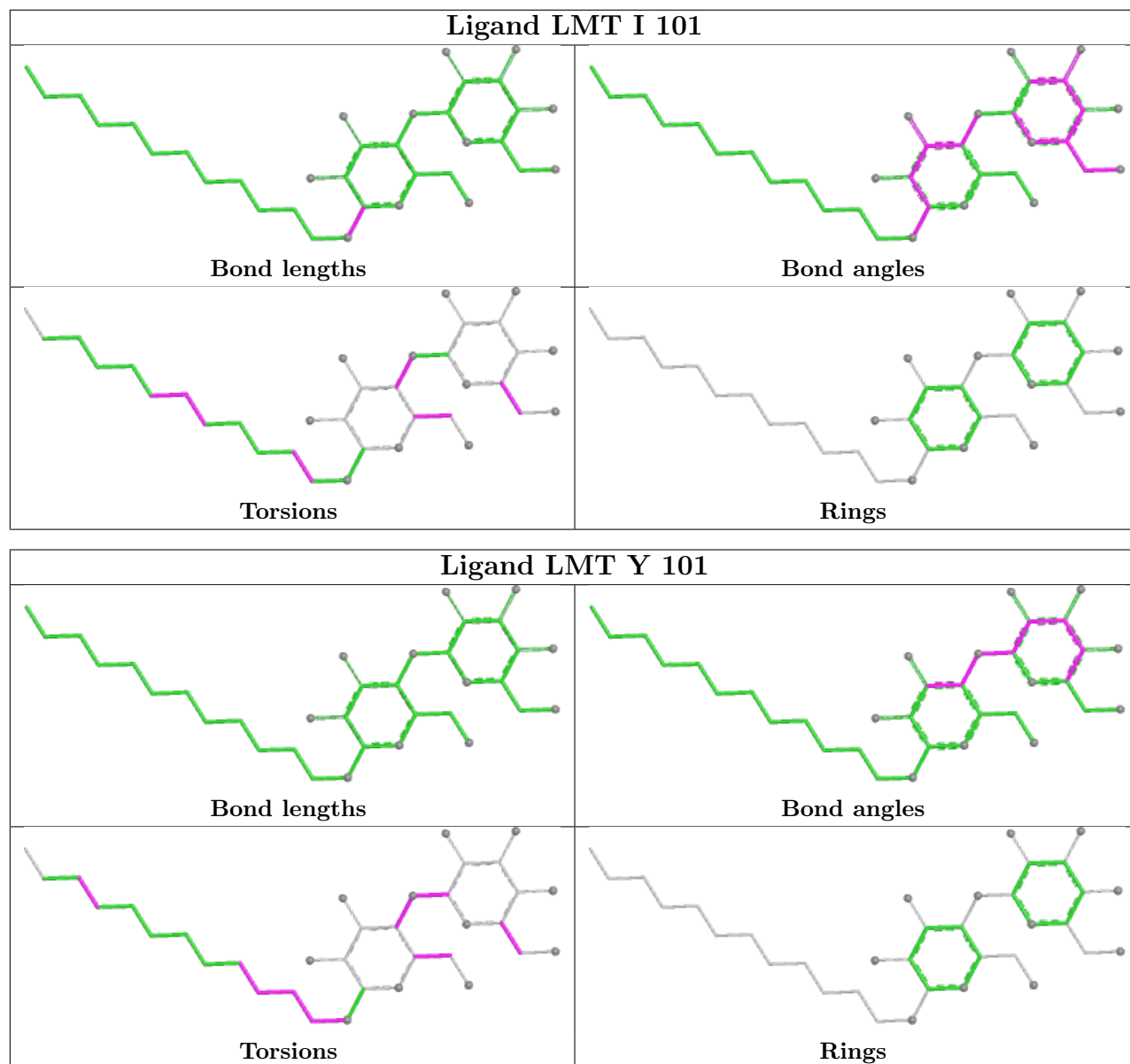


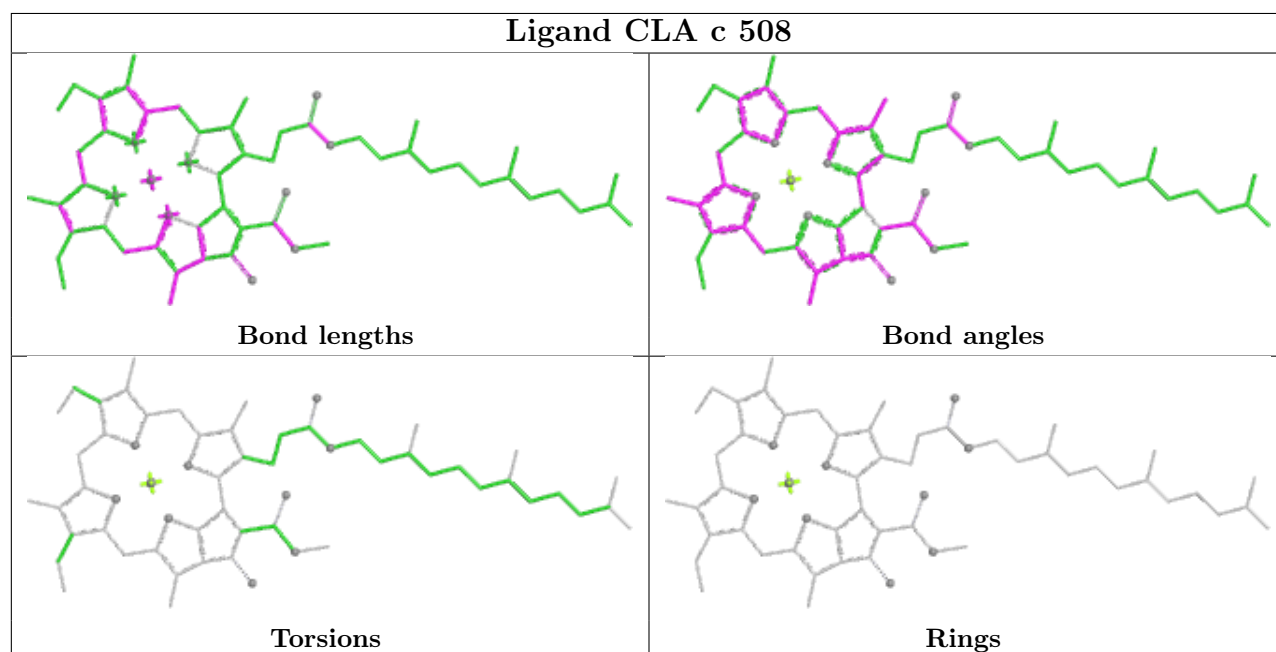
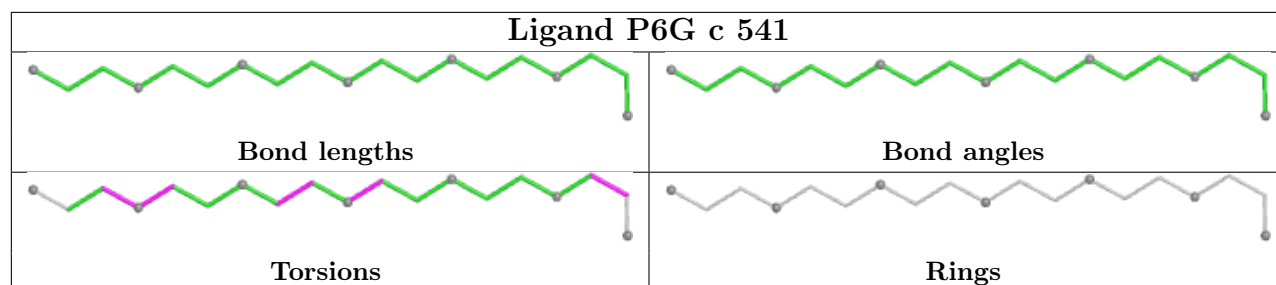
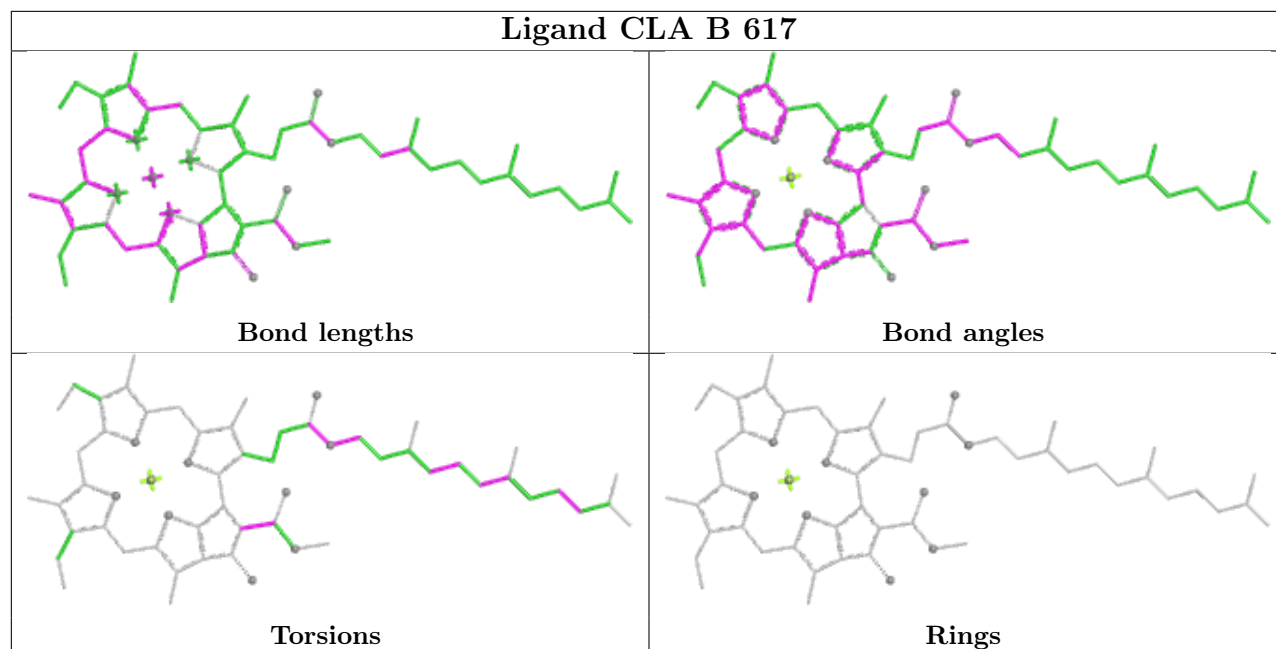
Ligand HTG b 632

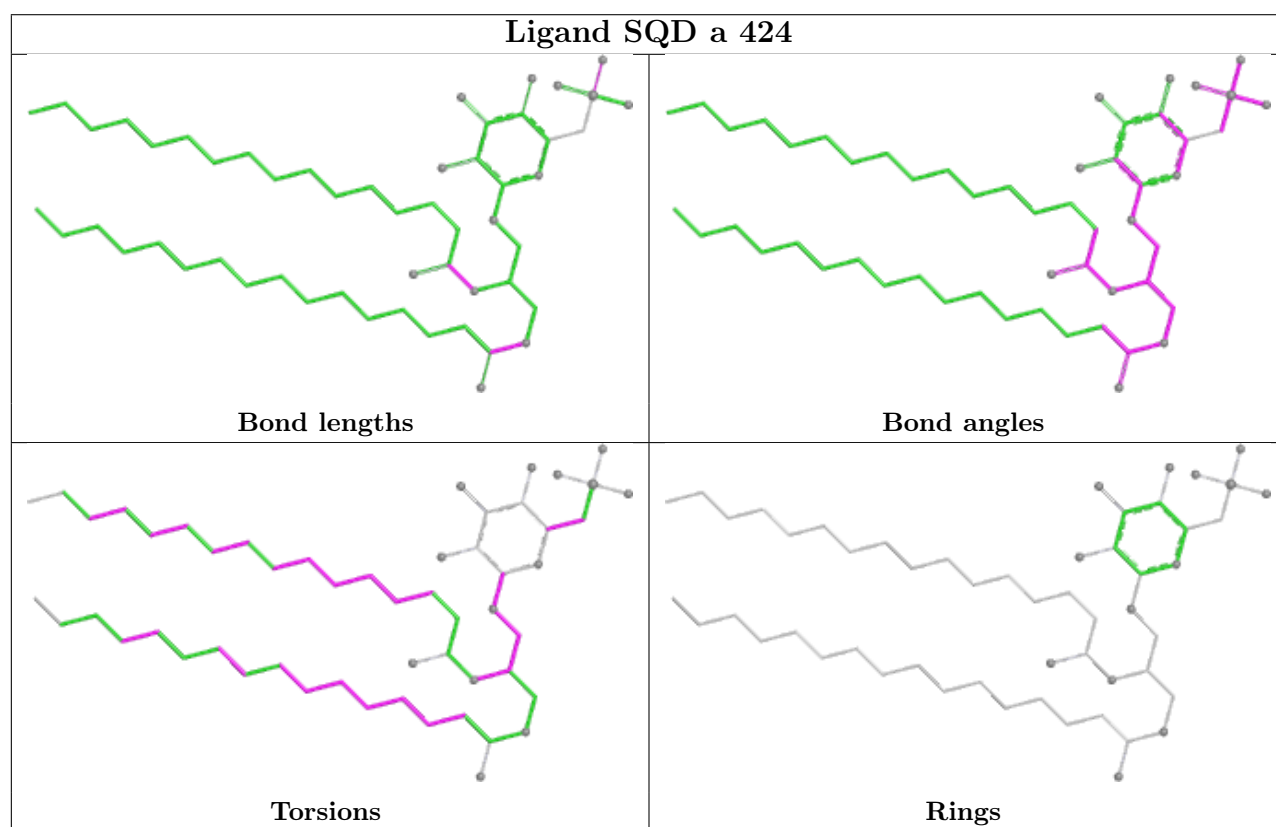
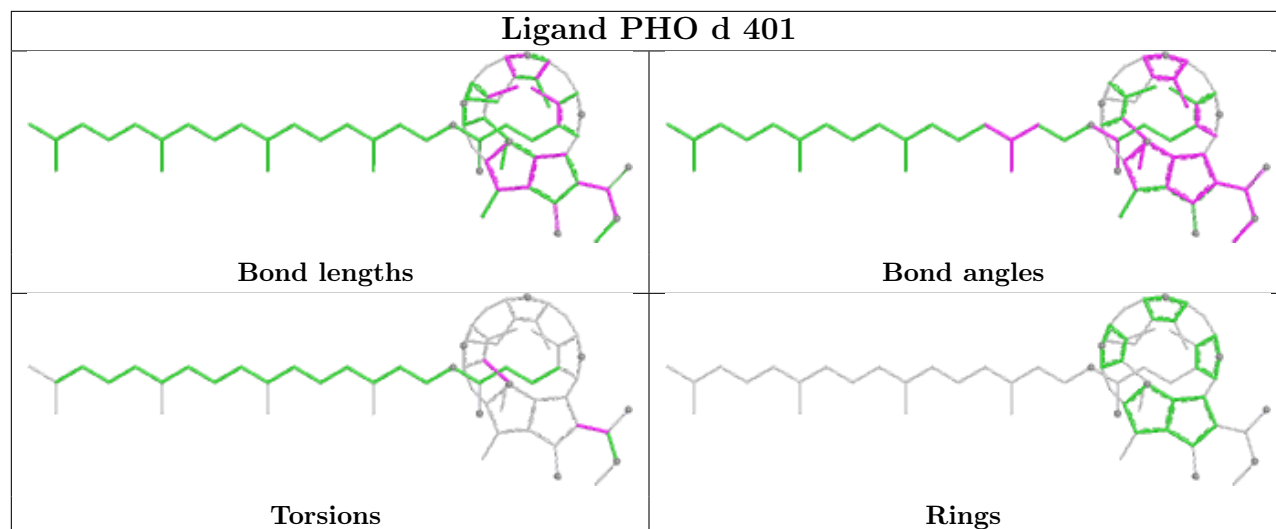


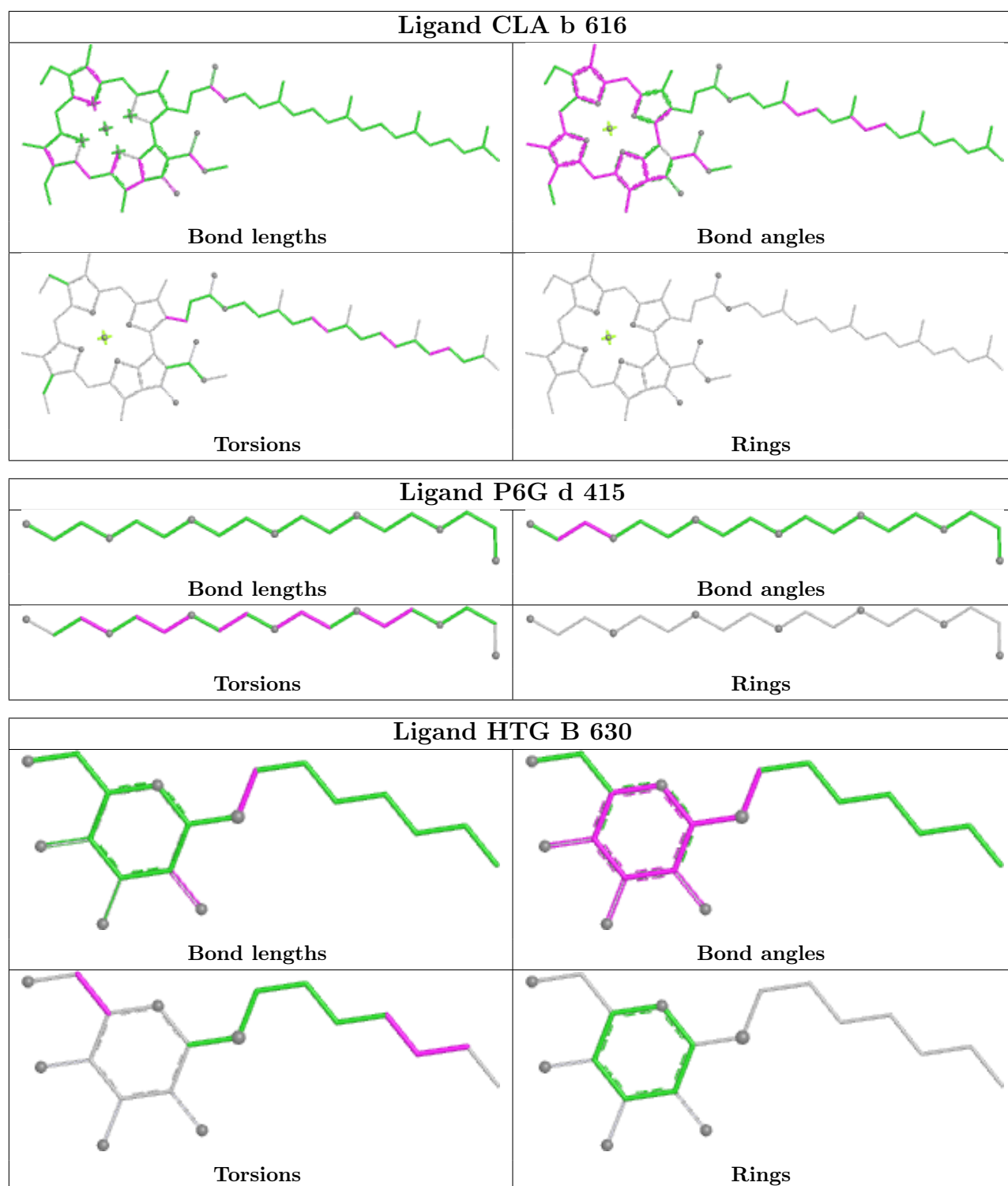


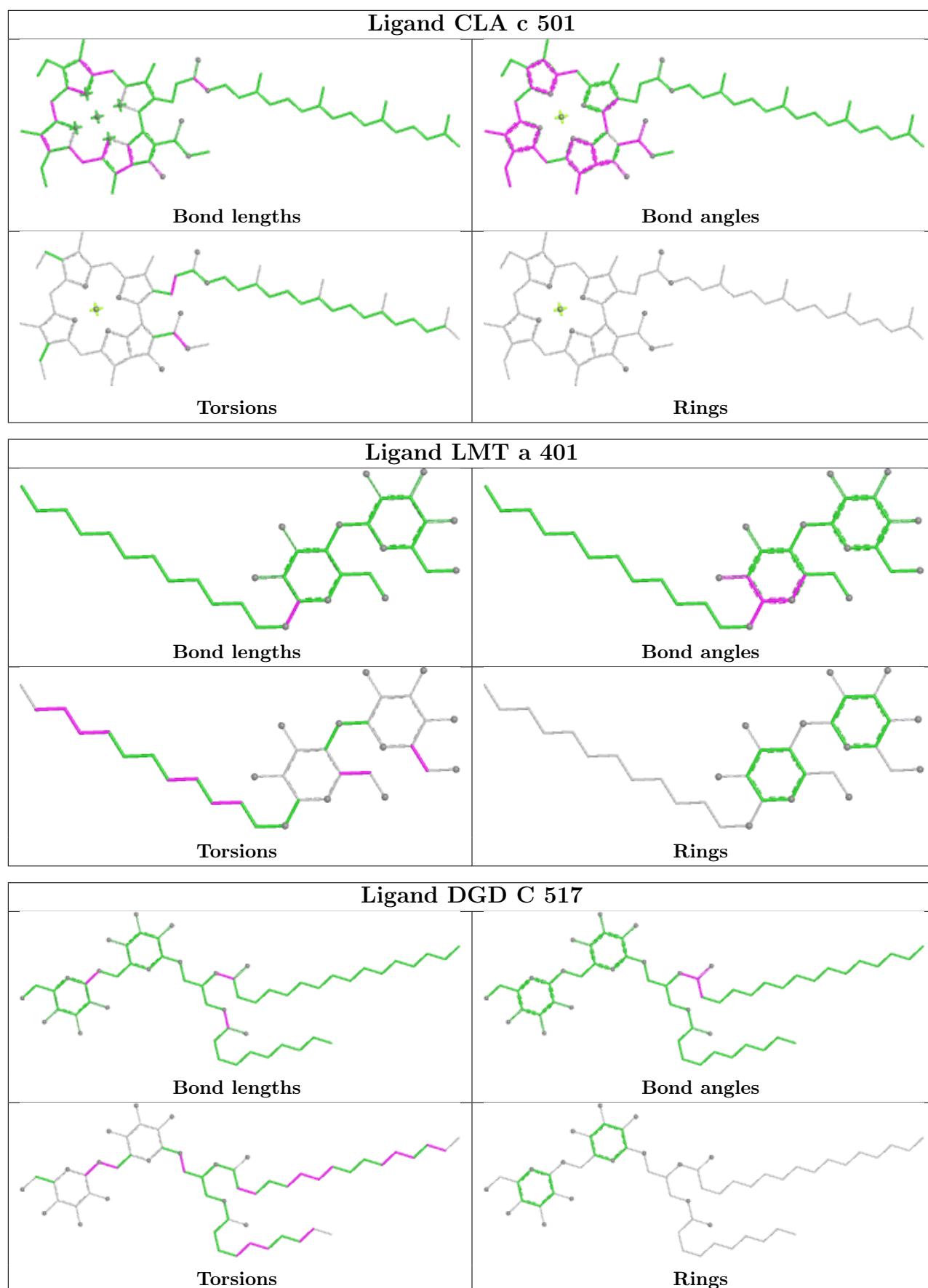


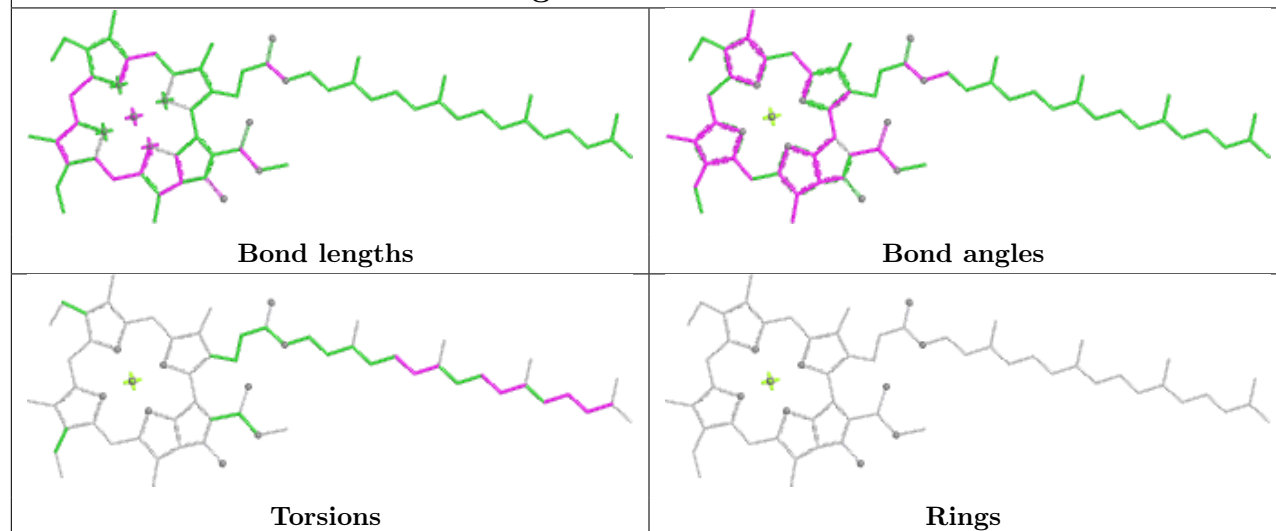
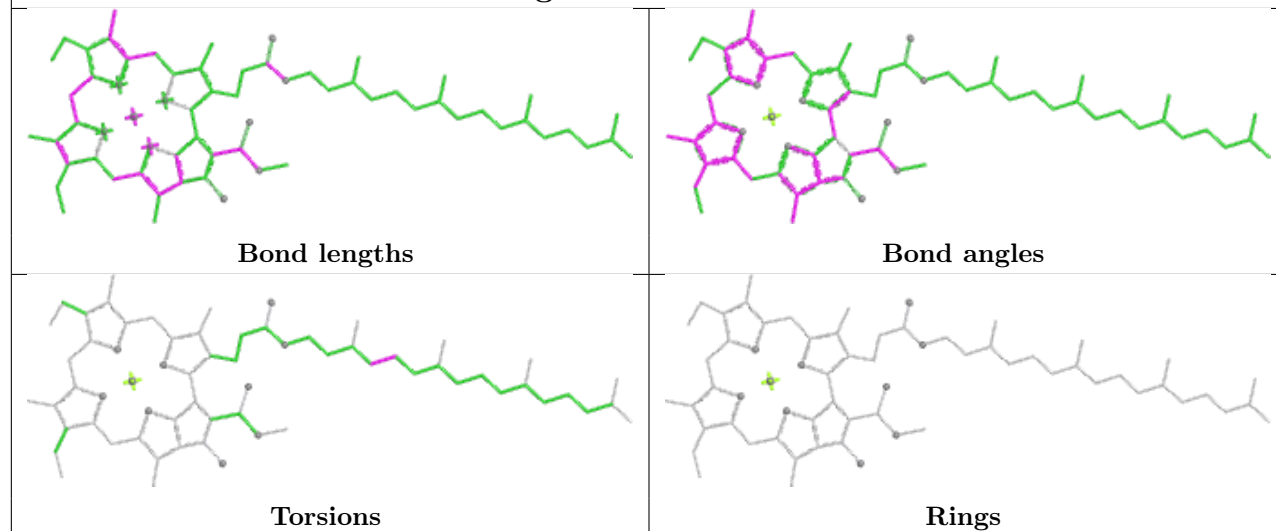


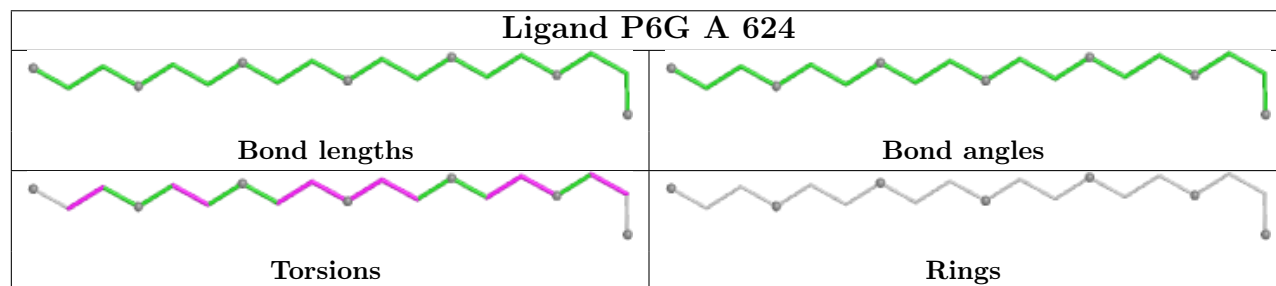
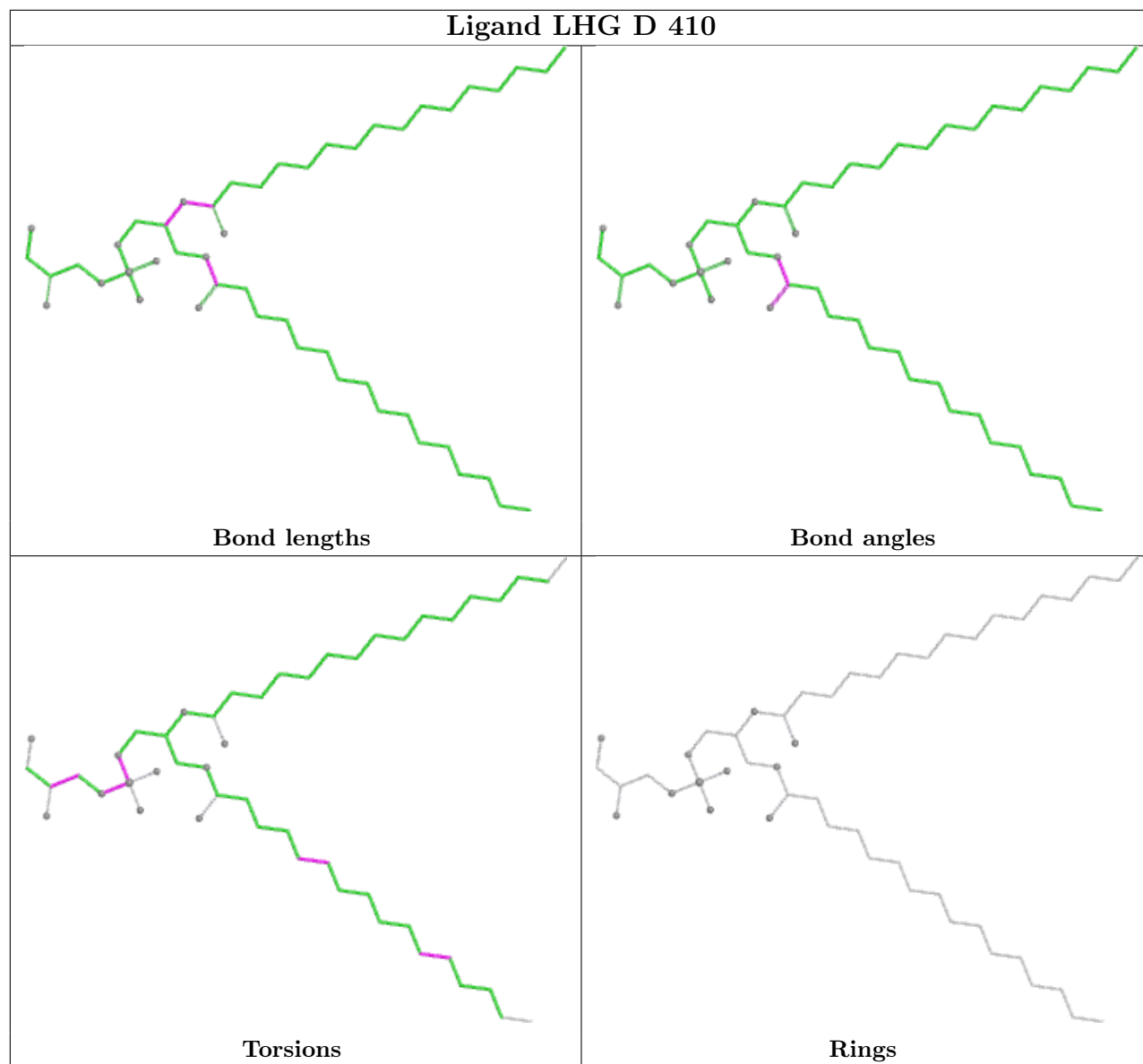


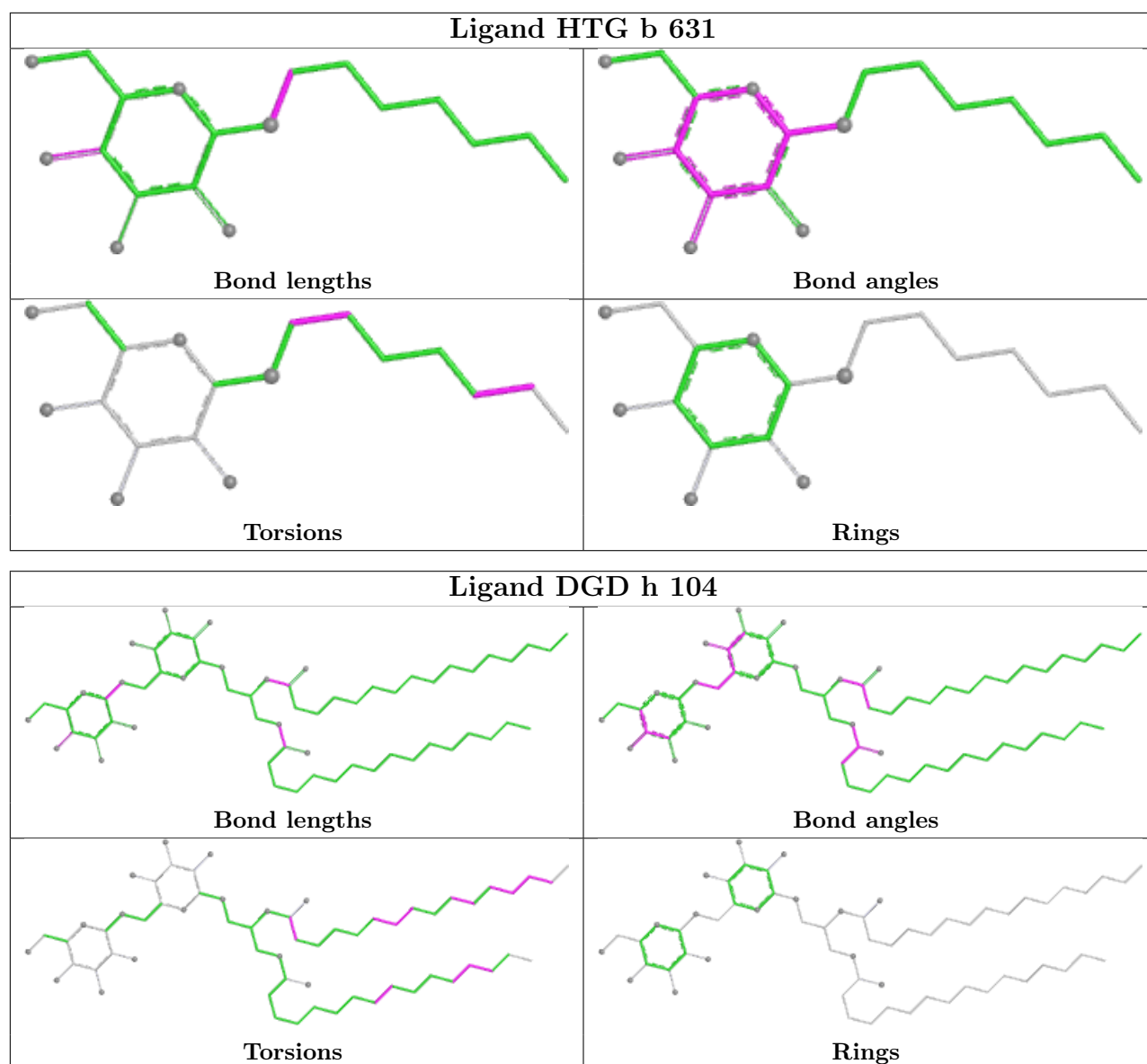






Ligand CLA C 506**Ligand CLA b 608**





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%)	-0.89	0 100 100	15, 22, 46, 78	4 (1%)
1	a	334/344 (97%)	-0.86	0 100 100	16, 24, 52, 89	4 (1%)
2	B	504/506 (99%)	-0.83	1 (0%) 91 92	14, 26, 57, 92	11 (2%)
2	b	506/506 (100%)	-0.75	2 (0%) 88 90	14, 29, 71, 129	10 (1%)
3	C	451/458 (98%)	-0.82	0 100 100	19, 31, 46, 87	5 (1%)
3	c	458/458 (100%)	-0.76	2 (0%) 88 90	20, 35, 50, 108	4 (0%)
4	D	341/342 (99%)	-0.96	0 100 100	16, 23, 40, 114	1 (0%)
4	d	341/342 (99%)	-0.90	0 100 100	17, 26, 44, 110	2 (0%)
5	E	81/83 (97%)	-0.57	0 100 100	19, 40, 66, 92	3 (3%)
5	e	81/83 (97%)	-0.45	0 100 100	22, 45, 75, 118	2 (2%)
6	F	34/44 (77%)	-0.68	0 100 100	26, 33, 63, 82	0
6	f	32/44 (72%)	-0.54	0 100 100	30, 38, 78, 117	0
7	H	65/65 (100%)	-0.72	1 (1%) 72 75	19, 33, 47, 123	2 (3%)
7	h	65/65 (100%)	-0.55	2 (3%) 51 55	26, 38, 56, 116	1 (1%)
8	I	37/38 (97%)	-0.72	0 100 100	28, 35, 75, 91	0
8	i	37/38 (97%)	-0.70	0 100 100	27, 34, 67, 89	0
9	J	39/40 (97%)	-0.42	0 100 100	20, 36, 108, 130	2 (5%)
9	j	39/40 (97%)	-0.43	0 100 100	29, 43, 75, 89	0
10	K	37/37 (100%)	-0.63	0 100 100	31, 37, 56, 70	0
10	k	37/37 (100%)	-0.59	0 100 100	36, 44, 64, 75	0
11	L	37/37 (100%)	-0.89	0 100 100	11, 21, 70, 92	1 (2%)
11	l	37/37 (100%)	-0.81	0 100 100	13, 22, 70, 95	2 (5%)
12	M	33/36 (91%)	-0.86	0 100 100	11, 22, 44, 88	2 (6%)
12	m	34/36 (94%)	-0.79	0 100 100	12, 24, 75, 98	1 (2%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	245/245 (100%)	-0.70	1 (0%) 88 90	18, 32, 69, 128	6 (2%)
13	o	245/245 (100%)	-0.68	1 (0%) 88 90	18, 34, 84, 136	5 (2%)
14	T	29/32 (90%)	-0.93	0 100 100	18, 22, 47, 101	1 (3%)
14	t	29/32 (90%)	-0.77	0 100 100	19, 22, 44, 81	1 (3%)
15	U	97/104 (93%)	-0.82	0 100 100	21, 31, 58, 95	2 (2%)
15	u	97/104 (93%)	-0.85	0 100 100	24, 31, 47, 84	0
16	V	137/137 (100%)	-0.85	0 100 100	16, 29, 46, 66	2 (1%)
16	v	137/137 (100%)	-0.74	0 100 100	20, 38, 58, 73	1 (0%)
17	Y	29/30 (96%)	-0.02	1 (3%) 48 51	36, 47, 76, 109	1 (3%)
17	y	29/30 (96%)	-0.10	0 100 100	40, 56, 81, 92	1 (3%)
18	X	40/41 (97%)	-0.39	0 100 100	23, 40, 100, 118	1 (2%)
18	x	40/41 (97%)	-0.24	0 100 100	36, 43, 112, 132	0
19	Z	62/62 (100%)	-0.38	0 100 100	37, 47, 86, 94	0
19	z	62/62 (100%)	0.14	2 (3%) 50 54	50, 62, 101, 117	0
All	All	5272/5362 (98%)	-0.76	13 (0%) 91 92	11, 30, 65, 136	78 (1%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	z	62	VAL	3.5
7	h	65	LEU	3.2
7	h	66	GLY	2.9
3	c	17	ALA	2.4
19	z	3	ILE	2.4

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
4	MHS	D	336	11/12	0.97	0.05	23,28,37,38	0
8	FME	I	1	10/11	0.98	0.06	26,32,40,44	0
12	FME	M	1	10/11	0.98	0.05	27,32,64,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	FME	T	1[A]	10/11	0.98	0.05	21,25,47,47	7
14	FME	T	1[B]	10/11	0.98	0.05	21,25,32,35	7
12	FME	m	1[A]	10/11	0.98	0.07	24,30,61,84	7
12	FME	m	1[B]	10/11	0.98	0.07	30,33,55,66	7
14	FME	t	1[A]	10/11	0.98	0.04	20,24,39,42	7
14	FME	t	1[B]	10/11	0.98	0.04	20,24,31,36	7
4	MHS	d	336	11/12	0.99	0.05	27,32,44,44	0
8	FME	i	1	10/11	0.99	0.04	30,33,36,37	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
39	1PE	B	653	16/16	0.70	0.12	103,121,137,148	0
38	HTG	C	530	19/19	0.71	0.10	98,124,143,150	0
34	PGE	f	105	10/10	0.73	0.10	91,98,114,127	0
34	PGE	D	415	10/10	0.75	0.11	86,105,110,122	0
34	PGE	o	307	10/10	0.75	0.11	90,112,130,142	0
34	PGE	c	536	10/10	0.76	0.13	87,105,124,125	0
31	LMT	C	533	35/35	0.77	0.11	72,121,170,191	0
34	PGE	E	108	10/10	0.78	0.15	52,65,68,73	10
34	PGE	E	105	10/10	0.78	0.12	90,96,116,118	0
36	EDO	B	656	4/4	0.80	0.22	78,87,100,107	0
36	EDO	c	542	4/4	0.80	0.15	88,91,102,107	0
34	PGE	H	110	10/10	0.80	0.08	91,103,116,118	0
33	PG4	B	643	13/13	0.80	0.10	75,92,114,118	0
34	PGE	V	215	10/10	0.81	0.12	66,90,103,111	0
38	HTG	C	529	19/19	0.81	0.11	70,102,136,144	0
28	SQD	h	105	54/54	0.81	0.11	76,100,195,214	0
38	HTG	a	418	19/19	0.81	0.12	53,84,123,124	0
34	PGE	c	540	10/10	0.81	0.10	82,92,110,113	0
39	1PE	V	217	16/16	0.81	0.12	63,93,120,133	0
36	EDO	V	218	4/4	0.82	0.12	87,88,88,96	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	PGE	J	107	10/10	0.82	0.09	87,137,168,170	0
34	PGE	O	310	10/10	0.82	0.12	58,81,122,137	0
31	LMT	j	103	35/35	0.82	0.09	68,114,162,168	0
35	P6G	C	541	19/19	0.82	0.11	79,103,127,142	0
30	GOL	O	307	6/6	0.82	0.10	116,117,120,123	0
36	EDO	H	112	4/4	0.82	0.13	70,85,94,95	0
30	GOL	v	205	6/6	0.83	0.13	102,122,135,152	0
34	PGE	b	646	10/10	0.83	0.10	70,102,120,121	0
38	HTG	C	531	19/19	0.83	0.10	72,109,139,142	0
34	PGE	h	109	10/10	0.83	0.10	84,97,111,113	0
34	PGE	o	306	10/10	0.83	0.11	70,92,102,103	0
30	GOL	C	527	6/6	0.83	0.10	96,108,112,135	0
31	LMT	u	203	35/35	0.84	0.13	42,77,115,137	0
35	P6G	D	418	19/19	0.84	0.10	68,99,126,131	0
34	PGE	E	107	10/10	0.84	0.11	73,106,142,143	0
39	1PE	x	104	16/16	0.84	0.11	85,105,130,136	0
44	2PE	V	216	28/28	0.84	0.11	44,91,110,123	0
33	PG4	e	103	13/13	0.85	0.08	72,107,125,136	0
34	PGE	J	106	10/10	0.85	0.09	85,121,129,138	0
34	PGE	B	650	10/10	0.85	0.10	88,109,126,128	0
34	PGE	O	309	10/10	0.85	0.12	62,86,111,111	0
31	LMT	Y	101	35/35	0.85	0.09	61,118,170,188	0
33	PG4	C	534	13/13	0.85	0.10	81,103,119,119	0
34	PGE	b	645	10/10	0.85	0.09	106,110,126,134	0
35	P6G	E	110	19/19	0.85	0.11	49,95,111,122	0
39	1PE	j	107	16/16	0.85	0.09	74,106,155,159	0
33	PG4	E	102	13/13	0.85	0.12	62,81,106,120	0
33	PG4	H	104	13/13	0.85	0.10	83,98,117,119	0
34	PGE	b	647	10/10	0.86	0.08	77,97,109,109	0
33	PG4	c	535	13/13	0.86	0.10	69,89,109,115	0
33	PG4	B	640	13/13	0.86	0.09	66,86,95,99	0
33	PG4	e	104	13/13	0.86	0.10	78,94,120,120	0
33	PG4	B	642	13/13	0.86	0.11	66,86,115,120	0
34	PGE	C	540	10/10	0.86	0.09	74,83,102,111	0
28	SQD	A	622	54/54	0.86	0.11	63,85,136,187	0
34	PGE	V	214	10/10	0.86	0.12	50,86,96,98	0
33	PG4	V	212	13/13	0.86	0.12	82,96,120,123	0
34	PGE	E	106	10/10	0.86	0.10	85,95,111,116	0
35	P6G	c	541	19/19	0.86	0.11	43,61,68,72	19
40	DGD	d	408	66/66	0.86	0.10	57,89,155,184	0
33	PG4	b	634	13/13	0.86	0.10	78,90,111,123	0
33	PG4	C	538	13/13	0.87	0.10	65,93,115,123	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	PGE	h	108	10/10	0.87	0.10	70,75,101,105	0
33	PG4	b	637	13/13	0.87	0.10	74,97,124,130	0
34	PGE	b	639	10/10	0.87	0.09	79,97,111,119	0
34	PGE	b	644	10/10	0.87	0.09	83,100,113,125	0
34	PGE	H	111	10/10	0.87	0.08	82,100,121,127	0
38	HTG	c	530	19/19	0.87	0.11	66,104,128,145	0
33	PG4	c	534	13/13	0.87	0.13	69,85,99,112	0
33	PG4	H	107	13/13	0.87	0.09	68,83,105,110	0
35	P6G	b	649	19/19	0.87	0.09	71,103,125,128	0
33	PG4	V	211	13/13	0.87	0.12	54,89,114,120	0
34	PGE	c	539	10/10	0.87	0.10	80,90,104,104	0
31	LMT	F	102	35/35	0.87	0.10	43,81,105,126	0
33	PG4	V	213	13/13	0.88	0.09	68,80,103,112	0
33	PG4	X	102	13/13	0.88	0.11	77,95,113,114	0
33	PG4	X	103	13/13	0.88	0.09	78,99,111,115	0
36	EDO	o	311	4/4	0.88	0.09	81,83,83,86	0
33	PG4	a	420	13/13	0.88	0.08	79,94,105,106	0
34	PGE	i	106	10/10	0.88	0.08	78,95,100,103	0
34	PGE	j	105	10/10	0.88	0.10	73,109,124,125	0
33	PG4	D	414	13/13	0.88	0.12	86,95,105,110	0
38	HTG	c	523	19/19	0.88	0.09	65,86,104,106	0
34	PGE	b	640	10/10	0.88	0.08	61,88,103,118	0
38	HTG	c	531	19/19	0.88	0.09	59,99,122,124	0
38	HTG	h	101	19/19	0.88	0.10	62,86,123,141	0
31	LMT	m	101	35/35	0.88	0.10	45,62,75,92	0
31	LMT	c	521	35/35	0.88	0.10	54,77,95,101	0
33	PG4	A	619	13/13	0.88	0.09	83,96,112,112	0
33	PG4	C	535	13/13	0.88	0.13	66,74,108,121	0
40	DGD	D	408	66/66	0.88	0.10	56,88,142,175	0
30	GOL	y	101	6/6	0.88	0.08	82,90,98,101	0
34	PGE	B	646	10/10	0.88	0.09	83,95,114,119	0
34	PGE	H	109	10/10	0.89	0.08	84,95,102,105	0
36	EDO	B	658	4/4	0.89	0.07	82,84,89,110	0
36	EDO	E	111	4/4	0.89	0.10	66,83,90,97	0
33	PG4	J	105	13/13	0.89	0.10	75,88,110,115	0
34	PGE	c	537	10/10	0.89	0.09	96,106,120,123	0
33	PG4	d	414	13/13	0.89	0.09	65,79,85,87	0
34	PGE	I	105	10/10	0.89	0.12	60,83,95,99	0
38	HTG	C	522	19/19	0.89	0.09	50,83,100,110	0
28	SQD	a	424	54/54	0.89	0.10	63,83,134,198	0
30	GOL	e	102	6/6	0.89	0.10	79,91,112,117	0
30	GOL	o	303	6/6	0.89	0.10	79,96,110,126	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
38	HTG	H	101	19/19	0.89	0.09	50,94,122,122	0
34	PGE	h	110	10/10	0.89	0.09	71,99,111,117	0
33	PG4	E	103	13/13	0.89	0.07	59,76,89,105	0
32	LHG	e	101	42/49	0.89	0.10	60,105,123,171	0
33	PG4	H	105	13/13	0.89	0.11	72,87,126,147	0
34	PGE	a	423	10/10	0.89	0.08	78,91,107,107	0
34	PGE	t	104	10/10	0.89	0.07	60,79,99,100	0
39	1PE	B	654	16/16	0.89	0.09	46,68,92,105	0
31	LMT	f	101	35/35	0.89	0.09	54,85,110,119	0
39	1PE	e	105	16/16	0.89	0.09	77,93,116,121	0
33	PG4	I	103	13/13	0.89	0.09	73,97,121,129	0
33	PG4	c	533	13/13	0.89	0.10	77,90,105,109	0
33	PG4	J	104	13/13	0.89	0.10	74,82,107,108	0
34	PGE	H	108	10/10	0.89	0.10	66,86,129,136	0
35	P6G	j	106	19/19	0.89	0.09	50,74,98,112	0
33	PG4	B	641	13/13	0.90	0.09	74,97,107,115	0
32	LHG	A	618	42/49	0.90	0.09	49,90,145,167	0
34	PGE	x	103	10/10	0.90	0.09	81,98,110,112	0
32	LHG	a	419	41/49	0.90	0.11	52,85,176,193	0
33	PG4	x	102	13/13	0.90	0.09	79,95,107,108	0
34	PGE	A	621	10/10	0.90	0.08	66,116,120,129	0
33	PG4	H	106	13/13	0.90	0.12	38,53,67,74	13
30	GOL	f	104	6/6	0.90	0.07	94,115,135,150	0
34	PGE	J	108	10/10	0.90	0.07	80,98,116,120	0
30	GOL	T	103	6/6	0.90	0.11	62,79,91,111	0
36	EDO	B	657	4/4	0.90	0.10	93,95,100,102	0
33	PG4	b	635	13/13	0.90	0.08	58,76,103,109	0
36	EDO	D	419	4/4	0.90	0.14	66,70,78,97	0
33	PG4	B	637	13/13	0.90	0.10	68,82,106,106	0
33	PG4	B	638	13/13	0.90	0.10	66,84,114,130	0
33	PG4	V	209	13/13	0.90	0.11	51,84,95,101	0
29	LMG	d	412	55/55	0.90	0.11	47,77,119,137	0
34	PGE	E	109	10/10	0.90	0.10	51,93,103,106	0
38	HTG	B	624	19/19	0.90	0.08	47,103,125,143	0
33	PG4	i	101	13/13	0.91	0.08	71,84,95,98	0
33	PG4	j	104	13/13	0.91	0.09	78,97,113,116	0
31	LMT	J	103	35/35	0.91	0.08	47,78,115,134	0
29	LMG	c	520	51/55	0.91	0.08	47,76,100,124	0
36	EDO	a	425	4/4	0.91	0.07	74,78,96,120	0
34	PGE	B	645	10/10	0.91	0.09	68,81,89,93	0
33	PG4	a	421	13/13	0.91	0.07	76,89,99,102	0
34	PGE	i	105	10/10	0.91	0.09	70,81,89,92	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	PGE	B	649	10/10	0.91	0.09	66,82,101,105	0
28	SQD	F	104	54/54	0.91	0.11	55,80,110,135	0
33	PG4	C	536	13/13	0.91	0.11	66,72,93,103	0
34	PGE	a	422	10/10	0.91	0.09	72,75,85,92	0
34	PGE	o	308	10/10	0.91	0.10	48,87,100,104	0
34	PGE	o	309	10/10	0.91	0.08	53,78,92,97	0
38	HTG	b	624	19/19	0.91	0.09	54,91,117,133	0
33	PG4	b	636	13/13	0.91	0.08	71,79,90,93	0
27	PL9	a	412	55/55	0.91	0.09	46,69,101,108	0
35	P6G	B	652	19/19	0.91	0.09	42,84,105,109	0
33	PG4	c	532	13/13	0.91	0.09	70,78,98,101	0
34	PGE	b	641	10/10	0.91	0.07	99,104,114,125	0
33	PG4	K	102	13/13	0.91	0.09	56,70,102,109	0
39	1PE	L	101	16/16	0.91	0.09	56,72,99,100	0
35	P6G	I	106	19/19	0.91	0.09	56,81,119,121	0
27	PL9	A	611	55/55	0.91	0.10	39,63,96,107	0
33	PG4	B	639	13/13	0.91	0.09	64,79,104,115	0
29	LMG	C	526	55/55	0.91	0.10	47,83,115,124	0
30	GOL	b	626	6/6	0.91	0.09	42,46,50,54	0
30	GOL	c	529	6/6	0.91	0.20	27,31,39,40	6
34	PGE	c	538	10/10	0.91	0.11	68,102,115,129	0
45	PE8	i	107	25/25	0.91	0.11	44,66,104,122	0
33	PG4	X	101	13/13	0.92	0.09	63,89,105,108	0
30	GOL	u	201	6/6	0.92	0.08	43,70,71,77	0
34	PGE	b	643	10/10	0.92	0.10	70,85,103,116	0
33	PG4	h	106	13/13	0.92	0.07	67,76,106,108	0
38	HTG	B	631	19/19	0.92	0.08	46,90,129,147	0
28	SQD	x	101	54/54	0.92	0.09	62,84,132,147	0
35	P6G	A	624	19/19	0.92	0.08	70,85,105,113	0
33	PG4	i	102	13/13	0.92	0.07	65,71,81,82	0
29	LMG	z	101	55/55	0.92	0.10	49,95,120,160	0
38	HTG	C	532	19/19	0.92	0.08	57,85,128,156	0
32	LHG	E	101	42/49	0.92	0.10	54,80,100,127	0
30	GOL	B	633	6/6	0.92	0.09	69,71,84,97	0
34	PGE	B	644	10/10	0.92	0.10	58,71,117,137	0
38	HTG	b	632	19/19	0.92	0.09	49,79,119,135	0
35	P6G	b	648	19/19	0.92	0.09	59,66,80,84	0
30	GOL	B	635	6/6	0.92	0.08	46,67,79,83	0
30	GOL	d	413	6/6	0.92	0.08	74,88,114,116	0
35	P6G	d	415	19/19	0.92	0.09	51,64,88,97	0
34	PGE	O	308	10/10	0.92	0.11	31,62,83,96	0
36	EDO	A	625	4/4	0.92	0.08	70,71,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	PGE	B	648	10/10	0.92	0.10	55,75,82,93	0
33	PG4	U	202	13/13	0.92	0.09	52,80,100,102	0
29	LMG	B	634	55/55	0.92	0.10	39,69,141,167	0
36	EDO	C	542	4/4	0.92	0.07	77,84,88,96	0
33	PG4	V	210	13/13	0.92	0.09	53,84,115,120	0
30	GOL	D	413	6/6	0.92	0.09	58,67,76,84	0
30	GOL	m	103	6/6	0.92	0.09	47,69,88,116	0
36	EDO	J	109	4/4	0.92	0.10	78,79,85,96	0
30	GOL	O	305	6/6	0.92	0.08	55,65,71,77	0
28	SQD	l	102	54/54	0.93	0.08	46,71,104,172	0
34	PGE	B	647	10/10	0.93	0.07	78,92,122,122	0
30	GOL	v	207	6/6	0.93	0.08	63,73,86,86	0
30	GOL	c	528	6/6	0.93	0.09	78,79,88,89	0
31	LMT	B	622	35/35	0.93	0.08	46,73,107,123	0
30	GOL	D	412	6/6	0.93	0.07	55,80,95,102	0
33	PG4	B	636	13/13	0.93	0.08	71,98,116,121	0
33	PG4	I	102	13/13	0.93	0.07	62,73,97,112	0
30	GOL	B	626	6/6	0.93	0.10	34,41,49,61	0
33	PG4	I	104	13/13	0.93	0.08	65,73,90,93	0
31	LMT	I	101	35/35	0.93	0.09	57,83,111,113	0
30	GOL	O	304	6/6	0.93	0.07	60,69,79,88	0
31	LMT	M	101	35/35	0.93	0.07	34,51,70,73	0
31	LMT	M	102	35/35	0.93	0.07	43,59,82,96	0
38	HTG	c	522	19/19	0.93	0.08	60,74,96,106	0
35	P6G	d	416	19/19	0.93	0.09	43,61,100,111	0
28	SQD	b	633	54/54	0.93	0.08	46,66,104,116	0
31	LMT	b	622	35/35	0.93	0.07	49,76,124,132	0
36	EDO	B	655	4/4	0.93	0.09	45,50,57,88	0
28	SQD	a	417	54/54	0.93	0.08	40,64,93,101	0
33	PG4	i	103	13/13	0.93	0.07	74,85,98,105	0
30	GOL	C	523	6/6	0.93	0.16	35,46,56,62	0
30	GOL	a	416	6/6	0.93	0.08	39,57,72,77	0
34	PGE	A	620	7/10	0.93	0.07	68,77,83,87	0
33	PG4	C	537	13/13	0.93	0.08	67,76,92,108	0
36	EDO	E	112	4/4	0.93	0.11	84,94,96,100	0
30	GOL	u	202	6/6	0.93	0.09	50,56,61,63	0
34	PGE	T	104	7/10	0.93	0.09	76,77,96,103	0
30	GOL	v	203	6/6	0.93	0.10	66,79,82,98	0
36	EDO	X	104	4/4	0.93	0.08	73,80,83,88	0
38	HTG	V	204	19/19	0.94	0.08	36,52,89,102	0
31	LMT	a	401	35/35	0.94	0.07	37,52,75,83	0
35	P6G	T	105	19/19	0.94	0.09	42,59,85,88	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	EDO	I	107	4/4	0.94	0.07	84,89,91,96	0
30	GOL	O	302	6/6	0.94	0.06	51,55,67,70	0
28	SQD	A	616	54/54	0.94	0.07	39,65,102,107	0
30	GOL	C	528	6/6	0.94	0.19	24,27,36,38	6
34	PGE	C	539	10/10	0.94	0.10	56,73,94,96	0
34	PGE	Y	102	10/10	0.94	0.08	61,84,103,104	0
36	EDO	i	108	4/4	0.94	0.08	70,71,76,87	0
30	GOL	v	206	6/6	0.94	0.07	50,54,66,75	0
29	LMG	a	414	51/55	0.94	0.07	42,64,80,90	0
34	PGE	E	104	10/10	0.94	0.07	67,76,99,106	0
38	HTG	C	521	19/19	0.94	0.08	53,65,84,85	0
31	LMT	t	103	35/35	0.94	0.08	32,75,110,117	0
35	P6G	B	651	19/19	0.94	0.07	49,63,77,81	0
34	PGE	h	107	10/10	0.94	0.07	67,78,92,95	0
30	GOL	o	304	6/6	0.94	0.07	45,53,55,62	0
34	PGE	b	642	10/10	0.94	0.07	51,65,87,92	0
29	LMG	C	520	51/55	0.94	0.08	38,79,108,121	0
35	P6G	D	416	19/19	0.95	0.07	38,60,84,87	0
34	PGE	b	638	10/10	0.95	0.07	55,77,90,93	0
31	LMT	A	617	35/35	0.95	0.08	37,55,92,105	0
30	GOL	t	101	6/6	0.95	0.10	44,49,56,62	0
33	PG4	i	104	13/13	0.95	0.07	56,71,90,91	0
24	CLA	b	602	65/65	0.95	0.07	28,47,99,111	0
30	GOL	U	201	6/6	0.95	0.08	40,67,78,98	0
34	PGE	t	105	7/10	0.95	0.06	58,79,84,87	0
26	BCR	C	514	40/40	0.95	0.06	31,41,50,57	0
35	P6G	A	623	19/19	0.95	0.08	48,60,95,96	0
26	BCR	c	514	40/40	0.95	0.06	39,51,58,60	0
30	GOL	O	306	6/6	0.95	0.09	39,45,55,97	0
30	GOL	A	615	6/6	0.95	0.07	34,54,62,66	0
30	GOL	o	305	6/6	0.95	0.07	51,56,61,62	0
36	EDO	o	310	4/4	0.95	0.07	60,65,77,90	0
30	GOL	a	415	6/6	0.96	0.06	29,39,45,45	0
26	BCR	t	102	40/40	0.96	0.06	21,29,48,53	0
31	LMT	m	102	35/35	0.96	0.06	28,50,66,82	0
26	BCR	D	406	40/40	0.96	0.06	23,28,60,65	0
29	LMG	c	519	51/55	0.96	0.06	34,67,104,112	0
30	GOL	D	402	6/6	0.96	0.10	31,37,43,44	0
30	GOL	d	402	6/6	0.96	0.07	35,39,45,48	0
35	P6G	D	417	19/19	0.96	0.08	35,56,89,111	0
26	BCR	a	411	40/40	0.96	0.05	20,25,31,32	0
38	HTG	b	631	19/19	0.96	0.07	41,48,77,98	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	c	513	65/65	0.96	0.07	37,51,89,99	0
36	EDO	O	311	4/4	0.96	0.12	42,54,57,72	0
30	GOL	F	101	6/6	0.96	0.08	43,48,50,54	0
33	PG4	l	103	13/13	0.96	0.06	48,64,71,74	0
26	BCR	d	406	40/40	0.96	0.05	28,36,70,82	0
30	GOL	A	614	6/6	0.96	0.06	33,37,38,44	0
36	EDO	d	417	4/4	0.96	0.09	46,49,52,58	0
29	LMG	A	613	51/55	0.96	0.06	45,60,82,95	0
30	GOL	B	625	6/6	0.96	0.06	32,36,38,50	0
26	BCR	h	103	40/40	0.96	0.06	25,35,50,53	0
37	CA	B	601	1/1	0.96	0.11	82,82,82,82	0
37	CA	h	102	1/1	0.96	0.05	97,97,97,97	0
38	HTG	B	623	19/19	0.96	0.09	28,40,74,88	0
29	LMG	C	519	51/55	0.96	0.08	29,59,104,117	0
38	HTG	B	630	19/19	0.96	0.07	38,50,78,82	0
26	BCR	k	101	40/40	0.96	0.06	34,40,51,54	0
30	GOL	V	208	6/6	0.96	0.06	65,70,82,83	0
24	CLA	C	512	65/65	0.97	0.05	31,39,74,85	0
30	GOL	T	101	6/6	0.97	0.06	52,52,56,59	0
26	BCR	H	102	40/40	0.97	0.05	23,33,52,55	0
29	LMG	B	621	51/55	0.97	0.05	27,39,54,88	0
30	GOL	V	201	6/6	0.97	0.06	28,30,35,39	0
36	EDO	e	106	4/4	0.97	0.06	72,76,79,89	0
30	GOL	V	205	6/6	0.97	0.05	26,34,37,43	0
30	GOL	V	207	6/6	0.97	0.06	44,49,52,55	0
26	BCR	K	101	40/40	0.97	0.05	27,36,45,47	0
26	BCR	T	102	40/40	0.97	0.05	20,29,45,60	0
24	CLA	C	513	65/65	0.97	0.05	33,44,73,92	0
30	GOL	b	625	6/6	0.97	0.05	34,39,44,54	0
26	BCR	b	618	40/40	0.97	0.04	19,26,33,37	0
32	LHG	D	409	49/49	0.97	0.05	25,35,45,55	0
30	GOL	b	627	6/6	0.97	0.05	40,47,52,54	0
30	GOL	b	628	6/6	0.97	0.07	32,34,35,44	0
30	GOL	b	629	6/6	0.97	0.12	36,42,45,50	0
30	GOL	c	525	6/6	0.97	0.06	47,49,64,80	0
26	BCR	b	619	40/40	0.97	0.05	21,28,47,57	0
29	LMG	b	621	51/55	0.97	0.05	28,39,53,103	0
26	BCR	b	620	40/40	0.97	0.05	24,32,45,48	0
24	CLA	B	602	65/65	0.97	0.07	27,39,92,115	0
26	BCR	c	515	40/40	0.97	0.05	26,35,47,55	0
29	LMG	j	101	47/55	0.97	0.06	26,35,80,91	0
38	HTG	b	623	19/19	0.97	0.08	26,42,77,81	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	BCR	c	527	40/40	0.97	0.05	34,42,53,59	0
24	CLA	b	613	65/65	0.97	0.05	20,25,32,41	0
24	CLA	c	503	65/65	0.97	0.05	26,35,42,52	0
24	CLA	c	504	60/65	0.97	0.05	25,31,67,75	0
24	CLA	c	506	65/65	0.97	0.06	26,37,83,95	0
30	GOL	B	627	6/6	0.97	0.06	35,44,48,48	0
24	CLA	c	507	65/65	0.97	0.06	28,34,50,59	0
27	PL9	D	407	55/55	0.97	0.05	17,22,33,48	0
24	CLA	c	511	65/65	0.97	0.05	28,36,47,52	0
28	SQD	A	612	54/54	0.97	0.06	31,55,78,87	0
24	CLA	c	512	65/65	0.97	0.05	30,44,74,79	0
24	CLA	C	503	65/65	0.97	0.05	26,30,38,43	0
25	PHO	d	401	64/64	0.97	0.04	20,25,31,41	0
28	SQD	a	413	54/54	0.97	0.06	33,54,92,96	0
26	BCR	A	610	40/40	0.97	0.04	20,25,32,35	0
26	BCR	B	619	40/40	0.97	0.05	20,26,50,62	0
40	DGD	H	103	62/66	0.97	0.05	21,31,45,54	0
40	DGD	c	517	57/66	0.97	0.05	27,34,75,108	0
24	CLA	C	506	65/65	0.97	0.06	28,39,97,106	0
40	DGD	h	104	62/66	0.97	0.06	25,35,49,55	0
26	BCR	C	515	40/40	0.97	0.04	28,33,52,59	0
26	BCR	C	525	40/40	0.97	0.05	26,33,39,41	0
24	CLA	b	609	65/65	0.98	0.04	22,27,37,44	0
24	CLA	b	610	65/65	0.98	0.04	23,30,35,44	0
24	CLA	b	611	65/65	0.98	0.04	23,28,38,44	0
24	CLA	b	612	65/65	0.98	0.04	18,24,37,42	0
24	CLA	A	609	65/65	0.98	0.06	19,24,109,130	0
24	CLA	b	614	65/65	0.98	0.04	19,23,48,54	0
24	CLA	b	615	65/65	0.98	0.05	18,26,94,117	0
24	CLA	b	616	65/65	0.98	0.05	22,29,47,56	0
29	LMG	J	101	47/55	0.98	0.05	23,29,74,83	0
24	CLA	b	617	60/65	0.98	0.06	26,31,82,92	0
24	CLA	c	501	65/65	0.98	0.04	27,35,49,53	0
24	CLA	c	502	65/65	0.98	0.04	24,30,41,50	0
22	CL	V	202	1/1	0.98	0.05	68,68,68,68	0
24	CLA	B	603	65/65	0.98	0.04	21,26,33,38	0
24	CLA	c	505	65/65	0.98	0.04	25,29,44,50	0
24	CLA	B	604	65/65	0.98	0.04	19,23,34,41	0
24	CLA	B	605	65/65	0.98	0.04	17,21,55,58	0
24	CLA	c	508	60/65	0.98	0.04	23,29,52,62	0
24	CLA	c	509	65/65	0.98	0.04	25,33,52,53	0
24	CLA	c	510	65/65	0.98	0.04	26,32,41,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	B	606	65/65	0.98	0.04	18,22,34,38	0
30	GOL	B	628	6/6	0.98	0.06	34,40,48,49	0
32	LHG	B	632	49/49	0.98	0.05	20,30,52,61	0
30	GOL	B	629	6/6	0.98	0.07	31,39,60,64	0
32	LHG	D	411	49/49	0.98	0.06	23,31,81,89	0
24	CLA	B	607	55/65	0.98	0.04	19,25,33,49	0
24	CLA	B	608	65/65	0.98	0.04	16,20,32,38	0
32	LHG	d	409	49/49	0.98	0.05	27,37,48,52	0
32	LHG	d	410	49/49	0.98	0.04	21,27,42,51	0
32	LHG	d	411	49/49	0.98	0.05	26,31,79,84	0
24	CLA	d	403	65/65	0.98	0.03	17,20,29,38	0
32	LHG	l	101	49/49	0.98	0.04	23,30,49,62	0
24	CLA	d	404	65/65	0.98	0.04	17,21,37,43	0
24	CLA	d	405	65/65	0.98	0.06	25,33,91,101	0
25	PHO	A	608	64/64	0.98	0.04	17,19,26,26	0
25	PHO	D	401	64/64	0.98	0.04	17,23,31,41	0
25	PHO	a	409	64/64	0.98	0.04	17,21,26,32	0
24	CLA	B	609	65/65	0.98	0.04	19,24,33,40	0
24	CLA	B	610	65/65	0.98	0.04	22,27,33,37	0
26	BCR	B	618	40/40	0.98	0.04	21,25,33,34	0
37	CA	O	301	1/1	0.98	0.05	53,53,53,53	0
37	CA	b	601	1/1	0.98	0.09	72,72,72,72	0
24	CLA	B	611	65/65	0.98	0.04	20,24,38,51	0
26	BCR	B	620	40/40	0.98	0.04	22,31,46,50	0
24	CLA	B	612	65/65	0.98	0.04	16,21,35,39	0
24	CLA	B	613	65/65	0.98	0.04	17,23,30,39	0
24	CLA	B	614	65/65	0.98	0.04	17,21,48,64	0
24	CLA	B	615	55/65	0.98	0.04	17,23,55,82	0
24	CLA	B	616	65/65	0.98	0.04	21,27,48,56	0
24	CLA	C	501	65/65	0.98	0.04	25,30,48,57	0
30	GOL	V	206	6/6	0.98	0.07	33,35,42,42	0
24	CLA	C	502	65/65	0.98	0.04	21,27,37,54	0
23	BCT	A	605	4/4	0.98	0.05	27,31,35,52	0
24	CLA	C	504	60/65	0.98	0.04	20,26,70,81	0
38	HTG	O	303	19/19	0.98	0.06	27,31,50,65	0
24	CLA	C	505	65/65	0.98	0.05	23,29,47,52	0
23	BCT	a	406	4/4	0.98	0.05	27,28,31,49	0
24	CLA	C	507	65/65	0.98	0.04	27,33,48,64	0
24	CLA	C	508	60/65	0.98	0.04	23,29,51,61	0
24	CLA	C	509	65/65	0.98	0.05	27,33,50,57	0
24	CLA	C	510	65/65	0.98	0.05	22,29,41,48	0
30	GOL	b	630	6/6	0.98	0.06	30,39,52,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	C	511	65/65	0.98	0.05	26,33,40,45	0
30	GOL	c	526	6/6	0.98	0.04	24,28,29,32	0
23	BCT	m	104[A]	4/4	0.98	0.05	18,34,38,38	4
23	BCT	m	104[B]	4/4	0.98	0.05	7,13,18,19	4
38	HTG	o	301	19/19	0.98	0.05	25,32,41,63	0
24	CLA	D	403	65/65	0.98	0.04	14,18,28,44	0
24	CLA	D	404	65/65	0.98	0.04	13,18,35,40	0
24	CLA	D	405	65/65	0.98	0.05	22,29,91,98	0
30	GOL	f	103	6/6	0.98	0.04	50,53,56,56	0
27	PL9	d	407	55/55	0.98	0.04	19,24,31,39	0
24	CLA	a	407	65/65	0.98	0.04	17,20,27,41	0
24	CLA	a	410	65/65	0.98	0.06	20,25,98,113	0
40	DGD	C	516	62/66	0.98	0.05	20,31,90,104	0
40	DGD	C	517	56/66	0.98	0.05	21,31,74,88	0
40	DGD	C	518	62/66	0.98	0.05	20,30,71,80	0
24	CLA	A	606	65/65	0.98	0.04	14,18,27,44	0
24	CLA	b	603	65/65	0.98	0.04	21,28,39,43	0
40	DGD	c	516	62/66	0.98	0.05	23,35,77,86	0
24	CLA	b	604	65/65	0.98	0.04	22,28,38,45	0
40	DGD	c	518	62/66	0.98	0.05	25,36,65,81	0
24	CLA	b	605	65/65	0.98	0.04	17,23,53,59	0
24	CLA	b	606	65/65	0.98	0.04	20,25,33,39	0
41	HEM	e	107	43/43	0.98	0.06	40,47,74,103	0
24	CLA	b	607	55/65	0.98	0.04	22,27,36,49	0
24	CLA	b	608	65/65	0.98	0.04	17,22,31,37	0
24	CLA	a	408	60/65	0.99	0.04	18,25,73,85	0
30	GOL	v	204	6/6	0.99	0.05	30,36,41,50	0
24	CLA	A	607	60/65	0.99	0.04	17,20,66,78	0
37	CA	c	524	1/1	0.99	0.06	45,45,45,45	0
22	CL	v	201	1/1	0.99	0.03	72,72,72,72	0
37	CA	o	302	1/1	0.99	0.04	55,55,55,55	0
24	CLA	B	617	60/65	0.99	0.05	21,27,90,107	0
41	HEM	E	113	43/43	0.99	0.05	35,42,61,68	0
30	GOL	C	524	6/6	0.99	0.03	21,22,24,26	0
42	MG	J	102	1/1	0.99	0.05	27,27,27,27	0
42	MG	j	102	1/1	0.99	0.08	35,35,35,35	0
43	HEC	V	203	43/43	0.99	0.04	20,24,27,29	0
43	HEC	v	202	43/43	0.99	0.04	26,31,34,38	0
32	LHG	D	410	49/49	0.99	0.04	21,27,41,48	0
22	CL	A	604	1/1	0.99	0.02	21,21,21,21	0
22	CL	A	603	1/1	1.00	0.04	23,23,23,23	0
42	MG	F	103	1/1	1.00	0.03	32,32,32,32	0

Continued on next page...

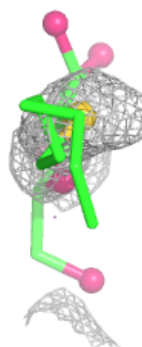
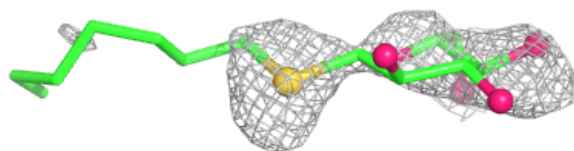
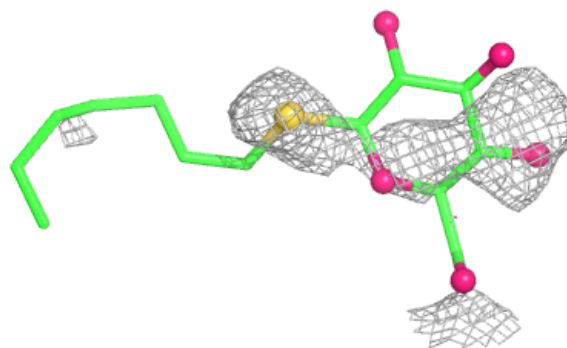
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	OEX	A	601	10/10	1.00	0.02	20,21,24,26	0
42	MG	f	102	1/1	1.00	0.01	45,45,45,45	0
20	OEX	a	402	10/10	1.00	0.02	23,24,26,27	0
22	CL	a	404	1/1	1.00	0.04	28,28,28,28	0
22	CL	a	405	1/1	1.00	0.02	25,25,25,25	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

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.

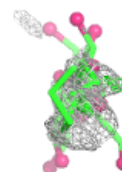
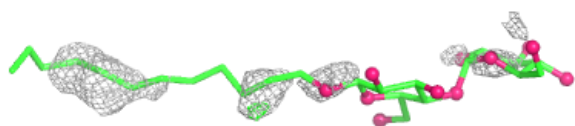
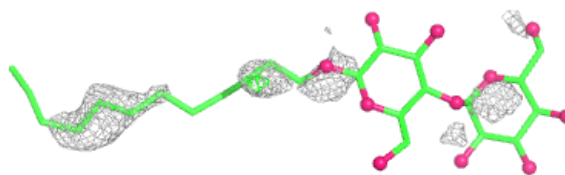
Electron density around HTG C 530:

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

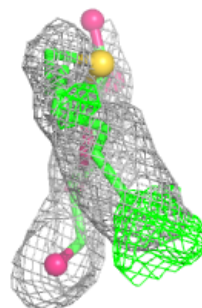
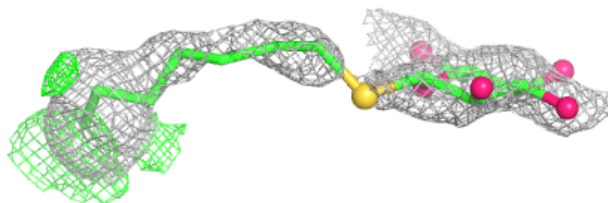
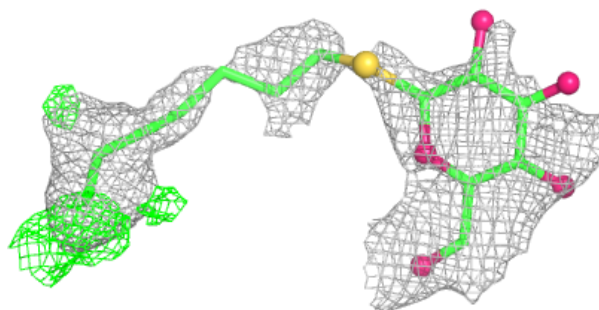


Electron density around LMT C 533:

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

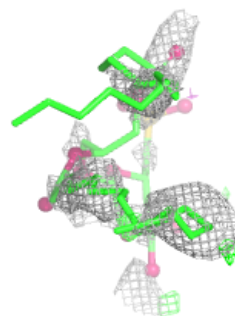
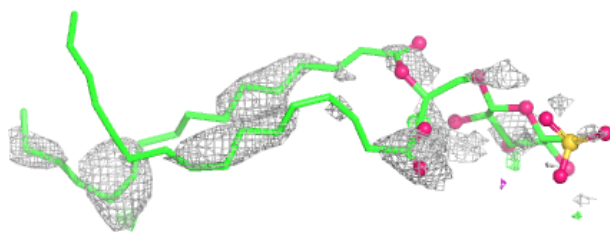
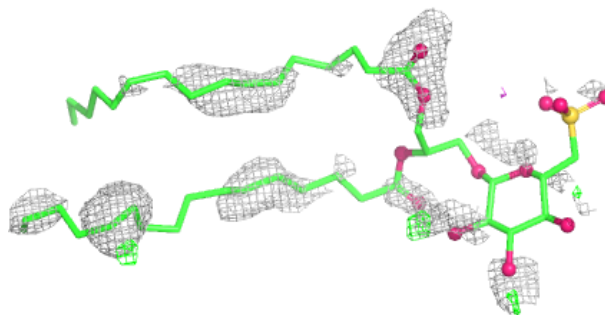
**Electron density around HTG C 529:**

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

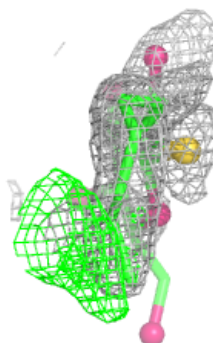
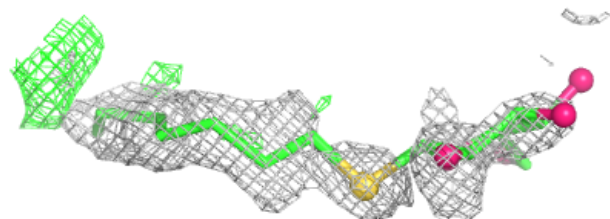
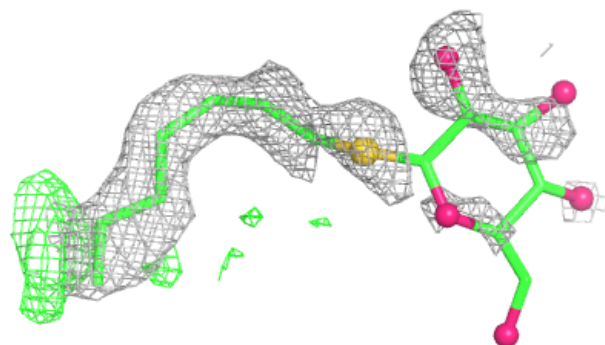


Electron density around SQD h 105:

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

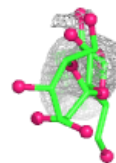
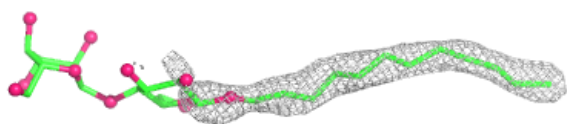
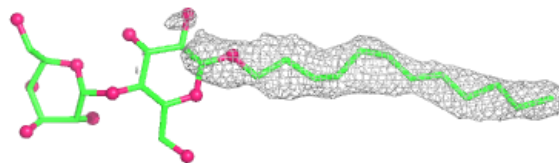
**Electron density around HTG a 418:**

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

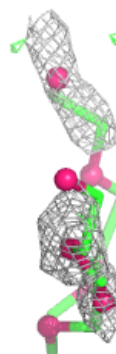
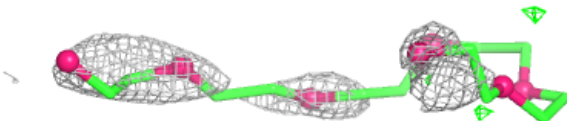
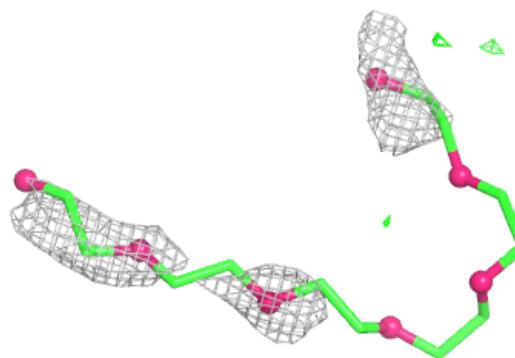


Electron density around LMT j 103:

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

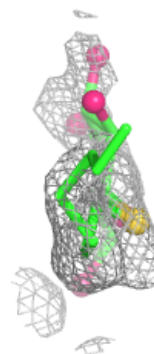
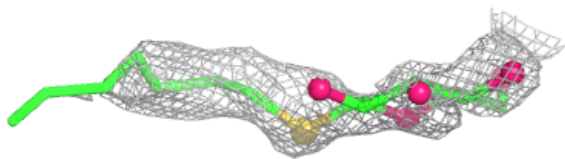
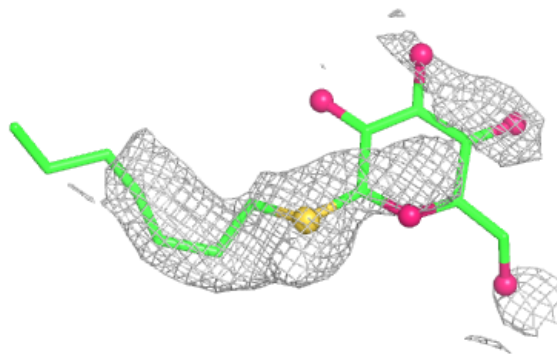
**Electron density around P6G C 541:**

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

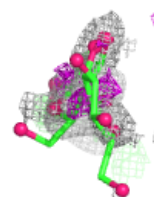
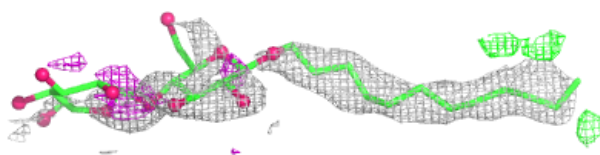
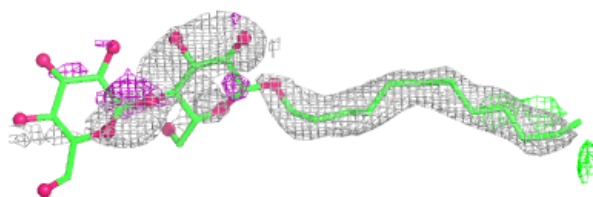


Electron density around HTG C 531:

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

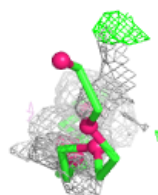
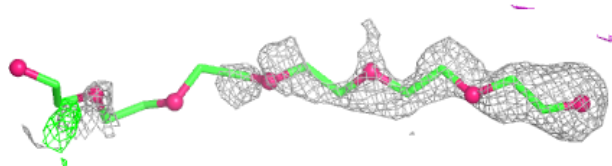
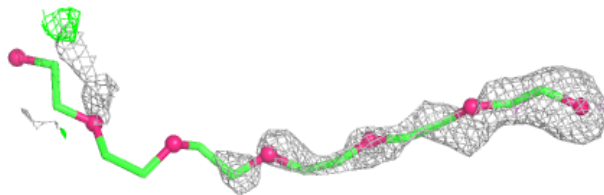
**Electron density around LMT u 203:**

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

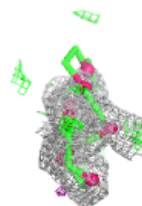
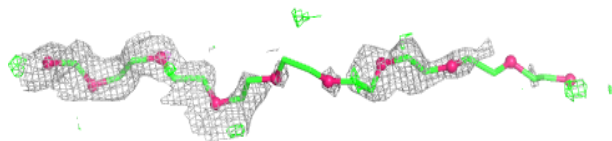
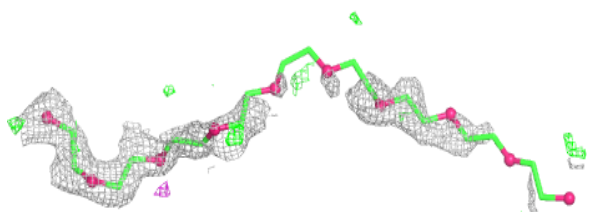


Electron density around P6G D 418:

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

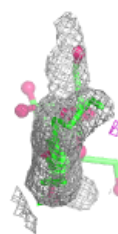
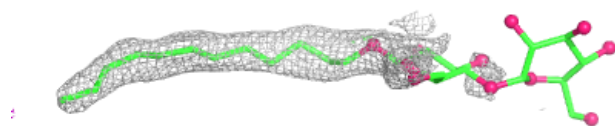
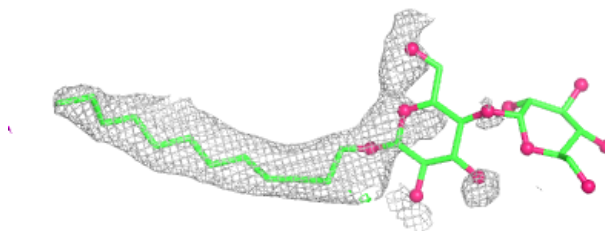
**Electron density around 2PE V 216:**

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

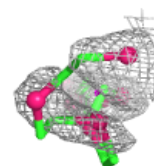
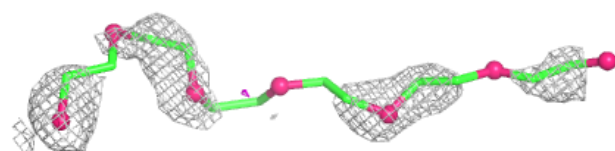
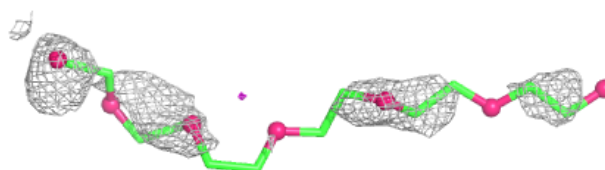


Electron density around LMT Y 101:

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

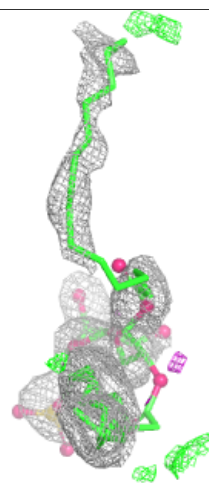
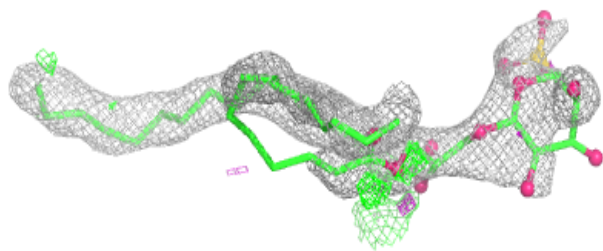
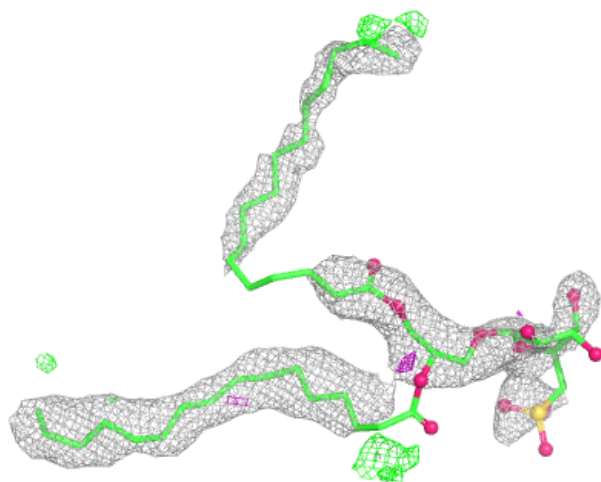
**Electron density around P6G E 110:**

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



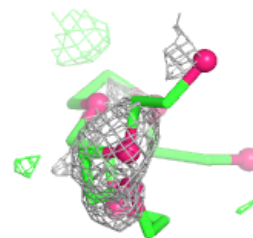
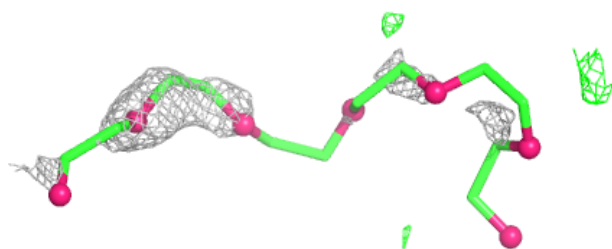
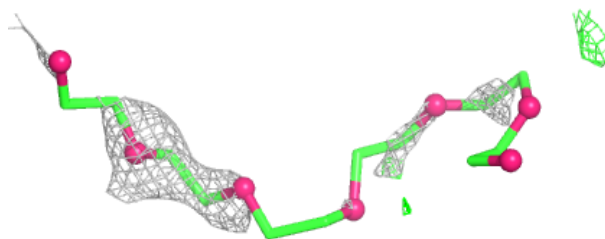
Electron density around SQD A 622:

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

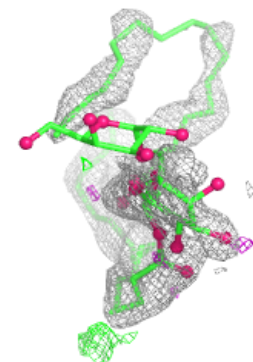
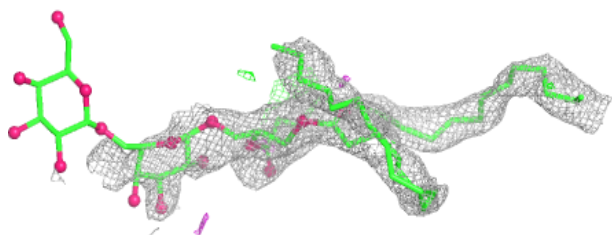
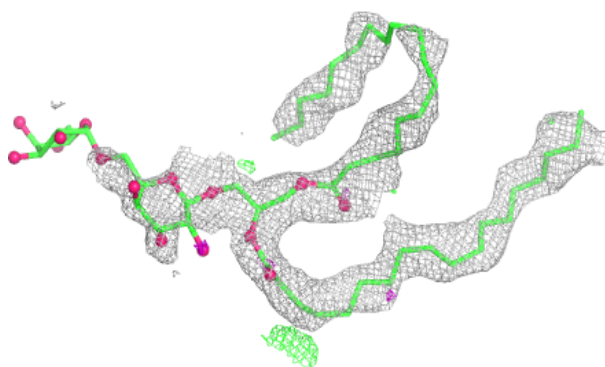


Electron density around P6G c 541:

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

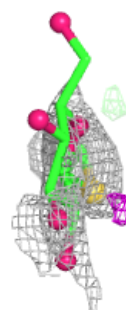
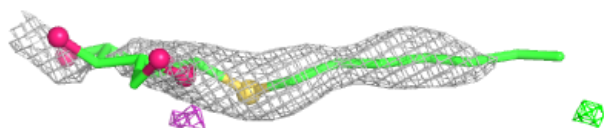
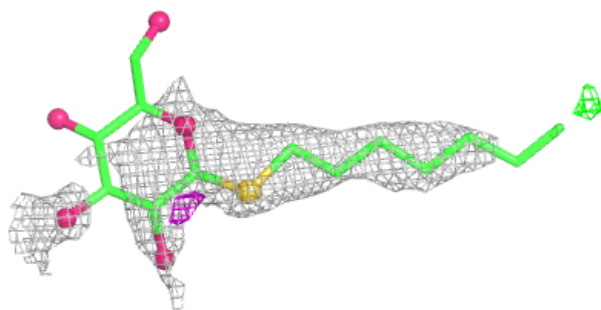
**Electron density around DGD d 408:**

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

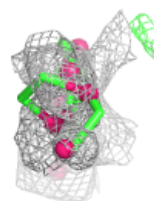
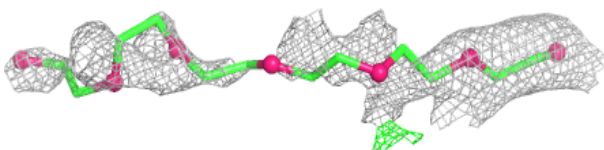
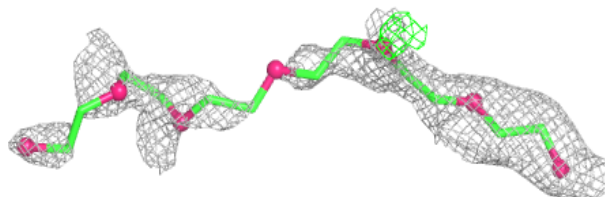


Electron density around HTG c 530:

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

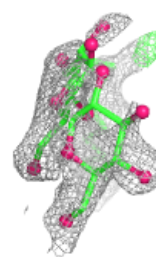
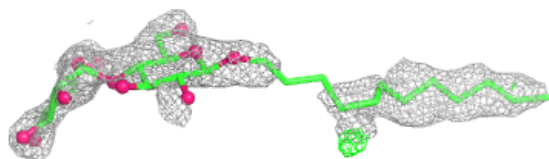
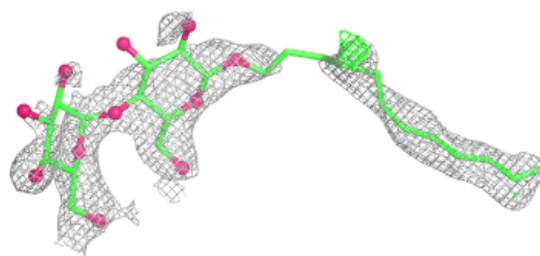
**Electron density around P6G b 649:**

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

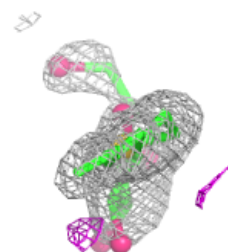
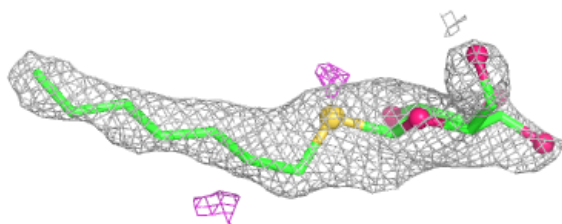
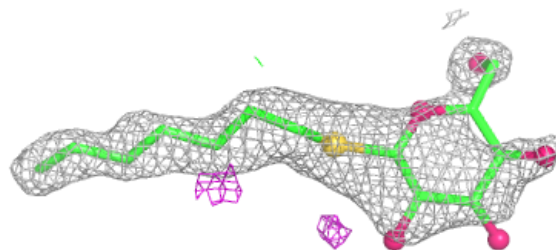


Electron density around LMT F 102:

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

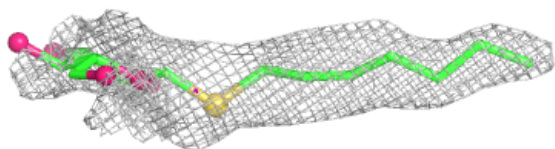
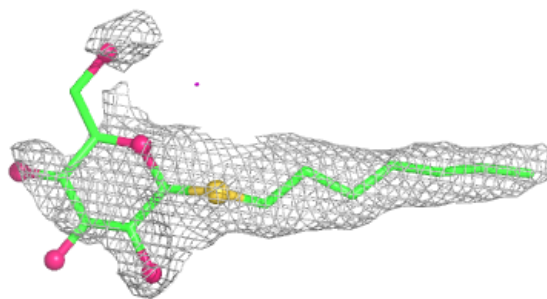
**Electron density around HTG c 523:**

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

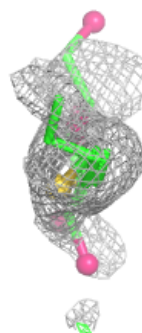
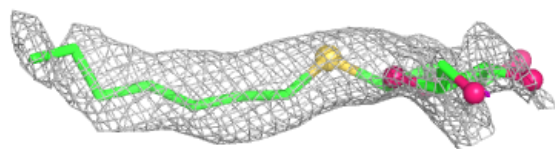
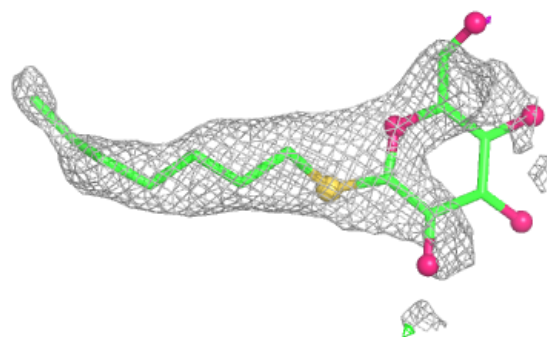


Electron density around HTG c 531:

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

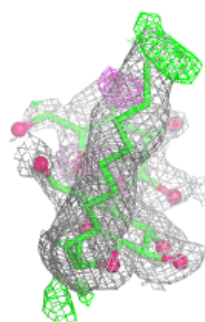
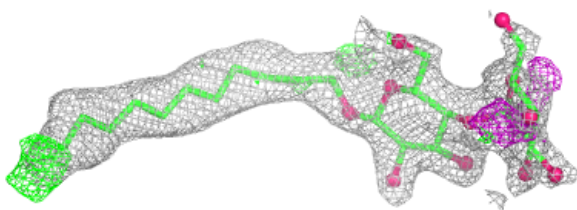
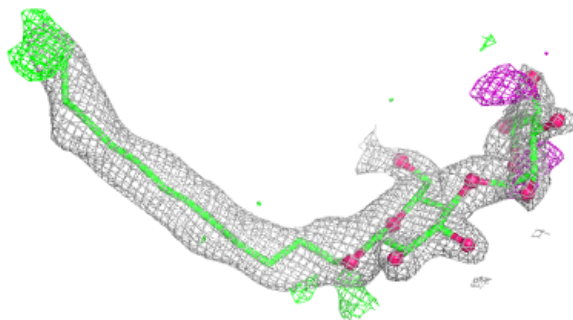
**Electron density around HTG h 101:**

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

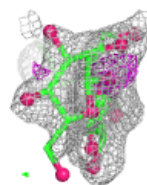
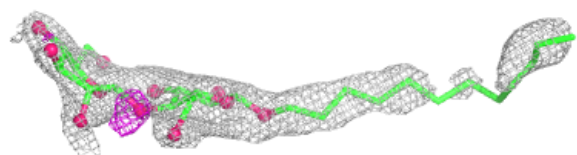
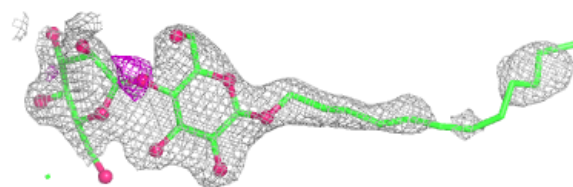


Electron density around LMT m 101:

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

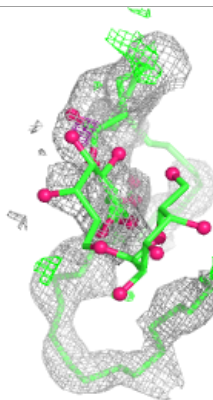
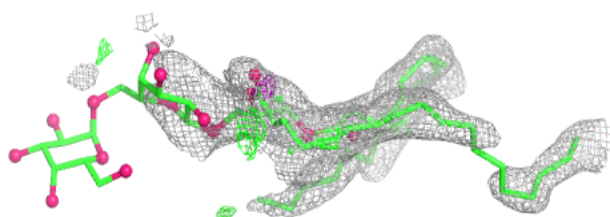
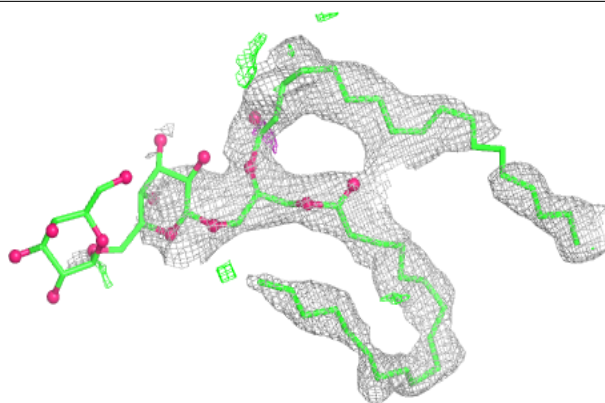
**Electron density around LMT c 521:**

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

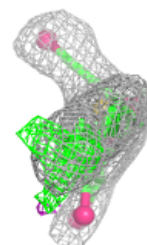
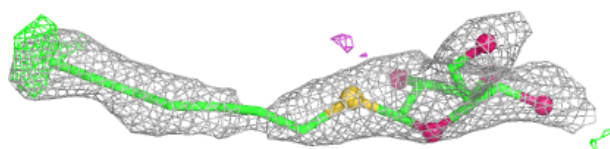
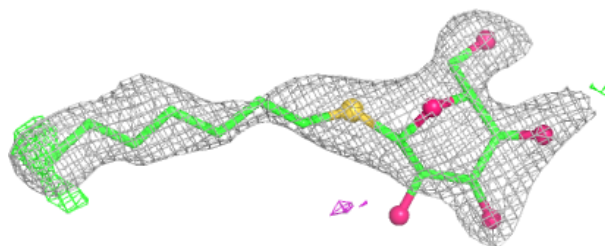


Electron density around DGD D 408:

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

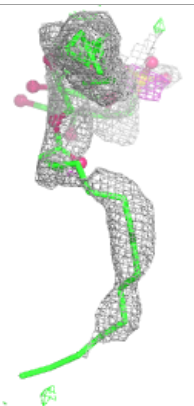
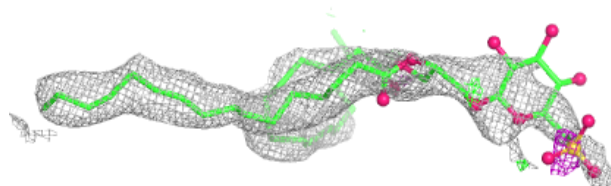
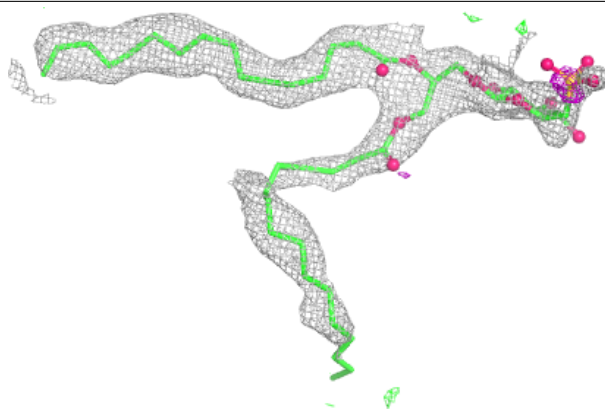
**Electron density around HTG C 522:**

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

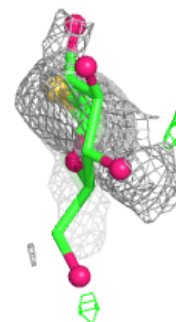
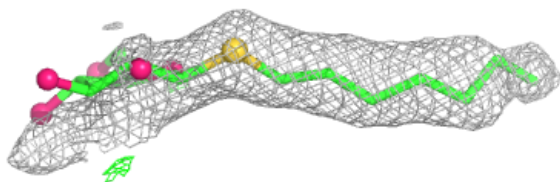
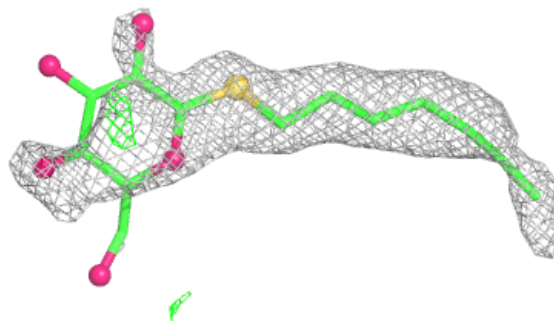


Electron density around SQD a 424:

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

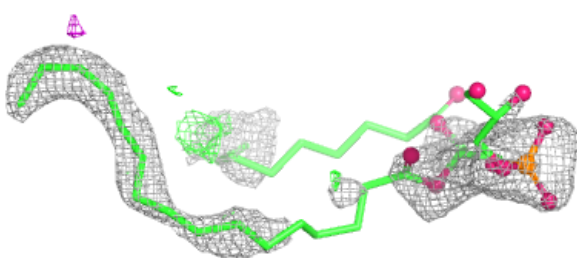
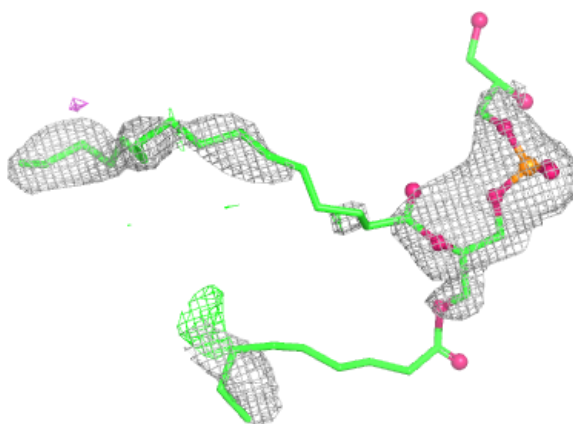
**Electron density around HTG H 101:**

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

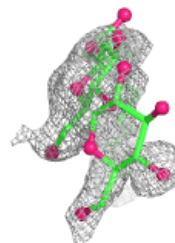
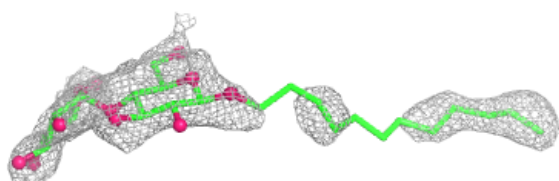
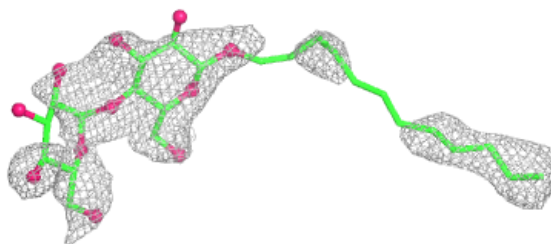


Electron density around LHG e 101:

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

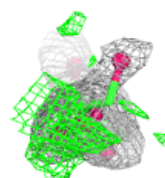
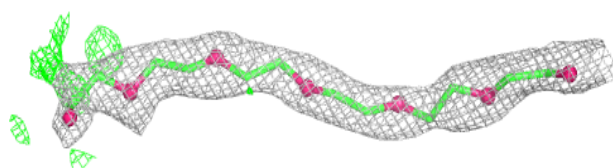
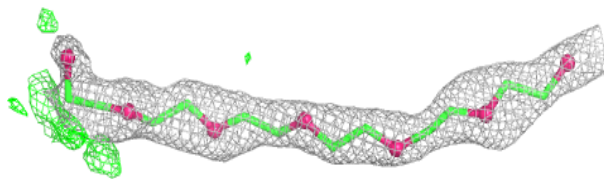
**Electron density around LMT f 101:**

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

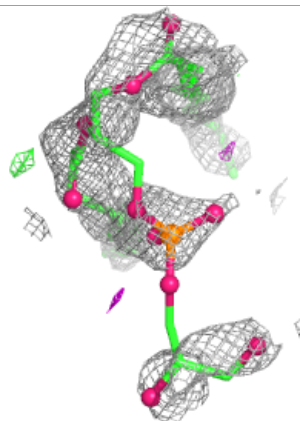
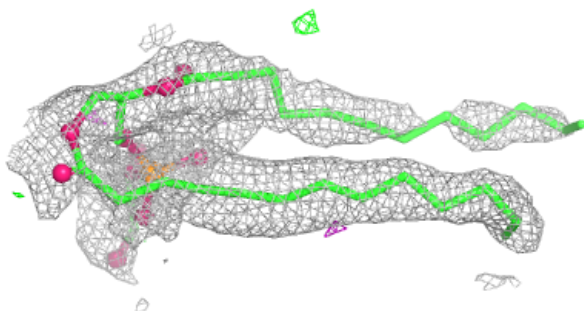
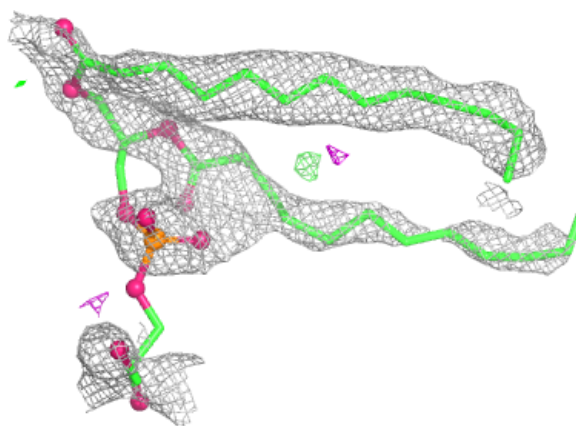


Electron density around P6G j 106:

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

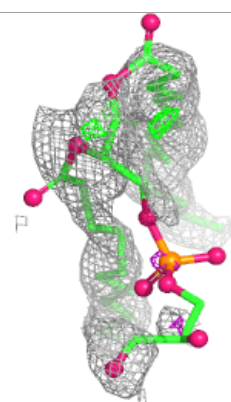
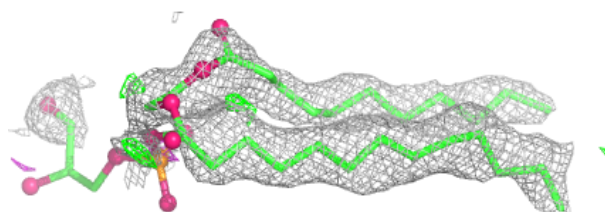
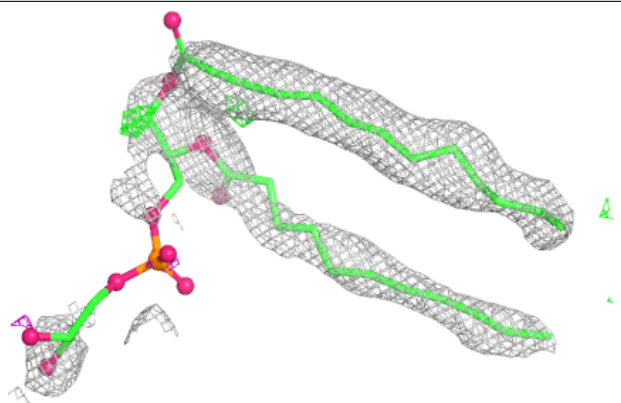
**Electron density around LHG A 618:**

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

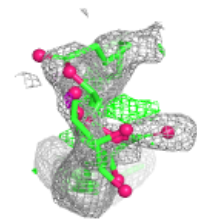
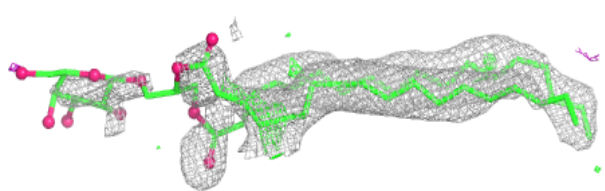
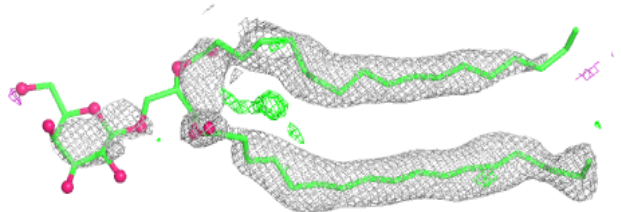


Electron density around LHG a 419:

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

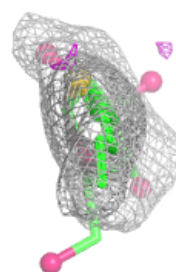
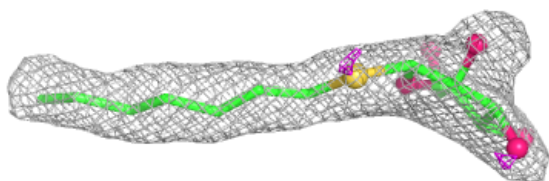
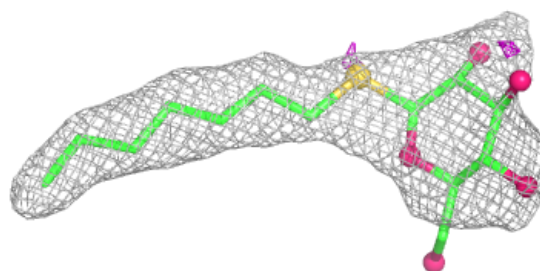
**Electron density around LMG d 412:**

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

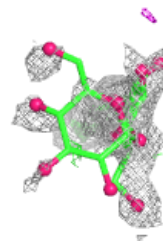
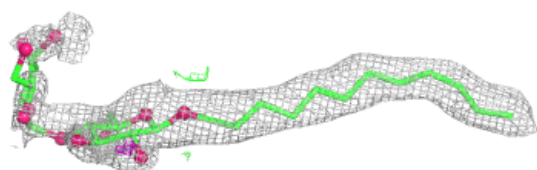
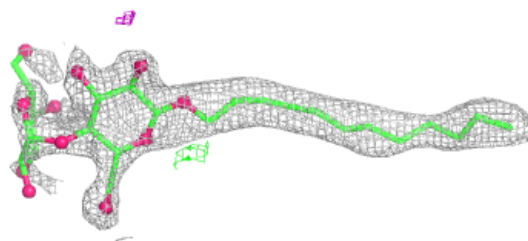


Electron density around HTG B 624:

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

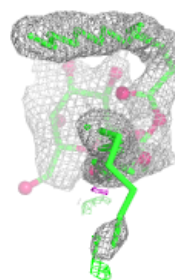
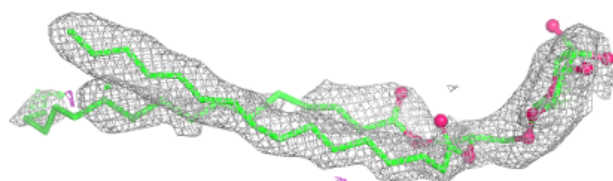
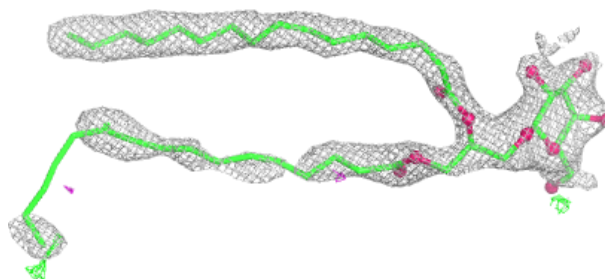
**Electron density around LMT J 103:**

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

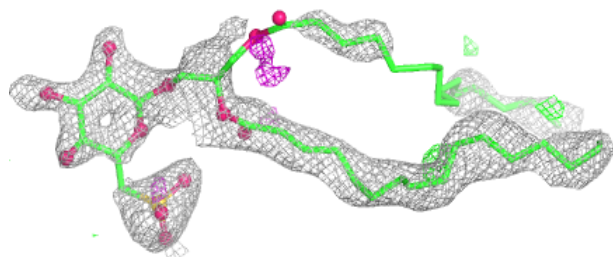
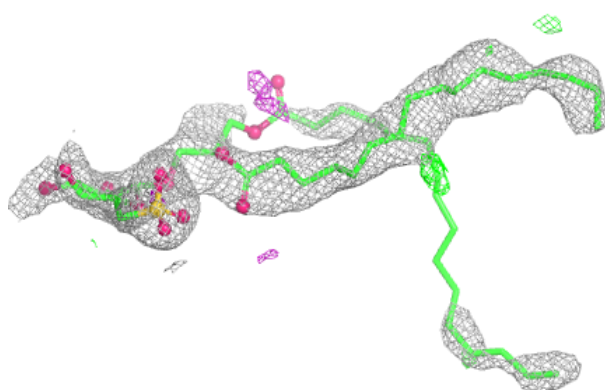


Electron density around LMG c 520:

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

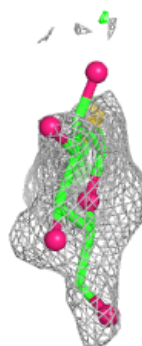
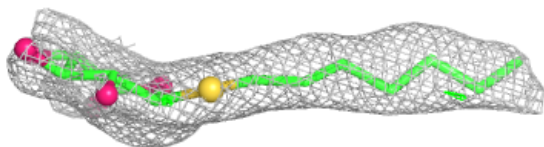
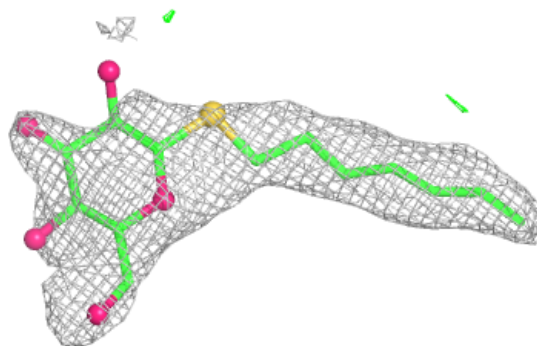
**Electron density around SQD F 104:**

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

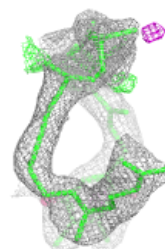
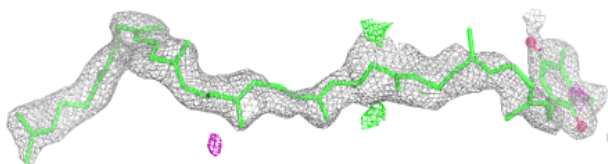
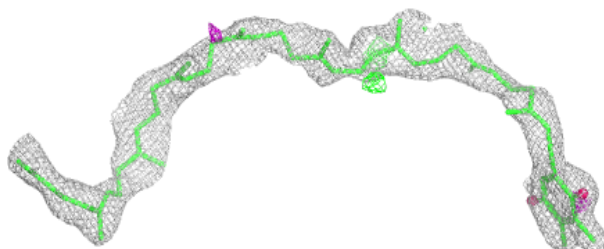


Electron density around HTG b 624:

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

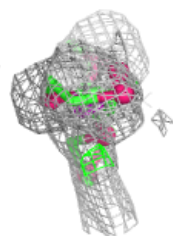
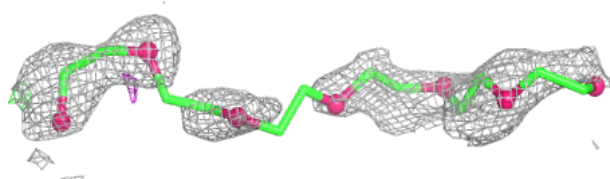
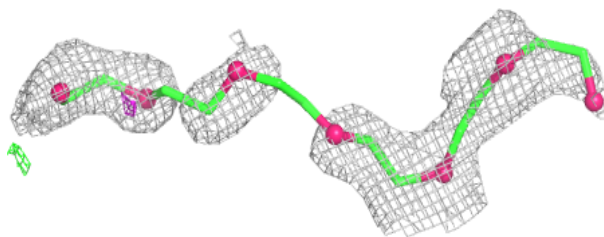
**Electron density around PL9 a 412:**

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

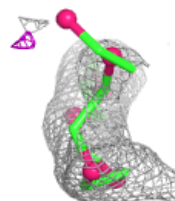
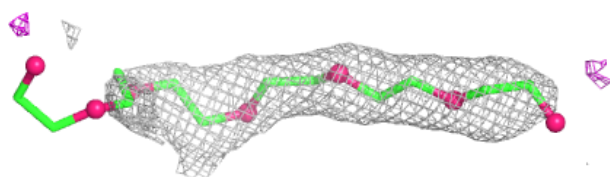
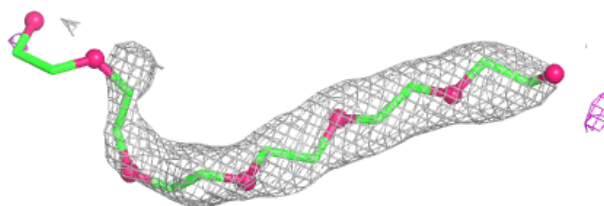


Electron density around P6G B 652:

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

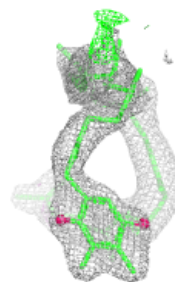
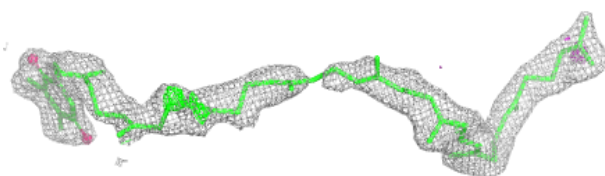
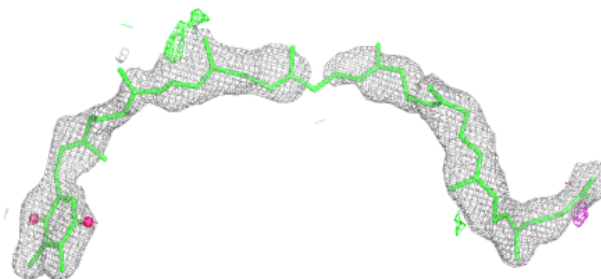
**Electron density around P6G I 106:**

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

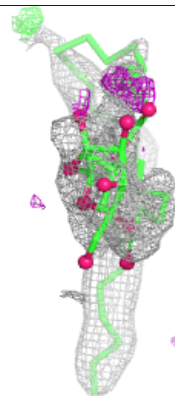
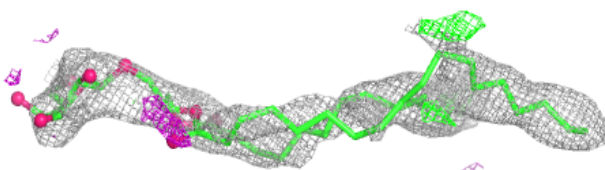
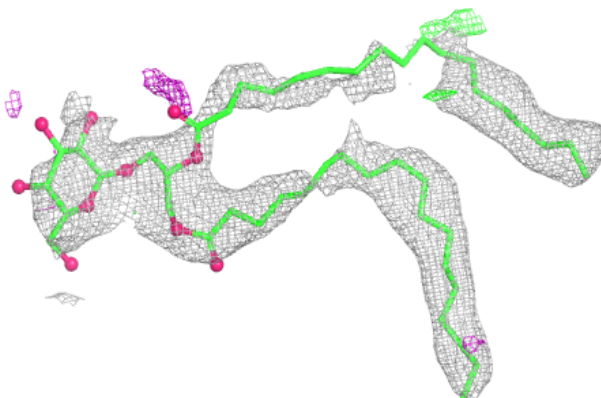


Electron density around PL9 A 611:

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

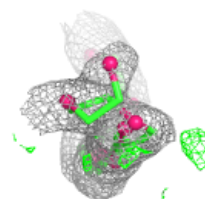
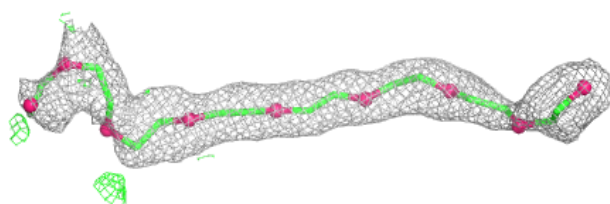
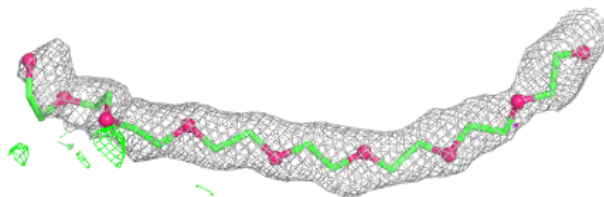
**Electron density around LMG C 526:**

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

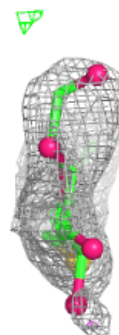
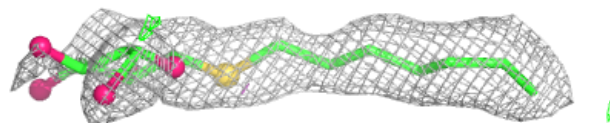
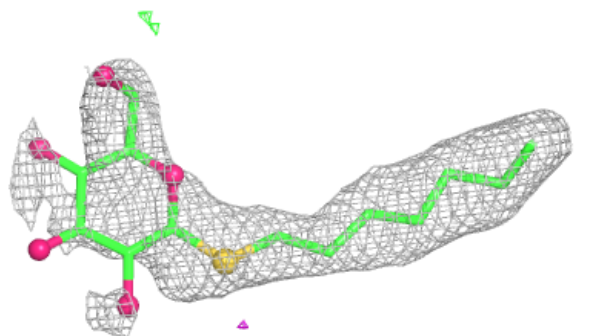


Electron density around PE8 i 107:

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

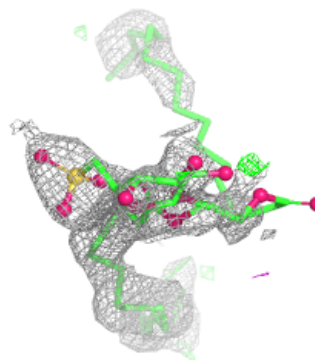
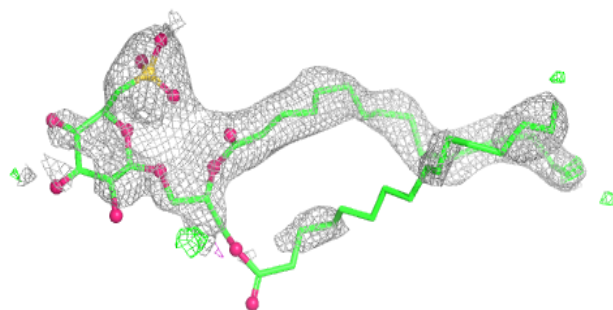
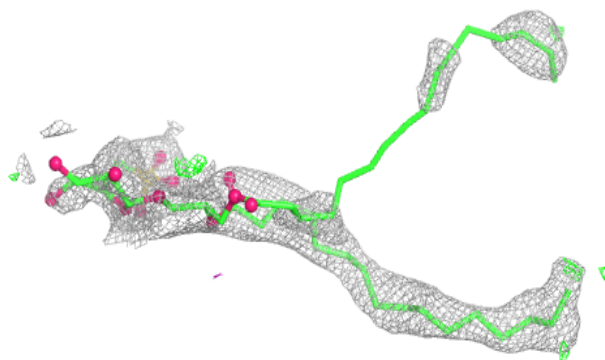
**Electron density around HTG B 631:**

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

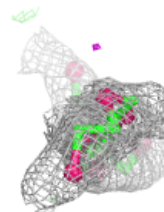
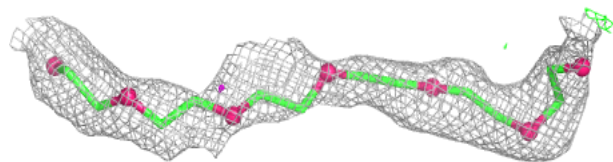
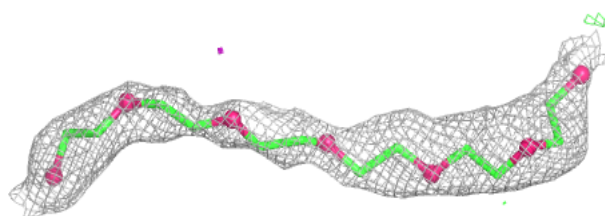


Electron density around SQD x 101:

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

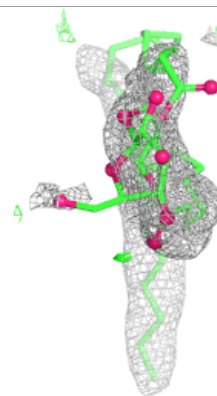
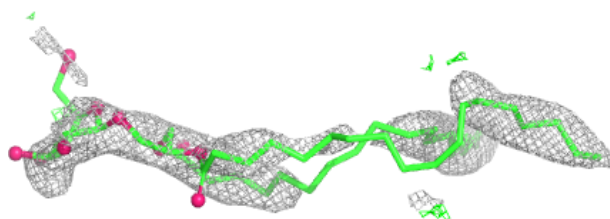
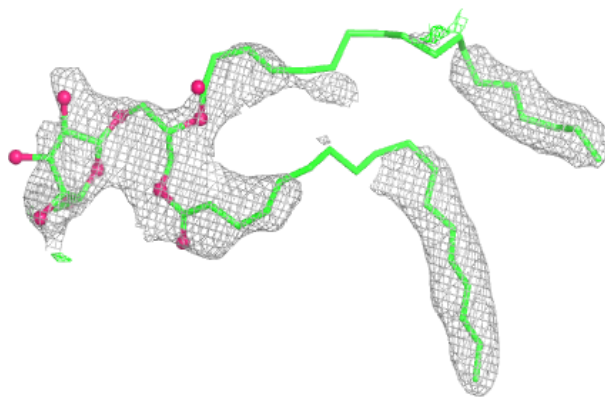
**Electron density around P6G A 624:**

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

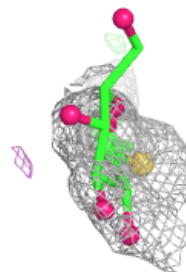
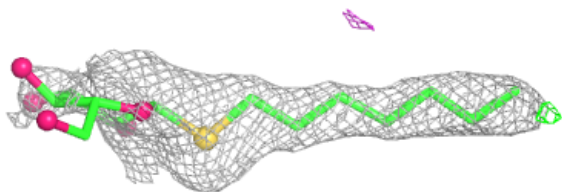
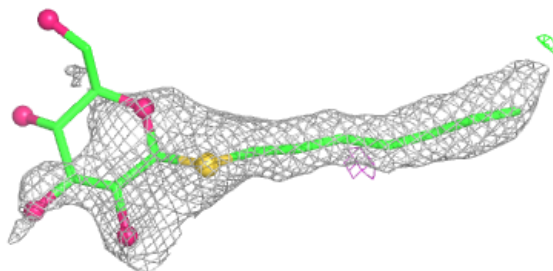


Electron density around LMG z 101:

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

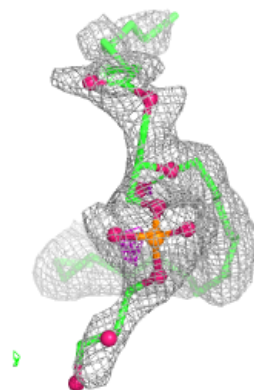
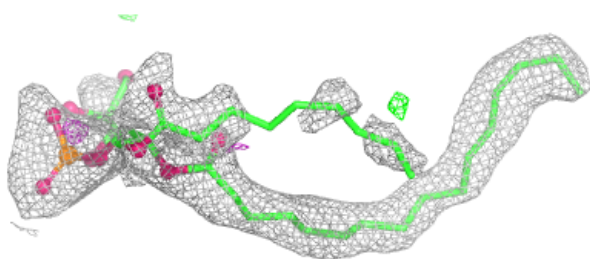
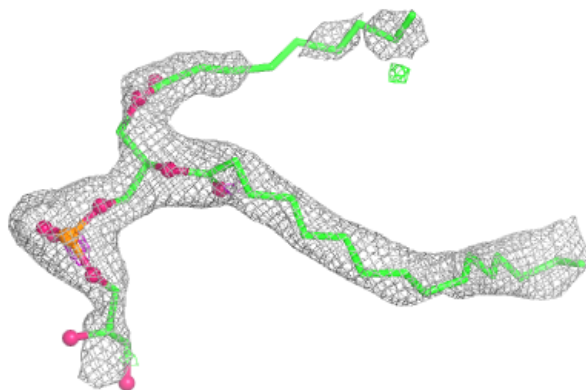
**Electron density around HTG C 532:**

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

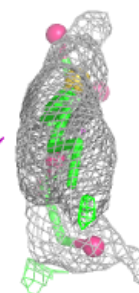
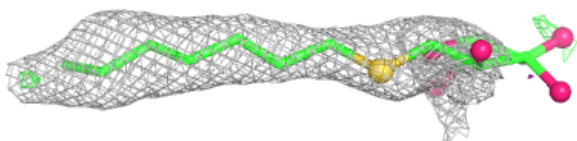
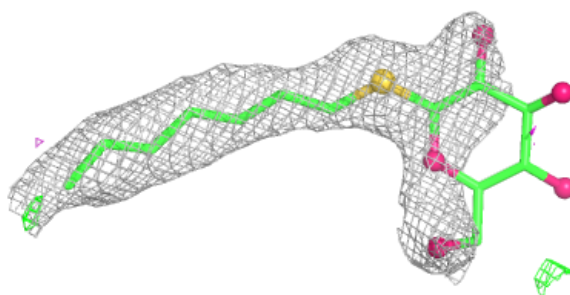


Electron density around LHG E 101:

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

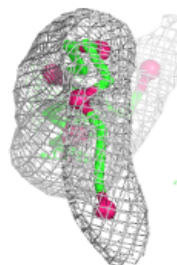
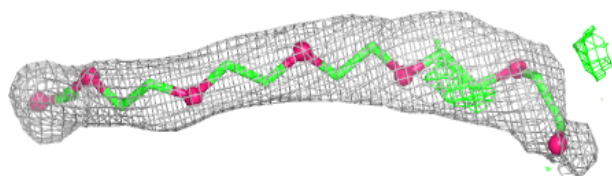
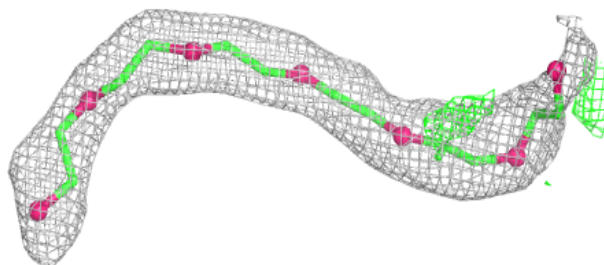
**Electron density around HTG b 632:**

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

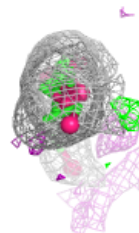
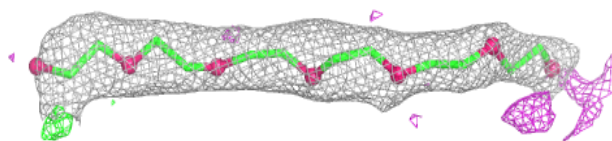
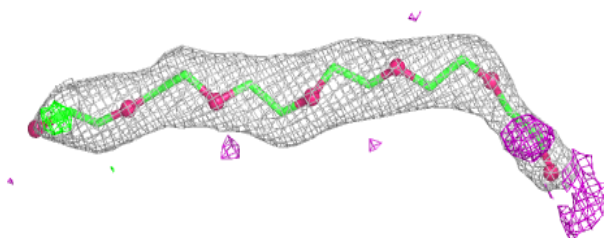


Electron density around P6G b 648:

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

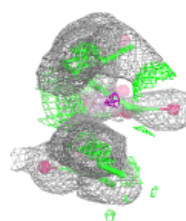
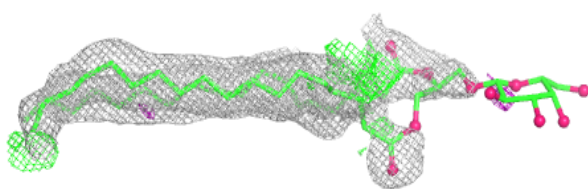
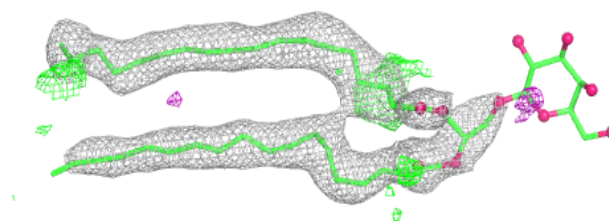
**Electron density around P6G d 415:**

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

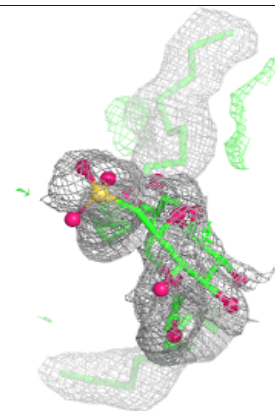
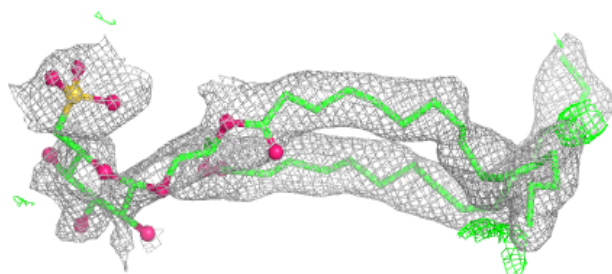
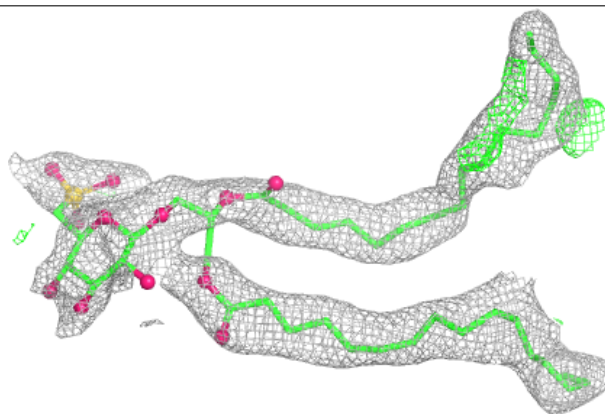


Electron density around LMG B 634:

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

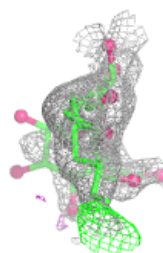
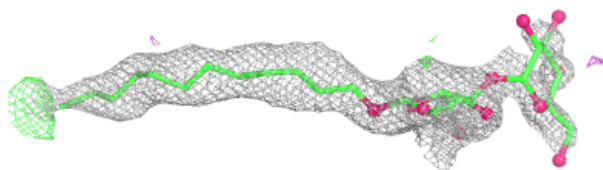
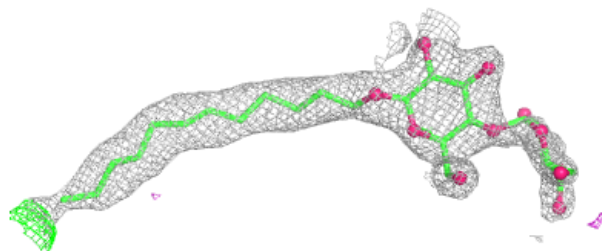
**Electron density around SQD 1 102:**

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

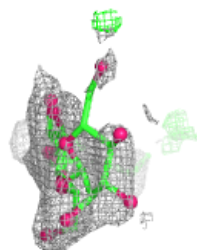
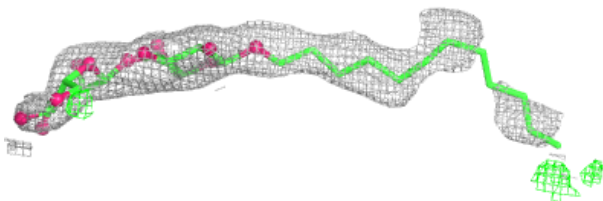
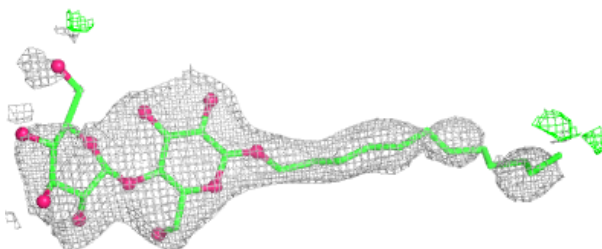


Electron density around LMT B 622:

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

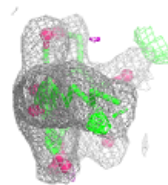
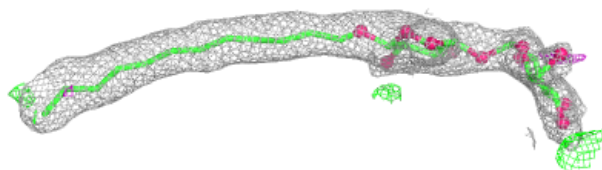
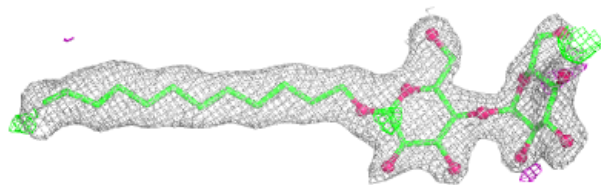
**Electron density around LMT I 101:**

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

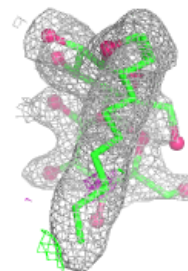
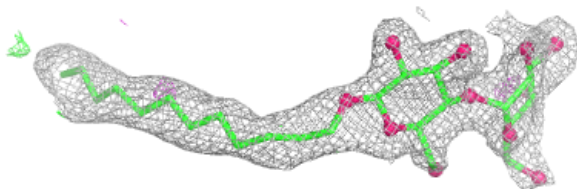
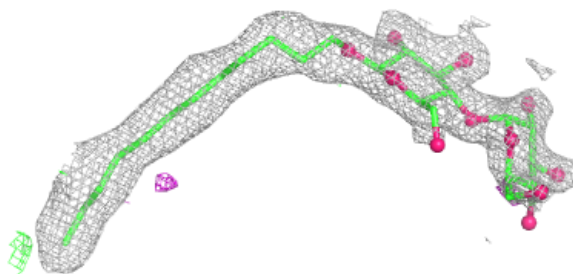


Electron density around LMT M 101:

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

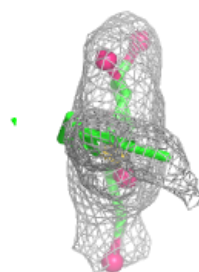
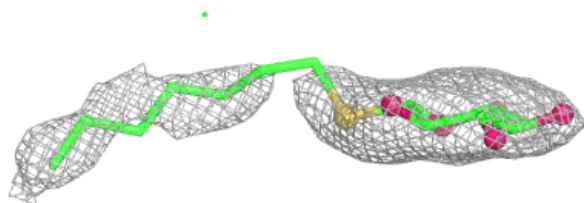
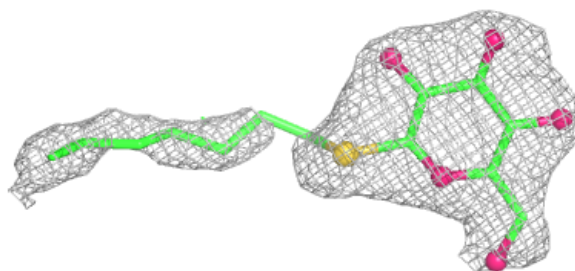
**Electron density around LMT M 102:**

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

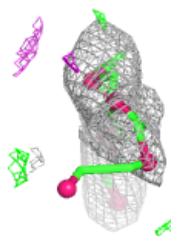
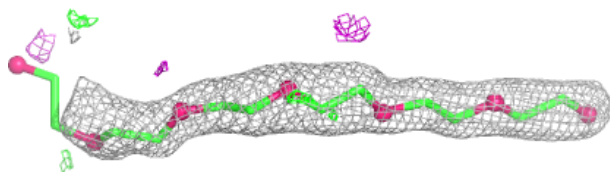
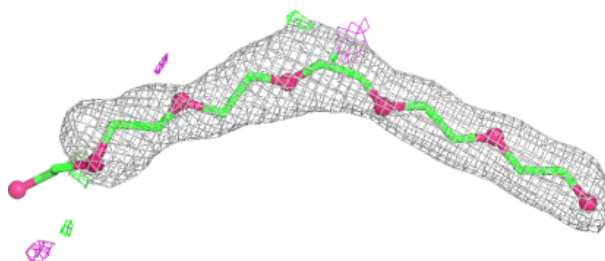


Electron density around HTG c 522:

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

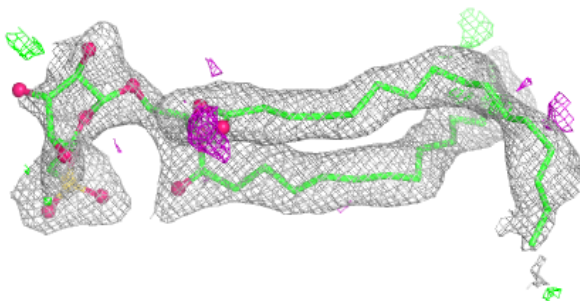
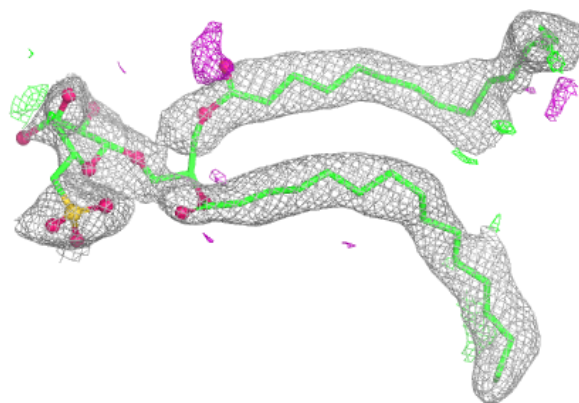
**Electron density around P6G d 416:**

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

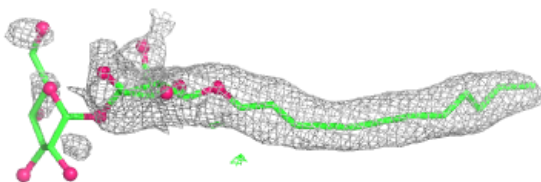
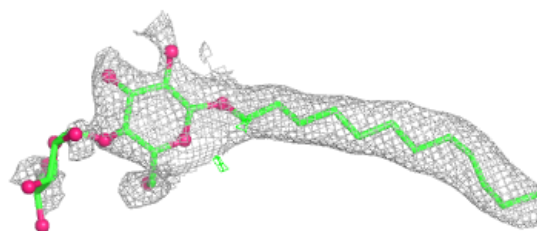


Electron density around SQD b 633:

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

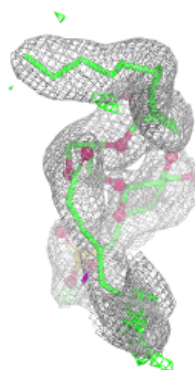
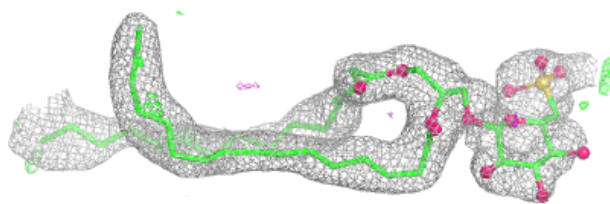
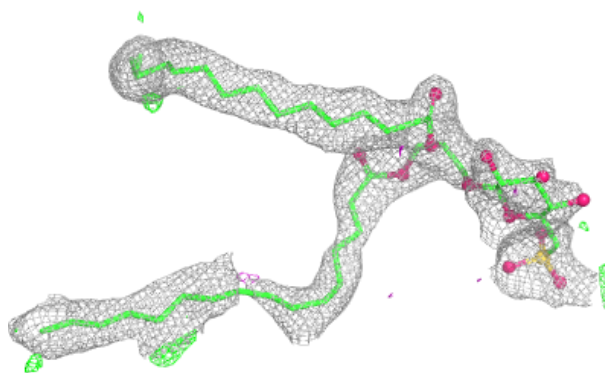
**Electron density around LMT b 622:**

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

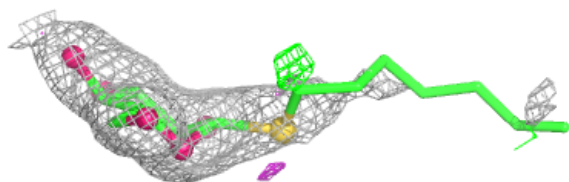
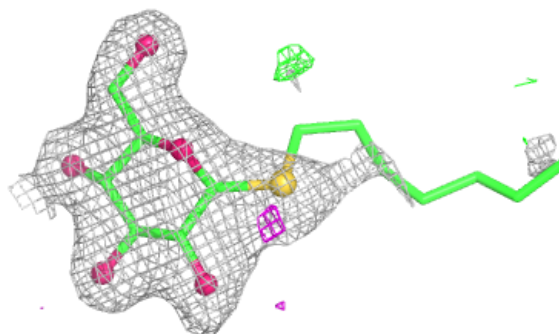


Electron density around SQD a 417:

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

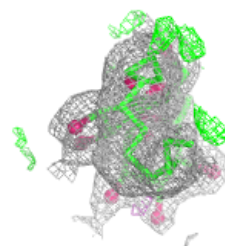
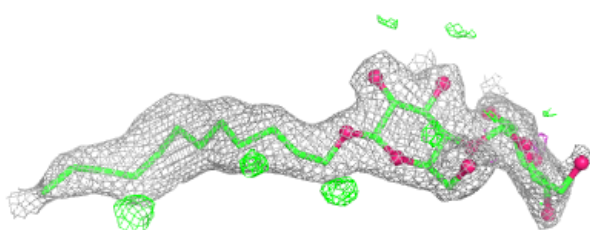
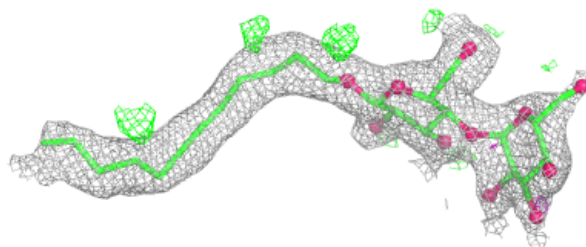
**Electron density around HTG V 204:**

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

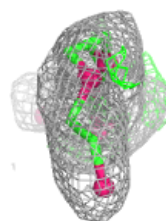
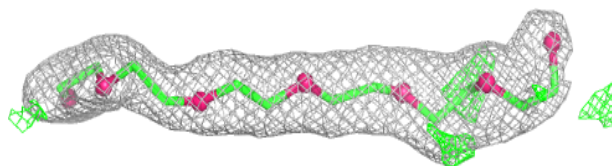
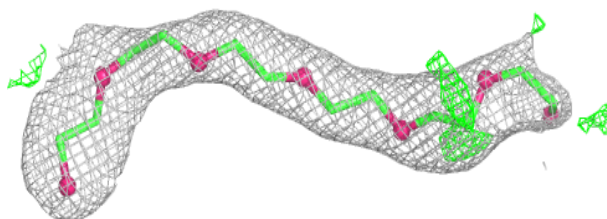


Electron density around LMT a 401:

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

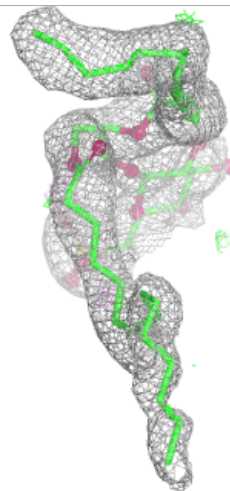
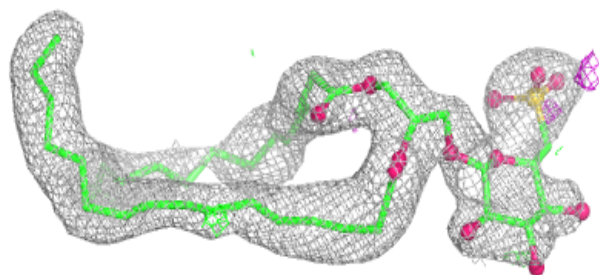
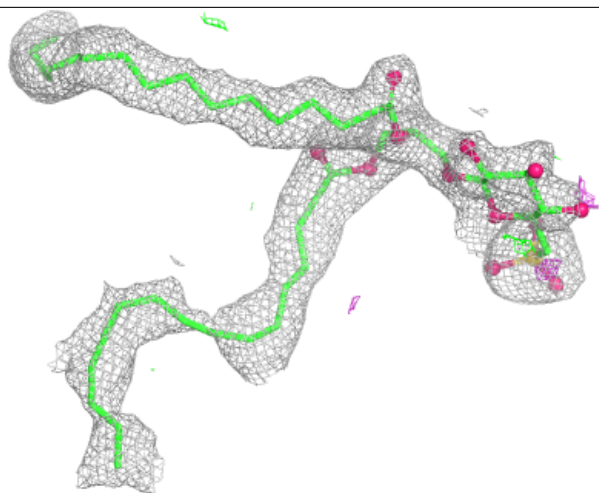
**Electron density around P6G T 105:**

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



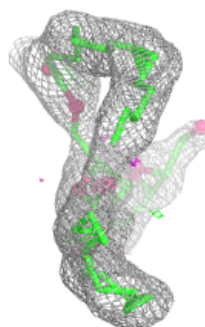
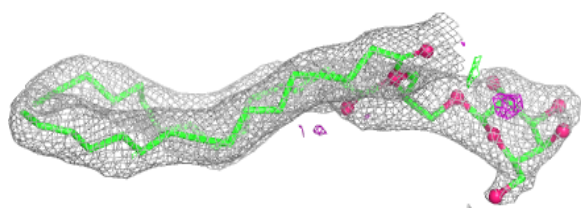
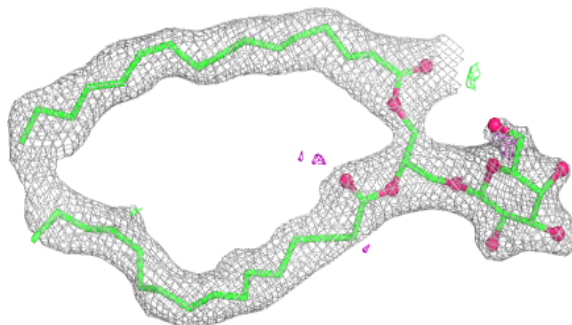
Electron density around SQD A 616:

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

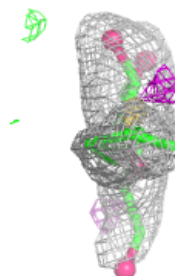
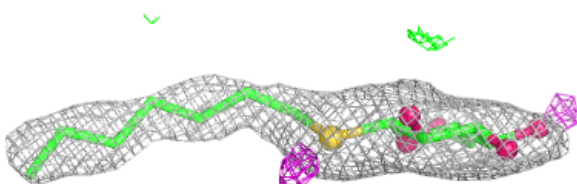
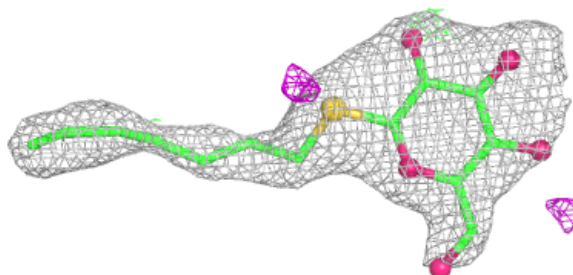


Electron density around LMG a 414:

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

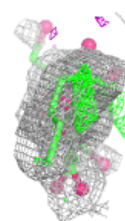
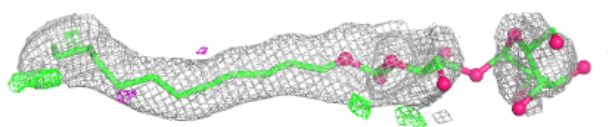
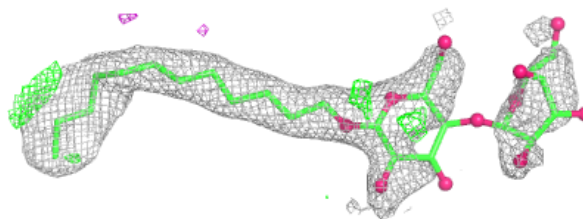
**Electron density around HTG C 521:**

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

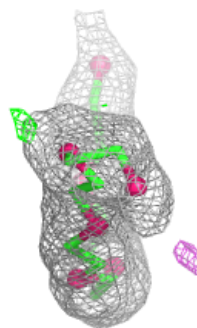
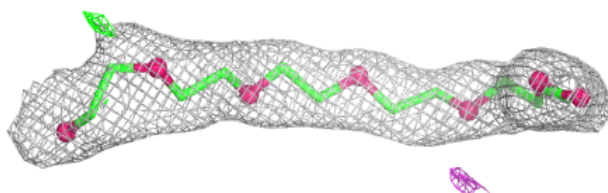
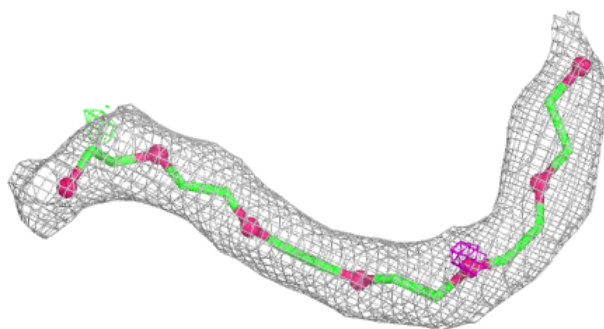


Electron density around LMT t 103:

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

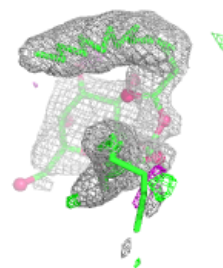
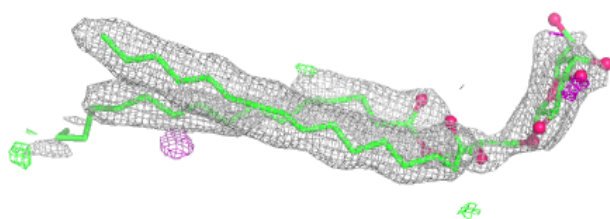
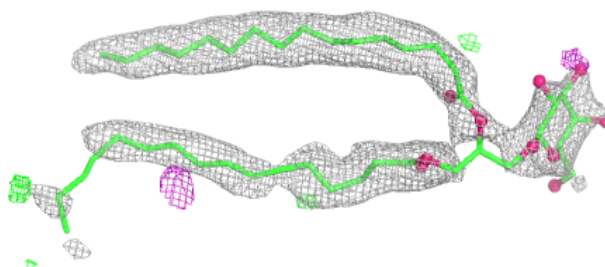
**Electron density around P6G B 651:**

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

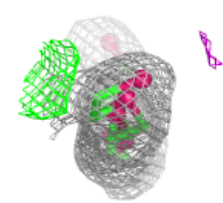
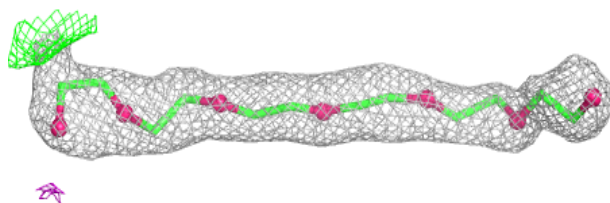
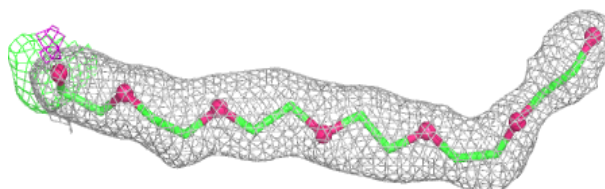


Electron density around LMG C 520:

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

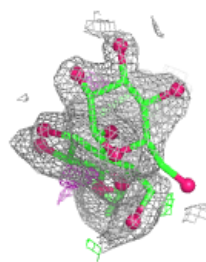
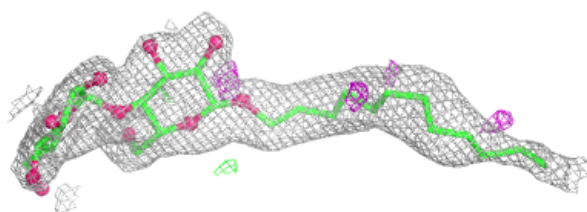
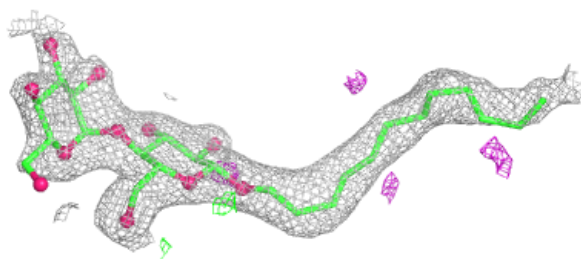
**Electron density around P6G D 416:**

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



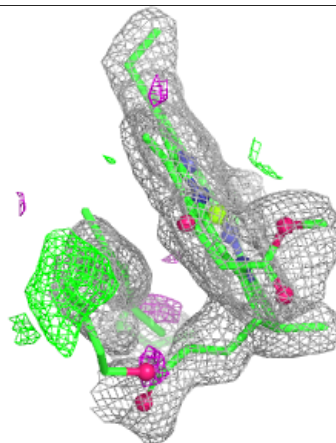
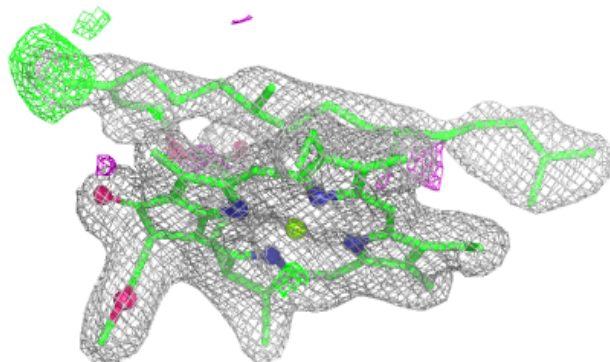
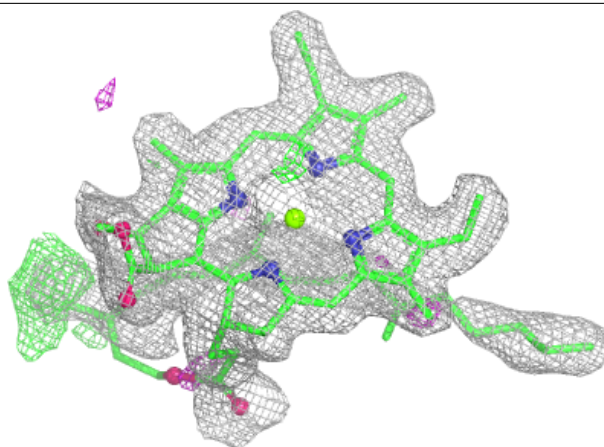
Electron density around LMT A 617:

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

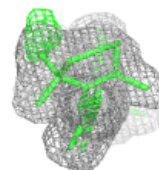
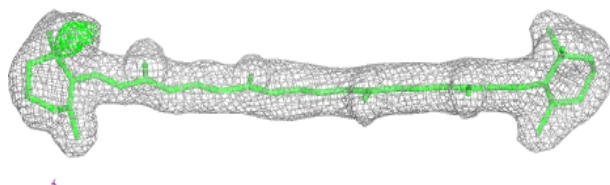
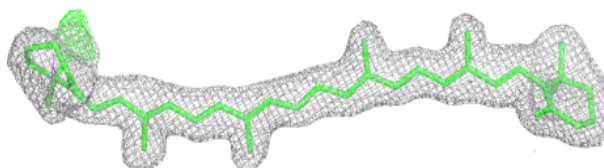


Electron density around CLA b 602:

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

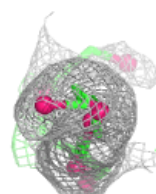
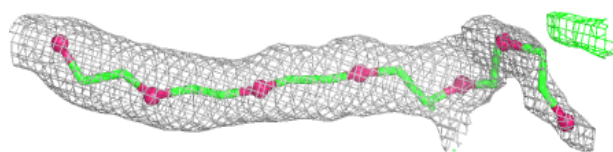
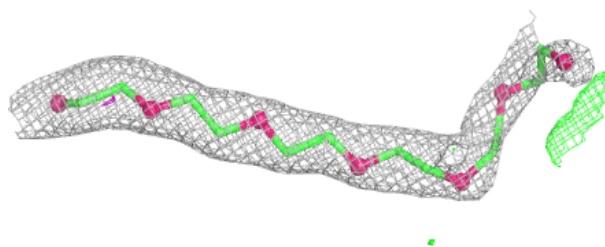
**Electron density around BCR C 514:**

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

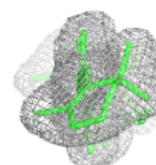
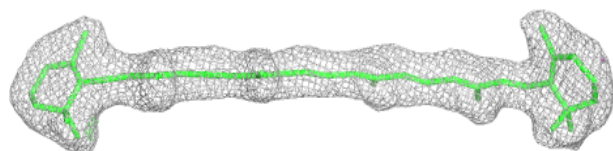
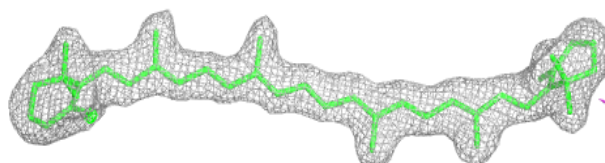


Electron density around P6G A 623:

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

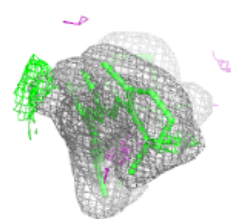
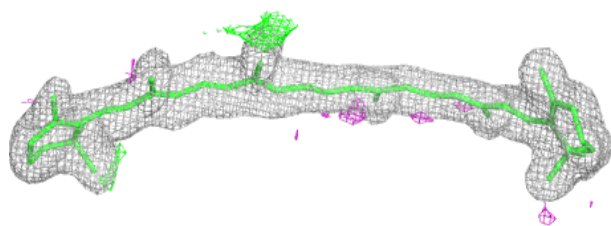
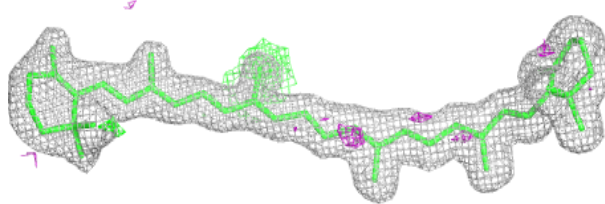
**Electron density around BCR c 514:**

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

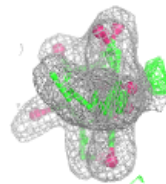
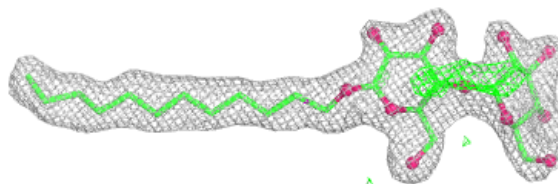


Electron density around BCR t 102:

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

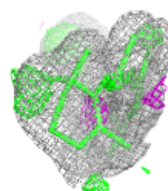
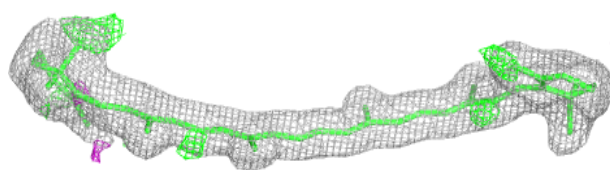
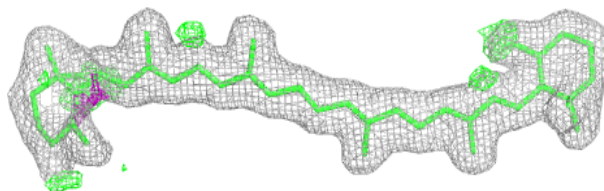
**Electron density around LMT m 102:**

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

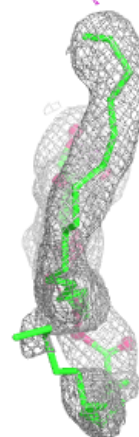
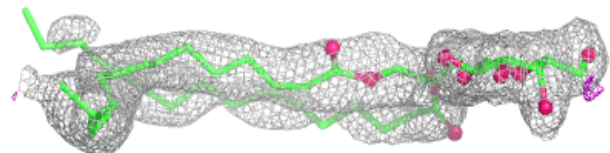
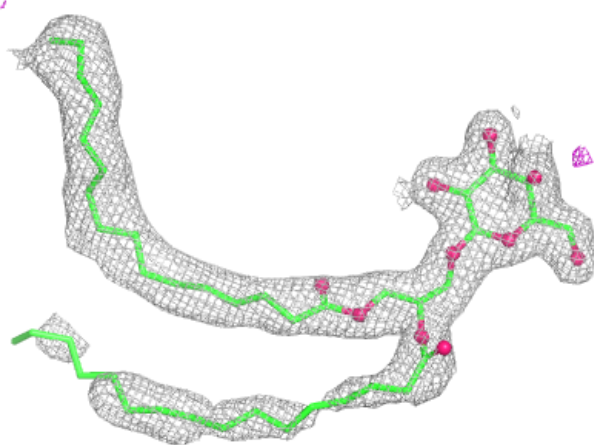


Electron density around BCR D 406:

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

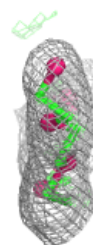
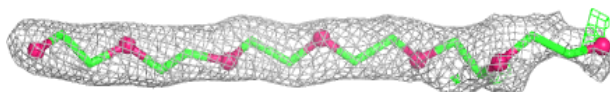
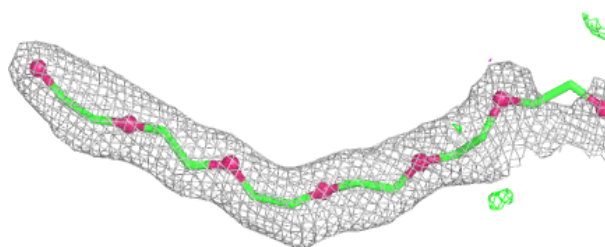
**Electron density around LMG c 519:**

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

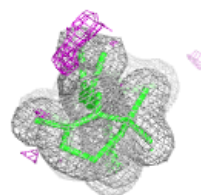
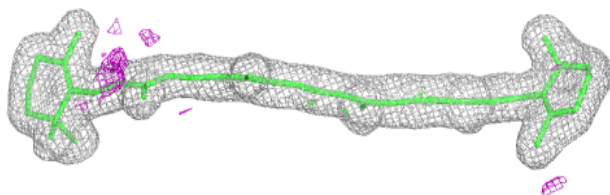
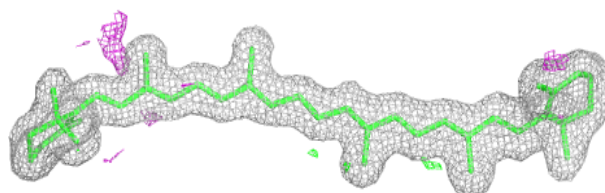


Electron density around P6G D 417:

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

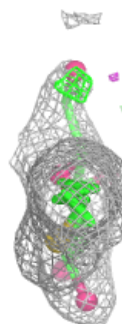
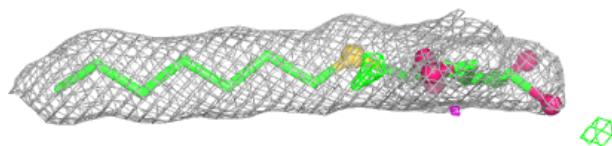
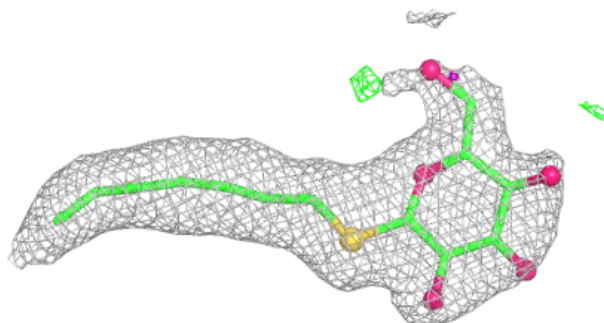
**Electron density around BCR a 411:**

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

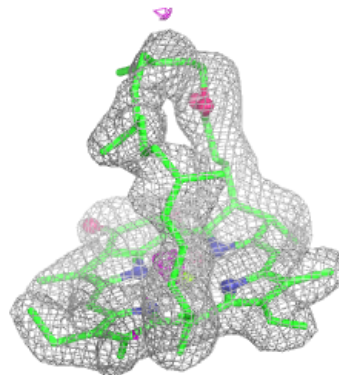
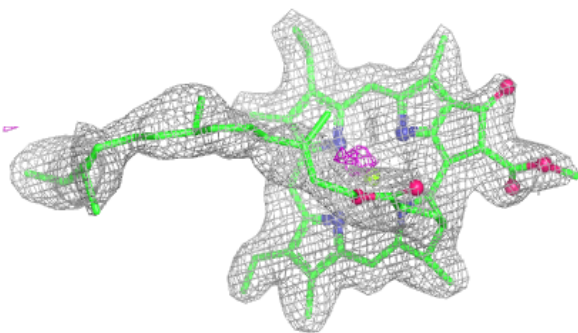
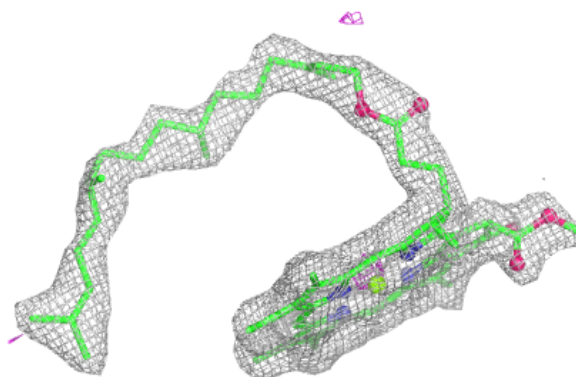


Electron density around HTG b 631:

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

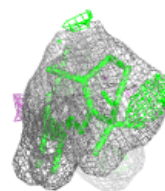
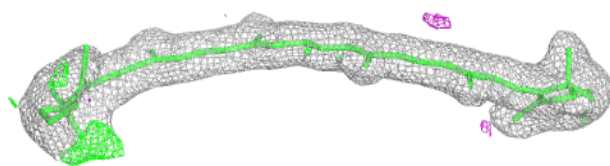
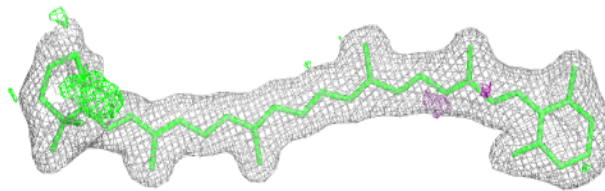
**Electron density around CLA c 513:**

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

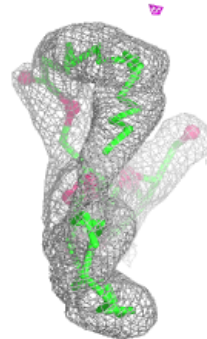
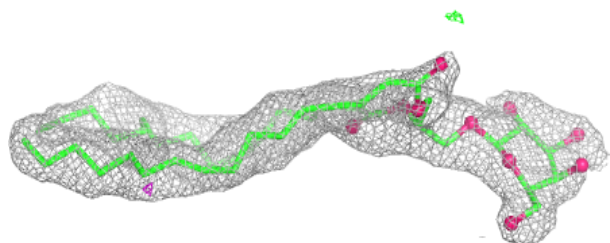


Electron density around BCR d 406:

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

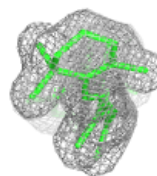
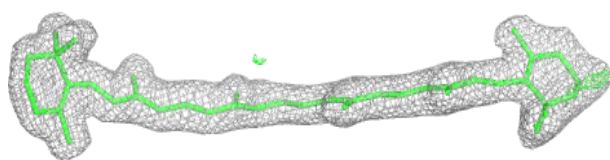
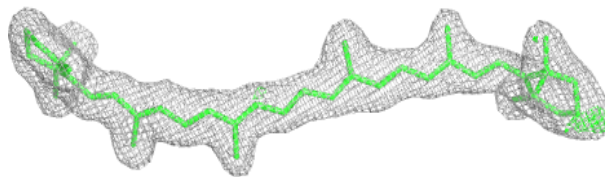
**Electron density around LMG A 613:**

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

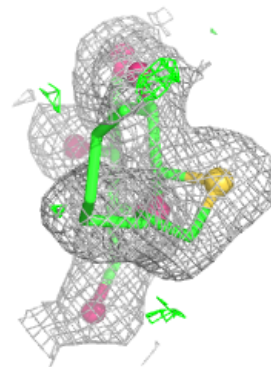
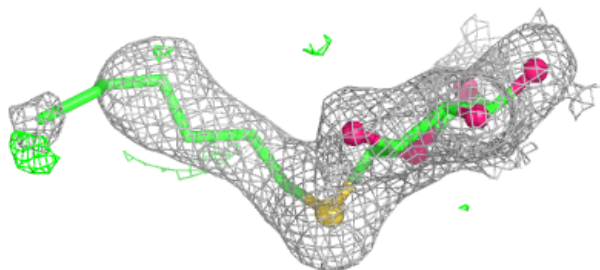
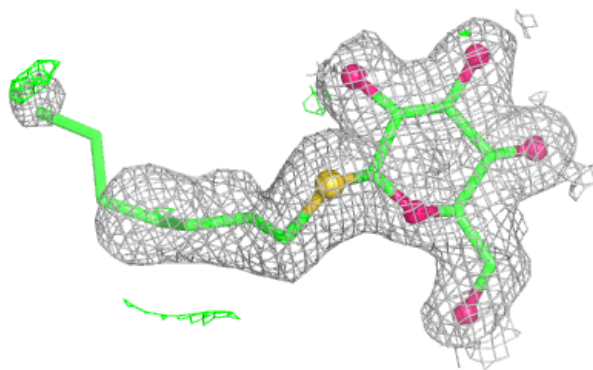


Electron density around BCR h 103:

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

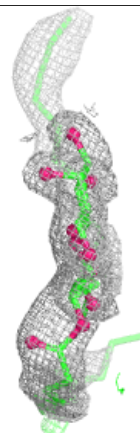
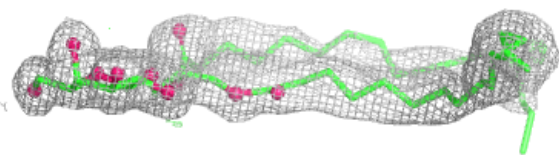
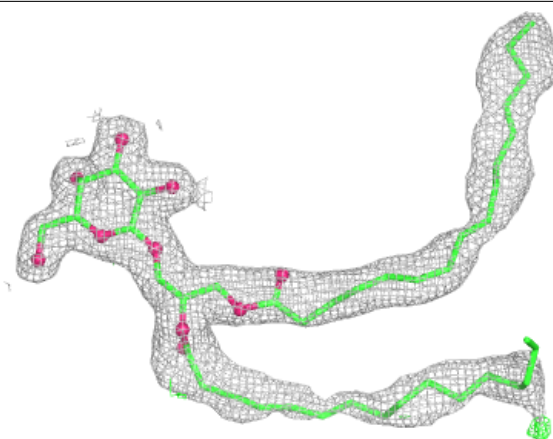
**Electron density around HTG B 623:**

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

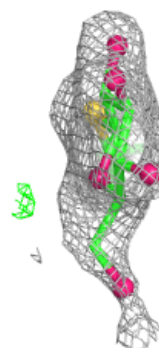
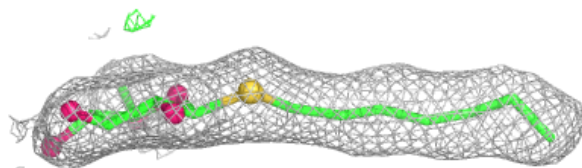
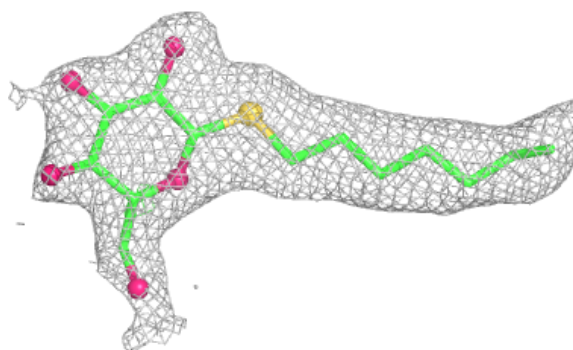


Electron density around LMG C 519:

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

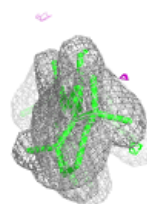
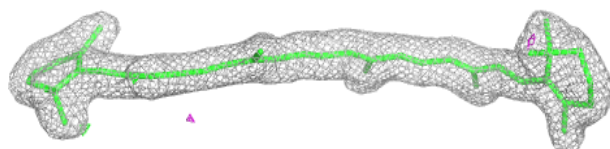
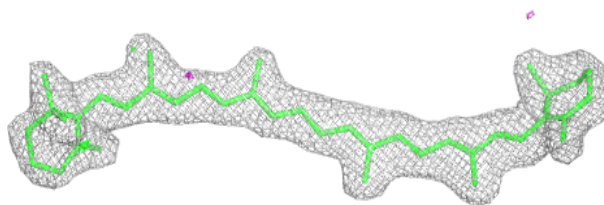
**Electron density around HTG B 630:**

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



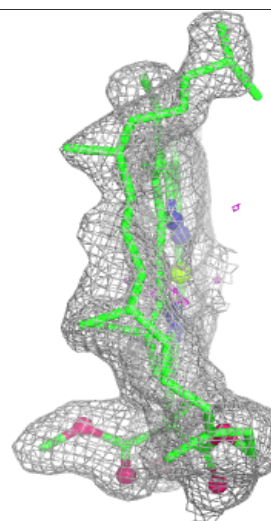
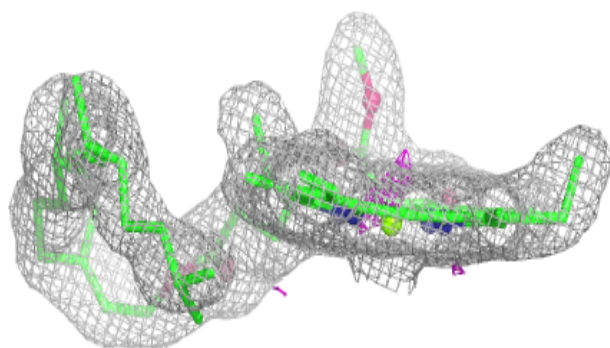
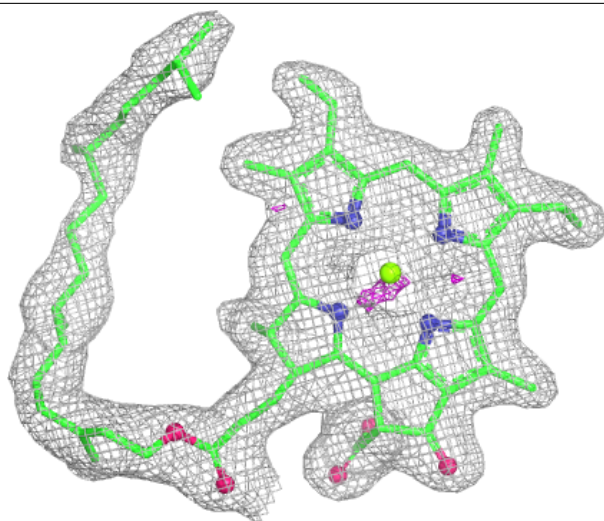
Electron density around BCR k 101:

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



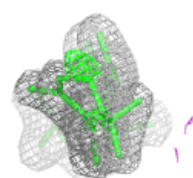
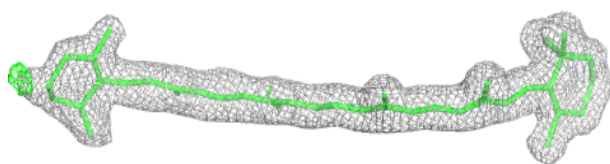
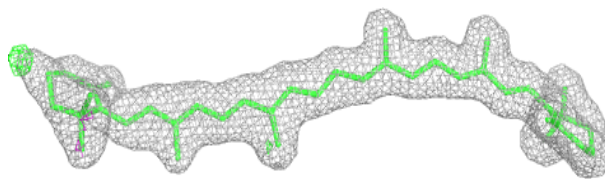
Electron density around CLA C 512:

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

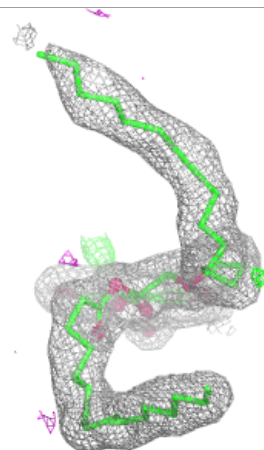
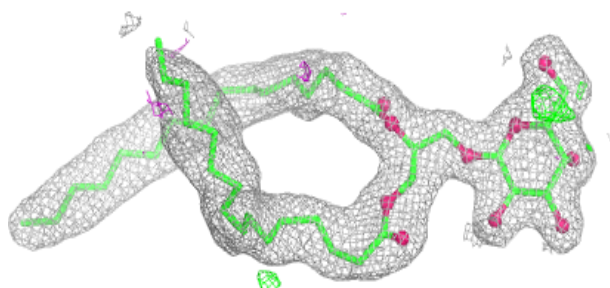
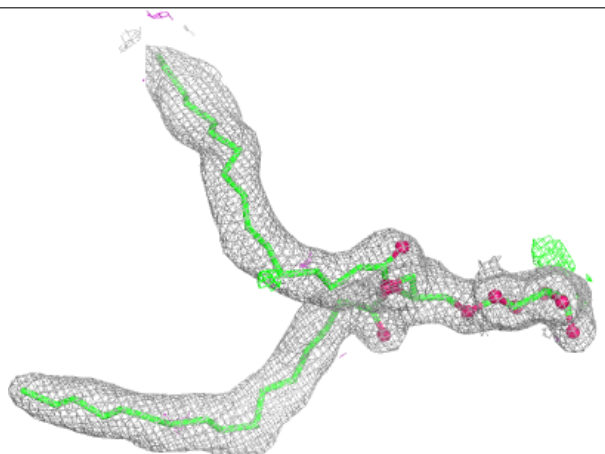


Electron density around BCR H 102:

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

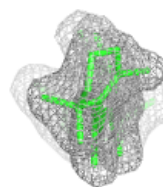
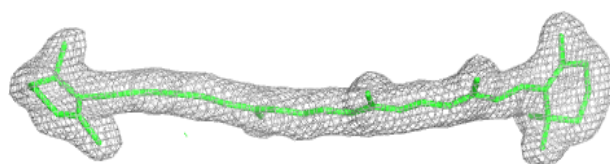
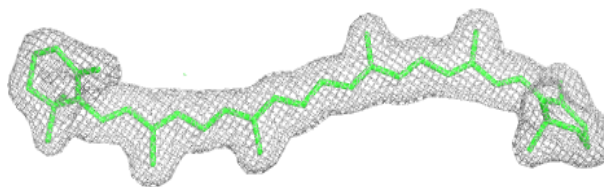
**Electron density around LMG B 621:**

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

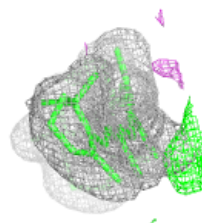
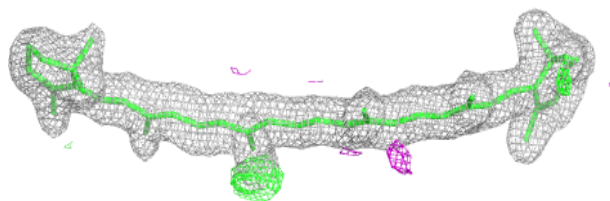
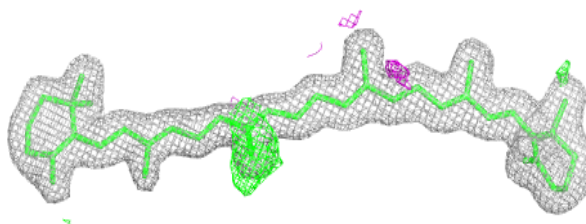


Electron density around BCR K 101:

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

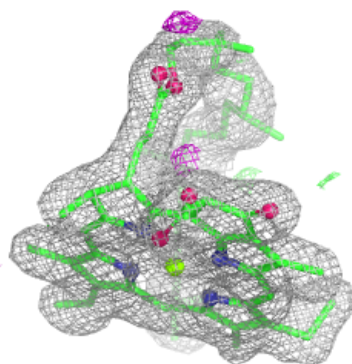
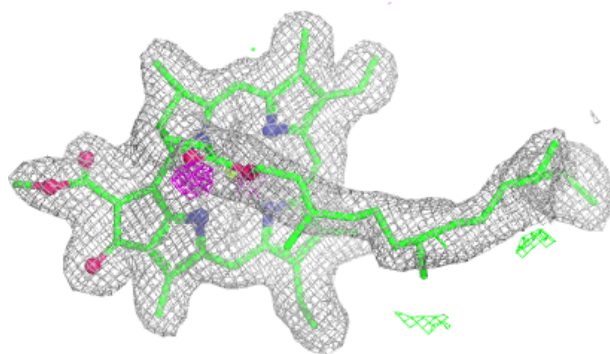
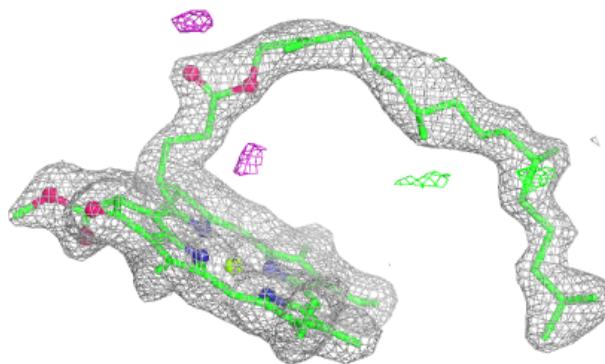
**Electron density around BCR T 102:**

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

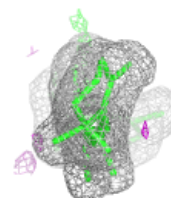
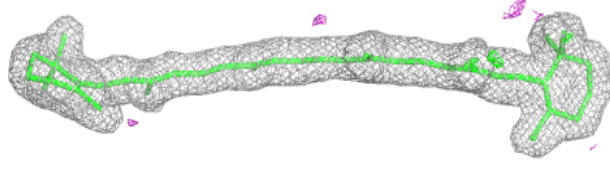
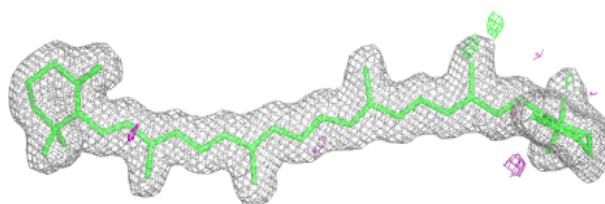


Electron density around CLA C 513:

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

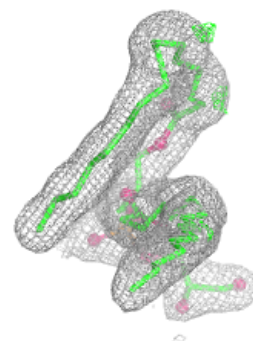
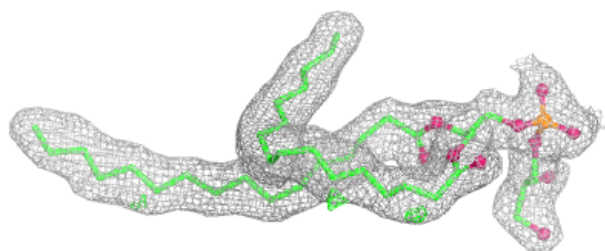
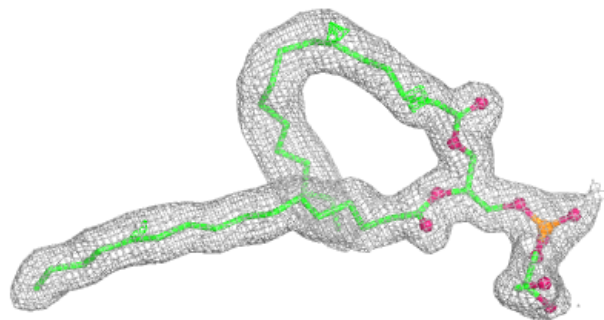
**Electron density around BCR b 618:**

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

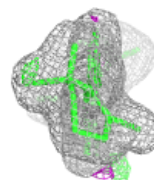
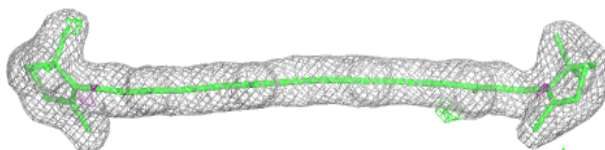
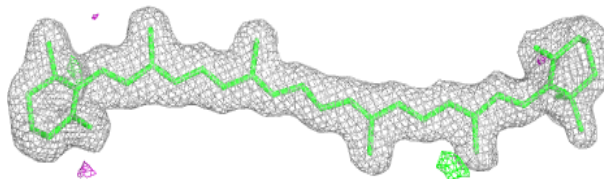


Electron density around LHG D 409:

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

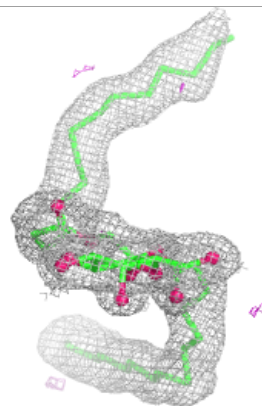
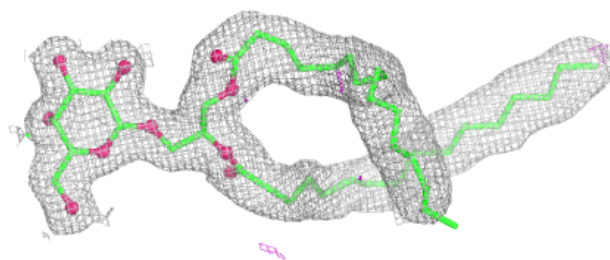
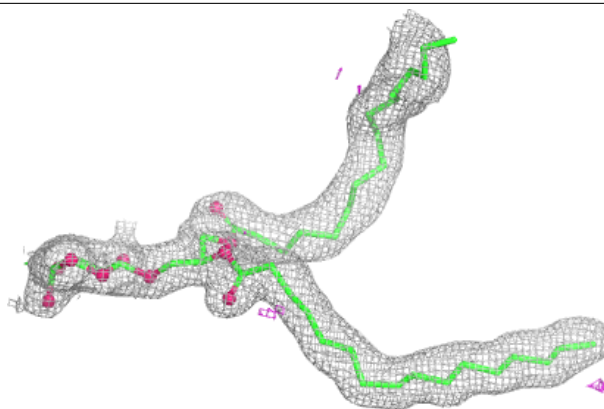
**Electron density around BCR b 619:**

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

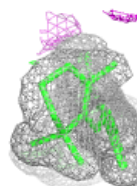
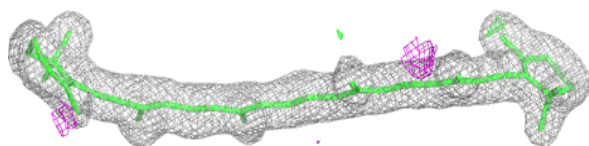
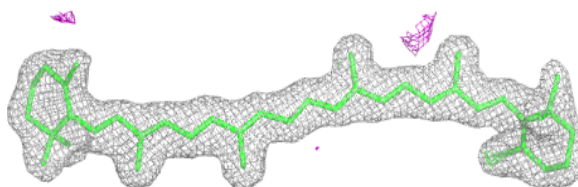


Electron density around LMG b 621:

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

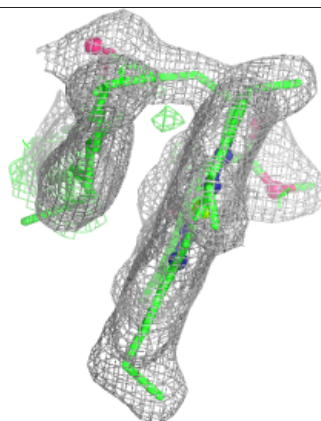
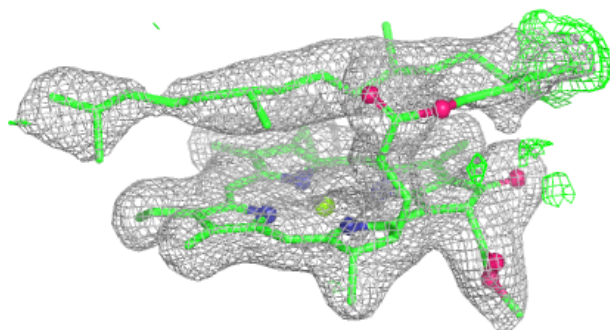
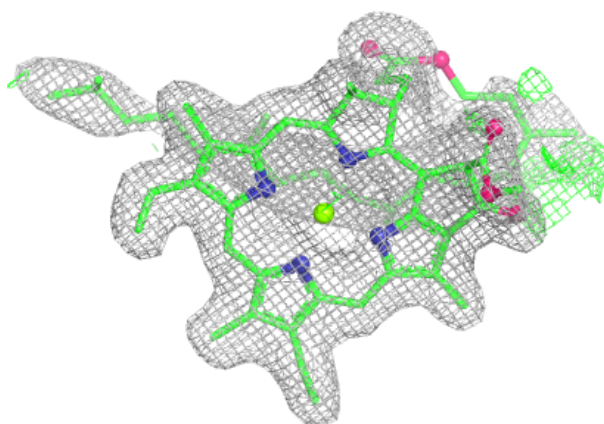
**Electron density around BCR b 620:**

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

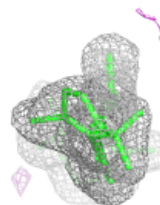
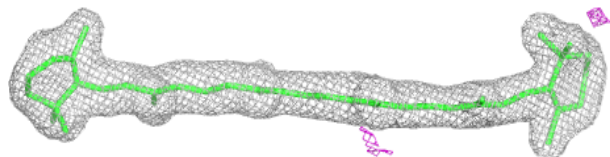
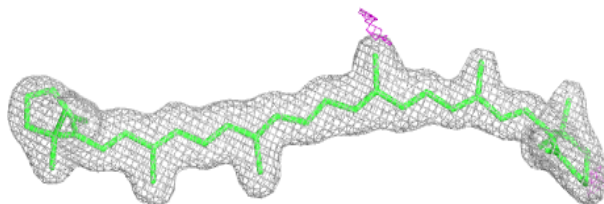


Electron density around CLA B 602:

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

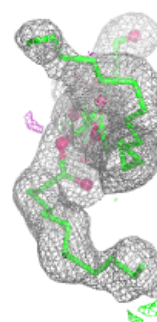
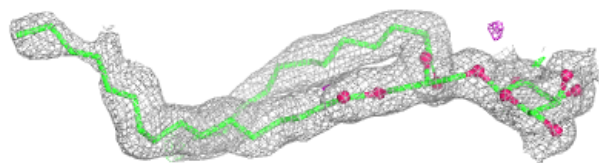
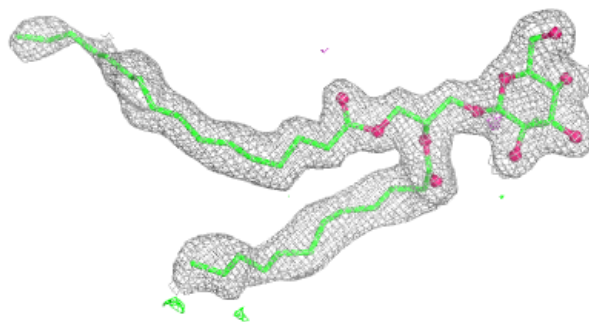
**Electron density around BCR c 515:**

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

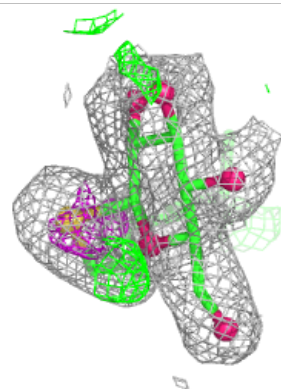
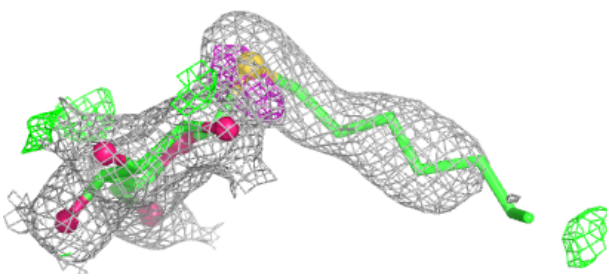
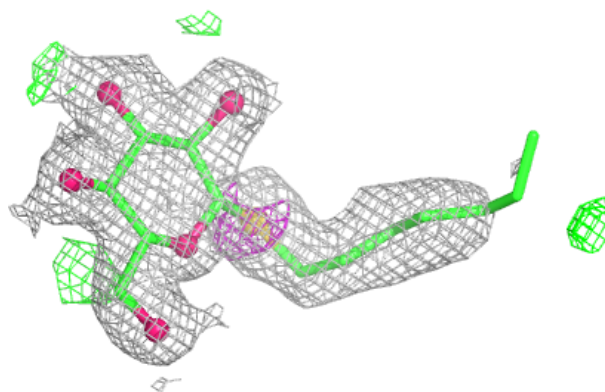


Electron density around LMG j 101:

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

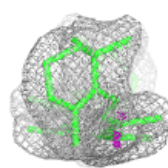
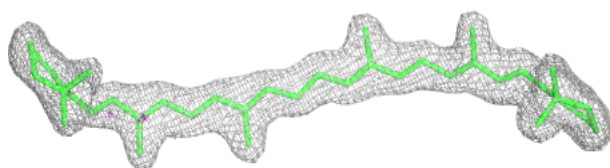
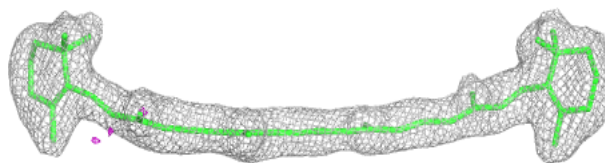
**Electron density around HTG b 623:**

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

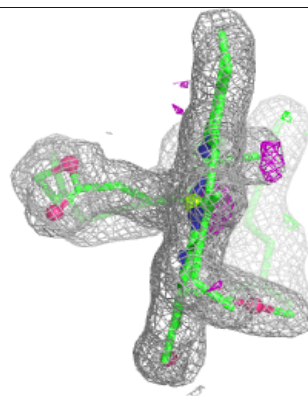
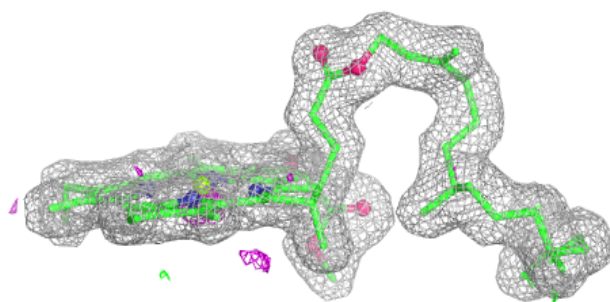
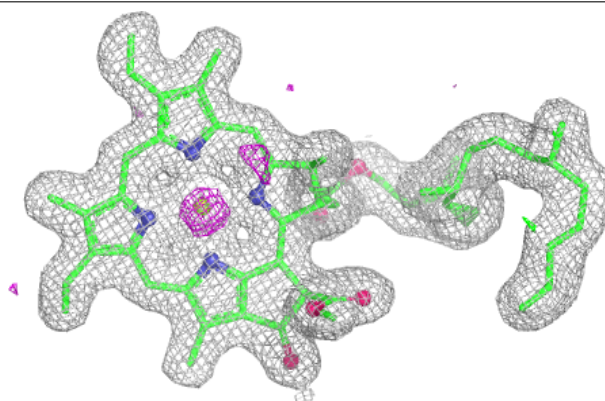


Electron density around BCR c 527:

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

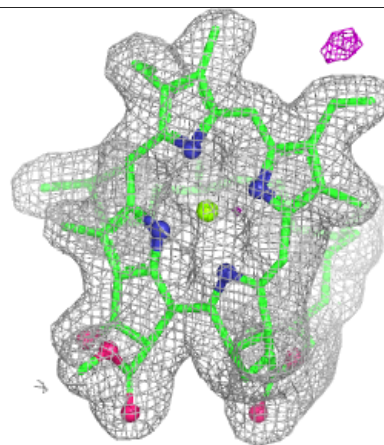
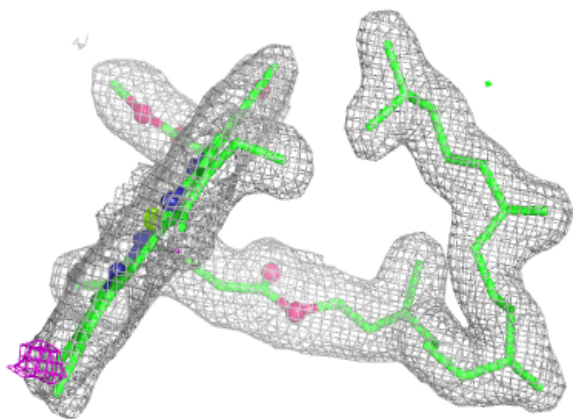
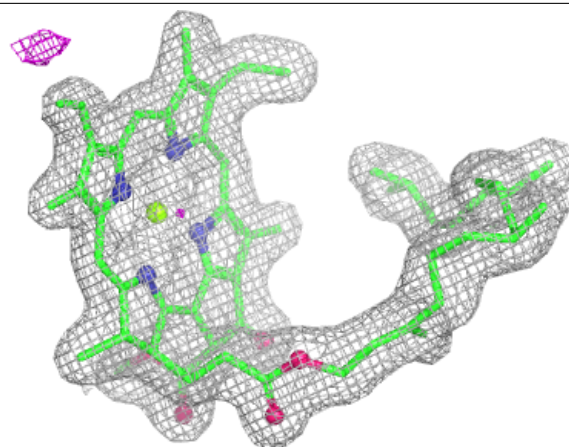
**Electron density around CLA b 613:**

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

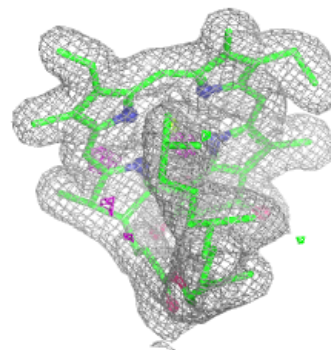
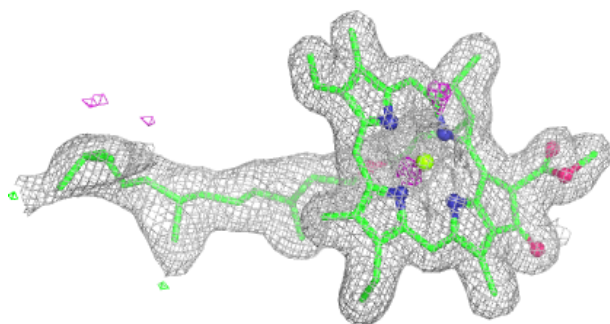
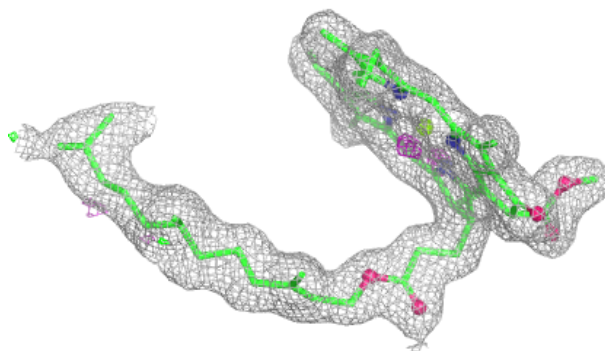


Electron density around CLA c 503:

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

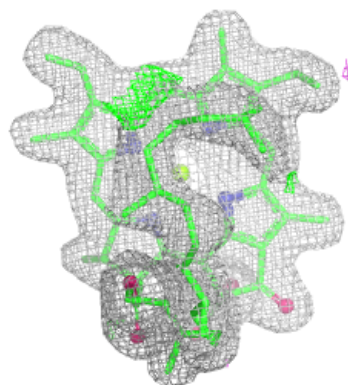
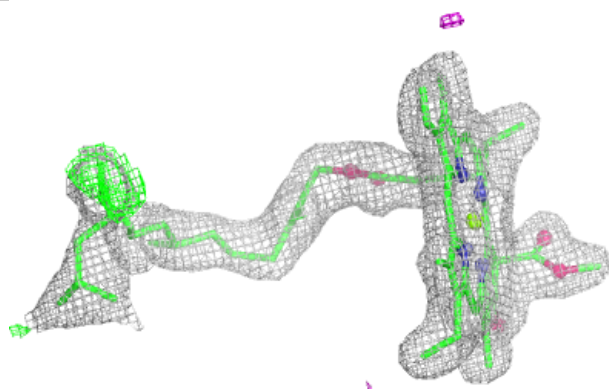
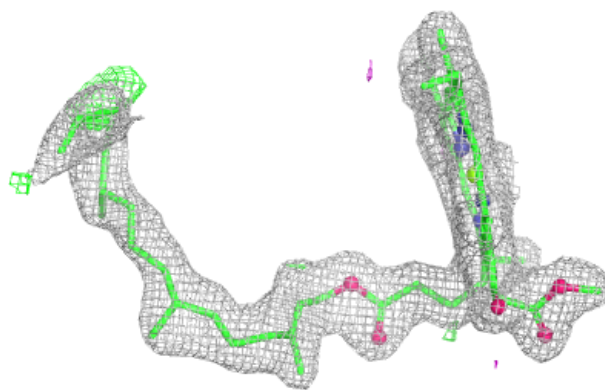
**Electron density around CLA c 504:**

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



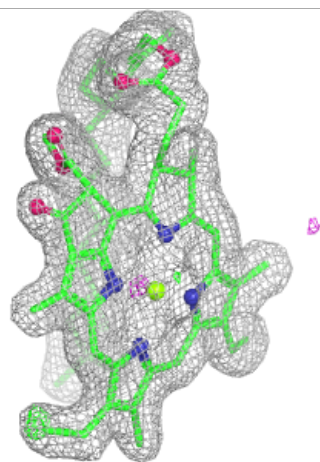
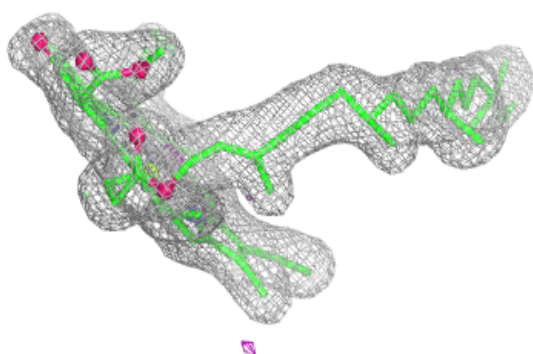
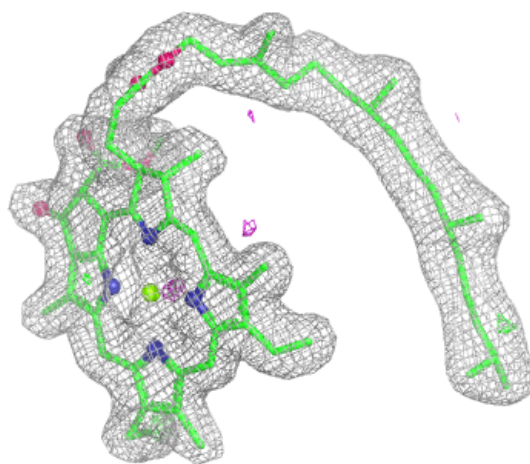
Electron density around CLA c 506:

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



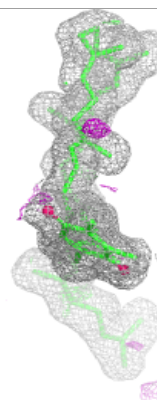
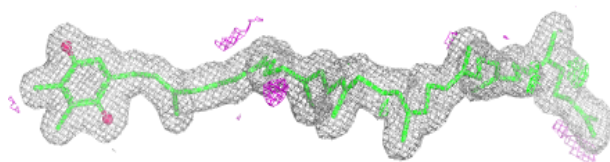
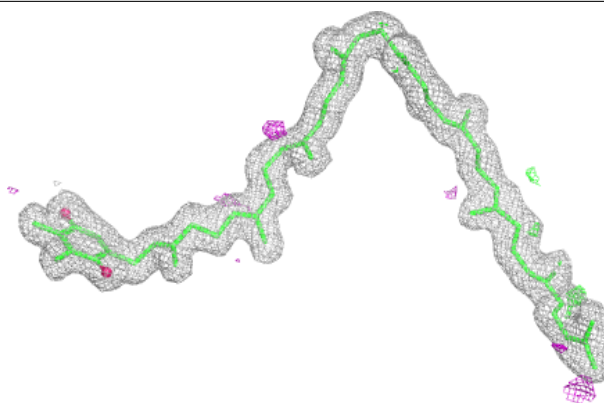
Electron density around CLA c 507:

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

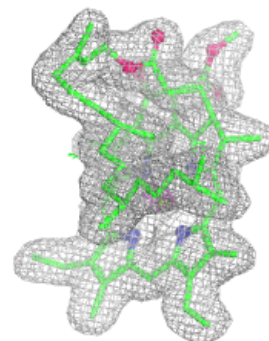
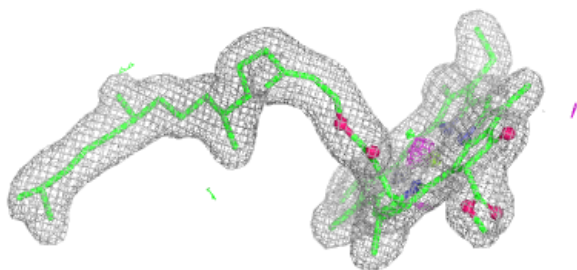
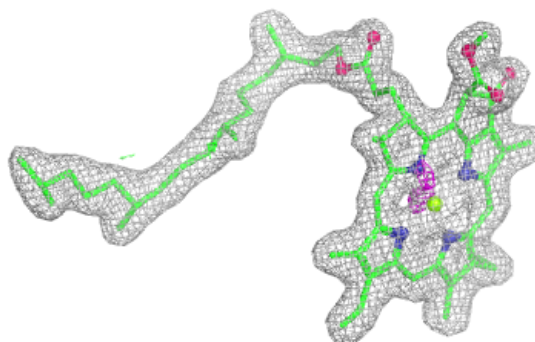


Electron density around PL9 D 407:

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

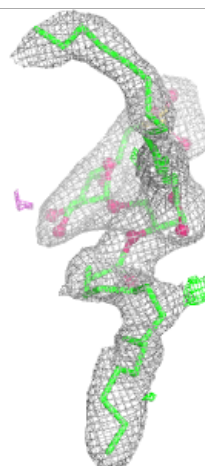
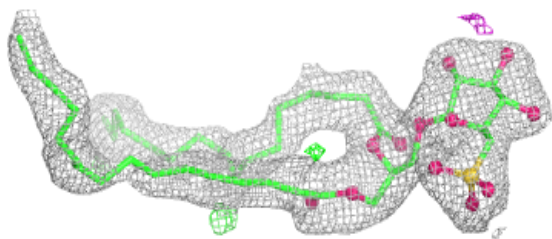
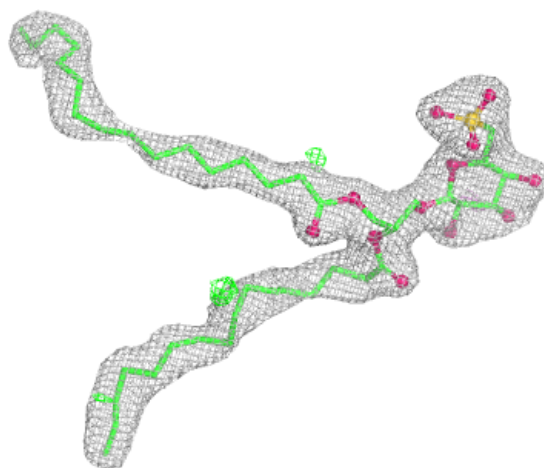
**Electron density around CLA c 511:**

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



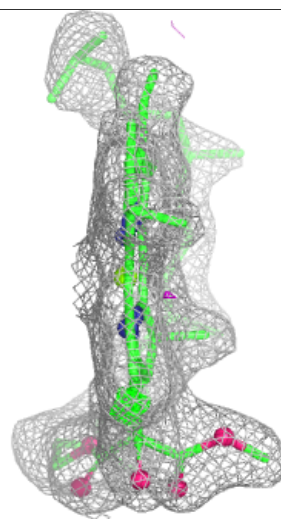
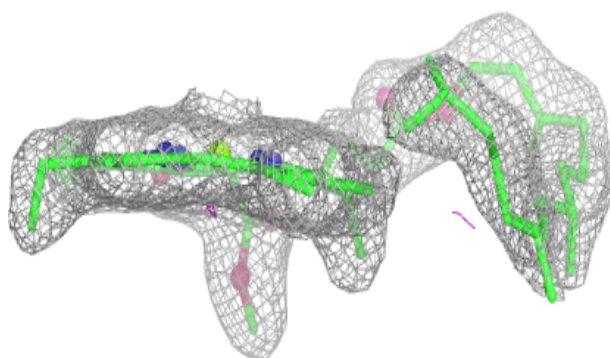
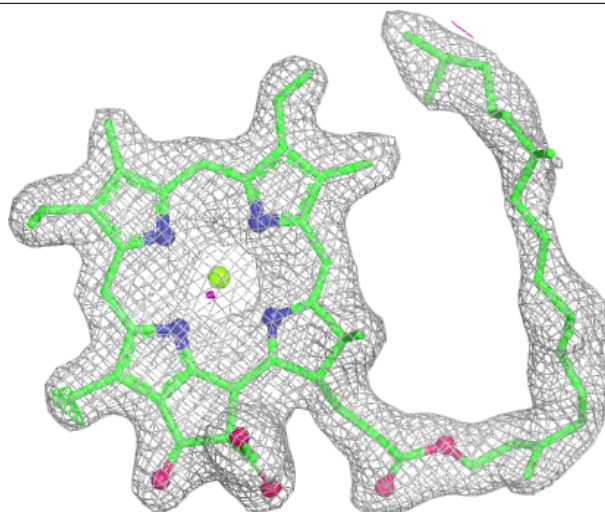
Electron density around SQD A 612:

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



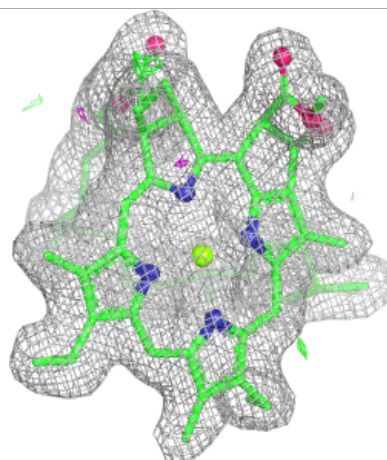
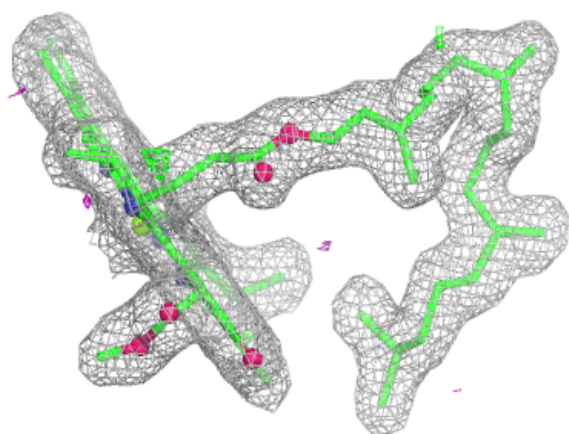
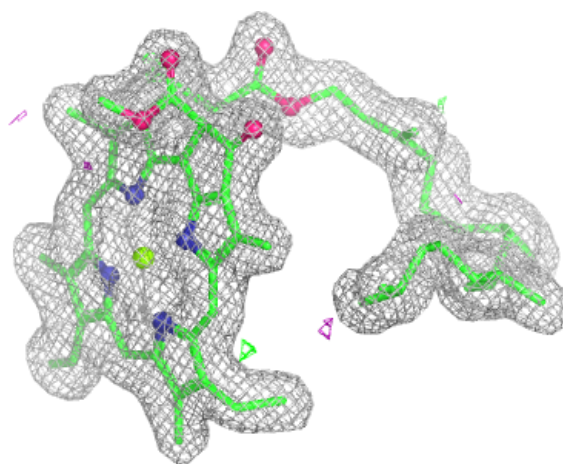
Electron density around CLA c 512:

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



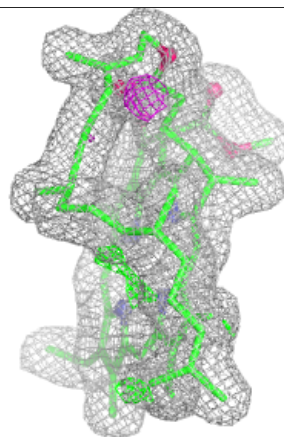
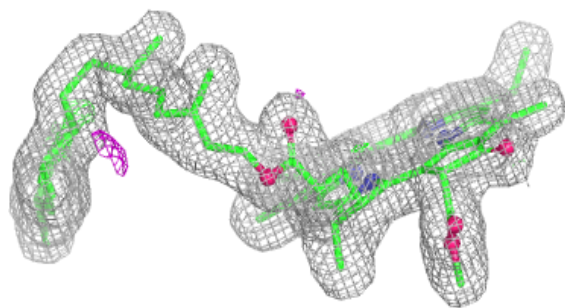
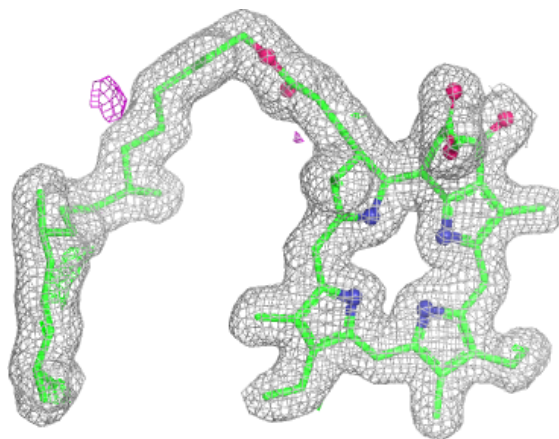
Electron density around CLA C 503:

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



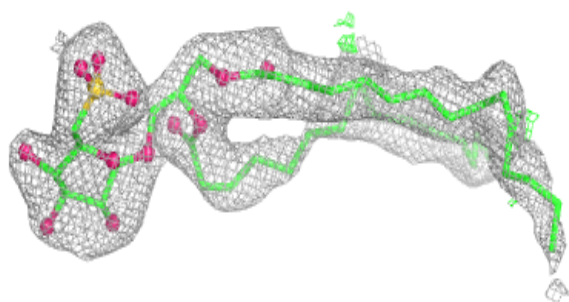
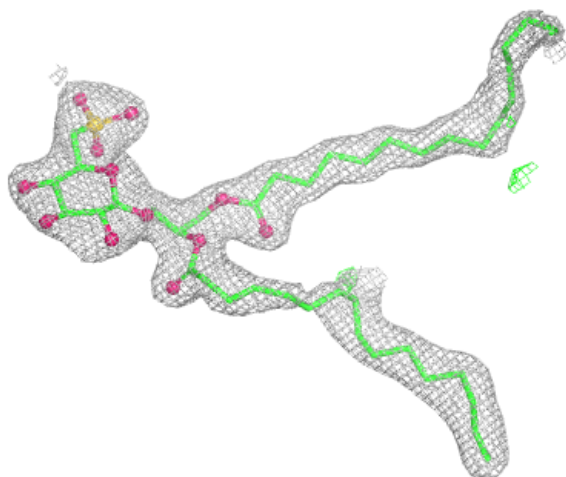
Electron density around PHO d 401:

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



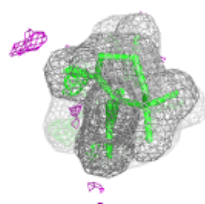
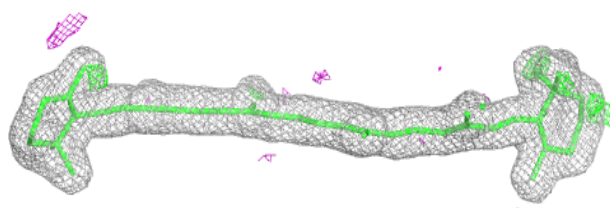
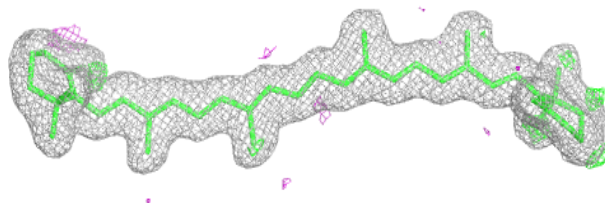
Electron density around SQD a 413:

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

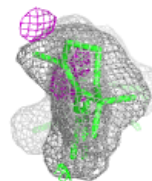
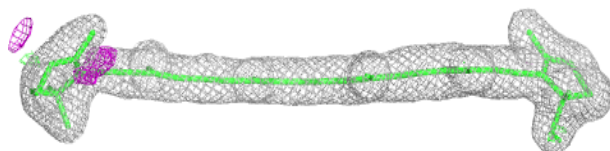
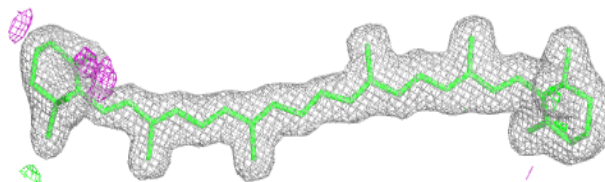


Electron density around BCR A 610:

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

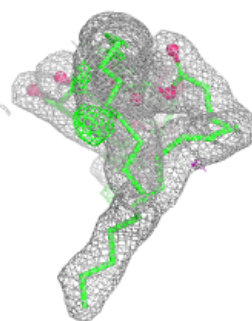
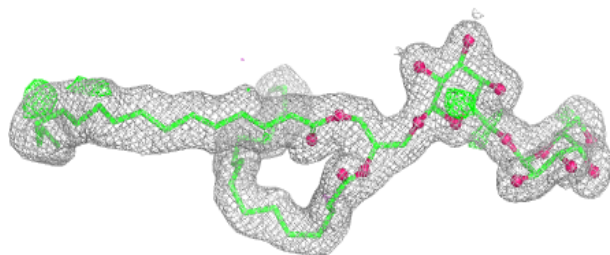
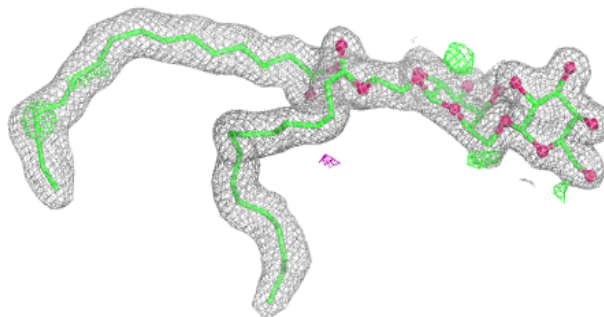
**Electron density around BCR B 619:**

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

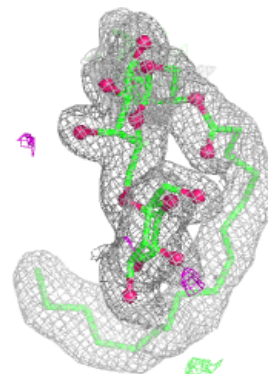
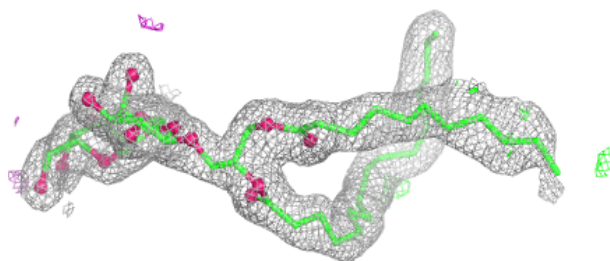
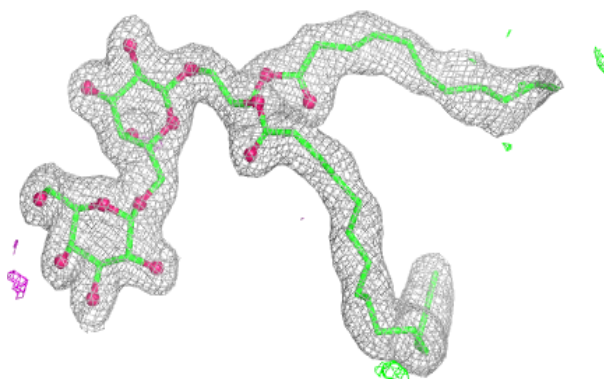


Electron density around DGD H 103:

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

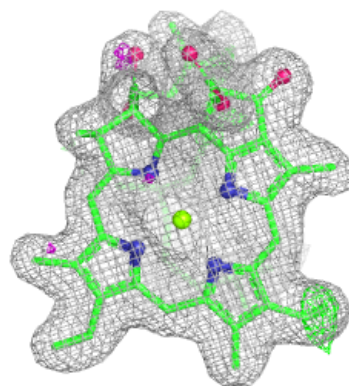
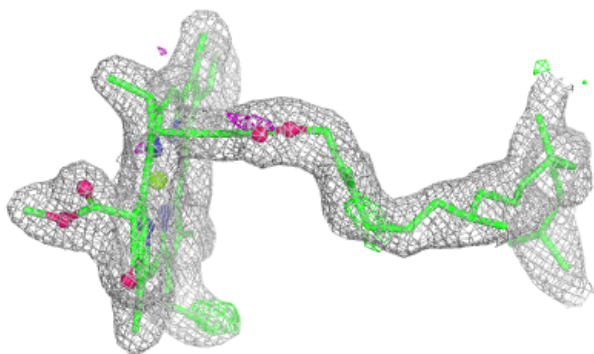
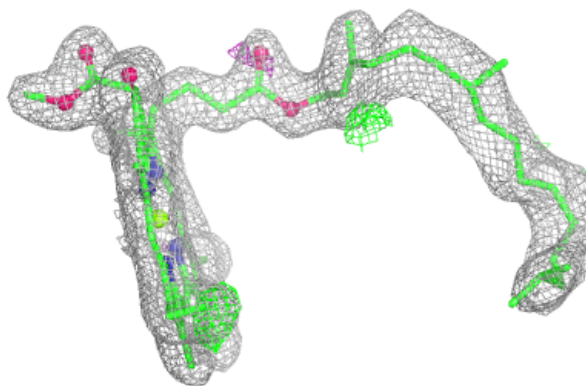
**Electron density around DGD c 517:**

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

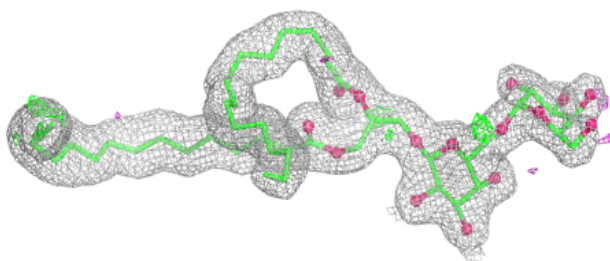
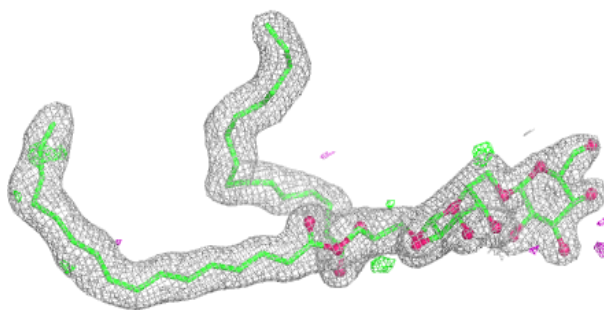


Electron density around CLA C 506:

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

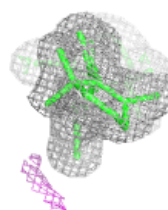
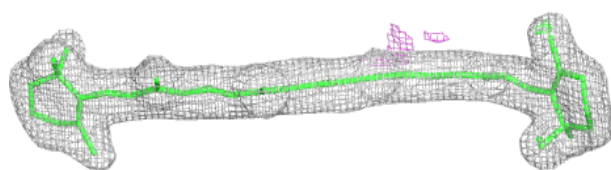
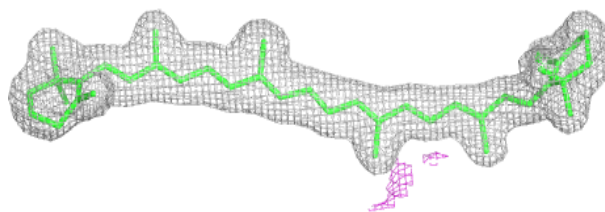
**Electron density around DGD h 104:**

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

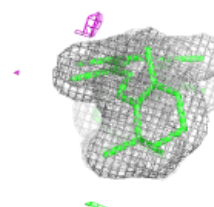
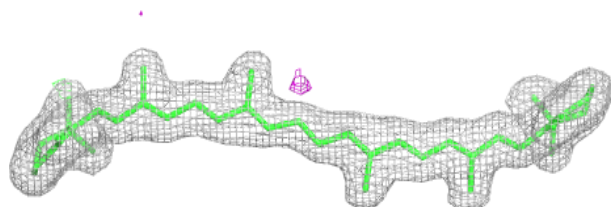
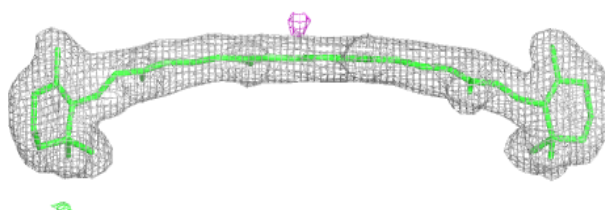


Electron density around BCR C 515:

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

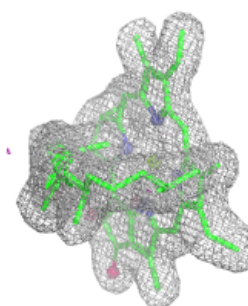
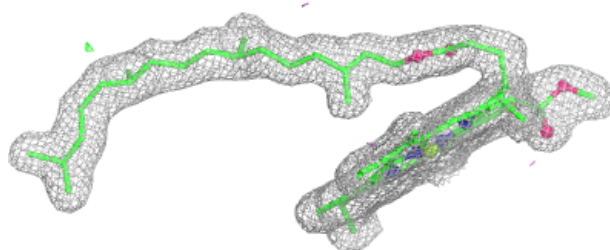
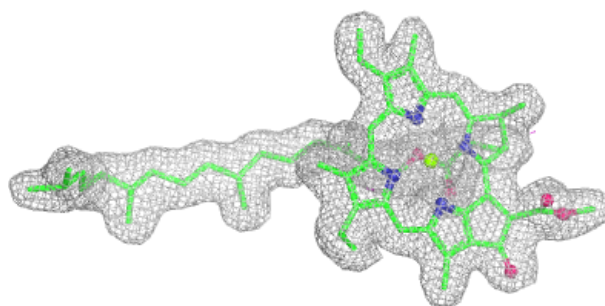
**Electron density around BCR C 525:**

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

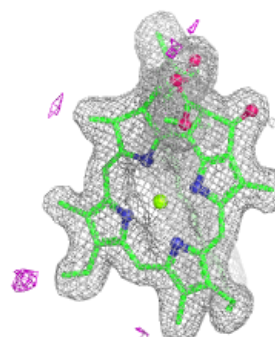
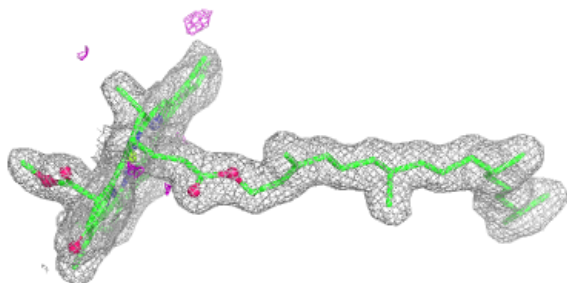
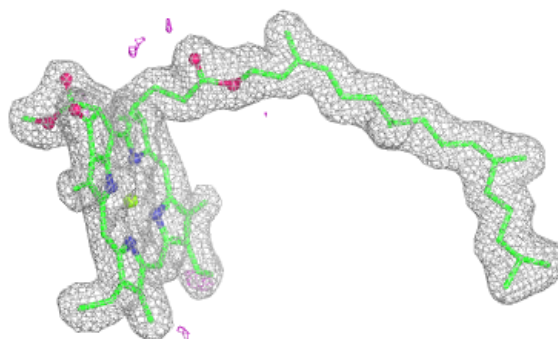


Electron density around CLA b 609:

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

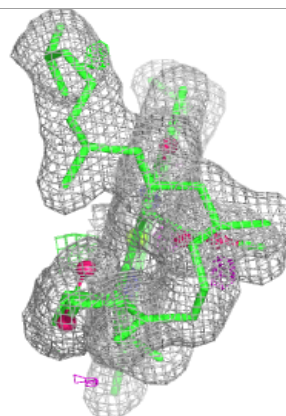
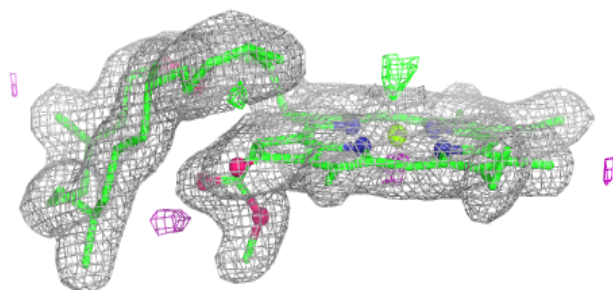
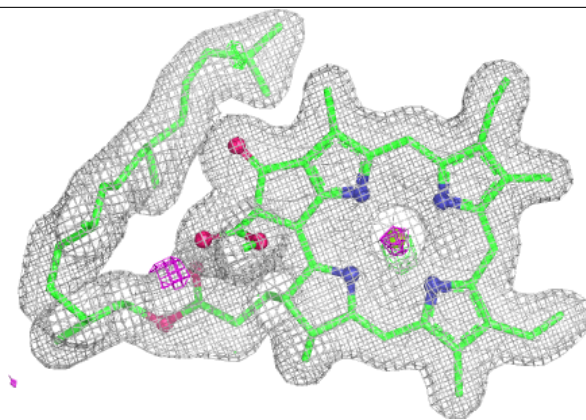
**Electron density around CLA b 610:**

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



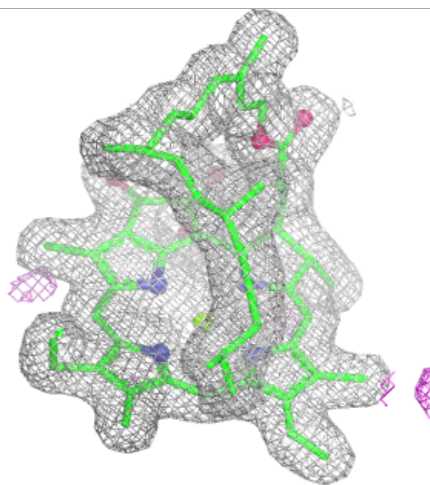
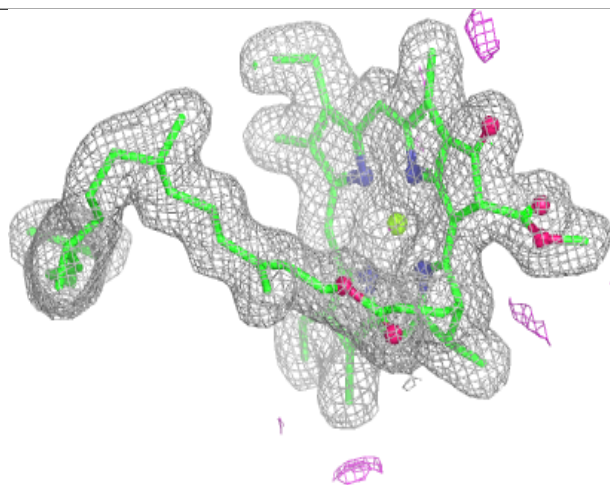
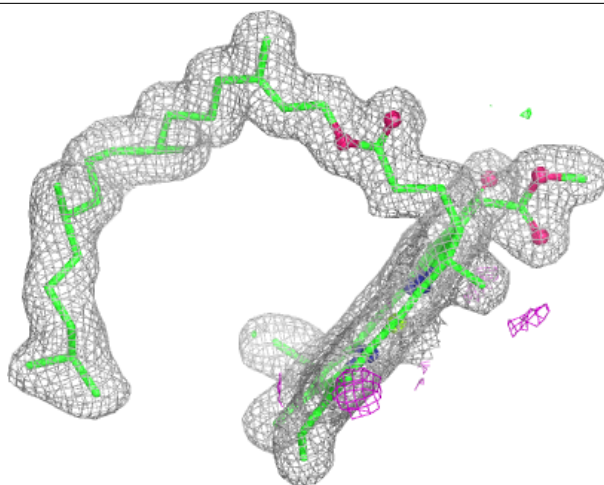
Electron density around CLA b 611:

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



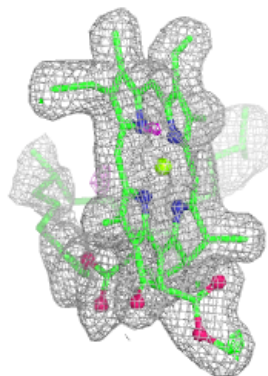
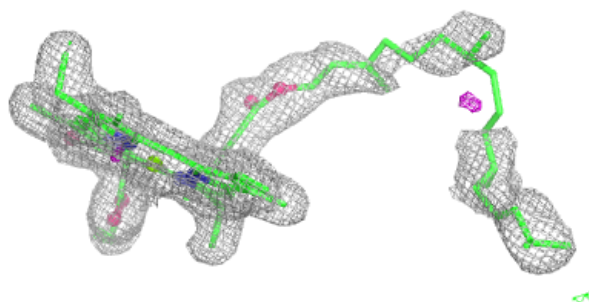
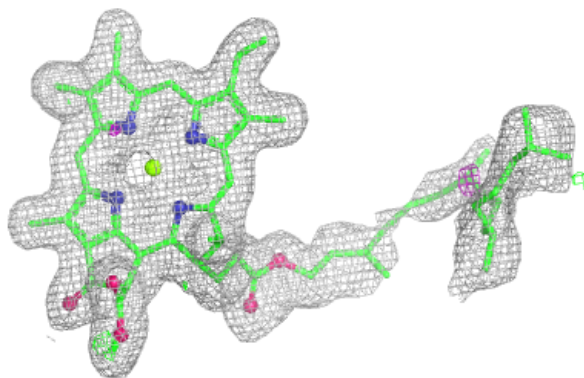
Electron density around CLA b 612:

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



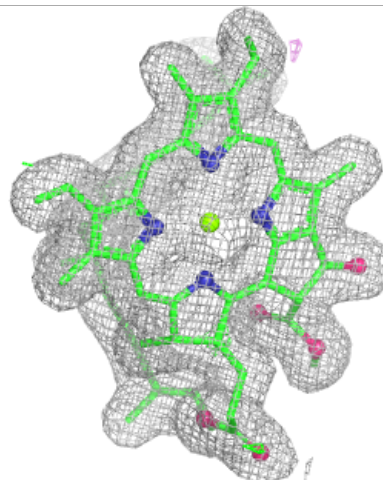
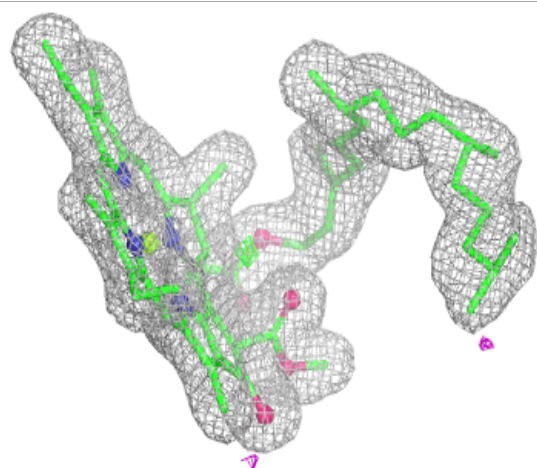
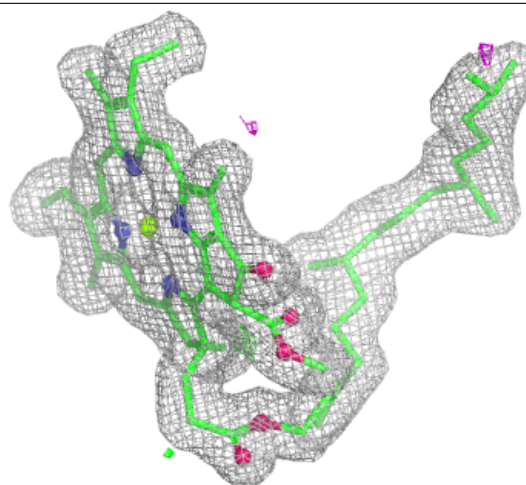
Electron density around CLA A 609:

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



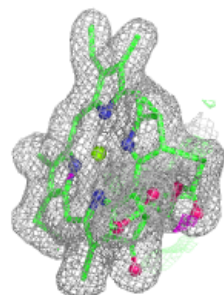
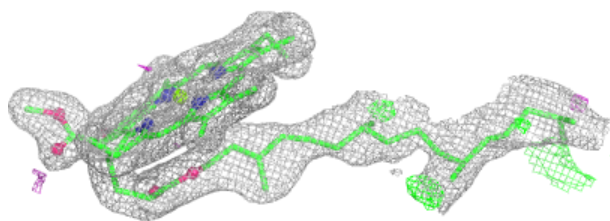
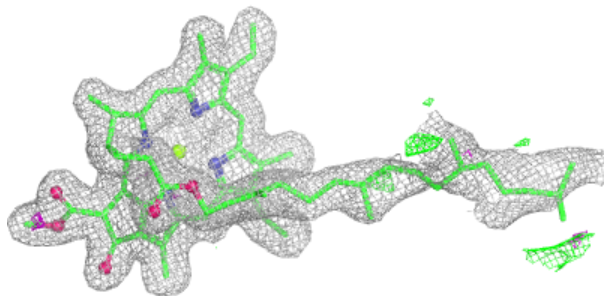
Electron density around CLA b 614:

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



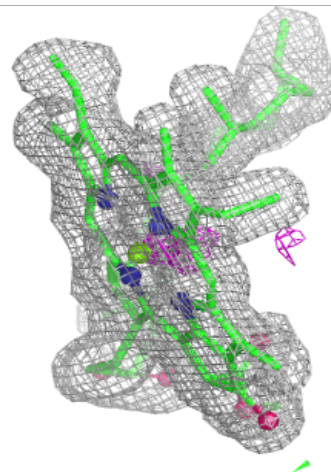
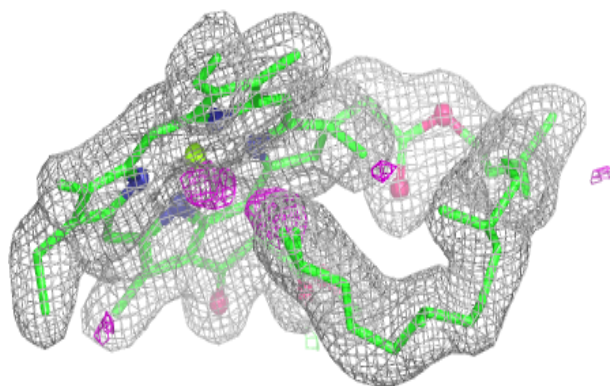
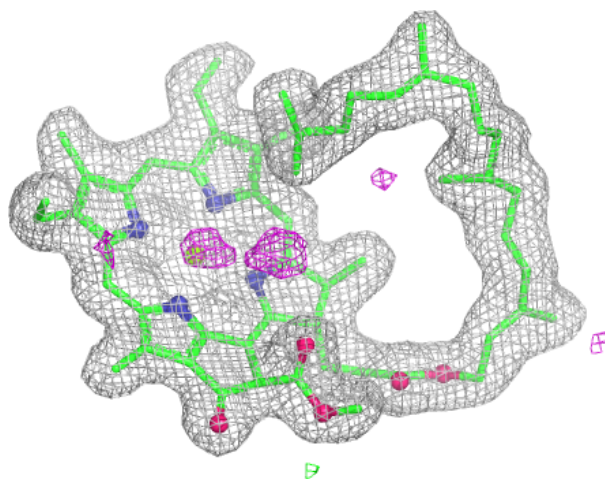
Electron density around CLA b 615:

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



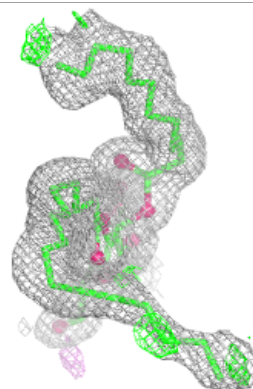
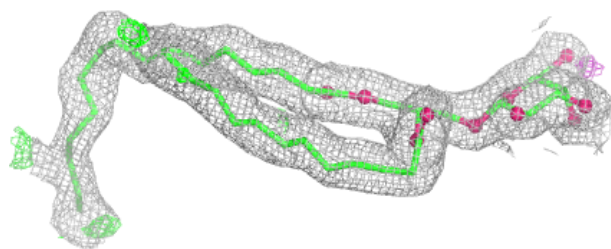
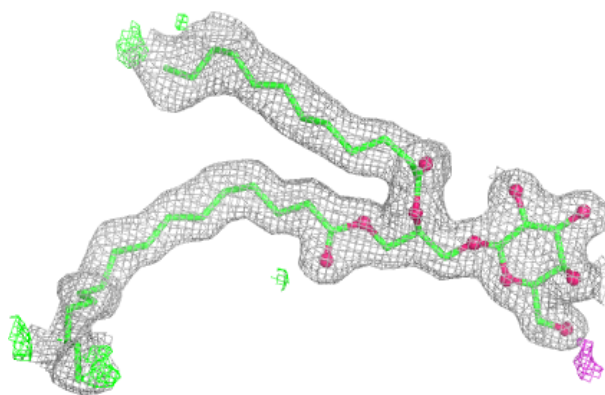
Electron density around CLA b 616:

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

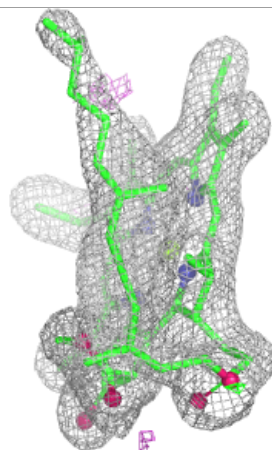
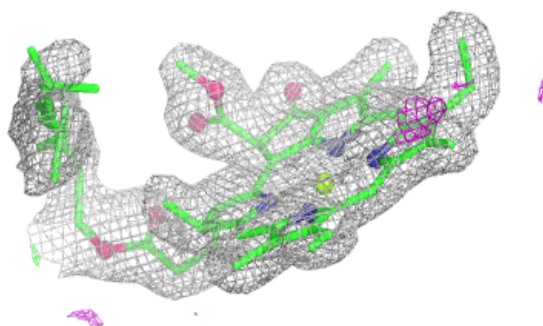
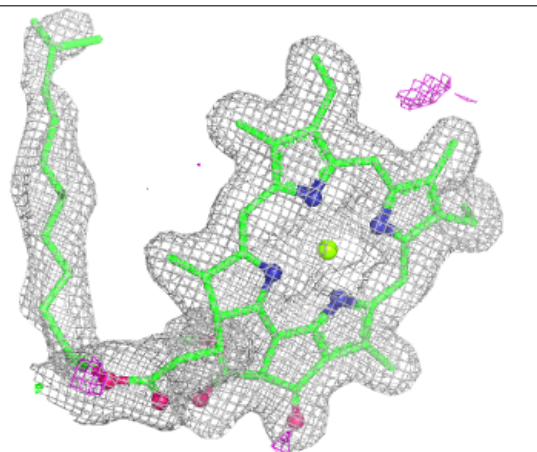


Electron density around LMG J 101:

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

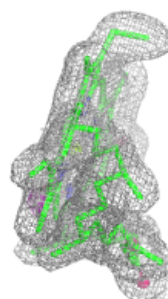
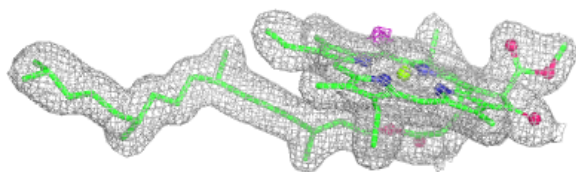
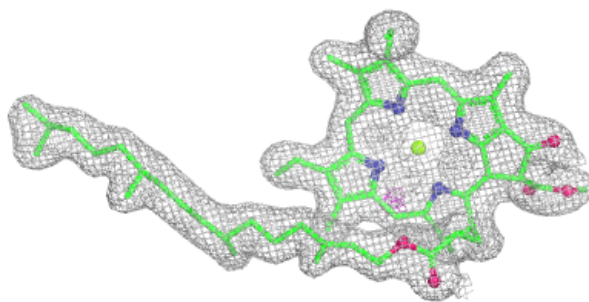
**Electron density around CLA b 617:**

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

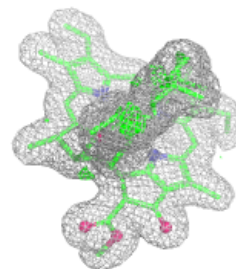
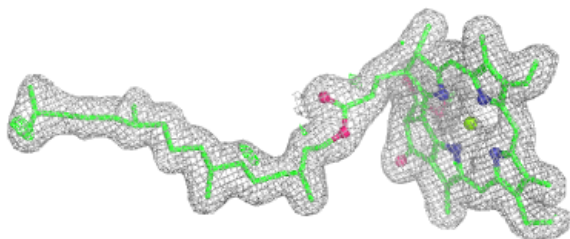
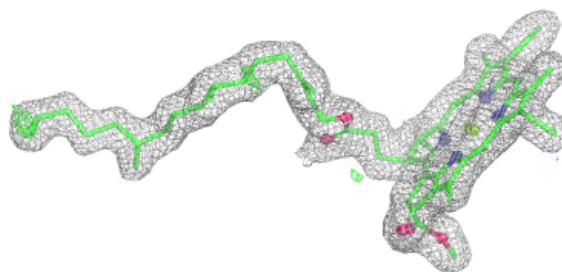


Electron density around CLA c 501:

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

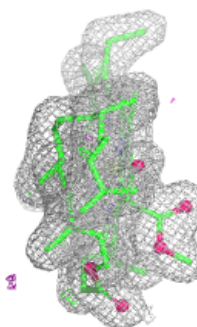
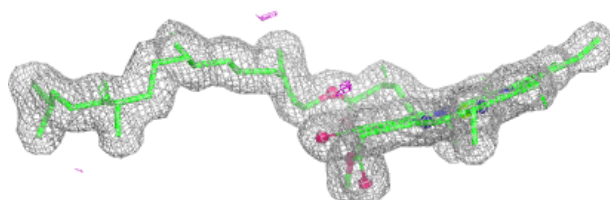
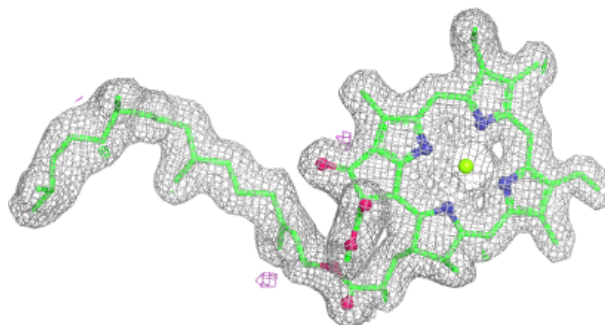
**Electron density around CLA c 502:**

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

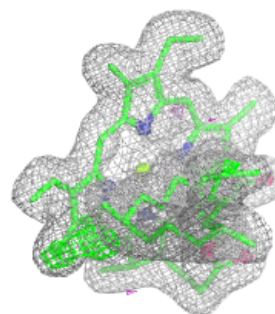
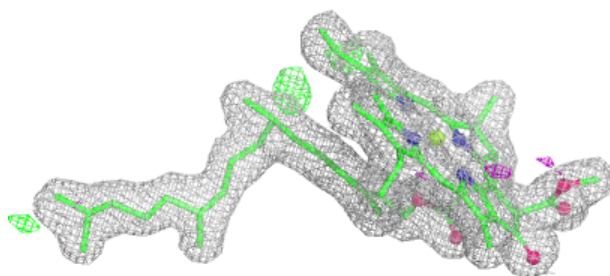
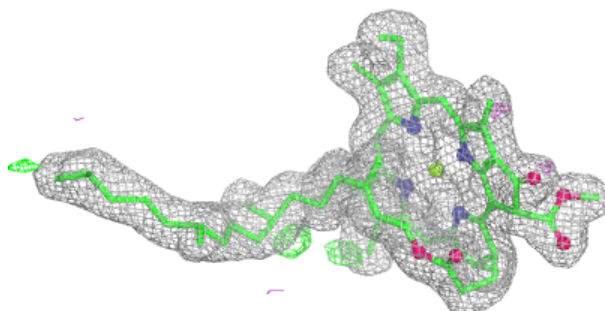


Electron density around CLA B 603:

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

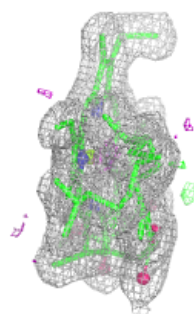
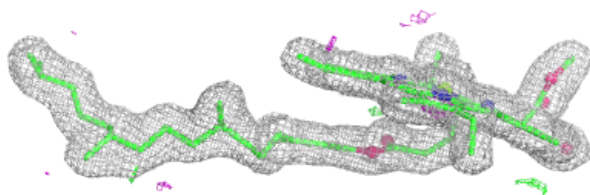
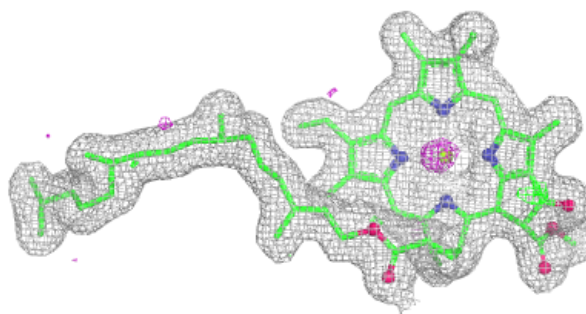
**Electron density around CLA c 505:**

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

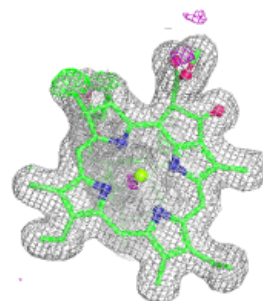
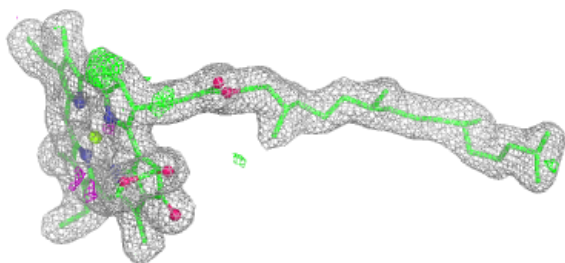
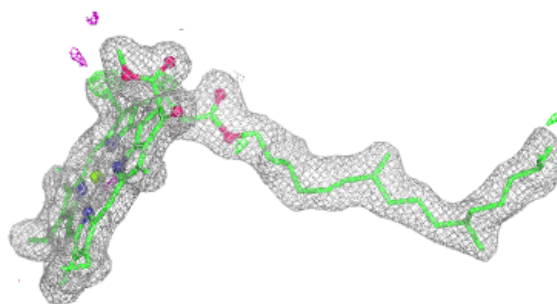


Electron density around CLA B 604:

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

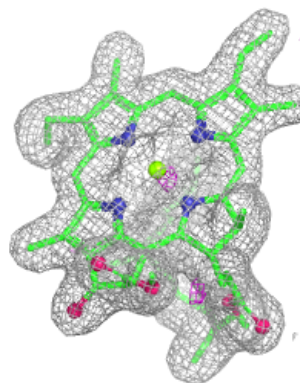
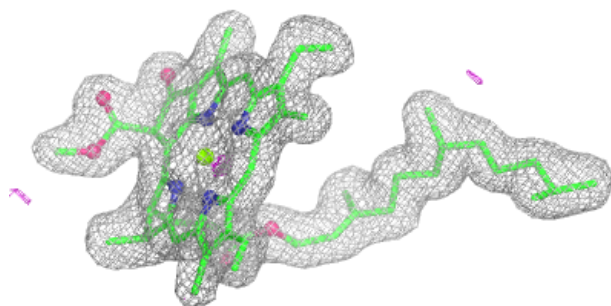
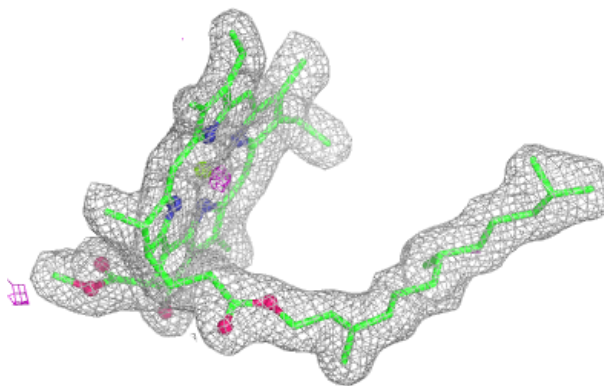
**Electron density around CLA B 605:**

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



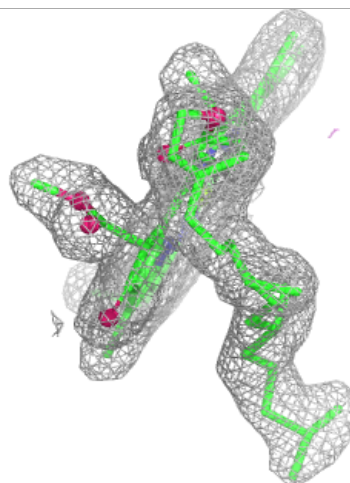
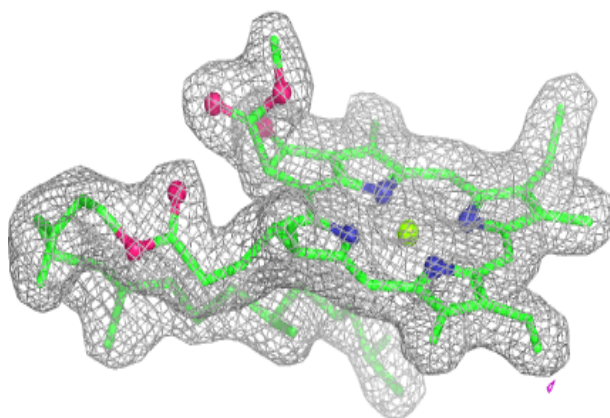
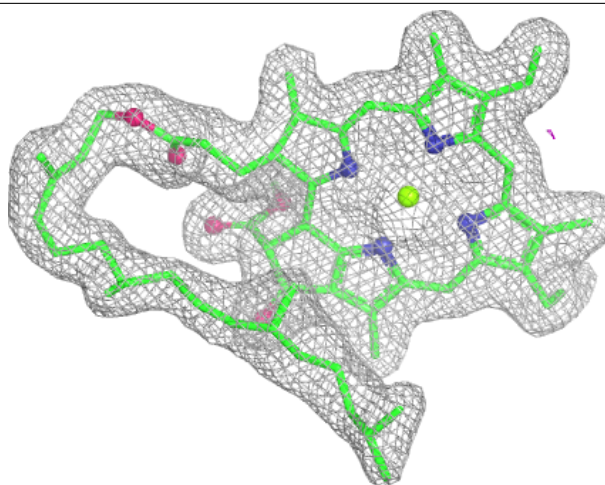
Electron density around CLA c 508:

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



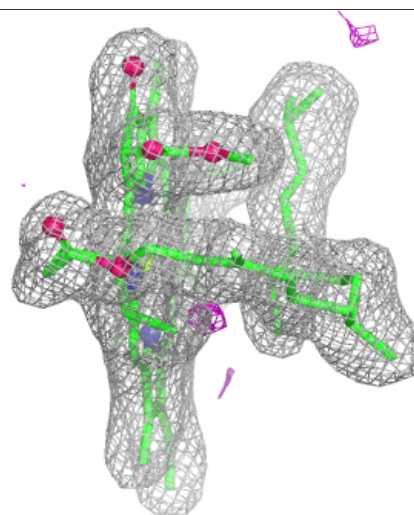
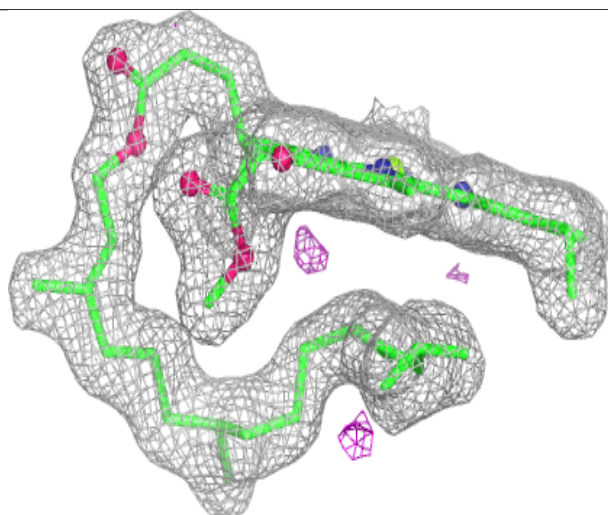
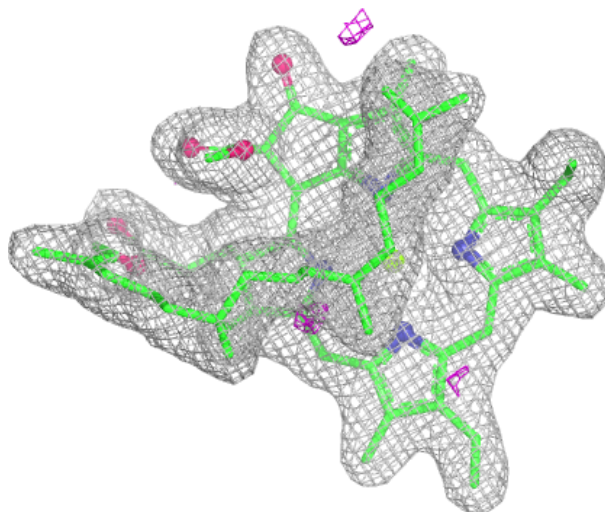
Electron density around CLA c 509:

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



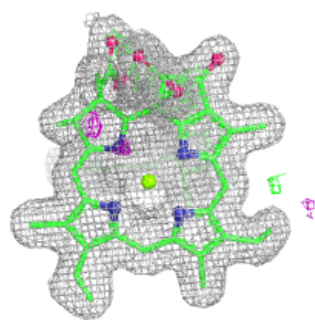
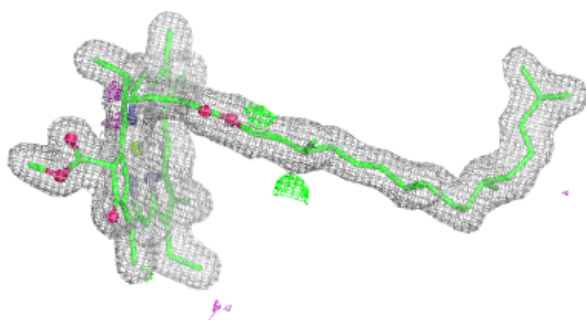
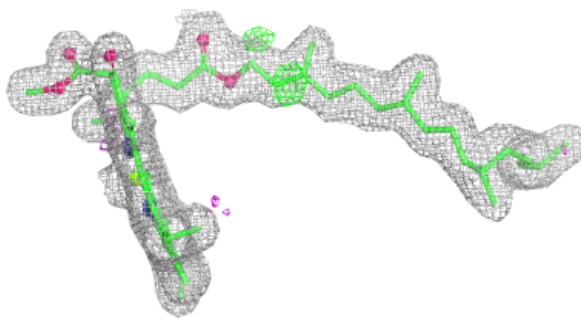
Electron density around CLA c 510:

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



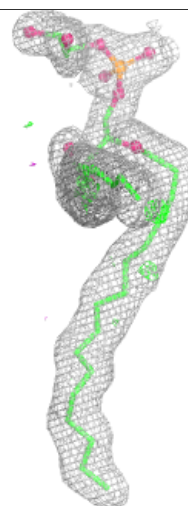
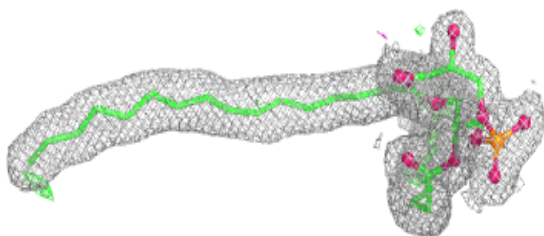
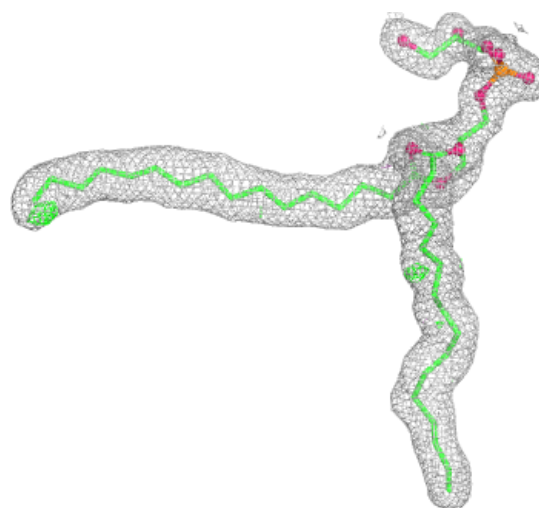
Electron density around CLA B 606:

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



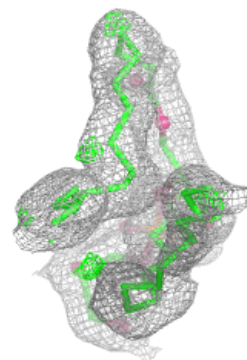
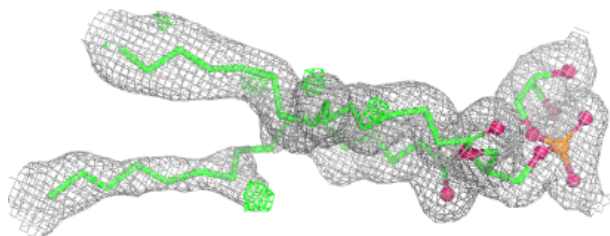
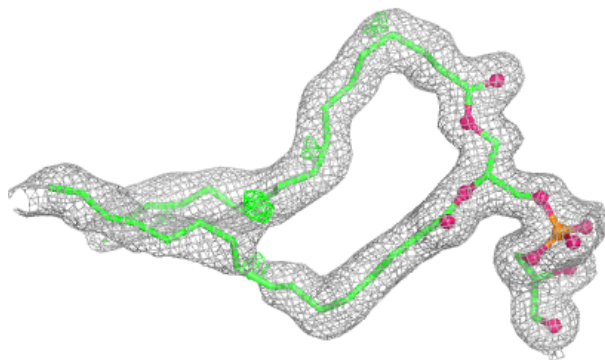
Electron density around LHG B 632:

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

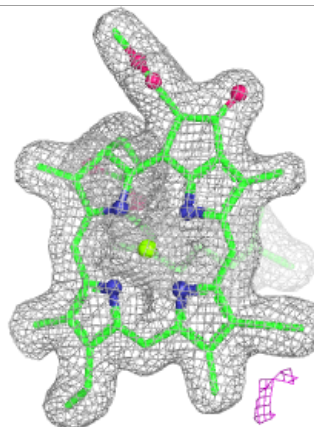
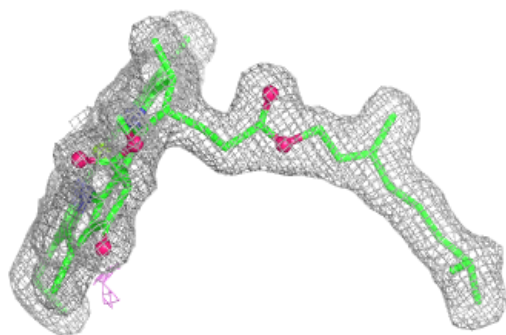


Electron density around LHG D 411:

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

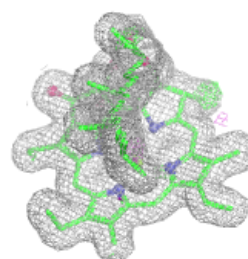
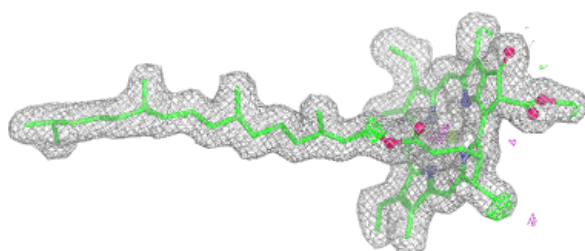
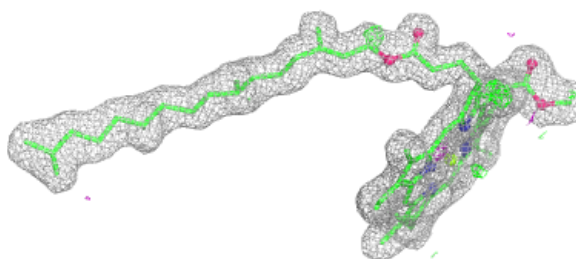
**Electron density around CLA B 607:**

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

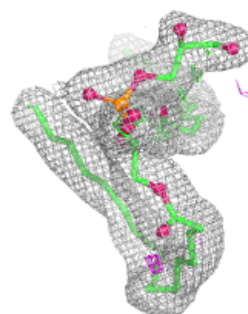
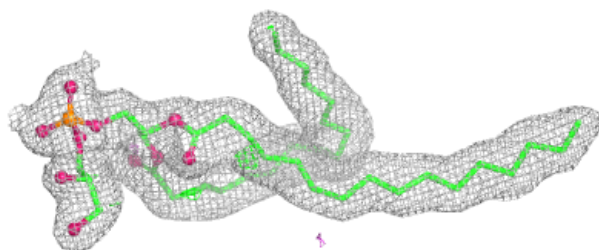
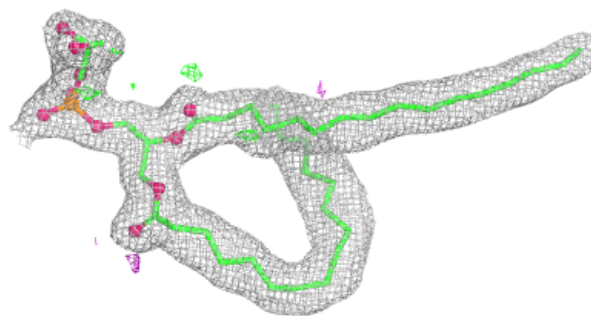


Electron density around CLA B 608:

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

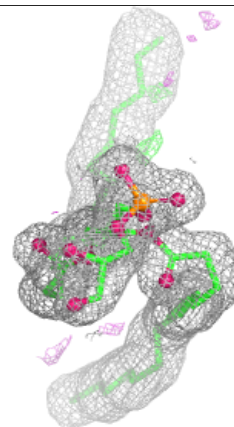
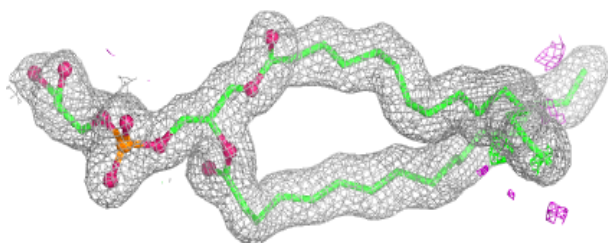
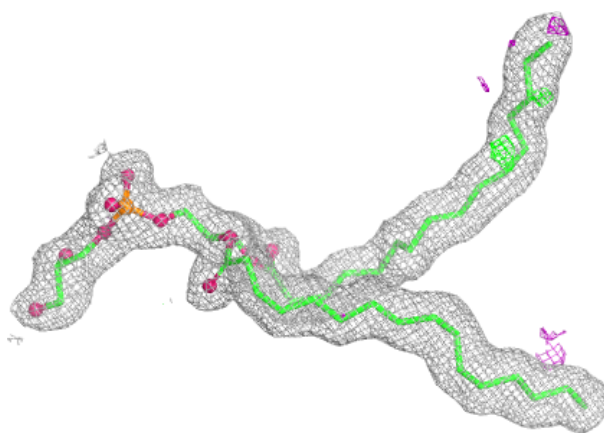
**Electron density around LHG d 409:**

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

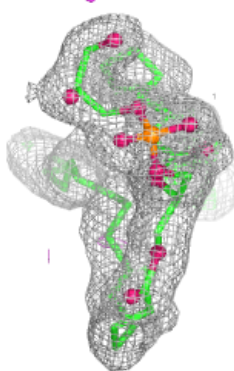
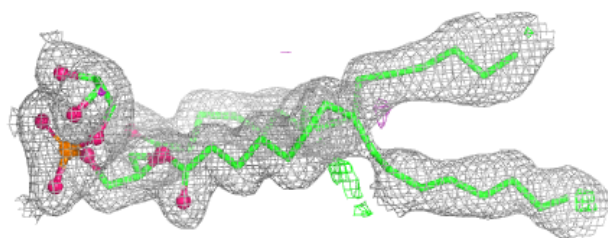
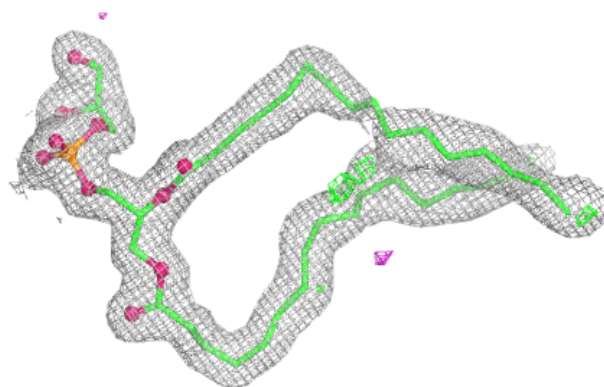


Electron density around LHG d 410:

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

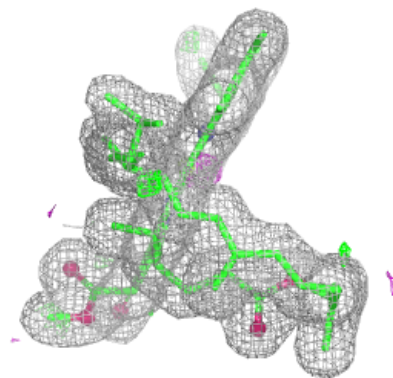
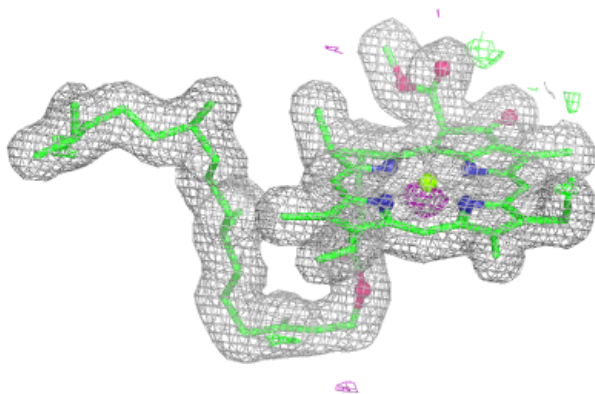
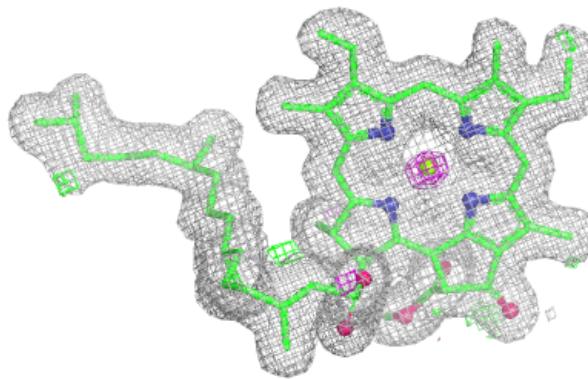
**Electron density around LHG d 411:**

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



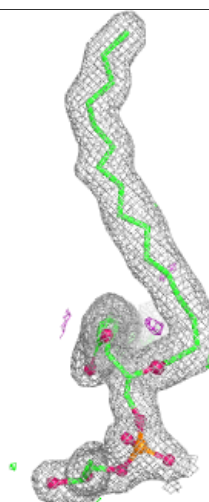
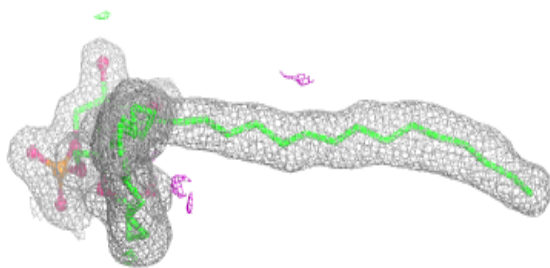
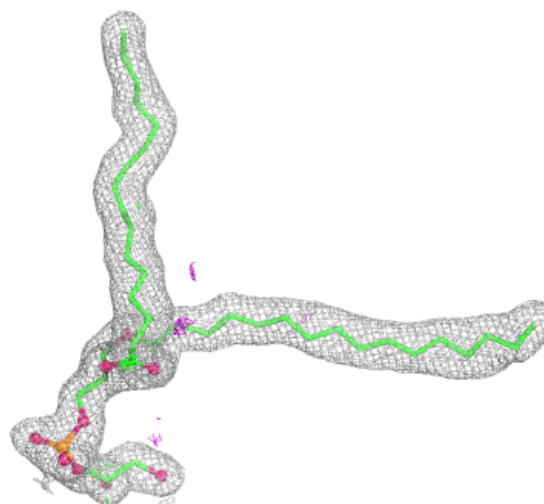
Electron density around CLA d 403:

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



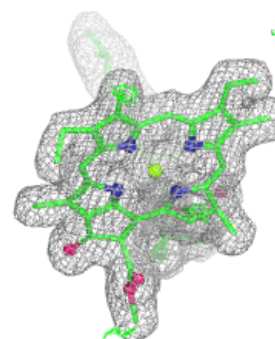
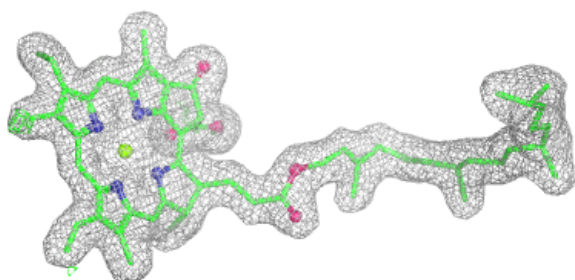
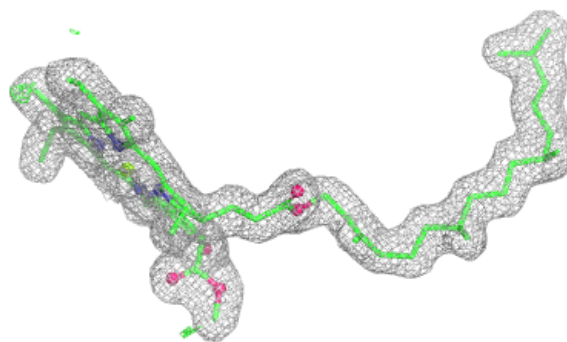
Electron density around LHG 1 101:

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

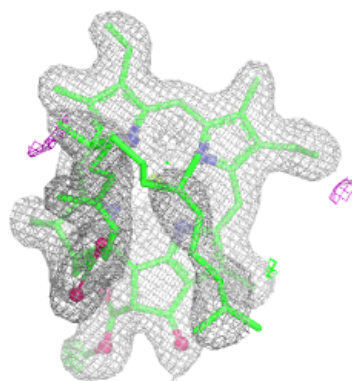
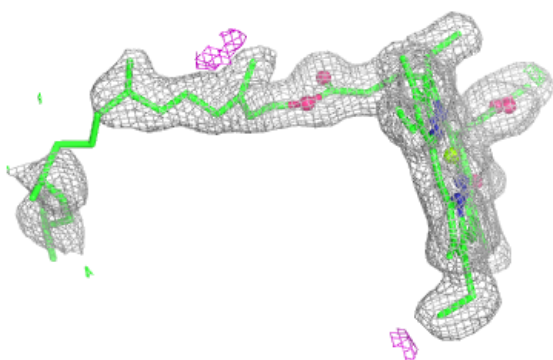
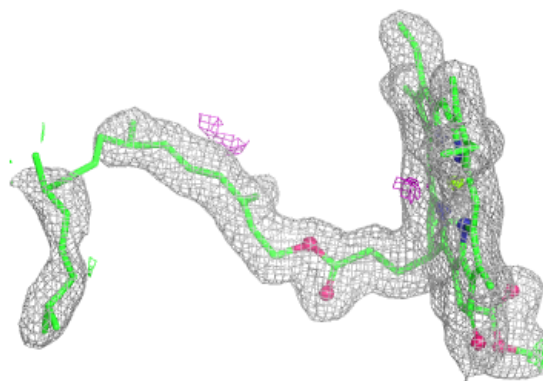


Electron density around CLA d 404:

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

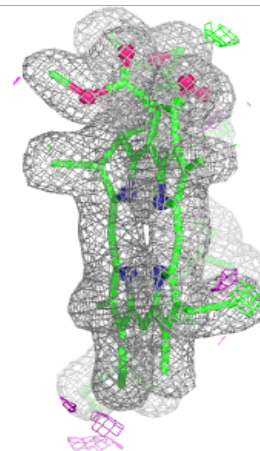
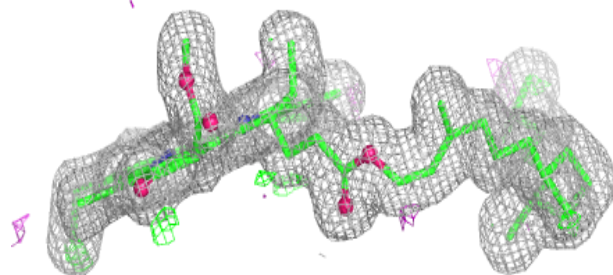
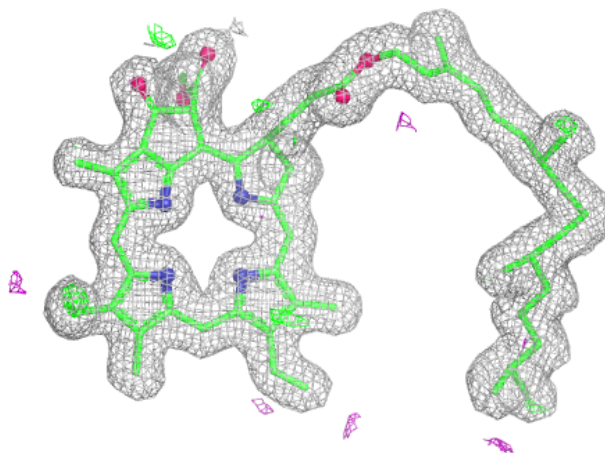
**Electron density around CLA d 405:**

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



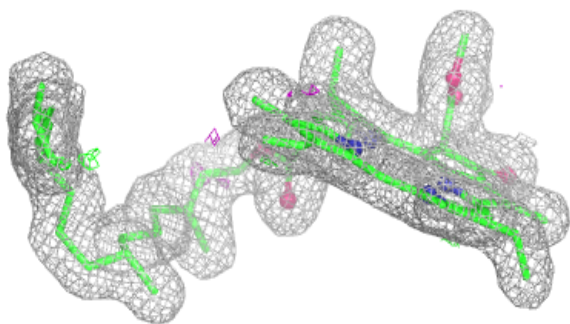
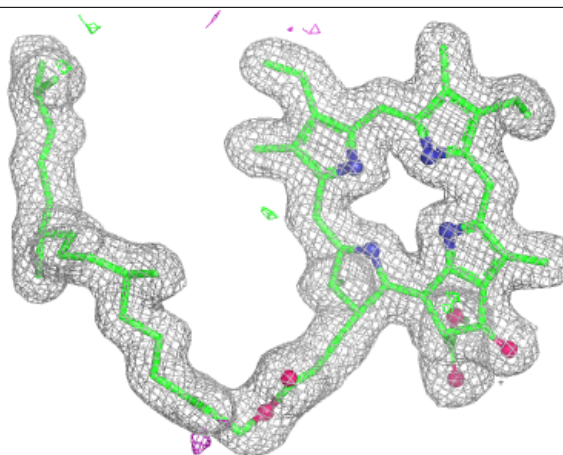
Electron density around PHO A 608:

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



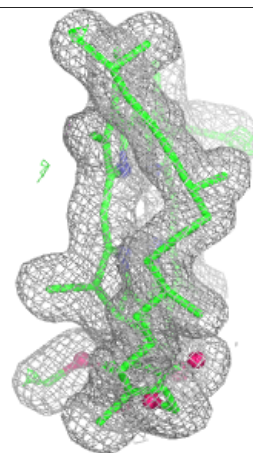
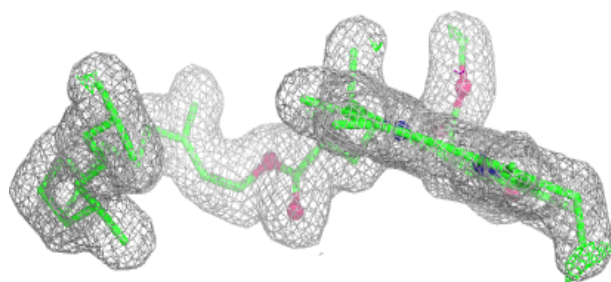
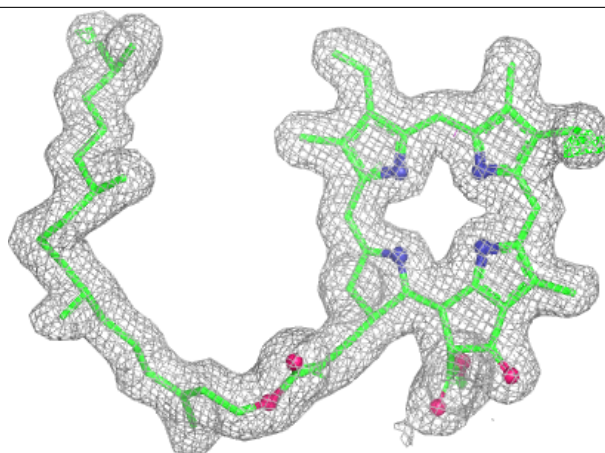
Electron density around PHO D 401:

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



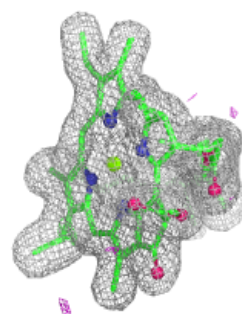
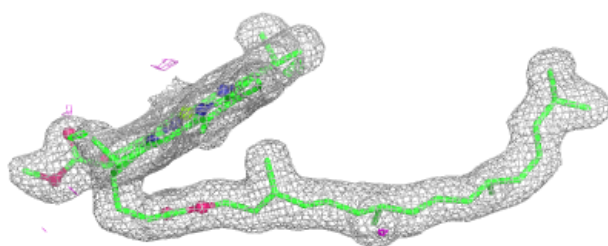
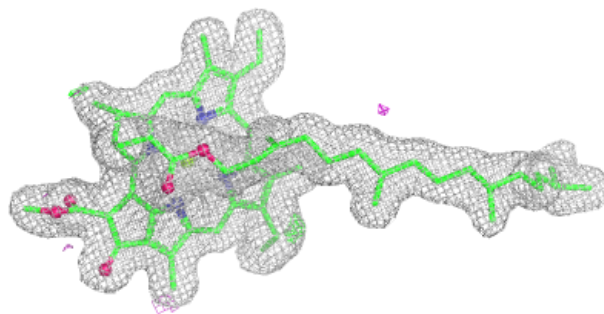
Electron density around PHO a 409:

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

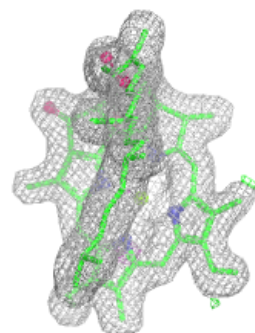
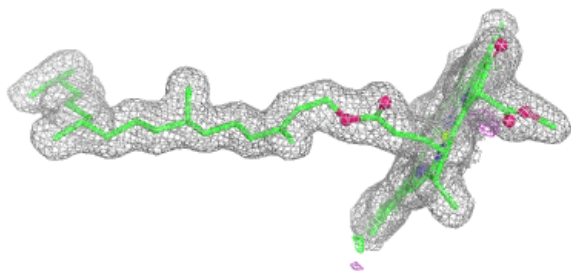
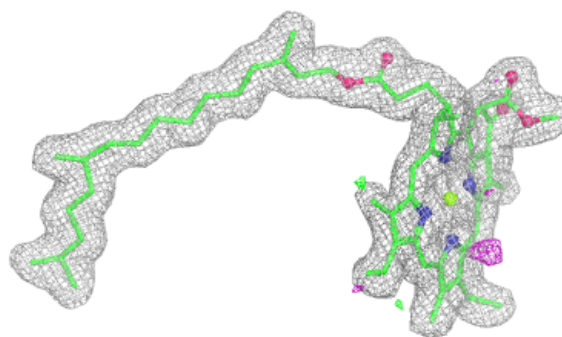


Electron density around CLA B 609:

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

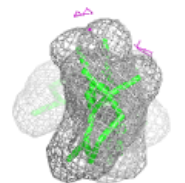
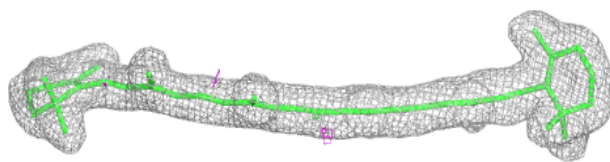
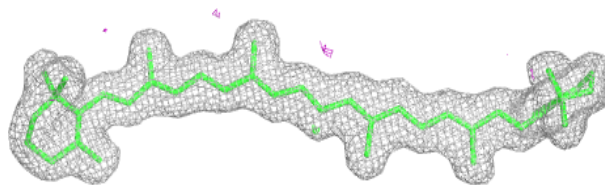
**Electron density around CLA B 610:**

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



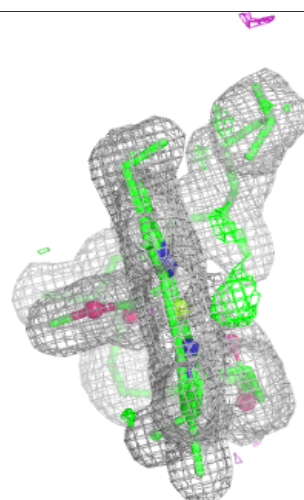
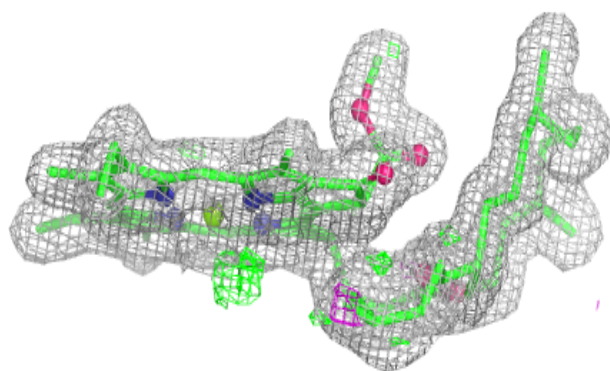
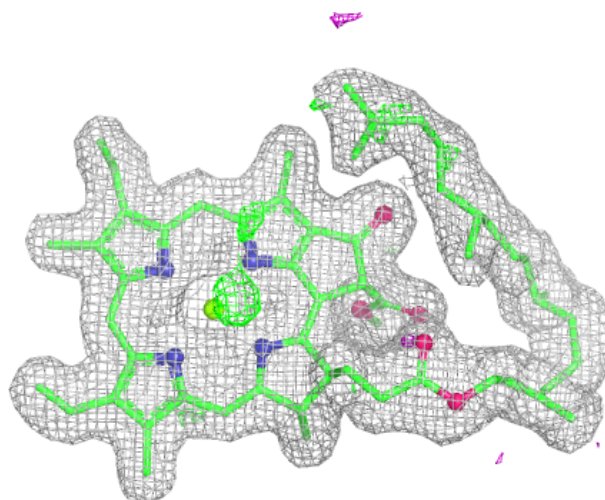
Electron density around BCR B 618:

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



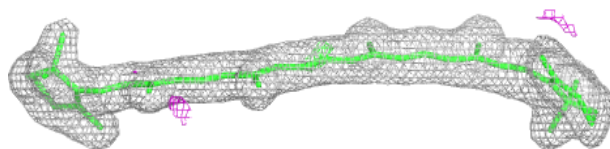
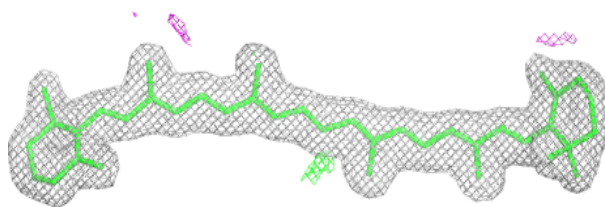
Electron density around CLA B 611:

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



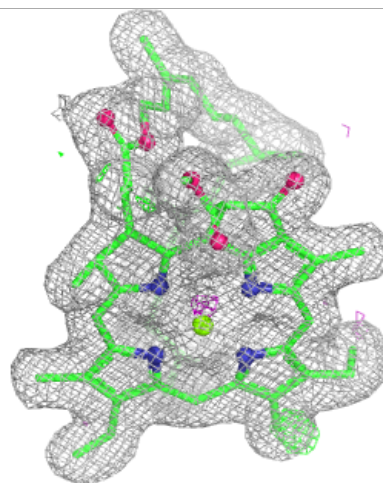
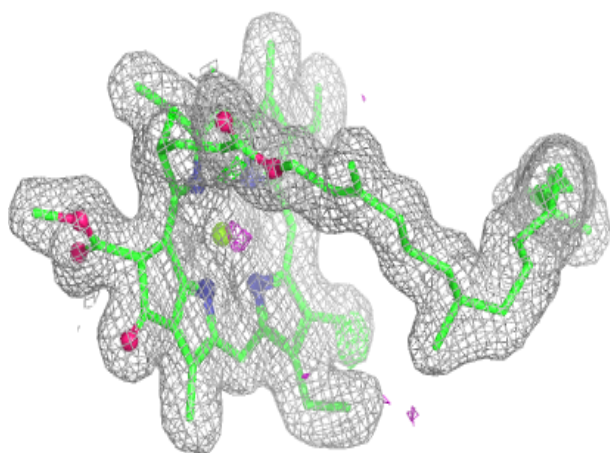
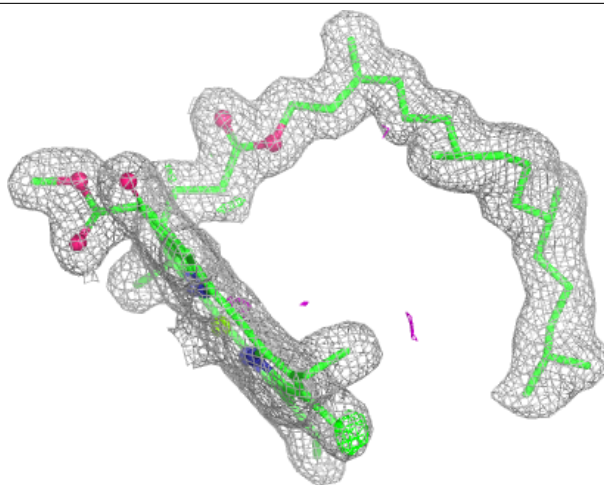
Electron density around BCR B 620:

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



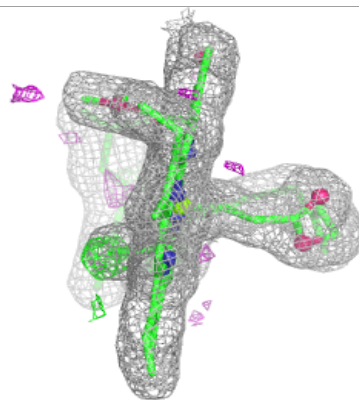
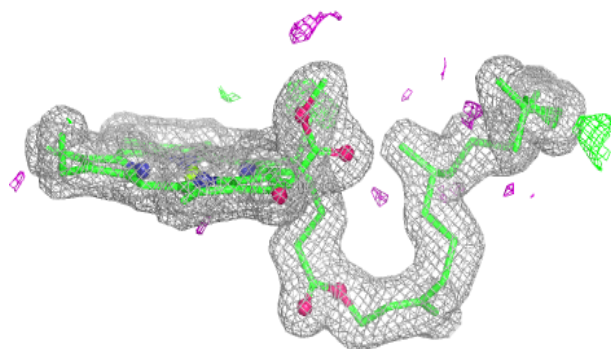
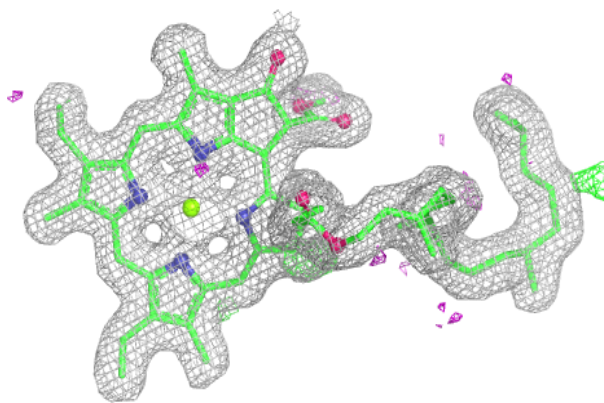
Electron density around CLA B 612:

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



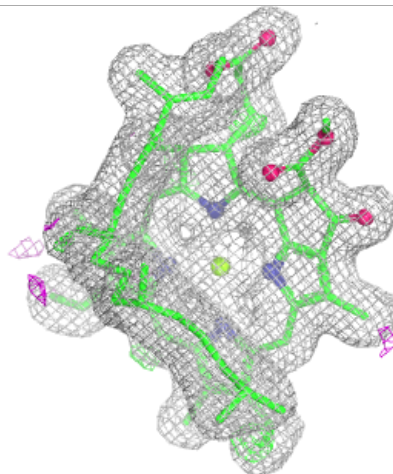
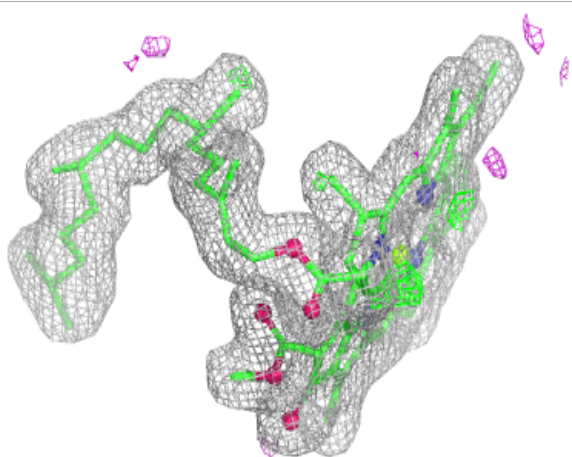
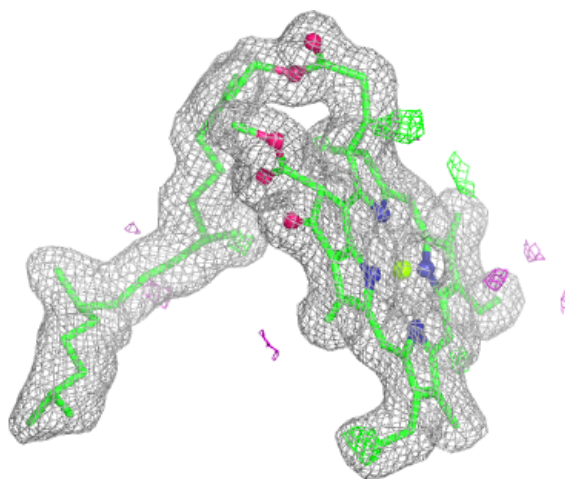
Electron density around CLA B 613:

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



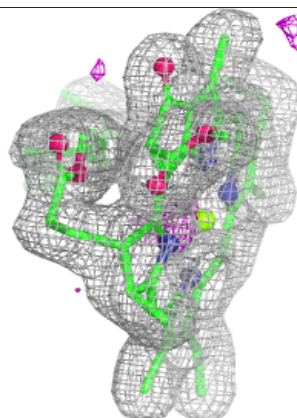
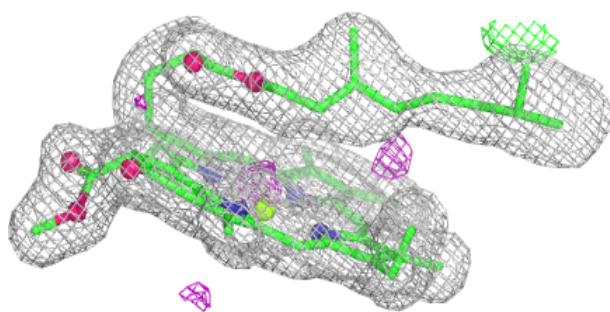
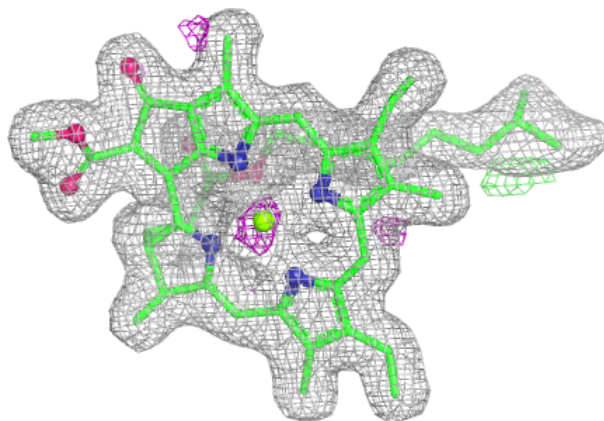
Electron density around CLA B 614:

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



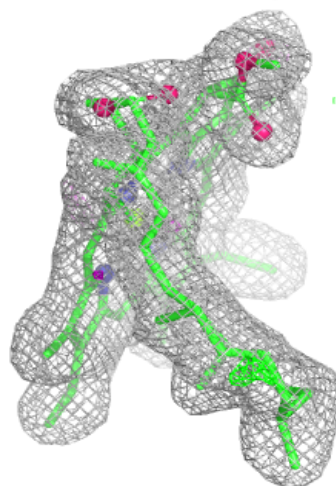
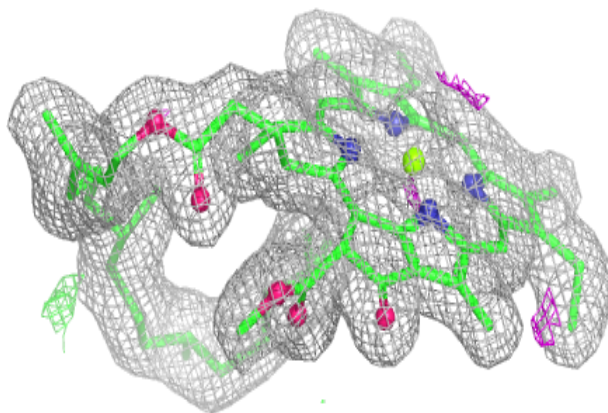
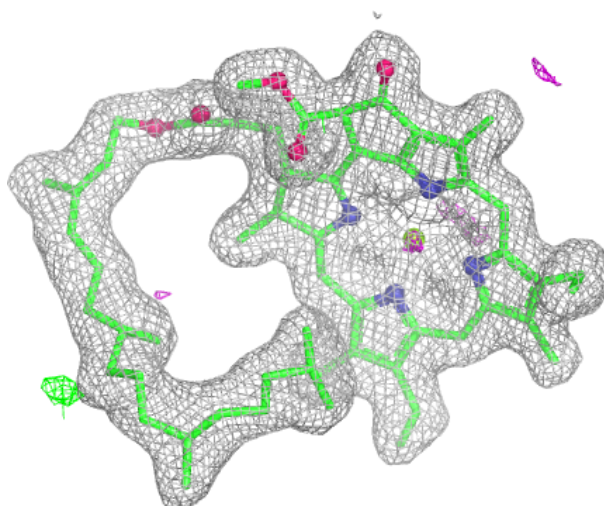
Electron density around CLA B 615:

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



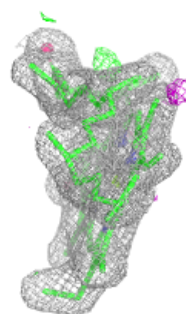
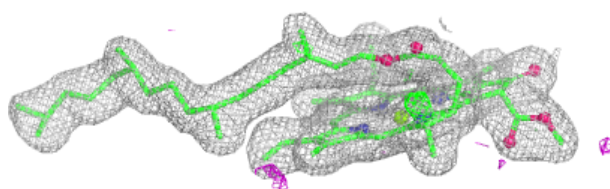
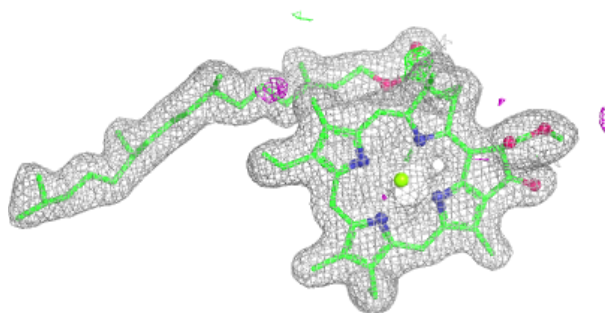
Electron density around CLA B 616:

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

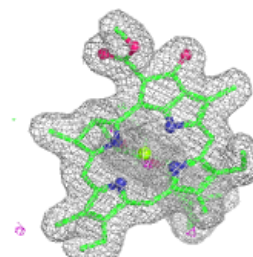
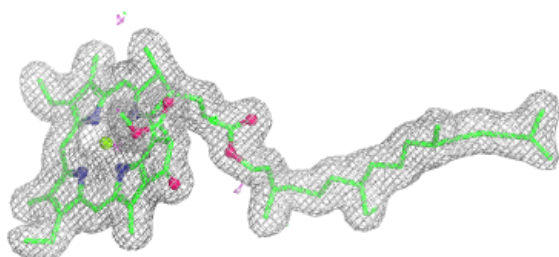
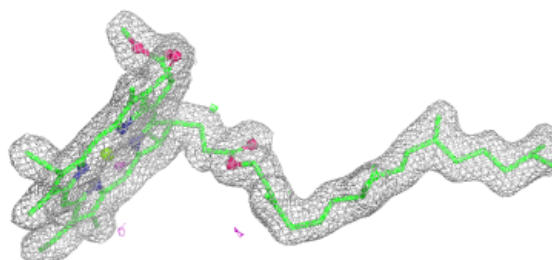


Electron density around CLA C 501:

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

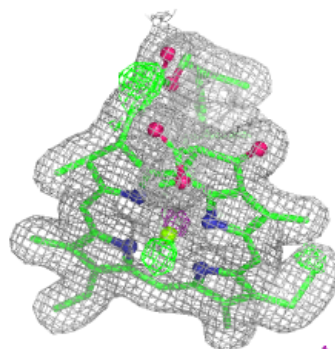
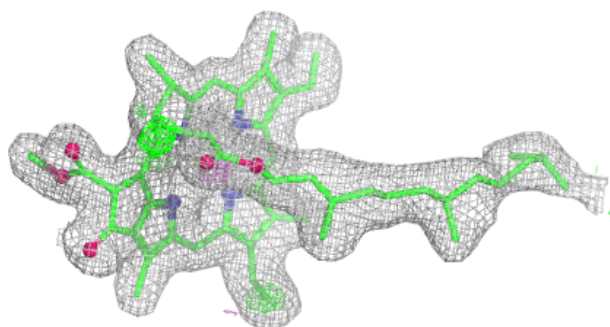
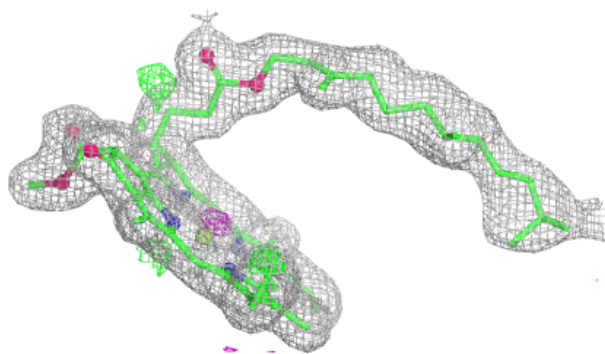
**Electron density around CLA C 502:**

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

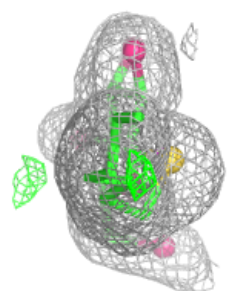
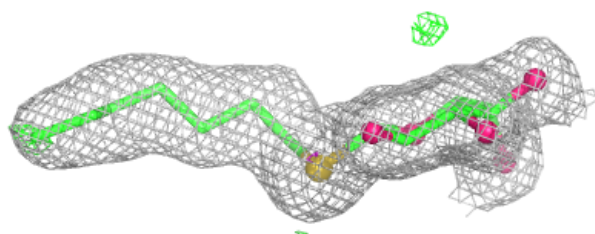
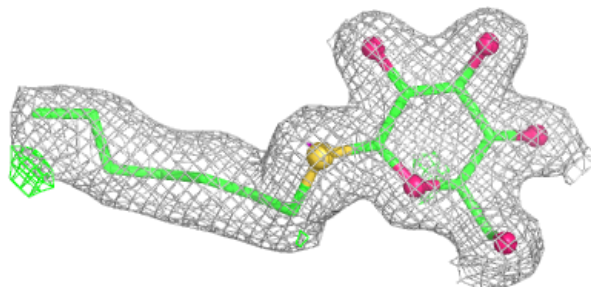


Electron density around CLA C 504:

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

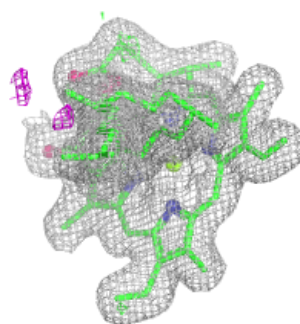
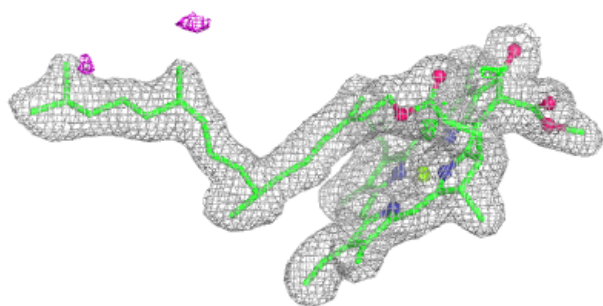
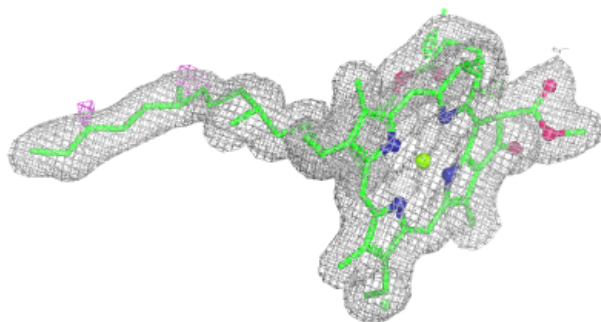
**Electron density around HTG O 303:**

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



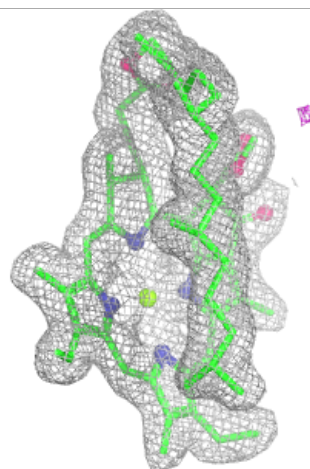
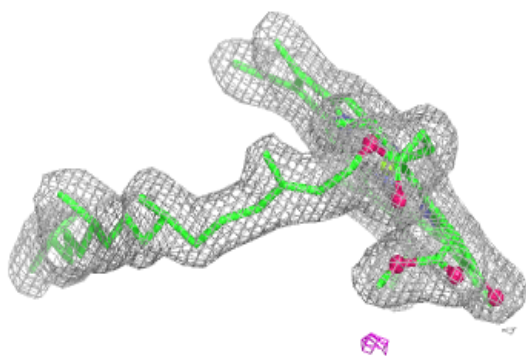
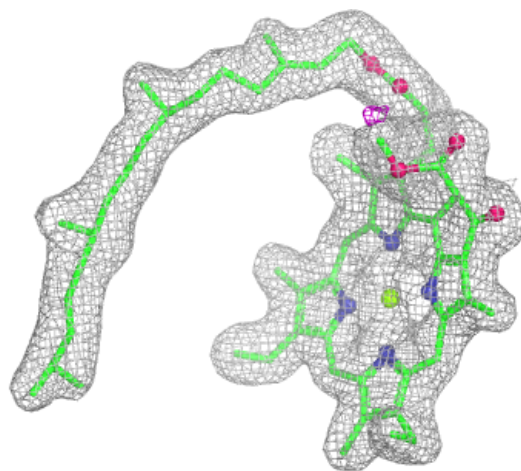
Electron density around CLA C 505:

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



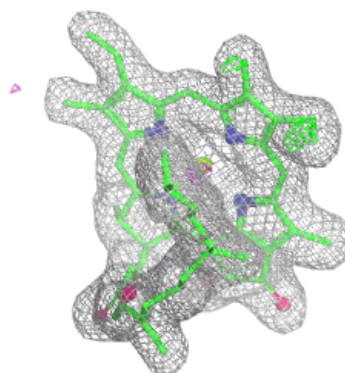
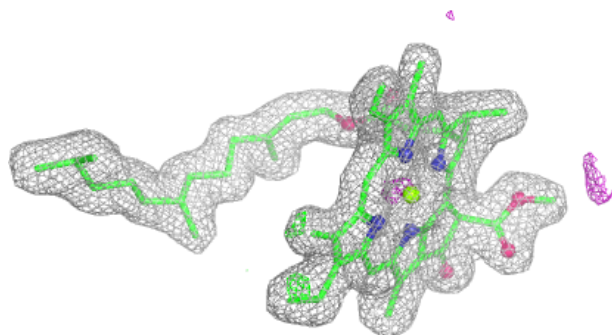
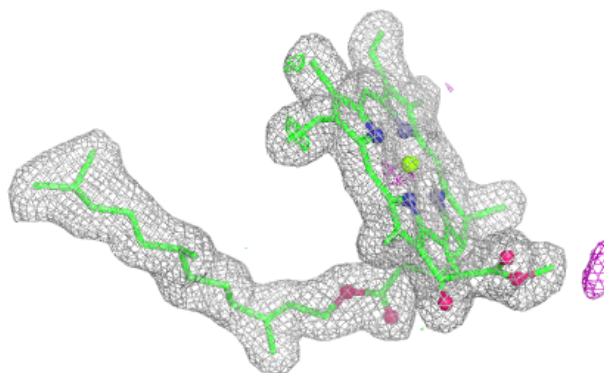
Electron density around CLA C 507:

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



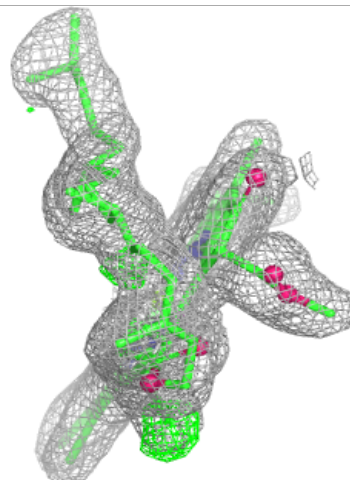
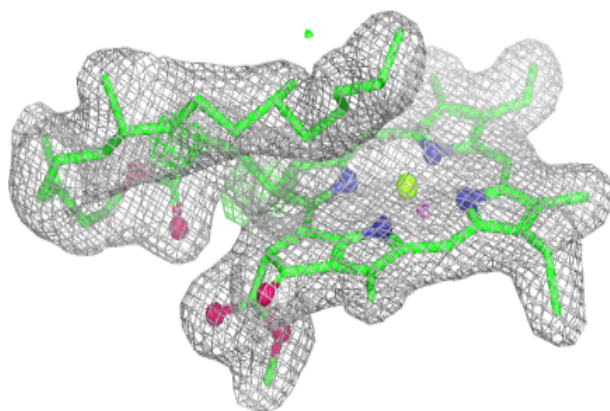
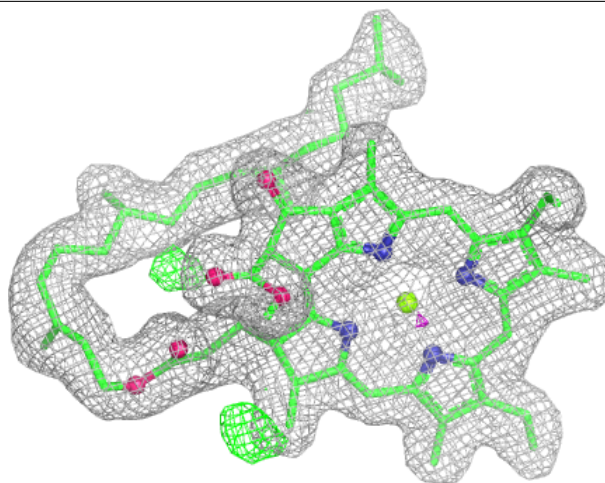
Electron density around CLA C 508:

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



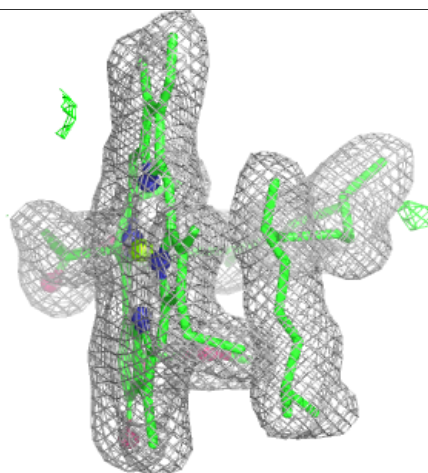
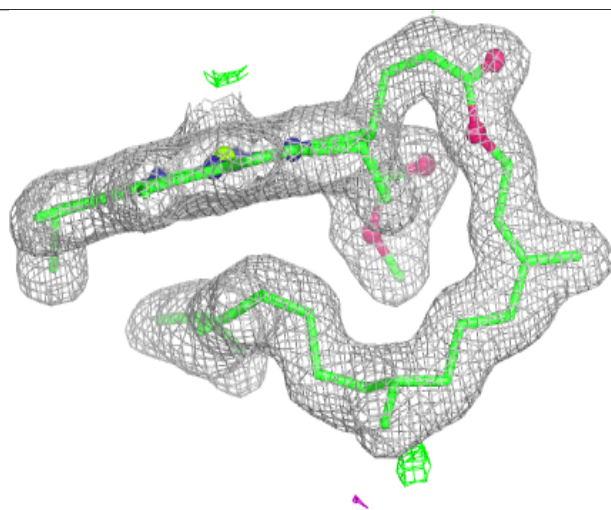
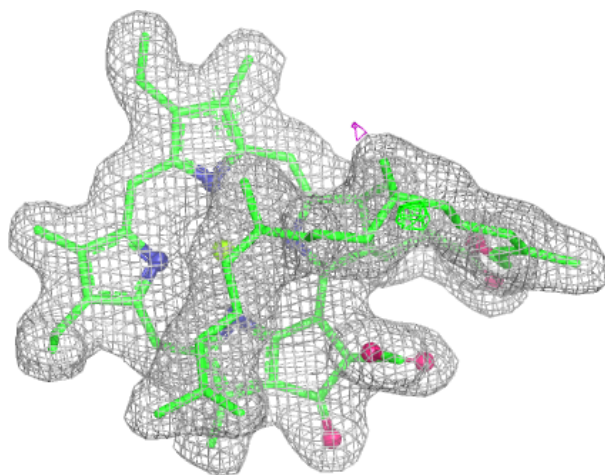
Electron density around CLA C 509:

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



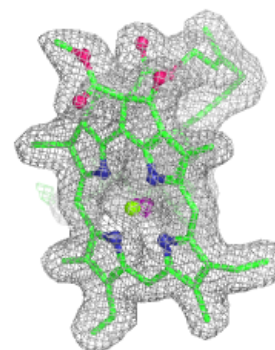
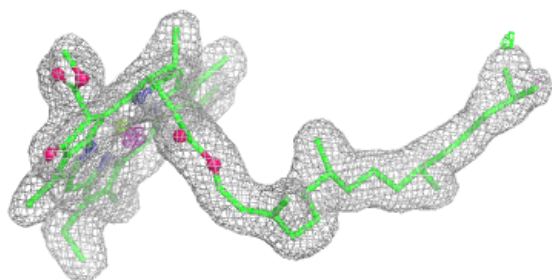
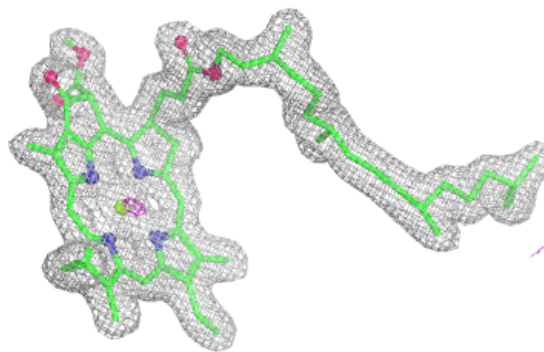
Electron density around CLA C 510:

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

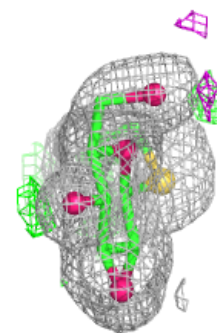
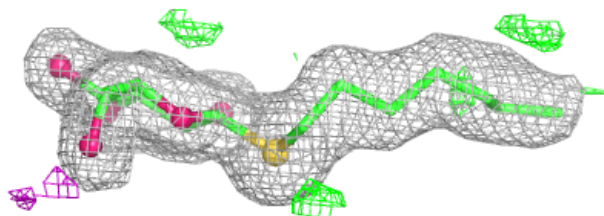
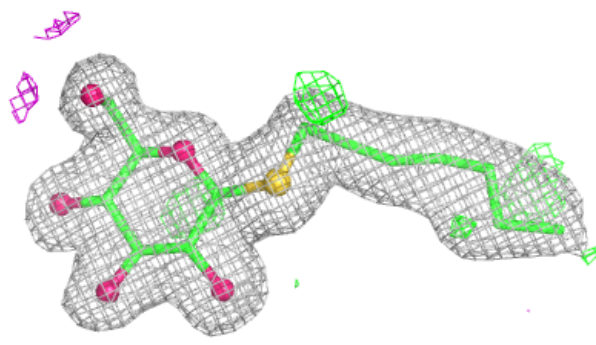


Electron density around CLA C 511:

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

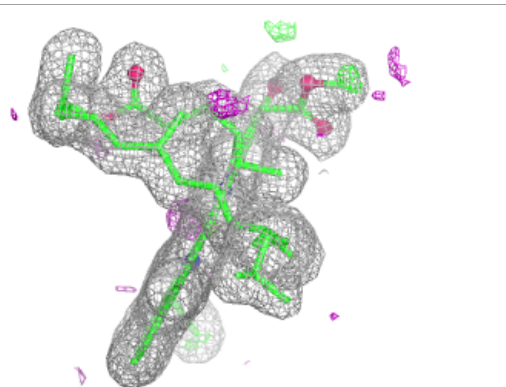
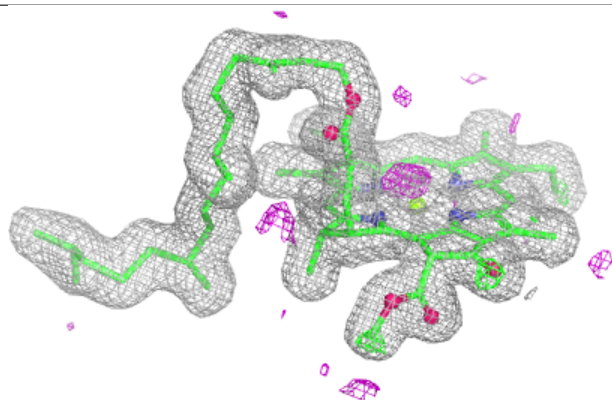
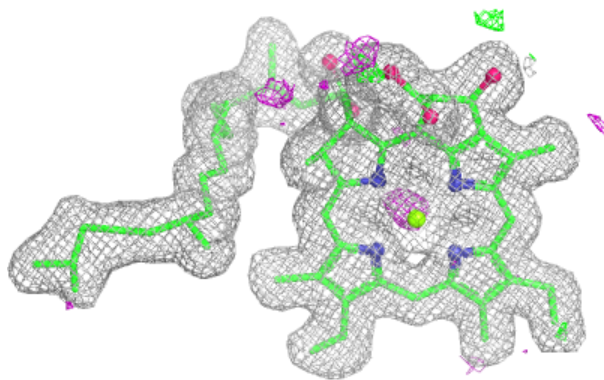
**Electron density around HTG o 301:**

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

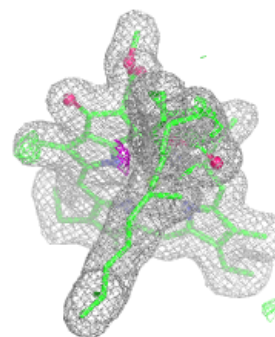
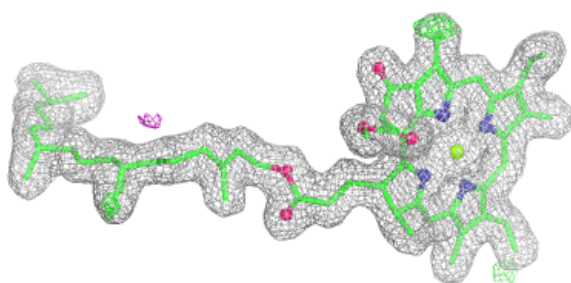
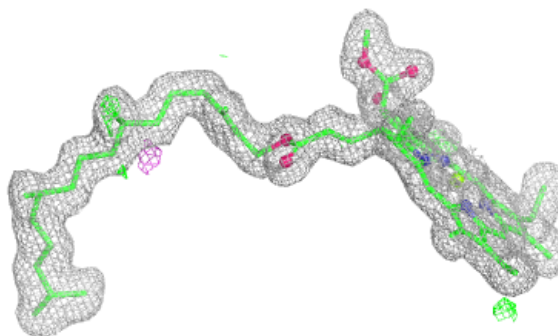


Electron density around CLA D 403:

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

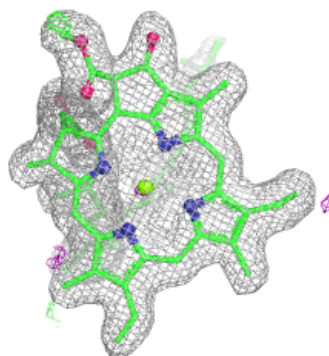
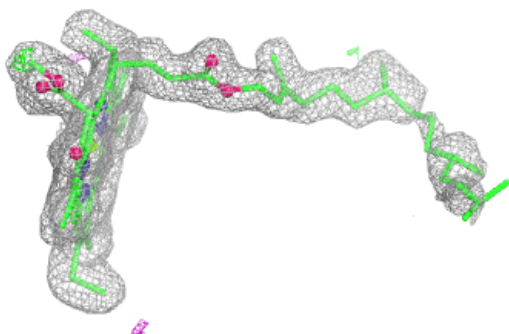
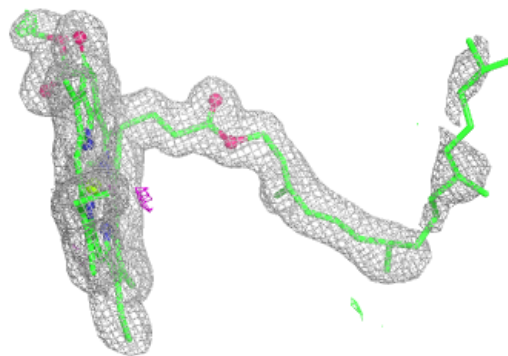
**Electron density around CLA D 404:**

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

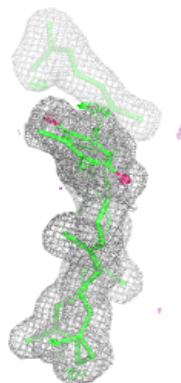
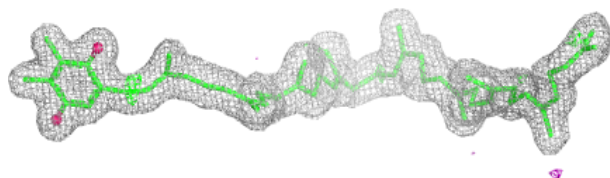
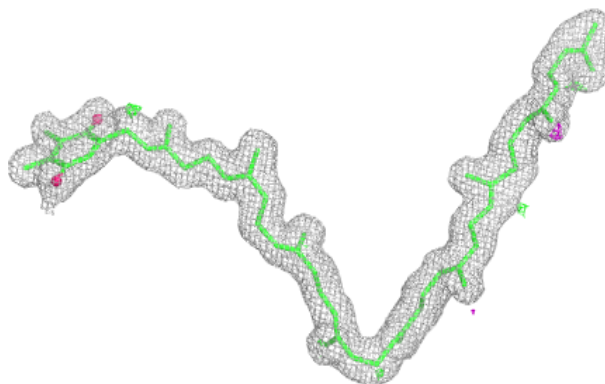


Electron density around CLA D 405:

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

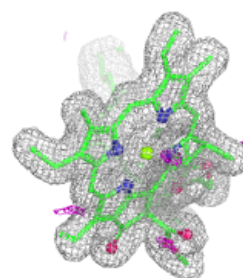
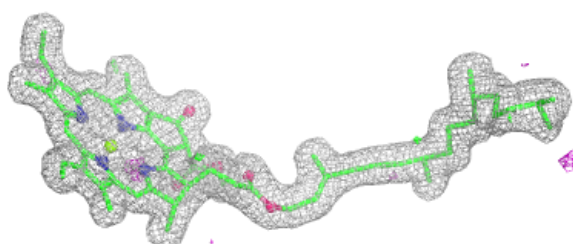
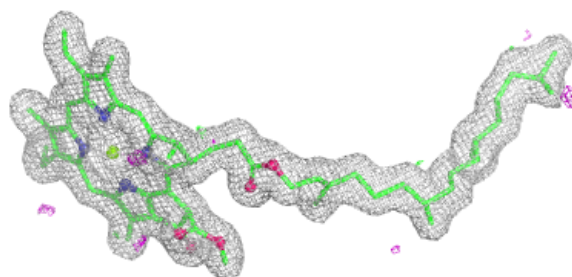
**Electron density around PL9 d 407:**

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

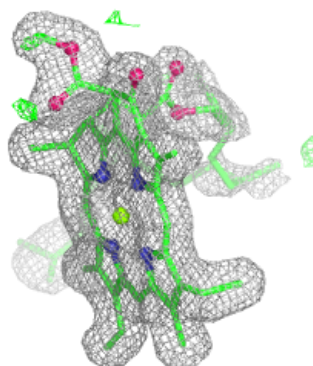
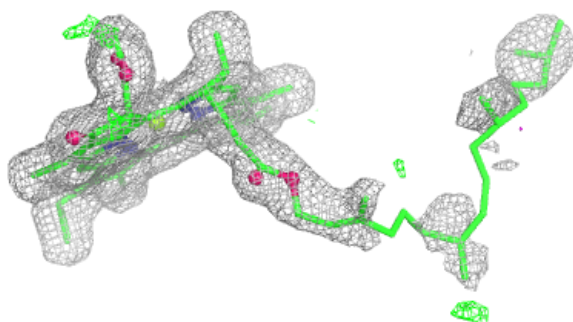
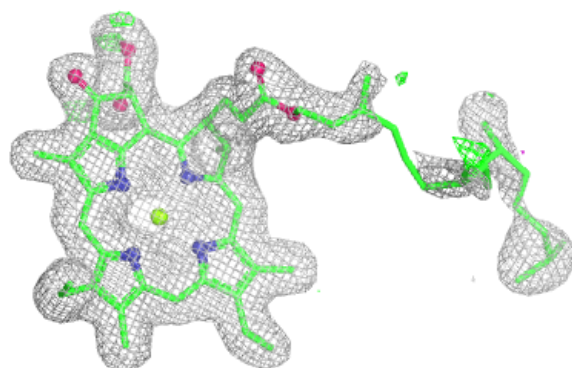


Electron density around CLA a 407:

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

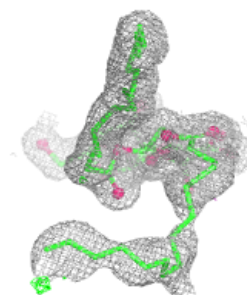
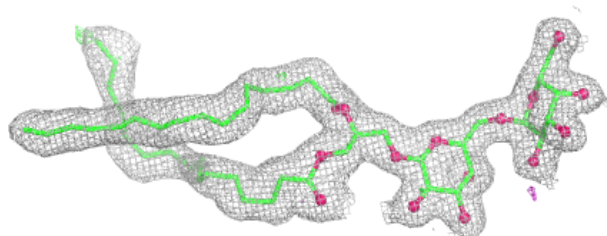
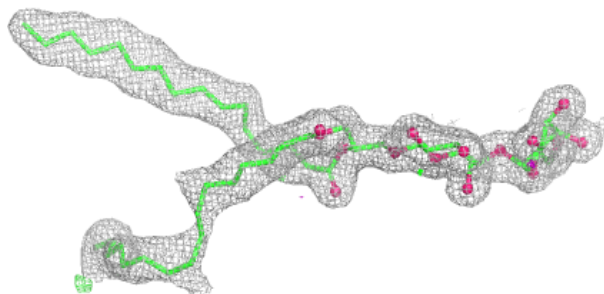
**Electron density around CLA a 410:**

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

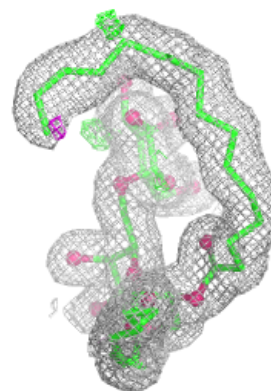
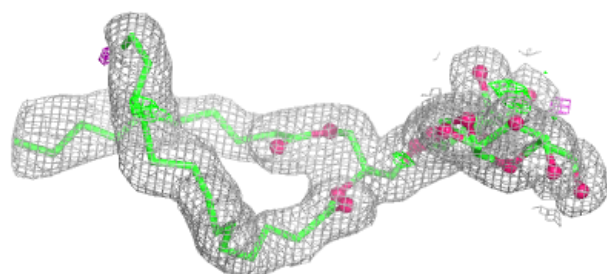
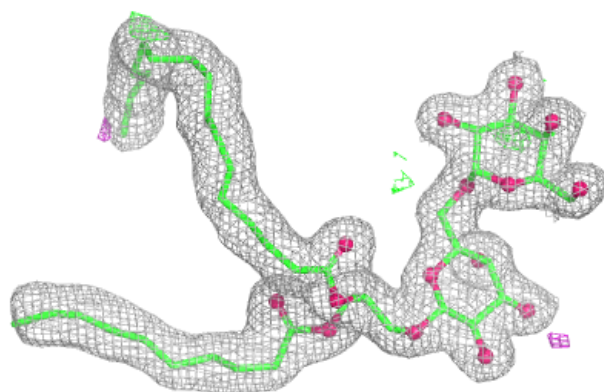


Electron density around DGD C 516:

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

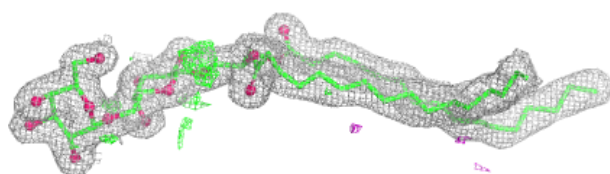
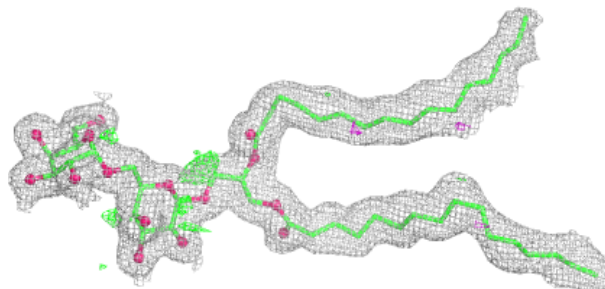
**Electron density around DGD C 517:**

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

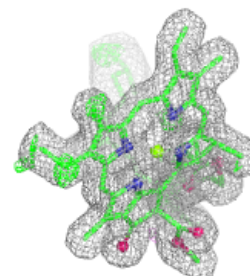
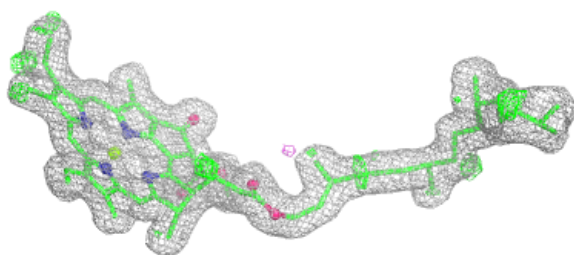
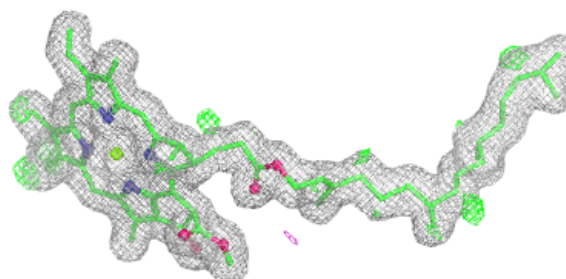


Electron density around DGD C 518:

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

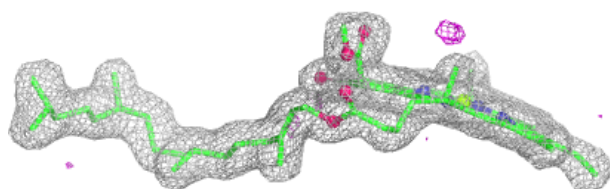
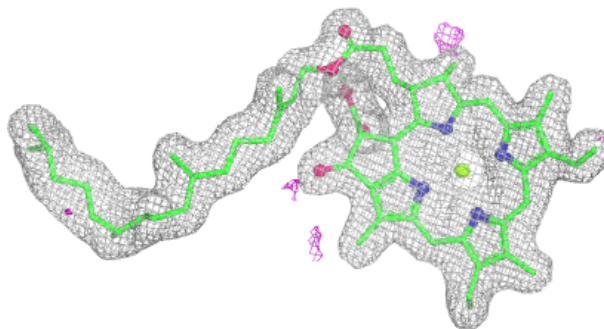
**Electron density around CLA A 606:**

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

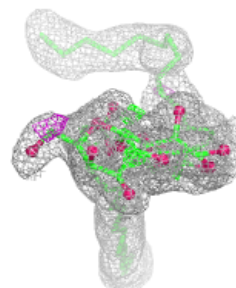
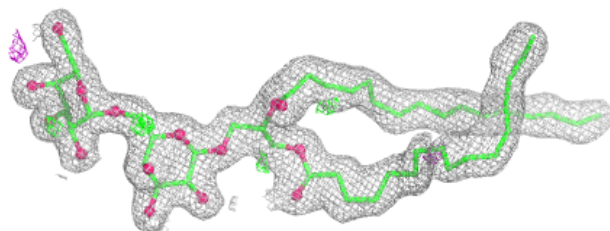
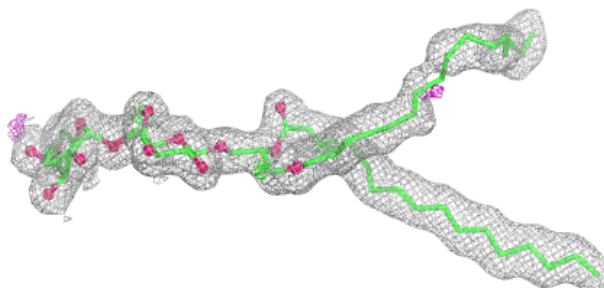


Electron density around CLA b 603:

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

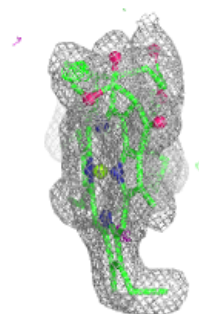
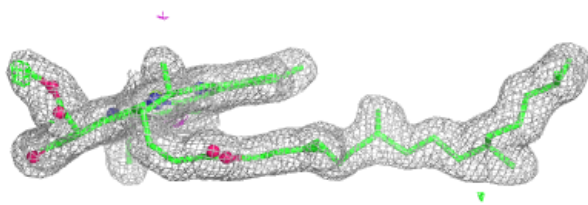
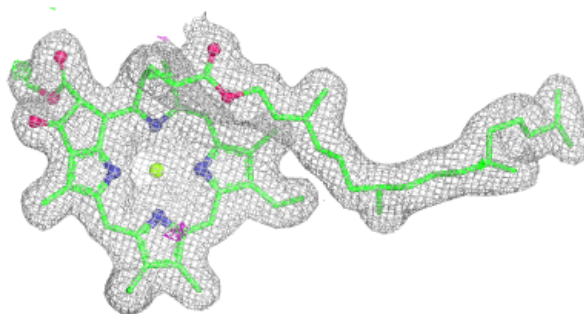
**Electron density around DGD c 516:**

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

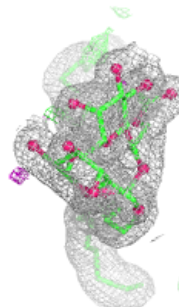
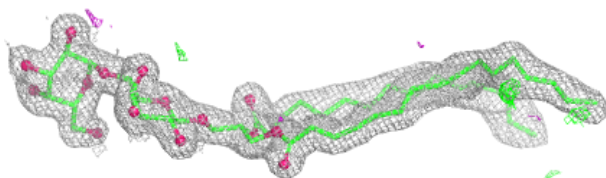
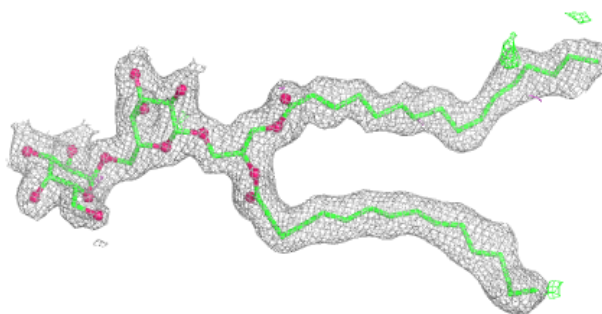


Electron density around CLA b 604:

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

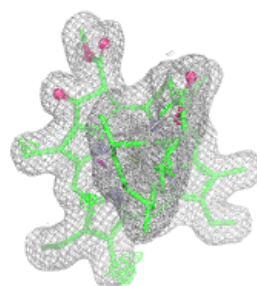
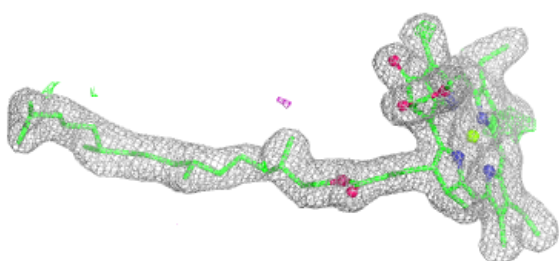
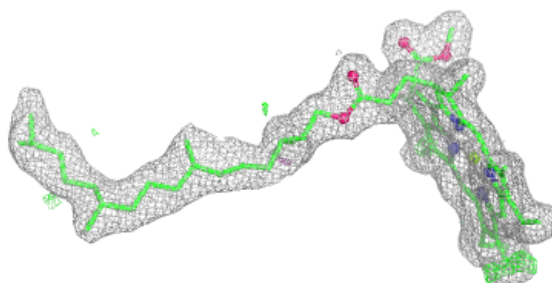
**Electron density around DGD c 518:**

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

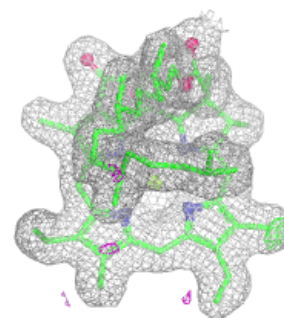
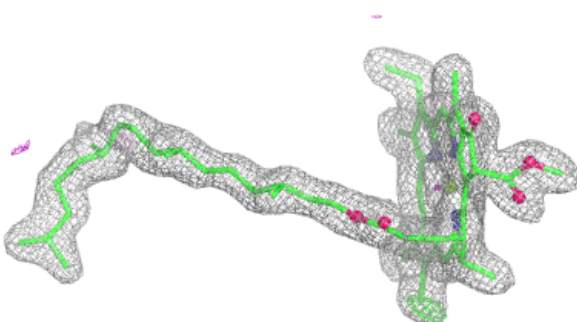
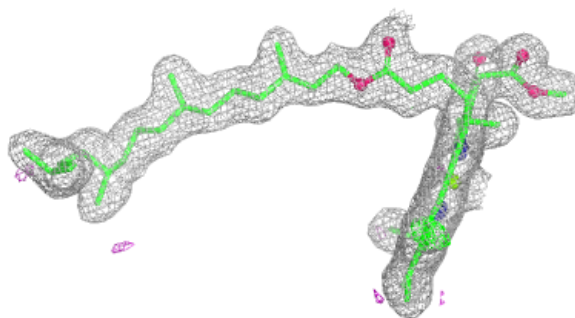


Electron density around CLA b 605:

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

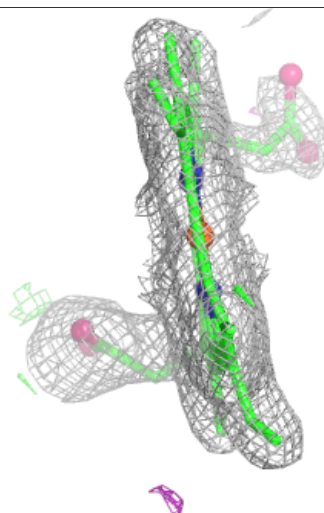
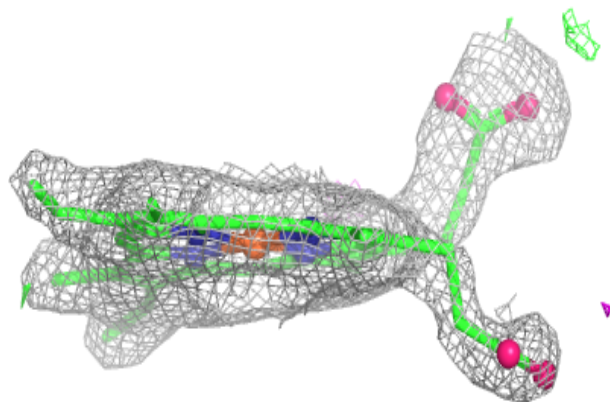
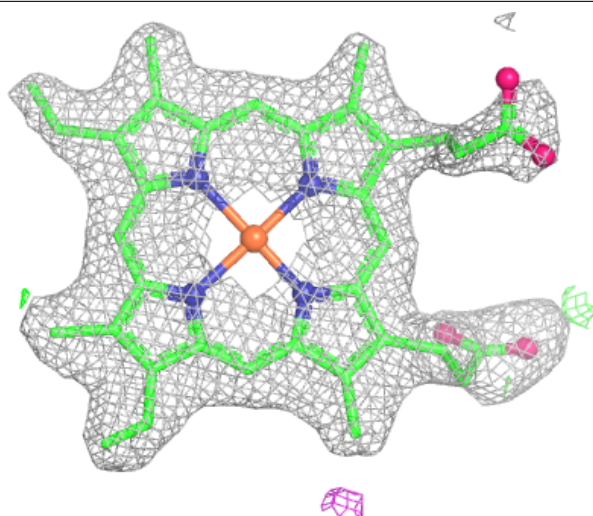
**Electron density around CLA b 606:**

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



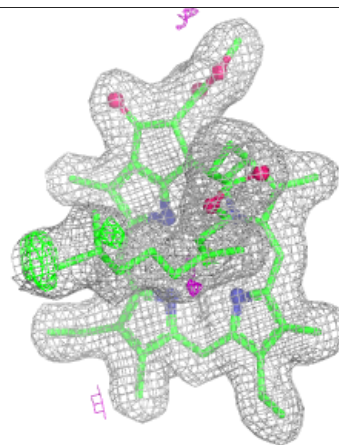
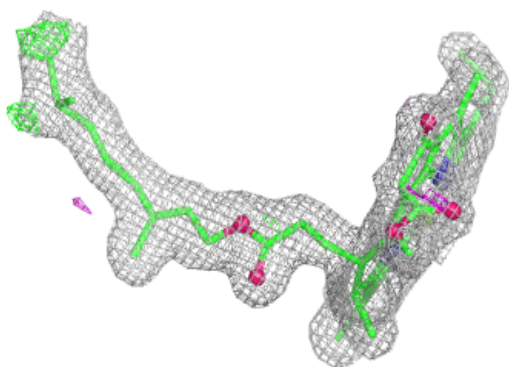
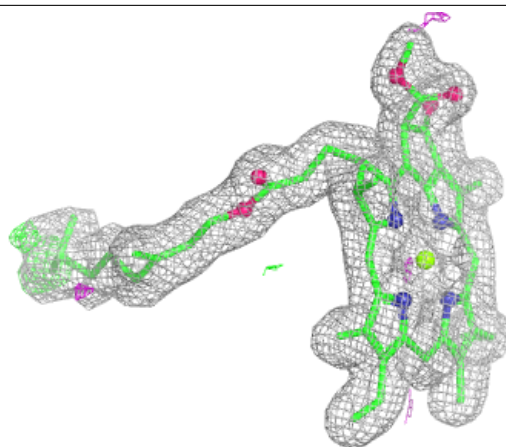
Electron density around HEM e 107:

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



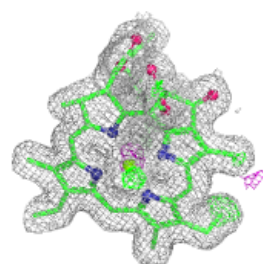
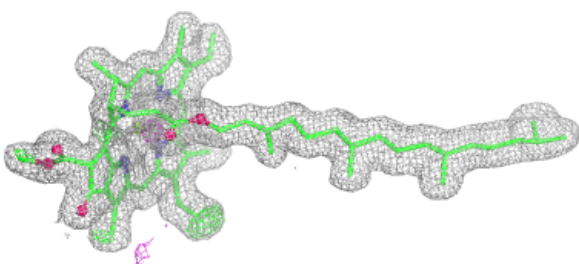
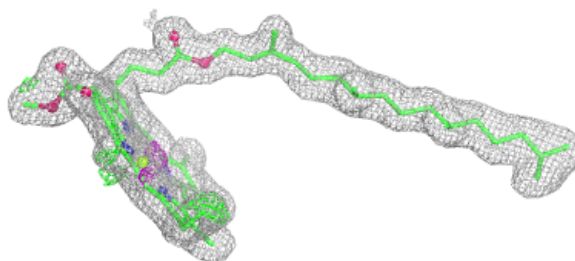
Electron density around CLA b 607:

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

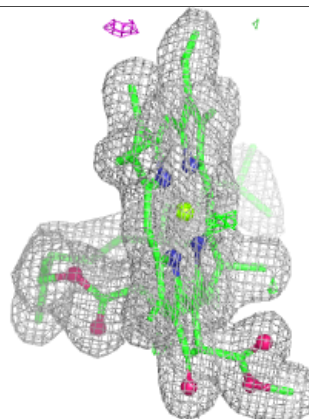
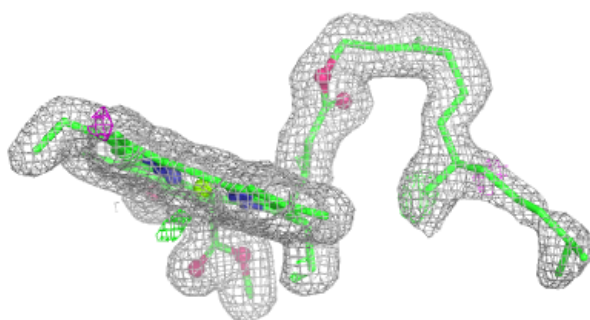
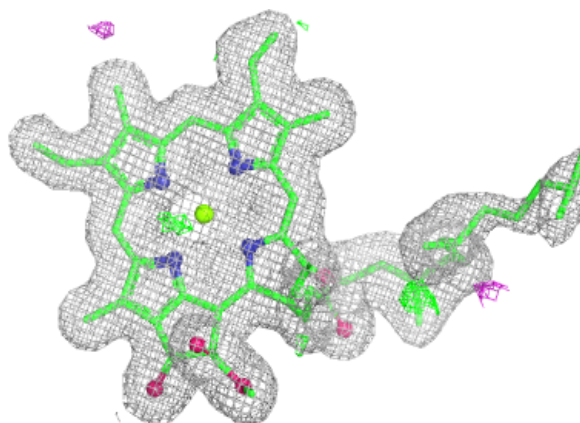


Electron density around CLA b 608:

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

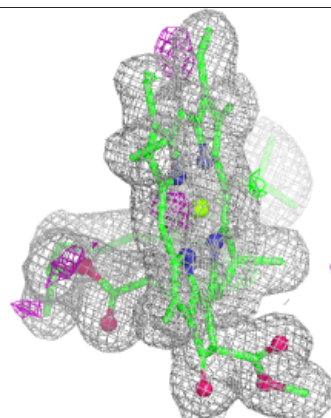
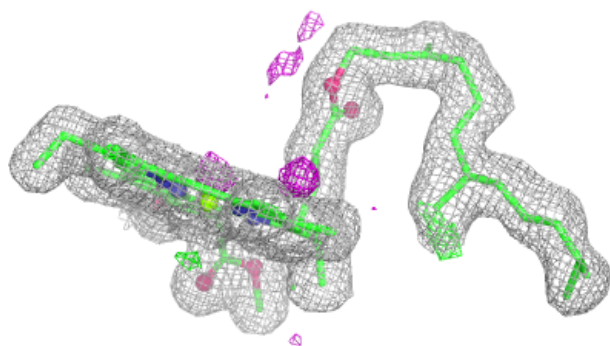
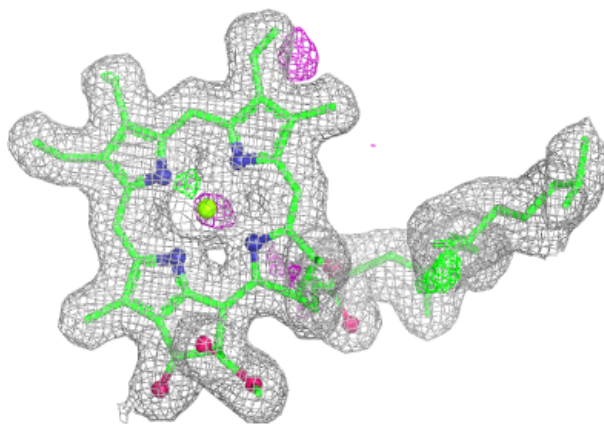
**Electron density around CLA a 408:**

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



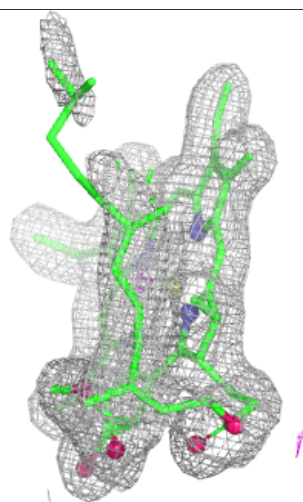
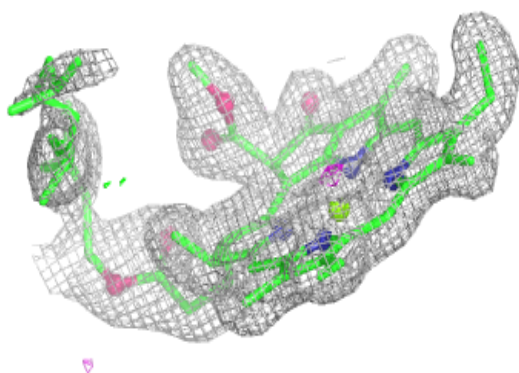
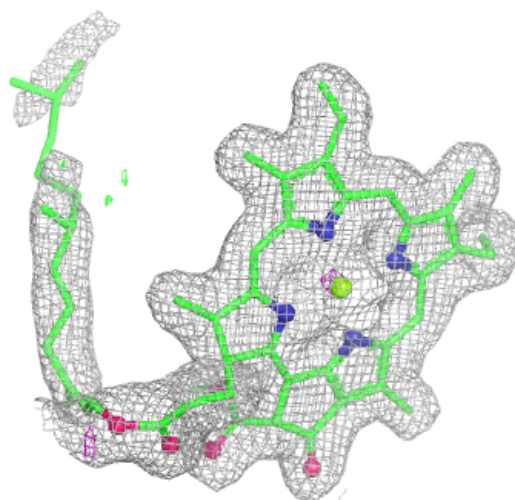
Electron density around CLA A 607:

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



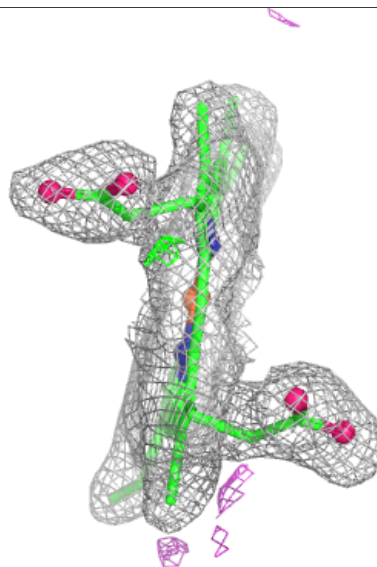
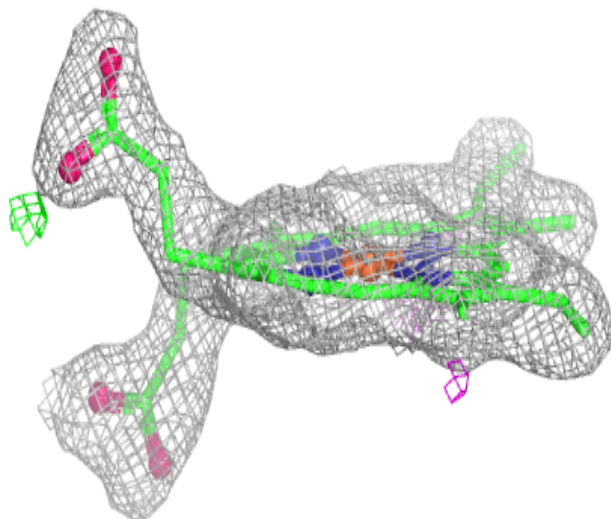
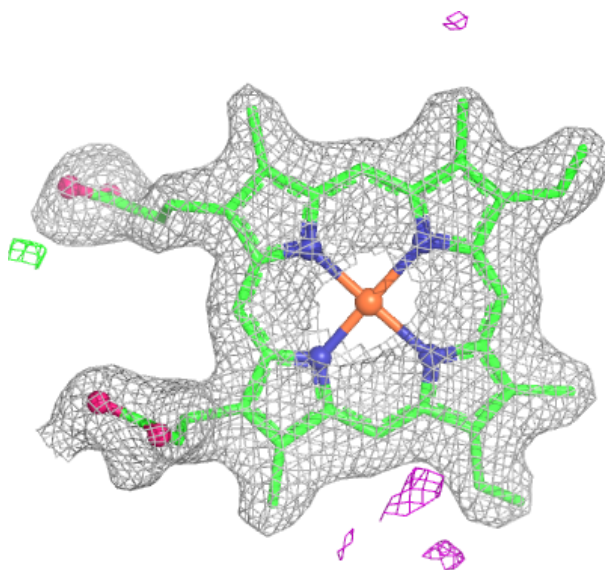
Electron density around CLA B 617:

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



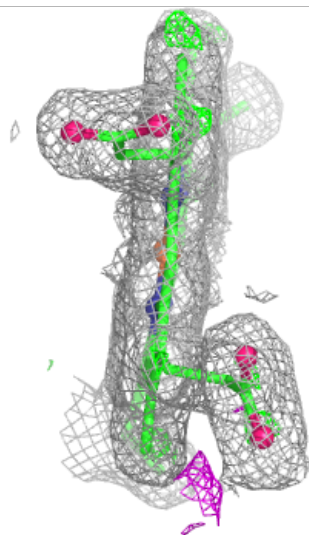
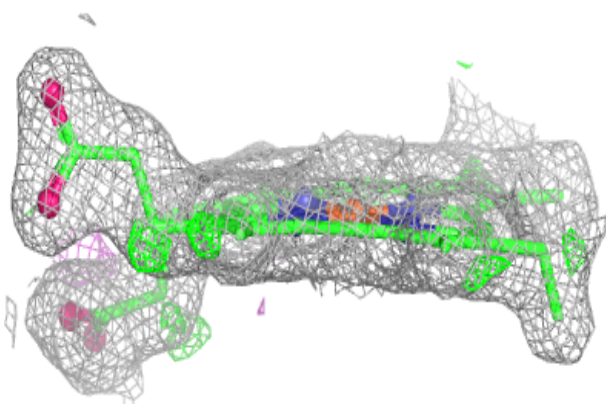
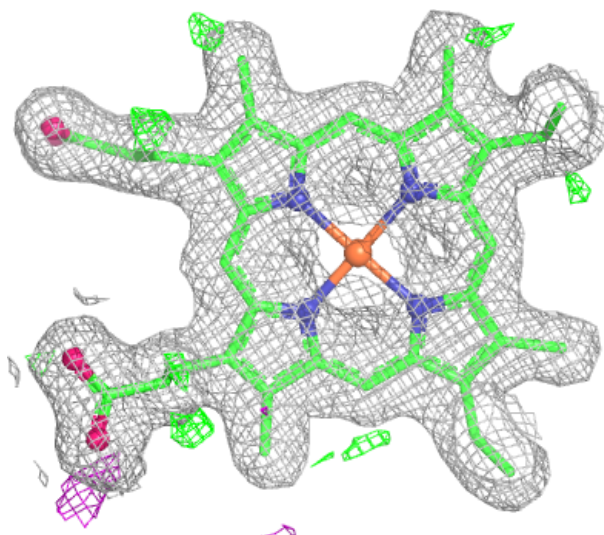
Electron density around HEM E 113:

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



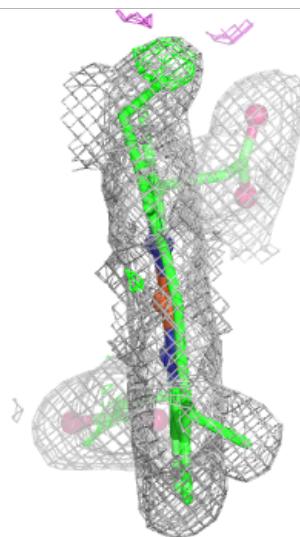
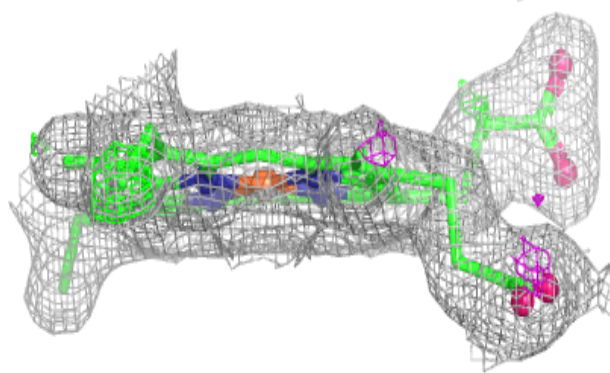
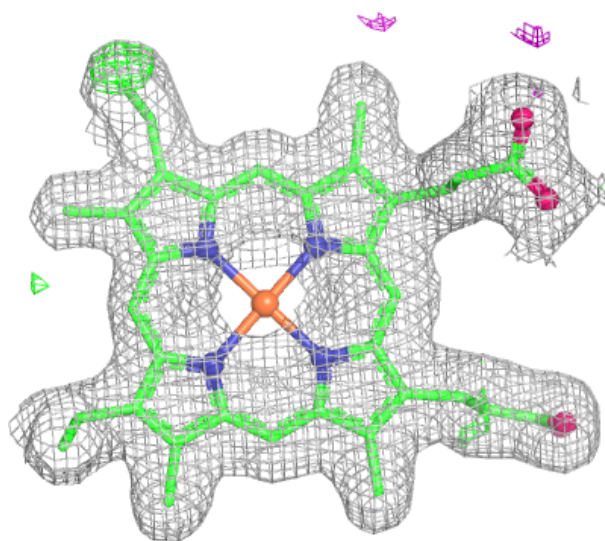
Electron density around HEC V 203:

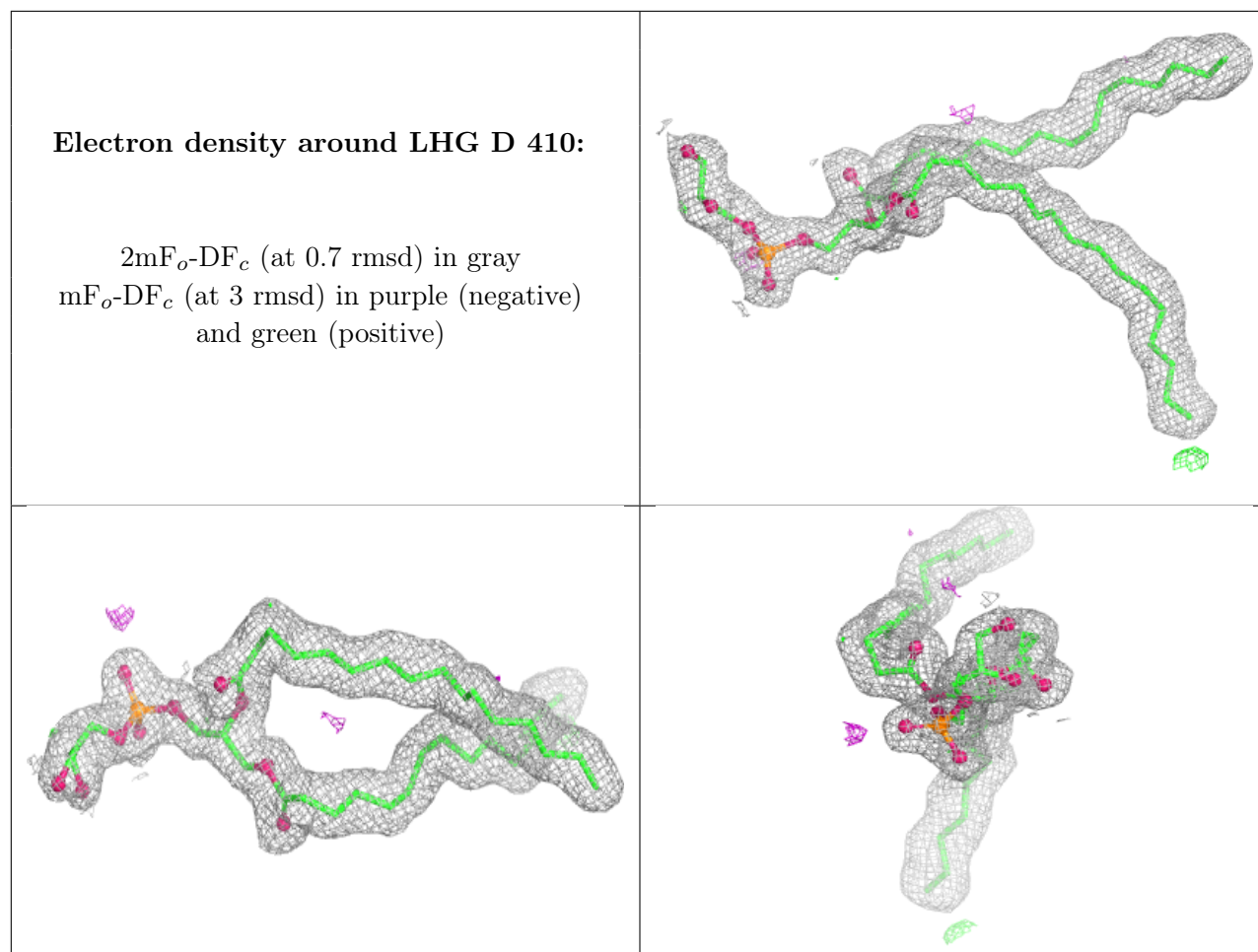
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.