



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 3, 2026 – 09:44 AM EDT

PDB ID : 5KAF / pdb_00005kaf
Title : RT XFEL structure of Photosystem II in the dark state at 3.0 Å resolution
Authors : Young, I.D.; Ibrahim, M.; Chatterjee, R.; Gul, S.; Koroidov, S.; Brewster, A.S.; Tran, R.; Alonso-Mori, R.; Fuller, F.; Kroll, T.; Michels-Clark, T.; Laksmono, H.; Sierra, R.G.; Stan, C.A.; Saracini, C.; Bean, M.A.; Seuffert, I.; Sokaras, D.; Weng, T.-C.; Hunter, M.S.; Aquila, A.; Koglin, J.E.; Robinson, J.; Liang, M.; Boutet, S.; Lyubimov, A.Y.; Uervirojnangkoorn, M.; Moriarty, N.W.; Liebschner, D.; Afonine, P.V.; Waterman, D.G.; Evans, G.; Dobbek, H.; Weis, W.I.; Brunger, A.T.; Zwart, P.H.; Adams, P.D.; Zouni, A.; Messinger, J.; Bergmann, U.; Sauter, N.K.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on : 2016-06-01
Resolution : 3.00 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)

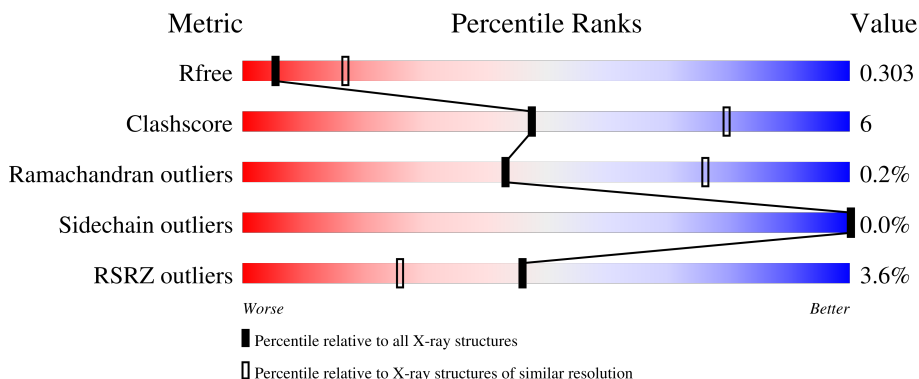
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

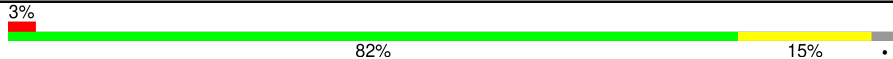
The reported resolution of this entry is 3.00 Å.

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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	
1	a	344	

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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

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Mol	Chain	Length	Quality of chain
2	B	510	
2	b	510	
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	

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Mol	Chain	Length	Quality of chain
14	t	32	
15	U	134	
15	u	134	
16	V	163	
16	v	163	
17	Y	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	R	41	
20	r	41	

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
32	BCT	A	620	-	X	-	-
35	HEC	V	201	X	-	-	-
35	HEC	v	201	X	-	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 50162 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2618	1715	431	457	15			
1	a	334	Total	C	N	O	S	0	0	0
			2613	1713	428	457	15			

- 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	0	0
			3953	2596	658	686	13			
2	b	504	Total	C	N	O	S	3	1	0
			3960	2600	658	689	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	0	0
			3486	2281	584	608	13			
3	c	451	Total	C	N	O	S	0	0	0
			3486	2281	584	608	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	0	0
			2716	1800	444	460	12			
4	d	341	Total	C	N	O	S	0	0	0
			2709	1798	441	458	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	0	0
			657	429	106	122			
5	e	82	Total	C	N	O	0	0	0
			665	434	108	123			

- 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
			274	187	45	41	1			
6	f	34	Total	C	N	O	S	0	0	0
			274	187	45	41	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			
7	h	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total	C	N	O	S	0	0	0
			296	200	46	49	1			
8	i	36	Total	C	N	O	S	0	0	0
			296	200	46	49	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	FME	-	expression tag	UNP Q8DJZ6
i	1	FME	-	expression tag	UNP Q8DJZ6

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			257	174	40	42	1			
9	j	36	Total	C	N	O	S	0	0	0
			257	174	40	42	1			

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

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

- 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	0	0	0
			301	200	48	53			
11	l	37	Total	C	N	O	0	0	0
			301	200	48	53			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	0	0
			256	171	37	47	1			
12	m	33	Total	C	N	O	S	0	0	0
			256	171	37	47	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	1	FME	-	expression tag	UNP Q8DHA7
m	1	FME	-	expression tag	UNP Q8DHA7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	N	O	S	0	0	0
			1845	1154	309	378	4			
13	o	244	Total	C	N	O	S	0	0	0
			1853	1160	312	377	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	1	FME	-	expression tag	UNP Q8DIQ0
t	1	FME	-	expression tag	UNP Q8DIQ0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	30	Total	C	N	O	S	0	0	0
			224	147	38	36	3			
17	y	30	Total	C	N	O	S	0	0	0
			224	147	38	36	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O		0	0	0
			279	187	45	47				
18	x	38	Total	C	N	O		0	0	0
			281	188	45	48				

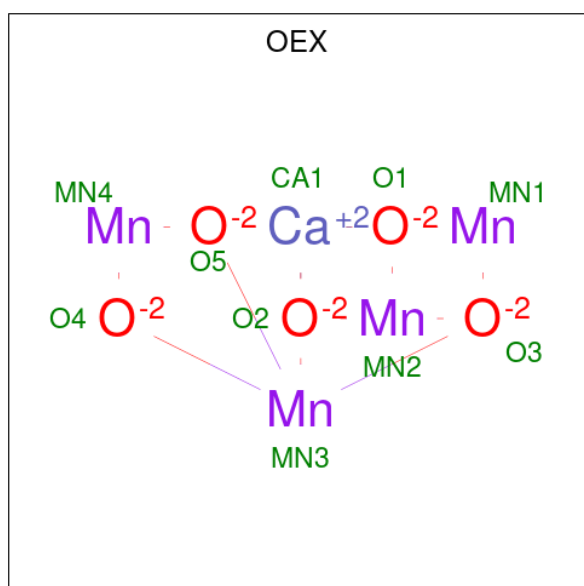
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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

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

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

- Molecule 21 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



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

- Molecule 22 is FE (II) ION (CCD ID: FE2) (formula: Fe).

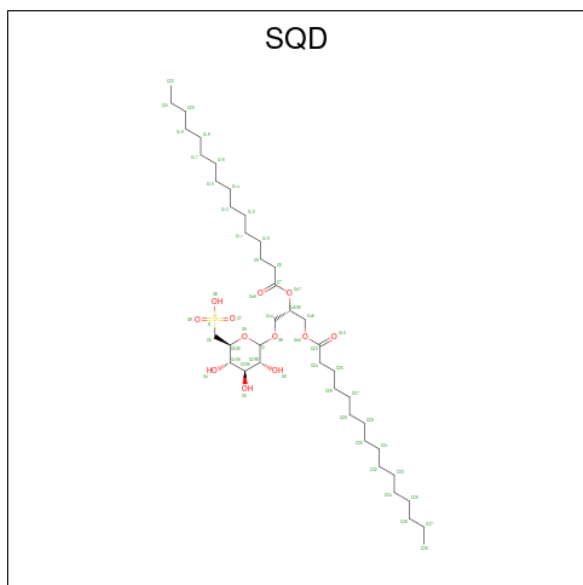
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	1	Total	Fe	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	a	1	Total	Fe	0	0
			1	1		

- Molecule 23 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).

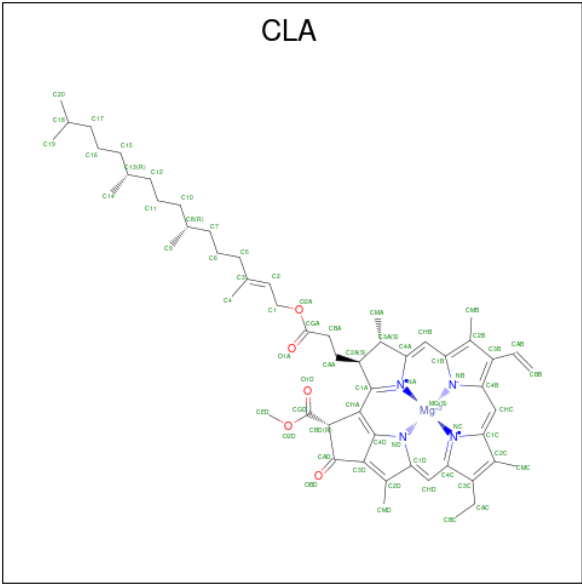


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	O	S	0	0
			52	39	12	1		
23	A	1	Total	C	O		0	0
			40	35	5			
23	B	1	Total	C	O	S	0	0
			54	41	12	1		
23	D	1	Total	C	O	S	0	0
			47	34	12	1		
23	D	1	Total	C	O	S	0	0
			43	30	12	1		
23	I	1	Total	C	O		0	0
			40	35	5			
23	b	1	Total	C	O	S	0	0
			54	41	12	1		
23	c	1	Total	C	O	S	0	0
			54	41	12	1		
23	f	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 24 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	2	Total Cl 2 2	0	0
24	a	2	Total Cl 2 2	0	0

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C Mg N O 65 55 1 4 5	0	0
25	A	1	Total C Mg N O 57 47 1 4 5	0	0
25	A	1	Total C Mg N O 65 55 1 4 5	0	0
25	A	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0

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

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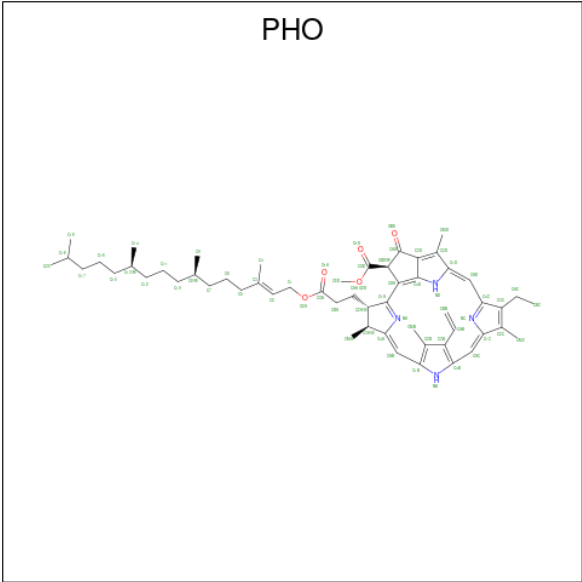
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 59	C 49	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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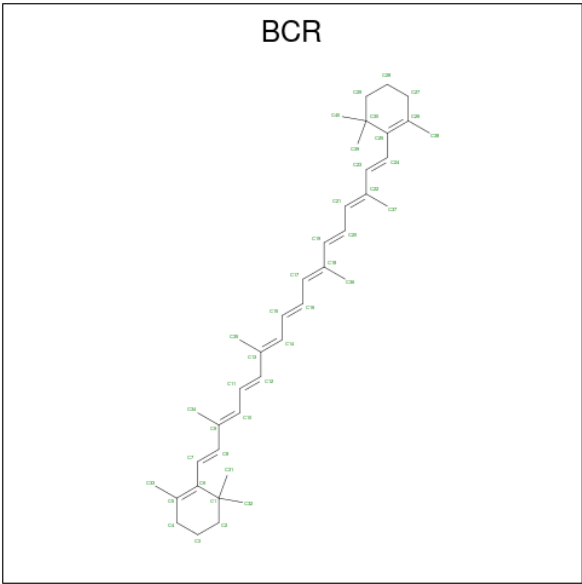
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 26 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



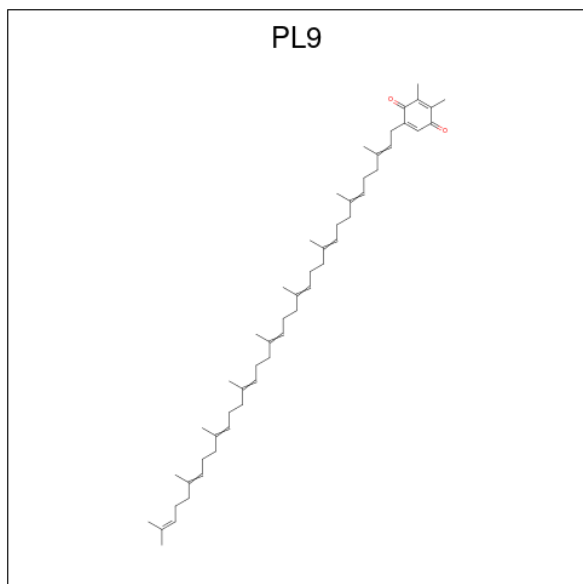
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	N	O	0	0
			64	55	4	5		
26	D	1	Total	C	N	O	0	0
			64	55	4	5		
26	a	1	Total	C	N	O	0	0
			64	55	4	5		
26	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 27 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



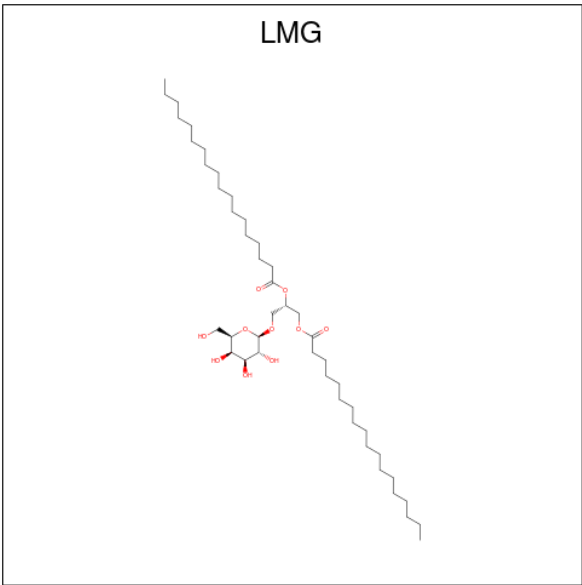
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	T	1	Total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

- Molecule 28 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
28	A	1	Total	C	O	0	0
			55	53	2		
28	D	1	Total	C	O	0	0
			55	53	2		
28	a	1	Total	C	O	0	0
			55	53	2		
28	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			51	41	10		
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
			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
			51	41	10		
29	b	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		0	0
			9	9			
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
			51	41	10		

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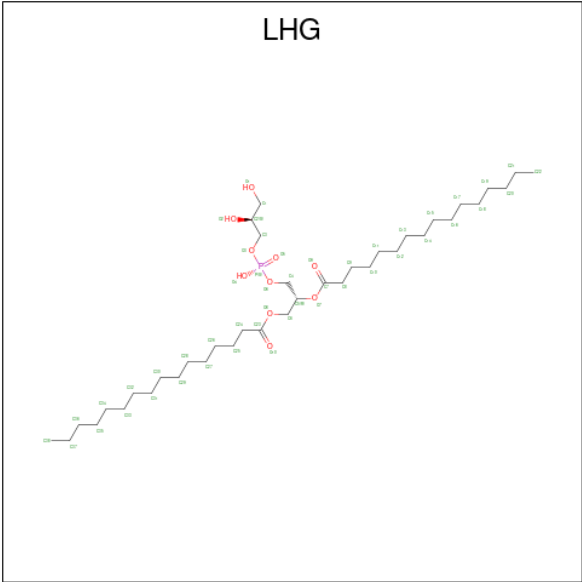
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	d	1	Total	C	O	0	0
			42	32	10		
29	d	1	Total	C	O	0	0
			40	35	5		

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

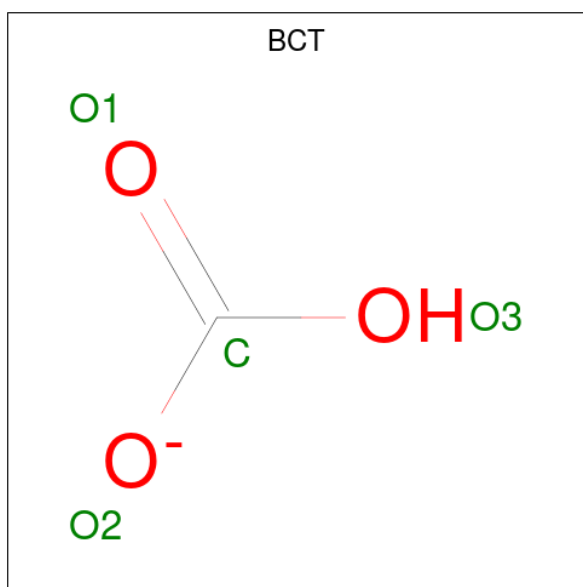
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C		0	0
			7	7			
30	B	3	Total	C		0	0
			28	28			
30	C	1	Total	C		0	0
			9	9			
30	H	1	Total	C		0	0
			8	8			
30	M	2	Total	C		0	0
			23	23			
30	b	2	Total	C		0	0
			26	26			
30	d	1	Total	C		0	0
			22	22			
30	i	1	Total	C		0	0
			12	12			
30	j	1	Total	C		0	0
			9	9			
30	m	2	Total	C		0	0
			21	21			
30	t	1	Total	C		0	0
			10	10			
30	z	1	Total	C		0	0
			11	11			

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



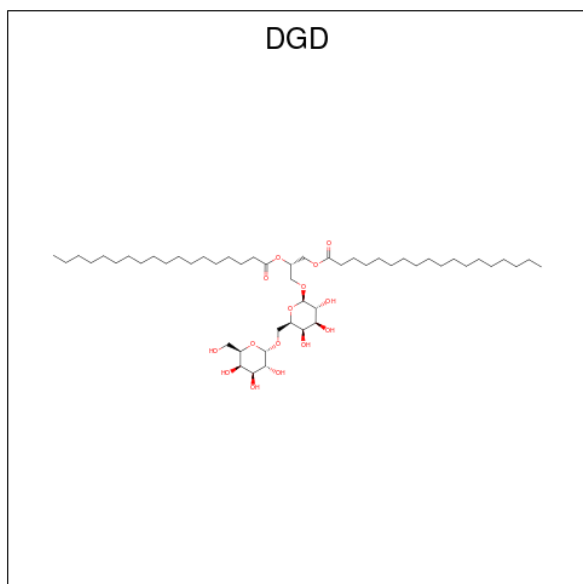
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	L	1	Total	C	O	P	0	0
			49	38	10	1		
31	a	1	Total	C	O	P	0	0
			49	38	10	1		
31	a	1	Total	C	O	P	0	0
			35	24	10	1		
31	a	1	Total	C	O	P	0	0
			42	31	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 32 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			4	1	3		
32	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



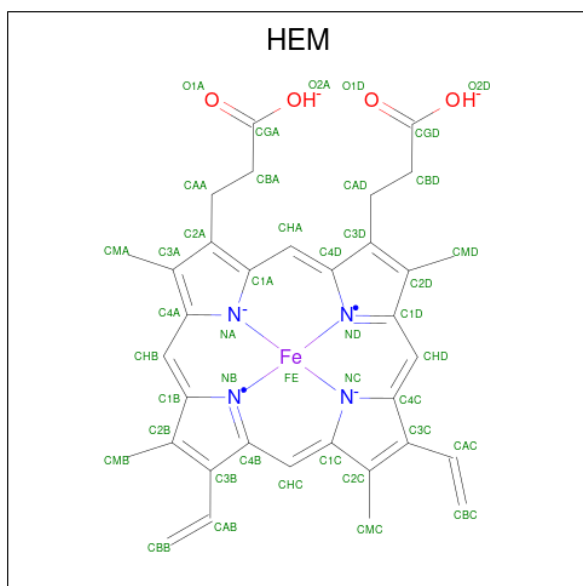
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	C	1	Total	C	O	0	0
			62	47	15		

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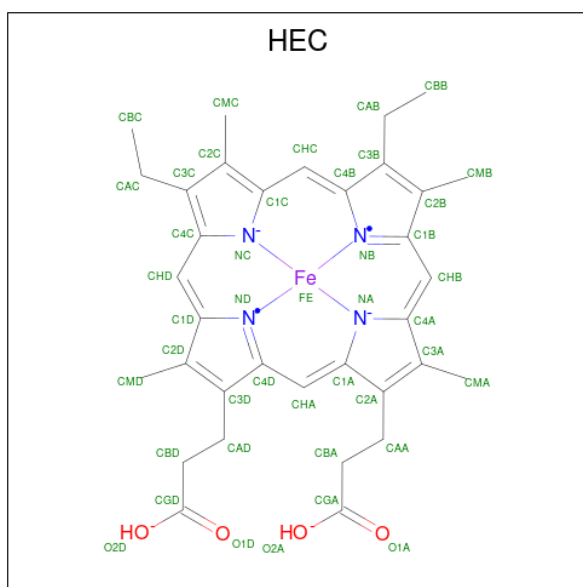
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	C	1	Total	C	O	0	0
			62	47	15		
33	C	1	Total	C	O	0	0
			62	47	15		
33	H	1	Total	C	O	0	0
			62	47	15		
33	c	1	Total	C	O	0	0
			62	47	15		
33	c	1	Total	C	O	0	0
			62	47	15		
33	c	1	Total	C	O	0	0
			62	47	15		
33	h	1	Total	C	O	0	0
			62	47	15		

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



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

- Molecule 35 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 36 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	A	10	Total O 10 10	0	0
36	B	17	Total O 17 17	0	0
36	C	11	Total O 11 11	0	0
36	D	9	Total O 9 9	0	0
36	E	3	Total O 3 3	0	0
36	L	2	Total O 2 2	0	0
36	M	2	Total O 2 2	0	0
36	O	5	Total O 5 5	0	0
36	T	1	Total O 1 1	0	0
36	V	2	Total O 2 2	0	0

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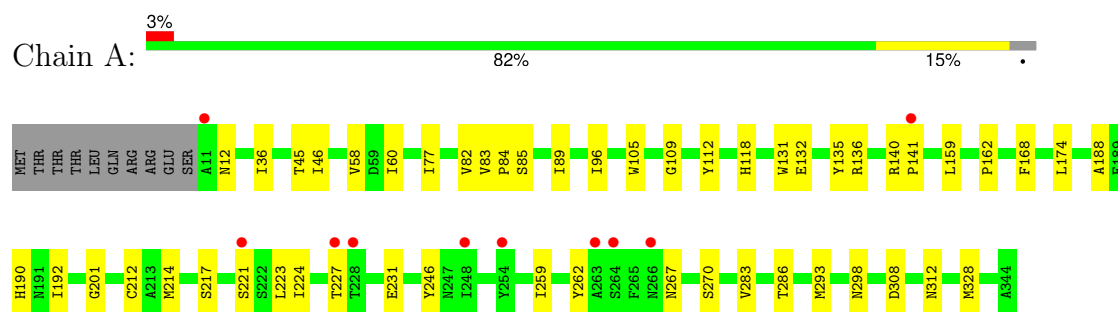
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	X	1	Total 1	O 1	0	0
36	Z	1	Total 1	O 1	0	0
36	a	11	Total 11	O 11	0	0
36	b	12	Total 12	O 12	0	0
36	c	11	Total 11	O 11	0	0
36	d	9	Total 9	O 9	0	0
36	i	1	Total 1	O 1	0	0
36	l	2	Total 2	O 2	0	0
36	o	9	Total 9	O 9	0	0
36	u	2	Total 2	O 2	0	0
36	v	3	Total 3	O 3	0	0

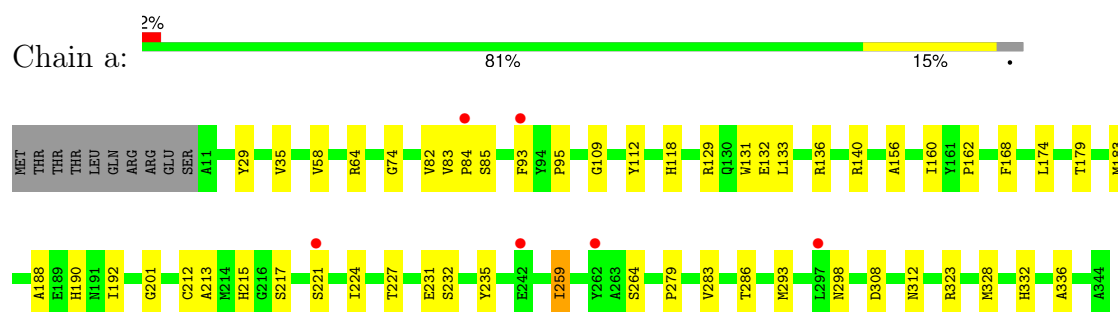
3 Residue-property plots [i](#)

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.

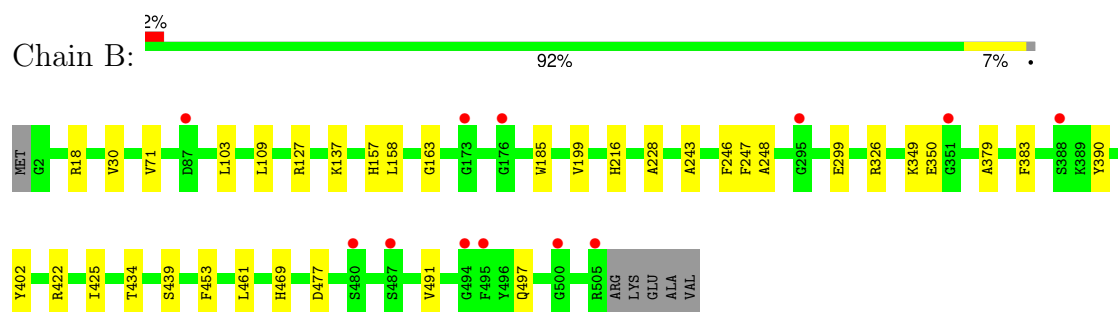
- Molecule 1: Photosystem II protein D1 1



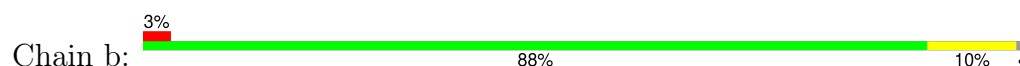
- Molecule 1: Photosystem II protein D1 1

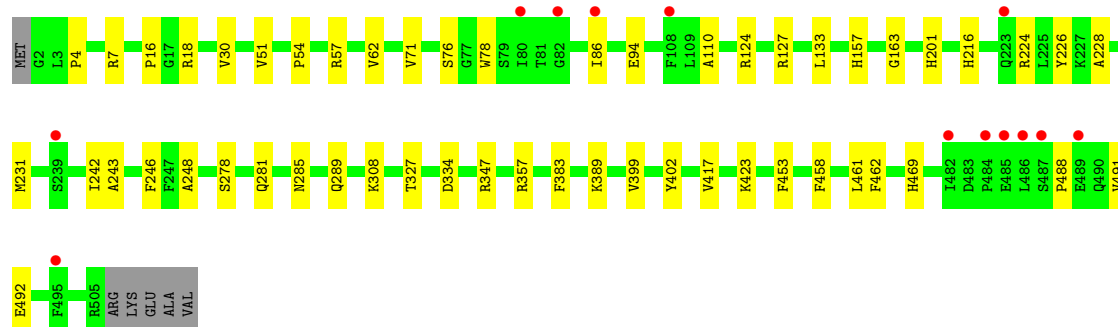


- Molecule 2: Photosystem II CP47 reaction center protein

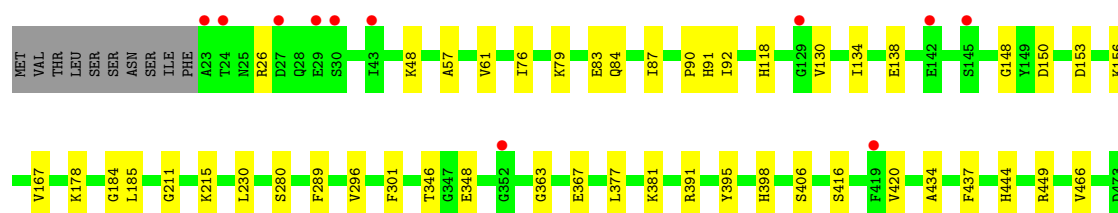
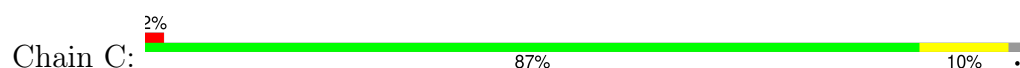


- Molecule 2: Photosystem II CP47 reaction center protein

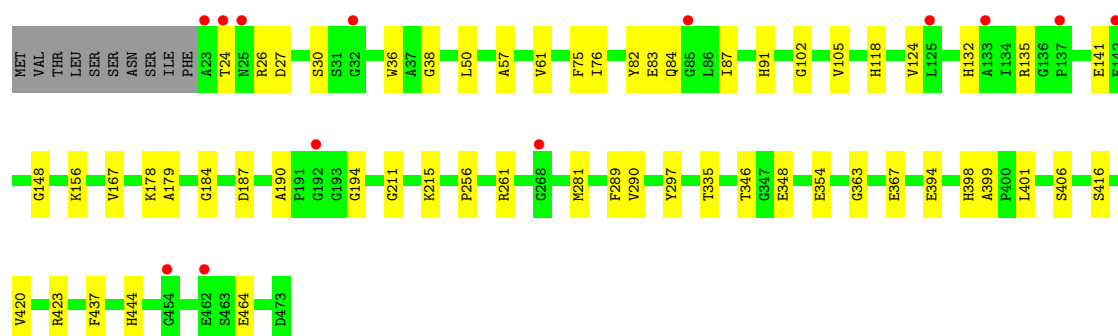
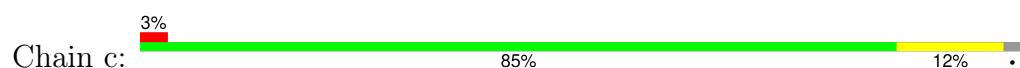




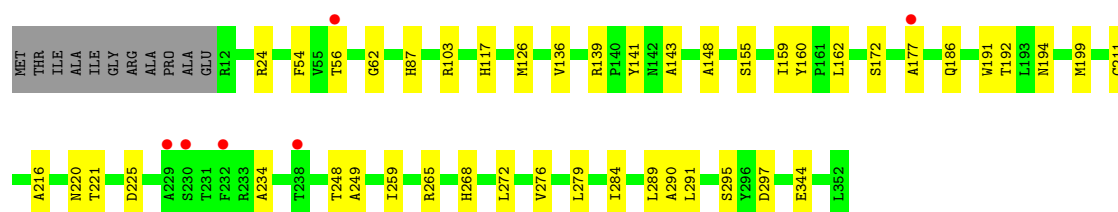
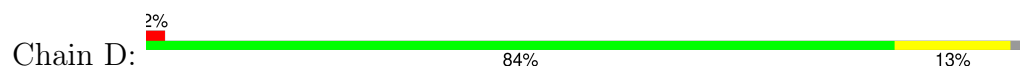
• Molecule 3: Photosystem II CP43 reaction center protein



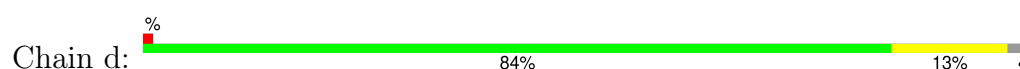
• Molecule 3: Photosystem II CP43 reaction center protein

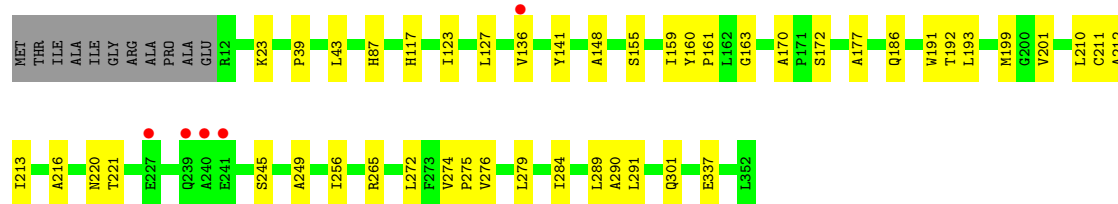


• Molecule 4: Photosystem II D2 protein

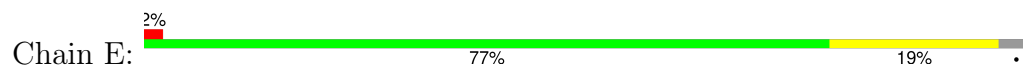


• Molecule 4: Photosystem II D2 protein

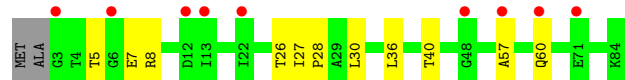
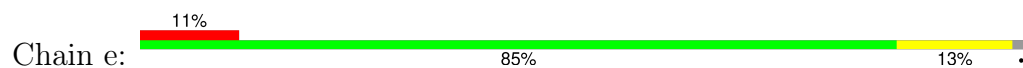




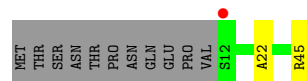
• Molecule 5: Cytochrome b559 subunit alpha



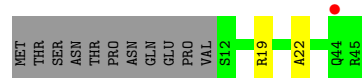
• Molecule 5: Cytochrome b559 subunit alpha



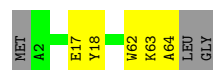
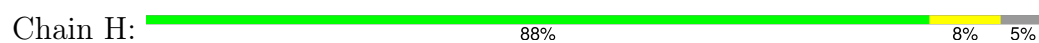
• Molecule 6: Cytochrome b559 subunit beta



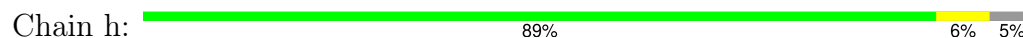
• Molecule 6: Cytochrome b559 subunit beta



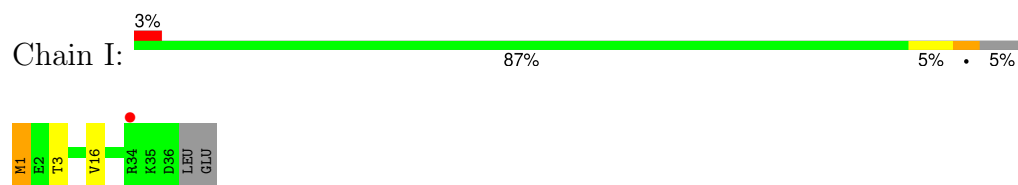
• Molecule 7: Photosystem II reaction center protein H



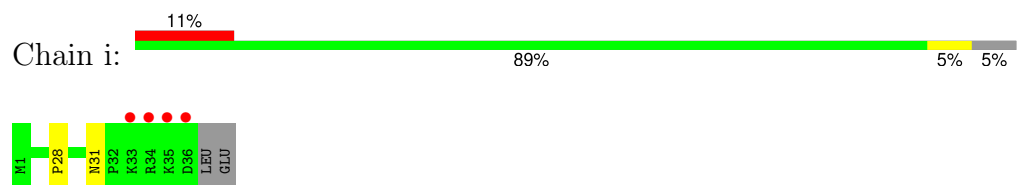
• Molecule 7: Photosystem II reaction center protein H



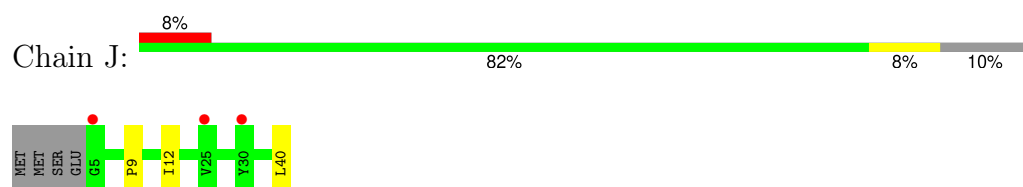
- Molecule 8: Photosystem II reaction center protein I



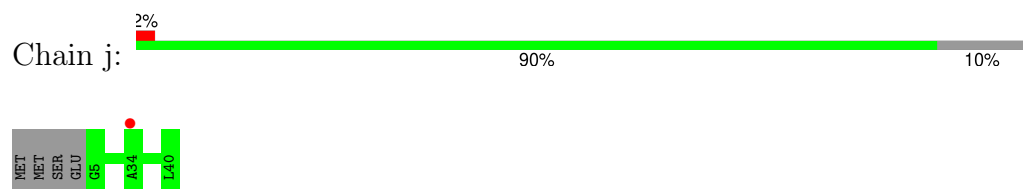
- Molecule 8: Photosystem II reaction center protein I



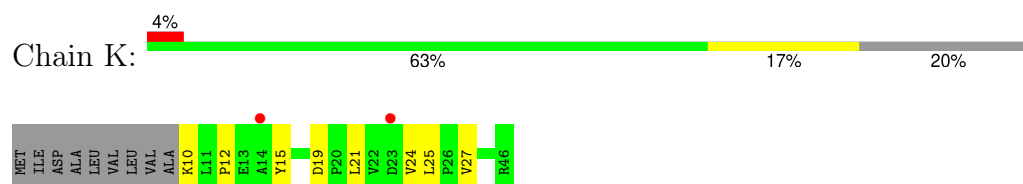
- Molecule 9: Photosystem II reaction center protein J



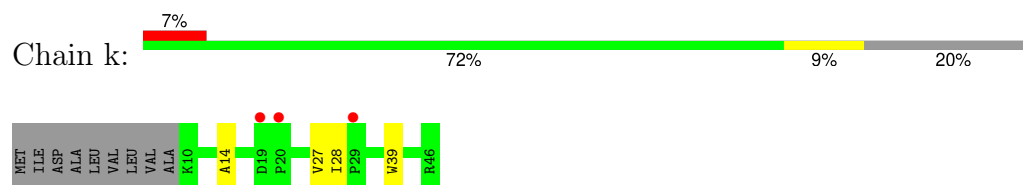
- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K

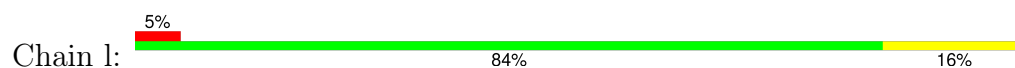


- Molecule 11: Photosystem II reaction center protein L

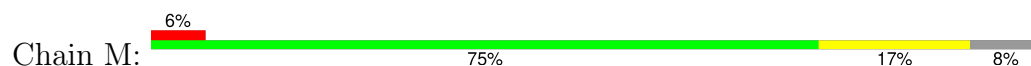




- Molecule 11: Photosystem II reaction center protein L



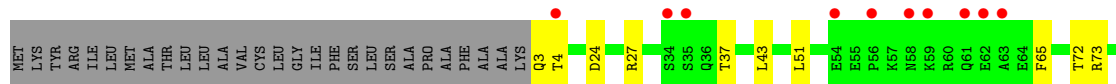
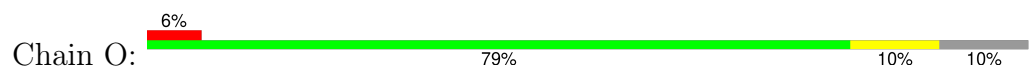
- Molecule 12: Photosystem II reaction center protein M



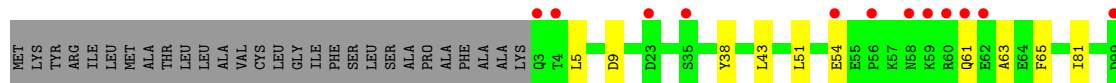
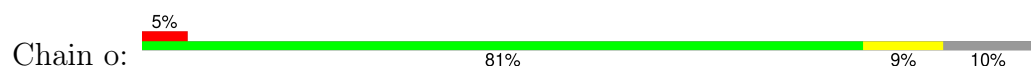
- Molecule 12: Photosystem II reaction center protein M



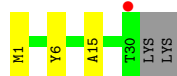
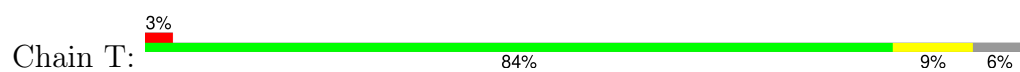
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



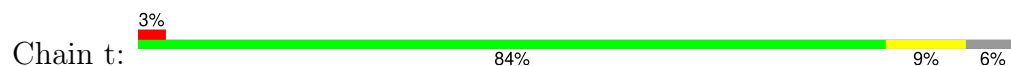
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



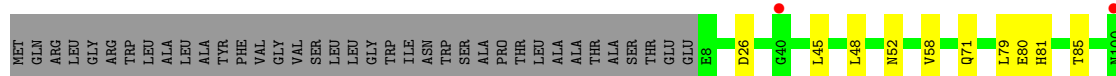
- Molecule 14: Photosystem II reaction center protein T



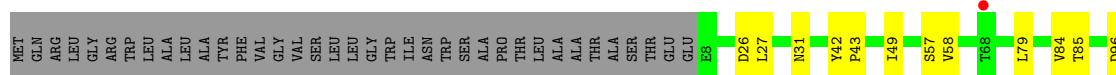
- Molecule 14: Photosystem II reaction center protein T



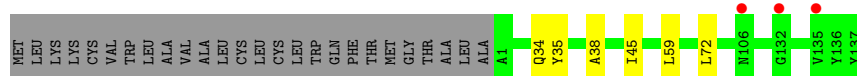
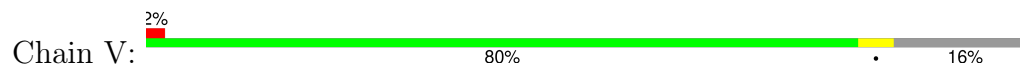
- Molecule 15: Photosystem II 12 kDa extrinsic protein



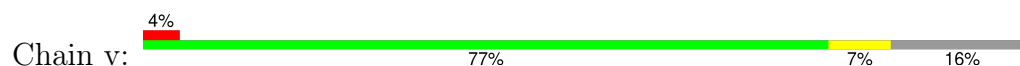
- Molecule 15: Photosystem II 12 kDa extrinsic protein



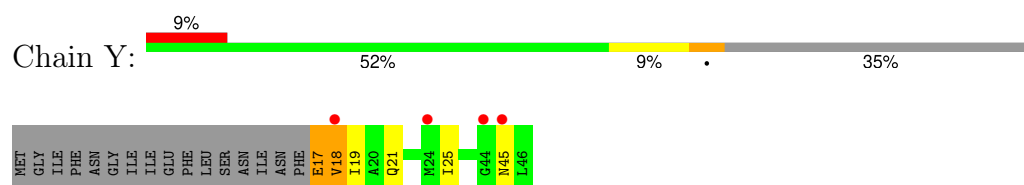
- Molecule 16: Cytochrome c-550



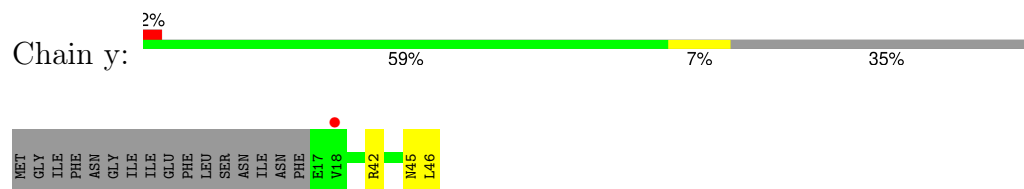
- Molecule 16: Cytochrome c-550



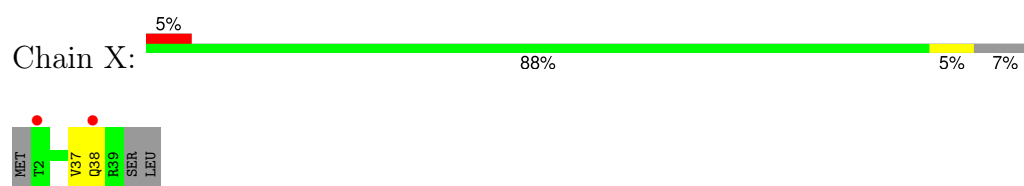
- Molecule 17: Photosystem II reaction center protein Ycf12



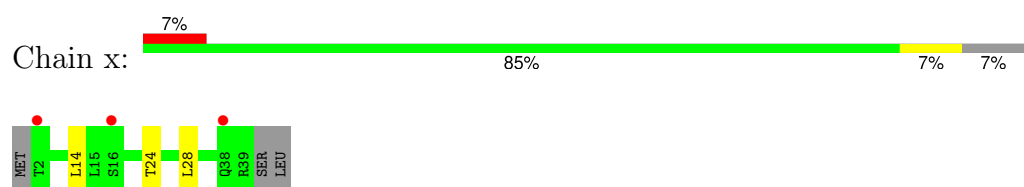
- Molecule 17: Photosystem II reaction center protein Ycf12



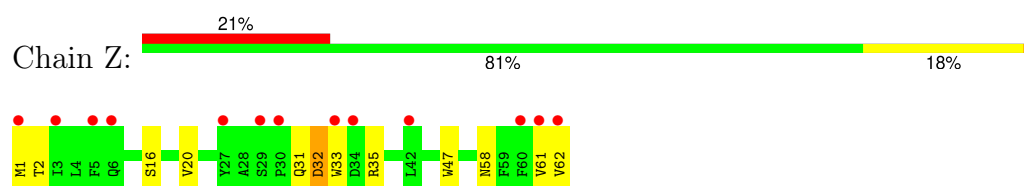
- Molecule 18: Photosystem II reaction center X protein



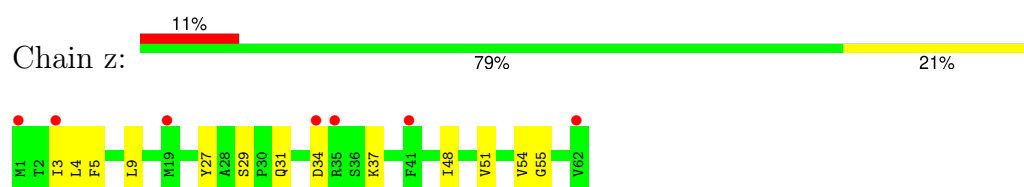
- Molecule 18: Photosystem II reaction center X protein



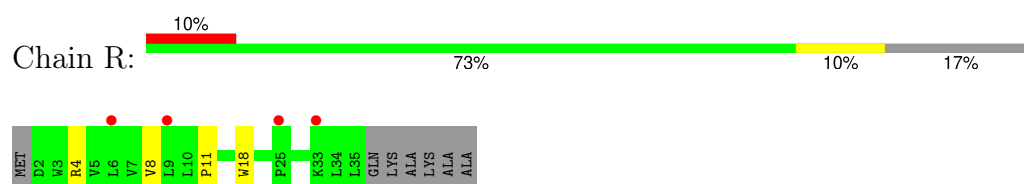
- Molecule 19: Photosystem II reaction center protein Z



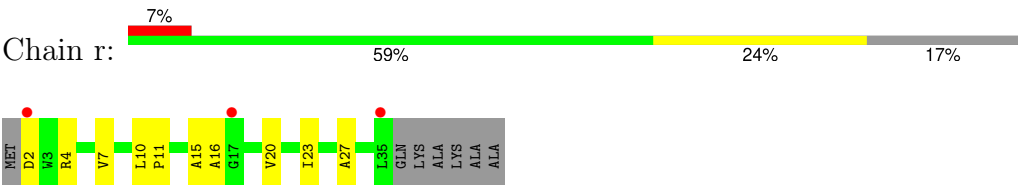
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



● Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.73Å 223.81Å 330.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.12 – 3.00 43.12 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.0 (43.12-3.00) 86.2 (43.12-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 3.01Å)	Xtriage
Refinement program	PHENIX dev_2411	Depositor
R, R_{free}	0.264 , 0.303 0.266 , 0.303	Depositor DCC
R_{free} test set	1446 reflections (0.83%)	wwPDB-VP
Wilson B-factor (Å ²)	48.4	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	50162	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% 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: LHG, UNL, OEX, FME, PHO, SQD, DGD, CL, BCR, BCT, LMG, HEM, PL9, HEC, CLA, FE2

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.08	0/2703	0.24	0/3687
1	a	0.08	0/2698	0.24	0/3681
2	B	0.09	0/4093	0.24	0/5580
2	b	0.08	0/4103	0.24	0/5593
3	C	0.08	0/3599	0.23	0/4900
3	c	0.09	0/3599	0.24	0/4900
4	D	0.08	0/2811	0.24	0/3830
4	d	0.09	0/2804	0.25	0/3821
5	E	0.17	0/676	0.26	0/924
5	e	0.10	0/684	0.27	0/933
6	F	0.08	0/283	0.23	0/386
6	f	0.08	0/283	0.24	0/386
7	H	0.09	0/511	0.25	0/697
7	h	0.11	0/511	0.25	0/697
8	I	0.09	0/293	0.23	0/396
8	i	0.09	0/293	0.24	0/396
9	J	0.09	0/263	0.28	0/356
9	j	0.07	0/263	0.22	0/356
10	K	0.12	0/303	0.31	0/416
10	k	0.11	0/303	0.30	0/416
11	L	0.09	0/308	0.24	0/419
11	l	0.07	0/308	0.22	0/419
12	M	0.08	0/249	0.21	0/341
12	m	0.08	0/249	0.26	0/341
13	O	0.09	0/1876	0.28	0/2549
13	o	0.08	0/1884	0.27	0/2557
14	T	0.07	0/257	0.24	0/349
14	t	0.08	0/257	0.24	0/349
15	U	0.08	0/785	0.26	0/1064
15	u	0.11	0/785	0.27	0/1064
16	V	0.09	0/1085	0.23	0/1473
16	v	0.11	0/1085	0.24	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.18	0/225	0.61	2/301 (0.7%)
17	y	0.10	0/225	0.29	0/301
18	X	0.06	0/282	0.16	0/381
18	x	0.11	0/284	0.26	0/384
19	Z	0.08	0/490	0.27	0/669
19	z	0.10	0/490	0.28	0/669
20	R	0.09	0/279	0.26	0/383
20	r	0.10	0/279	0.29	0/383
All	All	0.09	0/42758	0.25	2/58220 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Y	17	GLU	CA-C-N	6.13	132.74	121.70
17	Y	17	GLU	C-N-CA	6.13	132.74	121.70

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	2618	0	2515	38	0
1	a	2613	0	2506	40	0
2	B	3953	0	3802	33	0
2	b	3960	0	3811	40	0
3	C	3486	0	3407	29	0
3	c	3486	0	3407	39	0
4	D	2716	0	2621	36	0
4	d	2709	0	2612	38	0
5	E	657	0	637	14	0
5	e	665	0	651	9	0
6	F	274	0	279	3	0
6	f	274	0	279	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	498	0	518	3	0
7	h	498	0	518	4	0
8	I	296	0	311	2	0
8	i	296	0	311	1	0
9	J	257	0	268	2	0
9	j	257	0	268	0	0
10	K	293	0	305	7	0
10	k	293	0	305	4	0
11	L	301	0	309	3	0
11	l	301	0	309	6	0
12	M	256	0	269	5	0
12	m	256	0	269	6	0
13	O	1845	0	1793	15	0
13	o	1853	0	1817	15	0
14	T	258	0	261	4	0
14	t	258	0	261	2	0
15	U	774	0	773	5	0
15	u	774	0	773	7	0
16	V	1064	0	1073	4	0
16	v	1064	0	1073	8	0
17	Y	224	0	252	5	0
17	y	224	0	252	4	0
18	X	279	0	307	2	0
18	x	281	0	312	2	0
19	Z	479	0	516	7	0
19	z	479	0	516	9	0
20	R	273	0	305	3	0
20	r	273	0	305	7	0
21	A	10	0	0	0	0
21	a	10	0	0	0	0
22	A	1	0	0	0	0
22	a	1	0	0	0	0
23	A	92	0	138	4	0
23	B	54	0	78	7	0
23	D	90	0	111	1	0
23	I	40	0	67	0	0
23	b	54	0	77	1	0
23	c	54	0	78	1	0
23	f	43	0	53	0	0
24	A	2	0	0	0	0
24	a	2	0	0	1	0
25	A	252	0	269	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	B	1040	0	1152	35	0
25	C	845	0	936	27	0
25	D	130	0	144	5	0
25	a	254	0	274	9	0
25	b	1040	0	1152	31	0
25	c	838	0	919	23	0
25	d	130	0	144	10	0
26	A	64	0	74	1	0
26	D	64	0	74	3	0
26	a	64	0	74	1	0
26	d	64	0	74	4	0
27	A	40	0	56	3	0
27	B	160	0	224	11	0
27	C	80	0	112	3	0
27	D	40	0	56	3	0
27	H	40	0	56	4	0
27	K	40	0	56	2	0
27	T	40	0	56	7	0
27	Y	40	0	56	1	0
27	a	40	0	56	3	0
27	b	120	0	168	8	0
27	c	80	0	112	7	0
27	d	40	0	56	2	0
27	h	40	0	56	2	0
27	k	40	0	56	2	0
27	y	40	0	56	3	0
28	A	55	0	80	4	0
28	D	55	0	80	2	0
28	a	55	0	80	4	0
28	d	55	0	80	5	0
29	A	102	0	144	2	0
29	B	153	0	216	3	0
29	C	102	0	144	3	0
29	D	51	0	72	2	0
29	b	111	0	158	5	0
29	c	153	0	216	5	0
29	d	82	0	115	3	0
30	A	7	0	0	0	0
30	B	28	0	0	0	0
30	C	9	0	0	0	0
30	H	8	0	0	0	0
30	M	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	b	26	0	0	0	0
30	d	22	0	0	0	0
30	i	12	0	0	0	0
30	j	9	0	0	0	0
30	m	21	0	0	0	0
30	t	10	0	0	0	0
30	z	11	0	0	0	0
31	A	147	0	222	12	0
31	D	49	0	74	1	0
31	L	49	0	74	3	0
31	a	126	0	171	4	0
31	d	49	0	74	2	0
31	l	49	0	74	5	0
32	A	4	0	0	1	0
32	a	4	0	0	0	0
33	C	186	0	246	5	0
33	H	62	0	82	2	0
33	c	186	0	246	3	0
33	h	62	0	82	3	0
34	E	43	0	30	3	0
34	e	43	0	30	3	0
35	V	43	0	30	1	0
35	v	43	0	29	2	0
36	A	10	0	0	0	0
36	B	17	0	0	0	0
36	C	11	0	0	0	0
36	D	9	0	0	0	0
36	E	3	0	0	0	0
36	L	2	0	0	0	0
36	M	2	0	0	0	0
36	O	5	0	0	0	0
36	T	1	0	0	0	0
36	V	2	0	0	0	0
36	X	1	0	0	0	0
36	Z	1	0	0	0	0
36	a	11	0	0	0	0
36	b	12	0	0	0	0
36	c	11	0	0	0	0
36	d	9	0	0	0	0
36	i	1	0	0	0	0
36	l	2	0	0	0	0
36	o	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	u	2	0	0	0	0
36	v	3	0	0	0	0
All	All	50162	0	51045	563	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 563 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:613:LHG:O4	4:d:141:TYR:OH	1.90	0.88
2:B:157:HIS:HE1	25:B:606:CLA:NA	1.76	0.83
31:A:618:LHG:HC31	5:E:9:PRO:HB3	1.61	0.81
31:A:616:LHG:O4	4:D:141:TYR:OH	1.98	0.80
25:a:607:CLA:HAB	25:d:403:CLA:H72	1.69	0.74

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/344 (96%)	320 (96%)	11 (3%)	1 (0%)	36	70
1	a	332/344 (96%)	320 (96%)	11 (3%)	1 (0%)	36	70
2	B	502/510 (98%)	483 (96%)	19 (4%)	0	100	100
2	b	503/510 (99%)	486 (97%)	17 (3%)	0	100	100
3	C	449/461 (97%)	436 (97%)	12 (3%)	1 (0%)	43	76
3	c	449/461 (97%)	430 (96%)	17 (4%)	2 (0%)	30	65
4	D	339/352 (96%)	328 (97%)	11 (3%)	0	100	100
4	d	339/352 (96%)	324 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	79/84 (94%)	78 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	78 (98%)	2 (2%)	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	61/66 (92%)	57 (93%)	3 (5%)	1 (2%)	7	34
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
8	i	34/38 (90%)	31 (91%)	3 (9%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
12	M	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
12	m	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
13	O	242/272 (89%)	228 (94%)	14 (6%)	0	100	100
13	o	242/272 (89%)	232 (96%)	9 (4%)	1 (0%)	30	65
14	T	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
15	u	95/134 (71%)	90 (95%)	5 (5%)	0	100	100
16	V	135/163 (83%)	128 (95%)	7 (5%)	0	100	100
16	v	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
17	Y	28/46 (61%)	25 (89%)	2 (7%)	1 (4%)	2	16
17	y	28/46 (61%)	28 (100%)	0	0	100	100
18	X	36/41 (88%)	36 (100%)	0	0	100	100
18	x	36/41 (88%)	32 (89%)	4 (11%)	0	100	100
19	Z	60/62 (97%)	55 (92%)	3 (5%)	2 (3%)	3	17
19	z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
20	R	32/41 (78%)	32 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	r	32/41 (78%)	32 (100%)	0	0	100	100
All	All	5240/5700 (92%)	5040 (96%)	190 (4%)	10 (0%)	43	76

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	Y	18	VAL
19	Z	32	ASP
13	o	61	GLN
3	C	416	SER
7	H	63	LYS

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	269/280 (96%)	269 (100%)	0	100	100
1	a	268/280 (96%)	268 (100%)	0	100	100
2	B	398/407 (98%)	398 (100%)	0	100	100
2	b	400/407 (98%)	400 (100%)	0	100	100
3	C	352/362 (97%)	351 (100%)	1 (0%)	86	91
3	c	352/362 (97%)	351 (100%)	1 (0%)	86	91
4	D	276/283 (98%)	276 (100%)	0	100	100
4	d	274/283 (97%)	274 (100%)	0	100	100
5	E	71/73 (97%)	71 (100%)	0	100	100
5	e	72/73 (99%)	72 (100%)	0	100	100
6	F	27/39 (69%)	27 (100%)	0	100	100
6	f	27/39 (69%)	27 (100%)	0	100	100
7	H	53/55 (96%)	53 (100%)	0	100	100
7	h	53/55 (96%)	53 (100%)	0	100	100
8	I	32/34 (94%)	32 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	24 (100%)	0	100	100
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	30 (100%)	0	100	100
11	L	34/35 (97%)	34 (100%)	0	100	100
11	l	34/35 (97%)	34 (100%)	0	100	100
12	M	28/32 (88%)	28 (100%)	0	100	100
12	m	28/32 (88%)	28 (100%)	0	100	100
13	O	200/228 (88%)	200 (100%)	0	100	100
13	o	202/228 (89%)	202 (100%)	0	100	100
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	84/112 (75%)	84 (100%)	0	100	100
15	u	84/112 (75%)	84 (100%)	0	100	100
16	V	117/138 (85%)	117 (100%)	0	100	100
16	v	117/138 (85%)	117 (100%)	0	100	100
17	Y	23/37 (62%)	23 (100%)	0	100	100
17	y	23/37 (62%)	23 (100%)	0	100	100
18	X	30/34 (88%)	30 (100%)	0	100	100
18	x	31/34 (91%)	31 (100%)	0	100	100
19	Z	52/52 (100%)	52 (100%)	0	100	100
19	z	52/52 (100%)	52 (100%)	0	100	100
20	R	29/33 (88%)	29 (100%)	0	100	100
20	r	29/33 (88%)	29 (100%)	0	100	100
All	All	4313/4654 (93%)	4311 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	289	PHE
3	c	289	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
4	d	332	GLN
13	o	231	HIS
4	d	334	GLN
13	o	104	GLN
13	O	231	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	FME	I	1	8	8,9,10	0.88	0	8,9,11	1.65	2 (25%)
12	FME	M	1	12	8,9,10	0.97	0	8,9,11	1.02	1 (12%)
12	FME	m	1	12	8,9,10	0.97	0	8,9,11	1.00	0
14	FME	t	1	14	8,9,10	0.97	0	8,9,11	1.12	1 (12%)
14	FME	T	1	14	8,9,10	0.96	0	8,9,11	1.08	0
8	FME	i	1	8	8,9,10	0.96	0	8,9,11	1.04	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	-	2/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1	FME	C-CA-N	3.42	116.10	109.50
8	I	1	FME	CA-N-CN	2.44	126.57	122.82
14	t	1	FME	CB-CA-N	2.28	114.67	110.52
12	M	1	FME	CB-CA-N	2.03	114.22	110.52

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O-C-CA-CB
12	m	1	FME	N-CA-CB-CG
12	m	1	FME	C-CA-CB-CG
14	T	1	FME	CA-CB-CG-SD
12	M	1	FME	CA-CB-CG-SD

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	1	FME	1	0
14	T	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 174 ligands modelled in this entry, 6 are monoatomic and 17 are unknown - leaving 151 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	$\# Z > 2$
28	PL9	a	611	-	55,55,55	0.93	4 (7%)	68,69,69	1.50	12 (17%)
25	CLA	B	604	2	69,73,73	1.14	7 (10%)	82,113,113	1.27	7 (8%)
25	CLA	C	506	3	69,73,73	1.14	6 (8%)	82,113,113	1.17	6 (7%)
25	CLA	B	601	36	69,73,73	1.12	7 (10%)	82,113,113	1.20	6 (7%)
33	DGD	h	102	-	63,63,67	0.86	1 (1%)	77,77,81	1.33	8 (10%)
28	PL9	D	407	-	55,55,55	0.98	4 (7%)	68,69,69	1.51	13 (19%)
23	SQD	A	619	-	39,39,54	0.89	2 (5%)	41,41,65	1.18	2 (4%)
29	LMG	b	623	-	51,51,55	0.72	0	59,59,63	1.36	7 (11%)
27	BCR	B	619	-	41,41,41	1.13	2 (4%)	56,56,56	1.25	8 (14%)
25	CLA	C	504	36	69,73,73	1.12	7 (10%)	82,113,113	1.17	5 (6%)
27	BCR	b	620	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	6 (10%)
25	CLA	c	510	3	62,66,73	1.19	7 (11%)	73,104,113	1.25	7 (9%)
25	CLA	c	504	3	69,73,73	1.13	8 (11%)	82,113,113	1.20	6 (7%)
25	CLA	C	507	36	69,73,73	1.13	6 (8%)	82,113,113	1.24	4 (4%)
23	SQD	I	101	-	39,39,54	0.87	2 (5%)	41,41,65	1.20	2 (4%)
25	CLA	b	617	2	69,73,73	1.13	6 (8%)	82,113,113	1.17	4 (4%)
25	CLA	B	616	2	69,73,73	1.13	7 (10%)	82,113,113	1.20	5 (6%)
25	CLA	C	513	3	69,73,73	1.13	5 (7%)	82,113,113	1.16	6 (7%)
32	BCT	a	605	22	3,3,3	3.24	1 (33%)	2,3,3	2.64	1 (50%)
29	LMG	B	625	-	51,51,55	0.83	3 (5%)	59,59,63	1.41	8 (13%)
29	LMG	d	406	-	42,42,55	0.79	1 (2%)	50,50,63	1.31	6 (12%)
23	SQD	D	409	-	41,43,54	1.07	3 (7%)	51,54,65	1.56	10 (19%)
25	CLA	B	611	2	69,73,73	1.13	7 (10%)	82,113,113	1.21	6 (7%)
27	BCR	k	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	6 (10%)
23	SQD	B	626	-	52,54,54	0.95	3 (5%)	62,65,65	1.60	12 (19%)
25	CLA	c	508	3	69,73,73	1.13	6 (8%)	82,113,113	1.16	6 (7%)
25	CLA	c	509	36	69,73,73	1.14	6 (8%)	82,113,113	1.23	4 (4%)
25	CLA	A	609	1	69,73,73	1.12	6 (8%)	82,113,113	1.21	7 (8%)
25	CLA	b	611	2	69,73,73	1.12	7 (10%)	82,113,113	1.15	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	BCR	b	621	-	41,41,41	1.12	2 (4%)	56,56,56	1.20	4 (7%)
25	CLA	C	501	3	69,73,73	1.13	5 (7%)	82,113,113	1.20	5 (6%)
27	BCR	B	617	-	41,41,41	1.16	2 (4%)	56,56,56	1.27	8 (14%)
25	CLA	a	606	1	69,73,73	1.13	6 (8%)	82,113,113	1.15	7 (8%)
25	CLA	C	511	3	69,73,73	1.14	5 (7%)	82,113,113	1.23	6 (7%)
25	CLA	C	510	3	69,73,73	1.13	7 (10%)	82,113,113	1.15	6 (7%)
23	SQD	A	603	-	50,52,54	0.97	3 (6%)	60,63,65	1.53	11 (18%)
25	CLA	B	608	2	69,73,73	1.14	7 (10%)	82,113,113	1.17	6 (7%)
29	LMG	b	624	-	51,51,55	0.74	0	59,59,63	1.31	6 (10%)
31	LHG	a	614	-	34,34,48	0.73	1 (2%)	37,40,54	1.22	3 (8%)
25	CLA	C	503	3	69,73,73	1.14	6 (8%)	82,113,113	1.23	5 (6%)
33	DGD	c	520	-	63,63,67	0.87	2 (3%)	77,77,81	1.40	11 (14%)
25	CLA	C	508	3	69,73,73	1.13	6 (8%)	82,113,113	1.19	6 (7%)
25	CLA	A	607	36	61,65,73	1.20	7 (11%)	72,103,113	1.25	7 (9%)
21	OEX	a	601	36,1,3	0,14,14	-	-	-	-	-
25	CLA	C	509	3	69,73,73	1.13	6 (8%)	82,113,113	1.20	5 (6%)
25	CLA	a	607	36	63,67,73	1.19	7 (11%)	74,105,113	1.20	7 (9%)
25	CLA	b	610	36	69,73,73	1.13	5 (7%)	82,113,113	1.14	6 (7%)
25	CLA	B	610	36	69,73,73	1.14	7 (10%)	82,113,113	1.10	6 (7%)
26	PHO	A	608	-	58,69,69	2.18	9 (15%)	55,99,99	1.42	6 (10%)
32	BCT	A	620	22	3,3,3	3.24	1 (33%)	2,3,3	2.76	2 (100%)
35	HEC	V	201	16	50,50,50	1.56	8 (16%)	68,82,82	1.45	9 (13%)
27	BCR	y	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.17	5 (8%)
25	CLA	b	604	36	69,73,73	1.14	6 (8%)	82,113,113	1.22	6 (7%)
25	CLA	A	615	36	69,73,73	1.12	7 (10%)	82,113,113	1.17	5 (6%)
25	CLA	B	603	2	69,73,73	1.12	7 (10%)	82,113,113	1.13	6 (7%)
29	LMG	A	613	-	51,51,55	0.70	0	59,59,63	1.48	9 (15%)
33	DGD	c	519	-	63,63,67	0.89	2 (3%)	77,77,81	1.38	8 (10%)
25	CLA	c	512	3	69,73,73	1.13	6 (8%)	82,113,113	1.18	5 (6%)
31	LHG	d	407	-	48,48,48	0.63	1 (2%)	51,54,54	1.28	6 (11%)
25	CLA	B	609	2	69,73,73	1.14	6 (8%)	82,113,113	1.17	6 (7%)
25	CLA	B	606	2	69,73,73	1.14	6 (8%)	82,113,113	1.21	6 (7%)
25	CLA	D	403	4	69,73,73	1.13	7 (10%)	82,113,113	1.18	6 (7%)
25	CLA	c	514	3	69,73,73	1.13	6 (8%)	82,113,113	1.24	7 (8%)
25	CLA	B	614	2	69,73,73	1.12	6 (8%)	82,113,113	1.15	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	D	402	4	69,73,73	1.13	7 (10%)	82,113,113	1.14	6 (7%)
25	CLA	a	612	36	69,73,73	1.12	7 (10%)	82,113,113	1.17	6 (7%)
27	BCR	H	102	-	41,41,41	1.08	2 (4%)	56,56,56	1.26	7 (12%)
25	CLA	c	507	3	69,73,73	1.13	7 (10%)	82,113,113	1.16	6 (7%)
34	HEM	E	101	5,6	50,50,50	1.47	9 (18%)	67,82,82	1.06	5 (7%)
23	SQD	f	101	-	41,43,54	1.07	3 (7%)	51,54,65	1.58	11 (21%)
25	CLA	B	607	36	69,73,73	1.13	6 (8%)	82,113,113	1.10	7 (8%)
23	SQD	b	601	-	52,54,54	0.96	3 (5%)	62,65,65	1.39	9 (14%)
25	CLA	b	613	36	69,73,73	1.13	5 (7%)	82,113,113	1.12	6 (7%)
27	BCR	A	610	-	41,41,41	1.12	2 (4%)	56,56,56	1.19	6 (10%)
27	BCR	d	405	-	41,41,41	1.11	2 (4%)	56,56,56	1.22	6 (10%)
33	DGD	H	103	-	63,63,67	0.87	1 (1%)	77,77,81	1.34	7 (9%)
25	CLA	B	613	2	69,73,73	1.13	6 (8%)	82,113,113	1.22	5 (6%)
29	LMG	D	405	-	51,51,55	0.72	1 (1%)	59,59,63	1.32	6 (10%)
25	CLA	C	505	3	69,73,73	1.13	7 (10%)	82,113,113	1.17	6 (7%)
23	SQD	c	501	-	52,54,54	0.95	3 (5%)	62,65,65	1.45	9 (14%)
25	CLA	c	515	3	69,73,73	1.13	6 (8%)	82,113,113	1.17	6 (7%)
33	DGD	C	516	-	63,63,67	0.86	2 (3%)	77,77,81	1.42	9 (11%)
25	CLA	B	615	2	69,73,73	1.14	6 (8%)	82,113,113	1.23	5 (6%)
26	PHO	a	608	-	58,69,69	2.18	9 (15%)	55,99,99	1.43	7 (12%)
27	BCR	c	517	-	41,41,41	1.13	2 (4%)	56,56,56	1.21	6 (10%)
31	LHG	a	613	-	48,48,48	0.63	1 (2%)	51,54,54	1.30	6 (11%)
31	LHG	l	101	-	48,48,48	0.63	1 (2%)	51,54,54	1.26	6 (11%)
25	CLA	B	602	2	69,73,73	1.12	6 (8%)	82,113,113	1.13	6 (7%)
25	CLA	c	513	3	69,73,73	1.13	5 (7%)	82,113,113	1.25	5 (6%)
28	PL9	d	408	-	55,55,55	0.99	4 (7%)	68,69,69	1.48	11 (16%)
29	LMG	C	519	-	51,51,55	0.72	1 (1%)	59,59,63	1.33	6 (10%)
27	BCR	C	514	-	41,41,41	1.14	2 (4%)	56,56,56	1.25	7 (12%)
23	SQD	D	408	-	45,47,54	1.01	2 (4%)	55,58,65	1.72	11 (20%)
31	LHG	D	406	-	48,48,48	0.63	2 (4%)	51,54,54	1.26	6 (11%)
31	LHG	a	615	-	41,41,48	0.68	2 (4%)	44,47,54	1.33	6 (13%)
25	CLA	c	511	3	69,73,73	1.13	6 (8%)	82,113,113	1.22	5 (6%)
27	BCR	B	618	-	41,41,41	1.13	2 (4%)	56,56,56	1.22	5 (8%)
25	CLA	b	616	2	69,73,73	1.14	7 (10%)	82,113,113	1.21	6 (7%)
25	CLA	c	506	36	69,73,73	1.12	7 (10%)	82,113,113	1.19	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PHO	D	401	-	58,69,69	2.18	9 (15%)	55,99,99	1.44	6 (10%)
28	PL9	A	611	-	55,55,55	1.00	3 (5%)	68,69,69	1.51	14 (20%)
25	CLA	b	609	2	69,73,73	1.12	6 (8%)	82,113,113	1.19	4 (4%)
27	BCR	b	622	-	41,41,41	1.11	2 (4%)	56,56,56	1.24	7 (12%)
27	BCR	C	515	-	41,41,41	1.14	2 (4%)	56,56,56	1.23	7 (12%)
29	LMG	c	521	-	51,51,55	0.71	0	59,59,63	1.34	6 (10%)
27	BCR	a	610	-	41,41,41	1.11	2 (4%)	56,56,56	1.19	5 (8%)
29	LMG	d	409	-	39,39,55	0.58	1 (2%)	41,41,63	1.30	3 (7%)
35	HEC	v	201	16	50,50,50	1.58	7 (14%)	68,82,82	1.48	10 (14%)
27	BCR	h	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.32	8 (14%)
27	BCR	c	516	-	41,41,41	1.11	2 (4%)	56,56,56	1.28	6 (10%)
25	CLA	b	614	2	69,73,73	1.13	6 (8%)	82,113,113	1.22	6 (7%)
25	CLA	d	404	4	69,73,73	1.13	5 (7%)	82,113,113	1.19	6 (7%)
25	CLA	C	512	3	69,73,73	1.13	6 (8%)	82,113,113	1.22	5 (6%)
27	BCR	T	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.27	6 (10%)
25	CLA	b	608	2	69,73,73	1.13	7 (10%)	82,113,113	1.16	6 (7%)
25	CLA	c	505	3	69,73,73	1.14	6 (8%)	82,113,113	1.23	5 (6%)
29	LMG	B	620	-	51,51,55	0.73	0	59,59,63	1.34	6 (10%)
25	CLA	b	606	2	69,73,73	1.13	7 (10%)	82,113,113	1.12	5 (6%)
25	CLA	a	609	1	69,73,73	1.12	7 (10%)	82,113,113	1.14	7 (8%)
29	LMG	c	502	-	51,51,55	0.76	2 (3%)	59,59,63	1.34	6 (10%)
27	BCR	Y	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.17	4 (7%)
25	CLA	c	503	3	69,73,73	1.12	6 (8%)	82,113,113	1.19	7 (8%)
29	LMG	b	625	-	8,8,55	0.14	0	7,7,63	0.94	0
33	DGD	C	518	-	63,63,67	0.87	2 (3%)	77,77,81	1.40	8 (10%)
25	CLA	d	403	4	69,73,73	1.13	6 (8%)	82,113,113	1.14	4 (4%)
29	LMG	B	621	-	51,51,55	0.72	0	59,59,63	1.39	6 (10%)
25	CLA	b	619	2	69,73,73	1.13	7 (10%)	82,113,113	1.16	6 (7%)
33	DGD	c	518	-	63,63,67	0.86	2 (3%)	77,77,81	1.42	9 (11%)
27	BCR	B	627	-	41,41,41	1.13	2 (4%)	56,56,56	1.28	6 (10%)
29	LMG	A	612	-	51,51,55	0.72	1 (1%)	59,59,63	1.31	4 (6%)
25	CLA	A	606	1	69,73,73	1.13	6 (8%)	82,113,113	1.13	7 (8%)
31	LHG	A	616	-	48,48,48	0.63	2 (4%)	51,54,54	1.29	6 (11%)
25	CLA	C	502	3	69,73,73	1.13	7 (10%)	82,113,113	1.20	6 (7%)
27	BCR	D	404	-	41,41,41	1.14	2 (4%)	56,56,56	1.22	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	b	618	2	69,73,73	1.14	7 (10%)	82,113,113	1.23	7 (8%)
26	PHO	d	401	-	58,69,69	2.18	9 (15%)	55,99,99	1.43	6 (10%)
31	LHG	A	618	-	48,48,48	0.66	2 (4%)	51,54,54	1.27	7 (13%)
25	CLA	B	605	2	69,73,73	1.13	7 (10%)	82,113,113	1.15	4 (4%)
29	LMG	C	520	-	51,51,55	0.78	1 (1%)	59,59,63	1.35	6 (10%)
31	LHG	L	101	-	48,48,48	0.64	1 (2%)	51,54,54	1.26	6 (11%)
33	DGD	C	517	-	63,63,67	0.90	3 (4%)	77,77,81	1.35	9 (11%)
27	BCR	K	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.27	7 (12%)
31	LHG	A	617	-	48,48,48	0.62	0	51,54,54	1.26	6 (11%)
34	HEM	e	101	5,6	50,50,50	1.46	10 (20%)	67,82,82	1.09	5 (7%)
25	CLA	b	607	2	69,73,73	1.14	7 (10%)	82,113,113	1.27	7 (8%)
29	LMG	c	522	-	51,51,55	0.79	1 (1%)	59,59,63	1.37	6 (10%)
25	CLA	b	605	2	69,73,73	1.13	6 (8%)	82,113,113	1.13	5 (6%)
25	CLA	b	612	2	69,73,73	1.14	7 (10%)	82,113,113	1.19	6 (7%)
25	CLA	b	615	2	69,73,73	1.13	8 (11%)	82,113,113	1.20	6 (7%)
25	CLA	B	612	2	69,73,73	1.12	7 (10%)	82,113,113	1.21	6 (7%)
21	OEX	A	601	36,1,3	0,14,14	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PL9	a	611	-	-	16/53/73/73	0/1/1/1
25	CLA	B	604	2	-	5/39/115/115	-
25	CLA	C	506	3	-	17/39/115/115	-
25	CLA	B	601	36	-	15/39/115/115	-
33	DGD	h	102	-	-	10/51/91/95	0/2/2/2
28	PL9	D	407	-	-	9/53/73/73	0/1/1/1
23	SQD	A	619	-	-	27/41/41/69	-
29	LMG	b	623	-	-	11/46/66/70	0/1/1/1
27	BCR	B	619	-	-	4/29/63/63	0/2/2/2
25	CLA	C	504	36	-	5/39/115/115	-
27	BCR	b	620	-	-	3/29/63/63	0/2/2/2
25	CLA	c	510	3	-	3/31/107/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c	504	3	-	6/39/115/115	-
25	CLA	C	507	36	-	6/39/115/115	-
23	SQD	I	101	-	-	22/41/41/69	-
25	CLA	b	617	2	-	10/39/115/115	-
25	CLA	B	616	2	-	15/39/115/115	-
25	CLA	C	513	3	-	6/39/115/115	-
29	LMG	B	625	-	-	21/46/66/70	0/1/1/1
29	LMG	d	406	-	-	5/37/57/70	0/1/1/1
23	SQD	D	409	-	-	17/38/58/69	0/1/1/1
25	CLA	B	611	2	-	4/39/115/115	-
27	BCR	k	101	-	-	5/29/63/63	0/2/2/2
23	SQD	B	626	-	-	27/49/69/69	0/1/1/1
25	CLA	c	508	3	-	18/39/115/115	-
25	CLA	c	509	36	-	13/39/115/115	-
25	CLA	A	609	1	-	8/39/115/115	-
25	CLA	b	611	2	-	5/39/115/115	-
27	BCR	b	621	-	-	6/29/63/63	0/2/2/2
25	CLA	C	501	3	-	6/39/115/115	-
27	BCR	B	617	-	-	3/29/63/63	0/2/2/2
25	CLA	a	606	1	-	3/39/115/115	-
25	CLA	C	511	3	-	5/39/115/115	-
25	CLA	C	510	3	-	7/39/115/115	-
23	SQD	A	603	-	-	15/47/67/69	0/1/1/1
25	CLA	B	608	2	-	4/39/115/115	-
29	LMG	b	624	-	-	23/46/66/70	0/1/1/1
31	LHG	a	614	-	-	16/39/39/53	-
25	CLA	C	503	3	-	3/39/115/115	-
33	DGD	c	520	-	-	12/51/91/95	0/2/2/2
25	CLA	C	508	3	-	3/39/115/115	-
25	CLA	A	607	36	-	9/30/106/115	-
25	CLA	C	509	3	-	10/39/115/115	-
25	CLA	a	607	36	-	6/32/108/115	-
25	CLA	b	610	36	-	10/39/115/115	-
26	PHO	A	608	-	-	8/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	610	36	-	9/39/115/115	-
35	HEC	V	201	16	1/1/3/7	5/14/54/54	-
27	BCR	y	101	-	-	5/29/63/63	0/2/2/2
25	CLA	b	604	36	-	18/39/115/115	-
25	CLA	A	615	36	-	3/39/115/115	-
25	CLA	B	603	2	-	10/39/115/115	-
29	LMG	A	613	-	-	15/46/66/70	0/1/1/1
33	DGD	c	519	-	-	19/51/91/95	0/2/2/2
25	CLA	c	512	3	-	8/39/115/115	-
31	LHG	d	407	-	-	15/53/53/53	-
25	CLA	B	609	2	-	12/39/115/115	-
25	CLA	B	606	2	-	7/39/115/115	-
25	CLA	D	403	4	-	3/39/115/115	-
25	CLA	c	514	3	-	7/39/115/115	-
25	CLA	B	614	2	-	19/39/115/115	-
25	CLA	D	402	4	-	9/39/115/115	-
25	CLA	a	612	36	-	2/39/115/115	-
27	BCR	H	102	-	-	4/29/63/63	0/2/2/2
25	CLA	c	507	3	-	11/39/115/115	-
34	HEM	E	101	5,6	-	5/14/54/54	-
23	SQD	f	101	-	-	18/38/58/69	0/1/1/1
25	CLA	B	607	36	-	10/39/115/115	-
23	SQD	b	601	-	-	17/49/69/69	0/1/1/1
25	CLA	b	613	36	-	10/39/115/115	-
27	BCR	A	610	-	-	5/29/63/63	0/2/2/2
27	BCR	d	405	-	-	6/29/63/63	0/2/2/2
33	DGD	H	103	-	-	13/51/91/95	0/2/2/2
25	CLA	B	613	2	-	2/39/115/115	-
29	LMG	D	405	-	-	15/46/66/70	0/1/1/1
25	CLA	C	505	3	-	16/39/115/115	-
23	SQD	c	501	-	-	21/49/69/69	0/1/1/1
25	CLA	c	515	3	-	5/39/115/115	-
33	DGD	C	516	-	-	10/51/91/95	0/2/2/2
25	CLA	B	615	2	-	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PHO	a	608	-	-	7/37/103/103	0/5/6/6
27	BCR	c	517	-	-	6/29/63/63	0/2/2/2
31	LHG	a	613	-	-	19/53/53/53	-
31	LHG	l	101	-	-	19/53/53/53	-
25	CLA	B	602	2	-	11/39/115/115	-
25	CLA	c	513	3	-	4/39/115/115	-
28	PL9	d	408	-	-	10/53/73/73	0/1/1/1
29	LMG	C	519	-	-	21/46/66/70	0/1/1/1
27	BCR	C	514	-	-	3/29/63/63	0/2/2/2
23	SQD	D	408	-	-	19/42/62/69	0/1/1/1
31	LHG	D	406	-	-	20/53/53/53	-
31	LHG	a	615	-	-	21/46/46/53	-
25	CLA	c	511	3	-	9/39/115/115	-
27	BCR	B	618	-	-	4/29/63/63	0/2/2/2
25	CLA	b	616	2	-	8/39/115/115	-
25	CLA	c	506	36	-	7/39/115/115	-
26	PHO	D	401	-	-	7/37/103/103	0/5/6/6
28	PL9	A	611	-	-	10/53/73/73	0/1/1/1
25	CLA	b	609	2	-	6/39/115/115	-
27	BCR	b	622	-	-	6/29/63/63	0/2/2/2
27	BCR	C	515	-	-	5/29/63/63	0/2/2/2
29	LMG	c	521	-	-	24/46/66/70	0/1/1/1
27	BCR	a	610	-	-	5/29/63/63	0/2/2/2
35	HEC	v	201	16	1/1/3/7	6/14/54/54	-
29	LMG	d	409	-	-	21/41/41/70	-
27	BCR	h	101	-	-	4/29/63/63	0/2/2/2
27	BCR	c	516	-	-	6/29/63/63	0/2/2/2
25	CLA	b	614	2	-	6/39/115/115	-
25	CLA	d	404	4	-	5/39/115/115	-
25	CLA	C	512	3	-	15/39/115/115	-
27	BCR	T	101	-	-	10/29/63/63	0/2/2/2
25	CLA	b	608	2	-	8/39/115/115	-
25	CLA	c	505	3	-	6/39/115/115	-
29	LMG	B	620	-	-	16/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b	606	2	-	7/39/115/115	-
25	CLA	a	609	1	-	11/39/115/115	-
29	LMG	c	502	-	-	27/46/66/70	0/1/1/1
27	BCR	Y	101	-	-	7/29/63/63	0/2/2/2
25	CLA	c	503	3	-	7/39/115/115	-
29	LMG	b	625	-	-	1/6/6/70	-
33	DGD	C	518	-	-	14/51/91/95	0/2/2/2
25	CLA	d	403	4	-	9/39/115/115	-
29	LMG	B	621	-	-	18/46/66/70	0/1/1/1
25	CLA	b	619	2	-	14/39/115/115	-
33	DGD	c	518	-	-	15/51/91/95	0/2/2/2
27	BCR	B	627	-	-	10/29/63/63	0/2/2/2
29	LMG	A	612	-	-	17/46/66/70	0/1/1/1
25	CLA	A	606	1	-	3/39/115/115	-
31	LHG	A	616	-	-	17/53/53/53	-
25	CLA	C	502	3	-	6/39/115/115	-
27	BCR	D	404	-	-	6/29/63/63	0/2/2/2
25	CLA	b	618	2	-	10/39/115/115	-
26	PHO	d	401	-	-	6/37/103/103	0/5/6/6
31	LHG	A	618	-	-	23/53/53/53	-
25	CLA	B	605	2	-	10/39/115/115	-
29	LMG	C	520	-	-	16/46/66/70	0/1/1/1
31	LHG	L	101	-	-	17/53/53/53	-
33	DGD	C	517	-	-	16/51/91/95	0/2/2/2
27	BCR	K	101	-	-	6/29/63/63	0/2/2/2
31	LHG	A	617	-	-	14/53/53/53	-
34	HEM	e	101	5,6	-	3/14/54/54	-
25	CLA	b	607	2	-	8/39/115/115	-
29	LMG	c	522	-	-	15/46/66/70	0/1/1/1
25	CLA	b	605	2	-	10/39/115/115	-
25	CLA	b	612	2	-	11/39/115/115	-
25	CLA	b	615	2	-	11/39/115/115	-
25	CLA	B	612	2	-	7/39/115/115	-

The worst 5 of 643 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d	401	PHO	C1B-C2B	9.67	1.50	1.39
26	D	401	PHO	C1B-C2B	9.66	1.50	1.39
26	A	608	PHO	C1B-C2B	9.64	1.50	1.39
26	a	608	PHO	C1B-C2B	9.63	1.50	1.39
26	D	401	PHO	C3B-C4B	8.74	1.50	1.41

The worst 5 of 942 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	507	CLA	C4A-NA-C1A	6.35	109.58	106.68
25	C	503	CLA	C4A-NA-C1A	6.25	109.53	106.68
25	B	604	CLA	C4A-NA-C1A	6.25	109.53	106.68
25	b	607	CLA	C4A-NA-C1A	6.23	109.52	106.68
25	c	513	CLA	C4A-NA-C1A	6.21	109.51	106.68

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	V	201	HEC	NA
35	v	201	HEC	NA

5 of 1526 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	603	SQD	C5-C6-S-O7
23	A	603	SQD	C5-C6-S-O8
23	A	603	SQD	C5-C6-S-O9
23	A	619	SQD	O6-C44-C45-C46
23	B	626	SQD	C2-C1-O6-C44

There are no ring outliers.

139 monomers are involved in 279 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	a	611	PL9	4	0
25	B	604	CLA	2	0
25	C	506	CLA	2	0
25	B	601	CLA	3	0
33	h	102	DGD	3	0
28	D	407	PL9	2	0
23	A	619	SQD	2	0
29	b	623	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B	619	BCR	2	0
25	C	504	CLA	3	0
27	b	620	BCR	2	0
25	c	510	CLA	3	0
25	C	507	CLA	2	0
25	b	617	CLA	2	0
25	B	616	CLA	2	0
25	C	513	CLA	1	0
29	B	625	LMG	1	0
25	B	611	CLA	2	0
27	k	101	BCR	2	0
23	B	626	SQD	7	0
25	c	508	CLA	2	0
25	c	509	CLA	3	0
25	A	609	CLA	4	0
25	b	611	CLA	2	0
27	b	621	BCR	2	0
25	C	501	CLA	5	0
27	B	617	BCR	2	0
25	a	606	CLA	1	0
25	C	511	CLA	1	0
25	C	510	CLA	1	0
23	A	603	SQD	2	0
25	B	608	CLA	3	0
29	b	624	LMG	2	0
31	a	614	LHG	1	0
25	C	503	CLA	4	0
25	C	508	CLA	5	0
25	A	607	CLA	1	0
25	C	509	CLA	1	0
25	a	607	CLA	1	0
25	b	610	CLA	2	0
25	B	610	CLA	2	0
26	A	608	PHO	1	0
32	A	620	BCT	1	0
35	V	201	HEC	1	0
27	y	101	BCR	3	0
25	b	604	CLA	1	0
25	A	615	CLA	1	0
25	B	603	CLA	1	0
29	A	613	LMG	2	0
33	c	519	DGD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	c	512	CLA	1	0
31	d	407	LHG	2	0
25	B	609	CLA	4	0
25	B	606	CLA	3	0
25	D	403	CLA	2	0
25	c	514	CLA	2	0
25	B	614	CLA	4	0
25	D	402	CLA	3	0
25	a	612	CLA	1	0
27	H	102	BCR	4	0
25	c	507	CLA	3	0
34	E	101	HEM	3	0
25	B	607	CLA	2	0
23	b	601	SQD	1	0
25	b	613	CLA	1	0
27	A	610	BCR	3	0
27	d	405	BCR	2	0
33	H	103	DGD	2	0
25	B	613	CLA	2	0
29	D	405	LMG	2	0
25	C	505	CLA	5	0
23	c	501	SQD	1	0
25	c	515	CLA	3	0
33	C	516	DGD	1	0
25	B	615	CLA	1	0
26	a	608	PHO	1	0
27	c	517	BCR	4	0
31	a	613	LHG	2	0
31	l	101	LHG	5	0
25	B	602	CLA	4	0
25	c	513	CLA	1	0
28	d	408	PL9	5	0
29	C	519	LMG	1	0
23	D	408	SQD	1	0
31	D	406	LHG	1	0
31	a	615	LHG	1	0
25	c	511	CLA	2	0
27	B	618	BCR	2	0
25	b	616	CLA	3	0
26	D	401	PHO	3	0
28	A	611	PL9	4	0
25	b	609	CLA	1	0

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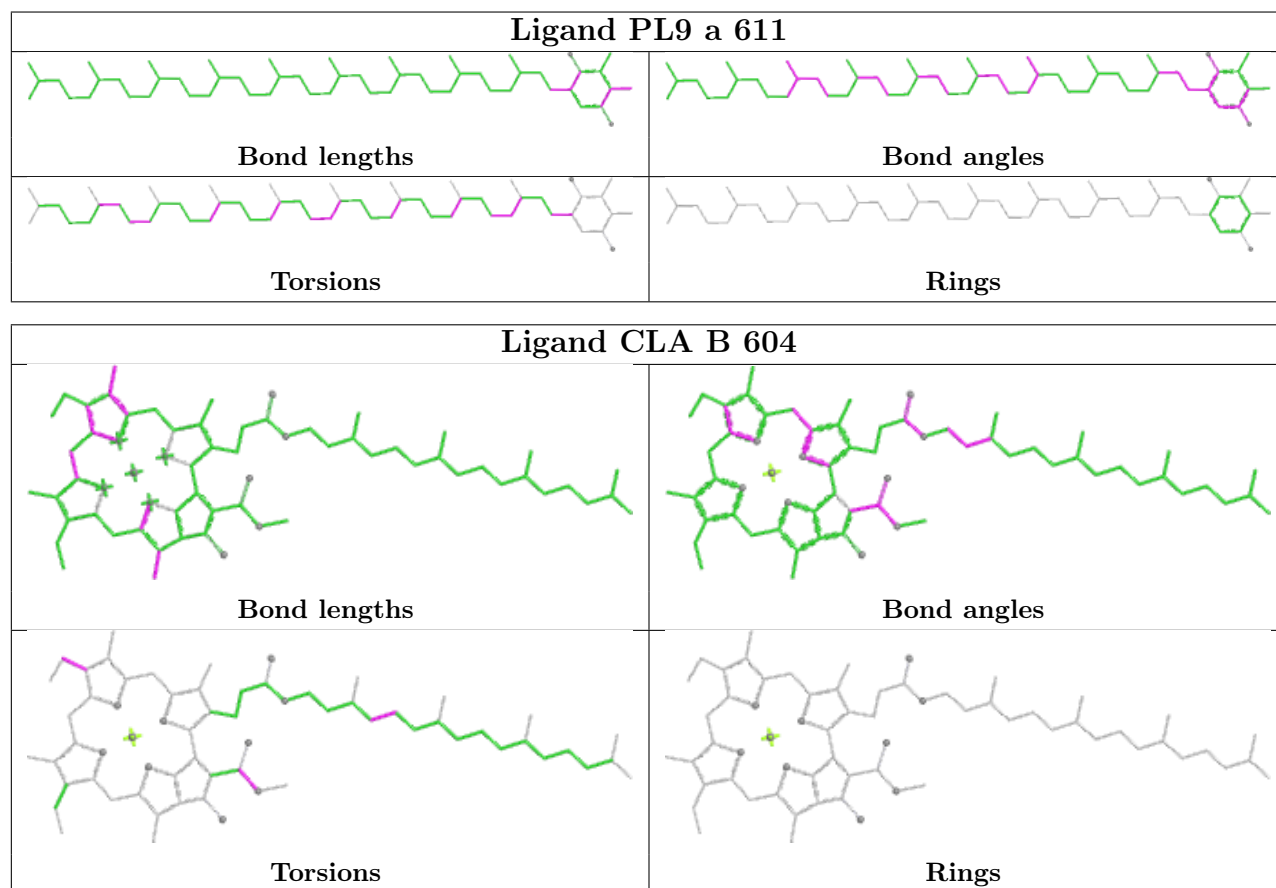
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	b	622	BCR	4	0
27	C	515	BCR	3	0
29	c	521	LMG	1	0
27	a	610	BCR	3	0
29	d	409	LMG	3	0
35	v	201	HEC	2	0
27	h	101	BCR	2	0
27	c	516	BCR	3	0
25	b	614	CLA	2	0
25	d	404	CLA	4	0
25	C	512	CLA	2	0
27	T	101	BCR	7	0
25	b	608	CLA	2	0
25	c	505	CLA	3	0
29	B	620	LMG	1	0
25	b	606	CLA	2	0
25	a	609	CLA	6	0
29	c	502	LMG	3	0
27	Y	101	BCR	1	0
25	c	503	CLA	5	0
29	b	625	LMG	2	0
33	C	518	DGD	2	0
25	d	403	CLA	6	0
29	B	621	LMG	1	0
25	b	619	CLA	4	0
33	c	518	DGD	1	0
27	B	627	BCR	5	0
25	A	606	CLA	1	0
31	A	616	LHG	2	0
25	C	502	CLA	1	0
27	D	404	BCR	3	0
25	b	618	CLA	1	0
26	d	401	PHO	4	0
31	A	618	LHG	3	0
25	B	605	CLA	2	0
29	C	520	LMG	2	0
31	L	101	LHG	3	0
33	C	517	DGD	2	0
27	K	101	BCR	2	0
31	A	617	LHG	7	0
34	e	101	HEM	3	0
25	b	607	CLA	2	0

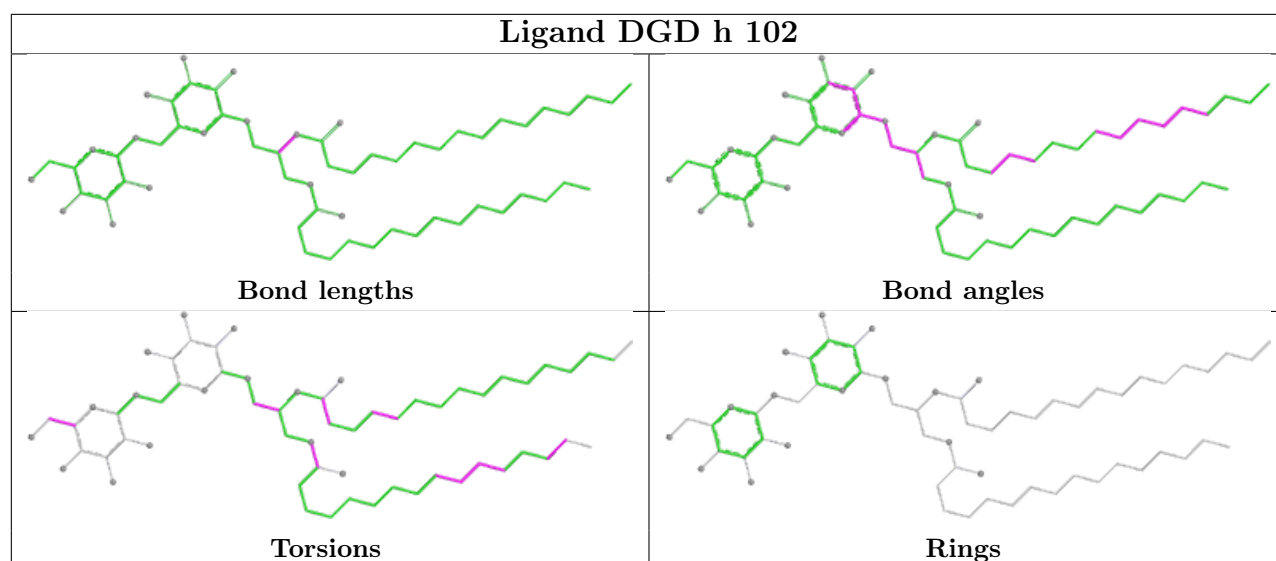
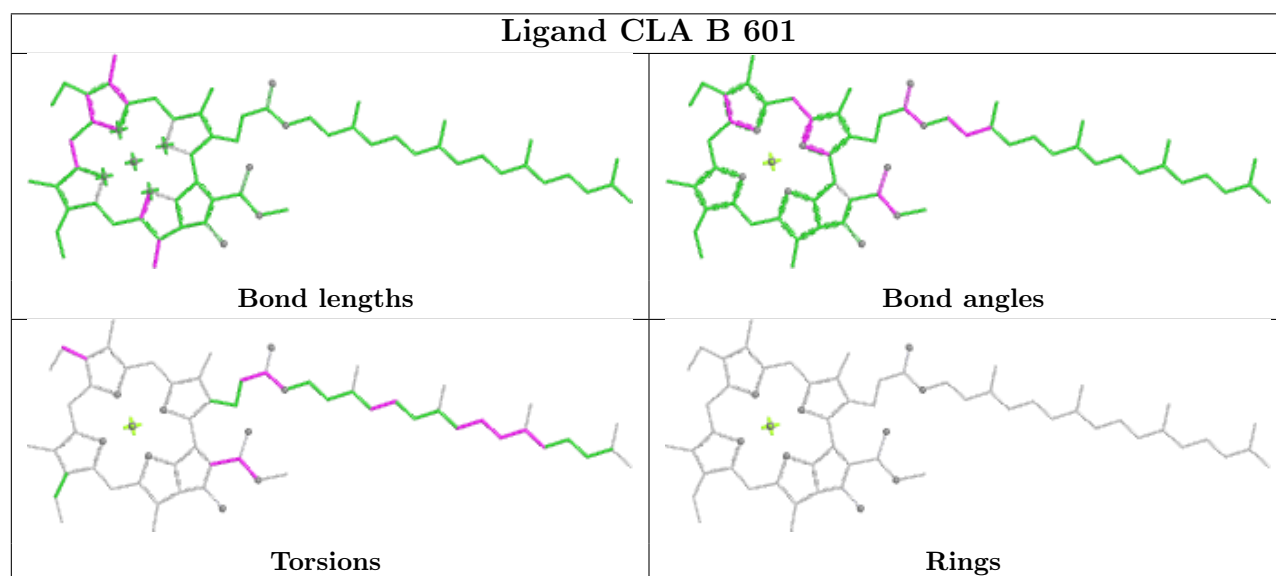
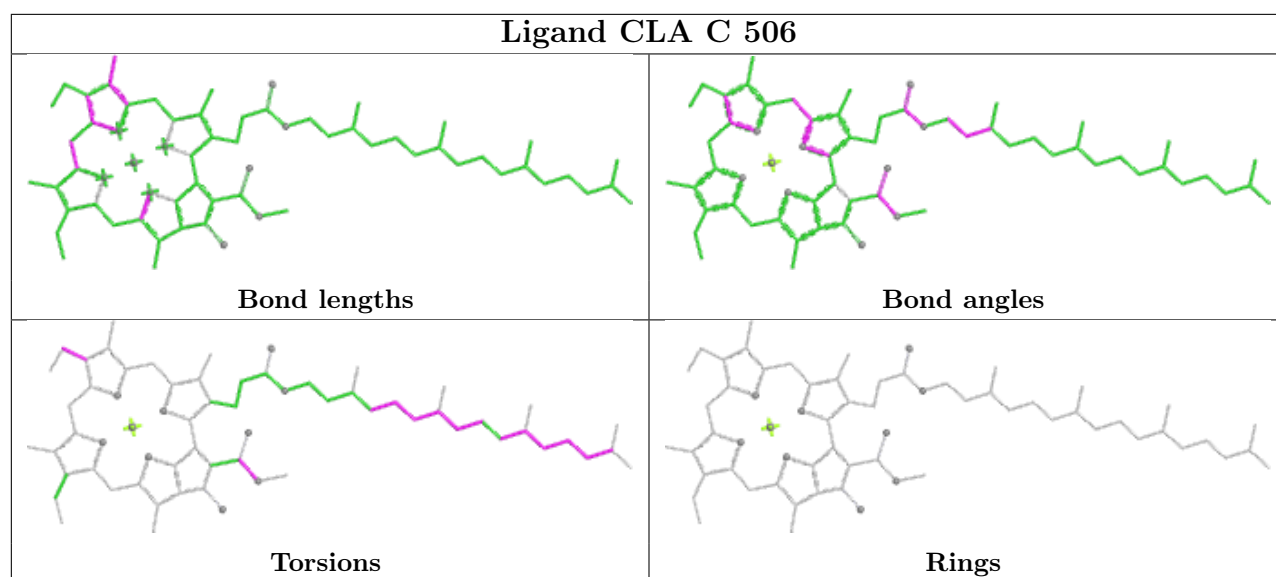
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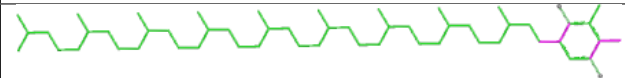
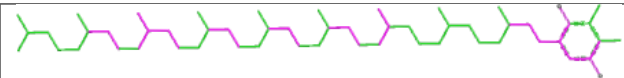
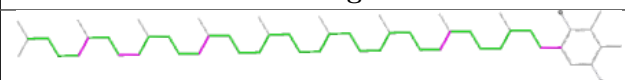
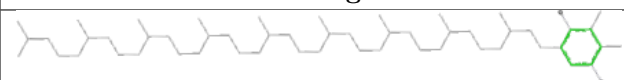
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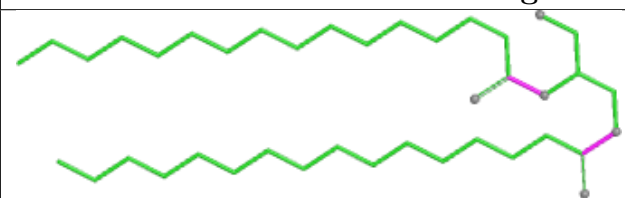
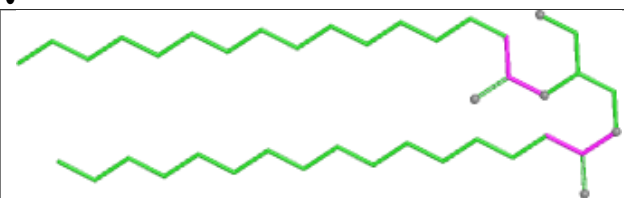
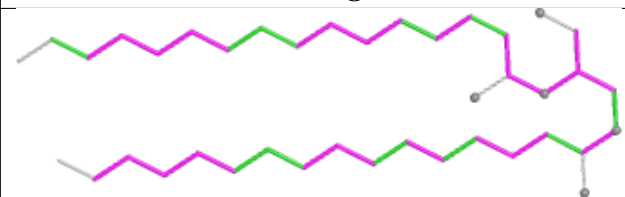
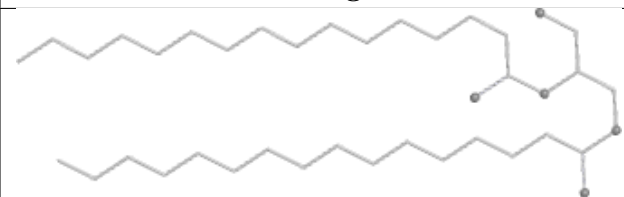
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	c	522	LMG	1	0
25	b	605	CLA	2	0
25	b	612	CLA	4	0
25	b	615	CLA	5	0
25	B	612	CLA	3	0

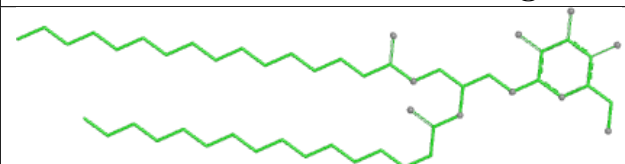
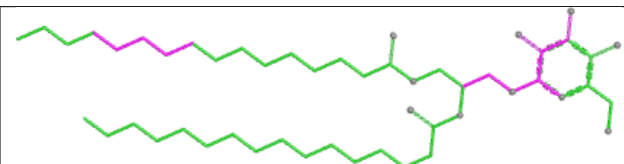
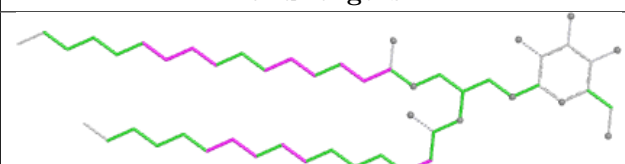
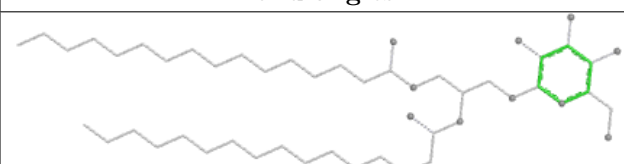
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

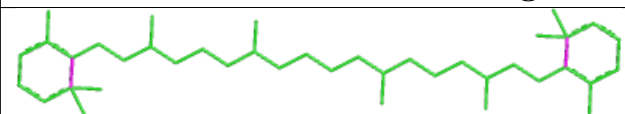
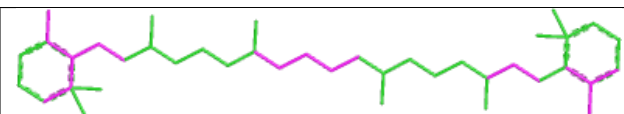
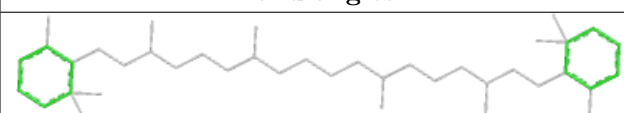


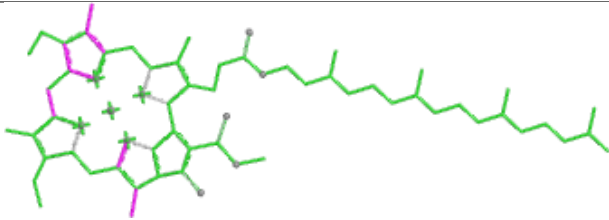
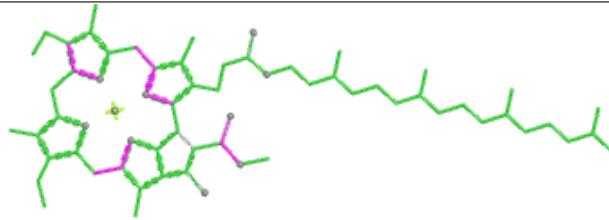
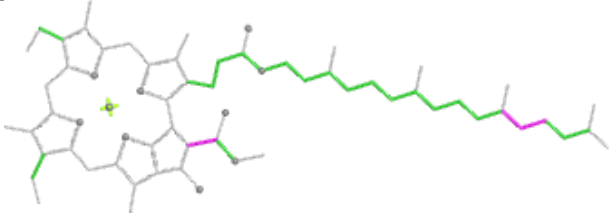
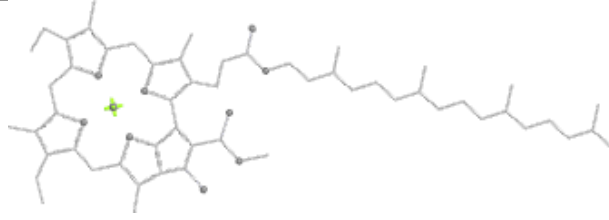


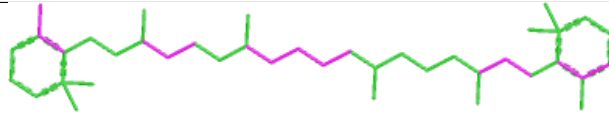
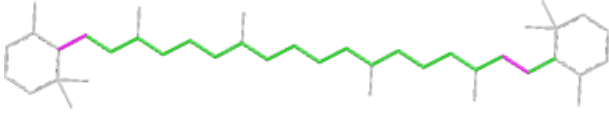
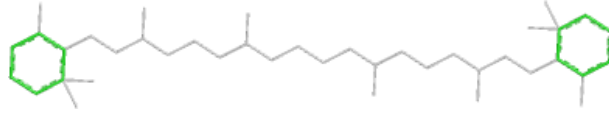
Ligand PL9 D 407	
 Bond lengths	 Bond angles
 Torsions	 Rings

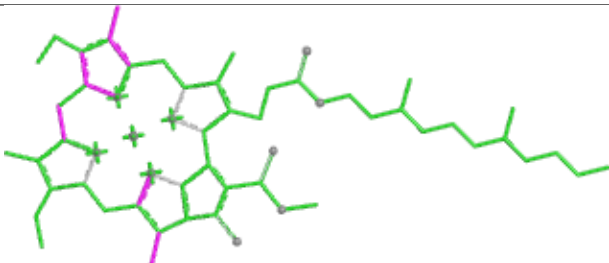
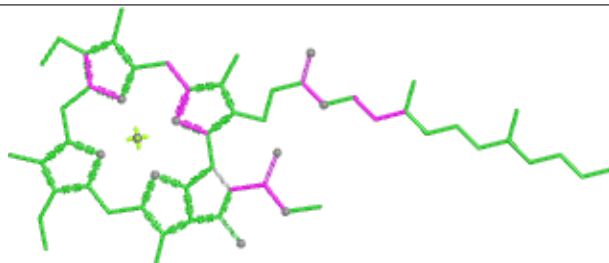
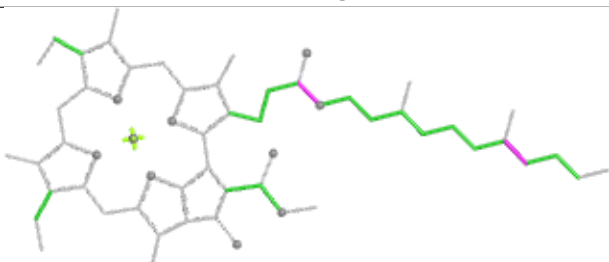
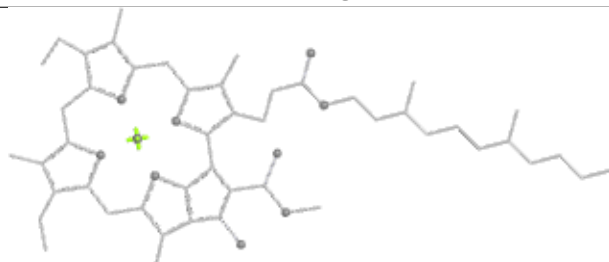
Ligand SQD A 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

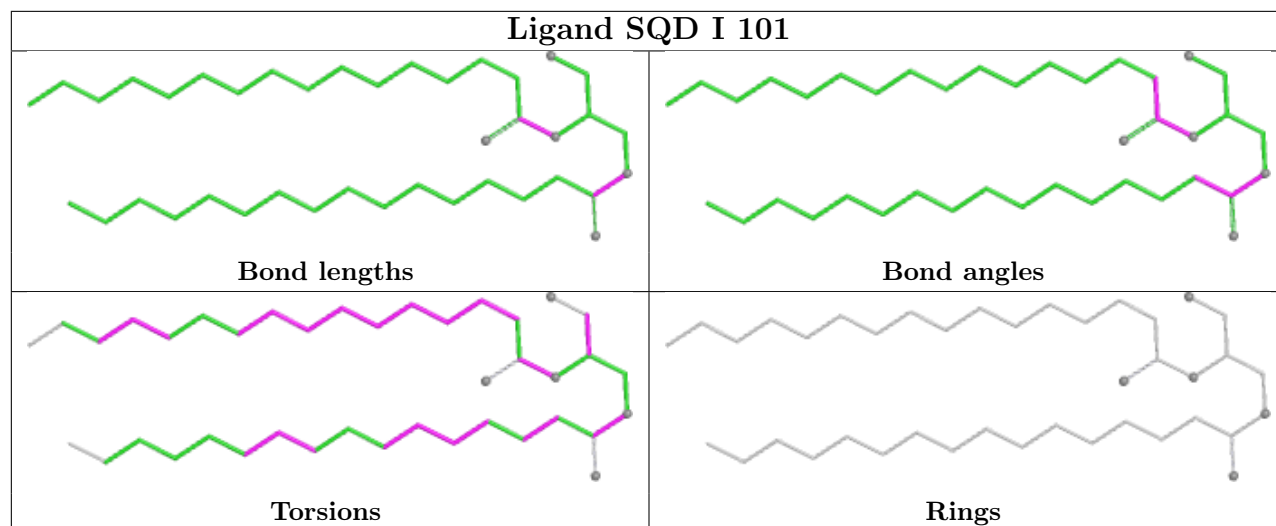
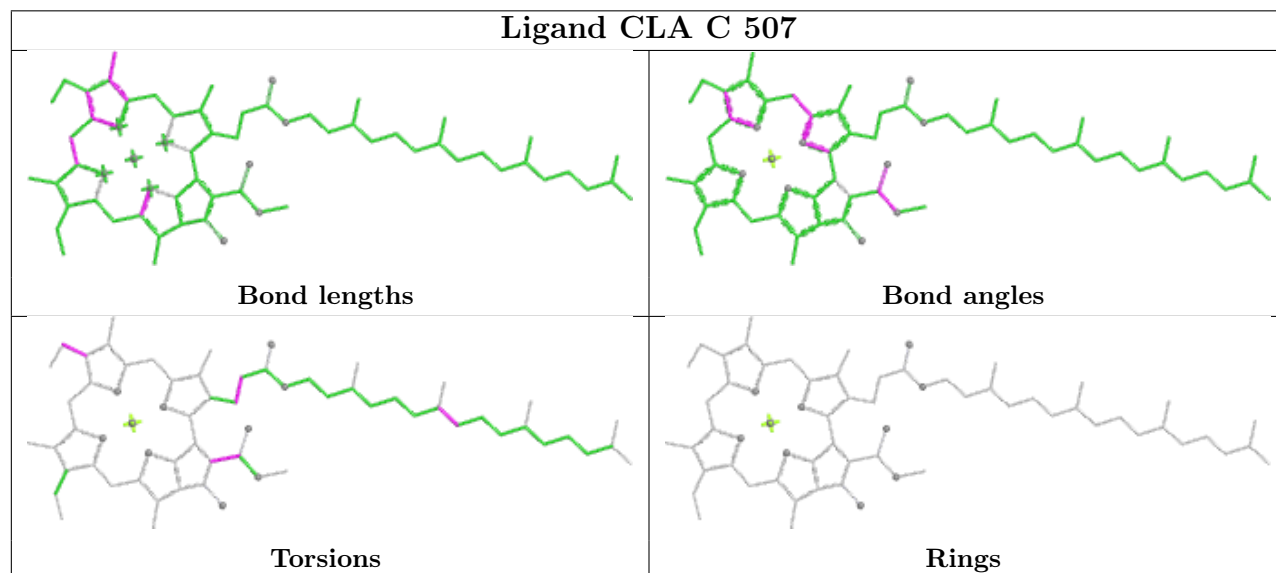
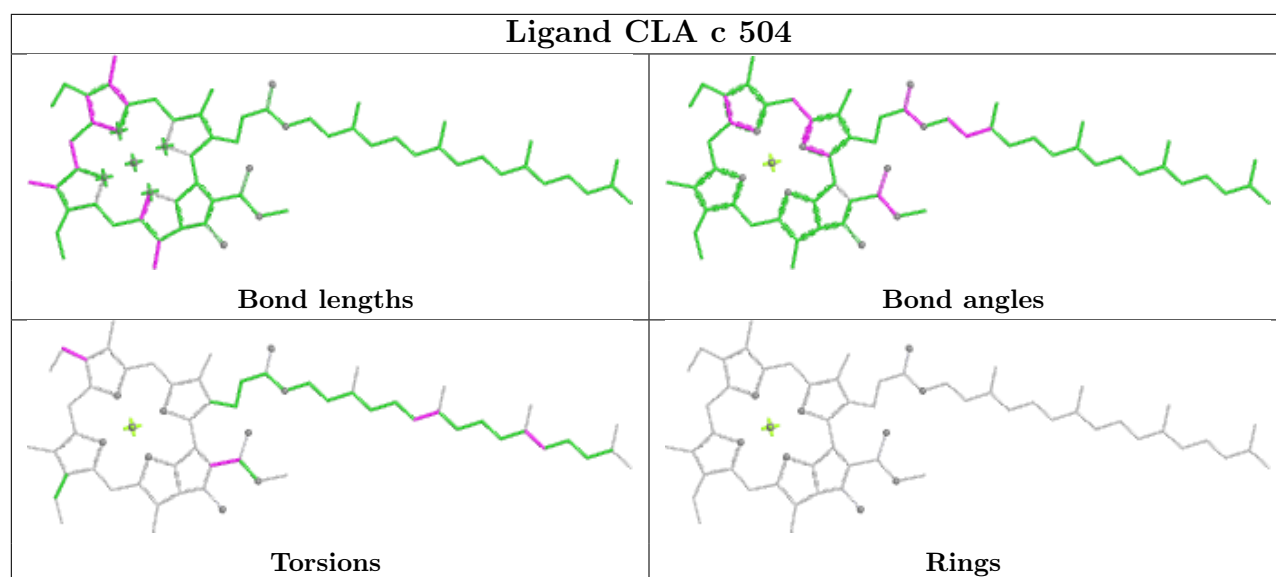
Ligand LMG b 623	
 Bond lengths	 Bond angles
 Torsions	 Rings

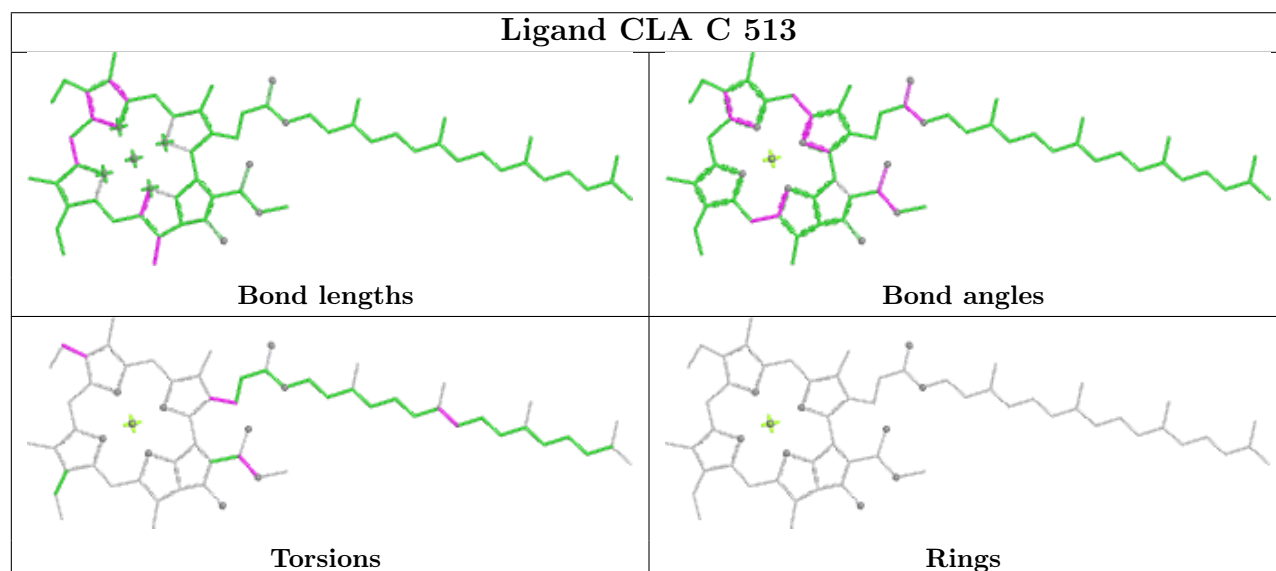
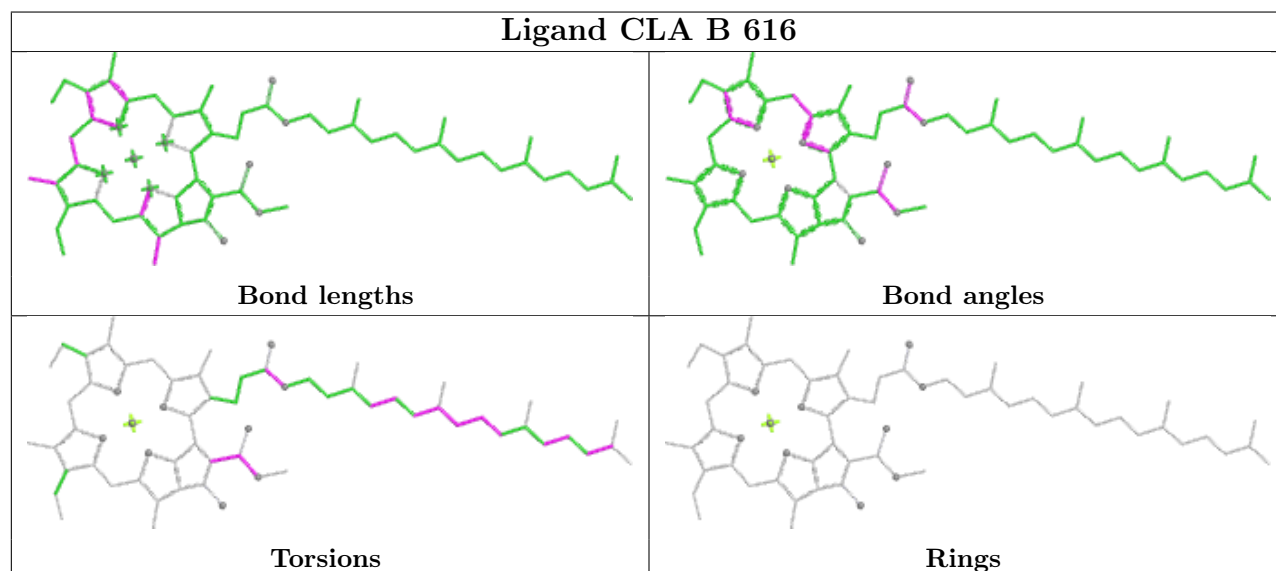
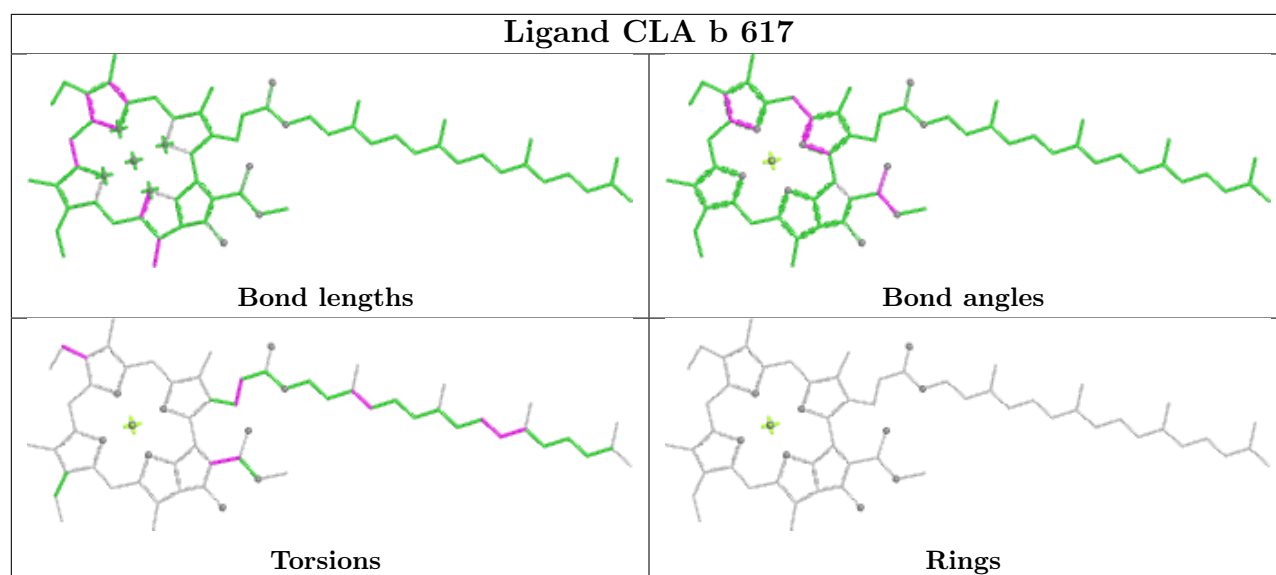
Ligand BCR B 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

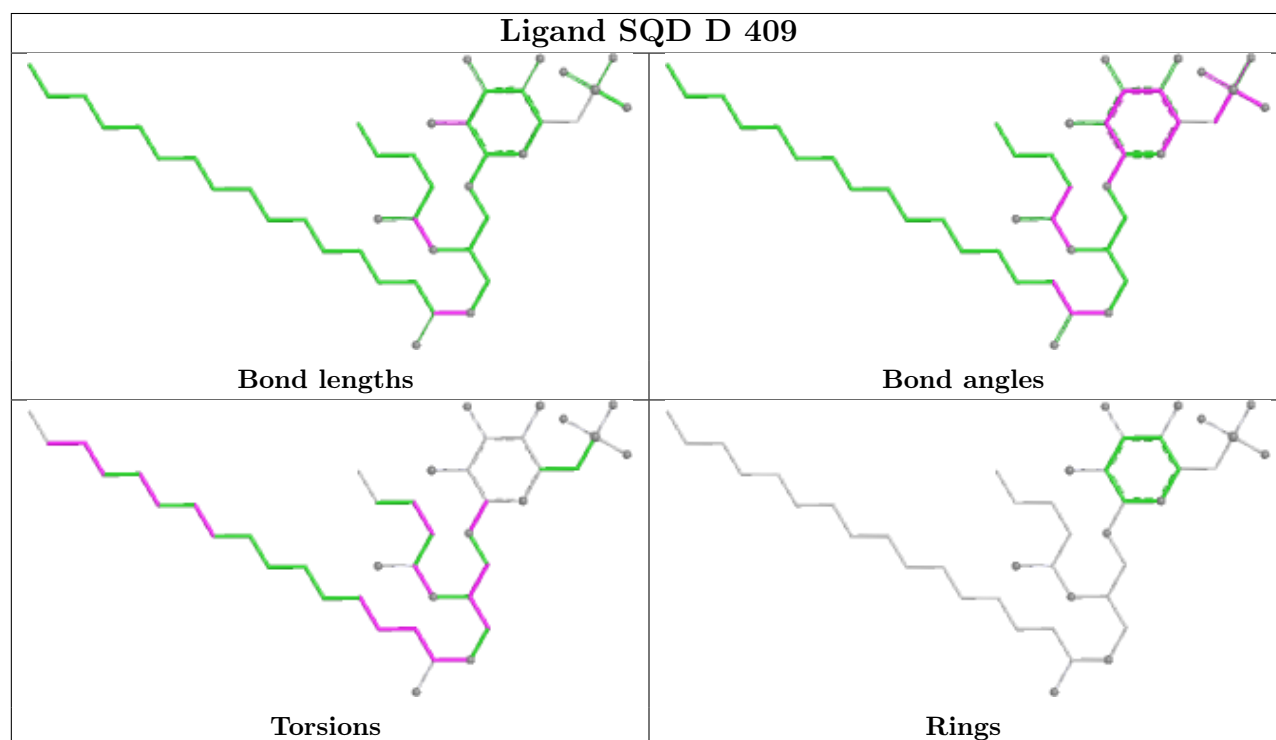
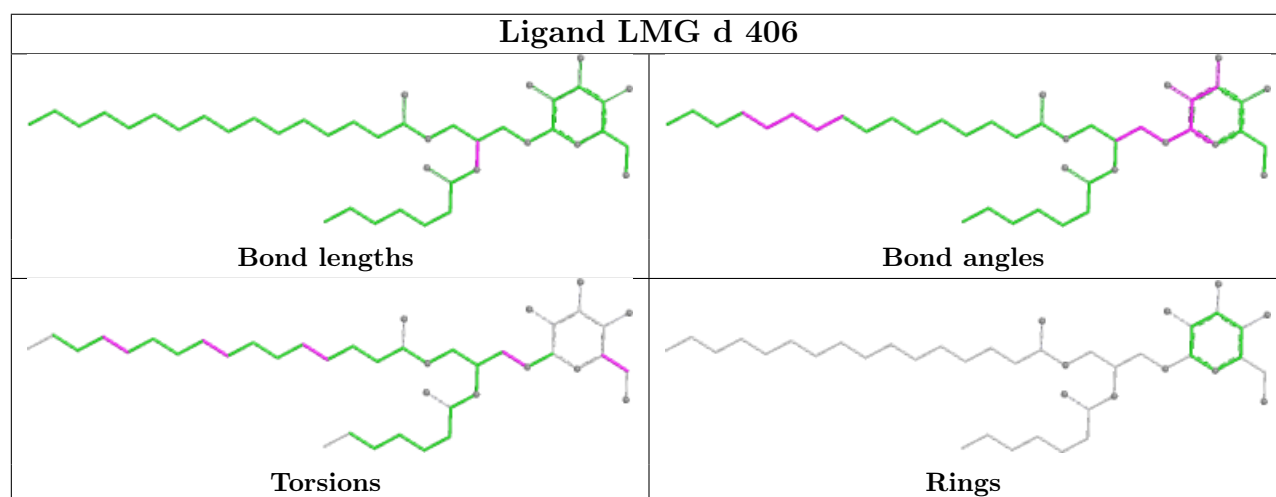
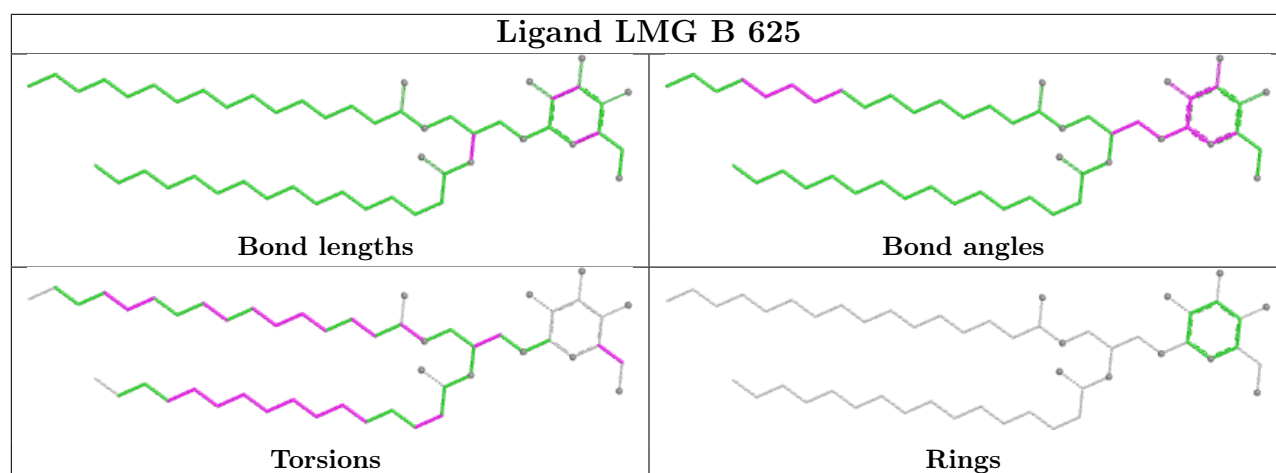
Ligand CLA C 504	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR b 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

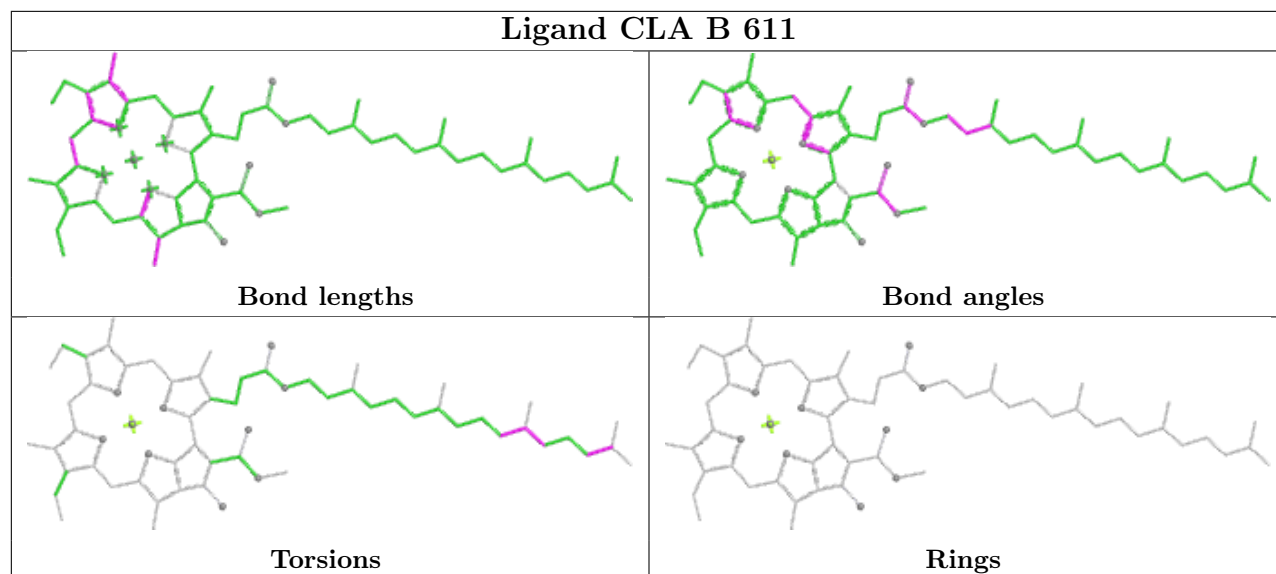
Ligand CLA c 510	
	
Bond lengths	Bond angles
	
Torsions	Rings



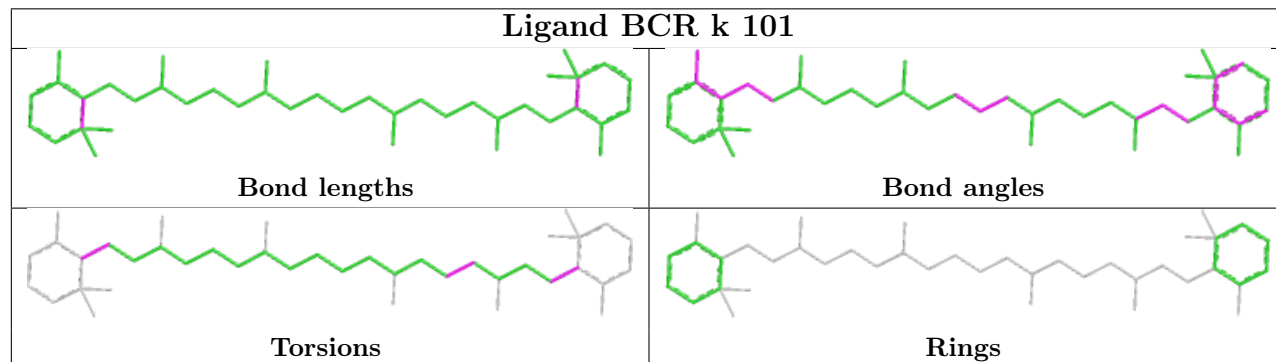




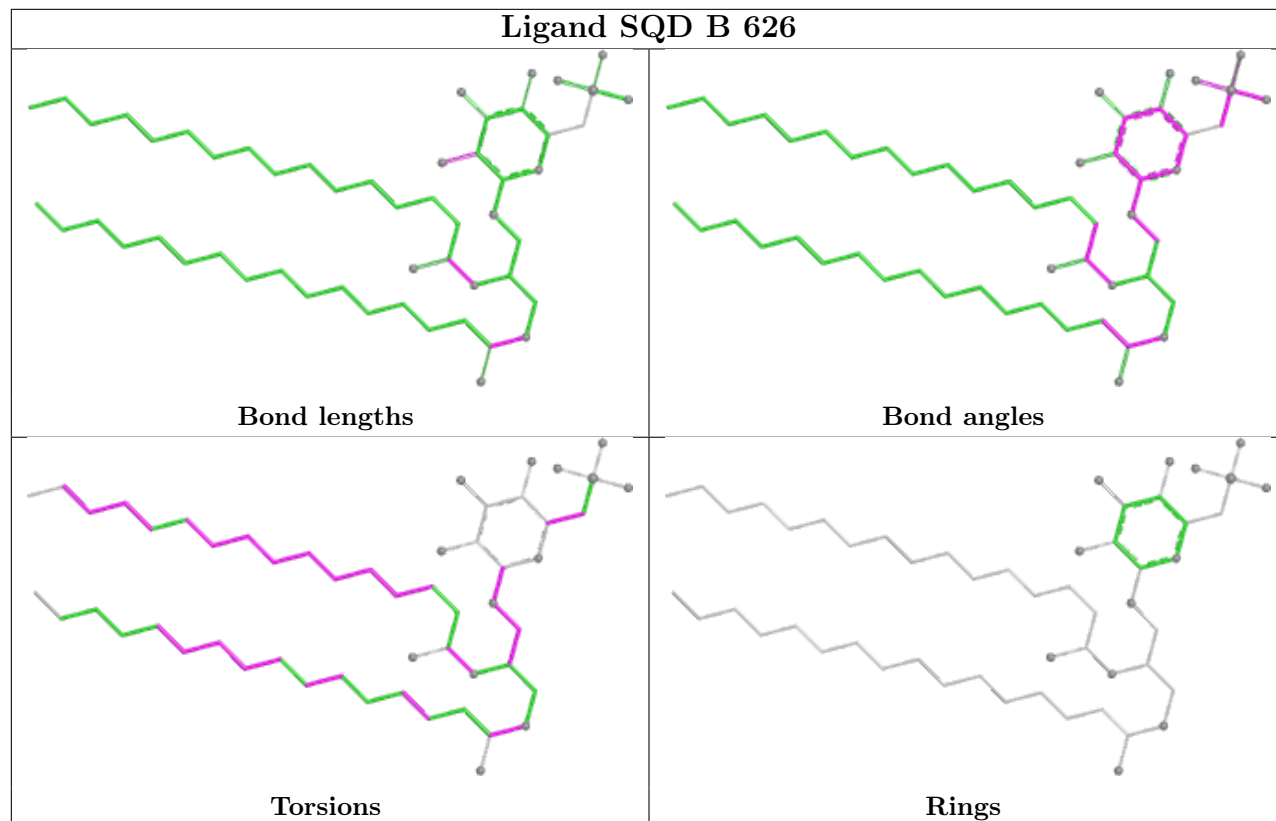
Ligand CLA B 611



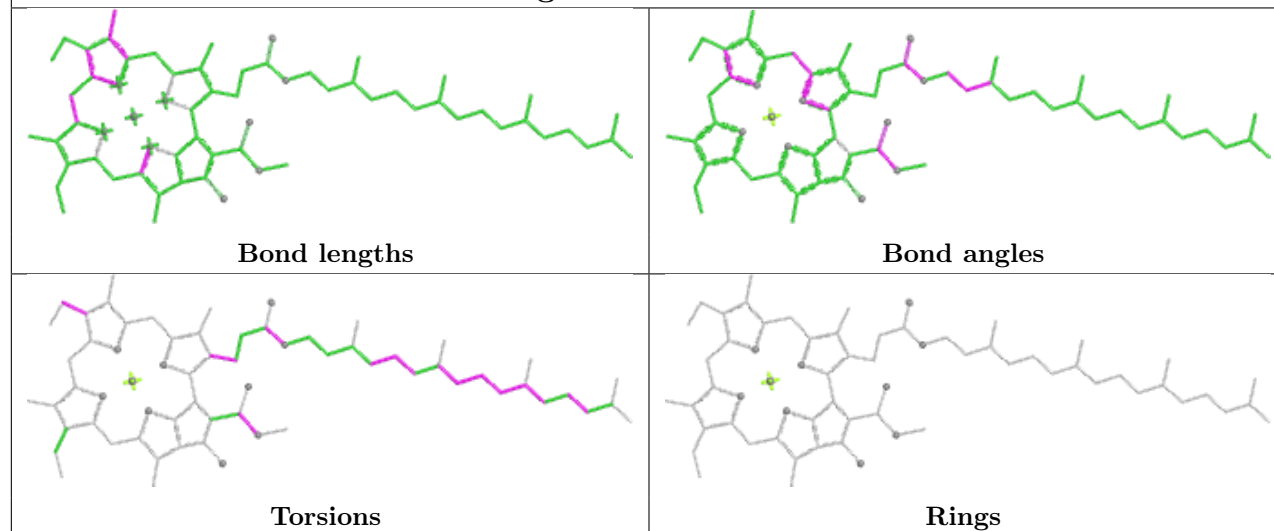
Ligand BCR k 101



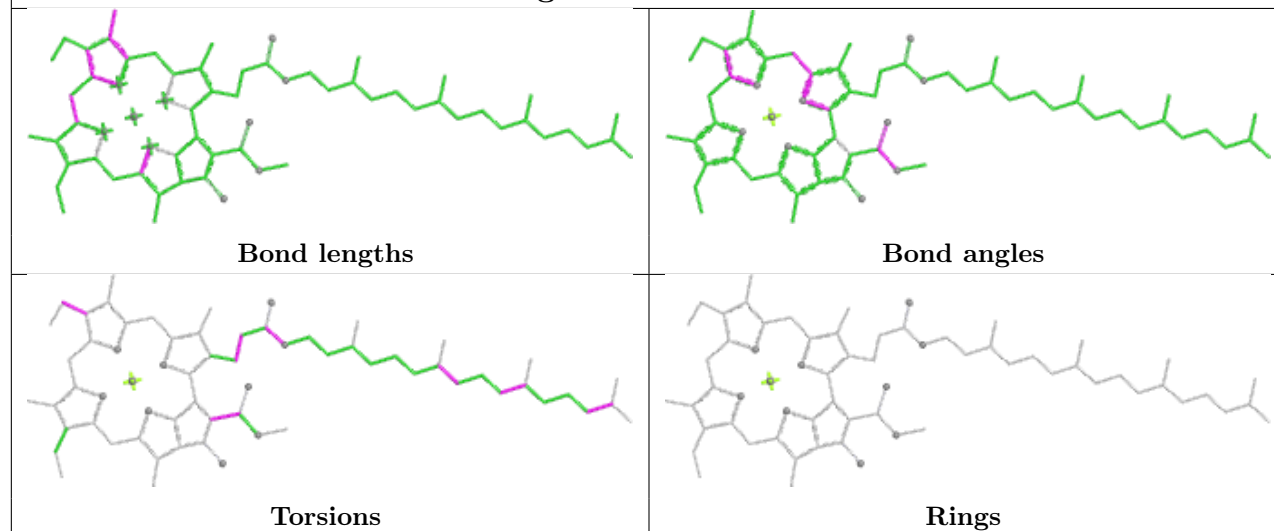
Ligand SQD B 626



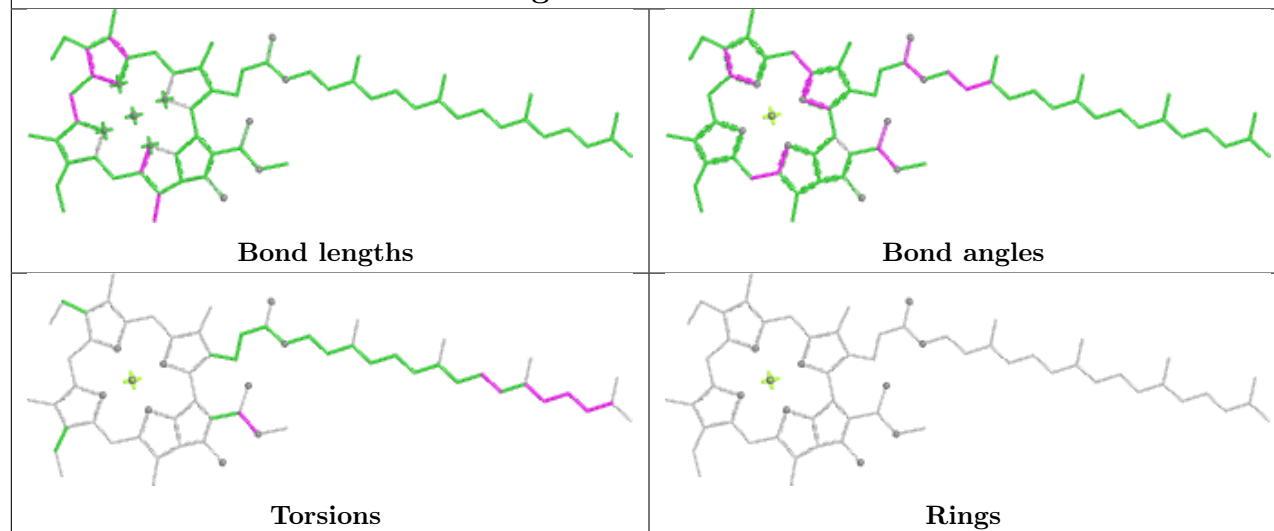
Ligand CLA c 508

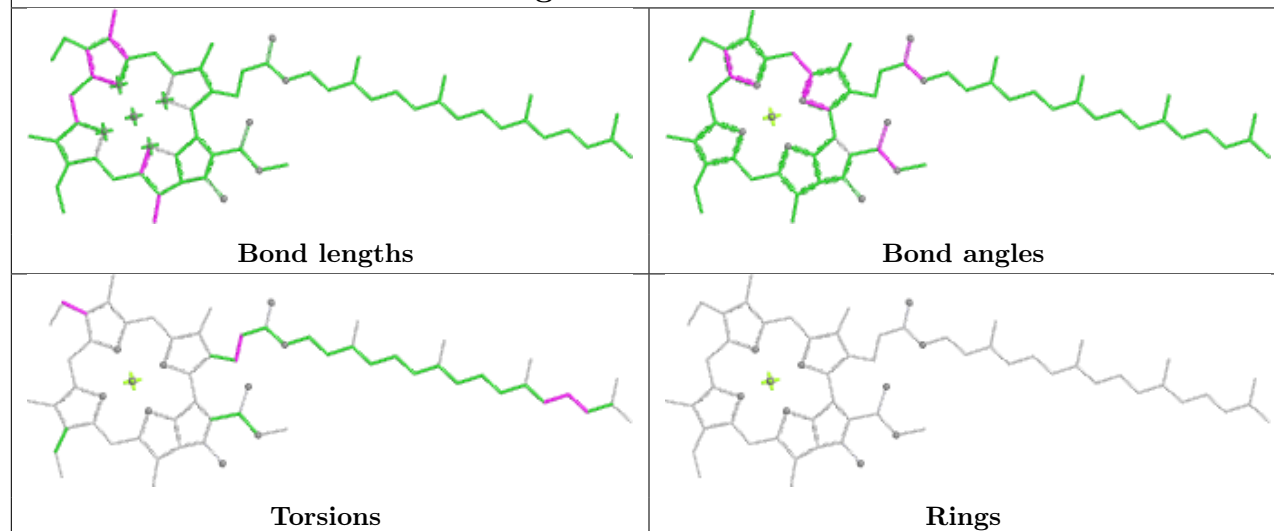
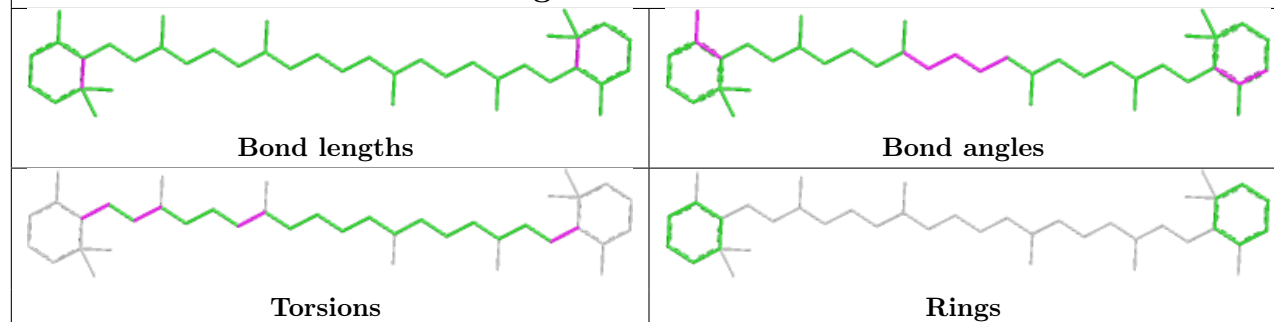
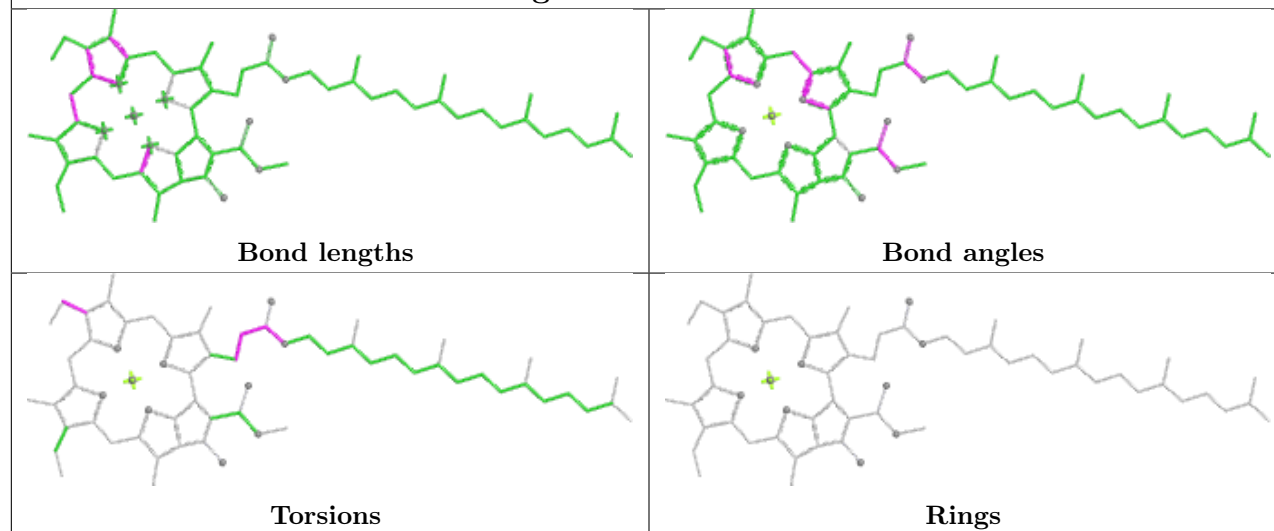


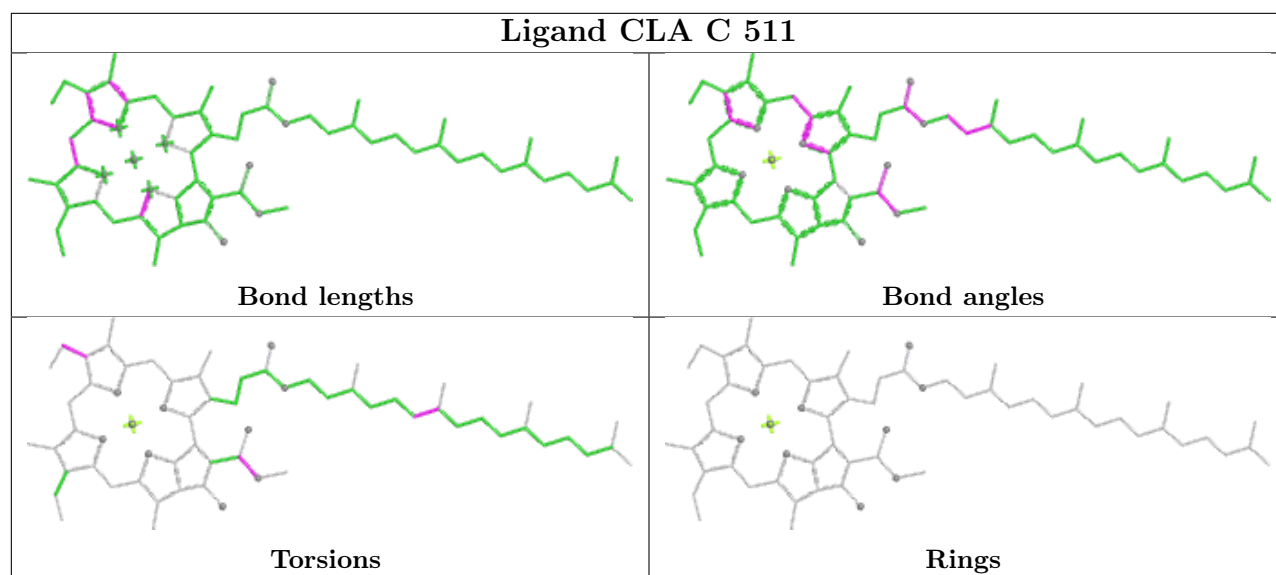
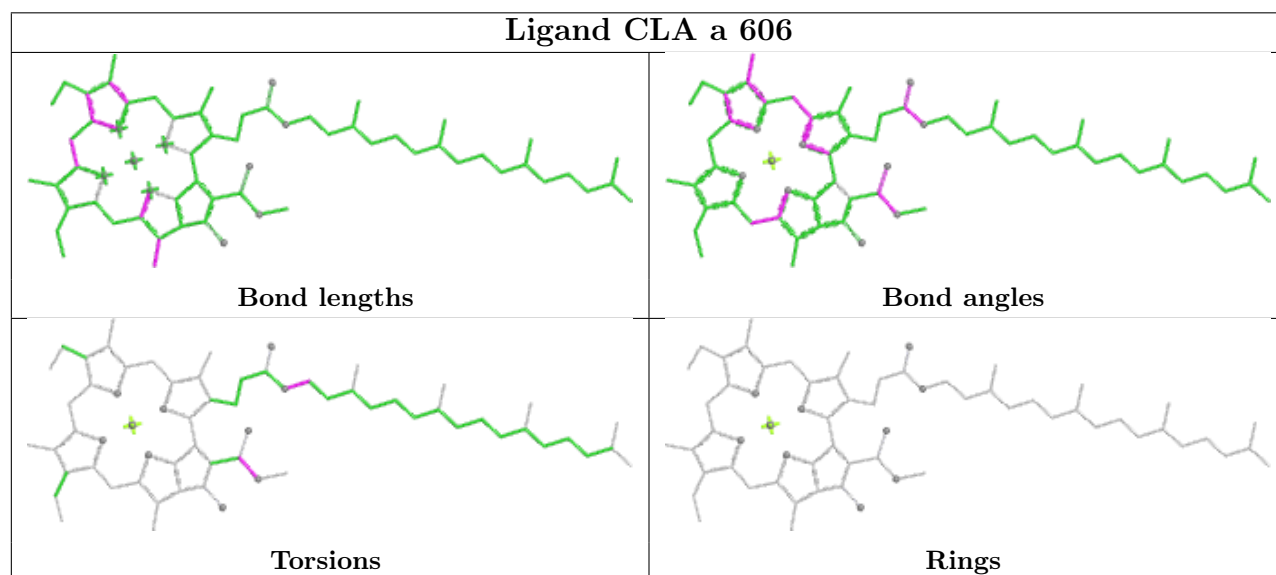
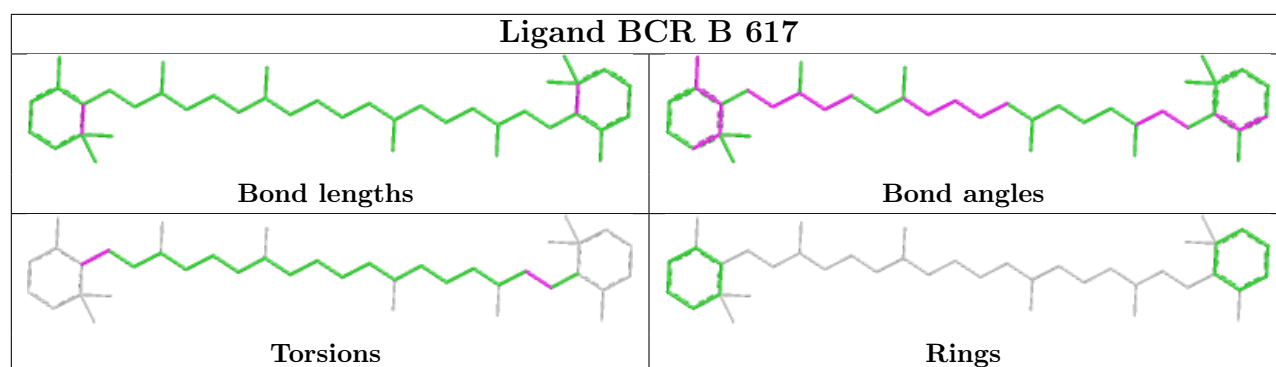
Ligand CLA c 509



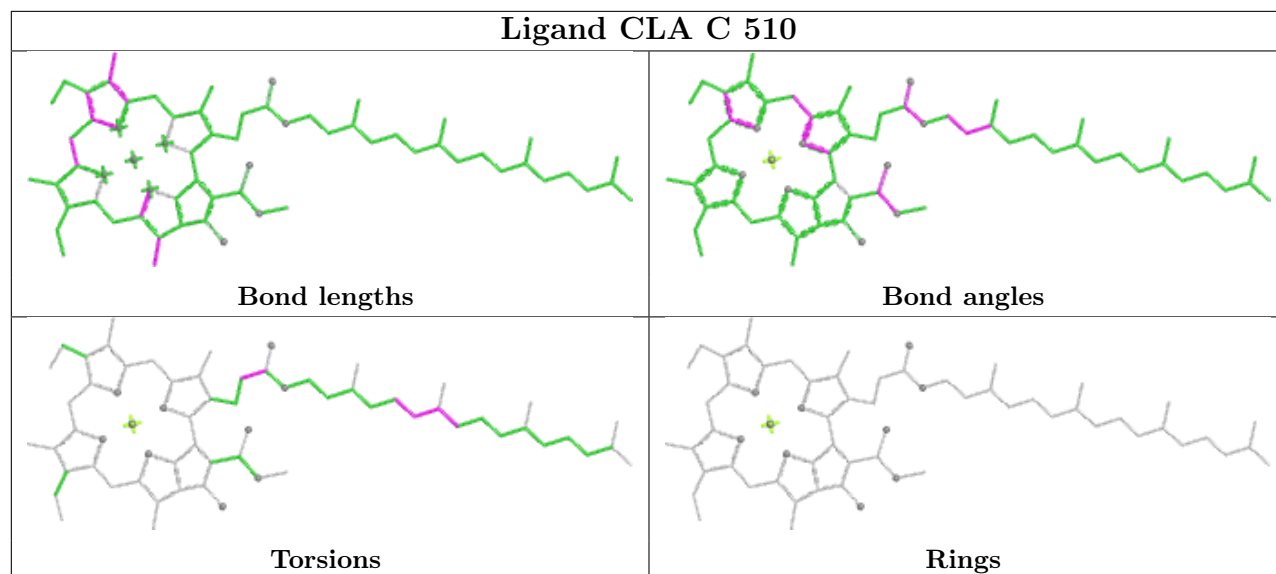
Ligand CLA A 609



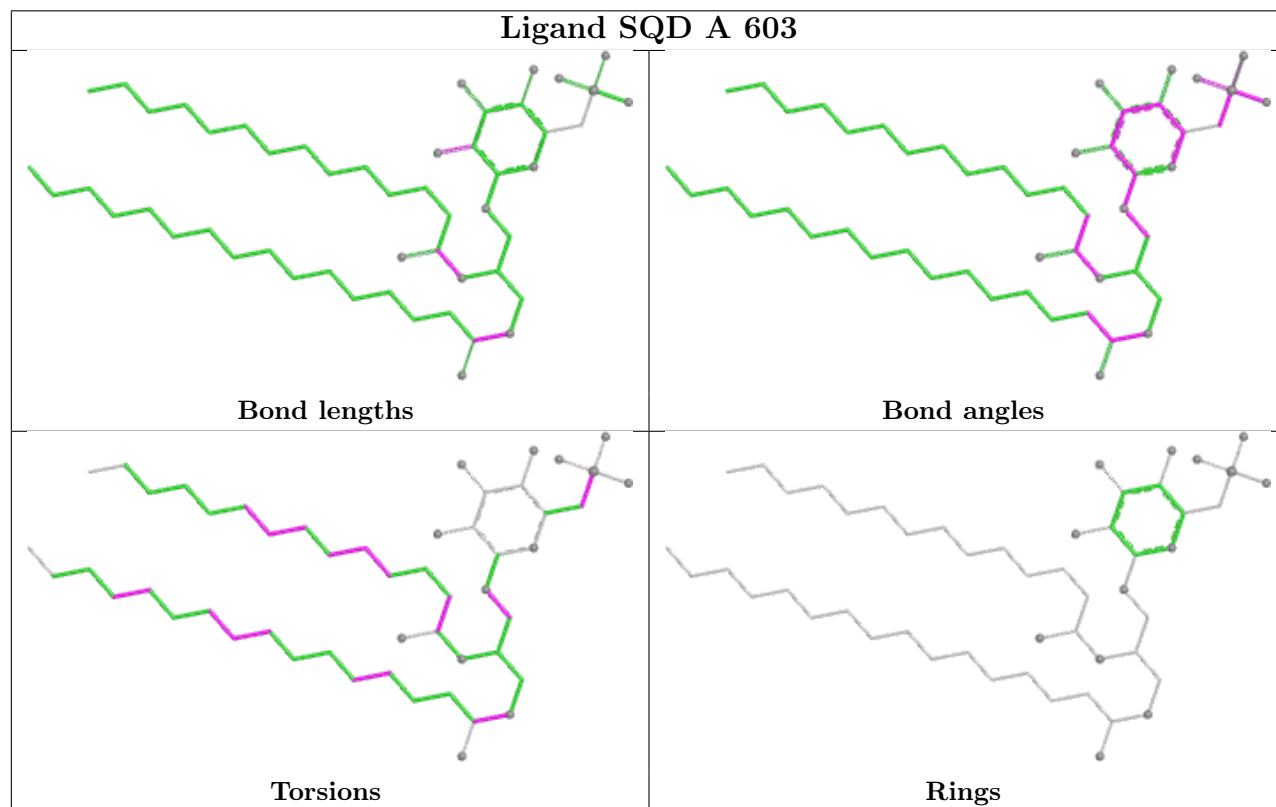
Ligand CLA b 611**Ligand BCR b 621****Ligand CLA C 501**

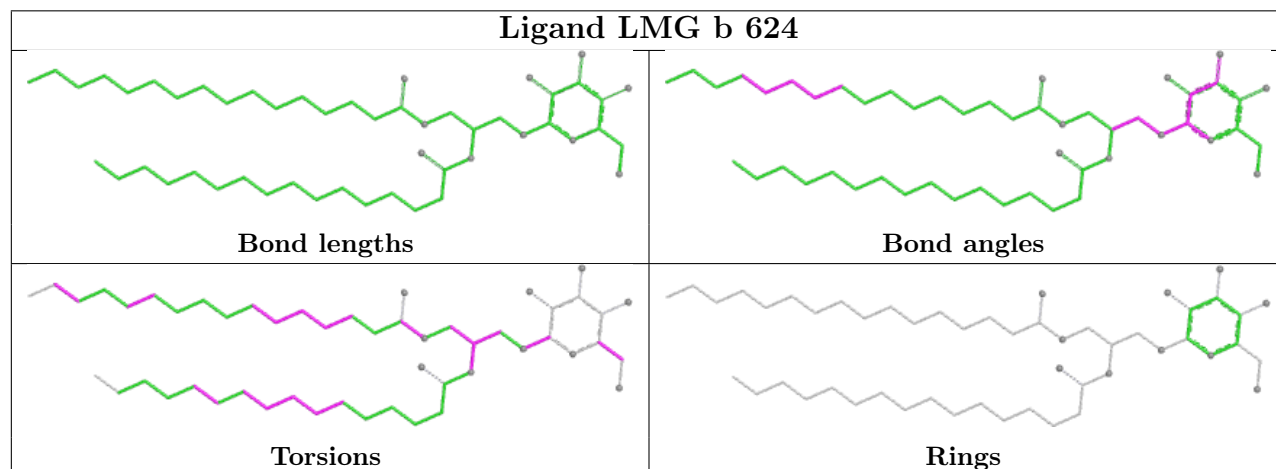
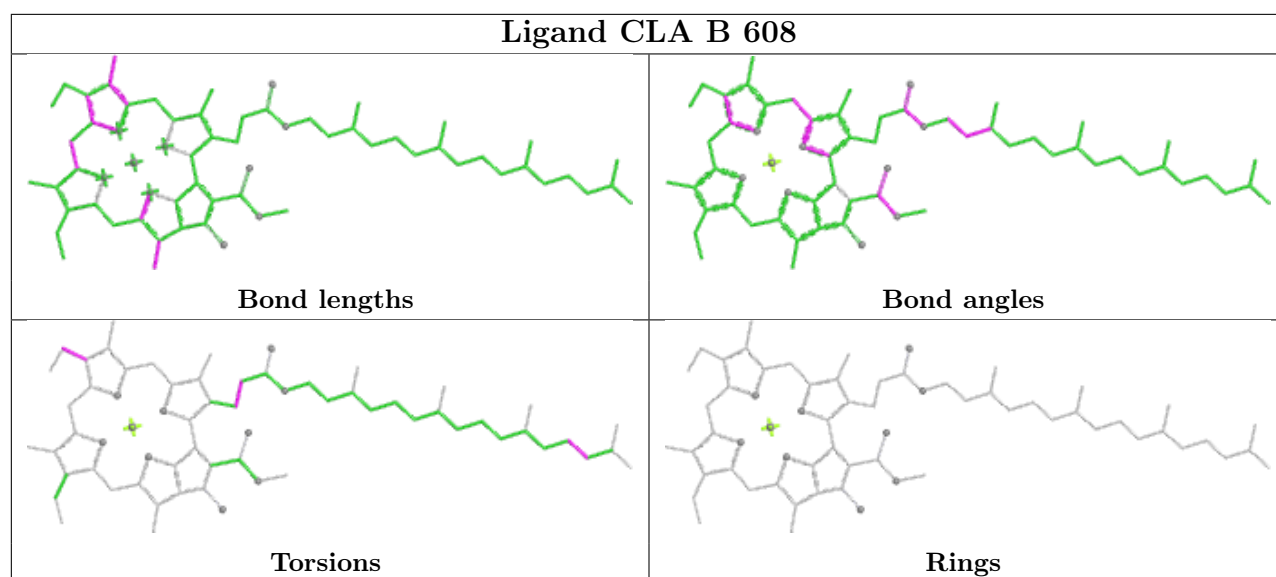


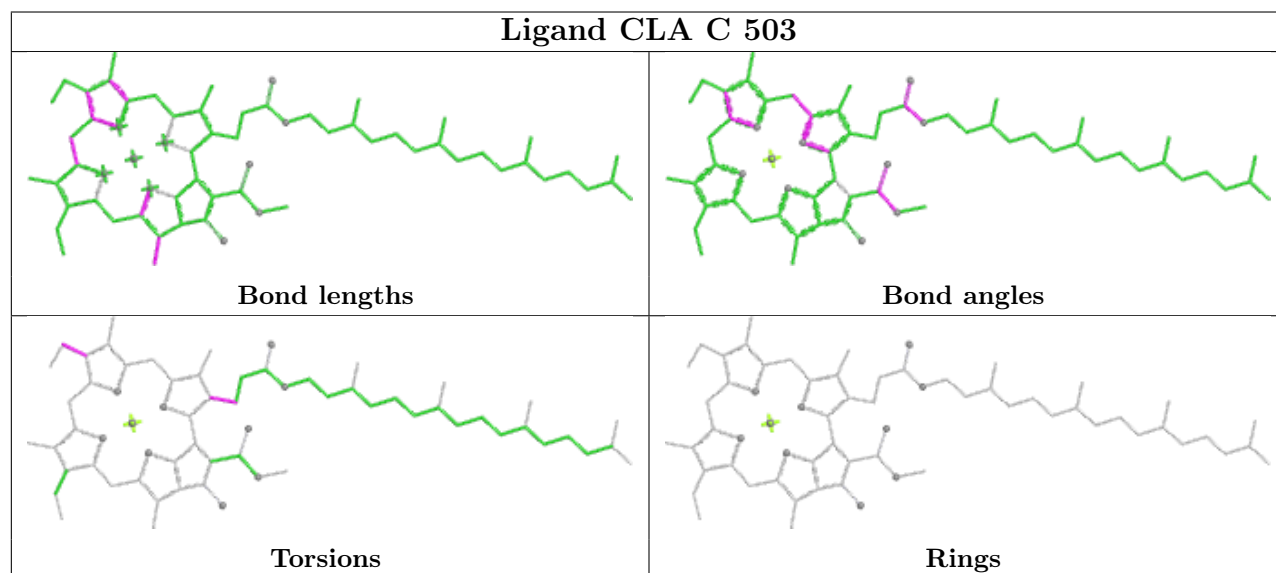
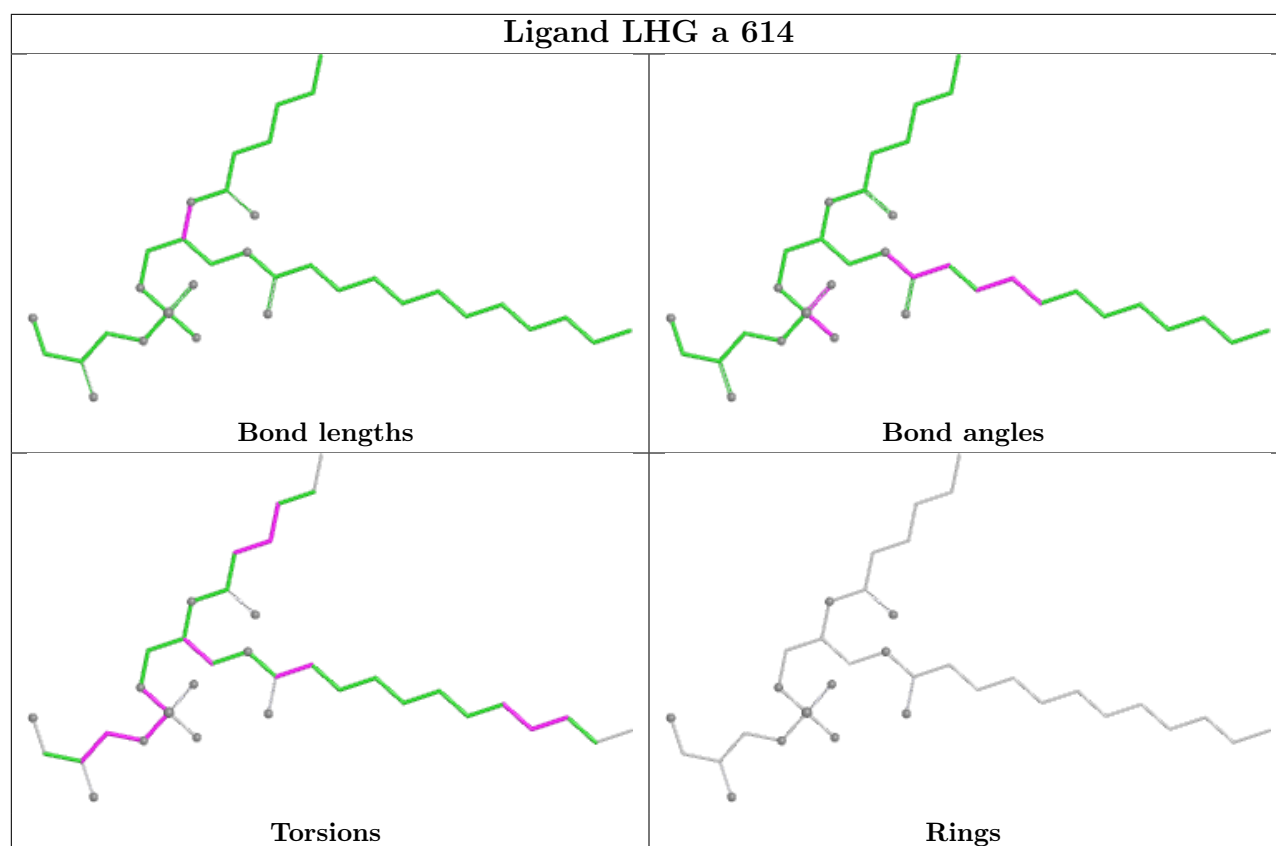
Ligand CLA C 510

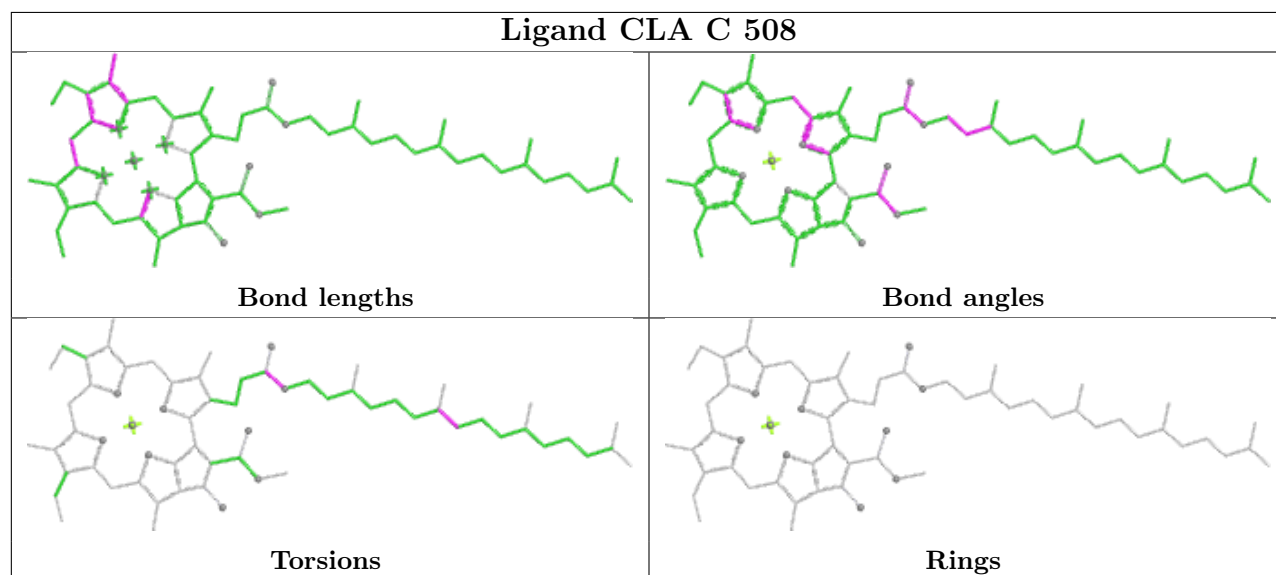
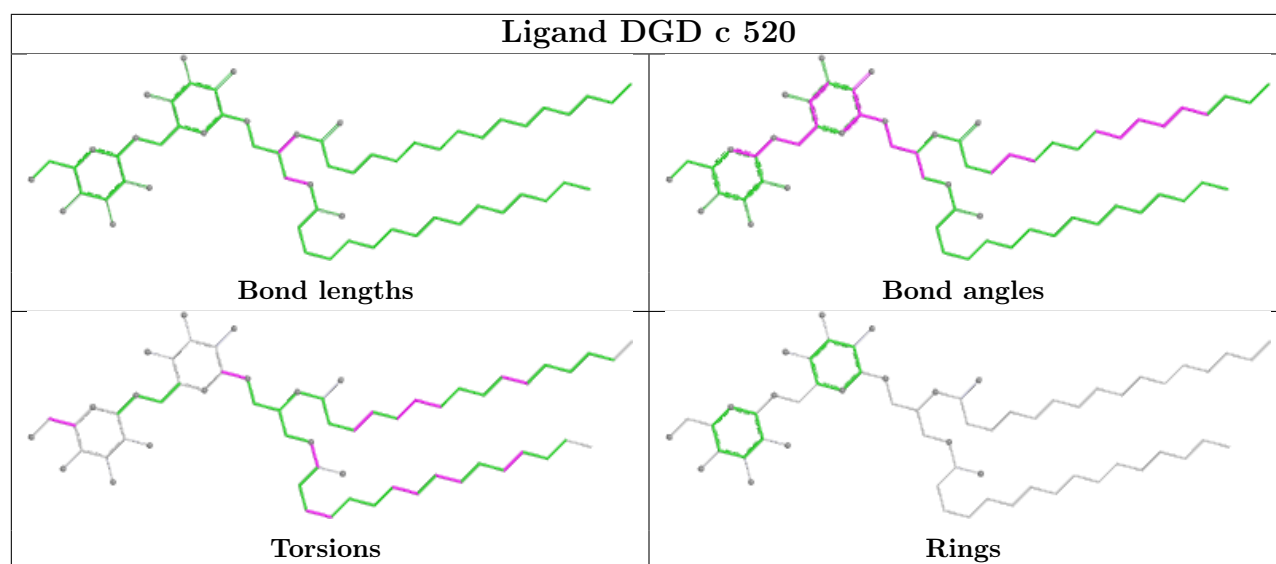


Ligand SQD A 603

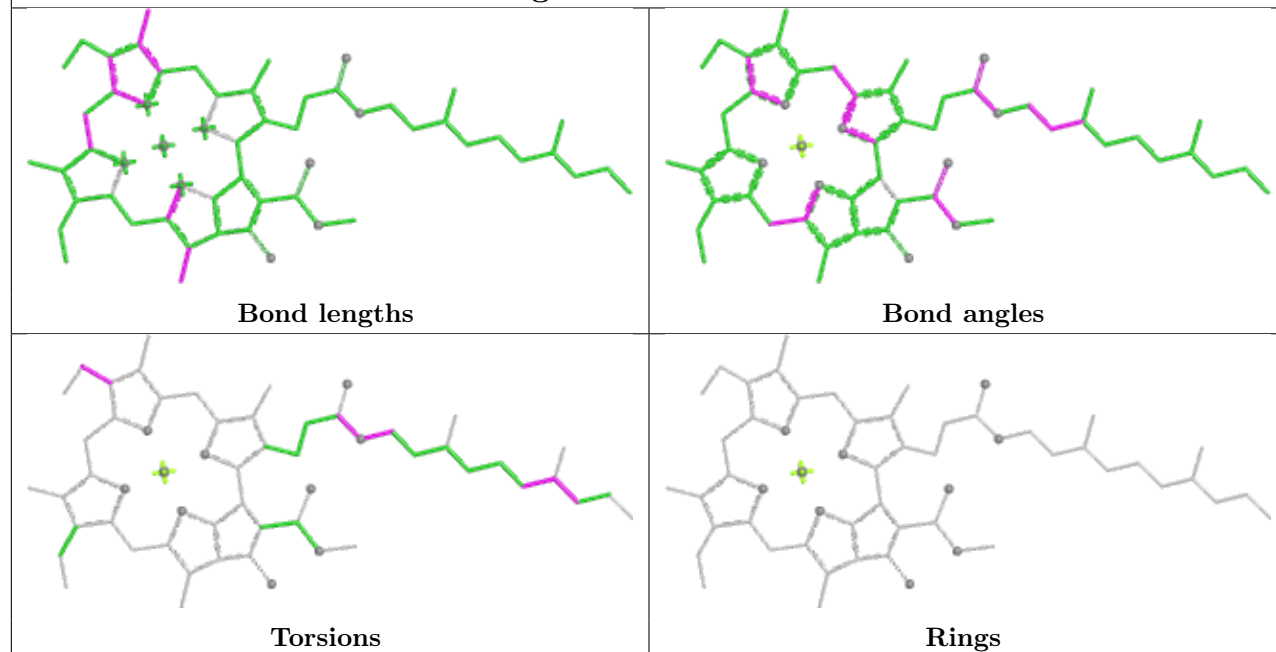




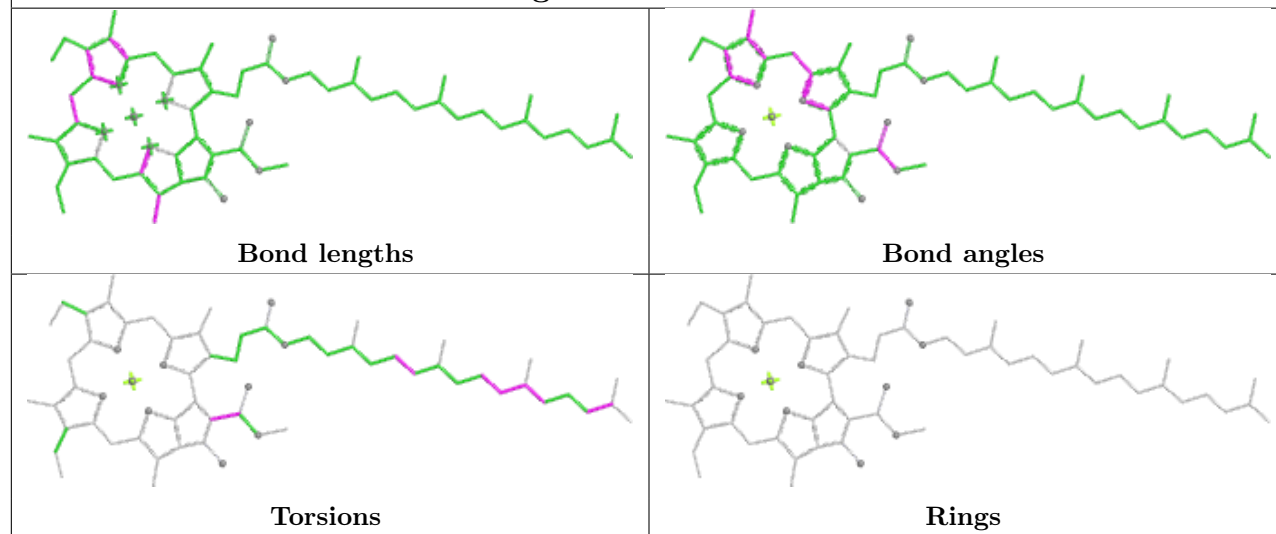




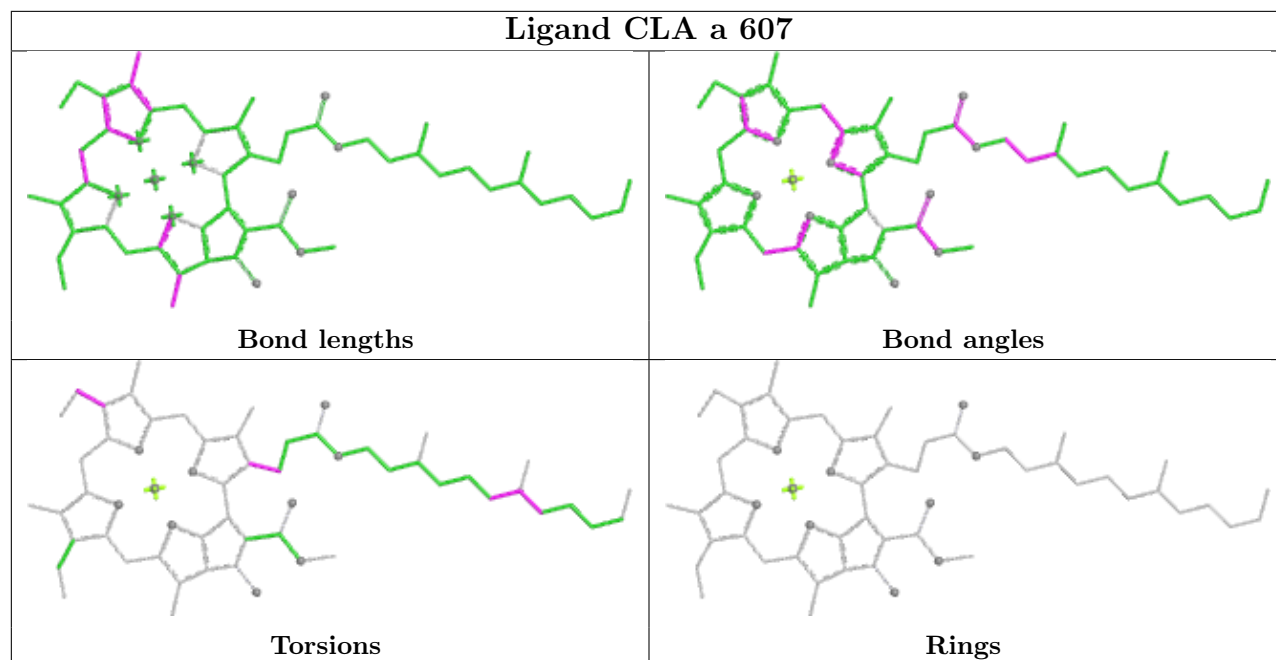
Ligand CLA A 607



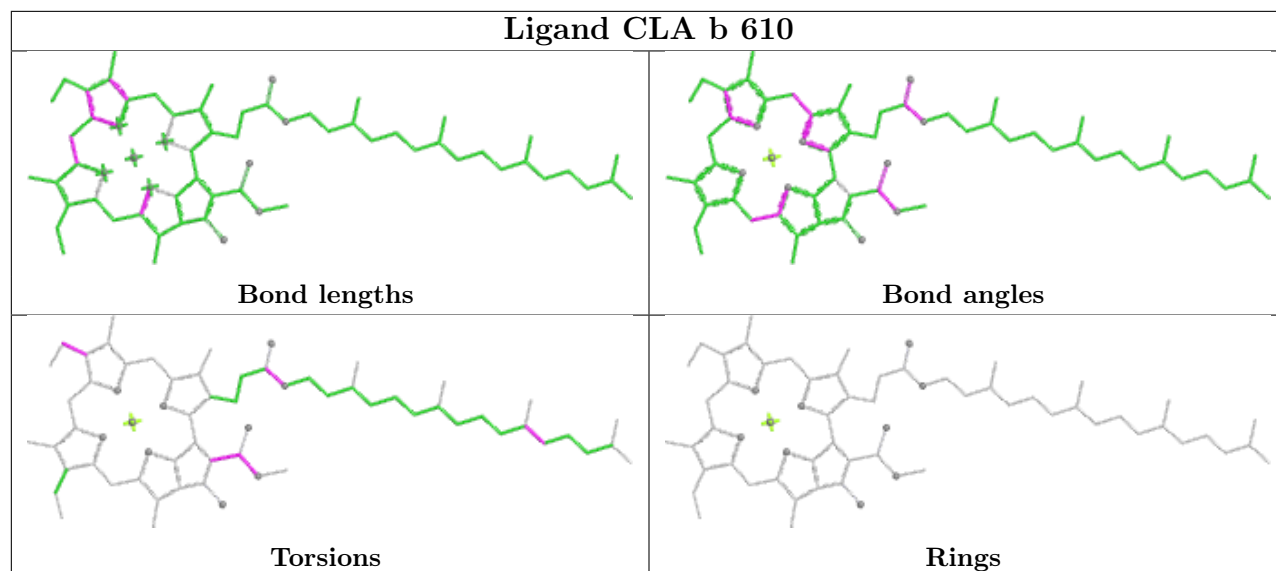
Ligand CLA C 509

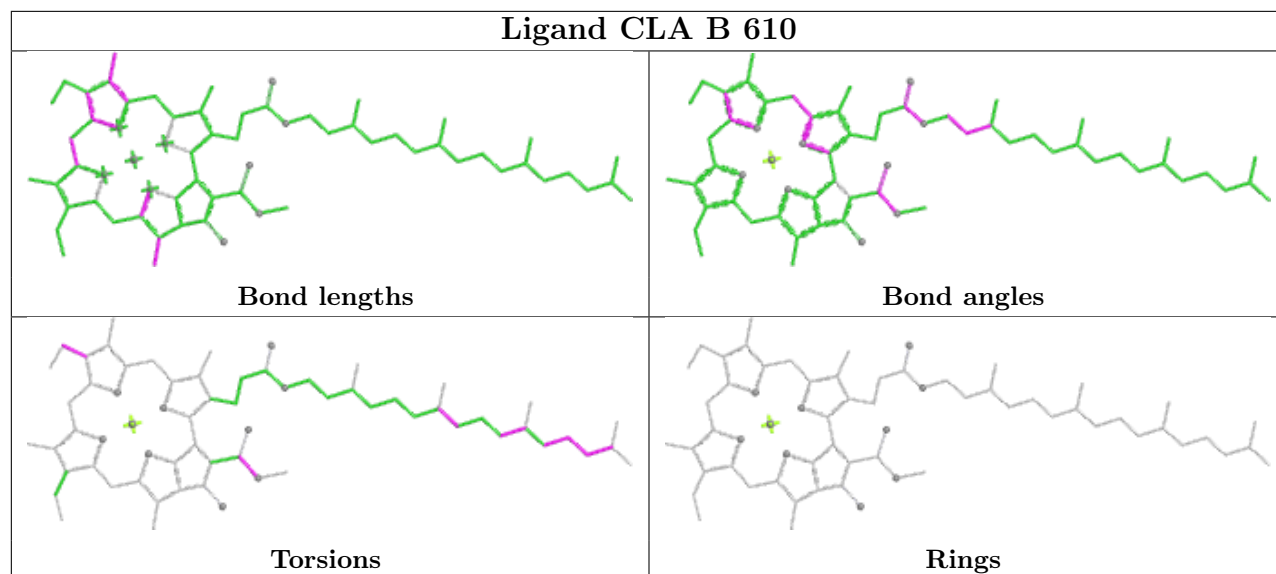
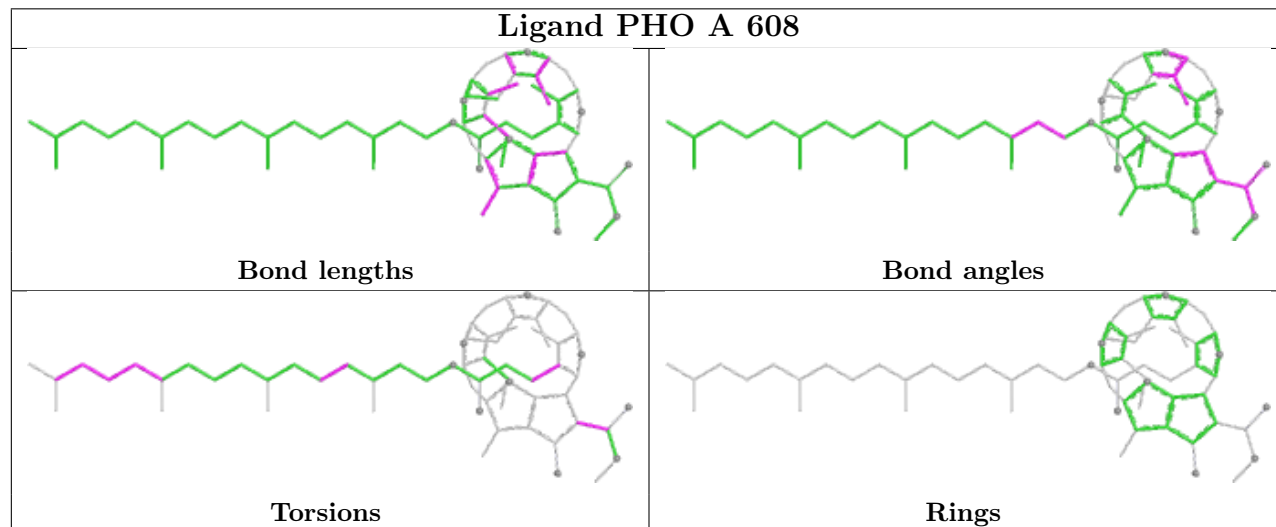


Ligand CLA a 607

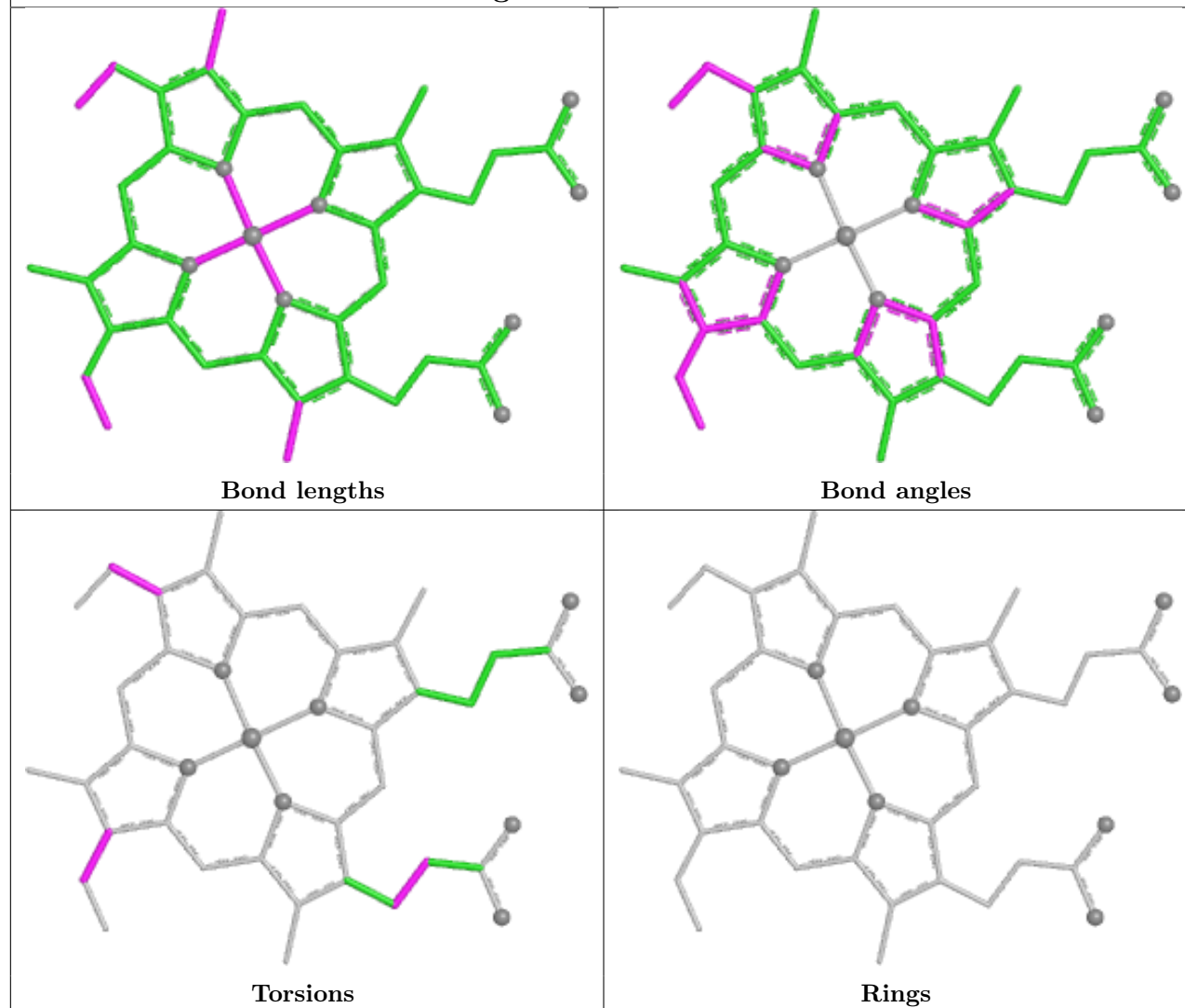


Ligand CLA b 610

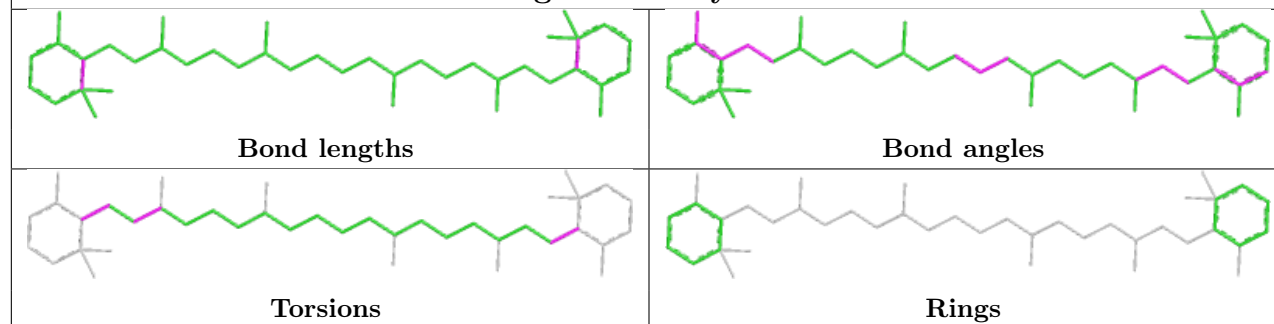


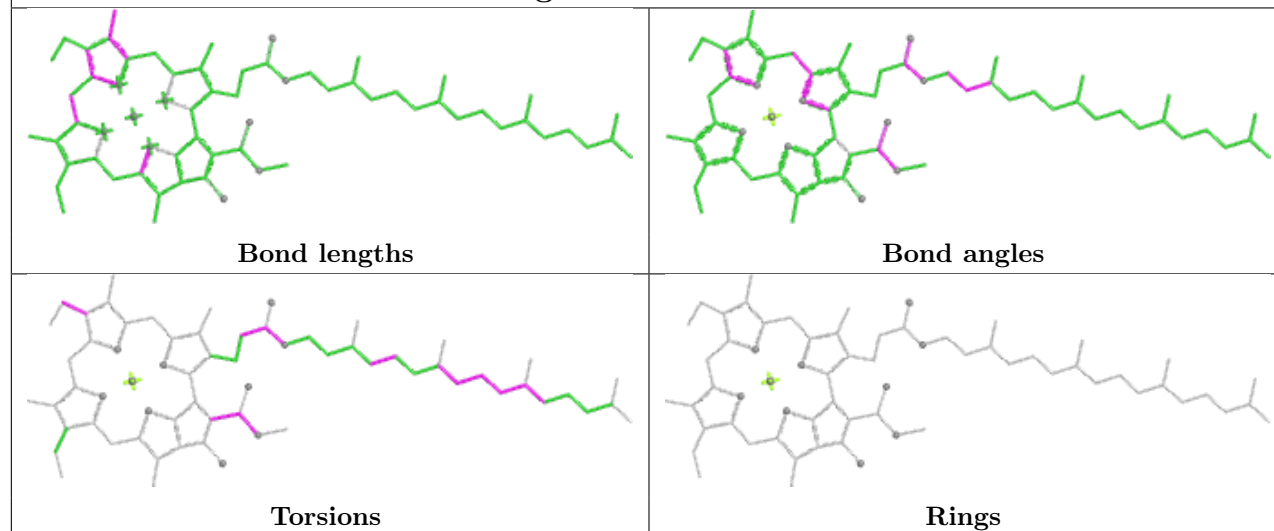
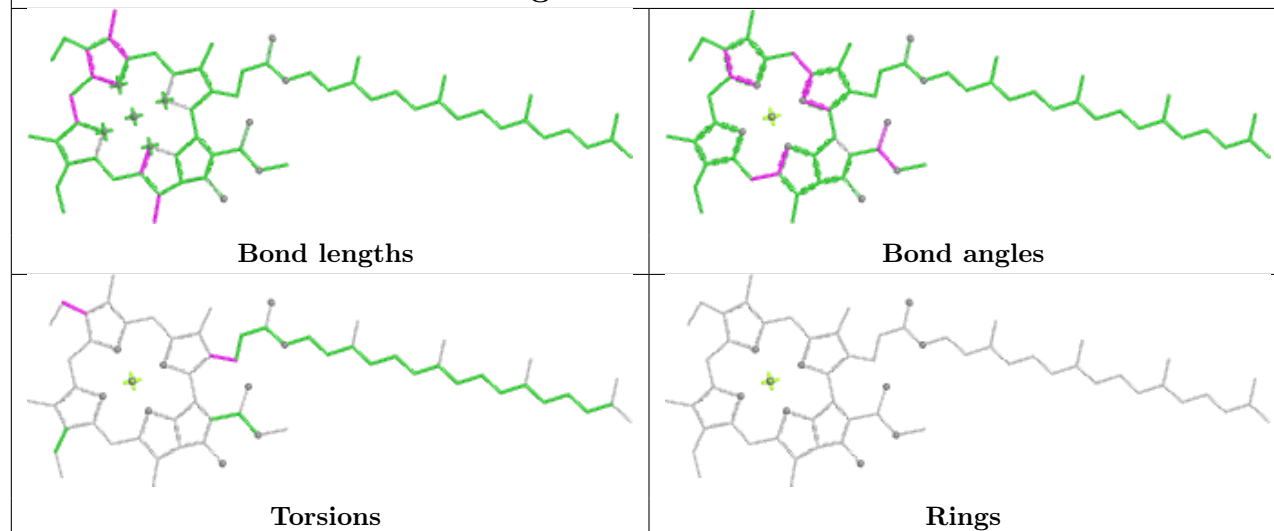
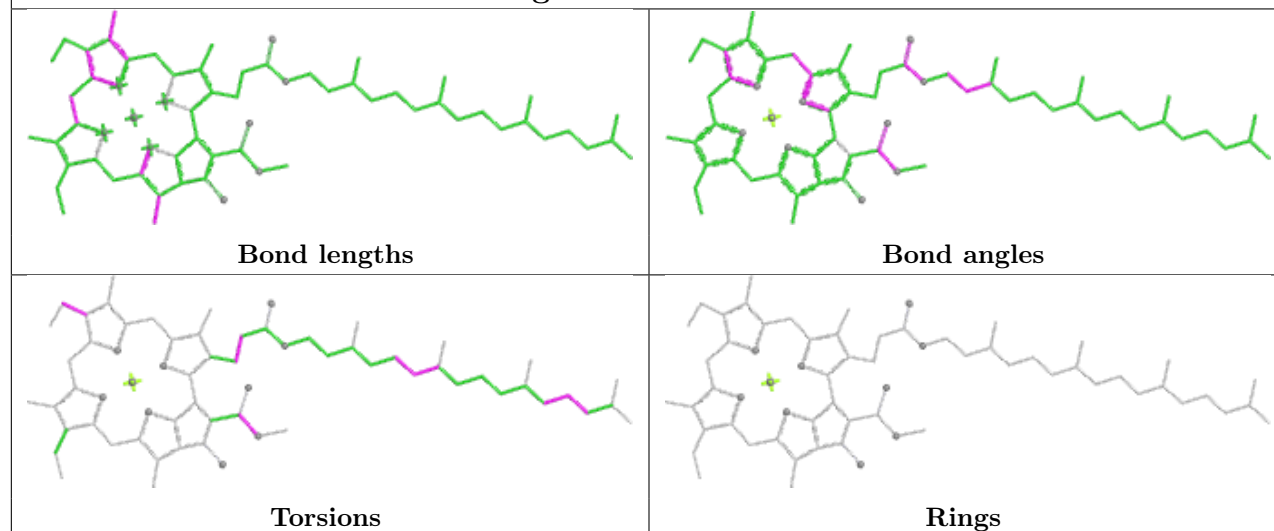
Ligand CLA B 610**Ligand PHO A 608**

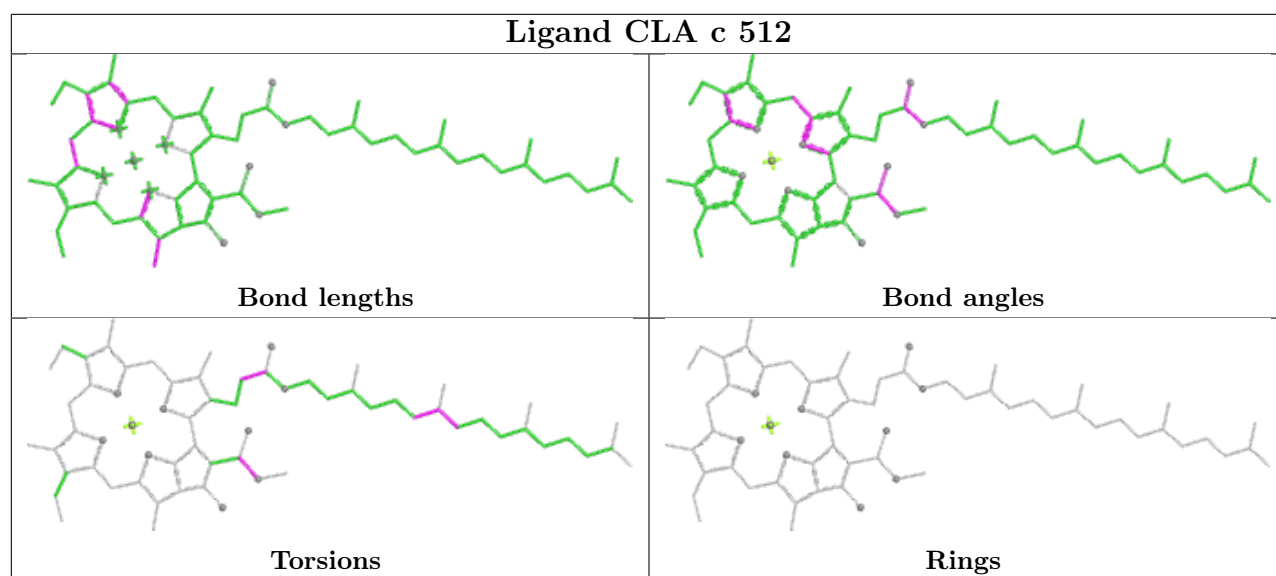
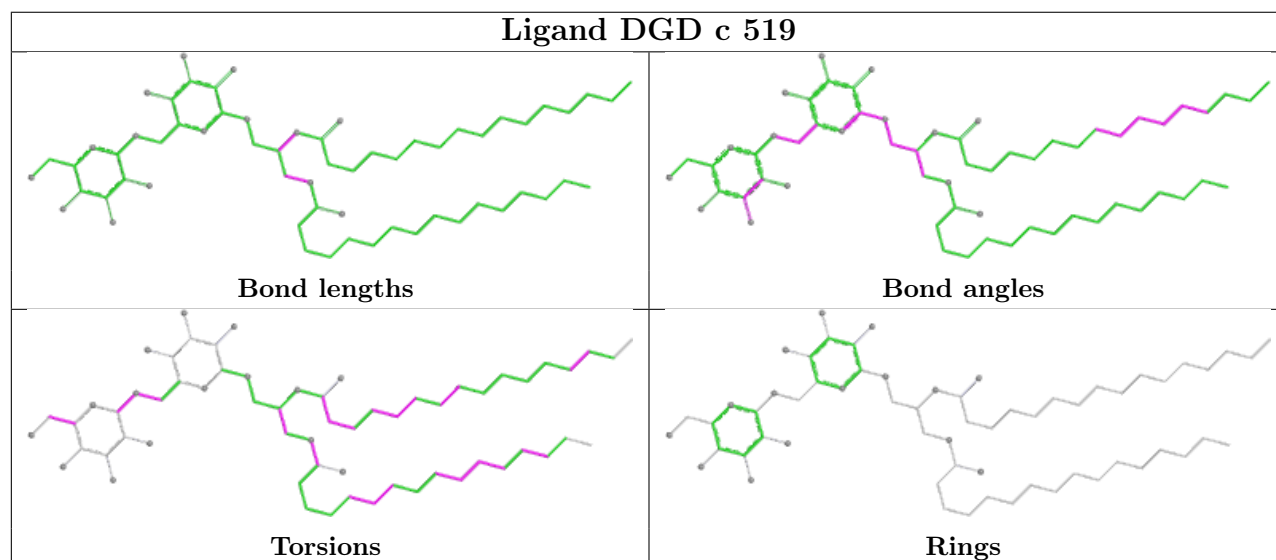
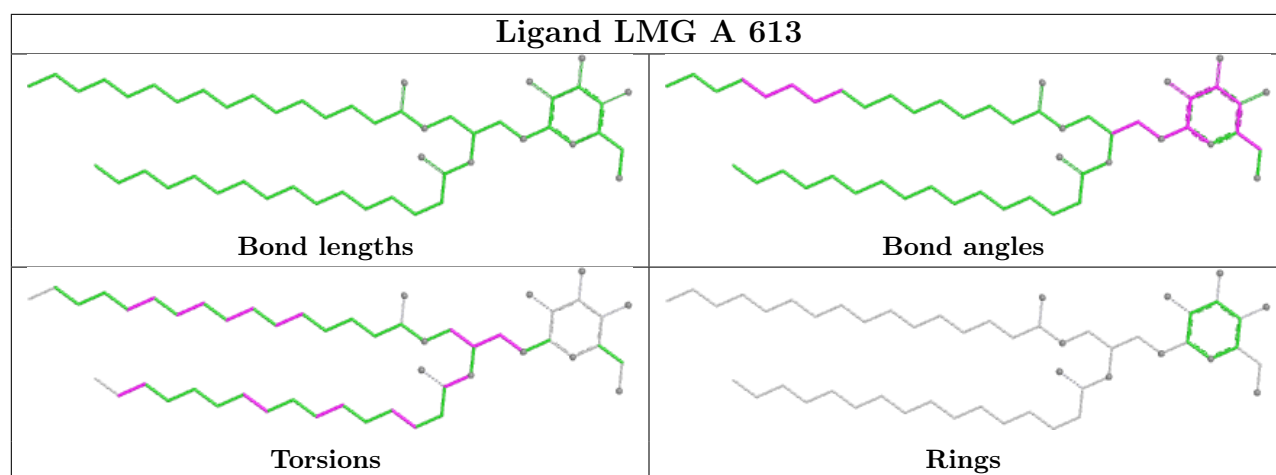
Ligand HEC V 201

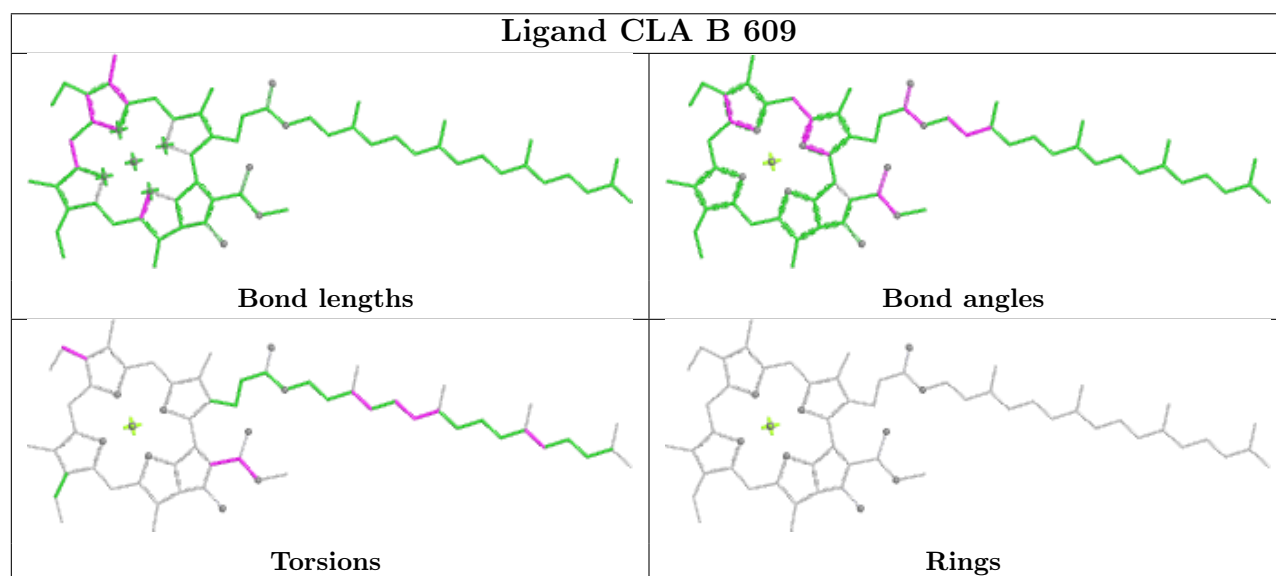
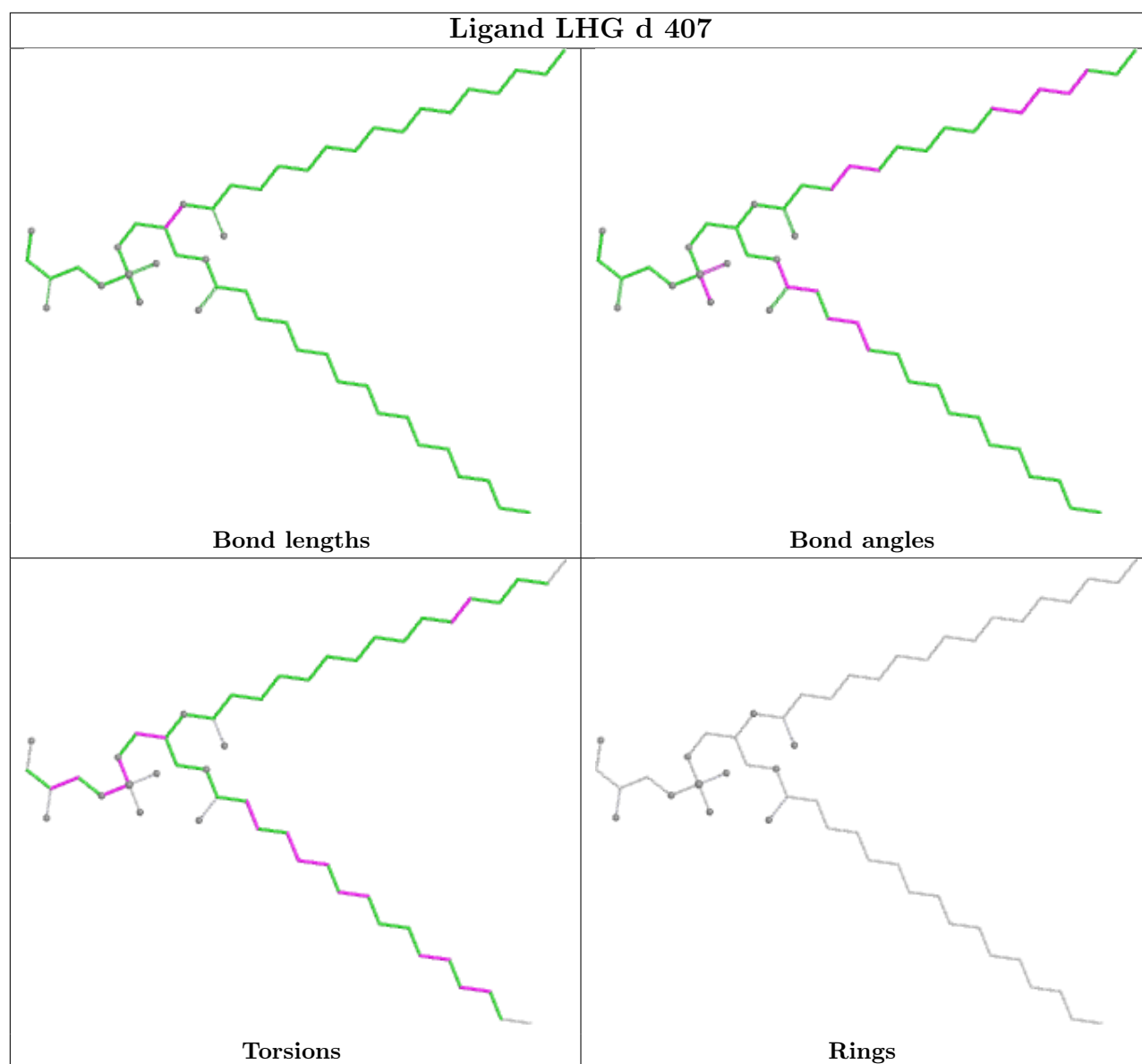


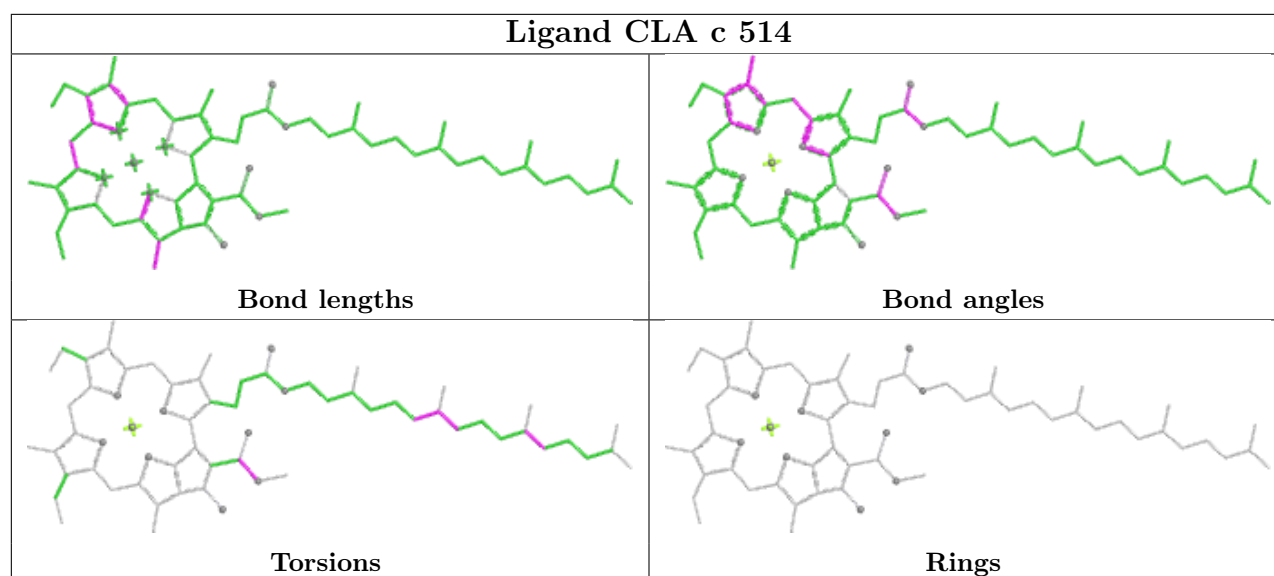
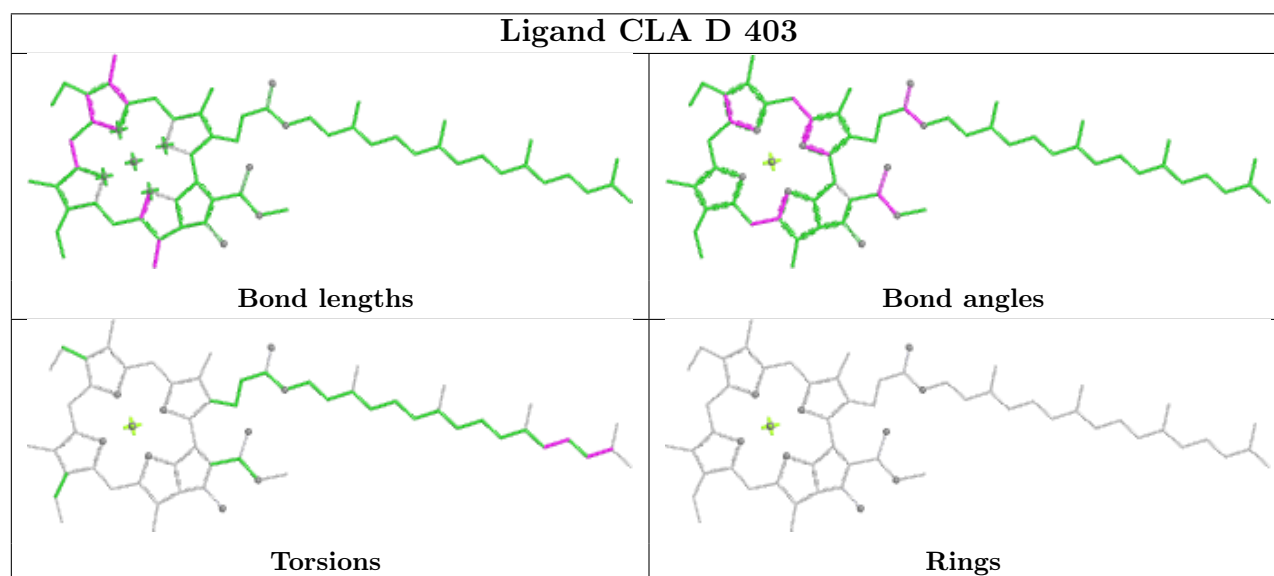
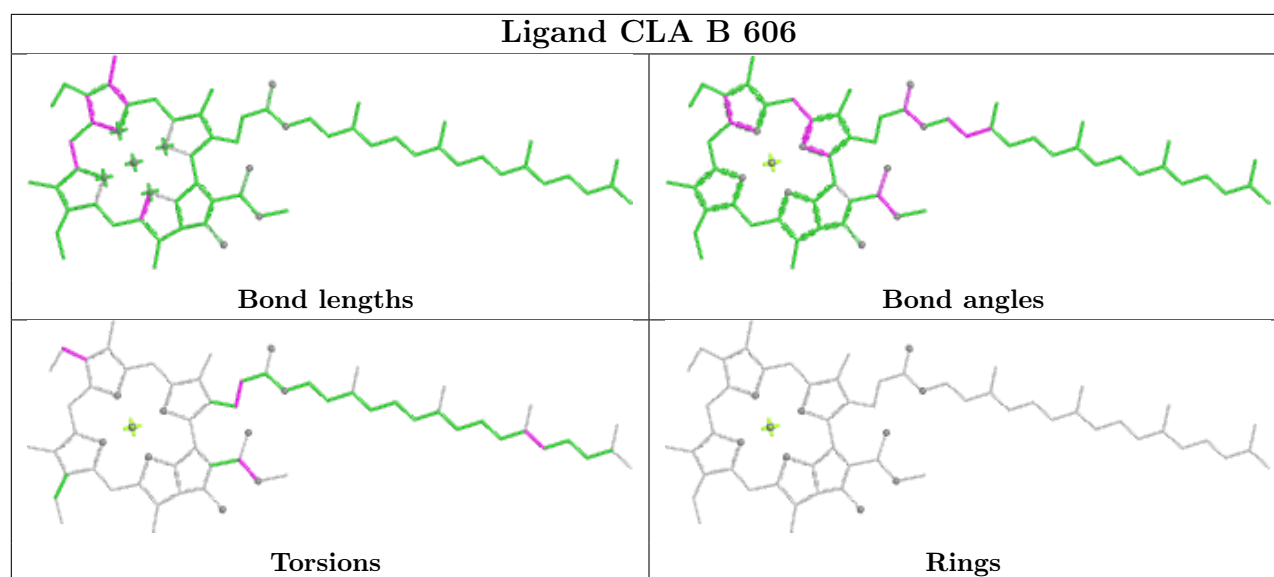
Ligand BCR y 101

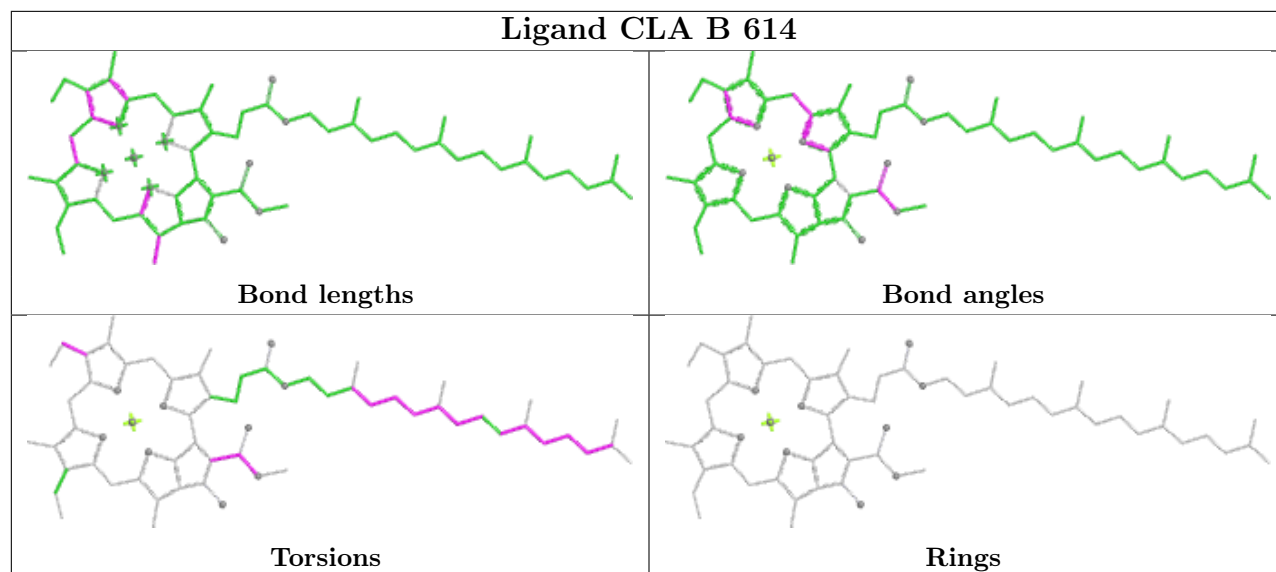
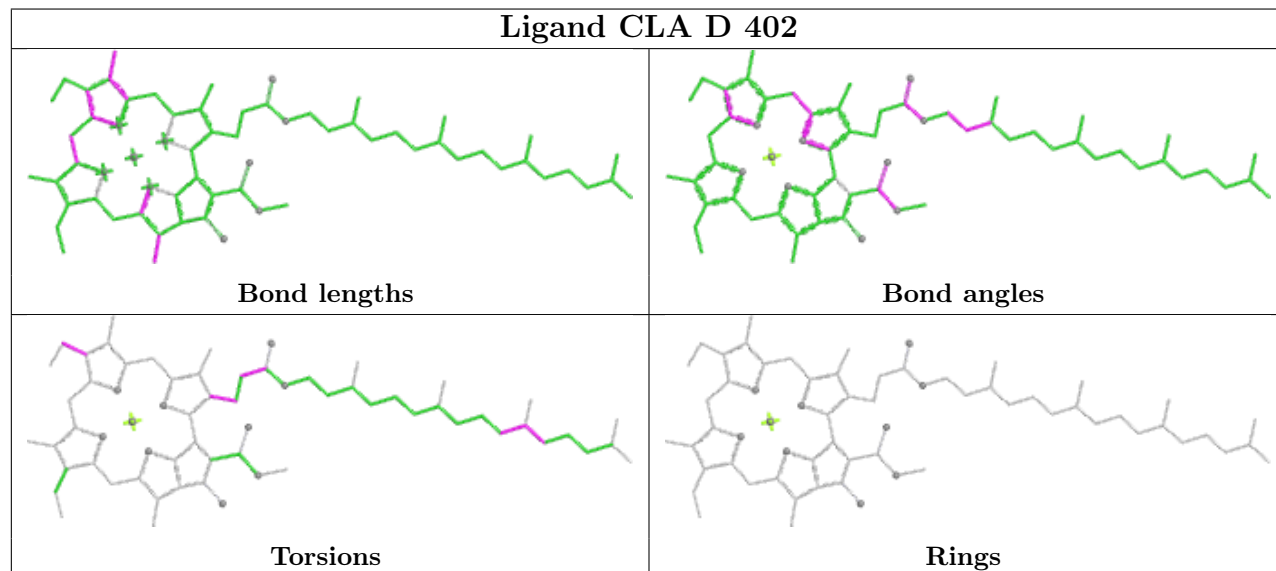
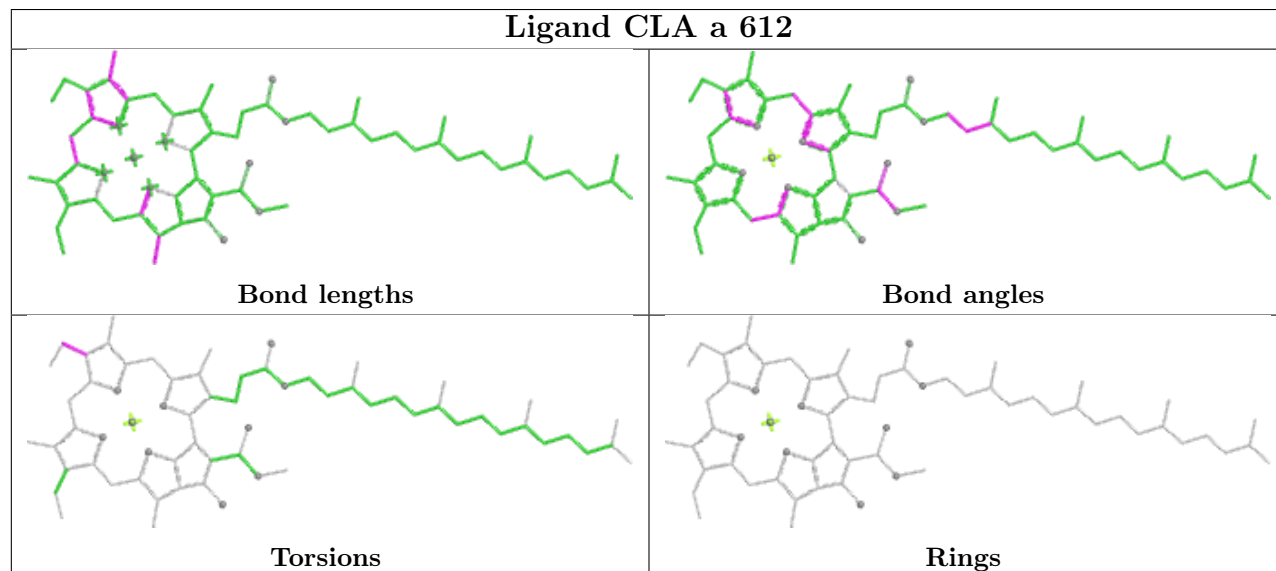


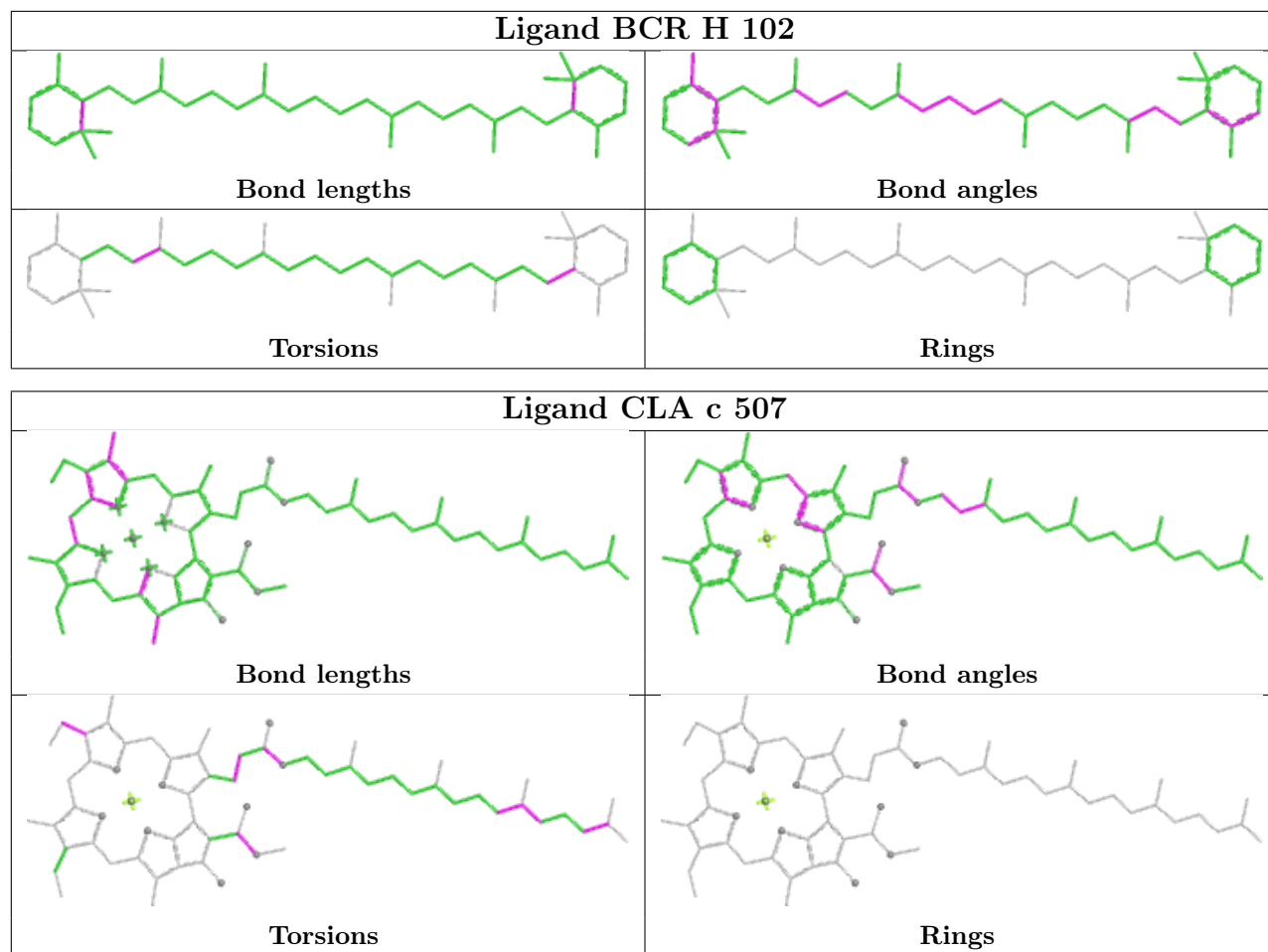
Ligand CLA b 604**Ligand CLA A 615****Ligand CLA B 603**

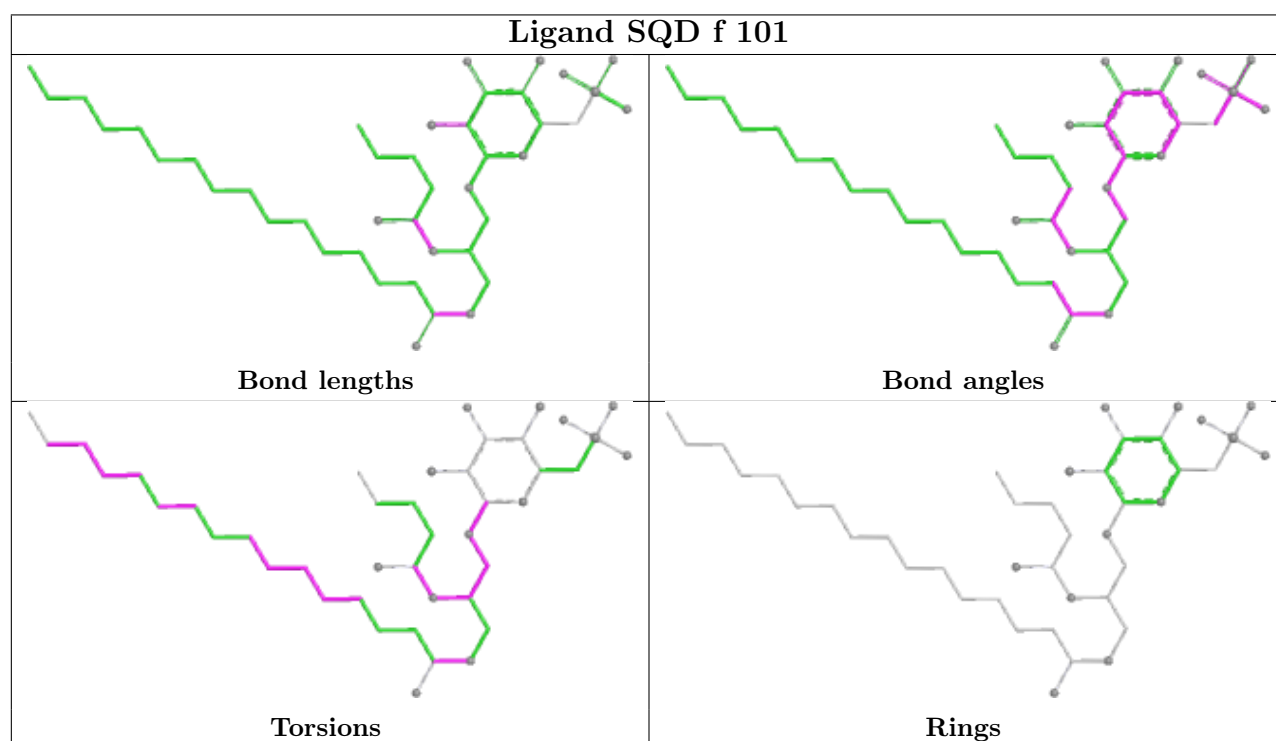
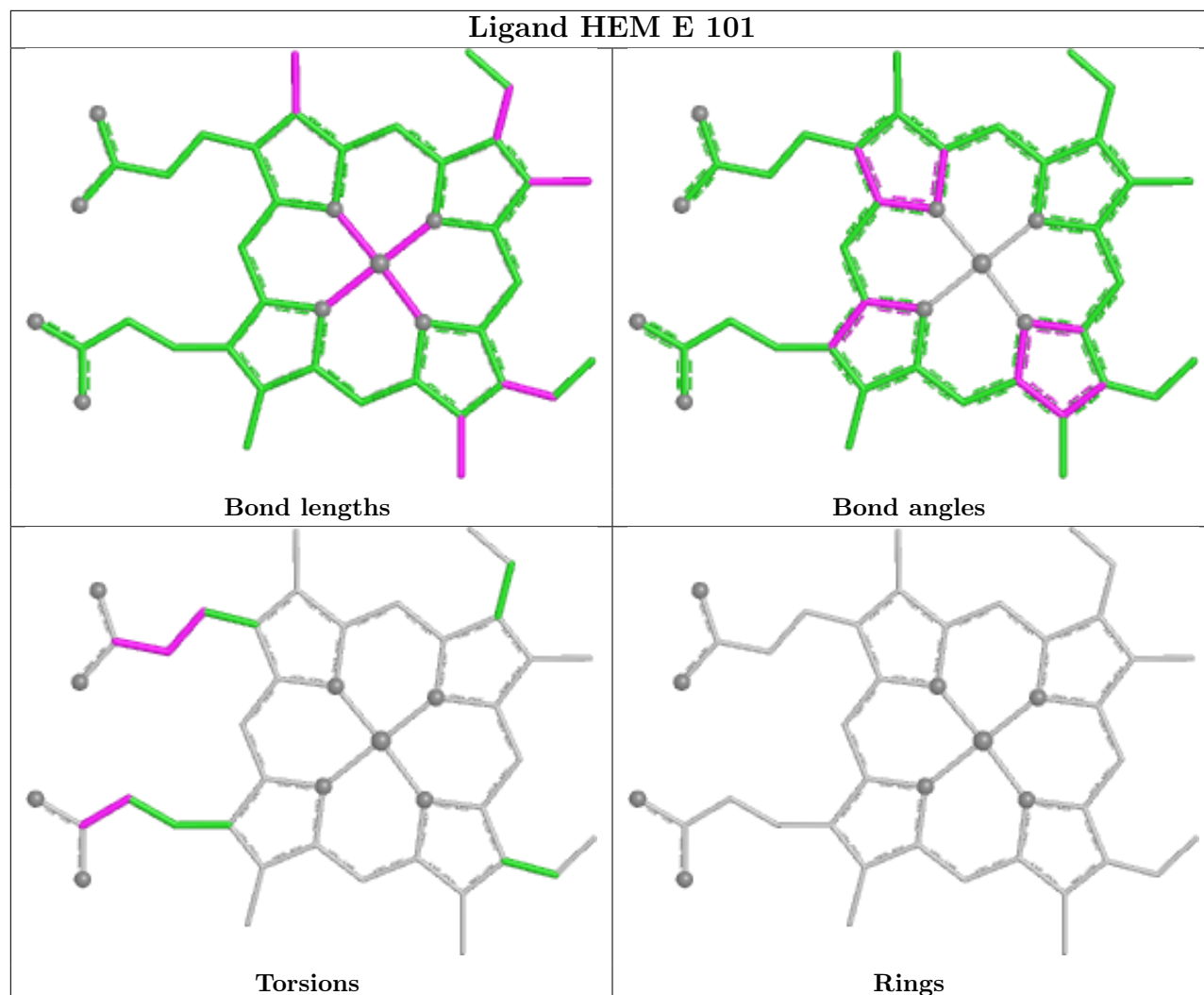


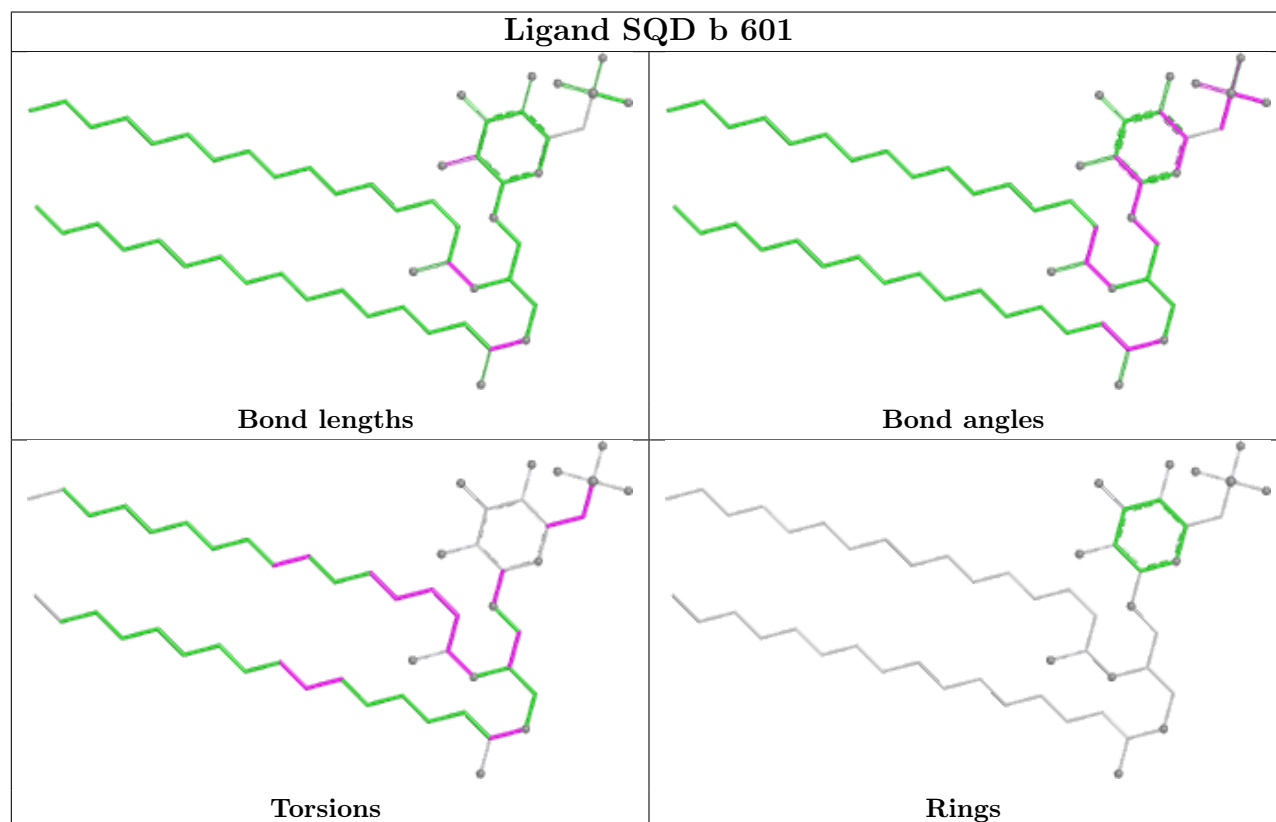
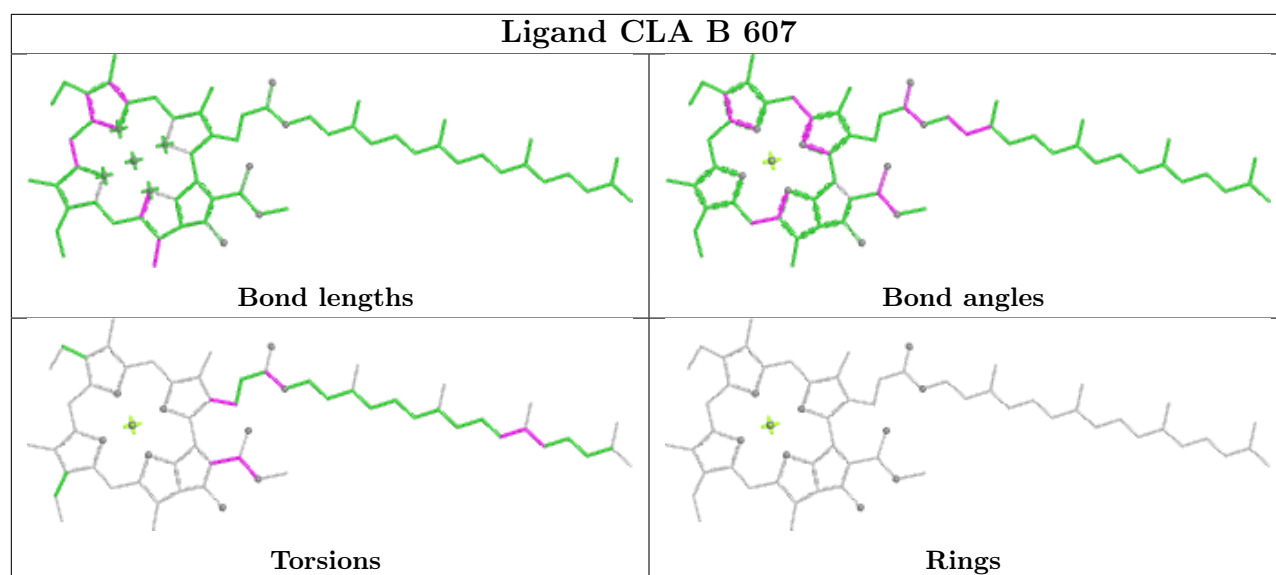


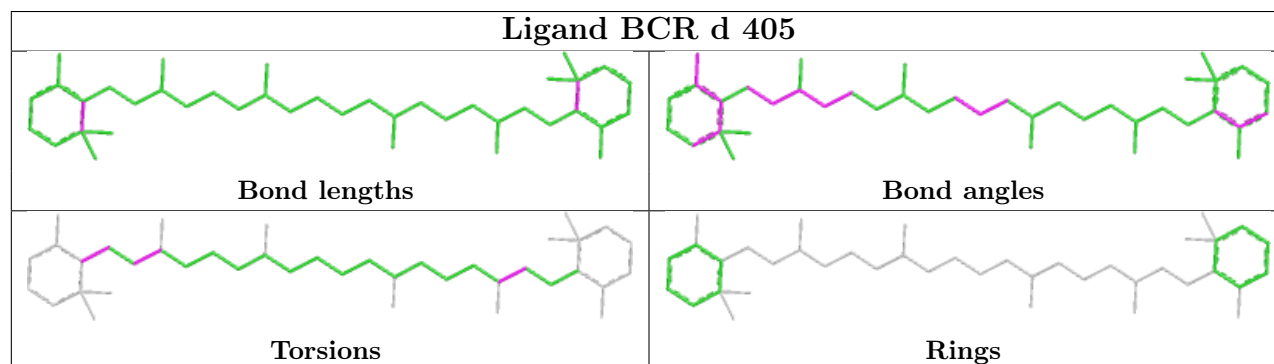
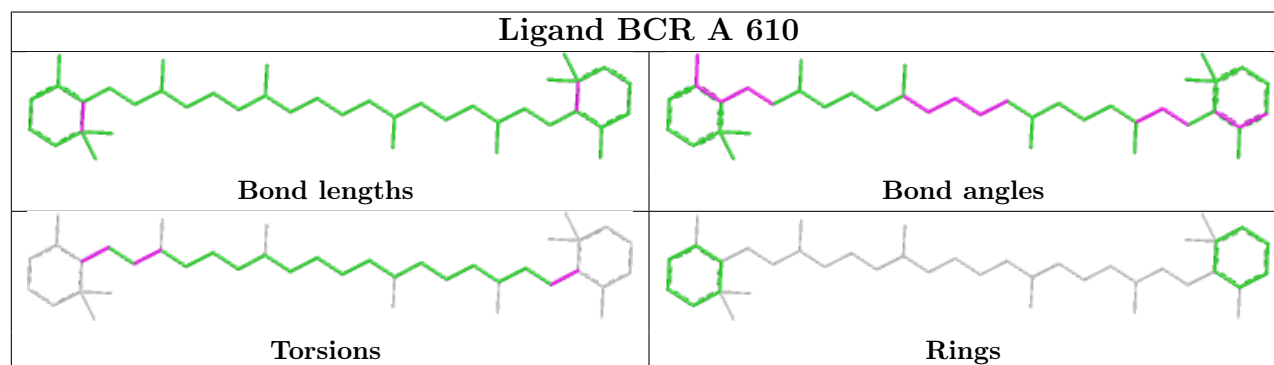
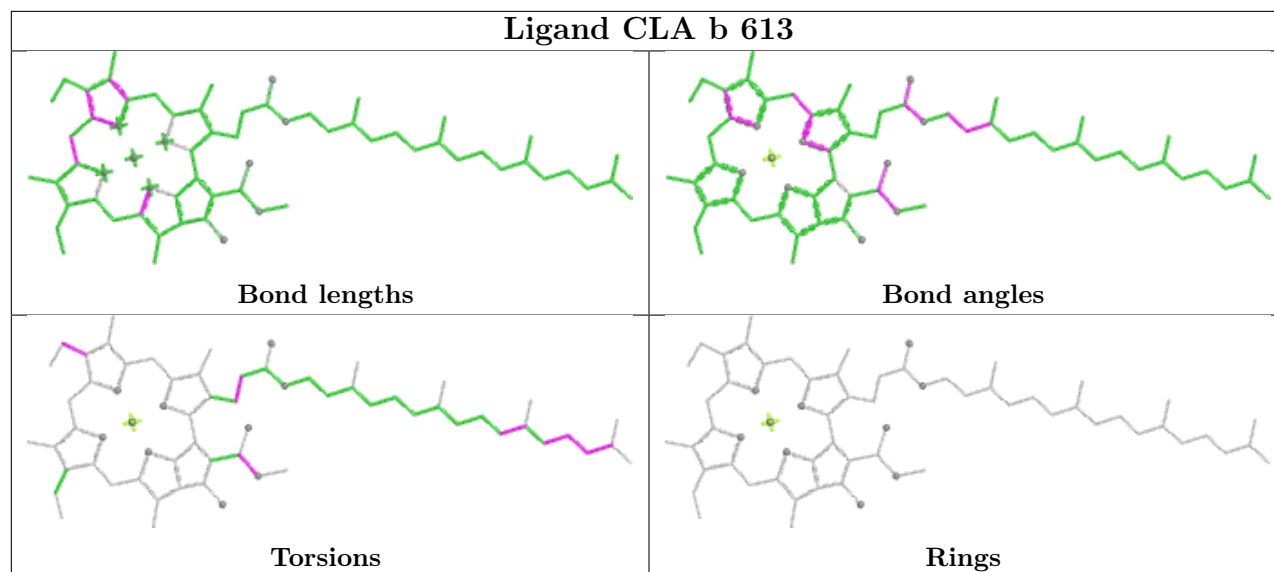


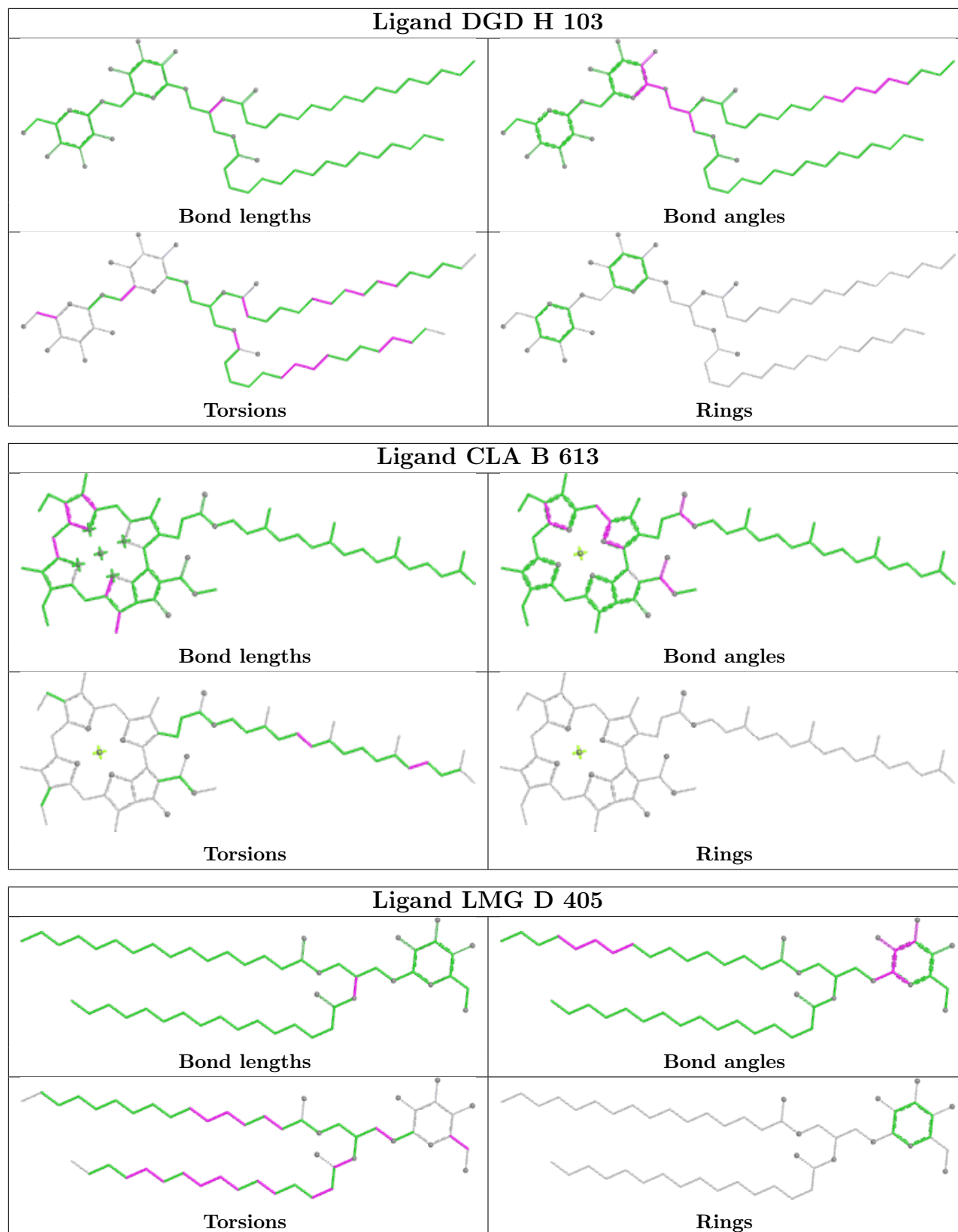
Ligand CLA B 614**Ligand CLA D 402****Ligand CLA a 612**

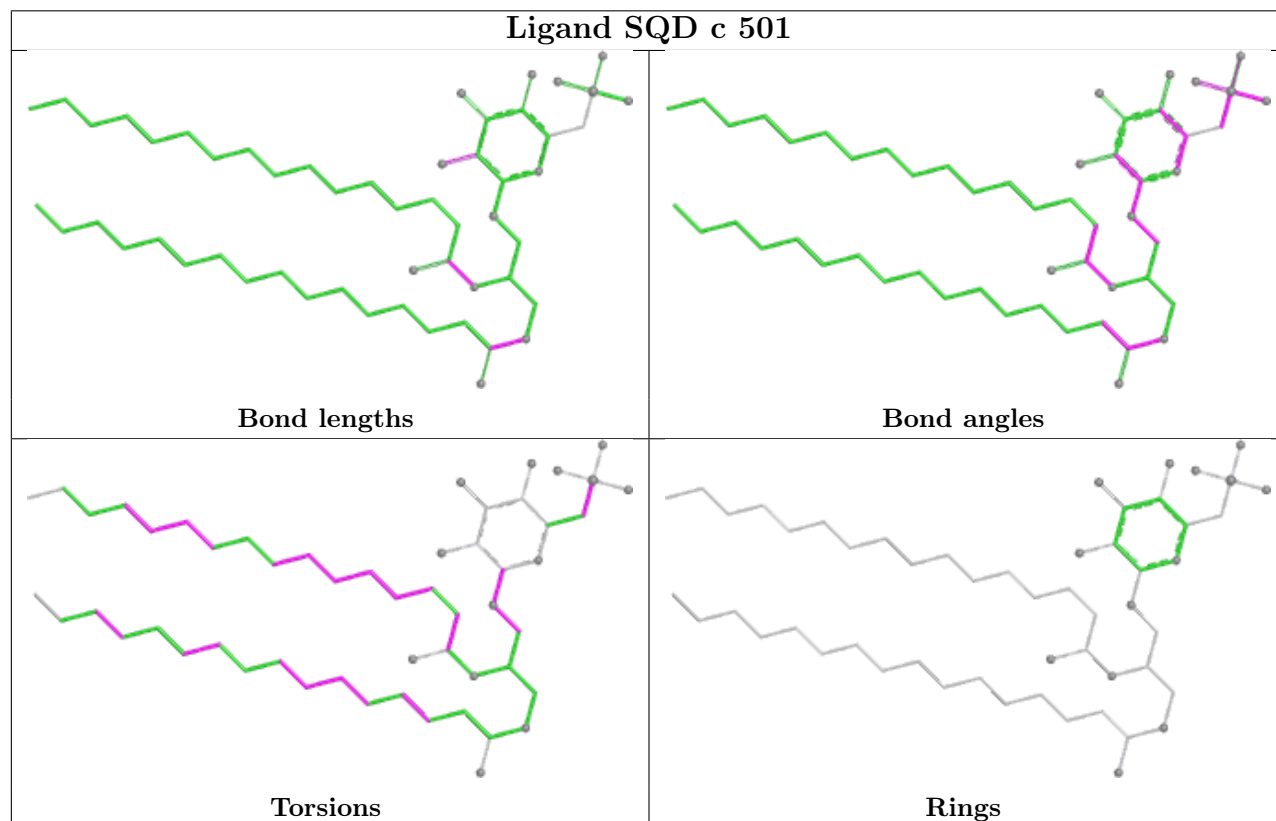
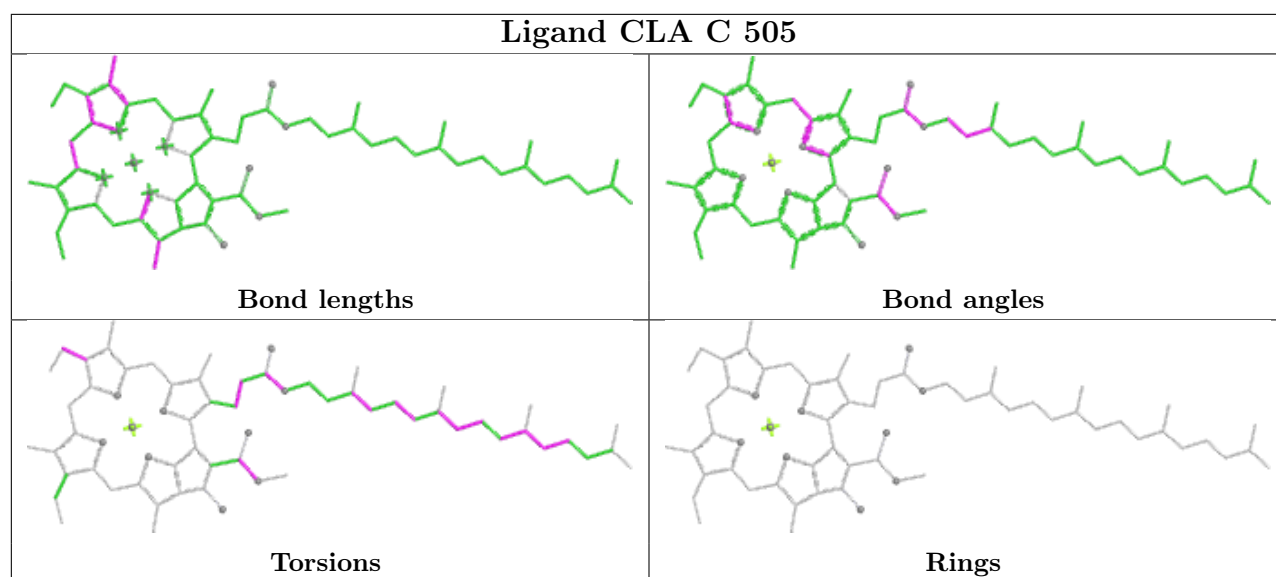


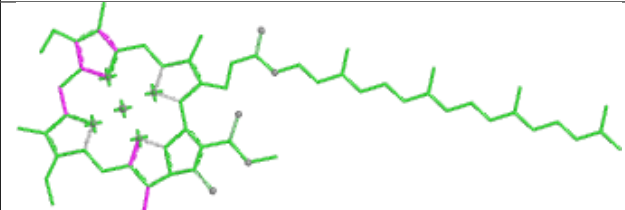
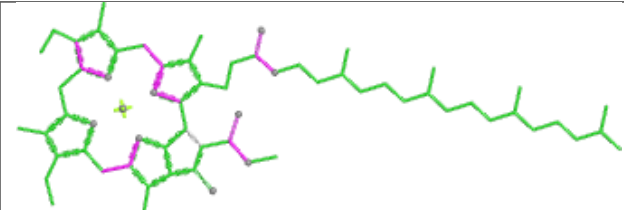
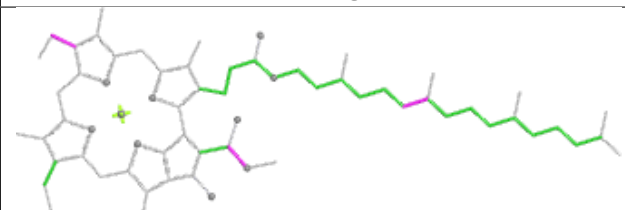
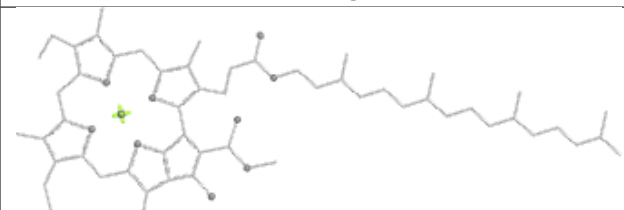


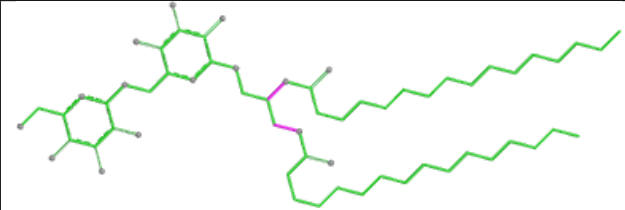
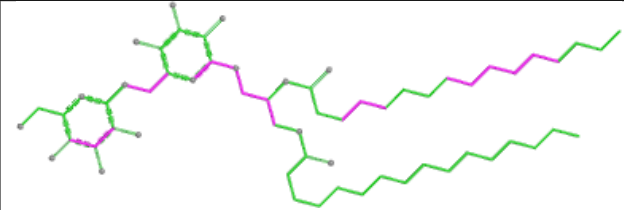
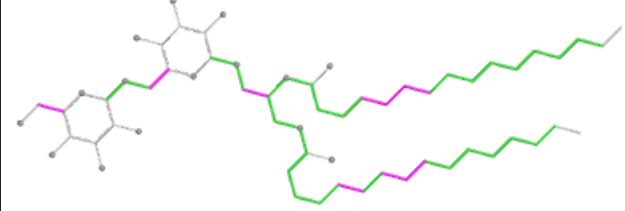
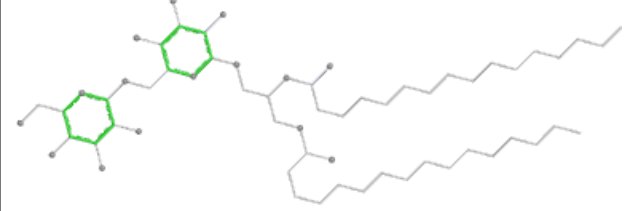


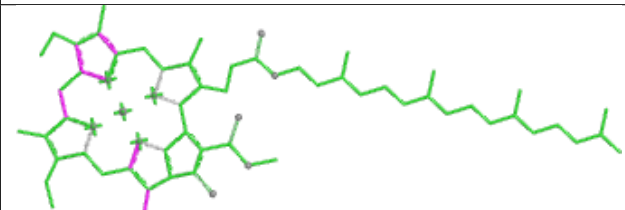
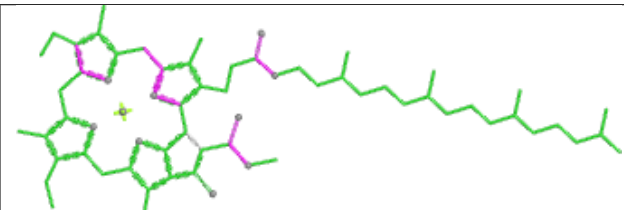
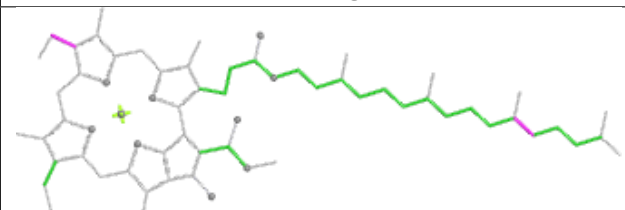
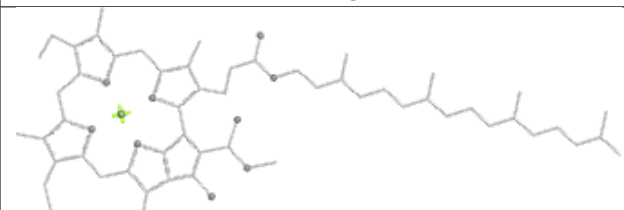


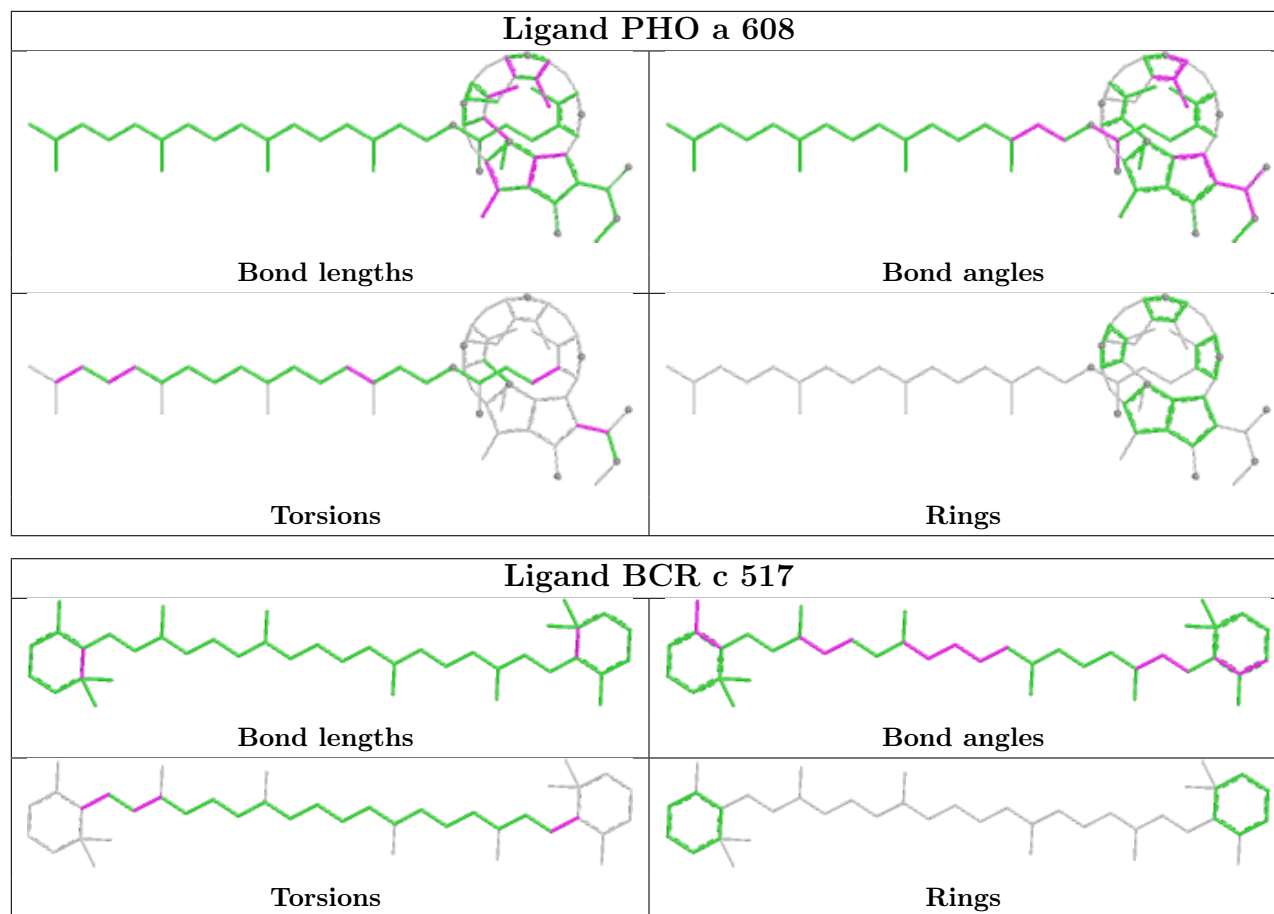


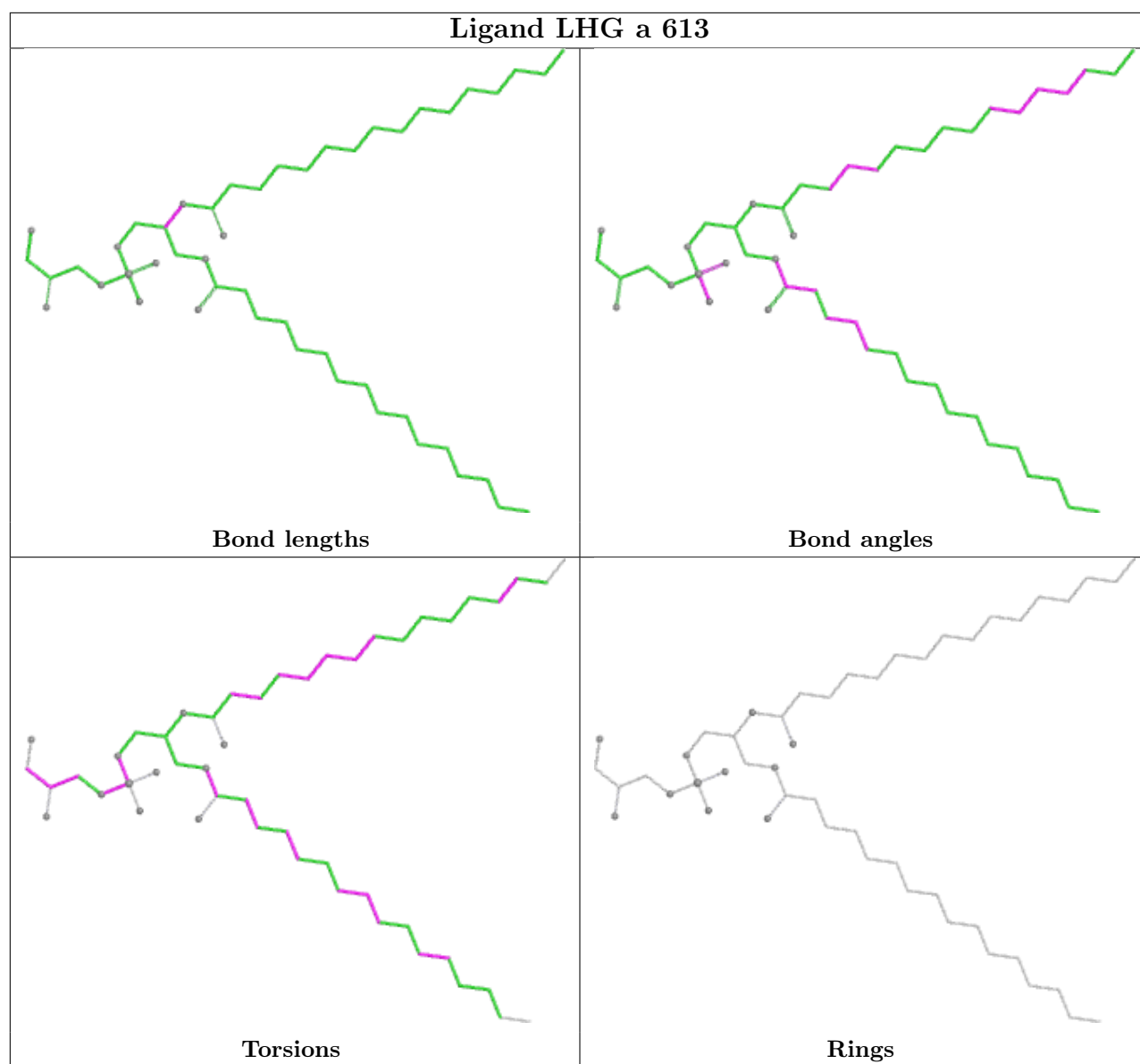


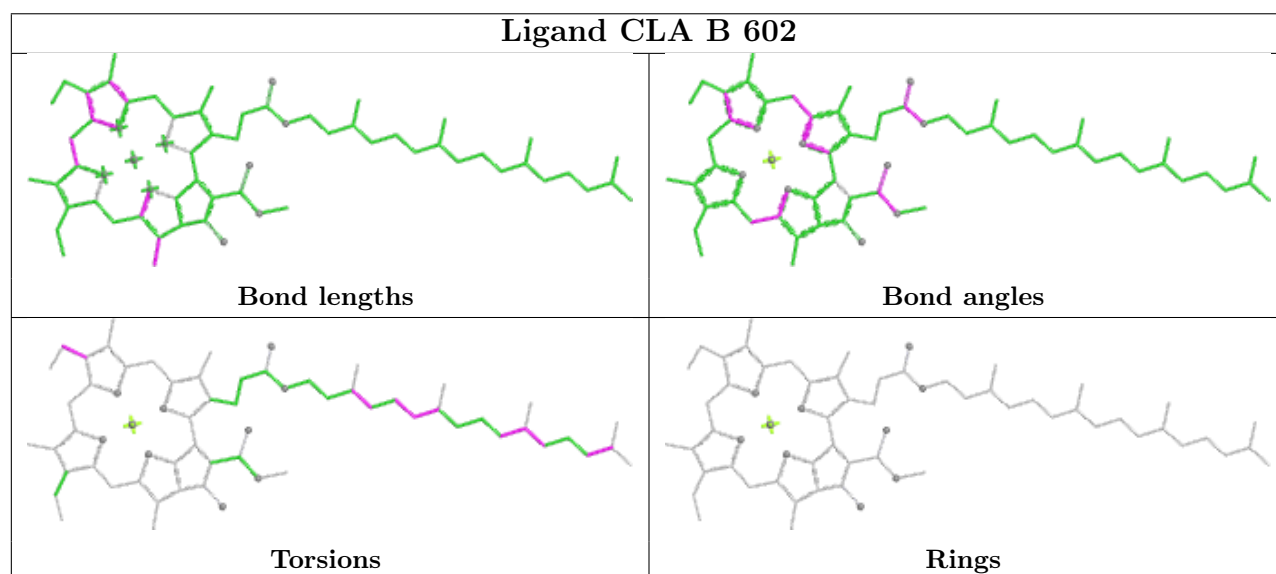
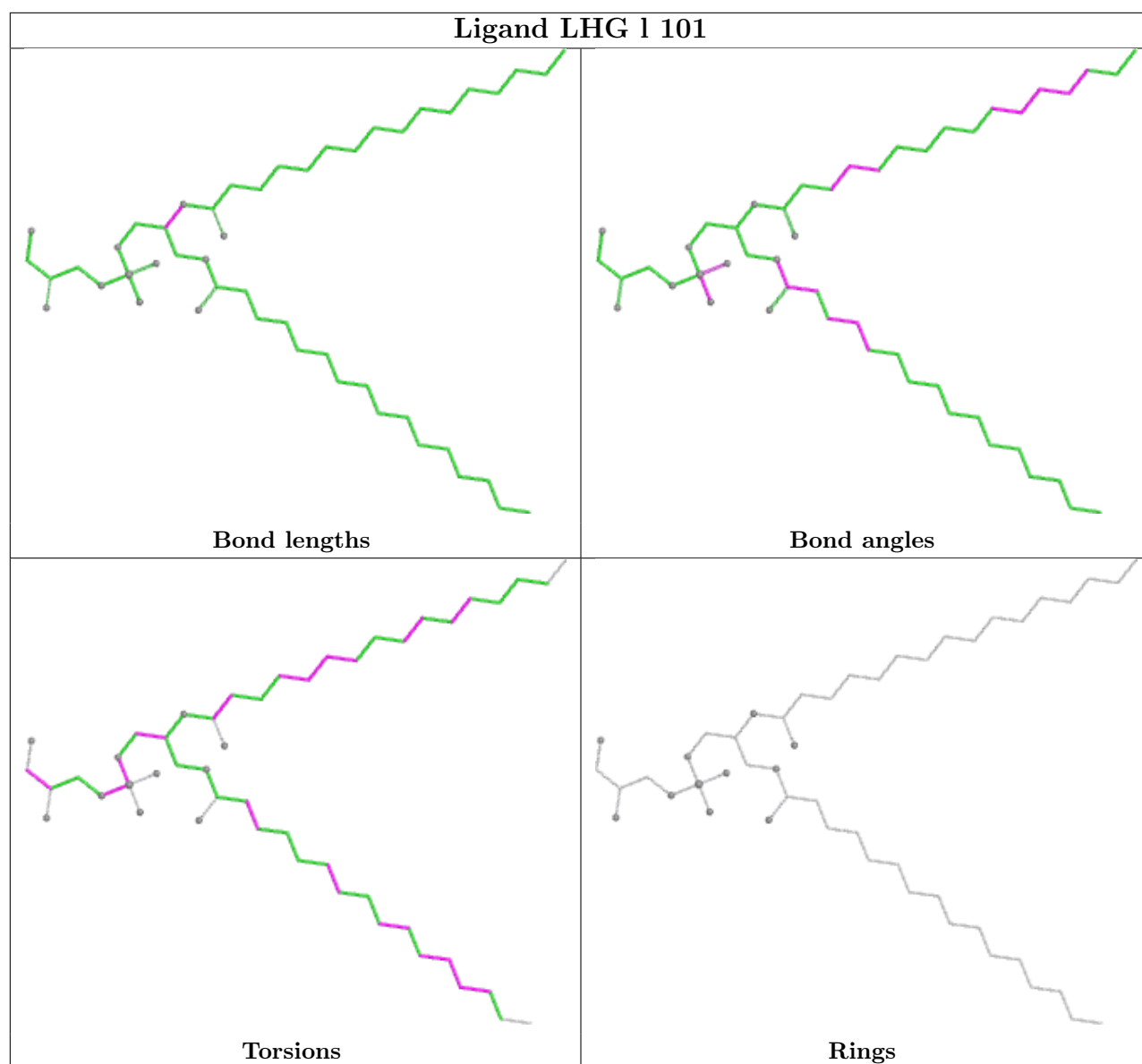
Ligand CLA c 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

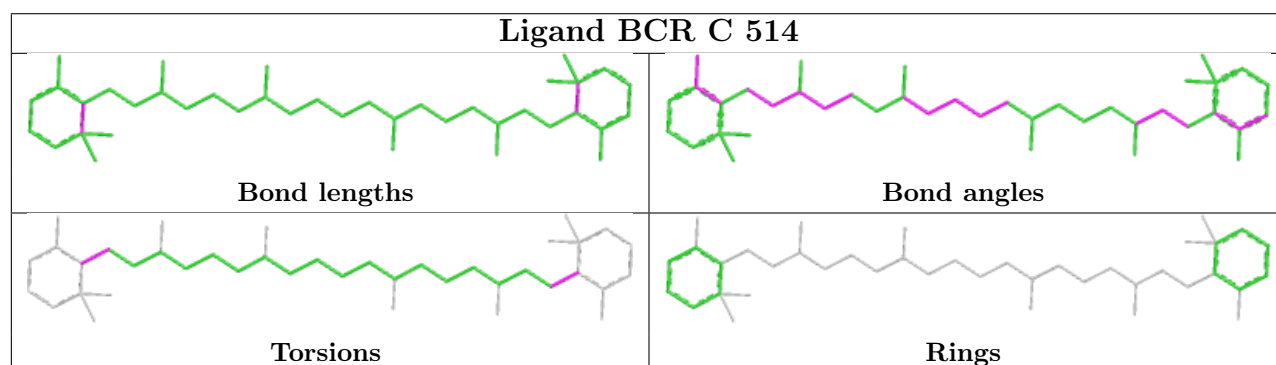
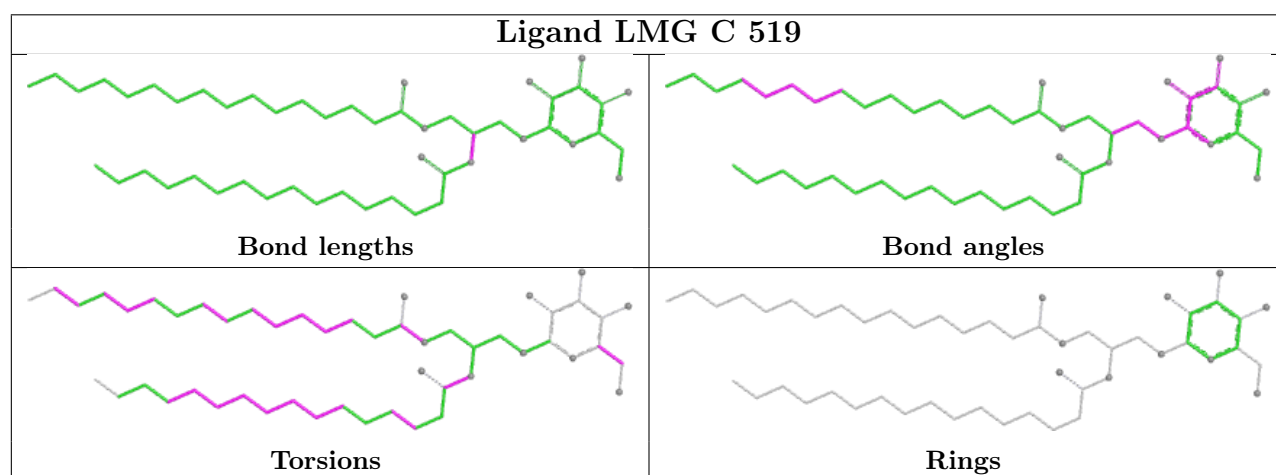
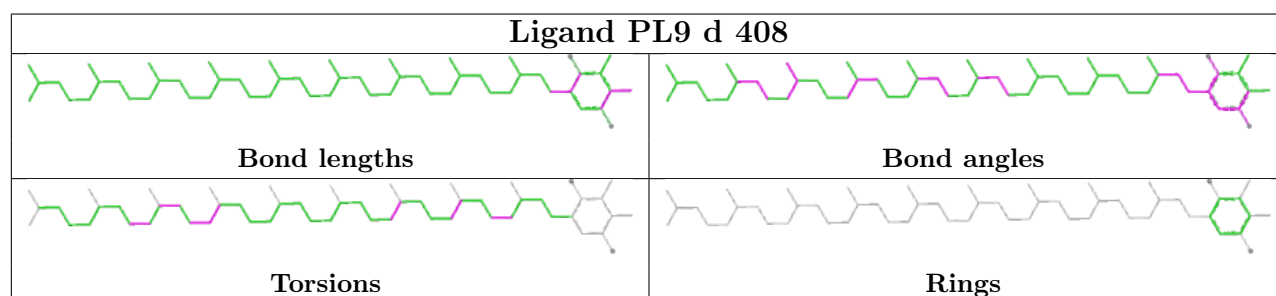
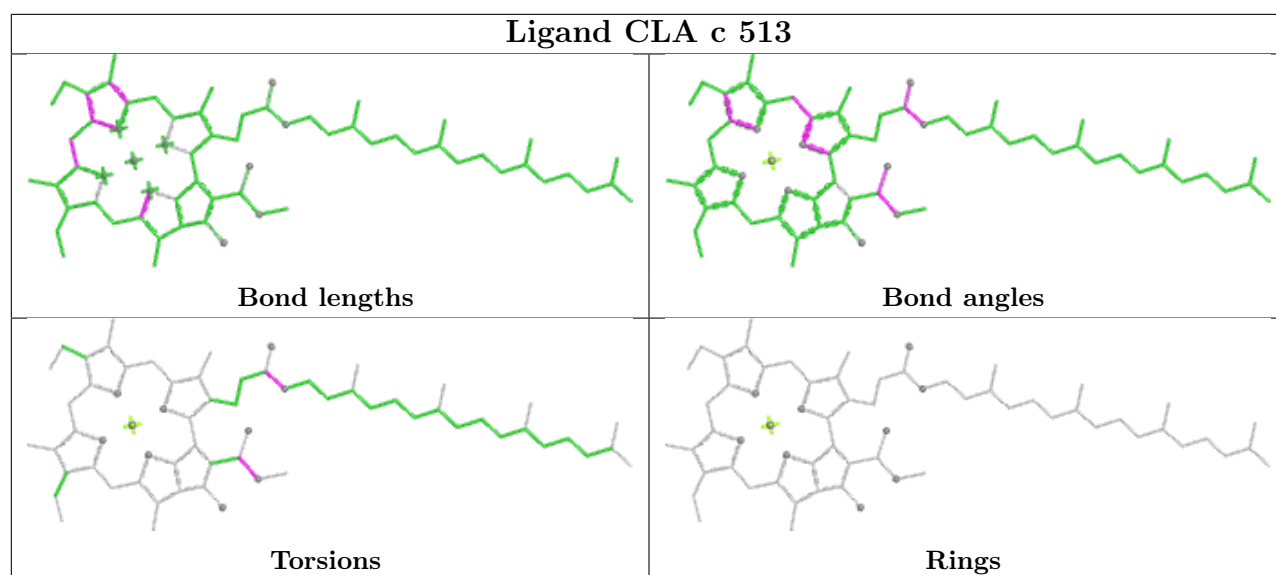
Ligand DGD C 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

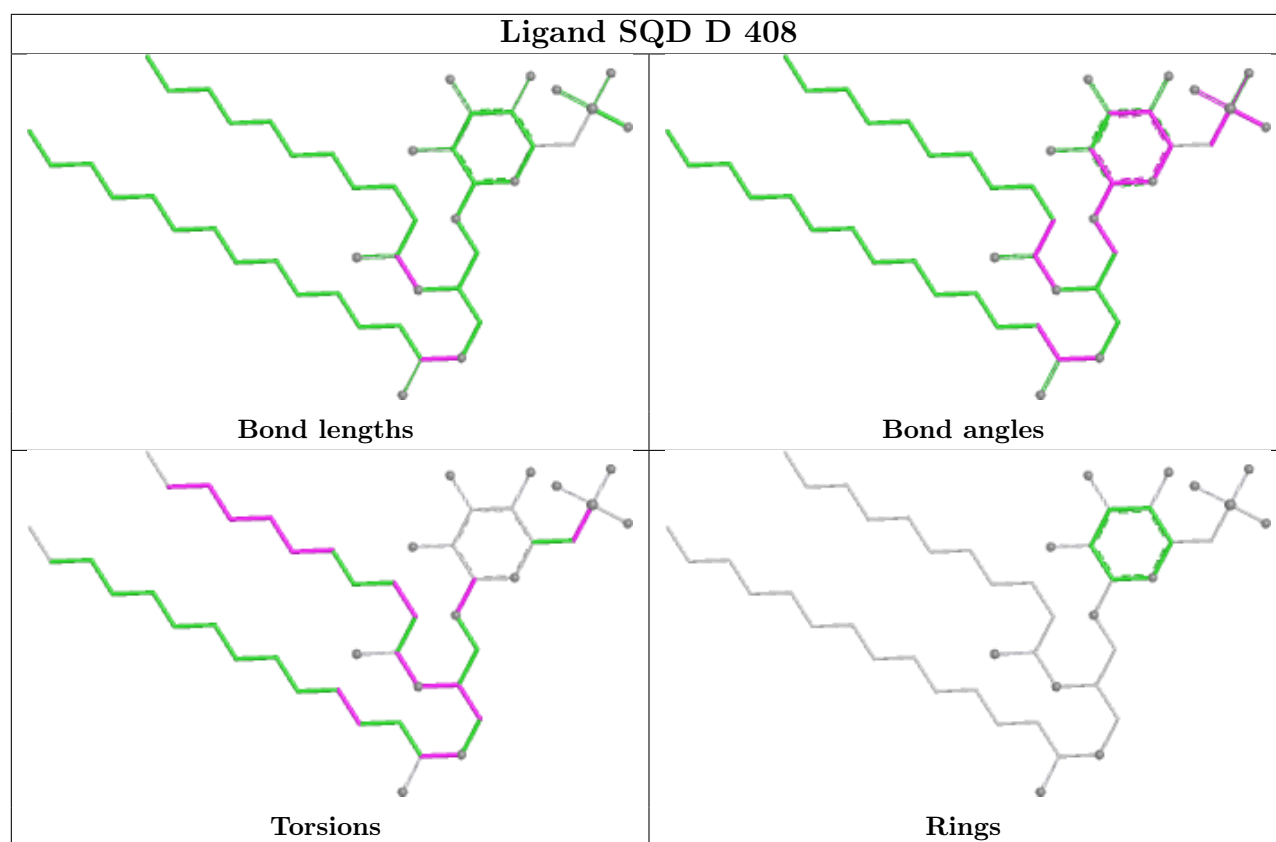
Ligand CLA B 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

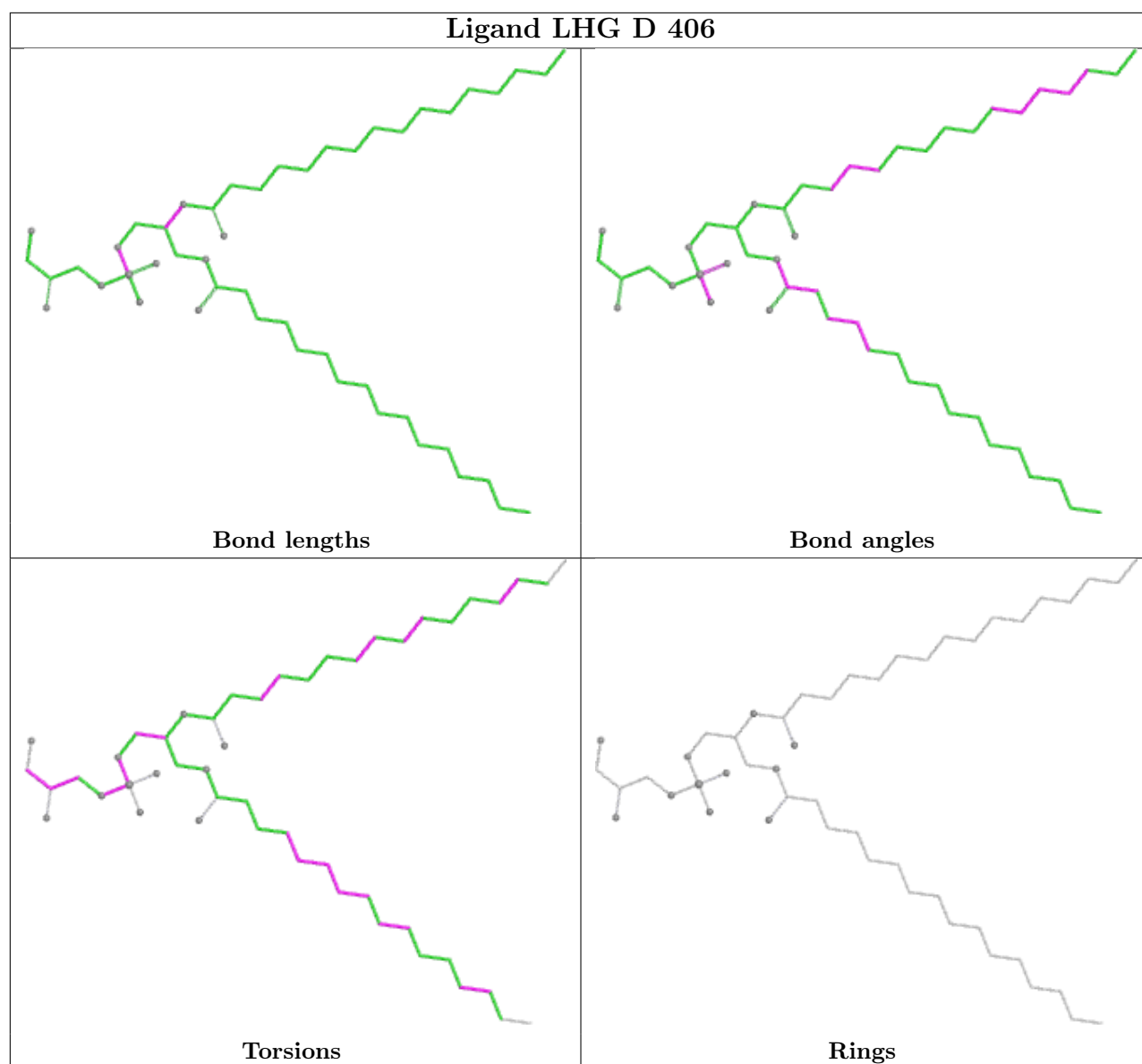


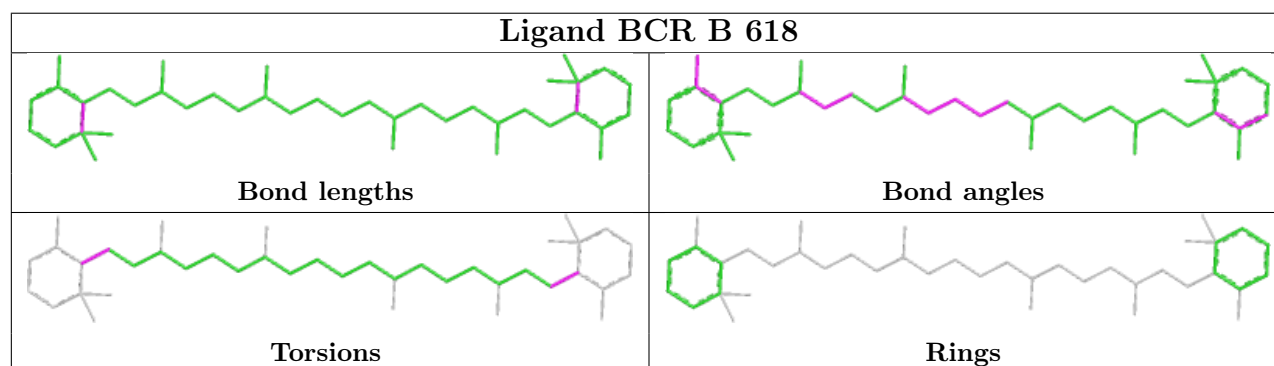
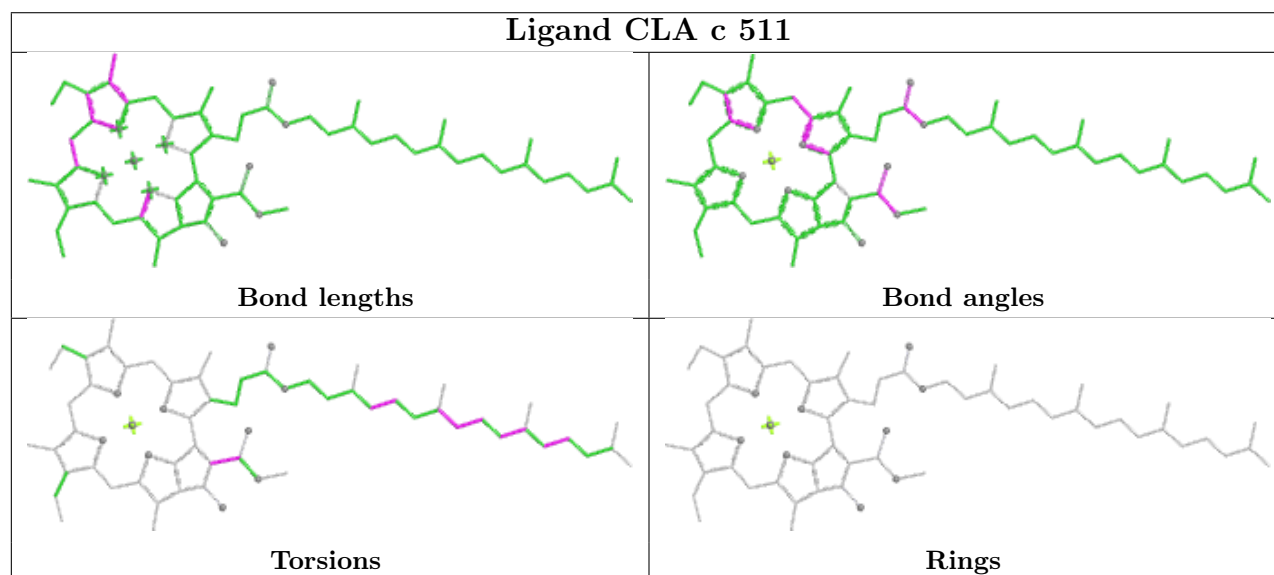
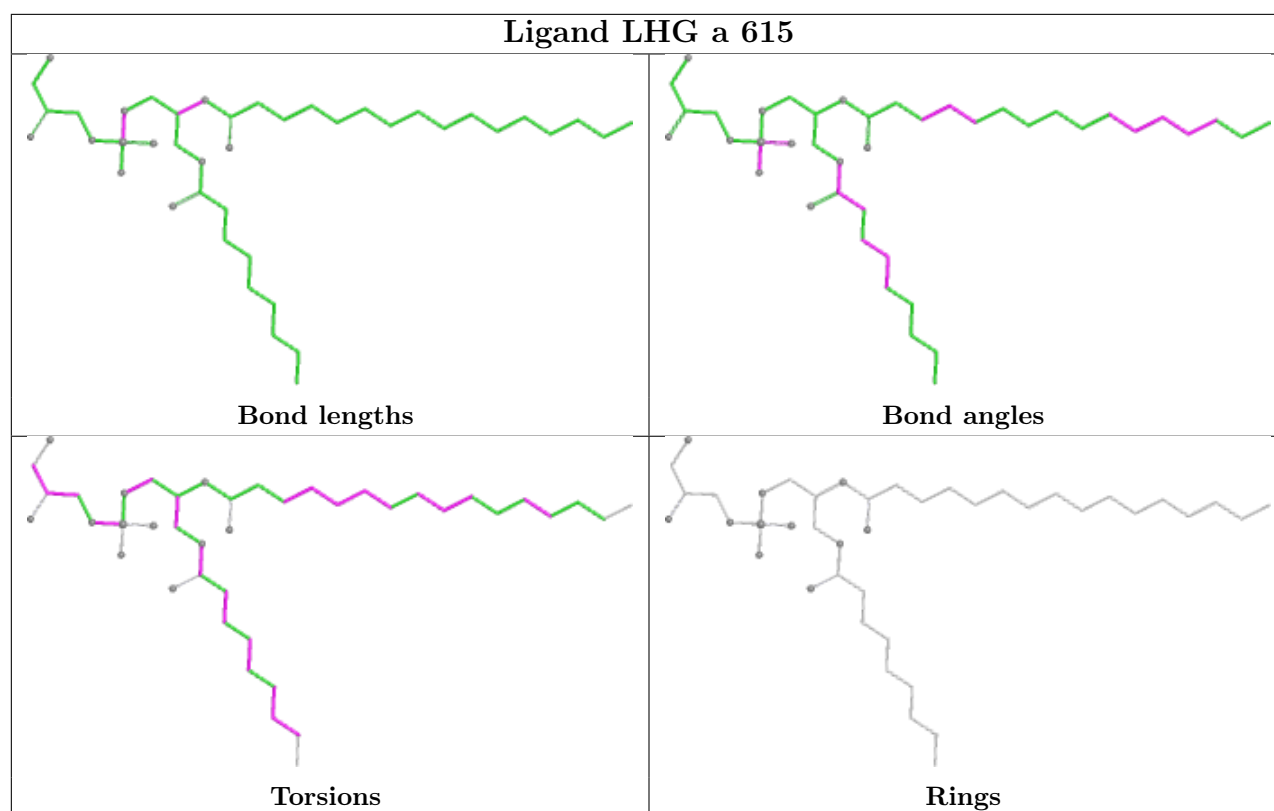




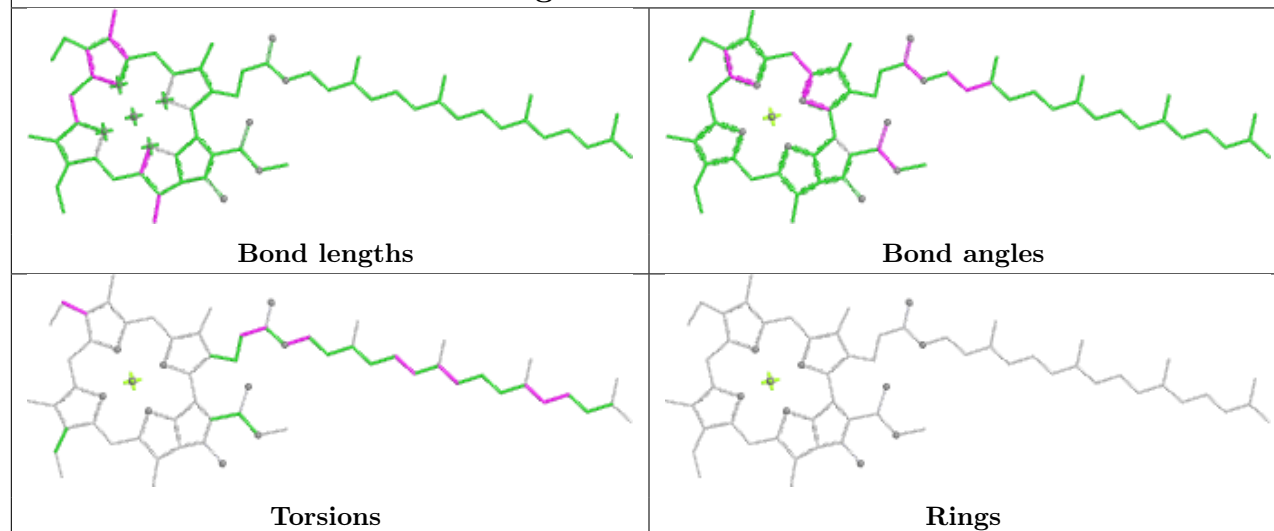




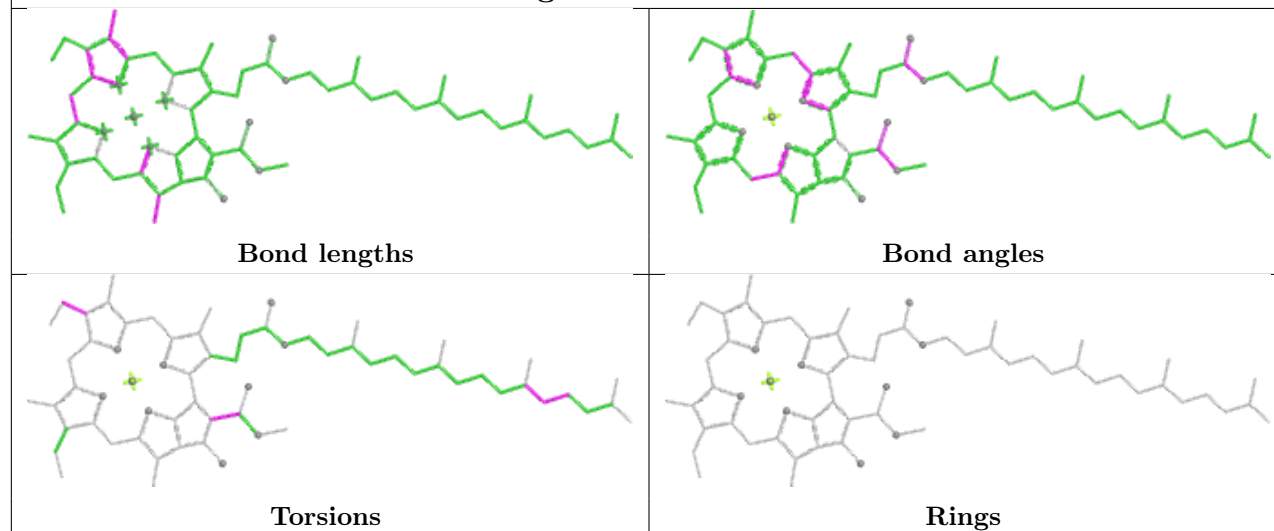




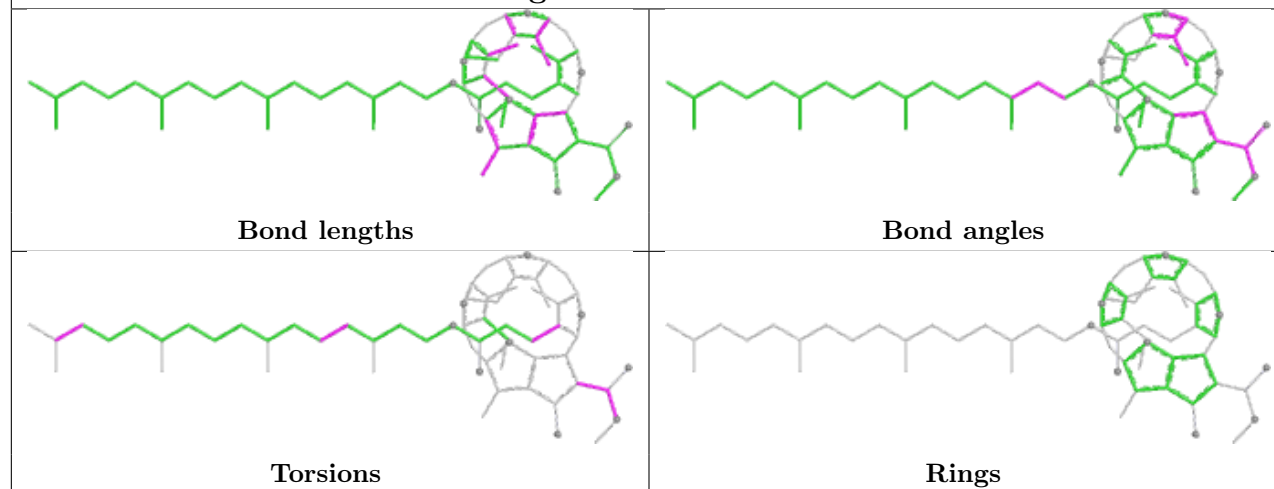
Ligand CLA b 616

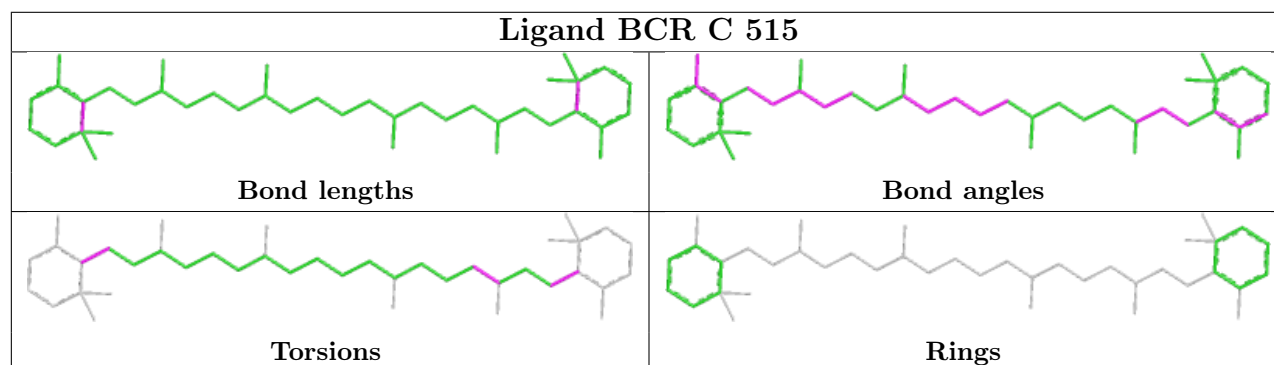
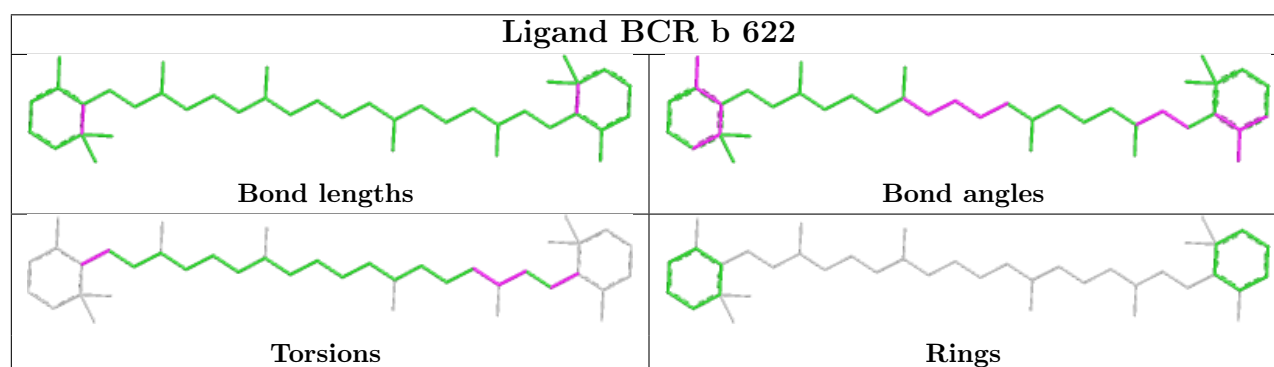
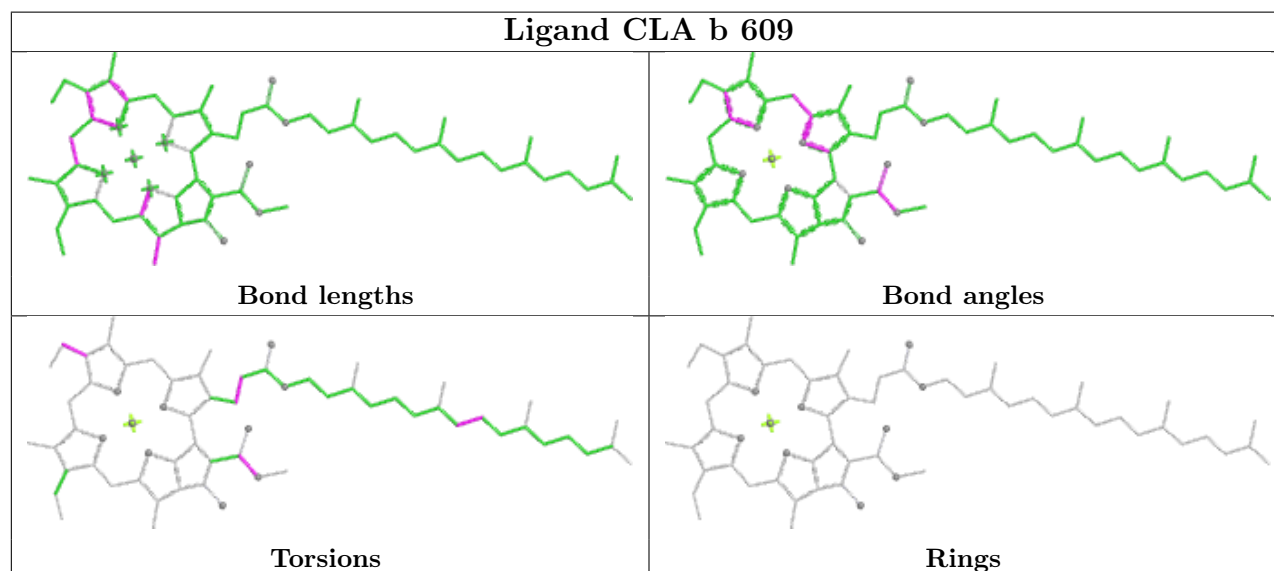
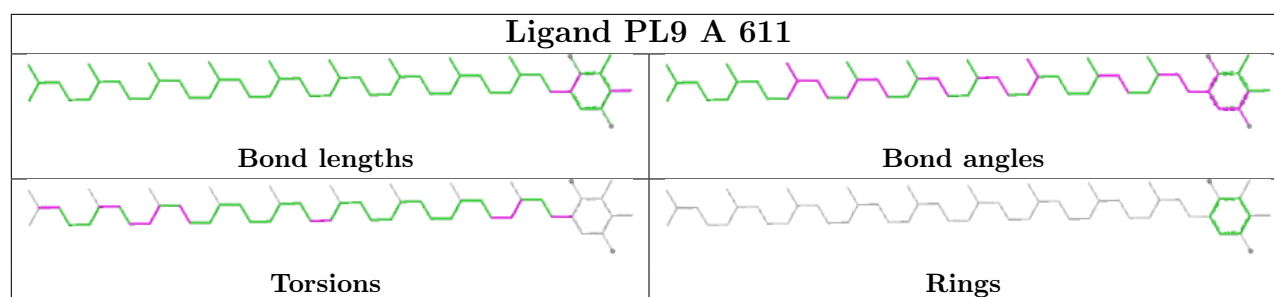


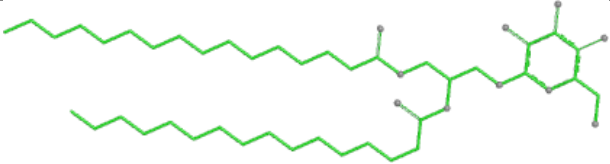
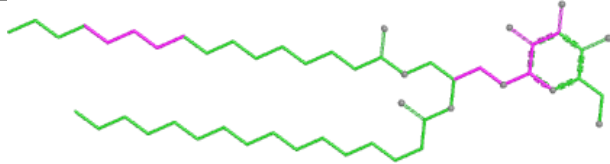
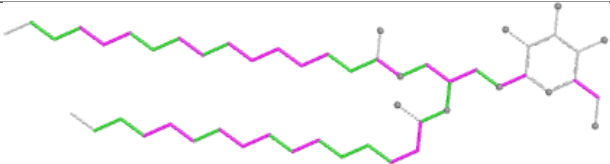
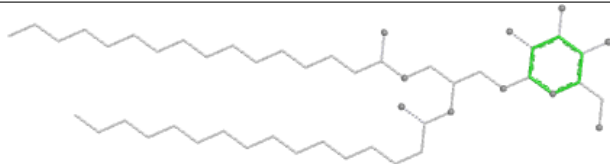
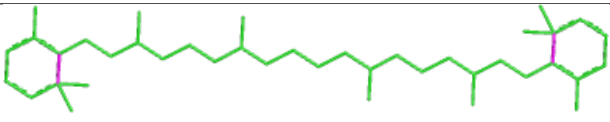
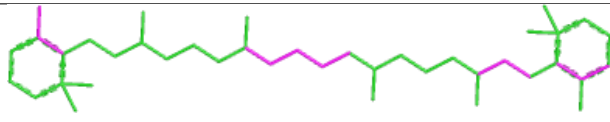
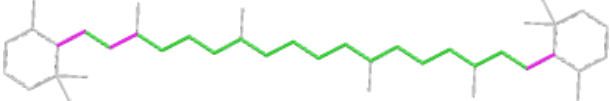
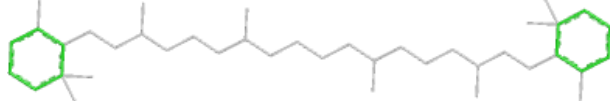
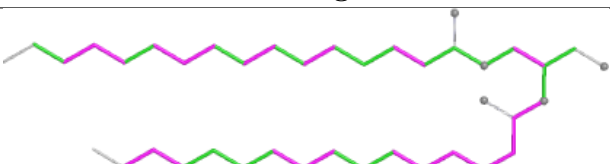
Ligand CLA c 506



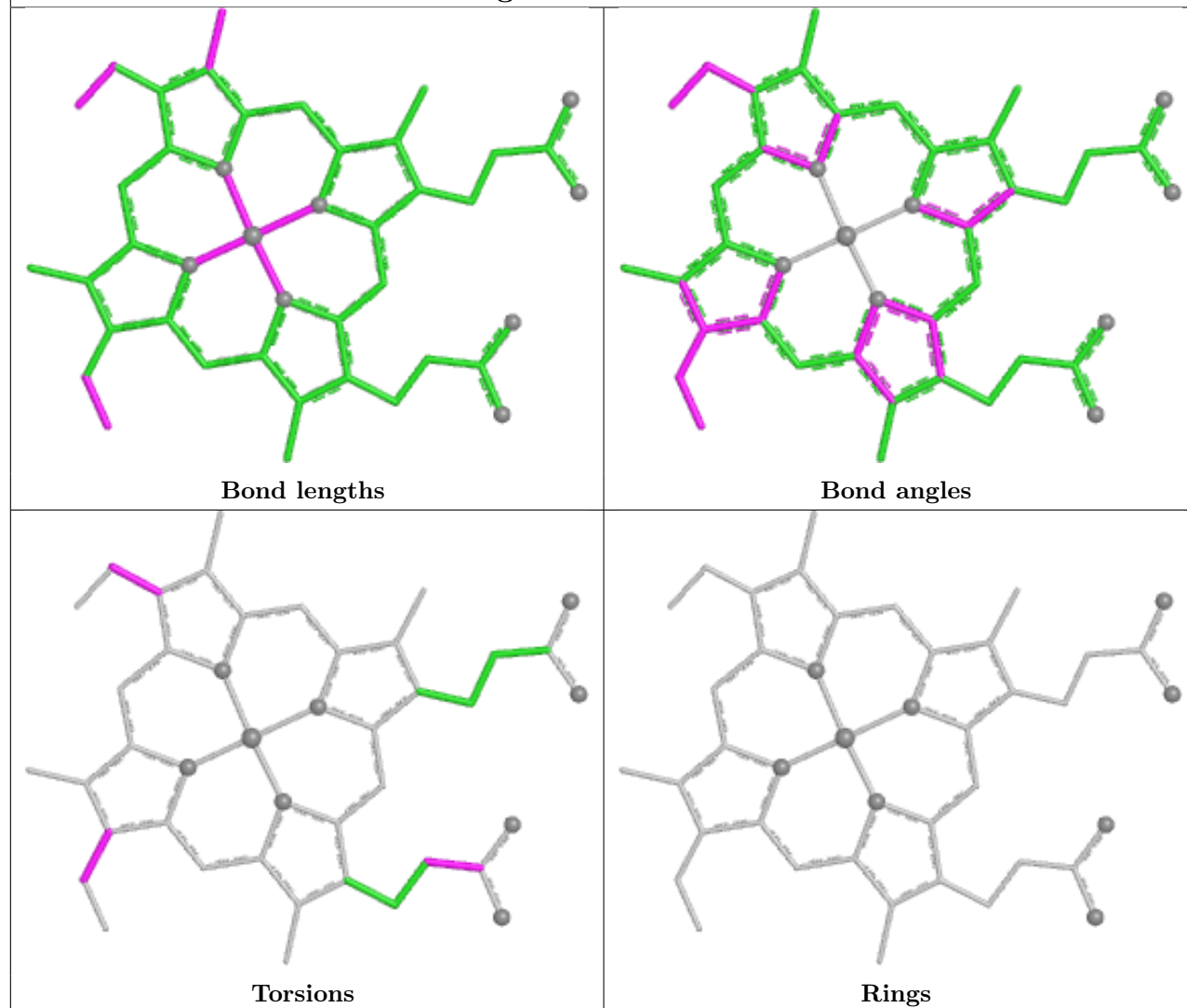
Ligand PHO D 401



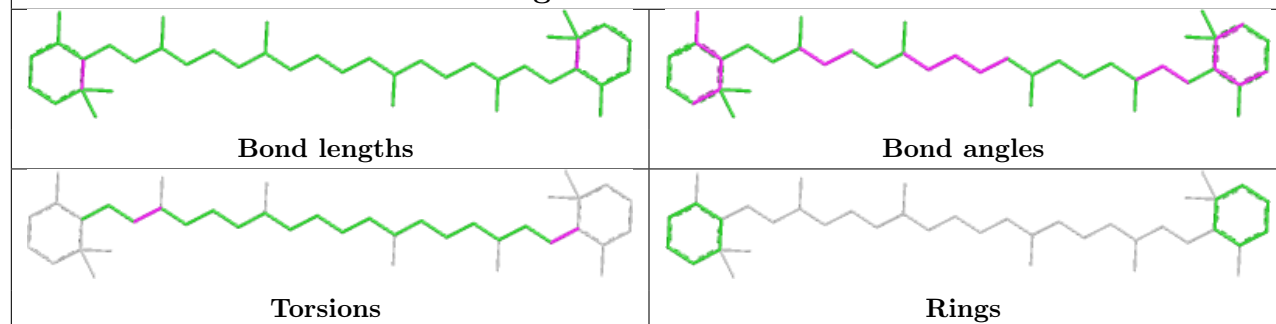


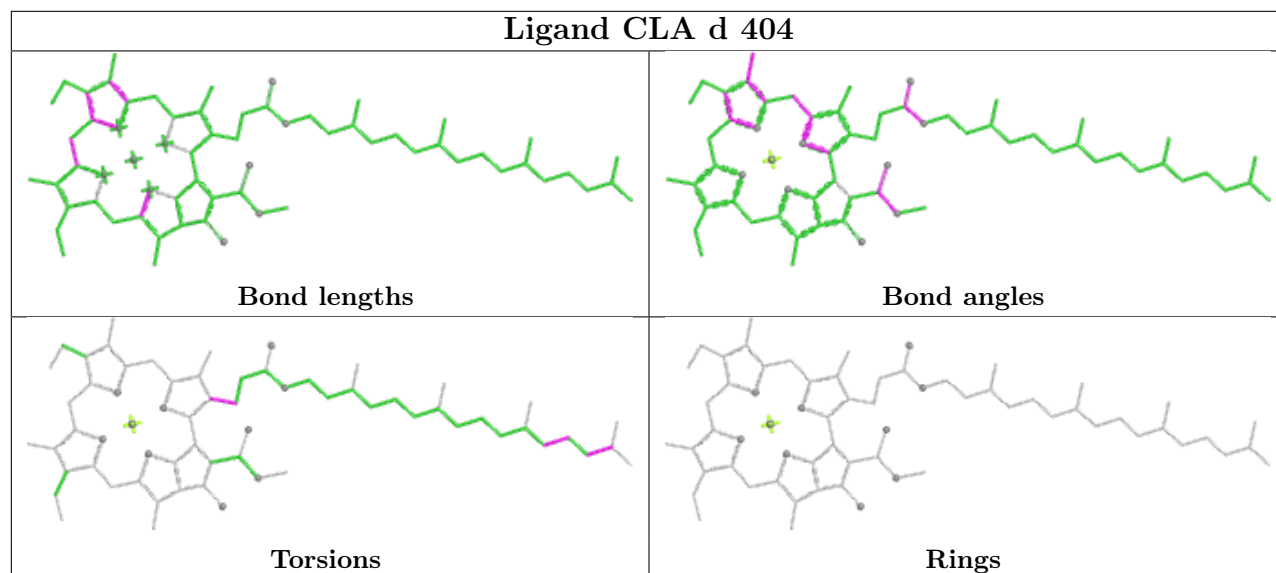
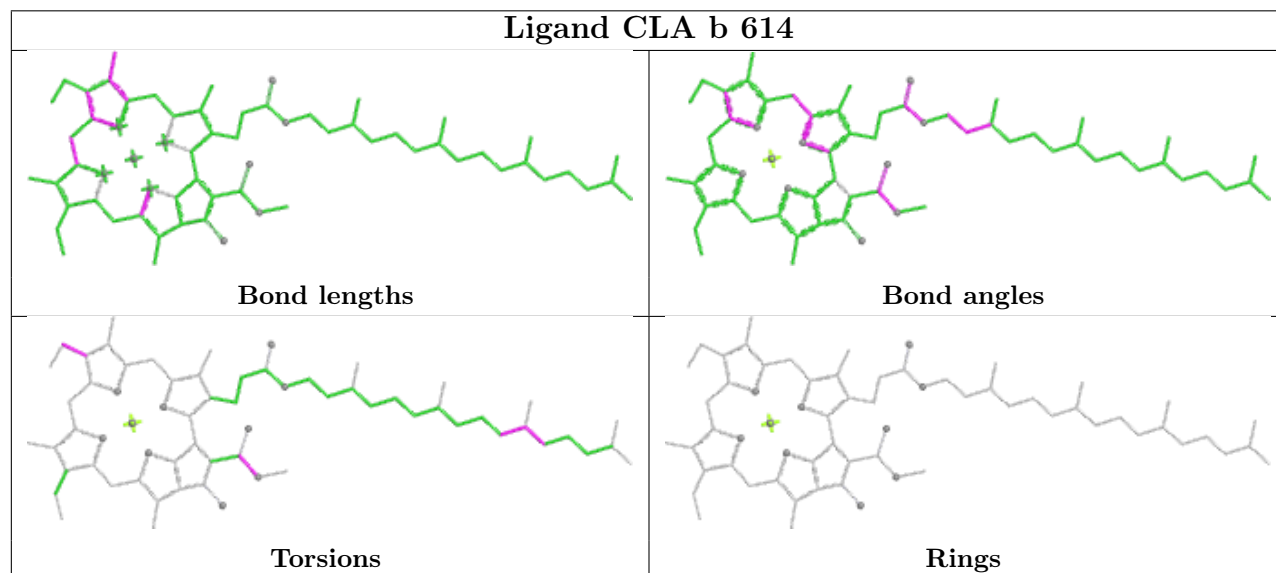
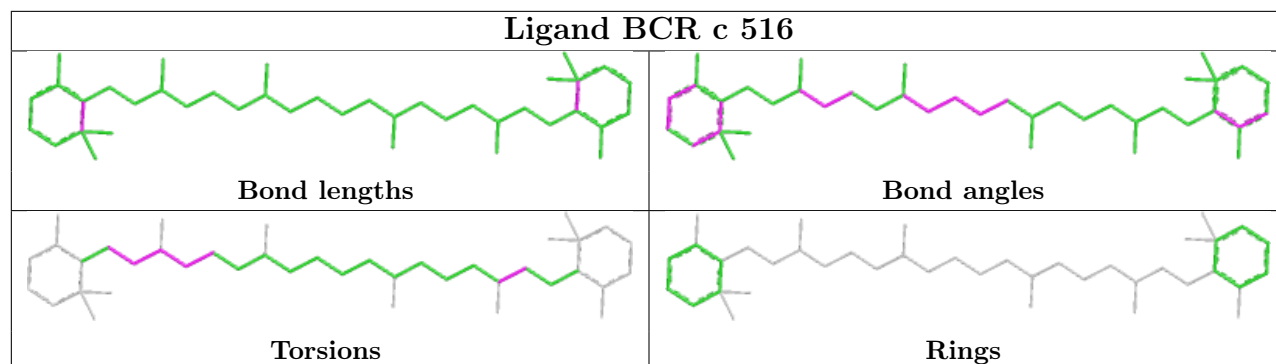
Ligand LMG c 521	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR a 610	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG d 409	
 Bond lengths	 Bond angles
 Torsions	 Rings

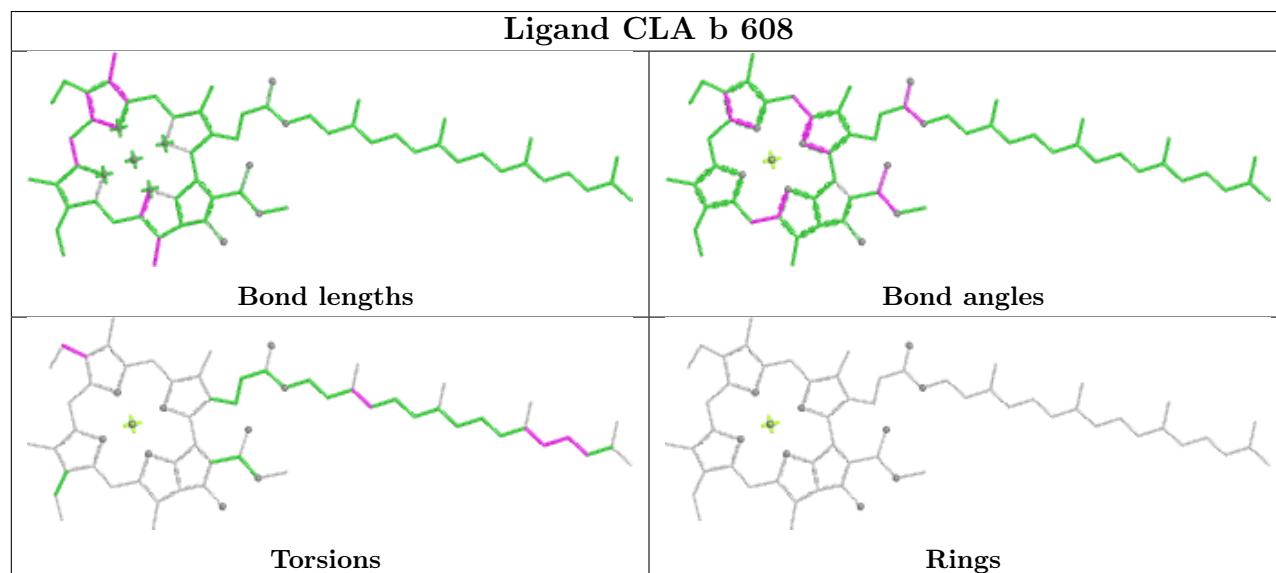
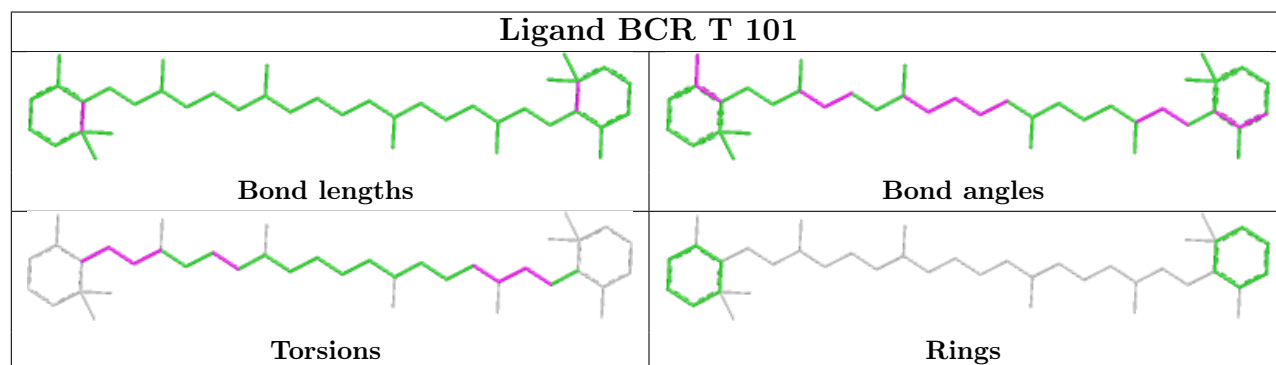
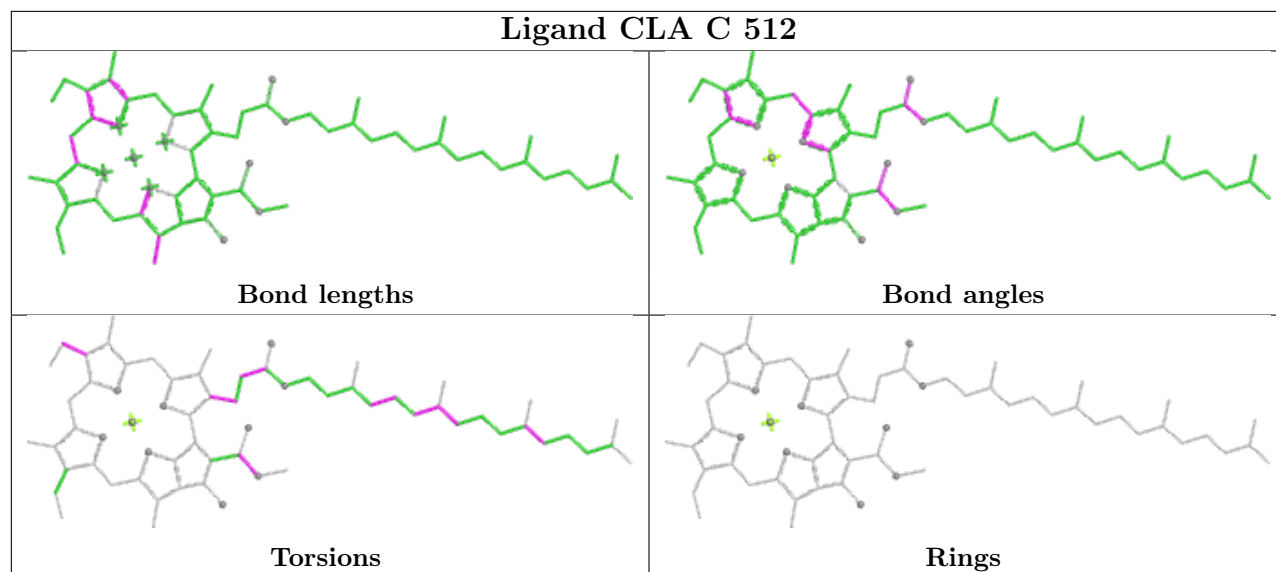
Ligand HEC v 201

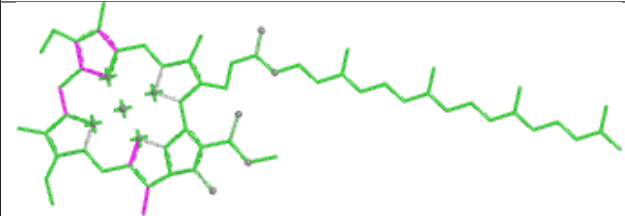
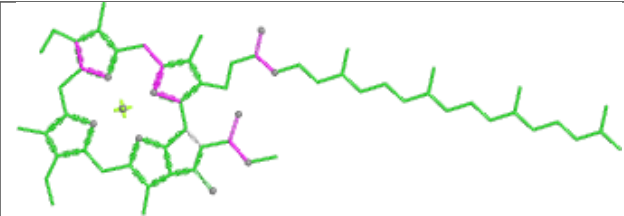
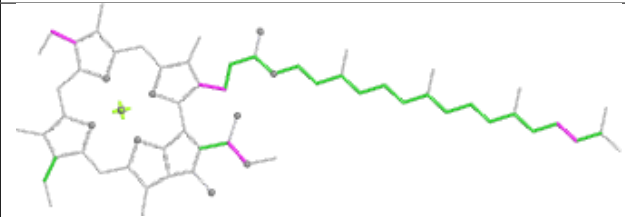
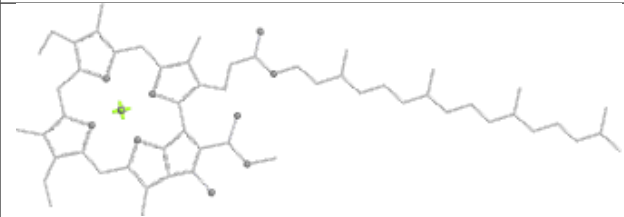


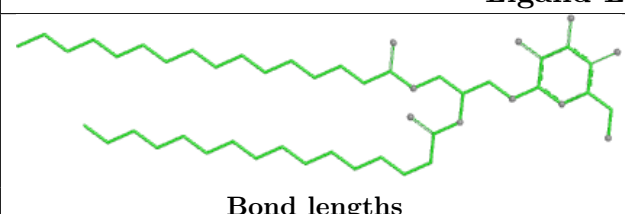
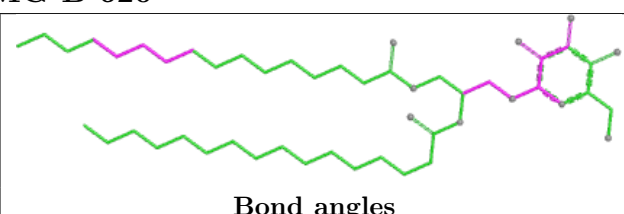
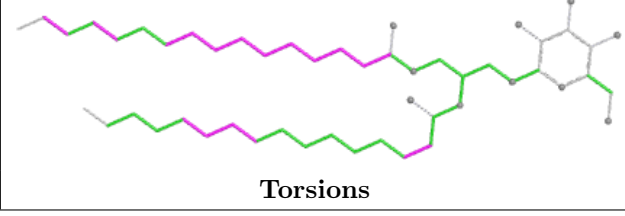
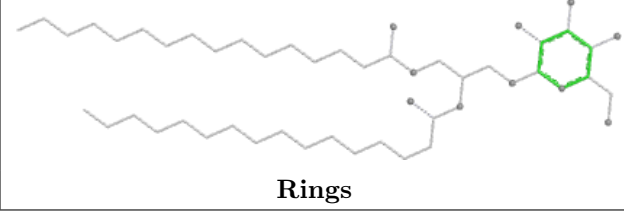
Ligand BCR h 101

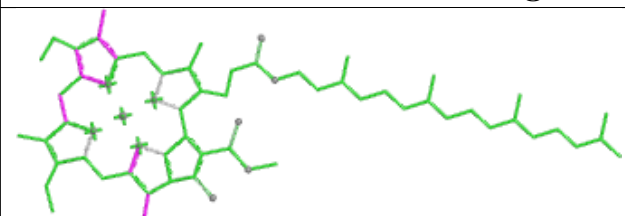
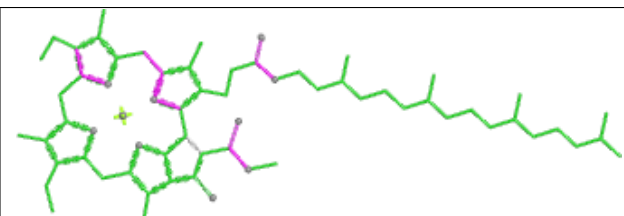
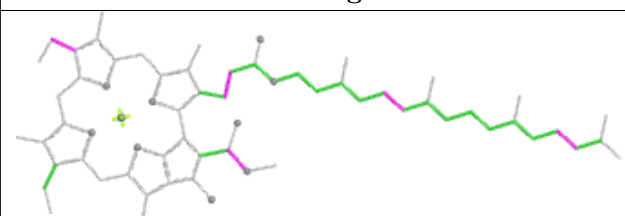
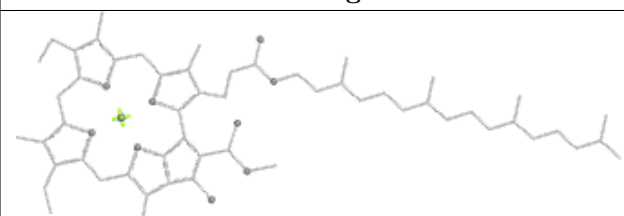




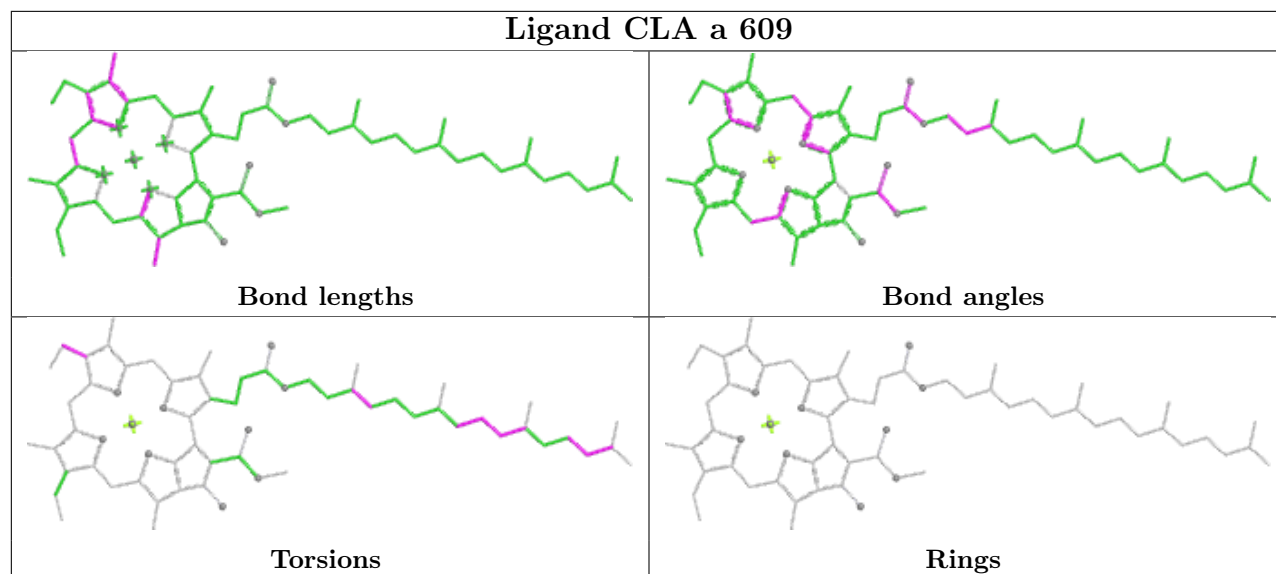


Ligand CLA c 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

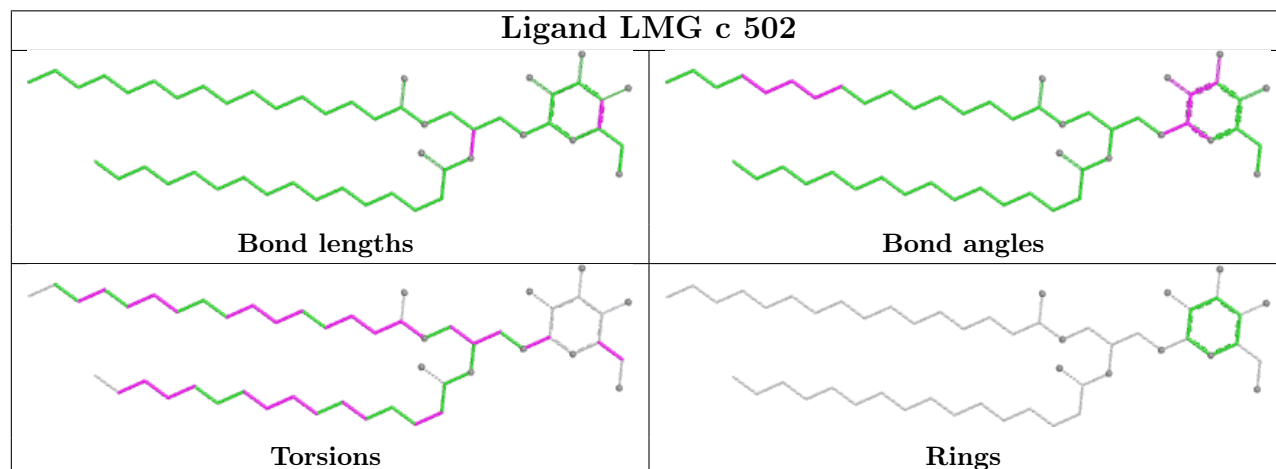
Ligand LMG B 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

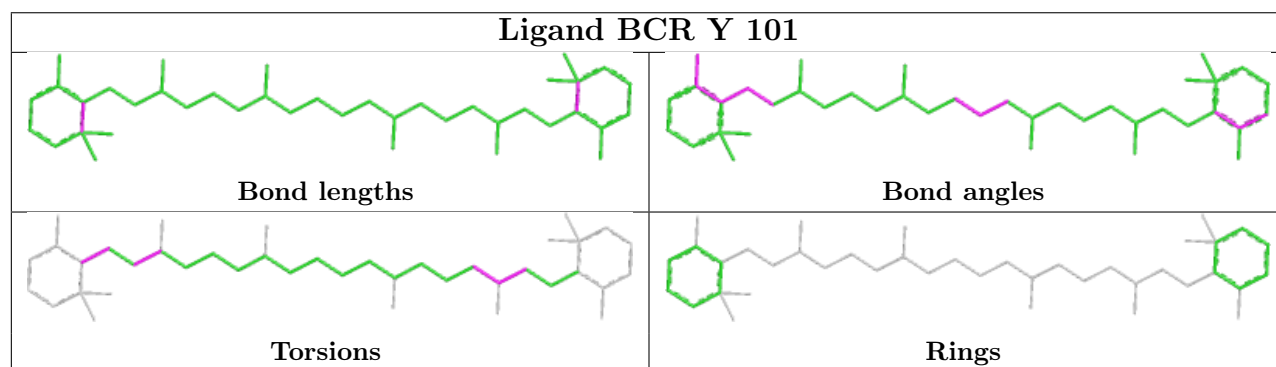
Ligand CLA a 609



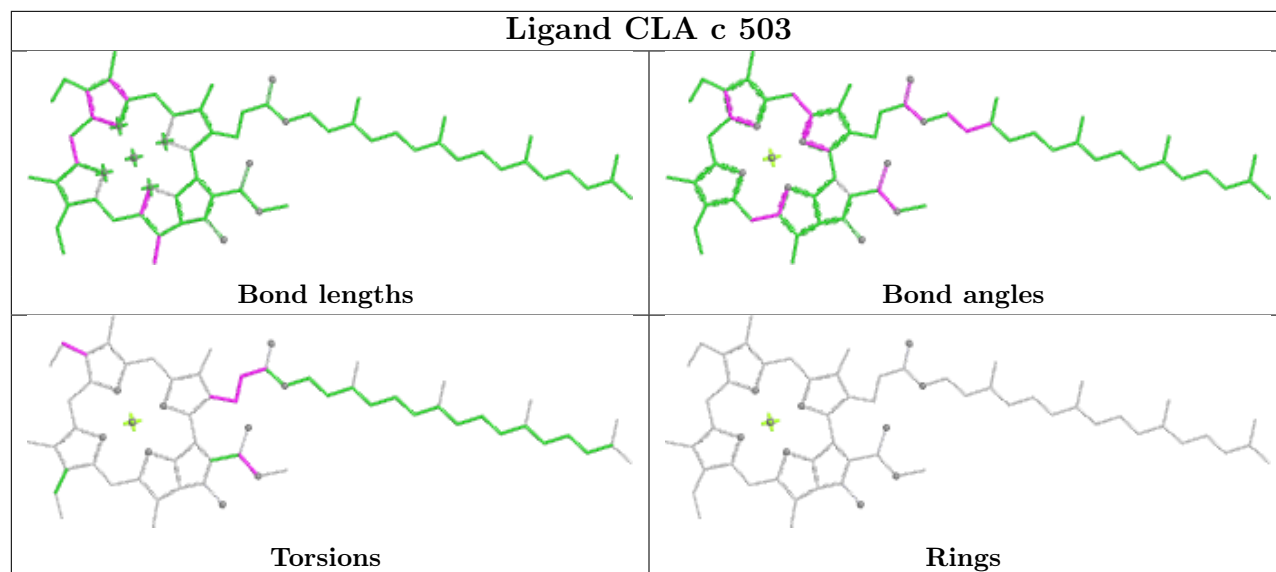
Ligand LMG c 502



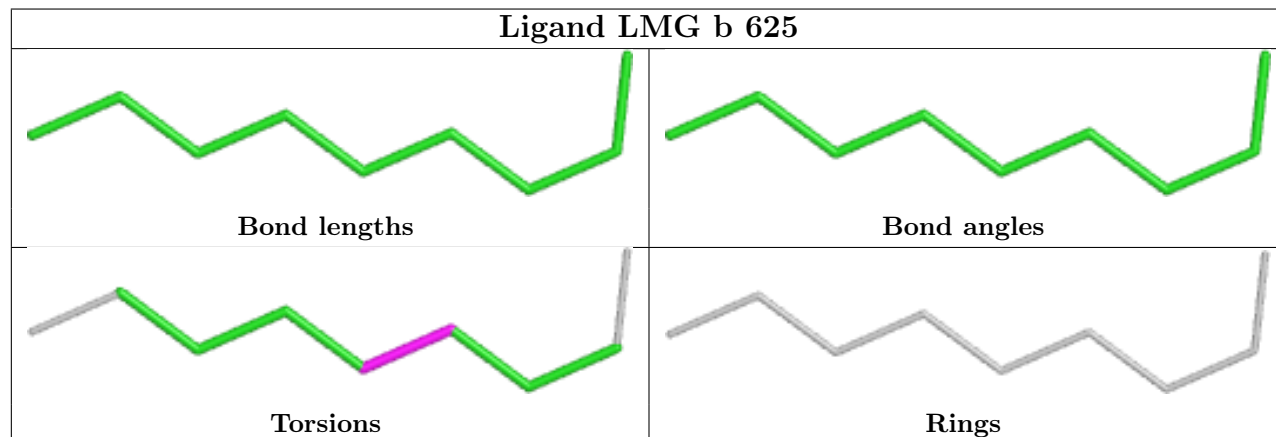
Ligand BCR Y 101



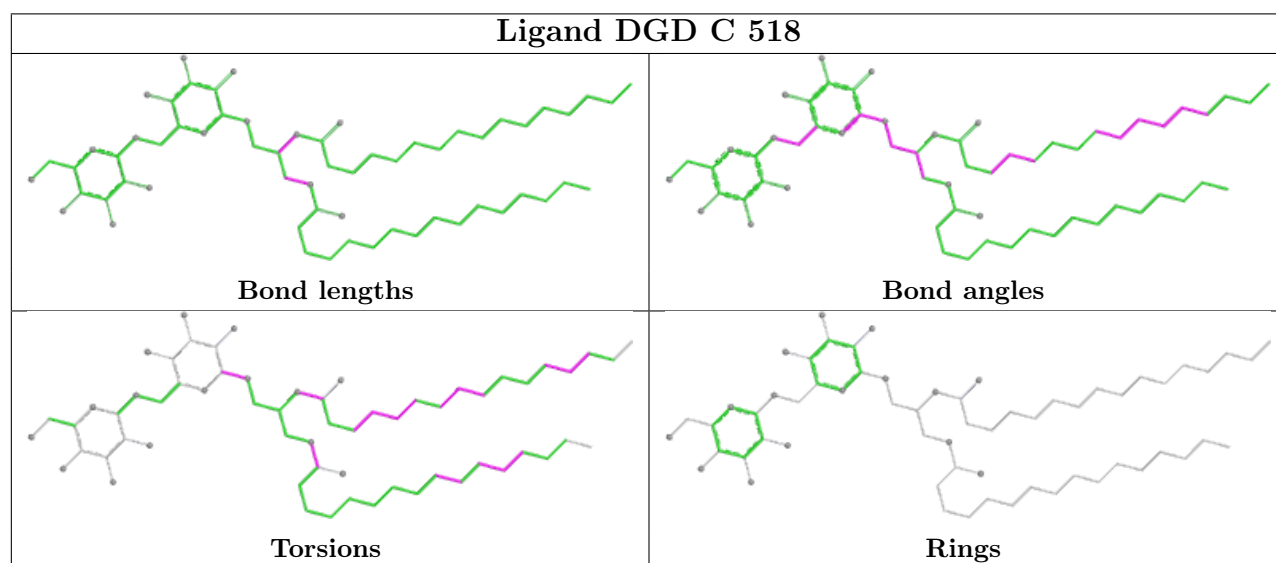
Ligand CLA c 503



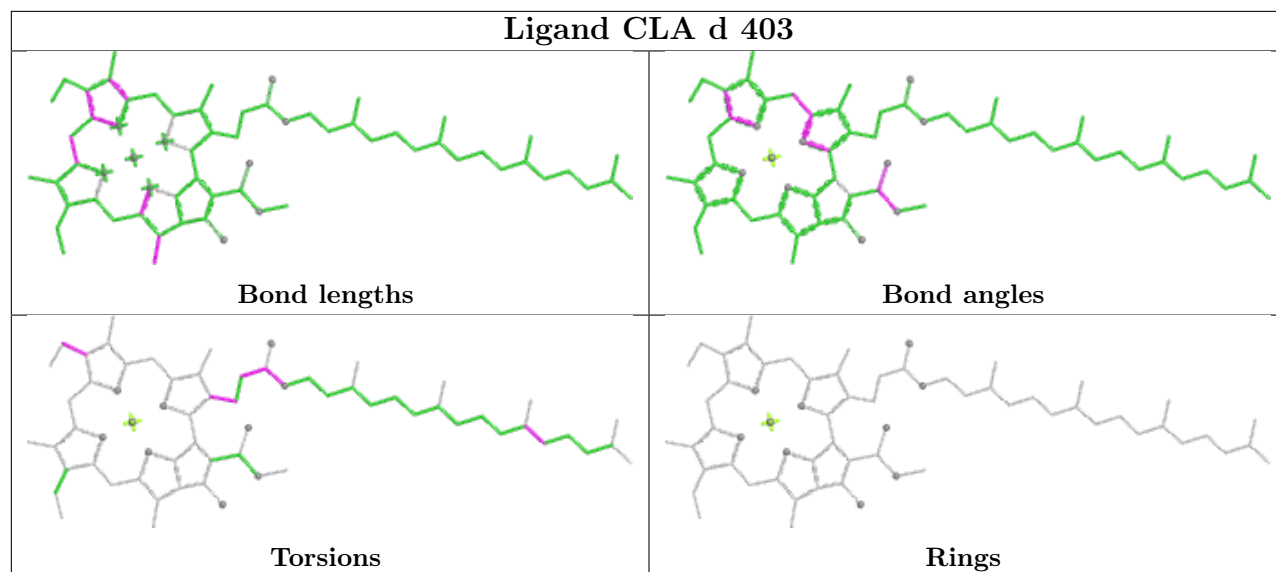
Ligand LMG b 625



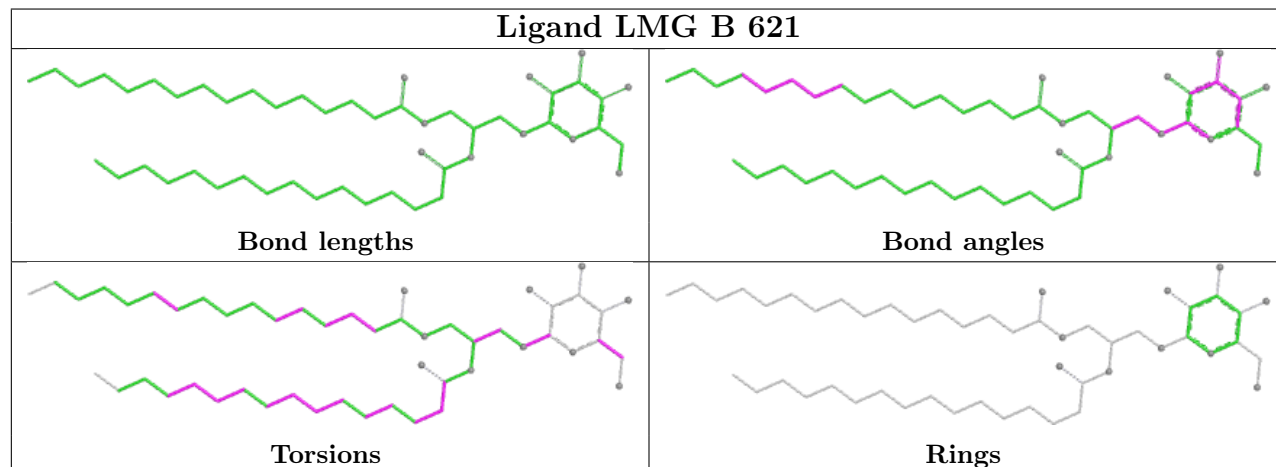
Ligand DGD C 518



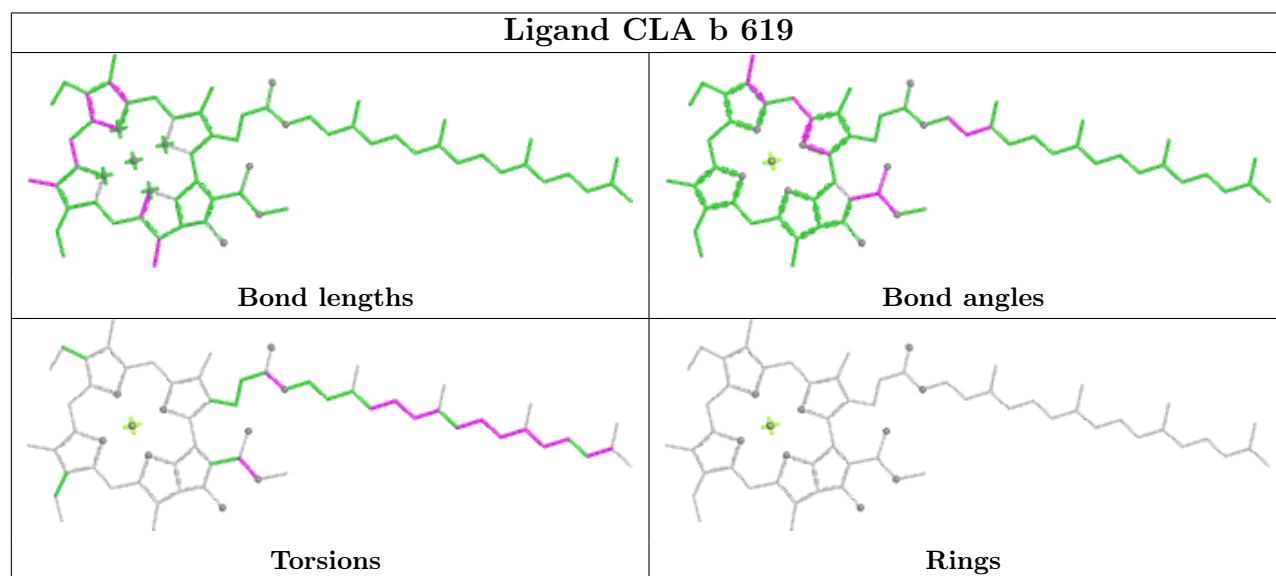
Ligand CLA d 403

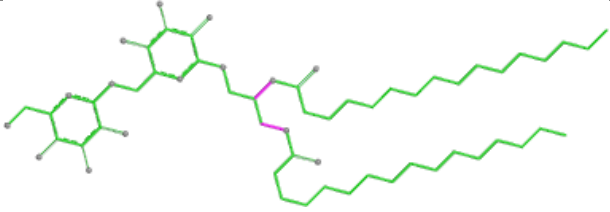
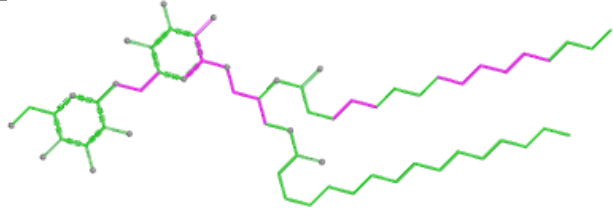
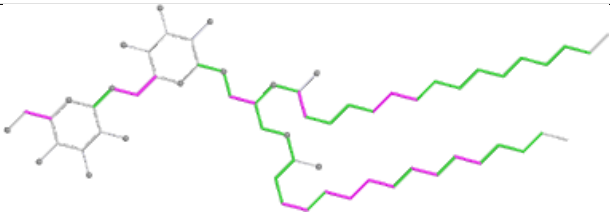
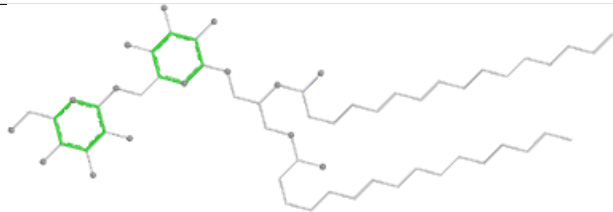
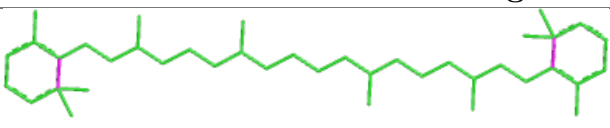
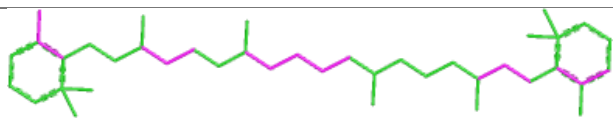
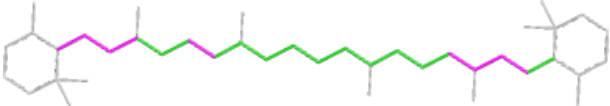
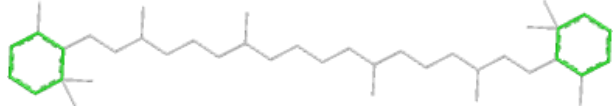
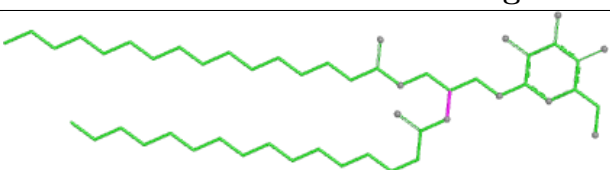
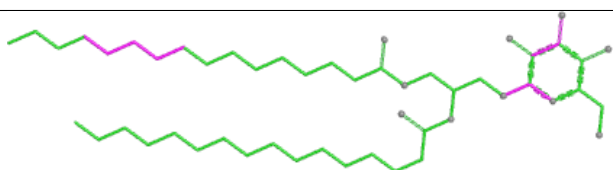
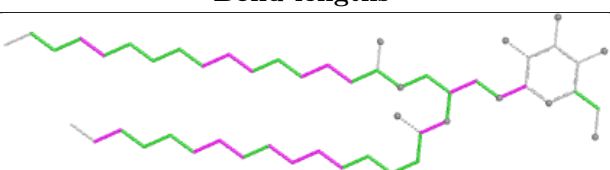
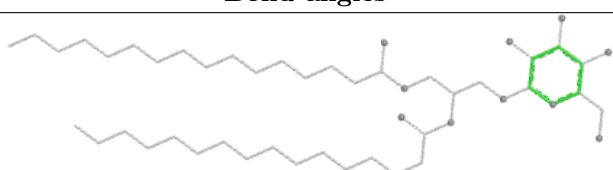


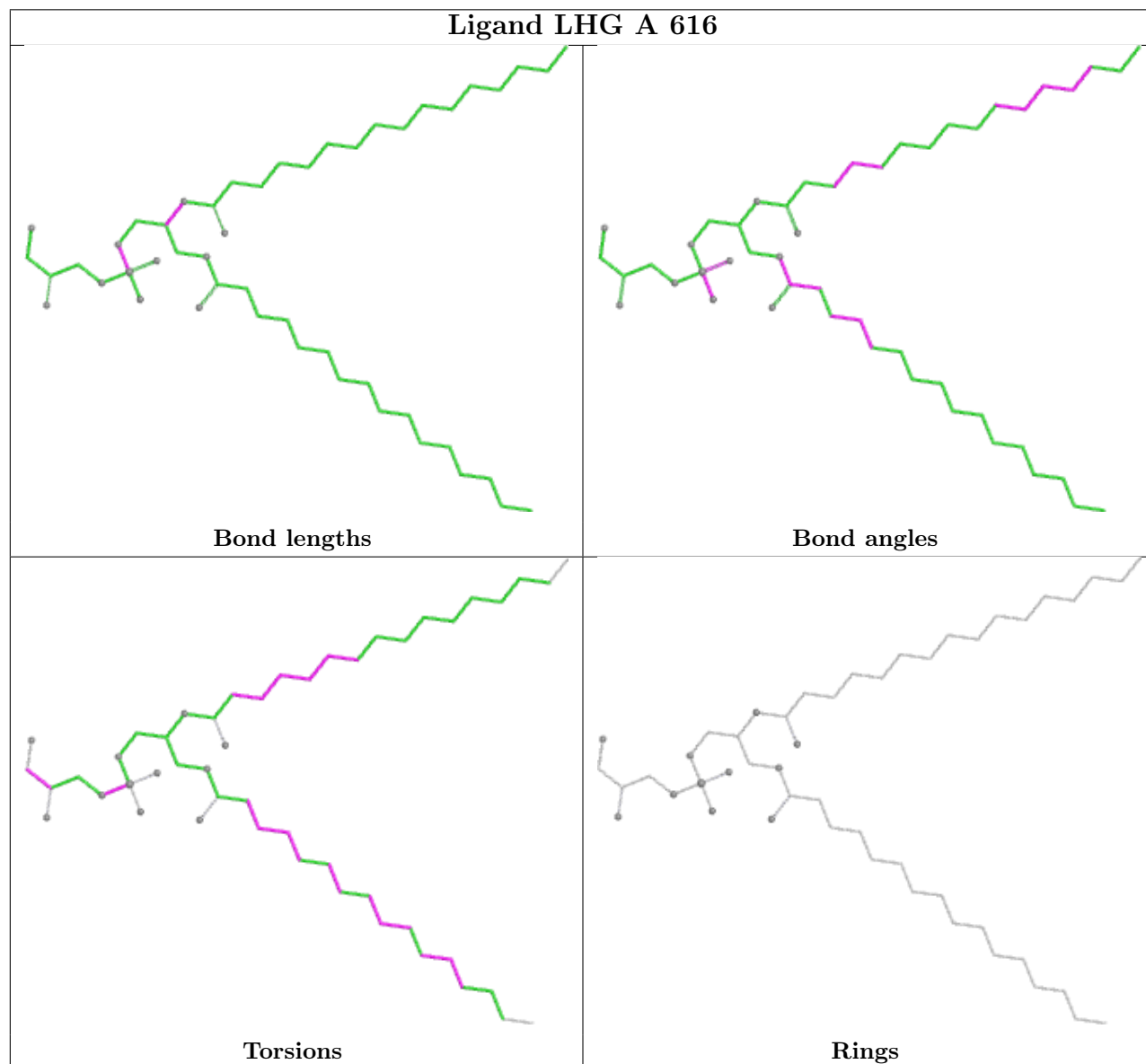
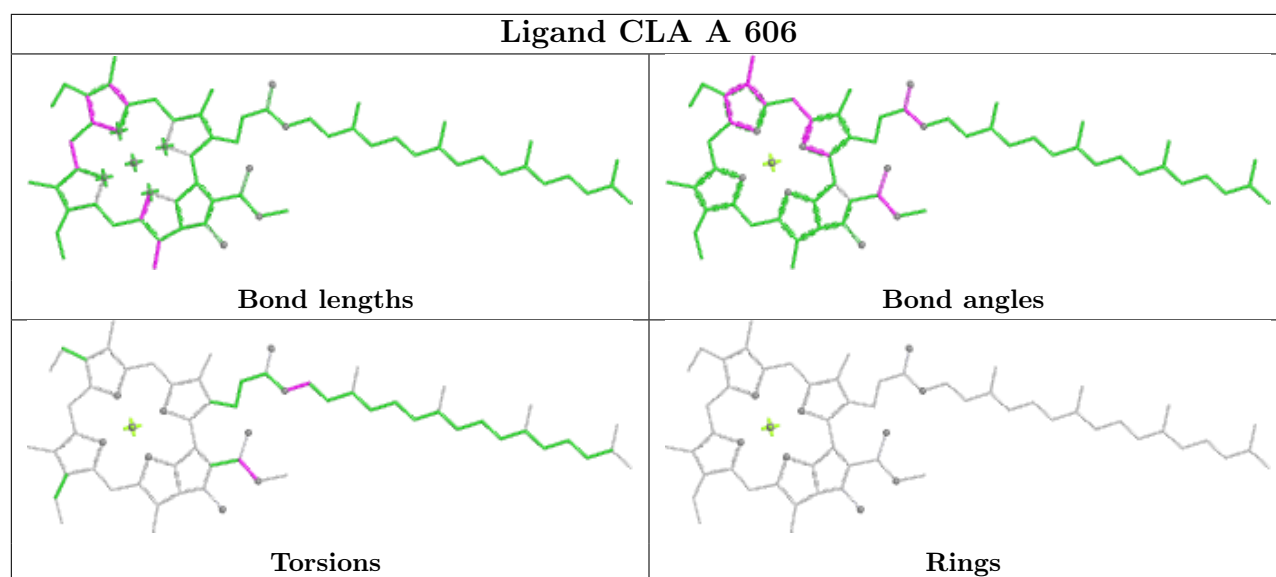
Ligand LMG B 621

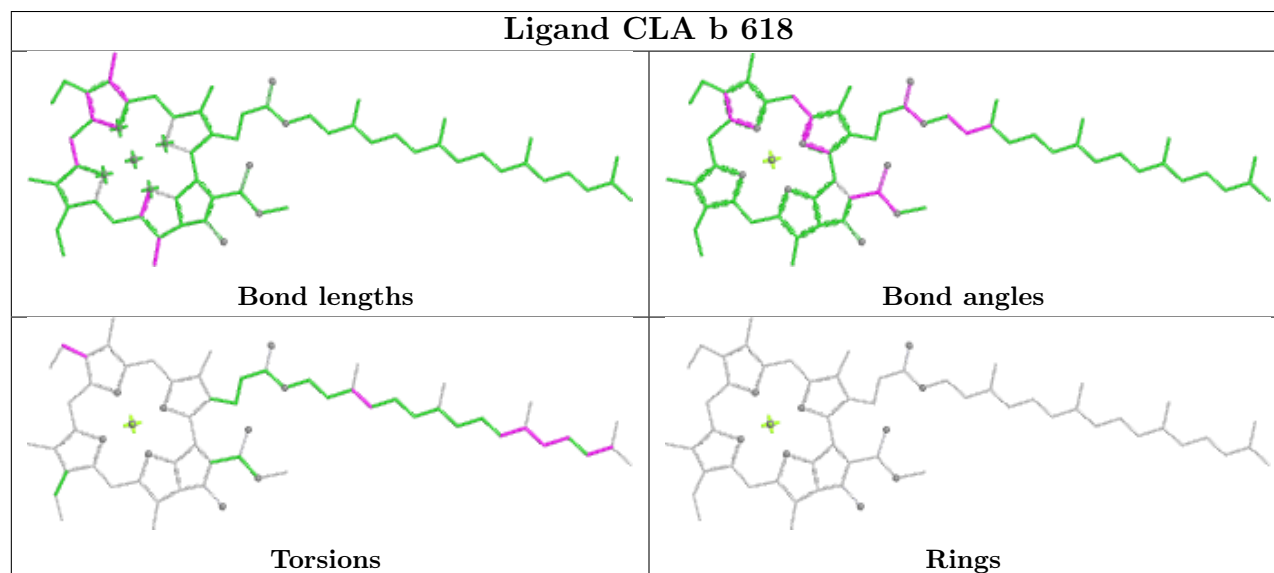
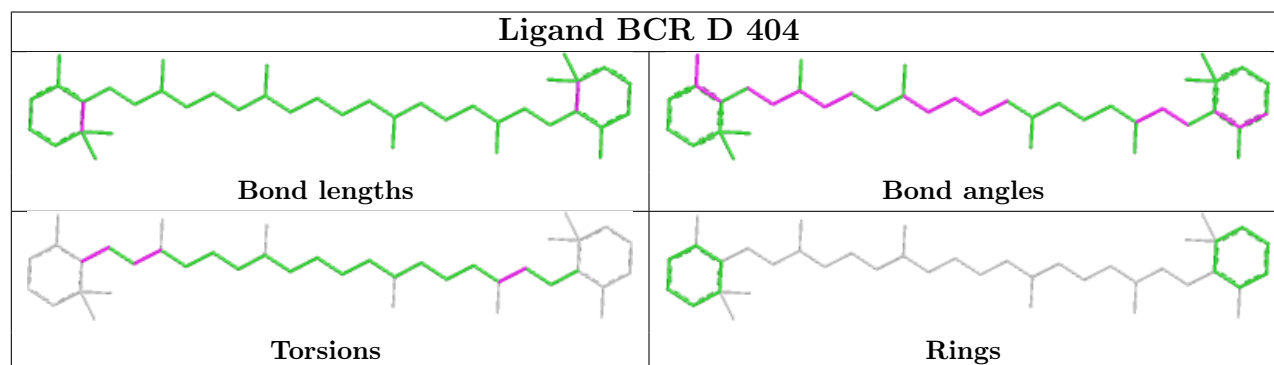
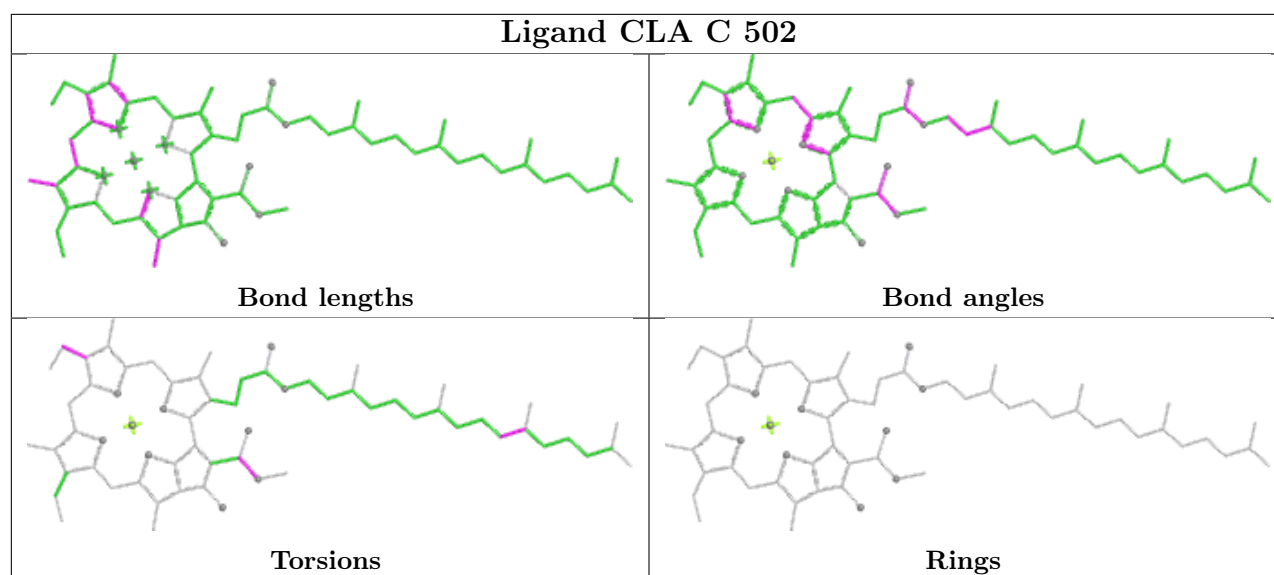


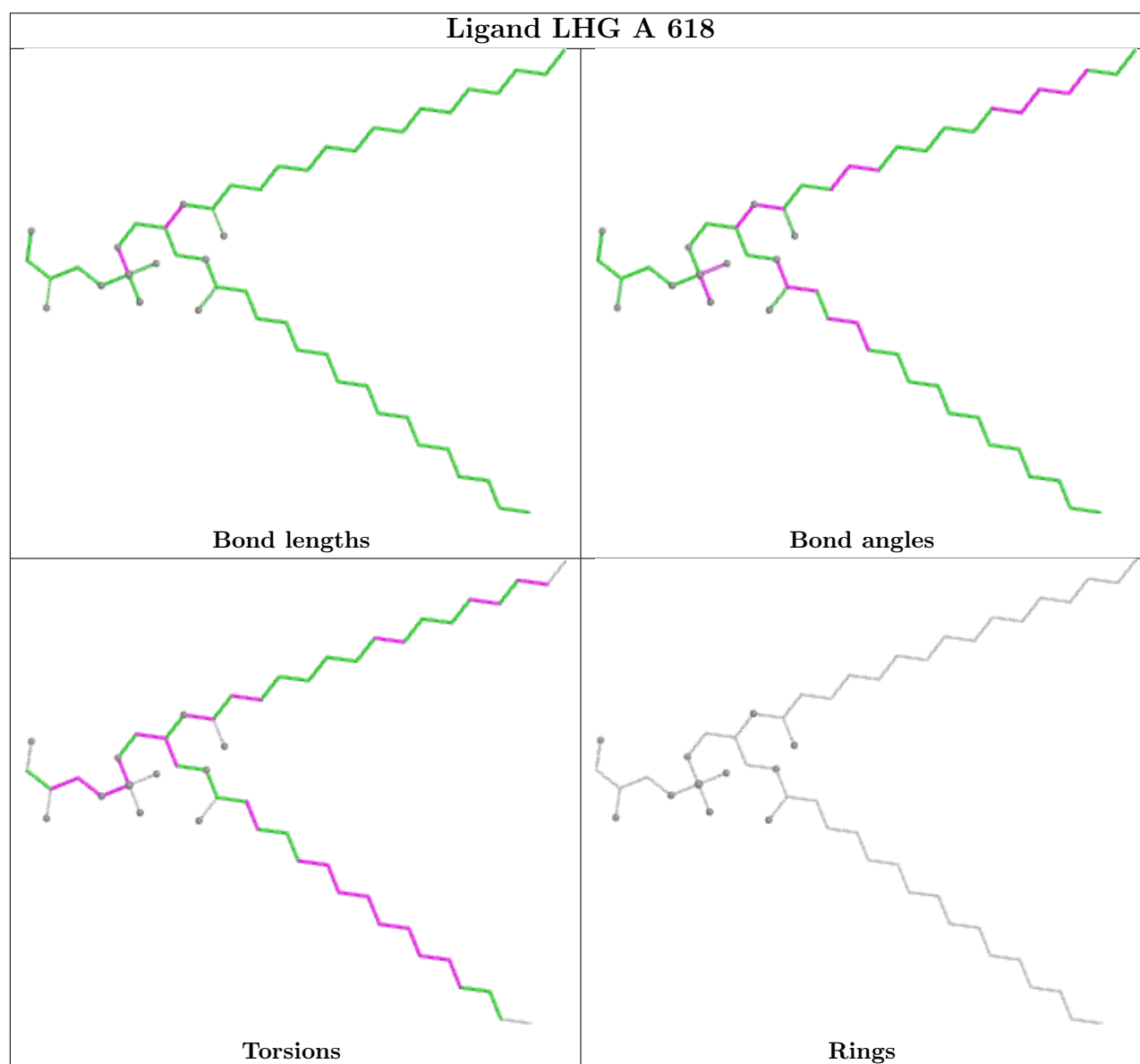
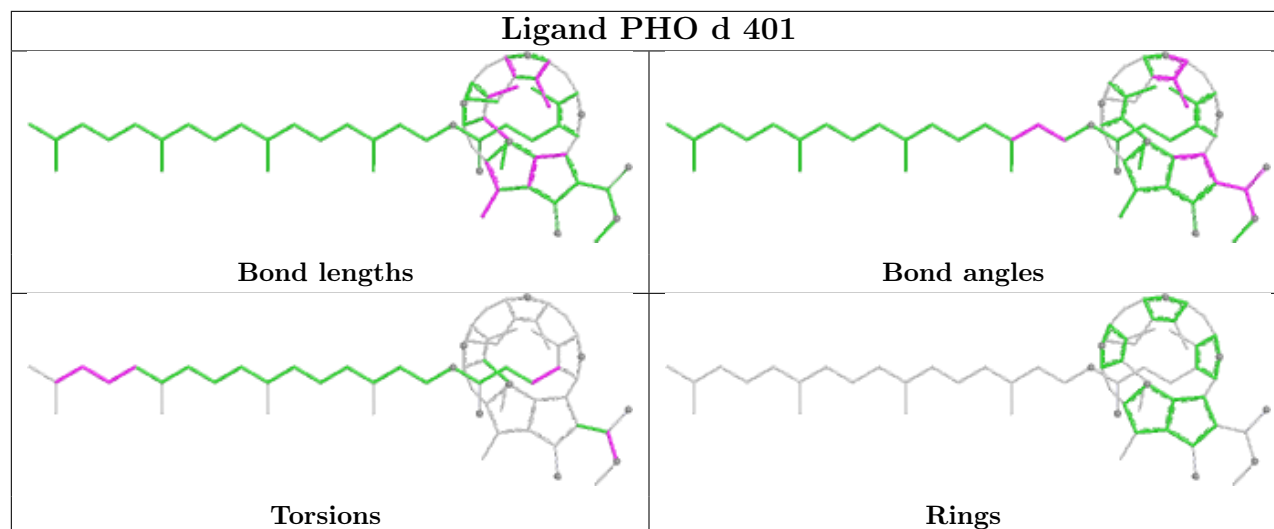
Ligand CLA b 619

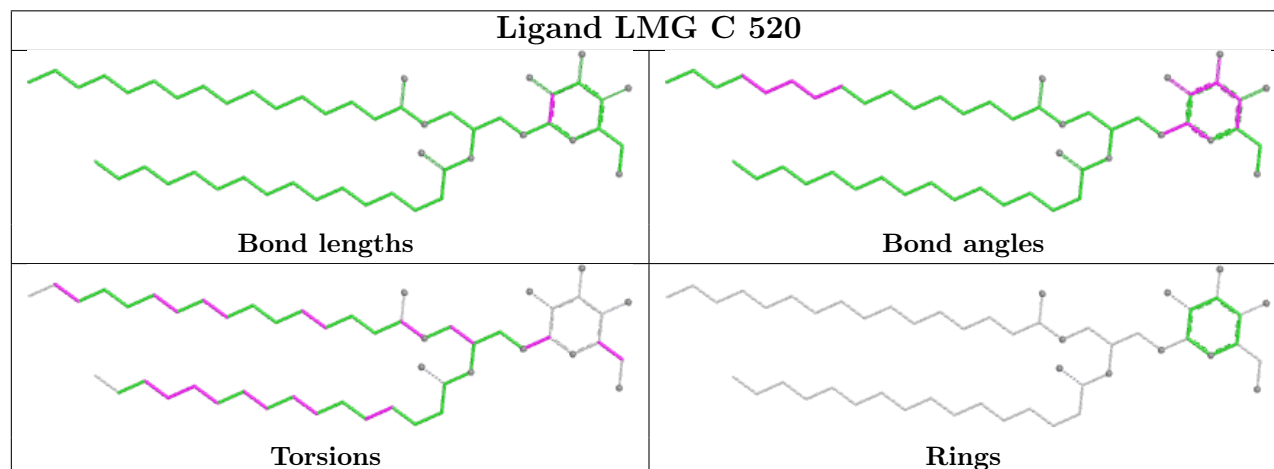
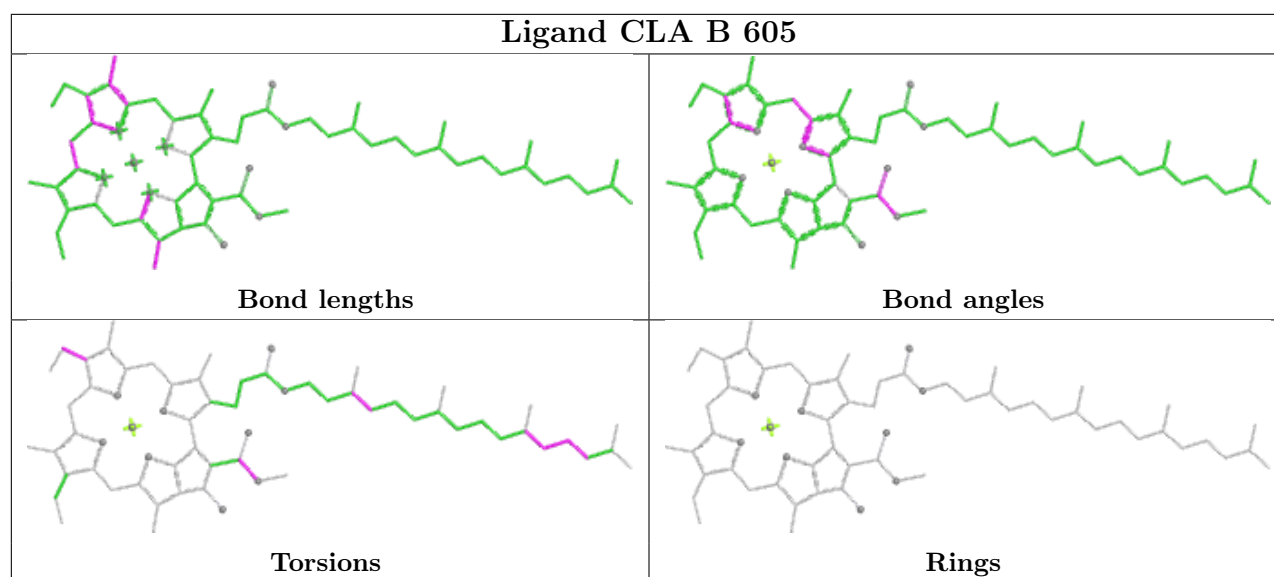


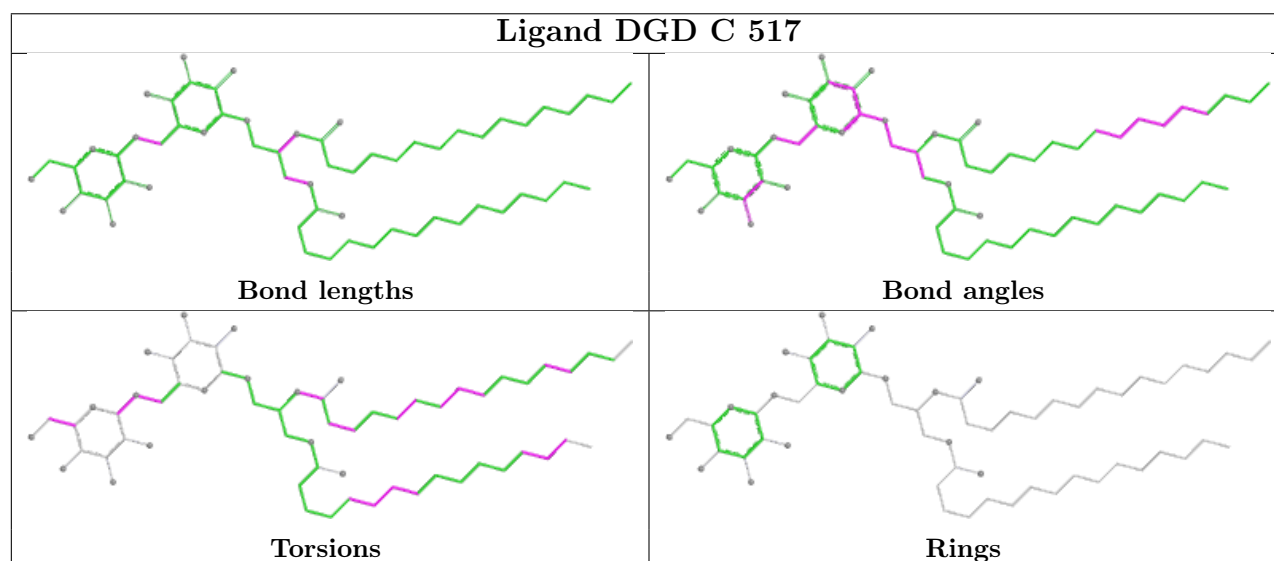
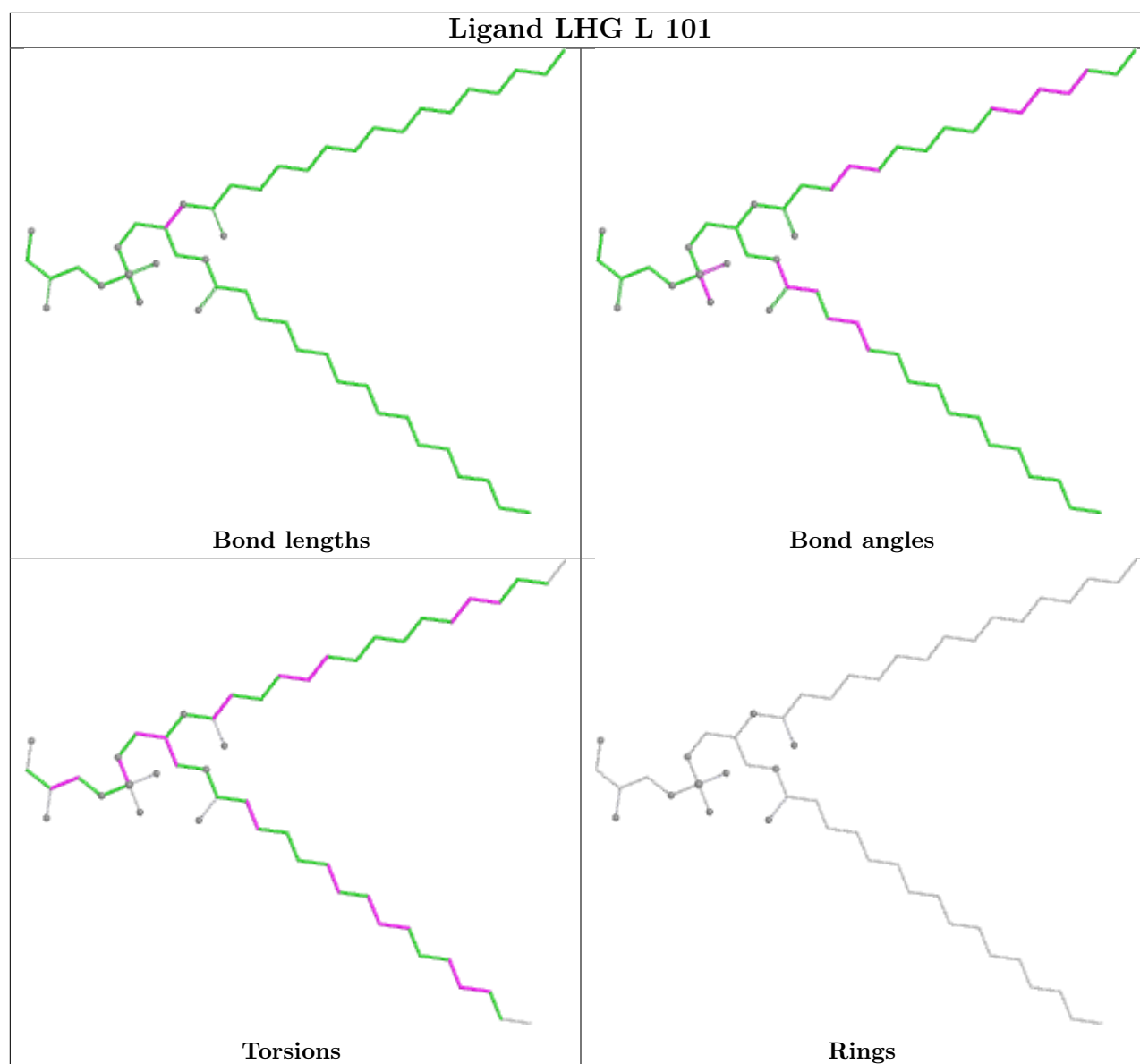
Ligand DGD c 518	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 627	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG A 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

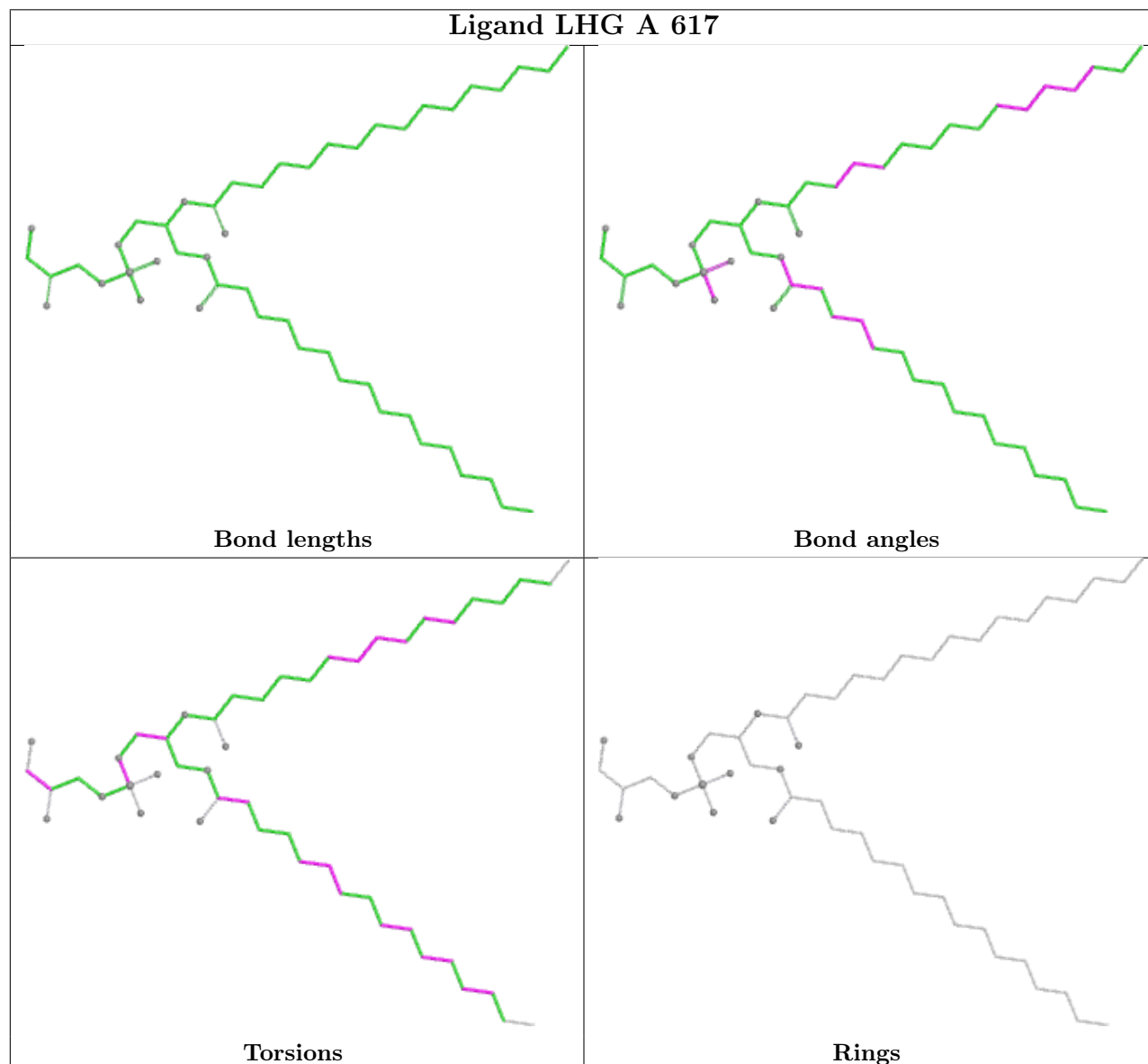
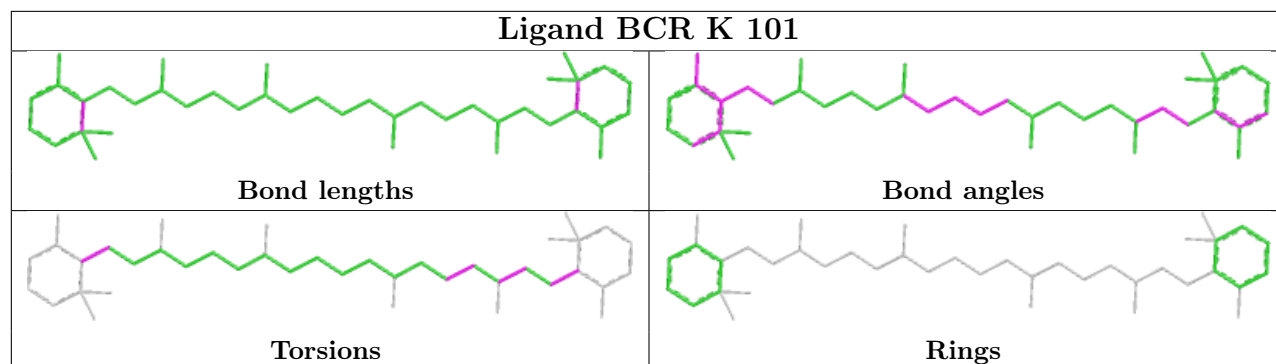




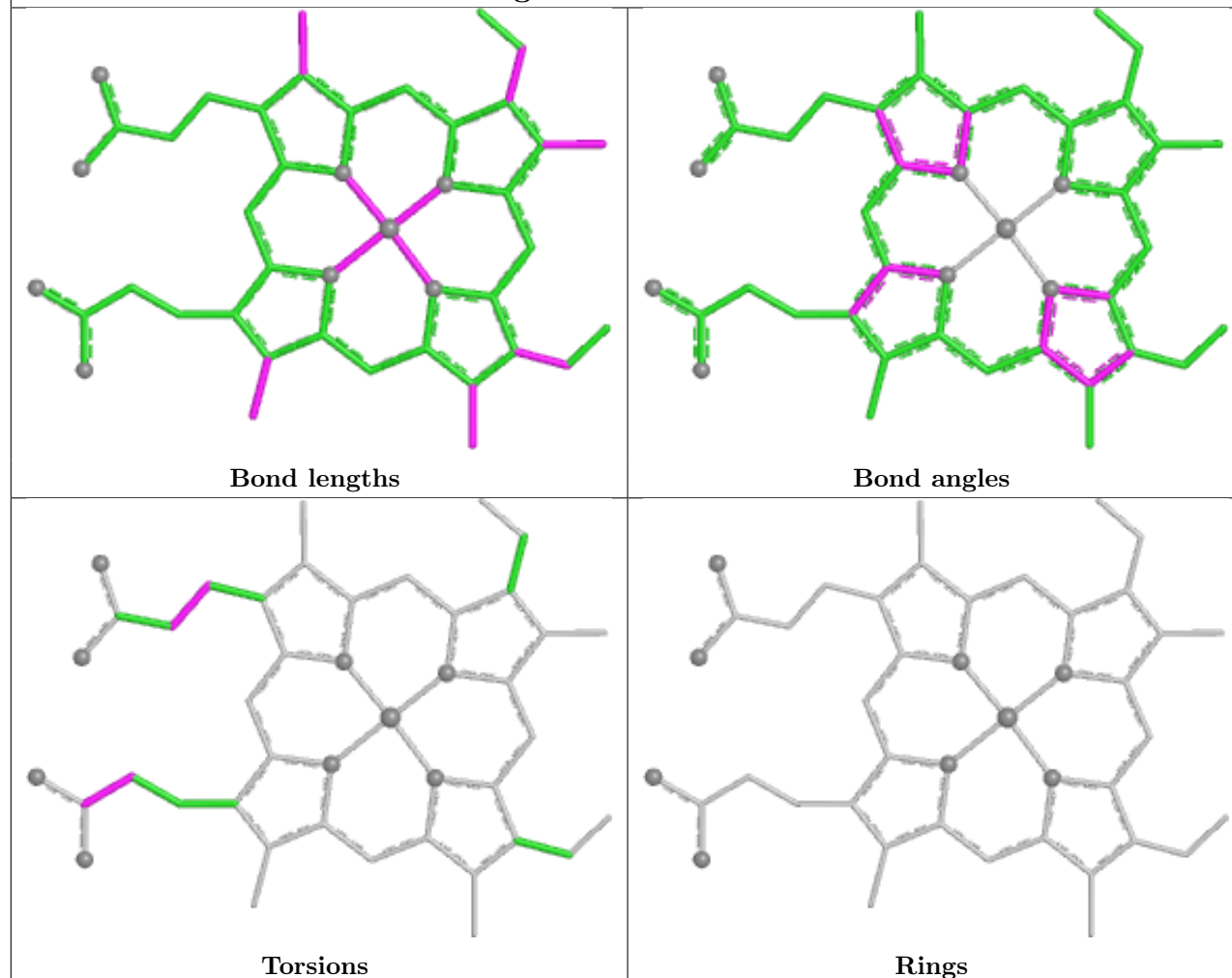




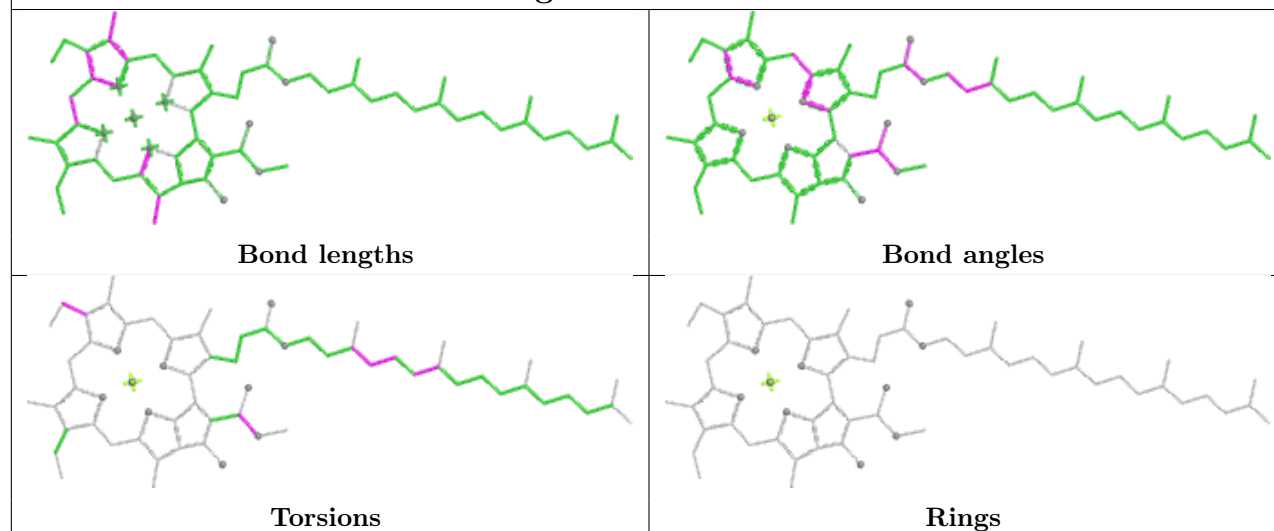


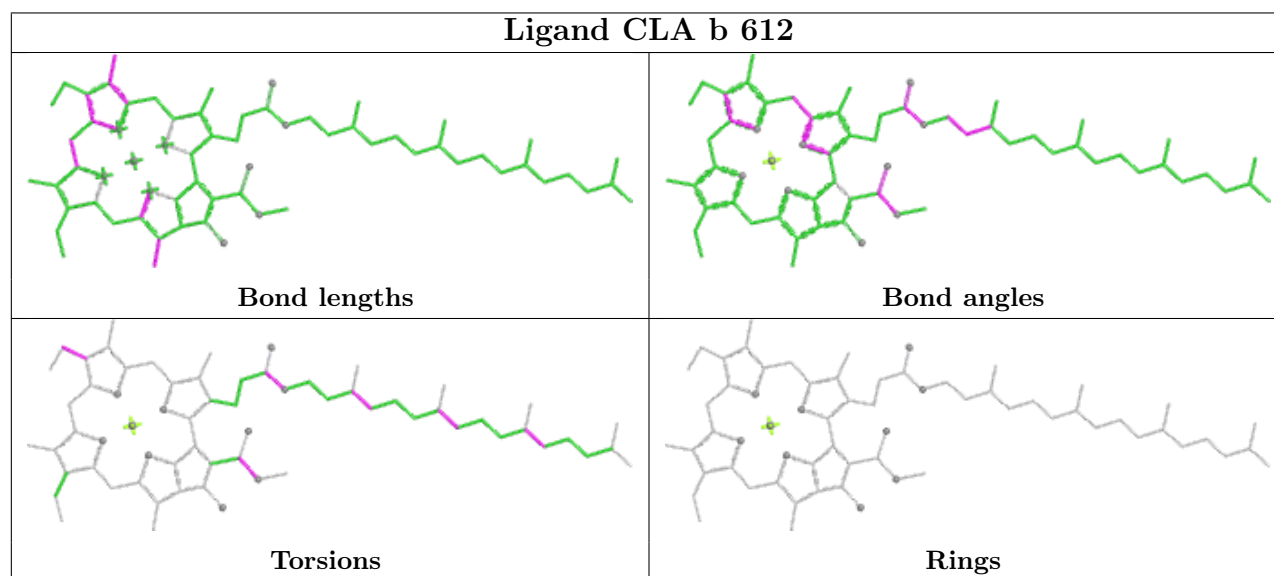
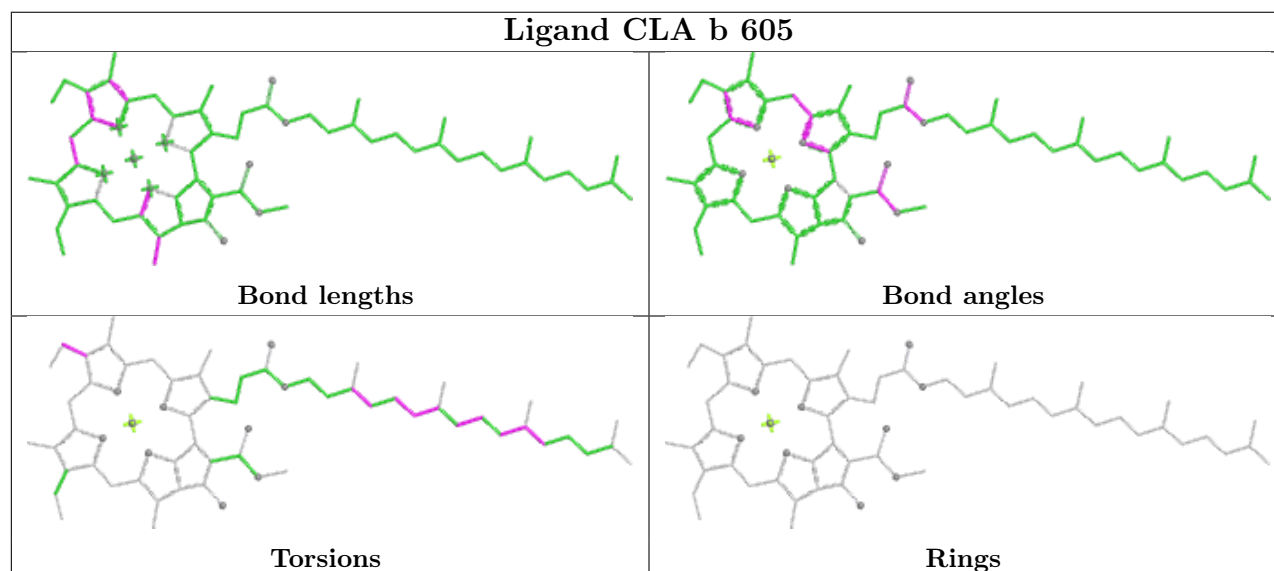
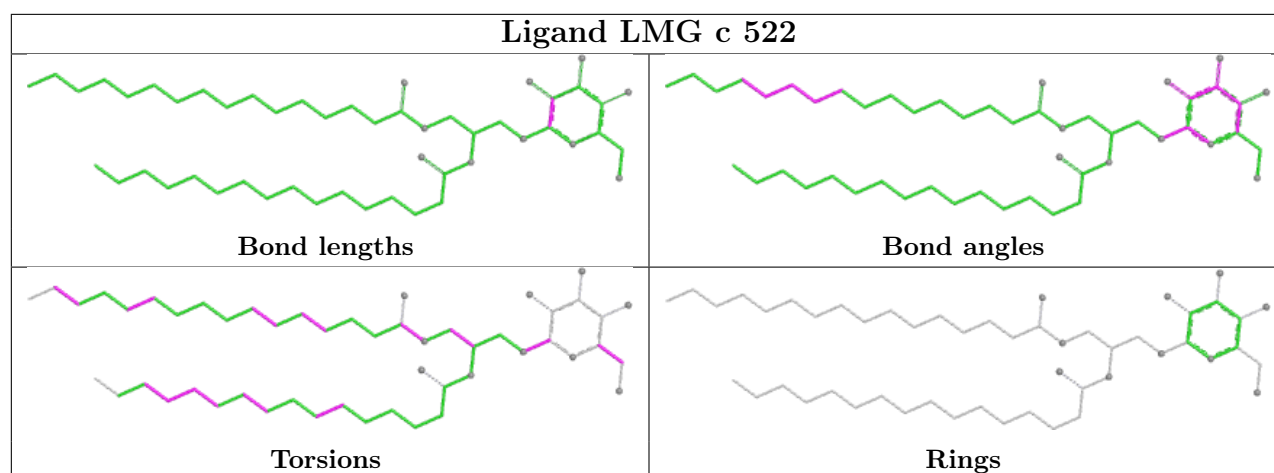


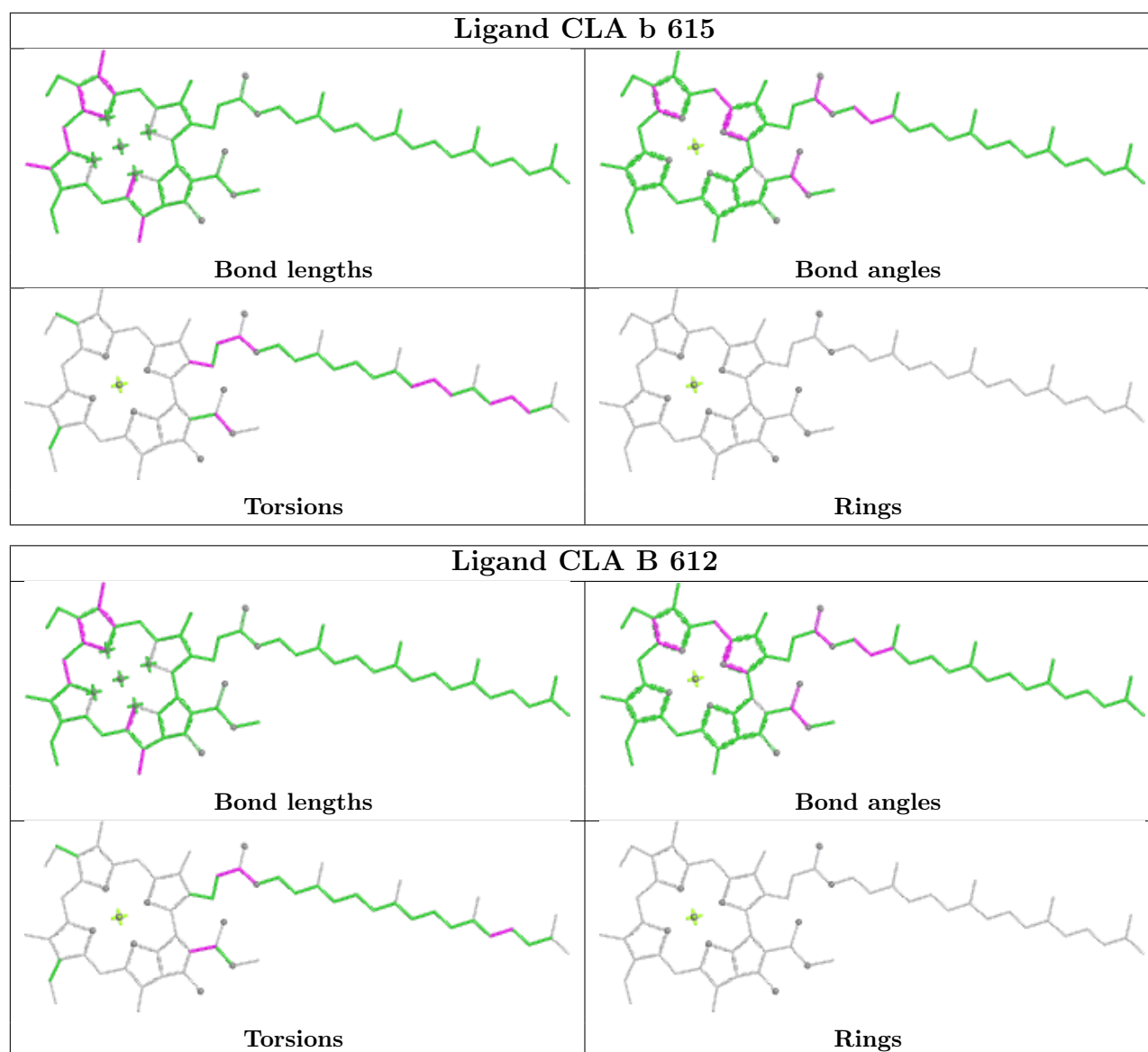
Ligand HEM e 101



Ligand CLA b 607







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%)	0.52	10 (2%) 52 30	28, 38, 60, 76	0
1	a	334/344 (97%)	0.48	6 (1%) 67 44	28, 38, 60, 76	0
2	B	504/510 (98%)	0.50	12 (2%) 59 36	27, 41, 66, 86	0
2	b	504/510 (98%)	0.53	13 (2%) 57 34	29, 42, 67, 85	1 (0%)
3	C	451/461 (97%)	0.58	11 (2%) 59 36	30, 45, 61, 75	0
3	c	451/461 (97%)	0.62	13 (2%) 53 31	31, 46, 63, 93	0
4	D	341/352 (96%)	0.45	6 (1%) 67 44	28, 39, 56, 67	0
4	d	341/352 (96%)	0.49	5 (1%) 72 49	29, 40, 55, 78	0
5	E	81/84 (96%)	0.75	2 (2%) 58 35	39, 54, 72, 89	0
5	e	82/84 (97%)	0.95	9 (10%) 10 6	43, 61, 75, 80	0
6	F	34/45 (75%)	0.67	1 (2%) 53 31	40, 50, 63, 77	0
6	f	34/45 (75%)	0.64	1 (2%) 53 31	39, 51, 69, 72	0
7	H	63/66 (95%)	0.60	0 100 100	39, 47, 57, 63	0
7	h	63/66 (95%)	0.43	0 100 100	35, 47, 58, 68	0
8	I	35/38 (92%)	0.48	1 (2%) 53 31	29, 44, 71, 73	0
8	i	35/38 (92%)	0.63	4 (11%) 10 6	33, 43, 74, 94	0
9	J	36/40 (90%)	0.86	3 (8%) 17 9	44, 58, 68, 75	0
9	j	36/40 (90%)	0.79	1 (2%) 55 32	49, 57, 72, 79	0
10	K	37/46 (80%)	0.95	2 (5%) 31 16	45, 59, 75, 89	0
10	k	37/46 (80%)	0.96	3 (8%) 18 9	47, 56, 72, 79	0
11	L	37/37 (100%)	0.25	1 (2%) 56 33	32, 38, 62, 84	0
11	l	37/37 (100%)	0.35	2 (5%) 31 16	29, 38, 69, 81	0
12	M	32/36 (88%)	0.35	2 (6%) 26 13	33, 38, 56, 74	0
12	m	32/36 (88%)	0.59	3 (9%) 14 7	31, 41, 59, 64	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	0.69	16 (6%) 24 12	30, 47, 81, 111	0
13	o	244/272 (89%)	0.75	14 (5%) 29 15	31, 46, 80, 127	0
14	T	29/32 (90%)	0.33	1 (3%) 48 27	30, 39, 60, 74	0
14	t	29/32 (90%)	0.26	1 (3%) 48 27	31, 36, 63, 66	0
15	U	97/134 (72%)	0.56	2 (2%) 63 40	36, 49, 69, 75	0
15	u	97/134 (72%)	0.54	1 (1%) 79 59	32, 44, 58, 76	0
16	V	137/163 (84%)	0.65	3 (2%) 62 39	34, 47, 59, 74	0
16	v	137/163 (84%)	0.80	7 (5%) 33 17	34, 54, 67, 81	0
17	Y	30/46 (65%)	1.25	4 (13%) 7 4	60, 73, 84, 87	0
17	y	30/46 (65%)	0.96	1 (3%) 49 28	49, 65, 78, 83	0
18	X	38/41 (92%)	0.56	2 (5%) 32 16	41, 50, 65, 79	0
18	x	38/41 (92%)	0.79	3 (7%) 18 10	46, 55, 74, 76	0
19	Z	62/62 (100%)	1.37	13 (20%) 2 1	52, 69, 88, 98	0
19	z	62/62 (100%)	1.20	7 (11%) 10 6	51, 72, 97, 105	0
20	R	34/41 (82%)	1.27	4 (11%) 9 5	65, 73, 83, 86	0
20	r	34/41 (82%)	1.29	3 (8%) 15 8	65, 78, 86, 90	0
All	All	5313/5700 (93%)	0.61	193 (3%) 46 26	27, 44, 72, 127	1 (0%)

The worst 5 of 193 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	m	31	SER	4.8
13	O	35	SER	4.7
16	v	18	THR	4.7
13	o	60	ARG	4.5
3	C	29	GLU	4.4

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
8	FME	I	1	10/11	0.87	0.14	43,56,63,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	FME	m	1	10/11	0.88	0.16	26,45,55,64	0
14	FME	t	1	10/11	0.88	0.13	39,42,63,72	0
12	FME	M	1	10/11	0.89	0.14	30,43,53,54	0
8	FME	i	1	10/11	0.89	0.11	35,50,56,61	0
14	FME	T	1	10/11	0.90	0.10	44,47,53,54	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
30	UNL	H	101	8/-	0.52	0.24	29,35,43,47	0
29	LMG	b	625	9/55	0.63	0.25	40,46,52,55	0
29	LMG	b	624	51/55	0.64	0.23	45,64,76,86	0
30	UNL	j	101	9/-	0.67	0.23	40,49,60,63	0
31	LHG	a	615	42/49	0.67	0.21	54,78,89,100	0
31	LHG	A	618	49/49	0.68	0.22	41,72,85,94	0
30	UNL	b	603	13/-	0.69	0.20	39,48,61,62	0
30	UNL	A	614	7/-	0.69	0.24	32,38,42,42	0
30	UNL	B	622	6/-	0.71	0.22	26,42,50,56	0
29	LMG	B	621	51/55	0.71	0.20	32,56,71,74	0
29	LMG	C	520	51/55	0.72	0.22	49,62,82,100	0
30	UNL	t	101	10/-	0.72	0.19	26,41,47,47	0
28	PL9	A	611	55/55	0.73	0.24	39,58,75,79	0
30	UNL	B	623	11/-	0.73	0.19	35,40,47,48	0
29	LMG	c	522	51/55	0.75	0.21	36,68,83,90	0
30	UNL	z	101	11/-	0.75	0.23	31,53,58,60	0
30	UNL	i	101	12/-	0.75	0.20	24,39,51,51	0
29	LMG	d	409	40/55	0.75	0.20	40,55,76,77	0
29	LMG	A	613	51/55	0.76	0.19	31,53,78,84	0
23	SQD	I	101	40/54	0.76	0.18	31,52,84,89	0
23	SQD	D	409	43/54	0.77	0.19	37,68,89,98	0
30	UNL	B	624	11/-	0.77	0.18	26,31,38,41	0
23	SQD	A	619	40/54	0.77	0.20	25,48,67,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	UNL	m	102	16/-	0.77	0.18	37,45,51,54	0
27	BCR	y	101	40/40	0.78	0.20	50,63,70,74	0
25	CLA	b	604	65/65	0.78	0.17	44,59,76,88	0
23	SQD	D	408	47/54	0.79	0.16	17,53,103,121	0
29	LMG	B	625	51/55	0.79	0.17	28,52,74,78	0
29	LMG	C	519	51/55	0.79	0.19	42,61,73,85	0
23	SQD	B	626	54/54	0.80	0.15	33,52,85,90	0
30	UNL	b	602	13/-	0.80	0.18	30,36,41,45	0
29	LMG	c	521	51/55	0.80	0.21	33,65,83,88	0
27	BCR	Y	101	40/40	0.80	0.19	46,60,72,76	0
23	SQD	b	601	54/54	0.80	0.16	39,60,90,97	0
23	SQD	c	501	54/54	0.80	0.19	38,58,76,77	0
28	PL9	a	611	55/55	0.80	0.20	40,59,72,73	0
29	LMG	b	623	51/55	0.80	0.18	29,48,71,74	0
29	LMG	A	612	51/55	0.80	0.17	34,59,76,85	0
30	UNL	C	521	9/-	0.80	0.20	36,42,46,49	0
29	LMG	c	502	51/55	0.81	0.19	34,57,80,83	0
27	BCR	D	404	40/40	0.81	0.18	28,46,63,67	0
30	UNL	m	101	5/-	0.81	0.16	26,32,37,41	0
25	CLA	C	512	65/65	0.81	0.17	42,58,68,79	0
27	BCR	k	101	40/40	0.81	0.18	37,53,59,61	0
25	CLA	B	601	65/65	0.81	0.17	41,59,84,96	0
27	BCR	C	514	40/40	0.81	0.19	45,56,64,66	0
30	UNL	d	402	22/-	0.81	0.19	26,43,60,78	0
33	DGD	c	519	62/66	0.81	0.19	37,57,86,95	0
33	DGD	h	102	62/66	0.81	0.18	35,47,63,73	0
23	SQD	f	101	43/54	0.82	0.17	51,70,77,84	0
25	CLA	C	504	65/65	0.82	0.19	33,51,70,78	0
25	CLA	c	515	65/65	0.82	0.18	45,60,78,81	0
27	BCR	h	101	40/40	0.82	0.17	31,45,55,62	0
32	BCT	a	605	4/4	0.82	0.11	44,47,49,50	0
27	BCR	B	627	40/40	0.82	0.17	30,41,49,53	0
29	LMG	B	620	51/55	0.82	0.16	27,46,67,75	0
27	BCR	b	622	40/40	0.83	0.18	33,43,52,54	0
24	CL	a	603	1/1	0.83	0.13	59,59,59,59	0
25	CLA	C	511	65/65	0.83	0.17	45,57,66,70	0
27	BCR	H	102	40/40	0.83	0.17	34,51,59,65	0
23	SQD	A	603	52/54	0.83	0.17	38,60,78,82	0
27	BCR	B	618	40/40	0.84	0.16	28,40,48,52	0
25	CLA	B	606	65/65	0.84	0.16	29,44,65,84	0
25	CLA	C	510	65/65	0.84	0.15	41,51,58,60	0
25	CLA	b	617	65/65	0.84	0.15	34,45,63,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	c	505	65/65	0.84	0.16	32,51,62,68	0
27	BCR	K	101	40/40	0.84	0.18	45,53,60,66	0
27	BCR	T	101	40/40	0.84	0.18	31,43,58,62	0
25	CLA	c	506	65/65	0.84	0.16	36,49,70,74	0
31	LHG	A	617	49/49	0.84	0.20	33,55,78,82	0
25	CLA	c	514	65/65	0.84	0.17	45,59,78,83	0
27	BCR	c	516	40/40	0.84	0.19	33,63,70,72	0
27	BCR	d	405	40/40	0.84	0.17	29,43,56,62	0
33	DGD	C	518	62/66	0.84	0.16	33,48,65,74	0
29	LMG	D	405	51/55	0.84	0.19	34,53,88,92	0
25	CLA	C	503	65/65	0.84	0.16	37,49,58,65	0
25	CLA	C	513	65/65	0.85	0.15	41,62,74,83	0
25	CLA	d	404	65/65	0.85	0.16	32,46,73,91	0
25	CLA	c	508	65/65	0.85	0.16	34,49,72,78	0
27	BCR	B	619	40/40	0.85	0.15	33,44,58,60	0
30	UNL	M	101	6/-	0.85	0.20	41,46,52,65	0
33	DGD	H	103	62/66	0.85	0.16	26,41,53,61	0
25	CLA	c	510	58/65	0.85	0.17	34,46,59,67	0
33	DGD	c	520	62/66	0.85	0.17	36,47,72,80	0
25	CLA	C	502	65/65	0.85	0.16	35,51,62,69	0
30	UNL	M	102	17/-	0.86	0.15	31,37,49,51	0
25	CLA	B	614	65/65	0.86	0.14	32,42,63,82	0
29	LMG	d	406	42/55	0.86	0.16	38,48,63,73	0
25	CLA	C	508	65/65	0.86	0.16	38,49,82,90	0
27	BCR	b	621	40/40	0.86	0.15	31,42,57,59	0
25	CLA	c	507	65/65	0.86	0.15	32,44,61,64	0
31	LHG	a	614	35/49	0.86	0.15	36,47,56,58	0
25	CLA	B	608	65/65	0.87	0.14	29,37,47,52	0
25	CLA	C	509	65/65	0.87	0.15	33,46,59,67	0
25	CLA	B	609	65/65	0.87	0.14	24,44,52,58	0
25	CLA	b	611	65/65	0.87	0.14	27,41,54,57	0
25	CLA	c	509	65/65	0.87	0.14	30,39,51,55	0
31	LHG	l	101	49/49	0.87	0.15	30,45,54,56	0
25	CLA	C	505	65/65	0.87	0.14	33,41,55,62	0
27	BCR	C	515	40/40	0.87	0.17	32,42,52,53	0
25	CLA	c	511	65/65	0.87	0.15	38,46,55,57	0
33	DGD	c	518	62/66	0.87	0.15	28,46,63,79	0
25	CLA	c	513	65/65	0.87	0.16	42,52,58,60	0
25	CLA	c	504	65/65	0.87	0.15	32,46,59,65	0
28	PL9	D	407	55/55	0.87	0.15	26,35,45,50	0
25	CLA	B	615	65/65	0.88	0.13	27,41,51,57	0
25	CLA	D	402	65/65	0.88	0.15	24,36,48,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	D	403	65/65	0.88	0.13	21,37,63,69	0
27	BCR	b	620	40/40	0.88	0.15	33,45,53,54	0
25	CLA	C	506	65/65	0.88	0.14	32,47,64,68	0
25	CLA	b	605	65/65	0.88	0.14	31,43,56,58	0
33	DGD	C	516	62/66	0.88	0.15	21,39,63,71	0
33	DGD	C	517	62/66	0.88	0.14	39,51,74,83	0
25	CLA	b	609	65/65	0.88	0.15	21,35,59,81	0
27	BCR	c	517	40/40	0.88	0.14	19,39,50,52	0
25	CLA	C	507	65/65	0.88	0.14	32,42,52,67	0
25	CLA	B	604	65/65	0.88	0.14	28,37,57,65	0
25	CLA	c	512	65/65	0.88	0.14	31,47,56,64	0
25	CLA	b	619	65/65	0.88	0.14	30,44,72,80	0
34	HEM	e	101	43/43	0.88	0.16	50,62,69,70	0
31	LHG	D	406	49/49	0.89	0.13	25,40,50,59	0
31	LHG	L	101	49/49	0.89	0.14	29,41,51,57	0
31	LHG	a	613	49/49	0.89	0.14	26,43,56,60	0
28	PL9	d	408	55/55	0.89	0.14	21,33,43,45	0
25	CLA	b	612	65/65	0.89	0.14	28,41,55,61	0
25	CLA	b	614	65/65	0.89	0.12	25,35,41,50	0
25	CLA	B	616	65/65	0.89	0.13	32,44,70,76	0
25	CLA	b	618	65/65	0.89	0.14	28,40,47,56	0
25	CLA	B	603	65/65	0.89	0.14	28,37,45,47	0
25	CLA	b	607	65/65	0.89	0.12	24,34,48,53	0
25	CLA	b	608	65/65	0.89	0.13	30,40,46,51	0
25	CLA	B	607	65/65	0.89	0.13	26,36,44,54	0
25	CLA	a	609	65/65	0.89	0.15	19,34,71,81	0
31	LHG	A	616	49/49	0.89	0.13	24,41,54,58	0
26	PHO	D	401	64/64	0.89	0.13	27,37,47,54	0
26	PHO	d	401	64/64	0.89	0.14	24,39,45,49	0
25	CLA	b	616	65/65	0.90	0.13	25,33,51,62	0
25	CLA	A	606	65/65	0.90	0.14	26,34,45,48	0
25	CLA	A	607	57/65	0.90	0.13	29,37,49,67	0
27	BCR	A	610	40/40	0.90	0.13	22,34,44,47	0
27	BCR	B	617	40/40	0.90	0.13	32,41,49,50	0
24	CL	a	604	1/1	0.90	0.13	42,42,42,42	0
25	CLA	B	610	65/65	0.90	0.12	25,33,39,45	0
25	CLA	B	613	65/65	0.90	0.14	19,33,48,69	0
25	CLA	b	613	65/65	0.90	0.13	24,35,43,45	0
34	HEM	E	101	43/43	0.90	0.14	42,54,67,69	0
25	CLA	b	606	65/65	0.90	0.13	24,36,50,58	0
31	LHG	d	407	49/49	0.91	0.12	20,37,47,51	0
25	CLA	A	609	65/65	0.91	0.15	17,29,79,89	0

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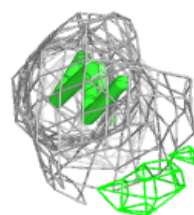
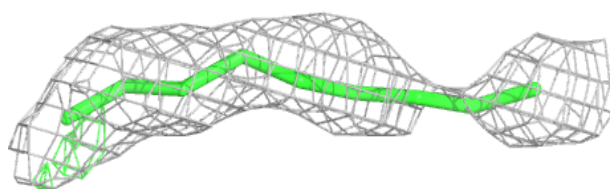
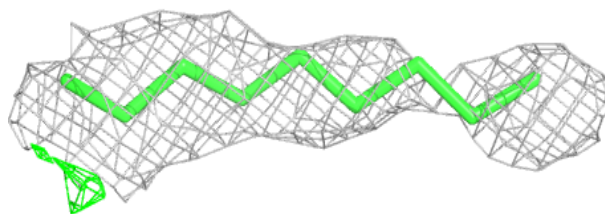
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	PHO	A	608	64/64	0.91	0.12	23,32,37,43	0
25	CLA	b	615	65/65	0.91	0.12	22,32,41,50	0
25	CLA	B	611	65/65	0.91	0.12	21,31,38,44	0
25	CLA	a	606	65/65	0.91	0.12	23,31,38,39	0
27	BCR	a	610	40/40	0.91	0.12	19,32,45,47	0
25	CLA	C	501	65/65	0.91	0.12	34,42,49,54	0
25	CLA	b	610	65/65	0.91	0.12	23,37,51,54	0
25	CLA	a	612	65/65	0.91	0.12	17,29,37,39	0
25	CLA	B	605	65/65	0.91	0.12	24,34,40,42	0
25	CLA	A	615	65/65	0.91	0.12	22,34,43,47	0
25	CLA	d	403	65/65	0.91	0.13	24,36,45,50	0
35	HEC	V	201	43/43	0.91	0.13	31,44,52,56	0
25	CLA	c	503	65/65	0.92	0.12	27,40,46,52	0
26	PHO	a	608	64/64	0.92	0.12	19,28,38,42	0
25	CLA	B	612	65/65	0.92	0.12	26,35,42,46	0
25	CLA	B	602	65/65	0.93	0.12	29,39,47,52	0
25	CLA	a	607	59/65	0.93	0.11	27,37,55,72	0
24	CL	A	605	1/1	0.93	0.11	44,44,44,44	0
22	FE2	a	602	1/1	0.93	0.07	62,62,62,62	0
35	HEC	v	201	43/43	0.93	0.11	32,41,48,52	0
32	BCT	A	620	4/4	0.94	0.10	26,36,37,44	0
22	FE2	A	602	1/1	0.95	0.08	46,46,46,46	0
24	CL	A	604	1/1	0.97	0.08	43,43,43,43	0
21	OEX	a	601	10/10	0.98	0.05	40,44,48,51	0
21	OEX	A	601	10/10	0.99	0.06	33,40,45,46	0

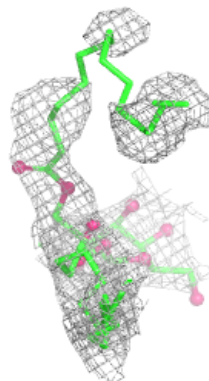
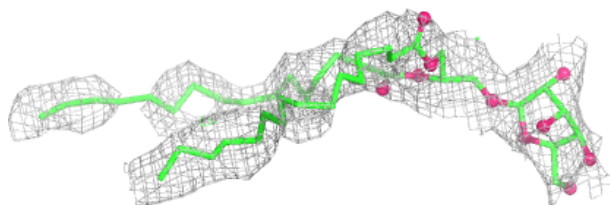
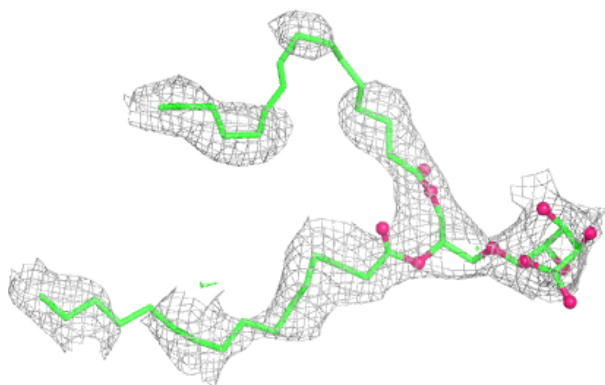
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMG b 625:

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

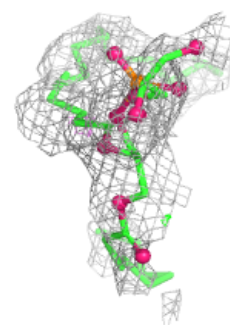
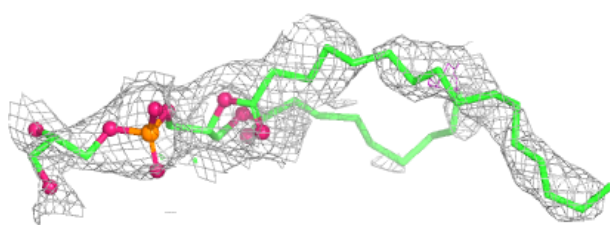
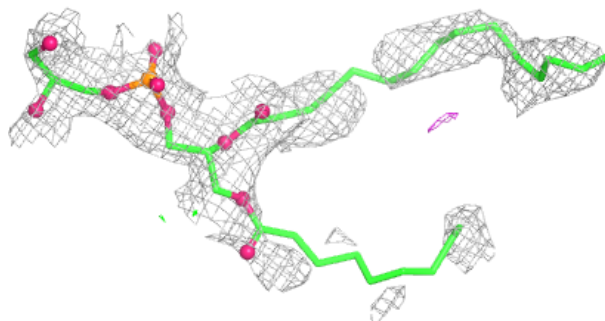
**Electron density around LMG b 624:**

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

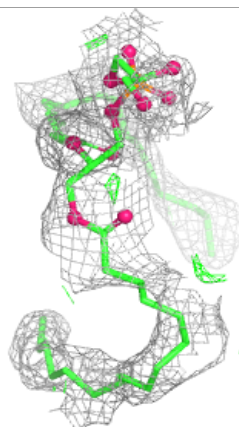
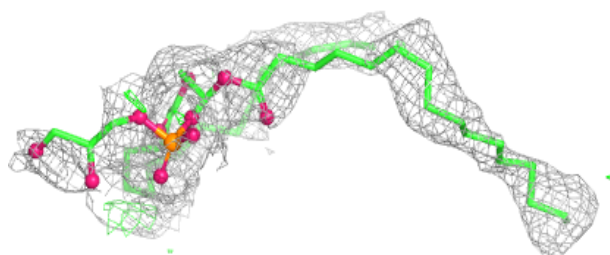
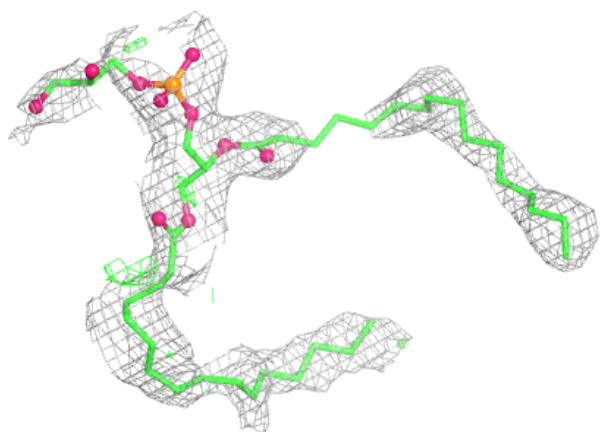


Electron density around LHG a 615:

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

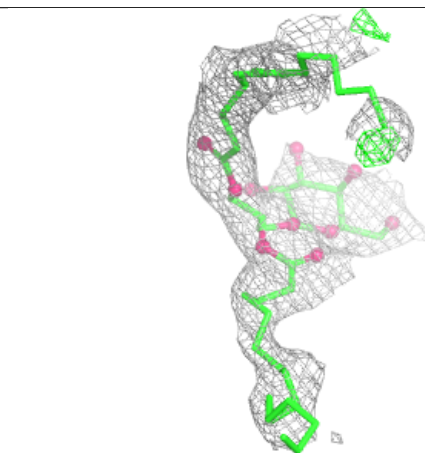
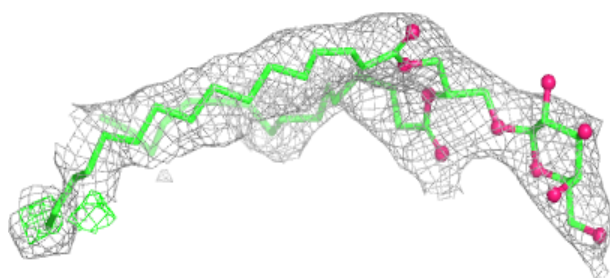
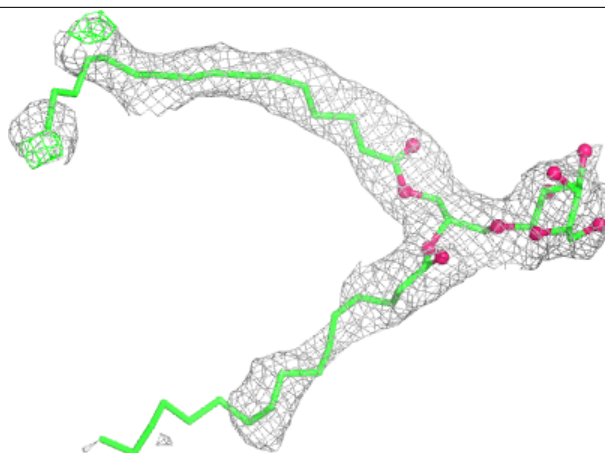
**Electron density around LHG A 618:**

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

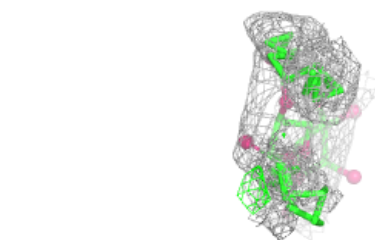
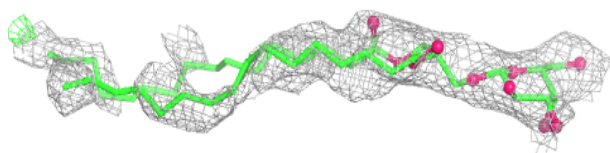
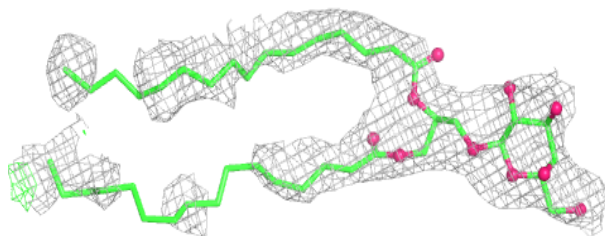


Electron density around LMG B 621:

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

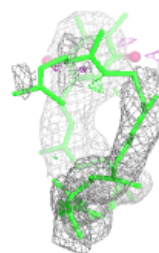
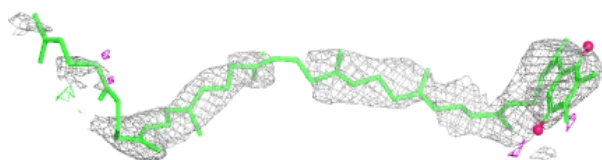
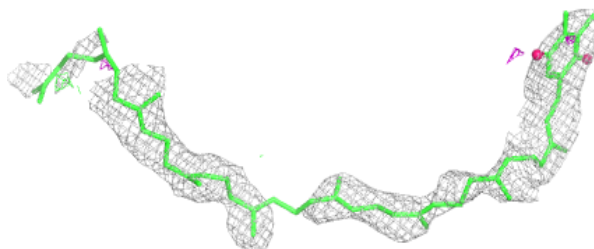
**Electron density around LMG C 520:**

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

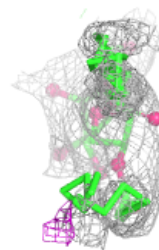
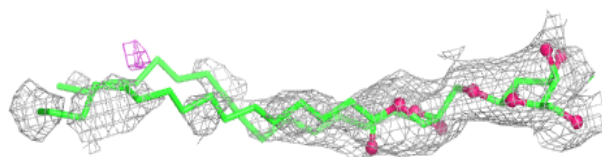
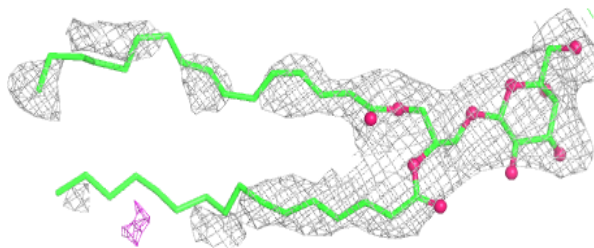


Electron density around PL9 A 611:

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

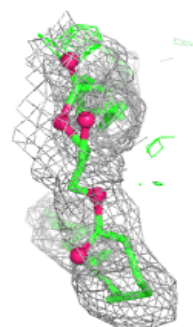
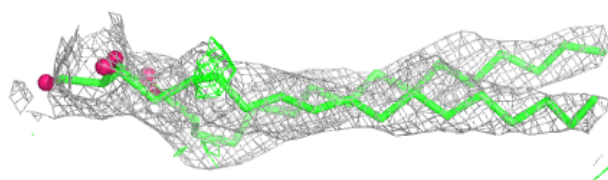
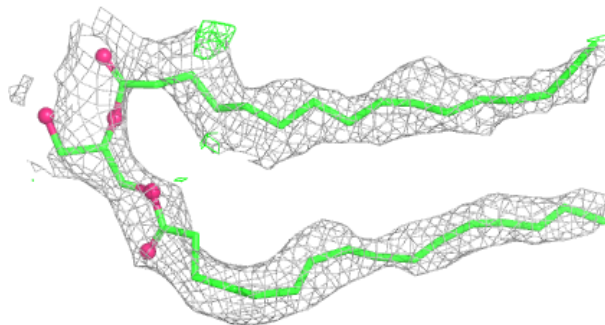
**Electron density around LMG c 522:**

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

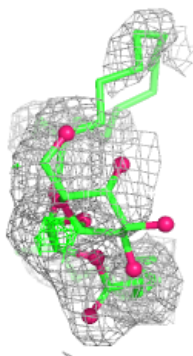
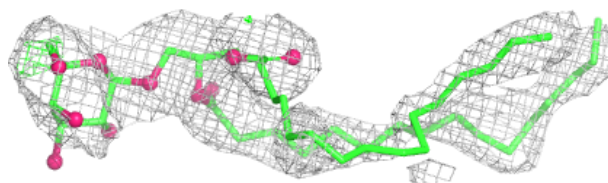
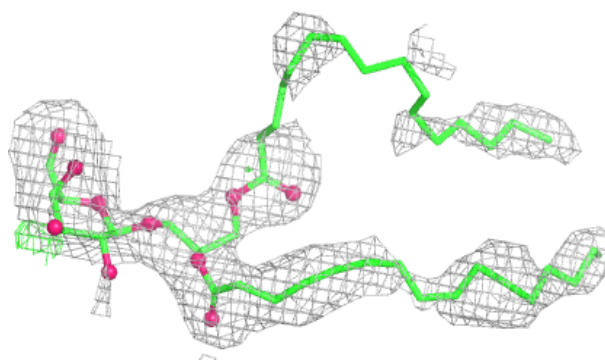


Electron density around LMG d 409:

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

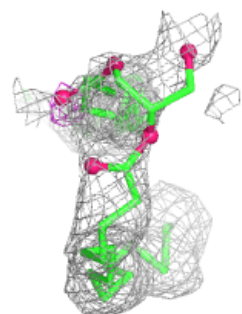
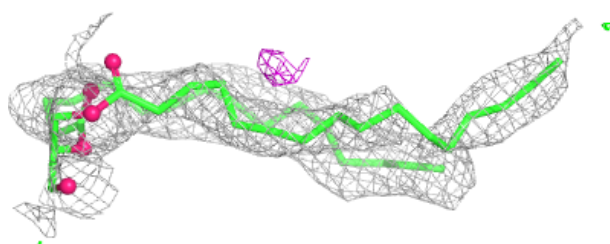
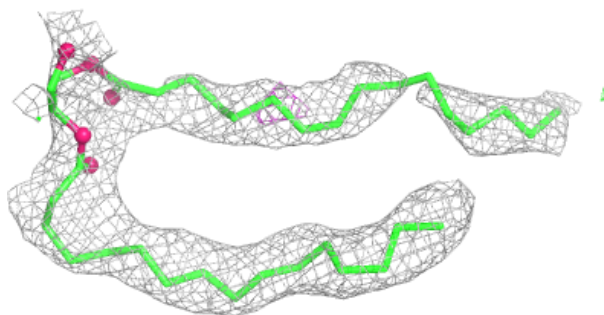
**Electron density around LMG A 613:**

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

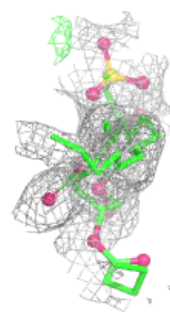
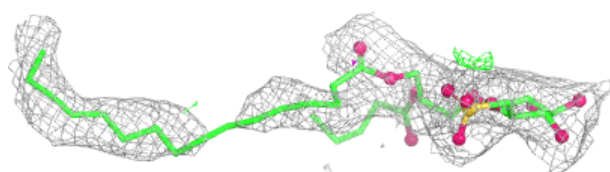
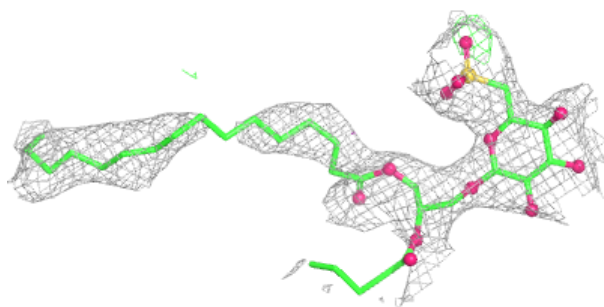


Electron density around SQD I 101:

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

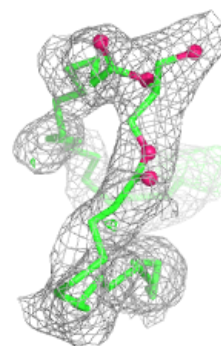
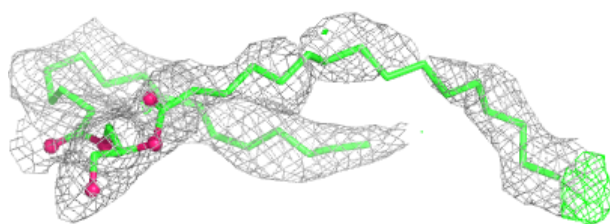
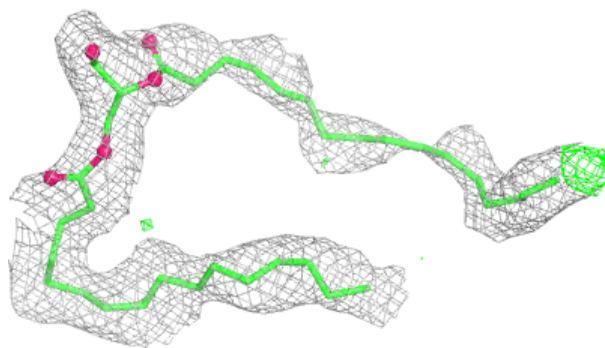
**Electron density around SQD D 409:**

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

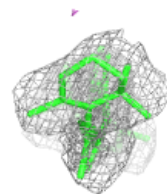
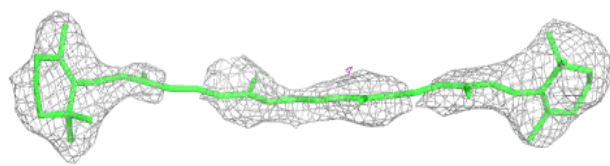
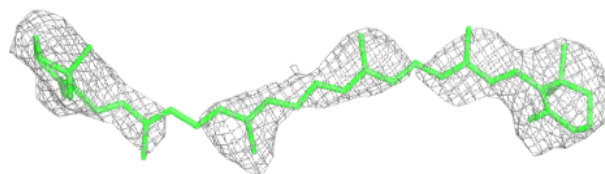


Electron density around SQD A 619:

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

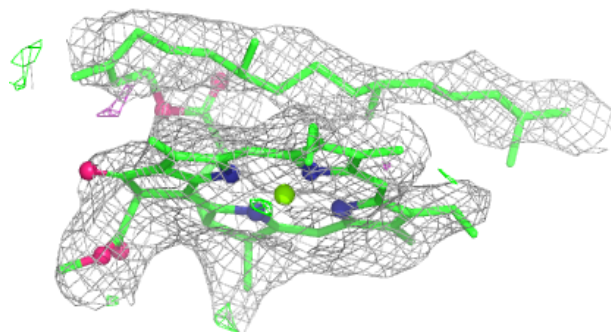
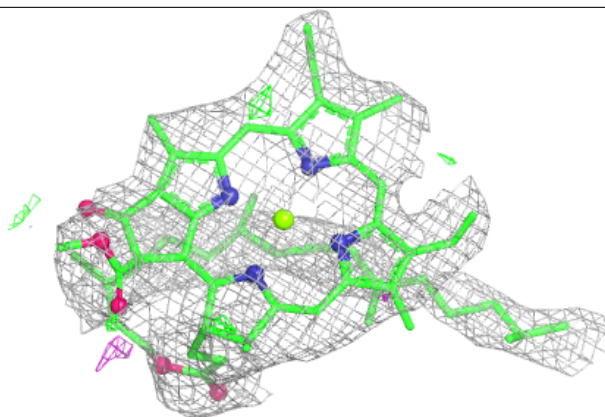
**Electron density around BCR y 101:**

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

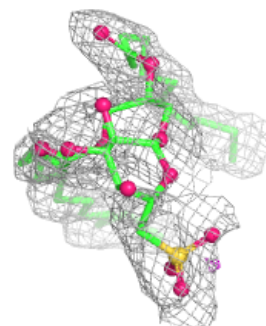
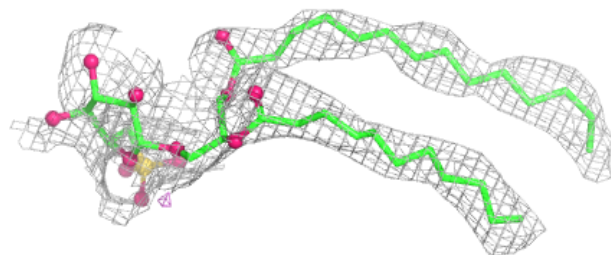
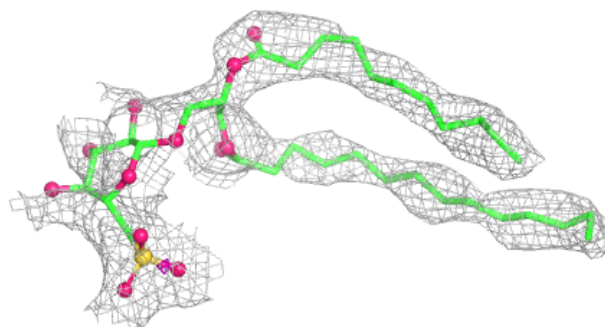


Electron density around CLA b 604:

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

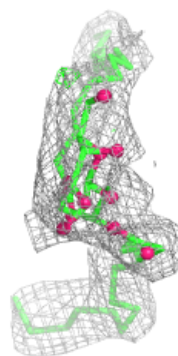
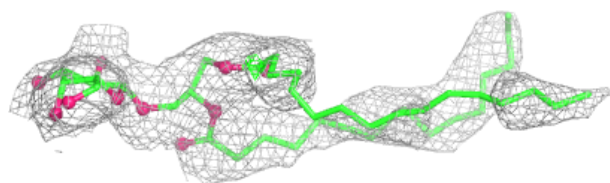
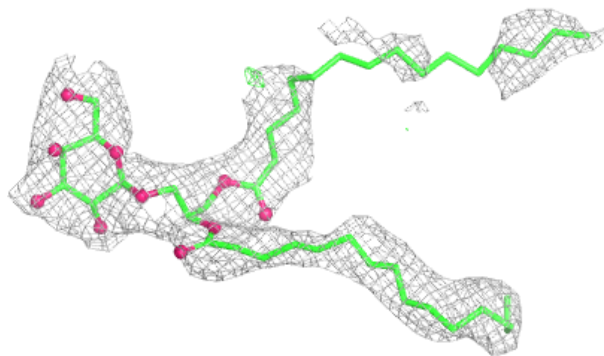
**Electron density around SQD D 408:**

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

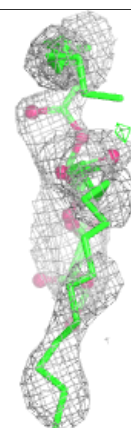
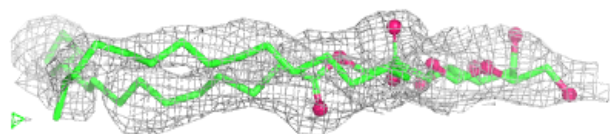
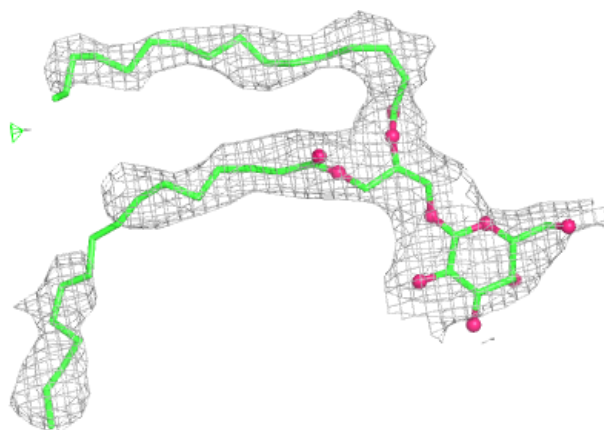


Electron density around LMG B 625:

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

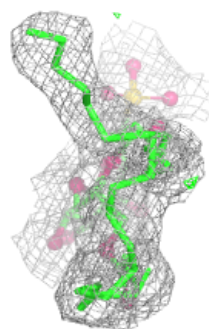
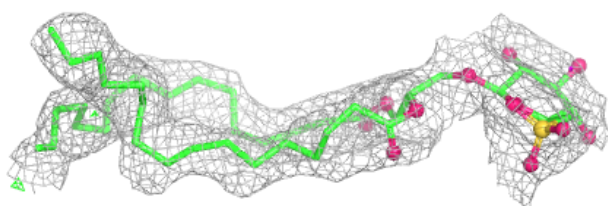
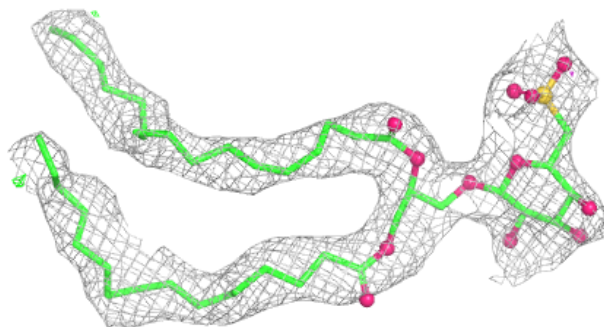
**Electron density around LMG C 519:**

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

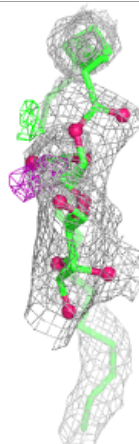
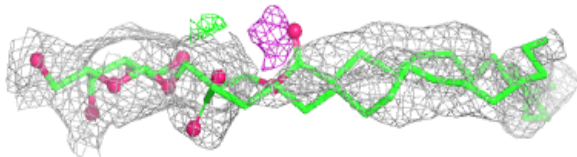
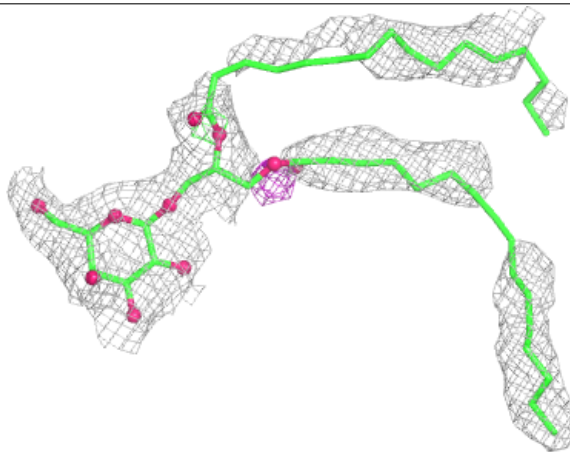


Electron density around SQD B 626:

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

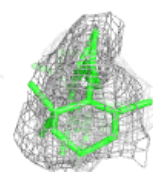
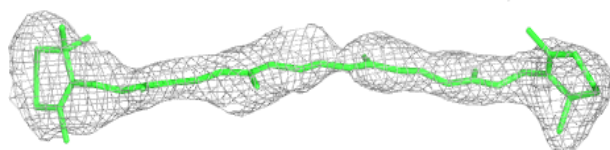
**Electron density around LMG c 521:**

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

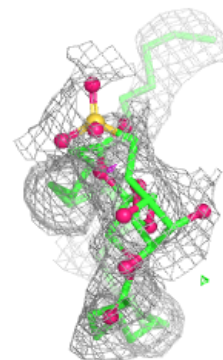
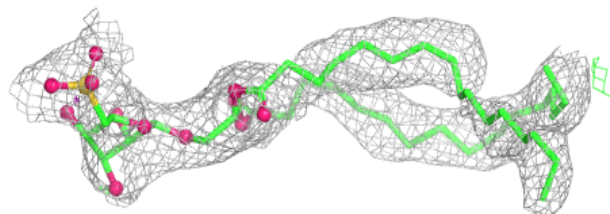
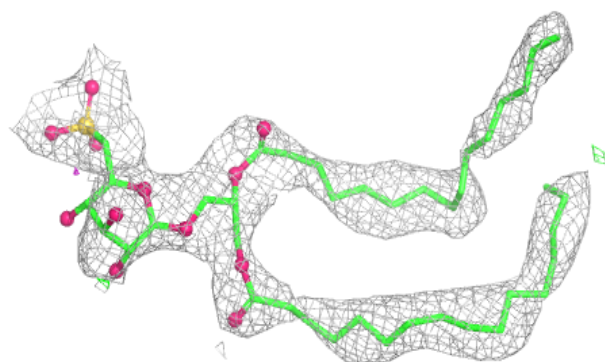


Electron density around BCR Y 101:

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

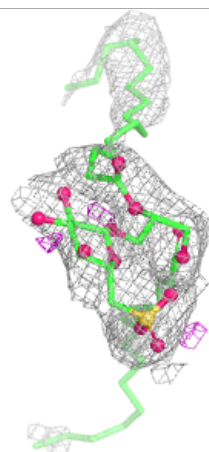
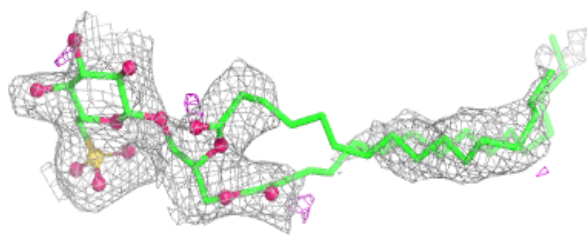
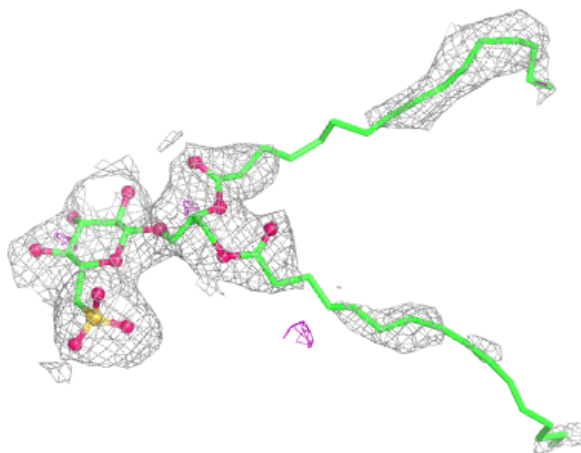
**Electron density around SQD b 601:**

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



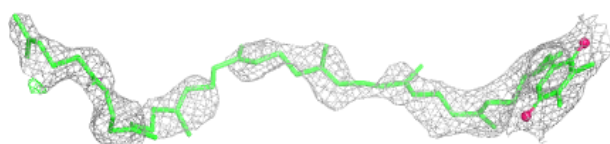
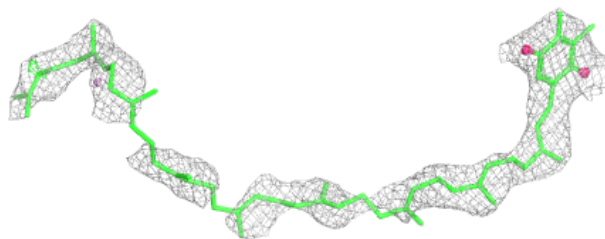
Electron density around SQD c 501:

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

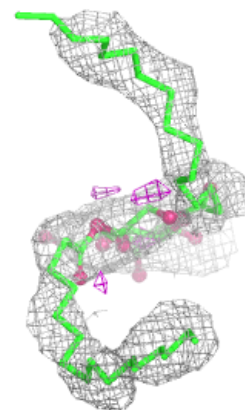
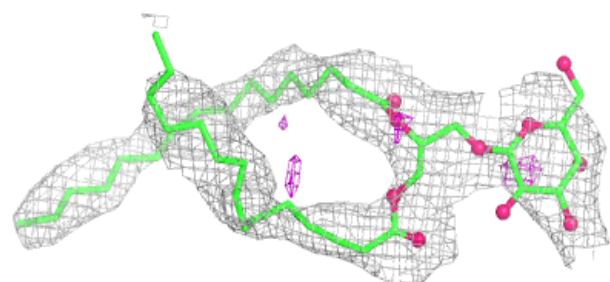


Electron density around PL9 a 611:

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

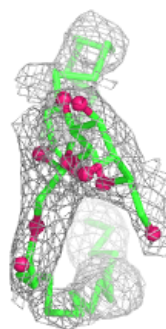
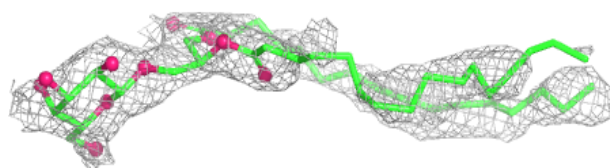
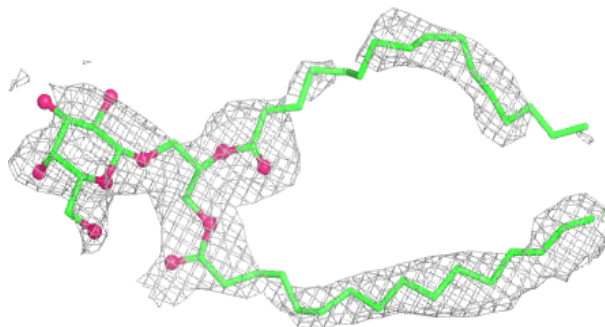
**Electron density around LMG b 623:**

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

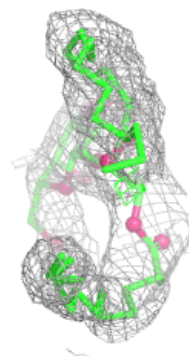
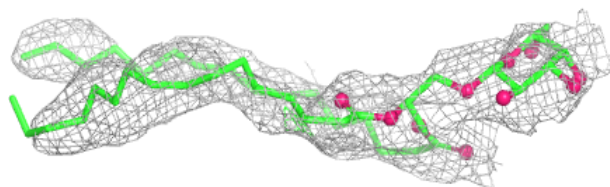
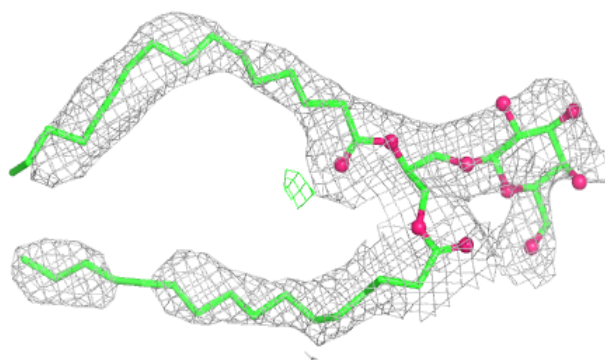


Electron density around LMG A 612:

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

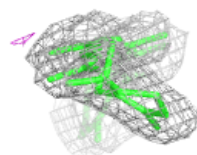
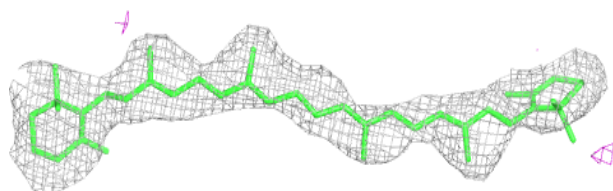
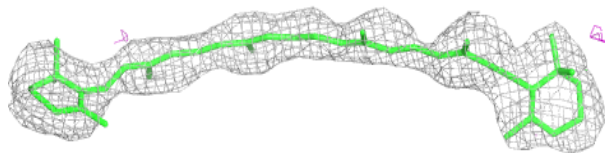
**Electron density around LMG c 502:**

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



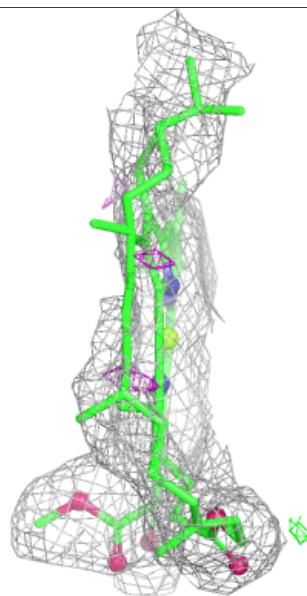
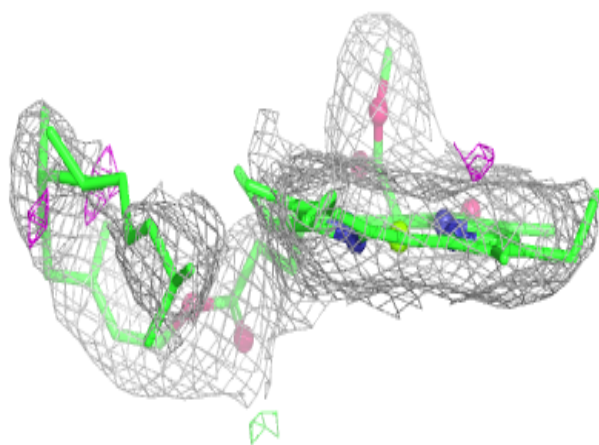
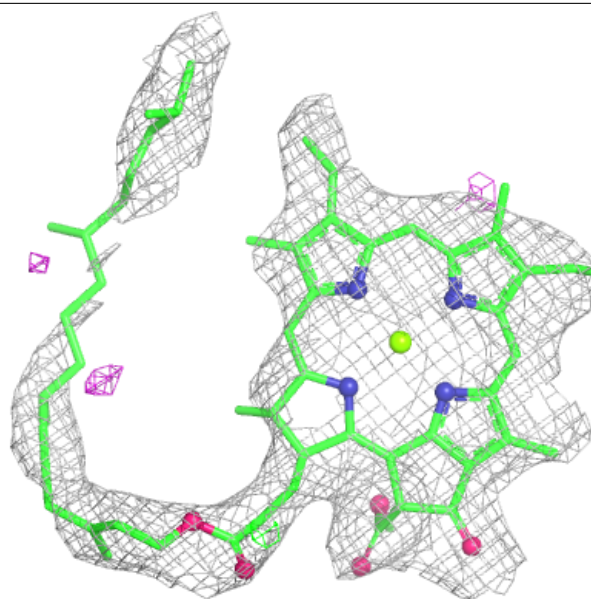
Electron density around BCR D 404:

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



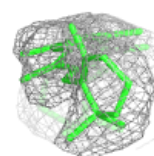
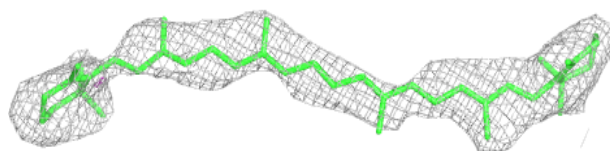
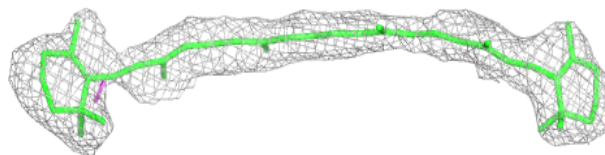
Electron density around CLA C 512:

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

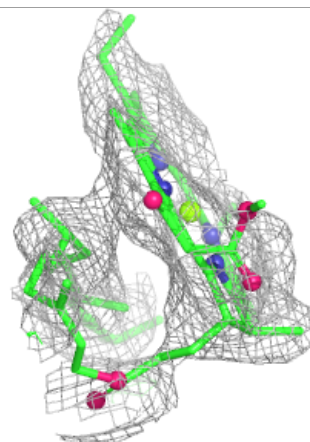
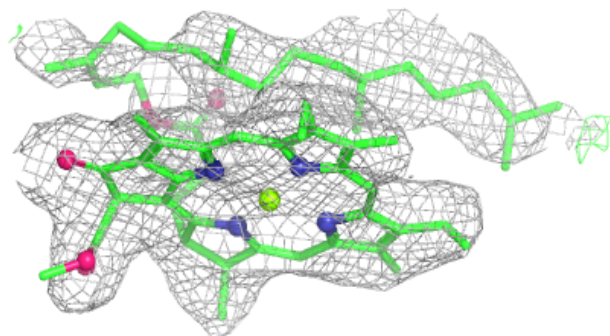
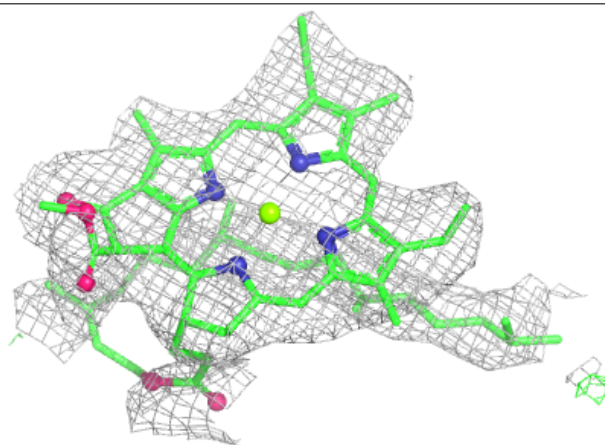


Electron density around BCR k 101:

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

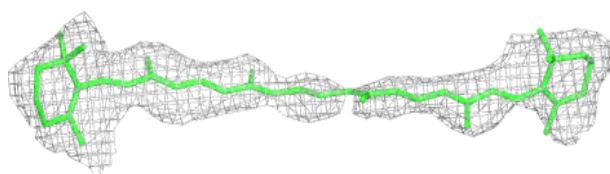
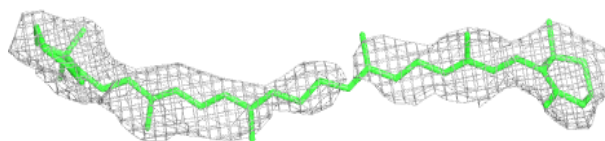
**Electron density around CLA B 601:**

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

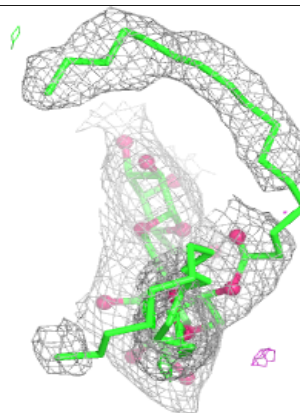
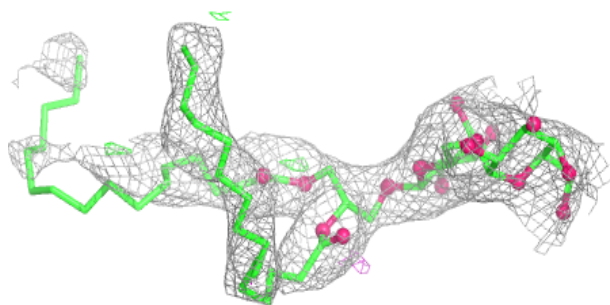
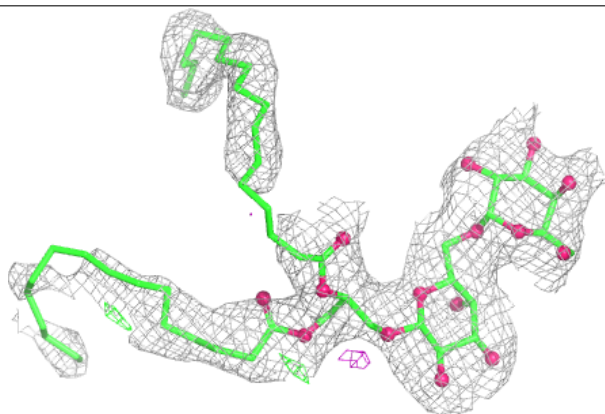


Electron density around BCR C 514:

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

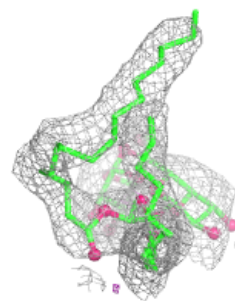
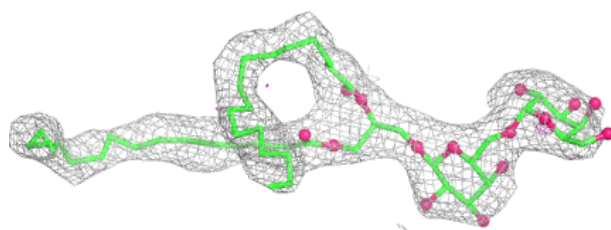
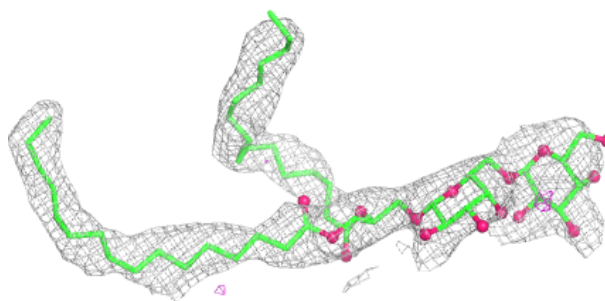
**Electron density around DGD c 519:**

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

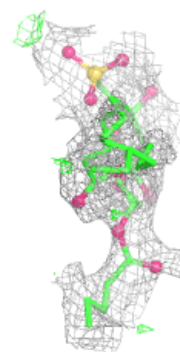
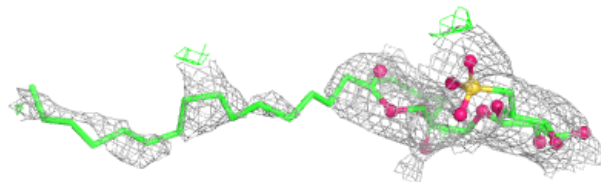
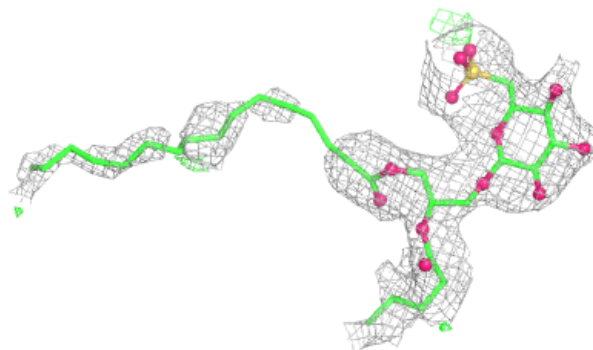


Electron density around DGD h 102:

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

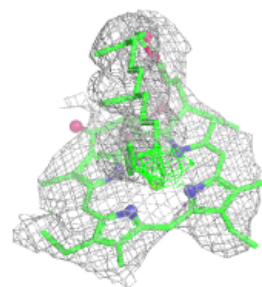
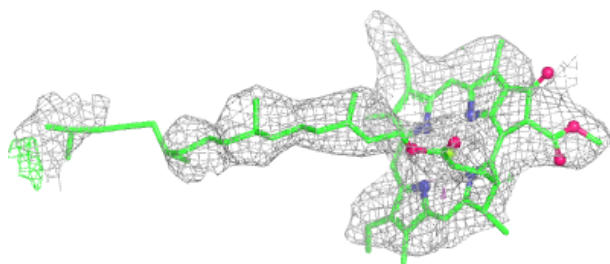
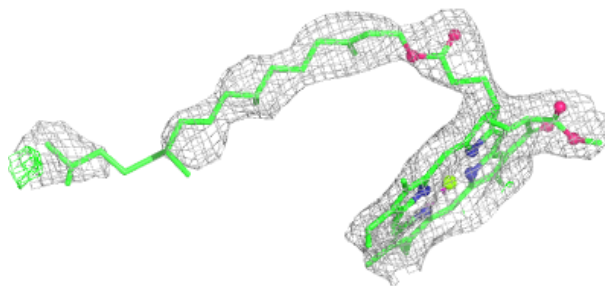
**Electron density around SQD f 101:**

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

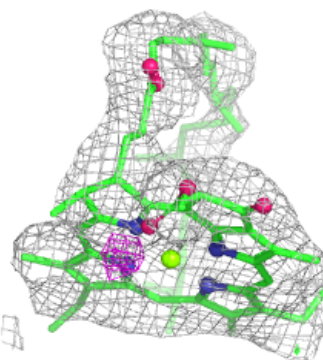
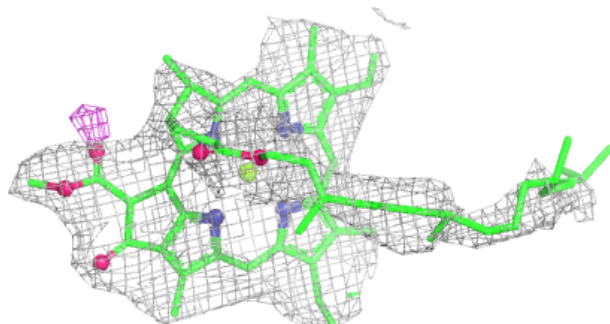
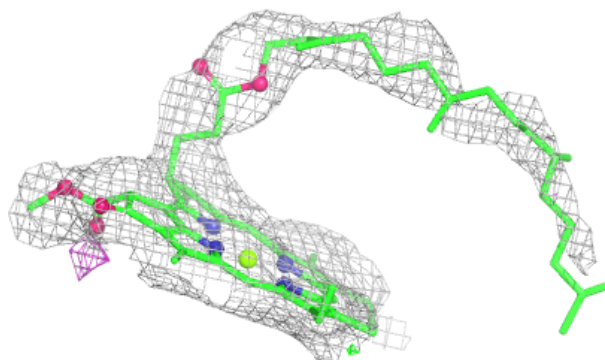


Electron density around CLA C 504:

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

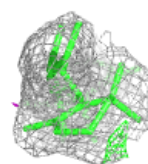
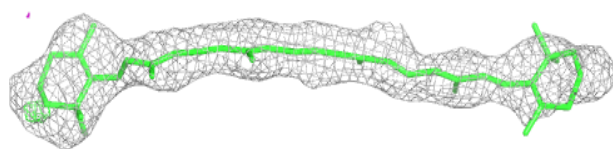
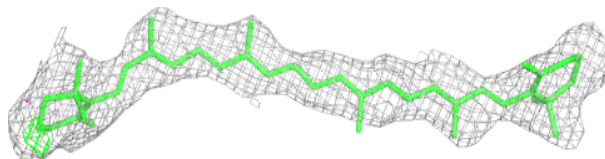
**Electron density around CLA c 515:**

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

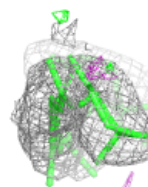
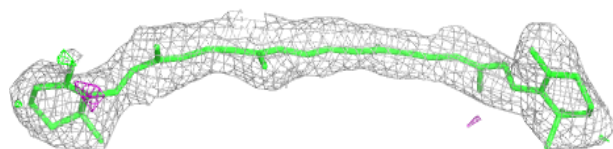
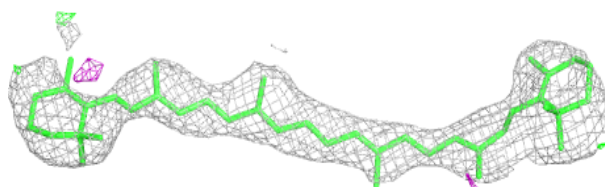


Electron density around BCR h 101:

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

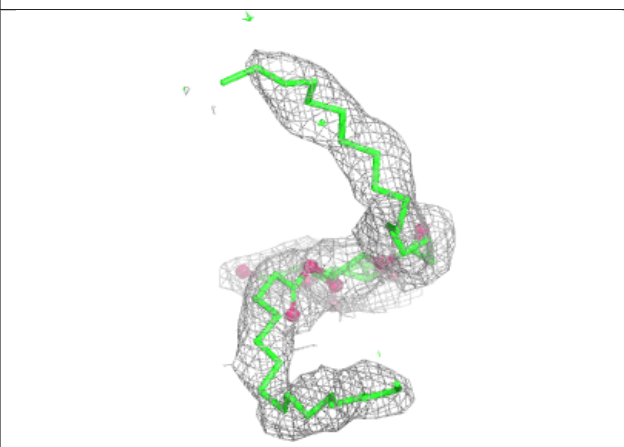
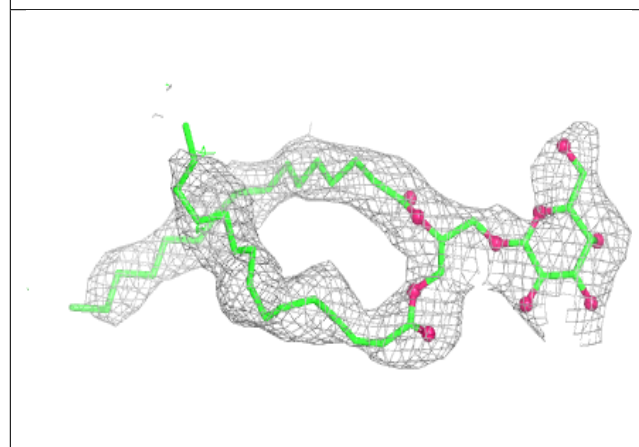
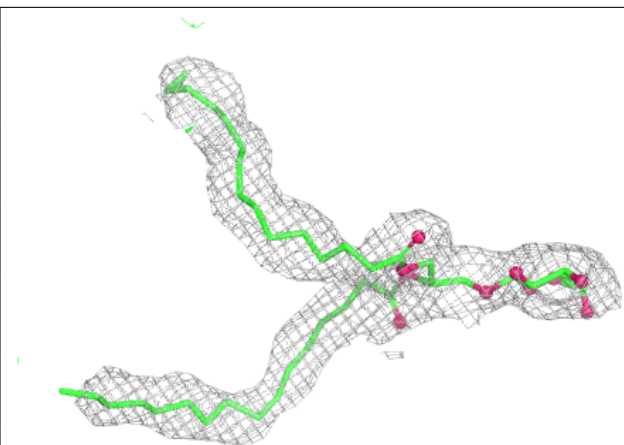
**Electron density around BCR B 627:**

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

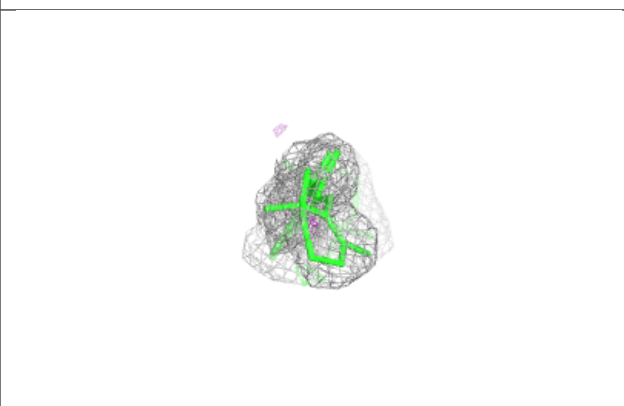
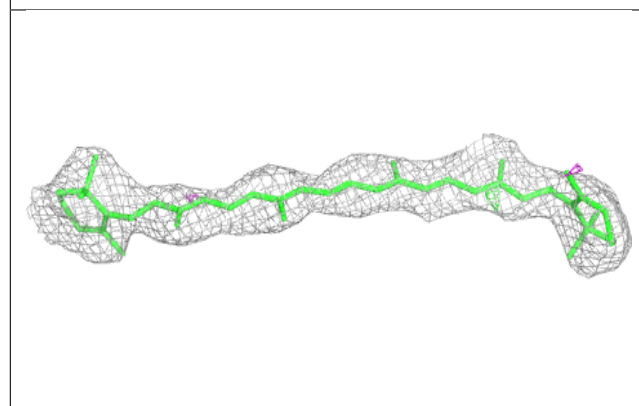
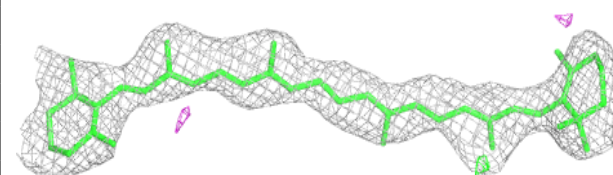


Electron density around LMG B 620:

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

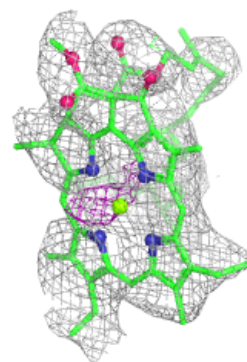
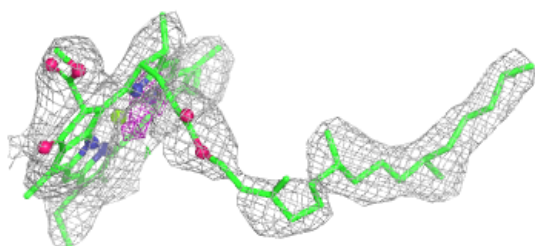
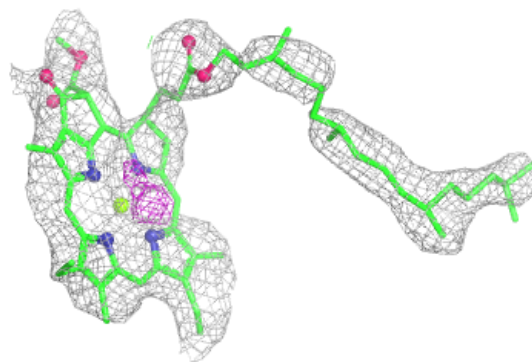
**Electron density around BCR b 622:**

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

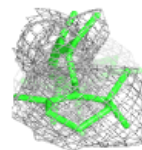
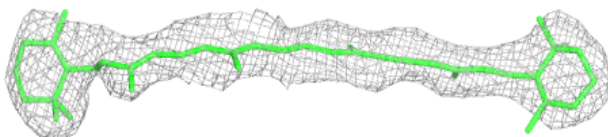
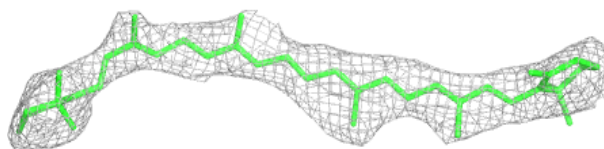


Electron density around CLA C 511:

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

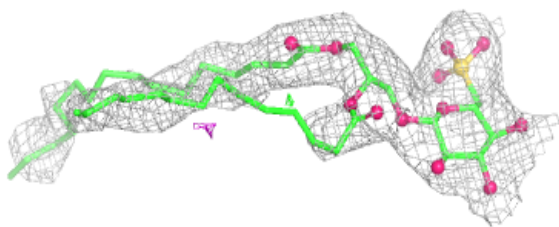
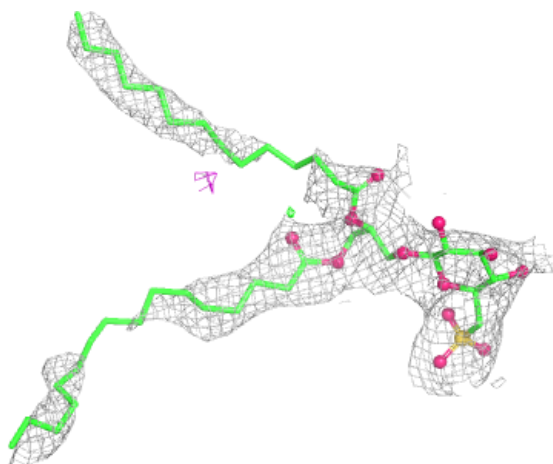
**Electron density around BCR H 102:**

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



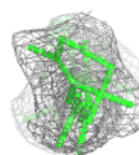
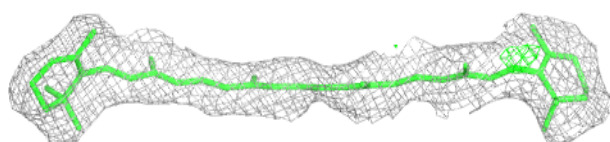
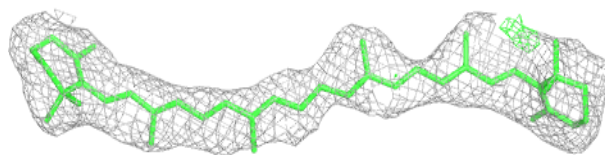
Electron density around SQD A 603:

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

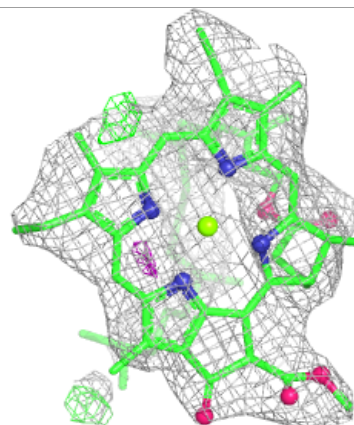
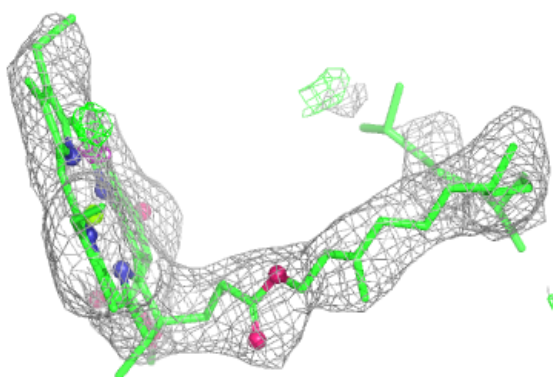
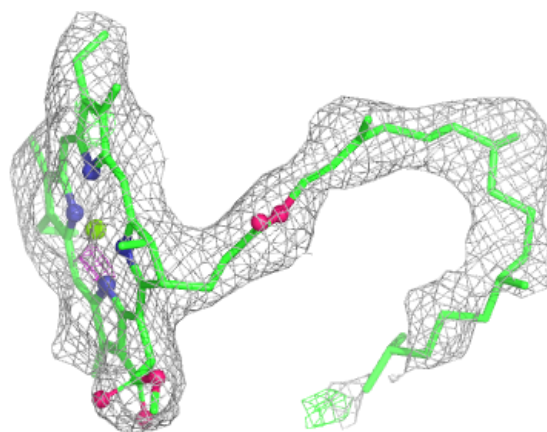


Electron density around BCR B 618:

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

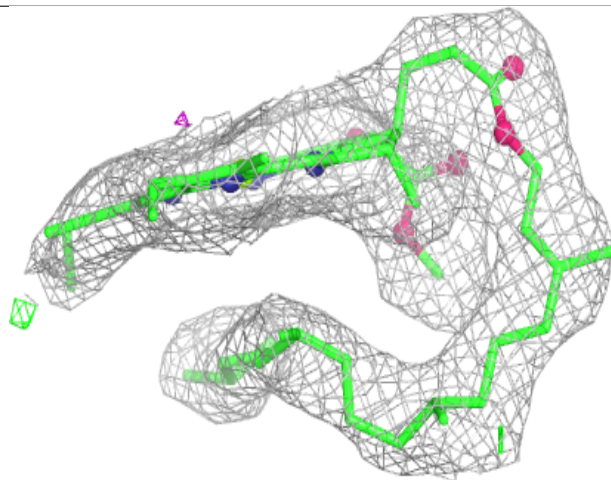
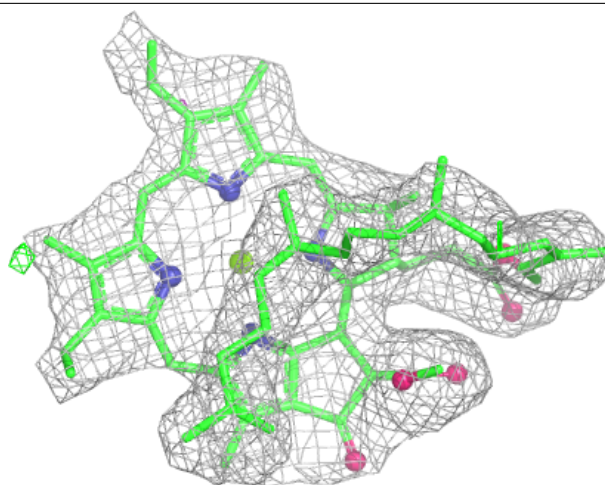
**Electron density around CLA B 606:**

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



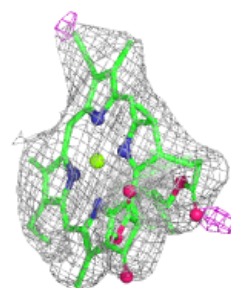
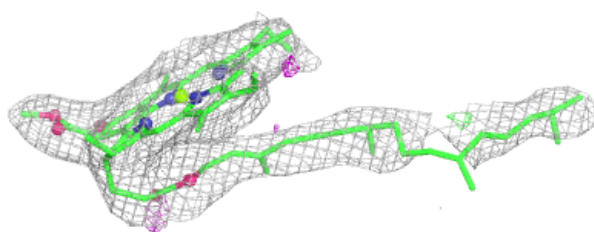
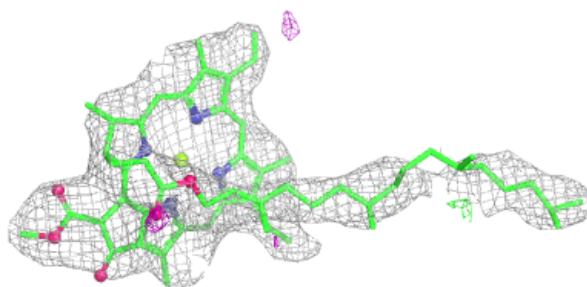
Electron density around CLA C 510:

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



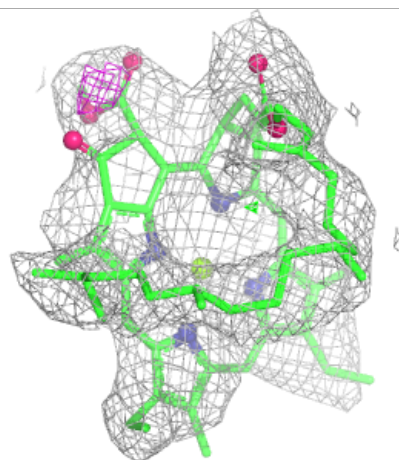
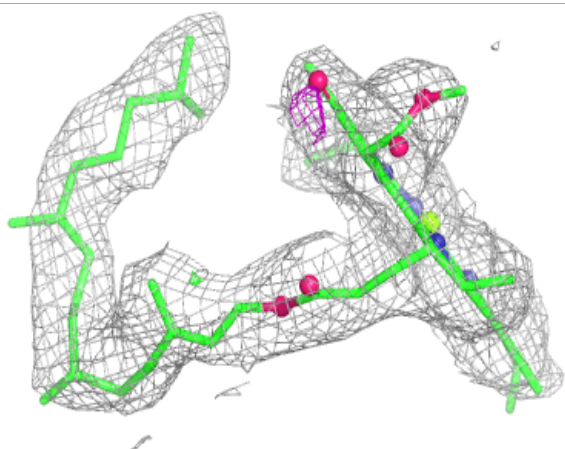
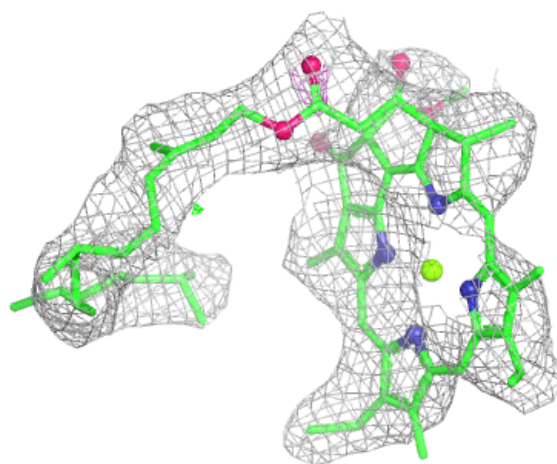
Electron density around CLA b 617:

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



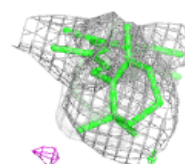
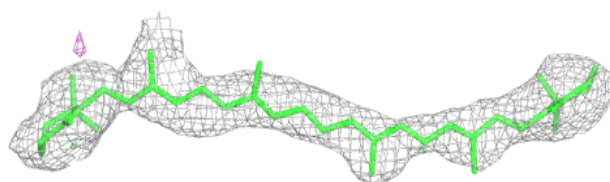
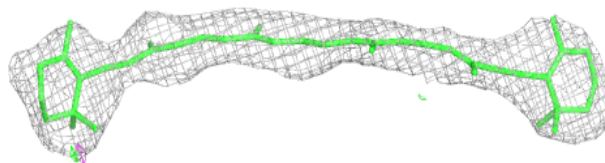
Electron density around CLA c 505:

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

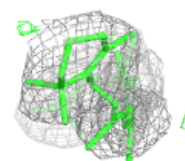
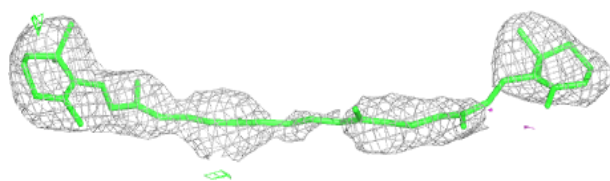
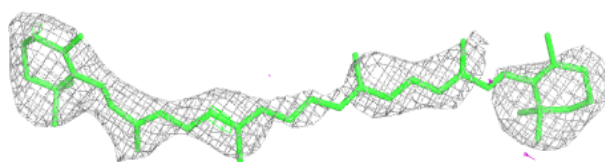


Electron density around BCR K 101:

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

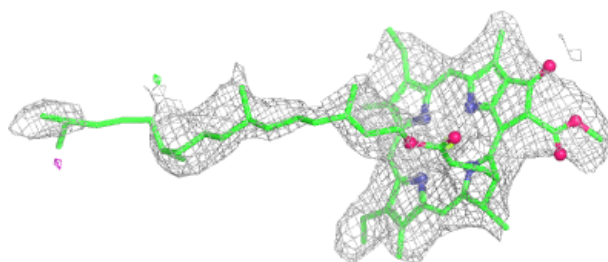
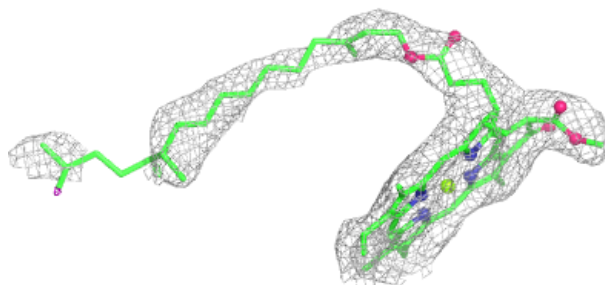
**Electron density around BCR T 101:**

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

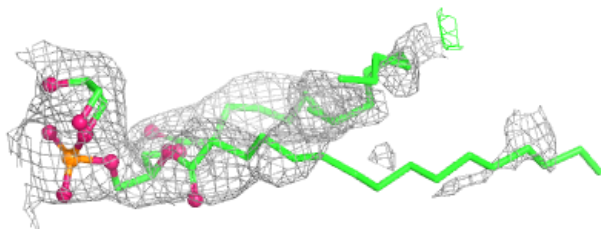
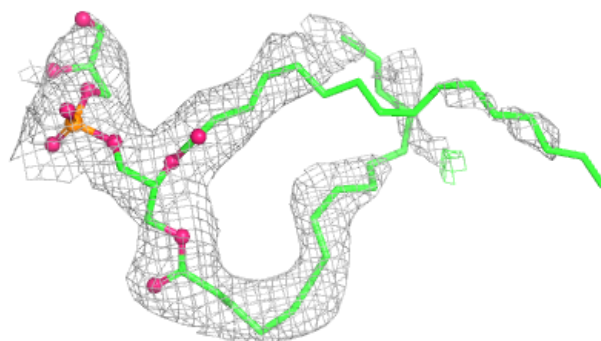


Electron density around CLA c 506:

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

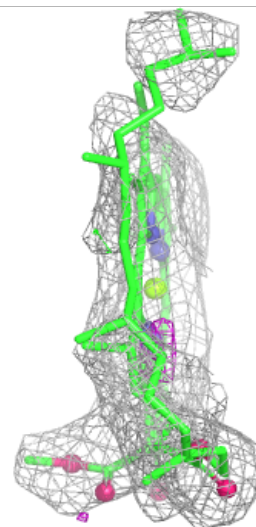
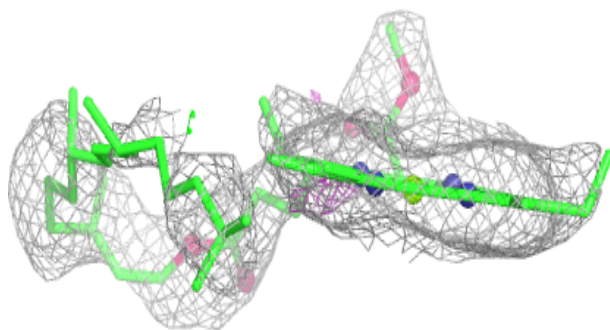
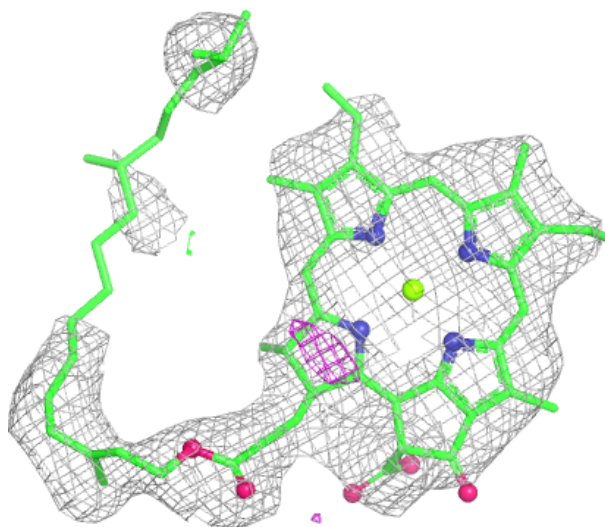
**Electron density around LHG A 617:**

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



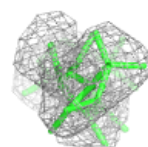
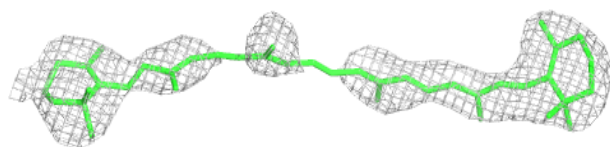
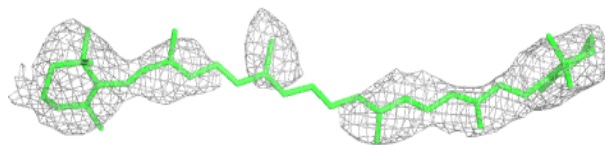
Electron density around CLA c 514:

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

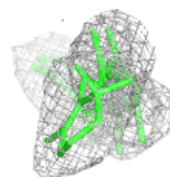
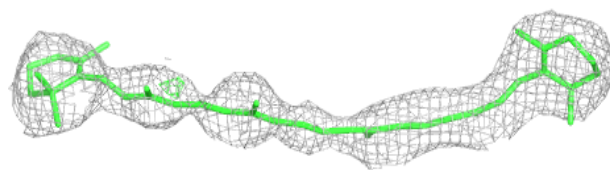
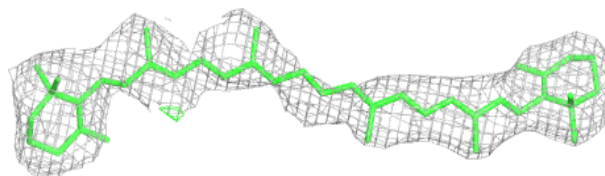


Electron density around BCR c 516:

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

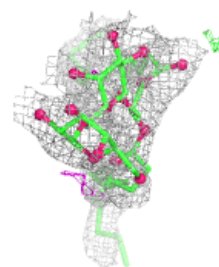
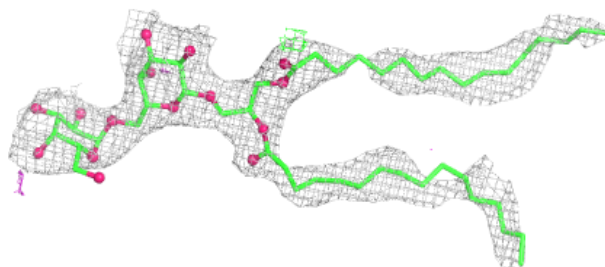
**Electron density around BCR d 405:**

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

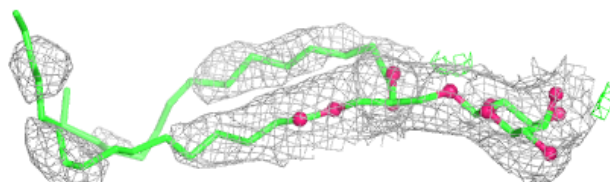
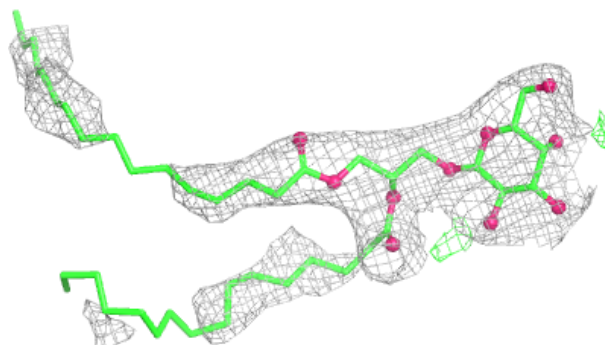


Electron density around DGD C 518:

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

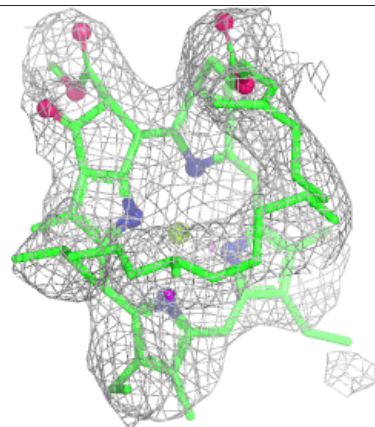
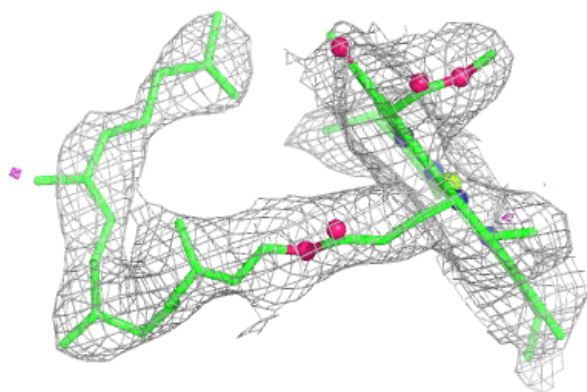
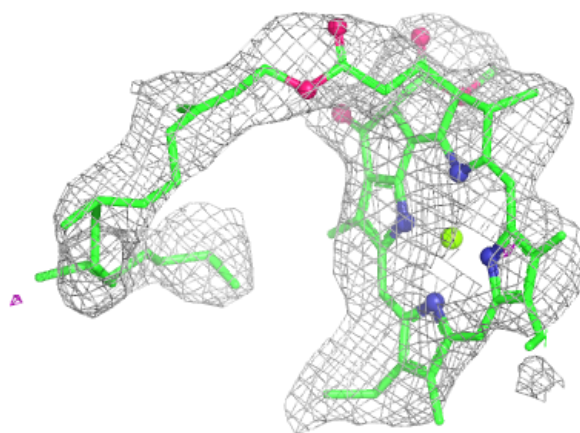
**Electron density around LMG D 405:**

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

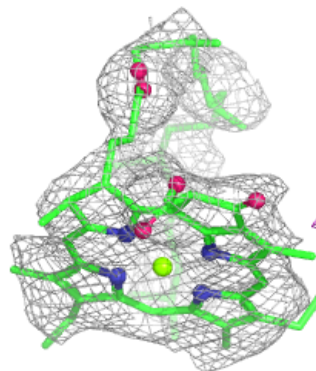
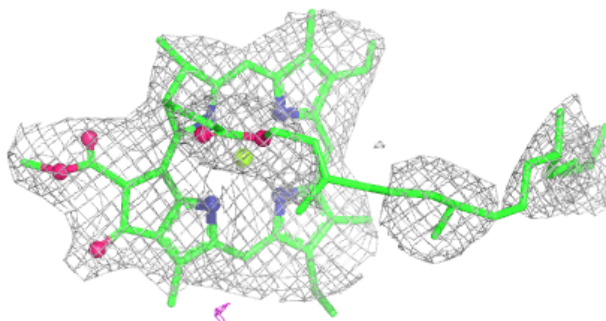
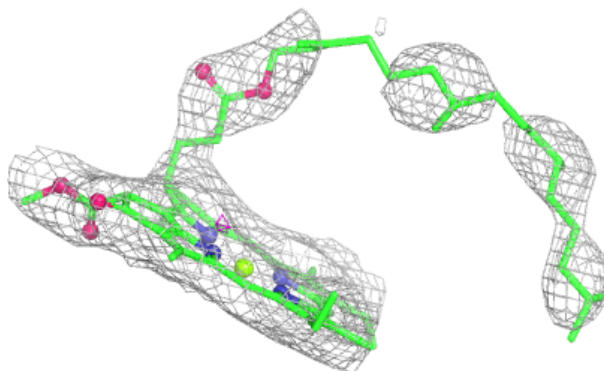


Electron density around CLA C 503:

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

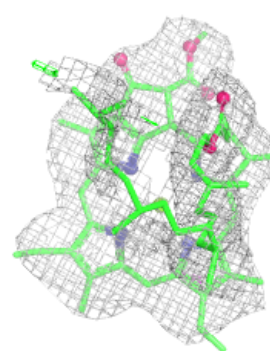
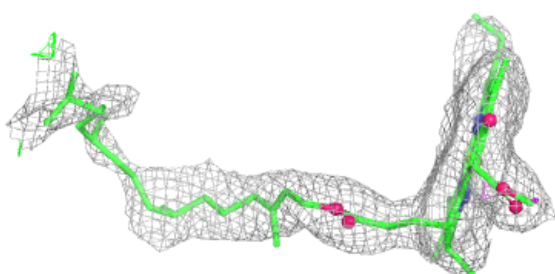
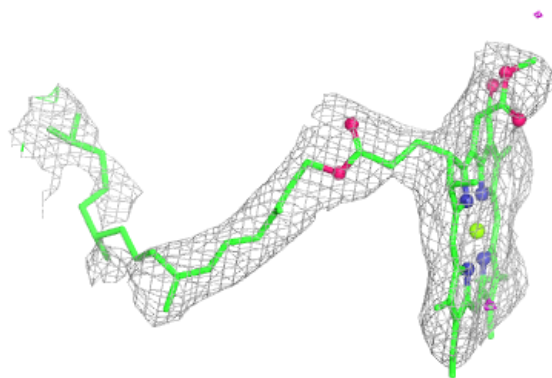
**Electron density around CLA C 513:**

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

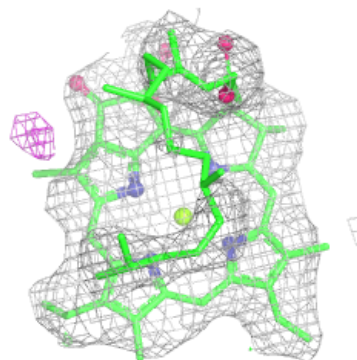
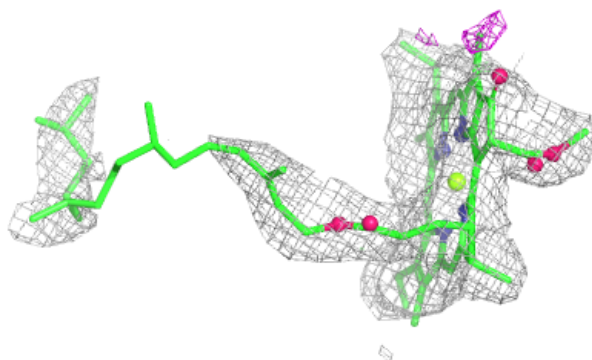
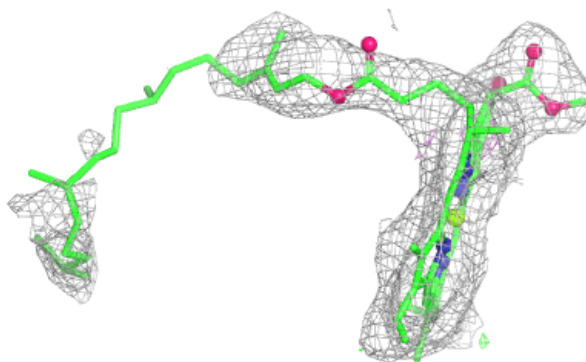


Electron density around CLA d 404:

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

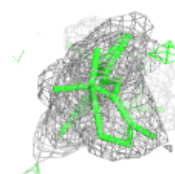
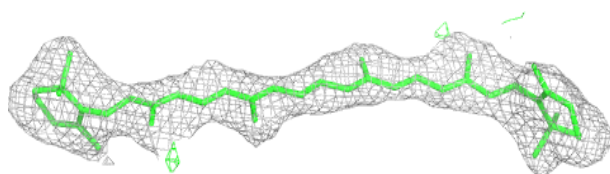
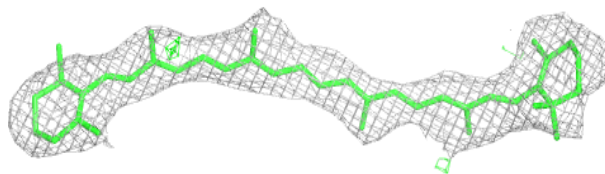
**Electron density around CLA c 508:**

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

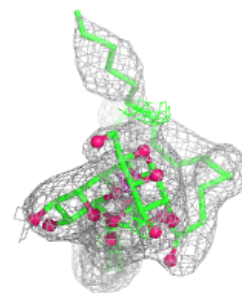
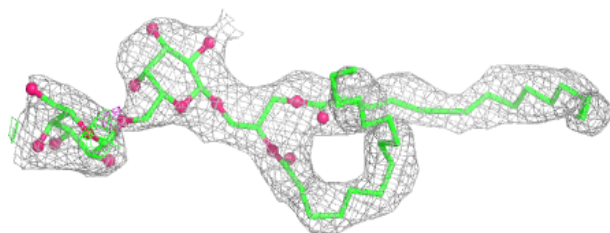
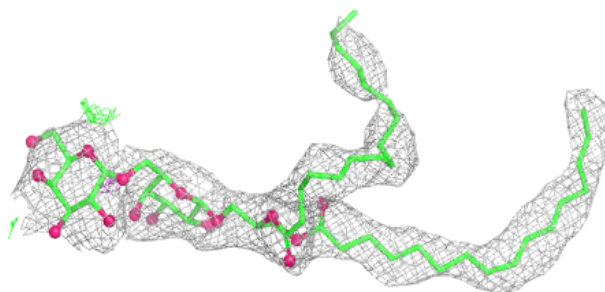


Electron density around BCR B 619:

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

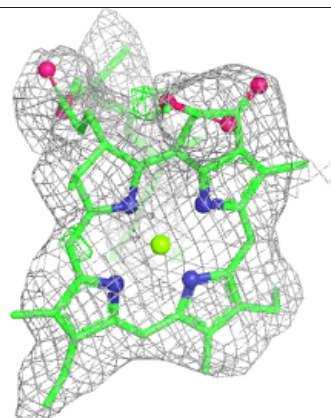
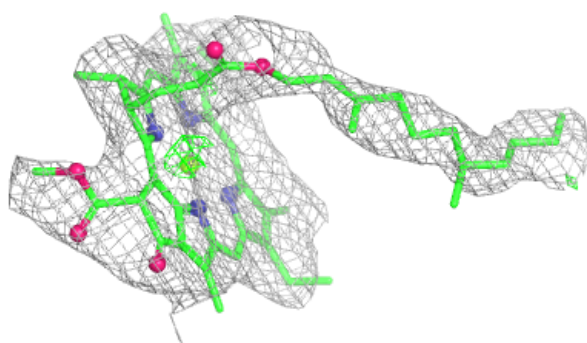
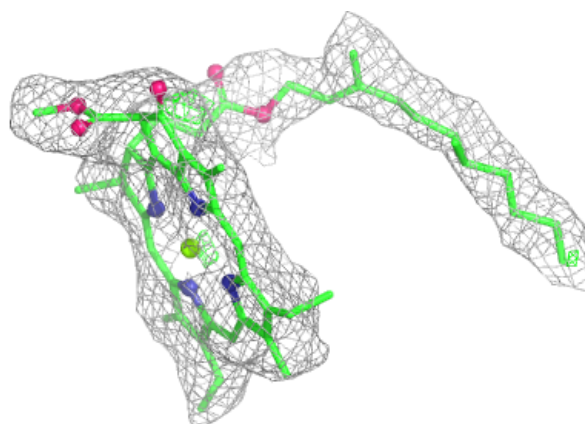
**Electron density around DGD H 103:**

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

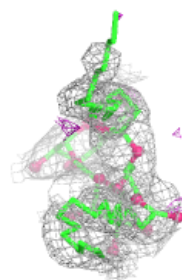
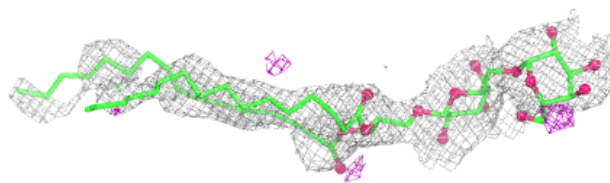
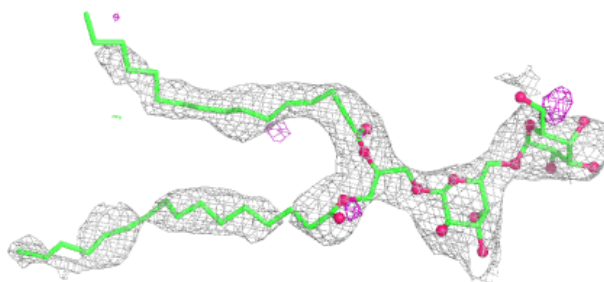


Electron density around CLA c 510:

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

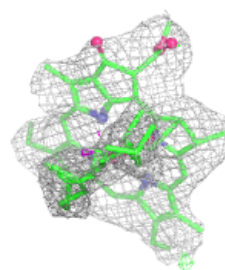
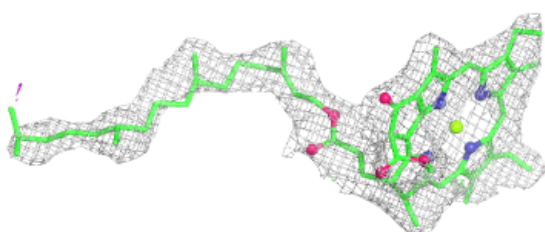
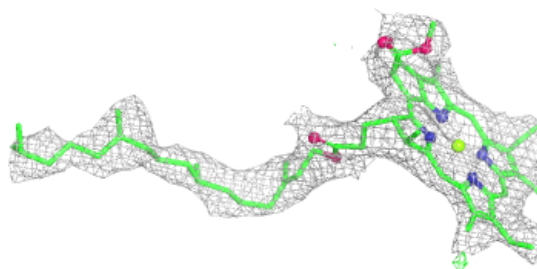
**Electron density around DGD c 520:**

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

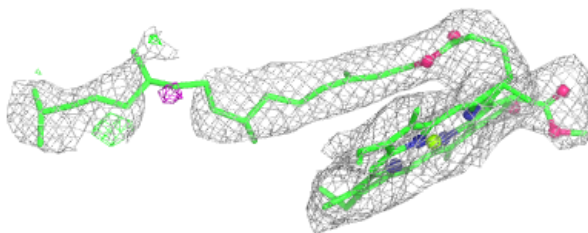
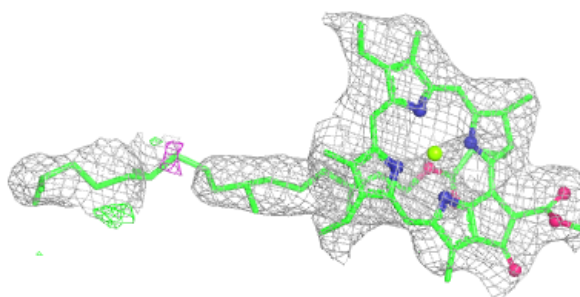


Electron density around CLA C 502:

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

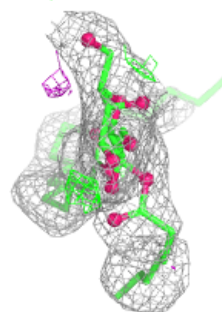
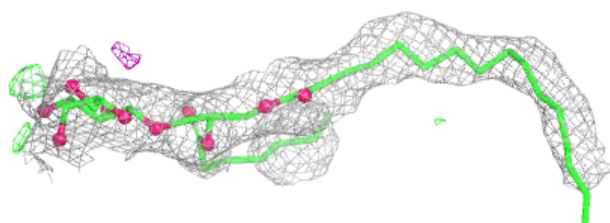
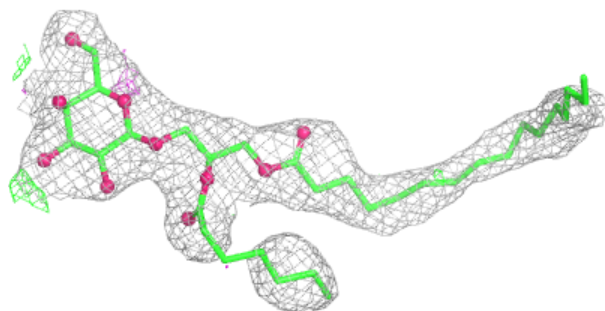
**Electron density around CLA B 614:**

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

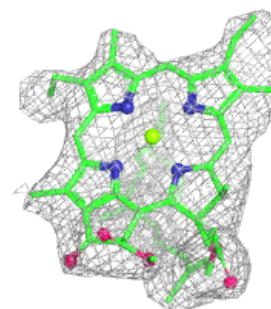
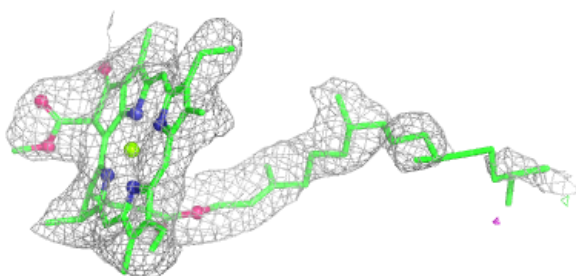
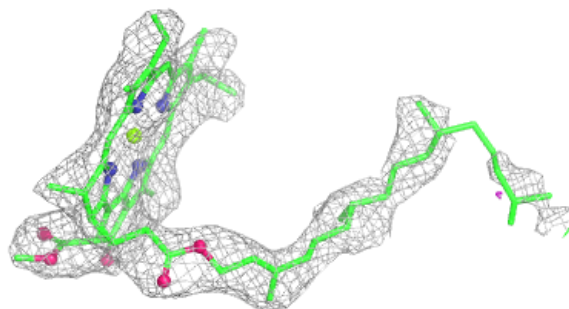


Electron density around LMG d 406:

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

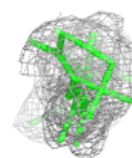
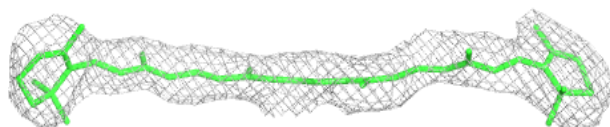
**Electron density around CLA C 508:**

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

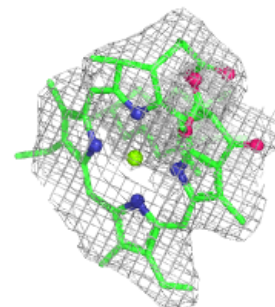
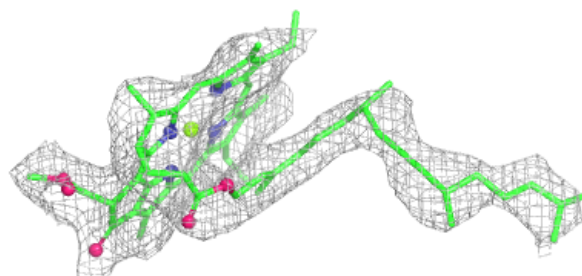
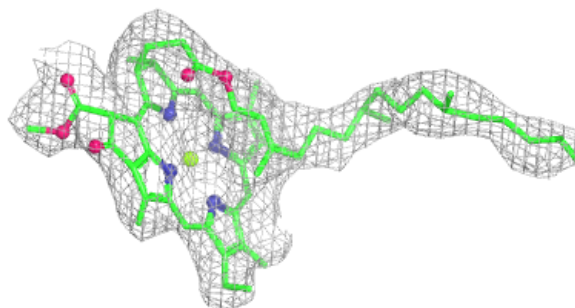


Electron density around BCR b 621:

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

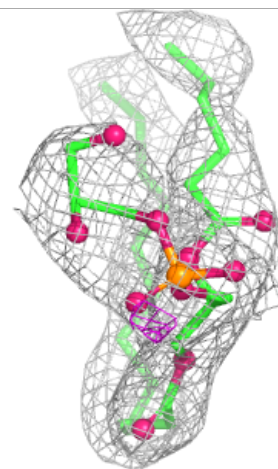
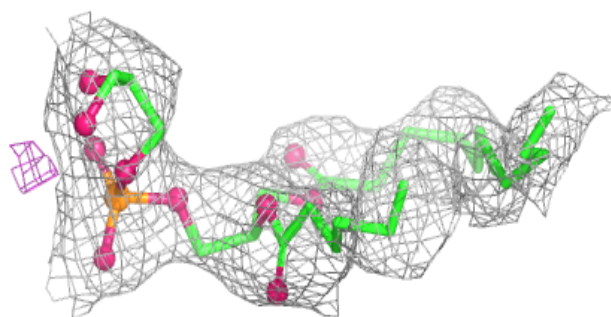
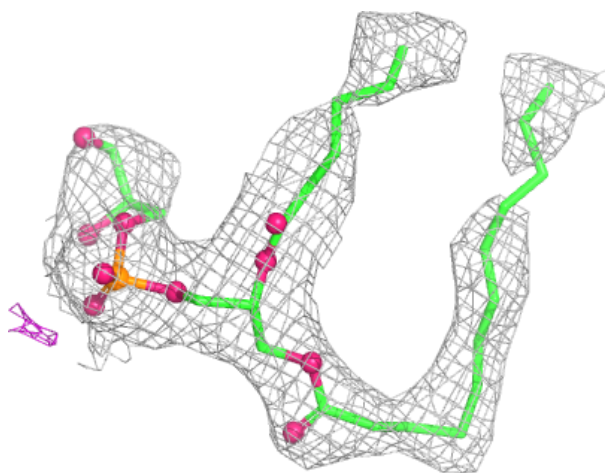
**Electron density around CLA c 507:**

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



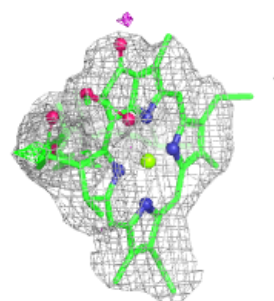
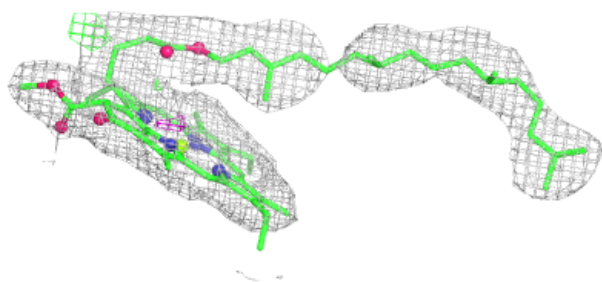
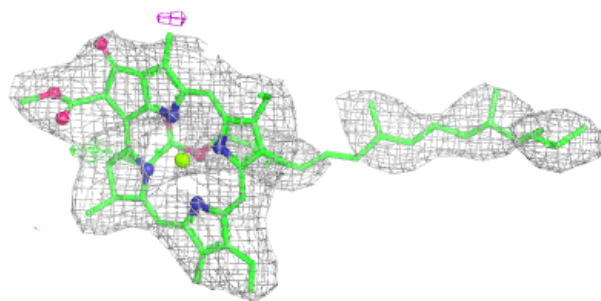
Electron density around LHG a 614:

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



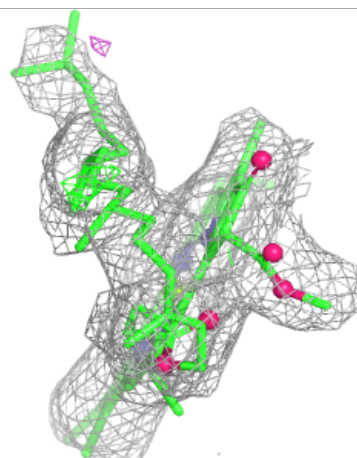
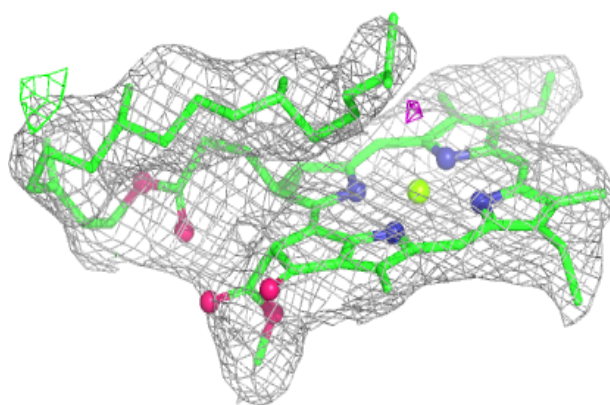
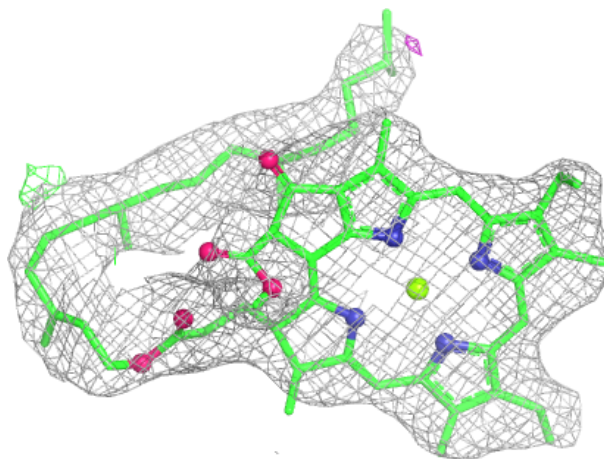
Electron density around CLA B 608:

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



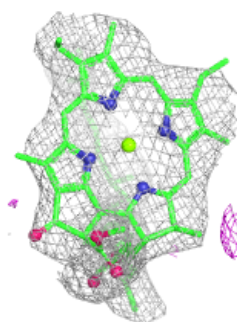
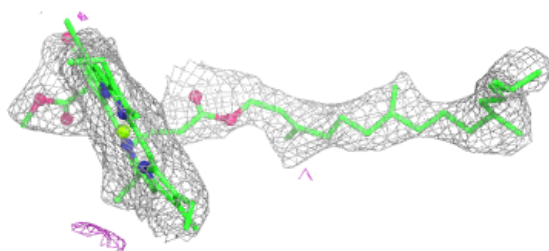
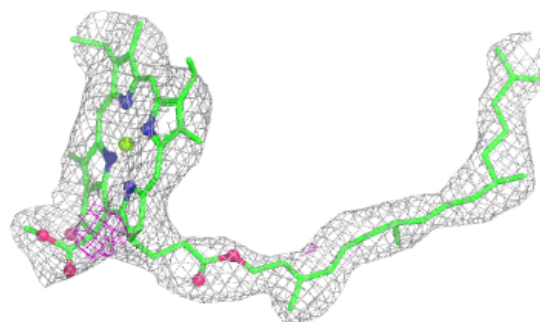
Electron density around CLA C 509:

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

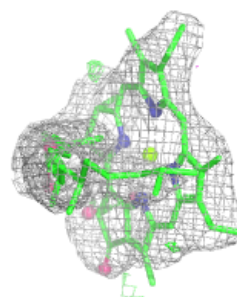
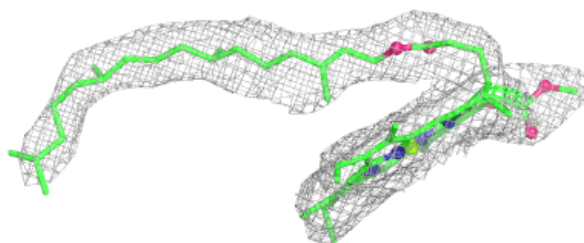
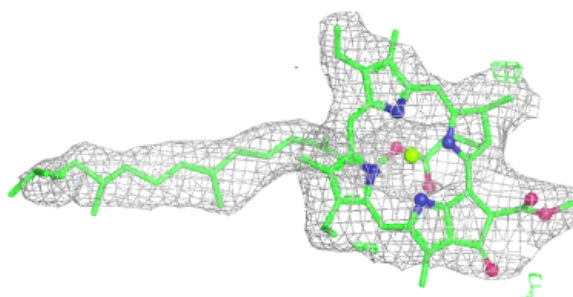


Electron density around CLA B 609:

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

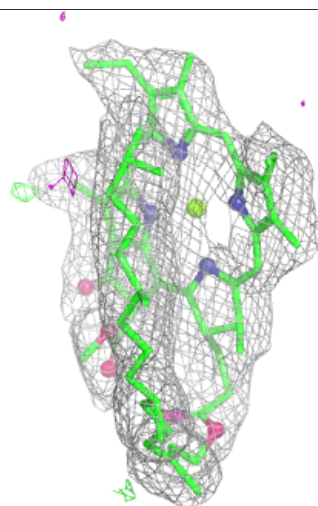
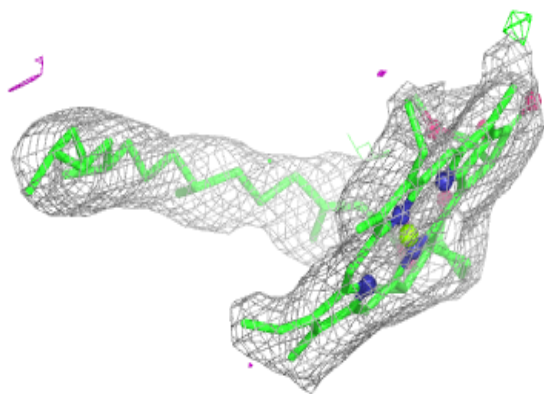
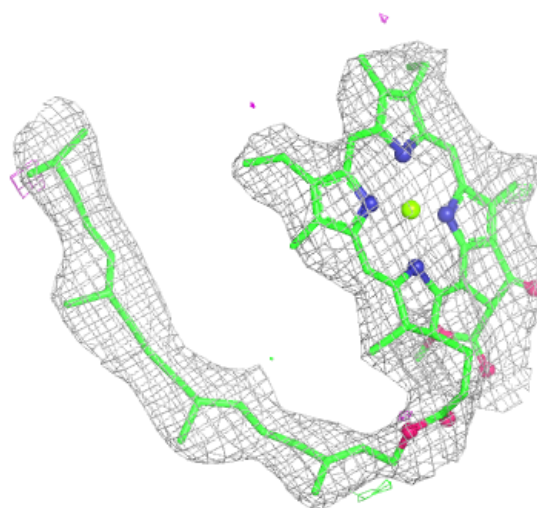
**Electron density around CLA b 611:**

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



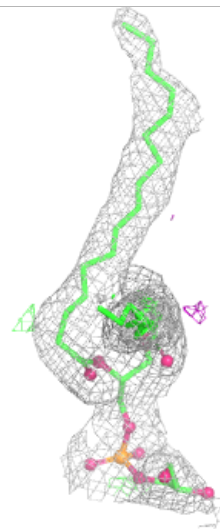
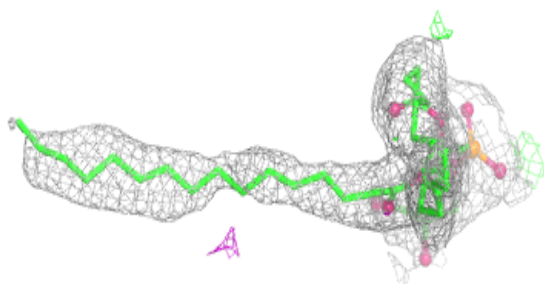
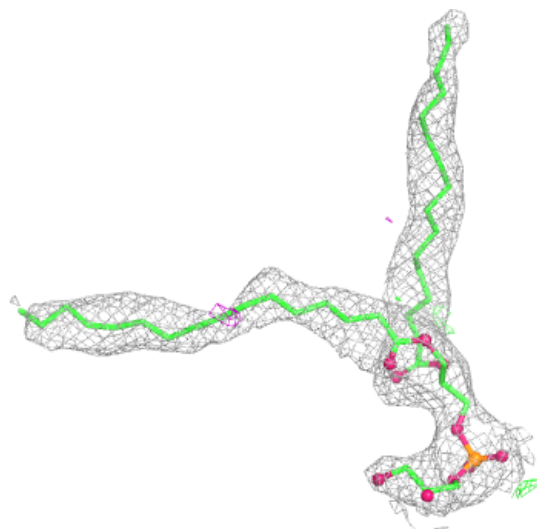
Electron density around CLA c 509:

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



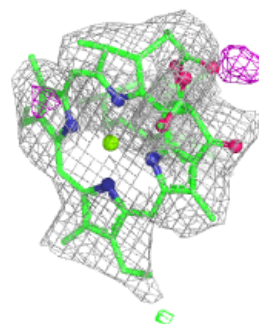
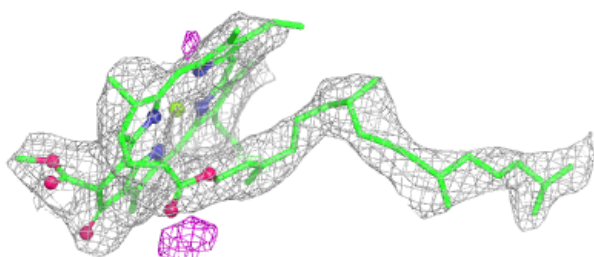
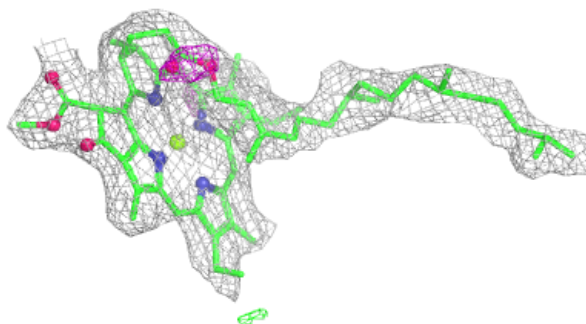
Electron density around LHG 1 101:

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

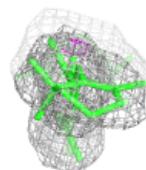
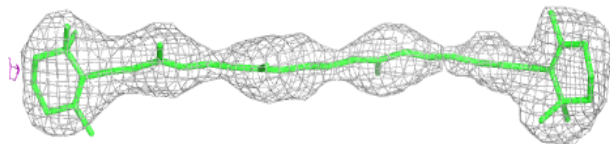
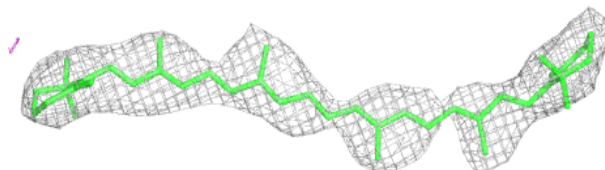


Electron density around CLA C 505:

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

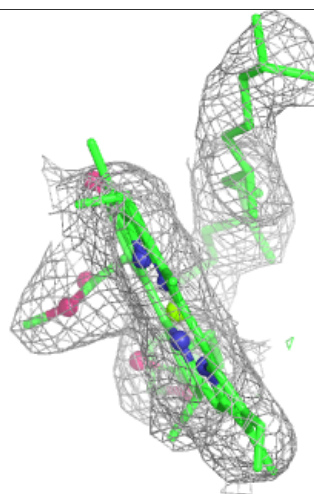
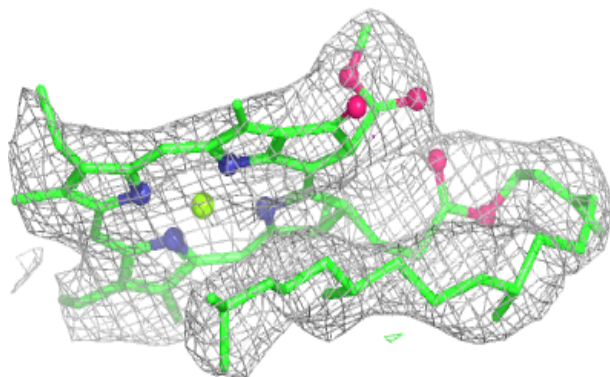
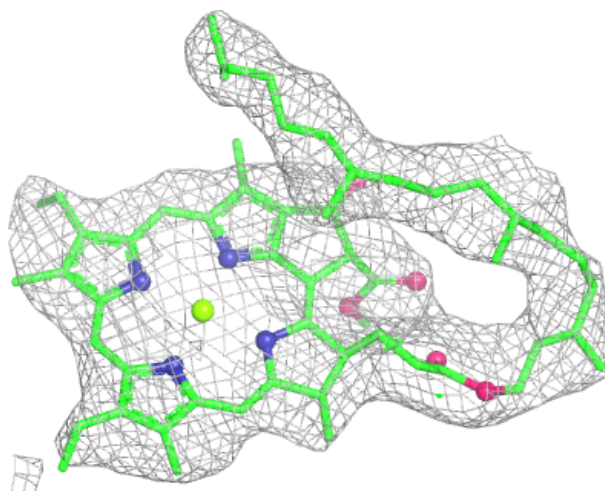
**Electron density around BCR C 515:**

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



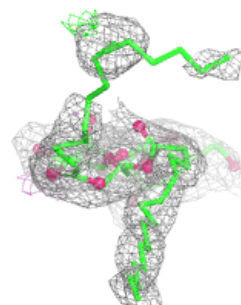
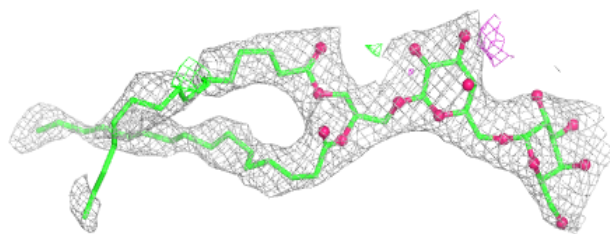
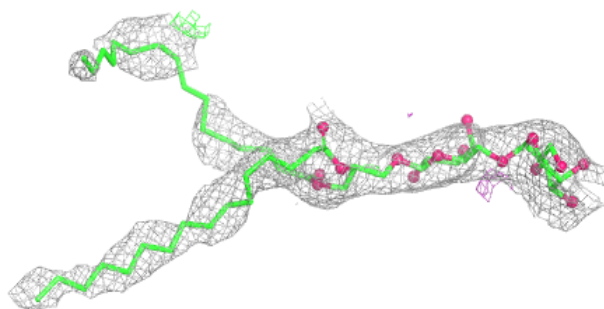
Electron density around CLA c 511:

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

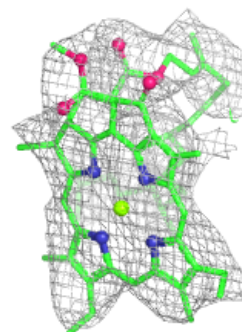
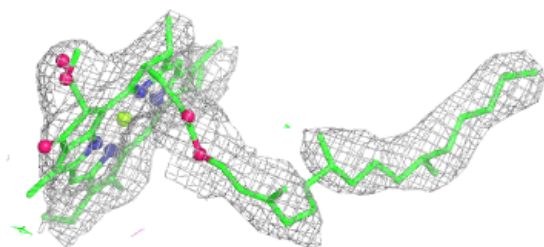
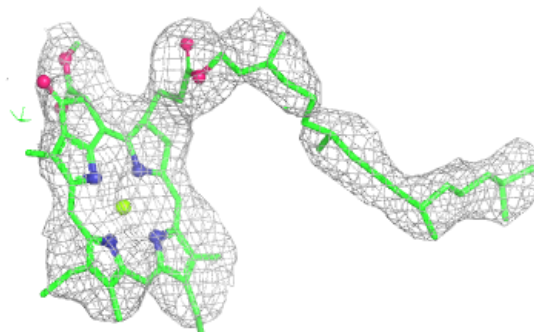


Electron density around DGD c 518:

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

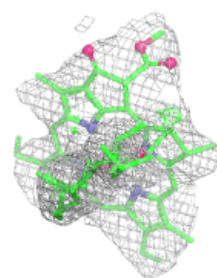
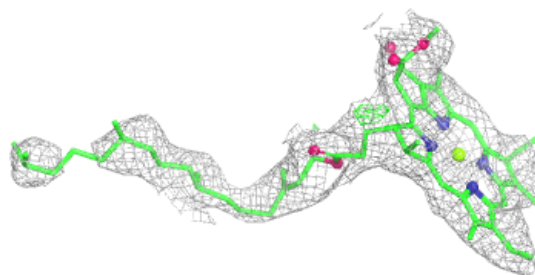
**Electron density around CLA c 513:**

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

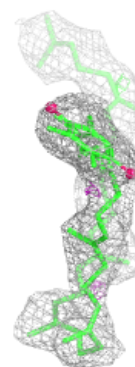
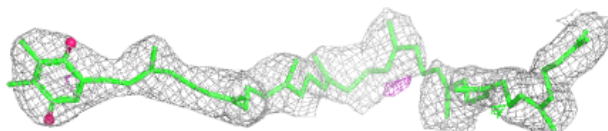
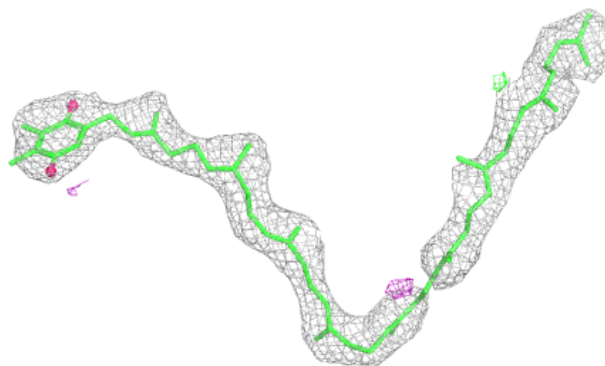


Electron density around CLA c 504:

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

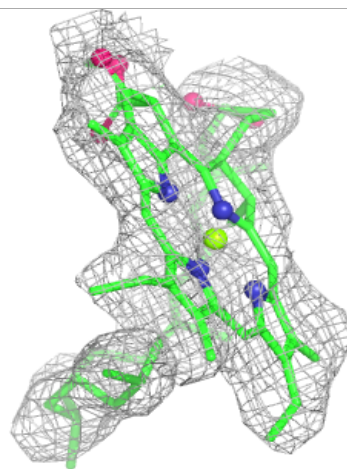
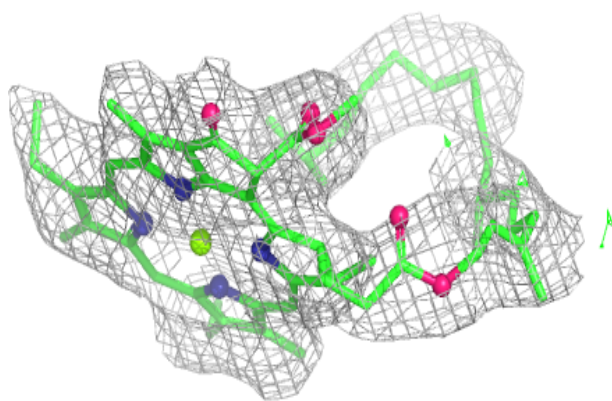
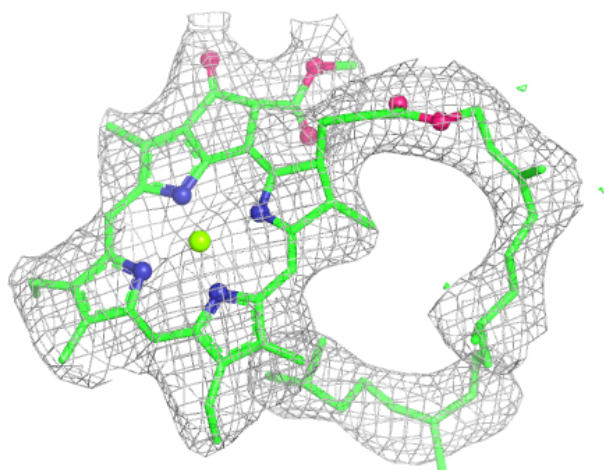
**Electron density around PL9 D 407:**

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



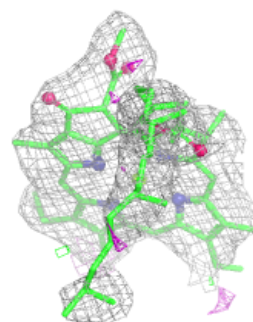
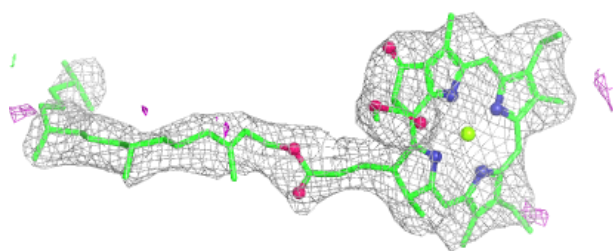
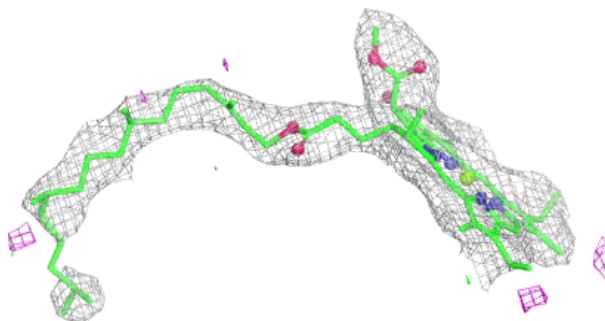
Electron density around CLA B 615:

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

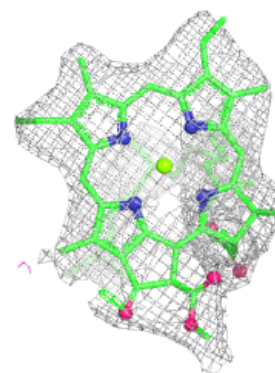
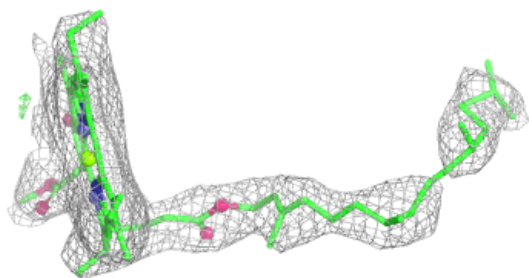
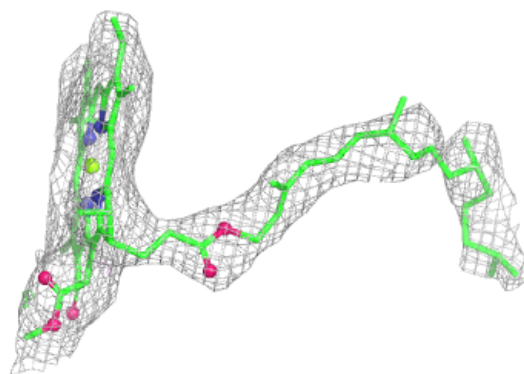


Electron density around CLA D 402:

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

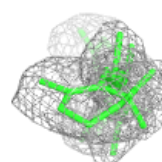
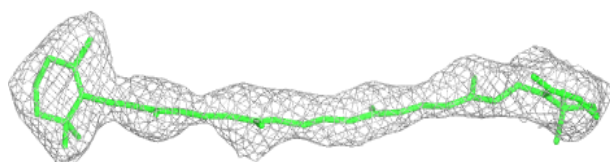
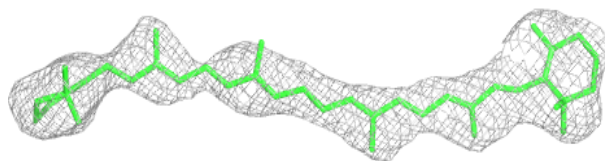
**Electron density around CLA D 403:**

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

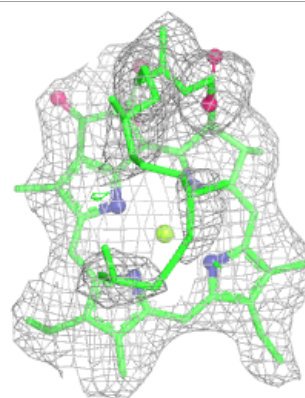
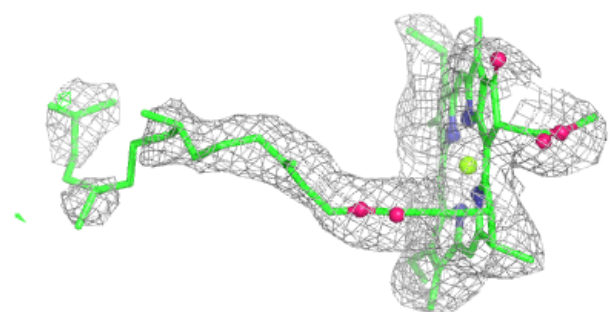
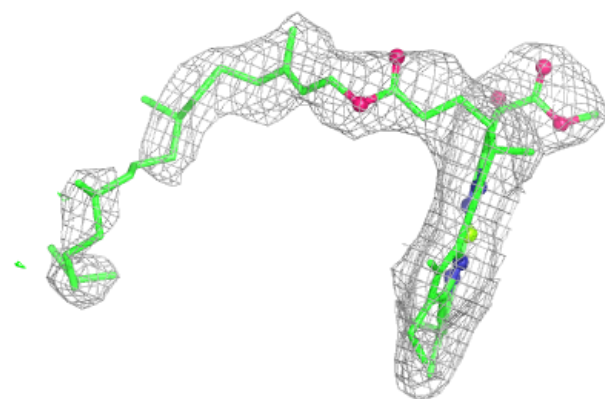


Electron density around BCR b 620:

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

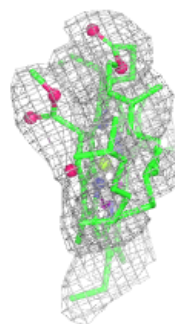
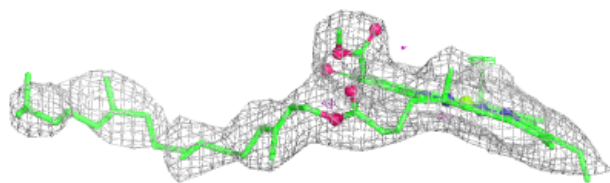
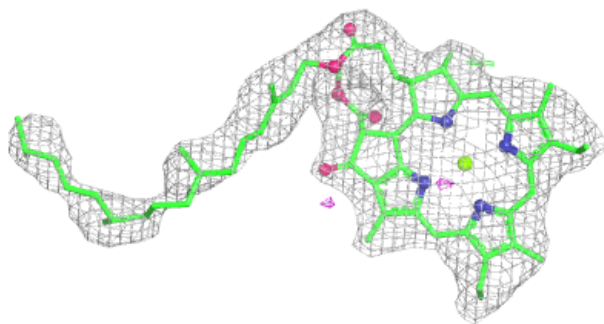
**Electron density around CLA C 506:**

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

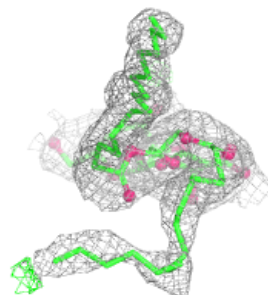
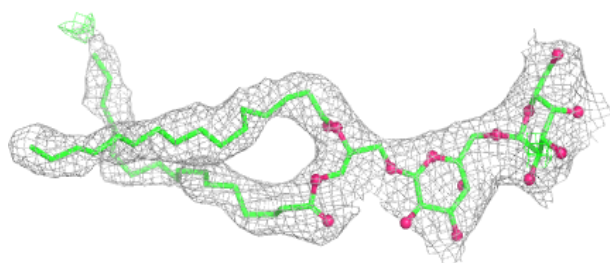
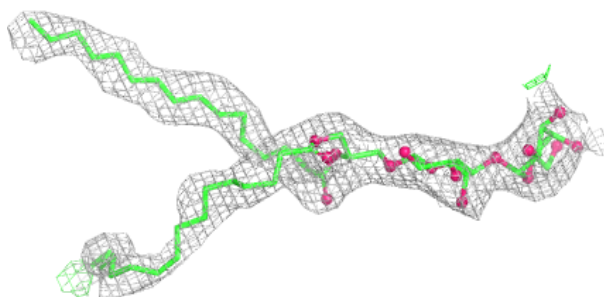


Electron density around CLA b 605:

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

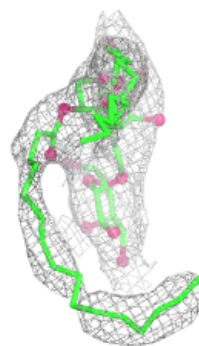
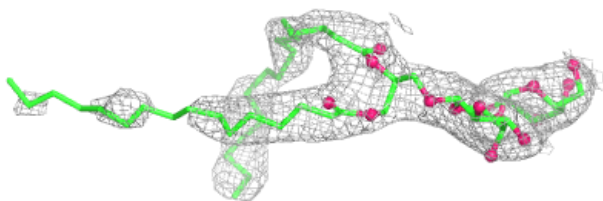
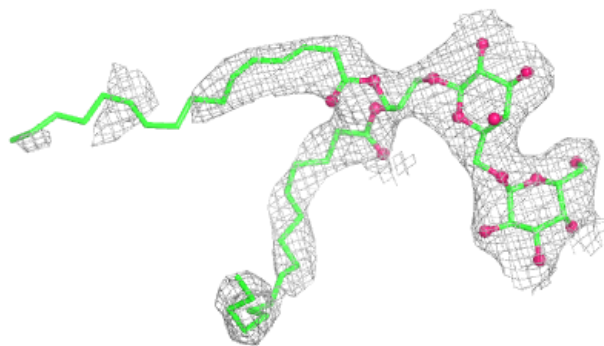
**Electron density around DGD C 516:**

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



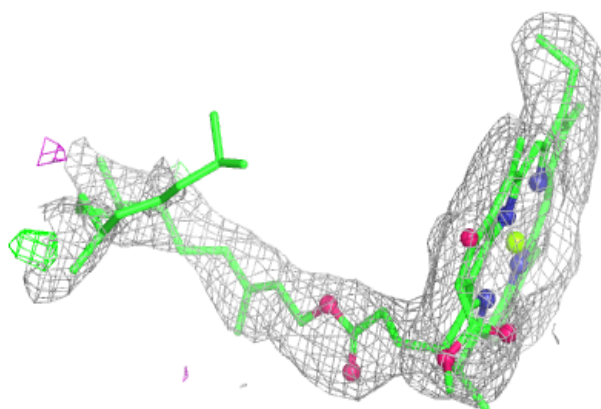
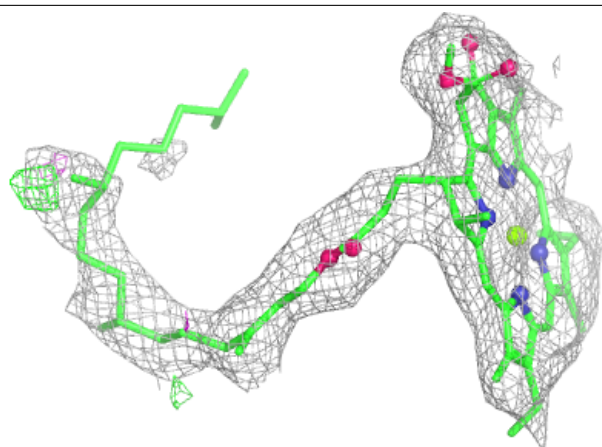
Electron density around DGD C 517:

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

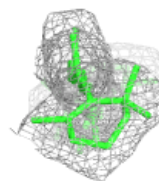
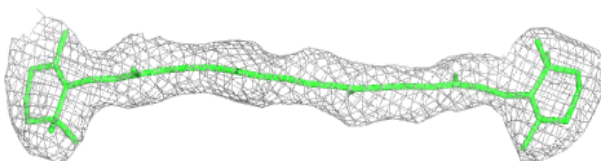
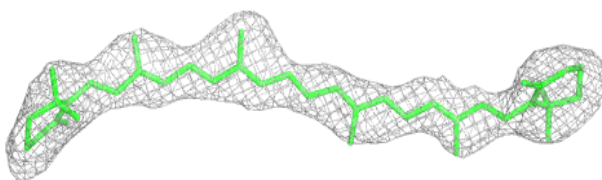


Electron density around CLA b 609:

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

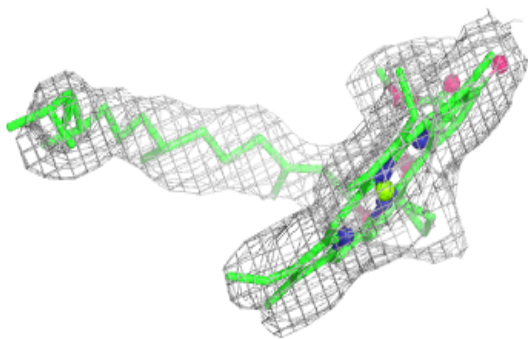
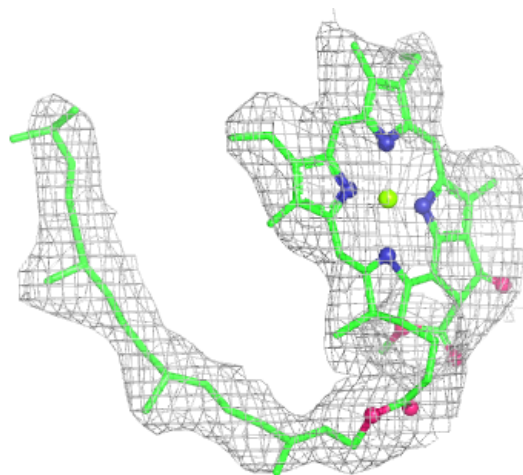
**Electron density around BCR c 517:**

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



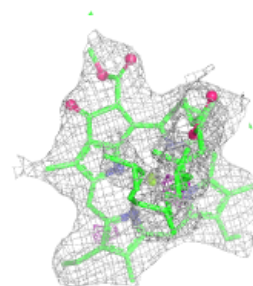
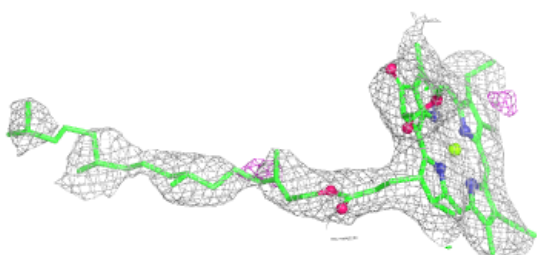
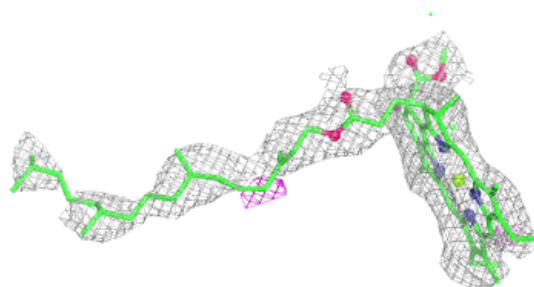
Electron density around CLA C 507:

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



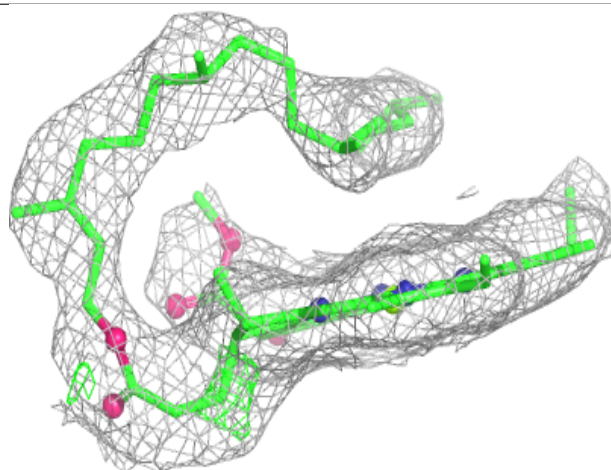
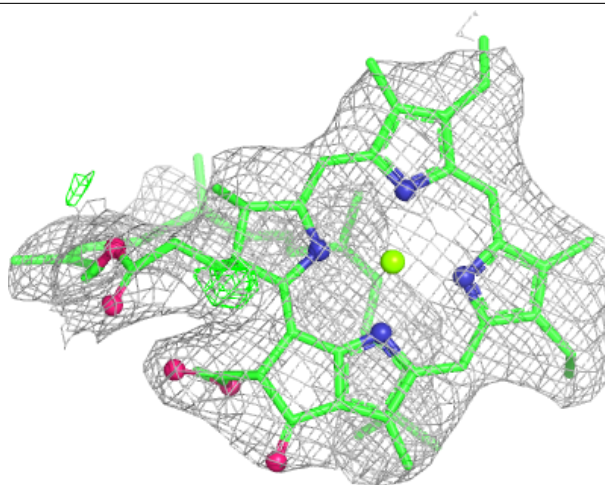
Electron density around CLA B 604:

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



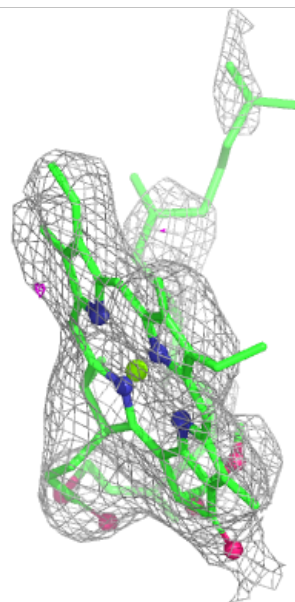
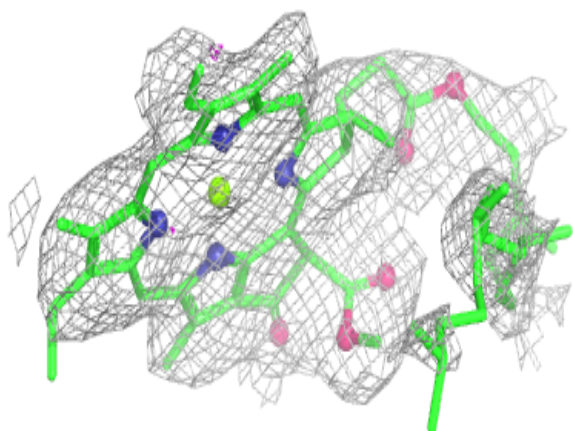
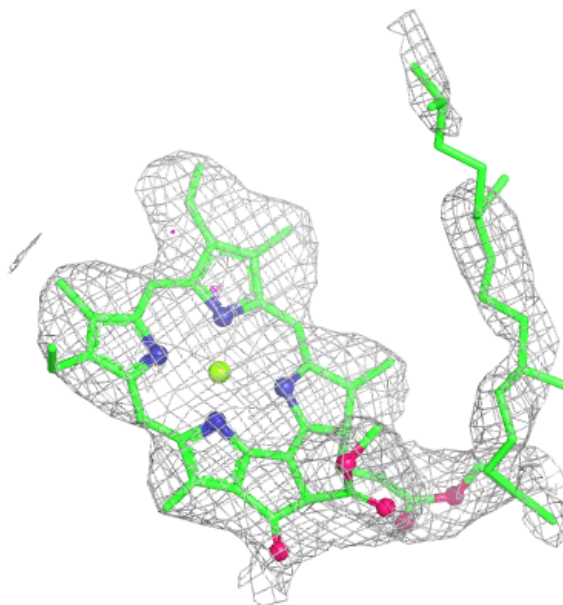
Electron density around CLA c 512:

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



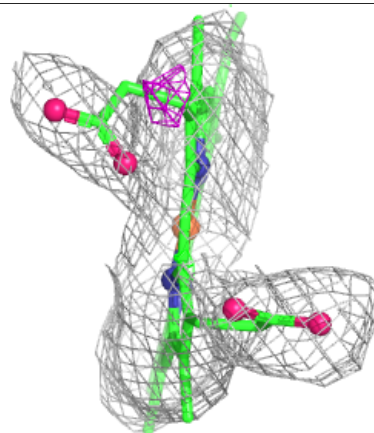
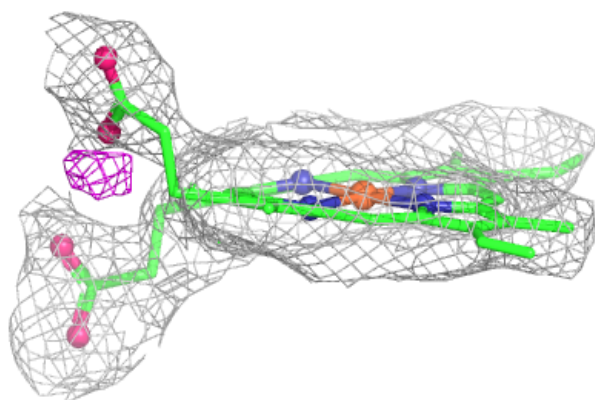
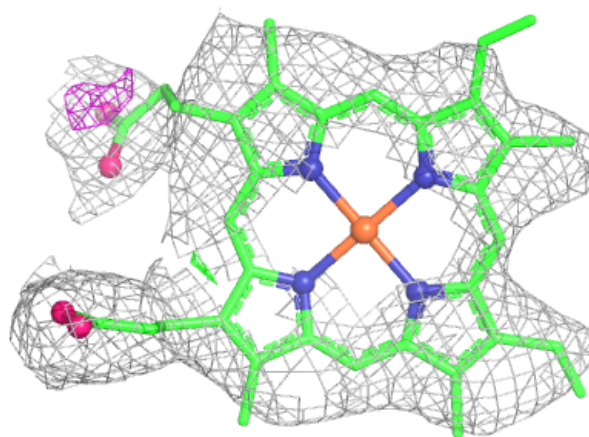
Electron density around CLA b 619:

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



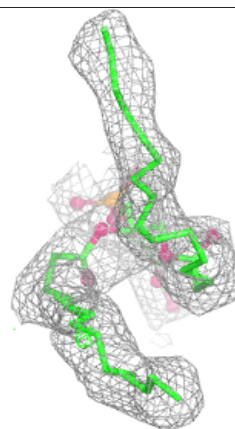
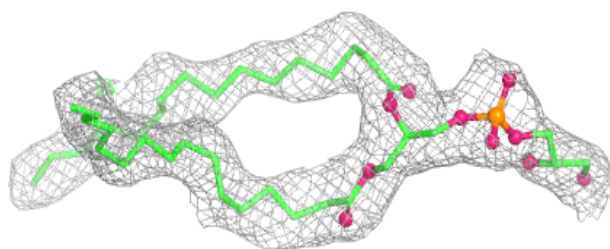
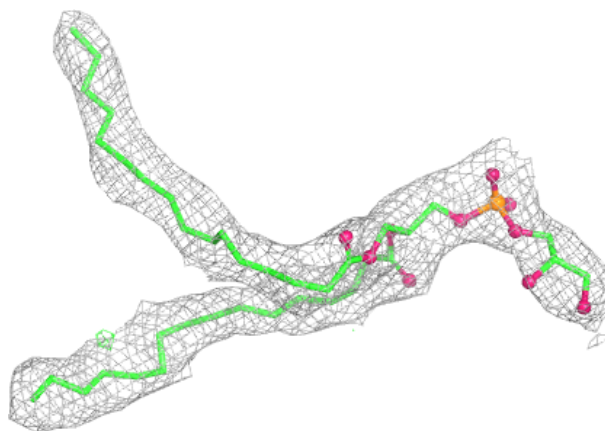
Electron density around HEM e 101:

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



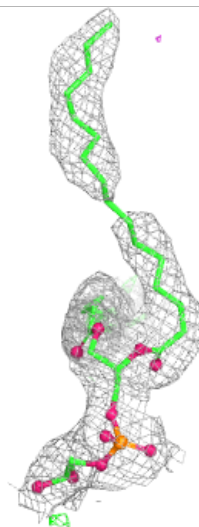
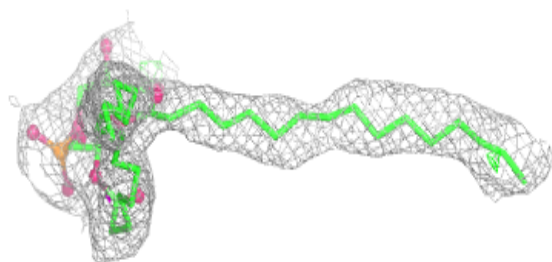
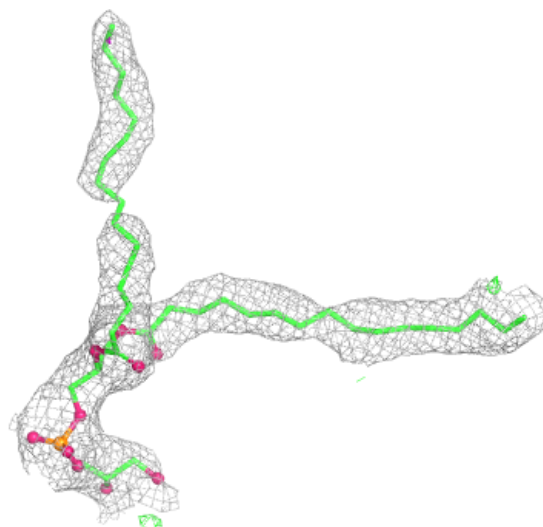
Electron density around LHG D 406:

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



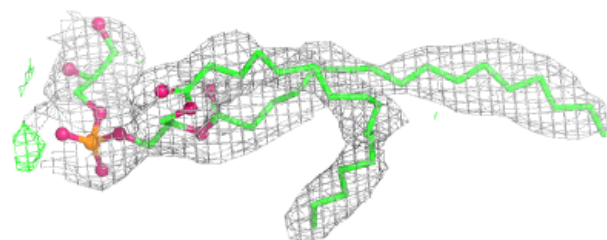
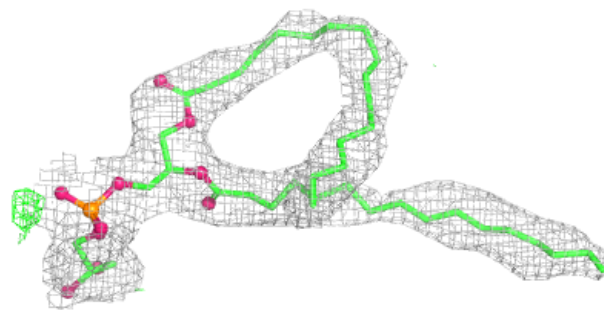
Electron density around LHG L 101:

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

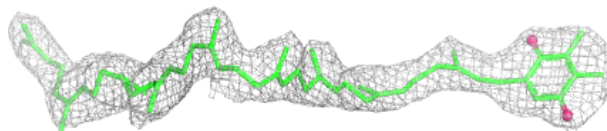
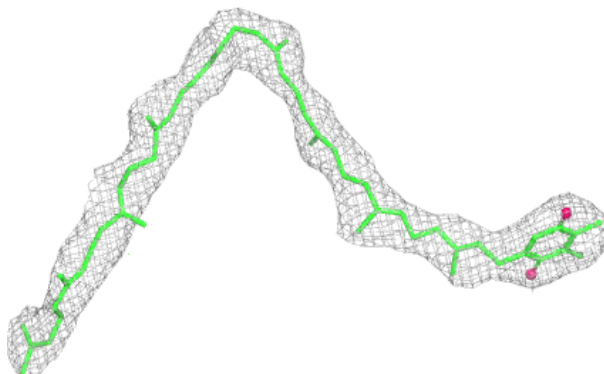


Electron density around LHG a 613:

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

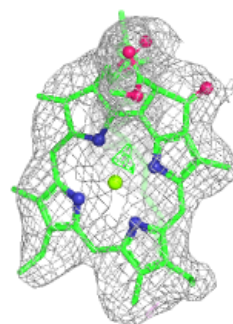
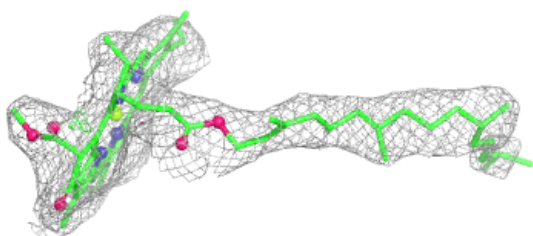
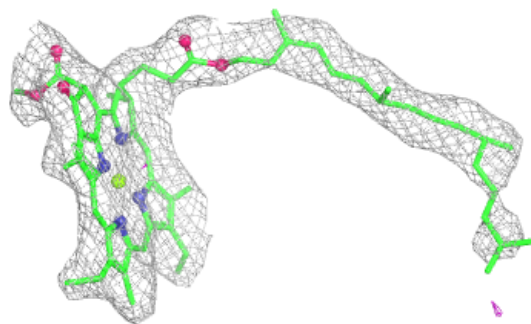
**Electron density around PL9 d 408:**

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



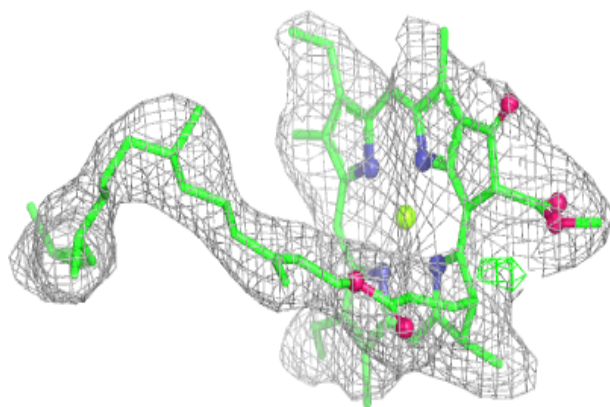
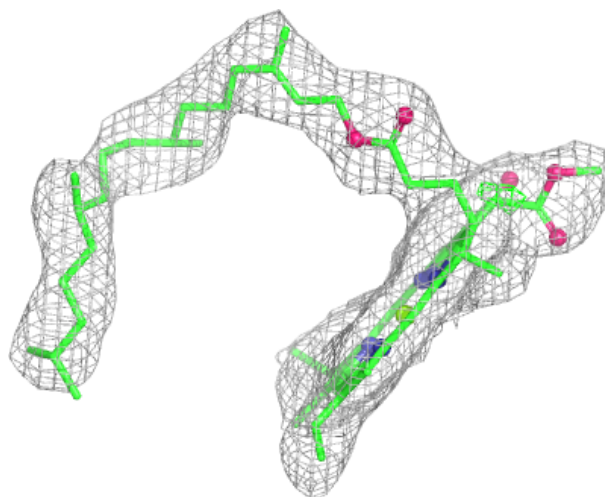
Electron density around CLA b 612:

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



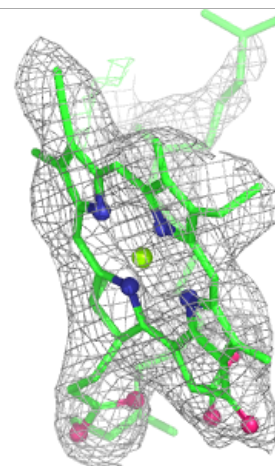
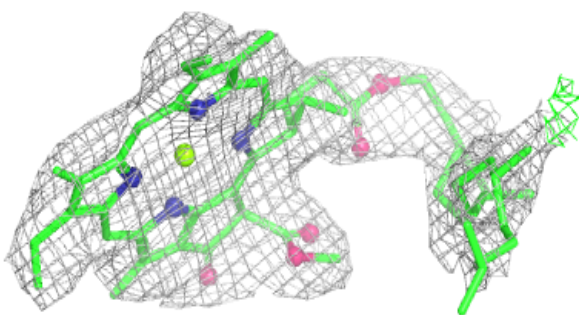
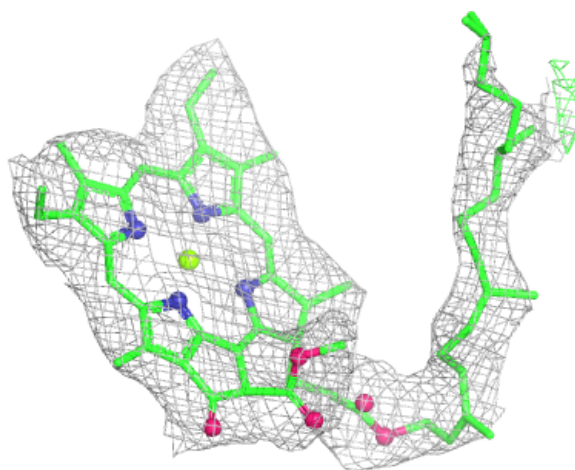
Electron density around CLA b 614:

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



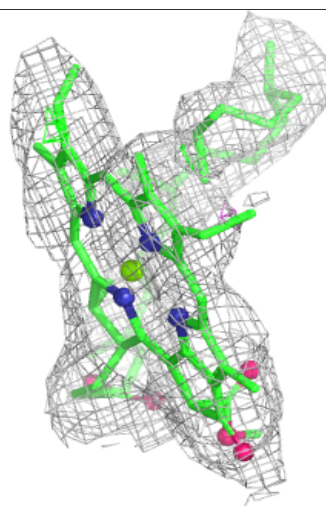
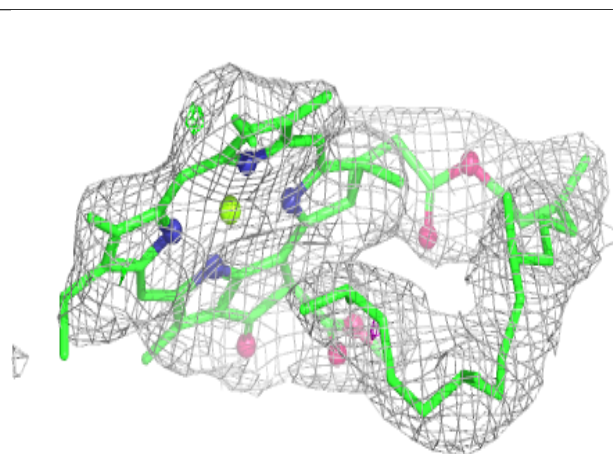
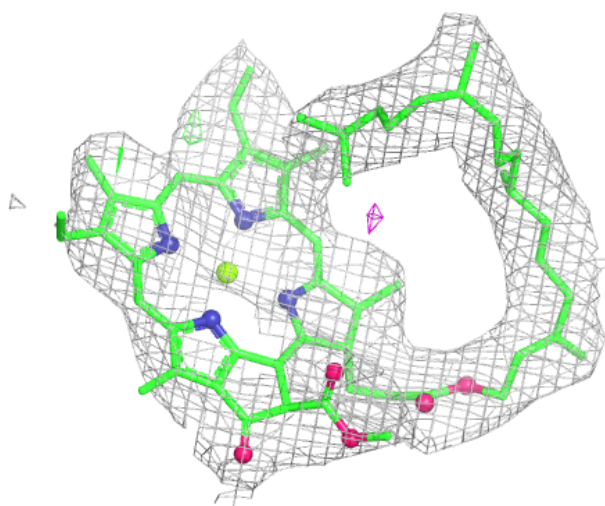
Electron density around CLA B 616:

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



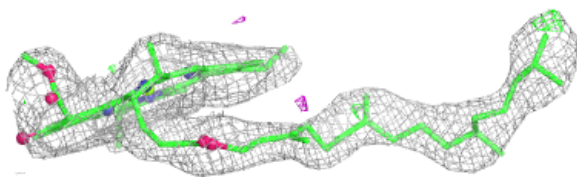
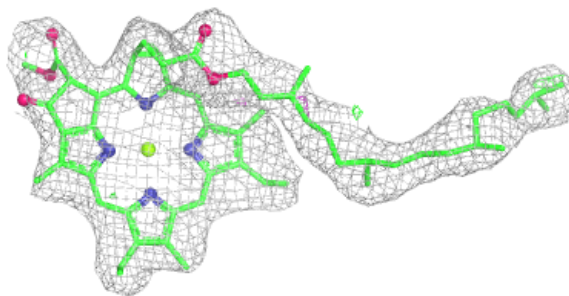
Electron density around CLA b 618:

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

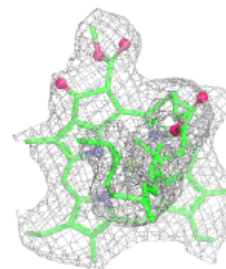
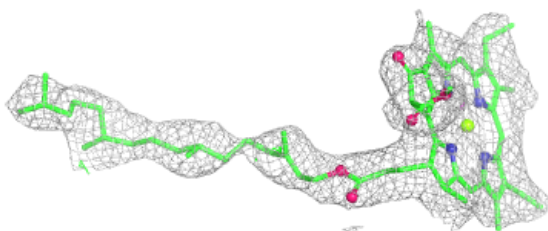
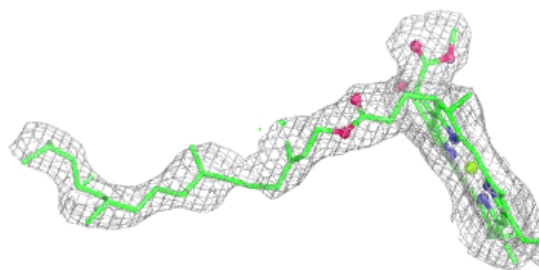


Electron density around CLA B 603:

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

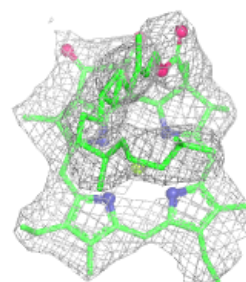
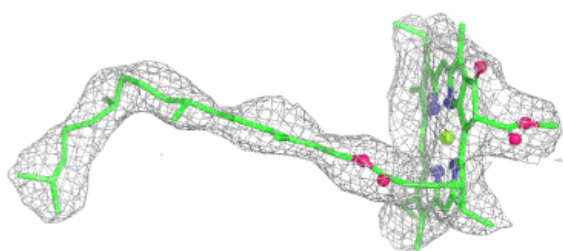
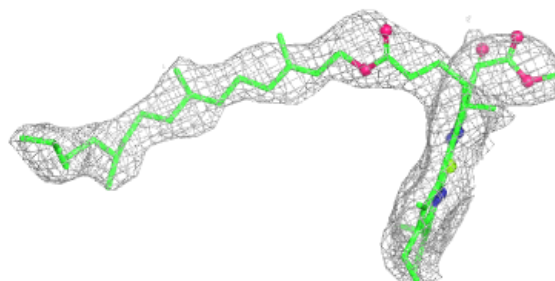
**Electron density around CLA b 607:**

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

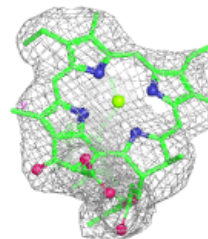
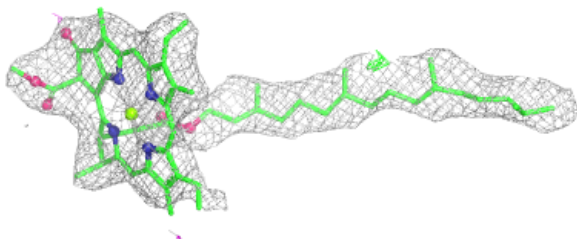
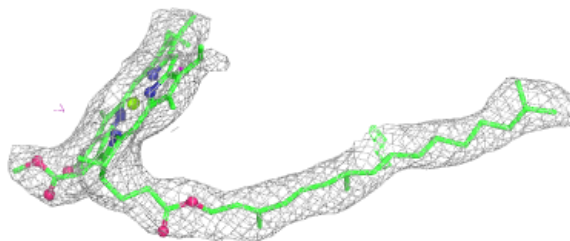


Electron density around CLA b 608:

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

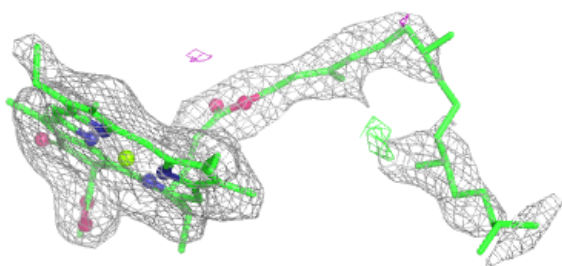
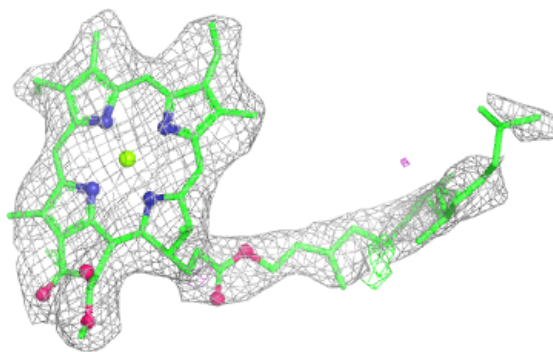
**Electron density around CLA B 607:**

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

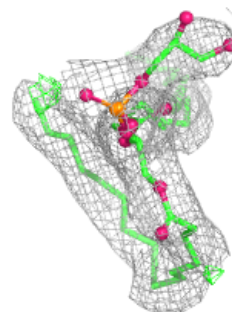
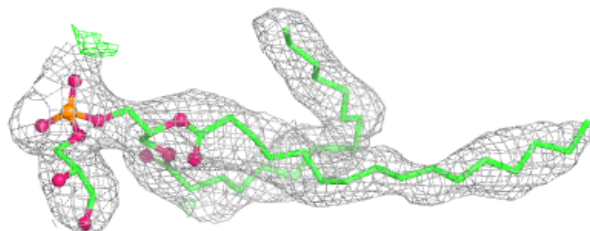
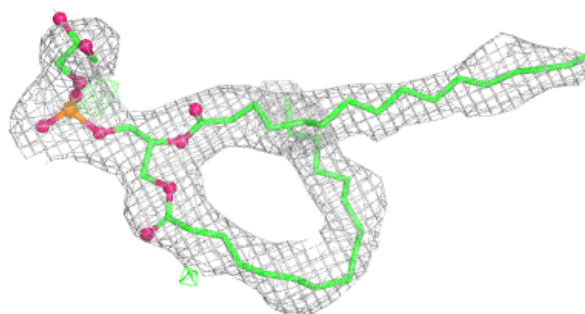


Electron density around CLA a 609:

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

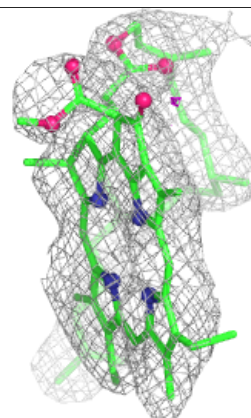
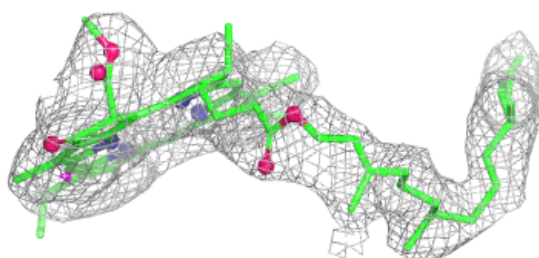
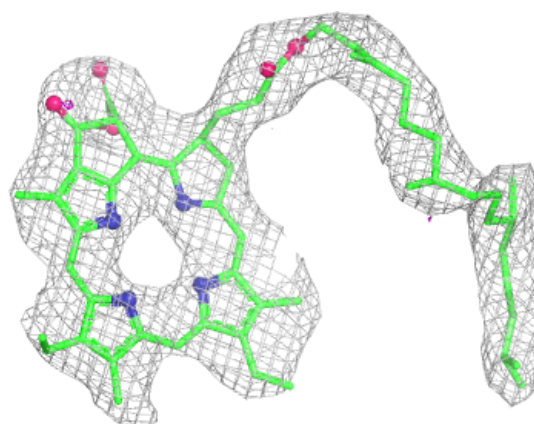
**Electron density around LHG A 616:**

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

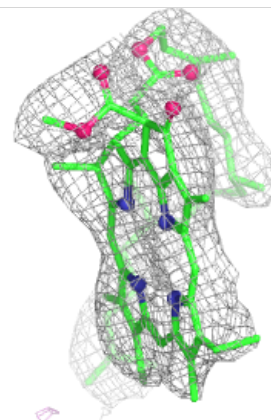
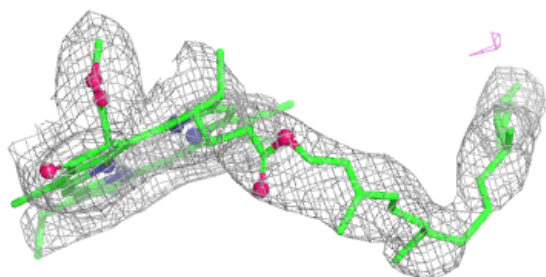
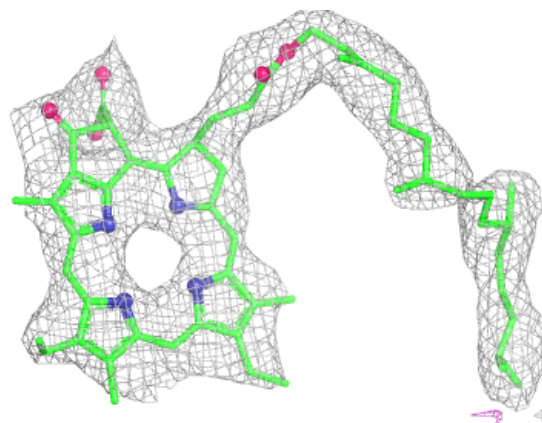


Electron density around PHO D 401:

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

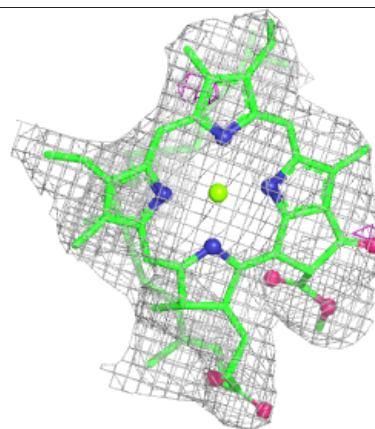
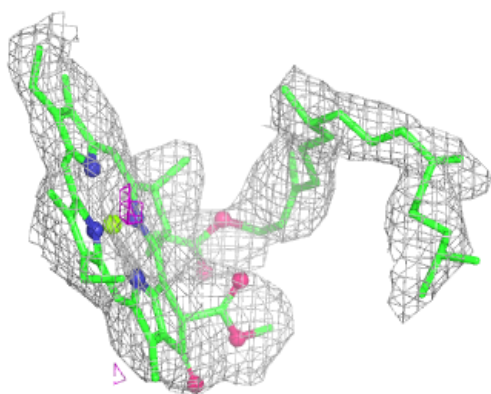
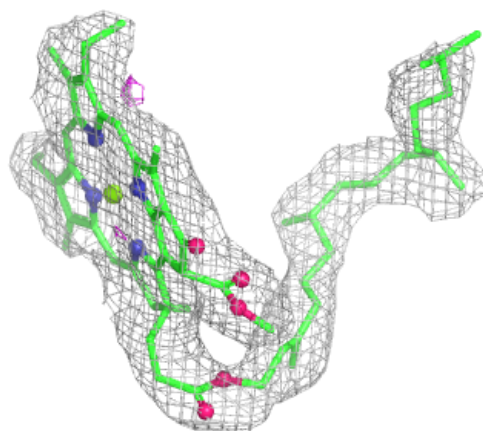
**Electron density around PHO d 401:**

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

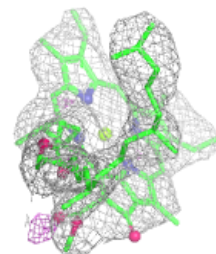
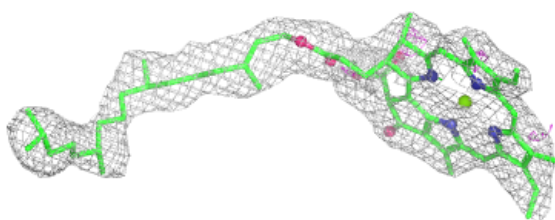
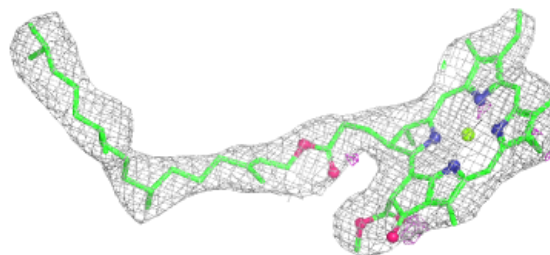


Electron density around CLA b 616:

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

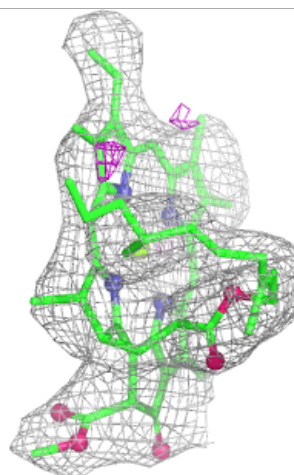
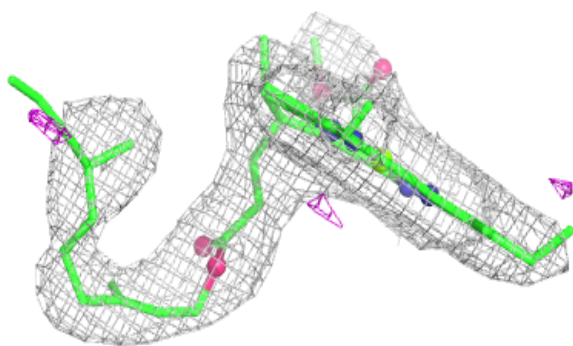
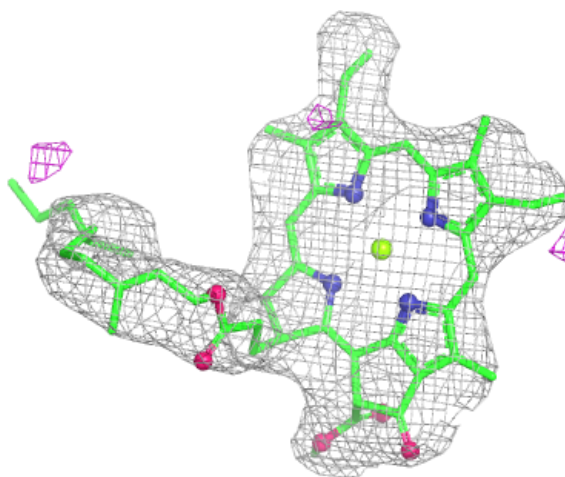
**Electron density around CLA A 606:**

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



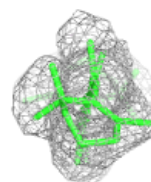
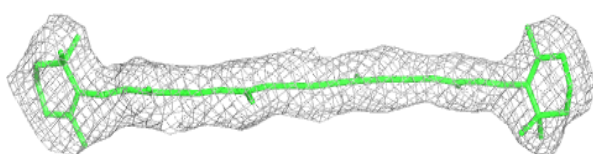
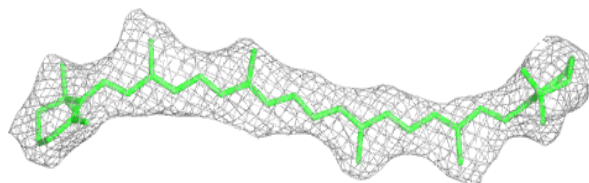
Electron density around CLA A 607:

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

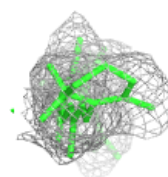
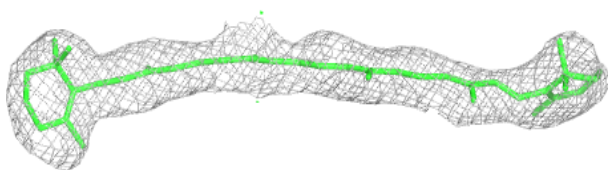
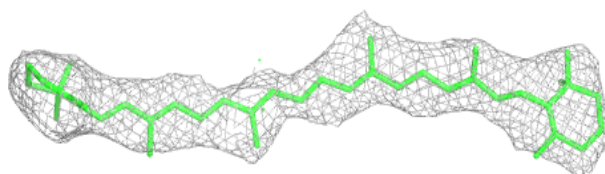


Electron density around BCR A 610:

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

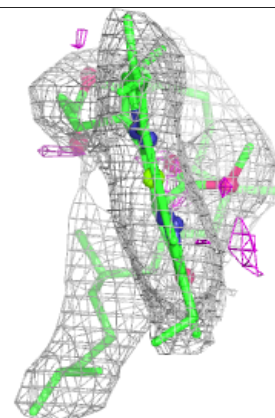
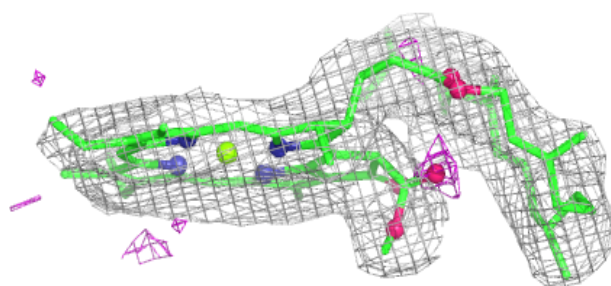
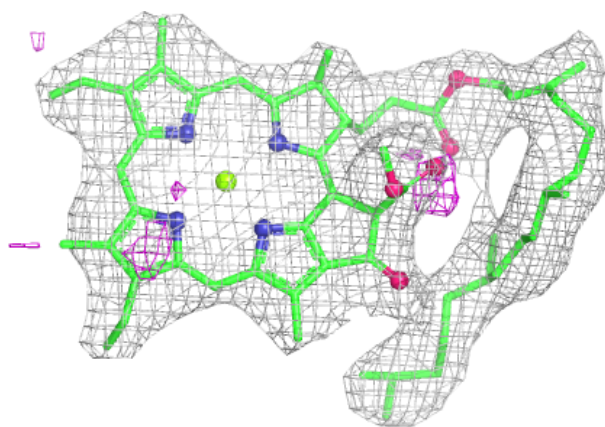
**Electron density around BCR B 617:**

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



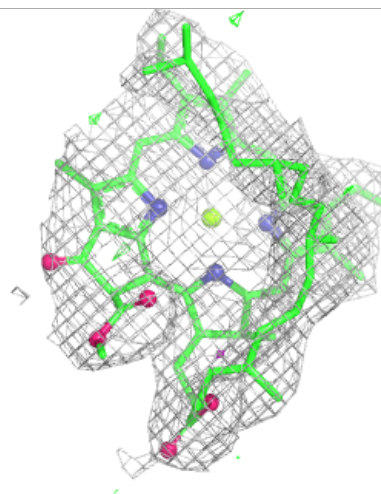
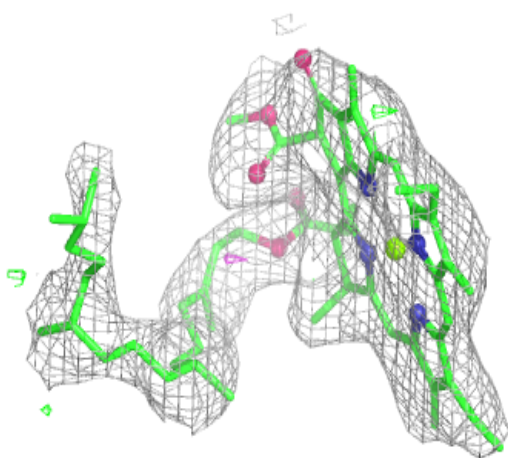
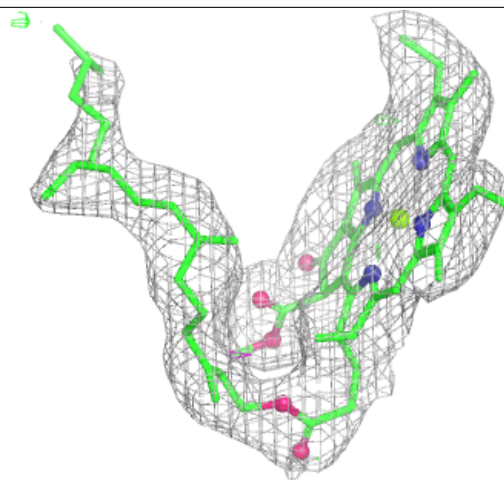
Electron density around CLA B 610:

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



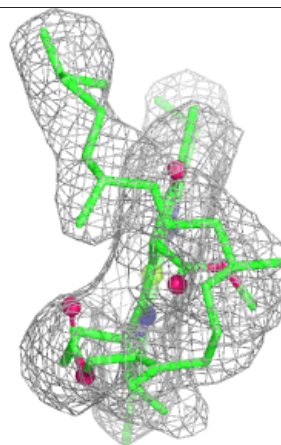
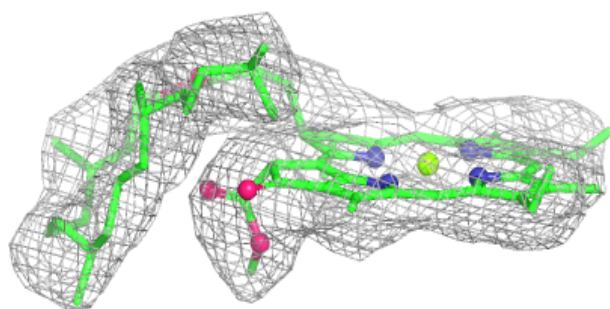
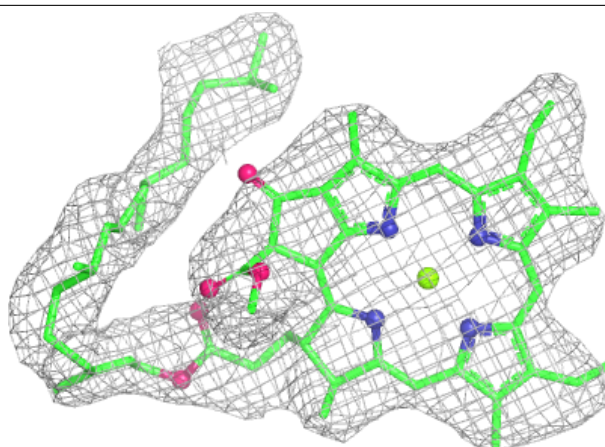
Electron density around CLA B 613:

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



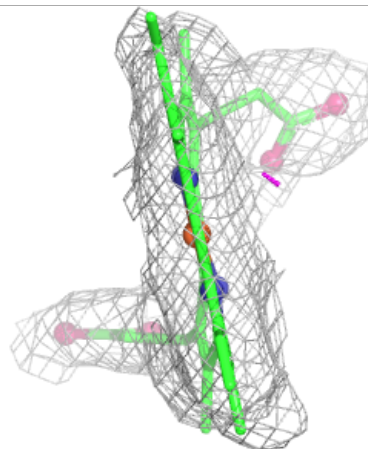
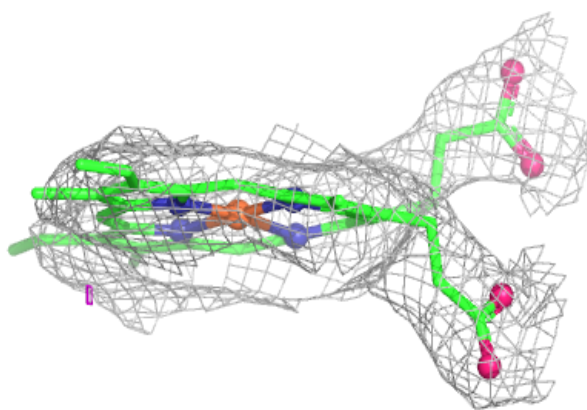
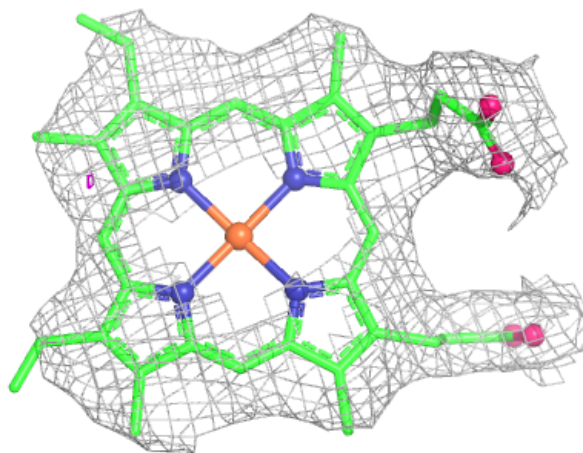
Electron density around CLA b 613:

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



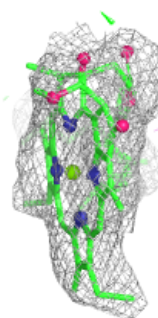
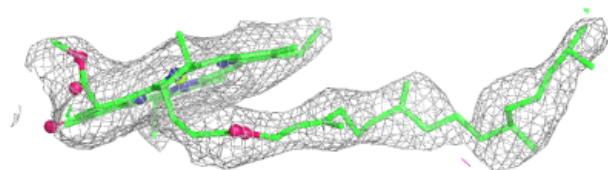
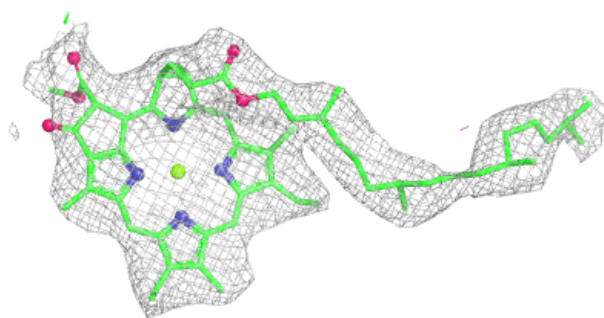
Electron density around HEM E 101:

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

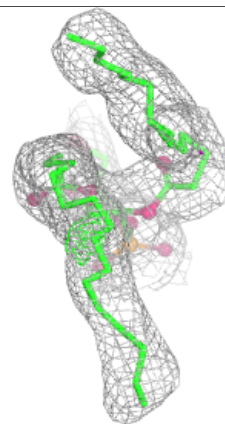
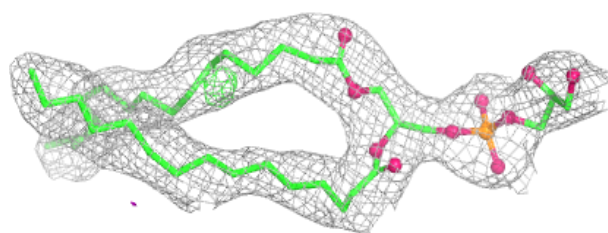
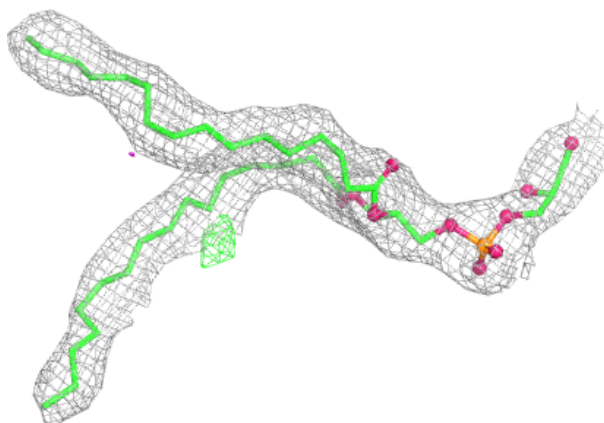


Electron density around CLA b 606:

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

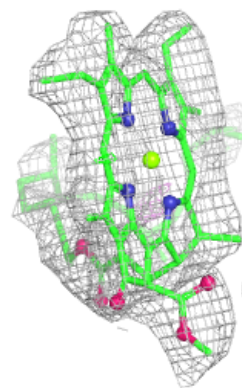
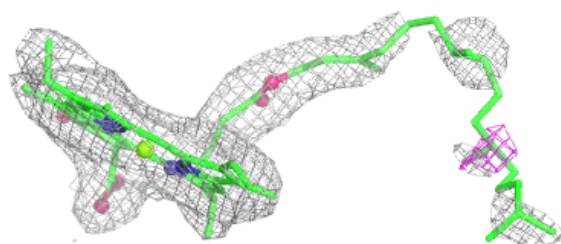
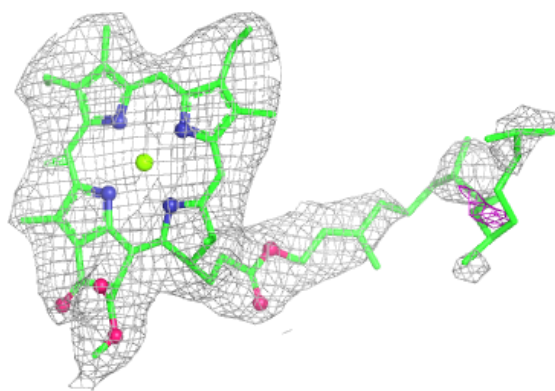
**Electron density around LHG d 407:**

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



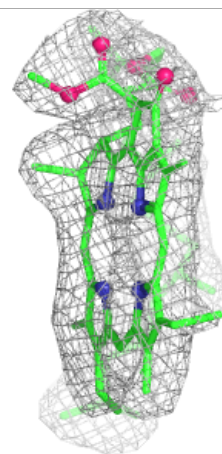
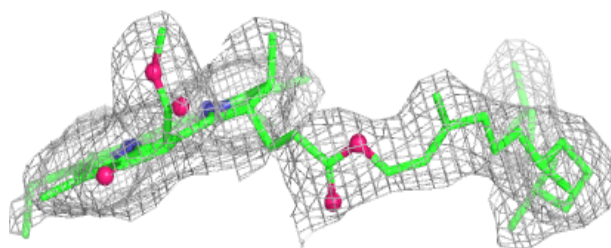
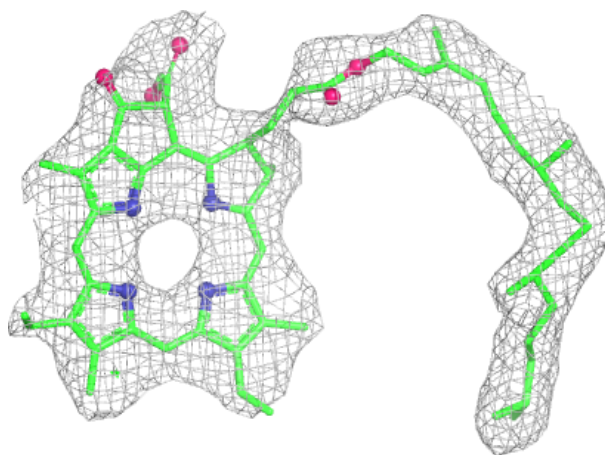
Electron density around CLA A 609:

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



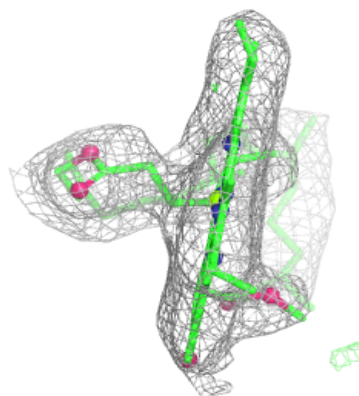
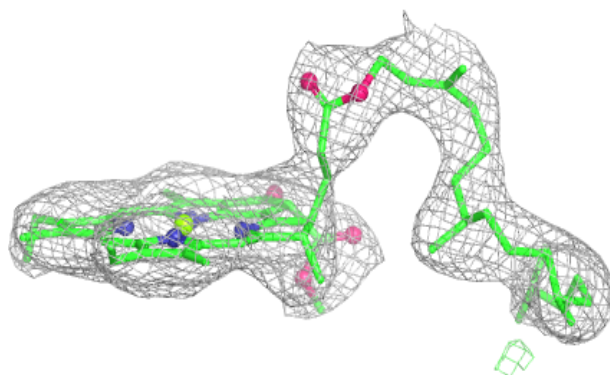
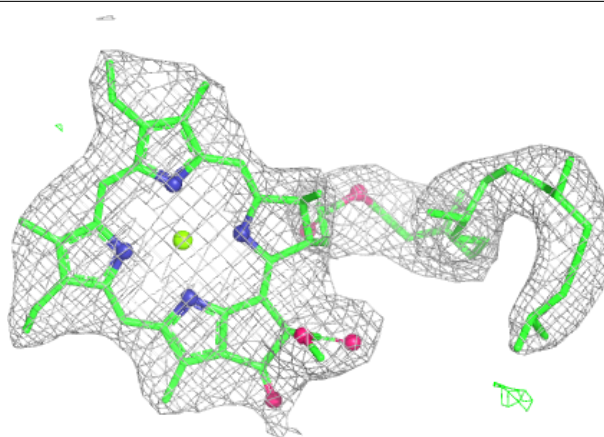
Electron density around PHO A 608:

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



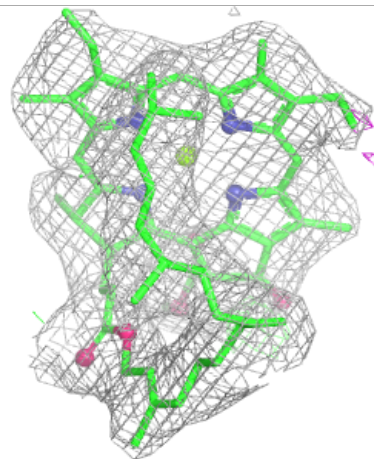
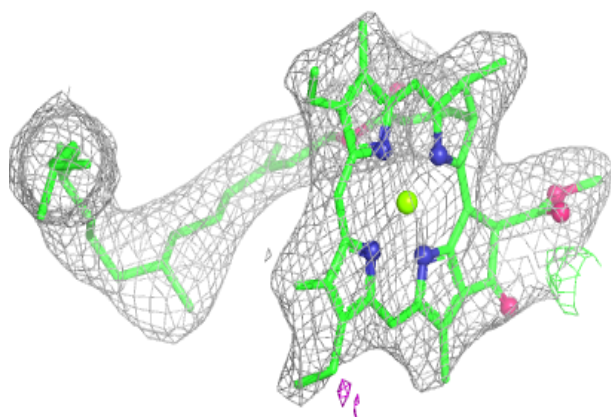
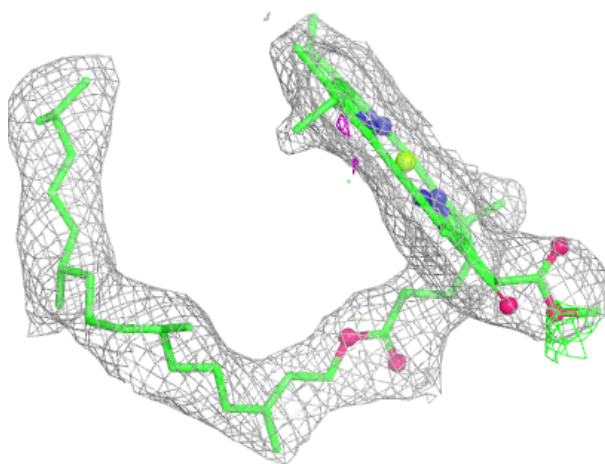
Electron density around CLA b 615:

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



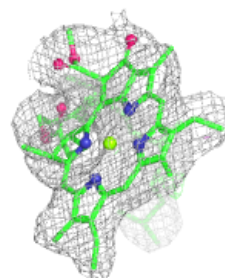
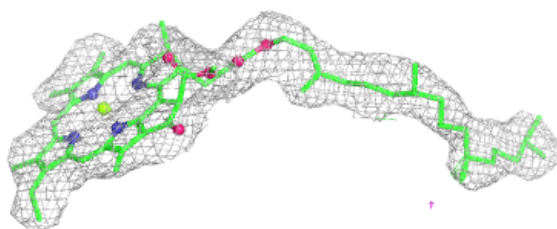
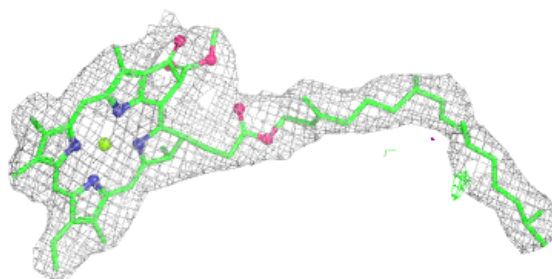
Electron density around CLA B 611:

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

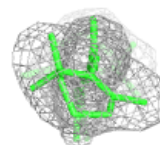
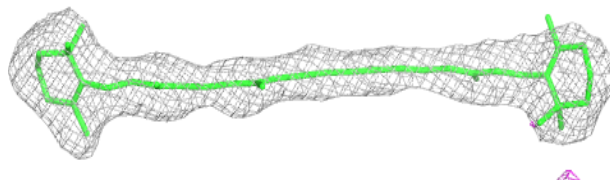
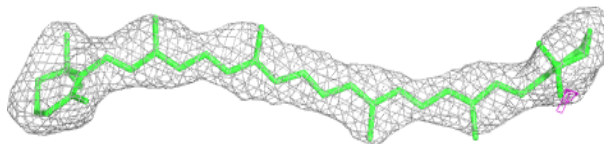


Electron density around CLA a 606:

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

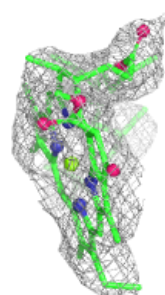
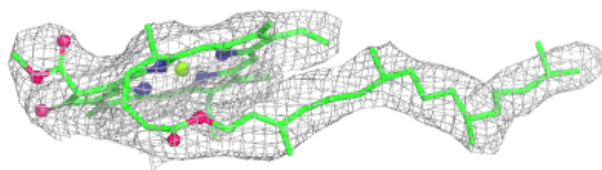
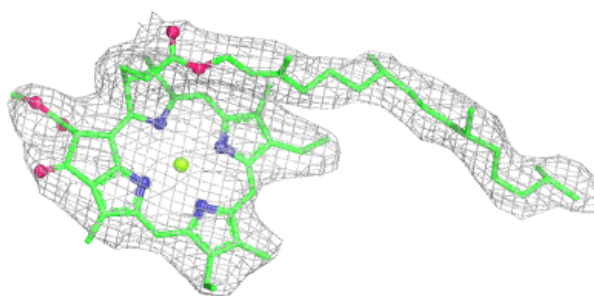
**Electron density around BCR a 610:**

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

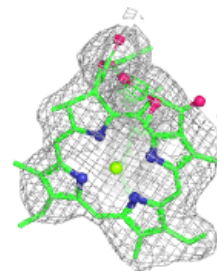
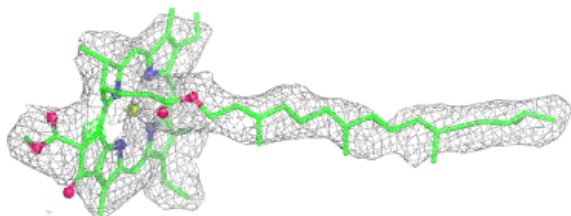
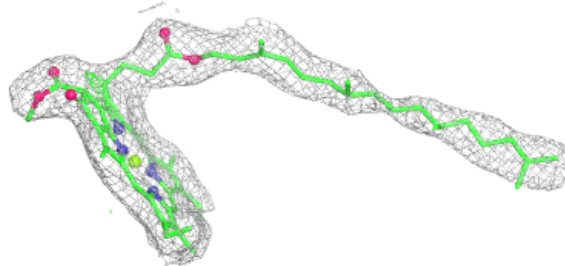


Electron density around CLA C 501:

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

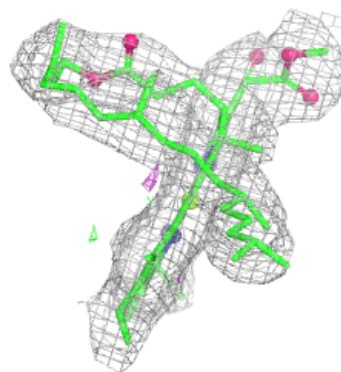
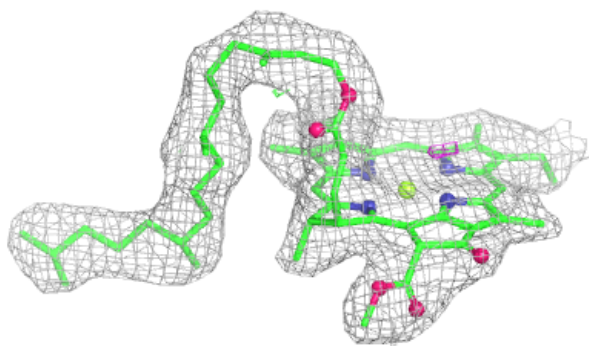
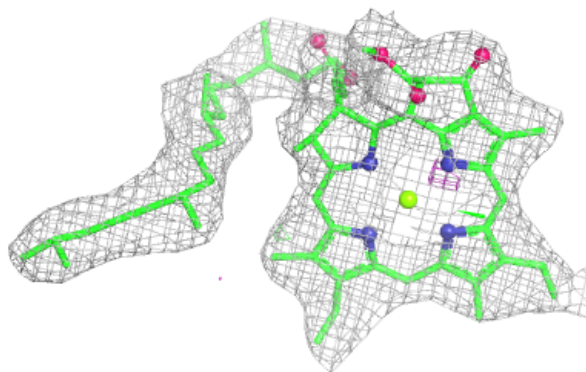
**Electron density around CLA b 610:**

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

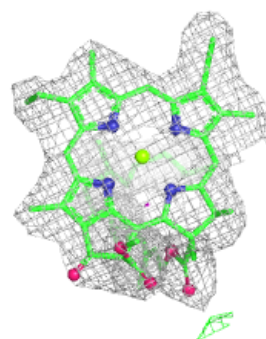
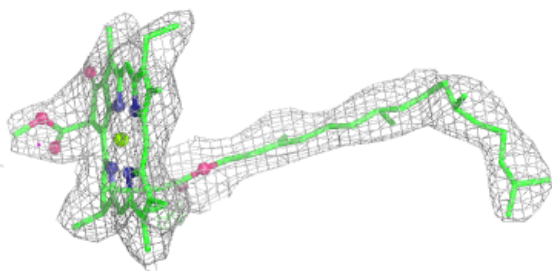
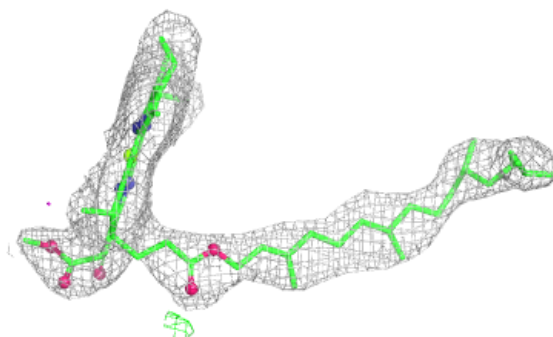


Electron density around CLA a 612:

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

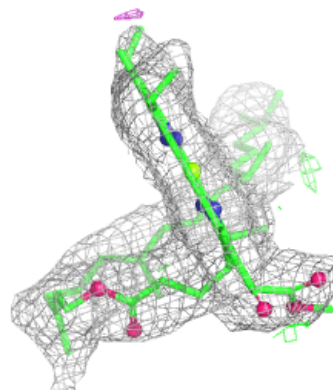
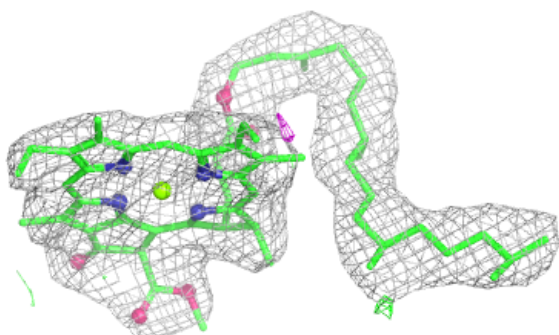
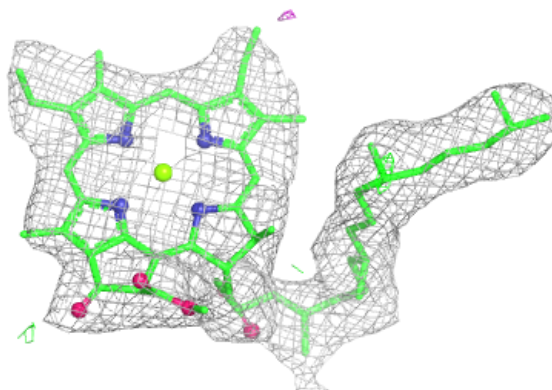
**Electron density around CLA B 605:**

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

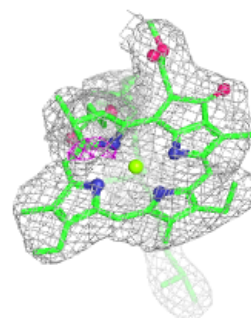
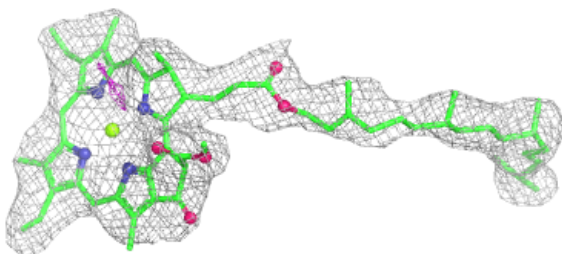
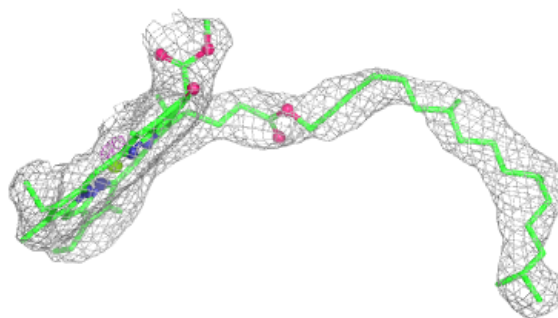


Electron density around CLA A 615:

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

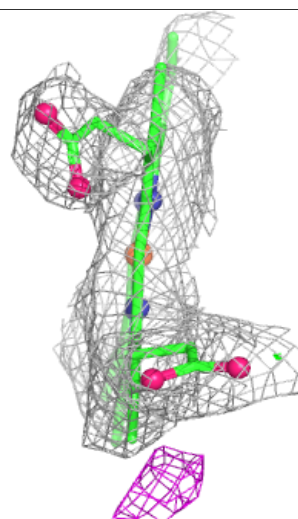
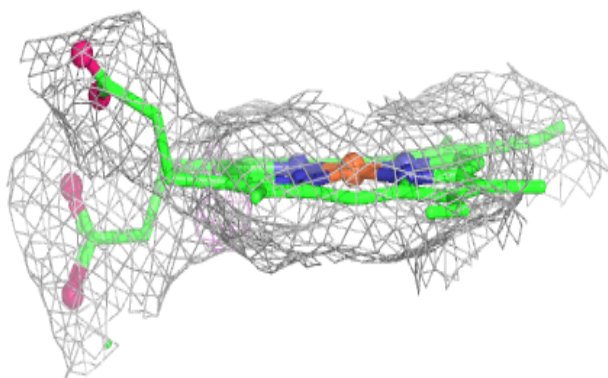
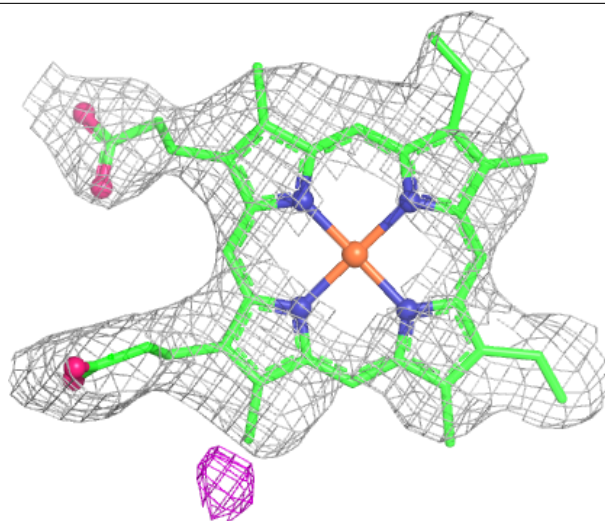
**Electron density around CLA d 403:**

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



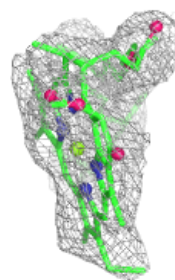
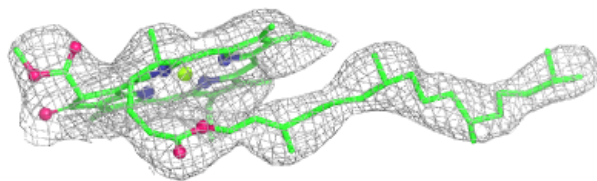
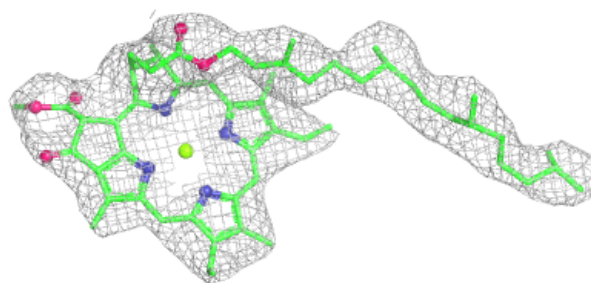
Electron density around HEC V 201:

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



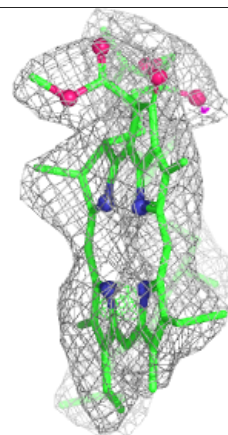
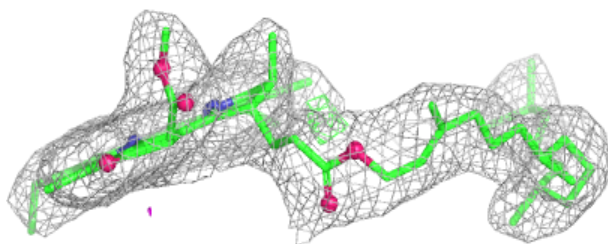
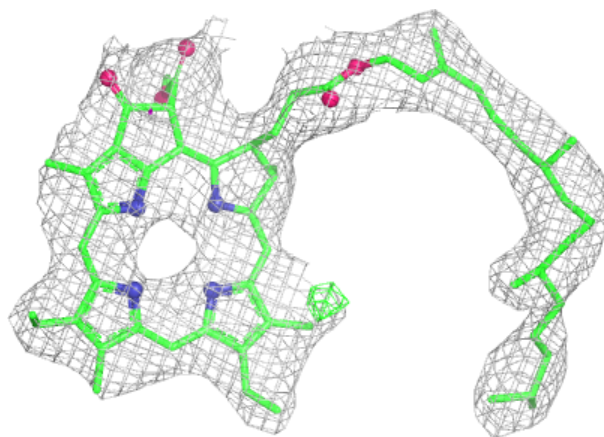
Electron density around CLA c 503:

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

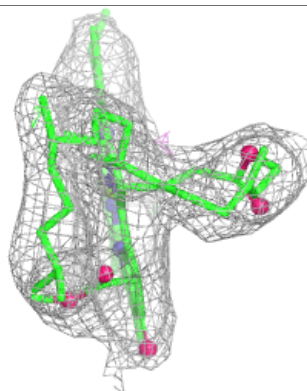
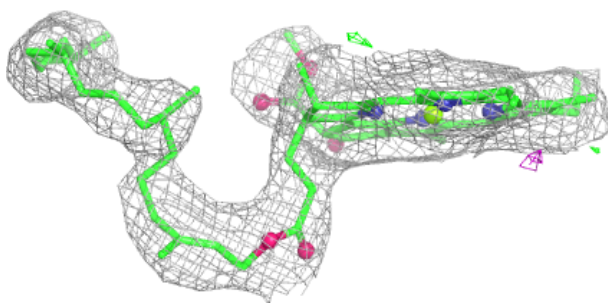
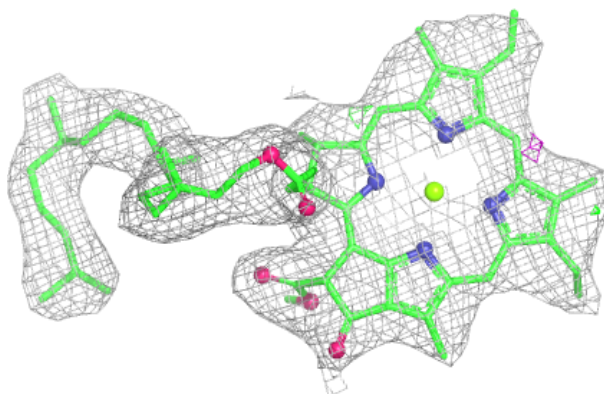


Electron density around PHO a 608:

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

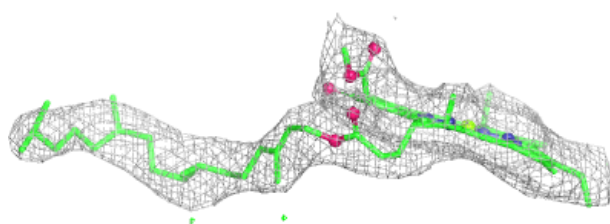
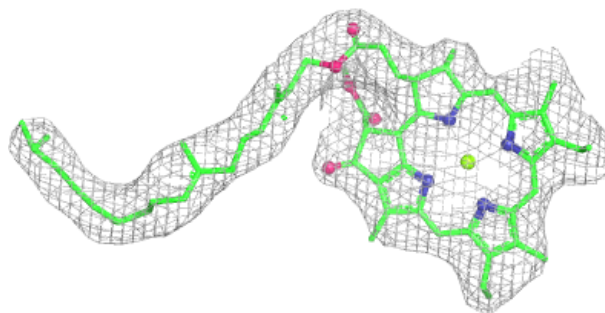
**Electron density around CLA B 612:**

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

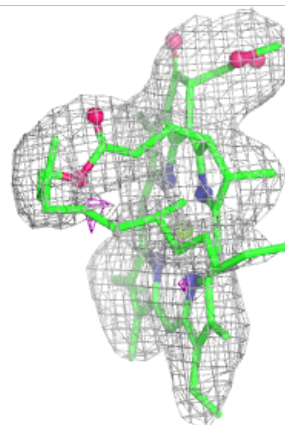
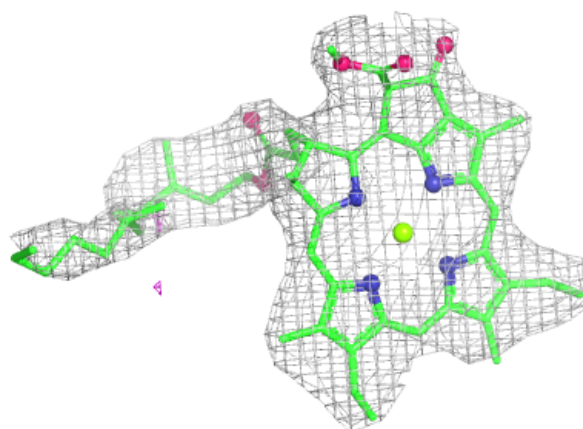


Electron density around CLA B 602:

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

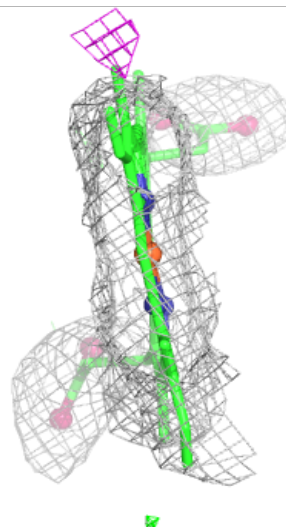
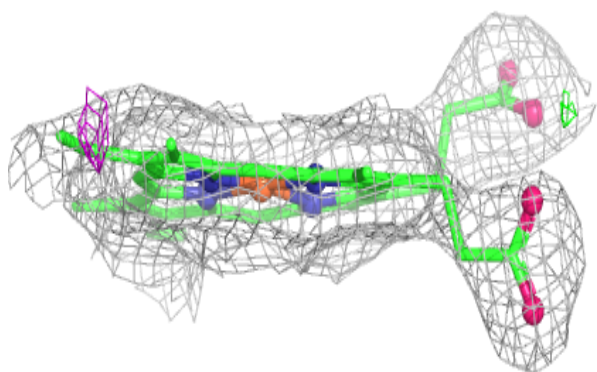
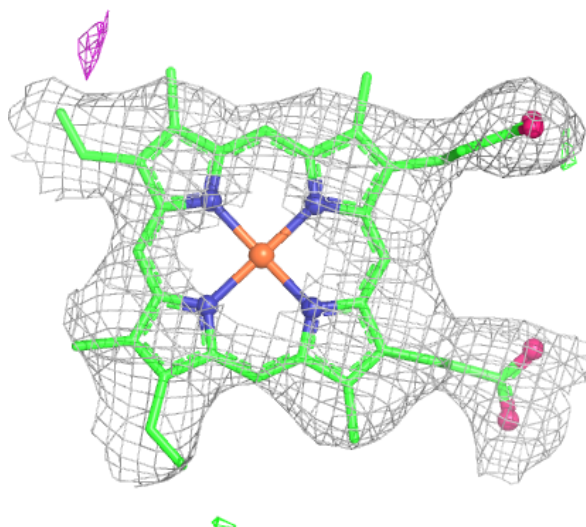
**Electron density around CLA a 607:**

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



Electron density around HEC v 201:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.